Supporting Information

Chiral-at-Ruthenium-SEGPHOS Catalysts Display Diastereomer-Dependent Regioselectivity: Enantioselective Isoprene-Mediated Carbonyl *tert*-Prenylation via Halide Counterion Effects

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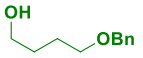
General Information:

All reactions were run under an atmosphere of argon, unless otherwise indicated. Resealable pressure tubes (13x100 mm) were purchased from Fischer Scientific (catalog number 14–959–35C) and were flame dried followed by cooling in a desiccator or under a stream of argon prior to use. All commercial reagents $RuHCl(CO)(PPh_3)_3$, (*R*)-SEGPHOS, (*S*)-SEGPHOS, rac-BINAP, and anhydrous solvents were used as received from vendors (Strem Chemicals, Fischer Scientific, Sigma Aldrich, and Combi-Blocks) without further purification. Purification of reaction products was carried out by flash column chromatography using 40-63 μm silica gel. Analytical thin-layer chromatography (TLC) was carried out using 0.25 mm commercial silica gel plates (Dynamic Absorbents F254).

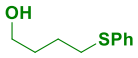
Spectroscopy, Spectrometry, and Data Collection:

Infrared spectra were recorded on a Perkin-Elmer 1600 spectrometer. High-resolution mass spectra (HRMS) were isolated on a Karatos MS9 and are reported as m/z (relative intensity). Accurate masses are reported for the molecular ion (M+, M+H, M+Na), or a suitable fragment ion. Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded with a Varian INOVA (400, 500 MHz) spectrometer equipped with a Bruker AVANCE III cryoprobe. Data reported as multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet). Integration and coupling constants were reported in Hertz (Hz). Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra were recorded with a Varian INOVA (100, 125 MHz) spectrometer and were routinely run with broadband decoupling. Fluorine-19 nuclear magnetic resonance (^{19}F NMR) spectra were recorded with a Varian INOVA (390, 470 MHz) spectrometer. Decoupled Proton Phosphorus-31 nuclear magnetic resonance (^{31}P{^{1}H} NMR) spectra were recorded with a Varian INOVA (202 MHz) spectrometer. Solid State Phosphorus-31 nuclear magnetic resonance (^{31}P NMR) spectra were recorded with a Broker Avance III 500 HD (162 MHz). Deuterium nuclear magnetic resonance (^{2}H NMR) spectra were recorded in $CHCl_3$ and C_6H_6 solutions with a Varian Gemini 500 (92 MHz) spectrometer (relaxation delay 2.00s).

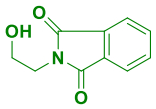
Known Alcohols:



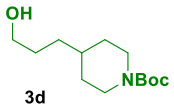
3a
commercial



3b
Ref. 1



3c
commercial



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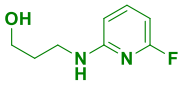
commercial



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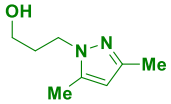

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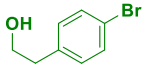
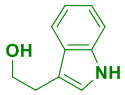
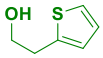
Ref. 3



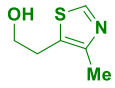
3g
commercial



3h
commercial



3i
commercial



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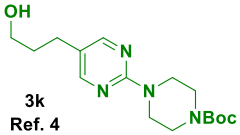
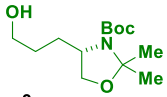


