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Synthesis and conformational analysis of 2,2,6,6-tetramethyl piperdine masked 1,2- diols: Synthesis of oxylipins from Dracontium lortense

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Synthesis and conformational analysis of 2,2,6,6-tetramethyl piperdine masked 1,2-diols: Synthesis of oxylipins from *Dracontium lortense*

by

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NOMENCLATURE

BINOL	1,1'-Bi-2-napthol
BH_3.THF	Trihydridoborane in Tetrahydrofuran
Bu_3Sn	Tributyl stannane
BuLi	Butyl lithium
CBS cat.	Corey-Bakshi-Shibata catalyst
$CeCl_3$	Cerium(III) chloride
n-C_8H_{17}	octyl
$CuCl_2$	Copper(II) chloride
DIBAL-H	Diisobutylaluminum hydride
DCM	Dichloromathane
DMF	*N*, *N*,-Dimethylformamide
DMSO	Dimethyl sulfoxide
dr	Diastereomeric ratio
er	Enatiomeric ratio
ESI	Electrospray ionization
HBF_4	Tetrafluroboric acid
HETLOC	Hetero half filtered total correlation spectroscopy
PS-HMBC	Phase sensitive hetero multi-bond correlation spectroscopy
HOAc	Acetic Acid
HPLC	High-performance liquid chromatography
IBX	2-Iodoxybenzoic acid

LiOH	Lithium hydroxide
Me	Methyl
MeOH	Methanol
m/z	Mass/charge ratio
$NaBH_4$	Sodium borohydride
NOE	Nuclear Overhauser effect
NMR	Nuclear magnetic resonance
PCy_3	Tricyclohexylphosphine
$Pd_2(dba)_3$	Tris(dibenzylideneacetone)dipalladium(0)
PhMe	Toluene
Q-TOF	Quadrapole time-of-flight mass spectrometer
TES	Triethylsilyl
THF	Tetrahydrofuran
TLC	Thin layer chromatography
TMP	Tetramethyl piperdine
TEMPO	2,2,6,6-Tetramethylpiperdinyloxy
Zn	Zinc

ABSTRACT

Various natural products have been isolated with promising bioactivities but in very small quantities, impeding structure elucidation and structure activity relationship studies. Therefore, synthesis of such natural products in laboratory becomes very important for structure determination and biological studies. Two isomeric oxylipins (a trihydroxy fatty acid) were isolated from the Peruvian plant *Dracontium lortense* in very minute quantities (1 mg of each). One of the oxylipins have shown promising activity as an immunostimulant. Although the relative stereochemistry of the natural product was assigned, due to scarcity the absolute configuration was unknown. The current work describes the synthesis and structural assignment of these unnamed isolated oxylipins.

The first chapter describes a synthesis of all stereoisomers of this natural product using a method develop to synthesize chiral 1,2-diols. *Anti* 1,2-diols were prepared from simple inexpensive aldehydes via aldehyde α-oxygenation followed by organomagnesium or organolithium addition. All the diastereomers were synthesized and the stereochemistry of the naturally occurring oxylipins were unambiguously assigned using NMR spectroscopy.

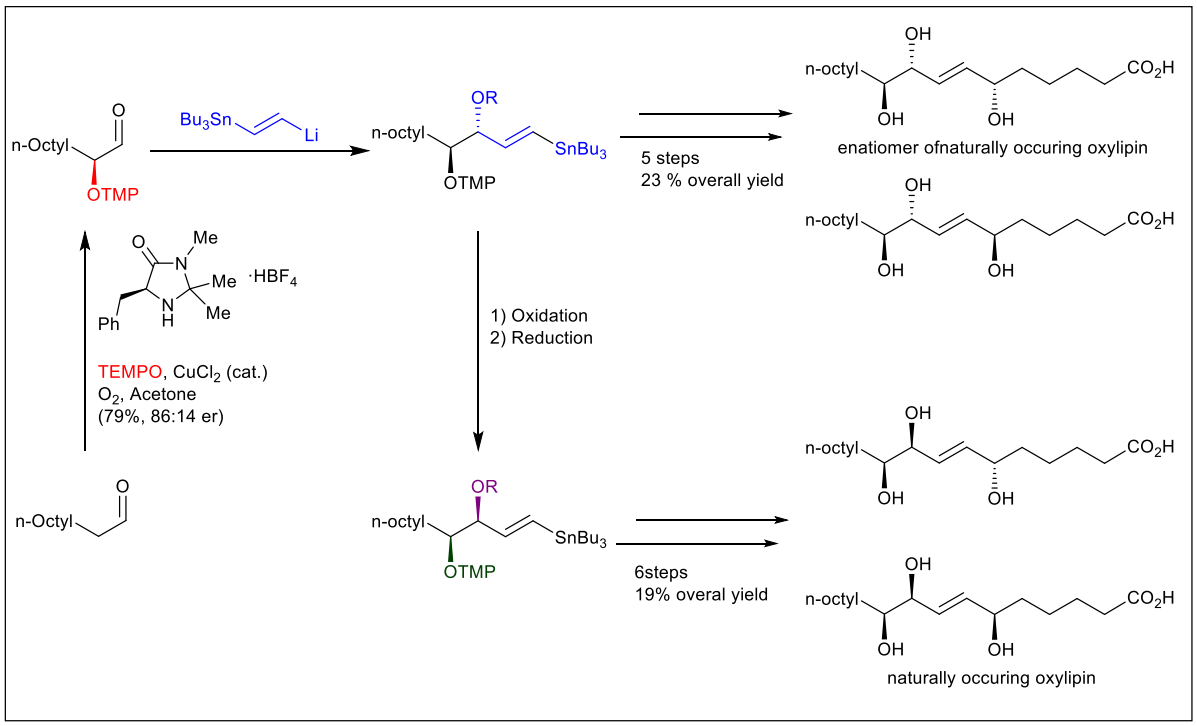
The second chapter describes a more direct and convergent synthesis of this natural product using an olefin cross metathesis approach. The natural product was synthesized in just three steps starting from cheap and readily available starting materials in 33% overall yield. Our synthesis is by far the shortest synthesis of this class of natural products containing the 3-ene-1,2,5 triol moiety.

The third chapter describes the studies towards structure elucidation of different diastereomers of 2,2,6,6-tetramethylpiperdine singly masked 1,2-diols. Observed disparity in

the hydroxyl proton ^{1}H-NMR chemical shifts of diastereomers of singly masked 1,2-diols led us to collaborate with computational chemists at Iowa State University (Professor Theresa Windus) to determine conformations of singly masked 1,2 diols. Computational (RHF, DFT, MP2) and 1D (decoupling experiments) and 2D NMR (HETLOC, HMBC) spectroscopic analysis revealed different hydrogen bonded ground state conformations of different diastereomers. This chemical shift difference was observed in various solvents and could be used as an stereochemical probe. The sterics of the gem dimethyl groups of the 2,2,6,6-tetramethylpiperdine moiety appears to be the reason behind this conformational preference.

CHAPTER I: FIRST GENERATION SYNTHESIS OF OXYLIPINS FROM *DRACONTIUM LORTENSE*

Paper published in *Organic letters*



Abstract

A stereochemically flexible synthesis was designed to make all the diastereomers of oxylipin isolated from *D. lortense* using a method developed to access chiral 1,2-diols. The key steps involve enantioselective organocatalytic α-oxygenation of decanal, Grignard addition, Stille cross coupling and asymmetric ketone reduction. This 7-step linear synthesis furnishes a single diastereomer of the biologically active natural product in 23% overall yield. The stereochemistry of the natural product was unambiguously assigned. Our synthesis is tied for the shortest synthesis to oxylipins containing the 3-en-1,2,5-triol moiety and the shortest synthesis of related oxylipins containing an anti-1,2-diol moiety.

Introduction

Oxylipins[2] are a group of oxygenated natural products formed from polyeneoic fatty acids involving atleast one mono or dioxygenase dependant oxidation.[3] Such polyhydroxy unsauturated fatty acids and their derivatives are commonly found in nature and have diverse bio-activities.[4] Acyclic trihydroxy fatty acids like **1** (fig 1) have shown immunomodulatory activity,[5] oxylpin **3** has been used as an oral adjuvant for influenza vaccines.[6] Bioactivity of these natural product is often dependent on its structure. Like, oxylipin **1**[5] was found to be an immunostimulant and the C-10 epimer **2** was found to be biologically inactive. Pinellic acid **3** with 9S and 13S configuration were more potent as oral adjuvants for influenza vaccines than the other isomers.[7] These observations underline the importance of stereochemistry in biological activity. Stereochemistry dependent diverse biological functions creates a demand to design stereoselective routes to these natural products.

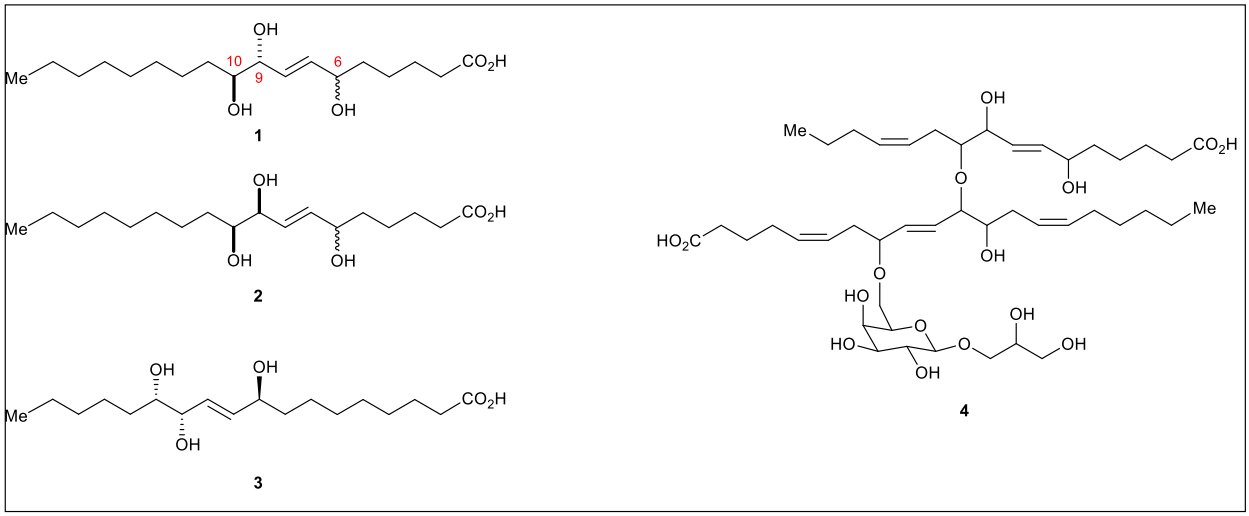
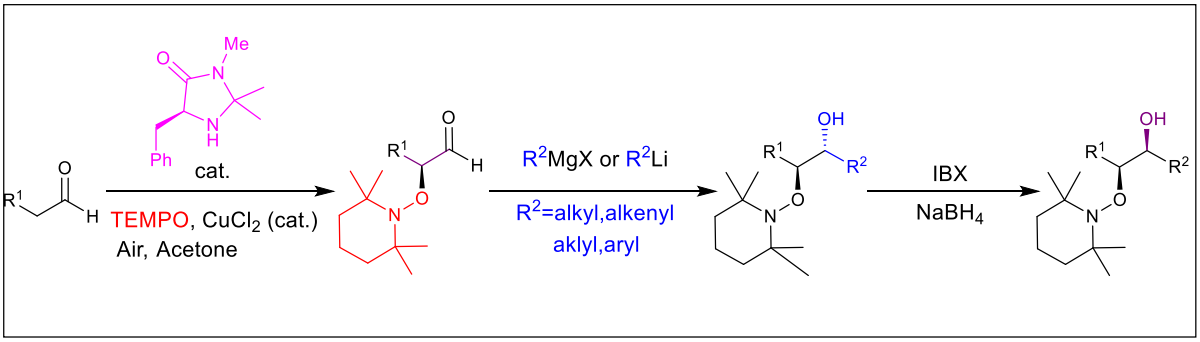


Fig 1: Oxylipins from *D. lortense*, Pinellic acid, Nigricanoside A

Our interest in Nigricanoside A **4** (fig 1),[8] a unique galactolipid containing hydroxylated fatty acid chains joined by ether linkage with misappropriated bioactivity,[9] drew our attention towards oxylipins **1** and **2**. Containing the same stereochemical triad like Nigricanoside A,

oxylipins could serve as ideal model system in the synthesis of Nigricanoside A. Furthermore, the isolation chemists were only able to assign the relative stereochemistry of the C-9 and C-10 carbinol positions and the configuration of both the isomer was unknown.[5] So far five total syntheses[10] have been reported of this natural product. Two groups synthesized a single isomer of the immunostimulant[10a] and biologiacally inactive natural product[10b] but made no attempts to assign the stereochemistry of these oxylipins. Two groups synthesized both diastereomers of immunostimulant but one compared the NMR spectroscopy data of their synthetic material in a solvent ($CDCl_3$) different from the isolation team (CD_3OD)[11] whereas the other compared their spectroscopic data with other synthetic oxylipins.[12] Hence stereochemistry of this natural product was ambiguous. Our goal was to devise a synthesis to make all four diastereomer of this trioxygenated fatty acids and unambiguously assign the stereochemistry of both the naturally occurring isomers.

Towards that end, we developed a method to synthesize the 1,2-diol moiety of the natural product in a stereochemically flexible manner from inexpensive aldehydes[1] (**Scheme 1**). Readily available α-oxyaldehydes were chosen as stereoflexible precursors, because substrate controlled stereoinduction (polar Felkin Anh and chelation control nucleophilic addition pathway) is possible, furnishing both diastereomers from a common precursor. The α-oxoaldehydes were prepared in a single step via organocatalytic oxidative incorporation of TEMPO onto aldehydes. Polar Felkin Anh addition of various nucleophiles, with different branching and hybridization, proceeded with good selectivities (upto dr> 20:1) to furnish anti-1,2-diols in two steps. The *syn* diastereomers were accessed by oxidation and reduction of *anti*-1,2-diols.



Scheme 1: Synthesis of chiral 1,2-diols

The above method was successfully applied in the synthesis of oxylipins **1** and **2**. All the diastereomers were synthesized and the stereochemistry was unambiguously assigned.

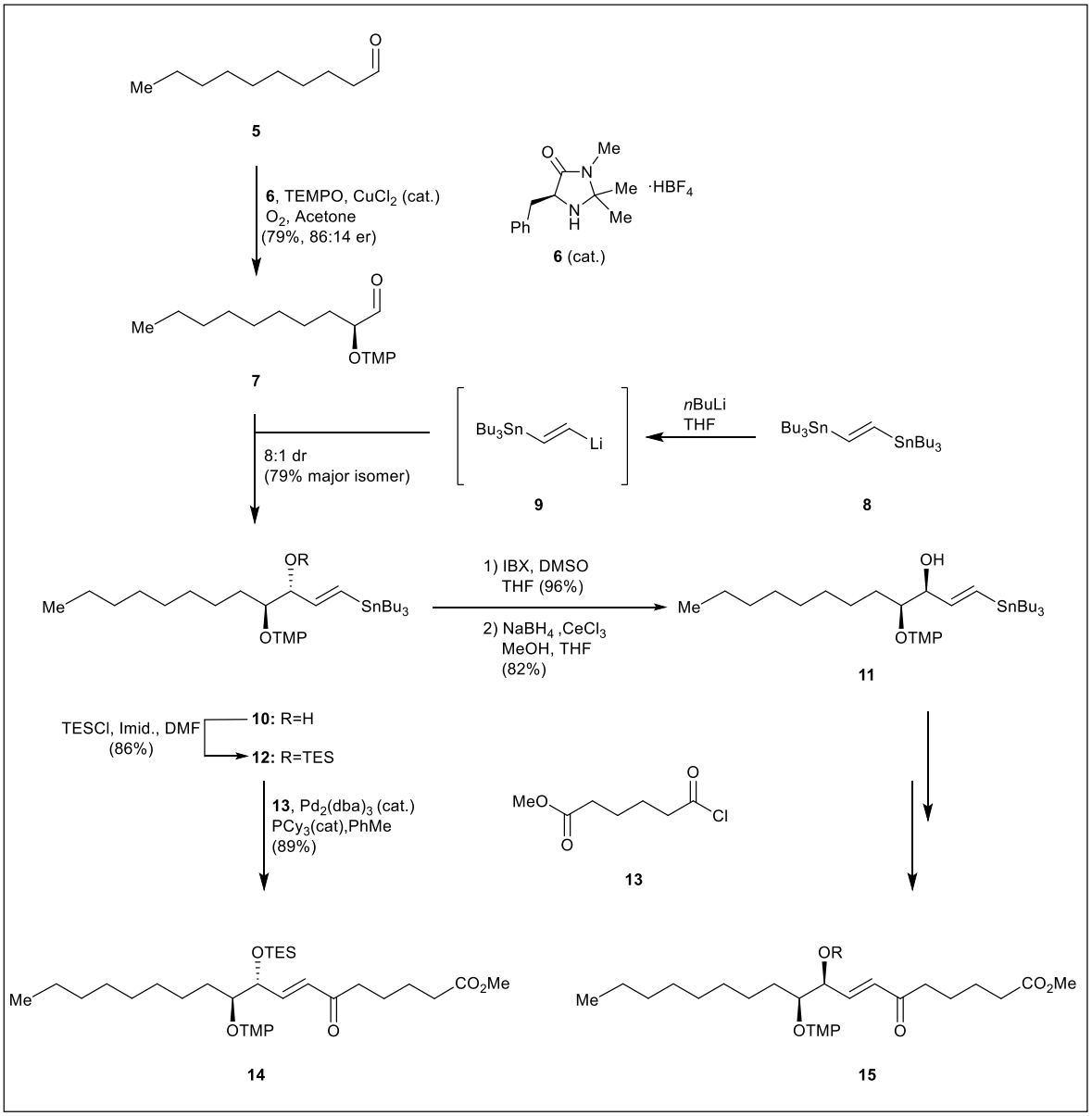
Results and Discussion

Our synthesis (**Scheme 2**) began with phenylalanine based imidazolidinone catalyst **6** promoted oxidative incorporation of TEMPO[13] onto decanal **5**, giving α-oxygenated aldehyde **7** in 79% yield and 86:14 er (20 mmol scale and 20 mol% catalyst loading). The enantiomeric ratio for α-oxyaldehyde **7** observed is lower than that reported by MacMillan for similar compounds because we avoided using a complex tryptophan-derived catalyst (five steps from tryptophan and additional chromatographic purification) using instead the more-readily prepared phenylalanine-derived catalyst **6** (two steps from phenylalanaine hydrochloride, no chromatography). Furthermore, the low cost of decanal and presence of a subsequent enantio-enriching step encouraged us to use catalyst **6**. *In situ* generation of lithio species **9** from distatanane **8** and diastereoselective addition onto aldehyde **7** generated anti 1,2-diol **10**. Distannane **8** has been extensively used generate the lithio species **9** to add onto various aldehydes,[14] forming synthetically important intermediates. But, we discovered that addition of lithio species **9** onto α-oxyaldehyde **7** in the presence of oxygen led to decomposition of the reaction mixture and gas formation. Freshly deoxygenated distannane **8**

and low temperature was essential to obtain and 8:1 diastereomeric mixture of diol **10** and **11** in 89% yield (15 mmol scale). The major diastereomer **10** was obtained after chromatographic purification in 79% yield with no degradation in enantiomeric ratio.

Attempted conversion of α-oxyaldehyde **7** to *syn*-diol **11** via a Lewis acid promoted chelation pathway was not met with any success other than degradation of diastereoselectivity using LiCl (dr 2:1, *anti*-1,2 diol still being the major product). Since the polar Felkin-Anh control is always predominating in this system, hydride addition to the corresponding ketone should also occur from the least hindered site inverting the stereocenter of the free alcohol. Therefore, oxidation of the free alcohol moiety of the *anti*-diol **10** to a ketone and reduction of the corresponding ketone is a viable route to access *syn*-diol **11**. Therefore, diol **10** was oxidized using IBX to furnish intermediate enone in 96% yield. Luche reduction of enone furnished *syn* diol **11** with good selectivity (12:1 dr) but with poor yield due to 1,4 conjugate addition and poor solubility of intermediate enone in methanol. Use of excess $CeCl_3$ (suppress 1,4-conjugate addition) and THF as a co-solvent (to promote solubility) improved the yield, furnishing diol **11** in 86% yield.

With both the diastereomer of the diol moiety in hand the next step was to form the carbon backbone of the natural product. Stille cross coupling[15] between vinyl stannane **10** and acid choride **13** was outcompeted by esterification. Cross coupling with less electrophilic thioesters[16] derived from acid chloride **13** also led to esterification. Hence the alcohol was now protected with TESCl to form protected stannane **12** in 86% yield. Stille cross coupling between stannane **12** and acid chloride furnished enone **14** in 89% yield. Similarly, stannane **11** was converted to enone **15** in 84% yield over two steps.

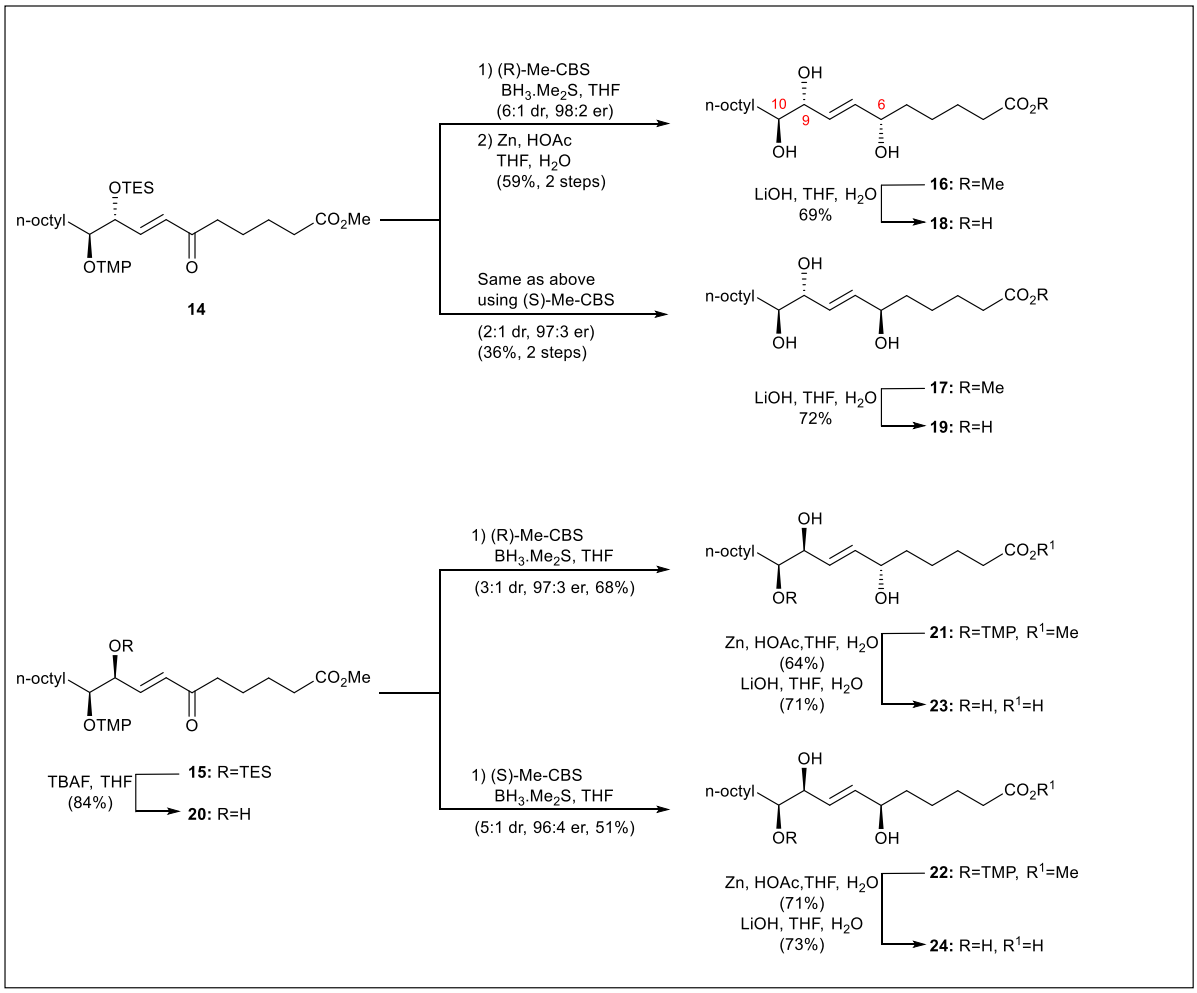


Scheme 2: Synthesis of carbon long chain of oxylipins

After synthesizing the carbon chain of the natural product, an asymmetric ketone reduction was envisioned to set the final stereocenter of the molecule and help improve the enatiopurity of the final product. The diastereoselectivity of this step was not expected to be high due to the modest enatioselectivity (86:14) of the previous α-oxygenation step. When enone **14** was subjected to diastereoselective reduction using borane-dimethyl sulfide complex in the presence of Me-CBS-oxazoborolidinone chiral ligand[17], a substrate bias was

observed. R-Me-CBS chiral ligand gave better diastereoselectivities (5:1 dr) compared to its enantiomer S-Me-CBS (2:1 dr), but with high isolated yields. This substrate bias could be overcome by diasteroselective reduction of corresponding silyl deprotected enone, but the yields plummeted (~30%). Reductive cleavage of the N-O bond using Zn-acetic acid also led to cleavage of the silyl protecting group to form triol **16** in a single step. Single diastereomer **16** was obtained after chromatographic purification in 59% yield after two steps with enhanced enatiopurity (98:2 er) as expected from the second asymmetric step. Single diastereomer of triol **17** was also obtained in 36% yield over two steps and 97:3 er. Ester hydrolysis using aq LiOH furnished C-6 epimers **18** and **19**, containing the *anti*-1,2-diol moiety, in 69% and 71% yield. This seven steps synthesis is the tied for the shortest synthesis of oxylipins containing the 3-ene-1,2,5-triol moiety. Furthermore, it is by far the shortest synthesis compared to the synthesis of related oxylipins containing the *anti*-1,2-diol moiety (11-19 steps).

Similarly, when the enone **15** was subjected to optimized condition for above mentioned asymmetric ketone reduction, very poor diastereoselectivities were obtained (~2:1dr). But, optimum distereoselectivity was obtained when silyl deprotected enone **20** was employed. Chiral reduction using R-Me-CBS and S-Me-CBS oxazoborolidinone ligand furnished a 3:1 and 5:1 diastereomeric mixture of enols which after chromatographic purification furnished a single diastereomer of enol **21** (68% yield, 97:3 er) enol **22** (51% yield, 96:4 er). Reductive cleavage of the TMP group and ester hydrolysis using the same above mentioned condition furnished the C-6 epimers **23** and **24** containing the *syn*-diol moiety.



Scheme 3: Synthesis of all diastereomers of oxylipins from *D. lortense*

With all the diastereomers prepared we compared the spectroscopic data, now taken in methanol, and the optical rotation data with that published by the isolation chemists. Stereochemistry of oxylipins from *D. lortense* containing the *anti*-diol moiety was found to be (6R,9S,10R)-**18** (enantiomer of compound shown in scheme 3) and that containg the *syn*-diol moiety was found to be (6R,9S,10S)-**24** (same as synthesized **24** in scheme 3). Thus, the two oxylipins isolated from *D. lortense* were found to be C-10 epimers.

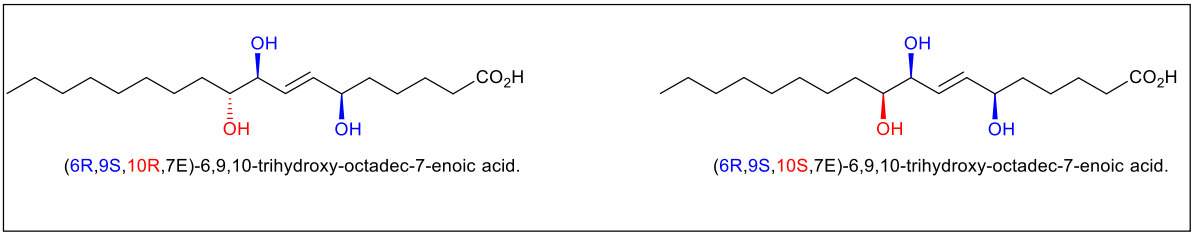


Fig 2: Naturally occurring oxylipins from *D. lortense*

Conclusion

In conclusion, synthesis of all the diastereomers of oxylipins **1** and **2** was accomplished. Enantioselective α-oxygenation of decanal followed by vinyl lithium addition was used to set the stereochemistry of the diol moiety of the natural product. Stille cross coupling furnished the carbon backbone and asymmetric ketone reduction was used to set the final stereocenter. This synthetic work led to the unambiguous stereochemical assignment of natural oxylipins. The major drawback would be the moderate enantioselectivity of the α-oxygenation step and the substrate bias in daistereoselective ketone reduction. Further shorter second generation synthesis addressing the aforementioned problems has been developed.

Experimental Section

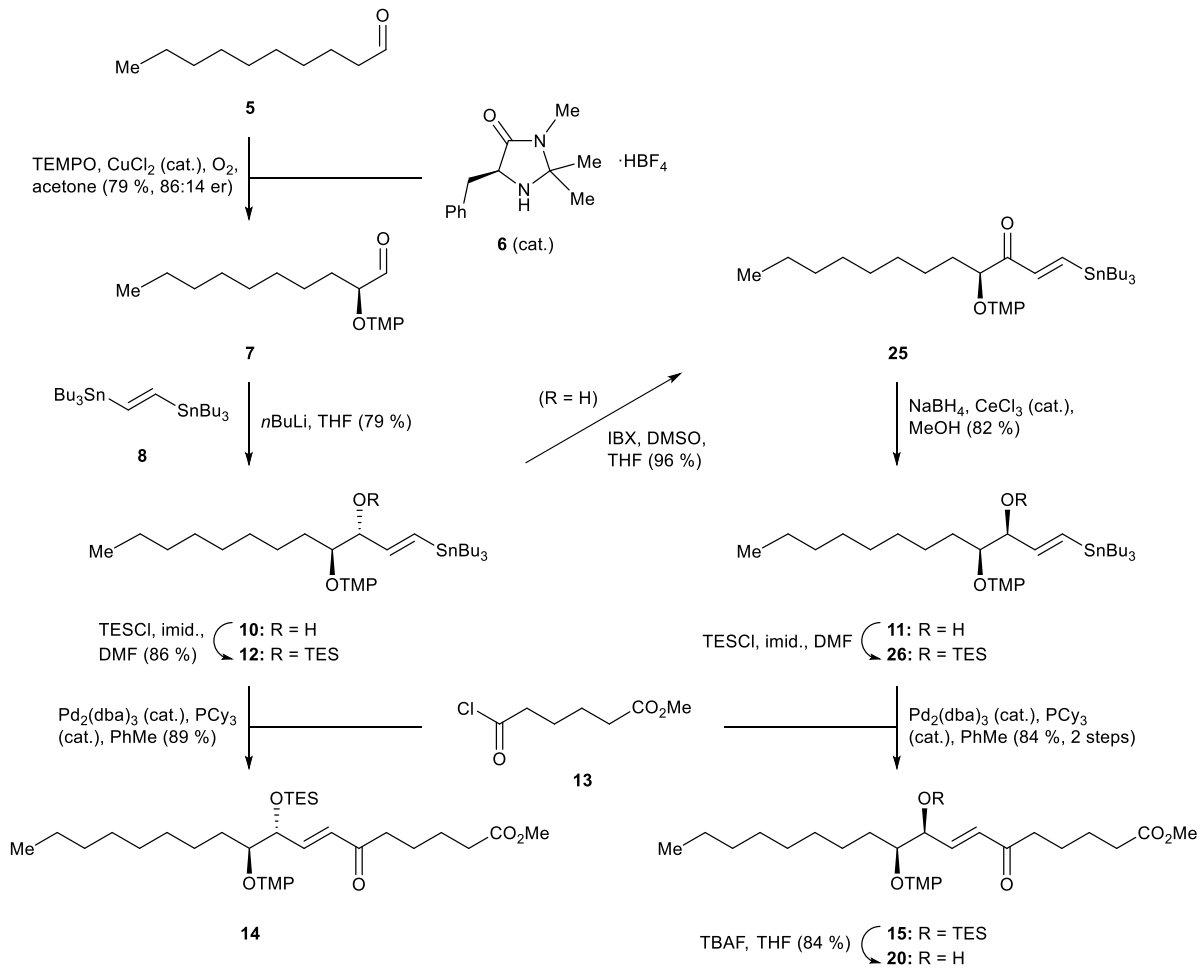
General methods

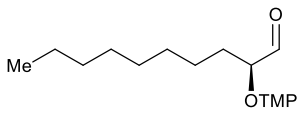
Unless otherwise noted, all reactions were performed with stirring under an argon atmosphere under anhydrous conditions. Organomagnesium and -lithium reagents were purchased from Aldrich. All other reagents were purchased at the most-economical grade. Dry tetrahydrofuran (THF), *N*,*N*-dimethylformamide (DMF), dichloromethane, and toluene were obtained by passing HPLC grade solvents through commercial solvent purification systems. All other chemicals were used as received, without purification. Flash column chromatography was performed using Grace Davison Davisil silica gel (60 Å, 35 – 70 □m). Unless otherwise noted, yields refer to chromatographically- and spectroscopically- (1H

NMR) homogeneous samples of single diastereomers. Thin-layer chromatography (TLC) was performed on Grace Davison Davisil silica TLC plates using UV light and common stains for visualization. NMR spectra were calibrated using residual undeuterated solvent as an internal reference. Apparent couplings were determined for multiplets that could be deconvoluted visually. Enantiomeric ratios were determined by chiral HPLC. Authentic peaks were identified by injecting a racemic reference sample prepared by mixing a 1:1 ratio of synthetic enantiomeric compounds.

Synthesis and characterization

Scheme 1: Oxylipins synthesis part 1

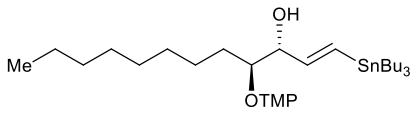




7

α-Oxyaldehyde 7: To a mixture of activated 4 Å molecular sieves (500 mg, powdered) and imidazolidinone catalyst **6** (1.22 g, 4 mmol, 0.2 equiv.) in 12 mL acetone was added $CuCl_2 \cdot 2H_2O$ (340 mg, 2 mmol, 0.1 equiv.). The green reaction mixture was stirred open to air for 5 minutes until the copper salt dissolved and the mixture turned dark orange. The reaction was cooled to -10 °C for 10 minutes, then decanal (**5**; 2.50 mL, 20 mmol, 1.0 equiv.) was added dropwise over 2 minutes. The reaction was stirred at -10 °C for 10 minutes, then a solution of TEMPO (3.75 g, 24 mmol, 1.2 equiv.) in 6 mL of acetone was added dropwise over 3 minutes. The reaction mixture was capped with a rubber septum and an air inlet line was attached via an 18-gauge needle. The reaction was stirred at -10 °C for 24 hours, then partitioned between ether (50 mL) and saturated NH_4Cl (150 mL). The aqueous layer was extracted with ether (2 × 150 mL) and the combined organic layers were washed with brine (300 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated to give an orange oil.. Flash column chromatography (3 % EtOAc / hexanes) gave α-oxygenated aldehyde **7** (79 % yield) as a colorless oil. A sample was derivatized [1. $NaBH_4$, MeOH; 2. *m*-nitrobenzoyl chloride, Et_3N, DMAP (cat.), CH_2Cl_2; 3. Zn, AcOH, THF, H_2O] and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 10 % *i*PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 10.7 (major), 12.3 (minor) minutes] to have 86:14 er. Another sample was converted into (*S*)-1,2-decanediol (1. $NaBH_4$, MeOH; 2. Zn, AcOH, THF, H_2O) and its optical rotation was compared with that of the commercial substance in order to confirm the absolute configuration. **3:** R_f = 0.37 (5 % EtOAc / hexanes); $[\alpha]_D^{23} = -102.5$ ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 2931, 1727 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 9.77 (d, *J* = 4.5 Hz, 1H), 4.07 (dt, *J* = 9.8, 5.0 Hz, 1H),

1.73 (m, 1H), 1.65 (m, 1H), 1.48 – 1.41 (m, 4H), 1.37 – 1.22 (m, 14H), 1.20 – 1.10 (m, 12H), 0.88 (t, J = 7.0 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 204.8, 88.7, 40.3, 32.0, 30.1, 29.8, 29.5, 29.3, 24.4, 22.8, 17.3, 14.2 ppm; HRMS (ESI-QTOF) calcd for $C_{19}H_{38}NO_2^+$ [M + H^+]: 312.2903, found: 312.2904.



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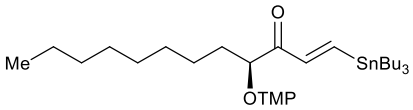
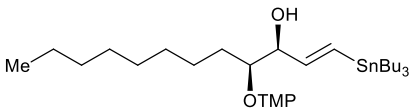
Vinylstannane 10: To a deoxygenated solution (3 × freeze–pump–thaw) of *trans*-1,2-bis(tributylstannyl)ethene (**8**) (16.4 g, 27 mmol, 1.8 equiv.) in 50 mL of THF at 0 °C was added *n*- BuLi (2.5 M in hexanes, 10.8 mL, 27 mmol, 1.8 equiv.) dropwise over 5 minutes. The resultant yellow solution was stirred at 0 °C for 30 minutes, cooled to –78 °C, then transferred by cannula to a deoxygenated solution (3 × freeze–pump–thaw) of aldehyde **7** (4.67 g, 15 mmol, 1.0 equiv.) in 15 mL of THF at –78 °C. The reaction was warmed to ambient temperature by removing the cooling bath, then partitioned between saturated NH_4Cl (50 mL) and EtOAc (50 mL). The organic phase was washed with water (2 × 50 mL) and brine (50 mL), dried over Na_2SO_4, and concentrated to give a yellow oil. Flash column chromatography (2% ether / hexanes) gave vinylstannane **10** (7.43 g, 79% yield) as a colorless oil as well as epimeric vinylstannane **11** contaminated with a trace of vinylstannane **10** (752 mg, 8% yield). A small sample was elaborated to oxylipin (6*R*,9*S*,10*S*)-**23** using a Luche reduction ($NaBH_4$, $CeCl_3$, MeOH) instead of a CBS reduction and determined to have 86:14 er. **5:** R_f = 0.35 (5% EtOAc / hexanes); $[\alpha]^{D23}$ = +16.4 ° (c = 1.34, $CHCl_3$); IR (thin film): ν_{max} = 3683, 3019, 2928, 1465 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 6.19 (dd, J = 19.1, 1.0 Hz, 1H), 6.08 (dd, J = 19.2, 5.6, 1H), 4.39 (dt, J= 5.0, 1.3 Hz, 1H), 3.98 (m, 1H), 2.47 (d, J = 6.9 Hz, 1H), 1.80 (m, 1H), 1.60 – 1.41 (m, 11H) 1.39 – 1.20 (m, 23H), 1.16 – 1.09 (m, 9H), 0.88 (m, 18H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 147.2, 129.2, 84.7, 76.3,

60.3, 40.8, 34.5, 32.0, 30.3, 29.7, 29.5, 29.3, 29.0, 27.4, 26.7, 22.8, 20.8, 20.6, 17.4, 14.2, 13.8, 9.6 ppm; HRMS (ESI-QTOF) calcd for $C_{33}H_{68}NO_2Sn^+$ [M + H^+]: 630.4272, found: 630.4308.



25

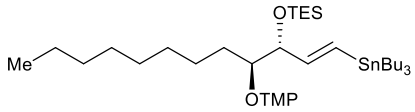
Enone 25: To a solution of vinylstannane **10** (654 mg, 1.04 mmol, 1.0 equiv.) in 3 mL of THF was added a solution of IBX (378 mg, 1.36 mmol, 1.3 equiv.) in 1 mL of DMSO. The reaction mixture was stirred for 1.5 hours, then diluted with 50 mL of ether and filtered. The organic phase was washed with water (3 × 50 mL) and brine (30 mL), dried over Na_2SO_4, and concentrated to give enone **25** (627 mg, 96 %) as a yellow oil. **25:** R_f = 0.46 (5 % EtOAc / hexanes); $[\alpha]_D^{23}$ = –47.0 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 2927, 1697, 1464 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.77 (d, *J* = 19.5 Hz, 1H), 6.99 (d, *J* = 19.5 Hz, 1H), 4.28 (dd, *J* = 9.9, 3.8 Hz, 1H), 1.89 (m, 1H), 1.74 (m, 1H), 1.59 – 1.06 (m, 39H), 1.04 – 0.91 (m, 9H), 0.87 (m, 12H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 198.8, 150.9, 142.3, 90.6, 59.8, 40.5, 29.8, 29.3, 27.5, 24.5, 22.8, 17.3, 14.2, 13.8, 9.9 ppm; HRMS (ESI-QTOF) calcd for $C_{33}H_{66}NO_2Sn^+$ [M + H^+]: 628.4116, found: 628.4116.



11

Allylic alcohol 11: To a solution of enone **25** (700 mg, 1.11 mmol, 1.0 equiv.) in 2.7 mL of THF and 8.3 mL of MeOH was added $CeCl_3 \cdot 7H_2O$ (834 mg, 2.24 mmol, 2.0 equiv.). The reaction mixture was stirred for 15 minutes, then cooled to –20 °C. $NaBH_4$ (43 mg, 1.11 mmol, 1.0 equiv.) was added, and since TLC analysis showed remaining enone **25** additional $NaBH_4$ (22 mg, 0.56 mmol, 0.5 equiv.) was added. The reaction mixture was partitioned between ether (50 mL) and water (100 mL). The aqueous layer was extracted with ether (100 mL), and the combined organic layers were washed with brine (50 mL), dried

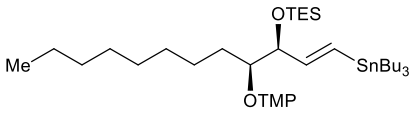
over Na_2SO_4, and concentrated to give a colorless oil. Flash column chromatography (2% ether / hexanes) gave allylic alcohol **11** (573 mg, 82% yield) as a colorless oil as well as epimeric allylic alcohol **10** (43 mg, 6% yield). A small sample was elaborated to oxylipin (6*R*,9*S*,10*S*)-**23** using a Luche reduction (NaBH4, CeCl3, MeOH) instead of a CBS reduction and determined to have 86:14 er. **11:** R_f = 0.34 (5% EtOAc / hexanes); $[\alpha]^{D23}$ = –20.0 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max}= 3576, 3018, 2925, 1465 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.48 (br s, 1H), 6.27 (d, *J* = 19.0 Hz, 1H), 5.87 (dd, *J* = 18.9, 6.4 Hz, 1H), 4.31 (t, *J* = 7.6 Hz, 1H), 3.87 (td, *J* = 8.4, 2.5 Hz, 1H), 1.63 – 1.24 (m, 38H), 1.18 (br s, 3H), 1.13 (br s, 3H), 0.88 (t, *J* = 7.5 Hz, 18H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 147.5, 131.0, 82.8, 80.8, 61.8, 60.2, 40.5, 40.0, 34.6, 32.1, 32.0, 31.4, 30.0, 29.6, 29.4, 29.2, 27.4, 25.6, 22.8, 17.3, 14.2, 13.8, 9.6 ppm; HRMS (ESI-QTOF) calcd for $C_{33}H_{68}NO_2Sn^+$ [M + H^+]: 630.4272, found: 630.4286.



12

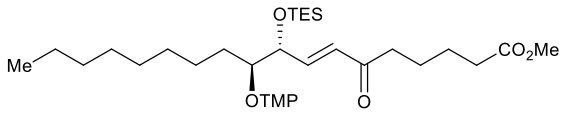
Silyl ether 8: To a solution of alcohol **10** (1.25 g, 2 mmol, 1.0 equiv.) and imidazole (204 mg, 3 mmol, 1.5 equiv.) in 8 mL of DMF was added TESCl (402 μL, 2.4 mmol, 1.2 equiv.) dropwise over 2 minutes. The reaction mixture was stirred for 45 minutes, then partitioned between water (50mL) and ether (100 mL). The organic phase was washed with water (3 × 50 mL) and brine (50 mL), dried over Na_2SO_4, and concentrated to give a colorless oil**.** Flash column chromatography (1% ether / hexanes) gave silyl ether **12** (1.48 g, 86% yield) as a colorless oil. **12:** R_f = 0.56 (5% EtOAc / hexanes); $[\alpha]^{D23}$ = –17.0 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3054, 2957, 1421 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 6.10 (dd, *J* = 19.0, 6.8 Hz, 1H), 6.03 (d, *J* = 19.2 Hz, 1H), 4.20 (dd, *J* = 6.4, 2.7 Hz, 1H), 3.83 (m, 1H), 1.94 (m, 1H), 1.62 – 1.13 (m, 37H), 1.07 (m, 6H), 0.95 (t, *J* = 7.9 Hz, 9H), 0.88 (t, *J* =

7.4 Hz , 18H), 0.59 (q, J = 7.8 Hz, 6H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 149.4, 128.6, 86.3, 79.3, 60.9, 59.4, 40.6, 34.6, 32.1, 30.4, 30.1, 29.8, 29.5, 29.4, 27.5, 27.0, 22.9, 20.8, 17.5, 14.3, 13.9, 9.6, 7.1, 5.4 ppm; HRMS (ESI-QTOF) calcd for $C_{39}H_{82}NO_2SnSi^+$ [M + H^+]: 744.5137, found: 744.5185.



26

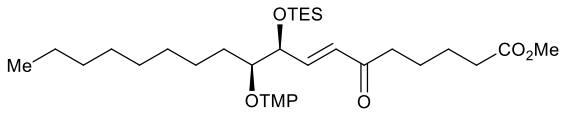
Silyl ether 26 was prepared in the same manner as TES ether **12**. Flash column chromatography (1% EtOAc / hexanes) gave a colorless oil that was contaminated with TESOH.



14

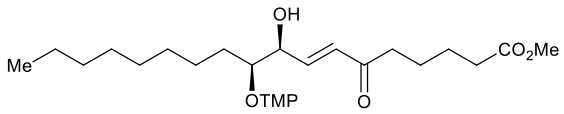
Enone 10: To a deoxygenated solution (3 × freeze–pump–thaw) of vinylstannane **10** (1.27 g, 1.7 mmol, 1.0 equiv.), $PCy_3{\cdot}HBF_4$ (31 mg, 85 µmol, 0.05 equiv.), *i*-Pr_2NEt (15 µL, 85 µmol, 0.05 equiv.), and $Pd_2(dba)_3$ (38 mg, 43 µmol, 0.025 equiv.) in 34 mL of toluene was added acid chloride **13** (528 µL, 3.4 mmol, 2.0 equiv.) dropwise over 2 minutes. The reaction mixture was heated at 50 °C for 45 minutes, then cooled and diluted with 75 mL EtOAc. The organic phase was washed with 3% aq. NH_4OH (85 mL), water (2 × 75 mL), and brine (75 mL), dried over Na_2SO_4, and concentrated to give a yellow oil. Flash column chromatography (8% EtOAc / hexanes) gave enone **14** (914 mg, 89% yield) as a colorless oil. **14:** R_f = 0.36 (10% EtOAc / hexanes); $[\alpha]^{D23}$ = +21.0 ° (c = 1.10, $CHCl_3$); IR (thin film): ν_{max} = 3022, 2929, 1733, 1670 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 6.91 (dd, J = 16.1, 5.9 Hz, 1H), 6.20 (dd, J = 16.0, 1.4 Hz, 1H), 4.40 (ddd, 5.8, 2.6, 1.4 Hz, 1H), 3.91 (m, 1H), 3.67 (s, 3H), 2.59 (m, 2H), 2.33 (m, 2H), 2.03 (m, 1H), 1.70 – 1.62 (m, 4H), 1.51 – 1.37 (m, 4H), 1.35 – 1.23 (m, 15H), 1.19 (br s, 3H), 1.15 (br s, 3H), 1.05 (br s, 3H), 1.03 (br s, 3H), 0.96 (t, 8.0 Hz, 9H), 0.88 (t, 6.9 Hz, 3H), 0.60 (q, 7.9

Hz, 6H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.3, 174.0, 147.3, 129.3, 86.3, 74.6, 61.0, 59.4, 51.6, 40.7, 40.4, 39.5, 34.6, 34.4, 34.0, 32.0, 30.21, 30.17, 29.7, 29.4, 27.0, 24.7, 23.8, 22.8, 20.8, 20.6, 17.4, 14.2, 7.0, 5.1 ppm; HRMS (ESI-QTOF) calcd for $C_{34}H_{66}NO_5Si^+$ [M + H^+]: 596.4705, found: 596.4704.



15

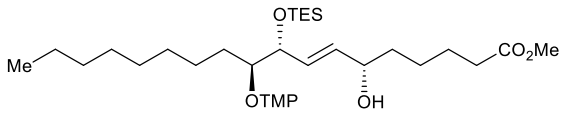
Enone 15 was prepared in the same manner as enone **14**. Flash column chromatography (8% EtOAc / hexanes) gave enone **12** (84% yield over two steps) as a colorless oil. **12:** R_f = 0.38 (10% EtOAc / hexanes); $[\alpha]^{D23}$ = −60.0 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3022, 2955, 1737, 1695, 1678, 1458 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.02 (dd, *J* = 15.9, 3.6 Hz, 1H), 6.32 (d, *J* = 15.9 Hz, 1H), 4.70 (m, 1H), 3.86 (m, 1H), 3.67 (s, 3H), 2.60 (m, 2H), 2.34 (m, 2H), 1.66 (m, 5H), 1.58 – 1.18 (m, 19H), 1.12 (br s, 12H), 0.96 (t, *J* = 8.0 Hz, 9H), 0.88 (t, *J* = 7.0 Hz, 3H), 0.61 (q, *J* = 7.9 Hz, 6H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.1, 174.0, 147.8, 129.1, 85.3, 72.3, 60.2, 51.6, 40.8, 39.8, 34.0, 32.0, 30.2, 29.7, 29.4, 26.9, 24.7, 23.8, 22.8, 20.6, 17.4, 14.2, 7.0, 5.0 ppm; HRMS (ESI-QTOF) calcd for $C_{34}H_{66}NO_5Si^+$ [M + H^+]: 596.4705, found: 596.4712.



20

Alcohol 20: To a solution of silyl ether **15** (380 mg, 0.64 mmol, 1.0 eqiv.) in 2.5 mL of THF was added TBAF (1.0 M in THF, 1.92 mL, 1.92 mmol, 3.0 equiv) over 2 minutes. The reaction mixture was stirred for 10 minutes, then partitioned between water (20mL) and EtOAc (20 mL). The organic phase was washed with water (3 × 10 mL) and brine (10 mL), dried over Na_2SO_4, and concentrated to give a colorless oil. Flash column chromatography (13% EtOAc / hexanes) gave alcohol **20** (256 mg, 84% yield) as a colorless oil. **20:** R_f = 0.26 (20% EtOAc / hexanes); $[\alpha]^{D23}$ = −24.0 ° (*c* =

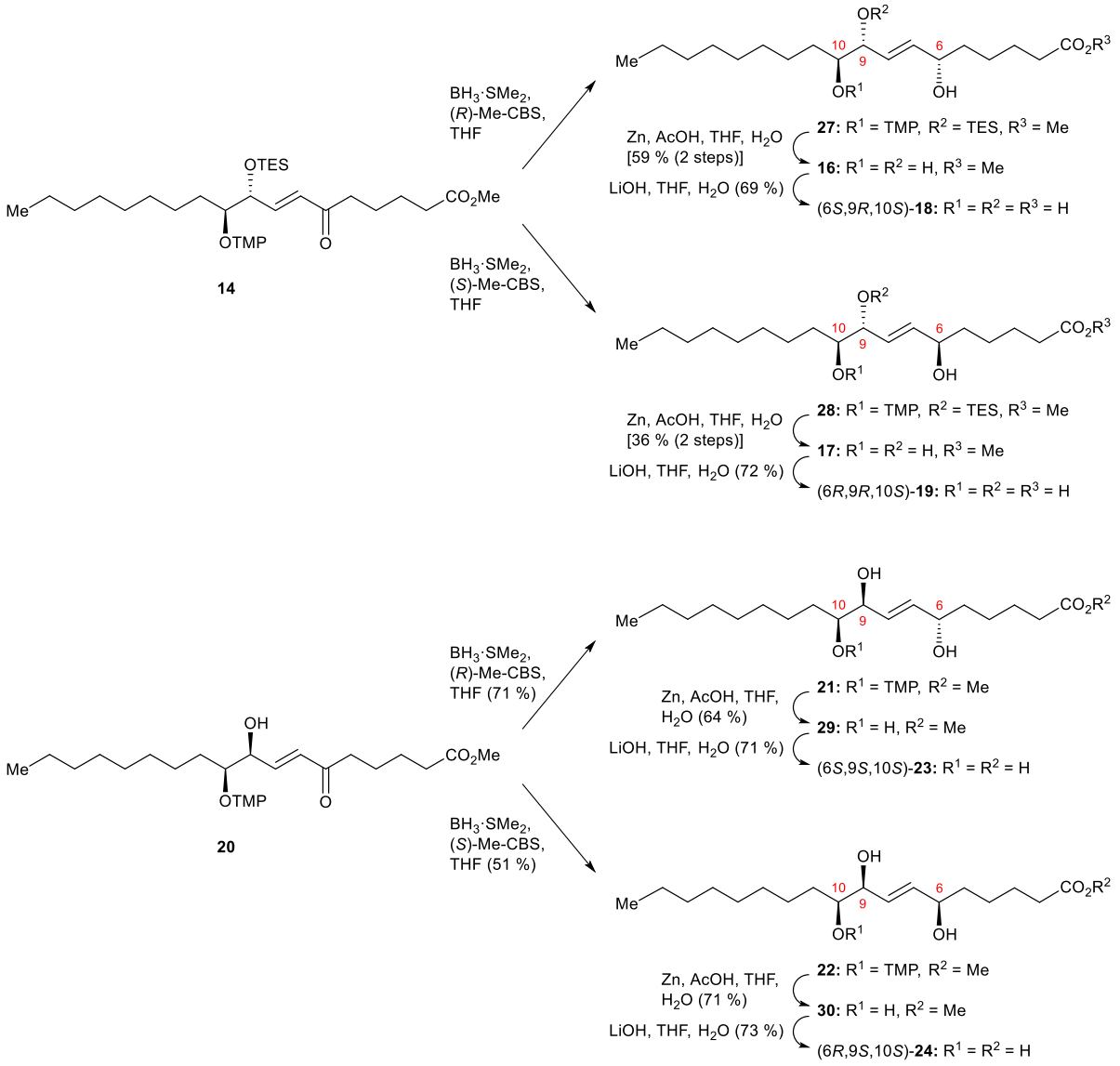
1.00, $CHCl_3$); IR (thin film): ν_{max} = 3674, 3054, 2929, 1695, 1677, 1633 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.86 (br s, 1H), 6.72 (dd, *J* = 15.7, 5.1 Hz, 1H), 6.45 (d, *J* = 15.8 Hz, 1H), 4.57 (m, 1H), 3.89 (m, 1H), 3.66 (s, 3H), 2.57 (m, 2H), 2.33 (m, 2H), 1.67 – 1.63 (m, 4H), 1.54 – 1.22 (m, 26H), 1.19 (br s, 3H), 1.14 (br s, 3H), 0.88 (t, *J* = 7.0 Hz, 3H), ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 199.8, 173.9, 144.2, 129.7, 82.7, 76.2, 62.0, 60.4, 51.6, 40.8, 40.5, 40.0, 34.6, 34.0, 31.99, 31.95, 31.3, 29.9, 29.6, 29.4, 25.4, 24.6, 23.5, 22.8, 20.72, 20.66, 17.2, 14.2 ppm; HRMS (ESI-QTOF) calcd for $C_{28}H_{52}NO_5^+$ [M + H^+]: 482.3840, found: 482.3844.



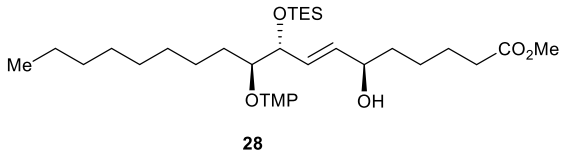
27

Allylic alcohol 27: To a solution of enone **14** (200 mg, 0.34 mmol, 1.0 equiv.) in 150 µL of THF at −78 °C was added a pre-mixed solution of (*R*)-Me- CBS (122 mg, 0.44 mmol, 1.3 equiv.) and $BH_3{\cdot}SMe_2$ (2 M in THF, 220 µL, 0.44 mmol, 1.3 equiv.) dropwise over 1 minute. After 5 minutes the reaction mixture was warmed to 0 °C and quenched by adding 50 µL of methanol and 10 µL of 4 *N* HCl. After stirring at ambient temperature for 30 minutes, the reaction mixture was diluted with EtOAc (10 mL). The organic layer was washed with water (2 × 10 mL), brine (10 mL), and saturated $NaHCO_3$ (10 mL), dried over Na_2SO_4, and concentrated to give a yellow oil as a 5.7:1 mixture of diastereomers. Flash column chromatography (40% EtOAc / hexanes) gave allylic alcohol **27** as a mixture of diastereomers that was a colorless oil. A sample was converted into methyl (*S*)-6,7-dihydroxyheptanoate (1. O_3, MeOH, THF; then Me_2S; 2. $NaBH_4$, EtOH) and its optical rotation was compared with that of the known substance[18] to confirm the absolute configuration.

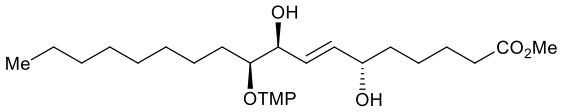
Scheme 2: Synthesis of oxylipins



Allylic alcohols 21, 22, 28 were prepared in the same manner as allylic alcohol **27**.

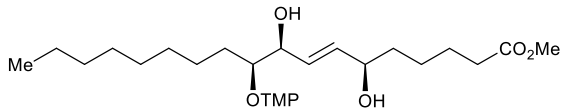


Allylic alcohol 28: Flash column chromatography (40% EtOAc / hexanes) gave allylic alcohol **17** (2.0:1 mixture of diastereomers) as a colorless oil.



21

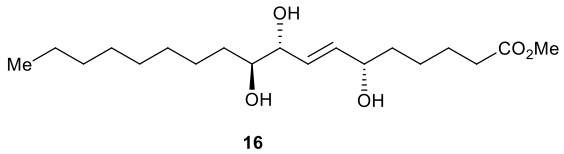
Allylic alcohol 21: Flash column chromatography (40% EtOAc / $CHCl_3$) gave allylic alcohol **21** in 68% yield as a colorless oil and epimeric alcohol **22** in 13% yield. **21:** R_f = 0.38 (40% EtOAc / $CHCl_3$); $[\alpha]^{D23}$ = −40.4 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3457, 3014, 2924, 1729 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.66 (br s, 1H), 5.80 (dd, *J* = 15.4 Hz, 6.0 Hz, 1H), 5.59 (dd, *J* = 15.4 Hz, 6.7 Hz, 1H), 4.35 (t, *J* = 7.7 Hz, 1H), 4.13 (m, 1H), 3.86 (t, *J* = 8.2 Hz, 1H), 3.66 (s, 3H), 2.31 (t, *J* = 7.5 Hz, 2H), 1.78 – 1.20 (m, 33H), 1.17 (s, 3H), 1.12 (s, 3H), 0.87 (t, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 174.3, 135.6, 130.0, 82.9, 72.1, 61.9, 60.3, 51.6, 40.5, 40.0, 36.9, 34.6, 34.1, 32.1, 32.0, 31.4, 30.0, 29.7, 29.4, 25.6, 25.1, 25.0, 22.8, 20.74, 20.67, 17.3, 14.2 ppm; HRMS (ESI-QTOF) calcd for $C_{28}H_{54}NO_5^+$ [M + H^+]: 484.3997, found: 484.4002.



22

Allylic alcohol 22: Flash column chromatography (40% EtOAc / $CHCl_3$) gave allylic alcohol **22** in 51% yield as a colorless oil, epimeric alcohol **21** in 7% yield, and a mixture of the two epimers in 7% yield. **22:** R_f = 0.33 (40% EtOAc / hexanes); $[\alpha]^{D23}$ = −20.2 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3357, 3924, 1739 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.70 (br s, 1H), 5.80 (dd, *J* = 15.6 Hz, 7.0 Hz, 1H), 5.58 (dd, *J* = 15.4 Hz, 6.8 Hz, 1H), 4.36 (t, *J* = 7.7 Hz, 1H), 4.11 (m, 1H), 3.88 (t, *J* = 8.2 Hz, 1H), 3.66 (s, 3H), 2.30 (t, *J* = 7.5 Hz, 2H), 1.70 – 1.20 (m, 33H), 1.18 (s, 3H), 1.13 (s, 3H), 0.88 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 174.2, 135.5, 130.5, 83.0, 72.5, 51.6, 40.5, 40.0, 36.9, 34.59, 34.56, 34.1, 32.0, 31.5, 30.0, 29.7, 29.4, 25.5, 25.2,

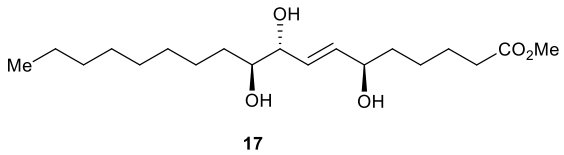
25.0, 22.8, 20.8, 20.7, 17.3, 14.2 ppm; HRMS (ESI-QTOF) calcd for $C_{28}H_{54}NO_5^+$ [M + H^+]: 484.3997, found: 484.4002.



16

Triol 16. To a solution of alcohol **27** (240 mg, 0.77 mmol, 1.0 equiv) in 5 mL of a 3:1:1 solvent mixture (HOAc:H_2O:THF) was added zinc (500mg, 7.7 mmol, 10 equiv.). The reaction mixture was stirred at 70 °C for one hour. After cooling, the reaction mixture was filtered through Celite, concentrated, and azeotroped dried with toluene to give a white solid. Flash column chromatography (85% EtOAc / hexanes) gave triol **16** (59% yield over two steps) as a white solid as well as epimeric triol **17** (11% yield). **16:** R_f = 0.21 (80% EtOAc / hexanes); $[\alpha]^{D23}$ = +8.2 ° (*c* = 0.6, MeOH); IR (thin film): ν_{max} = 3332, 2920, 2844, 1732, cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 5.73 (dd, *J* = 15.6 Hz, 6.3 Hz, 1H), 5.67 (dd, *J* = 15.8 Hz, 6.4 Hz, 1H), 4.05 (q, *J* = 6.3 Hz, 1H), 3.92 (dd, *J* = 6.3 Hz, 4.7 Hz, 1H), 3.65 (s, 3H), 3.49 (m, 1H), 2.33 (t, *J* = 7.4 Hz, 2H), 1.63 (m, 2H), 1.59 – 1.26 (m, 18H), 0.90 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (150 MHz, CD_3OD): δ = 175.9, 136.4, 131.0, 76.5, 75.7, 73.0, 52.0, 38.0, 34.8, 33.8, 33.1, 30.9, 30.7, 30.4, 27.0, 26.1, 26.0, 23.7, 14.4 ppm; HRMS (ESI-QTOF) calcd for $C_{19}H_{36}O_5Na^+$ [M + Na^+]: 367.2460, found: 367.2455.

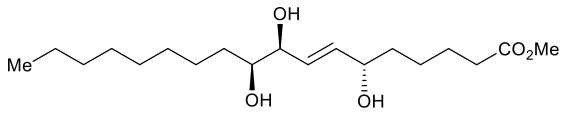
Triols 17, 29, 30 were prepared in the same manner as triol **16**.



17

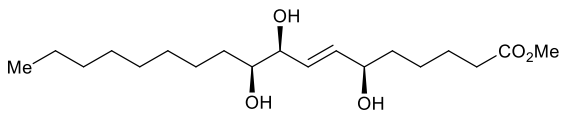
Triol 17. Flash column chromatography (85% EtOAc / hexanes) gave triol **17** (36% yield over two steps) as a white solid as well as epimeric triol **16** (23% yield). **17:** R_f = 0.26 (80% EtOAc / hexanes); $[\alpha]^{D23}$ = −6.8 ° (*c* = 0.25, MeOH); IR (thin film): ν_{max} = 3278, 2929, 2847, 1730 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ

= 5.73 (dd, *J* = 15.7 Hz, 6.1 Hz, 1H), 5.69 (dd, *J* = 15.6 Hz, 5.9 Hz, 1H), 4.06 (q, *J* = 6.0 Hz, 1H), 3.92 (t, *J* = 5.4 Hz, 1H), 3.65 (s, 3H), 3.47 (m, 1H), 2.33 (t, *J* = 7.4 Hz, 2H), 1.63 (m, 2H), 1.57 – 1.20 (m, 18H), 0.90 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (150 MHz, CD_3OD): δ = 175.9, 136.4, 131.1, 76.5, 75.7, 72.9, 52.0, 37.9, 34.8, 33.6, 33.1, 30.9, 30.7, 30.5, 27.0, 26.1, 26.0, 23.7, 14.4 ppm; HRMS (ESI-QTOF) calcd for $C_{19}H_{36}O_5Na^+$ [M + Na^+]: 367.2460, found: 367.2464.



29

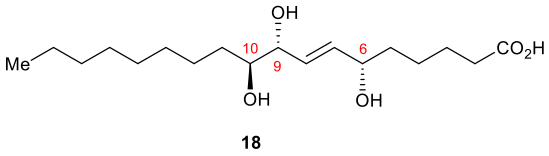
Triol 29: Flash column chromatography (85% EtOAc / hexanes) gave triol **29** (64% yield) as a white solid. **29:** R_f = 0.36 (80% EtOAc / hexanes); $[\alpha]^{D23}$ = −11.4° (*c* = 0.50, MeOH); IR (thin film): ν_{max} = 3357, 3313, 2924, 2841, 1739 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 5.70 (m, 2H), 4.05 (q, *J* = 6.1 Hz, 1H), 3.90 (t, *J* = 5.6 Hz, 1H), 3.65 (s, 3H), 3.41 (m, 1H), 2.33 (t, *J* = 7.5 Hz, 2H), 1.63 (m, 2H), 1.58 – 1.25 (m, 18H), 0.90 (t, *J* = 6.22, 3H) ppm; ^{13}C NMR (150 MHz, CD_3OD): δ = 175.9, 136.4, 131.2, 76.5, 75.8, 72.8, 52.0, 38.0, 34.8, 33.6, 33.1, 30.9, 30.7, 30.5, 26.9, 26.1, 26.0, 23.7, 14.4 ppm; HRMS (ESI-QTOF) calcd for $C_{19}H_{36}O_5Na^+$ [M + Na^+]: 367.2460, found: 367.2461.



30

Triol 30: Flash column chromatography (85% EtOAc / hexanes) gave triol **30** (71% yield) as a white solid. **30:** R_f = 0.29 (80% EtOAc / hexanes); $[\alpha]^{D23}$ = −36.3° (*c* = 0.30, MeOH); IR (thin film): ν_{max} = 3537, 3313, 2924, 2841, 1739 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 5.70 (dd, *J* = 15.6 Hz, 6.0 Hz, 1H), 5.65 (dd, *J* = 15.6 Hz, 6.2 Hz, 1H), 4.04 (q, *J* = 6.4 Hz, 1H), 3.88 (t, *J* = 6.1 Hz, 1H), 3.65 (s, 3H), 3.40 (m, 1H), 2.33 (t, *J* = 7.4 Hz, 2H), 1.63 (m, 2H), 1.59 – 1.21 (m, 18H) 0.90 (t, *J* = 6.4 Hz, 3H)

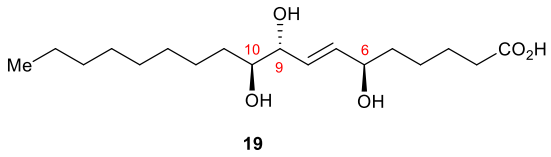
ppm; ^{13}C NMR (150 MHz, CD_3OD): δ = 175.9, 136.6, 131.4, 76.6, 75.7, 72.9, 52.0, 37.9, 34.8, 33.8, 33.1, 30.9, 30.7, 30.4, 26.8, 26.1, 26.0, 23.8, 14.5 ppm; HRMS (ESI-QTOF) calcd for $C_{19}H_{36}O_5Na^+$ [M + Na^+]: 367.2460, found: 367.2460.



18

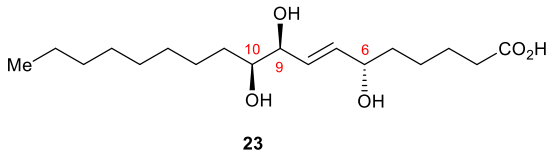
Oxylipin 18: To a solution of triol **16** (20 mg, 0.056 mmol, 1.0 equiv.) in THF (2.7 mL) was added 0.3 mL of an aqueous 1.0 M LiOH solution over one minute. The reaction mixture was stirred overnight, then partitioned between EtOAc (5 mL) and 1 *N* HCl (5 mL). The organic phase was washed with water (2 × 5 mL) and brine (5 mL), dried over Na_2SO_4, and concentrated to give a white solid. Flash column chromatography (0 – 10% MeOH / EtOAc) gave oxylipin **18** (13 mg, 69% yield) as a white solid. A sample was derivatized (*p*-nitrobenzyl amine·HCl, BOP–BF_4, HOBt, *i*-Pr_2NEt, DMF) and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 12% *i*-PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 11.3 (major), 12.7 (minor) minutes] to have 98:2 er.**18:** R_f = 0.29 (100% EtOAc); $[\alpha]^{D23}$ = +4.4 ° (*c* = 0.9, MeOH); IR (thin film): ν_{max}= 3386, 3019, 2941, 1712 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 5.73 (dd, *J* = 15.6 Hz, 6.4 Hz, 1H), 5.67 (dd, *J* = 15.6 Hz, 6.2 Hz, 1H), 4.06 (q, *J* = 6.2 Hz, 1H), 3.92 (t, *J* = 5.3 Hz, 1H), 3.49 (m, 1H), 2.29 (t, *J* = 7.2 Hz, 2H), 1.62 (m, 2H) 1.59 – 1.22 (m, 18H), 0.90 (t, *J* = 6.5 Hz, 3H) ppm; ^{13}C NMR (150 MHz, CD_3OD): δ = 177.7, 136.5, 131.0, 76.5, 75.7, 73.1, 38.0, 35.1, 33.8, 33.1, 30.9, 30.7, 30.4, 27.0, 26.2, 26.1, 23.7, 14.4 ppm; HRMS (ESI-QTOF) calcd for $C_{18}H_{34}O_5Na^+$ [M + Na^+]: 353.2304, found: 353.2301.

The other diastereomers of oxylipins from *D. lortense* were prepared in the same manner as oxylipin **18**.



19

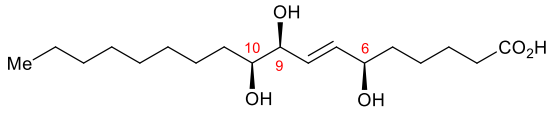
Oxylipin 19: Flash column chromatography (0 – 5% MeOH / EtOAc) gave oxylipin **20** (72% yield) as a white solid. A sample was derivatized (*p*-nitrobenzyl amine·HCl, BOP–BF_4, HOBt, *i*-Pr_2NEt, DMF) and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 12% *i*-PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 11.8 (major), 9.9 (minor) minutes] to have 97:3 er. **20:** R_f = 0.18 (5% MeOH / $CHCl_3$); $[\alpha]^{D23}$ = −14.6 ° (*c* = 0.15, MeOH); IR (thin film): ν_{max} = 3312, 2923, 1701 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 5.74 (dd, *J* = 15.6 Hz, 6.1 Hz, 1H), 5.69 (dd, *J* = 15.6 Hz, 6.0 Hz, 1H), 4.06 (q, 6.0 Hz, 1H), 3.92 (t, *J* = 6.0 Hz, 1H), 3.47 (ddd, *J* = 9.0, 4.9, 3.0 Hz, 1H), 2.29 (t, *J* = 7.5 Hz, 2H), 1.62 (m, 2H), 1.59 – 1.23 (m, 18H), 0.90 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (150 MHz, CD_3OD): 136.4, 131.1, 76.6, 75.7, 73.0, 38.0, 35.1, 33.6, 33.1, 30.9, 30.8, 30.5, 27.0, 26.2, 26.1, 23.7, 14.4 ppm; HRMS (ESI-QTOF) calcd for $C_{18}H_{34}O_5Na^+$ [M + Na^+]: 353.2304, found: 353.2304.



23

Oxylipin 23: Flash column chromatography (0 – 5% MeOH / EtOAc) gave oxylipin **23** (71% yield) as a white solid. A sample was derivatized (*p*-nitrobenzyl amine·HCl, BOP–BF_4, HOBt, *i*-Pr_2NEt, DMF) and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 12% *i*-PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 11.3 (major), 14.0 (minor) minutes] to have 97:3 er. **23:** R_f = 0.23 (10% MeOH / $CHCl_3$); $[\alpha]^{D23}$ = −21.2 ° (*c* = 0.25, MeOH); IR (thin film): ν_{max} = 3338, 2914, 1700 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 5.72 (dd, *J* = 15.6 Hz, 5.6 Hz, 1H), 5.68 (dd, *J* = 15.6 Hz, 5.9 Hz, 1H), 4.06 (q, *J* = 6.1 Hz, 1H), 3.91 (t, *J* = 5.6 Hz, 1H), 3.42 (ddd, *J* = 8.9, 5.9, 3.2 Hz, 1H), 2.28 (t, *J* = 7.4 Hz, 2H), 1.62 (m, 2H), 1.58 – 1.22 (m,

18H), 0.90 (t, J = 7.0 Hz, 3H) ppm; ^{13}C NMR (150 MHz, CD_3OD): δ = 136.3, 131.0, 76.4, 75.6, 72.7, 37.9, 35.3, 33.4, 32.9, 30.7, 30.6, 30.3, 26.8, 26.1, 26.0, 23.6, 14.3 ppm; HRMS (ESI-QTOF) calcd for $C_{18}H_{34}O_5Na^+$ [M + Na^+]: 353.2304 found: 353.2302.



24

Oxylipin 24: Flash column chromatography (0 – 5% MeOH / EtOAc) gave oxylipin **24** (73% yield) as a white solid. A sample was derivatized (*p*-nitrobenzyl amine·HCl, BOP–BF_4, HOBt, *i*-Pr_2NEt, DMF) and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 12% *i*-PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 14.4 (major), 11.8 (minor) minutes] to have 96:4 er. **24:** R_f = 0.19 (10% MeOH / $CHCl_3$); $[\alpha]^{D23}$ = −30.4 ° (c = 0.25, MeOH); IR (thin film): ν_{max} = 3395, 2917, 1686 cm^{-1}; ^{1}H NMR (600 MHz, CD3OD): δ = 5.71 (dd, J = 15.6 Hz, 6.1 Hz, 1H), 5.66 (dd, J = 15.6 Hz, 6.3 Hz, 1H), 4.05 (q, J = 6.3 Hz, 1H), 3.88 (t, J = 6.11, 1H), 3.40 (m, 1H), 2.29 (t, J = 7.5 Hz, 2H), 1.62 (m, 2H), 1.59 – 1.21 (m, 18H), 0.90 (t, J = 6.9 Hz, 3H) ppm; ^{13}C NMR (150 MHz, CD3OD): δ = 136.6, 131.4, 76.9, 75.6, 72.8, 38.2, 35.0, 33.8, 33.0, 30.9, 30.7, 30.4, 26.8, 26.2, 26.1, 23.7, 14.4 ppm; HRMS (ESI-QTOF) calcd for $C_{18}H_{34}O_5Na^+$ [M + Na^+]: 353.2304, found: 353.2303.

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11) Barua and co-workers[10c] apparently interpreted the reported relative configuration (9R*,10S*,7E)18 as an absolute assignment. They synthesized a pair of C6 epimers which have opposite signs of optical rotation and incorrectly assigned the stereochemistry of the natural oxylipin based on optical rotation. They did not notice any NMR discrepancies because their spectra were obtained in a different solvent(CDCl3) from that used by the isolation team (CD3OD).

12) Yadav and co-workers[10d] prepared (6S,9R,10S)-16 (enantiomer of the natural product) and obtained NMR spectra in CD3OD but only compared their synthetic product against the material prepared in the Sharma synthesis (NMR spectra in CDCl3, and no comparisonmade against the natural product).24a They do not address the opposite sign of optical rotation as compared with the natural oxylipin18 or the discrepancy with the Barua group's stereochemical assignment.[10c]

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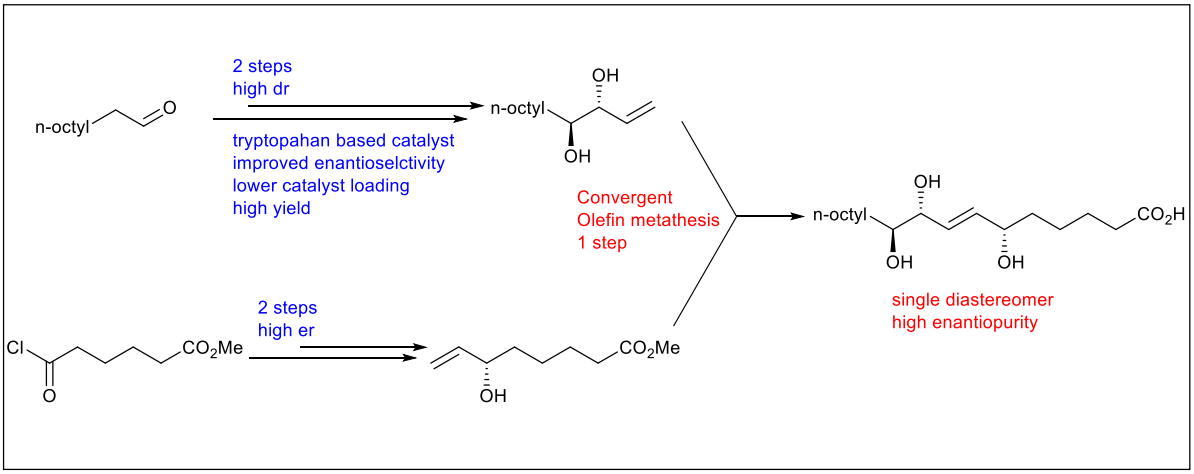
CHAPTER II: THREE STEP CONVERGENT SYNTHESIS OF OXYLIPINS FROM *DRACONTIUM LORTENSE*

Manuscript in preparation



Abstract

A much shorter convergent synthesis was developed using an olefin cross metatheis approach. Alkene diol fragment was prepared using the method developed to make chiral diol. Bulkier tryptophan based organocatalysts were now used for oxidative incorporation of TEMPO onto decanal with enhanced enantioselectivity and yield and much lower catalyst loading (now 5 mol% compared to 20 mol% of phenylalanine based organocatalyst). Nucleophilic addition to the α-oxoaldehyde and reductive cleavage of the masking group was carried out in one pot to furnish alkene fragment in just two steps. Alkene mono-ol fragment was also prepared in two steps via Stille cross coupling and enantioselective ketone reduction. The alkene fragments undergo cross metathesis and hydrolysis in one pot (scheme 2) to deliver single diastereomer of the natural product in only 3 steps with 33% overall yield.