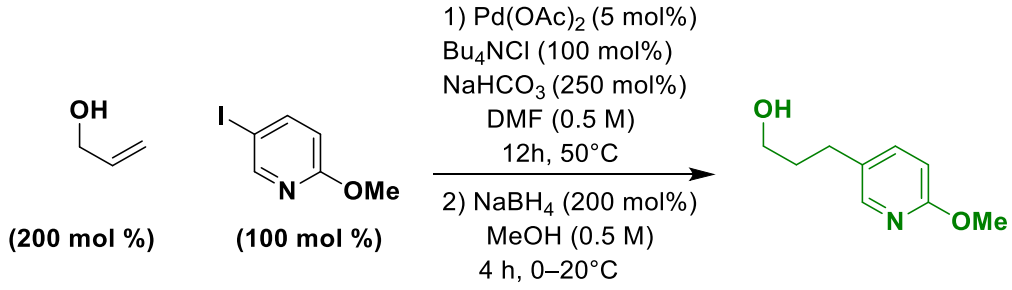
3k
Ref. 4



3m
Ref. 5

Alcohol 2l

General Procedure



To a flame dried 25 mL round bottom flask equipped with a magnetic stir-bar was added $Pd(OAc)_2$ (22.5 mg, 0.1 mmol), Bu_4NCl (555.0 mg, 2.0 mmol), $NaHCO_3$ (420.0 mg, 5.0 mmol), and DMF (4 mL) under an atmosphere of argon. The solution was sparged with argon and placed in an oil bath at 50 °C. 5-Iodo-2-methoxypyridine (500.0 mg, 2.0 mmol) and allyl alcohol (232.0 mg, 4.0 mmol) were added via syringe. The reaction was allowed to stir for 12 hours. The reaction vessel was removed from the oil bath and the reaction mixture was allowed to reach ambient temperature. Saturated NH_4Cl (aq) was added and the reaction mixture was transferred to a separatory funnel. The organic layer was collected, and the aqueous layer was extracted with ether (3 x 8 mL). The combined organic extracts were washed with water, dried (Na_2SO_4) and concentrated *in vacuo*. The crude residue was transferred to a 10 mL round bottom flask equipped with a magnetic stir bar. Methanol (4 mL) was added and the reaction vessel was placed in an ice water bath. Solid $NaBH_4$ (151.0 mg, 2.0 mmol) was slowly added. The reaction was allowed to stir for 30 minutes. The reaction vessel was removed from the ice bath and the reaction mixture was allowed to stir for 4 hours. Water was added and the reaction mixture was transferred to a separatory funnel. The organic layer was collected and the aqueous layer was extracted with ethyl acetate (3 x 5 mL). The combined organic extracts were washed with water, dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was subjected to flash column chromatography (SiO_2: 15:85 EtOAc:hexanes) to furnish the title compound as a clear oil in 81% yield (270.8 mg, 1.6 mmol).

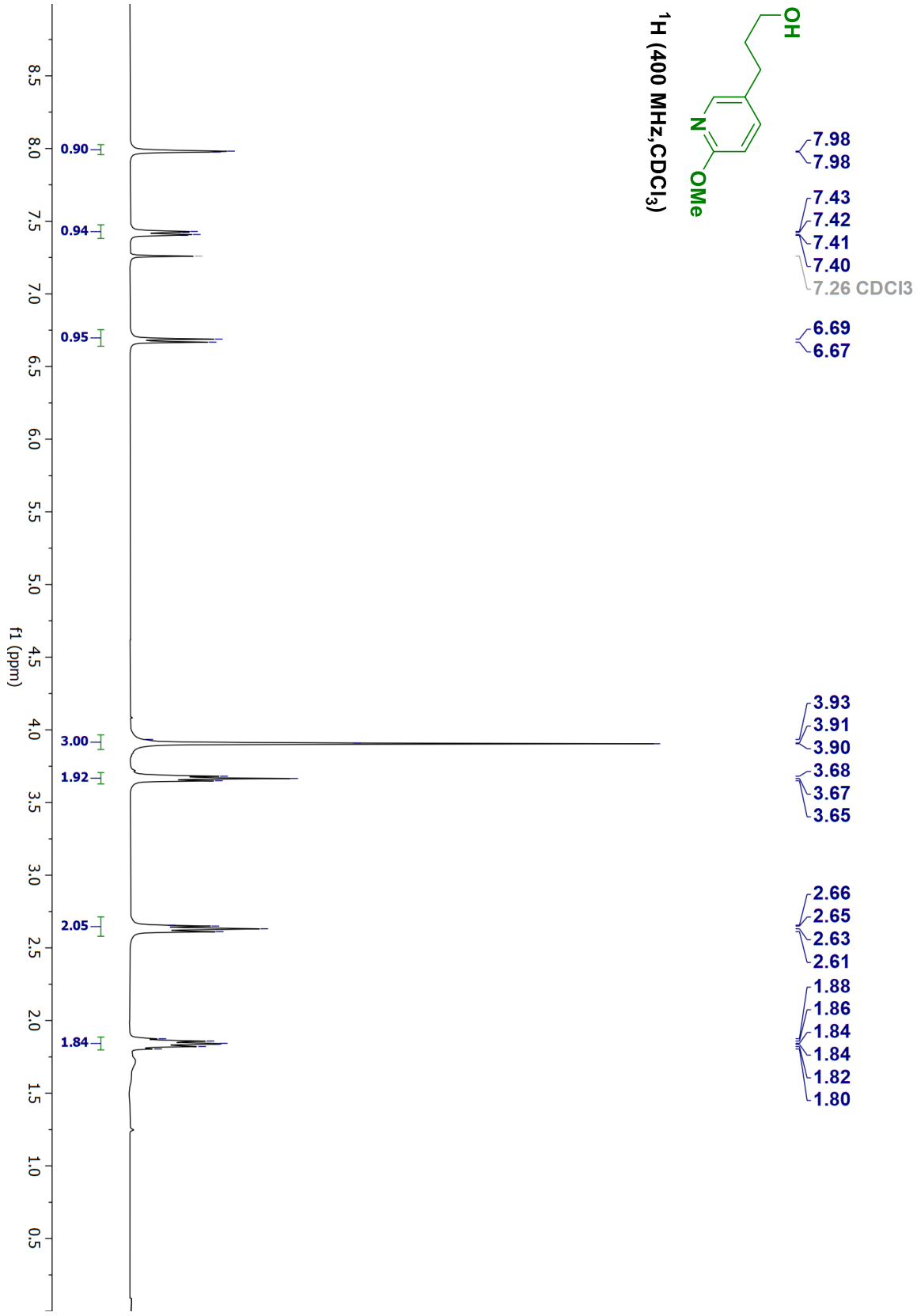
TLC (SiO_2): R_f = 0.13 (1:1 EtOAc:hexanes).

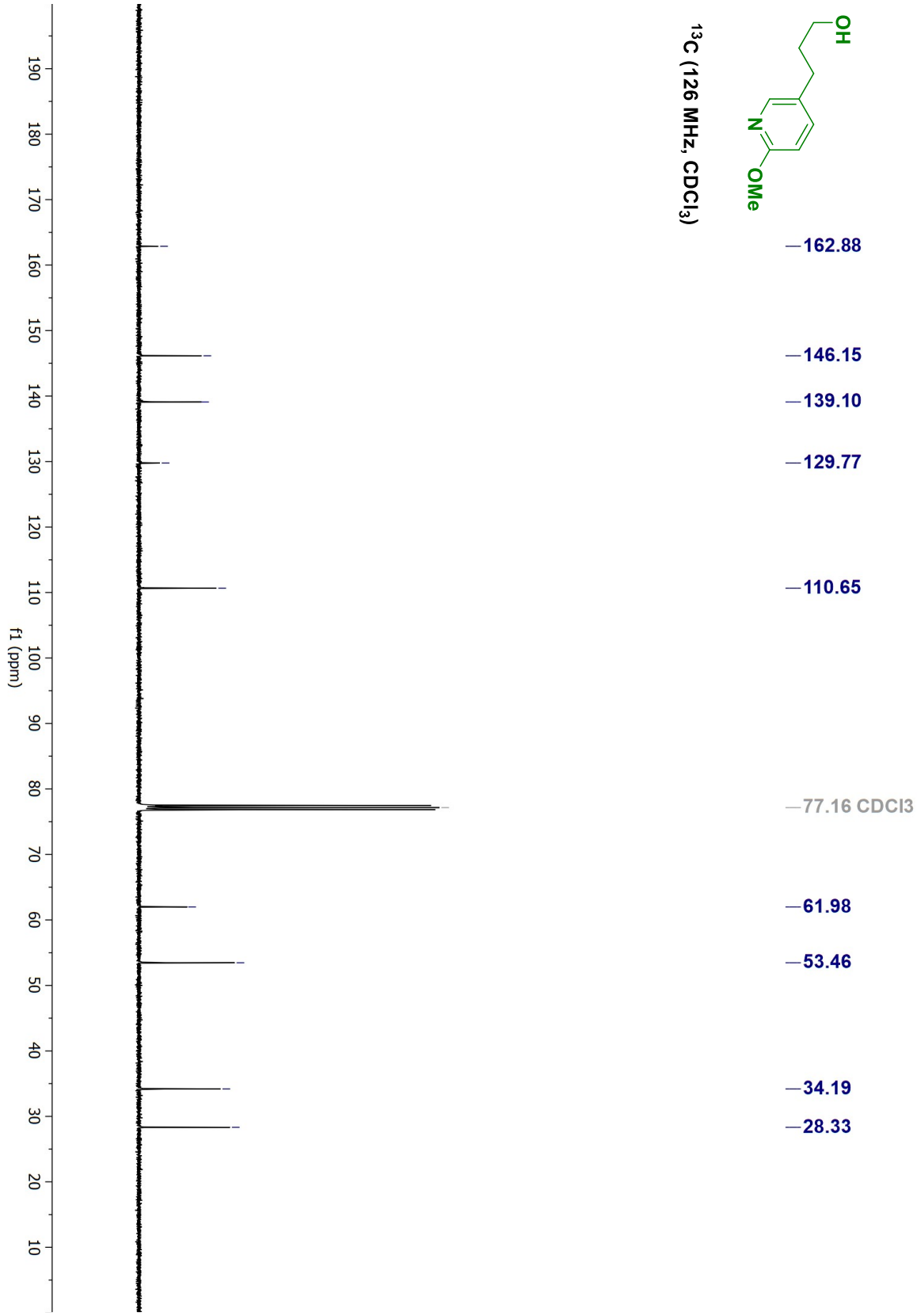
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, J = 2.5 Hz, 1H), 7.42 (dd, J = 8.5, 2.6 Hz, 1H), 6.68 (d, J = 8.4 Hz, 1H), 3.90 (s, 3H), 3.67 (t, J = 6.3 Hz, 2H), 2.63 (t, J = 7.7 Hz, 2H), 1.89 – 1.79 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.9, 146.1, 139.1, 129.8, 110.6, 62.0, 53.5, 34.2, 28.3.

HRMS (H+, *m/z*) for $C_{13}H_{19}NO_2$: calcd. = 168.1019; found = 168.1020.

FTIR (neat): 3054, 2957, 1661, 1572, 1510, 1307, 1113, 899, 778 cm^{-1}.