Introduction

Our first generation synthesis of oxylipins required 7 steps. This was tied for the shortest synthesis of oxylipins containing the 3-en-1,2,5-triol moiety. We have subsequently envisioned a shorter synthesis. Furthermore, a significant shorter synthesis will allow us to consider using a bulkier tryptophan based catalyst to improve the enantioselectivity of the α-oxygenation step despite the catalyst multistep synthesis. The presence of multiple double bonds in the fatty acid chains of Nigricanoside A discouraged us from using an olefin cross metathesis approach which can introduce convergency. Furthermore, a convergent synthesis allows us to set chiral centers independently on individual fragments overcoming problems faced due to substrate bias in setting stereocenters. A highly efficient convergent synthesis was developed that furnished the natural product in just three steps.

Results and Discussion

In our previous oxylipins synthesis we used an HBF_4 salt of a phenylalanine based chiral imidazolidinone catalyst **3** in organocatalytic, enantioselective α-oxygenation of decanal. A subsequent chiral enhancing step from CBS reduction followed by a 5 step laborious synthesis of a tryptophan-based sterically demanding imidazolidinone catalyst led us to use a more accessible phenylalanine-based chiral imidazolidinone despite the moderate enantioselectivity in the α-oxygenation step. The significantly shorter current oxylipins synthesis and the need for superior enantioselectivity in α-oxygenation, led us to consider a more sterically demanding chiral imidazolidinone catalyst despite its multi-step synthesis (**Table 1**). Salts of tryptophan-based chiral imidazolidinone **4** were our default choice because it is the optimum catalyst in MacMillan's aldehyde α-oxygenation approach.[1] Also, recently our group successfully employed this tryptophan-based chiral imidazolidinone **4** as

the catalyst in the enantiomeric enrichment in catalytic, enantioselective α,β,γ-trioxygenation of enals.[2] The HBF_4 salt of tryptophan-based imidazolidinones **4** in acetone at -10 °C gave superior enantioselectivity and yield compared to phenylalanine-based imidazolidinone **3**. Fast reaction rates (20 mol% of **4**, 6 hours), high yields and the lengthy synthesis of catalyst **4** encouraged us to screen lower catalyst loadings. It was found that the catalyst loading can be lowered to 5 mol% when using imidazolidinones **4** with no meaningful reduction of both enantioselectivity (er = 89:11) and yield. Screening lower temperatures revealed that enantioselectivity at 5 mol% can be further improved when the temperature was lowered to -10 °C. However, at this catalyst loading the yield suffered when the temperature was decreased to – 78 °C. A further decrease in the catalyst loading to 2 mol% at 0 °C degraded the yield significantly but highest turnover number (40.0) for the catalyst was observed while retaining the enantioselectivity. Further lowering of temperature to -10 °C at 2 mol% catalyst loading degraded the yield although enantioselectivity was retained. Therefore, the tryptophan-based catalyst was now used for oxidative incorporation of TEMPO into decanal furnishing α-oxyaldehyde 2 (**Scheme 1**) in 94% yield and 93:7 er.

Table 1: Optimization of α-oxygenation[a]

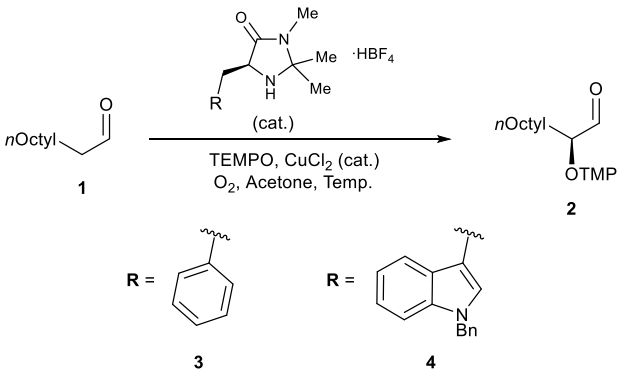
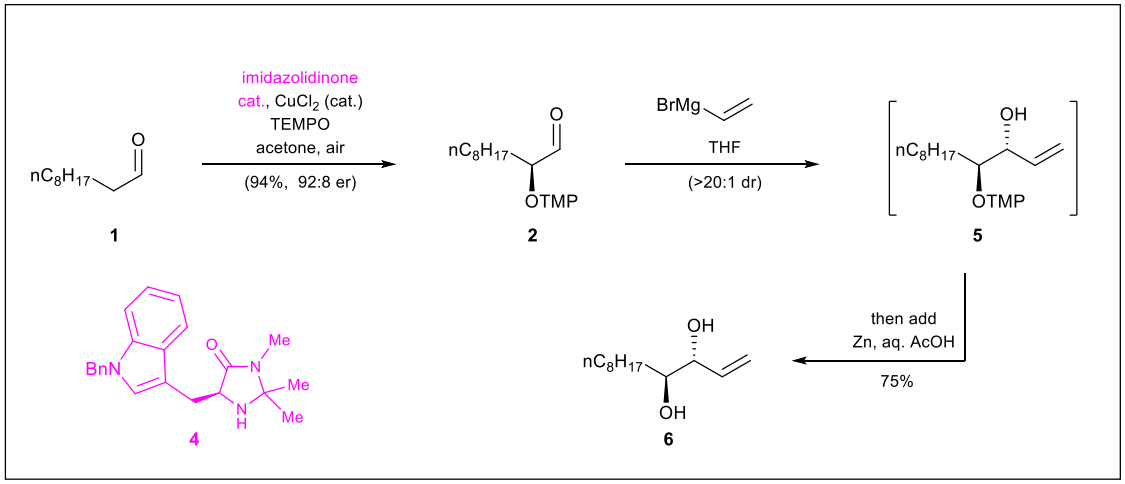


Table 1: continued

R	Cat. loading	Temp (°C)	yield[b] (%)	er[c]	Turnover number
3	20	-10	90	88:12	4.5
4	20	0	96	92:8	4.8
4	10	0	94	88:12	9.4
4	5	0	92	89:11	18.4
4	5	-10	94	92:8	18.8
4	2	0	80	91:9	40.0
4	2	-10	66	92:8	33.0

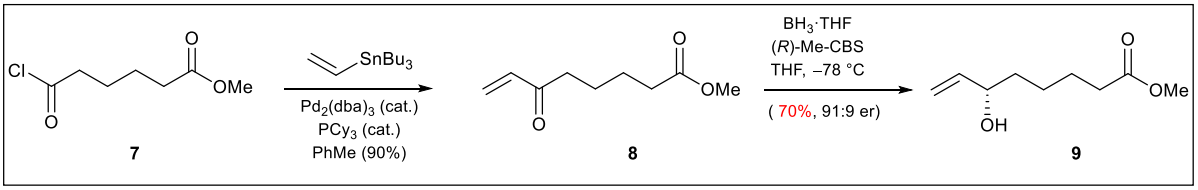
[a]2 mmol scale. [b]Isolated yield. [c]Determined by chiral HPLC analysis.

Nucleophilic vinyl Grignard addition to aldehyde **2** proceeded with high diastereoselectivities, consistent with earlier observation of high diastereoselectivity obtained with sp^2 nucleophiles (**Scheme 1**). Since the alcohol group protection did not influence the stereoselectivity in the cross metathesis reaction, the masking TMP group could be cleaved. Furthermore, since the nucleophilic addition was carried out in THF, a one pot nucleophilic addition and cleavage of the masking group was possible, reduceing the step count. In situ Grignard addition to form singly masked diol **5** and reductive cleavage of the masking group furnished the diol **6** in 75 % yield. The diol fragment was prepared in just two steps from readily available decanal **1**.



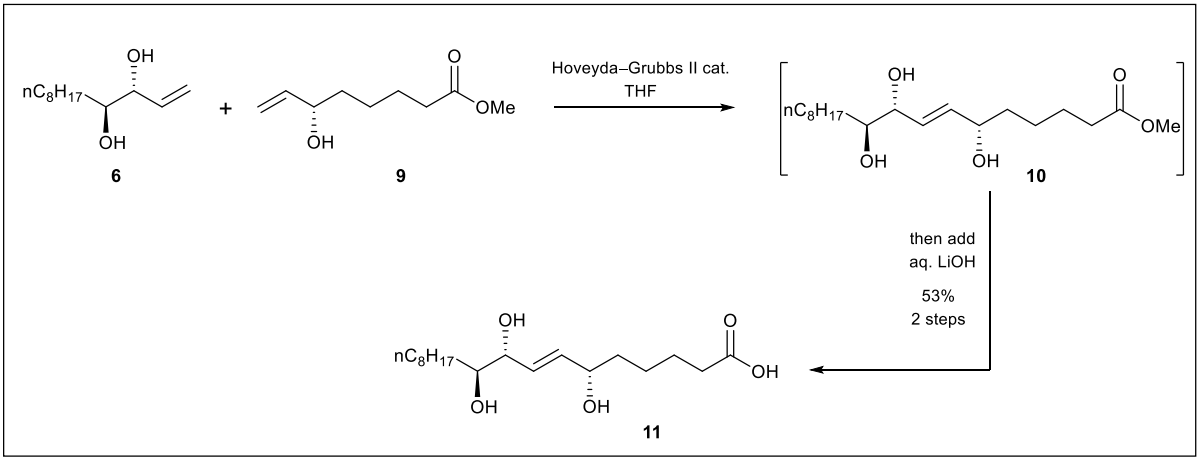
Scheme 1: Two step synthesis of diol fragment

Three routes, enantioselective allylic oxidation,[3] addition to aldehydes[4] and ketone reduction[5] were considered to synthesize mono-ol **9** (**Scheme 2**) in two steps. Enzyme mediated enantioselective allylic hydroxylation[3(b)] could furnish mono-ol **9** from readily available ethyl oct-7-enoate in just one step, but only produced the undesired enantiomer. Preliminary investigation of enantioselective vinyl bromide addition to methyl-6-oxohexanoate (prepared in one step from cyclohexene) did not yield promising results. Therefore, we pursued enantioselective ketone reductions. Stille cross coupling was used to couple tributylvinylstannane and acid chloride **7**, providing enone **8** in 90% yield. Reduction of enone **8** using BH_3•THF in the presence of chiral Me-CBS-oxazoborolidinone ligand furnished monol **9** in 90:10 er and 70% yield. Competitive 1,4-conjugate hydride addition to the terminal enone lowered the yield of the asymmetric ketone reduction step. Noyori reduction[6] and chiral hydride reductions using chelating BINOL ligands with LAH[7] produced the 1,4 conjugate addition adduct as the major product.



Scheme 2: Two step synthesis of mono-ol fragment

Olefin metathesis to join the two alkene fragments (**Scheme 3**) was expected to be challenging because both the coupling fragments were classified as type II alkenes.[8] However, it was found that mono-ol **9** behaved as a type I alkene and diol **6** behaved as a type II alkene. But, when mono-ol **9** was used in excess, it was difficult to purify the readily formed homodimer from the desired cross metathesis adduct. Therefore, diol **9** was used in excess, since it is readily prepared in catalytic and high yielding steps. In-situ olefin metathesis and basic ester hydrolysis yielded a single diastereomer of natural oxylipin **11** in 53% yield and and 98:2 er. Thus, the natural product was synthesized in just three steps from cheap and readily available starting materials in 33% yield.



Scheme 3: One pot olefin cross metathesis and ester hydrolysis

Conclusion

A straightforward synthesis of oxylipins from *Dracontium lortense* was developed using an olefin cross metathesis approach. This synthesis is not only considerably shorter, but also addresses the shortcoming of the previous synthesis. Successful integration of additional deprotection steps helped in reducing the step count. This three step synthesis is by far the shortest synthesis of oxylipins containing the 3-ene-1,2,3 trihydroxy stereochemical triad.

Experimental Section

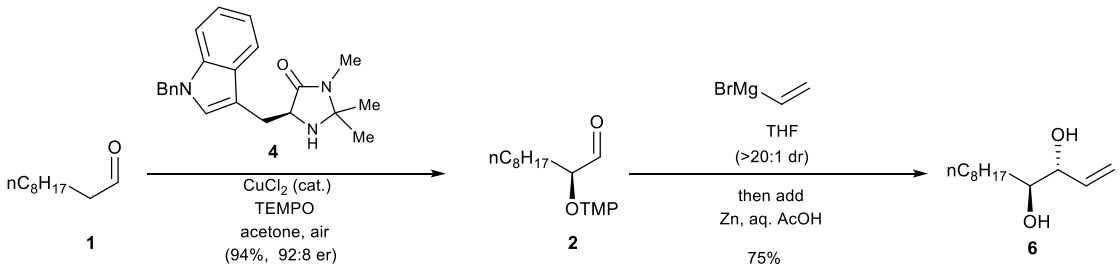
General protocols

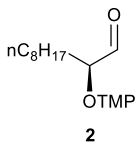
Unless otherwise noted, all reactions were performed with stirring under an argon atmosphere under anhydrous conditions. Organomagnesium and -lithium reagents were purchased from Aldrich. All other reagents were purchased at the most-economical grade. Dry tetrahydrofuran (THF), *N*,*N*-dimethylformamide (DMF), dichloromethane, and toluene were obtained by passing HPLC grade solvents through commercial solvent purification systems. All other chemicals were used as received, without purification. Flash column chromatography was performed using Grace Davison Davisil silica gel (60 Å, 35 – 70 µm). Unless otherwise noted, yields refer to chromatographically- and spectroscopically- (^{1}H NMR) homogeneous samples of single diastereomers. Thin-layer chromatography (TLC) was performed on Grace Davison Davisil silica TLC plates using UV light and common stains for visualization. NMR spectra were calibrated using residual undeuterated solvent as

an internal reference. Apparent couplings were determined for multiplets that could be deconvoluted visually.

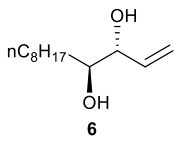
Synthesis and Characterization

Scheme 1: Sythesis of diol fragment





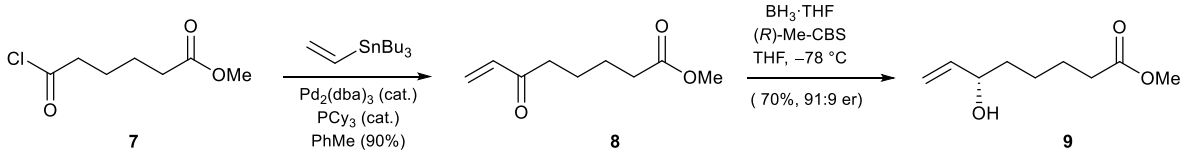
α-Oxyaldehyde 2: Prepared by following the same procedure as before as described in chapter 1. A sample was derivatized [1. $NaBH_4$, MeOH; 2. *m*-nitrobenzoyl chloride, Et_3N, DMAP (cat.), CH_2Cl_2; 3. Zn, AcOH, THF, H_2O] and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 10 % *i*PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 9.3 (major), 10.6 (minor) minutes] to have 93:7 er. Characterization reported in chapter I.

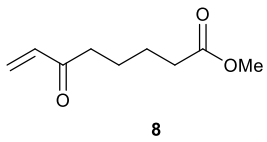


Diol 6: To a solution of aldehyde **2** (562 mg, 1.80 mmol, 1.0 equiv.) in 1.80 mL of THF at –78 °C was added vinylmagnesium bromide (1.0 M in THF, 2.33 mmol, 1.3 equiv.) dropwise over 3 minutes. The resultant solution was stirred at –78 °C for 30 minutes, then warmed to room temperature and was diluted with 20 mL of a 3:1:1 solvent mixture (HOAc:H_2O:THF). To the resulting solution was added zinc (1.18 g, 18.0 mmol, 10 equiv.) and refluxed at 70 °C for 6 hours. After cooling, the reaction mixture was filtered through Celite, concentrated, and azeotrope dried with toluene to give a

white solid. Flash column chromatography (30 % EtOAc / hexanes) gave **6** (270 mg, 75 % yield, >20:1 mixture diastereomers) as a white solid. **6**: R_f = 0.29 (35% EtOAc / hexanes); $[\alpha]_D^{23}$ = –3.5 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3305, 3212, 2916, 2849 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 5.93 (ddd, *J* = 17.1, 10.6, 6.5 Hz, 1H), 5.34 (td, *J* = 17.3, 1.5 Hz, 1H), 5.28 (td, *J* = 10.5, 1.3 Hz, 1H), 4.10 (m, 1H), 3.69 (td, *J* = 8.7, 4.2 Hz, 1H), 1.79 (brs, 2H), 1.54 – 1.19 (m, 13H), 0.88 (t, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 136.2, 117.9, 76.1, 74.2, 32.3, 32.0, 29.8, 29.7, 29.4, 26.0, 22.8, 14.3 ppm; HRMS (ESI-QTOF) calcd for $C_{12}H_{24}O_2^+$ [M^+]: 200.1776, found: 200.1776.

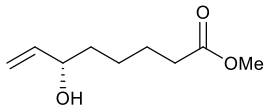
Scheme 2: synthesis of mono-ol





Enone 8: To a deoxygenated solution of tributyl(vinyl)tin (1.58 g, 5 mmol, 1.0 equiv.), $PCy_3 \cdot HBF_4$ (368 mg, 1 mmol, 0.2 equiv.), i-Pr_2NEt (170 μL, 1 mmol, 0.2equiv.), and $Pd_2(dba)_3$ (457 mg, 0.5 mmol, 0.1 equiv.) in 50 mL of toluene was added methyl adipoyl chloride (1.6 mL, 10 mmol, 2.0 equiv.) dropwise over 2 minutes and stirred for one hour at room temperature. The reaction mixture was diluted with EtOAc (75 mL) organic phase was washed with 3% aq. NH_4OH (75 mL), water (2 × 75 mL), and brine (75 mL), dried over Na_2SO_4, and concentrated to give a yellow oil. Flash column chromatography (20% EtOAc / hexanes) gave enone **8** (770 mg, 90.6% yield) as yellow oil. **8:** R_f = 0.32 (20% EtOAc / hexanes); IR (thin film): ν_{max} = 2953, 1732, 1699 cm^{-1}; ^1H NMR

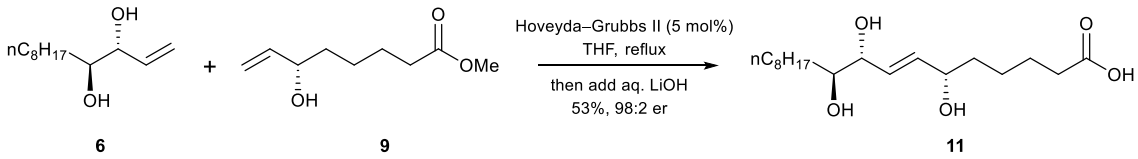
(600 MHz, $CDCl_3$): δ = 6.34 (dd, *J* = 17.7, 10.6 Hz, 1H), 6.21 (d, *J* = 17.6 Hz, 1H), *5*.82 (d, *J*= 10.6 Hz, 1H), 3.66 (s, 3H), 2.61 (m, 2H), 2.34 (m, 2H) ppm, 1.65 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.5, 174.0, 136.6, 128.2, 51.7, 39.3, 34.0, 24.6, 23.4ppm; HRMS (ESI-QTOF) calcd for $C_9H_{15}O_3^+$ [M + H^+]: 171.1000, found: 171.1017.

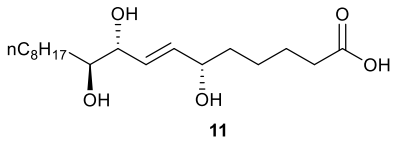


9

Allylic monol 9: To enone **8** (50 mg, 0.29 mmol, 1.0 equiv.) was added a solution of (R)-Me-CBS (163.35 mg, 0.59 mmol, 2.0 equiv.) in 300 µL THF and cooled to -78 °C. Then BH_3·THF (1 M in THF, 0.3 mL, 0.3 mmol, 1.0 equiv.) was added dropwise over 1 minute. The reaction was quenched by adding 50 µL of methanol and 10 µL of 4 N HCl and warmed to room temperature. The reaction mixture was diluted with EtOAc (10 mL). The organic layer was washed with water (2 × 10 mL), brine (10 mL), and saturated $NaHCO_3$ (10 mL), dried over Na_2SO_4, and concentrated to give a yellow oil. Flash column chromatography (30% EtOAc / hexanes) gave allylic monol **9** a colorless oil (34 mg, 69.5% yield). A sample was derivatized [1. DIBAL-H, THF; 2. *m*-nitrobenzoyl chloride, Et_3N, DMAP (cat.), CH_2Cl_2] and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 2.5 % *i*PrOH / hexanes, 0.2 mL / min, 40 °C; 280 nm UV detection; R_t = 9.3 (minor), 10.0 (major) minutes] to have 92:8 er.**9:** R_f = 0.33 (30% EtOAc / hexanes); $[\alpha]^{D23}$ = –90.5 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3433, 2936, 1735 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 5.86 (ddd, *J* = 17.3. 10.5, 6.2 Hz, 1H), 5.22 (dd, *J* = 17.3, 1.0 Hz, 1H), 5.11 (dd, *J* = 10.4, 1.0 Hz,1H), 4.10 (m, 1H), 3.66 (s, 3H), 2.32 (t, *J* = 7.6 Hz, 2H), 1.71–1.33 (m, 6H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 174.3, 141.2, 114.9, 73.1, 51.7, 36.7, 34.1, 25.0, 24.9 ppm; HRMS (ESI-QTOF) calcd for $C_9H_{17}O_3^+$ [M + H^+]: 173.1200, found: 173.1172.

Scheme 3: Synthesis of oxylipins





Oxylipin 11: Allylic monol **9** (85 mg, 0.49 mmol, 1 equiv) and allylic diol **6** (313 mg, 1.48 mmol, 3 equiv) was dissolved in 9 mL of THF and then Hoveyda Grubbs catalyst (21.1 mg, 0.026 mmol, 0.05 quiv) was added and heated to reflux for 24 hours. The reaction mixture was cooled to room temperature then LiOH (450 mg, 9.8 mmol, 20 equiv) dissolved in 1 mL water was added and stirred for another 24 hours. Reaction mixture was partitioned between EtOAc (20 mL) and 1N HCl (20 mL). The organic layer was washed with water (20 mL) and brine (20 mL) and dried over Na_2SO_4 and concentrated to give a white solid. Flash column chromatography (90 % EtOAc/hexanes) gave oxylipin **11** (86 mg, 53% yield) as a white solid. A sample was derivatized (*p*-nitrobenzyl amine·HCl, BOP–BF_4, HOBt, *i*-Pr_2NEt, DMF) and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 12% *i*- PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 11.8 (major), 13.3 (minor) minutes] to have 98:2 er. Characterization reported in chapter I.

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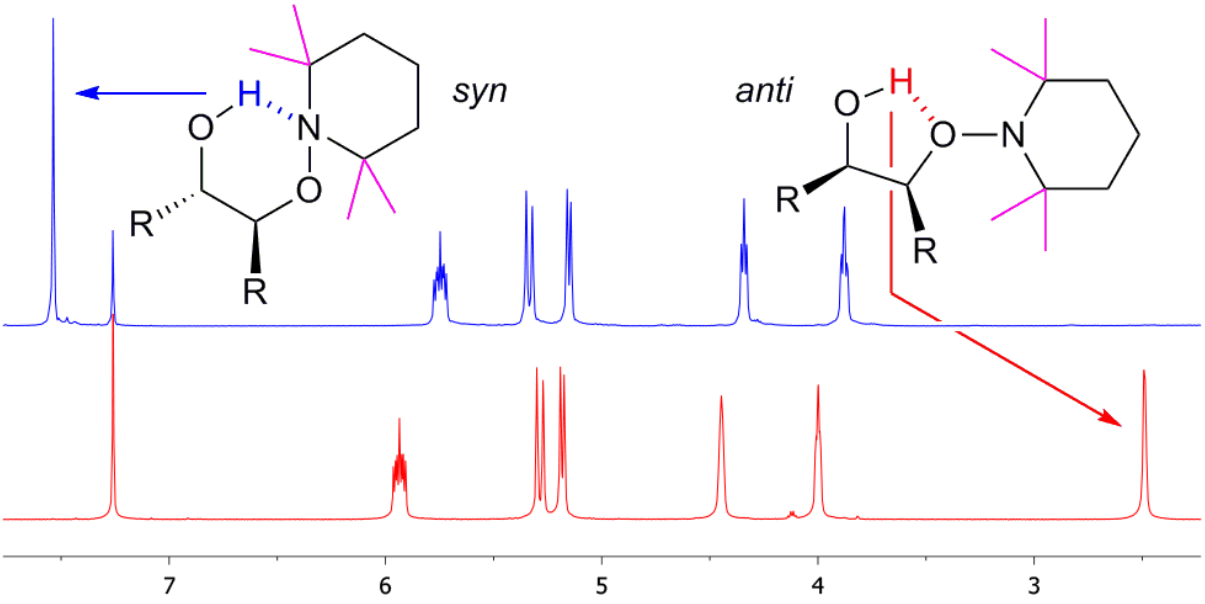
CHAPTER 3: CONFROMATIONAL ANALYSIS OF 2,2,6,6 TETRAMETHYLPIPERDINE 1,2- DIOLS

Paper published in *Journal of Organic Chemistry*[1]



Abstract

2,2,6,6-Tetramethylpiperidinyl-masked 1,2-diols exhibited stereochemistry-dependent hydroxyl proton chemical shifts: ca. 7 ppm for the *syn* diastereomer and ca. 2 ppm for the *anti* diastereomer. A computational search for low energy geometries revealed that the *syn* isomer favors a six-membered ring hydrogen bond to nitrogen and the *anti* isomer favors a five-membered ring hydrogen bond to oxygen. The computed low energy conformations were found to have a large difference in hydroxyl proton shielding that was reflected in the experimental chemical shift difference. This chemical shift difference was observed in a broad range of solvents, and thus may be useful as a stereochemical probe. The stereochemistry-dependent conformation and chemical shift signature appeared to be due to a *syn* pentane interaction between the *gem*-dimethyl groups on the 2,2,6,6-tetramethylpiperidinyl moiety.

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Introduction

Stereochemically-defined polyols are commonly found in natural products and bioactive molecules. Oxidative strategies for introducing alcohols or masked alcohols are appealing because they install additional functional groups. Many oxidants have been used to introduce alcohols, including osmium tetroxide,[1] selenium dioxide,[2] singlet oxygen,[3] and oxaziridine reagents.[4] More recently, the readily-available stable oxygen radical 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) has become increasingly popular as a precursor to an electrophilic oxygen reagent. TEMPO has been used to install 2,2,6,6-tetramethylpiperidinyl-masked alcohols through α-functionalization reactions of carbonyl compounds[5] and β-dicarbonyls[6] and vicinal difunctionalization reactions of alkenes[7] and α,β-unsaturated carbonyl compounds.[8]

We recently reported that α-oxyaldehydes generated by oxidative incorporation of TEMPO can react with diverse organomagnesium or -lithium reagents to yield differentially-masked *anti*-1,2-diols, in many cases with >20:1 diastereomeric ratio.[9] In the course of that study, we noticed that the NMR chemical shift of the hydroxyl proton in 2,2,6,6-tetramethylpiperidinyl-masked 1,2-diols is strongly dependent on the stereochemistry of the diol. (For clarity, throughout this paper 2,2,6,6-tetramethylpiperidinyl-masked 1,2-diols are referred to simply as diols. There are no unprotected diols in this paper.) The hydroxyl chemical shift in $CDCl_3$ is ca. 6 ppm for primary alcohols **1** (**Figure 1**), ca. 7 ppm for *syn* diols **2**, and ca. 2 ppm for *anti* diols **3**. Herein we provide computational and NMR spectroscopic evidence that this chemical shift anomaly reflects differences in the ground state conformations of such compounds.

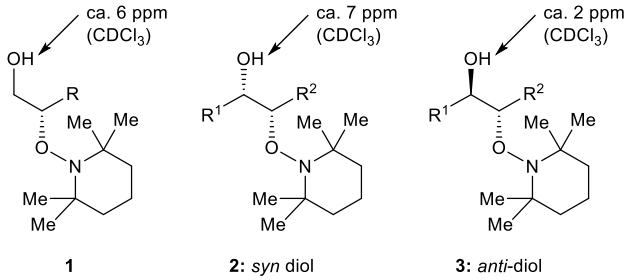


Figure 1: 2,2,6,6-Tetramethylpiperidinyl-masked diols.

Results and Discussion

The ^{1}H NMR spectra for differentially-masked diols **1a**, **2a**, and **3a** are shown in **Figure 2**. Diols **2a** (*syn*) and **3a** (*anti*) were synthesized containing an alkene in order to spread out the NMR signals. The identity of the hydroxyl protons was confirmed by deuterium exchange with D_2O. Whereas hydroxyl protons in $CDCl_3$ typically display variable chemical shifts and often are absent due to the rapid exchange of protons with adventitious water, the hydroxyl protons in diols **1**–**3** had reproducible chemical shifts and did not undergo rapid proton exchange with water. The slow rate of proton exchange suggested the presence of intramolecular hydrogen bonding. The hydroxyl proton could hydrogen bond to the oxygen of the masked alcohol to form a five-membered ring or to the nitrogen of the piperidine ring to form a six-membered ring. The large chemical shift differences between *syn* diols **2** and *anti* diols **3** suggested that these diastereomeric compounds may adopt different ground state conformations.

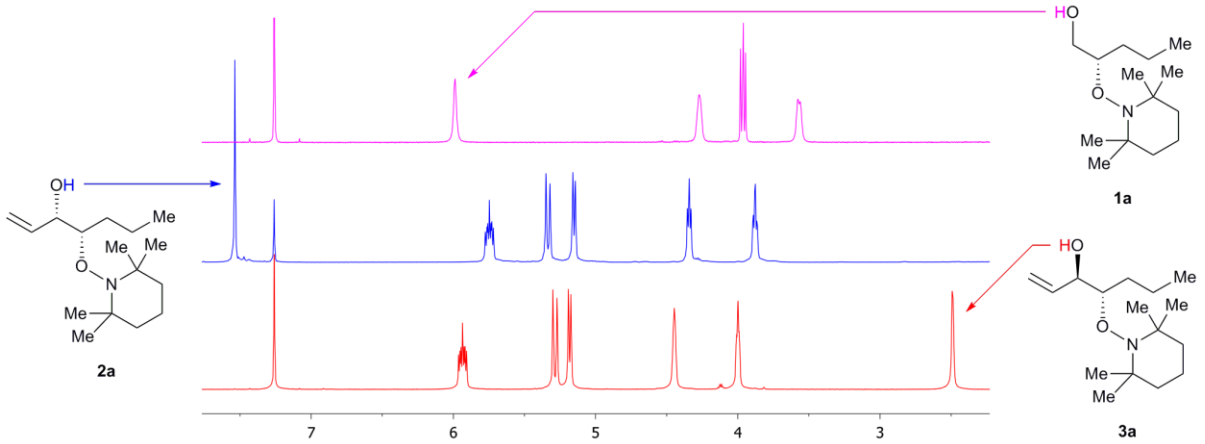


Figure 2: Partial ^{1}H NMR spectra of diols **1a**, **2a**, and **3a**. See Supporting Information for full-width spectra.

Since the unusual hydroxyl proton NMR chemical shifts were observed across all compounds of structures **1**–**3** that we have characterized thus far,[9] computational studies could be performed using the simplest possible carbon backbones. The computational analysis of primary alcohol **1b**, *syn* diol **2b**, and *anti* diol **3b** (all with R = R^1 = R^2 = Me) began with a systematic identification of the low energy conformations. Three to five of the lowest energy conformations were chosen for each compound as starting points for higher-level analysis. All structures shown in this paper are at the MP2/6-311G(d,p) level and all energies include zero point energy (ZPE) corrections. The element colors in the figures are as follows: nitrogen is blue, oxygen is red, carbon is grey, and hydrogen is white.

After the final round of geometry optimizations, a low energy geometry emerged for each of the compounds (**1b**–**3b**). The structures shown in Figures 3 and 4 do not emphasize visualization of the piperidinyl ring, but in all cases this ring possesses a chair conformation with the oxygen substituent in an equatorial position.

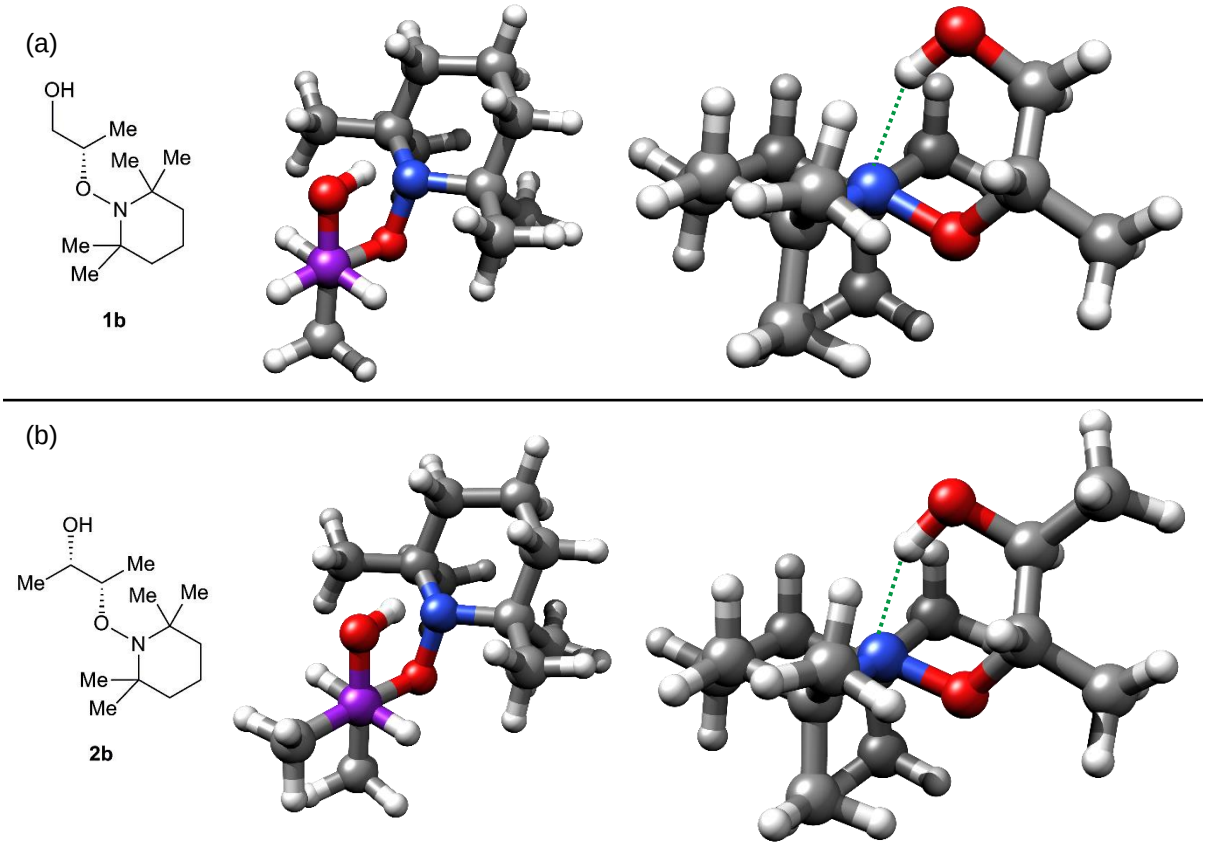


Figure 3: Computed ground state conformations of (a) primary diol **1b** and (b) *syn* diol **2b**. Two different views are given for each conformation. The purple atom is a carbon directly in front of another carbon in a Newman projection-like view.

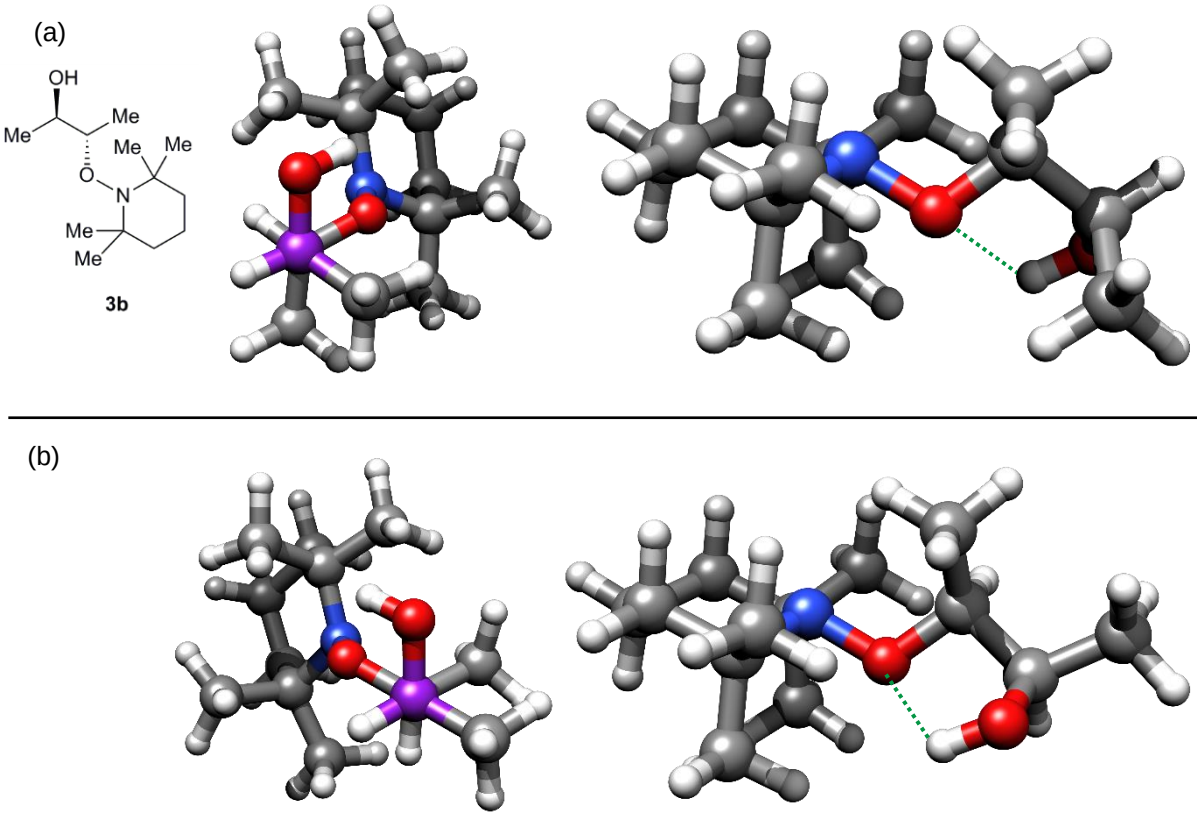


Figure 4: Computed geometries for (a) the lowest energy conformation of *anti* diol **3b** and (b) the second-lowest energy conformation of diol **3b**. Two different views are given for each conformation. The purple atom is a carbon directly in front of another carbon in a Newman projection-like view.

The computed geometry of primary alcohol **1b** (**Figure 3a**) shows an intramolecular hydrogen bond between the hydroxyl proton and the piperidine nitrogen (1.85 Å). The six-membered ring formed by hydrogen bonding adopts a twist boat conformation, and the alkyl chain of the diol backbone is *anti* to the free hydroxyl group. While the lowest energy conformation contains a six-membered ring hydrogen bond, the lowest energy conformation with a five-membered ring hydrogen bond is only 3.3 kcal mol^{-1} higher in energy (see **Table 1**). The Boltzmann ratios between the different five- and six- membered rings are also given to show the populations of the different conformations at room temperature.

Table 1: Relative energy and Boltzmann populations of five- and six-membered ring hydrogen bond conformations

Compound	ΔE / kcal mol^{-1} [a]	Boltzman population ratios at 298 K[b]
1b	+3.3	99.6 : 0.4
2b	+3.4	99.7 : 0.3
3b	–2.7	80.3 : 18.8 : 0.9
1b′	+1.2	88.5 : 11.5
2b′	+0.9	82.0 : 18.0
3b′	+0.6	57.5 : 42.5

[a] The energy difference is calculated for the lowest energy five- and six-membered ring hydrogen bond conformations. A positive energy indicates that the six-membered ring hydrogen bond conformation is lower in energy. [b] The ratios are for the six- to five-membered ring for all compounds except **3b**). This ratio for the lowest and next lowest five-membered ring to the six-membered ring.

The computed geometry of *syn* diol **2b** (**Figure 3b**) is virtually identical to that of primary alcohol **1b** (1.85 Å hydrogen bond for **1b**; 1.81 Å for **2b**) save for the presence of an additional alkyl group *anti* to the masked hydroxyl group. The *anti* relationship between the two methine protons (and thus the gauche relationship of the diol alkyl groups) was experimentally validated by the observation of a large $^{3}J_{H–H}$ coupling constant (8.7 Hz) between these two protons in the ^{1}H NMR spectrum of *syn* diol **2a**.[10] The lowest energy five-membered ring hydrogen bond conformation is 3.4 kcal mol^{-1} higher in energy than the lowest six-membered ring structure.

As shown in **Figure 4**, the two lowest energy computed geometries of *anti* diol **3b** possess a five-membered ring hydrogen bond between the hydroxyl proton and the oxygen of the masked hydroxyl. The two five-membered ring geometries were calculated to have similar energies (separated by only 0.9 kcal mol^{-1}) and hydrogen bond distances (2.21 Å for

the lower energy geometry; 2.25 Å for the higher energy geometry). This hydrogen bond length is significantly longer than those for **1b** and **2b**, and is likely due to the need to minimize torsional strain in the five-membered ring. A transition state between these two geometries was located computationally at 6.3 kcal mol^{-1} above the lower energy geometry, suggesting that these two structures rapidly equilibrate at ambient temperature. The hydrogen bond to oxygen shortens in the transition state to 1.87 Å. HETLOC NMR spectroscopy of *anti* diol **3a** revealed a 4 Hz $^{3}J_{H-H}$ coupling constant between the methine protons, consistent with a gauche relationship between these two protons (and thus a gauche relationship between the diol alkyl groups). Measurement of $^{2}J_{C-H}$ and $^{3}J_{C-H}$ coupling constants by HETLOC and PS-HMBC NMR spectroscopy, respectively,[10] did not allow unambiguous identification of the major conformation, but 1D NOE data provided evidence for the presence of both conformations shown in Figure 4. The lowest energy six-membered ring hydrogen bond conformation is 2.7 kcal mol^{-1} higher in energy than the lowest energy five-membered ring.

Isotropic chemical shifts were calculated for the lowest energy conformations of diols **1b**–**3b** (see **Table 2**). The KT2 functional was favored over B3LYP because KT2 was designed specifically for the calculation of magnetic properties. The computed hydroxyl proton chemical shifts for diols **1b**–**3b** are in good qualitative agreement with the experimental chemical shifts for diols **1a**–**3a** in $CDCl_3$. Interestingly, even though the computed low energy geometries of diols **1b** and **2b** are very similar, the computed hydroxyl proton chemical shifts nonetheless correctly reflect not only the experimentally-observed relative shielding of the hydroxyl protons, but even the magnitude of the difference. This

close agreement provides strong evidence that the computed gas phase conformations of diols **1b**–**3b** are relevant in solution.

Table 2: Computed and experimental hydroxyl proton chemical shifts

Solvent	Primary alcohol / ppm	*syn* Diol / ppm	*anti* Diol / ppm
Gas phase (computed)	5.51 (**1b**)[a]	6.98 (**2b**)[a]	0.00 (**3b**)[b] 2.05 (**3b**)[a][c]
$CDCl_3$	5.99 (**1a**)	7.55 (**2a**)	2.49 (**3a**)
Benzene-d_6	5.40 (**1a**)	7.16 (**2a**)[d]	1.87 (**3a**)
Cyclohexane-d_{12}	4.68 (**1a**)	6.49 (**2a**)	1.75 (**3a**)
CD_3CN	5.94 (**1a**)	6.66 (**2a**)	2.71 (**3a**)
THF-d_8	4.44 (**1a**)	6.36 (**2a**)	3.54 (**3a**)
Acetone-d_6	4.75 (**1a**)	6.93 (**2a**)	3.46 (**3a**)
DMF-d_7	4.58 (**1a**)	6.00 (**2a**)	4.50 (**3a**)
DMSO-d_6	4.59 (**1a**)	6.42 (**2a**)	4.51 (**3a**)
Pyridine-d_5	5.94 (**1a**)	7.17 (**2a**)	6.06 (**3a**)
CD_3OH:$CDCl_3$ (1:1)	5.51 (**1a**)	6.98 (**2a**)	[e]

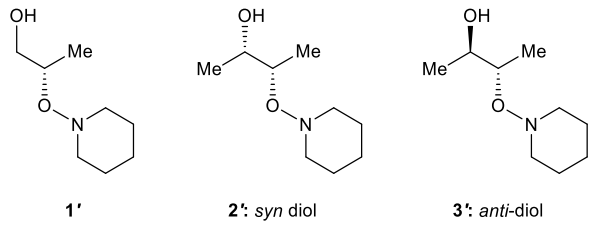
[a] Referenced to the calculated isotropic chemical shift of the lower energy conformation of diol**3b**. [b] The calculated isotropic chemical shift for the lower energy conformation of diol **3b** was set to 0.00 ppm. [c] Calculated for the higher

energy conformation of diol **3b**. [d] Hydroxyl proton signal is hidden under the solvent residual peak. Blending in a small amount of $CDCl_3$ shifts the hydroxyl proton signal downfield. [e] Hydroxyl proton signal is either hidden under the CD_3OH hydroxyl proton signal or rapidly exchanging with the CD_3OH hydroxyl proton signal.

Similar differences in shielding between the hydroxyl protons of diols **1a**–**3a** are observed in other solvents with weak Lewis basicity, suggesting that the calculated conformational preferences are retained. The chemical shift of the hydroxyl protons of primary alcohol **1a** and *syn* diol **2a** are little affected by solvents with stronger Lewis basicity, but the hydroxyl proton of *anti* diol **3a** shifts downfield. This change might be due to a competition between intramolecular hydrogen bonding and hydrogen bonding to the more Lewis basic solvents; alternatively, these solvents might reduce the energy gap between the five- and the six-membered ring intramolecular hydrogen bond conformations. Nonetheless, the relative shielding as compared with *syn* diol **2a** is preserved, and thus this chemical shift difference is a useful stereochemical probe across a broad range of solvents. Interestingly, despite the ability to compensate for loss of intramolecular hydrogen bond by hydrogen bonding to CD_3OH, the proton exchange for diols **1a** and **2a** is sufficiently slow that their characteristic hydroxyl proton chemical shifts can be observed even in a 1:1 CD_3OH:$CDCl_3$ mixture. ($CDCl_3$ was added in order to improve solubility.) Therefore, the 6-membered ring hydrogen bond conformation of primary alcohol **1a** and *syn* diol **2a** appears to be surprisingly stable even in protic solvent.

To try to understand why diastereomeric diols **2** and **3** favor different conformations, we investigated the role of the *gem*-dimethyl groups on the 2,2,6,6-tetramethylpiperidinyl moiety by computing the low energy geometries for diols **1′**–**3′** (**Figure 5**). In all cases, a six-membered ring hydrogen bond conformation is favored, but the energy difference between five- and six-membered ring hydrogen bond conformations is smaller than the corresponding

energy difference for diols **1b**–**3b** (see Table 1). The *syn* pentane interaction between the axial methyl groups on the piperidine ring of diols **1**–**3** forces these methyl groups apart (N–C–C_{axial} angle for **1b**: 115.0° and 115.3°; N–C–H_{axial} angles for **1′**: 109.6° and 109.9°; all angles measured on the lowest energy conformation) and flattens the chair conformation at nitrogen (C–N–C angle for **1b**: 117.2°; for **1′**: 110.9°). Similar angles are observed for all five- and six-membered ring conformations of diols **1b**–**3b** and for diols **1′**–**3′**. This *syn* pentane-induced distortion does not consistently favor a five- or six-membered ring hydrogen bond conformation, but nonetheless appears to be causing diols **1**–**3** to have distinct preferred conformations and NMR spectroscopic signatures.



1′ **2′**: *syn* diol **3′**: *anti*-diol

Figure 5: Diols masked by unmethylated piperidinyl moieties.

Conclusion

The stereochemistry-dependent hydroxyl proton chemical shift of 2,2,6,6-tetramethylpiperidinyl-masked 1,2-diols was shown by a combination of computational and NMR spectroscopic methods to be the result of differences in ground state conformations. Primary alcohols **1** and *syn* diols **2** favor a six-membered ring hydrogen bond, but *anti* diols **3** favor a five-membered ring hydrogen bond. Computed isotropic chemical shifts of the hydroxyl protons show good correlation with experimental chemical shifts. The hydroxyl proton of *syn* diols **2** is downfield of the hydroxyl proton of *anti* diols **3** in a broad range of solvents, making this difference in chemical shift useful for assigning relative

stereochemistry. These stereochemistry-dependent conformational and spectroscopic differences appear to stem from a *syn* pentane interaction on the tetramethylpiperidine ring.

The internal hydrogen bonding forces the carbon chain of the diol to adopt a gauche conformation in both *syn* diols **2** and *anti* diols **3**. This bending of the carbon chain is expected to enhance ring closure rates of substrates containing a 2,2,6,6-tetramethylpiperidinyl-masked 1,2-diol. Furthermore, the predictable direction of the bend for *syn* diols **2** may be useful for remote stereoinduction in cyclization reactions. Studies to explore these potential synthetic consequences of the conformational preferences discovered herein are under way.

Experimental Section

Computation

The General Atomic and Molecular Electronic Structure System (GAMESS) software package[11] was used for all structure analysis calculations. The systematic identification of low energy conformations was performed using Restricted Hartree-Fock (RHF) and the small basis set 3-21G(d).[12] The optimization process began by finding a stable, low-energy conformation for the tetramethylpiperidine ring by twisting the ring in the known conformations (boat, chair, twisted chair for example). A systematic rotor search around all of the rotatable chain bonds then followed for each diol's required stereochemistry. Between 15 and 20 different conformations of each compound were found in the optimization process. All equilibrium coordinates are provided in the Supporting Information. The lowest energy geometries within a 4 kcal/mol window (three to five geometries) were used in higher-level calculations. Further optimizations were performed using both B3LYP[13] density functional

theory and Møller–Plesset second-order perturbation theory (MP2)[14] using the 6-311G(d,p) basis set.[15] Since the B3LYP and MP2 geometries were very similar, Hessians were only computed at the B3LYP/6-311G(d,p) level to confirm that minima were found and to obtain the zero point energy (ZPE) corrections. The images in the paper were generated using Chimera.[16]

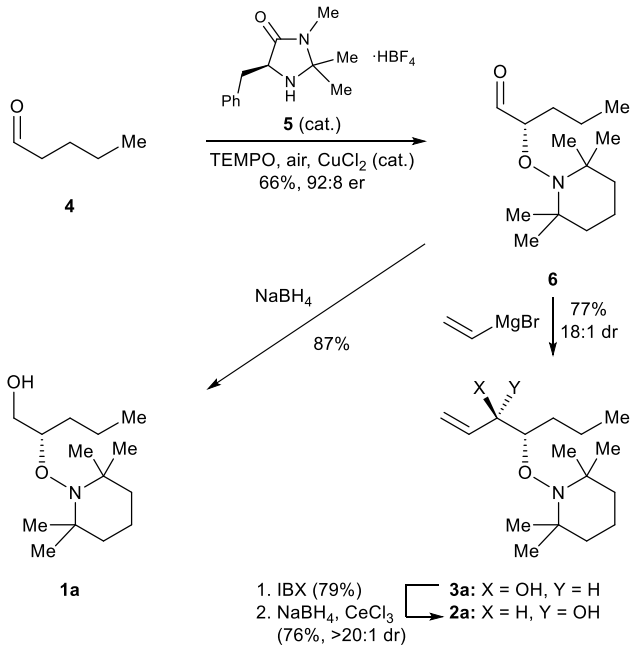
Chemical shielding calculations were performed using the NWChem computational software package with a fine grid and a wavefunction DIIS error vector of less of $1.0x10^{-5}$.[17] The Gauge-Independent Atomic Orbital (GIAO) method[18] was employed with the KT2 functional[19] and the aug-cc-pVTZ basis set[20] using the MP2/6-311G(d,p) optimized geometries. Shielding tensors of the B3LYP optimized structures for each compound were calculated and the isotropic shielding values were then used to calculate the chemical shifts. For completeness, shielding calculations for the lowest energy structures were also performed using the B3LYP functional. The results using B3LYP provided the same trend in chemical shifts and are available in the Supporting Information. In this paper, only the shifts for the lowest energy structure for each compound are reported in the text and the others are available in the Supporting Information. The higher energy compounds have the same trends as those for the lowest energy conformations with respect to the different compounds and the formation of a five- or six-membered ring.

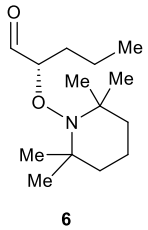
Synthesis

See Scheme 1. All reactions were performed with stirring under an argon atmosphere under anhydrous conditions. Vinylmagnesium bromide solution was purchased from Aldrich. All other reagents were purchased at the most economical grade. Dry tetrahydrofuran (THF), was

obtained by passing HPLC grade solvent through a commercial solvent purification system. All other chemicals were used as received, without purification. Flash column chromatography was performed using Grace Davison Davisil silica gel (60 Å, 35–70 μm). Yields refer to chromatographically- and spectroscopically- (1H NMR) homogeneous samples of single diastereomers. Thin-layer chromatography (TLC) was performed on Grace Davison Davisil silica TLC plates using UV light and common stains for visualization. NMR spectra were calibrated using residual undeuterated solvent as an internal reference. Apparent couplings were determined for multiplets that could be deconvoluted visually.

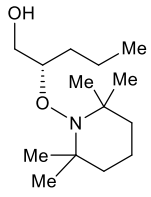
Scheme 1: Synthesis of diols **1a**–**3a**.




6

α-Oxyaldehyde 6: To a mixture of activated 4 Å molecular sieves (100 mg, powdered) and imidazolidinone catalyst **5** (500 mg, 1.6 mmol, 0.2 equiv.) in 5 mL of acetone was added $CuCl_2 \cdot 2H_2O$ (139 mg, 0.81 mmol, 0.1 equiv.). The

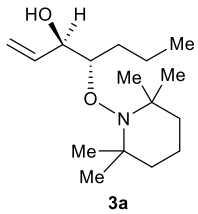
green reaction mixture was stirred open to air for 5 minutes until the copper salt dissolved and the mixture turned dark orange. The reaction was cooled to 0 °C for 10 minutes, then pentanal (**4**, 0.87 mL, 8.1 mmol, 1.0 equiv.) was added dropwise over 2 minutes. The reaction was stirred at 0 °C for 10 minutes, then a solution of TEMPO (1.51 g, 9.7 mmol, 1.2 equiv.) in 2 mL of acetone was added dropwise over 3 minutes. The reaction mixture was capped with a rubber septum and an air inlet line was attached via an 18-gauge needle. The reaction was stirred at 0 °C for 24 hours, then partitioned between ether (15 mL) and saturated NH_4Cl (45 mL). The aqueous layer was extracted with ether (2 × 45 mL) and the combined organic layers were washed with brine (90 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated to give an orange oil. Flash column chromatography (5% EtOAc / hexanes) gave α-oxyaldehyde **6** (1.30 g, 66% yield) as a colorless oil. A sample was derivatized [1. $NaBH_4$, MeOH; 2. *m*-nitrobenzoyl chloride, Et_3N, DMAP (cat.), CH_2Cl_2; 3. Zn, AcOH, THF, H_2O] and determined by chiral HPLC [Chiraltech IC column, 2.1 × 100 mm, 3 µm; 10% *i*-PrOH / hexanes, 0.2 mL / min, 25 °C; 280 nm UV detection; R_t = 8.8 (major), 9.9 (minor) minutes] to have 92:8 er. **6:** R_f = 0.47 (5% EtOAc / hexanes); $[\alpha]_D^{23}$ = –90.5 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 2933, 1732 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 9.77 (d, *J* = 4.5 Hz, 1H), 4.08 (m, 1H), 1.70 (m, 1H), 1.64 (m, 1H), 1.50–1.08 (m, 20H), 0.92 (t, *J* = 7.4Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 204.6, 88.5, 40.2, 34.5, 33.9, 32.2, 20.5, 20.3, 17.8, 17.3, 14.3 ppm; HRMS (ESI-QTOF) calcd for $C_{14}H_{28}NO_2^+$ [M + H^+]: 242.2100, found: 242.2102.



1a

Primary alcohol 1a: To a solution of α-oxyaldehyde **6** (96 mg, 0.4 mmol, 1.0 equiv.) in 5 mL ethanol was added sodium borohydride (101 mg, 3.6 mmol, 9.0 equiv.). The reaction mixture was stirred for five minutes, then partitioned

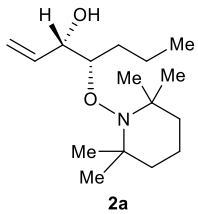
between ether (20 mL) and water (20 mL). The aqueous layer was extracted with ether (20 mL), and the combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, and concentrated to give a colorless oil. Flash column chromatography (5% EtOAc / hexanes) gave primary alcohol **1a** (85 mg, 87%) as a colorless oil. **1a:** R_f = 0.27 (10% EtOAc / hexanes) [□]$_D^{23}$ = –62.3 ° (*c* = 1.00, $CHCl_3$); IR (thin film): □$_{max}$ = 3576, 3018, 2925, 1465 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): □ = 5.99 (s, 1H), 4.27 (s, 1H), 3.96 (dd, *J* = 11.9, 10.0 Hz, 1H), 3.57 (d, *J* = 9.5 Hz, 1H), 1.70–1.01 (m, 22H), 0.93 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): □ = 68.8, 40.5, 39.8, 34.8, 33.5, 32.5, 20.6, 19.3, 17.3, 14.4 ppm; HRMS (ESI-QTOF) calcd for $C_{14}H_{30}NO_2^+$ [M + H^+]: 244.2300, found: 244.2271.



3a

***anti* Diol 3a** : To a solution of aldehyde **6** (100 mg, 0.4 mmol, 1.0 equiv.) in 400 µL of THF at –78 °C was added vinylmagnesium bromide (1.0 m in THF, 600 µL, 0.6 mmol, 1.5 equiv.) dropwise over 3 minutes. The resultant solution was stirred at –78 °C for 30 minutes, then warmed to ambient temperature. The reaction mixture was partitioned between saturated NH_4Cl (5 mL) and ether (10 mL). The organic phase was washed with water (2 × 10 mL) and brine (10 mL), dried over Na_2SO_4, and concentrated to give a colorless oil. Flash column chromatography (5% EtOAc / hexanes) gave alcohol **3a** (77 mg, 71% yield) and a mixture of alcohol **3a** and the epimeric alcohol **2a** (7 mg, 6% yield) as colorless oils. **3a:** R_f = 0.42 (10% EtOAc / hexanes); [α]$_D^{23}$ = –10.3 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3450, 1642 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 5.93 (ddd, *J* = 17.4 , 10.5, 6.2 Hz, 1H), 5.28 (d, *J* = 17.3 Hz, 1H), 5.18 (d, *J* = 10.7 Hz, 1H), 4.44 (s, 1H), 3.98 (m, 1H), 2.49 (d, *J* = 3.6 Hz, 1H), 1.76 (m, 1H), 1.63–1.04 (m, 21 H), 0.90 (t, *J* = 7.3 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ = 137.5, 115.9, 84.2, 73.9, 60.4, 40.8, 34.4, 31.1, 19.9, 17.3, 14.7, 14.3 ppm; $^3J_{H3–H4}$ = 4 Hz, $^2J_{H3-C4}$ = –3.1

Hz, $^{2}J_{H4–C3}$ = –1.0 Hz, $^{3}J_{H3–C5}$ = +1.2 Hz, $^{3}J_{H4–C2}$ = +3.1 Hz; HRMS (ESI-QTOF) calcd for $C_{16}H_{32}NO_2^+$ [M + H+]: 270.2400, found: 270.2431.



2a

***syn* Diol 2a**: To alcohol **3a** (1.56 g, 5.8 mmol, 1.0 equiv.) in 12 mL of THF was added a solution of IBX (2.45 g, 8.7 mmol, 1.5 equiv.) in 10 mL of DMSO. The reaction mixture was stirred for 1.5 hours, then diluted with 20 mL of ether and filtered. The organic phase was washed with water (2 × 20 mL) and brine (20 mL), dried over Na_2SO_4, and concentrated to give an enone (1.20 g, 79%) as a colorless oil. The enone was used without purification in the next reaction.

To this enone (1.20 g, 4.5 mmol, 1.0 equiv.) in 6 mL of THF and 18 mL of MeOH was added $CeCl_3 \cdot 7H_2O$ (3.36 g, 9.0 mmol, 2.0 equiv.). The reaction mixture was stirred for 15 minutes, then cooled to –20 °C. $NaBH_4$ (513 mg, 13.6 mmol, 3.0 equiv.) was added, and the resultant mixture was stirred for 2 hours. The reaction mixture was partitioned between ether (50 mL) and water (100 mL). The aqueous layer was extracted with ether (100 mL), and the combined organic layers were washed with brine (50 mL), dried over Na_2SO_4, and concentrated to give a colorless oil. Flash column chromatography (5% EtOAc / hexanes) gave allylic alcohol **2a** (800 mg, 67%) and a mixture of alcohol **2a** and epimeric alcohol **3a** (110 mg, 9%) as colorless oils. **2a:** R_f = 0.36 (10% EtOAc / hexanes); $[\alpha]_D^{23}$ = –28.6 ° (*c* = 1.00, $CHCl_3$); IR (thin film): ν_{max} = 3438, 1641 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ= 7.55 (br s, 1H), 5.74 (ddd, *J* = 17.1, 10.5, 6.8 Hz, 1H), 5.33 (d, *J* = 17.0 Hz, 1H), 5.14 (d, *J* = 10.4 Hz, 1H), 4.33 (t, *J* = 7.7 Hz, 1H), 3.87 (dt, *J* = 2.8, 8.7 Hz, 1H), 1.65–1.08 (m, 22H), 0.90 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ= 137.8, 116.8, 82.7, 78.1, 61.8, 60.3, 40.5, 40.0, 34.6, 33.6, 32.0, 20.73, 20.67, 18.9, 17.3, 14.5 ppm; HRMS (ESI-QTOF) calcd for $C_{16}H_{32}NO_2^+$ [M + H^+]: 270.2400, found: 270.2434.

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CHAPTER IV: CONCLUSION AND FUTURE DIRECTIONS

Synthesis has always been a valuable tool for structure elucidation of natural products isolated in minute quantities. This dissertation describes the synthesis and stereochemical assignment of two naturally occurring oxylipins isolated from *Dracontium lortense*. Despite five previous reported syntheses, the stereochemistry of the trihydroxy fatty acids was ambiguous. The first-generation synthesis generated all stereoisomers using a method developed to synthesize chiral 1,2-diols. The key steps involved organocatalytic α-oxygenation of decanal followed by Grignard addition, Stille cross coupling and asymmetric ketone reduction. This seven step synthesis (23% overall yield) to the biologically active natural product is tied for the shortest synthesis of this class of natural products containing the 3-en-1,2,5 triol moiety. The stereochemistry of both the naturally occurring oxylipins were unambiguously assigned using NMR spectroscopy and optical rotation.

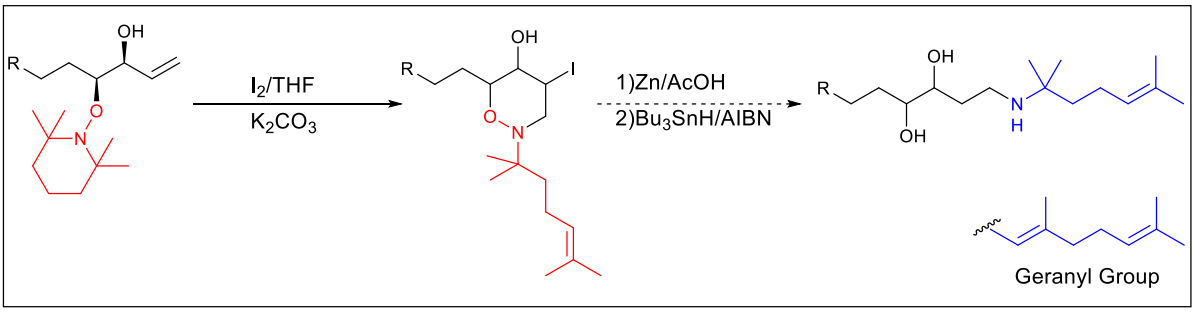
A substantially more direct synthesis was developed using an olefin cross metatheis approach. Bulkier tryptophan based organocatalysts were used for oxidative incorporation of TEMPO onto decanal with enhanced enantioselectivity and yield and much lower catalyst loading (now 5 mol%). The step count was considerably reduced by telescoping additional protecting group deprotection steps. The natural product can now be made in just three steps in 33% overall yield. This synthesis is by far the shortest synthesis of acyclic fatty acid natural products containing the 3-en-1,2,5-triol moiety.

Observed disparity in the hydroxyl proton ^{1}H-NMR chemical shifts of diastereomers of singly masked 1,2-diols led us to collaborate with computational chemists at Iowa State University (Professor Theresa Windus) to determine conformations of singly masked 1,2

diols. Computational (RHF, DFT, MP2) and 1D (decoupling experiments) and 2D NMR (HETLOC, HMBC) spectroscopic analysis revealed different hydrogen bonded ground state conformations of different diastereomers. The primary alcohol and *syn* diastereomer adopt a ground state conformation where hydroxyl proton hydrogen bonds with the nitrogen of the piperdine ring forming a six member ring whereas the hydroxyl proton of the anti diastereomer hydrogen bonds with the oxygen forming a five membered ring. The anti diastereomer was 2.2 kcal/mol higher in energy. The chemical shift difference was found to hold in various solvents and hence can be used as a stereochemical probe. This conformational preference is lost for piperdinyl masked 1,2 diols. Hence the stereochemistry-dependent conformation and chemical shift signature appeared to be due to a *syn* pentane interaction between the *gem*-dimethyl groups on the 2,2,6,6-tetramethylpiperidinyl moiety

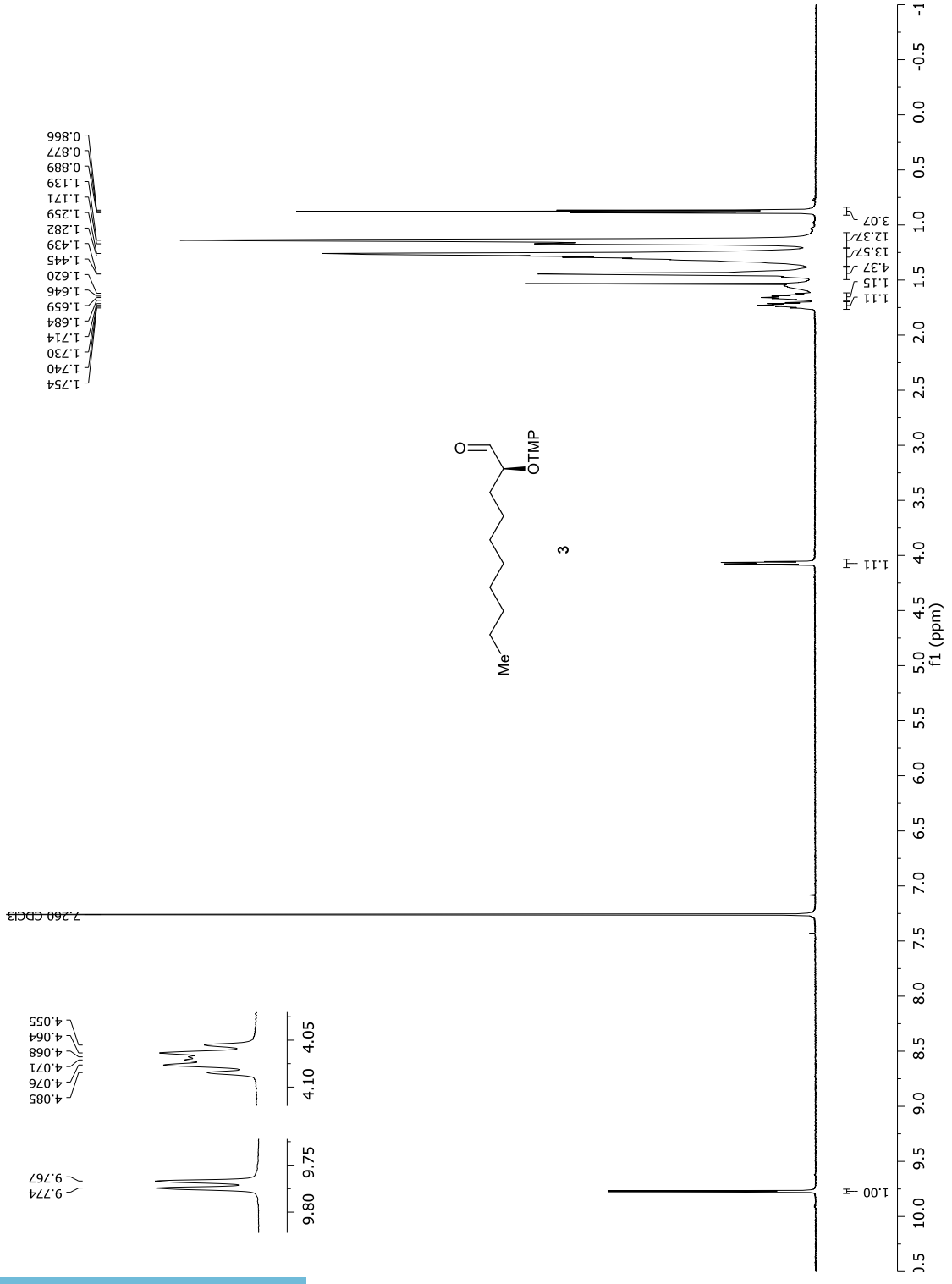
The discovered conformational bias in singly masked 1,2 diols was hypothesized to be useful for diastereoselective cyclizations. Instead, attempted iodoetherification of the singly masked 1,2-diols tethered to an alcohol led to fragmentation of the piperdine ring of the masking group. Preliminary investigations reveal that simple chain diols, irrespective of the relative stereochemistry of the 1,2 diol, undergo ring fragmentation. The corresponding enone fails to undergo fragmentation. The fragmented product resembles nitrogen containing geranyl moiety. In future, this novel fragmentation reaction can be used to synthesize nitrogen containing geranyl mimics of natural products as novel drug candidates.