¹H (400 MHz,CDCl₃)
OH
N
OMe
7.98
7.98
7.43
7.42
7.41
7.40
7.26 CDCl3
6.69
6.67
3.93
3.91
3.90
3.68
3.67
3.65
2.66
2.65
2.63
2.61
1.88
1.86
1.84
1.84
1.82
1.80
0.90
0.94
0.95
3.00
1.92
2.05
1.84
f1 (ppm)


^{13}C (126 MHz, $CDCl_3$)
OH
N
OMe
162.88
146.15
139.10
129.77
110.65
77.16 CDCl3
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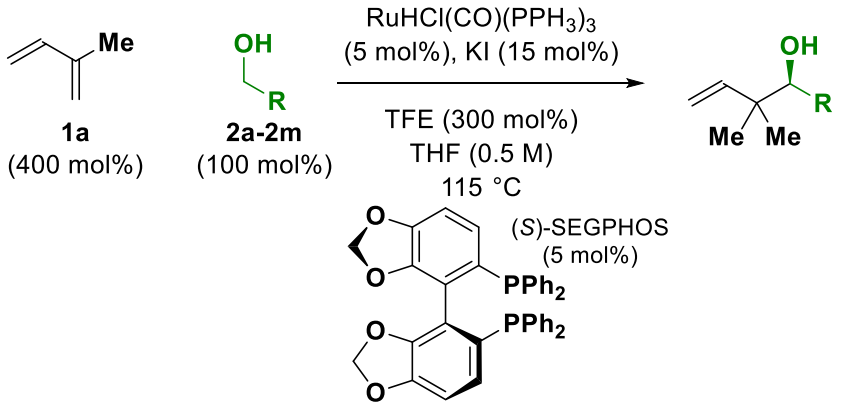
53.46
34.19
28.33
f1 (ppm)

Products 3a-3m

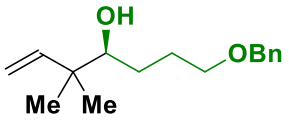
General Procedure



To an oven-dried pressure tube equipped with a magnetic stir bar under an argon atmosphere charged with alcohol **2a-2m** (0.2 mmol, 100 mol%), $RuHCl(CO)(PPh_3)_3$ (9.5 mg, 0.01 mmol, 5 mol%), **(*S*)-SEGPHOS** (6.1 mg, 0.01 mmol, 5 mol%), KI (5.0 mg, 0.03 mmol, 15 mol%) and trifluoroethanol (43 µL, 0.6 mmol, 300 mol%) was added THF (0.4 mL, 0.5 M) and isoprene (80 µL, 0.8 mmol, 400 mol%). The tube was sealed with a PTFE lined cap and the reaction vessel was placed in a 115 °C oil bath and was allowed to stir for 48 hours, at which point the reaction vessel was removed from the oil batch and the reaction mixture was allowed to reach ambient temperature. The solvent was removed *in vacuo* and the residue was subjected to flash column chromatography (SiO_2) under the noted conditions to furnish products **3a**-**3m**. Diastereomeric ratios were determined by ^1H NMR of crude reaction mixtures, regioisomeric ratios were determined by ^1H NMR of a purified mixture of regioisomers, and enantiomeric excesses were determined by chiral stationary phase HPLC.

Racemic reactions were performed using *rac*-BINAP (6.2 mg, 0.01 mmol, 5 mol%) as ligand.

(*S*)-7-(benzyloxy)-3,3-dimethylhept-1-en-4-ol (3a)



Alcohol **2a** (36.0 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h). Flash column chromatography (SiO_2: 8:92 EtOAc:hexanes) provided the title compound **3a** as a yellow oil in 75% yield (37.4 mg, 0.15 mmol, 17:1 rr, 90% ee).

Aldehyde *dehydro*-**2a** (36.0 mg, 0.2 mmol) was subjected to standard reaction conditions (115°C, 48 h) with 2-PrOH (22 µL, 0.3 mmol, 150 mol%). Flash column chromatography (SiO_2: 8:92 EtOAc:hexanes) provided title compound **3a** as a yellow oil in 76% Yield (37.7 mg, 0.15 mmol, 15:1 rr, 90% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 2:98 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.5 (1:3 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 – 7.31 (m, 4H), 7.28 (td, J = 5.9, 2.5 Hz, 1H), 5.83 (dd, J = 17.5, 10.8 Hz, 1H), 5.07 (dd, J = 10.8, 1.4 Hz, 1H), 5.04 (dd, J = 17.5, 1.4 Hz, 1H), 4.52 (s, 2H), 3.51 (t, J = 6.0 Hz, 2H), 3.27 (ddd, J = 10.7, 4.6, 1.7 Hz, 1H), 2.04 (d, J = 4.6 Hz, 1H), 1.83 (dt, J = 10.7, 5.8 Hz, 1H), 1.69 (m, 2H), 1.29 (td, J = 10.7, 5.8 Hz, 1H), 1.01 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 145.7, 138.6, 128.5, 127.9, 127.7, 113.2, 78.2, 73.1, 70.5, 41.8, 28.7, 27.4, 23.2, 22.5.