Scheme 1: Novel Fragmentation Reaction

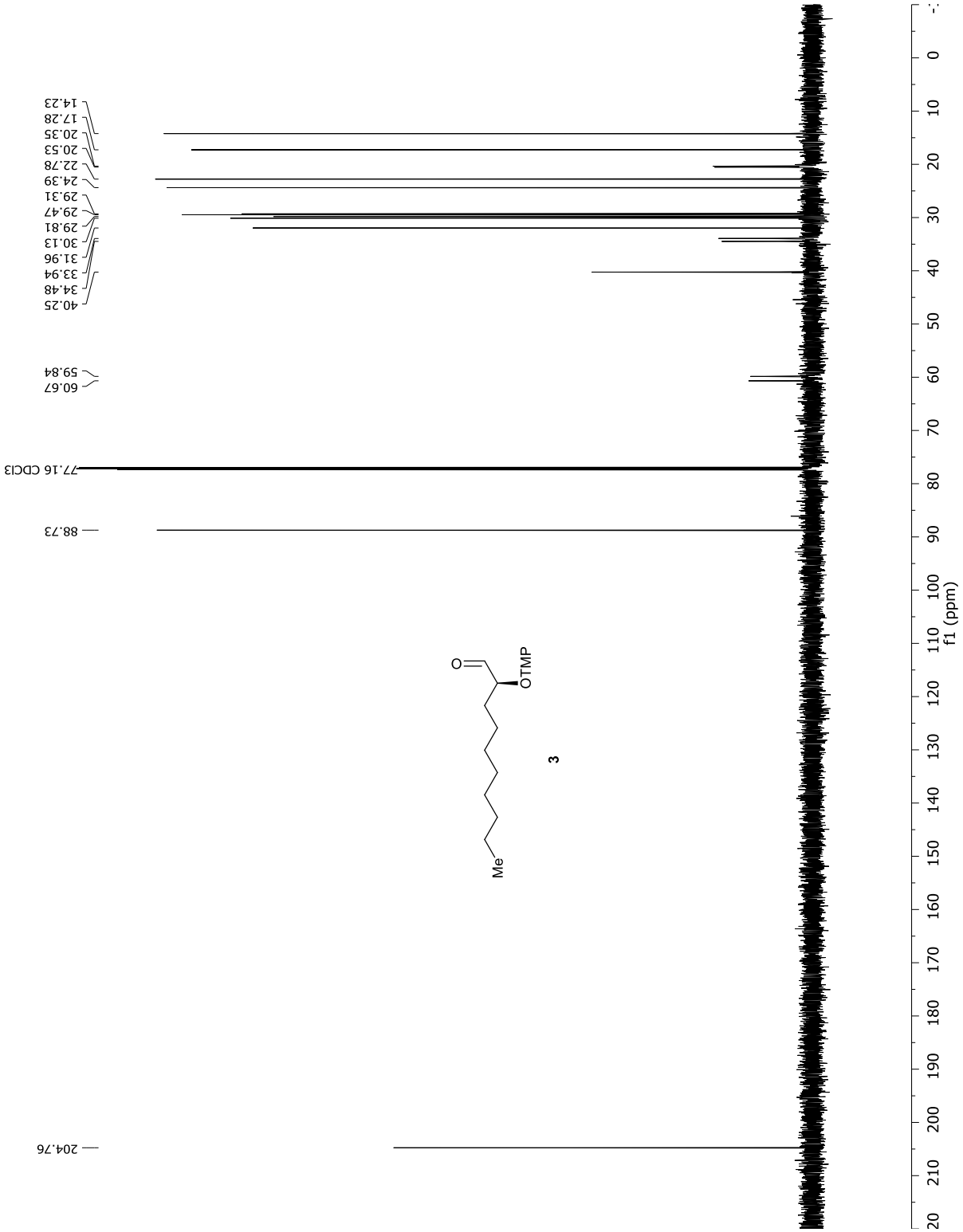


APENDIX A: CHAPTER I 1D & 2D NMR SPECTRA

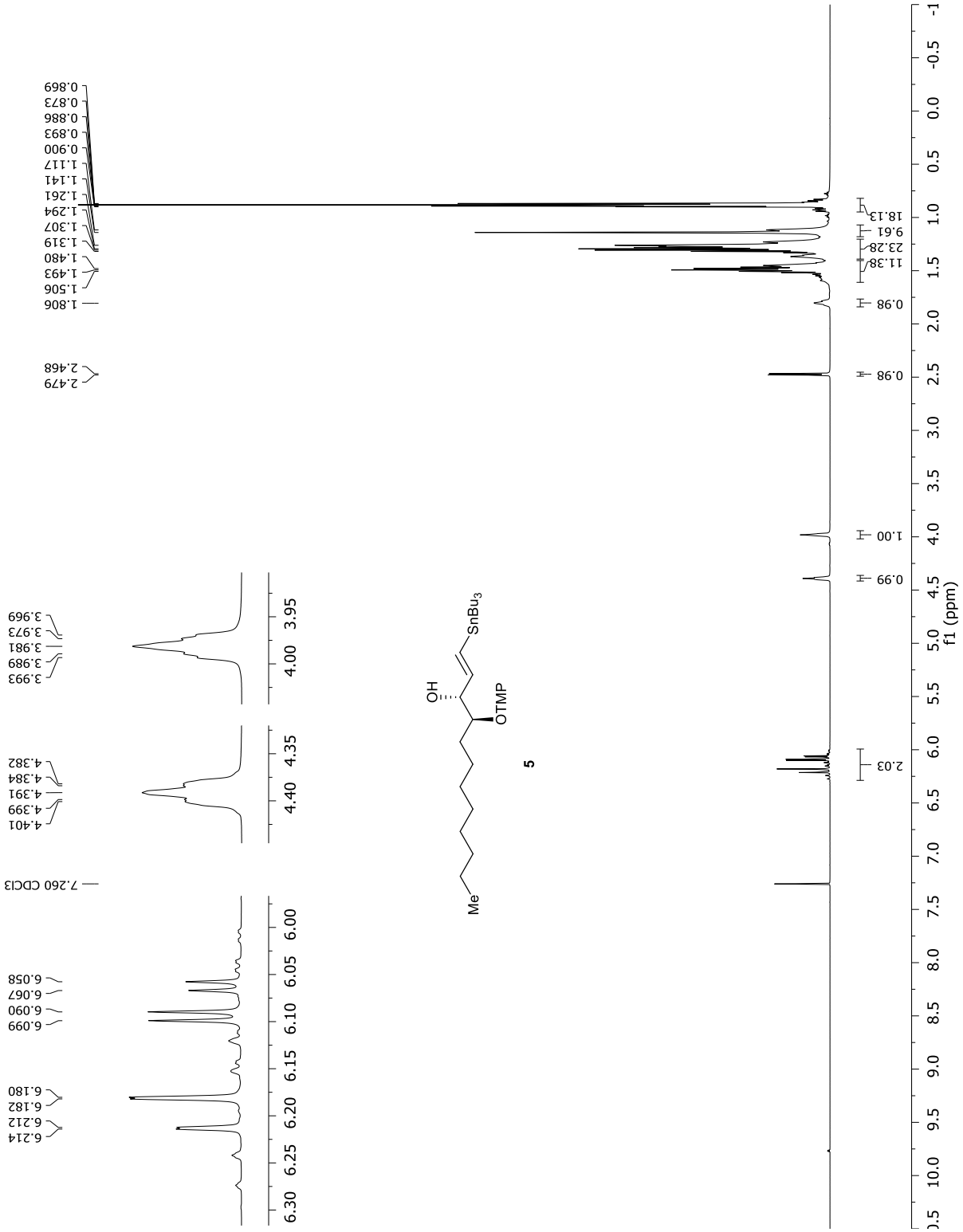
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of α-oxyaldehyde **3:**



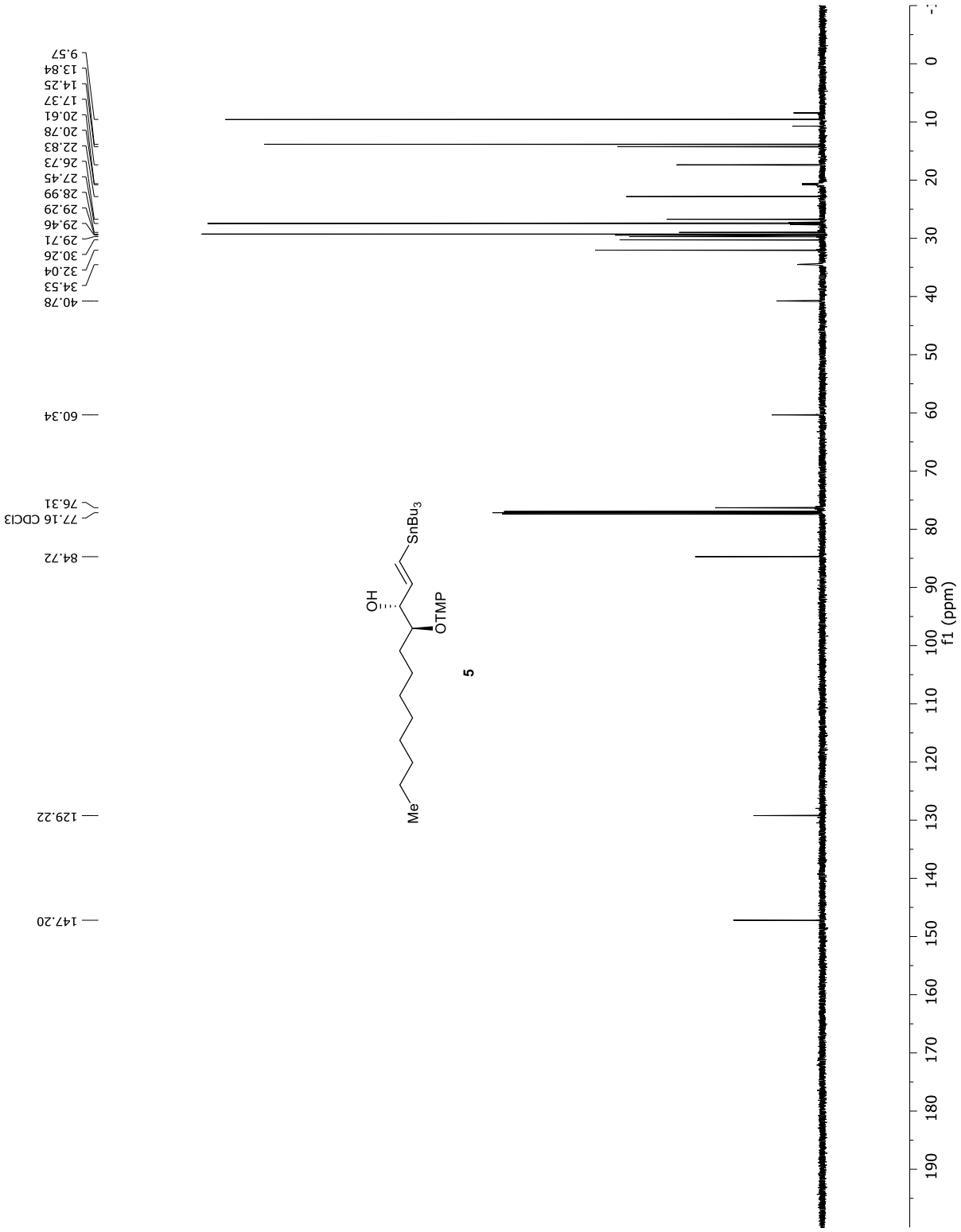
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of α-oxyaldehyde **3:**



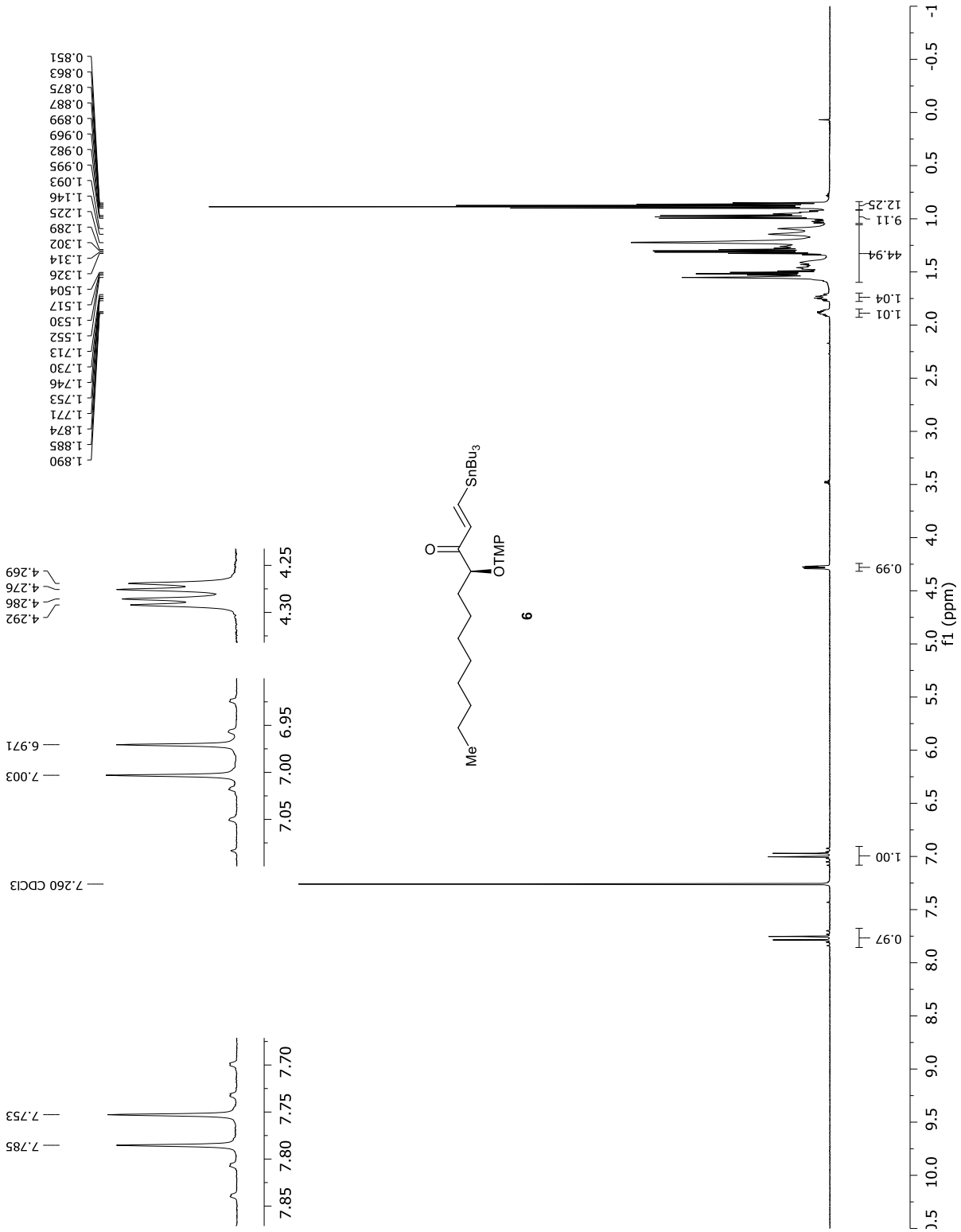
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of vinylstannane **5:**



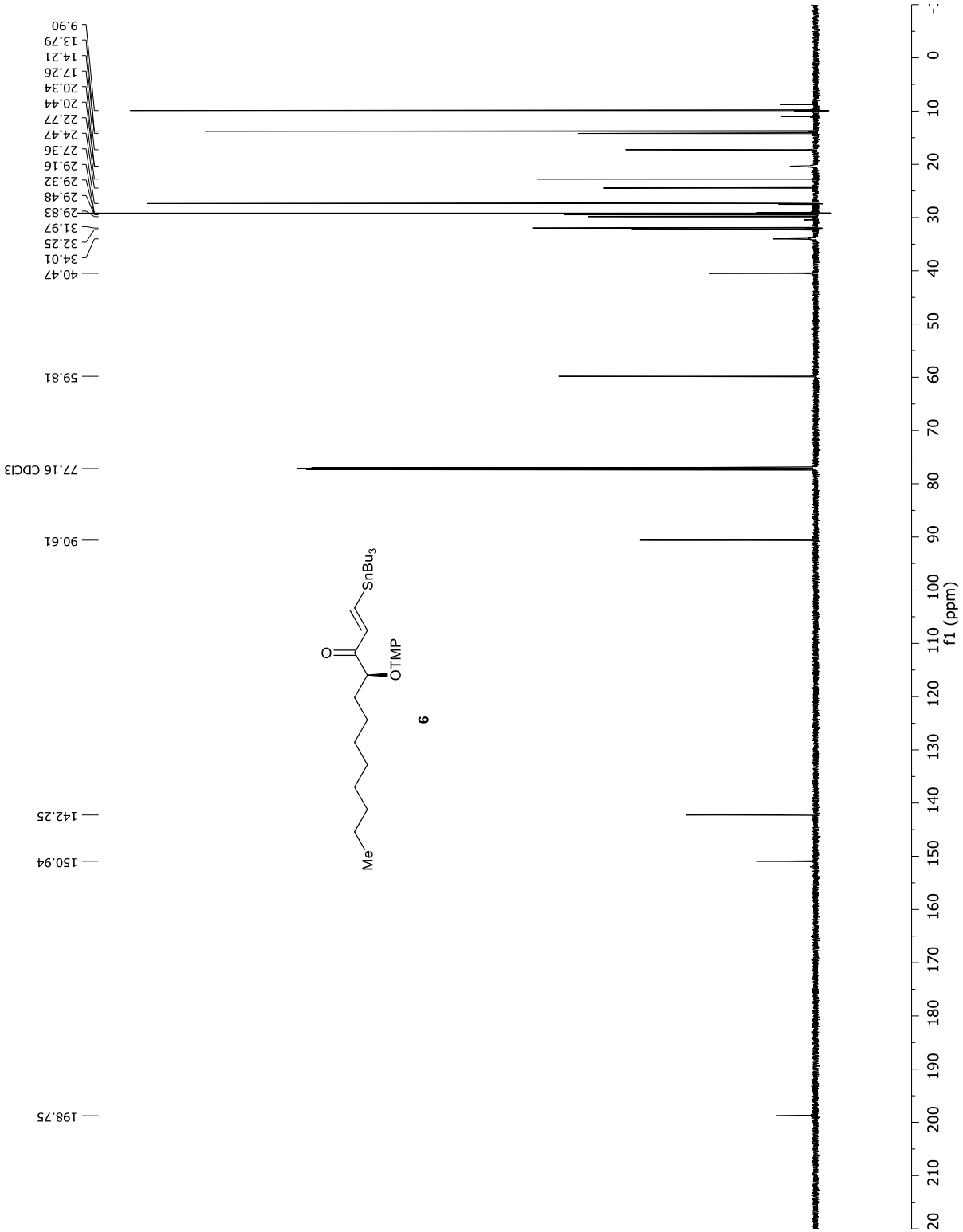
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of vinylstannane **5:**



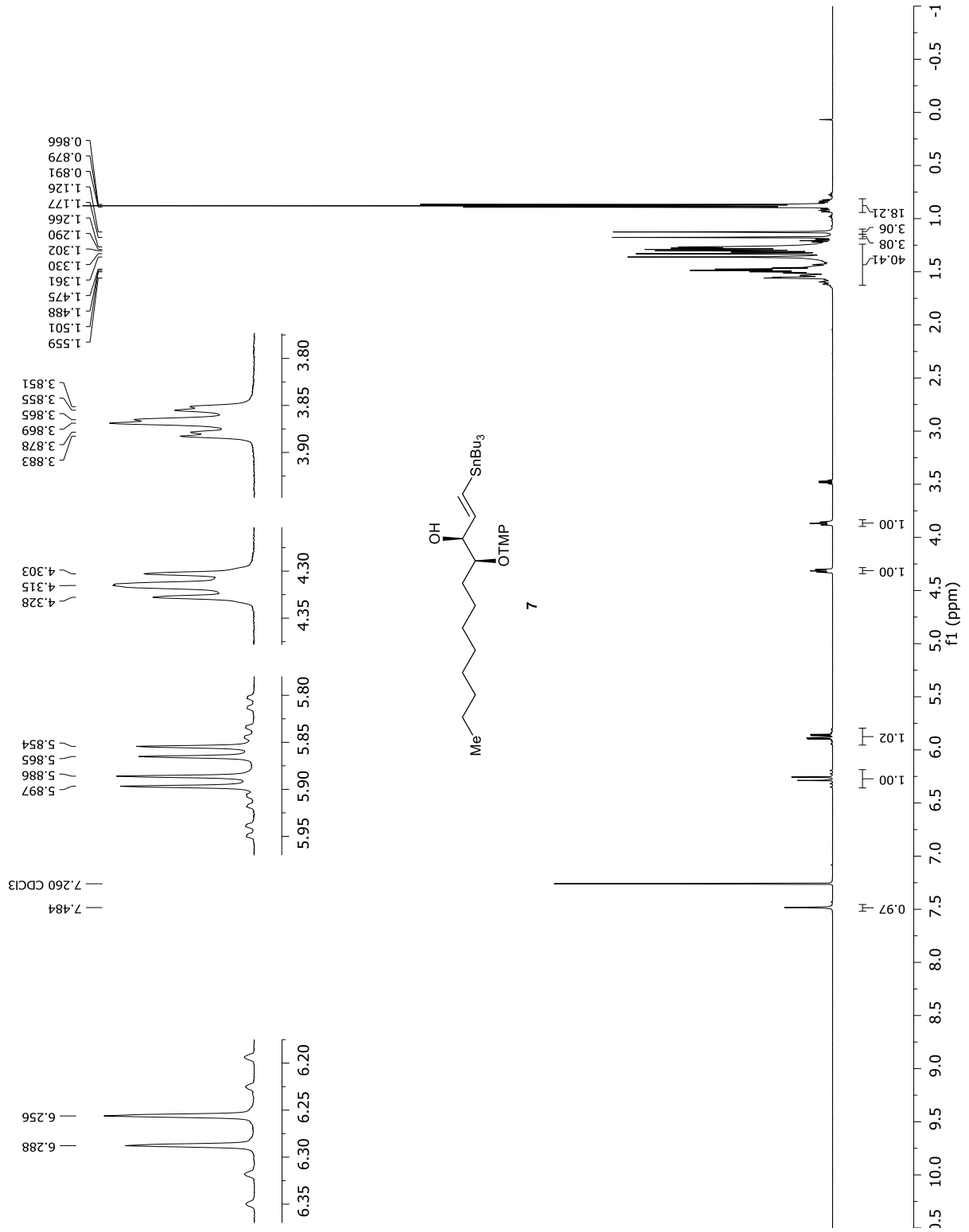
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of enone **6:**



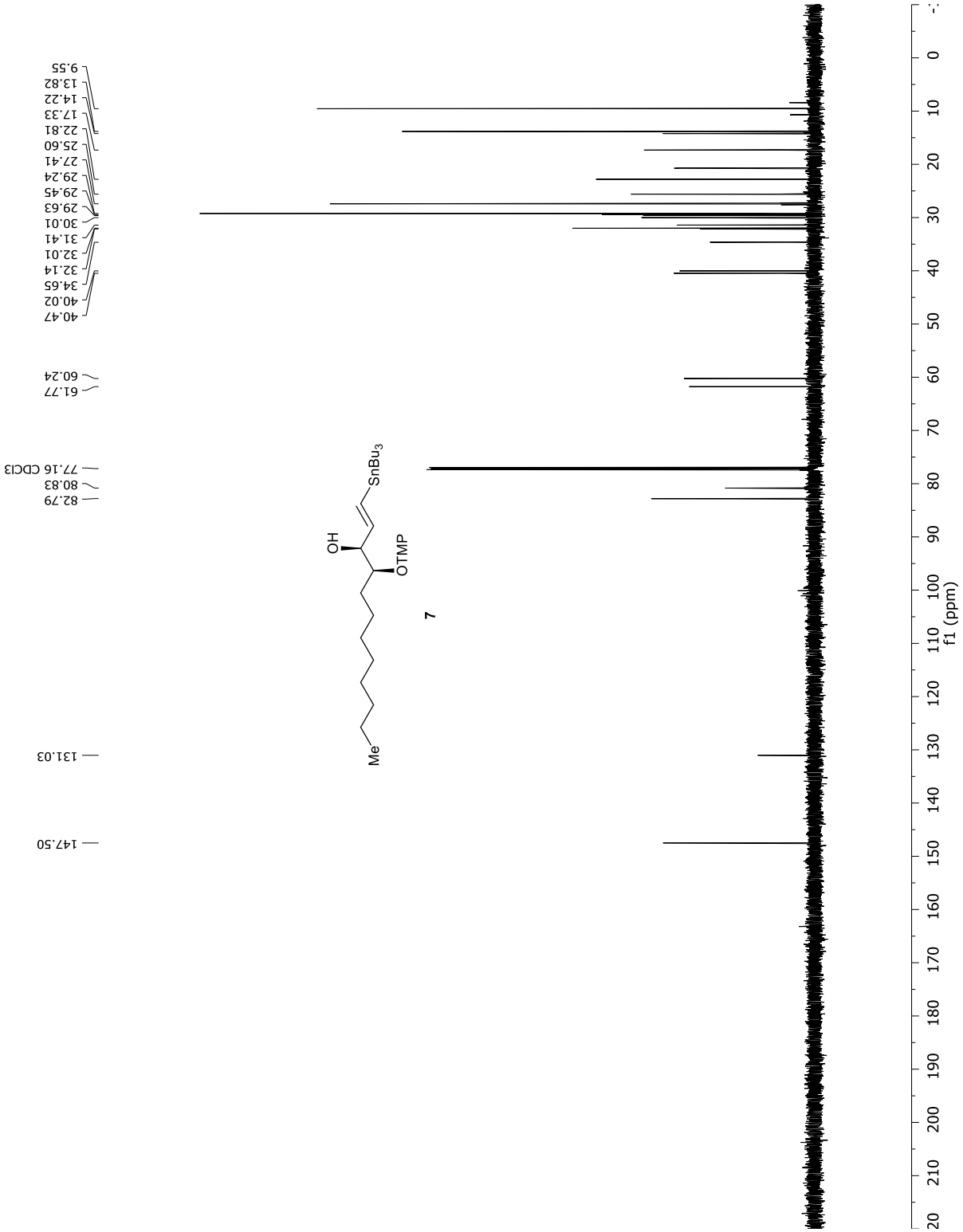
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of enone **6:**



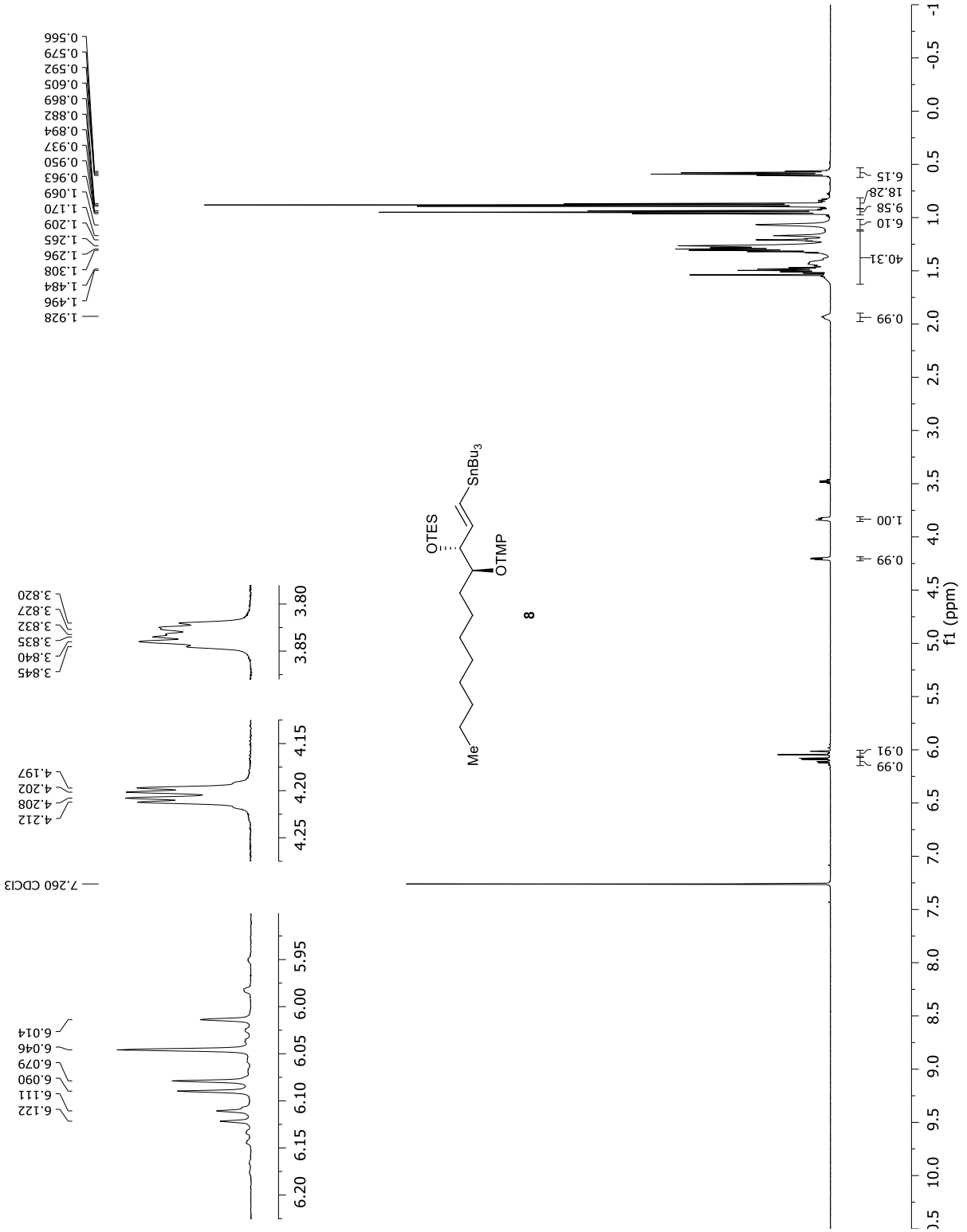
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of allylic alcohol **7:**



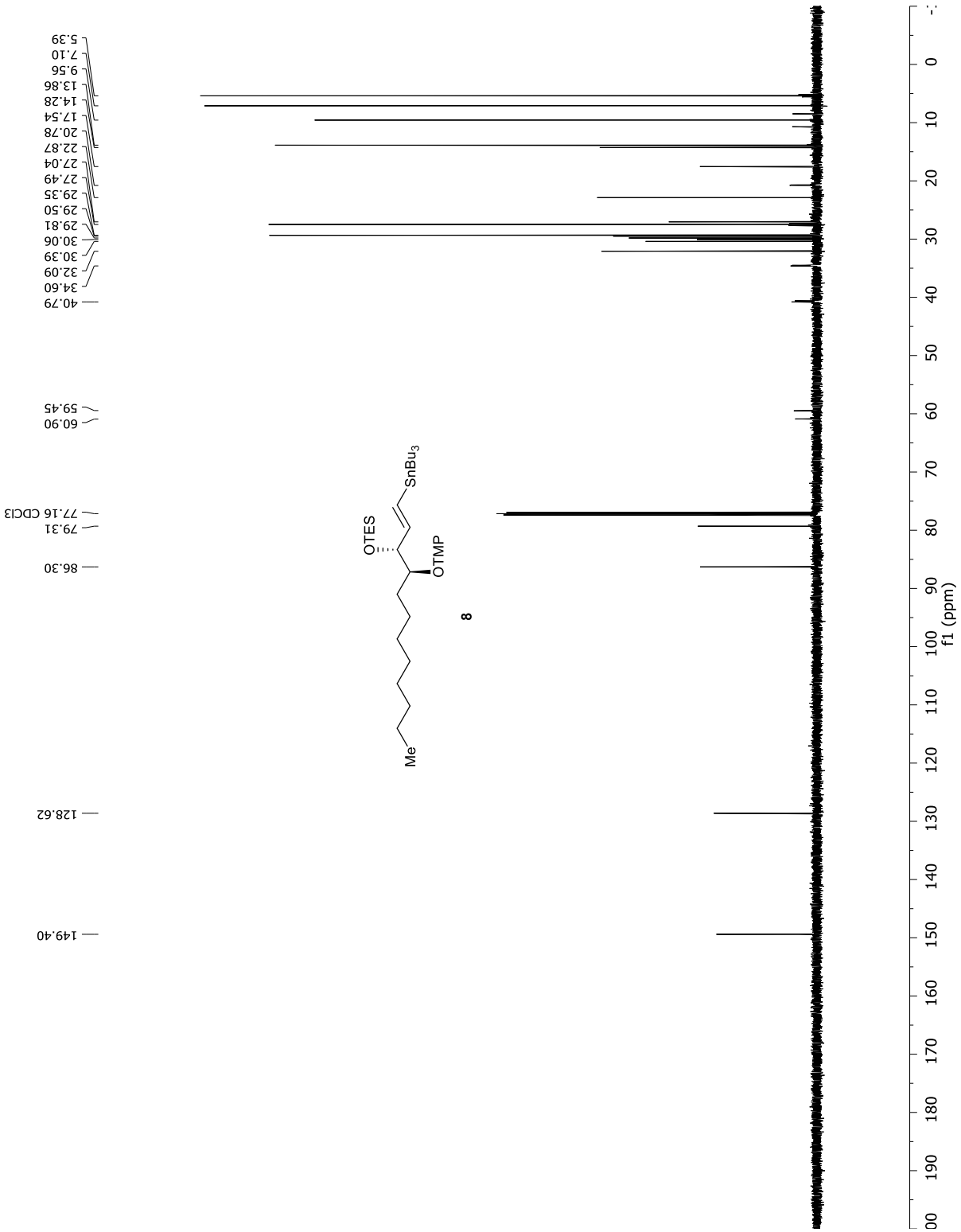
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of allylic alcohol **7:**



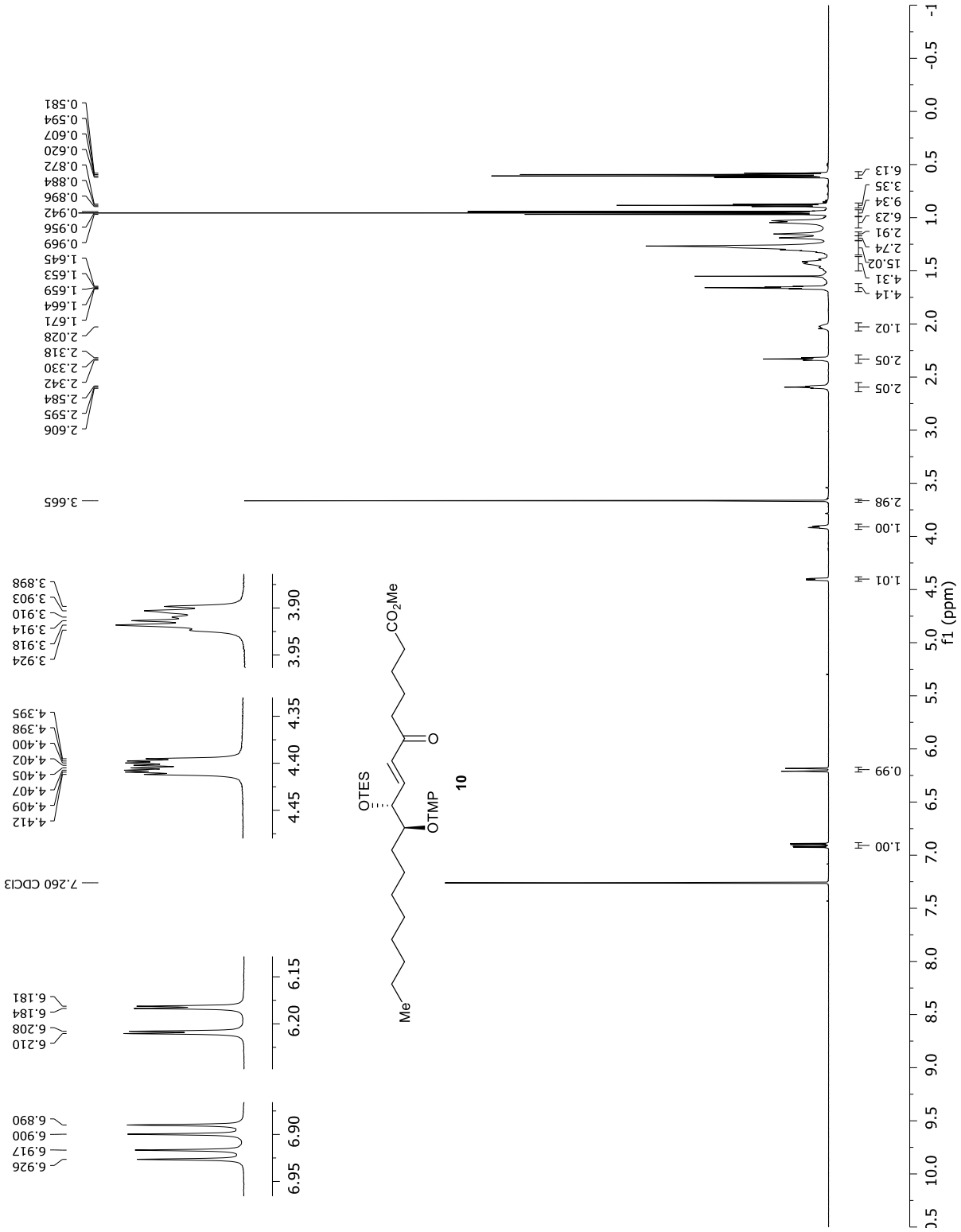
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of silyl ether **8:**



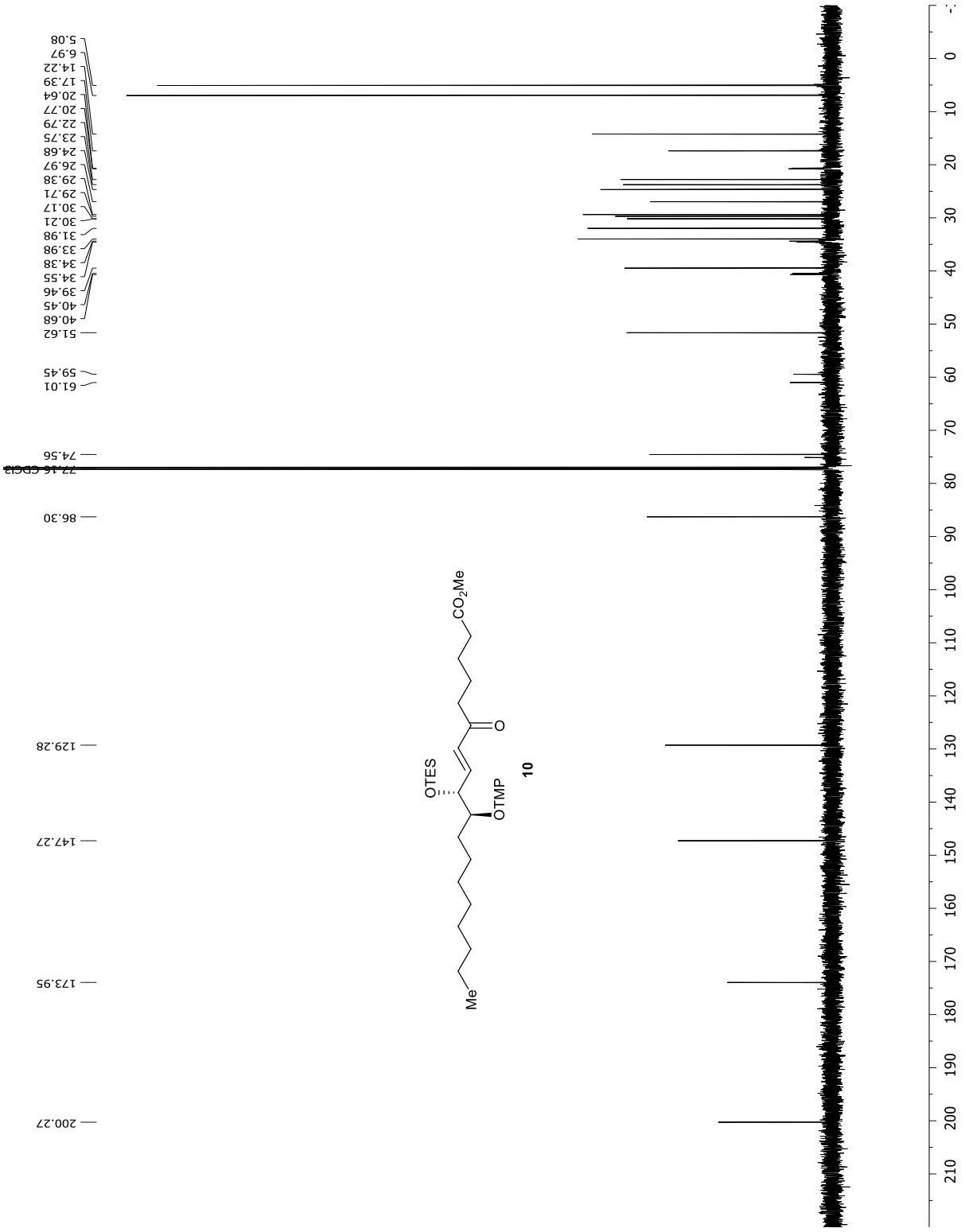
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of silyl ether **8:**



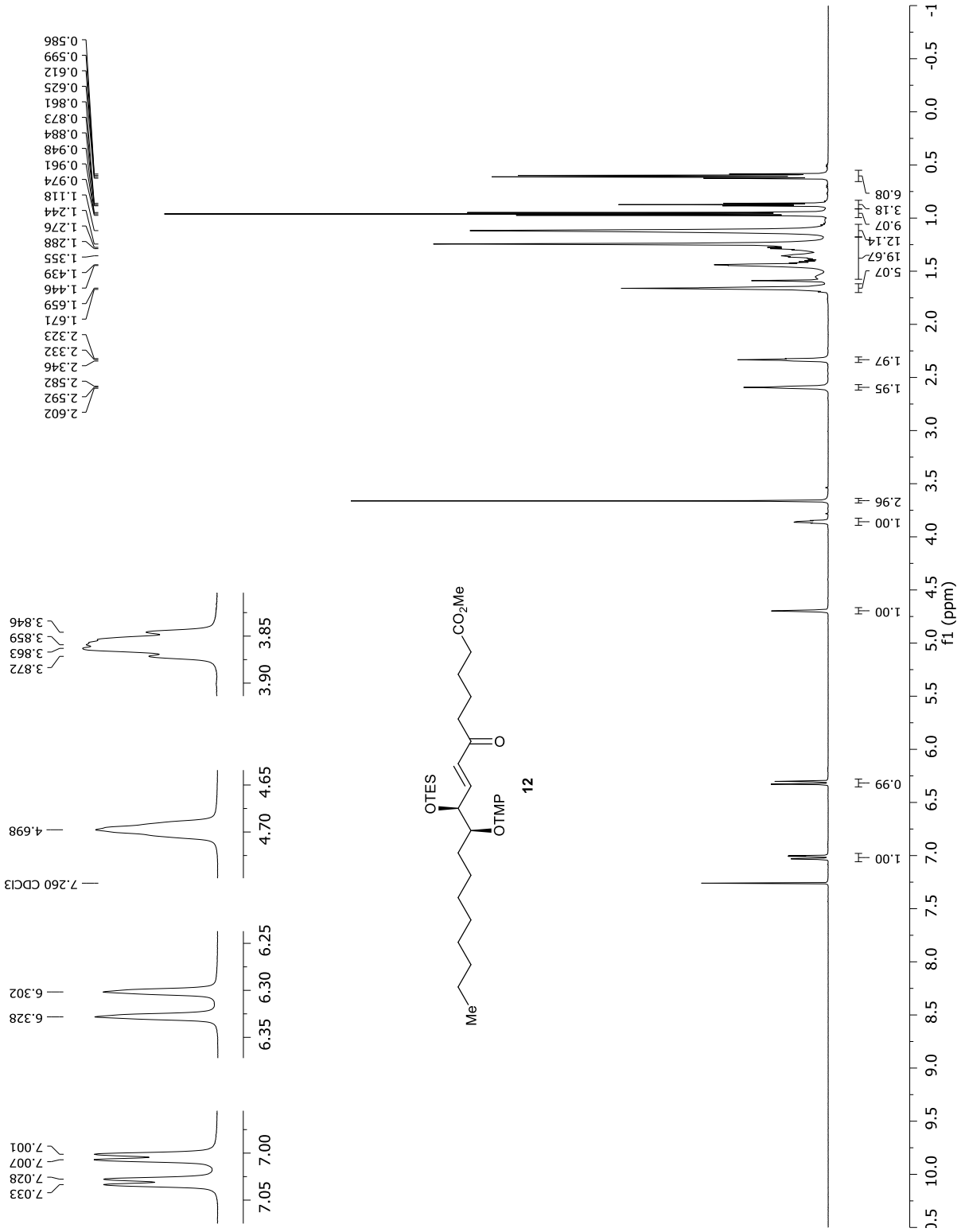
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of enone **10:**



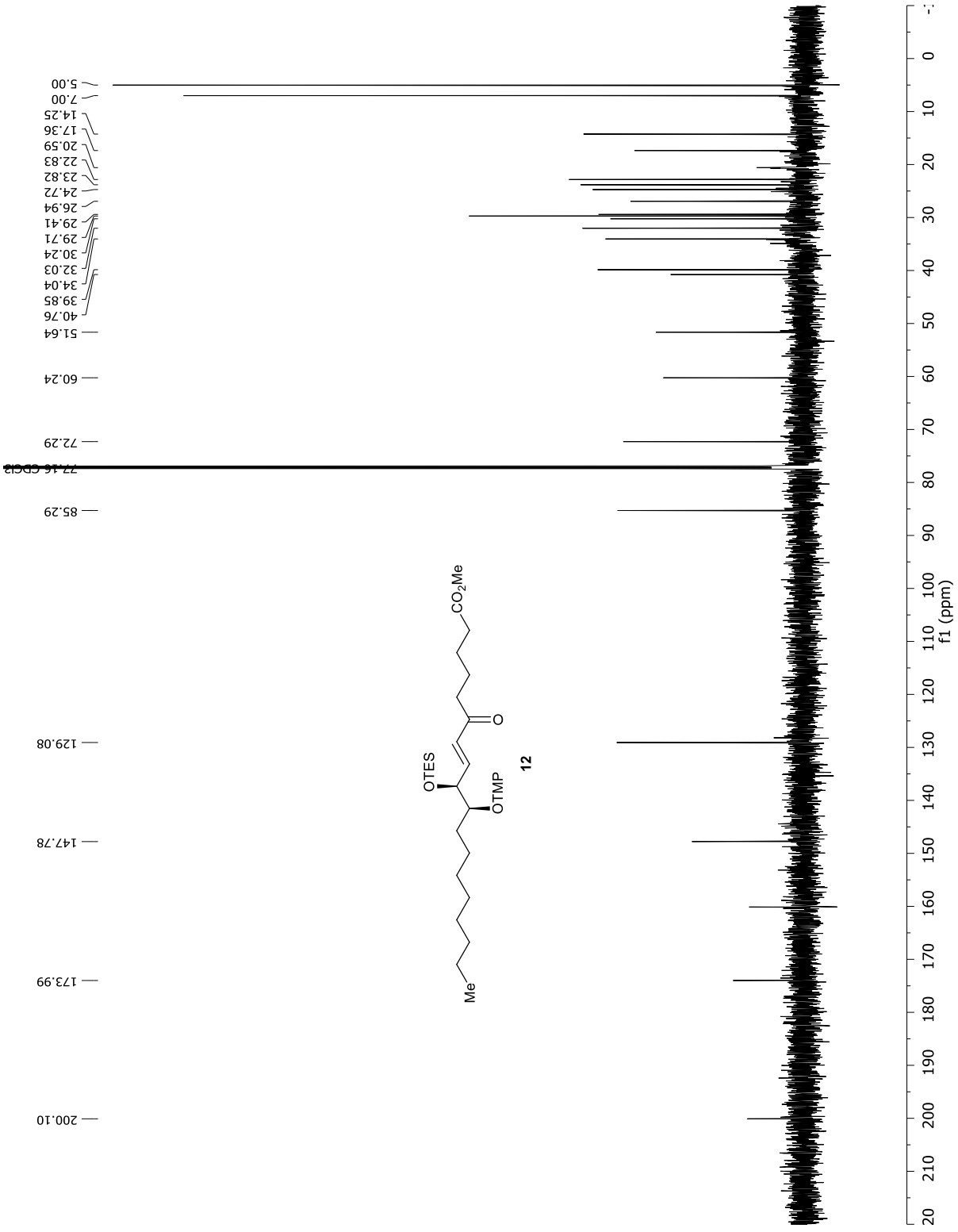
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of enone **10:**



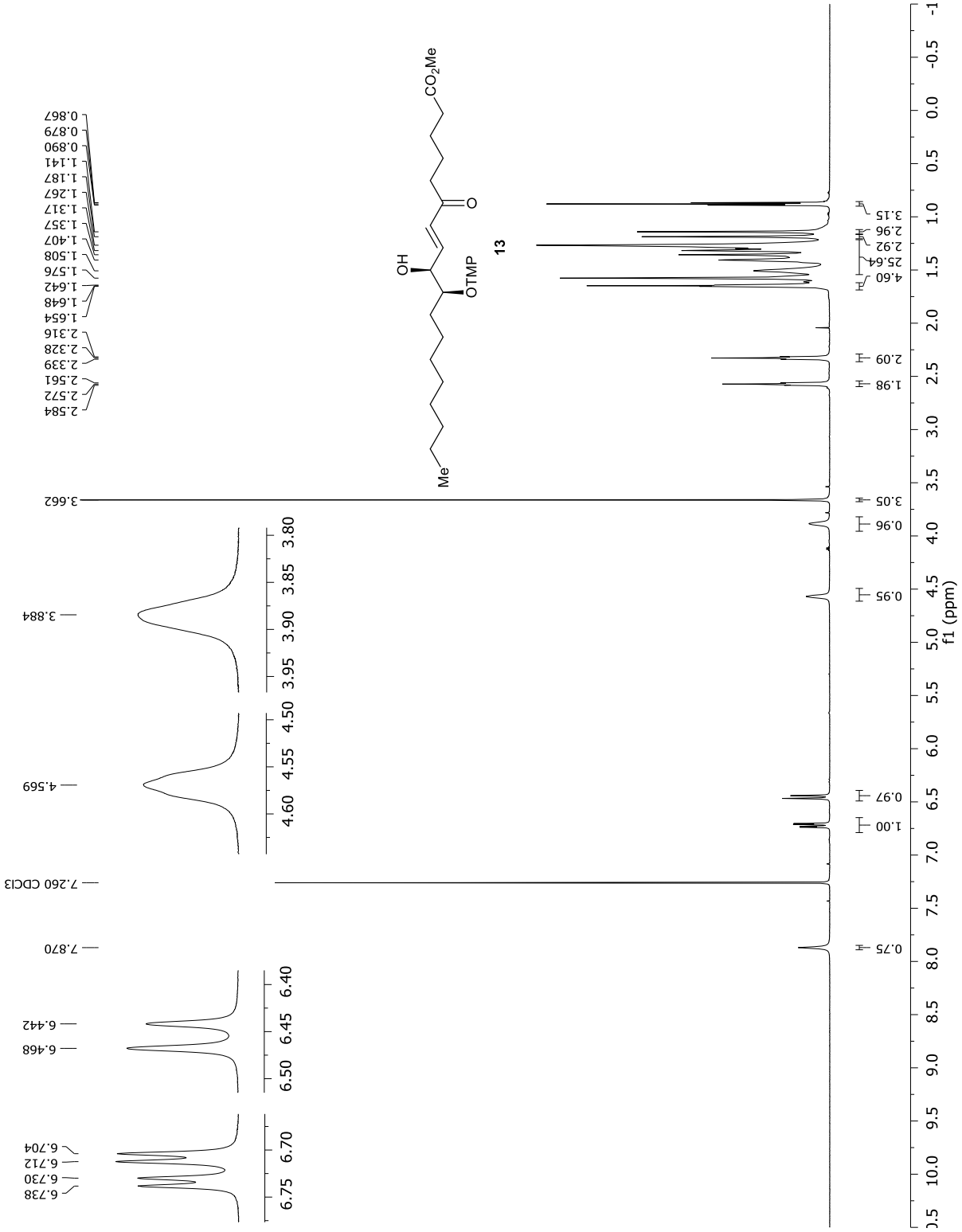
^{1}H-NMR spectrum (600 MHz, $CDCl_3$) of enone **12:**



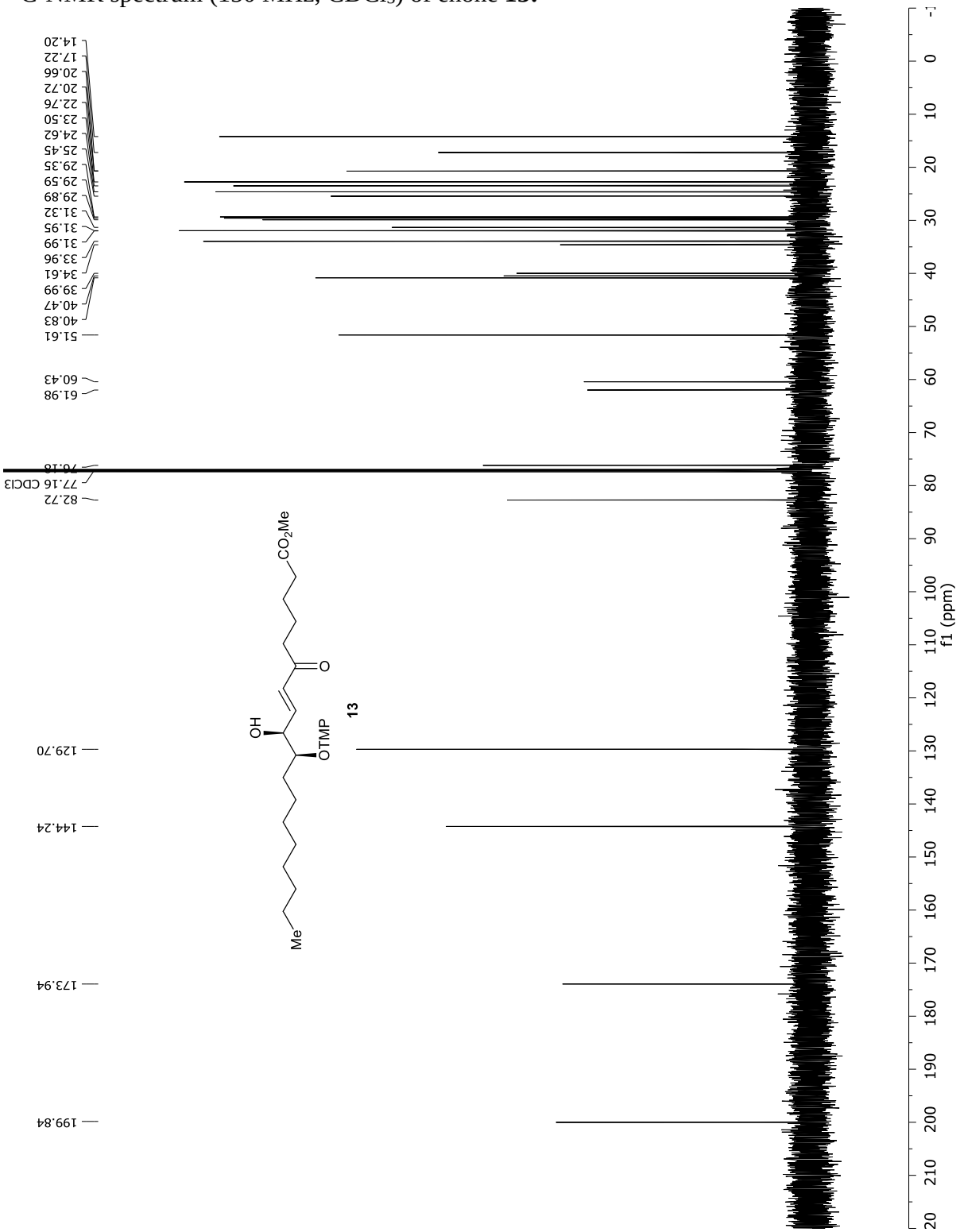
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of enone **12:**



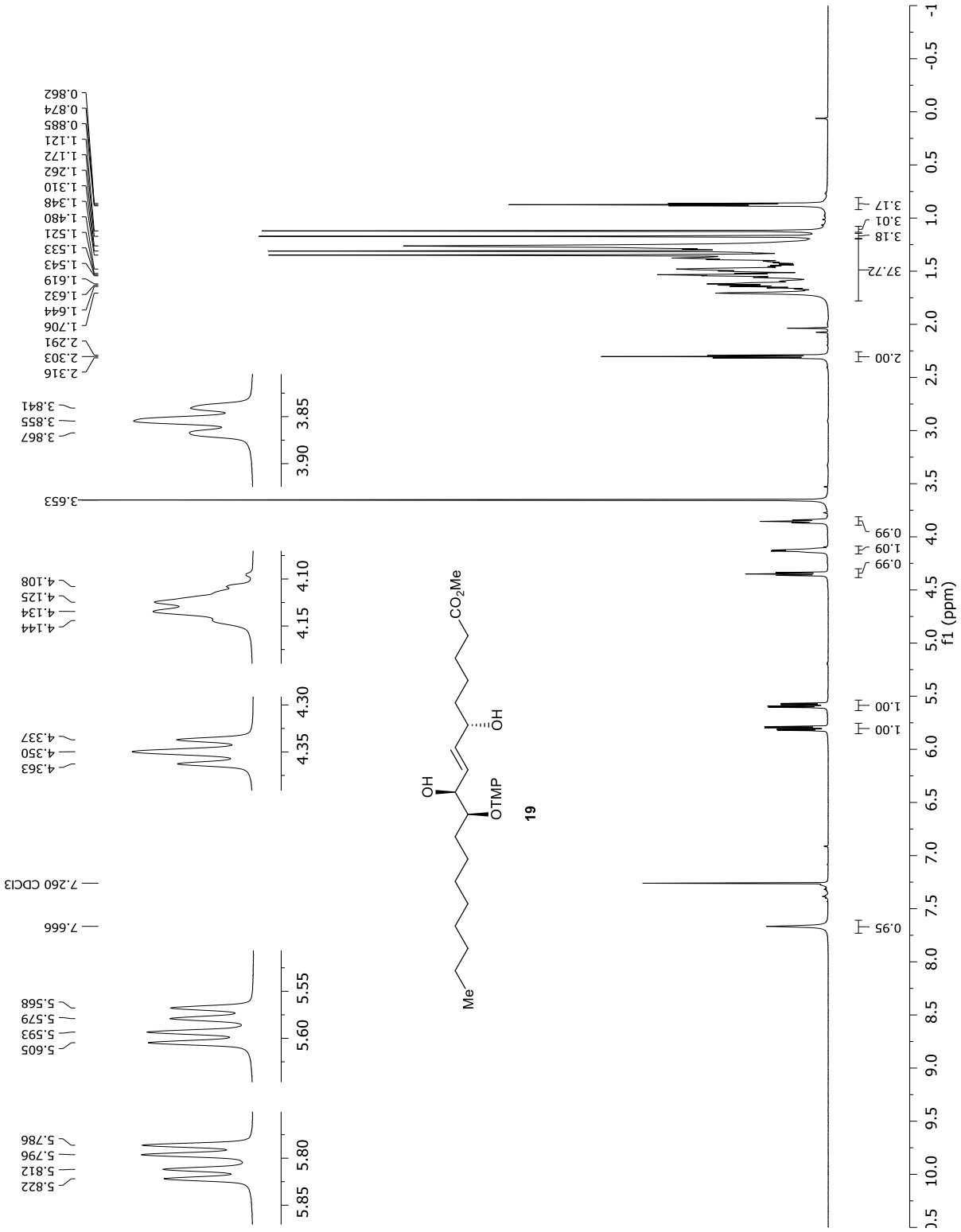
^{1}H-NMR spectrum (600 MHz, $CDCl_3$) of enone **13:**



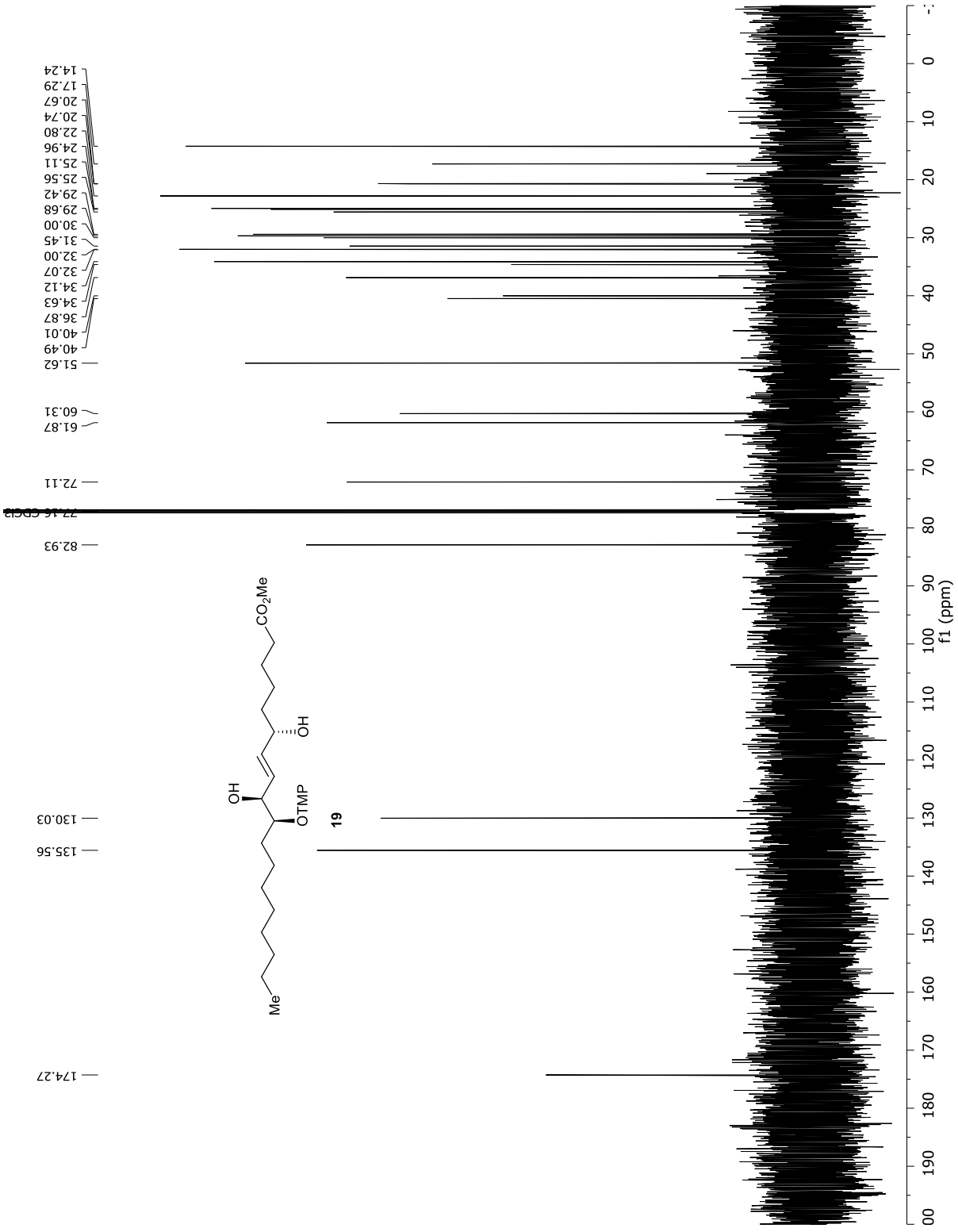
^{13}C-NMR spectrum (150 MHz, $CDCl_3$) of enone **13:**



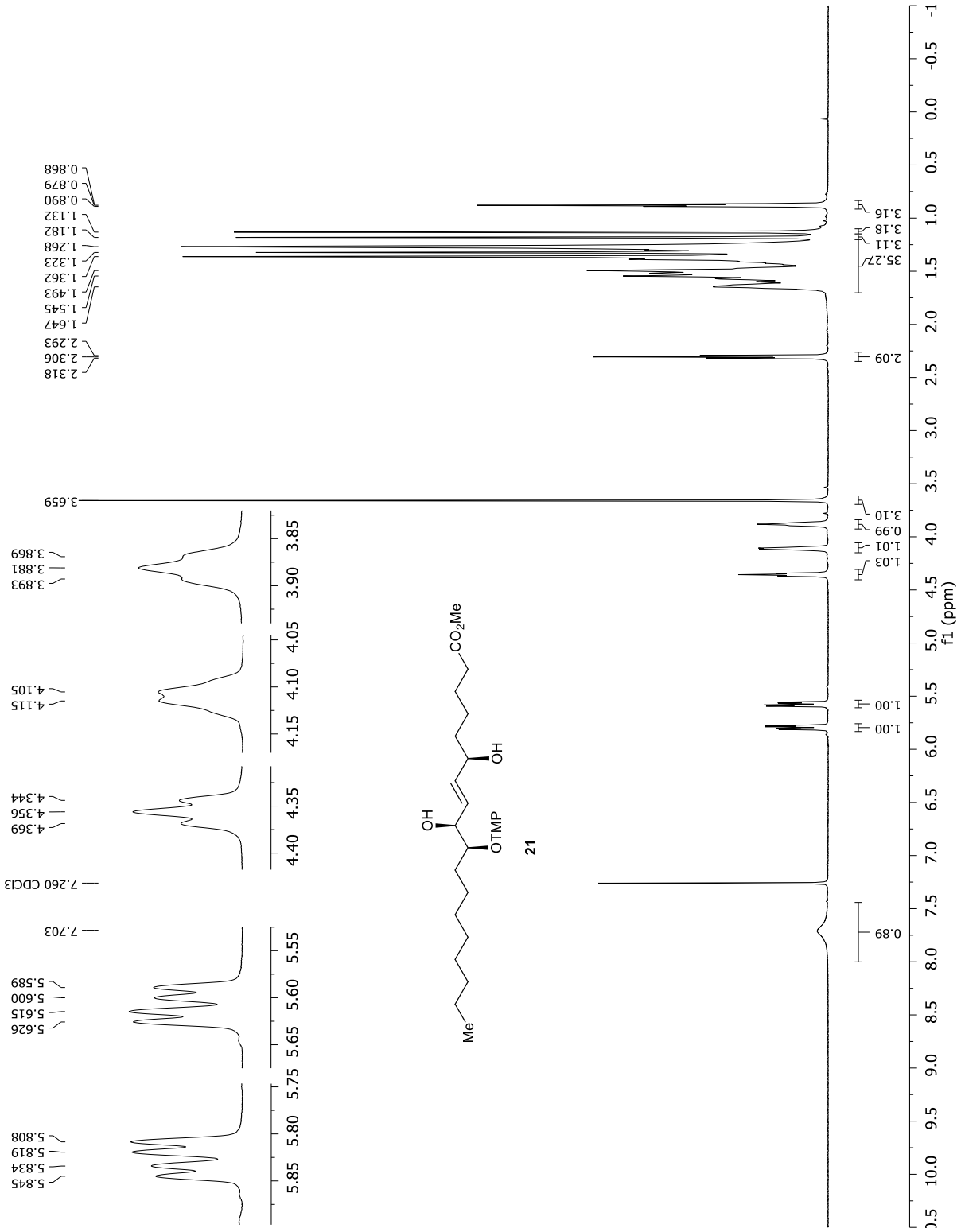
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of allylic alcohol **19:**



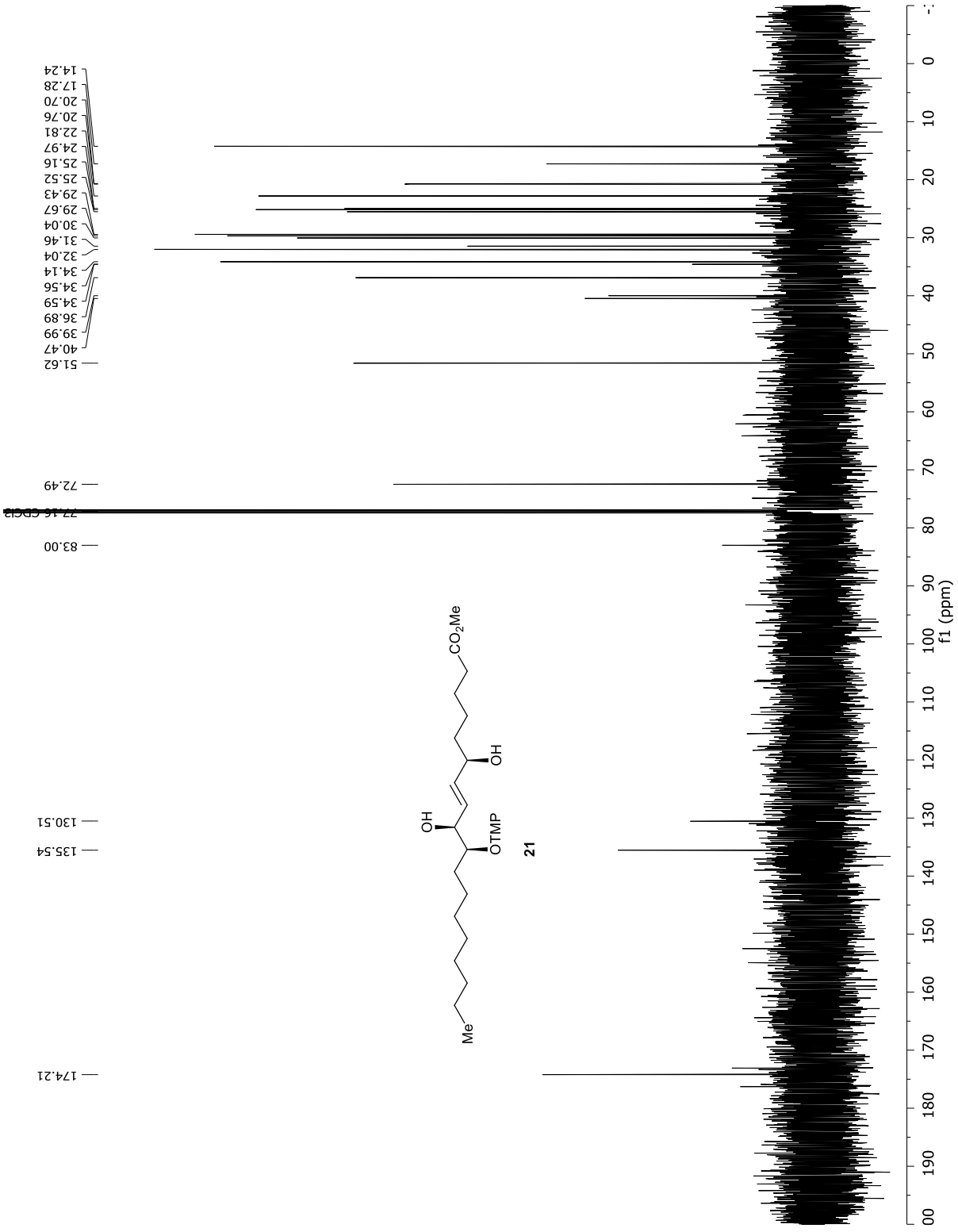
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of allylic alcohol **19:**



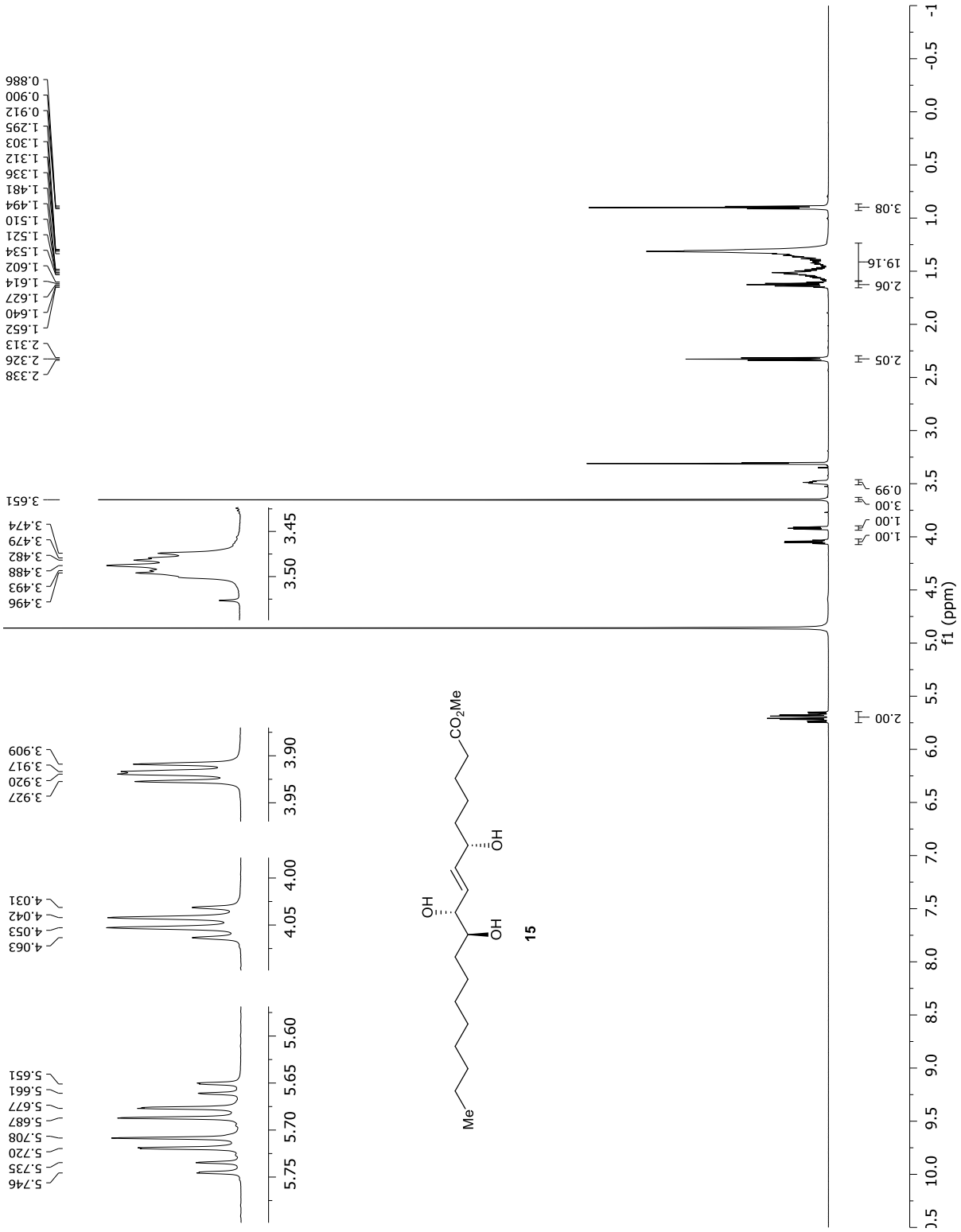
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of allylic alcohol **21:**



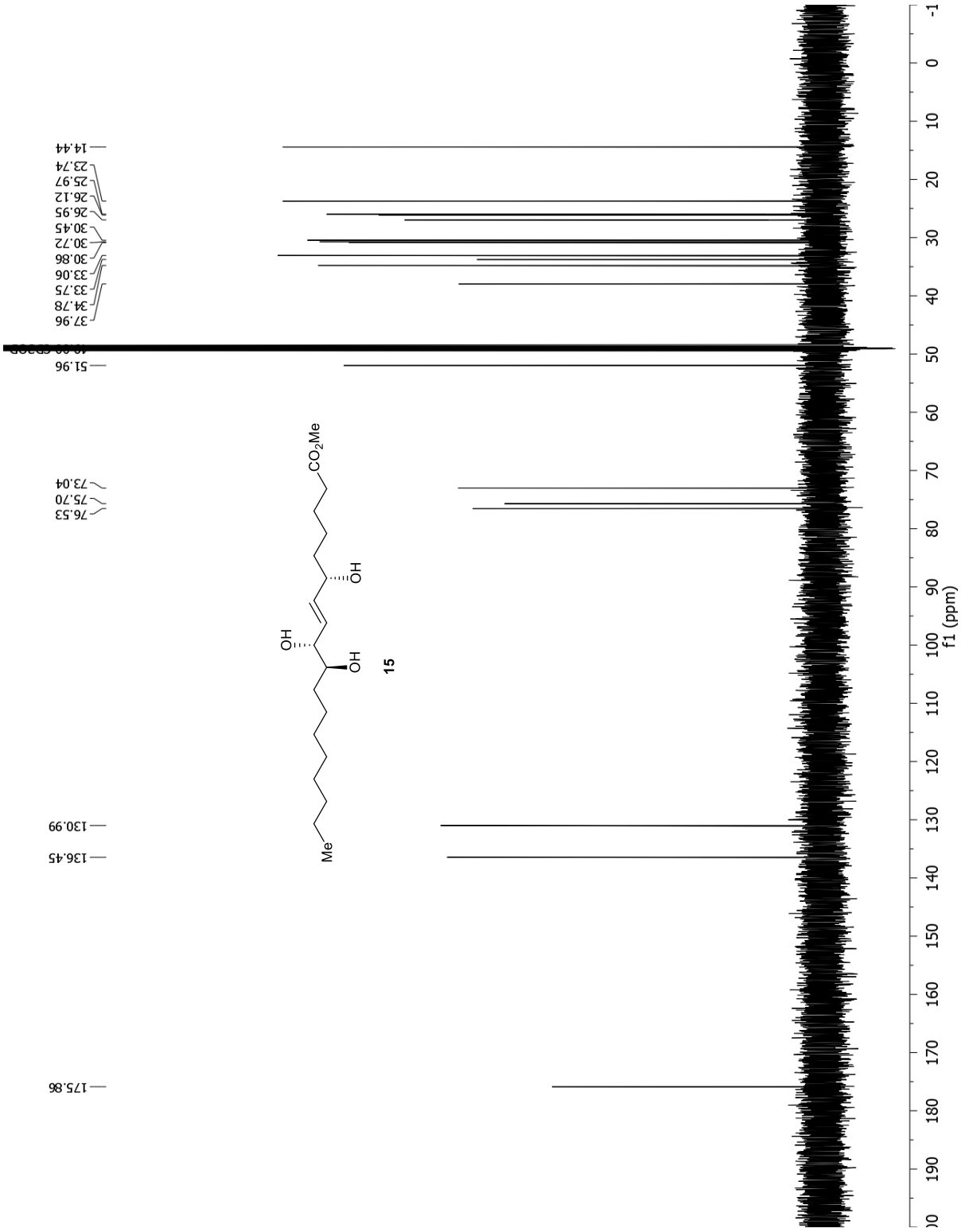
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of allylic alcohol **21:**



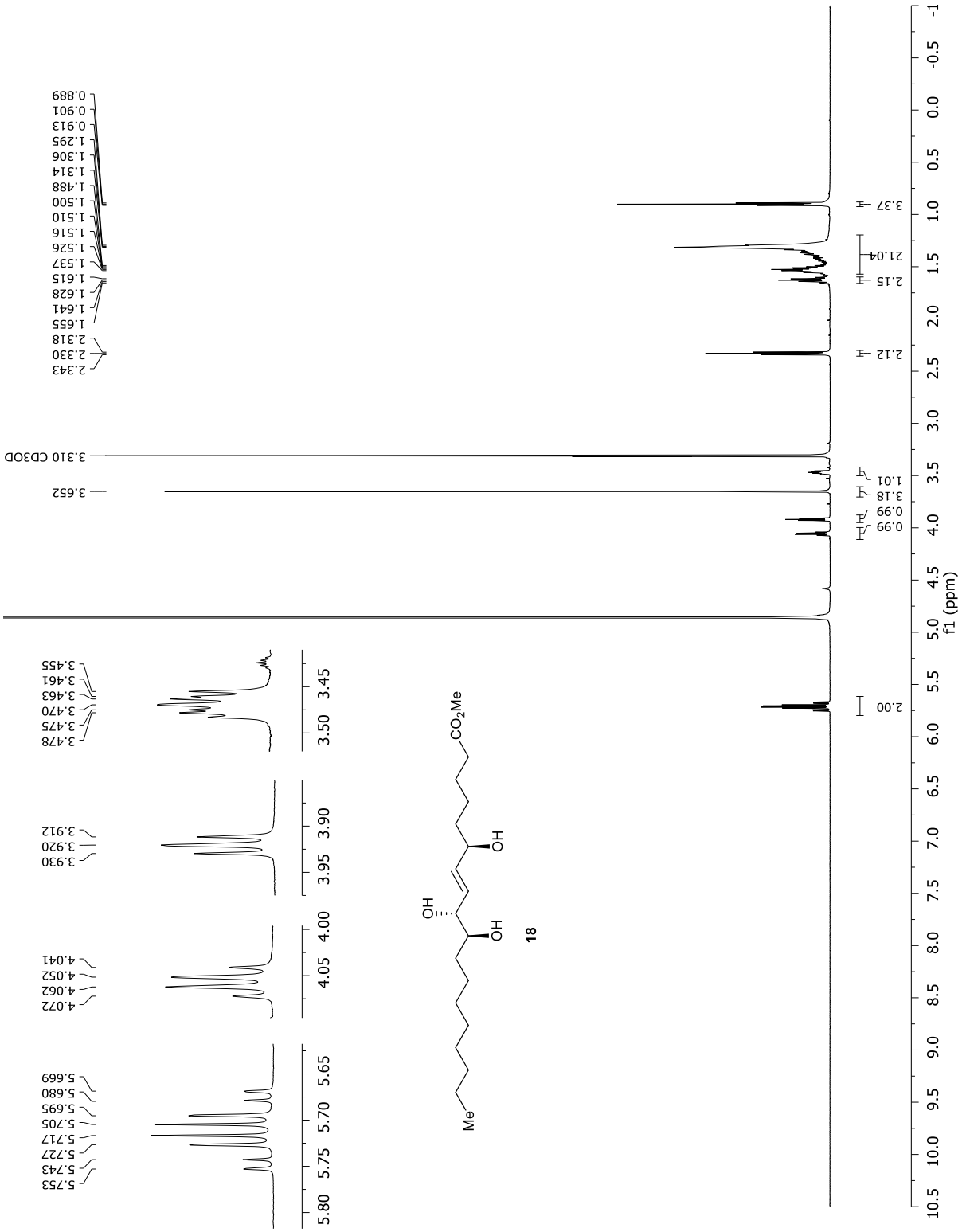
^{1}H NMR spectrum (600 MHz, CD_3OD) of triol **15:**



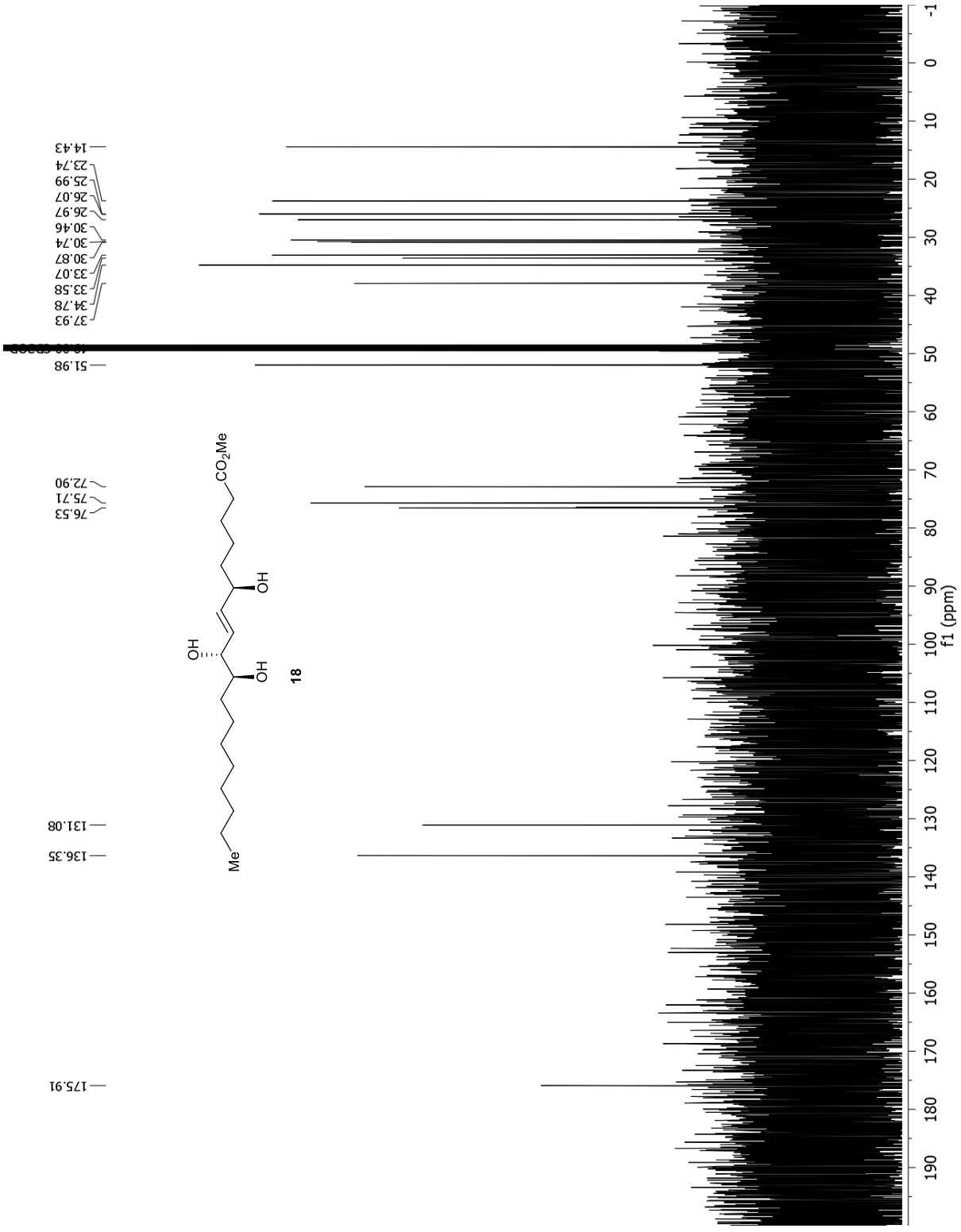
^{13}C NMR spectrum (150 MHz, CD_3OD) of triol **15:**