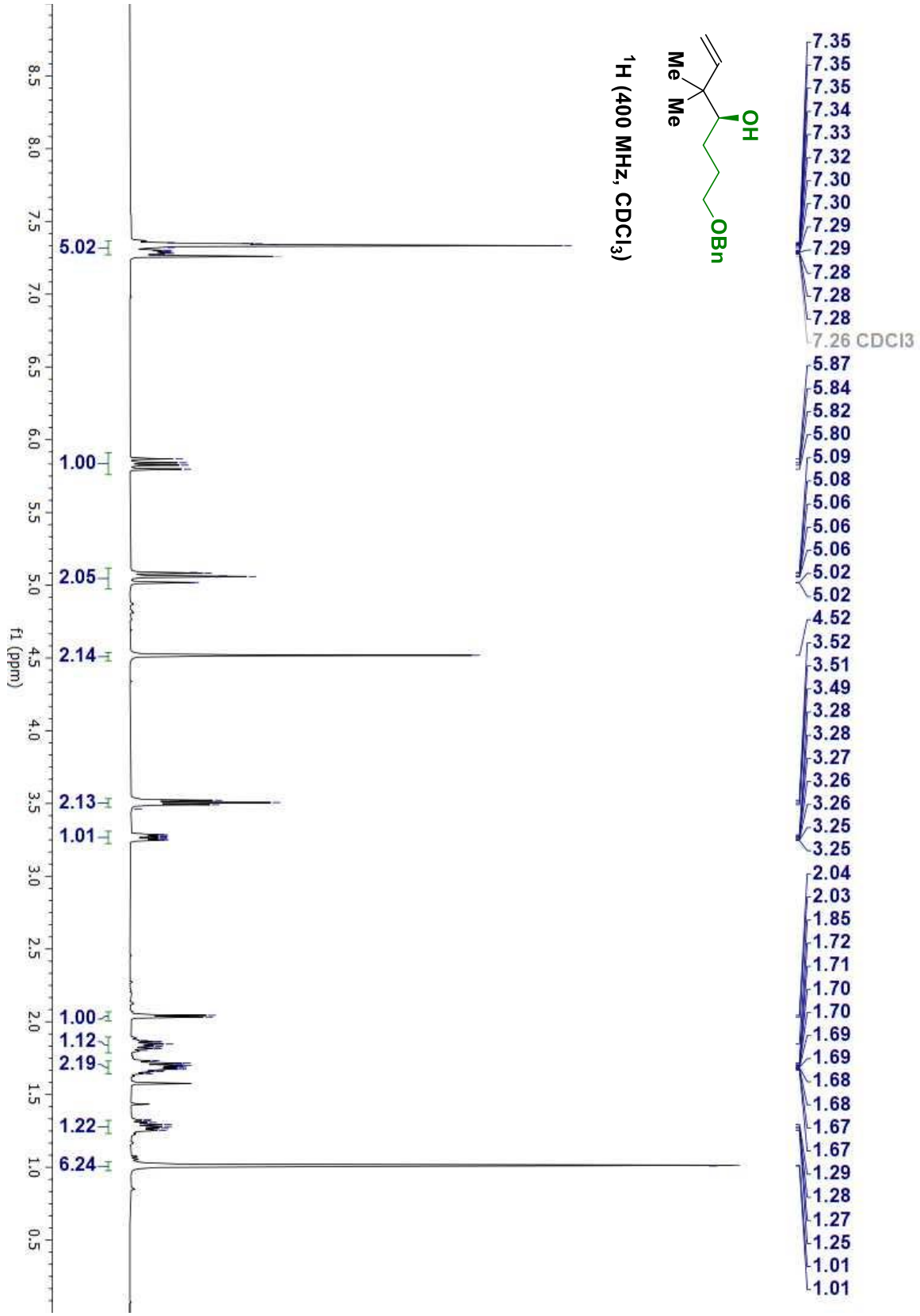
HRMS (Na+, *m/z*) for $C_{16}H_{24}O_2$: calcd. = 271.1669; found = 271.1669.

FTIR (neat): 3478, 2959, 2862, 1637, 1496, 1454, 1414, 1361, 1274, 1204, 1091, 1028, 1005, 972, 910, 734, 696 cm^{-1}.

HPLC (Alcohol **2a**): (Chiralcel columns Amylose 3-1 + Amylose 3-2, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm).

HPLC (Aldehyde *dehydro*-**2a**): (Chiralcel column Amylose 3-1, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm).

$[\alpha]_D^{24}$ = -20.9 (c = 0.1, $CHCl_3$).