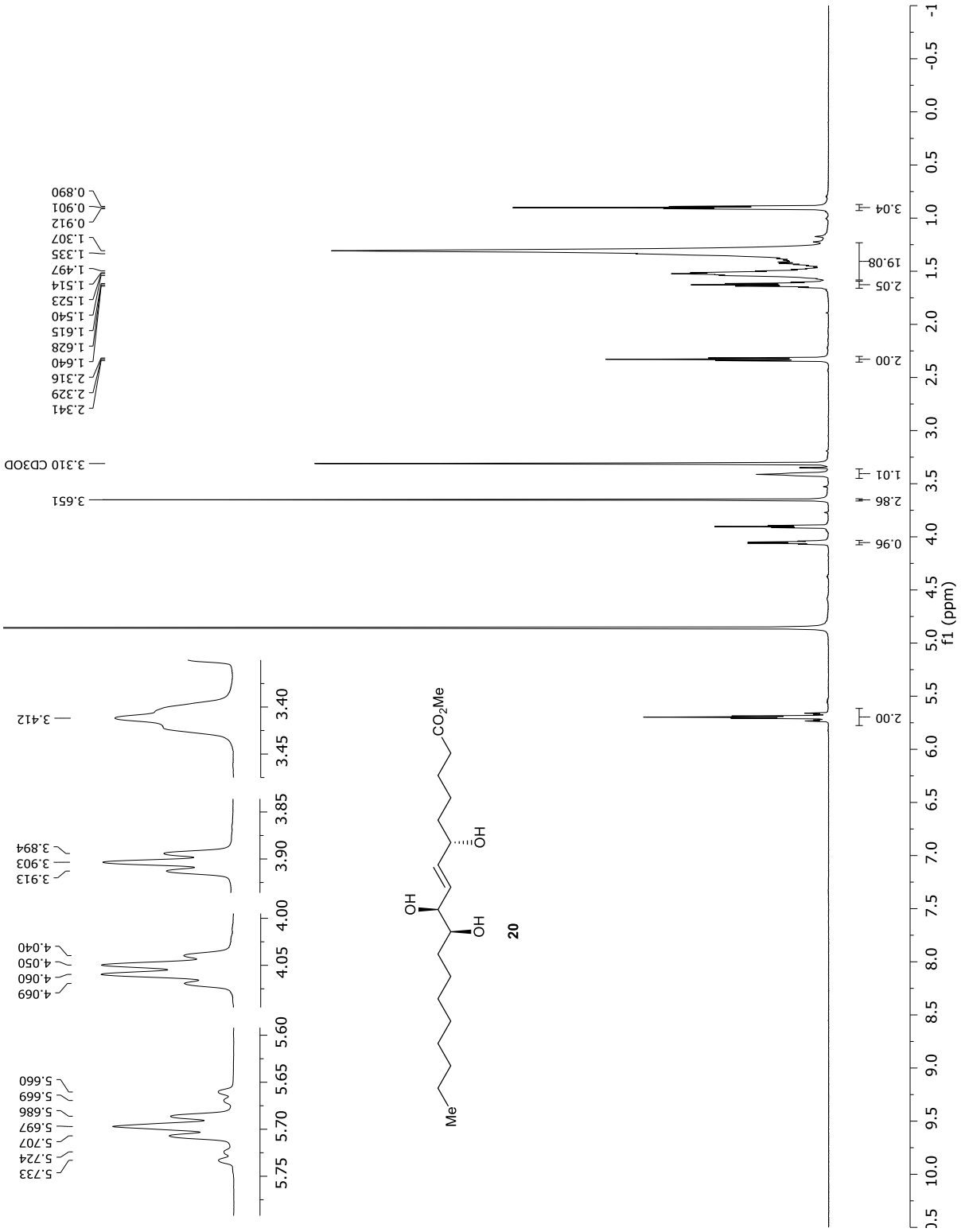
^{1}H NMR spectrum (600 MHz, CD_3OD) of triol **18:**



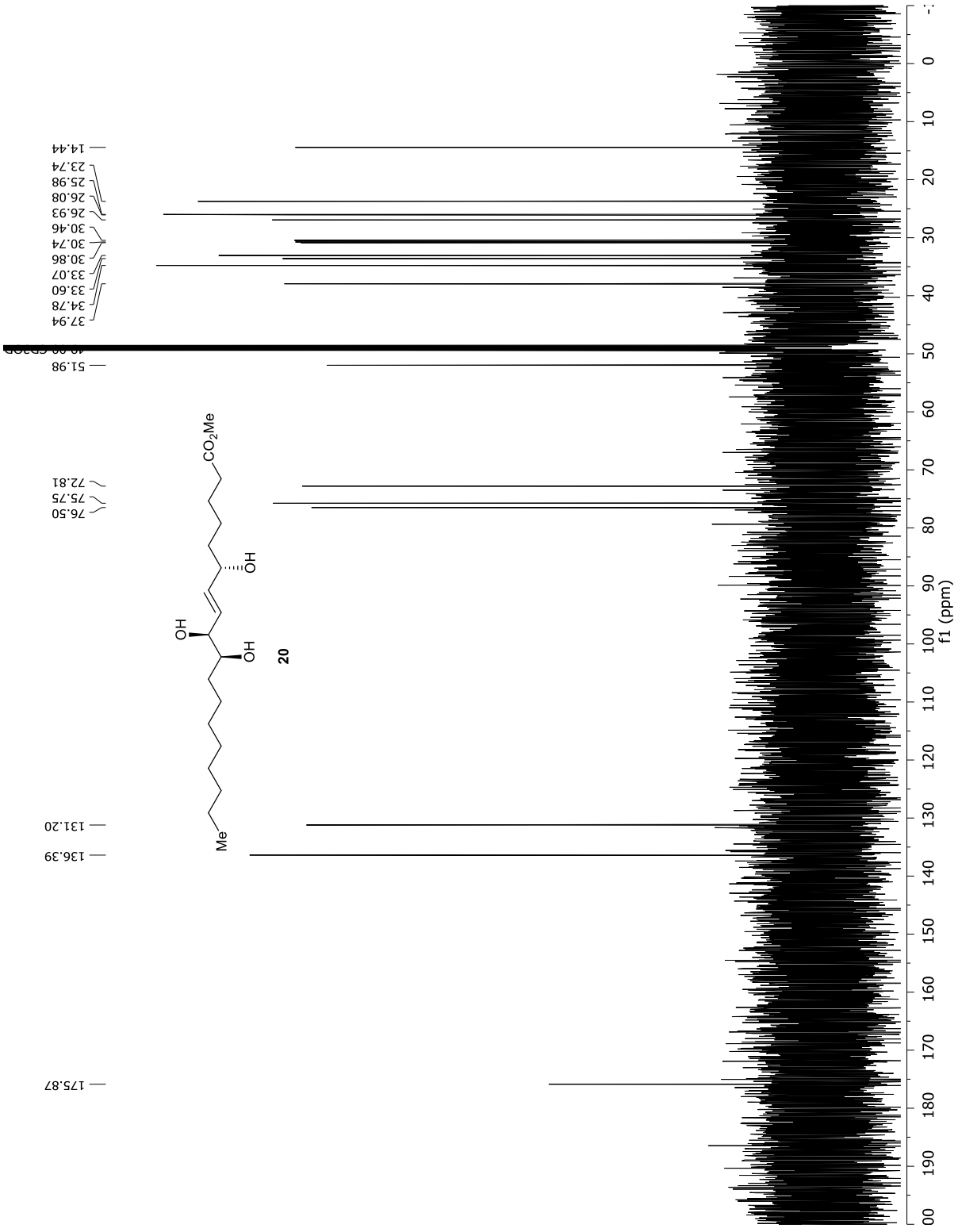
^{13}C NMR spectrum (150 MHz, CD_3OD) of triol **18:**



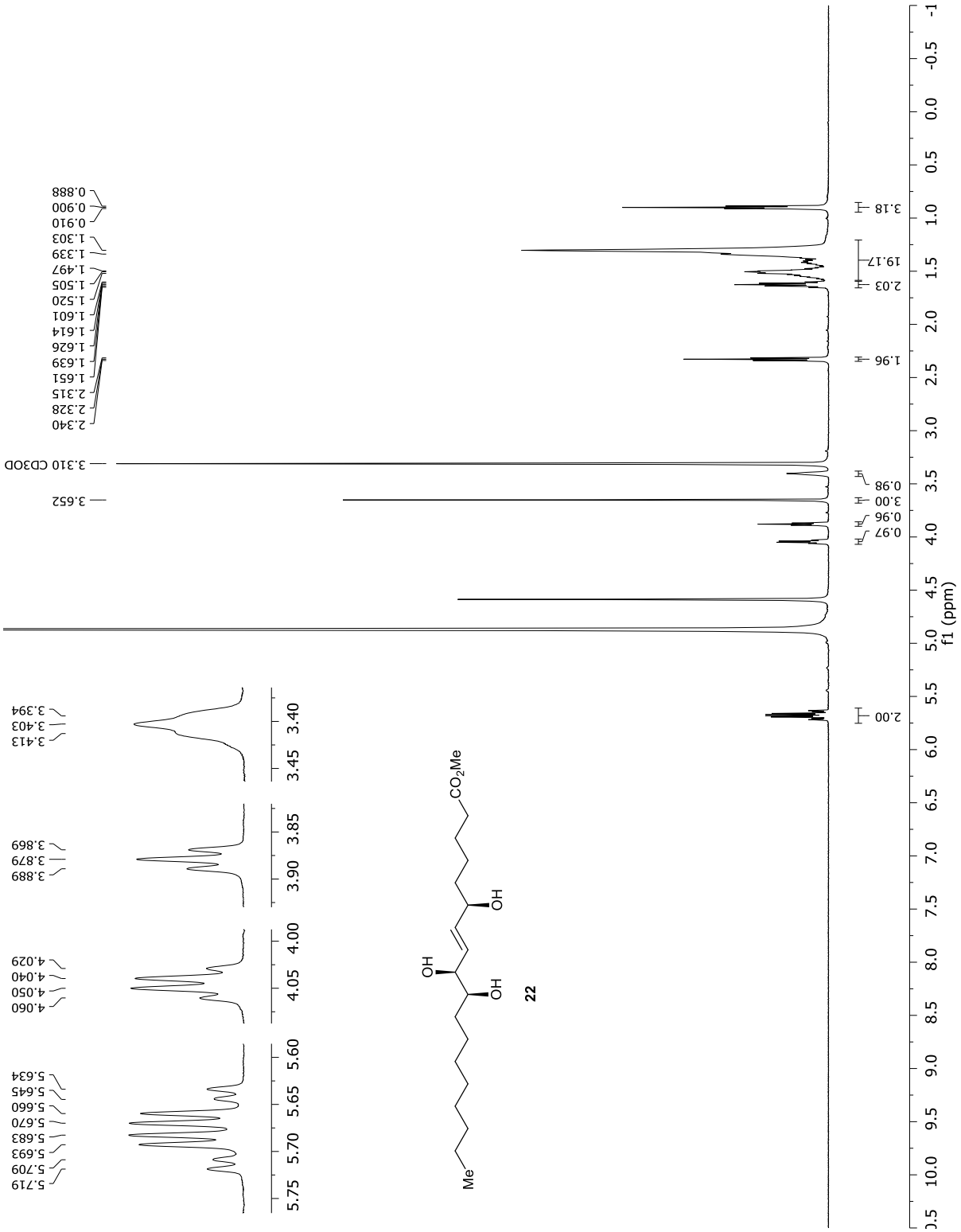
^{1}H NMR spectrum (600 MHz, CD_3OD) of triol **20:**



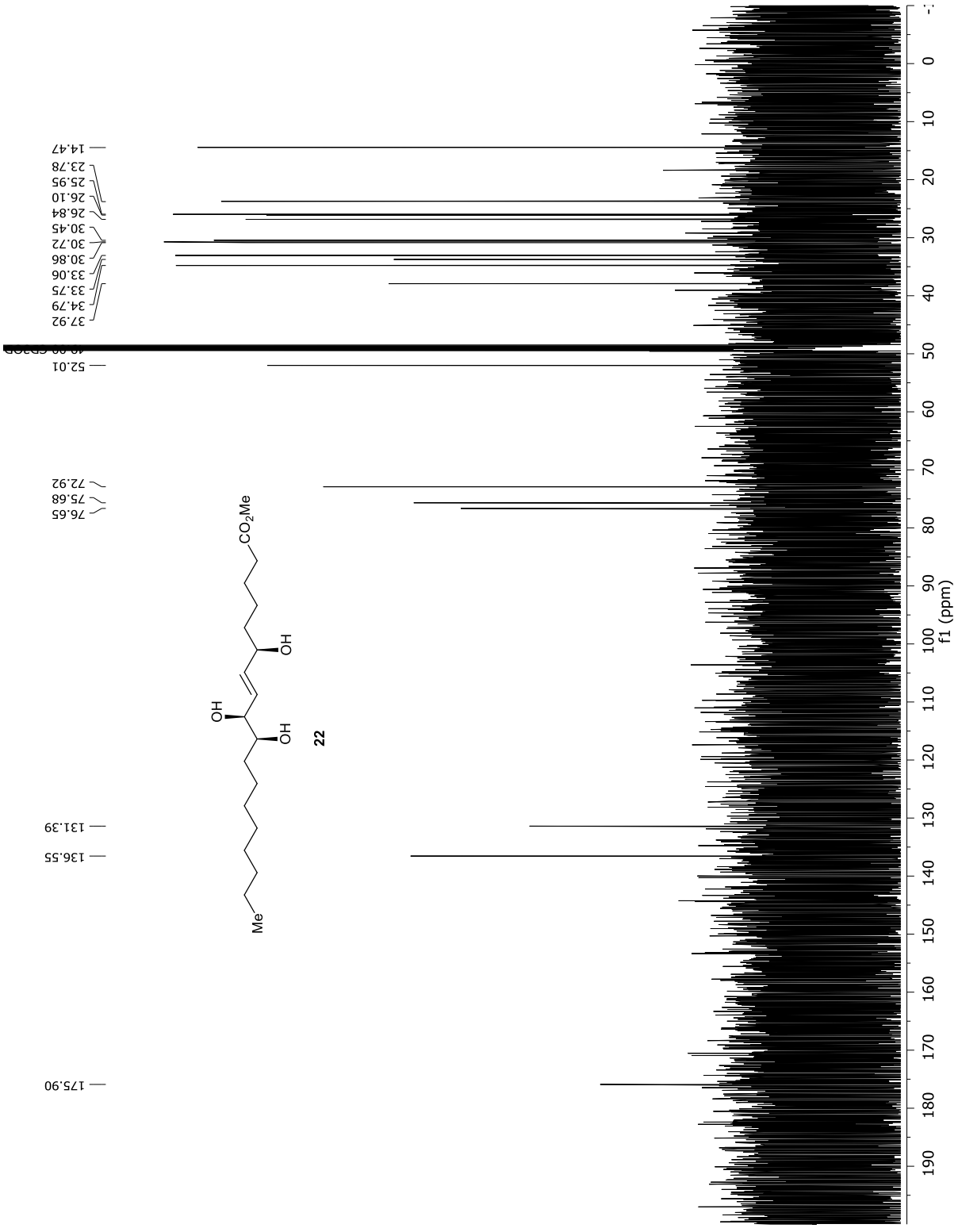
^{13}C NMR spectrum (150 MHz, CD_3OD) of triol **20:**



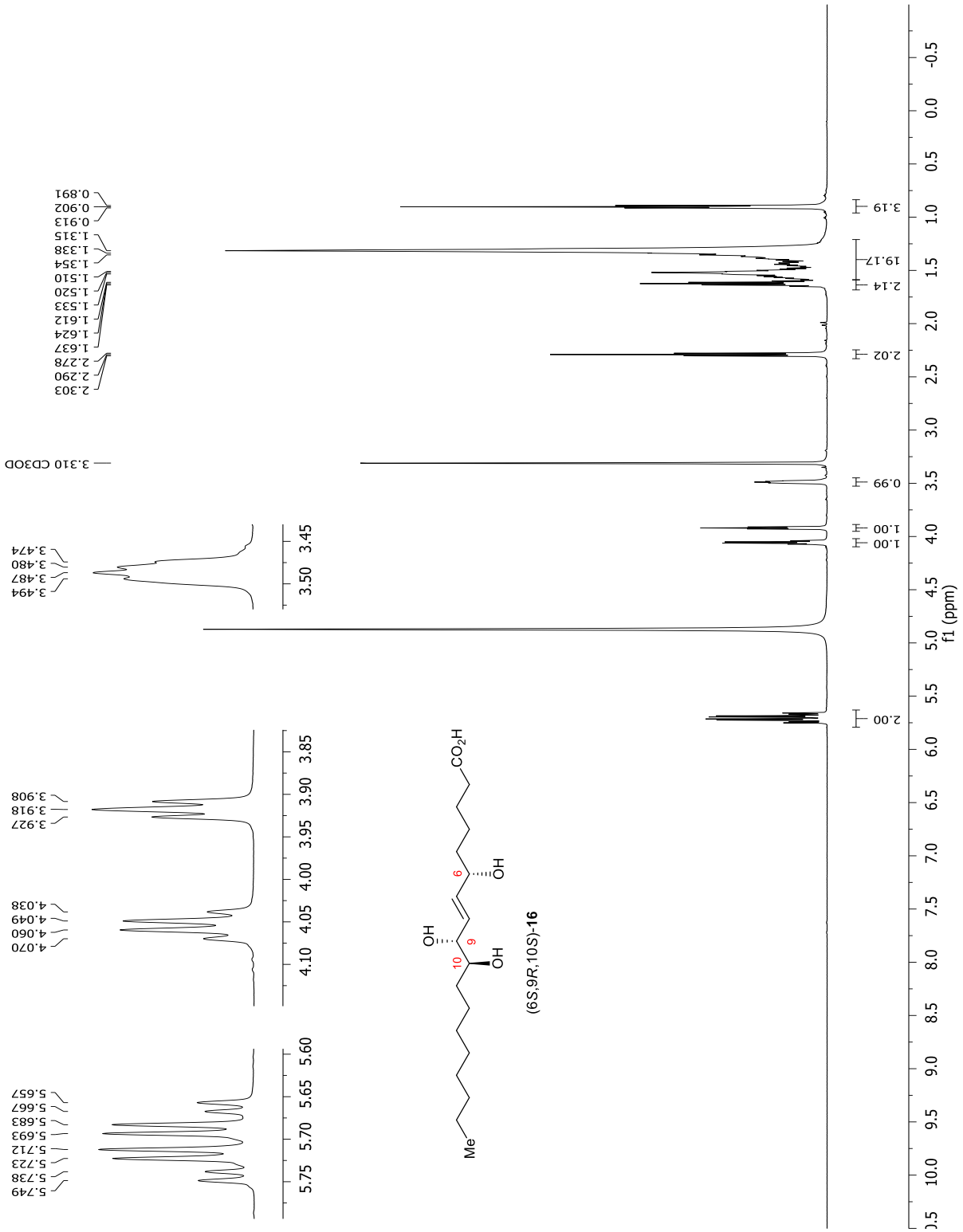
^{1}H NMR spectrum (600 MHz, CD_3OD) of triol **22:**



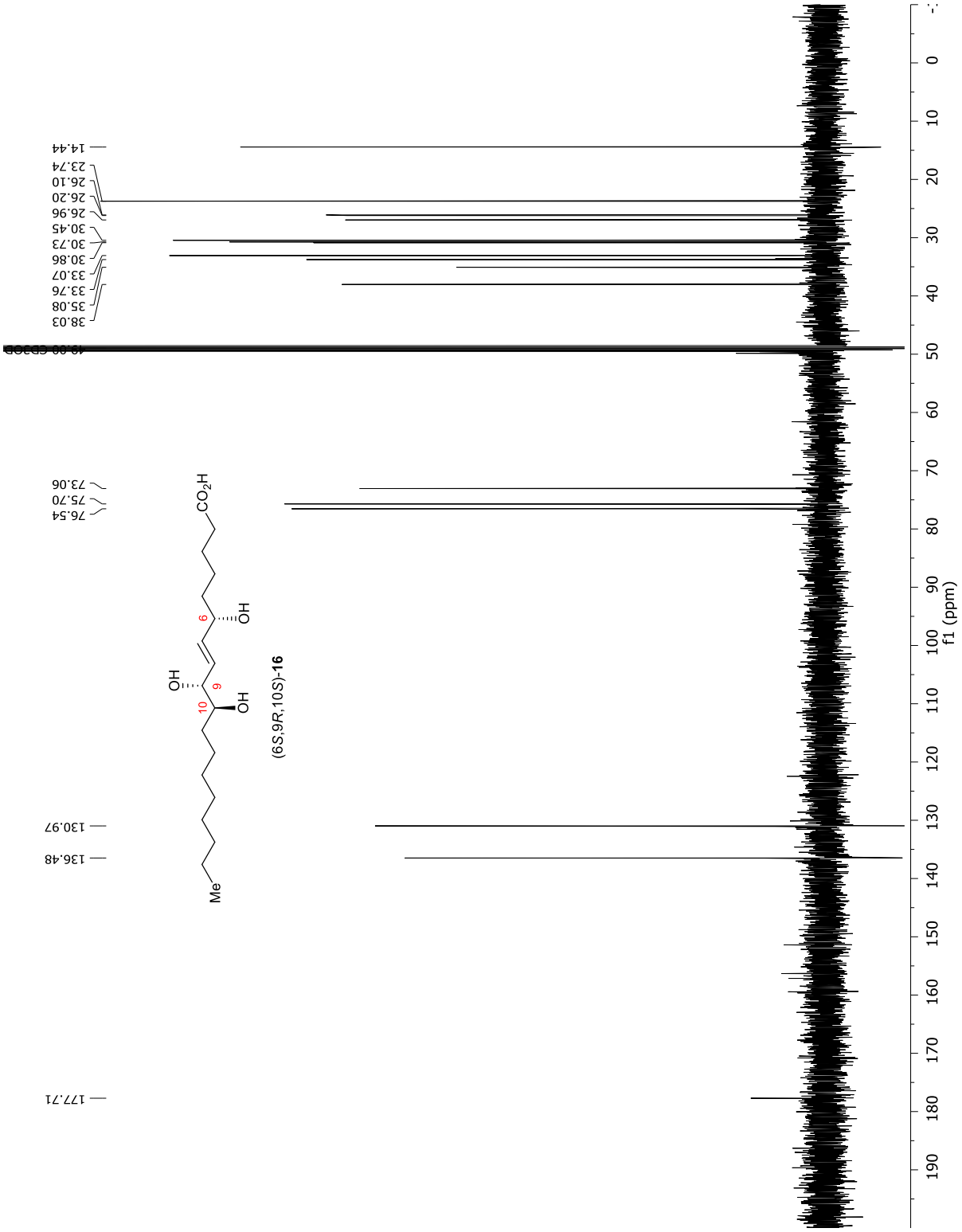
^{13}C-NMR Spectrum (150 MHz, CD_3OD) of triol **22:**



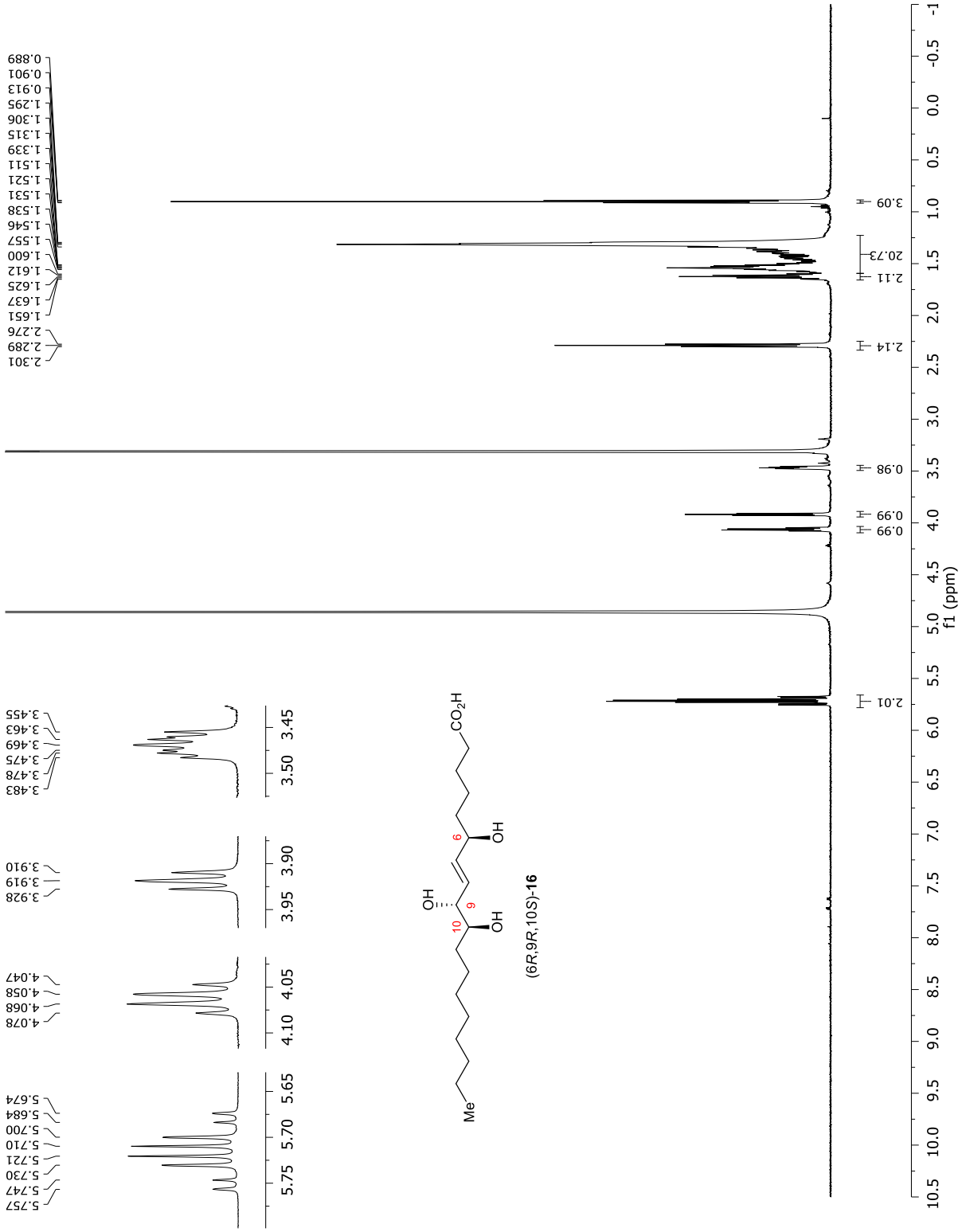
^{1}H NMR spectrum (600 MHz, CD_3OD) of oxylipin (6*S*,9*R*,10*S*)-**16:**



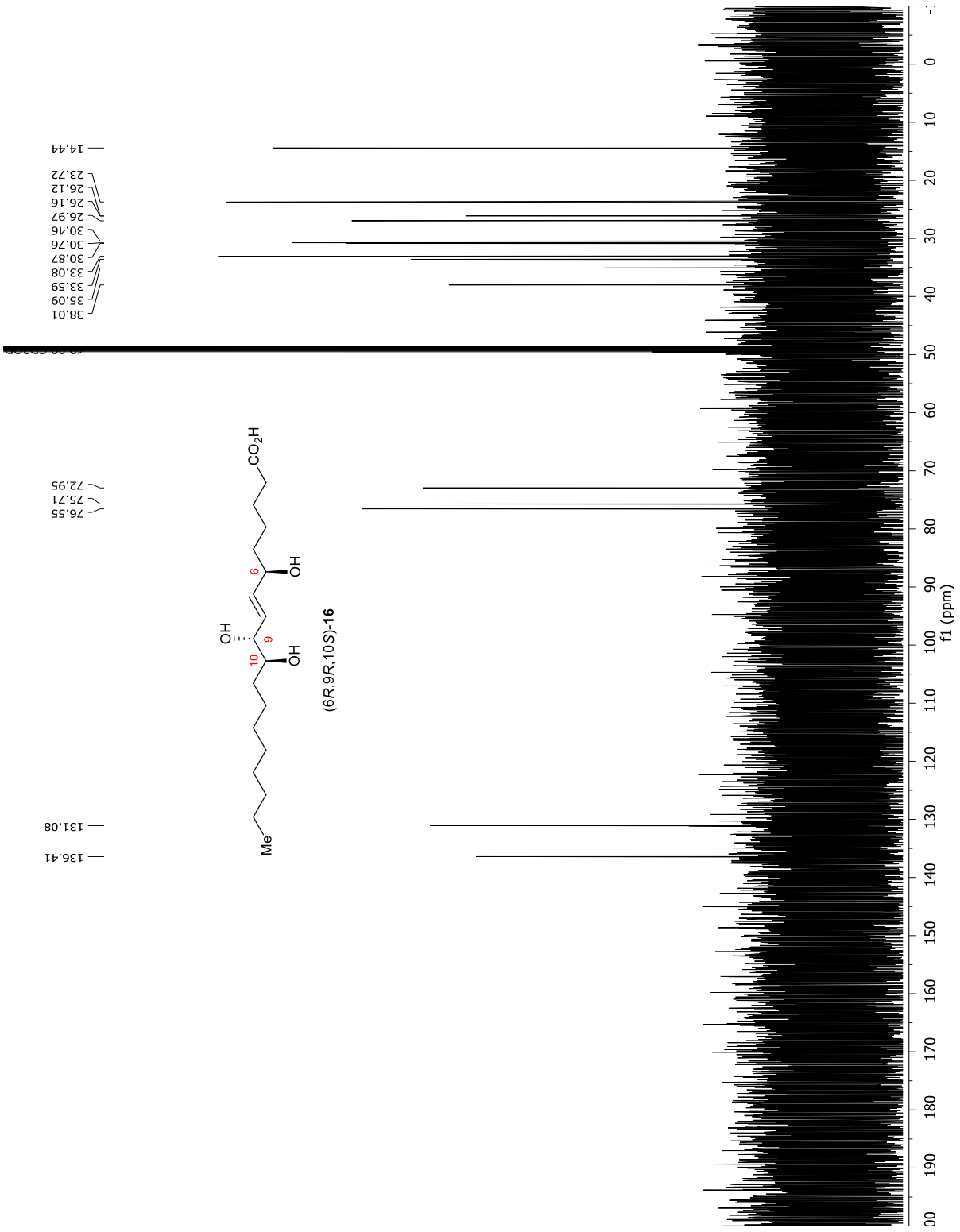
^{13}C NMR spectrum (150 MHz, CD_3OD) of oxylipin (6*S*,9*R*,10*S*)-**16:**



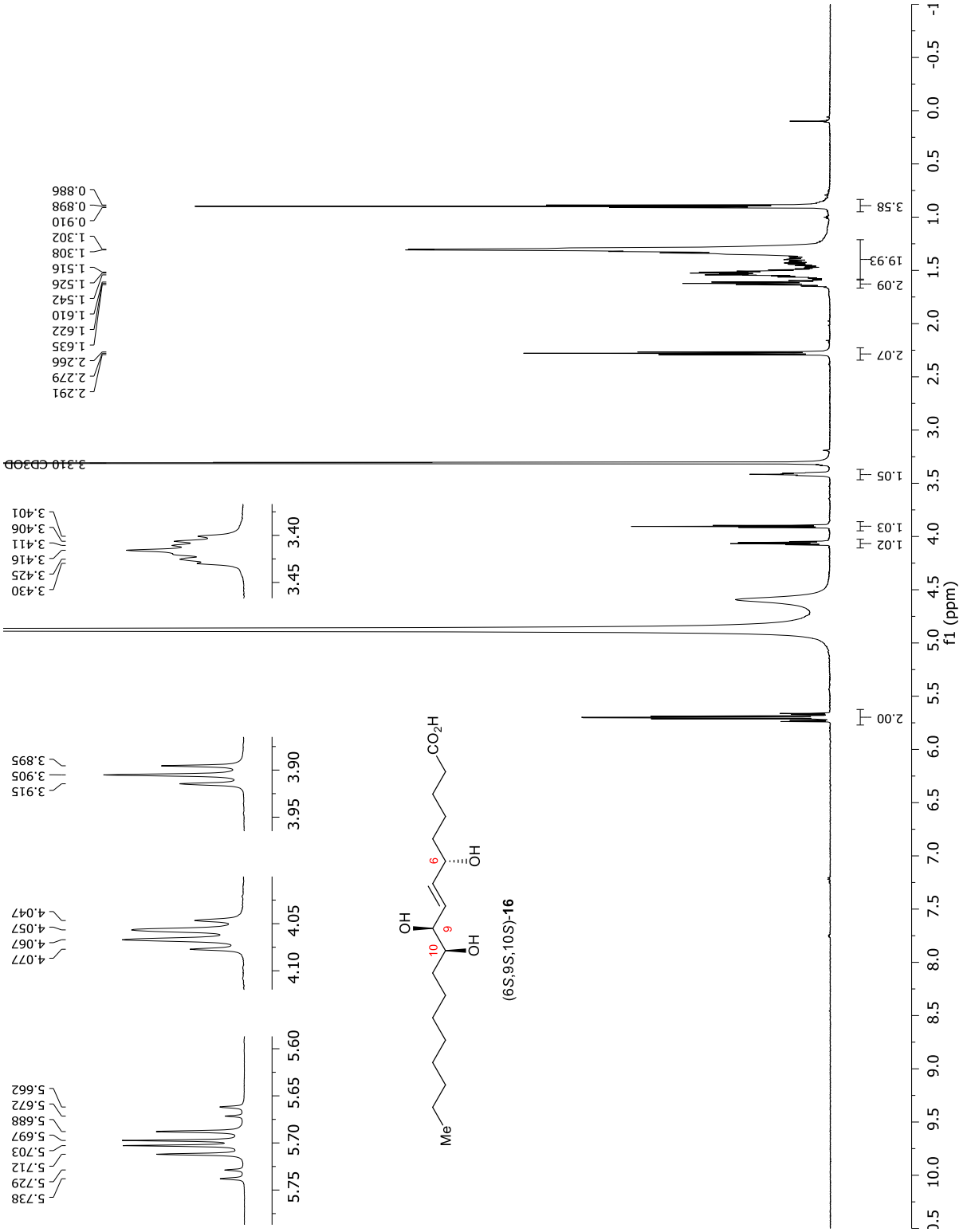
^{1}H NMR spectrum (600 MHz, CD_3OD) of oxylipin (6*R*,9*R*,10*S*)-**16:**



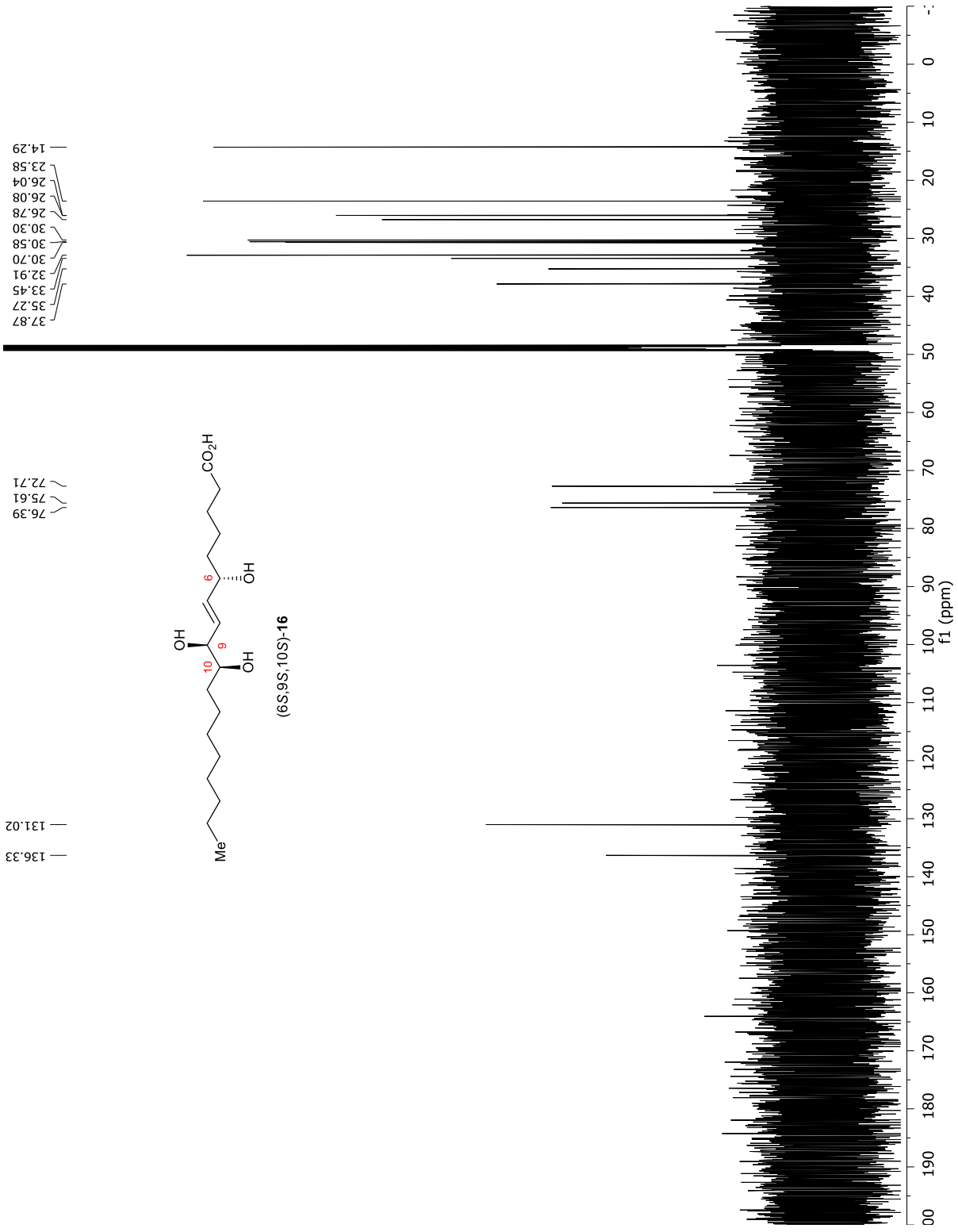
^{13}C NMR spectrum (150 MHz, CD_3OD) of oxylipin (6*R*,9*R*,10*S*)-**16:**



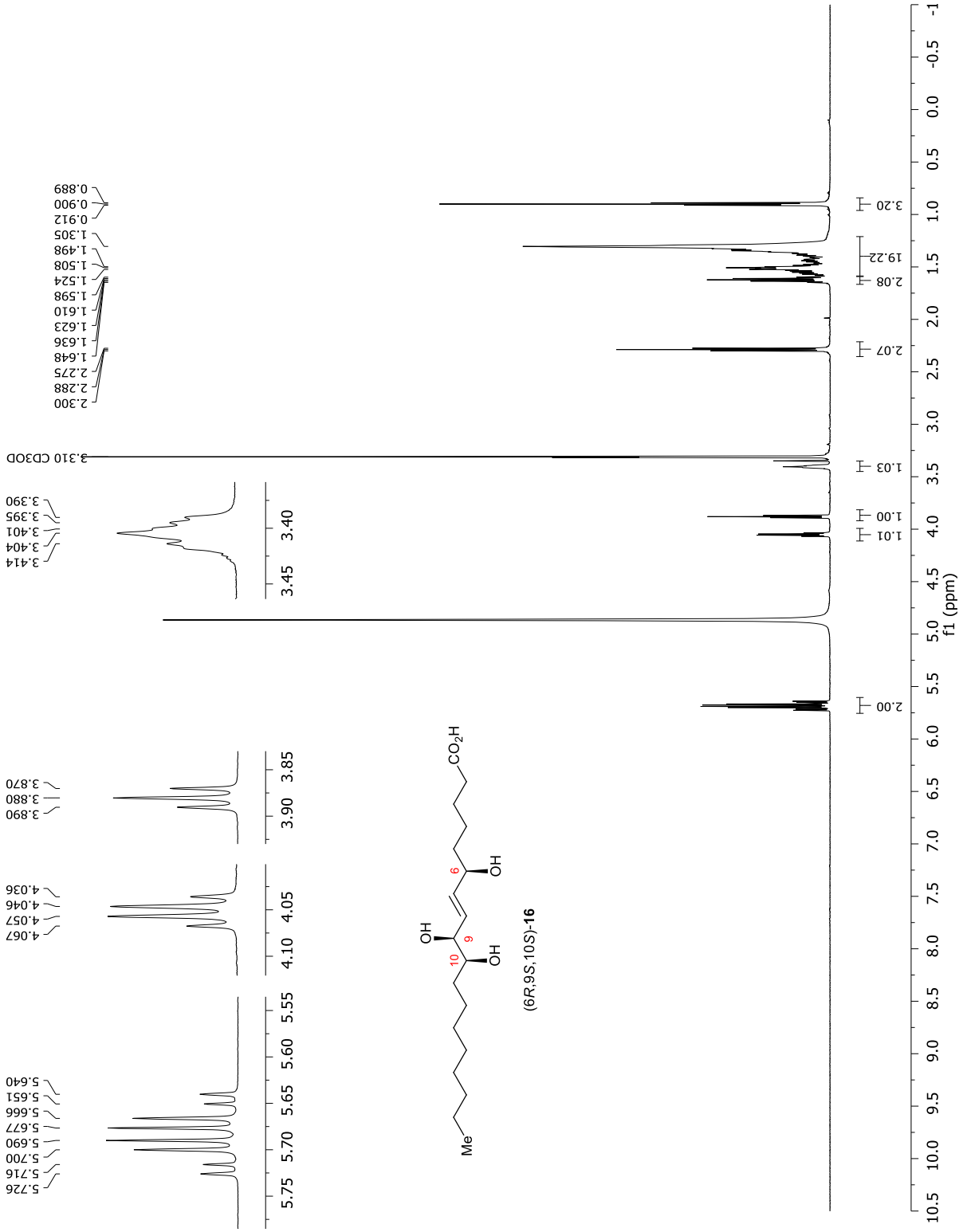
^{1}H NMR spectrum (600 MHz, CD_3OD) of oxylipin (6*S*,9*S*,10*S*)-**16:**



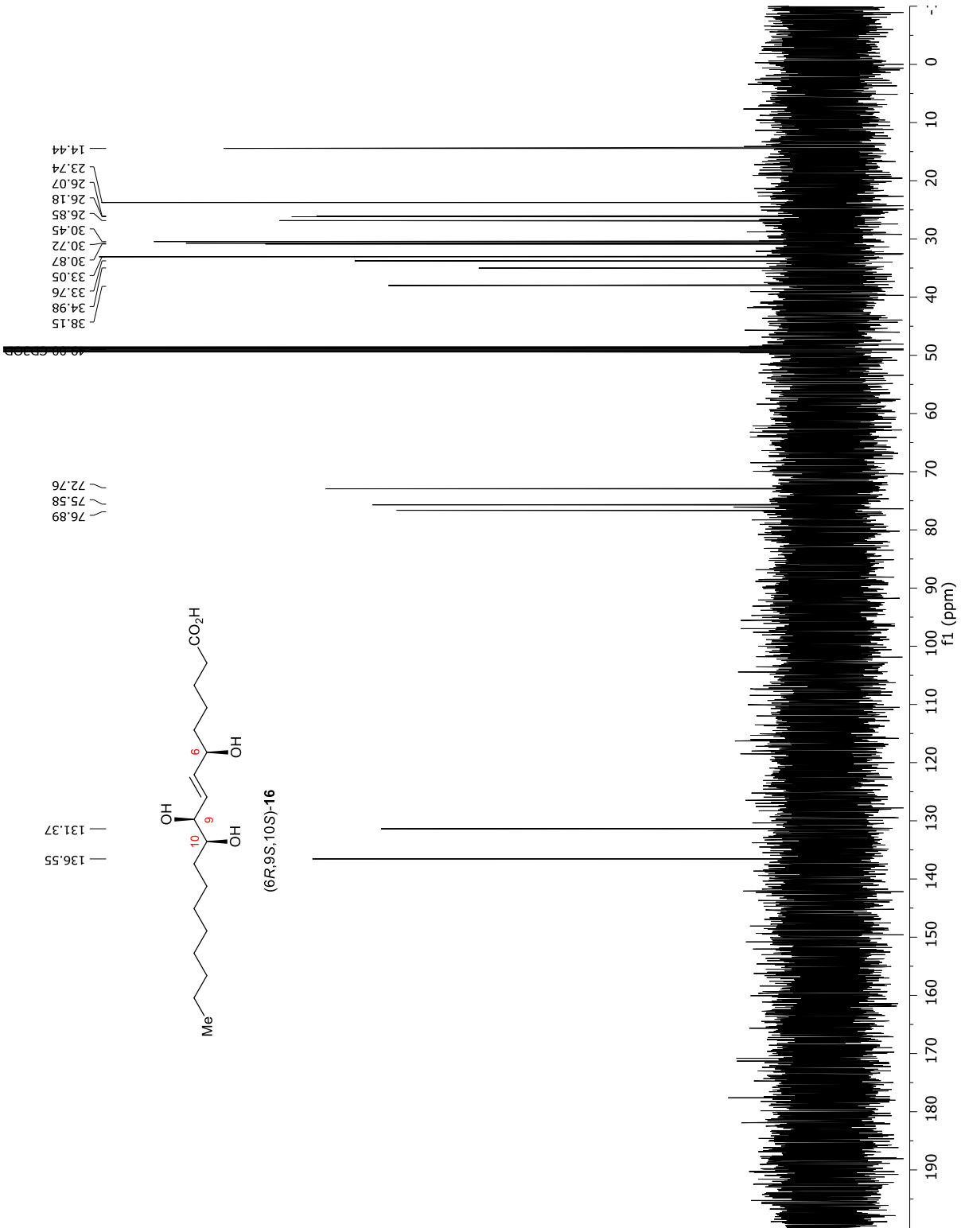
^{13}C NMR spectrum (150 MHz, CD_3OD) of oxylipin (6*S*,9*S*,10*S*)-**16:**



^{1}H NMR spectrum (600 MHz, CD_3OD) of oxylipin (6*R*,9*S*,10*S*)-**16:**

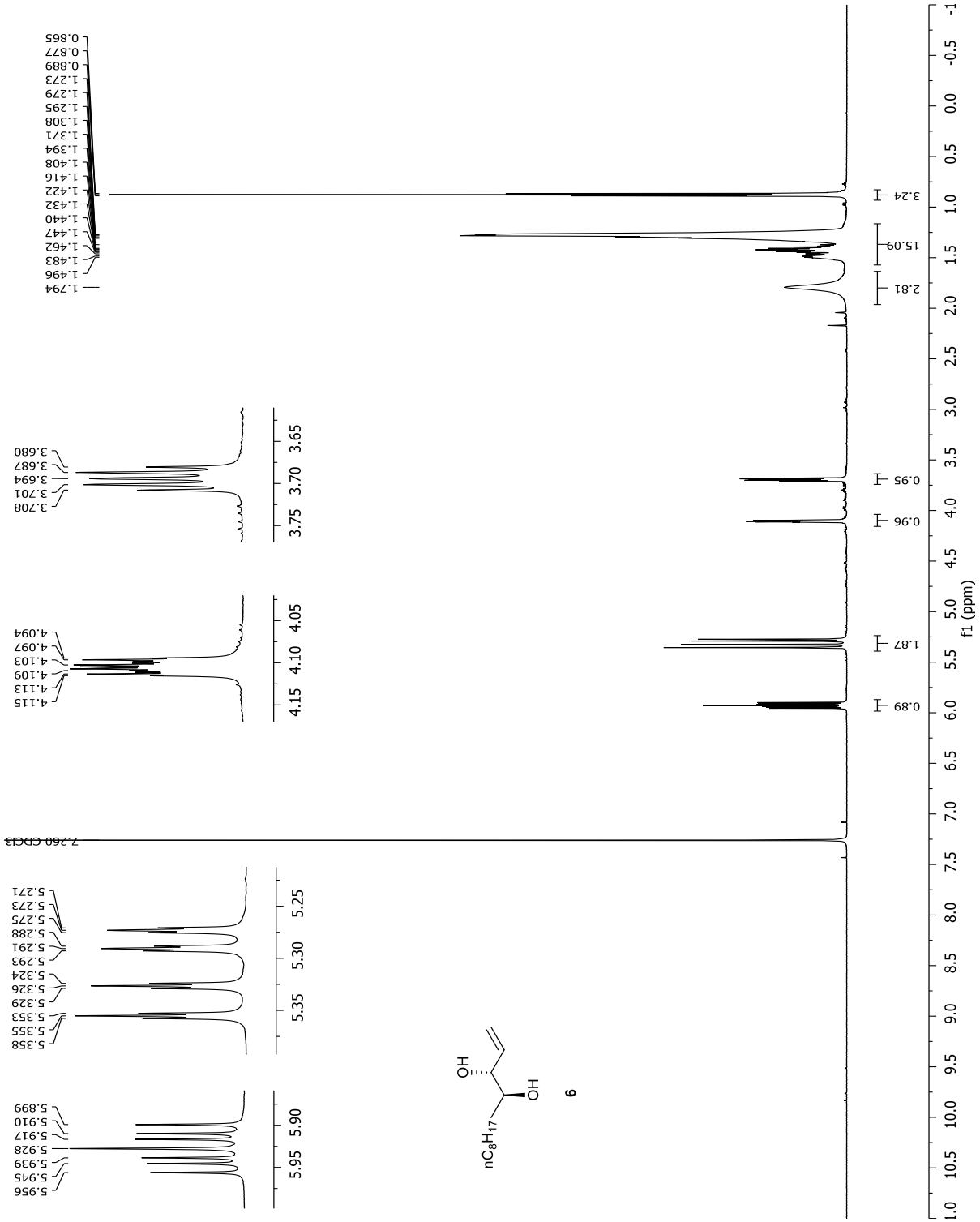


^{13}C NMR spectrum (150 MHz, CD_3OD) of oxylipin (6*R*,9*S*,10*S*)-**16:**

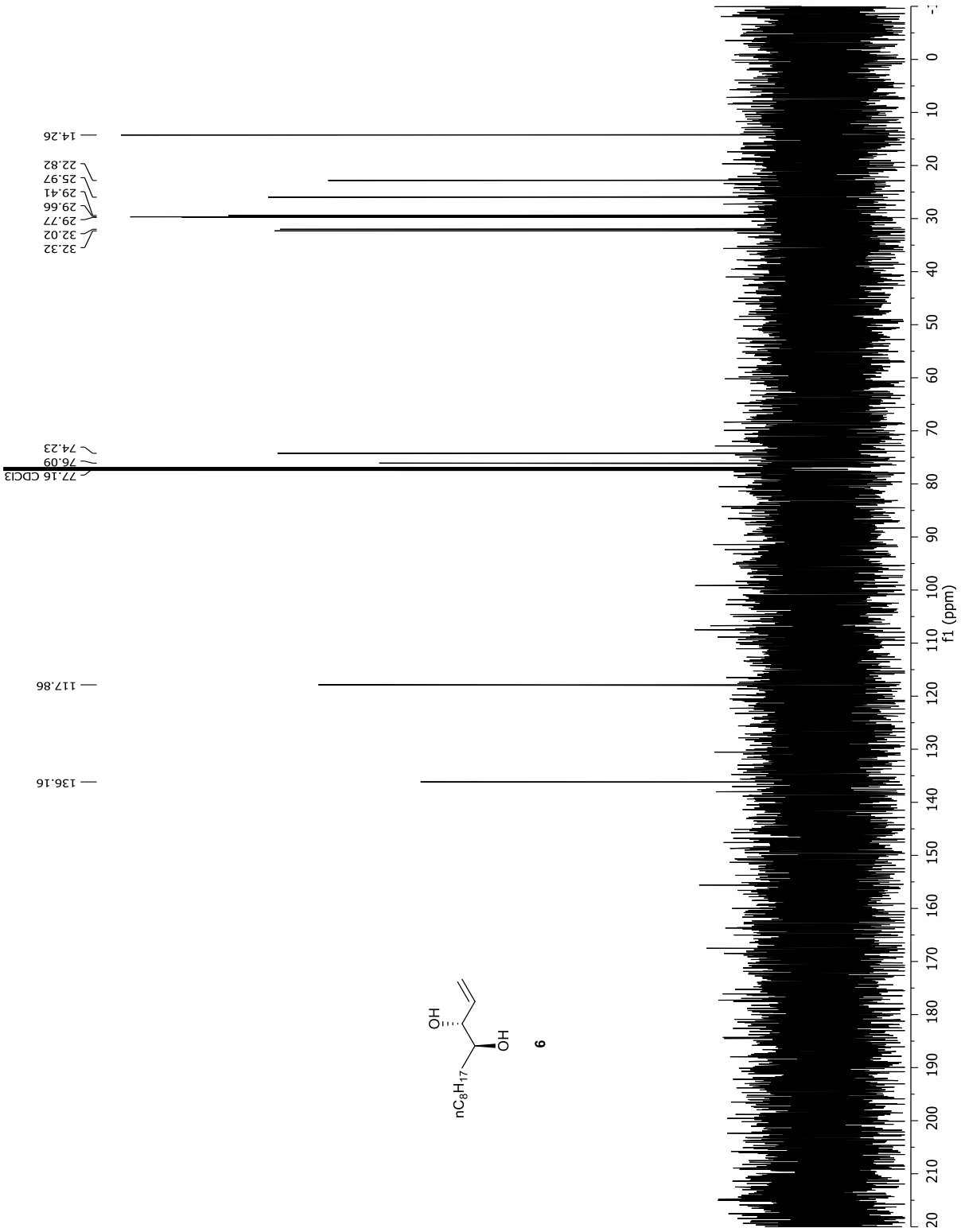


APENDIX B: CHAPTER II 1D & 2D NMR SPECTRA

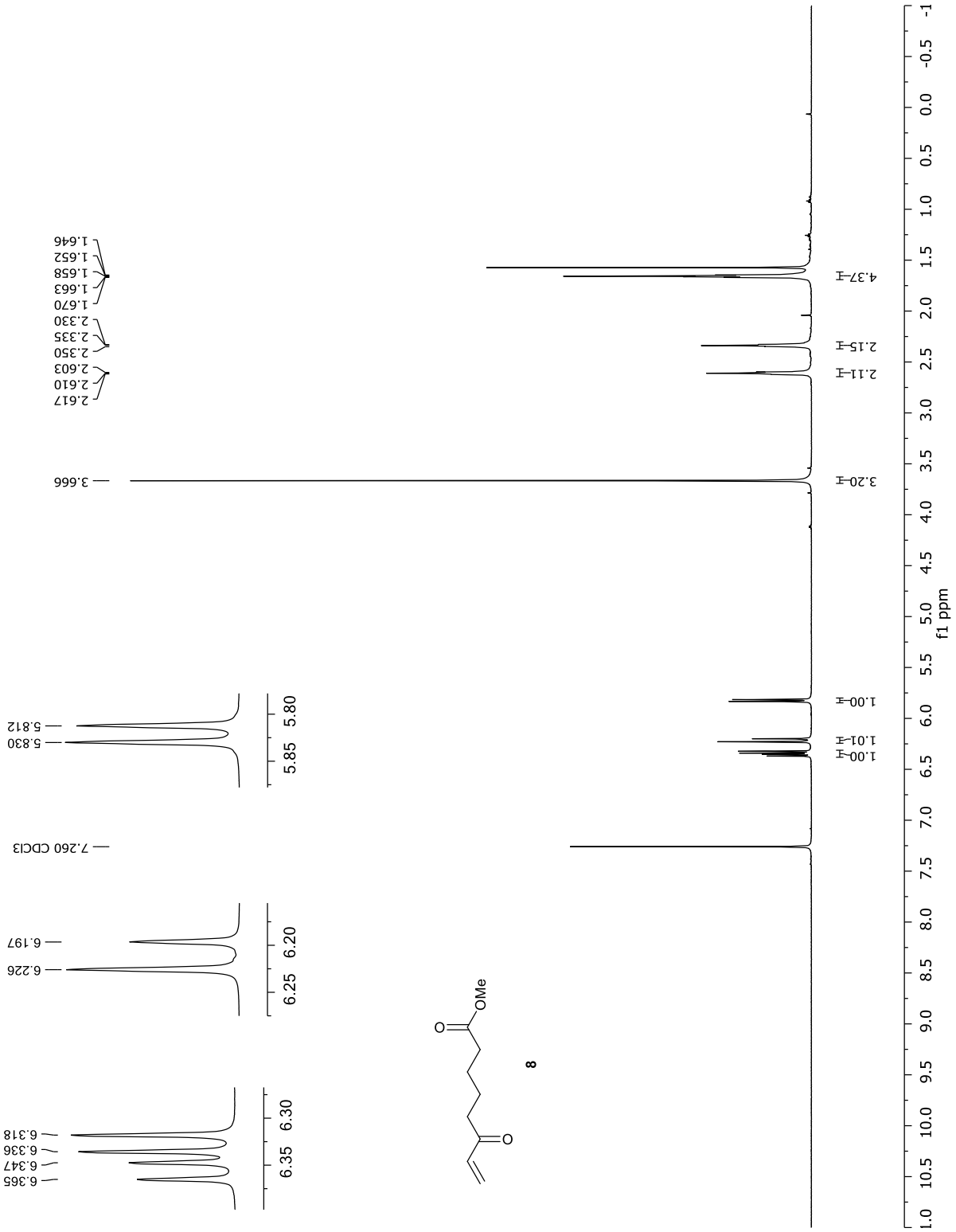
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of diol **6:**



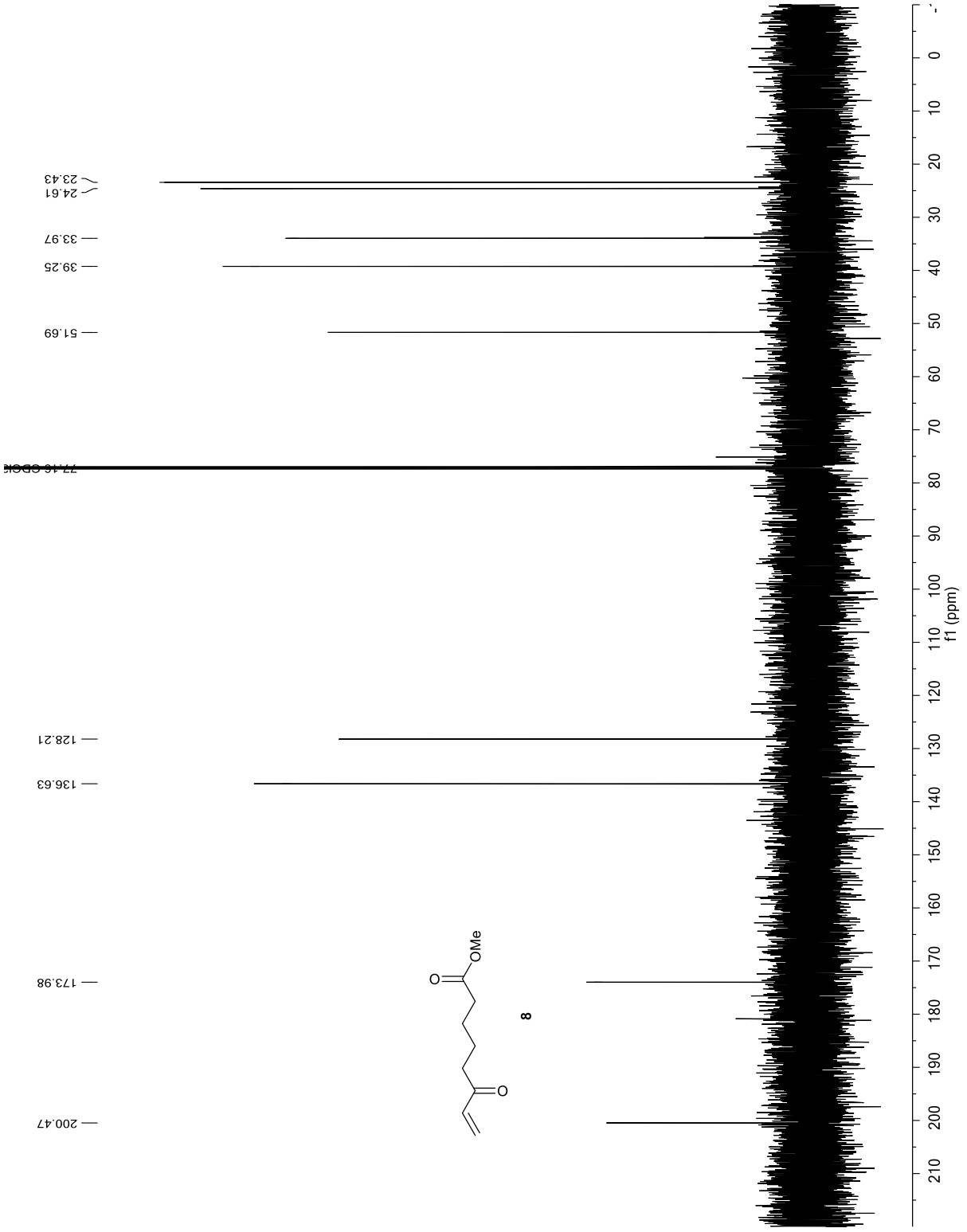
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of diol **6:**



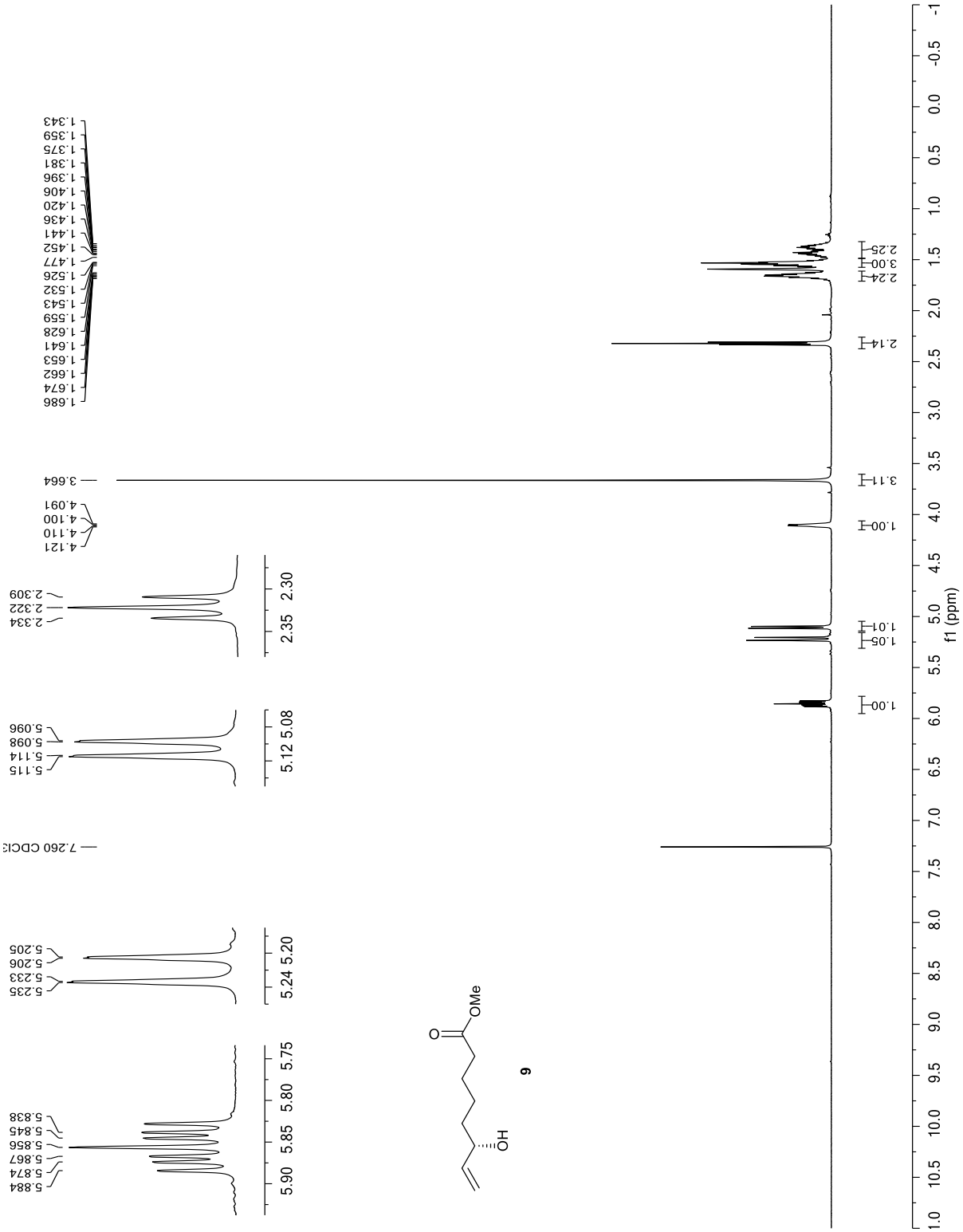
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of enone **8:**



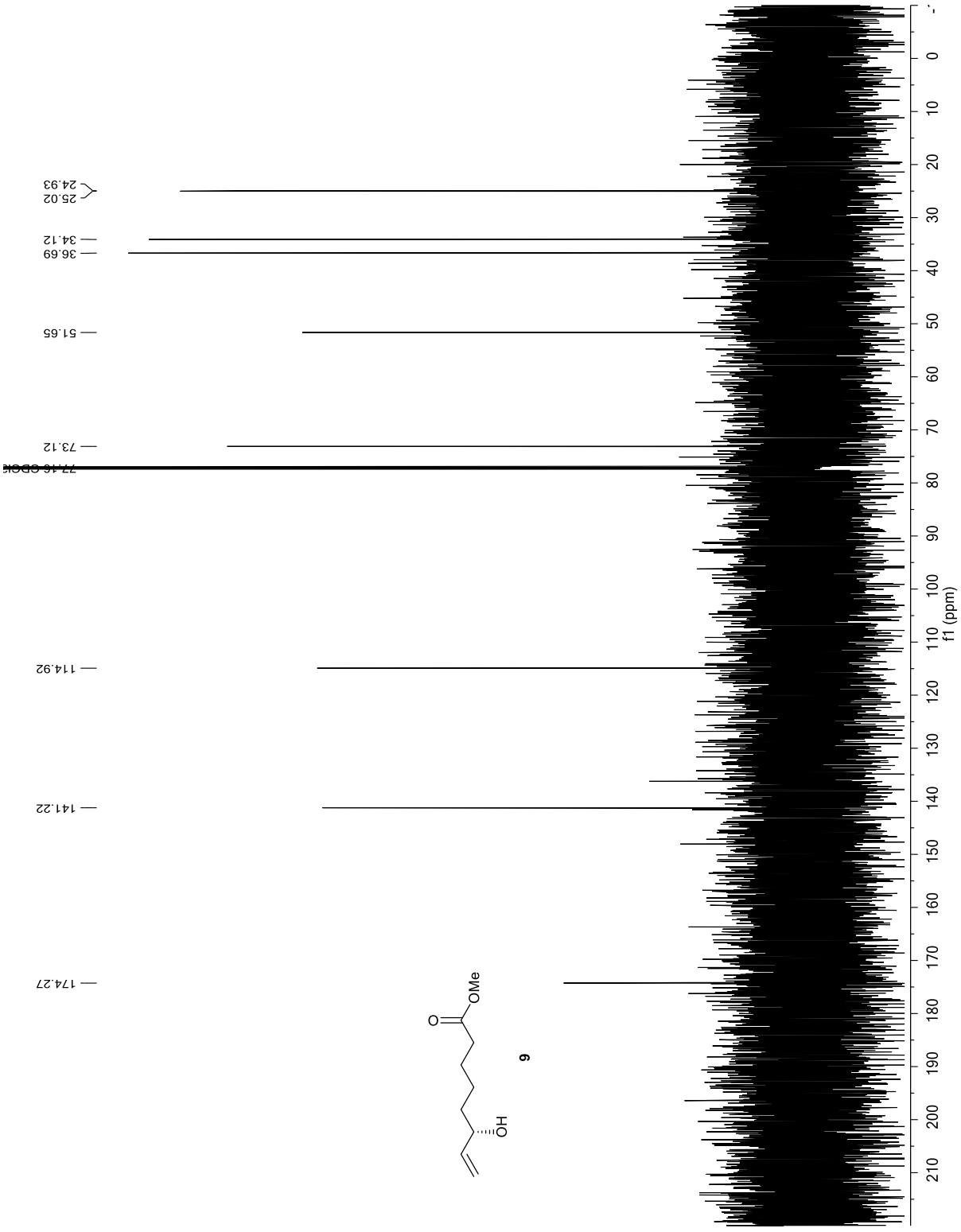
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of enone **8:**



^{1}H NMR spectrum (600 MHz, $CDCl_3$) of mono-ol **9:**

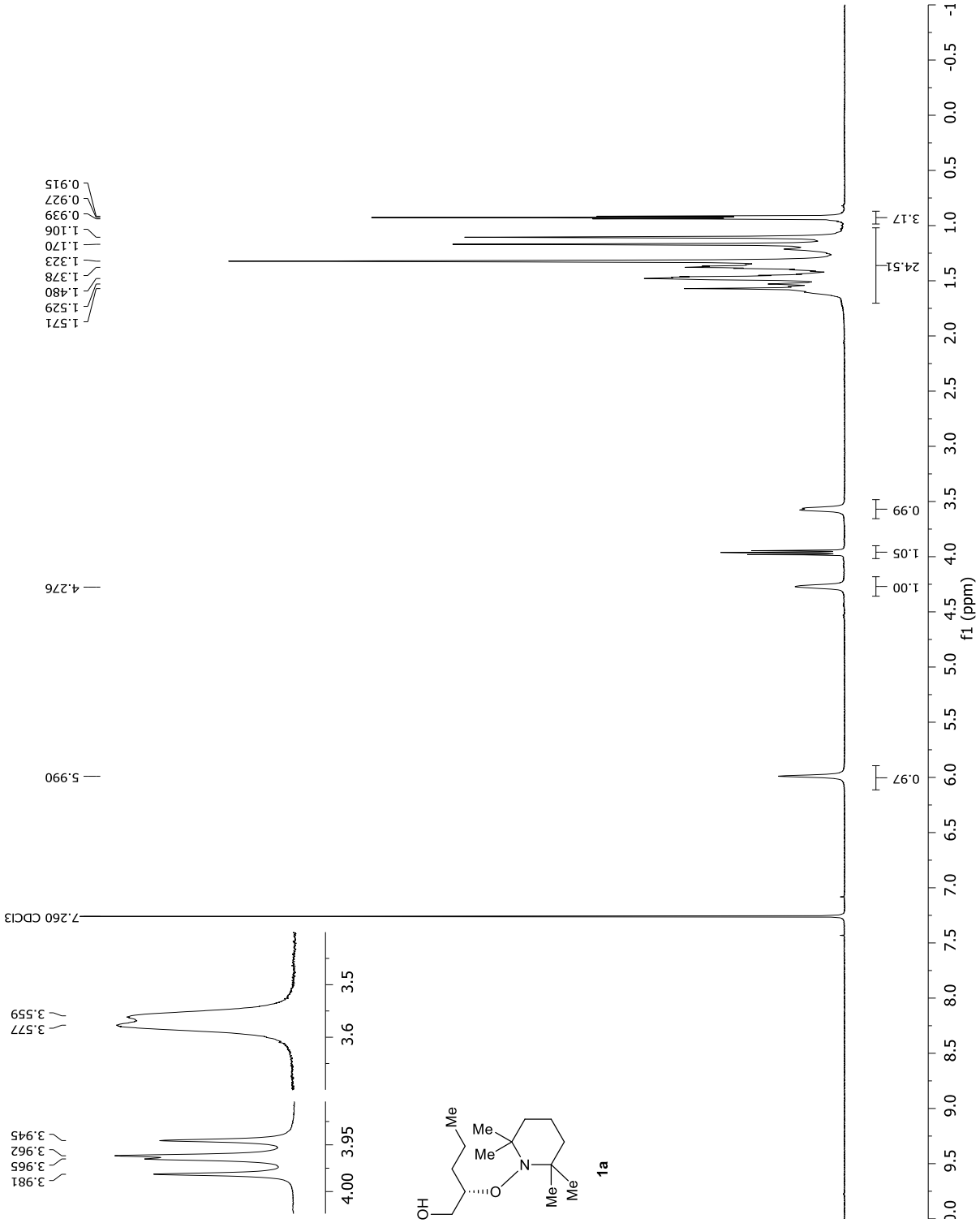


^{13}C NMR spectrum (150 MHz, $CDCl_3$) of mono-ol **9:**

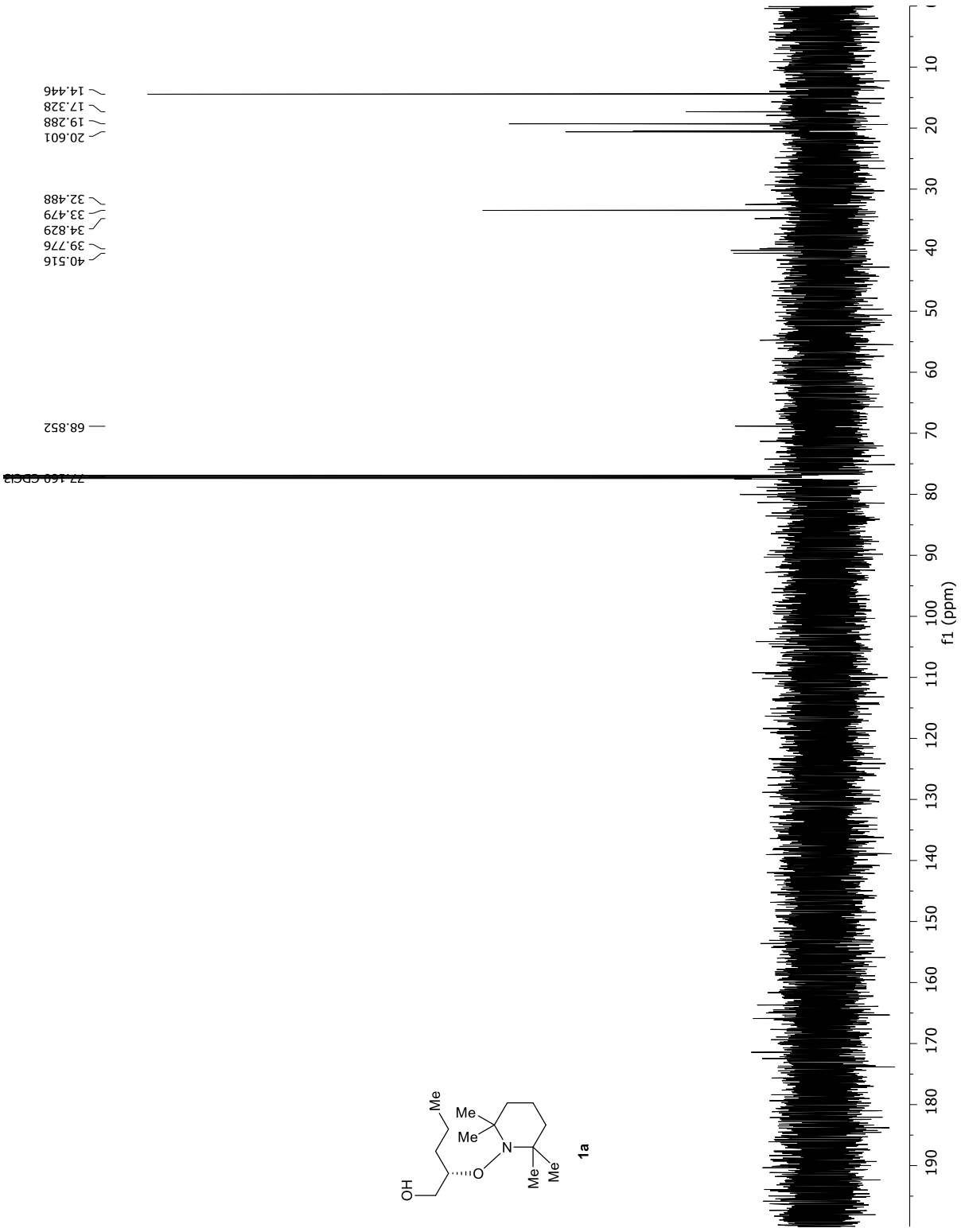


APENDIX C: CHAPTER III 1D & 2D NMR SPECTRA COMPUTATION DATA

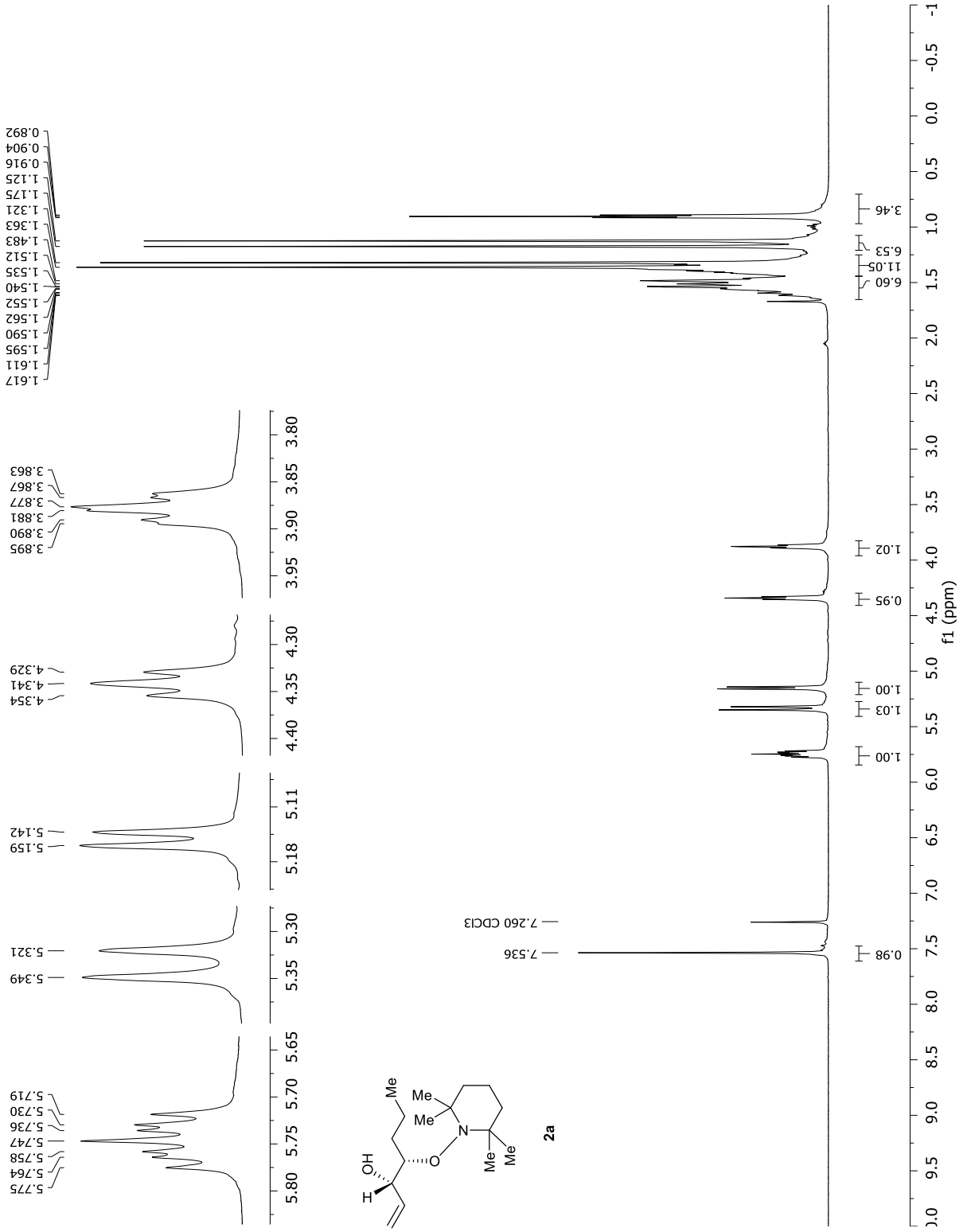
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of primary alcohol **1a**:



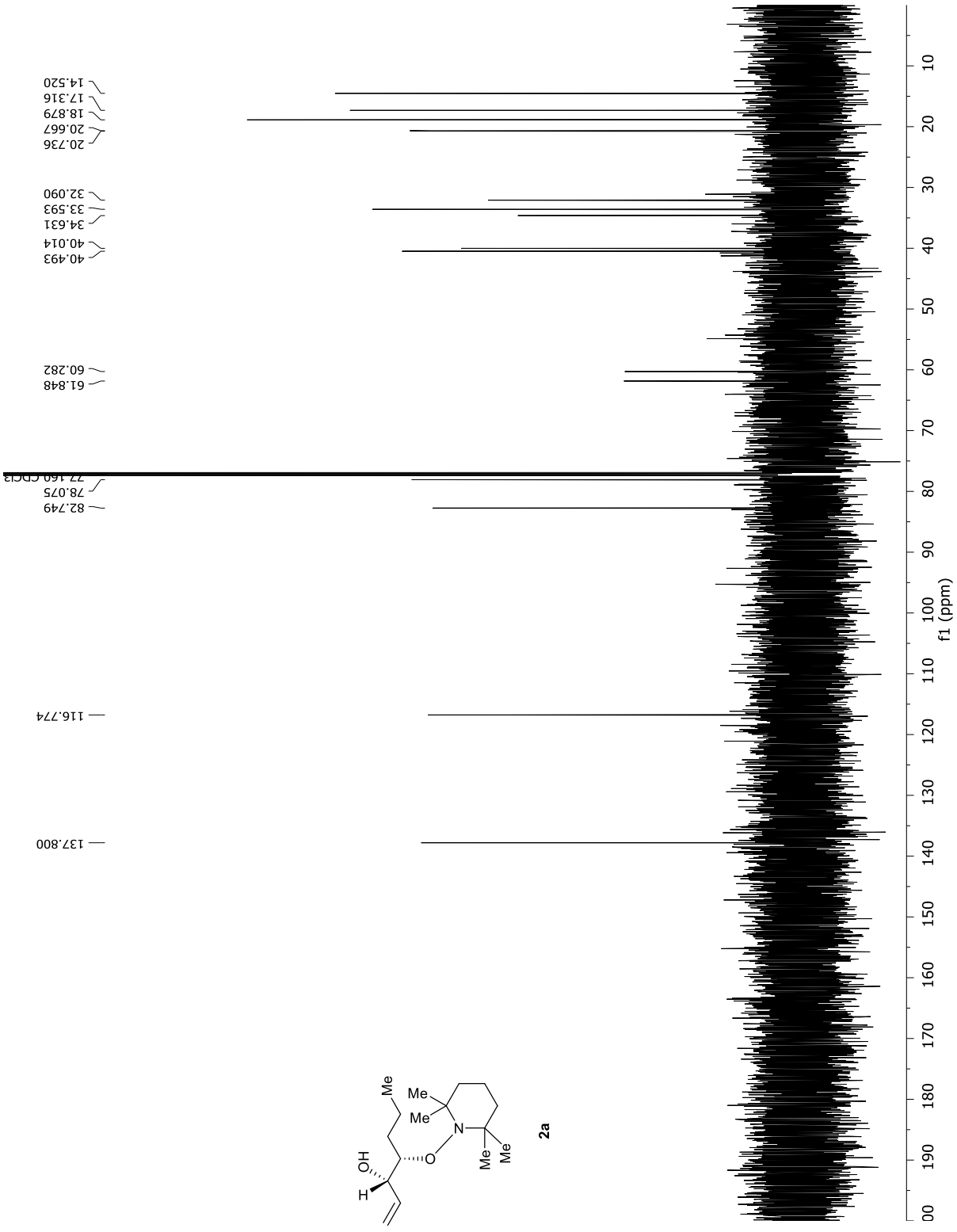
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of primary alcohol **1a**:



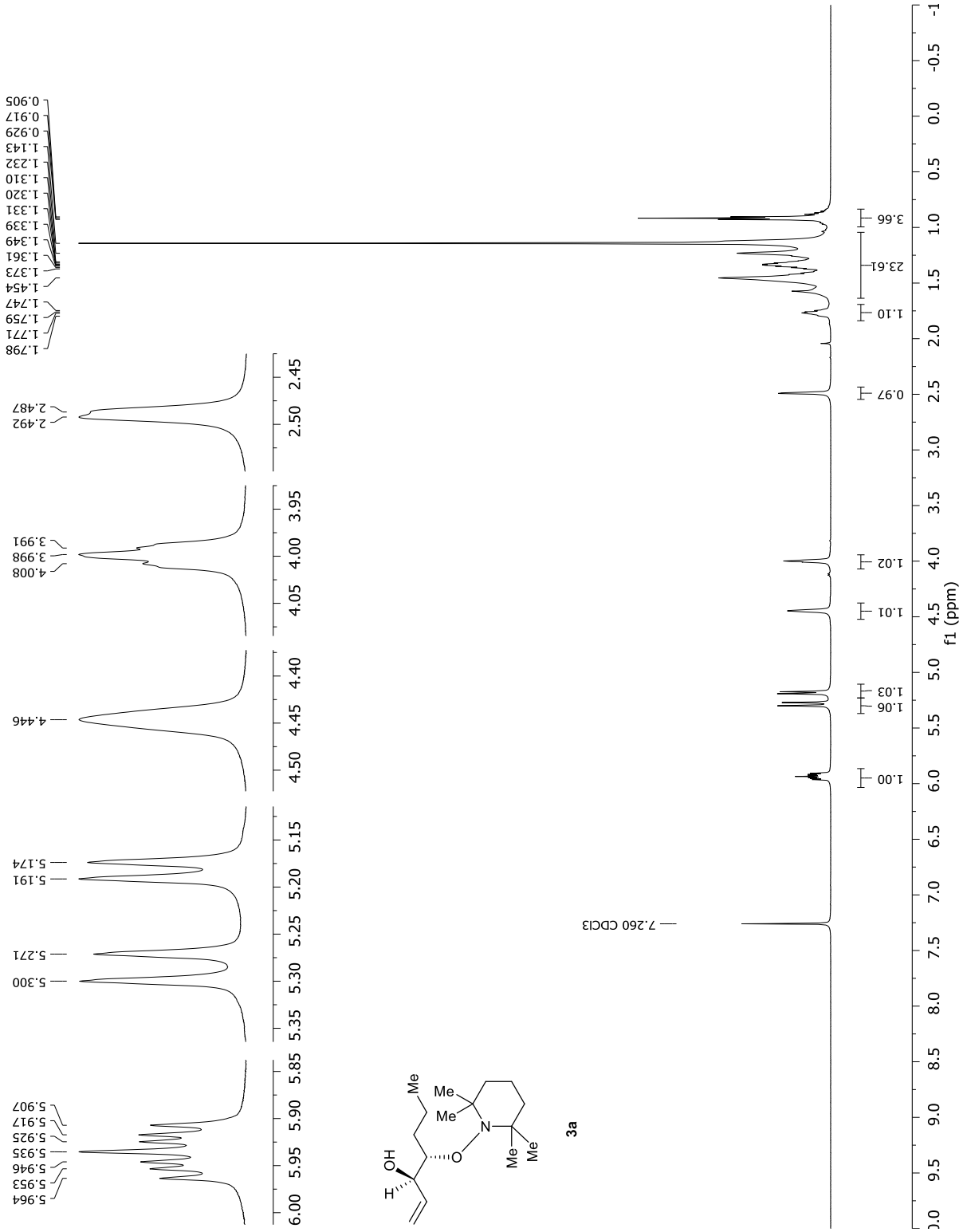
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of *syn* diol **2a**:



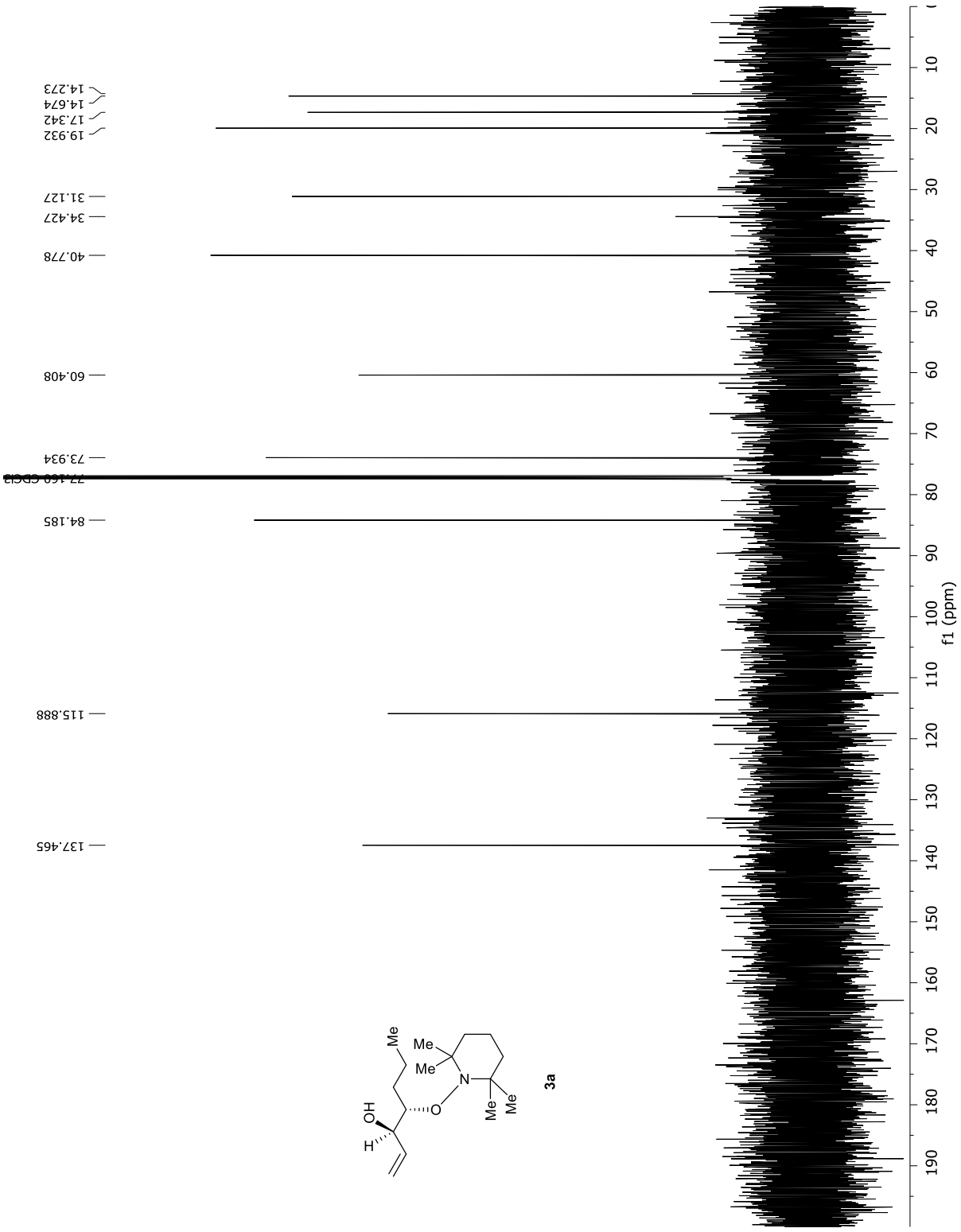
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of *syn* diol **2a**:



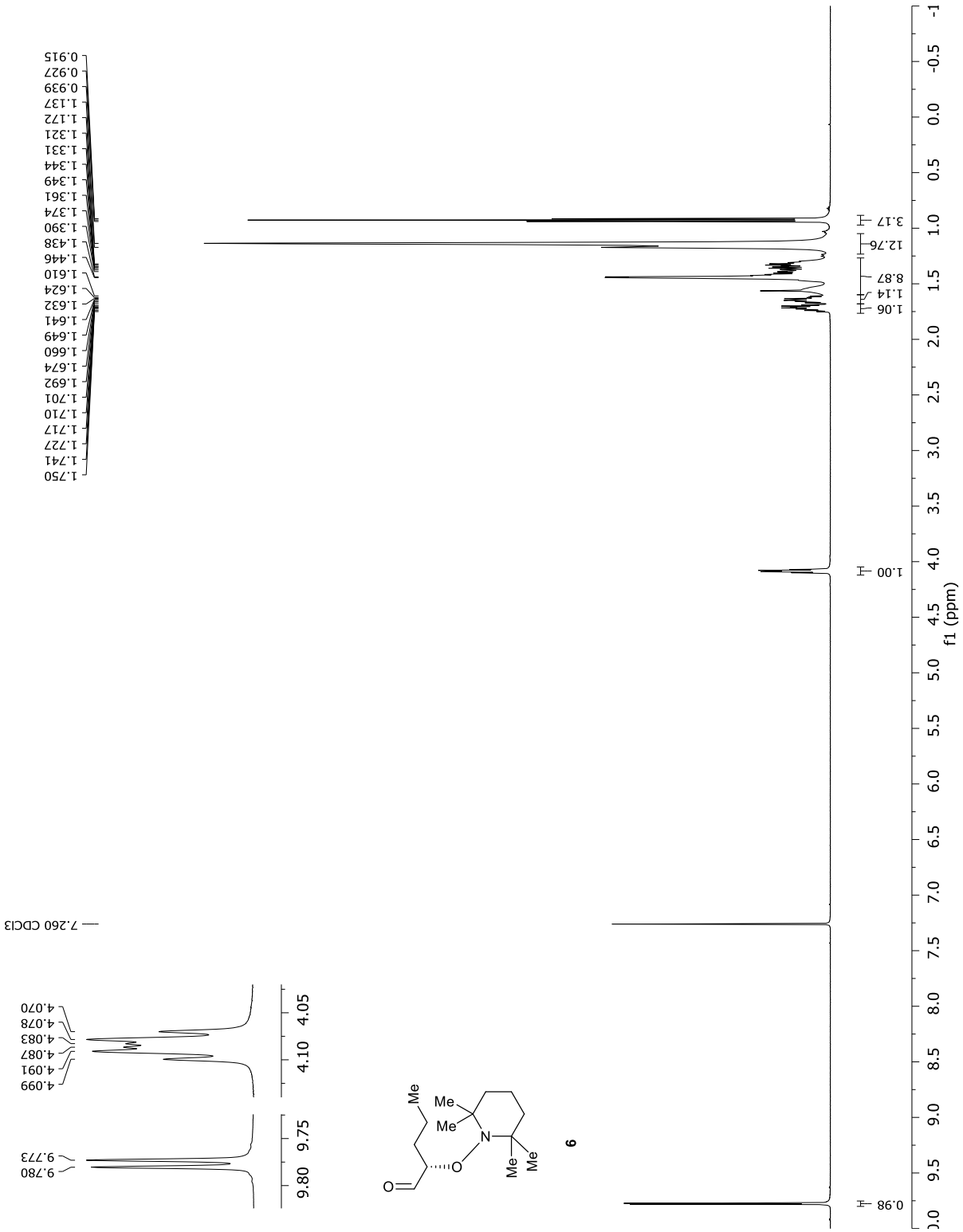
^{1}H NMR spectrum (600 MHz, $CDCl_3$) of *anti* diol **3a**:



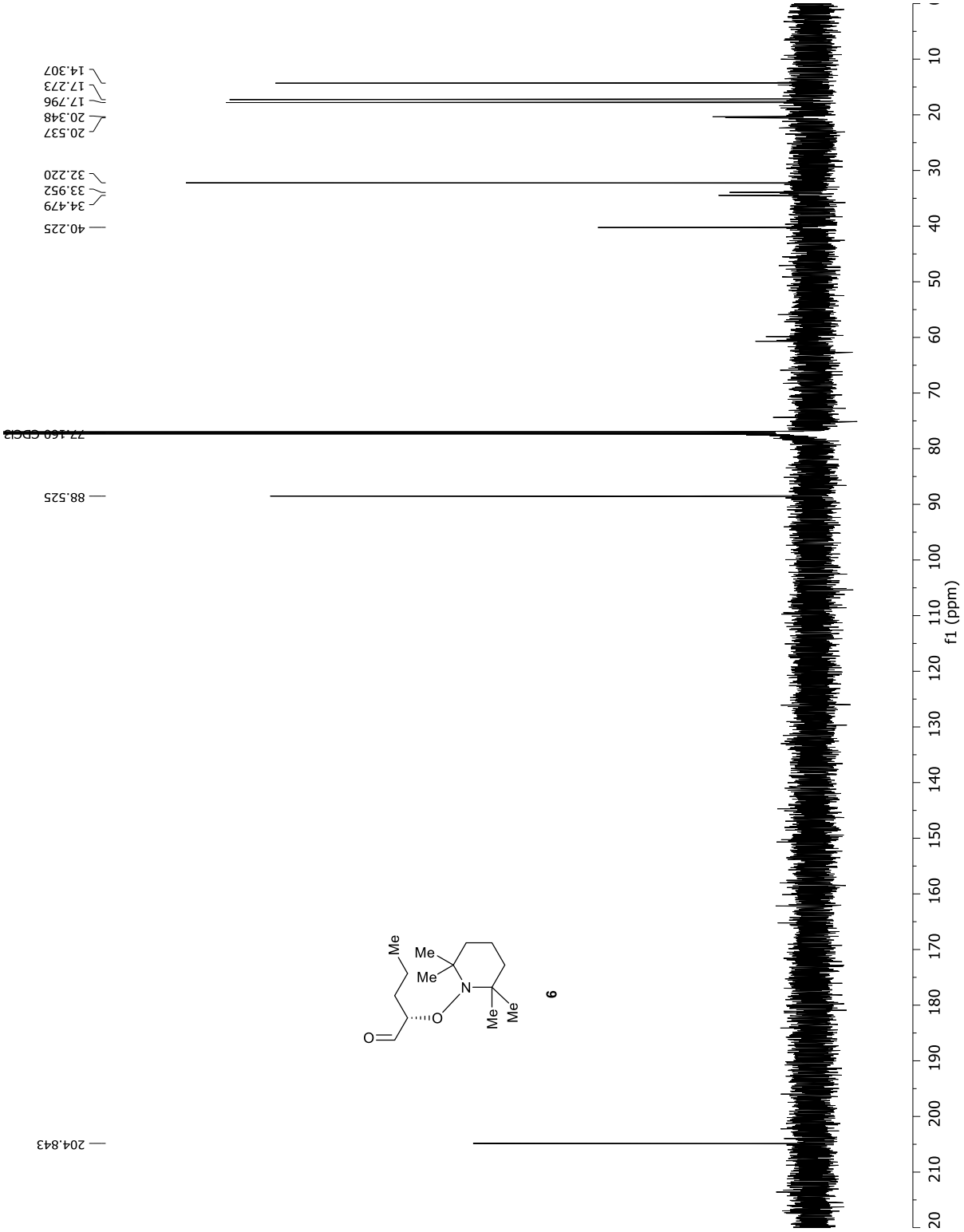
^{13}C NMR spectrum (150 MHz, $CDCl_3$) of *anti* diol **3a**:



^{1}H NMR spectrum (600 MHz, $CDCl_3$) of α-oxyaldehyde **6**:



^{13}C NMR spectrum (150 MHz, $CDCl_3$) of α-oxyaldehyde **6**:



MP2 optimized Cartesian coordinates

The lowest energy structures of **1b**–**3b** were optimized using MP2 with a 6-311G(d,p) basis. Coordinates are in angstroms and energies are in hartree.

Primary alcohol **1b** E= -675.6819676697

ATOM	CHARGE	X	Y	Z
C	6.0	0.0350552326	-0.9948554678	0.0625494124
C	6.0	0.3272557518	-2.4268320087	-0.3616931230
O	8.0	-0.8336369208	-3.2365858915	-0.4126817429
O	8.0	-0.4074869993	-0.8446207137	1.4333296612
C	6.0	1.2760287712	-0.1208575031	-0.0054934539
N	7.0	-1.4600521196	-1.7640265851	1.8189668332
C	6.0	-1.0121685387	-2.3852003949	3.1053731480
C	6.0	-2.7550923988	-1.0136792369	1.8356062617
C	6.0	-3.8300542677	-1.9913843097	2.3328352957
C	6.0	-2.7529435506	0.2829356176	2.6590933152
C	6.0	-2.1397381672	-3.3169644388	3.5726600472
C	6.0	-0.6182150515	-1.3868243837	4.2053613712
C	6.0	0.2154591233	-3.2498757931	2.8032161512
C	6.0	-3.0953746180	-0.6411094295	0.3871610236
C	6.0	-3.4907898784	-2.6196008995	3.6794688652
H	1.0	-0.7368382070	-0.6031026474	-0.6078306476
H	1.0	1.0955342615	-2.8503337008	0.2995264478
H	1.0	0.7443780068	-2.3898433600	-1.3744566826
H	1.0	-1.2947609092	-2.9870258879	0.4097397014
H	1.0	2.0714581350	-0.5414163103	0.6164397044
H	1.0	1.0477823653	0.8849326586	0.3543104203
H	1.0	1.6315173537	-0.0519268493	-1.0373874385
H	1.0	-3.9458004982	-2.7877966612	1.5848042246
H	1.0	-4.7809862693	-1.4458979460	2.3781663198
H	1.0	-1.8360870042	0.8453366374	2.4677985881
H	1.0	-2.8487542002	0.1132287727	3.7311108016
H	1.0	-3.6046102530	0.8957898691	2.3443629969
H	1.0	-1.8390745080	-3.7475938151	4.5359389295
H	1.0	-2.2219847172	-4.1457009721	2.8561876322
H	1.0	-1.4755718571	-0.9300242122	4.6985152923
H	1.0	0.0145671276	-0.5992412650	3.7900187389
H	1.0	-0.0437587662	-1.9216920307	4.9692577150
H	1.0	0.4504045637	-3.8488936503	3.6891840439
H	1.0	1.0826696144	-2.6281215544	2.5706139771
H	1.0	0.0175239382	-3.9267541416	1.9681483405
H	1.0	-2.9311364865	-1.4885896516	-0.2833555740
H	1.0	-2.4962894091	0.2073904497	0.0471528899
H	1.0	-4.1491153274	-0.3468391449	0.3374155388
H	1.0	-4.2643828336	-3.3433619373	3.9607546046
H	1.0	-3.4727204882	-1.8588512111	4.4675603690

syn Diol **2b** E= -714.8850755986

C	6.0	0.2056288729	0.1052791483	1.7072219945
C	6.0	-0.0991656502	1.2004139169	2.7284799780

O	8.0	-0.6456015407	0.6493906709	3.9192613101
O	8.0	-0.9577695761	-0.5962081659	1.1961349054
C	6.0	0.8544212327	0.6367015019	0.4387969493
N	7.0	-1.8770518421	-1.0634521528	2.2137348311
C	6.0	-1.6725180025	-2.5351132320	2.3942806265
C	6.0	-3.2359811896	-0.6073097088	1.7810286235
C	6.0	-4.2396835505	-1.1417568834	2.8128108810
C	6.0	-3.2585634177	0.9226645193	1.8515864058
C	6.0	-2.7194090479	-3.0074877073	3.4139737556
C	6.0	-0.2863179802	-2.7395578674	3.0183211652
C	6.0	-1.7282650338	-3.3689840887	1.1056903606
C	6.0	-3.6308507032	-1.0125651060	0.3521292687
C	6.0	-4.1467582201	-2.6494478558	3.0166874015
C	6.0	1.1634683839	1.9482154619	3.1310131125
H	1.0	0.8707114754	-0.6137042015	2.1990161094
H	1.0	-0.8044619291	1.9091158812	2.2693437439
H	1.0	-1.2622416805	-0.0321173676	3.5834645484
H	1.0	0.8917942317	-0.1582602507	-0.3100424434
H	1.0	1.8736624017	0.9751714977	0.6367971068
H	1.0	0.2736774534	1.4706423076	0.0328476666
H	1.0	-5.2444176369	-0.8477811443	2.4843806470
H	1.0	-4.0493719770	-0.6397009693	3.7712350861
H	1.0	-4.2893065426	1.2653876147	1.7131199657
H	1.0	-2.6434509719	1.3579576896	1.0610900811
H	1.0	-2.9021648419	1.2718044871	2.8239656724
H	1.0	-2.4904759625	-2.5443969041	4.3836753684
H	1.0	-2.6014951493	-4.0917336389	3.5341541808
H	1.0	-0.1168116272	-2.0329697893	3.8349938917
H	1.0	0.5034053234	-2.6224288102	2.2718881060
H	1.0	-0.2248326724	-3.7597051003	3.4120837489
H	1.0	-1.2567448515	-4.3387052915	1.2988510856
H	1.0	-1.1696977043	-2.8678691918	0.3116749149
H	1.0	-2.7435795044	-3.5604298735	0.7597293999
H	1.0	-3.9303851299	-2.0567224808	0.2682902402
H	1.0	-2.8032293100	-0.8233114599	-0.3352276024
H	1.0	-4.4826469187	-0.3983097762	0.0410730837
H	1.0	-4.4397908977	-3.1822938935	2.1054219872
H	1.0	-4.8439961626	-2.9646832098	3.8014862529
H	1.0	0.9255803544	2.5788574526	3.9909746395
H	1.0	1.5416130348	2.5808203543	2.3243888709
H	1.0	1.9422844608	1.2403236172	3.4325720790

anti Diol **3b** (lowest energy) E= -714.8791740110

C	6.0	-3.0515112368	0.0083881787	0.6569451213
C	6.0	-2.1894035075	1.2619506235	0.4830759262
O	8.0	-2.9898782736	2.3628646864	0.0659201208
O	8.0	-3.9896175495	0.4383685484	1.6735034364
C	6.0	-3.6876701779	-0.4784736817	-0.6317887050
N	7.0	-5.1004596171	-0.4541303354	1.8860997155
C	6.0	-4.8587096737	-1.1832737913	3.1653074630
C	6.0	-6.3307775323	0.3870906768	1.8008215699
C	6.0	-7.5277494428	-0.5239975750	2.1100471382
C	6.0	-6.3390255148	1.6318518275	2.7061595332
C	6.0	-6.0936520555	-2.0579913542	3.4250881179
C	6.0	-4.5340942669	-0.3053030399	4.3850528426

C	6.0	-3.6639124837	-2.1171526685	2.9393234242
C	6.0	-6.4722914374	0.8616474379	0.3514498345
C	6.0	-7.3943134574	-1.2632492167	3.4362390400
C	6.0	-1.0880253475	1.0870475493	-0.5455169850
H	1.0	-2.4188603859	-0.7862760507	1.0704797762
H	1.0	-1.7408086915	1.4802547003	1.4645677952
H	1.0	-3.6913924784	2.4093774142	0.7250924497
H	1.0	-4.4668187173	-1.2063547400	-0.4029229302
H	1.0	-2.9245668257	-0.9675222771	-1.2446470389
H	1.0	-4.1135357512	0.3514677939	-1.1972608625
H	1.0	-7.6129800639	-1.2616795384	1.3011052571
H	1.0	-8.4345900578	0.0934239290	2.0883733698
H	1.0	-5.3810903671	2.1543640795	2.6481182815
H	1.0	-6.5422229919	1.3990996915	3.7511530026
H	1.0	-7.1229324628	2.3142594543	2.3605913478
H	1.0	-5.9396580194	-2.5813624229	4.3771860052
H	1.0	-6.1477305754	-2.8194150570	2.6353468453
H	1.0	-5.4145082993	0.1644804975	4.8230543369
H	1.0	-3.8186280347	0.4717371981	4.1059019692
H	1.0	-4.0761756888	-0.9326448220	5.1578376623
H	1.0	-3.6274371440	-2.8550092642	3.7480825126
H	1.0	-2.7213884503	-1.5641667590	2.9493116854
H	1.0	-3.7658531084	-2.6424822644	1.9853031960
H	1.0	-6.4507960054	0.0105389697	-0.3325217458
H	1.0	-5.6752051140	1.5546748894	0.0758956378
H	1.0	-7.4316639282	1.3774026746	0.2382629076
H	1.0	-8.2461796466	-1.9389110600	3.5758780985
H	1.0	-7.4117521894	-0.5607837051	4.2767633450
H	1.0	-0.4707639747	0.2150559364	-0.3092678984
H	1.0	-0.4523082924	1.9753815607	-0.5547848050
H	1.0	-1.5175411612	0.9630713059	-1.5420977946

anti Diol **3b** (next lowest energy) E= -714.8788499577

C	6.0	-3.2093746730	-0.0256394496	0.4670616059
C	6.0	-1.9585697270	0.8447498787	0.6188630259
O	8.0	-1.4073935151	0.6688366164	1.9221140848
O	8.0	-4.1014860404	0.4774754967	1.4830077245
C	6.0	-3.7876082145	-0.0205391585	-0.9371851557
N	7.0	-5.1514056042	-0.4626345859	1.8138992273
C	6.0	-4.8016318316	-1.0931056844	3.1261426817
C	6.0	-6.4290367584	0.3116682073	1.7659816881
C	6.0	-7.5555519499	-0.6394545667	2.1958341288
C	6.0	-6.4468618154	1.6050325528	2.5988119595
C	6.0	-5.9726189039	-2.0082943089	3.5143771386
C	6.0	-4.4719847838	-0.1153218307	4.2695265172
C	6.0	-3.5754533969	-1.9900176622	2.9135563432
C	6.0	-6.6919875184	0.7036860081	0.3105385581
C	6.0	-7.3127611042	-1.2850640857	3.5538755230
C	6.0	-2.2054562147	2.3223644258	0.3298405216
H	1.0	-2.9262231774	-1.0478046533	0.7267791502
H	1.0	-1.2009199069	0.4557311924	-0.0703435897
H	1.0	-2.1427870527	0.8616393165	2.5147257024
H	1.0	-4.6150381727	-0.7277139177	-1.0036042373
H	1.0	-3.0086280379	-0.3364837366	-1.6403445804
H	1.0	-4.1411403895	0.9692536806	-1.2315211827
H	1.0	-7.6411653448	-1.4294228470	1.4377351154

H	1.0	-8.4947533743	-0.0721363602	2.1871120005
H	1.0	-5.5438743396	2.1898254660	2.4075597909
H	1.0	-6.5309241825	1.4272873580	3.6702552612
H	1.0	-7.3118458556	2.2040885976	2.2938896647
H	1.0	-5.7345820927	-2.4595665642	4.4860106796
H	1.0	-6.0285971804	-2.8218013603	2.7788013474
H	1.0	-5.3593260458	0.2615229690	4.7786440568
H	1.0	-3.9037145086	0.7389435073	3.8944532331
H	1.0	-3.8593399127	-0.6326335935	5.0154360105
H	1.0	-3.4413109067	-2.6146231510	3.8033700182
H	1.0	-2.6633196926	-1.4066468342	2.7707208021
H	1.0	-3.7289283238	-2.6430240244	2.0494842910
H	1.0	-6.6357888664	-0.1737480951	-0.3375418636
H	1.0	-5.9758423595	1.4529271951	-0.0310888643
H	1.0	-7.6982824533	1.1293644656	0.2351692058
H	1.0	-8.1161638856	-1.9951807945	3.7818172335
H	1.0	-7.3264204402	-0.5319873483	4.3494234404
H	1.0	-2.4931617115	2.4873593129	-0.7122348104
H	1.0	-1.2891521597	2.8819759382	0.5318936754
H	1.0	-3.0013275751	2.7039224279	0.9754028768

Structures of **1b**–**3b** containing less favorable hydrogen bond patterns were optimized using MP2 with a 6-311G(d,p) basis.

Primary alcohol **1b** (five-membered ring hydrogen bond)

E= -675.6760637477

C	6.0	-3.0557912531	0.0059431263	0.6670360622
C	6.0	-2.1962095531	1.2500294351	0.4736930494
O	8.0	-2.9632142180	2.3541734422	0.0192970284
O	8.0	-3.9905524694	0.4391218211	1.6818194544
C	6.0	-3.6832716506	-0.4754009178	-0.6286247262
N	7.0	-5.1016836214	-0.4540062752	1.8912115435
C	6.0	-4.8625896727	-1.1844269489	3.1702981275
C	6.0	-6.3321847228	0.3868444076	1.8055229228
C	6.0	-7.5293025660	-0.5256481854	2.1095166470
C	6.0	-6.3429256029	1.6296595746	2.7134084752
C	6.0	-6.0972402397	-2.0608920710	3.4253975108
C	6.0	-4.5422208489	-0.3076616844	4.3920405328
C	6.0	-3.6661806291	-2.1168693349	2.9470728676
C	6.0	-6.4702750769	0.8651174255	0.3572503427
C	6.0	-7.3988401012	-1.2676890148	3.4344226373
H	1.0	-2.4229940267	-0.7904038172	1.0769442142
H	1.0	-1.6864962402	1.4851262264	1.4181143216
H	1.0	-3.6481608285	2.4542892573	0.6882558711
H	1.0	-4.4313203696	-1.2422100763	-0.4253104238
H	1.0	-2.8942469661	-0.9089567857	-1.2523880842
H	1.0	-4.1395697939	0.3518157505	-1.1724604495
H	1.0	-7.6119508052	-1.2615051255	1.2986399638
H	1.0	-8.4364635989	0.0912695297	2.0869462955
H	1.0	-5.3839037854	2.1506004403	2.6596666933
H	1.0	-6.5510128717	1.3954421549	3.7571012499
H	1.0	-7.1244320661	2.3137047947	2.3656040736
H	1.0	-5.9452201211	-2.5857279687	4.3770142003

H	1.0	-6.1483223502	-2.8210077958	2.6341929988
H	1.0	-5.4242803633	0.1602522358	4.8286633058
H	1.0	-3.8272072279	0.4707771081	4.1156769601
H	1.0	-4.0851796376	-0.9354039205	5.1650110589
H	1.0	-3.6318158412	-2.8557541177	3.7549443651
H	1.0	-2.7241035886	-1.5632919586	2.9612075394
H	1.0	-3.7645823458	-2.6411468439	1.9921284905
H	1.0	-6.4390594308	0.0161332946	-0.3289834149
H	1.0	-5.6766667395	1.5648172842	0.0887684323
H	1.0	-7.4327150570	1.3744912602	0.2412532858
H	1.0	-8.2503140750	-1.9446131473	3.5702433920
H	1.0	-7.4194881107	-0.5670020709	4.2763813931
H	1.0	-1.4393815332	1.0518994913	-0.2899982082

syn Diol **2b** (five-membered ring hydrogen bond)

E= -714.8789264577

C	6.0	-3.0640772714	0.0372465590	0.6934260632
C	6.0	-2.2053141273	1.2924319529	0.5036082304
O	8.0	-3.0098036131	2.3846525892	0.0690233344
O	8.0	-4.0076153569	0.4484253704	1.7077847315
C	6.0	-3.6794381343	-0.4378690415	-0.6103118719
N	7.0	-5.1111150650	-0.4593560666	1.8996785386
C	6.0	-4.8724168630	-1.1995662962	3.1728488303
C	6.0	-6.3495856372	0.3693175156	1.8142019706
C	6.0	-7.5385015352	-0.5601470574	2.0991372273
C	6.0	-6.3805385983	1.6018427703	2.7355648372
C	6.0	-6.0978254541	-2.0946328033	3.4078837685
C	6.0	-4.5747258988	-0.3332114787	4.4080636208
C	6.0	-3.6611594584	-2.1126637680	2.9499325846
C	6.0	-6.4821354991	0.8625750387	0.3705322242
C	6.0	-7.4092141762	-1.3173711722	3.4157000571
H	1.0	-2.4266639121	-0.7582585720	1.0982635448
H	1.0	-3.6776158471	2.4724659492	0.7585611874
H	1.0	-4.4210129900	-1.2143360482	-0.4197804810
H	1.0	-2.8815514016	-0.8578507249	-1.2323194812
H	1.0	-4.1392981189	0.3912546599	-1.1486627865
H	1.0	-7.6072507974	-1.2866759100	1.2786392615
H	1.0	-8.4523779803	0.0468090430	2.0777421430
H	1.0	-5.4279687431	2.1355933107	2.6918486202
H	1.0	-6.5907265199	1.3541669161	3.7757369413
H	1.0	-7.1687321702	2.2797856929	2.3909481721
H	1.0	-5.9468819146	-2.6285131297	4.3546308533
H	1.0	-6.1330190775	-2.8459838573	2.6075258593
H	1.0	-5.4670888530	0.1151039340	4.8443212685
H	1.0	-3.8696144440	0.4599621227	4.1485453133
H	1.0	-4.1135383362	-0.9638234874	5.1762528835
H	1.0	-3.6217316079	-2.8582306876	3.7514402323
H	1.0	-2.7277587911	-1.5447987656	2.9756841495
H	1.0	-3.7450454252	-2.6296462852	1.9896333409
H	1.0	-6.4408334831	0.0213516037	-0.3246637428
H	1.0	-5.6913806511	1.5702240061	0.1148580494
H	1.0	-7.4475642014	1.3662310800	0.2540726995
H	1.0	-8.2533721472	-2.0063301628	3.5359015417
H	1.0	-7.4456098941	-0.6277924716	4.2662988989
C	6.0	-1.4176477755	1.6535762276	1.7580084002
H	1.0	-1.5117540286	1.0947461634	-0.3212094386

H	1.0	-0.8096453918	2.5415704400	1.5693628124
H	1.0	-0.7602976362	0.8293070022	2.0540342748
H	1.0	-2.1017911727	1.8630478386	2.5845013355

anti Diol **3b** (six-membered ring hydrogen bond)

E= -714.8760599918

C	6.0	0.1014401381	0.1257190237	1.7011588793
C	6.0	-0.0603738651	1.2430494020	2.7405876810
O	8.0	-0.8209031172	0.7969916565	3.8577478750
O	8.0	-1.1159369708	-0.4778436812	1.1941872266
C	6.0	0.8067641192	0.5880173652	0.4367593928
N	7.0	-1.9858825503	-1.0459158576	2.2163273355
C	6.0	-1.6805982465	-2.5063719959	2.3849562485
C	6.0	-3.3761641890	-0.7019270459	1.7675848589
C	6.0	-4.3518534645	-1.3127829353	2.7825029683
C	6.0	-3.5277377518	0.8193131053	1.8311619445
C	6.0	-2.7148928354	-3.0670655323	3.3759164496
C	6.0	-0.3089742956	-2.6531619683	3.0616546321
C	6.0	-1.6451999496	-3.3234886851	1.0855529327
C	6.0	-3.7236132391	-1.1363800178	0.3337941967
C	6.0	-4.1586396725	-2.8115384105	2.9672296579
H	1.0	0.7006655723	-0.6489331889	2.1815300976
H	1.0	-1.4053868611	0.1010064127	3.4970570671
H	1.0	1.0324262917	-0.2691132114	-0.2022144035
H	1.0	1.7436779179	1.0916842688	0.6925065534
H	1.0	0.1730462445	1.2813845712	-0.1210260643
H	1.0	-5.3691695896	-1.0823607963	2.4427062318
H	1.0	-4.2070766918	-0.8092507911	3.7480263707
H	1.0	-4.5905046661	1.0693639284	1.7458189761
H	1.0	-2.9982853181	1.2916507012	1.0026366296
H	1.0	-3.1476973820	1.2141050175	2.7758076802
H	1.0	-2.5343486739	-2.6045794663	4.3559921454
H	1.0	-2.5167813308	-4.1410162230	3.4812001467
H	1.0	-0.1846844673	-1.9162022888	3.8593501288
H	1.0	0.5088381413	-2.5564067472	2.3437785620
H	1.0	-0.2443019646	-3.6571381954	3.4948741208
H	1.0	-1.1116781684	-4.2605707674	1.2785291511
H	1.0	-1.1039637544	-2.7725746085	0.3125219087
H	1.0	-2.6352331368	-3.5800129565	0.7103534042
H	1.0	-3.9571198669	-2.1968908876	0.2474950444
H	1.0	-2.9018786451	-0.8957339780	-0.3442121381
H	1.0	-4.6086730570	-0.5773543062	0.0113488763
H	1.0	-4.4033011700	-3.3515976748	2.0460446849
H	1.0	-4.8382380788	-3.1873602038	3.7407235547
C	6.0	-0.5653834229	2.5808327195	2.2047425716
H	1.0	0.9630662185	1.4133884743	3.1093891899
H	1.0	-0.7484206722	3.2399447950	3.0573755975
H	1.0	-1.4921174417	2.4794903705	1.6420131050
H	1.0	0.1835598634	3.0520406091	1.5608085280

Structures of **1′**–**3′** containing five- and six-membered ring hydrogen bonds were optimized using MP2 with a 6-311G(d,p) basis.

Primary alcohol **1′** (six-membered ring hydrogen bond)

E= -518.8845807425

C	6.0	0.0105759916	-1.0766873396	0.0809059586
C	6.0	0.5065500237	-2.4885765725	-0.2068874306
O	8.0	-0.5389458513	-3.4422072716	-0.2531603560
O	8.0	-0.3682415524	-0.9144764699	1.4586180380
C	6.0	1.0833146320	-0.0268874415	-0.1477911857
N	7.0	-1.4620436271	-1.8056570866	1.7688818876
C	6.0	-1.0831277760	-2.4700637302	3.0190674204
C	6.0	-2.6389693031	-0.9550268492	1.9661389338
C	6.0	-3.8299124336	-1.8266933214	2.3579704460
C	6.0	-2.2163504752	-3.3954769558	3.4572874153
C	6.0	-3.5162964971	-2.6094883357	3.6339220671
H	1.0	-0.8673970360	-0.8817149624	-0.5525964095
H	1.0	1.2573474575	-2.7410342098	0.5592141203
H	1.0	1.0031937559	-2.4973770931	-1.1835533347
H	1.0	-1.1476671463	-3.1309128014	0.4363247863
H	1.0	1.9691609561	-0.2578770125	0.4506590629
H	1.0	0.7138779000	0.9582468552	0.1442354763
H	1.0	1.3666311261	-0.0007664191	-1.2030590716
H	1.0	-4.0449918312	-2.5228084779	1.5384000800
H	1.0	-4.7118723372	-1.1913965085	2.4931424312
H	1.0	-1.9295884748	-3.8948353980	4.3889851832
H	1.0	-2.3519513587	-4.1730624296	2.6958296492
H	1.0	-4.3425039991	-3.2813402828	3.8892134337
H	1.0	-3.3990278615	-1.9041176174	4.4671411715
H	1.0	-0.8705792876	-1.7156411340	3.7943175767
H	1.0	-0.1666053683	-3.0345570473	2.8268218303
H	1.0	-2.8258361819	-0.4259422986	1.0270625236
H	1.0	-2.4285834442	-0.2081617890	2.7492182963

Primary alcohol **1′** (five-membered ring hydrogen bond)

E= -518.8822327945

C	6.0	-3.0393164937	-0.2610742327	0.5005604177
C	6.0	-1.8317489541	0.6591717466	0.5408841827
O	8.0	-1.4065669606	0.8858627803	1.8730294501
O	8.0	-4.0393391181	0.4490427057	1.2468090648
C	6.0	-3.5237897864	-0.5801212581	-0.9011933286
N	7.0	-5.0547981937	-0.4821585278	1.6677966333
C	6.0	-4.8874064357	-0.6312513712	3.1150429579
C	6.0	-6.3312909743	0.1656110216	1.3665284935
C	6.0	-7.4691509459	-0.7428264921	1.8291188926
C	6.0	-5.9607043341	-1.5784323035	3.6468260481
C	6.0	-7.3525882975	-1.0306716527	3.3269805366
H	1.0	-2.7943121526	-1.1804667974	1.0476183568
H	1.0	-2.2123167870	1.1532392119	2.3277008391
H	1.0	-4.4263715498	-1.1924663621	-0.8444753864
H	1.0	-2.7606360717	-1.1348843292	-1.4564773250
H	1.0	-3.7524150281	0.3443003617	-1.4400031419
H	1.0	-7.4180059789	-1.6827593304	1.2670516187
H	1.0	-8.4276926719	-0.2669018009	1.5952303942
H	1.0	-5.8275344994	-1.7078673552	4.7263448174
H	1.0	-5.8293156411	-2.5586918199	3.1740642178

H	1.0	-8.1290506626	-1.7336432694	3.6470453859
H	1.0	-7.5070615926	-0.0975402403	3.8847914072
H	1.0	-4.9644056465	0.3529271344	3.6100221198
H	1.0	-3.8836818754	-1.0288506368	3.2949591988
H	1.0	-6.3717887010	0.3323883910	0.2867531374
H	1.0	-6.3921895001	1.1465597181	1.8694338521
H	1.0	-2.0859397355	1.6011399261	0.0323111838
H	1.0	-0.9974914118	0.1934347823	0.0098259755

syn Diol **2′** (six-membered ring hydrogen bond)

E= -558.0875997321

C	6.0	0.1046108475	0.1893487582	1.6860467170
C	6.0	-0.2057845539	1.3548757643	2.6282040169
O	8.0	-0.7675390989	0.8897673126	3.8485111534
O	8.0	-1.0982671554	-0.4042339312	1.1612025026
C	6.0	0.8813671259	0.5961669640	0.4453736543
N	7.0	-1.8658788933	-1.0006142641	2.2285261693
C	6.0	-1.7785987117	-2.4508962241	2.0368638948
C	6.0	-3.2397789970	-0.5276409491	2.0346981981
C	6.0	-4.1397159319	-1.1587939748	3.0949053349
C	6.0	-2.6202044361	-3.1500480086	3.1021396450
C	6.0	-4.0747970047	-2.6848824184	3.0180813183
C	6.0	1.0324622428	2.1589312728	2.9934906609
H	1.0	0.6549742024	-0.5738607610	2.2583268125
H	1.0	-0.9244429754	2.0033358544	2.0979591455
H	1.0	-1.2539539396	0.0866238088	3.5916711516
H	1.0	0.9286357569	-0.2483011000	-0.2458054494
H	1.0	1.8984914242	0.8963371234	0.7044863622
H	1.0	0.3821170503	1.4296932565	-0.0576542853
H	1.0	-5.1650891767	-0.8015263767	2.9514842635
H	1.0	-3.8089756666	-0.8211139431	4.0844812810
H	1.0	-2.2105619333	-2.9110745983	4.0907795562
H	1.0	-2.5454413196	-4.2342233245	2.9653172676
H	1.0	-4.5018248006	-3.0149723768	2.0619322131
H	1.0	-4.6728067945	-3.1378156944	3.8158362253
H	1.0	0.7666292105	2.8553101509	3.7922779678
H	1.0	1.4186616598	2.7279632019	2.1443043200
H	1.0	1.8149511643	1.4927863772	3.3708069538
H	1.0	-0.7243929953	-2.7321224205	2.1158483988
H	1.0	-2.1329863825	-2.7123648147	1.0263266434
H	1.0	-3.5850646379	-0.7869396389	1.0205779615
H	1.0	-3.2268652796	0.5616249746	2.1284299457

syn Diol **2′** (five-membered ring hydrogen bond)

E= -558.0875997321

C	6.0	0.1046108475	0.1893487582	1.6860467170
C	6.0	-0.2057845539	1.3548757643	2.6282040169
O	8.0	-0.7675390989	0.8897673126	3.8485111534
O	8.0	-1.0982671554	-0.4042339312	1.1612025026
C	6.0	0.8813671259	0.5961669640	0.4453736543
N	7.0	-1.8658788933	-1.0006142641	2.2285261693
C	6.0	-1.7785987117	-2.4508962241	2.0368638948
C	6.0	-3.2397789970	-0.5276409491	2.0346981981
C	6.0	-4.1397159319	-1.1587939748	3.0949053349
C	6.0	-2.6202044361	-3.1500480086	3.1021396450

C	6.0	-4.0747970047	-2.6848824184	3.0180813183
C	6.0	1.0324622428	2.1589312728	2.9934906609
H	1.0	0.6549742024	-0.5738607610	2.2583268125
H	1.0	-0.9244429754	2.0033358544	2.0979591455
H	1.0	-1.2539539396	0.0866238088	3.5916711516
H	1.0	0.9286357569	-0.2483011000	-0.2458054494
H	1.0	1.8984914242	0.8963371234	0.7044863622
H	1.0	0.3821170503	1.4296932565	-0.0576542853
H	1.0	-5.1650891767	-0.8015263767	2.9514842635
H	1.0	-3.8089756666	-0.8211139431	4.0844812810
H	1.0	-2.2105619333	-2.9110745983	4.0907795562
H	1.0	-2.5454413196	-4.2342233245	2.9653172676
H	1.0	-4.5018248006	-3.0149723768	2.0619322131
H	1.0	-4.6728067945	-3.1378156944	3.8158362253
H	1.0	0.7666292105	2.8553101509	3.7922779678
H	1.0	1.4186616598	2.7279632019	2.1443043200
H	1.0	1.8149511643	1.4927863772	3.3708069538
H	1.0	-0.7243929953	-2.7321224205	2.1158483988
H	1.0	-2.1329863825	-2.7123648147	1.0263266434
H	1.0	-3.5850646379	-0.7869396389	1.0205779615
H	1.0	-3.2268652796	0.5616249746	2.1284299457

anti Diol **3′** (six-membered ring hydrogen bond)

E= -558.0862082567

C	6.0	0.0872473518	0.2083178340	2.1549055658
C	6.0	-0.1413095257	1.2983604968	3.2064640072
O	8.0	-0.8718300793	0.7872088093	4.3166569827
O	8.0	-1.1401542271	-0.2158704290	1.5360342381
C	6.0	0.9710708431	0.6494644512	1.0009469220
N	7.0	-1.9236180926	-0.9693350440	2.4909853568
C	6.0	-1.8062949560	-2.3764376214	2.0957782196
C	6.0	-3.3009289129	-0.4959026668	2.3265734129
C	6.0	-4.2165822000	-1.2881497078	3.2577152453
C	6.0	-2.6596638025	-3.2347248451	3.0266025282
C	6.0	-4.1204578476	-2.7863018929	2.9667344054
H	1.0	0.5327209768	-0.6579676442	2.6660633282
C	6.0	-0.8247562843	2.5394741070	2.6417520381
H	1.0	-1.3328010336	0.0046744919	3.9692002823
H	1.0	1.2073110650	-0.2033323322	0.3607850767
H	1.0	1.9029529294	1.0780855311	1.3799503064
H	1.0	0.4565746501	1.4003437646	0.3969472728
H	1.0	-5.2442112596	-0.9295129206	3.1353793580
H	1.0	-3.9208988810	-1.0910883673	4.2951563901
H	1.0	-2.2809858904	-3.1319191830	4.0504499948
H	1.0	-2.5583117013	-4.2867568412	2.7391726218
H	1.0	-4.5150643702	-2.9836973918	1.9613574993
H	1.0	-4.7305720944	-3.3573293946	3.6744474213
H	1.0	-0.7496050845	-2.6526451211	2.1606181885
H	1.0	-2.1318144916	-2.4937308137	1.0492758449
H	1.0	-3.6146167079	-0.6111878831	1.2762202981
H	1.0	-3.3141727759	0.5666613441	2.5804947338
H	1.0	0.8531188133	1.5825142279	3.5808579348
H	1.0	-1.7455422687	2.2635429585	2.1222084532
H	1.0	-0.1760933357	3.0759825490	1.9424227209
H	1.0	-1.0732608067	3.2083195343	3.4688933521

anti Diol **3′** (five-membered ring hydrogen bond)

E= -558.0842899175

C	6.0	-2.9366408863	-0.4048762616	0.7746561547
C	6.0	-1.8975446982	0.6877243712	0.5175631908
O	8.0	-1.2229272451	1.0203900690	1.7254192407
O	8.0	-3.7952118419	0.1930470047	1.7603953287
N	7.0	-4.9625284113	-0.6264473303	1.9501397194
C	6.0	-5.0828443854	-0.8174210043	3.3960460989
C	6.0	-6.0879080758	0.1622737471	1.4430484283
C	6.0	-7.3811777942	-0.6231076141	1.6501134116
C	6.0	-6.3382406752	-1.6371374703	3.6885995540
C	6.0	-7.5788739456	-0.9350366767	3.1342753024
H	1.0	-1.9276315380	1.1751558346	2.3644223571
H	1.0	-7.3206360972	-1.5572361078	1.0795105923
H	1.0	-8.2231712269	-0.0444372359	1.2548190014
H	1.0	-6.4244306118	-1.7900209056	4.7699549573
H	1.0	-6.2310236381	-2.6229316303	3.2208908688
H	1.0	-8.4720352280	-1.5505195609	3.2859476653
H	1.0	-7.7334318801	0.0049303750	3.6804055229
H	1.0	-5.1331926220	0.1597180880	3.9080453165
H	1.0	-4.1835053788	-1.3367142243	3.7384057510
H	1.0	-5.9078890144	0.3518711760	0.3805601271
H	1.0	-6.1384420649	1.1340545078	1.9639150852
C	6.0	-0.8408049359	0.2826964649	-0.4927342016
H	1.0	-2.4462025489	1.5657126445	0.1436111188
H	1.0	-0.2336246014	-0.5349381312	-0.0979642691
H	1.0	-0.1824949381	1.1313394996	-0.6924763889
H	1.0	-1.3032665489	-0.0331673030	-1.4326657690
C	6.0	-2.3521991775	-1.7127380996	1.2777143984
H	1.0	-3.5194146919	-0.5708393066	-0.1432761444
H	1.0	-1.6817767640	-1.5174753696	2.1178750895
H	1.0	-1.7911245637	-2.2175918207	0.4861953806
H	1.0	-3.1645239707	-2.3696277296	1.5951771116

For the purposes of structural analysis, piperidine and 2,2,6,6-tetramethylpiperidine were optimized using MP2 with a 6-311G(d,p) basis.

Piperidine

C	6.0	-0.7165441808	-0.4651675883	0.0684311434
C	6.0	0.4579231564	-0.8692511597	-0.8270695829
C	6.0	1.3175906593	0.3518222019	-1.1654973038
C	6.0	0.4485996854	1.4608034918	-1.7536619025
C	6.0	-1.4982082513	0.6788525028	-0.5727951582
N	7.0	-0.5973461742	1.8118764416	-0.7914519740
H	1.0	-0.3395940139	-0.1232106484	1.0393389622
H	1.0	-1.3802755578	-1.3192193270	0.2452028434
H	1.0	0.0637088599	-1.2962204561	-1.7596309915
H	1.0	1.0616815564	-1.6470274267	-0.3467438559
H	1.0	2.1106760719	0.0829104261	-1.8725187023
H	1.0	1.7922628395	0.7329395465	-0.2538253202
H	1.0	0.0294459551	1.1108149782	-2.7170002086

H	1.0	1.0517675462	2.3520995760	-1.9548447669
H	1.0	-2.3116984894	1.0011458230	0.0852724132
H	1.0	-1.9494840008	0.3158953143	-1.5166227427
H	1.0	-1.1346856618	2.5917663039	-1.1608728528

2,2,6,6-Tetramethylpiperidine

C	6.0	-0.7530337856	-0.5154923243	-0.0276903015
C	6.0	0.4338302981	-0.8855193593	-0.9177257067
C	6.0	1.2693440746	0.3627009952	-1.2032682272
C	6.0	0.4452403488	1.4819300903	-1.8514526363
C	6.0	-1.6278391304	0.5816979042	-0.6464375152
N	7.0	-0.7500228344	1.7026416435	-1.0208242785
H	1.0	-0.3690300375	-0.1456344452	0.9322775593
H	1.0	-1.3774105488	-1.3935708492	0.1805278193
H	1.0	0.0863709642	-1.3383132118	-1.8537589022
H	1.0	1.0521289064	-1.6402269495	-0.4178335877
H	1.0	2.1211961663	0.1256637270	-1.8531835514
H	1.0	1.6709257130	0.7401722376	-0.2535104283
H	1.0	-1.3137357085	2.4427962306	-1.4376827879
C	6.0	-2.5771013407	1.1359403251	0.4197911984
C	6.0	-2.4857178701	0.0100152576	-1.7909583953
C	6.0	1.2364643690	2.7919383685	-1.7968057920
C	6.0	0.1648750567	1.1612070996	-3.3317193024
H	1.0	-1.9976012362	1.5896098219	1.2277395360
H	1.0	-3.2104692046	0.3401588224	0.8264892066
H	1.0	-3.2311166498	1.9039663725	-0.0112188029
H	1.0	-3.2409211911	-0.6728326244	-1.3849286342
H	1.0	-1.8979693342	-0.5424258348	-2.5253381176
H	1.0	-3.0081096500	0.8210989639	-2.3112838056
H	1.0	1.4141767464	3.0707696796	-0.7551216084
H	1.0	0.6740017869	3.5998815912	-2.2807768294
H	1.0	2.1953531435	2.6877197369	-2.3159457007
H	1.0	-0.2634710282	0.1684204138	-3.4760505900
H	1.0	1.0970317237	1.2100881641	-3.9063302468
H	1.0	-0.5299797477	1.8977581530	-3.7514395716

3. B3LYP computed isotropic shift values

To provide a comparison to the shifts calculated using the KT2 functional, isotropic shifts were calculated using the B3LYP functional and the Dunning aug-cc-pVTZ basis.

Compound	Isotropic shift / ppm
1b	5.44
2b	5.56
3b (lowest energy geometry)	0.00 [reference]
3b (next lowest energy geometry)	1.03

4. Saddle point geometry, energy, and number of imaginary modes

Coordinates are in angstroms and energies are in hartree.

Saddle point between lowest energy geometries (**3b**)

E= -716.1268001

Contains 1 imaginary frequency

ATOM	CHARGE	X	Y	Z
C	6.0	-1.81346	-0.29349	-0.73136
C	6.0	-2.91404	0.72281	-0.20461
O	8.0	-2.51438	1.33126	1.02134
O	8.0	-0.73935	-0.33657	0.24935
C	6.0	-2.33741	-1.69720	-1.01444
N	7.0	0.58902	-0.17236	-0.31862
C	6.0	1.07615	1.23242	-0.06811
C	6.0	1.42605	-1.31658	0.18238
C	6.0	2.85214	-1.12930	-0.38628
C	6.0	1.45522	-1.48579	1.71934
C	6.0	2.50283	1.31776	-0.65775
C	6.0	1.07380	1.69966	1.40586
C	6.0	0.18845	2.20495	-0.86859
C	6.0	0.87235	-2.61870	-0.41907
C	6.0	3.45112	0.24872	-0.12125
C	6.0	-4.32177	0.15568	-0.01593
H	1.0	-1.38391	0.11044	-1.64691
H	1.0	-2.97911	1.52179	-0.95437
H	1.0	-1.71144	0.86347	1.29139
H	1.0	-1.56563	-2.30180	-1.48708
H	1.0	-3.19069	-1.65590	-1.69575
H	1.0	-2.65939	-2.19772	-0.09805
H	1.0	2.81252	-1.29279	-1.46956
H	1.0	3.48450	-1.92022	0.02995
H	1.0	0.44429	-1.43415	2.12538
H	1.0	2.06983	-0.74201	2.22446
H	1.0	1.86614	-2.46932	1.96550
H	1.0	2.89108	2.32222	-0.46013
H	1.0	2.43053	1.21298	-1.74643
H	1.0	1.85915	1.24125	2.00387
H	1.0	0.11754	1.49808	1.88823
H	1.0	1.22820	2.78186	1.43427
H	1.0	0.66443	3.18958	-0.88745
H	1.0	-0.79211	2.32598	-0.40886
H	1.0	0.07353	1.86565	-1.90039
H	1.0	0.72078	-2.50840	-1.49498
H	1.0	-0.06975	-2.90802	0.04546
H	1.0	1.58957	-3.42755	-0.25312
H	1.0	4.42632	0.33307	-0.61188
H	1.0	3.63479	0.39322	0.94823
H	1.0	-4.76870	-0.16978	-0.95918
H	1.0	-4.94863	0.94682	0.40093
H	1.0	-4.32861	-0.68167	0.68582

5. MP2 optimized Cartesian coordinates

The lowest energy structures of **1b**–**3b** were optimized using MP2 with a 6-311G(d,p) basis. Coordinates are in angstroms and energies are in hartree.

Primary alcohol **1b** E= -675.6819676697

ATOM	CHARGE	X	Y	Z
C	6.0	0.0350552326	-0.9948554678	0.0625494124
C	6.0	0.3272557518	-2.4268320087	-0.3616931230
O	8.0	-0.8336369208	-3.2365858915	-0.4126817429
O	8.0	-0.4074869993	-0.8446207137	1.4333296612
C	6.0	1.2760287712	-0.1208575031	-0.0054934539
N	7.0	-1.4600521196	-1.7640265851	1.8189668332
C	6.0	-1.0121685387	-2.3852003949	3.1053731480
C	6.0	-2.7550923988	-1.0136792369	1.8356062617
C	6.0	-3.8300542677	-1.9913843097	2.3328352957
C	6.0	-2.7529435506	0.2829356176	2.6590933152
C	6.0	-2.1397381672	-3.3169644388	3.5726600472
C	6.0	-0.6182150515	-1.3868243837	4.2053613712
C	6.0	0.2154591233	-3.2498757931	2.8032161512
C	6.0	-3.0953746180	-0.6411094295	0.3871610236
C	6.0	-3.4907898784	-2.6196008995	3.6794688652
H	1.0	-0.7368382070	-0.6031026474	-0.6078306476
H	1.0	1.0955342615	-2.8503337008	0.2995264478
H	1.0	0.7443780068	-2.3898433600	-1.3744566826
H	1.0	-1.2947609092	-2.9870258879	0.4097397014
H	1.0	2.0714581350	-0.5414163103	0.6164397044
H	1.0	1.0477823653	0.8849326586	0.3543104203
H	1.0	1.6315173537	-0.0519268493	-1.0373874385
H	1.0	-3.9458004982	-2.7877966612	1.5848042246
H	1.0	-4.7809862693	-1.4458979460	2.3781663198
H	1.0	-1.8360870042	0.8453366374	2.4677985881
H	1.0	-2.8487542002	0.1132287727	3.7311108016
H	1.0	-3.6046102530	0.8957898691	2.3443629969
H	1.0	-1.8390745080	-3.7475938151	4.5359389295
H	1.0	-2.2219847172	-4.1457009721	2.8561876322
H	1.0	-1.4755718571	-0.9300242122	4.6985152923
H	1.0	0.0145671276	-0.5992412650	3.7900187389
H	1.0	-0.0437587662	-1.9216920307	4.9692577150
H	1.0	0.4504045637	-3.8488936503	3.6891840439
H	1.0	1.0826696144	-2.6281215544	2.5706139771
H	1.0	0.0175239382	-3.9267541416	1.9681483405
H	1.0	-2.9311364865	-1.4885896516	-0.2833555740
H	1.0	-2.4962894091	0.2073904497	0.0471528899
H	1.0	-4.1491153274	-0.3468391449	0.3374155388
H	1.0	-4.2643828336	-3.3433619373	3.9607546046
H	1.0	-3.4727204882	-1.8588512111	4.4675603690

syn Diol **2b** E= -714.8850755986

C	6.0	0.2056288729	0.1052791483	1.7072219945
C	6.0	-0.0991656502	1.2004139169	2.7284799780

O	8.0	-0.6456015407	0.6493906709	3.9192613101
O	8.0	-0.9577695761	-0.5962081659	1.1961349054
C	6.0	0.8544212327	0.6367015019	0.4387969493
H	1.0	-0.1339472803	-2.4703183121	1.0958837273
H	1.0	-3.7720471325	-1.6139925867	0.4603606557
H	1.0	-3.3925685014	0.0440679776	0.0421443071
H	1.0	-4.9398404243	-0.3392195959	0.7837327835
H	1.0	-4.5814122879	-3.1371559323	2.4050495208
H	1.0	-3.9712628630	-3.1823695256	4.0345267364
H	1.0	1.8851545916	2.4729250382	3.9150422842
H	1.0	2.2972905385	0.9201669973	3.1882179934
H	1.0	0.8289080809	1.0825458811	4.1447834295

synfive3 E= -708.1846776719

C	6.0	0.1986852907	-0.2363146282	0.4893373404
C	6.0	1.1662538759	0.9468577781	0.6180490482
O	8.0	0.4034486252	2.1674565764	0.7008596610
O	8.0	-0.6189461191	-0.1230214265	1.6968788424
C	6.0	-0.6092012197	-0.1497410657	-0.7986572829
N	7.0	-1.7075572920	-1.0906976274	1.7726593676
C	6.0	-1.3451936766	-2.1085283757	2.8110069983
C	6.0	-3.0473799286	-0.3822613243	1.8989482426
C	6.0	-3.7344920651	-0.6714961877	3.2505875086
C	6.0	-2.8991234410	1.1418030682	1.7725318741
C	6.0	-2.6027657238	-2.9639046334	3.0376238757
C	6.0	-0.8050882776	-1.5256496268	4.1314405185
C	6.0	-0.2552127267	-3.0166807206	2.2119110273
C	6.0	-3.9396690306	-0.8946248204	0.7524682710
C	6.0	-3.8007600200	-2.1713395154	3.6116384524
C	6.0	2.1003715646	0.8135753203	1.8225863501
H	1.0	0.7495002733	-1.1617364283	0.5156268401
H	1.0	1.7454482357	1.0225648057	-0.2903048957
H	1.0	-0.2208248177	2.0678915094	1.4322842810
H	1.0	-1.3817905586	-0.9022814704	-0.8098140474
H	1.0	0.0510105538	-0.3148896864	-1.6433242387
H	1.0	-1.0443840496	0.8344317014	-0.8939927378
H	1.0	-4.7369405522	-0.2614178097	3.2041645292
H	1.0	-3.2129912671	-0.1280784213	4.0253333336
H	1.0	-2.2965720476	1.5364525601	2.5789218313
H	1.0	-3.8860230358	1.5867887491	1.8287971621
H	1.0	-2.4498221887	1.4221310168	0.8335183759
H	1.0	-2.8742680232	-3.4028910884	2.0851442233
H	1.0	-2.3434148093	-3.7778741729	3.7044032138
H	1.0	-1.5509576099	-0.9796962665	4.6875517013
H	1.0	0.0191836190	-0.8617124708	3.9215915151
H	1.0	-0.4494991141	-2.3381862184	4.7561779235
H	1.0	-0.1057794268	-3.8811456041	2.8495245511
H	1.0	0.6862255317	-2.4907098869	2.1369583829
H	1.0	-0.5550845007	-3.3502277759	1.2268702954
H	1.0	-4.0601163130	-1.9682872097	0.8005449063
H	1.0	-3.4993193387	-0.6465397903	-0.2028942144
H	1.0	-4.9197857186	-0.4337718453	0.8111038794
H	1.0	-3.8264187329	-2.2697867933	4.6905993454
H	1.0	-4.7204692038	-2.6025343830	3.2346531309

H	1.0	1.5189966300	0.7104756469	2.7284140284
H	1.0	2.7185680057	1.6990105241	1.8998763456
H	1.0	2.7416586234	-0.0550819829	1.7200202428

synfive4 E= -708.1875707499

C	6.0	0.1452704333	-0.4182017589	0.6654003612
C	6.0	1.0240472845	0.8289723320	0.7598985005
O	8.0	1.3893090764	1.0237383174	2.1419476102
O	8.0	-0.9015269117	-0.1256577876	1.6410635360
C	6.0	-0.4043770363	-0.6891760760	-0.7268194825
N	7.0	-1.9000102302	-1.1751936643	1.8262810189
C	6.0	-1.4884281101	-2.0511074217	2.9915736616
C	6.0	-3.2115954870	-0.4489553590	1.9070465362
C	6.0	-4.3473793458	-1.5049659604	2.0637612423
C	6.0	-3.2618160244	0.5993218051	3.0387746472
C	6.0	-2.7631461113	-2.6103563353	3.6686020454
C	6.0	-0.6139127766	-1.3295767608	4.0314652569
C	6.0	-0.6948969032	-3.2388208710	2.4095857135
C	6.0	-3.4163348779	0.2911705013	0.5756293949
C	6.0	-3.8665467730	-2.8524008552	2.6355226480
C	6.0	2.3345700956	0.6966679005	-0.0051888408
H	1.0	0.7242329366	-1.2568845693	1.0127452651
H	1.0	0.4525070674	1.6760400989	0.3957081961
H	1.0	0.5756664356	1.0294353238	2.6631133586
H	1.0	-1.1430167588	-1.4755434962	-0.6750678642
H	1.0	0.3935593877	-1.0042739781	-1.3877312113
H	1.0	-0.8699670330	0.1978558068	-1.1385465757
H	1.0	-4.8122446327	-1.6757817860	1.1003815283
H	1.0	-5.1045218682	-1.0864309627	2.7172013708
H	1.0	-2.4142045437	1.2640229657	2.9549306962
H	1.0	-3.2591563610	0.1483727304	4.0205516730
H	1.0	-4.1718212033	1.1816561096	2.9437311936
H	1.0	-3.1246923663	-1.9226809728	4.4230349823
H	1.0	-2.4982033561	-3.5305494305	4.1760122055
H	1.0	-1.1198536320	-0.4675978760	4.4428964245
H	1.0	0.3213974237	-1.0047809841	3.6012538700
H	1.0	-0.3997661221	-2.0184285615	4.8416304216
H	1.0	-0.4532301301	-3.9420810831	3.1988790885
H	1.0	0.2309620059	-2.9073955191	1.9647628978
H	1.0	-1.2743175730	-3.7457851183	1.6498334689
H	1.0	-3.3361270316	-0.4033416961	-0.2497461827
H	1.0	-2.6784792756	1.0694342280	0.4568806051
H	1.0	-4.4050086433	0.7368381305	0.5614415904
H	1.0	-3.4873334853	-3.4756433408	1.8361782383
H	1.0	-4.7018151567	-3.3751939608	3.0879077765
H	1.0	2.8712995724	-0.1786279662	0.3399521580
H	1.0	2.9461298338	1.5661008904	0.1964935921
H	1.0	2.1697482076	0.6227370116	-1.0722126167

synsix1 E= -708.1991976300

C	6.0	0.2749056825	0.0285342820	1.4601162152
C	6.0	0.1014270024	1.1582400689	2.4780458438
O	8.0	-0.4041445922	0.6425732485	3.7257651079

O	8.0	-0.9795134584	-0.6515500549	1.0967370780
C	6.0	0.7809904750	0.5157087085	0.1033417580
N	7.0	-1.8622411090	-1.0649608242	2.1908009630
C	6.0	-1.6546957693	-2.5334298249	2.4500942995
C	6.0	-3.2361734744	-0.5778784340	1.8104583436
C	6.0	-4.2095310674	-1.0667372013	2.9000992718
C	6.0	-3.1987472222	0.9596967802	1.8486817223
C	6.0	-2.6882112922	-2.9482575353	3.5170960495
C	6.0	-0.2496596731	-2.7056211861	3.0649791530
C	6.0	-1.7369049110	-3.4222877372	1.1960660561
C	6.0	-3.6947622029	-1.0043642175	0.4030678184
C	6.0	-4.1275989705	-2.5795531679	3.1378270427
C	6.0	1.4368245067	1.8153275658	2.8215225379
H	1.0	0.9545139889	-0.6935598324	1.8795117146
H	1.0	-0.5739230947	1.8968069521	2.0665365117
H	1.0	-1.1182212729	0.0148537015	3.5139674361
H	1.0	0.7645181680	-0.3079315472	-0.5978151277
H	1.0	1.7921044564	0.8925964321	0.1749227592
H	1.0	0.1334343254	1.2972749665	-0.2755866101
H	1.0	-5.2129587145	-0.7736523585	2.6111898300
H	1.0	-3.9707935798	-0.5574070509	3.8286175368
H	1.0	-2.5967362800	1.3381103851	1.0354664220
H	1.0	-2.7845712026	1.3052527604	2.7860985793
H	1.0	-4.2051991404	1.3483550993	1.7436145368
H	1.0	-2.4369154321	-2.4502769401	4.4485161304
H	1.0	-2.5926105228	-4.0165856639	3.6778542556
H	1.0	-0.0577885905	-1.9309406376	3.7940429047
H	1.0	0.5138008116	-2.6647734845	2.3004642401
H	1.0	-0.1855762470	-3.6753801630	3.5458863136
H	1.0	-1.3031351313	-4.3898733296	1.4240636466
H	1.0	-1.1713380821	-2.9639266482	0.3982959543
H	1.0	-2.7482828600	-3.5856726072	0.8590176376
H	1.0	-3.9800380424	-2.0429308255	0.3487469093
H	1.0	-2.8987686163	-0.8210171610	-0.3029120229
H	1.0	-4.5571012742	-0.4094269974	0.1226314018
H	1.0	-4.7983938048	-2.8583678448	3.9436874533
H	1.0	-4.4437682197	-3.1238835554	2.2570788410
H	1.0	1.2746431681	2.4922073195	3.6497041138
H	1.0	1.8459161761	2.3703930195	1.9878056916
H	1.0	2.1475650897	1.0619055404	3.1406236800

synsix2 E= -708.1991977008

C	6.0	0.2935772805	0.0409335496	1.4901872667
C	6.0	0.1267724995	1.1659754785	2.5144730865
O	8.0	-0.3773020293	0.6455667608	3.7606786018
O	8.0	-0.9640601906	-0.6339803486	1.1277574999
C	6.0	0.7958863248	0.5340011038	0.1342263374
N	7.0	-1.8446517812	-1.0498868088	2.2226444196
C	6.0	-1.6386908507	-2.5195025258	2.4766396351
C	6.0	-3.2186449633	-0.5595023819	1.8471801270
C	6.0	-4.1905018123	-1.0506433501	2.9372384446
C	6.0	-3.1788167382	0.9776964874	1.8907159256
C	6.0	-2.6704612039	-2.9362602011	3.5445677772
C	6.0	-0.2325842752	-2.6956624244	3.0882221536
C	6.0	-1.7254646371	-3.4040021038	1.2199149547
C	6.0	-3.6807640136	-0.9803995173	0.4394048302

C	6.0	-4.1102532718	-2.5643874044	3.1697395388
C	6.0	1.4656296176	1.8163611393	2.8582201797
H	1.0	0.9726830879	-0.6851243031	1.9033325758
H	1.0	-0.5468705018	1.9094251442	2.1085468321
H	1.0	-1.0947248093	0.0222191636	3.5474302882
H	1.0	0.7735509523	-0.2856466544	-0.5714819755
H	1.0	1.8089474953	0.9060808400	0.2037098686
H	1.0	0.1498339768	1.3200860236	-0.2375895789
H	1.0	-5.1940627297	-0.7551676040	2.6512621634
H	1.0	-3.9491307838	-0.5447544193	3.8669316693
H	1.0	-2.5756575984	1.3578590579	1.0791933549
H	1.0	-2.7648035616	1.3193636381	2.8296401001
H	1.0	-4.1846197595	1.3682459799	1.7864664027
H	1.0	-2.4164055987	-2.4416337231	4.4770245779
H	1.0	-2.5758717810	-4.0052024853	3.7016298222
H	1.0	-0.0373379598	-1.9219165581	3.8173253148
H	1.0	0.5294193407	-2.6561406380	2.3220886373
H	1.0	-0.1698429658	-3.6659151704	3.5683687173
H	1.0	-1.2921803838	-4.3729055226	1.4432181190
H	1.0	-1.1616790286	-2.9435560354	0.4220267505
H	1.0	-2.7380233231	-3.5648140945	0.8853117732
H	1.0	-3.9670708209	-2.0184921480	0.3819224032
H	1.0	-2.8861820807	-0.7952812139	-0.2676362480
H	1.0	-4.5432446138	-0.3837556833	0.1630778413
H	1.0	-4.7794949222	-2.8448667320	3.9763467058
H	1.0	-4.4292721360	-3.1055654277	2.2880926258
H	1.0	1.3078440684	2.4898802658	3.6899021834
H	1.0	1.8754069110	2.3738177161	2.0264841816
H	1.0	2.1737695710	1.0585131311	3.1722641157

synsix3 E= -708.1991978863

C	6.0	0.2268202905	0.1206082688	1.6508170728
C	6.0	-0.0364376002	1.1982026928	2.7054223092
O	8.0	-0.5909957026	0.6129793627	3.9005263627
O	8.0	-0.9840195792	-0.5802276292	1.1912649917
C	6.0	0.7875723754	0.6830707647	0.3456830781
N	7.0	-1.9113122343	-1.0656752977	2.2167850036
C	6.0	-1.6705483437	-2.5367644344	2.4284858672
C	6.0	-3.2773472951	-0.6051107863	1.7797087433
C	6.0	-4.2924753999	-1.1679597273	2.7929084317
C	6.0	-3.2917011468	0.9298408661	1.8811225540
C	6.0	-2.7465751833	-3.0264351457	3.4189379653
C	6.0	-0.2960845829	-2.6915185385	3.1131836804
C	6.0	-1.6560398918	-3.3747774889	1.1373830739
C	6.0	-3.6438861796	-0.9865632250	0.3329769613
C	6.0	-4.1743850391	-2.6860996903	2.9747892705
C	6.0	1.2573223306	1.8784145481	3.1493918153
H	1.0	0.9064785349	-0.5986877700	2.0749158640
H	1.0	-0.7121002946	1.9343519281	2.2897259179
H	1.0	-1.2744718379	-0.0233055881	3.6234952551
H	1.0	0.8336556548	-0.1083272738	-0.3904172236
H	1.0	1.7814424285	1.0849649917	0.4876153085
H	1.0	0.1367010866	1.4618918619	-0.0329853070
H	1.0	-5.2876204034	-0.8939268600	2.4600474489
H	1.0	-4.1216708161	-0.6904811159	3.7527593372
H	1.0	-4.3024606310	1.2925534407	1.7333373964

H	1.0	-2.6568551040	1.3592908151	1.1199578437
H	1.0	-2.9428939720	1.2483053456	2.8540704920
H	1.0	-2.5627430019	-2.5601539746	4.3820170081
H	1.0	-2.6251560478	-4.0971124194	3.5421705549
H	1.0	-0.1685402602	-1.9406136358	3.8801980379
H	1.0	0.5059425267	-2.5978809896	2.3940639086
H	1.0	-0.2273636001	-3.6771250949	3.5600685017
H	1.0	-1.2023190491	-4.3367444809	1.3496573445
H	1.0	-1.0649767995	-2.8658117274	0.3903975888
H	1.0	-2.6420513652	-3.5559674469	0.7398758859
H	1.0	-3.8903493650	-2.0304326884	0.2212488288
H	1.0	-2.8172406921	-0.7487907269	-0.3194660740
H	1.0	-4.5092812704	-0.4079149885	0.0288129057
H	1.0	-4.4241426770	-3.2030658220	2.0570245833
H	1.0	-4.8786328891	-3.0181840586	3.7303647334
H	1.0	1.0298320764	2.5117529012	3.9963432706
H	1.0	1.6923064853	2.4825718546	2.3643961507
H	1.0	1.9737844655	1.1325989829	3.4732872572

synfive5 E= -708.1875708408

C	6.0	0.1327254686	-0.4423541078	0.6874622234
C	6.0	1.0192063835	0.7974932249	0.8031040549
O	8.0	1.3846735932	0.9676869699	2.1883602340
O	8.0	-0.9128062088	-0.1599618480	1.6673303157
C	6.0	-0.4180739055	-0.6862099141	-0.7092950653
N	7.0	-1.9163684652	-1.2075425226	1.8352679533
C	6.0	-1.5089827817	-2.1046093001	2.9857786969
C	6.0	-3.2245512208	-0.4764630626	1.9283395892
C	6.0	-4.3652326913	-1.5297591245	2.0666421555
C	6.0	-3.2702956611	0.5524336909	3.0779201872
C	6.0	-2.7864963973	-2.6692743782	3.6531214197
C	6.0	-0.6312267873	-1.4044084607	4.0375971860
C	6.0	-0.7206664524	-3.2862209457	2.3844492383
C	6.0	-3.4252665172	0.2873881707	0.6098726741
C	6.0	-3.8907633143	-2.8888065972	2.6159952223
C	6.0	2.3294518360	0.6695191611	0.0369078999
H	1.0	0.7062272106	-1.2903690018	1.0206956738
H	1.0	0.4533755348	1.6541320806	0.4524271574
H	1.0	0.5707842345	0.9713484333	2.7092409036
H	1.0	-1.1614928687	-1.4688475312	-0.6709983156
H	1.0	0.3781171694	-0.9950080772	-1.3752382673
H	1.0	-0.8782323721	0.2104641386	-1.1060001499
H	1.0	-4.8303461086	-1.6822560482	1.1002813066
H	1.0	-5.1208814846	-1.1187735897	2.7266419658
H	1.0	-2.4198605737	1.2148455771	3.0056146922
H	1.0	-3.2699907255	0.0846202048	4.0518040155
H	1.0	-4.1777962014	1.1402288714	2.9927079944
H	1.0	-3.1450660703	-1.9927121383	4.4189348681
H	1.0	-2.5259547691	-3.5990583468	4.1450605788
H	1.0	-1.1332338361	-0.5470694550	4.4632982549
H	1.0	0.3055413104	-1.0766471127	3.6128356985
H	1.0	-0.4202145462	-2.1075775367	4.8362335638
H	1.0	-0.4828562373	-4.0035822657	3.1621176220
H	1.0	0.2071748717	-2.9518896614	1.9459968509
H	1.0	-1.3019441721	-3.7778240059	1.6160769049
H	1.0	-3.3475609846	-0.3929970841	-0.2274027408

H	1.0	-2.6839837629	1.0643505417	0.5049551518
H	1.0	-4.4119903006	0.7375229800	0.6028330318
H	1.0	-3.5142401938	-3.5002976635	1.8063616197
H	1.0	-4.7285363446	-3.4151459595	3.0596025054
H	1.0	2.8615901121	-0.2130952791	0.3705739232
H	1.0	2.9451754433	1.5331632047	0.2504408512
H	1.0	2.1647087872	0.6107537683	-1.0311196457

synfive6 E= -708.1917773064

C	6.0	-0.6179169861	-1.0173727254	-0.1175039545
C	6.0	0.0669024582	-1.6148492830	-2.4984574768
O	8.0	-1.7216193955	-2.7323084685	-1.4185523911
O	8.0	-1.3620396296	-1.6973550015	0.9421722635
C	6.0	-0.4361351023	-2.1282211115	-1.1550168928
N	7.0	-1.8974264415	-0.7863713599	1.9646801791
C	6.0	-1.5067033833	-1.4307475009	3.2835234088
C	6.0	-3.3885873396	-0.6902084906	1.6889307503
C	6.0	-4.1135222425	-2.0176152355	1.9820670648
C	6.0	-3.9839356806	0.4740545422	2.5090428513
C	6.0	-2.2787560745	-2.7424122629	3.5231684407
C	6.0	-1.7147470908	-0.4262321014	4.4373276170
C	6.0	-0.0021981849	-1.7518892079	3.2616155723
C	6.0	-3.6197810717	-0.3253438427	0.2090510117
C	6.0	-3.7974729961	-2.5769879960	3.3758495088
C	6.0	0.6928437084	-0.4061065412	0.3577145217
H	1.0	-1.2405069594	-0.2491664752	-0.5387238518
H	1.0	0.0738671175	-2.4334314290	-3.2058793304
H	1.0	1.0667102527	-1.2077419575	-2.4229732385
H	1.0	-0.6070609592	-0.8534131354	-2.8713525270
H	1.0	-2.0940400242	-3.0040794208	-0.5692853020
H	1.0	0.2473798161	-2.8673229349	-0.7501551403
H	1.0	-3.8046968847	-2.7472206475	1.2422721995
H	1.0	-5.1807696281	-1.8615263481	1.8636303968
H	1.0	-3.3349404372	1.3372468207	2.4348371696
H	1.0	-4.1346163330	0.2396488651	3.5486369207
H	1.0	-4.9500841203	0.7318765172	2.0912122045
H	1.0	-2.0283780195	-3.1153292970	4.5110688105
H	1.0	-1.9384350810	-3.4707527353	2.7960015634
H	1.0	-2.7390273510	-0.3391332156	4.7566075579
H	1.0	-1.3560988554	0.5499006663	4.1377101873
H	1.0	-1.1369102404	-0.7583833608	5.2919076426
H	1.0	0.2648898408	-2.2187832834	4.2029041302
H	1.0	0.5782186930	-0.8456592423	3.1555202437
H	1.0	0.2354290199	-2.4249438158	2.4563540658
H	1.0	-3.2420609170	-1.0784015597	-0.4616880609
H	1.0	-3.1566016578	0.6269636668	-0.0200057681
H	1.0	-4.6871769244	-0.2256679897	0.0467840988
H	1.0	-4.2817450273	-3.5405064930	3.4985029830
H	1.0	-4.1898555439	-1.9264390273	4.1481550989
H	1.0	0.4973645422	0.2822294670	1.1668466606
H	1.0	1.1544332253	0.1441175639	-0.4532405803
H	1.0	1.3832279086	-1.1660946119	0.7003793911

synsix4 E= -708.1991976437

C	6.0	-0.2962987749	-0.8600936712	0.1878641397
C	6.0	0.8299598177	-2.5834804990	-1.2814620039
O	8.0	-0.9242899110	-3.2215570784	0.1664960245
O	8.0	-0.9361823600	-0.5363720774	1.4739131442
C	6.0	0.1872540145	-2.3078681569	0.0768954999
N	7.0	-1.9515500536	-1.4671846457	1.9736920632
C	6.0	-1.5892062675	-1.7293420125	3.4121897749
C	6.0	-3.3144274603	-0.9126887625	1.6540188985
C	6.0	-4.3443540083	-1.8579050666	2.3056704612
C	6.0	-3.5265297356	0.5499397479	2.0841261845
C	6.0	-2.6838530443	-2.6420680074	3.9976920911
C	6.0	-1.3932407861	-0.4584350862	4.2602354751
C	6.0	-0.2609040516	-2.5053843968	3.4106711449
C	6.0	-3.5046822267	-0.9925768457	0.1245095502
C	6.0	-4.0970291242	-2.0791140389	3.8028980820
C	6.0	0.8408450387	0.1583949522	0.1292230171
H	1.0	-1.0013997852	-0.6847869654	-0.6066097843
H	1.0	1.0067873034	-3.6478688021	-1.3589357149
H	1.0	1.7690264560	-2.0603579708	-1.4038260201
H	1.0	0.1496258571	-2.2994974668	-2.0757201433
H	1.0	-1.4941246947	-2.9170744130	0.8953696156
H	1.0	0.9037815866	-2.4970241773	0.8656051957
H	1.0	-4.2951944402	-2.8178430955	1.8009434423
H	1.0	-5.3324739992	-1.4450724454	2.1341256608
H	1.0	-2.6623677775	1.1322943239	1.8003368127
H	1.0	-3.6895804861	0.6593839038	3.1445821028
H	1.0	-4.3985932960	0.9423999134	1.5723504933
H	1.0	-2.4686155642	-2.7933757825	5.0498341225
H	1.0	-2.6258324285	-3.6081931004	3.5060363506
H	1.0	-0.7720639627	0.2397754324	3.7196540200
H	1.0	-0.8944420518	-0.7297740438	5.1842586613
H	1.0	-2.3223561760	0.0246486145	4.5175737144
H	1.0	-0.0471134973	-2.8580496296	4.4131429306
H	1.0	0.5462399982	-1.8619326997	3.0923148239
H	1.0	-0.3199556201	-3.3552436662	2.7443852944
H	1.0	-3.1284520495	-1.9320094173	-0.2552865893
H	1.0	-2.9888472975	-0.1819378323	-0.3712871734
H	1.0	-4.5598165071	-0.9066636612	-0.1100838118
H	1.0	-4.8259505134	-2.7826174491	4.1914282072
H	1.0	-4.2212510876	-1.1550202180	4.3529654033
H	1.0	1.5847261389	-0.0719703748	0.8823728930
H	1.0	0.4450628451	1.1441409368	0.3340114361
H	1.0	1.3091599829	0.1663057314	-0.8454754904

synsix5 E= -708.1991973722

C	6.0	-0.4159866824	-0.8934707238	0.0706973313
C	6.0	0.6111764180	-2.6361456433	-1.4479321321
O	8.0	-1.0793581302	-3.2454615180	0.0857550208
O	8.0	-0.9888373857	-0.5585672239	1.3851659336
C	6.0	0.0399517761	-2.3486988984	-0.0606682704
N	7.0	-1.9910268540	-1.4745102459	1.9364261993
C	6.0	-1.5628908098	-1.7372383443	3.3567110791
C	6.0	-3.3603764511	-0.9030933459	1.6807968515
C	6.0	-4.3696472279	-1.8331546234	2.3844941561
C	6.0	-3.5327891811	0.5634503886	2.1155580480
C	6.0	-2.6395112026	-2.6339075131	3.9975569026

C	6.0	-1.3091908195	-0.4664659148	4.1896363010
C	6.0	-0.2464550876	-2.5306112852	3.2932354009
C	6.0	-3.6250309708	-0.9850645504	0.1624667588
C	6.0	-4.0531889431	-2.0535200787	3.8687280825
C	6.0	0.7325782897	0.1075467389	-0.0437233441
H	1.0	-1.1552504737	-0.7081068537	-0.6897562470
H	1.0	0.7698039783	-3.7029717294	-1.5309644112
H	1.0	1.5501541128	-2.1262315217	-1.6174496883
H	1.0	-0.1034020670	-2.3445636657	-2.2087269260
H	1.0	-1.6073751264	-2.9315177322	0.8417234126
H	1.0	0.7915190030	-2.5473650354	0.6922248606
H	1.0	-4.3573947739	-2.7949015855	1.8808560046
H	1.0	-5.3595988588	-1.4080766261	2.2595873218
H	1.0	-2.6752388554	1.1334351124	1.7896600894
H	1.0	-3.6444858470	0.6779793107	3.1820922853
H	1.0	-4.4226210971	0.9660747990	1.6439075292
H	1.0	-2.3759895190	-2.7845526912	5.0387420301
H	1.0	-2.6174399497	-3.6023317478	3.5074625283
H	1.0	-0.7043292064	0.2209662552	3.6178108539
H	1.0	-0.7716358967	-0.7420892451	5.0903095121
H	1.0	-2.2183446500	0.0306292967	4.4883274079
H	1.0	0.0129223503	-2.8808110260	4.2857630806
H	1.0	0.5518586391	-1.8993340902	2.9311628414
H	1.0	-0.3495476980	-3.3830141401	2.6355463717
H	1.0	-3.2793795016	-1.9302915722	-0.2316158624
H	1.0	-3.1233874990	-0.1825741374	-0.3605081028
H	1.0	-4.6890623272	-0.8861601470	-0.0214943376
H	1.0	-4.7715066818	-2.7463412768	4.2943362377
H	1.0	-4.1389022324	-1.1263504119	4.4210006393
H	1.0	1.5081377810	-0.1334856257	0.6731979853
H	1.0	0.3618198406	1.0993891226	0.1778145756
H	1.0	1.1540398182	0.1075197464	-1.0396943108

antiopen1 E= -708.1832947861

C	6.0	0.1643026992	-0.5431767573	0.5962227643
C	6.0	0.8342873199	0.7819671797	0.2139839794
O	8.0	1.8037232394	0.5366248824	-0.8307291424
O	8.0	-0.7807067319	-0.1644370983	1.6331366891
C	6.0	-0.4602539372	-1.2204175448	-0.6168063537
N	7.0	-1.7682441835	-1.1779783617	1.9962598103
C	6.0	-1.2820349879	-1.9198327967	3.2185284857
C	6.0	-3.0737010265	-0.4422181327	2.0795859533
C	6.0	-4.1935604001	-1.4747324406	2.4172388038
C	6.0	-3.0586299884	0.7191081459	3.0954992164
C	6.0	-2.5105625230	-2.4372329228	4.0054683240
C	6.0	-0.3804267045	-1.0816103789	4.1405789054
C	6.0	-0.4829548519	-3.1386130855	2.7156853708
C	6.0	-3.3623068430	0.1508304315	0.6918315189
C	6.0	-3.6619724782	-2.7722057716	3.0540186868
C	6.0	1.4772473041	1.4810943232	1.4111776272
H	1.0	0.9181536699	-1.1927141113	1.0227017360
H	1.0	0.0876577228	1.4213409531	-0.2297402902
H	1.0	2.6073931825	0.1534236808	-0.4528573469
H	1.0	-0.9634551136	-2.1314002547	-0.3298557774
H	1.0	0.3236017952	-1.4357483647	-1.3285043258
H	1.0	-1.1769129110	-0.5616402698	-1.0882853044

H	1.0	-4.8928106012	-1.0021560379	3.0981416124
H	1.0	-4.7387336497	-1.7204516434	1.5141275166
H	1.0	-2.2109292712	1.3595725683	2.8991154857
H	1.0	-3.0084980381	0.3712927005	4.1176608825
H	1.0	-3.9691208134	1.2987435302	2.9872679802
H	1.0	-2.2061635096	-3.3094005903	4.5724359894
H	1.0	-2.8442226448	-1.6925204606	4.7182213214
H	1.0	-0.8744118983	-0.1790740747	4.4671941190
H	1.0	0.5340531693	-0.8037441194	3.6390608190
H	1.0	-0.1300111020	-1.6745792274	5.0141045572
H	1.0	-0.1476426936	-3.7337449234	3.5581511133
H	1.0	0.3872230100	-2.8266206744	2.1570882134
H	1.0	-1.0960924351	-3.7546066432	2.0714310456
H	1.0	-3.3315995136	-0.6301335700	-0.0556648934
H	1.0	-2.6351558505	0.9084806259	0.4434399039
H	1.0	-4.3507744843	0.5971275440	0.6909406002
H	1.0	-3.3147883533	-3.4453715177	2.2810441167
H	1.0	-4.4632876899	-3.2713445537	3.5875128093
H	1.0	1.9571611605	2.3967470822	1.0880576454
H	1.0	2.2284996291	0.8390630916	1.8649103811
H	1.0	0.7283413272	1.7046295881	2.1551894504

antiopen2 E= -708.1895383357

C	6.0	-0.0159987528	-1.4347649381	0.4841530269
C	6.0	1.3355207421	-0.7263523807	0.5626892153
O	8.0	0.4412736501	-2.2405181952	-1.6642112467
O	8.0	-0.9260532851	-0.7068484589	1.3607764685
C	6.0	-0.5515827071	-1.4649973547	-0.9478757334
N	7.0	-1.8396710327	-1.5523879659	2.1386254759
C	6.0	-1.2794536656	-1.6663746731	3.5318099940
C	6.0	-3.2125384812	-0.9643224248	1.9649296916
C	6.0	-4.1768973201	-1.7255523775	2.8970204584
C	6.0	-3.2953813939	0.5571915682	2.2012189987
C	6.0	-2.3238045202	-2.3949693358	4.4032027024
C	6.0	-0.8570136402	-0.3264245660	4.1639773527
C	6.0	-0.0394638460	-2.5788181723	3.4686275643
C	6.0	-3.6561089162	-1.2473912617	0.5207186102
C	6.0	-3.7095887943	-1.7466656568	4.3547260389
C	6.0	-0.7204511681	-0.0775224196	-1.5666228285
H	1.0	0.0674735589	-2.4536759044	0.8164933579
H	1.0	1.9991567051	-1.1427254823	-0.1803330373
H	1.0	1.7728565107	-0.8485304141	1.5443888986
H	1.0	1.2094059473	0.3336045297	0.3860605267
H	1.0	0.1919653801	-2.3423092967	-2.5918435652
H	1.0	-1.4952384454	-1.9897108410	-0.9492335420
H	1.0	-4.2542657216	-2.7498254351	2.5465032909
H	1.0	-5.1567339379	-1.2689718587	2.8078690500
H	1.0	-2.4887119456	1.0463935303	1.6767411477
H	1.0	-3.2404523670	0.8222312241	3.2455459103
H	1.0	-4.2413229544	0.9225582330	1.8159084907
H	1.0	-1.9440409939	-2.4288456320	5.4186307676
H	1.0	-2.4115691917	-3.4168308638	4.0480093531
H	1.0	-1.6984425640	0.2674868069	4.4858229537
H	1.0	-0.2855190293	0.2416478000	3.4459189557
H	1.0	-0.2388199290	-0.5237579286	5.0331667648
H	1.0	0.2646535989	-2.8406334194	4.4763580079

H	1.0	0.7912641208	-2.0840922748	2.9898357595
H	1.0	-0.2756693941	-3.4860463306	2.9279331852
H	1.0	-3.5006211005	-2.2932222393	0.2890895298
H	1.0	-3.1022014651	-0.6399466203	-0.1769271173
H	1.0	-4.7098646346	-1.0151161943	0.4116950752
H	1.0	-3.6840122191	-0.7464030461	4.7677513584
H	1.0	-4.4054355063	-2.3239574577	4.9548645895
H	1.0	-1.2641552454	0.5689648235	-0.8924763049
H	1.0	-1.2625154170	-0.1346483967	-2.5059778853
H	1.0	0.2514093712	0.3550313013	-1.7626513104

antiopen3 E= -708.1849376606

C	6.0	0.2158060342	-0.8457287841	0.4666182925
C	6.0	0.2293058240	0.5823362629	-0.0624733533
O	8.0	1.7602654238	-1.5805998880	-1.2635537179
O	8.0	-1.0425182808	-1.2879292520	1.0462202075
C	6.0	0.5002945636	-1.8898586707	-0.6234823617
N	7.0	-1.3706687782	-0.6146808913	2.3146862286
C	6.0	-1.1598764142	-1.6666515247	3.3884221348
C	6.0	-2.8016740843	-0.1398122123	2.1348083043
C	6.0	-3.7852096235	-1.3230107921	2.0544486553
C	6.0	-3.1745097643	0.8383392881	3.2698999455
C	6.0	-2.1828865041	-2.8112437594	3.2708618426
C	6.0	-1.1980035273	-1.0015768167	4.7813346109
C	6.0	0.2528249725	-2.2619773530	3.2464785494
C	6.0	-2.9038296656	0.6661348944	0.8295437509
C	6.0	-3.6324112734	-2.3085266125	3.2214811403
C	6.0	-0.5481035616	-1.9243006132	-1.7256963890
H	1.0	0.9883911595	-0.9256594903	1.2156650164
H	1.0	-0.5429645174	0.7473920129	-0.7979452531
H	1.0	1.1898507831	0.7544918943	-0.5285978135
H	1.0	0.0931069540	1.2816840426	0.7508418838
H	1.0	2.5013057531	-1.7618665737	-0.6698195971
H	1.0	0.5427299246	-2.8627888988	-0.1463814470
H	1.0	-3.5956937602	-1.8542464245	1.1291676695
H	1.0	-4.7961876584	-0.9302213864	2.0145520453
H	1.0	-2.3561593157	1.5262028939	3.4395032698
H	1.0	-3.4214481236	0.3528073126	4.1981232213
H	1.0	-4.0439987187	1.4072467008	2.9617964101
H	1.0	-2.0405574155	-3.4932486730	4.1032432243
H	1.0	-1.9760888414	-3.3508131641	2.3541282177
H	1.0	-2.1932241658	-0.7961552895	5.1350369946
H	1.0	-0.6361173129	-0.0766749462	4.7571440618
H	1.0	-0.7327310583	-1.6696211698	5.4969316473
H	1.0	0.4106686366	-2.9740365377	4.0482779557
H	1.0	1.0026802962	-1.4850917812	3.3295323812
H	1.0	0.3654979172	-2.7796814779	2.3078218375
H	1.0	-2.6439685585	0.0595384997	-0.0199212757
H	1.0	-2.2537715770	1.5294057955	0.8661240757
H	1.0	-3.9252423837	1.0114725103	0.7154877153
H	1.0	-3.9101812349	-1.8415352067	4.1588143933
H	1.0	-4.3030368811	-3.1493897419	3.0765111876
H	1.0	-1.5267564150	-2.0813006121	-1.2958786313
H	1.0	-0.3214388923	-2.7275435329	-2.4153674055
H	1.0	-0.5352499345	-0.9954900313	-2.2790196256

antiopen4 E= -708.1888912904

C	6.0	-0.0129400433	-1.5174102619	0.5195465921
C	6.0	1.3459383912	-0.8246782895	0.6094054891
O	8.0	0.4366372564	-2.2678363793	-1.7323486928
O	8.0	-0.9248432171	-0.7791180481	1.3842709762
C	6.0	-0.5276980451	-1.5460379236	-0.9242758745
N	7.0	-1.8585438363	-1.6134526955	2.1503669746
C	6.0	-1.3233340579	-1.7202775745	3.5541717507
C	6.0	-3.2242878510	-1.0152818594	1.9497941926
C	6.0	-4.2093536834	-1.7652589486	2.8691773725
C	6.0	-3.2987359357	0.5078549288	2.1774856852
C	6.0	-2.3864928922	-2.4375737329	4.4119511553
C	6.0	-0.9043973395	-0.3783553649	4.1845508313
C	6.0	-0.0866190163	-2.6385892479	3.5184781891
C	6.0	-3.6450385395	-1.3002903788	0.4993267577
C	6.0	-3.7674281575	-1.7814974097	4.3349646999
C	6.0	-0.6566073803	-0.1645417208	-1.5517307154
H	1.0	0.0552882890	-2.5338467294	0.8729677584
H	1.0	1.7909009954	-0.9722614535	1.5842623235
H	1.0	1.2251951552	0.2391863360	0.4563916251
H	1.0	2.0012471967	-1.2240829128	-0.1507520127
H	1.0	0.3941731316	-3.2162292176	-1.5504280959
H	1.0	-1.4803444452	-2.0543249632	-0.9452545626
H	1.0	-4.2879003686	-2.7908883766	2.5226148900
H	1.0	-5.1844742542	-1.3028931882	2.7608534725
H	1.0	-2.4808178478	0.9880804689	1.6622991684
H	1.0	-3.2576880628	0.7781908567	3.2210040763
H	1.0	-4.2357593670	0.8783087491	1.7757205736
H	1.0	-2.0247535691	-2.4669708310	5.4340713105
H	1.0	-2.4741823050	-3.4612722198	4.0618736131
H	1.0	-1.7477696706	0.2204227318	4.4915382863
H	1.0	-0.3207507993	0.1833758425	3.4712570851
H	1.0	-0.2989959103	-0.5730764846	5.0632384569
H	1.0	0.2024843688	-2.8908521833	4.5329747182
H	1.0	0.7524055169	-2.1515902468	3.0459645513
H	1.0	-0.3197053860	-3.5513087450	2.9853420130
H	1.0	-3.4966454252	-2.3487286015	0.2741048546
H	1.0	-3.0736092177	-0.7009326556	-0.1911381068
H	1.0	-4.6945277581	-1.0589839281	0.3711293854
H	1.0	-4.4771601193	-2.3509950020	4.9261873178
H	1.0	-3.7430102130	-0.7790871383	4.7427191668
H	1.0	-1.1762587193	-0.2334368532	-2.4993296448
H	1.0	0.3289754694	0.2374496250	-1.7406385839
H	1.0	-1.1948423369	0.5007720269	-0.8914890240

antiopen5 E= -708.1807003759

C	6.0	-0.1857079271	-1.6779546397	0.5564294858
C	6.0	1.2606753539	-1.2135524604	0.7280782686
O	8.0	0.2933152693	-2.4051930302	-1.7073600766
O	8.0	-1.0506990558	-0.8186441749	1.3578671316
C	6.0	-0.6169267637	-1.6014001576	-0.9157190638
N	7.0	-1.9351677043	-1.5442835579	2.2717413544
C	6.0	-1.3454844511	-1.4648424061	3.6609715611
C	6.0	-3.3172305492	-1.0021415356	2.0629637152

C	6.0	-4.2928581579	-1.8111872745	2.9755136309
C	6.0	-3.4320285258	0.5145436146	2.3192718444
C	6.0	-2.4855543372	-1.6357912089	4.6941555411
C	6.0	-0.5718413018	-0.1658787232	3.9452215017
C	6.0	-0.3825045835	-2.6594317938	3.8022844435
C	6.0	-3.7110482825	-1.2622045546	0.6018231924
C	6.0	-3.5906454434	-2.5355184319	4.1374124408
C	6.0	-0.5534755876	-0.1919159648	-1.4881610796
H	1.0	-0.3074230189	-2.6940448877	0.9006279601
H	1.0	1.6388019888	-1.4628243036	1.7102938380
H	1.0	1.3145506228	-0.1395101702	0.6112763801
H	1.0	1.8766904385	-1.6854167916	-0.0231974154
H	1.0	0.1342926511	-3.3473460902	-1.5601258676
H	1.0	-1.6218636064	-1.9872497831	-1.0050079197
H	1.0	-4.8254361778	-2.5382550291	2.3744423251
H	1.0	-5.0285413422	-1.1221040685	3.3752866661
H	1.0	-4.3992804156	0.8638402803	1.9737400424
H	1.0	-2.6560378425	1.0309171821	1.7720260393
H	1.0	-3.3476215023	0.7616880057	3.3678847286
H	1.0	-2.0614776876	-2.0504914706	5.6011747640
H	1.0	-2.9098708990	-0.6722642687	4.9509393727
H	1.0	-1.2008215007	0.7046750752	3.8358842635
H	1.0	0.2653540050	-0.0625260632	3.2744389713
H	1.0	-0.2039577364	-0.1978555564	4.9656174924
H	1.0	0.0374039452	-2.6795592777	4.8019573370
H	1.0	0.4323902864	-2.5832313561	3.0983732432
H	1.0	-0.9051205301	-3.5894806838	3.6207624693
H	1.0	-3.5334620857	-2.3016729115	0.3551103849
H	1.0	-3.1480645108	-0.6317749620	-0.0672520236
H	1.0	-4.7661635957	-1.0486995462	0.4714637751
H	1.0	-4.3139969903	-2.7742926333	4.9091387995
H	1.0	-3.1648883016	-3.4668408705	3.7870118671
H	1.0	-0.9955041518	-0.1743544656	-2.4764990013
H	1.0	0.4784564340	0.1174993805	-1.5784689700
H	1.0	-1.0804164284	0.4962715647	-0.8423834139

antiopen6 E= -708.1911739112

C	6.0	0.1015378547	-0.7511165341	0.6536538871
C	6.0	0.8594882057	0.5154438502	0.2373820616
O	8.0	1.7681311774	0.1898833392	-0.8396382548
O	8.0	-0.7773561259	-0.2881875046	1.7193146423
C	6.0	-0.5971543677	-1.3975246998	-0.5364545625
N	7.0	-1.8664695850	-1.1853091325	2.1008872326
C	6.0	-1.4800645401	-1.8909338849	3.3690743324
C	6.0	-3.1091318412	-0.3397468664	2.0948933039
C	6.0	-4.2703951282	-1.2252114984	2.5869770557
C	6.0	-3.0067461097	0.9616656945	2.9163066282
C	6.0	-2.7018458464	-2.7201581682	3.8154961202
C	6.0	-0.9756201785	-0.9735797524	4.5000189302
C	6.0	-0.3510961975	-2.8826177135	3.0282159198
C	6.0	-3.3917536990	0.0500447457	0.6356519583
C	6.0	-3.9825877771	-1.8870126053	3.9394613240
C	6.0	1.6002572463	1.1663495146	1.4052198273
H	1.0	0.8134716828	-1.4528034966	1.0642538885
H	1.0	0.1505825026	1.2106706081	-0.1838211926
H	1.0	2.5492689233	-0.2599733383	-0.4888418242

H	1.0	-1.1937787589	-2.2388954731	-0.2176057068
H	1.0	0.1598142794	-1.7230747674	-1.2353679563
H	1.0	-1.2369775993	-0.6871598080	-1.0408838060
H	1.0	-4.4393805892	-2.0051181612	1.8516022180
H	1.0	-5.1649021677	-0.6136450051	2.6356541609
H	1.0	-3.8439527458	1.6028425841	2.6629628314
H	1.0	-2.0885810358	1.4717083195	2.6668141998
H	1.0	-3.0337899993	0.7920530200	3.9809140049
H	1.0	-2.4572615890	-3.1981074825	4.7580453860
H	1.0	-2.8696283929	-3.5004879114	3.0801646916
H	1.0	-1.7701221098	-0.4331159378	4.9897100852
H	1.0	-0.2687307875	-0.2642863778	4.0959232201
H	1.0	-0.4765633587	-1.5787300523	5.2494309384
H	1.0	-0.2226960951	-3.5792657287	3.8495793925
H	1.0	0.5874978587	-2.3686674335	2.8792314656
H	1.0	-0.6018053523	-3.4372555909	2.1335224922
H	1.0	-3.4325260977	-0.8341254767	0.0148651799
H	1.0	-2.6181823834	0.7066768030	0.2660377428
H	1.0	-4.3434118613	0.5663744449	0.5757182651
H	1.0	-4.8110534852	-2.5314153560	4.2150412922
H	1.0	-3.8840737212	-1.1426631903	4.7193910376
H	1.0	0.8996224063	1.4611394436	2.1709499743
H	1.0	2.1455610592	2.0345541477	1.0560144447
H	1.0	2.3085263300	0.4657624324	1.8408831681

antisix1 E= -708.1894604087

C	6.0	0.1437963370	0.1252163252	1.6346001390
C	6.0	0.0729395637	1.1769647263	2.7578035695
O	8.0	-0.6482696417	0.6613119650	3.8953312348
O	8.0	-1.1361508536	-0.4436895981	1.1945626755
C	6.0	0.7454390082	0.6664797658	0.3391586016
N	7.0	-2.0183944300	-1.0229319443	2.2217429742
C	6.0	-1.6768626799	-2.4804212593	2.4409677646
C	6.0	-3.4119629219	-0.6803424008	1.7499034260
C	6.0	-4.4092246346	-1.3202029862	2.7332429551
C	6.0	-3.5608288506	0.8452344823	1.8428890578
C	6.0	-2.7540731379	-3.0568665321	3.3868070370
C	6.0	-0.3330652056	-2.5692016381	3.2045580191
C	6.0	-1.5508094703	-3.3054008106	1.1482246489
C	6.0	-3.7114122613	-1.0919727487	0.2949111922
C	6.0	-4.1883760507	-2.8256858385	2.9041197812
C	6.0	-0.4651853712	2.5523655656	2.3494526590
H	1.0	0.7602516245	-0.6743230219	1.9991073118
H	1.0	1.0956946651	1.3120846401	3.0869180627
H	1.0	-1.3759740799	0.1024732715	3.5666051305
H	1.0	0.8680680917	-0.1428418456	-0.3684748849
H	1.0	1.7132953391	1.1165075983	0.5276606042
H	1.0	0.0880096959	1.4042246618	-0.0990596571
H	1.0	-5.4114830544	-1.1114501626	2.3754596439
H	1.0	-4.2959375213	-0.8404711209	3.7004470116
H	1.0	-2.9660246848	1.3223061683	1.0803404962
H	1.0	-3.2431084827	1.1990206576	2.8145830772
H	1.0	-4.5995917446	1.1167699506	1.6930582585
H	1.0	-2.6369870281	-2.5877426452	4.3588325048
H	1.0	-2.5523406386	-4.1157160844	3.5060291832
H	1.0	-0.2502369181	-1.7635533322	3.9187510107

H	1.0	0.5100195446	-2.5325050362	2.5290507038
H	1.0	-0.2862534375	-3.5188844926	3.7259911312
H	1.0	-1.0363006291	-4.2331419316	1.3736013791
H	1.0	-0.9716325793	-2.7500630797	0.4248271965
H	1.0	-2.5048357834	-3.5545871513	0.7115830783
H	1.0	-3.8716185163	-2.1518598606	0.1791862474
H	1.0	-2.8928328423	-0.7886209774	-0.3397082220
H	1.0	-4.6136445935	-0.5846844160	-0.0292315476
H	1.0	-4.3727295355	-3.3503286982	1.9753731367
H	1.0	-4.8856385956	-3.2178361081	3.6371414084
H	1.0	-0.5956860624	3.1372539126	3.2508062362
H	1.0	-1.4167430876	2.4794706940	1.8488146731
H	1.0	0.2314714545	3.0683713361	1.7002910901

antisix2 E= -708.1894606350

C	6.0	0.1894179140	0.0863260979	1.8598570542
C	6.0	0.0764392911	1.0643815078	3.0447339878
O	8.0	-0.7030460357	0.4861985151	4.1116408071
O	8.0	-1.0740418657	-0.4359687407	1.3247359352
C	6.0	0.8568625374	0.7019898907	0.6315858820
N	7.0	-2.0093803775	-1.0692305590	2.2697134329
C	6.0	-1.6932418885	-2.5422491881	2.4081370634
C	6.0	-3.3755226292	-0.6781971129	1.7574503899
C	6.0	-4.4245506644	-1.3680861256	2.6487922753
C	6.0	-3.5129852411	0.8399060043	1.9446259296
C	6.0	-2.8195820829	-3.1650497192	3.2628918206
C	6.0	-0.3878674989	-2.6980459720	3.2258052501
C	6.0	-1.5149513639	-3.2825426231	1.0710461385
C	6.0	-3.6097071664	-0.9891000290	0.2659254846
C	6.0	-4.2268998297	-2.8842728240	2.7299348408
C	6.0	-0.4270232746	2.4705657484	2.7023637000
H	1.0	0.7798994924	-0.7431993137	2.1995740108
H	1.0	1.0837612789	1.1637894147	3.4294752400
H	1.0	-1.4201925051	-0.0405519758	3.7142702916
H	1.0	1.8190873234	1.1267881267	0.8933238710
H	1.0	0.2281247363	1.4746487013	0.2118473382
H	1.0	1.0047722284	-0.0618067653	-0.1204265334
H	1.0	-5.4066210789	-1.1233433023	2.2592556919
H	1.0	-4.3524598899	-0.9543435290	3.6498318555
H	1.0	-3.2385601939	1.1246240109	2.9515424916
H	1.0	-4.5404658178	1.1348330561	1.7642562923
H	1.0	-2.8774433756	1.3581030658	1.2443145305
H	1.0	-2.7440239159	-2.7617936337	4.2680041696
H	1.0	-2.6342511058	-4.2319622753	3.3214543344
H	1.0	-0.3306121049	-1.9412919386	3.9939614704
H	1.0	0.4865353732	-2.6290991834	2.5940307244
H	1.0	-0.3754779098	-3.6798938754	3.6860529566
H	1.0	-1.0209831154	-4.2297396601	1.2582969050
H	1.0	-0.8970824723	-2.6888013125	0.4131538523
H	1.0	-2.4499830044	-3.4901896509	0.5755723040
H	1.0	-3.7748062095	-2.0368996109	0.0727889079
H	1.0	-2.7588603987	-0.6553777520	-0.3080343206
H	1.0	-4.4903906777	-0.4498300882	-0.0656889821
H	1.0	-4.9621463302	-3.3146055475	3.4018778497
H	1.0	-4.3719698487	-3.3443740450	1.7608877382
H	1.0	-0.5950657667	2.9972336307	3.6330171695

H	1.0	-1.3537937943	2.4436253926	2.1527765043
H	1.0	0.3059992588	3.0180431899	2.1227833441

antisix3 E= -708.1894599586

C	6.0	-0.2271777958	-1.5144857094	0.3192993642
C	6.0	1.0059173559	-0.6737960514	-0.0067681083
O	8.0	-1.1324543790	-3.7768865289	0.6169256480
O	8.0	-0.5883500363	-1.0650511996	1.6696247550
C	6.0	0.0046539654	-3.0270883559	0.1425179981
N	7.0	-1.7317805249	-1.7194733566	2.3279160207
C	6.0	-1.3365403661	-1.7791037051	3.7848907319
C	6.0	-3.0180965332	-1.0099252878	1.9656329414
C	6.0	-4.1348253264	-1.6351784806	2.8309439148
C	6.0	-2.9653024156	0.5202527469	2.1192991508
C	6.0	-2.5180265118	-2.3835710481	4.5656467270
C	6.0	-0.8980615415	-0.4272712808	4.3819245923
C	6.0	-0.1471510427	-2.7444934017	3.8939040034
C	6.0	-3.3713728191	-1.3367237604	0.4941741931
C	6.0	-3.8300915224	-1.6297433623	4.3312039767
C	6.0	1.3054961953	-3.5764738872	0.7373810007
H	1.0	-1.0219582550	-1.2438419777	-0.3496018410
H	1.0	1.7865708272	-0.8578835550	0.7179625967
H	1.0	0.7478607864	0.3763839965	0.0306206353
H	1.0	1.3754542670	-0.9083572344	-0.9984412851
H	1.0	-1.4865696090	-3.3263880880	1.4051756315
H	1.0	0.0429905852	-3.1866619716	-0.9278230258
H	1.0	-4.2757306139	-2.6628852613	2.5106740539
H	1.0	-5.0521713555	-1.0962789794	2.6208621343
H	1.0	-2.0427782361	0.8905798941	1.6962601106
H	1.0	-3.0310994193	0.8440725415	3.1458605297
H	1.0	-3.7995987768	0.9553299070	1.5799935700
H	1.0	-2.2549099056	-2.3896203423	5.6177216979
H	1.0	-2.6485940176	-3.4141786748	4.2506664625
H	1.0	-1.7242431748	0.2376759050	4.5762707450
H	1.0	-0.2084925692	0.0563457190	3.7070626709
H	1.0	-0.3949543752	-0.6126037720	5.3247867263
H	1.0	0.0494715532	-2.9592396728	4.9381718605
H	1.0	0.7335624129	-2.2967585412	3.4617459686
H	1.0	-0.3629181277	-3.6720040317	3.3805409391
H	1.0	-3.0944777838	-2.3527000852	0.2556793071
H	1.0	-2.8757728583	-0.6638252060	-0.1914538824
H	1.0	-4.4391378936	-1.2114385992	0.3521455114
H	1.0	-4.6359434097	-2.1203537182	4.8670808226
H	1.0	-3.7659339747	-0.6171647484	4.7085646365
H	1.0	1.4229478967	-3.3005284099	1.7726373400
H	1.0	2.1675956767	-3.2262116924	0.1831173585
H	1.0	1.2685036485	-4.6562907330	0.6719918156

antifive1 E= -708.1949416076

C	6.0	-0.1049651646	-0.9073420672	0.3992994762
C	6.0	1.1918006189	-0.1219669437	0.6213335746
O	8.0	1.6828327967	-0.3938542997	1.9542858233
O	8.0	-1.0074376831	-0.4041666443	1.4336853698
C	6.0	-0.6426728002	-0.7649671446	-1.0203417813
N	7.0	-2.0558894913	-1.3528645574	1.8241650483

C	6.0	-1.6607069165	-1.9718421966	3.1392194698
C	6.0	-3.3597869571	-0.6069056855	1.7562086998
C	6.0	-4.4629024131	-1.5676599478	2.2446272893
C	6.0	-3.3839559356	0.7251949854	2.5331340913
C	6.0	-2.8211319530	-2.8922038316	3.5683329055
C	6.0	-1.3106655025	-0.9669592507	4.2575718530
C	6.0	-0.4261455453	-2.8636430351	2.9006339063
C	6.0	-3.6414525219	-0.2884873341	0.2805650607
C	6.0	-4.1722011115	-2.1702719555	3.6232013964
C	6.0	1.0262774070	1.3874279416	0.4257002026
H	1.0	0.0960657501	-1.9439877853	0.5970753113
H	1.0	1.9489103156	-0.5064559879	-0.0454356406
H	1.0	1.0276860484	-0.0630805298	2.5819146089
H	1.0	-1.4921285462	-1.4143874318	-1.1696762933
H	1.0	0.1314897717	-1.0526585879	-1.7244706779
H	1.0	-0.9424207704	0.2516621319	-1.2309670492
H	1.0	-4.5474157969	-2.3775363346	1.5273929823
H	1.0	-5.4029932950	-1.0265164059	2.2476319228
H	1.0	-2.4976473586	1.2948846293	2.2955693457
H	1.0	-3.4374146977	0.5912416311	3.6015907464
H	1.0	-4.2556981739	1.2935960908	2.2278873914
H	1.0	-2.5703998437	-3.3208767597	4.5327188187
H	1.0	-2.8919898842	-3.7037438826	2.8516814791
H	1.0	-2.1816131752	-0.5363409355	4.7252931774
H	1.0	-0.7097647069	-0.1649039701	3.8570649626
H	1.0	-0.7414661717	-1.4771255906	5.0263568345
H	1.0	-0.2447173829	-3.4598426419	3.7885290520
H	1.0	0.4557390489	-2.2750880347	2.7003248160
H	1.0	-0.6110078245	-3.5324608304	2.0693893174
H	1.0	-3.5790955910	-1.1906484228	-0.3123574301
H	1.0	-2.9321904751	0.4333252663	-0.0928136169
H	1.0	-4.6395455799	0.1245046494	0.1846030783
H	1.0	-4.9533131808	-2.8767761449	3.8845271965
H	1.0	-4.1694842231	-1.4023374011	4.3862509655
H	1.0	0.8421133058	1.6370238282	-0.6110824720
H	1.0	1.9331753751	1.8846326271	0.7454931021
H	1.0	0.1963802353	1.7440887900	1.0221156855

antifive2 E= -708.1896509227

C	6.0	-0.8043573233	-1.8419346873	-0.1518117905
C	6.0	-0.0299240359	-3.2779602477	-2.1226983001
O	8.0	-0.0584883642	-4.1368680829	0.0972052038
O	8.0	-1.5269494515	-2.1203151042	1.0925941414
C	6.0	0.5728538291	-1.2274396715	0.0573364064
N	7.0	-1.6671209206	-0.9736923304	2.0012060599
C	6.0	-1.1732204987	-1.4924063430	3.3398835634
C	6.0	-3.1352077812	-0.6008805312	1.9365577787
C	6.0	-4.0255678416	-1.7063656368	2.5331577389
C	6.0	-3.3584787546	0.7585526950	2.6323825139
C	6.0	-2.1117064519	-2.5792489775	3.8983168428
C	6.0	-1.0082805076	-0.3211819769	4.3326963046
C	6.0	0.2334631193	-2.0913327867	3.1617832973
C	6.0	-3.5287093286	-0.3937630421	0.4632186273
C	6.0	-3.5810129748	-2.1330907395	3.9398339589
C	6.0	-0.7575324824	-3.2351544882	-0.7857050994
H	1.0	-1.4024140736	-1.1913101549	-0.7677437851

H	1.0	-0.0889077397	-4.2791831013	-2.5290586001
H	1.0	1.0140529599	-3.0341088607	-1.9839184874
H	1.0	-0.4721378001	-2.5848552501	-2.8293646204
H	1.0	-0.5487667525	-4.1812022973	0.9278875150
H	1.0	0.4968342114	-0.3876705638	0.7314257286
H	1.0	0.9575185320	-0.8727461039	-0.8914885656
H	1.0	1.2554170729	-1.9611635358	0.4582280349
H	1.0	-3.9694612576	-2.5689142892	1.8798698089
H	1.0	-5.0538428760	-1.3591304764	2.5441552133
H	1.0	-2.5806949645	1.4504253659	2.3354786697
H	1.0	-3.3785141235	0.6965458972	3.7064614039
H	1.0	-4.3145715737	1.1571773109	2.3137923389
H	1.0	-1.7686152548	-2.8580415116	4.8893665069
H	1.0	-2.0359211236	-3.4529431661	3.2615543858
H	1.0	-1.9317770045	0.0022788490	4.7810460976
H	1.0	-0.5474375976	0.5194679596	3.8301150580
H	1.0	-0.3543747715	-0.6420793514	5.1353615766
H	1.0	0.5561330237	-2.5017287903	4.1121803499
H	1.0	0.9362525362	-1.3231386985	2.8688203421
H	1.0	0.2447852382	-2.8708131483	2.4225536885
H	1.0	-3.4626165170	-1.3161574354	-0.0907241858
H	1.0	-2.8916451974	0.3526533908	0.0046830722
H	1.0	-4.5532054555	-0.0427685891	0.4206919798
H	1.0	-4.2001893462	-2.9565563017	4.2808305499
H	1.0	-3.7158545609	-1.3237851668	4.6472960055
H	1.0	-1.7821758156	-3.5666100297	-0.9150973287

antifive3 E= -708.1857577270

C	6.0	-0.4932193940	-1.1713201812	0.0846169621
C	6.0	0.6381168999	-0.1423743624	0.0161961374
O	8.0	1.2252141309	-0.0060333038	1.3316010821
O	8.0	-1.4428024426	-0.6074784565	1.0392453633
C	6.0	-1.1172559958	-1.4670514160	-1.2744692742
N	7.0	-2.2526755371	-1.6388429152	1.6823086398
C	6.0	-1.8050279157	-1.7457090793	3.1081331490
C	6.0	-3.7303468266	-1.4302172835	1.4042924173
C	6.0	-4.5351523803	-1.1610313751	2.6941389239
C	6.0	-3.9673680146	-0.2463808356	0.4538545585
C	6.0	-2.7965741507	-2.6960110400	3.7975791132
C	6.0	-1.6970539123	-0.4003237734	3.8554214865
C	6.0	-0.4156003533	-2.4111594608	3.1134496706
C	6.0	-4.2431543772	-2.7239878480	0.7440447997
C	6.0	-4.2482879858	-2.1610708289	3.8362828500
C	6.0	0.1815549545	1.2273976015	-0.4928697140
H	1.0	-0.0977681960	-2.0803769783	0.5026544827
H	1.0	1.4269318709	-0.5326922383	-0.6091813373
H	1.0	0.5544318434	0.3660862407	1.9178542036
H	1.0	-1.8752910951	-2.2306287254	-1.1768651499
H	1.0	-0.3538559039	-1.8340209845	-1.9525185634
H	1.0	-1.5681126973	-0.5835607347	-1.7038336277
H	1.0	-5.5877874265	-1.1936379443	2.4360758327
H	1.0	-4.3287295844	-0.1530856255	3.0243487355
H	1.0	-5.0359638959	-0.1328851960	0.3088930273
H	1.0	-3.5084221434	-0.4143016855	-0.5065210934
H	1.0	-3.5676420516	0.6669072538	0.8688692011
H	1.0	-2.4429401939	-2.8852459950	4.8044067995

H	1.0	-2.7662206710	-3.6378318544	3.2631242131
H	1.0	-2.6567533742	0.0441876202	4.0669298425
H	1.0	-1.1259509202	0.2991424752	3.2648894883
H	1.0	-1.1859203043	-0.5580287459	4.7986563398
H	1.0	-0.1205644338	-2.6274955140	4.1346767931
H	1.0	0.3288829253	-1.7667747325	2.6713148432
H	1.0	-0.4545057072	-3.3402343635	2.5583344118
H	1.0	-4.1160561637	-3.5737175432	1.4012464909
H	1.0	-3.6922575670	-2.9192502399	-0.1653108814
H	1.0	-5.2958683346	-2.6284816412	0.5001745427
H	1.0	-4.9329855860	-2.9985338137	3.7749216929
H	1.0	-4.4372829105	-1.6706581503	4.7841497123
H	1.0	-0.6771752889	1.5599756503	0.0760882822
H	1.0	-0.0870256276	1.1946932593	-1.5405349403
H	1.0	0.9894867382	1.9364647649	-0.3651995071

antifive4 E= -708.1857581834

C	6.0	-0.5672795787	-1.7872968847	-0.2193620116
C	6.0	0.6404677517	-0.8763654553	-0.4551318192
O	8.0	1.3132097497	-0.6582095791	0.8072552590
O	8.0	-1.4051217049	-1.0463944840	0.7188214800
C	6.0	-1.2968257935	-2.1606000201	-1.5047184688
N	7.0	-2.2580044405	-1.9297121433	1.5096785182
C	6.0	-1.7339824506	-1.9313301060	2.9134345840
C	6.0	-3.7270557886	-1.6172852756	1.2888442933
C	6.0	-4.4255377426	-1.1480760314	2.5832614899
C	6.0	-3.9208705149	-0.5182254314	0.2326581703
C	6.0	-2.7578824206	-2.7140151515	3.7509587218
C	6.0	-1.4680595801	-0.5322422945	3.5067672002
C	6.0	-0.4075749228	-2.7150520801	2.9168301001
C	6.0	-4.3867990187	-2.9192331014	0.7965907592
C	6.0	-4.1543322578	-2.0496364378	3.8081733916
C	6.0	0.2707257258	0.4688715197	-1.0859231783
H	1.0	-0.2247803344	-2.6815778991	0.2711905135
H	1.0	1.3555208582	-1.3982879544	-1.0732378171
H	1.0	0.7089614377	-0.1747487183	1.3846001822
H	1.0	-2.1092572373	-2.8387719223	-1.2873286918
H	1.0	-0.6106929509	-2.6612581458	-2.1798543568
H	1.0	-1.6970188182	-1.2874116074	-2.0002696588
H	1.0	-5.4909705401	-1.1114674873	2.3856727937
H	1.0	-4.1150635830	-0.1346652785	2.7936679327
H	1.0	-4.9828934423	-0.3237467356	0.1319339298
H	1.0	-3.5367941978	-0.8221103489	-0.7271973428
H	1.0	-3.4210460546	0.3922377806	0.5282506267
H	1.0	-2.3604760674	-2.8311963369	4.7524150177
H	1.0	-2.8394744048	-3.7040465847	3.3188884625
H	1.0	-2.3724707400	0.0147890705	3.7211266201
H	1.0	-0.8788388396	0.0505375662	2.8158163848
H	1.0	-0.9138095420	-0.6386877600	4.4325853084
H	1.0	-0.0703099521	-2.8529430496	3.9385876130
H	1.0	0.3603288270	-2.1881611073	2.3711595966
H	1.0	-0.5581393834	-3.6881920951	2.4660783681
H	1.0	-4.2927432080	-3.7060450302	1.5329575119
H	1.0	-3.9099899924	-3.2545823043	-0.1137159710
H	1.0	-5.4404211045	-2.7541060896	0.5979477792
H	1.0	-4.9094727522	-2.8240294916	3.8712441337

H	1.0	-4.2435236314	-1.4513718464	4.7075153145
H	1.0	-0.5248271210	0.9321053334	-0.5163571437
H	1.0	-0.0574397552	0.3523549848	-2.1104767313
H	1.0	1.1403055167	1.1136160146	-1.0728588660

antifive5 E= -708.1864715637

C	6.0	-0.5525113882	-1.9815026569	0.0419119969
C	6.0	0.3988732229	-0.9894808796	-0.6344538810
O	8.0	1.0416423181	-0.2150590936	0.4035568408
O	8.0	-1.4301079789	-1.1202865372	0.8238974986
C	6.0	-1.2965217242	-2.9030074094	-0.9131898380
N	7.0	-2.3568239561	-1.8315108056	1.7045367781
C	6.0	-1.7392374653	-1.9563558800	3.0838823524
C	6.0	-3.6587373345	-1.0963952738	1.5701034080
C	6.0	-4.7237680497	-1.8128659277	2.4545907696
C	6.0	-3.5531985512	0.4023451499	1.9240092674
C	6.0	-2.8684554547	-1.9431120629	4.1425841612
C	6.0	-0.7107824609	-0.8584419830	3.4039417272
C	6.0	-1.0401028232	-3.3303355679	3.1502512131
C	6.0	-4.1058991723	-1.2025838930	0.1034094985
C	6.0	-4.1238440437	-2.6371577590	3.6097502227
C	6.0	-0.2881177522	-0.0565353513	-1.6335187883
H	1.0	0.0440505121	-2.5696127206	0.7172584176
H	1.0	1.1896056220	-1.5411714820	-1.1209667370
H	1.0	0.3430062188	0.2280926774	0.9037535820
H	1.0	-1.9496954262	-3.5556704232	-0.3516610245
H	1.0	-0.5835067309	-3.5095772502	-1.4614293096
H	1.0	-1.8944895020	-2.3437665504	-1.6182232844
H	1.0	-5.3241768453	-2.4644988928	1.8316409710
H	1.0	-5.3850439109	-1.0542075022	2.8577463015
H	1.0	-4.4831251114	0.8961524261	1.6634723616
H	1.0	-2.7502984586	0.8527028892	1.3586171755
H	1.0	-3.3750694364	0.5667901709	2.9768116722
H	1.0	-2.4990951261	-2.4397129704	5.0321635750
H	1.0	-3.1130798480	-0.9265582382	4.4237399371
H	1.0	-1.1489031860	0.1265948917	3.3231889957
H	1.0	0.1402927913	-0.9126854077	2.7429525203
H	1.0	-0.3643875622	-0.9955762224	4.4228217319
H	1.0	-0.6696971624	-3.5061165050	4.1541737545
H	1.0	-0.1993541270	-3.3733455237	2.4749014347
H	1.0	-1.7298907684	-4.1200045658	2.8847626348
H	1.0	-4.1268596385	-2.2405469463	-0.2004002930
H	1.0	-3.4353133471	-0.6581859477	-0.5425960600
H	1.0	-5.1035617621	-0.7890671996	0.0024103646
H	1.0	-4.8594981986	-2.7491389843	4.3984864142
H	1.0	-3.8704875931	-3.6292525115	3.2593315918
H	1.0	-1.1322817847	0.4299875899	-1.1627928049
H	1.0	-0.6356808857	-0.5925451660	-2.5072621773
H	1.0	0.4202538813	0.6986162959	-1.9494049721

antifive6 E= -708.1949406949

C	6.0	-0.4288872887	-1.0143794252	0.0650959766
C	6.0	0.7644303129	-0.0536978478	0.0314667002
O	8.0	1.3858457745	-0.0316189086	1.3372497926
O	8.0	-1.3070610880	-0.4549910794	1.0915293047

C	6.0	-1.0895737018	-1.1777881708	-1.2993358247
N	7.0	-2.1844738624	-1.4426216008	1.7289887898
C	6.0	-1.6078101768	-1.7780770749	3.0793823317
C	6.0	-3.5781949640	-0.8809118820	1.6742276679
C	6.0	-4.5000055894	-1.8714468256	2.4142319582
C	6.0	-3.7209634826	0.5502197046	2.2311598448
C	6.0	-2.5961129341	-2.7460094682	3.7608562908
C	6.0	-1.3109746114	-0.5635016425	3.9851532526
C	6.0	-0.2864508034	-2.5418607255	2.8626394532
C	6.0	-4.0148500061	-0.8517165220	0.2021959271
C	6.0	-4.0241011345	-2.1936842482	3.8347826022
C	6.0	0.3840943013	1.3687786586	-0.3881283009
H	1.0	-0.0767049402	-1.9715776457	0.4025968309
H	1.0	1.5138023583	-0.4540567926	-0.6346886503
H	1.0	0.7389057534	0.3159953335	1.9642528323
H	1.0	-1.8527160406	-1.9406218756	-1.2611625020
H	1.0	-0.3406607122	-1.4837371402	-2.0227955774
H	1.0	-1.5389906398	-0.2542763213	-1.6351888173
H	1.0	-4.5297643087	-2.7948007890	1.8449681984
H	1.0	-5.5014968059	-1.4548866210	2.4252867609
H	1.0	-2.9415317595	1.1745059056	1.8196926216
H	1.0	-3.6709772280	0.5926562774	3.3072726279
H	1.0	-4.6829942450	0.9498951301	1.9295331423
H	1.0	-2.2155188332	-2.9722261202	4.7511693014
H	1.0	-2.6119831208	-3.6695041376	3.1915381212
H	1.0	-2.1923278537	-0.1723421490	4.4679077423
H	1.0	-0.8631650414	0.2283491616	3.4044248659
H	1.0	-0.6149180338	-0.8618544756	4.7609414830
H	1.0	0.0424059949	-2.9542163591	3.8104993946
H	1.0	0.4894999672	-1.8933138490	2.4865831986
H	1.0	-0.4434274625	-3.3579224769	2.1685727654
H	1.0	-3.8773213895	-1.8265068694	-0.2452247112
H	1.0	-3.4415680501	-0.1224641155	-0.3483429514
H	1.0	-5.0641518979	-0.5846827930	0.1424382261
H	1.0	-4.6797462167	-2.9350339903	4.2798690162
H	1.0	-4.0660636999	-1.3135367123	4.4637705767
H	1.0	-0.4402327882	1.7206816051	0.2187342754
H	1.0	0.0931774063	1.4127179051	-1.4295261176
H	1.0	1.2371988419	2.0184369733	-0.2392884207

antifive7 E= -708.1896506026

C	6.0	-0.6747226376	-1.0525580251	-0.1946095493
C	6.0	0.5477071356	-1.9391202565	-2.2601189955
O	8.0	0.3144166051	-3.2651437696	-0.2971571723
O	8.0	-1.5227394686	-1.6659693879	0.8313293285
C	6.0	-0.3615460652	-2.2609297157	-1.0818058445
N	7.0	-1.9367425871	-0.7657890278	1.9168583863
C	6.0	-1.5734111487	-1.5158371294	3.1860530285
C	6.0	-3.4170500182	-0.5315936515	1.6871633163
C	6.0	-4.2315027788	-1.8219554866	1.8922145230
C	6.0	-3.9106391018	0.6128256578	2.5972412923
C	6.0	-2.4325115037	-2.7841535546	3.3506164637
C	6.0	-1.7032977128	-0.5810417138	4.4080298023
C	6.0	-0.0900371395	-1.9223610272	3.1253781816
C	6.0	-3.6223257003	-0.0444093773	0.2418799297
C	6.0	-3.9382542865	-2.5022081413	3.2374542825

C	6.0	0.5692709854	-0.3710008138	0.3583810170
H	1.0	-1.2588386762	-0.3419653175	-0.7551462758
H	1.0	1.5228503131	-1.6382472790	-1.9033137070
H	1.0	0.1273701331	-1.1492683241	-2.8724695014
H	1.0	0.6722880746	-2.8259534565	-2.8677296590
H	1.0	-0.2780190311	-3.5356715333	0.4157052643
H	1.0	-1.3069769387	-2.6505924344	-1.4436366257
H	1.0	-3.9724806760	-2.5103019566	1.0965677085
H	1.0	-5.2873045829	-1.5867610278	1.8032357048
H	1.0	-3.1943333220	1.4242291078	2.5812380704
H	1.0	-4.0754861176	0.3132191555	3.6174911150
H	1.0	-4.8548878224	0.9787694854	2.2112275952
H	1.0	-2.1998664476	-3.2389422045	4.3080490505
H	1.0	-2.1549507489	-3.4855715277	2.5724951288
H	1.0	-2.7152217238	-0.4522602419	4.7515536365
H	1.0	-1.2860731515	0.3888612281	4.1698471402
H	1.0	-1.1357360420	-1.0072861708	5.2271960129
H	1.0	0.1470304076	-2.4952809327	4.0149756321
H	1.0	0.5412697791	-1.0442720910	3.1101207401
H	1.0	0.1252532026	-2.5185509133	2.2578816969
H	1.0	-3.3594923009	-0.8113946088	-0.4685253311
H	1.0	-3.0293998305	0.8427079327	0.0557875012
H	1.0	-4.6674345597	0.2064697796	0.1021667879
H	1.0	-4.4874118983	-3.4362717961	3.2981882645
H	1.0	-4.2751786239	-1.8847347952	4.0614173895
H	1.0	0.2923931782	0.2914314867	1.1646230256
H	1.0	1.0368488937	0.2158112698	-0.4233446534
H	1.0	1.2754239347	-1.1065274142	0.7122202983

antisix4 E= -708.1894600906

C	6.0	-0.4588686998	-0.6810042230	0.2022510951
C	6.0	1.4564217743	-2.4234678514	0.4624039461
O	8.0	-0.8768435271	-3.0989915990	0.1451462877
O	8.0	-0.9654746966	-0.5081173134	1.5693766873
C	6.0	0.0950061789	-2.0746737803	-0.1484831024
N	7.0	-1.9753513982	-1.4649434869	2.0528881375
C	6.0	-1.6411092680	-1.6500205104	3.5143344897
C	6.0	-3.3638848830	-0.9841359129	1.6928270027
C	6.0	-4.3633722660	-1.9351170526	2.3885140401
C	6.0	-3.6379730739	0.4888342763	2.0438392106
C	6.0	-2.7043063816	-2.5825595959	4.1234101234
C	6.0	-1.5200027341	-0.3365683608	4.3117865653
C	6.0	-0.2832942433	-2.3643937611	3.5829983925
C	6.0	-3.5761095990	-1.1664657900	0.1701180383
C	6.0	-4.1326014531	-2.0803811750	3.8949449781
C	6.0	0.5812853373	0.4303879635	0.0753910734
H	1.0	-1.2628458725	-0.4872477041	-0.4820234538
H	1.0	1.4679571101	-2.2759224838	1.5299531730
H	1.0	2.2470466870	-1.8299639359	0.0200447505
H	1.0	1.6528151375	-3.4681248783	0.2577536417
H	1.0	-1.3544186804	-2.8426055362	0.9550400809
H	1.0	0.2121521268	-2.0723580145	-1.2249703658
H	1.0	-4.2738801407	-2.9148218428	1.9294457407
H	1.0	-5.3625048620	-1.5661644624	2.1843402274
H	1.0	-2.7956448389	1.0920960455	1.7376885779
H	1.0	-3.8137183390	0.6466744325	3.0960362095

H	1.0	-4.5205802757	0.8183181111	1.5065681251
H	1.0	-2.4916821203	-2.6844988244	5.1819508271
H	1.0	-2.6040812371	-3.5634521203	3.6692355054
H	1.0	-0.9126125618	0.3642442288	3.7597219476
H	1.0	-1.0366445744	-0.5504415622	5.2588856159
H	1.0	-2.4739659338	0.1178977485	4.5257667771
H	1.0	-0.0935784828	-2.6825678279	4.6018764672
H	1.0	0.5040054556	-1.6930624365	3.2790061191
H	1.0	-0.2781884800	-3.2330536887	2.9381796255
H	1.0	-3.0835681495	-2.0631316656	-0.1753027927
H	1.0	-3.2015256250	-0.3191430212	-0.3867882257
H	1.0	-4.6391532158	-1.2391437613	-0.0312449810
H	1.0	-4.8416867220	-2.7926753383	4.3037342536
H	1.0	-4.2963556226	-1.1389435341	4.4035443230
H	1.0	1.3503118001	0.3105831679	0.8255135665
H	1.0	0.1049204189	1.3900274791	0.2267800198
H	1.0	1.0358359315	0.4163795980	-0.9084527206

antifive8 E= -708.1896509458

C	6.0	-0.4518943146	-1.5265563837	-0.0146266789
C	6.0	0.7122645969	-2.6585766102	-1.9918444369
O	8.0	-1.6170964532	-2.9498977610	-1.5965910064
O	8.0	-1.5503584825	-1.9070328566	0.8780198898
C	6.0	-0.3594802658	-2.7618287586	-0.9149861865
N	7.0	-1.9623475372	-0.8706336058	1.8351445212
C	6.0	-1.4895636404	-1.3744041748	3.1847963919
C	6.0	-3.4664544914	-0.7693559439	1.6552745463
C	6.0	-4.1720778499	-2.0594841294	2.1151962364
C	6.0	-4.0061547672	0.4689692387	2.4032165309
C	6.0	-2.2463668227	-2.6459197841	3.6103815896
C	6.0	-1.6159986388	-0.2495077722	4.2338955624
C	6.0	0.0111267999	-1.7027641663	3.0924020782
C	6.0	-3.7826477792	-0.5309383053	0.1678046604
C	6.0	-3.7715622150	-2.4824858767	3.5365222865
C	6.0	-0.6990576605	-0.2361434811	-0.7837616992
H	1.0	0.4542784135	-1.4379164039	0.5609392881
H	1.0	0.7536938457	-3.5880443834	-2.5446669846
H	1.0	1.6856534098	-2.4651012146	-1.5553164583
H	1.0	0.4647125118	-1.8673063818	-2.6855553310
H	1.0	-2.3000137832	-3.0927901045	-0.9290589852
H	1.0	-0.1559324910	-3.6139563520	-0.2755537388
H	1.0	-3.9033646860	-2.8559689369	1.4311481215
H	1.0	-5.2449403153	-1.9105614655	2.0488982531
H	1.0	-3.3460976999	1.3105832813	2.2370735194
H	1.0	-4.1236338978	0.3198474335	3.4626609423
H	1.0	-4.9825682546	0.7133358747	2.0010612449
H	1.0	-1.9375716211	-2.9165340658	4.6150470836
H	1.0	-1.9550263313	-3.4475045964	2.9421105367
H	1.0	-2.6196915447	-0.1047190472	4.5937001491
H	1.0	-1.2562605593	0.6810146608	3.8136453952
H	1.0	-0.9996895589	-0.5029600395	5.0886064957
H	1.0	0.3698080295	-1.9803228286	4.0767084470
H	1.0	0.5665335755	-0.8352667466	2.7574552494
H	1.0	0.1885297526	-2.5276584452	2.4215227743
H	1.0	-3.3753593707	-1.3048934002	-0.4560467175
H	1.0	-3.3844255333	0.4216055827	-0.1544287392

H	1.0	-4.8594903553	-0.5079603265	0.0436475777
H	1.0	-4.2491439529	-3.4255210843	3.7822423649
H	1.0	-4.1155198659	-1.7565054225	4.2634243727
H	1.0	-1.4548410349	-0.3874498341	-1.5392792525
H	1.0	0.2192677490	0.0784463575	-1.2652632781
H	1.0	-1.0106969096	0.5397382603	-0.1008166161

Higher level theory calculations. Optimizations, single point energies, and Hessians were all done for a select group of structures for each conformer. The 6-311G(d,p) basis set was used for all of the following calculations. Optimizations and single point energies were done using RHF, DFT with B3LYP, and MP2. Hessians were done using DFT with B3LYP.