^{1}H (400 MHz, CDCl$_3$)
Me Me
OH
OBn
7.35
7.35
7.35
7.34
7.33
7.32
7.30
7.30
7.29
7.29
7.28
7.28
7.28
7.26 CDCl3
5.87
5.84
5.82
5.80
5.09
5.08
5.06
5.06
5.06
5.02
5.02
4.52
3.52
3.51
3.49
3.28
3.28
3.27
3.26
3.26
3.25
3.25
2.04
2.03
1.85
1.72
1.71
1.70
1.70
1.69
1.69
1.68
1.68
1.67
1.67
1.29
1.28
1.27
1.25
1.01
1.01
5.02
1.00
2.05
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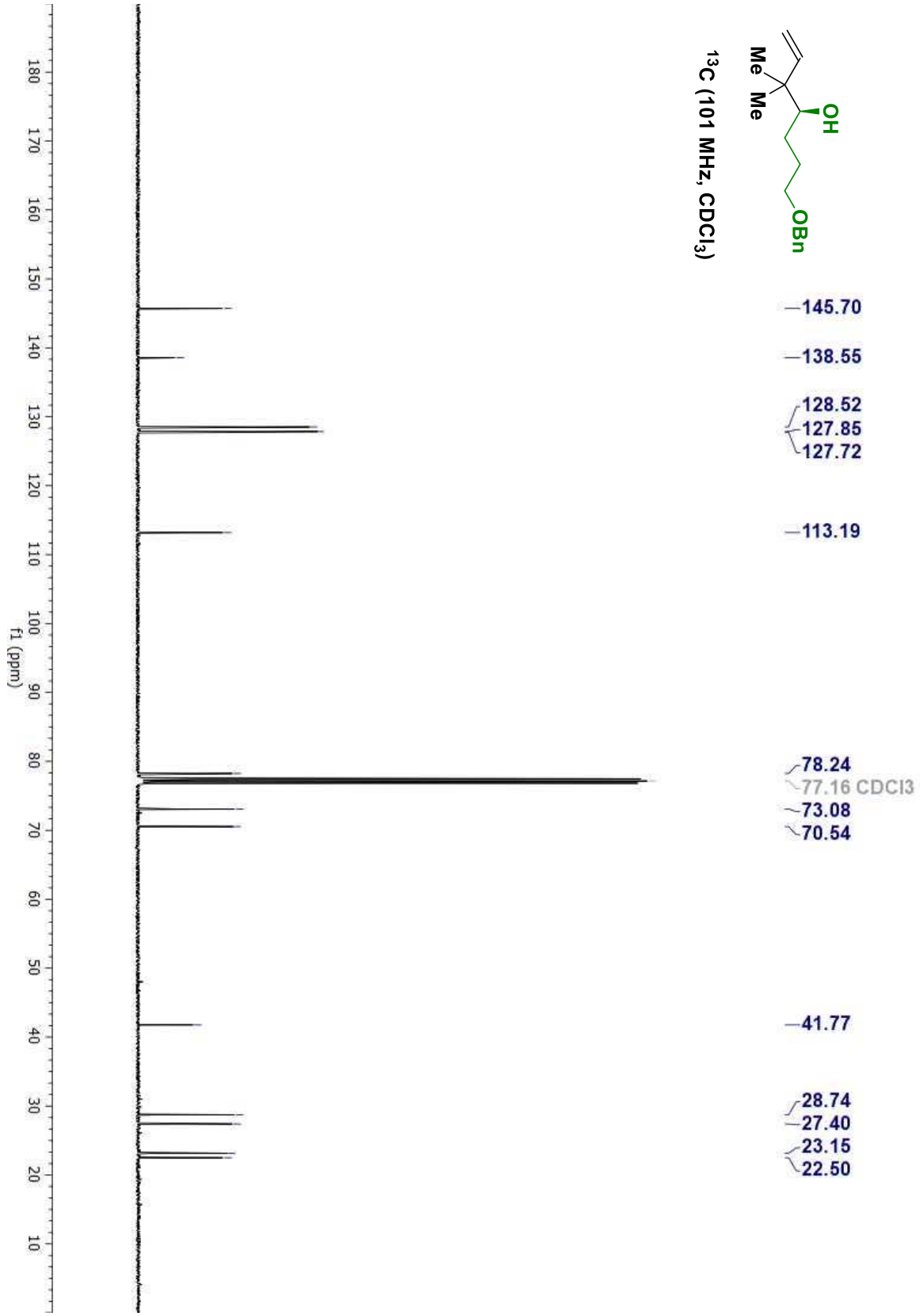
1.01
1.00
1.12
2.19
1.22
6.24
f1 (ppm)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Me
Me
OH
OBn
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138.55
128.52
127.85
127.72
113.19
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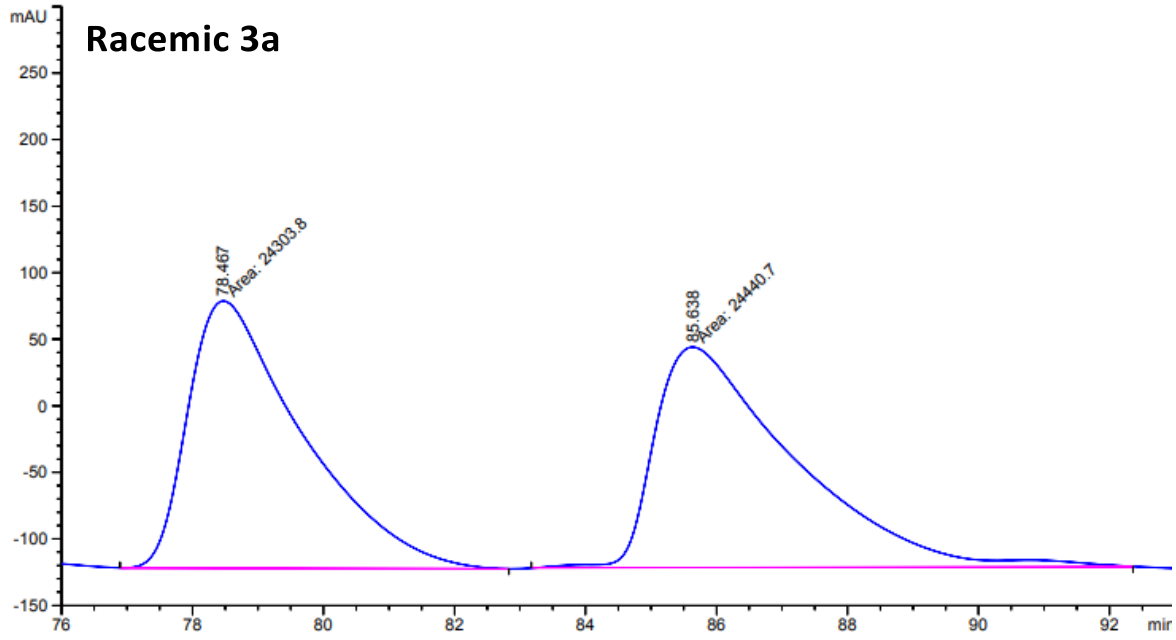
27.40
23.15
22.50
f1 (ppm)



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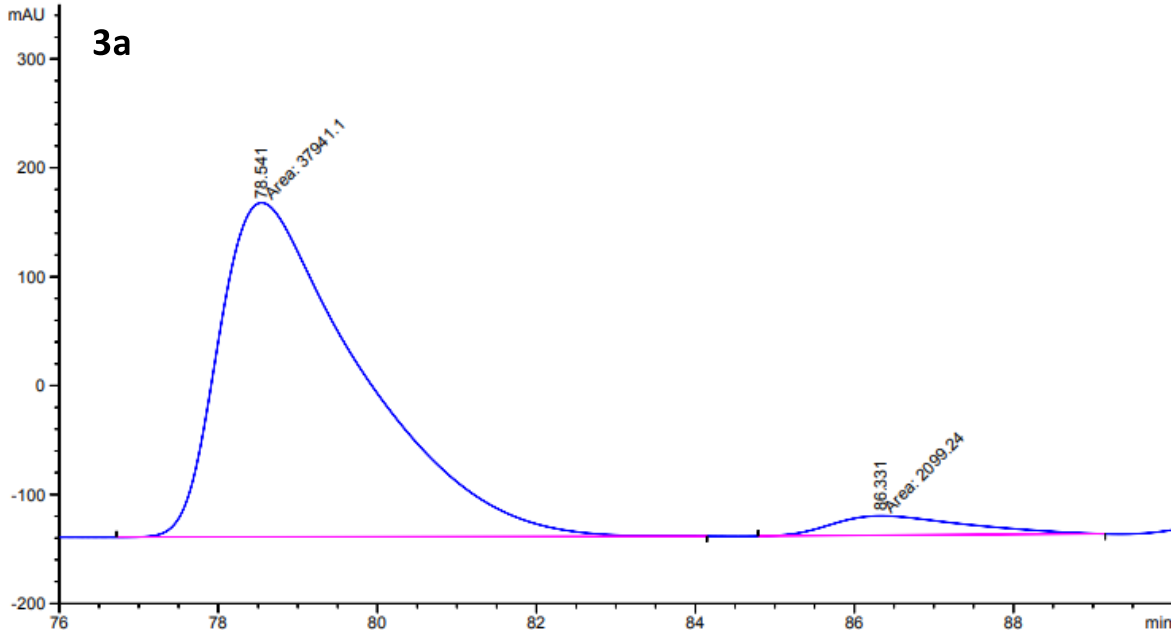

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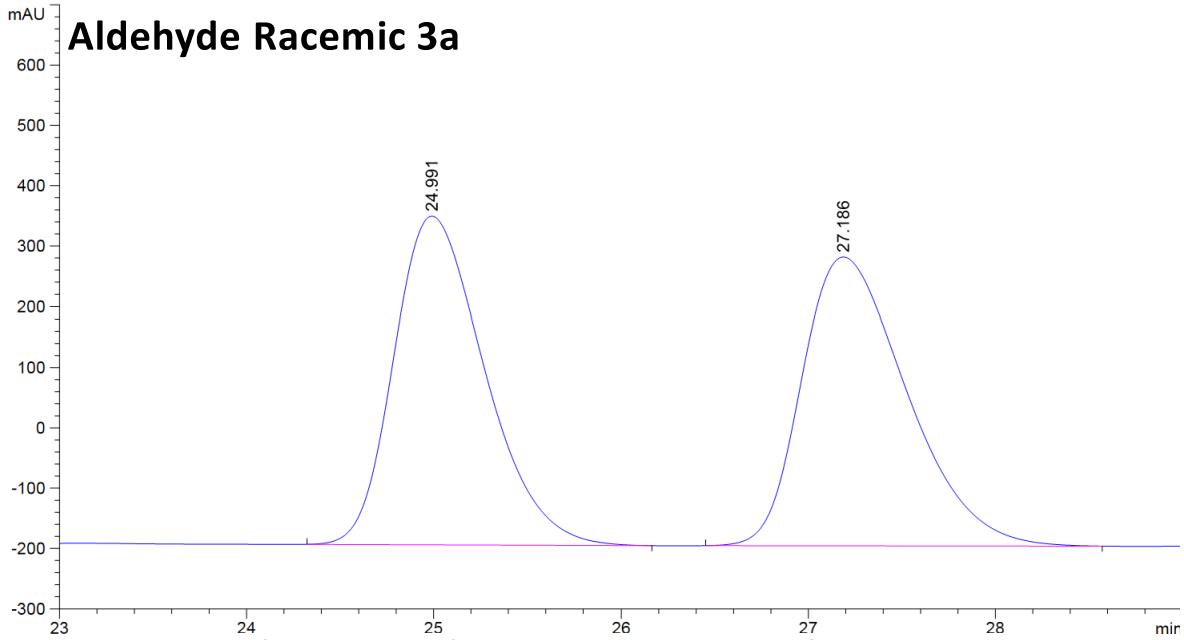
Aldehyde Racemic 3a