RHF Optimizations: **1b**–**3b**

primerhf1 E= -673.2447182432

C	6.0	0.0356033765	-0.9950908497	0.0836260586
C	6.0	0.3677966278	-2.4019820156	-0.3963167659
O	8.0	-0.7515925174	-3.2257998048	-0.5461478814
O	8.0	-0.4245903013	-0.8933969266	1.4281759661
C	6.0	1.2589187745	-0.0925378843	0.0345331915
N	7.0	-1.4556398589	-1.7495136080	1.8365018967
C	6.0	-1.0114627837	-2.3906979268	3.1108601733
C	6.0	-2.7535986910	-1.0103462917	1.8315163108
C	6.0	-3.8360311119	-1.9681950231	2.3604296575
C	6.0	-2.7512830706	0.3136750134	2.6199254105
C	6.0	-2.1486116424	-3.3028216192	3.6017277276
C	6.0	-0.5799801515	-1.4019659147	4.2123530486
C	6.0	0.1980047538	-3.2870764590	2.8135060504
C	6.0	-3.1272876918	-0.6693179354	0.3794269660
C	6.0	-3.4966054397	-2.6027683397	3.7018317982
H	1.0	-0.7215255593	-0.6019154655	-0.5822149778
H	1.0	1.1065535713	-2.8565503922	0.2570077845
H	1.0	0.8182105546	-2.3094879650	-1.3786074746
H	1.0	-1.2682265528	-3.1372701553	0.2383572661
H	1.0	2.0565360822	-0.4883617584	0.6559123305
H	1.0	1.0080820942	0.8973803740	0.3976222991
H	1.0	1.6246985226	-0.0021924859	-0.9833778832
H	1.0	-3.9837067994	-2.7587647151	1.6275833252
H	1.0	-4.7714892775	-1.4192726251	2.4211522779
H	1.0	-1.8638786396	0.8906223289	2.3937842546
H	1.0	-2.8090863569	0.1796874871	3.6900795943
H	1.0	-3.6168380315	0.8990210564	2.3238687004
H	1.0	-1.8588348287	-3.7188922488	4.5624638470
H	1.0	-2.2414478146	-4.1398301722	2.9129711067
H	1.0	-1.4084258448	-0.9046055447	4.6946138105
H	1.0	0.0853206656	-0.6493215755	3.8101134936
H	1.0	-0.0430166256	-1.9480609663	4.9822178914
H	1.0	0.4291564619	-3.8755260353	3.6959989143
H	1.0	1.0750243614	-2.7018543663	2.5695080097
H	1.0	-0.0057271427	-3.9738558092	2.0007994648
H	1.0	-2.9853667147	-1.5171617926	-0.2798124898
H	1.0	-2.5525451115	0.1672242758	0.0018317409

H	1.0	-4.1735719221	-0.3814052071	0.3424885184
H	1.0	-4.2651929659	-3.3212979995	3.9734175525
H	1.0	-3.4861023985	-1.8562726568	4.4900110345

primerhf2 E= -673.2437762849

C	6.0	-0.0325679481	-0.6749279035	0.3161190472
C	6.0	0.7055383232	0.6090354969	-0.0293340614
O	8.0	-0.1110785467	1.7395944580	0.0716315307
O	8.0	-0.4465897969	-0.4853973798	1.6631025597
C	6.0	0.8367756721	-1.8970848782	0.0674184535
N	7.0	-1.3832386410	-1.3958296839	2.1674473823
C	6.0	-0.8576263001	-1.9110283544	3.4637186198
C	6.0	-2.7399211155	-0.7767397789	2.1551228880
C	6.0	-3.7213514891	-1.7922545974	2.7666795079
C	6.0	-2.8511332880	0.5852935119	2.8720003567
C	6.0	-1.8982583502	-2.8845442323	4.0442997243
C	6.0	-0.4877953421	-0.8200155760	4.4904562173
C	6.0	0.4148717628	-2.7237165161	3.1975958912
C	6.0	-3.1785148600	-0.5557901544	0.6988383519
C	6.0	-3.3017343915	-2.3042997061	4.1368642499
H	1.0	-0.9037704137	-0.7452625429	-0.3171891494
H	1.0	1.0476863734	0.5614101735	-1.0559273580
H	1.0	1.5805734317	0.7044600219	0.6125948007
H	1.0	-0.4269904033	1.7893876285	0.9561753903
H	1.0	1.7613844446	-1.8629989926	0.6331797319
H	1.0	1.0881369764	-1.9360160368	-0.9892641836
H	1.0	0.3077377443	-2.8066802929	0.3142132366
H	1.0	-3.8034970211	-2.6384729946	2.0884890611
H	1.0	-4.7027338919	-1.3283070044	2.8130554866
H	1.0	-3.7673021342	1.0764260722	2.5587438627
H	1.0	-2.0240592034	1.2315013348	2.6091769624
H	1.0	-2.8849688340	0.5052010216	3.9483635418
H	1.0	-1.5506553243	-3.2098269879	5.0208883580
H	1.0	-1.9298371769	-3.7673750073	3.4100023361
H	1.0	-1.3446685557	-0.3576455133	4.9576396905
H	1.0	0.1085183606	-0.0454494805	4.0257039765
H	1.0	0.1051578934	-1.2672364637	5.2826247935
H	1.0	0.7178903351	-3.2190503937	4.1151408795
H	1.0	1.2329233868	-2.0923063190	2.8789716459
H	1.0	0.2425592405	-3.4848623718	2.4475288202
H	1.0	-3.0230334826	-1.4505288230	0.1064351626
H	1.0	-2.6554197327	0.2716296823	0.2367907121
H	1.0	-4.2381899924	-0.3196424736	0.6807426361
H	1.0	-3.9958852297	-3.0702272884	4.4724673694
H	1.0	-3.3443624798	-1.5108116543	4.8766915176

primerhf3 E= -673.2447183602

C	6.0	0.3379662303	-1.3654095507	0.5312110640
C	6.0	-0.4122609280	-2.0296850403	-0.6159349522
O	8.0	-0.9657255008	-3.2698584296	-0.2845509572
O	8.0	-0.4680366218	-0.9037129463	1.6115677320
C	6.0	1.0817597529	-0.1254682169	0.0591362209
N	7.0	-1.4070222098	-1.7892292460	2.1564315893
C	6.0	-0.8708705289	-2.3733369174	3.4222538963
C	6.0	-2.7118516811	-1.0632836059	2.2092432112

C	6.0	-3.7495262674	-2.0031082828	2.8462590426
C	6.0	-2.6654941130	0.2905567653	2.9454505387
C	6.0	-1.9668249412	-3.2741979779	4.0190283016
C	6.0	-0.3758499482	-1.3429743101	4.4555646900
C	6.0	0.3225590699	-3.2825482062	3.0852952194
C	6.0	-3.1729005965	-0.7783552145	0.7736870128
C	6.0	-3.3124968230	-2.5820732796	4.1844973663
H	1.0	1.0533134455	-2.0868190780	0.9041513333
H	1.0	0.3060154504	-2.2123786422	-1.4077986949
H	1.0	-1.1658219673	-1.3553346724	-1.0116892618
H	1.0	-1.4193791266	-3.1608220353	0.5355578587
H	1.0	1.5931673552	0.3434662198	0.8917101273
H	1.0	0.3942236926	0.5991871824	-0.3665128614
H	1.0	1.8191937325	-0.3872309732	-0.6930134796
H	1.0	-3.9407846108	-2.8235521505	2.1578650239
H	1.0	-4.6830383977	-1.4572153629	2.9495387351
H	1.0	-1.8156528560	0.8744096423	2.6174569993
H	1.0	-2.6223497192	0.1958959945	4.0203231130
H	1.0	-3.5669525951	0.8482204268	2.7098590930
H	1.0	-1.6099341619	-3.6528284034	4.9726308796
H	1.0	-2.0954941726	-4.1364369340	3.3680084705
H	1.0	-1.1736999661	-0.8527295819	4.9936530676
H	1.0	0.2316934215	-0.5853794989	3.9776469022
H	1.0	0.2398445777	-1.8525417639	5.1908873636
H	1.0	0.5420740245	-3.9096351814	3.9440746209
H	1.0	1.2166405767	-2.7103471110	2.8711076938
H	1.0	0.1088641198	-3.9265295560	2.2408351062
H	1.0	-3.1719319585	-1.6775471535	0.1694844514
H	1.0	-2.5497590265	-0.0325853950	0.2975319422
H	1.0	-4.1879977393	-0.3941908750	0.7966048332
H	1.0	-4.0523229143	-3.2961905069	4.5358441305
H	1.0	-3.2563560779	-1.8055001315	4.9410425765

synrhf1 E= -712.2807747130

C	6.0	0.2044361206	0.0137884050	1.8731520520
C	6.0	0.1171969645	1.4956907515	2.2577202143
O	8.0	-0.4311277915	1.5499372769	3.5536118788
O	8.0	-1.0296389586	-0.5101885695	1.4017368206
C	6.0	1.1838000409	-0.2452401030	0.7315561005
N	7.0	-1.8910121065	-1.1169012783	2.3257481899
C	6.0	-1.6896047517	-2.5929884448	2.2962118672
C	6.0	-3.2568609033	-0.5838502522	2.0637978113
C	6.0	-4.2395938983	-1.2906973181	3.0131158393
C	6.0	-3.2809789371	0.9047569922	2.4282241341
C	6.0	-2.7265157870	-3.2348080414	3.2365617995
C	6.0	-0.3109007578	-2.9202142369	2.8940354829
C	6.0	-1.7488484170	-3.2352637509	0.8954201923
C	6.0	-3.7283062454	-0.7061016605	0.5995661651
C	6.0	-4.1598752746	-2.8086439536	2.9604166039
C	6.0	1.4610821752	2.2231628678	2.2588594506
H	1.0	0.5114546581	-0.5157666437	2.7618202013
H	1.0	-0.5451056698	1.9851952381	1.5471073894
H	1.0	-0.6332624408	2.4418946002	3.7718629324
H	1.0	1.1495596566	-1.2904942143	0.4528645317
H	1.0	2.2018763191	-0.0012285053	1.0099355439
H	1.0	0.9154722094	0.3380270323	-0.1449212324

H	1.0	-5.2433583274	-0.9483766699	2.7766842535
H	1.0	-4.0252837561	-0.9667491580	4.0287934536
H	1.0	-2.7240008072	1.4970221284	1.7140199650
H	1.0	-2.8630565427	1.0614417291	3.4114533255
H	1.0	-4.3090038083	1.2569124500	2.4172597109
H	1.0	-2.4759094332	-2.9605140118	4.2585783111
H	1.0	-2.6233807989	-4.3141867057	3.1647833071
H	1.0	-0.1675295760	-2.4046586052	3.8365874684
H	1.0	0.5007568121	-2.6647042536	2.2250297841
H	1.0	-0.2479131160	-3.9886682048	3.0782435322
H	1.0	-1.3251613391	-4.2344587442	0.9440598209
H	1.0	-1.1711050845	-2.6593359552	0.1845050949
H	1.0	-2.7543678052	-3.3344128569	0.5125305952
H	1.0	-3.9954677965	-1.7133394221	0.3137063984
H	1.0	-2.9626596216	-0.3511174037	-0.0776897528
H	1.0	-4.6117895281	-0.0891656496	0.4617694491
H	1.0	-4.8227971952	-3.2407937535	3.7056419420
H	1.0	-4.4981431090	-3.1822889092	1.9986264400
H	1.0	1.3238462812	3.2282235095	2.6495925637
H	1.0	1.8815555912	2.3143744386	1.2643005801
H	1.0	2.1761727556	1.7157898567	2.8998197881

synrhf2 E= -712.2910394481

C	6.0	0.1919194329	0.1029184518	1.7164291151
C	6.0	-0.0564964440	1.2246494248	2.7310036302
O	8.0	-0.5476127337	0.7141531447	3.9432011241
O	8.0	-0.9807117793	-0.5755456753	1.2614963946
C	6.0	0.8314296953	0.5912104898	0.4236514045
N	7.0	-1.8888407838	-1.0709220388	2.2056928511
C	6.0	-1.6710129133	-2.5364984259	2.3957575564
C	6.0	-3.2465139316	-0.6052977084	1.7884189648
C	6.0	-4.2670100191	-1.1708494886	2.7905051919
C	6.0	-3.2962053588	0.9246855807	1.8974012875
C	6.0	-2.7412272372	-3.0402464703	3.3806091880
C	6.0	-0.3055372548	-2.7555657905	3.0683087736
C	6.0	-1.6741930662	-3.3682459180	1.0988068504
C	6.0	-3.6331523846	-0.9667814399	0.3404682124
C	6.0	-4.1655158332	-2.6773135091	2.9843368961
C	6.0	1.2165595010	1.9860674654	3.0748381032
H	1.0	0.8527025271	-0.6101611203	2.1924150790
H	1.0	-0.7720860156	1.9240027831	2.3065762329
H	1.0	-1.2121478562	0.0756160151	3.7358683189
H	1.0	0.8721761874	-0.2242990240	-0.2886757203
H	1.0	1.8412009162	0.9443925948	0.5937700492
H	1.0	0.2501627262	1.3955653580	-0.0178100545
H	1.0	-5.2619026368	-0.8923741959	2.4547328920
H	1.0	-4.1126984021	-0.6847369437	3.7514288183
H	1.0	-4.3195828865	1.2567004736	1.7523255887
H	1.0	-2.6867267176	1.3957679259	1.1373121203
H	1.0	-2.9706731555	1.2658265251	2.8724486516
H	1.0	-2.5328595675	-2.6161660923	4.3606578766
H	1.0	-2.6317047766	-4.1168530599	3.4756950372
H	1.0	-0.1535995210	-2.0744494927	3.8968429870
H	1.0	0.5116392850	-2.6415927681	2.3670064380
H	1.0	-0.2598103961	-3.7708922843	3.4502860742
H	1.0	-1.2341544365	-4.3395245053	1.3048009324

H	1.0	-1.0779548267	-2.8860699843	0.3349364064
H	1.0	-2.6625287154	-3.5448106421	0.7008304402
H	1.0	-3.9000237841	-2.0051492263	0.2111459444
H	1.0	-2.8253936653	-0.7320818744	-0.3400631108
H	1.0	-4.4976137905	-0.3765183099	0.0516701157
H	1.0	-4.4605712195	-3.2032407928	2.0815706043
H	1.0	-4.8553788442	-2.9958568566	3.7611084939
H	1.0	1.0056152883	2.6453037808	3.9087929741
H	1.0	1.5717384121	2.5866110694	2.2452081727
H	1.0	2.0054769820	1.3043125550	3.3805630937

synrhf3 E= -712.2853483171

C	6.0	-0.7159910760	-1.0220211621	-0.1444904159
C	6.0	0.2818155399	-1.7161016727	-2.3891760803
O	8.0	-1.5617561570	-2.8451931525	-1.4740680831
O	8.0	-1.4537672706	-1.6572992399	0.8937734627
C	6.0	-0.3873307694	-2.1698418151	-1.1027148566
N	7.0	-1.9306636496	-0.8202393822	1.9148788729
C	6.0	-1.5031627697	-1.4619986018	3.2052684227
C	6.0	-3.4115566396	-0.6626578490	1.7186027439
C	6.0	-4.1729427684	-1.9655623534	2.0297596161
C	6.0	-3.9363881843	0.5078662998	2.5734017663
C	6.0	-2.2963473777	-2.7537742162	3.4843570344
C	6.0	-1.6351466256	-0.4633216616	4.3717174240
C	6.0	-0.0122079931	-1.8243282529	3.1465256398
C	6.0	-3.7129542283	-0.2696847976	0.2647454729
C	6.0	-3.8080054620	-2.5739717888	3.3805526987
C	6.0	0.5135513870	-0.2600864984	0.3274623258
H	1.0	-1.3661961082	-0.3286100737	-0.6608019301
H	1.0	0.3851620294	-2.5678007725	-3.0513244805
H	1.0	1.2674933878	-1.3029009686	-2.2076623370
H	1.0	-0.3250026914	-0.9701391118	-2.8942476366
H	1.0	-2.0140729644	-3.0908682894	-0.6863295466
H	1.0	0.2753453036	-2.8602020874	-0.5796640782
H	1.0	-3.9515345577	-2.6896551344	1.2499433392
H	1.0	-5.2409877903	-1.7692115373	1.9768071295
H	1.0	-3.2646086284	1.3559533438	2.5051487209
H	1.0	-4.0806316617	0.2684844813	3.6143188087
H	1.0	-4.9028428024	0.8138368309	2.1872669645
H	1.0	-2.0256020244	-3.1248993711	4.4698397281
H	1.0	-1.9833343234	-3.5092559797	2.7684261396
H	1.0	-2.6381326227	-0.3525946803	4.7509907895
H	1.0	-1.2684352549	0.5137528915	4.0778843074
H	1.0	-1.0268111706	-0.8144271338	5.1985659472
H	1.0	0.2592486588	-2.3034678484	4.0819476457
H	1.0	0.6037969552	-0.9398149911	3.0396713778
H	1.0	0.2126117285	-2.5099253906	2.3440436423
H	1.0	-3.4059509691	-1.0229912700	-0.4447191339
H	1.0	-3.2410324980	0.6732047742	0.0076385825
H	1.0	-4.7850700692	-0.1388627718	0.1609299852
H	1.0	-4.2995546627	-3.5366660966	3.4924816764
H	1.0	-4.1766111330	-1.9529329007	4.1919876561
H	1.0	0.2450446590	0.4291867911	1.1160941414
H	1.0	0.9151481235	0.3194164487	-0.4969299665
H	1.0	1.2928351310	-0.9223730079	0.6887364831

synrhf4 E= -712.2910397022

C	6.0	-0.3449788098	-0.9180909279	0.1969308592
C	6.0	0.9499635358	-2.5827217920	-1.2153996350
O	8.0	-0.8435190115	-3.2896801462	0.1141436776
O	8.0	-0.9608865292	-0.5960514856	1.4456674051
C	6.0	0.1972981596	-2.3477050636	0.0872868313
N	7.0	-1.9482023284	-1.4481705565	1.9563019467
C	6.0	-1.5878782414	-1.7268203038	3.3798126931
C	6.0	-3.3011012053	-0.8851017438	1.6663947520
C	6.0	-4.3400471793	-1.8183279715	2.3138911837
C	6.0	-3.5086047318	0.5742106738	2.1158793298
C	6.0	-2.6807580535	-2.6315714674	3.9739287130
C	6.0	-1.3768719381	-0.4697814977	4.2476377008
C	6.0	-0.2725509535	-2.5172592321	3.4083139614
C	6.0	-3.5455553697	-0.9279672274	0.1487112994
C	6.0	-4.0914901191	-2.0898516430	3.7909468271
C	6.0	0.7341470321	0.1473048566	0.0594511020
H	1.0	-1.0688926520	-0.7951322824	-0.5983727040
H	1.0	1.1595851794	-3.6424770930	-1.3025625450
H	1.0	1.8901050405	-2.0440750743	-1.2485266160
H	1.0	0.3457411078	-2.2913341365	-2.0701693972
H	1.0	-1.4413143097	-3.0353298059	0.7998882978
H	1.0	0.8787111820	-2.5247120144	0.9154600676
H	1.0	-4.3314913586	-2.7656082456	1.7787824614
H	1.0	-5.3238510569	-1.3828696707	2.1638881723
H	1.0	-2.6606662920	1.1846776253	1.8333508854
H	1.0	-3.6679670265	0.6808637812	3.1787340895
H	1.0	-4.3888351323	0.9716862917	1.6191496629
H	1.0	-2.4601440573	-2.7826882353	5.0268087240
H	1.0	-2.6177459712	-3.6073208342	3.4969403250
H	1.0	-0.7488269096	0.2468582790	3.7351223966
H	1.0	-0.8752410927	-0.7593534306	5.1661304139
H	1.0	-2.2970769000	0.0202401757	4.5293138101
H	1.0	-0.0880095843	-2.8604141522	4.4216169149
H	1.0	0.5662156437	-1.9010778828	3.1119162251
H	1.0	-0.3160172114	-3.3874688053	2.7649241529
H	1.0	-3.2540596483	-1.8804654448	-0.2768853769
H	1.0	-3.0153615975	-0.1371047443	-0.3670276965
H	1.0	-4.6042095492	-0.7803941587	-0.0419445887
H	1.0	-4.8141874568	-2.8135681752	4.1579849257
H	1.0	-4.2382535540	-1.1890164647	4.3787932652
H	1.0	1.5389155541	-0.0206814381	0.7692437042
H	1.0	0.3059349721	1.1220947141	0.2611224084
H	1.0	1.1494684233	0.1591567502	-0.9408806258

antirhf1 E= -712.2873819003

C	6.0	0.0487648926	-0.7553159127	0.6462942683
C	6.0	0.8697196840	0.4798667554	0.2524050042
O	8.0	1.7829055608	0.1394536325	-0.7647214778
O	8.0	-0.7984065296	-0.3081813626	1.6940037480
C	6.0	-0.6558898615	-1.3749724072	-0.5514990207
N	7.0	-1.8387070843	-1.1482078759	2.1007253926
C	6.0	-1.4558363824	-1.8574999711	3.3508699832
C	6.0	-3.0865179349	-0.3365055152	2.0899560284

C	6.0	-4.2395299679	-1.2295801095	2.5781034489
C	6.0	-3.0163864513	0.9671960481	2.9118422549
C	6.0	-2.6615346379	-2.7042353804	3.7966470070
C	6.0	-0.9652238795	-0.9518159221	4.4977890596
C	6.0	-0.3176772999	-2.8406011353	3.0309302906
C	6.0	-3.3989395805	0.0573906552	0.6406780433
C	6.0	-3.9600839270	-1.9180784399	3.9062755079
C	6.0	1.5942549132	1.1302601665	1.4232587485
H	1.0	0.7417206932	-1.4922969881	1.0427751967
H	1.0	0.1982324125	1.2032885797	-0.1964433424
H	1.0	2.4915185024	-0.3575119251	-0.3947154868
H	1.0	-1.2972948465	-2.1887026679	-0.2418053339
H	1.0	0.0932847513	-1.7591682489	-1.2324856938
H	1.0	-1.2503748833	-0.6457868012	-1.0886634679
H	1.0	-4.4249352829	-1.9919783457	1.8250565038
H	1.0	-5.1380072980	-0.6218728708	2.6399184057
H	1.0	-3.8670950739	1.5920733689	2.6561767432
H	1.0	-2.1150750674	1.5183705628	2.6775860785
H	1.0	-3.0494913663	0.8056886309	3.9795348773
H	1.0	-2.4136820518	-3.1728313901	4.7450881548
H	1.0	-2.8014237592	-3.5061583136	3.0751708908
H	1.0	-1.7617301283	-0.4183185571	4.9958713256
H	1.0	-0.2465848160	-0.2293110112	4.1329358021
H	1.0	-0.4731249138	-1.5654869882	5.2471470742
H	1.0	-0.2160764646	-3.5490231260	3.8477384580
H	1.0	0.6348114150	-2.3369476431	2.9251923624
H	1.0	-0.5259716755	-3.3966576730	2.1237795737
H	1.0	-3.4191372172	-0.8130643471	-0.0026484179
H	1.0	-2.6747448467	0.7625777836	0.2536845174
H	1.0	-4.3756414864	0.5306338475	0.6010834035
H	1.0	-4.7775817631	-2.5905163497	4.1527220659
H	1.0	-3.9072608883	-1.1945492398	4.7141255603
H	1.0	0.8975548531	1.4924162702	2.1670836554
H	1.0	2.1896983874	1.9618811692	1.0610225865
H	1.0	2.2636213006	0.4190590477	1.9061602202

antirhf2 E= -712.2896347904

C	6.0	-0.0436214077	-0.9177581887	0.5220649913
C	6.0	1.1434634719	0.0486425726	0.5870992983
O	8.0	1.7512652296	-0.0287884037	1.8523161131
O	8.0	-0.9490964433	-0.4578769564	1.5172545723
C	6.0	-0.6269280761	-1.0640638805	-0.8756021809
N	7.0	-1.9976945684	-1.3222714410	1.8566997436
C	6.0	-1.6799681081	-2.0218908438	3.1348760819
C	6.0	-3.2662507734	-0.5437316231	1.7790043251
C	6.0	-4.4206590281	-1.4798051673	2.1770588945
C	6.0	-3.2869036099	0.7474815748	2.6235598155
C	6.0	-2.8812508980	-2.9179650843	3.4856953304
C	6.0	-1.3244309390	-1.1006687157	4.3208377122
C	6.0	-0.4797539080	-2.9564309369	2.9138044214
C	6.0	-3.5078555993	-0.1285656355	0.3229202716
C	6.0	-4.2128407982	-2.1816075514	3.5110919734
C	6.0	0.8150569564	1.4977552437	0.2396814384
H	1.0	0.3372368956	-1.8838385234	0.8153942688
H	1.0	1.8900497195	-0.3177414818	-0.1092166226
H	1.0	1.1080500977	0.2067276338	2.4977691268

H	1.0	-1.4041792214	-1.8161839707	-0.8841577472
H	1.0	0.1617508201	-1.3954285327	-1.5464344038
H	1.0	-1.0341161142	-0.1394399430	-1.2631945530
H	1.0	-4.5293859693	-2.2346220860	1.4018285358
H	1.0	-5.3400812734	-0.9008946709	2.1855593496
H	1.0	-2.3847612230	1.3238305143	2.4632864617
H	1.0	-3.3944326635	0.5697664405	3.6833593732
H	1.0	-4.1308892194	1.3571352811	2.3148955423
H	1.0	-2.6832844664	-3.3883599817	4.4449081251
H	1.0	-2.9385027912	-3.7152142217	2.7483506897
H	1.0	-2.1862541041	-0.6461902334	4.7869733818
H	1.0	-0.6539962057	-0.3094774360	4.0115567291
H	1.0	-0.8188838819	-1.6841878133	5.0841053865
H	1.0	-0.3911877577	-3.6243637500	3.7653781396
H	1.0	0.4521167159	-2.4120683705	2.8321157660
H	1.0	-0.6171884326	-3.5616258825	2.0246432748
H	1.0	-3.4563044185	-0.9820062652	-0.3407580702
H	1.0	-2.7946426215	0.6160982733	-0.0033108188
H	1.0	-4.4999512583	0.3046227520	0.2374492597
H	1.0	-5.0205052917	-2.8873710365	3.6859872265
H	1.0	-4.2475950399	-1.4714359239	4.3316367823
H	1.0	0.4627612319	1.5979313742	-0.7815750299
H	1.0	1.7110596662	2.0986283457	0.3501284485
H	1.0	0.0528353061	1.8929345459	0.9031885757

antirhf3 E= -712.2843697864

C	6.0	-0.7323016659	-1.8416145016	-0.0594273290
C	6.0	-0.1488117311	-3.1313914918	-2.1917904268
O	8.0	-0.1806208797	-4.2017578442	-0.0912097151
O	8.0	-1.4399762267	-2.1253813171	1.1425448151
C	6.0	0.6772586360	-1.3062433659	0.1437711416
N	7.0	-1.6490543871	-1.0367189566	2.0037551153
C	6.0	-1.1727768769	-1.4756736230	3.3602702326
C	6.0	-3.1026205668	-0.6708868093	1.9078716890
C	6.0	-4.0050059298	-1.7439245325	2.5466302992
C	6.0	-3.3454022382	0.7149016230	2.5372555327
C	6.0	-2.1092770176	-2.5356698298	3.9732004848
C	6.0	-1.0207402063	-0.2600629336	4.2961814885
C	6.0	0.2330599643	-2.0842941773	3.2581331163
C	6.0	-3.5123062960	-0.5227659269	0.4352790331
C	6.0	-3.5798485270	-2.1290614814	3.9603234918
C	6.0	-0.7974359041	-3.1706620847	-0.8193295093
H	1.0	-1.2879136948	-1.1076995229	-0.6286490762
H	1.0	-0.3313351637	-4.0699839462	-2.7027998754
H	1.0	0.9238253700	-2.9985200279	-2.1114503727
H	1.0	-0.5585001252	-2.3262214658	-2.7952855880
H	1.0	-0.6140416385	-4.2701426847	0.7411664546
H	1.0	0.6577163452	-0.4423249878	0.7942845201
H	1.0	1.0773865272	-0.9883353990	-0.8136567136
H	1.0	1.3402278924	-2.0548876561	0.5570647160
H	1.0	-3.9768493261	-2.6311861229	1.9199512597
H	1.0	-5.0324502044	-1.3878486703	2.5422439011
H	1.0	-2.5713761202	1.4095384422	2.2309984219
H	1.0	-3.3951301475	0.7111466799	3.6138282627
H	1.0	-4.2974087474	1.0958151529	2.1828949427
H	1.0	-1.7827992729	-2.7459444720	4.9887273309

H	1.0	-1.9977798219	-3.4594698989	3.4112986782
H	1.0	-1.9444585187	0.0835954058	4.7331516180
H	1.0	-0.5589776291	0.5678419415	3.7702742307
H	1.0	-0.3712329480	-0.5369488597	5.1198112214
H	1.0	0.5294038286	-2.4239052699	4.2455327991
H	1.0	0.9578216201	-1.3485862317	2.9323859779
H	1.0	0.2734522672	-2.9299750128	2.5902905232
H	1.0	-3.4107185123	-1.4463940090	-0.1154935781
H	1.0	-2.9371502234	0.2539654992	-0.0578677718
H	1.0	-4.5570968507	-0.2325679224	0.3969122776
H	1.0	-4.1910279626	-2.9552288879	4.3138499844
H	1.0	-3.7561876489	-1.3087936788	4.6504400861
H	1.0	-1.8539094413	-3.4051711419	-0.9430036899

antirhf4 E= -712.2843689838

C	6.0	-0.5486444185	-1.4714604901	-0.0397392780
C	6.0	0.8432343207	-2.6202161654	-1.8548396088
O	8.0	-1.4480261664	-3.1066914121	-1.5860678145
O	8.0	-1.6127390465	-1.8547315244	0.8246303279
C	6.0	-0.3008081087	-2.7395646643	-0.8631595233
N	7.0	-1.9887449309	-0.9106956145	1.7931650977
C	6.0	-1.4937120952	-1.4169796090	3.1175039268
C	6.0	-3.4781092608	-0.7511756179	1.6687315163
C	6.0	-4.2242267460	-2.0088172349	2.1565529646
C	6.0	-3.9500343936	0.5049860452	2.4277256213
C	6.0	-2.2743256651	-2.6618114210	3.5807339065
C	6.0	-1.5490041412	-0.2938107503	4.1714919453
C	6.0	-0.0101899574	-1.7999862515	3.0127710277
C	6.0	-3.8654413547	-0.5057150858	0.2031476624
C	6.0	-3.7881917749	-2.4763075479	3.5421405006
C	6.0	-0.8226285239	-0.2283863783	-0.8731354791
H	1.0	0.3364037465	-1.2854234884	0.5547800317
H	1.0	1.0211041332	-3.5847405800	-2.3164957438
H	1.0	1.7573492853	-2.3016889864	-1.3617357262
H	1.0	0.6044467116	-1.9132691194	-2.6409161816
H	1.0	-2.1491975025	-3.2379608175	-0.9724732451
H	1.0	-0.0607980346	-3.5288880436	-0.1519628780
H	1.0	-4.0464821856	-2.8116101178	1.4455971793
H	1.0	-5.2929137266	-1.8093914965	2.1425199364
H	1.0	-3.2698040471	1.3308984964	2.2534333256
H	1.0	-4.0579523856	0.3682539656	3.4916902629
H	1.0	-4.9262141134	0.7906303082	2.0503122842
H	1.0	-1.9492963286	-2.9281647635	4.5837064794
H	1.0	-2.0081726935	-3.4923105819	2.9326336313
H	1.0	-2.5303661832	-0.1157249122	4.5799092630
H	1.0	-1.1765224671	0.6346875436	3.7535922067
H	1.0	-0.9098460312	-0.5668532683	5.0045874071
H	1.0	0.3282556538	-2.1342888773	3.9879563900
H	1.0	0.5978147146	-0.9476292123	2.7280108559
H	1.0	0.1582303414	-2.6075682553	2.3154385880
H	1.0	-3.5475997140	-1.3017905597	-0.4511599553
H	1.0	-3.4561231864	0.4285134627	-0.1608591899
H	1.0	-4.9470628508	-0.4365522608	0.1442128961
H	1.0	-4.2780524864	-3.4162525291	3.7821159349
H	1.0	-4.1072554352	-1.7691111813	4.3025884882
H	1.0	-1.5887762959	-0.3999538526	-1.6176667604

H	1.0	0.0891851028	0.0648140179	-1.3837222397
H	1.0	-1.1182217584	0.5918088318	-0.2329960342

antirhf5 E= -712.2907767581

C	6.0	-3.0999265568	0.0243080415	0.6250663057
C	6.0	-2.1900216129	1.2508906165	0.5021209625
O	8.0	-2.9070762891	2.3734580796	0.0574498945
O	8.0	-4.0439333704	0.4317847858	1.6130079135
C	6.0	-3.7018232768	-0.4411523158	-0.6918962869
N	7.0	-5.1136940860	-0.4225562779	1.8927225560
C	6.0	-4.8397452899	-1.1720351267	3.1490757454
C	6.0	-6.3628563322	0.3826558964	1.7990244634
C	6.0	-7.5474602954	-0.5337781787	2.1492729324
C	6.0	-6.3796542197	1.6536029007	2.6748568390
C	6.0	-6.0727708302	-2.0413987169	3.4542077861
C	6.0	-4.4639610369	-0.3003324440	4.3637155782
C	6.0	-3.6678967393	-2.1364245050	2.9037189787
C	6.0	-6.5510872782	0.8281051079	0.3429335310
C	6.0	-7.3837043048	-1.2685726989	3.4719029275
C	6.0	-1.0174977269	1.0553987547	-0.4432495608
H	1.0	-2.4999252654	-0.7828048915	1.0258154092
H	1.0	-1.8017236537	1.4470152982	1.5005543653
H	1.0	-3.6039423277	2.5343911074	0.6685396321
H	1.0	-4.4479710074	-1.2038391636	-0.5169320118
H	1.0	-2.9177973786	-0.8767412937	-1.3029961688
H	1.0	-4.1472927278	0.3756571330	-1.2436215517
H	1.0	-7.6572901618	-1.2690457032	1.3557369574
H	1.0	-8.4530405446	0.0665906889	2.1507846520
H	1.0	-5.4541161202	2.2057654354	2.5744646831
H	1.0	-6.5361423378	1.4504828287	3.7242100412
H	1.0	-7.1905737780	2.2980214030	2.3493201211
H	1.0	-5.9075964141	-2.5408349179	4.4048490073
H	1.0	-6.1382844345	-2.8187087018	2.6962217488
H	1.0	-5.3072059318	0.2120930979	4.8036249311
H	1.0	-3.7218071031	0.4379228391	4.0880611988
H	1.0	-4.0361192610	-0.9341422618	5.1351652391
H	1.0	-3.6335133453	-2.8684904890	3.7051165649
H	1.0	-2.7145179192	-1.6231473357	2.8993687390
H	1.0	-3.7892225008	-2.6663543852	1.9655332640
H	1.0	-6.5205743514	-0.0194033165	-0.3297027423
H	1.0	-5.7967700309	1.5401940607	0.0362074797
H	1.0	-7.5201299819	1.3068469558	0.2387314797
H	1.0	-8.2135117294	-1.9550773883	3.6173190595
H	1.0	-7.4129164086	-0.5755075081	4.3071123921
H	1.0	-0.4389713410	0.1763160311	-0.1732900429
H	1.0	-0.3675697518	1.9216813537	-0.3942680378
H	1.0	-1.3568349468	0.9507652044	-1.4673269762

DFT Optimizations: **1b**–**3b**

primedft1 E= -677.2325106918

C	6.0	0.0611605595	-0.9683280883	0.0595089927
C	6.0	0.3598539730	-2.3935889266	-0.4031279430

O	8.0	-0.7921692905	-3.2192335779	-0.4623225041
O	8.0	-0.3963230027	-0.8545290967	1.4356037120
C	6.0	1.3001454458	-0.0822662658	0.0103779054
N	7.0	-1.4605730386	-1.7620607386	1.8307012523
C	6.0	-1.0100216890	-2.4042246626	3.1223560342
C	6.0	-2.7735483806	-1.0133870235	1.8261900454
C	6.0	-3.8512542568	-1.9870335199	2.3552536317
C	6.0	-2.7692560165	0.3090705767	2.6230592727
C	6.0	-2.1588902467	-3.3142712701	3.6117939176
C	6.0	-0.5797665643	-1.4069363908	4.2211625903
C	6.0	0.2000061315	-3.3034172272	2.8130705460
C	6.0	-3.1335214129	-0.6773285699	0.3654410590
C	6.0	-3.5081996479	-2.6066264295	3.7072410813
H	1.0	-0.7082259956	-0.5593371457	-0.6014361709
H	1.0	1.1374919488	-2.8310667509	0.2387465548
H	1.0	0.7683347366	-2.3374805362	-1.4175455951
H	1.0	-1.2723604597	-3.0213792034	0.3625799467
H	1.0	2.1068484851	-0.5067140784	0.6139263009
H	1.0	1.0716435170	0.9128876949	0.3969677566
H	1.0	1.6521603818	0.0216652273	-1.0192078576
H	1.0	-3.9813228936	-2.7896301084	1.6194864868
H	1.0	-4.8010000929	-1.4443927786	2.4002541991
H	1.0	-1.8747778973	0.8864148754	2.3860964465
H	1.0	-2.8124484264	0.1639143401	3.7012536614
H	1.0	-3.6429971780	0.9010824352	2.3365420441
H	1.0	-1.8669958932	-3.7336825815	4.5799999658
H	1.0	-2.2494447779	-4.1594370813	2.9188648547
H	1.0	-1.4167789432	-0.8995141479	4.6983372589
H	1.0	0.0919956181	-0.6548386868	3.8065057045
H	1.0	-0.0392555290	-1.9497550303	5.0018737751
H	1.0	0.4343924478	-3.9049947554	3.6955645607
H	1.0	1.0818652260	-2.7098001296	2.5702557331
H	1.0	-0.0103174442	-3.9819441762	1.9838469093
H	1.0	-2.9827916841	-1.5375824775	-0.2890373953
H	1.0	-2.5420180360	0.1581864222	-0.0125524571
H	1.0	-4.1850425590	-0.3810813561	0.3143275574
H	1.0	-4.2842338040	-3.3220441063	3.9981019184
H	1.0	-3.4901533104	-1.8411346541	4.4896782476

primedft2 E= -677.2288808160

C	6.0	0.0105547377	-0.7079165530	0.2979982115
C	6.0	0.6028003710	0.6385288167	-0.1186780818
O	8.0	-0.3363009297	1.7001008914	-0.0273524871
O	8.0	-0.4051310177	-0.4841351910	1.6685217189
C	6.0	1.0049925555	-1.8456518425	0.1091580776
N	7.0	-1.3886348243	-1.4267677321	2.1641018868
C	6.0	-0.8689863666	-1.9525587396	3.4765642521
C	6.0	-2.7395116125	-0.7555715309	2.1637029757
C	6.0	-3.7450411934	-1.7601080427	2.7702504818
C	6.0	-2.8093551608	0.6009342905	2.9048946872
C	6.0	-1.9443497529	-2.9001711171	4.0557112530
C	6.0	-0.4708327283	-0.8627949277	4.5015805970
C	6.0	0.3827418214	-2.8011836747	3.2003005380
C	6.0	-3.1597383322	-0.5084745388	0.7021091434
C	6.0	-3.3352896629	-2.2784260516	4.1464300113
H	1.0	-0.8743075348	-0.9038757095	-0.3089468888

H	1.0	0.9169264814	0.5875874103	-1.1636410160
H	1.0	1.4935852583	0.8430701862	0.4936473700
H	1.0	-0.6555012116	1.6904890960	0.8820228456
H	1.0	1.9147681601	-1.6925324049	0.6950286789
H	1.0	1.2855531665	-1.9062422020	-0.9473800158
H	1.0	0.5616387903	-2.7999605487	0.3900588122
H	1.0	-3.8369245702	-2.6098435791	2.0836867850
H	1.0	-4.7256793225	-1.2745796165	2.8084344840
H	1.0	-3.7034187344	1.1423584992	2.5841870864
H	1.0	-1.9411025963	1.2169142771	2.6674612412
H	1.0	-2.8615684327	0.4985152045	3.9877663482
H	1.0	-1.6006013330	-3.2376826810	5.0389566050
H	1.0	-1.9971412823	-3.7874917333	3.4143688832
H	1.0	-1.3251073792	-0.3776845376	4.9708651148
H	1.0	0.1393351516	-0.0988850328	4.0185438246
H	1.0	0.1249352787	-1.3174912086	5.2980582487
H	1.0	0.6863910983	-3.3054077976	4.1220448106
H	1.0	1.2155078540	-2.1849631153	2.8641188945
H	1.0	0.1771462003	-3.5630412770	2.4462483042
H	1.0	-3.0554224395	-1.4206386273	0.1097955922
H	1.0	-2.5739649508	0.2861939529	0.2385990864
H	1.0	-4.2101475451	-0.2042677427	0.6758150504
H	1.0	-4.0560926041	-3.0255444430	4.4943755455
H	1.0	-3.3521554072	-1.4712004261	4.8857910434

primedft3 E= -677.2324829457

C	6.0	0.3688575514	-1.3511647120	0.5050076556
C	6.0	-0.4151264752	-2.0266926890	-0.6194821044
O	8.0	-1.0190636099	-3.2479690886	-0.2232534772
O	8.0	-0.4403101110	-0.8665227047	1.6116727096
C	6.0	1.1119767380	-0.1110099172	0.0231027239
N	7.0	-1.4123168159	-1.8030689510	2.1507764842
C	6.0	-0.8697313358	-2.3866999913	3.4352095798
C	6.0	-2.7293703212	-1.0650038666	2.2065305564
C	6.0	-3.7631054194	-2.0206422988	2.8411469349
C	6.0	-2.6781963127	0.2843505410	2.9585346180
C	6.0	-1.9761041803	-3.2883092270	4.0300381508
C	6.0	-0.3775008719	-1.3458179838	4.4635854283
C	6.0	0.3235347214	-3.2976765316	3.0858444292
C	6.0	-3.1798498186	-0.7764237248	0.7645247404
C	6.0	-3.3248675620	-2.5905400152	4.1883164073
H	1.0	1.0893115168	-2.0810472889	0.8867834645
H	1.0	0.2884535414	-2.2644891786	-1.4242431414
H	1.0	-1.1535358528	-1.3227746974	-1.0270889643
H	1.0	-1.4070276437	-3.0539592039	0.6490952898
H	1.0	1.6085631369	0.3815863066	0.8612971025
H	1.0	0.4250939425	0.6052192405	-0.4356225640
H	1.0	1.8718266519	-0.3863662741	-0.7129101573
H	1.0	-3.9406478722	-2.8500401178	2.1461039915
H	1.0	-4.7102217600	-1.4795185145	2.9340956151
H	1.0	-1.8177218103	0.8671151625	2.6291308782
H	1.0	-2.6271160624	0.1724142962	4.0400620052
H	1.0	-3.5826204697	0.8552550972	2.7306980459
H	1.0	-1.6155227364	-3.6670386303	4.9917331774
H	1.0	-2.1027584520	-4.1596144294	3.3759174898
H	1.0	-1.1849819017	-0.8482983418	4.9986978197

H	1.0	0.2278818859	-0.5869638685	3.9668949723
H	1.0	0.2480146091	-1.8465001109	5.2080593467
H	1.0	0.5553912012	-3.9290340009	3.9481764402
H	1.0	1.2198857725	-2.7190825265	2.8564931122
H	1.0	0.0953813530	-3.9419018412	2.2349759535
H	1.0	-3.1753614133	-1.6841415665	0.1581794368
H	1.0	-2.5379285585	-0.0316874850	0.2935987363
H	1.0	-4.1990547581	-0.3808919263	0.7795797001
H	1.0	-4.0720274786	-3.3030456664	4.5526853136
H	1.0	-3.2651230184	-1.7993132738	4.9420020986

syndft1 E= -716.5319377704

C	6.0	0.2229455024	0.1197491028	1.6875839611
C	6.0	-0.0517646308	1.2323832362	2.7130208626
O	8.0	-0.6167777607	0.6984276898	3.9080358892
O	8.0	-0.9669639058	-0.5729282221	1.2047530945
C	6.0	0.8679766066	0.6205137582	0.4001017331
N	7.0	-1.8906412047	-1.0646791900	2.2116265584
C	6.0	-1.6698320781	-2.5482853823	2.4017257033
C	6.0	-3.2650367999	-0.6001436292	1.7888818933
C	6.0	-4.2718820826	-1.1645301319	2.8151534204
C	6.0	-3.3050051839	0.9351344602	1.8848994549
C	6.0	-2.7423090758	-3.0453770216	3.3985299998
C	6.0	-0.2959699236	-2.7512902725	3.0706991545
C	6.0	-1.6850252607	-3.3779072769	1.0999739534
C	6.0	-3.6591893218	-0.9886206046	0.3459183874
C	6.0	-4.1706247755	-2.6764564812	3.0050222154
C	6.0	1.2184384138	1.9720598430	3.1231546801
H	1.0	0.8824035808	-0.6075827490	2.1705192697
H	1.0	-0.7464224796	1.9525362050	2.2563211245
H	1.0	-1.2548516105	0.0212202015	3.6096058934
H	1.0	0.9128343436	-0.1906246123	-0.3293495082
H	1.0	1.8854778631	0.9697956509	0.5842057323
H	1.0	0.2896618645	1.4397765844	-0.0360231221
H	1.0	-5.2780107141	-0.8763643145	2.4941767563
H	1.0	-4.0938198045	-0.6726263884	3.7785991950
H	1.0	-4.3328084986	1.2767835952	1.7346520855
H	1.0	-2.6837456070	1.3945057579	1.1158130816
H	1.0	-2.9693601275	1.2811247860	2.8640387032
H	1.0	-2.5228060330	-2.6170035995	4.3837895081
H	1.0	-2.6298214792	-4.1299900787	3.4955492085
H	1.0	-0.1556781680	-2.0623965738	3.9057882950
H	1.0	0.5226051166	-2.6154108803	2.3623737401
H	1.0	-0.2309339788	-3.7748730479	3.4505298344
H	1.0	-1.2341002083	-4.3556208677	1.2928632527
H	1.0	-1.0964871109	-2.8805151537	0.3281991509
H	1.0	-2.6866794983	-3.5542954435	0.7109002843
H	1.0	-3.9243054139	-2.0390697724	0.2407436333
H	1.0	-2.8449141131	-0.7651534571	-0.3439543990
H	1.0	-4.5301801389	-0.4005774552	0.0434663493
H	1.0	-4.4681651822	-3.2019089174	2.0918625710
H	1.0	-4.8671651031	-3.0023434123	3.7841627971
H	1.0	0.9794841619	2.6243271040	3.9657882102
H	1.0	1.6204755611	2.5856600547	2.3142294007
H	1.0	1.9881842592	1.2683169062	3.4544679909

syndft2			E= -716.5235606292	
C	6.0	-0.6753086646	-1.0265215793	-0.1553680275
C	6.0	0.2437338597	-1.6842694202	-2.4517450591
O	8.0	-1.6187970305	-2.8106454147	-1.5162415466
O	8.0	-1.4199221483	-1.6981022727	0.8942906235
C	6.0	-0.3979882820	-2.1607454373	-1.1563523165
N	7.0	-1.9175807975	-0.8055707804	1.9315120145
C	6.0	-1.5024484766	-1.4536273115	3.2447987750
C	6.0	-3.4193633926	-0.6738378500	1.7143978007
C	6.0	-4.1665708048	-1.9894972612	2.0279249260
C	6.0	-3.9602095693	0.4973943658	2.5641052515
C	6.0	-2.2979586363	-2.7518163547	3.5222978802
C	6.0	-1.6602619674	-0.4390024138	4.3985811689
C	6.0	-0.0044557569	-1.8036407336	3.1981339842
C	6.0	-3.6973243913	-0.2881374703	0.2496518179
C	6.0	-3.8133700680	-2.5771700759	3.3963468045
C	6.0	0.5777755662	-0.3103105832	0.3280565359
H	1.0	-1.3344597756	-0.3005073043	-0.6372789451
H	1.0	0.2998764038	-2.5230631849	-3.1486737594
H	1.0	1.2543895873	-1.3042842444	-2.2891962280
H	1.0	-0.3603684654	-0.8994559055	-2.9160986490
H	1.0	-2.0580144899	-3.0195928082	-0.6832438998
H	1.0	0.2697852552	-2.8844738932	-0.6630577159
H	1.0	-3.9142300457	-2.7218715821	1.2531111562
H	1.0	-5.2445773678	-1.8109302734	1.9500069556
H	1.0	-3.2834906858	1.3522248851	2.5045685207
H	1.0	-4.1146923404	0.2523079521	3.6119297459
H	1.0	-4.9292417573	0.8028631347	2.1616722210
H	1.0	-2.0351044718	-3.1210412290	4.5198509389
H	1.0	-1.9673154157	-3.5137599226	2.8079314153
H	1.0	-2.6821218833	-0.3136804581	4.7475810756
H	1.0	-1.2754753318	0.5381896628	4.1000167474
H	1.0	-1.0727097200	-0.7872021556	5.2520606888
H	1.0	0.2716508968	-2.2722545448	4.1464656276
H	1.0	0.6050414672	-0.9064007171	3.0783633579
H	1.0	0.2256703295	-2.4984841036	2.3937196252
H	1.0	-3.3584244395	-1.0443781452	-0.4557668766
H	1.0	-3.2287281402	0.6672411831	-0.0009747271
H	1.0	-4.7766215538	-0.1709670281	0.1210297022
H	1.0	-4.3100293550	-3.5446239156	3.5225719383
H	1.0	-4.1948614692	-1.9371336798	4.1992442997
H	1.0	0.3201509373	0.3650248612	1.1440816208
H	1.0	0.9983702267	0.2889755963	-0.4834600382
H	1.0	1.3430221646	-1.0091915869	0.6748145688

syndft3			E= -716.5321867009	
C	6.0	-0.3086153582	-0.8827962457	0.1831631873
C	6.0	0.9010404492	-2.6073608362	-1.2449990594
O	8.0	-0.8873783775	-3.2574089502	0.1620948229
O	8.0	-0.9397325584	-0.5399722780	1.4527105730
C	6.0	0.1937563095	-2.3336292969	0.0798166923
N	7.0	-1.9478641608	-1.4559382054	1.9554416193
C	6.0	-1.5849974981	-1.7292945901	3.3969278707
C	6.0	-3.3186995142	-0.8935285899	1.6589035183

C	6.0	-4.3479790025	-1.8477630374	2.3068299311
C	6.0	-3.5356252571	0.5643112003	2.1192312420
C	6.0	-2.6824634419	-2.6442954476	3.9834888965
C	6.0	-1.3913641975	-0.4630684400	4.2620942823
C	6.0	-0.2595835081	-2.5109949130	3.4156604280
C	6.0	-3.5413354692	-0.9405008566	0.1341404659
C	6.0	-4.0981970739	-2.1057091310	3.7910094685
C	6.0	0.8038079587	0.1550090835	0.0690275359
H	1.0	-1.0347995155	-0.7334609924	-0.6220655273
H	1.0	1.0925037575	-3.6800361277	-1.3183712190
H	1.0	1.8545870154	-2.0808975313	-1.3248961297
H	1.0	0.2646943979	-2.3235750223	-2.0887567368
H	1.0	-1.4672345539	-2.9072208780	0.8664992963
H	1.0	0.9047542656	-2.5079230703	0.9006454144
H	1.0	-4.3188752136	-2.8032683576	1.7695092898
H	1.0	-5.3447690606	-1.4254758355	2.1443254454
H	1.0	-2.6766170291	1.1768030873	1.8435194794
H	1.0	-3.6995580038	0.6599516645	3.1914482639
H	1.0	-4.4181264443	0.9693141392	1.6160710778
H	1.0	-2.4618763392	-2.7943078701	5.0452342912
H	1.0	-2.6059912735	-3.6266769965	3.5031070624
H	1.0	-0.7632258126	0.2596126248	3.7409944287
H	1.0	-0.8869606149	-0.7419859773	5.1914839956
H	1.0	-2.3272410976	0.0224631439	4.5331936745
H	1.0	-0.0542847094	-2.8448364546	4.4362223063
H	1.0	0.5707858132	-1.8828919887	3.0925780324
H	1.0	-0.3090039549	-3.3910843097	2.7715265075
H	1.0	-3.2317061503	-1.8996765746	-0.2841546550
H	1.0	-2.9982222696	-0.1436298612	-0.3765646002
H	1.0	-4.6047992960	-0.7962969929	-0.0762816172
H	1.0	-4.8272806817	-2.8279805698	4.1720902100
H	1.0	-4.2452600140	-1.1889886710	4.3711736497
H	1.0	1.6031948919	-0.0494658476	0.7865861541
H	1.0	0.4039909892	1.1491352046	0.2783470031
H	1.0	1.2280516039	0.1622405991	-0.9363365719

antidft1 E= -716.5237338996

C	6.0	-2.4239320413	-1.5662153963	0.6168612505
C	6.0	-1.5376485786	-0.3534349280	0.2562671268
O	8.0	-0.6160882437	-0.7237429390	-0.7751740131
O	8.0	-3.2787888740	-1.0911635403	1.6817356870
C	6.0	-3.1450020585	-2.1305121113	-0.5985806690
N	7.0	-4.3358493610	-1.9944435654	2.0856733148
C	6.0	-3.9305700033	-2.6851372615	3.3604268022
C	6.0	-5.6069111417	-1.1875747676	2.0844001329
C	6.0	-6.7424253425	-2.1017725673	2.5961933109
C	6.0	-5.5419230288	0.1246169989	2.9026028487
C	6.0	-5.1305934247	-3.5454240622	3.8188524172
C	6.0	-3.4488644207	-1.7536901975	4.4957683615
C	6.0	-2.7776707994	-3.6561869529	3.0365106084
C	6.0	-5.9370126842	-0.8130802592	0.6297536309
C	6.0	-6.4372872315	-2.7656646725	3.9359108848
C	6.0	-0.8021377161	0.2442005975	1.4518883560
H	1.0	-1.7591517047	-2.3450396194	1.0152034924
H	1.0	-2.1743873106	0.4102269670	-0.2002211504
H	1.0	0.0470068090	-1.3003176908	-0.3786292962

H	1.0	-3.7909751719	-2.9593846605	-0.3097292189
H	1.0	-2.3999162223	-2.4861741097	-1.3118514466
H	1.0	-3.7488990769	-1.3683945430	-1.0949770559
H	1.0	-6.9175076840	-2.8837474317	1.8481978763
H	1.0	-7.6583062203	-1.5042030922	2.6512020911
H	1.0	-6.4032212139	0.7514659821	2.6537247705
H	1.0	-4.6369037544	0.6787791648	2.6526935920
H	1.0	-5.5596134955	-0.0403948755	3.9788322283
H	1.0	-4.8645527808	-4.0144854903	4.7718652460
H	1.0	-5.2686598660	-4.3561550637	3.0936432056
H	1.0	-4.2590896628	-1.2146506384	4.9849651592
H	1.0	-2.7348611836	-1.0261210951	4.1084914897
H	1.0	-2.9435670660	-2.3491278984	5.2623833086
H	1.0	-2.6442891646	-4.3516471435	3.8701974411
H	1.0	-1.8318816061	-3.1307334542	2.8965312599
H	1.0	-2.9997952163	-4.2345385647	2.1373185828
H	1.0	-5.9502523617	-1.6994406530	-0.0059698569
H	1.0	-5.2145664921	-0.1022638114	0.2276094685
H	1.0	-6.9254355291	-0.3459524365	0.5916911063
H	1.0	-7.2524483592	-3.4421786104	4.2134931416
H	1.0	-6.3735805184	-2.0198047581	4.7344495415
H	1.0	-1.5012433201	0.6081745009	2.2053794784
H	1.0	-0.1709967600	1.0707855037	1.1171069933
H	1.0	-0.1590101177	-0.5088708534	1.9239685017

antidft2 E= -716.5270809529

C	6.0	-3.2040607483	-0.0024767455	0.4539795096
C	6.0	-1.9364150364	0.8594308680	0.6076375648
O	8.0	-1.3644951482	0.6621754620	1.9033542463
O	8.0	-4.1079679931	0.4871309144	1.4759677872
C	6.0	-3.7735030086	0.0052679288	-0.9603473044
N	7.0	-5.1601764061	-0.4447000464	1.8351458524
C	6.0	-4.7997811478	-1.1018683545	3.1450747974
C	6.0	-6.4604713331	0.3124343757	1.7650921464
C	6.0	-7.5822142383	-0.6523207120	2.2137502741
C	6.0	-6.5000753846	1.6274974657	2.5795232999
C	6.0	-5.9827647854	-2.0163368508	3.5389513021
C	6.0	-4.4487544541	-0.1324374092	4.2974331676
C	6.0	-3.5803714772	-2.0162064981	2.9171619735
C	6.0	-6.7342956950	0.6746539641	0.2963857089
C	6.0	-7.3298140430	-1.3013424752	3.5709840599
C	6.0	-2.1397502415	2.3498799427	0.3258853886
H	1.0	-2.9235175767	-1.0255723087	0.7045746633
H	1.0	-1.1933473821	0.4597700693	-0.0895497978
H	1.0	-2.0493472201	0.9090968233	2.5359315760
H	1.0	-4.6045394920	-0.6948423196	-1.0383323151
H	1.0	-2.9966913784	-0.3158386314	-1.6618695183
H	1.0	-4.1198441045	0.9943792364	-1.2648506514
H	1.0	-7.6744965983	-1.4402709866	1.4574224699
H	1.0	-8.5260003145	-0.0974898629	2.2112073416
H	1.0	-5.6134376590	2.2286818968	2.3742156840
H	1.0	-6.5678109580	1.4690539984	3.6545503459
H	1.0	-7.3772166975	2.2074951680	2.2792971799
H	1.0	-5.7509792942	-2.4658737973	4.5100952818
H	1.0	-6.0326941207	-2.8367941033	2.8139280356
H	1.0	-5.3225968192	0.3278155156	4.7562380147

H	1.0	-3.7950059588	0.6660818101	3.9436029644
H	1.0	-3.9164903057	-0.6778126567	5.0818814206
H	1.0	-3.4364374962	-2.6472309721	3.7991472875
H	1.0	-2.6616078340	-1.4487883269	2.7651630810
H	1.0	-3.7432079407	-2.6697208520	2.0568858308
H	1.0	-6.6880243198	-0.2116413308	-0.3385451942
H	1.0	-6.0216254652	1.4120730050	-0.0710296060
H	1.0	-7.7368598222	1.1034604565	0.2111013174
H	1.0	-8.1278269374	-2.0153058797	3.7990980497
H	1.0	-7.3548327646	-0.5524715239	4.3698060431
H	1.0	-2.4438102281	2.5304235413	-0.7085526816
H	1.0	-1.2022497105	2.8798233246	0.5062184740
H	1.0	-2.9063104609	2.7655268770	0.9846349289

antidft3 E= -716.5219547490

C	6.0	-0.7558237875	-1.8576343050	-0.1136634600
C	6.0	-0.1128022823	-3.2350005768	-2.1818182042
O	8.0	-0.0787244100	-4.2067995436	-0.0122487853
O	8.0	-1.4807401563	-2.1374945782	1.1130619966
C	6.0	0.6285631726	-1.2557327687	0.0873277934
N	7.0	-1.6454406674	-0.9962498923	2.0010034212
C	6.0	-1.1716790791	-1.4827885738	3.3628467114
C	6.0	-3.1182120054	-0.6216455711	1.9222138513
C	6.0	-4.0219046119	-1.7170190186	2.5334870303
C	6.0	-3.3447692781	0.7467657982	2.6007885371
C	6.0	-2.1151909324	-2.5651089420	3.9388859967
C	6.0	-1.0313900661	-0.2886902383	4.3326411172
C	6.0	0.2424191202	-2.0761856655	3.2333265654
C	6.0	-3.5119893728	-0.4290400353	0.4469485923
C	6.0	-3.5889953964	-2.1496311773	3.9372541148
C	6.0	-0.7608566235	-3.2332587151	-0.8052571777
H	1.0	-1.3512981376	-1.1708075863	-0.7234108611
H	1.0	-0.2306428493	-4.2204779272	-2.6368228167
H	1.0	0.9560623696	-3.0222322388	-2.1113378659
H	1.0	-0.5781270705	-2.4932569238	-2.8371001831
H	1.0	-0.5214350724	-4.2110002387	0.8440497614
H	1.0	0.5609949598	-0.3782636437	0.7308233338
H	1.0	1.0275172644	-0.9338464638	-0.8785157136
H	1.0	1.3218736668	-1.9754090012	0.5231455858
H	1.0	-3.9922904301	-2.5879339467	1.8706624816
H	1.0	-5.0577034483	-1.3599116373	2.5425969916
H	1.0	-2.5544481421	1.4463349326	2.3207533323
H	1.0	-3.3952799103	0.6994120693	3.6853212517
H	1.0	-4.2974591245	1.1570948081	2.2560718056
H	1.0	-1.7873056104	-2.8158127136	4.9537864687
H	1.0	-2.0014436115	-3.4746369055	3.3387286536
H	1.0	-1.9694390694	0.0418418292	4.7718866643
H	1.0	-0.5660439747	0.5610414285	3.8287479946
H	1.0	-0.3814474404	-0.5864502797	5.1592885726
H	1.0	0.5567679978	-2.4422467935	4.2145163903
H	1.0	0.9598720673	-1.3179289637	2.9141630470
H	1.0	0.2836714060	-2.9059386989	2.5322239790
H	1.0	-3.4274644545	-1.3537258603	-0.1225173478
H	1.0	-2.8990903984	0.3423947925	-0.0266760693
H	1.0	-4.5547501939	-0.1042908973	0.4011531364
H	1.0	-4.2095258575	-2.9875675295	4.2715538069

H	1.0	-3.7604609952	-1.3443530175	4.6601223731
H	1.0	-1.8159575640	-3.5259247896	-0.9096828734

antidft4 E= -716.5221894362

C	6.0	-0.5087267822	-1.4964027402	-0.0522086934
C	6.0	0.8198405410	-2.6534091346	-1.9168182988
O	8.0	-1.4987958315	-3.0874419282	-1.6240064577
O	8.0	-1.5921307796	-1.8909498278	0.8298232119
C	6.0	-0.3082339032	-2.7646802326	-0.9025694389
N	7.0	-1.9766295142	-0.8819898243	1.8046984253
C	6.0	-1.4901641601	-1.3989738778	3.1509072466
C	6.0	-3.4883264225	-0.7488868212	1.6680868028
C	6.0	-4.2182562135	-2.0259074959	2.1503223422
C	6.0	-3.9760463783	0.5004806700	2.4347755387
C	6.0	-2.2653917801	-2.6598267524	3.5965288989
C	6.0	-1.5834367792	-0.2745179133	4.2056368155
C	6.0	0.0039667810	-1.7546692995	3.0489957222
C	6.0	-3.8533278868	-0.5006710515	0.1945211596
C	6.0	-3.7849269333	-2.4856827257	3.5440753061
C	6.0	-0.7757887274	-0.2325806242	-0.8593575335
H	1.0	0.3931567943	-1.3442238025	0.5484591734
H	1.0	0.9518904356	-3.6125812512	-2.4216719360
H	1.0	1.7619493761	-2.3842483365	-1.4312156356
H	1.0	0.5861791095	-1.9033179945	-2.6753105133
H	1.0	-2.1985254596	-3.1588085672	-0.9647354174
H	1.0	-0.0791015535	-3.5798483715	-0.2003007179
H	1.0	-4.0157039699	-2.8281224123	1.4321002466
H	1.0	-5.2985923558	-1.8456472637	2.1222152588
H	1.0	-3.2951126436	1.3378079837	2.2698334833
H	1.0	-4.0865116521	0.3506982852	3.5059473410
H	1.0	-4.9590579171	0.7837657452	2.0499830942
H	1.0	-1.9425608545	-2.9347283707	4.6068044067
H	1.0	-1.9795743736	-3.4856039625	2.9363292882
H	1.0	-2.5840854321	-0.1217558768	4.6013205390
H	1.0	-1.2274937002	0.6700594447	3.7886581077
H	1.0	-0.9421886681	-0.5347760922	5.0514014164
H	1.0	0.3549467220	-2.0740627330	4.0336730622
H	1.0	0.5977393878	-0.8876535499	2.7473897709
H	1.0	0.1827439196	-2.5718945388	2.3519278744
H	1.0	-3.5062107291	-1.2981812035	-0.4576894982
H	1.0	-3.4388435514	0.4444100985	-0.1608279729
H	1.0	-4.9420469628	-0.4410685708	0.1131078979
H	1.0	-4.2748171213	-3.4335890597	3.7898944447
H	1.0	-4.1171524303	-1.7700775669	4.3042036346
H	1.0	-1.5454369475	-0.3941957691	-1.6146640418
H	1.0	0.1428916747	0.0792282666	-1.3632540332
H	1.0	-1.0815563272	0.5735950486	-0.1922603215

MP2 Optimizations: **1b**–**3b**

primemp2-1 E= -675.6819676697

C	6.0	0.0350552326	-0.9948554678	0.0625494124
C	6.0	0.3272557518	-2.4268320087	-0.3616931230

O	8.0	-0.8336369208	-3.2365858915	-0.4126817429
O	8.0	-0.4074869993	-0.8446207137	1.4333296612
C	6.0	1.2760287712	-0.1208575031	-0.0054934539
N	7.0	-1.4600521196	-1.7640265851	1.8189668332
C	6.0	-1.0121685387	-2.3852003949	3.1053731480
C	6.0	-2.7550923988	-1.0136792369	1.8356062617
C	6.0	-3.8300542677	-1.9913843097	2.3328352957
C	6.0	-2.7529435506	0.2829356176	2.6590933152
C	6.0	-2.1397381672	-3.3169644388	3.5726600472
C	6.0	-0.6182150515	-1.3868243837	4.2053613712
C	6.0	0.2154591233	-3.2498757931	2.8032161512
C	6.0	-3.0953746180	-0.6411094295	0.3871610236
C	6.0	-3.4907898784	-2.6196008995	3.6794688652
H	1.0	-0.7368382070	-0.6031026474	-0.6078306476
H	1.0	1.0955342615	-2.8503337008	0.2995264478
H	1.0	0.7443780068	-2.3898433600	-1.3744566826
H	1.0	-1.2947609092	-2.9870258879	0.4097397014
H	1.0	2.0714581350	-0.5414163103	0.6164397044
H	1.0	1.0477823653	0.8849326586	0.3543104203
H	1.0	1.6315173537	-0.0519268493	-1.0373874385
H	1.0	-3.9458004982	-2.7877966612	1.5848042246
H	1.0	-4.7809862693	-1.4458979460	2.3781663198
H	1.0	-1.8360870042	0.8453366374	2.4677985881
H	1.0	-2.8487542002	0.1132287727	3.7311108016
H	1.0	-3.6046102530	0.8957898691	2.3443629969
H	1.0	-1.8390745080	-3.7475938151	4.5359389295
H	1.0	-2.2219847172	-4.1457009721	2.8561876322
H	1.0	-1.4755718571	-0.9300242122	4.6985152923
H	1.0	0.0145671276	-0.5992412650	3.7900187389
H	1.0	-0.0437587662	-1.9216920307	4.9692577150
H	1.0	0.4504045637	-3.8488936503	3.6891840439
H	1.0	1.0826696144	-2.6281215544	2.5706139771
H	1.0	0.0175239382	-3.9267541416	1.9681483405
H	1.0	-2.9311364865	-1.4885896516	-0.2833555740
H	1.0	-2.4962894091	0.2073904497	0.0471528899
H	1.0	-4.1491153274	-0.3468391449	0.3374155388
H	1.0	-4.2643828336	-3.3433619373	3.9607546046
H	1.0	-3.4727204882	-1.8588512111	4.4675603690

primemp2-2 E= -675.6767583815

C	6.0	-0.0081544203	-0.7177598654	0.3128275920
C	6.0	0.5637088530	0.6263003129	-0.1145061805
O	8.0	-0.3944088803	1.6674919592	-0.0200811323
O	8.0	-0.4056278945	-0.4847972614	1.6799080891
C	6.0	0.9979037777	-1.8401236198	0.1350869701
N	7.0	-1.3826339890	-1.4441813954	2.1480456031
C	6.0	-0.8752038934	-1.9492599482	3.4601953764
C	6.0	-2.7144116734	-0.7600142109	2.1649755606
C	6.0	-3.7259436172	-1.7491713019	2.7626811470
C	6.0	-2.7629123549	0.5853918376	2.9138802565
C	6.0	-1.9401174662	-2.8991248907	4.0283715245
C	6.0	-0.4985654849	-0.8610136568	4.4799175320
C	6.0	0.3807636617	-2.7815165419	3.1940708054
C	6.0	-3.1343206134	-0.5008986161	0.7124116096

C	6.0	-3.3196874627	-2.2632982881	4.1378671969
H	1.0	-0.8993212830	-0.9280727541	-0.2815352628
H	1.0	0.8723357150	0.5721223573	-1.1616535438
H	1.0	1.4514975489	0.8440307816	0.4981246740
H	1.0	-0.7254949077	1.5977445698	0.8812857628
H	1.0	1.9040000896	-1.6536181328	0.7181212572
H	1.0	1.2727849920	-1.9072971287	-0.9232033455
H	1.0	0.5672804848	-2.7944397876	0.4366392454
H	1.0	-3.8173708660	-2.6017037594	2.0764742942
H	1.0	-4.7017988108	-1.2482911775	2.7964705095
H	1.0	-3.5987468327	1.1788769787	2.5287481985
H	1.0	-1.8413555329	1.1496185200	2.7547555150
H	1.0	-2.9105783852	0.4704572125	3.9880003365
H	1.0	-1.5862819162	-3.2531106020	5.0048066581
H	1.0	-2.0048563174	-3.7726347680	3.3658554372
H	1.0	-1.3629815043	-0.3723977387	4.9280391005
H	1.0	0.1293847644	-0.1032150524	4.0053737729
H	1.0	0.0769981776	-1.3240505748	5.2888559984
H	1.0	0.6779925326	-3.2813521992	4.1221457416
H	1.0	1.2085099392	-2.1522866986	2.8628982604
H	1.0	0.1787015169	-3.5438717497	2.4380620273
H	1.0	-3.0294523002	-1.4139787066	0.1192738512
H	1.0	-2.5480541046	0.2987786564	0.2548191516
H	1.0	-4.1865010562	-0.1966181052	0.7015360430
H	1.0	-4.0473186869	-3.0022825000	4.4929734548
H	1.0	-3.3151717992	-1.4508221539	4.8727009117

primemp2-3 E= -675.6819673827

C	6.0	0.3515335796	-1.3778245490	0.5206465502
C	6.0	-0.4550149436	-2.0485338916	-0.5818323338
O	8.0	-1.0633663018	-3.2573063128	-0.1644118429
O	8.0	-0.4341096452	-0.8672972744	1.6247745050
C	6.0	1.0887451825	-0.1494746734	0.0144429887
N	7.0	-1.4069558506	-1.8087864956	2.1433921843
C	6.0	-0.8761148825	-2.3736267968	3.4238968133
C	6.0	-2.7043534502	-1.0646091595	2.2092913621
C	6.0	-3.7412508748	-2.0192898061	2.8188457940
C	6.0	-2.6504809717	0.2669245249	2.9748930128
C	6.0	-1.9661871500	-3.2955329614	3.9899299015
C	6.0	-0.4250399651	-1.3361203196	4.4628519774
C	6.0	0.3399582166	-3.2428475568	3.0800310104
C	6.0	-3.1385734706	-0.7561323451	0.7731126674
C	6.0	-3.3103291170	-2.5976242808	4.1615747464
H	1.0	1.0669185033	-2.1143897754	0.9005922362
H	1.0	0.2400136732	-2.2959060138	-1.3922058312
H	1.0	-1.1891198646	-1.3342123459	-0.9787959491
H	1.0	-1.4178860836	-3.0172677469	0.7119381996
H	1.0	1.6141637702	0.3395854513	0.8378128705
H	1.0	0.3834226745	0.5642123531	-0.4209911486
H	1.0	1.8192984807	-0.4362453901	-0.7470621936
H	1.0	-3.9083665036	-2.8440656338	2.1126549566
H	1.0	-4.6872389356	-1.4709074896	2.9090491521
H	1.0	-1.7678366937	0.8372472445	2.6768856443
H	1.0	-2.6429364012	0.1408611832	4.0570179895
H	1.0	-3.5399861620	0.8513181095	2.7164536155
H	1.0	-1.6019587371	-3.6946789511	4.9448475433

H	1.0	-2.0890121320	-4.1465390244	3.3059068245
H	1.0	-1.2522866705	-0.8889665532	5.0132147089
H	1.0	0.1482440269	-0.5441689381	3.9753695303
H	1.0	0.2252231832	-1.8334549019	5.1906707270
H	1.0	0.5727052866	-3.8793964362	3.9403088574
H	1.0	1.2190299066	-2.6270816681	2.8738167572
H	1.0	0.1345496232	-3.8772135111	2.2139222818
H	1.0	-3.1151013305	-1.6593421226	0.1580520289
H	1.0	-2.4959956660	0.0056558692	0.3263747558
H	1.0	-4.1641460042	-0.3728332202	0.7903611146
H	1.0	-4.0604808863	-3.3122661139	4.5192469850
H	1.0	-3.2427174132	-1.8091424766	4.9190890062

synmp2-1 E= -714.8850755986

C	6.0	0.2056288729	0.1052791483	1.7072219945
C	6.0	-0.0991656502	1.2004139169	2.7284799780
O	8.0	-0.6456015407	0.6493906709	3.9192613101
O	8.0	-0.9577695761	-0.5962081659	1.1961349054
C	6.0	0.8544212327	0.6367015019	0.4387969493
N	7.0	-1.8770518421	-1.0634521528	2.2137348311
C	6.0	-1.6725180025	-2.5351132320	2.3942806265
C	6.0	-3.2359811896	-0.6073097088	1.7810286235
C	6.0	-4.2396835505	-1.1417568834	2.8128108810
C	6.0	-3.2585634177	0.9226645193	1.8515864058
C	6.0	-2.7194090479	-3.0074877073	3.4139737556
C	6.0	-0.2863179802	-2.7395578674	3.0183211652
C	6.0	-1.7282650338	-3.3689840887	1.1056903606
C	6.0	-3.6308507032	-1.0125651060	0.3521292687
C	6.0	-4.1467582201	-2.6494478558	3.0166874015
C	6.0	1.1634683839	1.9482154619	3.1310131125
H	1.0	0.8707114754	-0.6137042015	2.1990161094
H	1.0	-0.8044619291	1.9091158812	2.2693437439
H	1.0	-1.2622416805	-0.0321173676	3.5834645484
H	1.0	0.8917942317	-0.1582602507	-0.3100424434
H	1.0	1.8736624017	0.9751714977	0.6367971068
H	1.0	0.2736774534	1.4706423076	0.0328476666
H	1.0	-5.2444176369	-0.8477811443	2.4843806470
H	1.0	-4.0493719770	-0.6397009693	3.7712350861
H	1.0	-4.2893065426	1.2653876147	1.7131199657
H	1.0	-2.6434509719	1.3579576896	1.0610900811
H	1.0	-2.9021648419	1.2718044871	2.8239656724
H	1.0	-2.4904759625	-2.5443969041	4.3836753684
H	1.0	-2.6014951493	-4.0917336389	3.5341541808
H	1.0	-0.1168116272	-2.0329697893	3.8349938917
H	1.0	0.5034053234	-2.6224288102	2.2718881060
H	1.0	-0.2248326724	-3.7597051003	3.4120837489
H	1.0	-1.2567448515	-4.3387052915	1.2988510856
H	1.0	-1.1696977043	-2.8678691918	0.3116749149
H	1.0	-2.7435795044	-3.5604298735	0.7597293999
H	1.0	-3.9303851299	-2.0567224808	0.2682902402
H	1.0	-2.8032293100	-0.8233114599	-0.3352276024
H	1.0	-4.4826469187	-0.3983097762	0.0410730837
H	1.0	-4.4397908977	-3.1822938935	2.1054219872
H	1.0	-4.8439961626	-2.9646832098	3.8014862529
H	1.0	0.9255803544	2.5788574526	3.9909746395
H	1.0	1.5416130348	2.5808203543	2.3243888709

H	1.0	1.9422844608	1.2403236172	3.4325720790

synmp2-2 E= -714.8759649245

C	6.0	-0.6984322940	-1.0506353597	-0.1387246467
C	6.0	0.2235092614	-1.7213798701	-2.4044759808
O	8.0	-1.6838978056	-2.7880749340	-1.5009300892
O	8.0	-1.4400330274	-1.7064122040	0.9116306473
C	6.0	-0.4464948986	-2.1888502681	-1.1250975558
N	7.0	-1.9046198121	-0.7751622121	1.9254092540
C	6.0	-1.5009424400	-1.4246942557	3.2263552741
C	6.0	-3.3944468128	-0.6637754513	1.7159540341
C	6.0	-4.1210097667	-1.9893100430	1.9911835230
C	6.0	-3.9557088841	0.4725072025	2.5852373285
C	6.0	-2.2574725965	-2.7407929105	3.4688856265
C	6.0	-1.7002208463	-0.4404856079	4.3893329167
C	6.0	0.0001947093	-1.7296355843	3.1898709952
C	6.0	-3.6659612294	-0.2527730707	0.2644238114
C	6.0	-3.7720395343	-2.5852311365	3.3528929124
C	6.0	0.5670637009	-0.3577585364	0.3325229126
H	1.0	-1.3497886870	-0.3186906163	-0.6272103077
H	1.0	0.2489358570	-2.5522908491	-3.1133078503
H	1.0	1.2466078612	-1.3856209565	-2.2216033971
H	1.0	-0.3500544641	-0.9041491360	-2.8520801295
H	1.0	-2.1322614660	-2.9478939839	-0.6624613184
H	1.0	0.1922286303	-2.9330691904	-0.6216922454
H	1.0	-3.8417652271	-2.7059773268	1.2081825402
H	1.0	-5.2020023209	-1.8197669045	1.9026134017
H	1.0	-3.2774414665	1.3301463770	2.5660942354
H	1.0	-4.1368012727	0.1882664026	3.6198022511
H	1.0	-4.9161906691	0.7837834581	2.1627752192
H	1.0	-1.9797502496	-3.1242790514	4.4593587233
H	1.0	-1.9151425272	-3.4737081621	2.7272333771
H	1.0	-2.7247048309	-0.3859761575	4.7519143254
H	1.0	-1.3738995994	0.5611409986	4.0954915969
H	1.0	-1.0785098414	-0.7724126515	5.2268617432
H	1.0	0.2704178525	-2.2149119190	4.1335018640
H	1.0	0.5818838451	-0.8084245996	3.1016594060
H	1.0	0.2556630497	-2.3996844858	2.3700327382
H	1.0	-3.3225010537	-1.0005525163	-0.4503728902
H	1.0	-3.1926764469	0.7086748065	0.0403429554
H	1.0	-4.7475105092	-0.1372859792	0.1399732549
H	1.0	-4.2575935924	-3.5612910777	3.4680753071
H	1.0	-4.1570228856	-1.9510924172	4.1599741195
H	1.0	0.3231404153	0.3215607008	1.1504895788
H	1.0	0.9865894465	0.2312042190	-0.4882112798
H	1.0	1.3181024281	-1.0772047405	0.6697518177

synmp2-3 E= -714.8850752808

C	6.0	-0.3364147632	-0.9061496236	0.1878372711
C	6.0	0.8820782240	-2.6283127528	-1.1871779737
O	8.0	-0.9124319001	-3.2685014527	0.2092707024
O	8.0	-0.9485870354	-0.5244419793	1.4472341167
C	6.0	0.1668481472	-2.3477515287	0.1262083608
N	7.0	-1.9425722814	-1.4546640662	1.9428180711
C	6.0	-1.5843682534	-1.7157505546	3.3730200550

C	6.0	-3.2995337410	-0.8858603948	1.6678964899
C	6.0	-4.3204056727	-1.8549805514	2.2824102650
C	6.0	-3.5221751091	0.5511359793	2.1624584029
C	6.0	-2.6586653677	-2.6538804810	3.9418713776
C	6.0	-1.4224544041	-0.4575247005	4.2404599183
C	6.0	-0.2485968679	-2.4652974924	3.3897076601
C	6.0	-3.5068000323	-0.8898723516	0.1480340625
C	6.0	-4.0762477215	-2.1230071450	3.7629306735
C	6.0	0.7752173956	0.1202217974	0.0365641201
H	1.0	-1.0703127028	-0.7895579974	-0.6177497143
H	1.0	1.0489927490	-3.7056288325	-1.2600655775
H	1.0	1.8462369622	-2.1178613736	-1.2475988416
H	1.0	0.2557091765	-2.3225350758	-2.0313984793
H	1.0	-1.4857367813	-2.8734995790	0.8968780529
H	1.0	0.8715204010	-2.4993247556	0.9574534512
H	1.0	-4.2686622989	-2.8050981412	1.7330756357
H	1.0	-5.3203514329	-1.4354322810	2.1151117061
H	1.0	-2.6508550151	1.1667220184	1.9269119560
H	1.0	-3.7225610998	0.6130933306	3.2316912023
H	1.0	-4.3894718269	0.9680958048	1.6391405478
H	1.0	-2.4290307861	-2.8205940464	5.0016952274
H	1.0	-2.5741170463	-3.6237531083	3.4329021381
H	1.0	-0.8269964897	0.2902970633	3.7118178670
H	1.0	-0.8900444680	-0.7349807457	5.1565009169
H	1.0	-2.3723630523	-0.0120831360	4.5341366037
H	1.0	-0.0577435855	-2.8205447701	4.4077858742
H	1.0	0.5714959003	-1.8059662887	3.0972600805
H	1.0	-0.2790847413	-3.3276107549	2.7189571474
H	1.0	-3.1825900979	-1.8381897251	-0.2883887069
H	1.0	-2.9606770517	-0.0706472996	-0.3265298098
H	1.0	-4.5720988354	-0.7469465033	-0.0622747494
H	1.0	-4.8004095224	-2.8569493182	4.1348077301
H	1.0	-4.2251914161	-1.2106538025	4.3508322589
H	1.0	1.5907555934	-0.0941724510	0.7339950596
H	1.0	0.3821801274	1.1158042802	0.2565924756
H	1.0	1.1680167240	0.1195547865	-0.9824136258

antimp2-1 E= -714.8749345431

C	6.0	-2.4410148264	-1.5885802645	0.6184662855
C	6.0	-1.5720754470	-0.3820640973	0.2475667128
O	8.0	-0.6407506617	-0.7582594909	-0.7657079560
O	8.0	-3.2708527996	-1.1028471597	1.6898274740
C	6.0	-3.1854833848	-2.1462019268	-0.5809892729
N	7.0	-4.3279192377	-2.0088858761	2.0714861451
C	6.0	-3.9297081994	-2.6677360014	3.3500012924
C	6.0	-5.5758772431	-1.1896462455	2.0907453049
C	6.0	-6.7127778395	-2.1033087696	2.5705691257
C	6.0	-5.5059793919	0.0963582107	2.9328284429
C	6.0	-5.1100686113	-3.5472295873	3.7886682624
C	6.0	-3.4882597058	-1.7267332725	4.4833984458
C	6.0	-2.7498426048	-3.5981717929	3.0424831968
C	6.0	-5.8857943674	-0.7790812365	0.6487803056
C	6.0	-6.4186357925	-2.7748351810	3.9066934062
C	6.0	-0.8556399283	0.2165542629	1.4490557486
H	1.0	-1.7666016759	-2.3665244014	1.0067256521
H	1.0	-2.2127503943	0.3729944780	-0.2211008195

H	1.0	-0.0138302090	-1.3501165127	-0.3371613891
H	1.0	-3.8578073258	-2.9470147407	-0.2705860630
H	1.0	-2.4522249950	-2.5371795419	-1.2898961481
H	1.0	-3.7611650256	-1.3638606998	-1.0807215037
H	1.0	-6.8708963030	-2.8802280309	1.8106944331
H	1.0	-7.6290735772	-1.5018133310	2.6216936485
H	1.0	-6.3431483439	0.7448518086	2.6524648516
H	1.0	-4.5757336207	0.6309910167	2.7271284501
H	1.0	-5.5777969200	-0.0875821270	4.0044165274
H	1.0	-4.8401965046	-4.0194918508	4.7417730479
H	1.0	-5.2347504937	-4.3482439433	3.0475540622
H	1.0	-4.3230770107	-1.2495581985	4.9961262326
H	1.0	-2.8243401841	-0.9531671702	4.0900595376
H	1.0	-2.9339743788	-2.3094741943	5.2276811105
H	1.0	-2.6175917672	-4.2954577215	3.8769209905
H	1.0	-1.8200525032	-3.0353685444	2.9284742007
H	1.0	-2.9421402144	-4.1704263968	2.1303583577
H	1.0	-5.8955044379	-1.6544439227	-0.0042442252
H	1.0	-5.1506183736	-0.0612647161	0.2783161439
H	1.0	-6.8737418850	-0.3072527453	0.6185999716
H	1.0	-7.2347040117	-3.4570364207	4.1720148715
H	1.0	-6.3588119883	-2.0319406622	4.7097428604
H	1.0	-1.5661087655	0.6110199165	2.1774999621
H	1.0	-0.1917696513	1.0179221191	1.1144117737
H	1.0	-0.2497293985	-0.5530250382	1.9438305432

antimp2-2 E= -714.8788499577

C	6.0	-3.2093746730	-0.0256394496	0.4670616059
C	6.0	-1.9585697270	0.8447498787	0.6188630259
O	8.0	-1.4073935151	0.6688366164	1.9221140848
O	8.0	-4.1014860404	0.4774754967	1.4830077245
C	6.0	-3.7876082145	-0.0205391585	-0.9371851557
N	7.0	-5.1514056042	-0.4626345859	1.8138992273
C	6.0	-4.8016318316	-1.0931056844	3.1261426817
C	6.0	-6.4290367584	0.3116682073	1.7659816881
C	6.0	-7.5555519499	-0.6394545667	2.1958341288
C	6.0	-6.4468618154	1.6050325528	2.5988119595
C	6.0	-5.9726189039	-2.0082943089	3.5143771386
C	6.0	-4.4719847838	-0.1153218307	4.2695265172
C	6.0	-3.5754533969	-1.9900176622	2.9135563432
C	6.0	-6.6919875184	0.7036860081	0.3105385581
C	6.0	-7.3127611042	-1.2850640857	3.5538755230
C	6.0	-2.2054562147	2.3223644258	0.3298405216
H	1.0	-2.9262231774	-1.0478046533	0.7267791502
H	1.0	-1.2009199069	0.4557311924	-0.0703435897
H	1.0	-2.1427870527	0.8616393165	2.5147257024
H	1.0	-4.6150381727	-0.7277139177	-1.0036042373
H	1.0	-3.0086280379	-0.3364837366	-1.6403445804
H	1.0	-4.1411403895	0.9692536806	-1.2315211827
H	1.0	-7.6411653448	-1.4294228470	1.4377351154
H	1.0	-8.4947533743	-0.0721363602	2.1871120005
H	1.0	-5.5438743396	2.1898254660	2.4075597909
H	1.0	-6.5309241825	1.4272873580	3.6702552612
H	1.0	-7.3118458556	2.2040885976	2.2938896647
H	1.0	-5.7345820927	-2.4595665642	4.4860106796
H	1.0	-6.0285971804	-2.8218013603	2.7788013474

H	1.0	-5.3593260458	0.2615229690	4.7786440568
H	1.0	-3.9037145086	0.7389435073	3.8944532331
H	1.0	-3.8593399127	-0.6326335935	5.0154360105
H	1.0	-3.4413109067	-2.6146231510	3.8033700182
H	1.0	-2.6633196926	-1.4066468342	2.7707208021
H	1.0	-3.7289283238	-2.6430240244	2.0494842910
H	1.0	-6.6357888664	-0.1737480951	-0.3375418636
H	1.0	-5.9758423595	1.4529271951	-0.0310888643
H	1.0	-7.6982824533	1.1293644656	0.2351692058
H	1.0	-8.1161638856	-1.9951807945	3.7818172335
H	1.0	-7.3264204402	-0.5319873483	4.3494234404
H	1.0	-2.4931617115	2.4873593129	-0.7122348104
H	1.0	-1.2891521597	2.8819759382	0.5318936754
H	1.0	-3.0013275751	2.7039224279	0.9754028768

antimp2-3 E= -714.8748580623

C	6.0	-0.7955282551	-1.8610813037	-0.1025392919
C	6.0	-0.0659402422	-3.2313532583	-2.1185819979
O	8.0	-0.1791563657	-4.2055813908	0.0388188906
O	8.0	-1.5133366739	-2.1456184329	1.1176309647
C	6.0	0.5921984830	-1.2809776211	0.1042947912
N	7.0	-1.6435712190	-0.9872150072	1.9831709794
C	6.0	-1.1688583171	-1.4742746279	3.3296908202
C	6.0	-3.1060394699	-0.6272838652	1.9256003088
C	6.0	-3.9961012886	-1.7275450483	2.5235435945
C	6.0	-3.3389169885	0.7257534236	2.6150558346
C	6.0	-2.0907529806	-2.5637353508	3.9013977770
C	6.0	-1.0366475550	-0.2912742700	4.3017296504
C	6.0	0.2435766710	-2.0510980159	3.1850470640
C	6.0	-3.5015628797	-0.4264413086	0.4590043005
C	6.0	-3.5592289346	-2.1439709541	3.9263269802
C	6.0	-0.8004055974	-3.2286402782	-0.7911678096
H	1.0	-1.3857076897	-1.1657193702	-0.7106731760
H	1.0	-0.1879707133	-4.2037523012	-2.6012556578
H	1.0	1.0009209527	-3.0588452803	-1.9606330408
H	1.0	-0.4608804758	-2.4564040815	-2.7824240294
H	1.0	-0.6583876745	-4.1508925047	0.8731314012
H	1.0	0.5306059770	-0.4282623612	0.7816587805
H	1.0	0.9808309809	-0.9283023673	-0.8558725904
H	1.0	1.2774062851	-2.0279899738	0.5074767030
H	1.0	-3.9468297022	-2.6015094852	1.8622902831
H	1.0	-5.0358631943	-1.3751701461	2.5257459706
H	1.0	-2.5441673617	1.4271482039	2.3456804872
H	1.0	-3.4011079364	0.6625802460	3.6994036255
H	1.0	-4.2913765247	1.1315996398	2.2599492542
H	1.0	-1.7415829947	-2.8212717706	4.9097788661
H	1.0	-1.9880726494	-3.4638536919	3.2817741860
H	1.0	-1.9742671594	0.0048134527	4.7679887889
H	1.0	-0.6067546261	0.5728666750	3.7875069706
H	1.0	-0.3549953974	-0.5860525500	5.1058325613
H	1.0	0.5541859811	-2.4373741749	4.1613752591
H	1.0	0.9504192898	-1.2732339857	2.8851943720
H	1.0	0.2851714600	-2.8641986859	2.4624420222
H	1.0	-3.4149028095	-1.3517107724	-0.1121178602
H	1.0	-2.8862814098	0.3512320496	-0.0046933533
H	1.0	-4.5469235259	-0.1033325154	0.4244547024

H	1.0	-4.1790065625	-2.9772265086	4.2774596032
H	1.0	-3.7121147043	-1.3236926538	4.6373245469
H	1.0	-1.8544762017	-3.5005377766	-0.9575015329

antimp2-4 E= -714.8748585729

C	6.0	-0.5049158113	-1.5299618364	-0.0127448150
C	6.0	0.7303506323	-2.6421141091	-1.9393372882
O	8.0	-1.5662625764	-3.0813984648	-1.5502106928
O	8.0	-1.5845454715	-1.9160926155	0.8651308993
C	6.0	-0.3457127495	-2.7827862991	-0.8790688600
N	7.0	-1.9546614223	-0.8717936342	1.8035056621
C	6.0	-1.4942752957	-1.3806493917	3.1454423703
C	6.0	-3.4514312328	-0.7537181610	1.6561933028
C	6.0	-4.1727057513	-2.0350175852	2.1050872679
C	6.0	-3.9625737309	0.4723371988	2.4290545967
C	6.0	-2.2496927513	-2.6482495366	3.5728336510
C	6.0	-1.6163987077	-0.2670994499	4.1966894333
C	6.0	-0.0013600859	-1.7128516673	3.0552699632
C	6.0	-3.7912720411	-0.4874701534	0.1858674247
C	6.0	-3.7664242990	-2.4830761002	3.5077021579
C	6.0	-0.7625700711	-0.2616870200	-0.8067349598
H	1.0	0.4085534495	-1.4006468819	0.5794985324
H	1.0	0.8601360191	-3.5955697248	-2.4566414130
H	1.0	1.6843830165	-2.3531822259	-1.4881280822
H	1.0	0.4391693907	-1.8898892248	-2.6758053584
H	1.0	-2.2208054726	-3.1338851000	-0.8448881051
H	1.0	-0.0837169273	-3.6108187589	-0.2018164114
H	1.0	-3.9329075516	-2.8345174187	1.3922482032
H	1.0	-5.2554635351	-1.8628652440	2.0488999648
H	1.0	-3.2746413753	1.3126954872	2.3004080595
H	1.0	-4.1096022913	0.2948975385	3.4926606354
H	1.0	-4.9337412005	0.7571229192	2.0118922006
H	1.0	-1.9288104742	-2.9231034453	4.5861665085
H	1.0	-1.9522423809	-3.4634926235	2.9016161477
H	1.0	-2.6223939727	-0.1427802003	4.5920134397
H	1.0	-1.2801491851	0.6852094188	3.7768214639
H	1.0	-0.9666104668	-0.5200104651	5.0404716971
H	1.0	0.3439733447	-2.0219231037	4.0470986419
H	1.0	0.5734737996	-0.8324450378	2.7503902437
H	1.0	0.1876942882	-2.5328009161	2.3611273022
H	1.0	-3.4138334423	-1.2678904243	-0.4725758932
H	1.0	-3.3871199908	0.4755342221	-0.1367427093
H	1.0	-4.8814811421	-0.4497560165	0.0910390133
H	1.0	-4.2554041948	-3.4334291653	3.7515890449
H	1.0	-4.1079890024	-1.7585534303	4.2562031671
H	1.0	-1.5239415250	-0.4212718526	-1.5716431608
H	1.0	0.1657302865	0.0519547790	-1.2938620759
H	1.0	-1.0772680987	0.5321257205	-0.1279911698

antimp2-5 E= -714.8791740110

C	6.0	-3.0515112368	0.0083881787	0.6569451213
C	6.0	-2.1894035075	1.2619506235	0.4830759262
O	8.0	-2.9898782736	2.3628646864	0.0659201208
O	8.0	-3.9896175495	0.4383685484	1.6735034364
C	6.0	-3.6876701779	-0.4784736817	-0.6317887050

N	7.0	-5.1004596171	-0.4541303354	1.8860997155
C	6.0	-4.8587096737	-1.1832737913	3.1653074630
C	6.0	-6.3307775323	0.3870906768	1.8008215699
C	6.0	-7.5277494428	-0.5239975750	2.1100471382
C	6.0	-6.3390255148	1.6318518275	2.7061595332
C	6.0	-6.0936520555	-2.0579913542	3.4250881179
C	6.0	-4.5340942669	-0.3053030399	4.3850528426
C	6.0	-3.6639124837	-2.1171526685	2.9393234242
C	6.0	-6.4722914374	0.8616474379	0.3514498345
C	6.0	-7.3943134574	-1.2632492167	3.4362390400
C	6.0	-1.0880253475	1.0870475493	-0.5455169850
H	1.0	-2.4188603859	-0.7862760507	1.0704797762
H	1.0	-1.7408086915	1.4802547003	1.4645677952
H	1.0	-3.6913924784	2.4093774142	0.7250924497
H	1.0	-4.4668187173	-1.2063547400	-0.4029229302
H	1.0	-2.9245668257	-0.9675222771	-1.2446470389
H	1.0	-4.1135357512	0.3514677939	-1.1972608625
H	1.0	-7.6129800639	-1.2616795384	1.3011052571
H	1.0	-8.4345900578	0.0934239290	2.0883733698
H	1.0	-5.3810903671	2.1543640795	2.6481182815
H	1.0	-6.5422229919	1.3990996915	3.7511530026
H	1.0	-7.1229324628	2.3142594543	2.3605913478
H	1.0	-5.9396580194	-2.5813624229	4.3771860052
H	1.0	-6.1477305754	-2.8194150570	2.6353468453
H	1.0	-5.4145082993	0.1644804975	4.8230543369
H	1.0	-3.8186280347	0.4717371981	4.1059019692
H	1.0	-4.0761756888	-0.9326448220	5.1578376623
H	1.0	-3.6274371440	-2.8550092642	3.7480825126
H	1.0	-2.7213884503	-1.5641667590	2.9493116854
H	1.0	-3.7658531084	-2.6424822644	1.9853031960
H	1.0	-6.4507960054	0.0105389697	-0.3325217458
H	1.0	-5.6752051140	1.5546748894	0.0758956378
H	1.0	-7.4316639282	1.3774026746	0.2382629076
H	1.0	-8.2461796466	-1.9389110600	3.5758780985
H	1.0	-7.4117521894	-0.5607837051	4.2767633450
H	1.0	-0.4707639747	0.2150559364	-0.3092678984
H	1.0	-0.4523082924	1.9753815607	-0.5547848050
H	1.0	-1.5175411612	0.9630713059	-1.5420977946

antimp2-6 E= -714.8760611173

C	6.0	0.1560304812	0.0955340223	1.9621550207
C	6.0	-0.0491866463	1.1402586054	3.0672876428
O	8.0	-0.8756839545	0.6296835601	4.1074445369
O	8.0	-1.0390575350	-0.4503203806	1.3480885561
C	6.0	0.9369088941	0.6329076100	0.7740917916
N	7.0	-1.9696195265	-1.0770483304	2.2784403992
C	6.0	-1.6912433556	-2.5505937327	2.3552821778
C	6.0	-3.3295205490	-0.6796798282	1.7829595428
C	6.0	-4.3657913856	-1.3473639036	2.6970235547
C	6.0	-3.4668846082	0.8351148794	1.9495673312
C	6.0	-2.7842709313	-3.1657084028	3.2458725545
C	6.0	-0.3601374765	-2.7680795660	3.0912477219
C	6.0	-1.5949273885	-3.2713200048	1.0029996768
C	6.0	-3.6038044501	-1.0034115259	0.3048065065
C	6.0	-4.2006539638	-2.8584492965	2.7809489715
C	6.0	-0.5076389875	2.5198954468	2.6001894396

H	1.0	0.7171843683	-0.7207581143	2.4188975973
H	1.0	0.9542926797	1.2681737571	3.5022398411
H	1.0	-1.4465279120	-0.0314066686	3.6680706582
H	1.0	1.8640866243	1.1024449597	1.1157640299
H	1.0	0.3440781140	1.3734686776	0.2322730385
H	1.0	1.1875303950	-0.1813692705	0.0899537767
H	1.0	-5.3604121165	-1.0767563243	2.3215985957
H	1.0	-4.2675099967	-0.9178326873	3.7032894510
H	1.0	-3.1333883822	1.1549072232	2.9390652239
H	1.0	-4.5206582171	1.1067543464	1.8270265542
H	1.0	-2.8886770928	1.3580080097	1.1866214951
H	1.0	-2.6517109965	-2.7787688043	4.2655421419
H	1.0	-2.6047926842	-4.2474387377	3.2822310308
H	1.0	-0.2706848317	-2.0939762216	3.9470767793
H	1.0	0.4964434171	-2.6315635651	2.4270752202
H	1.0	-0.3307618972	-3.8021032254	3.4514124805
H	1.0	-1.0828399077	-4.2277895173	1.1543987932
H	1.0	-1.0068628529	-2.6735575223	0.3024061260
H	1.0	-2.5660454102	-3.4851305613	0.5580939659
H	1.0	-3.8427627028	-2.0514501561	0.1283709040
H	1.0	-2.7444667526	-0.7252126440	-0.3091689196
H	1.0	-4.4646994966	-0.4101317630	-0.0218754491
H	1.0	-4.9255182667	-3.2788792280	3.4874768099
H	1.0	-4.4014257441	-3.3260055876	1.8108163188
H	1.0	-0.7298119952	3.1211000364	3.4856970195
H	1.0	-1.4030176059	2.4724586231	1.9822498426
H	1.0	0.2813706463	3.0226558132	2.0324612498

Structures of **1b**–**3b** containing less favorable hydrogen bond patterns were optimized using the same optimization methods described above.

RHF Optimizations: **1b**–**3b** (alternate hydrogen bond)

prime5tmp E= -673.2433032443

C	6.0	-3.0831908405	0.0210439923	0.6683504226
C	6.0	-2.1784261107	1.2370884957	0.5198503680
O	8.0	-2.8560627152	2.3646191639	0.0431308281
O	8.0	-4.0319403669	0.4283039907	1.6479367251
C	6.0	-3.6596311849	-0.4466187853	-0.6594291822
N	7.0	-5.1077577802	-0.4242793758	1.9099451369
C	6.0	-4.8521281010	-1.1799628310	3.1662874211
C	6.0	-6.3533724694	0.3843599764	1.8020464461
C	6.0	-7.5447528595	-0.5309545923	2.1321848787
C	6.0	-6.3791198289	1.6519065147	2.6822171765
C	6.0	-6.0912806783	-2.0475341379	3.4512315488
C	6.0	-4.4903225546	-0.3145076041	4.3897177958
C	6.0	-3.6792018137	-2.1452495852	2.9309743251
C	6.0	-6.5184264672	0.8358498499	0.3452399000
C	6.0	-7.4003136016	-1.2711721512	3.4541380140
H	1.0	-2.4770044432	-0.7806128734	1.0727774024
H	1.0	-1.7111247077	1.4492707052	1.4792192297
H	1.0	-3.5277829710	2.5836050172	0.6644578041

H	1.0	-4.3761979138	-1.2433100314	-0.5127830197
H	1.0	-2.8444265257	-0.8321159200	-1.2663090007
H	1.0	-4.1282628259	0.3621863356	-1.2028113835
H	1.0	-7.6452755064	-1.2628857946	1.3342819858
H	1.0	-8.4490228859	0.0713291938	2.1238989876
H	1.0	-5.4535221829	2.2055833647	2.5901402793
H	1.0	-6.5431979714	1.4448452346	3.7296751039
H	1.0	-7.1886663683	2.2961035632	2.3525012933
H	1.0	-5.9403101886	-2.5509843252	4.4021343925
H	1.0	-6.1485418140	-2.8217520118	2.6893796451
H	1.0	-5.3385124440	0.1963700940	4.8219002389
H	1.0	-3.7440983385	0.4243471247	4.1266983428
H	1.0	-4.0725033904	-0.9524647867	5.1633754108
H	1.0	-3.6560377331	-2.8814767462	3.7288692696
H	1.0	-2.7249511293	-1.6336204789	2.9412199674
H	1.0	-3.7897233165	-2.6699329798	1.9885704852
H	1.0	-6.4764667136	-0.0092115311	-0.3299653953
H	1.0	-5.7587218163	1.5490182913	0.0545899562
H	1.0	-7.4855970862	1.3152551443	0.2270582918
H	1.0	-8.2337766261	-1.9559594571	3.5861190104
H	1.0	-7.4387081059	-0.5809403272	4.2913322842
H	1.0	-1.3930096228	1.0163202742	-0.1931723865

syn5tmp E= -712.2904114082

C	6.0	-3.0858105485	0.0594691885	0.7007839667
C	6.0	-2.1964708668	1.2960620744	0.5274244719
O	8.0	-2.9466360705	2.3995792027	0.0895240209
O	8.0	-4.0452213882	0.4441207892	1.6788026949
C	6.0	-3.6548277062	-0.4210951797	-0.6259996772
N	7.0	-5.1141605695	-0.4241647921	1.9213511147
C	6.0	-4.8623377252	-1.1943774568	3.1693540728
C	6.0	-6.3684973733	0.3705451195	1.8108962835
C	6.0	-7.5519376469	-0.5635087898	2.1169615629
C	6.0	-6.4189656787	1.6260434017	2.7070804897
C	6.0	-6.0930768806	-2.0823897325	3.4269266892
C	6.0	-4.5279342904	-0.3438360699	4.4109236460
C	6.0	-3.6737539103	-2.1401962096	2.9338393408
C	6.0	-6.5264608112	0.8379442242	0.3583122877
C	6.0	-7.4117699980	-1.3225622866	3.4285491719
H	1.0	-2.4677327002	-0.7329597602	1.1041899053
H	1.0	-3.6060559595	2.5775066357	0.7376806203
H	1.0	-4.3591975353	-1.2280030253	-0.4771976634
H	1.0	-2.8339616375	-0.7964487361	-1.2314286619
H	1.0	-4.1355311056	0.3793106088	-1.1710838028
H	1.0	-7.6365891873	-1.2842207234	1.3071748009
H	1.0	-8.4629907210	0.0284365941	2.1090450101
H	1.0	-5.4999160317	2.1930133020	2.6315715265
H	1.0	-6.5906683693	1.4033219095	3.7501083823
H	1.0	-7.2332248219	2.2644747266	2.3778351350
H	1.0	-5.9455332889	-2.5993538430	4.3710966019
H	1.0	-6.1324356408	-2.8447963975	2.6521707489
H	1.0	-5.3882517203	0.1494834384	4.8394577963
H	1.0	-3.7874949776	0.4082433312	4.1709688822
H	1.0	-4.1126824553	-0.9887996762	5.1801275515
H	1.0	-3.6485373357	-2.8864120549	3.7223358061
H	1.0	-2.7270969957	-1.6154742028	2.9604997917

H	1.0	-3.7673498146	-2.6541480020	1.9837340680
H	1.0	-6.4707162303	0.0011710907	-0.3260823914
H	1.0	-5.7723336246	1.5618781948	0.0808119430
H	1.0	-7.4978884119	1.3082307463	0.2384581189
H	1.0	-8.2378777515	-2.0196222696	3.5409993717
H	1.0	-7.4674824019	-0.6463350918	4.2761698578
C	6.0	-1.3967125866	1.6448981065	1.7781807621
H	1.0	-1.5020589020	1.0811671207	-0.2777548021
H	1.0	-0.7672913380	2.5053394093	1.5782055927
H	1.0	-0.7606526879	0.8168567483	2.0795651036
H	1.0	-2.0550943025	1.8862283369	2.6057298086

anti6tmp E= -712.2817932033

C	6.0	0.0703628186	0.1349908194	1.7162927163
C	6.0	-0.0366603133	1.3063878779	2.7067733718
O	8.0	-0.7505431116	0.9367778952	3.8591923754
O	8.0	-1.1432026622	-0.4617986371	1.2617850385
C	6.0	0.8024171176	0.5064411976	0.4353015366
N	7.0	-1.9979951116	-1.0586663654	2.2068966879
C	6.0	-1.6748710230	-2.5116332763	2.3793302767
C	6.0	-3.3903298702	-0.7056406767	1.7815869791
C	6.0	-4.3726010039	-1.3545258747	2.7701104105
C	6.0	-3.5696707564	0.8126862860	1.8901977786
C	6.0	-2.7232240616	-3.1116313403	3.3371641342
C	6.0	-0.3195161089	-2.6701678402	3.0942752593
C	6.0	-1.5906845356	-3.3182323448	1.0696097928
C	6.0	-3.7375767822	-1.0911635091	0.3287014530
C	6.0	-4.1667003126	-2.8515472735	2.9372984657
H	1.0	0.6505878740	-0.6123296438	2.2315777706
H	1.0	-1.3720558000	0.2639798766	3.6292804187
H	1.0	1.0031101351	-0.3853253510	-0.1473596599
H	1.0	1.7489195082	0.9877980064	0.6614913431
H	1.0	0.2077615965	1.1788936868	-0.1720897944
H	1.0	-5.3820502183	-1.1393684747	2.4315969187
H	1.0	-4.2562831154	-0.8735783272	3.7390219495
H	1.0	-4.6241259140	1.0515273166	1.7909750108
H	1.0	-3.0416772955	1.3239283068	1.0984503347
H	1.0	-3.2289774054	1.1925190201	2.8447468956
H	1.0	-2.5570303427	-2.6936686127	4.3277100303
H	1.0	-2.5321219249	-4.1782519494	3.4115672237
H	1.0	-0.2137589633	-1.9665513768	3.9113069332
H	1.0	0.5185505783	-2.5582039455	2.4183470844
H	1.0	-0.2589938675	-3.6739251051	3.5033010874
H	1.0	-1.0852878010	-4.2586236173	1.2691527886
H	1.0	-1.0163567238	-2.7807618493	0.3258646580
H	1.0	-2.5549670139	-3.5585802685	0.6473604123
H	1.0	-3.9323256529	-2.1445742188	0.1936812937
H	1.0	-2.9435590283	-0.7984363795	-0.3451883534
H	1.0	-4.6386297892	-0.5608404905	0.0353465630
H	1.0	-4.4171969445	-3.3811855888	2.0233535216
H	1.0	-4.8343035452	-3.2347306606	3.7042891572
C	6.0	-0.5270561767	2.6442469569	2.1591878700
H	1.0	0.9897573439	1.4660889370	3.0318952632
H	1.0	-0.5951179002	3.3439802113	2.9851583818
H	1.0	-1.4995681871	2.5795529097	1.6939131980
H	1.0	0.1720622907	3.0485636934	1.4338554231

DFT Optimizations: **1b**–**3b** (alternate hydrogen bond)

prime5tmpdft E= -677.2277677612

C	6.0	-3.0404133437	0.0251849056	0.6618855300
C	6.0	-2.1676281699	1.2688627047	0.4813747356
O	8.0	-2.9038596476	2.3857390416	-0.0009071588
O	8.0	-3.9998741664	0.4554970089	1.6655821860
C	6.0	-3.6404810414	-0.4749120748	-0.6449109725
N	7.0	-5.1098957945	-0.4353443523	1.9046146898
C	6.0	-4.8568616139	-1.1946219446	3.1792520954
C	6.0	-6.3599423494	0.3948487566	1.8032187029
C	6.0	-7.5550222345	-0.5313168478	2.1212972919
C	6.0	-6.3812063970	1.6521576629	2.7058395702
C	6.0	-6.1073490200	-2.0617766127	3.4521722561
C	6.0	-4.5002154892	-0.3217304942	4.4044074557
C	6.0	-3.6792980922	-2.1582569821	2.9340139904
C	6.0	-6.5080613168	0.8621583721	0.3448012465
C	6.0	-7.4156983565	-1.2756940254	3.4469239672
H	1.0	-2.4150859695	-0.7647211704	1.0909452168
H	1.0	-1.6765601752	1.5048655580	1.4351593394
H	1.0	-3.6019298113	2.5389941680	0.6456754621
H	1.0	-4.3893938823	-1.2434969223	-0.4548908466
H	1.0	-2.8429560965	-0.9147355846	-1.2518176094
H	1.0	-4.0922441295	0.3388354677	-1.2120274797
H	1.0	-7.6436623251	-1.2647458875	1.3117685608
H	1.0	-8.4678741506	0.0731086175	2.1048599431
H	1.0	-5.4402703481	2.1987738288	2.6258815788
H	1.0	-6.5493379414	1.4228715235	3.7571223181
H	1.0	-7.1860319431	2.3181100663	2.3823785773
H	1.0	-5.9601113297	-2.5715924465	4.4100355438
H	1.0	-6.1577181870	-2.8406349406	2.6822244792
H	1.0	-5.3632162034	0.1757911641	4.8456648118
H	1.0	-3.7715749523	0.4392050689	4.1213387223
H	1.0	-4.0532371898	-0.9495596106	5.1807095215
H	1.0	-3.6374438774	-2.8965101366	3.7404319134
H	1.0	-2.7222101164	-1.6344527669	2.9235973195
H	1.0	-3.8038976087	-2.6892709488	1.9877167622
H	1.0	-6.4883859271	0.0132844213	-0.3399200975
H	1.0	-5.7138552847	1.5531227332	0.0616535886
H	1.0	-7.4649275131	1.3780814693	0.2246983483
H	1.0	-8.2611784932	-1.9576608301	3.5831232824
H	1.0	-7.4513505647	-0.5773728814	4.2897431092
H	1.0	-1.3910989469	1.0608049210	-0.2586379521

syn5tmpdft E= -716.5271437226

C	6.0	-3.0415014205	0.0576903415	0.7028643613
C	6.0	-2.1853631274	1.3241889738	0.5011325761
O	8.0	-2.9997691598	2.4197073420	0.0812745623
O	8.0	-4.0119808918	0.4626312202	1.7064538285
C	6.0	-3.6299661345	-0.4547036734	-0.6048120371
N	7.0	-5.1195266730	-0.4398199224	1.9200494838
C	6.0	-4.8768415373	-1.2156622216	3.1859164179

C	6.0	-6.3751372027	0.3802928995	1.8124311052
C	6.0	-7.5658499216	-0.5611020883	2.1016717047
C	6.0	-6.4233106168	1.6246954369	2.7313545834
C	6.0	-6.1220623384	-2.0994719900	3.4276849986
C	6.0	-4.5498431180	-0.3603939622	4.4317683430
C	6.0	-3.6857959965	-2.1629912957	2.9429765316
C	6.0	-6.5107688681	0.8658427929	0.3585285662
C	6.0	-7.4378375873	-1.3255425891	3.4170503779
H	1.0	-2.4030975085	-0.7216725894	1.1314137799
H	1.0	-3.6868543762	2.5095703389	0.7526837199
H	1.0	-4.3655054038	-1.2365164697	-0.4172955525
H	1.0	-2.8222153639	-0.8804764884	-1.2082651637
H	1.0	-4.0943071215	0.3505672867	-1.1739850675
H	1.0	-7.6392330233	-1.2828889512	1.2801025814
H	1.0	-8.4832900152	0.0361319204	2.0828815611
H	1.0	-5.4968187783	2.1964300067	2.6571748373
H	1.0	-6.5839625656	1.3783393518	3.7797749093
H	1.0	-7.2446873933	2.2745551124	2.4170743749
H	1.0	-5.9829322873	-2.6225229412	4.3796082286
H	1.0	-6.1552824726	-2.8674349869	2.6458500695
H	1.0	-5.4267483450	0.1148424607	4.8700948721
H	1.0	-3.8289451730	0.4166438525	4.1749469259
H	1.0	-4.1044279458	-0.9963155828	5.2022568587
H	1.0	-3.6459161780	-2.9105568757	3.7407507854
H	1.0	-2.7346998548	-1.6286186134	2.9499073790
H	1.0	-3.7935641741	-2.6836418891	1.9888698507
H	1.0	-6.4788204531	0.0258601912	-0.3366609926
H	1.0	-5.7192780480	1.5658297509	0.0906529987
H	1.0	-7.4702377730	1.3761704380	0.2354332709
H	1.0	-8.2785667459	-2.0177176231	3.5301316669
H	1.0	-7.4919737017	-0.6417482386	4.2705249524
C	6.0	-1.3488177437	1.6921569384	1.7280396013
H	1.0	-1.5121402595	1.1302419165	-0.3401692264
H	1.0	-0.7798826277	2.6018156076	1.5243420635
H	1.0	-0.6452838383	0.8915654474	1.9787313818
H	1.0	-1.9881762353	1.8686393654	2.5960939301

anti6tmpdft E= -716.5239820644

C	6.0	0.1103170639	0.1348311779	1.6627964904
C	6.0	-0.0172789282	1.2558140053	2.7191414469
O	8.0	-0.7606747431	0.8119832871	3.8527650982
O	8.0	-1.1252853655	-0.4707329905	1.1887541879
C	6.0	0.8025223108	0.5866174379	0.3824285035
N	7.0	-1.9988231590	-1.0508284855	2.2055848306
C	6.0	-1.6756804116	-2.5201409935	2.4008439649
C	6.0	-3.4045180627	-0.6993056821	1.7630344487
C	6.0	-4.3854217352	-1.3375842567	2.7699711901
C	6.0	-3.5710406356	0.8262968603	1.8526863316
C	6.0	-2.7341727215	-3.0941475260	3.3735323537
C	6.0	-0.3154132450	-2.6512794517	3.1220315485
C	6.0	-1.5992434600	-3.3452464040	1.0995429951
C	6.0	-3.7472028896	-1.1166568584	0.3148285478
C	6.0	-4.1783536902	-2.8376972967	2.9554240399
H	1.0	0.7130142429	-0.6441143308	2.1290101591
H	1.0	-1.3832315631	0.1328269823	3.5282190302
H	1.0	0.9949094512	-0.2682912550	-0.2688279562

H	1.0	1.7586639944	1.0617105846	0.6174024925
H	1.0	0.1850659677	1.3017737842	-0.1646204015
H	1.0	-5.4025768462	-1.1209355812	2.4283364581
H	1.0	-4.2631108234	-0.8380471621	3.7380147413
H	1.0	-4.6284251598	1.0766742566	1.7311124287
H	1.0	-3.0142062583	1.3246781435	1.0602435824
H	1.0	-3.2345181998	1.2103371832	2.8165931865
H	1.0	-2.5686550883	-2.6482290389	4.3611295146
H	1.0	-2.5390955116	-4.1666185451	3.4748445386
H	1.0	-0.2190272039	-1.9159838900	3.9226304730
H	1.0	0.5273708405	-2.5437221370	2.4379194042
H	1.0	-0.2440098464	-3.6513572925	3.5592940500
H	1.0	-1.0953481667	-4.2940599180	1.3053289336
H	1.0	-1.0198670888	-2.8108468267	0.3453064565
H	1.0	-2.5758035387	-3.5809229445	0.6801521730
H	1.0	-3.9191862237	-2.1853181047	0.2017355078
H	1.0	-2.9503372503	-0.8178072935	-0.3662023811
H	1.0	-4.6644314184	-0.6062757121	0.0067634512
H	1.0	-4.4187753154	-3.3808788798	2.0359558096
H	1.0	-4.8605250926	-3.2187390220	3.7222304956
C	6.0	-0.5135691251	2.6182382698	2.2235251971
H	1.0	1.0131621225	1.4074252611	3.0724471130
H	1.0	-0.6317231655	3.2722773927	3.0905901707
H	1.0	-1.4747235737	2.5563775958	1.7148686968
H	1.0	0.2077195131	3.0823256567	1.5449506972

MP2 Optimizations: **1b**–**3b** (alternate hydrogen bond)

prime5tmpmp2 E= -675.6760637477

C	6.0	-3.0557912531	0.0059431263	0.6670360622
C	6.0	-2.1962095531	1.2500294351	0.4736930494
O	8.0	-2.9632142180	2.3541734422	0.0192970284
O	8.0	-3.9905524694	0.4391218211	1.6818194544
C	6.0	-3.6832716506	-0.4754009178	-0.6286247262
N	7.0	-5.1016836214	-0.4540062752	1.8912115435
C	6.0	-4.8625896727	-1.1844269489	3.1702981275
C	6.0	-6.3321847228	0.3868444076	1.8055229228
C	6.0	-7.5293025660	-0.5256481854	2.1095166470
C	6.0	-6.3429256029	1.6296595746	2.7134084752
C	6.0	-6.0972402397	-2.0608920710	3.4253975108
C	6.0	-4.5422208489	-0.3076616844	4.3920405328
C	6.0	-3.6661806291	-2.1168693349	2.9470728676
C	6.0	-6.4702750769	0.8651174255	0.3572503427
C	6.0	-7.3988401012	-1.2676890148	3.4344226373
H	1.0	-2.4229940267	-0.7904038172	1.0769442142
H	1.0	-1.6864962402	1.4851262264	1.4181143216
H	1.0	-3.6481608285	2.4542892573	0.6882558711
H	1.0	-4.4313203696	-1.2422100763	-0.4253104238
H	1.0	-2.8942469661	-0.9089567857	-1.2523880842
H	1.0	-4.1395697939	0.3518157505	-1.1724604495
H	1.0	-7.6119508052	-1.2615051255	1.2986399638
H	1.0	-8.4364635989	0.0912695297	2.0869462955
H	1.0	-5.3839037854	2.1506004403	2.6596666933

H	1.0	-6.5510128717	1.3954421549	3.7571012499
H	1.0	-7.1244320661	2.3137047947	2.3656040736
H	1.0	-5.9452201211	-2.5857279687	4.3770142003
H	1.0	-6.1483223502	-2.8210077958	2.6341929988
H	1.0	-5.4242803633	0.1602522358	4.8286633058
H	1.0	-3.8272072279	0.4707771081	4.1156769601
H	1.0	-4.0851796376	-0.9354039205	5.1650110589
H	1.0	-3.6318158412	-2.8557541177	3.7549443651
H	1.0	-2.7241035886	-1.5632919586	2.9612075394
H	1.0	-3.7645823458	-2.6411468439	1.9921284905
H	1.0	-6.4390594308	0.0161332946	-0.3289834149
H	1.0	-5.6766667395	1.5648172842	0.0887684323
H	1.0	-7.4327150570	1.3744912602	0.2412532858
H	1.0	-8.2503140750	-1.9446131473	3.5702433920
H	1.0	-7.4194881107	-0.5670020709	4.2763813931
H	1.0	-1.4393815332	1.0518994913	-0.2899982082

syn5tmpmp2 E= -714.8789264577

C	6.0	-3.0640772714	0.0372465590	0.6934260632
C	6.0	-2.2053141273	1.2924319529	0.5036082304
O	8.0	-3.0098036131	2.3846525892	0.0690233344
O	8.0	-4.0076153569	0.4484253704	1.7077847315
C	6.0	-3.6794381343	-0.4378690415	-0.6103118719
N	7.0	-5.1111150650	-0.4593560666	1.8996785386
C	6.0	-4.8724168630	-1.1995662962	3.1728488303
C	6.0	-6.3495856372	0.3693175156	1.8142019706
C	6.0	-7.5385015352	-0.5601470574	2.0991372273
C	6.0	-6.3805385983	1.6018427703	2.7355648372
C	6.0	-6.0978254541	-2.0946328033	3.4078837685
C	6.0	-4.5747258988	-0.3332114787	4.4080636208
C	6.0	-3.6611594584	-2.1126637680	2.9499325846
C	6.0	-6.4821354991	0.8625750387	0.3705322242
C	6.0	-7.4092141762	-1.3173711722	3.4157000571
H	1.0	-2.4266639121	-0.7582585720	1.0982635448
H	1.0	-3.6776158471	2.4724659492	0.7585611874
H	1.0	-4.4210129900	-1.2143360482	-0.4197804810
H	1.0	-2.8815514016	-0.8578507249	-1.2323194812
H	1.0	-4.1392981189	0.3912546599	-1.1486627865
H	1.0	-7.6072507974	-1.2866759100	1.2786392615
H	1.0	-8.4523779803	0.0468090430	2.0777421430
H	1.0	-5.4279687431	2.1355933107	2.6918486202
H	1.0	-6.5907265199	1.3541669161	3.7757369413
H	1.0	-7.1687321702	2.2797856929	2.3909481721
H	1.0	-5.9468819146	-2.6285131297	4.3546308533
H	1.0	-6.1330190775	-2.8459838573	2.6075258593
H	1.0	-5.4670888530	0.1151039340	4.8443212685
H	1.0	-3.8696144440	0.4599621227	4.1485453133
H	1.0	-4.1135383362	-0.9638234874	5.1762528835
H	1.0	-3.6217316079	-2.8582306876	3.7514402323
H	1.0	-2.7277587911	-1.5447987656	2.9756841495
H	1.0	-3.7450454252	-2.6296462852	1.9896333409
H	1.0	-6.4408334831	0.0213516037	-0.3246637428
H	1.0	-5.6913806511	1.5702240061	0.1148580494
H	1.0	-7.4475642014	1.3662310800	0.2540726995
H	1.0	-8.2533721472	-2.0063301628	3.5359015417
H	1.0	-7.4456098941	-0.6277924716	4.2662988989

C	6.0	-1.4176477755	1.6535762276	1.7580084002
H	1.0	-1.5117540286	1.0947461634	-0.3212094386
H	1.0	-0.8096453918	2.5415704400	1.5693628124
H	1.0	-0.7602976362	0.8293070022	2.0540342748
H	1.0	-2.1017911727	1.8630478386	2.5845013355

anti6tmpmp2 E= -714.8760599918

C	6.0	0.1014401381	0.1257190237	1.7011588793
C	6.0	-0.0603738651	1.2430494020	2.7405876810
O	8.0	-0.8209031172	0.7969916565	3.8577478750
O	8.0	-1.1159369708	-0.4778436812	1.1941872266
C	6.0	0.8067641192	0.5880173652	0.4367593928
N	7.0	-1.9858825503	-1.0459158576	2.2163273355
C	6.0	-1.6805982465	-2.5063719959	2.3849562485
C	6.0	-3.3761641890	-0.7019270459	1.7675848589
C	6.0	-4.3518534645	-1.3127829353	2.7825029683
C	6.0	-3.5277377518	0.8193131053	1.8311619445
C	6.0	-2.7148928354	-3.0670655323	3.3759164496
C	6.0	-0.3089742956	-2.6531619683	3.0616546321
C	6.0	-1.6451999496	-3.3234886851	1.0855529327
C	6.0	-3.7236132391	-1.1363800178	0.3337941967
C	6.0	-4.1586396725	-2.8115384105	2.9672296579
H	1.0	0.7006655723	-0.6489331889	2.1815300976
H	1.0	-1.4053868611	0.1010064127	3.4970570671
H	1.0	1.0324262917	-0.2691132114	-0.2022144035
H	1.0	1.7436779179	1.0916842688	0.6925065534
H	1.0	0.1730462445	1.2813845712	-0.1210260643
H	1.0	-5.3691695896	-1.0823607963	2.4427062318
H	1.0	-4.2070766918	-0.8092507911	3.7480263707
H	1.0	-4.5905046661	1.0693639284	1.7458189761
H	1.0	-2.9982853181	1.2916507012	1.0026366296
H	1.0	-3.1476973820	1.2141050175	2.7758076802
H	1.0	-2.5343486739	-2.6045794663	4.3559921454
H	1.0	-2.5167813308	-4.1410162230	3.4812001467
H	1.0	-0.1846844673	-1.9162022888	3.8593501288
H	1.0	0.5088381413	-2.5564067472	2.3437785620
H	1.0	-0.2443019646	-3.6571381954	3.4948741208
H	1.0	-1.1116781684	-4.2605707674	1.2785291511
H	1.0	-1.1039637544	-2.7725746085	0.3125219087
H	1.0	-2.6352331368	-3.5800129565	0.7103534042
H	1.0	-3.9571198669	-2.1968908876	0.2474950444
H	1.0	-2.9018786451	-0.8957339780	-0.3442121381
H	1.0	-4.6086730570	-0.5773543062	0.0113488763
H	1.0	-4.4033011700	-3.3515976748	2.0460446849
H	1.0	-4.8382380788	-3.1873602038	3.7407235547
C	6.0	-0.5653834229	2.5808327195	2.2047425716
H	1.0	0.9630662185	1.4133884743	3.1093891899
H	1.0	-0.7484206722	3.2399447950	3.0573755975
H	1.0	-1.4921174417	2.4794903705	1.6420131050
H	1.0	0.1835598634	3.0520406091	1.5608085280

Structures of **1′**–**3′** containing five- and six-membered ring hydrogen bonds were optimized using the same optimization methods described above.

RHF Optimizations: **1′–3′**

prime5rhf E= -517.0889734181

C	6.0	-3.0435722050	-0.2648636928	0.5154262818
C	6.0	-1.8454194350	0.6685495475	0.5208011150
O	8.0	-1.3729916696	0.9040379980	1.8147936409
O	8.0	-4.0289059313	0.3958776468	1.2847763196
C	6.0	-3.5372219086	-0.5790608684	-0.8874923921
N	7.0	-5.0397540635	-0.4657422235	1.7050825395
C	6.0	-4.8901967205	-0.6506071629	3.1403388941
C	6.0	-6.3073814801	0.1599599567	1.3651522290
C	6.0	-7.4612394184	-0.7312051368	1.8166645374
C	6.0	-5.9846269054	-1.5778007408	3.6606374958
C	6.0	-7.3707950022	-1.0328793271	3.3133645936
H	1.0	-2.7686273720	-1.1835666522	1.0255180741
H	1.0	-2.0900840272	1.2386626626	2.3247384279
H	1.0	-4.4061552319	-1.2243507145	-0.8450573806
H	1.0	-2.7649026788	-1.0900224676	-1.4558065297
H	1.0	-3.8064352545	0.3323120627	-1.4139857913
H	1.0	-7.4293299545	-1.6607984832	1.2534944867
H	1.0	-8.4023825746	-0.2431236211	1.5796974454
H	1.0	-5.8746956859	-1.6933196424	4.7351311092
H	1.0	-5.8541741444	-2.5608544550	3.2149500282
H	1.0	-8.1419720695	-1.7395928188	3.6060140168
H	1.0	-7.5501128416	-0.1185179924	3.8771404764
H	1.0	-4.9338636199	0.3143163298	3.6524923460
H	1.0	-3.9104911781	-1.0757780044	3.3241298743
H	1.0	-6.3322614132	0.3041429895	0.2923377876
H	1.0	-6.3814865216	1.1455010378	1.8316728191
H	1.0	-2.1153415908	1.6026495757	0.0294680330
H	1.0	-1.0325191020	0.2191341967	-0.0368704777

prime6rhf E= -517.0880843616

C	6.0	0.0031760155	-1.0799550979	0.0944392632
C	6.0	0.5005992375	-2.4755526065	-0.2661638710
O	8.0	-0.5257100842	-3.4108825817	-0.4276320949
O	8.0	-0.3778392015	-0.9753327099	1.4541221719
C	6.0	1.0774063751	-0.0237299050	-0.1033123304
N	7.0	-1.4430339189	-1.8098119458	1.7943675589
C	6.0	-1.0783693448	-2.4608159244	3.0460443464
C	6.0	-2.6279063227	-0.9739681631	1.9426547018
C	6.0	-3.8217762208	-1.8273935534	2.3606025171
C	6.0	-2.2125222426	-3.3686847810	3.5137376409
C	6.0	-3.5215965412	-2.5900548622	3.6516801020
H	1.0	-0.8572759189	-0.8547838856	-0.5326638232
H	1.0	1.2125748628	-2.7983253418	0.4937188770
H	1.0	1.0281355790	-2.4257324044	-1.2122689026
H	1.0	-1.1423659359	-3.2757350950	0.2728058198
H	1.0	1.9604085408	-0.2616500960	0.4821512261
H	1.0	0.7117363150	0.9449754063	0.2163984535
H	1.0	1.3611616377	0.0404139346	-1.1486624260
H	1.0	-4.0523999923	-2.5302429659	1.5633919443
H	1.0	-4.6905137317	-1.1873454954	2.4846918081
H	1.0	-1.9341897693	-3.8238819878	4.4597337133

H	1.0	-2.3402954039	-4.1766034188	2.7967534146
H	1.0	-4.3392739375	-3.2615183395	3.8964856637
H	1.0	-3.4355320043	-1.8831777753	4.4755721843
H	1.0	-0.8507997159	-1.7089508146	3.8039394825
H	1.0	-0.1760763988	-3.0340142132	2.8725614883
H	1.0	-2.8191018925	-0.4907291424	0.9919388927
H	1.0	-2.4384599856	-0.1910662339	2.6792221776

syn5rhf E= -556.1365934915

C	6.0	-3.0326954548	-0.2675844551	0.5052315774
C	6.0	-1.8300502898	0.6754696324	0.5357303268
O	8.0	-1.4682883419	0.9405306501	1.8657895731
O	8.0	-4.0265424726	0.3971009203	1.2644788932
C	6.0	-3.5405828766	-0.5915893981	-0.8912765097
N	7.0	-5.0357818546	-0.4633271440	1.6908328192
C	6.0	-4.8749882129	-0.6547701424	3.1241814247
C	6.0	-6.3041284283	0.1684798926	1.3650897700
C	6.0	-7.4570726737	-0.7210821992	1.8221362267
C	6.0	-5.9673040204	-1.5816978574	3.6490656809
C	6.0	-7.3547945784	-1.0312902606	3.3163030484
H	1.0	-2.7625419875	-1.1837890154	1.0234226068
H	1.0	-2.2389355388	1.2310936500	2.3215514907
H	1.0	-4.4525684223	-1.1716874131	-0.8227274593
H	1.0	-2.8150034652	-1.1772155160	-1.4452400170
H	1.0	-3.7490259085	0.3185149347	-1.4471106900
H	1.0	-7.4332911536	-1.6477285361	1.2537363170
H	1.0	-8.3984406274	-0.2283967250	1.5959238029
H	1.0	-5.8483809705	-1.7031661125	4.7219236013
H	1.0	-5.8432983604	-2.5628267136	3.1973215208
H	1.0	-8.1255574580	-1.7373343372	3.6115631651
H	1.0	-7.5267135756	-0.1195152655	3.8865951771
H	1.0	-4.9129145544	0.3080728848	3.6408684443
H	1.0	-3.8946756573	-1.0823625203	3.2986659498
H	1.0	-6.3379302384	0.3186223910	0.2933896315
H	1.0	-6.3707537281	1.1518021531	1.8373814421
C	6.0	-0.5978800716	0.1144998121	-0.1532667630
H	1.0	-2.1235723380	1.6046424360	0.0462463105
H	1.0	-0.3275957566	-0.8482639269	0.2710085450
H	1.0	0.2324371436	0.7936320692	0.0011692894
H	1.0	-0.7502081272	-0.0017438879	-1.2204151956

syn6rhf E= -556.1347663558

C	6.0	0.1516419035	0.0877295956	1.8151927240
C	6.0	-0.1285546451	1.3279200945	2.6736295696
O	8.0	-0.7085761385	0.9719009788	3.9024246154
O	8.0	-1.0451875534	-0.4776191015	1.3032906141
C	6.0	0.9939215292	0.3665676252	0.5797216980
N	7.0	-1.8782019702	-1.0283139542	2.2772252236
C	6.0	-1.7536518726	-2.4783351797	2.1972293402
C	6.0	-3.2303123823	-0.5807057875	1.9672839091
C	6.0	-4.2200696545	-1.1733245792	2.9662994582
C	6.0	-2.6823564841	-3.1402375405	3.2109162663
C	6.0	-4.1305168496	-2.6997687962	2.9927387241
C	6.0	1.1180675545	2.1338490743	3.0071339022
H	1.0	0.6498308866	-0.6497420134	2.4421939958

H	1.0	-0.8184560399	1.9575066963	2.1097496652
H	1.0	-1.2777298938	0.2332588502	3.7569128584
H	1.0	1.0438327715	-0.5277959719	-0.0300770468
H	1.0	2.0025045958	0.6563729298	0.8479305345
H	1.0	0.5510214490	1.1575150792	-0.0182230374
H	1.0	-5.2233945008	-0.8514454141	2.7031118562
H	1.0	-4.0068660422	-0.7761962941	3.9561223492
H	1.0	-2.3629889845	-2.8697223692	4.2146771680
H	1.0	-2.5907725416	-4.2191099770	3.1254075635
H	1.0	-4.4893039437	-3.0989617258	2.0452182414
H	1.0	-4.7728772195	-3.1047634068	3.7691384067
H	1.0	0.8516863707	2.8971165984	3.7290924711
H	1.0	1.5379865388	2.6195964342	2.1333347933
H	1.0	1.8768660812	1.5000342422	3.4583677594
H	1.0	-0.7214528615	-2.7385242245	2.3995516520
H	1.0	-1.9871950770	-2.8136683341	1.1850895655
H	1.0	-3.4926996925	-0.8698021064	0.9480343687
H	1.0	-3.2405553334	0.5011385774	2.0141507906

anti5rhf E= -556.1356390492

C	6.0	-2.9231614876	-0.4444955262	0.8236621998
C	6.0	-1.9201458833	0.6723655411	0.5248687129
O	8.0	-1.2190753750	1.0404916177	1.6842834076
O	8.0	-3.7854238798	0.1226978808	1.7937470293
N	7.0	-4.9510577163	-0.6150202832	1.9810027848
C	6.0	-5.0926521922	-0.8445706543	3.4098205760
C	6.0	-6.0531634352	0.1676244153	1.4425914944
C	6.0	-7.3667702006	-0.5845124069	1.6354733176
C	6.0	-6.3695916887	-1.6339639763	3.6844536466
C	6.0	-7.5930512015	-0.9177986176	3.1107416224
H	1.0	-1.8479740728	1.2532183972	2.3521675792
H	1.0	-7.3362796135	-1.5020095084	1.0528100416
H	1.0	-8.1836666762	0.0172873447	1.2473695427
H	1.0	-6.4760479005	-1.7779251772	4.7559017146
H	1.0	-6.2779832407	-2.6195670447	3.2344274569
H	1.0	-8.4828004946	-1.5291012316	3.2309525649
H	1.0	-7.7652282191	0.0031750608	3.6659241904
H	1.0	-5.1112532588	0.1074752360	3.9466834353
H	1.0	-4.2230944579	-1.3936544131	3.7482919101
H	1.0	-5.8624369701	0.3353766100	0.3890354337
H	1.0	-6.0969333167	1.1448628071	1.9295185131
C	6.0	-0.8942621614	0.3155106124	-0.5359124643
H	1.0	-2.5048376720	1.5218969914	0.1740520979
H	1.0	-0.2350680707	-0.4722825601	-0.1899128824
H	1.0	-0.2864773155	1.1857617720	-0.7563849560
H	1.0	-1.3774196167	-0.0074994038	-1.4538962274
C	6.0	-2.3031675393	-1.7414511624	1.3216747198
H	1.0	-3.4992332207	-0.6382811886	-0.0785054827
H	1.0	-1.6605071665	-1.5543889087	2.1744062551
H	1.0	-1.7122753376	-2.2091317378	0.5410306460
H	1.0	-3.0836906186	-2.4354204856	1.6083111199

anti6rhf E= -556.1333357327

C	6.0	0.0734394136	0.0682290193	1.7880680242
C	6.0	-0.0989695990	1.3413852035	2.6258372150

O	8.0	-0.7238692562	1.0551480055	3.8524648231
O	8.0	-1.1503077475	-0.4421361378	1.2885164333
C	6.0	0.9650877632	0.2551535879	0.5705191891
N	7.0	-1.9482504164	-1.0275362995	2.2753528247
C	6.0	-1.7668191394	-2.4721125683	2.1909876178
C	6.0	-3.3224797265	-0.6418261286	1.9808985542
C	6.0	-4.2727224780	-1.2757995571	2.9933464936
C	6.0	-2.6494813881	-3.1729062125	3.2193268412
C	6.0	-4.1181588089	-2.7966874990	3.0219798088
H	1.0	0.5169701160	-0.6775385688	2.4433875608
C	6.0	-0.8216757959	2.4773916561	1.9091741725
H	1.0	-1.3129576937	0.3290472711	3.7256149689
H	1.0	1.1385837917	-0.7013988959	0.0909349829
H	1.0	1.9234775782	0.6758764891	0.8578785099
H	1.0	0.5002875136	0.9128130151	-0.1548538266
H	1.0	-5.2920340802	-0.9972566745	2.7423855748
H	1.0	-4.0643584246	-0.8675741781	3.9796457653
H	1.0	-2.3270910078	-2.8866421086	4.2176307790
H	1.0	-2.5117888146	-4.2468010771	3.1330407634
H	1.0	-4.4735760475	-3.2136142564	2.0808724128
H	1.0	-4.7311532937	-3.2262577708	3.8087697165
H	1.0	-0.7223810158	-2.6931715224	2.3751535407
H	1.0	-2.0044895430	-2.8149574046	1.1824296528
H	1.0	-3.5845334765	-0.9447594597	0.9655853269
H	1.0	-3.3847782871	0.4372733995	2.0278654259
H	1.0	0.9034130774	1.6797965447	2.8755415781
H	1.0	-1.8014969542	2.1673264623	1.5648112394
H	1.0	-0.2580784833	2.8342009122	1.0524665863
H	1.0	-0.9475177756	3.3031047534	2.6006074447

DFT Optimizations: **1′**–**3′**

prime5dft E= -520.0601084004

C	6.0	-3.0426695764	-0.2627284399	0.4534024192
C	6.0	-1.8077792371	0.6251359190	0.5701246000
O	8.0	-1.4179175136	0.8010707144	1.9234289100
O	8.0	-4.0574715999	0.4363273766	1.2043675788
C	6.0	-3.4842325430	-0.5168782679	-0.9814179070
N	7.0	-5.0718113428	-0.4798145701	1.6710544725
C	6.0	-4.8885114714	-0.6054380382	3.1229716259
C	6.0	-6.3653064399	0.1301854718	1.3479850576
C	6.0	-7.4954409416	-0.7717388424	1.8575153631
C	6.0	-5.9542453857	-1.5447857580	3.6949537594
C	6.0	-7.3624439519	-1.0324175480	3.3638446998
H	1.0	-2.8404353535	-1.2108543750	0.9632744842
H	1.0	-2.2097926986	1.1102170589	2.3795335342
H	1.0	-4.3986339613	-1.1129280825	-0.9892860968
H	1.0	-2.7156985999	-1.0683327502	-1.5320509181
H	1.0	-3.6750040018	0.4264321208	-1.5012539896
H	1.0	-7.4601020286	-1.7223263633	1.3134966906
H	1.0	-8.4573040002	-0.3037047106	1.6268971006
H	1.0	-5.8147702185	-1.6322839298	4.7767956685
H	1.0	-5.8134427405	-2.5430391661	3.2668190985

H	1.0	-8.1202638094	-1.7479203859	3.6972937080
H	1.0	-7.5444554858	-0.0993348756	3.9116140490
H	1.0	-4.9547678805	0.3860828550	3.6027944539
H	1.0	-3.8841845933	-0.9969661401	3.3020898108
H	1.0	-6.4196688391	0.2472718839	0.2638390933
H	1.0	-6.4449044885	1.1346974278	1.7976479437
H	1.0	-2.0085230302	1.5915019201	0.0834765771
H	1.0	-0.9671482670	0.1556294952	0.0533782127

prime6dft E= -520.0618076422

C	6.0	0.0322369124	-1.0570434469	0.0665075444
C	6.0	0.4936704772	-2.4683278746	-0.3001525129
O	8.0	-0.5751024288	-3.3956304744	-0.3922061374
O	8.0	-0.3551988922	-0.9533369942	1.4538602193
C	6.0	1.1289880225	-0.0146728674	-0.1043454859
N	7.0	-1.4529091550	-1.8409077879	1.7810709466
C	6.0	-1.0824830264	-2.4704763184	3.0575368509
C	6.0	-2.6521615476	-0.9997708148	1.9219691058
C	6.0	-3.8440468000	-1.8555862450	2.3624083838
C	6.0	-2.2189686233	-3.3769947012	3.5400969614
C	6.0	-3.5343694541	-2.5977709592	3.6686647641
H	1.0	-0.8323596311	-0.8060369738	-0.5635031378
H	1.0	1.2465888164	-2.7866323673	0.4391312518
H	1.0	0.9817762088	-2.4408694716	-1.2800153341
H	1.0	-1.1632405455	-3.1688791294	0.3478345211
H	1.0	2.0091893913	-0.2822514722	0.4864756517
H	1.0	0.7777799710	0.9628233447	0.2316493293
H	1.0	1.4224190952	0.0623730645	-1.1538770391
H	1.0	-4.0787954564	-2.5772827176	1.5719377971
H	1.0	-4.7204056173	-1.2105173818	2.4775351902
H	1.0	-1.9348979871	-3.8234897486	4.4978606750
H	1.0	-2.3440054642	-4.2010686143	2.8284971232
H	1.0	-4.3550724257	-3.2726429642	3.9301819631
H	1.0	-3.4466773165	-1.8725838210	4.4869553798
H	1.0	-0.8582038988	-1.6934919880	3.8052505768
H	1.0	-0.1689020800	-3.0438912288	2.8889445817
H	1.0	-2.8468092644	-0.5313880492	0.9544574813
H	1.0	-2.4578792805	-0.1981919973	2.6515833484

syn5dft E= -559.3603268282

C	6.0	-3.0311370107	-0.2592151329	0.4458533340
C	6.0	-1.8056756493	0.6602548972	0.5470317504
O	8.0	-1.4833146417	0.8750194287	1.9199120340
O	8.0	-4.0479263974	0.4340429636	1.2036635449
C	6.0	-3.5100021936	-0.5426552882	-0.9718972683
N	7.0	-5.0644115014	-0.4824804026	1.6639896796
C	6.0	-4.8765983790	-0.6254108938	3.1141171856
C	6.0	-6.3546938336	0.1419741203	1.3537235079
C	6.0	-7.4909731377	-0.7542659622	1.8592182005
C	6.0	-5.9488785893	-1.5604313606	3.6811998952
C	6.0	-7.3535549898	-1.0310453261	3.3622348921
H	1.0	-2.8024340474	-1.1965288499	0.9662576210
H	1.0	-2.3116390237	1.1334165120	2.3425519276
H	1.0	-4.4485846115	-1.0986237623	-0.9340251694
H	1.0	-2.7840068890	-1.1469210881	-1.5219046104

H	1.0	-3.6756492990	0.3897943814	-1.5196855454
H	1.0	-7.4675573020	-1.6996878467	1.3055337965
H	1.0	-8.4492895333	-0.2747278875	1.6374711322
H	1.0	-5.8051367470	-1.6604652686	4.7613968158
H	1.0	-5.8198784905	-2.5554542784	3.2420429447
H	1.0	-8.1169363628	-1.7420816247	3.6925602235
H	1.0	-7.5238003054	-0.1013171853	3.9194582914
H	1.0	-4.9322639375	0.3618643664	3.6039134175
H	1.0	-3.8752714900	-1.0275932233	3.2857826374
H	1.0	-6.4130227015	0.2715180652	0.2712163560
H	1.0	-6.4222709639	1.1423576027	1.8142749527
C	6.0	-0.5611312478	0.0956474499	-0.1211346041
H	1.0	-2.0711274288	1.6194972380	0.0741561767
H	1.0	-0.3150601129	-0.8875569948	0.2907614990
H	1.0	0.2818037159	0.7623428802	0.0717371373
H	1.0	-0.6886468985	0.0057924704	-1.2018517558

syn6dft E= -559.3616191177

C	6.0	0.1795479200	0.1076187407	1.7779943001
C	6.0	-0.1113416077	1.3313236155	2.6658332522
O	8.0	-0.7443633798	0.9366073487	3.8800056094
O	8.0	-1.0365804217	-0.4767021570	1.2541055824
C	6.0	0.9994912624	0.4150333982	0.5312207083
N	7.0	-1.8854018331	-1.0220786317	2.2920472129
C	6.0	-1.7517870965	-2.4864105491	2.2330582853
C	6.0	-3.2501078776	-0.5891835368	1.9555918596
C	6.0	-4.2454013356	-1.1776840906	2.9598155191
C	6.0	-2.6901845714	-3.1349456713	3.2555021987
C	6.0	-4.1432834533	-2.7072929339	3.0110661868
C	6.0	1.1410512869	2.1105697485	3.0557378067
H	1.0	0.6945351311	-0.6432461949	2.3940535756
H	1.0	-0.7802591544	1.9910400617	2.0879354476
H	1.0	-1.2912004479	0.1624825320	3.6555863302
H	1.0	1.0563460680	-0.4752933066	-0.0977440328
H	1.0	2.0136827918	0.7192793113	0.7946383295
H	1.0	0.5337453409	1.2143692299	-0.0520648599
H	1.0	-5.2559272689	-0.8624951165	2.6831377820
H	1.0	-4.0405586043	-0.7586031983	3.9515882967
H	1.0	-2.3818556150	-2.8370750295	4.2637265807
H	1.0	-2.5872049024	-4.2225973262	3.1950520762
H	1.0	-4.4894462854	-3.1266614495	2.0581556171
H	1.0	-4.7979199448	-3.1091380592	3.7902321358
H	1.0	0.8634070667	2.8692262049	3.7907020947
H	1.0	1.5990935507	2.6108627713	2.1995313958
H	1.0	1.8781130865	1.4489973919	3.5211430150
H	1.0	-0.7098873132	-2.7367326431	2.4456831847
H	1.0	-1.9825351591	-2.8375204217	1.2153339827
H	1.0	-3.5019575826	-0.9031473582	0.9302017964
H	1.0	-3.2661796502	0.5018773194	1.9839787304

anti5dft E= -559.3592945158

C	6.0	-2.9103293045	-0.4293685396	0.7746169754
C	6.0	-1.8797057177	0.6826465906	0.5147383272
O	8.0	-1.1896749082	1.0198505900	1.7186315448
O	8.0	-3.7888507188	0.1679322249	1.7534409865

N	7.0	-4.9736714474	-0.6265456076	1.9621622279
C	6.0	-5.0972636314	-0.8197079074	3.4114759089
C	6.0	-6.0995620547	0.1522940376	1.4304094939
C	6.0	-7.4065493820	-0.6159758864	1.6547492843
C	6.0	-6.3652083951	-1.6252930954	3.7146375964
C	6.0	-7.6081700487	-0.9302867574	3.1429321841
H	1.0	-1.8713034669	1.1857747333	2.3808940315
H	1.0	-7.3711430901	-1.5476976628	1.0794173716
H	1.0	-8.2412427483	-0.0257915936	1.2640751472
H	1.0	-6.4557965035	-1.7562580737	4.7973747611
H	1.0	-6.2640570315	-2.6235477136	3.2749770005
H	1.0	-8.4973021687	-1.5514431219	3.2878358565
H	1.0	-7.7810599959	0.0048288076	3.6899135106
H	1.0	-5.1308654469	0.1547331862	3.9278171378
H	1.0	-4.2069317228	-1.3488967399	3.7561804129
H	1.0	-5.9227452834	0.3132636251	0.3644850348
H	1.0	-6.1466178587	1.1413493125	1.9163188092
C	6.0	-0.8283853201	0.3207629556	-0.5237281451
H	1.0	-2.4487805623	1.5559247048	0.1632903264
H	1.0	-0.2164631394	-0.5158971203	-0.1805581533
H	1.0	-0.1687842044	1.1756284360	-0.6863091390
H	1.0	-1.2913795287	0.0537244420	-1.4778930244
C	6.0	-2.3206705003	-1.7403849470	1.2796621983
H	1.0	-3.4814952708	-0.6028251657	-0.1470449319
H	1.0	-1.6789531295	-1.5568710177	2.1435730556
H	1.0	-1.7251238990	-2.2249902103	0.5013892206
H	1.0	-3.1266435205	-2.4202424859	1.5591049898

anti6dft E= -559.3600893984

C	6.0	0.1023356190	0.0807925657	1.7749389651
C	6.0	-0.1132275686	1.3451767784	2.6275436862
O	8.0	-0.8302573760	1.0327320443	3.8216242899
O	8.0	-1.1320945366	-0.4530381333	1.2476465254
C	6.0	0.9937110140	0.2946531230	0.5585660858
N	7.0	-1.9452708486	-1.0399885003	2.2953848426
C	6.0	-1.7764966046	-2.4989813927	2.1990887754
C	6.0	-3.3292514072	-0.6397150168	2.0028649646
C	6.0	-4.2796646978	-1.2764189330	3.0226099592
C	6.0	-2.6640347419	-3.1950978545	3.2350422557
C	6.0	-4.1348367371	-2.8037637095	3.0426450675
H	1.0	0.5496920142	-0.6757720611	2.4332932692
C	6.0	-0.7920005811	2.4966514195	1.8814198485
H	1.0	-1.3441397045	0.2296521043	3.6291166333
H	1.0	1.1946819515	-0.6582194814	0.0651995355
H	1.0	1.9454521974	0.7408786305	0.8571171056
H	1.0	0.5109682454	0.9553119158	-0.1646196420
H	1.0	-5.3056457072	-0.9844983376	2.7795003800
H	1.0	-4.0593581819	-0.8704316547	4.0164131878
H	1.0	-2.3330442989	-2.9091716915	4.2395099667
H	1.0	-2.5316070483	-4.2778262248	3.1479142631
H	1.0	-4.4988173275	-3.2162079827	2.0933979180
H	1.0	-4.7542861197	-3.2368987057	3.8337178538
H	1.0	-0.7226733190	-2.7285483379	2.3735990867
H	1.0	-2.0305133999	-2.8326216331	1.1811457525
H	1.0	-3.6015426277	-0.9407859583	0.9788590798
H	1.0	-3.3766606509	0.4490294542	2.0569270200

H	1.0	0.8850978626	1.6787638788	2.9433518215
H	1.0	-1.7468717386	2.1789880535	1.4563334595
H	1.0	-0.1661623205	2.8831525990	1.0712406011
H	1.0	-0.9812013601	3.3099630419	2.5848774419

MP2 Optimizations: **1′**–**3′**

prime5mp2 E= -518.8822327945

C	6.0	-3.0393164937	-0.2610742327	0.5005604177
C	6.0	-1.8317489541	0.6591717466	0.5408841827
O	8.0	-1.4065669606	0.8858627803	1.8730294501
O	8.0	-4.0393391181	0.4490427057	1.2468090648
C	6.0	-3.5237897864	-0.5801212581	-0.9011933286
N	7.0	-5.0547981937	-0.4821585278	1.6677966333
C	6.0	-4.8874064357	-0.6312513712	3.1150429579
C	6.0	-6.3312909743	0.1656110216	1.3665284935
C	6.0	-7.4691509459	-0.7428264921	1.8291188926
C	6.0	-5.9607043341	-1.5784323035	3.6468260481
C	6.0	-7.3525882975	-1.0306716527	3.3269805366
H	1.0	-2.7943121526	-1.1804667974	1.0476183568
H	1.0	-2.2123167870	1.1532392119	2.3277008391
H	1.0	-4.4263715498	-1.1924663621	-0.8444753864
H	1.0	-2.7606360717	-1.1348843292	-1.4564773250
H	1.0	-3.7524150281	0.3443003617	-1.4400031419
H	1.0	-7.4180059789	-1.6827593304	1.2670516187
H	1.0	-8.4276926719	-0.2669018009	1.5952303942
H	1.0	-5.8275344994	-1.7078673552	4.7263448174
H	1.0	-5.8293156411	-2.5586918199	3.1740642178
H	1.0	-8.1290506626	-1.7336432694	3.6470453859
H	1.0	-7.5070615926	-0.0975402403	3.8847914072
H	1.0	-4.9644056465	0.3529271344	3.6100221198
H	1.0	-3.8836818754	-1.0288506368	3.2949591988
H	1.0	-6.3717887010	0.3323883910	0.2867531374
H	1.0	-6.3921895001	1.1465597181	1.8694338521
H	1.0	-2.0859397355	1.6011399261	0.0323111838
H	1.0	-0.9974914118	0.1934347823	0.0098259755

prime6mp2 E= -518.8845807425

C	6.0	0.0105759916	-1.0766873396	0.0809059586
C	6.0	0.5065500237	-2.4885765725	-0.2068874306
O	8.0	-0.5389458513	-3.4422072716	-0.2531603560
O	8.0	-0.3682415524	-0.9144764699	1.4586180380
C	6.0	1.0833146320	-0.0268874415	-0.1477911857
N	7.0	-1.4620436271	-1.8056570866	1.7688818876
C	6.0	-1.0831277760	-2.4700637302	3.0190674204
C	6.0	-2.6389693031	-0.9550268492	1.9661389338
C	6.0	-3.8299124336	-1.8266933214	2.3579704460
C	6.0	-2.2163504752	-3.3954769558	3.4572874153
C	6.0	-3.5162964971	-2.6094883357	3.6339220671
H	1.0	-0.8673970360	-0.8817149624	-0.5525964095
H	1.0	1.2573474575	-2.7410342098	0.5592141203
H	1.0	1.0031937559	-2.4973770931	-1.1835533347
H	1.0	-1.1476671463	-3.1309128014	0.4363247863

H	1.0	1.9691609561	-0.2578770125	0.4506590629
H	1.0	0.7138779000	0.9582468552	0.1442354763
H	1.0	1.3666311261	-0.0007664191	-1.2030590716
H	1.0	-4.0449918312	-2.5228084779	1.5384000800
H	1.0	-4.7118723372	-1.1913965085	2.4931424312
H	1.0	-1.9295884748	-3.8948353980	4.3889851832
H	1.0	-2.3519513587	-4.1730624296	2.6958296492
H	1.0	-4.3425039991	-3.2813402828	3.8892134337
H	1.0	-3.3990278615	-1.9041176174	4.4671411715
H	1.0	-0.8705792876	-1.7156411340	3.7943175767
H	1.0	-0.1666053683	-3.0345570473	2.8268218303
H	1.0	-2.8258361819	-0.4259422986	1.0270625236
H	1.0	-2.4285834442	-0.2081617890	2.7492182963

syn5mp2 E= -558.0853231865

C	6.0	-3.0354720402	-0.2463303210	0.4879986527
C	6.0	-1.8258023805	0.6798953317	0.5451577427
O	8.0	-1.4805162398	0.9173671985	1.9044306466
O	8.0	-4.0479366188	0.4638733542	1.2208772080
C	6.0	-3.5217556008	-0.5834641063	-0.9092913578
N	7.0	-5.0551063345	-0.4727805223	1.6506923714
C	6.0	-4.8718690285	-0.6244724994	3.0960883786
C	6.0	-6.3371050107	0.1709169257	1.3641464916
C	6.0	-7.4660783741	-0.7435535179	1.8365516872
C	6.0	-5.9348860610	-1.5783248114	3.6362893100
C	6.0	-7.3322805099	-1.0354368745	3.3322700876
H	1.0	-2.7871727181	-1.1592265016	1.0467744784
H	1.0	-2.3207524890	1.1380984470	2.3223748494
H	1.0	-4.4621649640	-1.1345167138	-0.8344354167
H	1.0	-2.7981535517	-1.2087229736	-1.4396168450
H	1.0	-3.6890578560	0.3338819304	-1.4826470372
H	1.0	-7.4174252300	-1.6814477996	1.2709190216
H	1.0	-8.4290598367	-0.2707591161	1.6147747330
H	1.0	-5.7899922233	-1.7098262415	4.7140706753
H	1.0	-5.8036345779	-2.5566652389	3.1595095708
H	1.0	-8.1025165117	-1.7425148069	3.6583445078
H	1.0	-7.4845730972	-0.1046022557	3.8944525873
H	1.0	-4.9491343989	0.3582812332	3.5941106681
H	1.0	-3.8640816007	-1.0169578377	3.2648570617
H	1.0	-6.3892674964	0.3401646809	0.2852102893
H	1.0	-6.3966578084	1.1505990456	1.8698542666
C	6.0	-0.6015063376	0.0907347443	-0.1309197772
H	1.0	-2.1040790276	1.6264156868	0.0536960687
H	1.0	-0.3885865748	-0.9011485273	0.2788512660
H	1.0	0.2577708324	0.7358902337	0.0657436658
H	1.0	-0.7402263336	0.0116618536	-1.2115958524

syn6mp2 E= -558.0875996483

C	6.0	0.1738316297	0.0806564526	1.7912647961
C	6.0	-0.1772294312	1.3050768496	2.6398393033
O	8.0	-0.8209179644	0.9217821039	3.8480362637
O	8.0	-1.0028868632	-0.5303160730	1.2283054878
C	6.0	1.0326345660	0.4019166446	0.5798445630
N	7.0	-1.8444325592	-1.0517569677	2.2790616290
C	6.0	-1.7665855840	-2.5119046671	2.1814547673

C	6.0	-3.1964808342	-0.5768218574	1.9703720300
C	6.0	-4.1699706603	-1.1319979457	3.0078439358
C	6.0	-2.6831150612	-3.1351942437	3.2318747494
C	6.0	-4.1226567347	-2.6604891298	3.0279149898
C	6.0	1.0477724129	2.1161008396	3.0334005891
H	1.0	0.6758069988	-0.6523550376	2.4422032197
H	1.0	-0.8515281112	1.9278920948	2.0270052826
H	1.0	-1.3026157154	0.1100911367	3.6097389828
H	1.0	1.1099063321	-0.4836595784	-0.0548287274
H	1.0	2.0360443603	0.7056480851	0.8843880004
H	1.0	0.5786002360	1.2088422907	-0.0031165051
H	1.0	-5.1790924430	-0.7731952153	2.7784909523
H	1.0	-3.8968232208	-0.7376900635	3.9940515178
H	1.0	-2.3324445150	-2.8403316155	4.2281006825
H	1.0	-2.6157364797	-4.2264835279	3.1660706570
H	1.0	-4.4937810749	-3.0440156567	2.0683652665
H	1.0	-4.7758738875	-3.0571512993	3.8122429850
H	1.0	0.7430407511	2.8628780109	3.7703911975
H	1.0	1.4945259904	2.6278627510	2.1774690742
H	1.0	1.7953097989	1.4656446477	3.4987766911
H	1.0	-0.7235514090	-2.7991607244	2.3436723411
H	1.0	-2.0610855483	-2.8310426826	1.1682213937
H	1.0	-3.4814055241	-0.8943149410	0.9540123773
H	1.0	-3.1736294550	0.5159793193	1.9984015068

anti5mp2 E= -558.0842899175

C	6.0	-2.9366408863	-0.4048762616	0.7746561547
C	6.0	-1.8975446982	0.6877243712	0.5175631908
O	8.0	-1.2229272451	1.0203900690	1.7254192407
O	8.0	-3.7952118419	0.1930470047	1.7603953287
N	7.0	-4.9625284113	-0.6264473303	1.9501397194
C	6.0	-5.0828443854	-0.8174210043	3.3960460989
C	6.0	-6.0879080758	0.1622737471	1.4430484283
C	6.0	-7.3811777942	-0.6231076141	1.6501134116
C	6.0	-6.3382406752	-1.6371374703	3.6885995540
C	6.0	-7.5788739456	-0.9350366767	3.1342753024
H	1.0	-1.9276315380	1.1751558346	2.3644223571
H	1.0	-7.3206360972	-1.5572361078	1.0795105923
H	1.0	-8.2231712269	-0.0444372359	1.2548190014
H	1.0	-6.4244306118	-1.7900209056	4.7699549573
H	1.0	-6.2310236381	-2.6229316303	3.2208908688
H	1.0	-8.4720352280	-1.5505195609	3.2859476653
H	1.0	-7.7334318801	0.0049303750	3.6804055229
H	1.0	-5.1331926220	0.1597180880	3.9080453165
H	1.0	-4.1835053788	-1.3367142243	3.7384057510
H	1.0	-5.9078890144	0.3518711760	0.3805601271
H	1.0	-6.1384420649	1.1340545078	1.9639150852
C	6.0	-0.8408049359	0.2826964649	-0.4927342016
H	1.0	-2.4462025489	1.5657126445	0.1436111188
H	1.0	-0.2336246014	-0.5349381312	-0.0979642691
H	1.0	-0.1824949381	1.1313394996	-0.6924763889
H	1.0	-1.3032665489	-0.0331673030	-1.4326657690
C	6.0	-2.3521991775	-1.7127380996	1.2777143984
H	1.0	-3.5194146919	-0.5708393066	-0.1432761444
H	1.0	-1.6817767640	-1.5174753696	2.1178750895
H	1.0	-1.7911245637	-2.2175918207	0.4861953806

H	1.0	-3.1645239707	-2.3696277296	1.5951771116

anti6mp2 E= -558.0862080660

C	6.0	0.0952900012	0.0670028658	1.7963080989
C	6.0	-0.1583055477	1.3252780974	2.6321047116
O	8.0	-0.9101136710	1.0151488140	3.8010635810
O	8.0	-1.1176731277	-0.4688148050	1.2385993136
C	6.0	1.0012574155	0.3017977508	0.5999766082
N	7.0	-1.9179177494	-1.0460424856	2.2968109730
C	6.0	-1.7874187579	-2.5001189917	2.1605595517
C	6.0	-3.2931259693	-0.6189612916	2.0238695076
C	6.0	-4.2252006199	-1.2395220226	3.0627660289
C	6.0	-2.6569623000	-3.1853051146	3.2122285528
C	6.0	-4.1178253166	-2.7648932213	3.0452033841
H	1.0	0.5326238518	-0.6914311589	2.4623629473
C	6.0	-0.8339887223	2.4411294667	1.8420875533
H	1.0	-1.3603875962	0.1796405457	3.5901378752
H	1.0	1.2531971319	-0.6497997164	0.1266869667
H	1.0	1.9238875276	0.7971547972	0.9148333895
H	1.0	0.4968601001	0.9298692542	-0.1378046861
H	1.0	-5.2513266827	-0.9156435106	2.8583172108
H	1.0	-3.9518348811	-0.8590026406	4.0542842141
H	1.0	-2.2998055976	-2.8996955884	4.2087883052
H	1.0	-2.5462050000	-4.2709264115	3.1183394684
H	1.0	-4.4914843333	-3.1409665091	2.0836670809
H	1.0	-4.7400402229	-3.2051849027	3.8313917702
H	1.0	-0.7313254156	-2.7526660742	2.2947965524
H	1.0	-2.0903344544	-2.8041025628	1.1452957558
H	1.0	-3.5848312506	-0.9210033007	1.0047306670
H	1.0	-3.3150492422	0.4716839616	2.0844894497
H	1.0	0.8273391121	1.6783066660	2.9693001308
H	1.0	-1.7439616194	2.0712931022	1.3634701334
H	1.0	-0.1732248215	2.8477121518	1.0701851003
H	1.0	-1.0998222411	3.2457928347	2.5314198039