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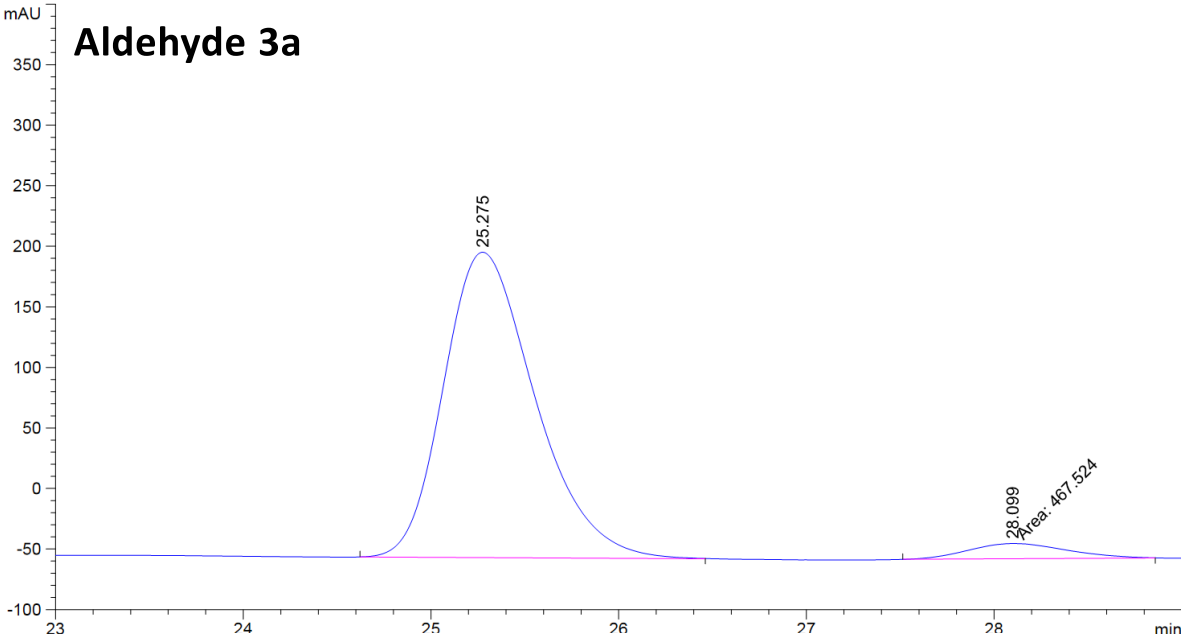
Aldehyde 3a



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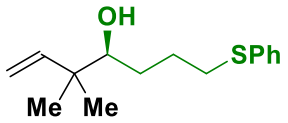
1	25.275	BB	0.5254	8551.91895	252.31773	94.8165
2	28.099	MM	0.6141	467.52444	12.68763	5.1835

(*S*)-3,3-dimethyl-7-(phenylthio)hept-1-en-4-ol (3b)



Alcohol **2b** (36.0 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h) with (*S*)-SEGPHOS (7.5 mol%), $RuHCl(CO)(PPh_3)_3$ (7.5 mol%), and KI (20 mol%). Flash column chromatography (SiO_2: 3:97 EtOAc:hexanes) provided the title compound **3b** as a yellow oil in 65% yield (32.4 mg, 0.13 mmol, 16:1 rr, 87% ee).

Aldehyde *dehydro*-**2b** (36.0 mg, 0.2 mmol) was subjected to standard reaction conditions (115°C, 48 h) with 2-PrOH (22 µL, 0.3 mmol, 150 mol%), (*S*)-SEGPHOS (7.5 mol%), $RuHCl(CO)(PPh_3)_3$ (7.5 mol%), and KI (20 mol%). Flash column chromatography (SiO_2: 3:97 EtOAc:hexanes) provided the title compound **3b** as a yellow oil in 69% Yield (34.2 mg, 0.14 mmol, 14:1 rr, 86% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 1:99 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.4 (1:3 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.32 (m, 2H), 7.30 – 7.26 (m, 2H), 7.20 – 7.14 (m, 1H), 5.80 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.11 (dd, *J* = 10.8, 1.4 Hz, 1H), 5.06 (dd, *J* = 17.5, 1.4 Hz, 1H), 3.25 (ddd, *J* = 10.8, 5.0, 1.6 Hz, 1H), 2.96 (t, *J* = 7.1 Hz, 2H), 2.00 – 1.88 (m, 1H), 1.74 – 1.64 (m, 2H), 1.47 (d, *J* = 5.0 Hz, 1H), 1.40 – 1.31 (m, 1H), 1.01 (s, 6H).

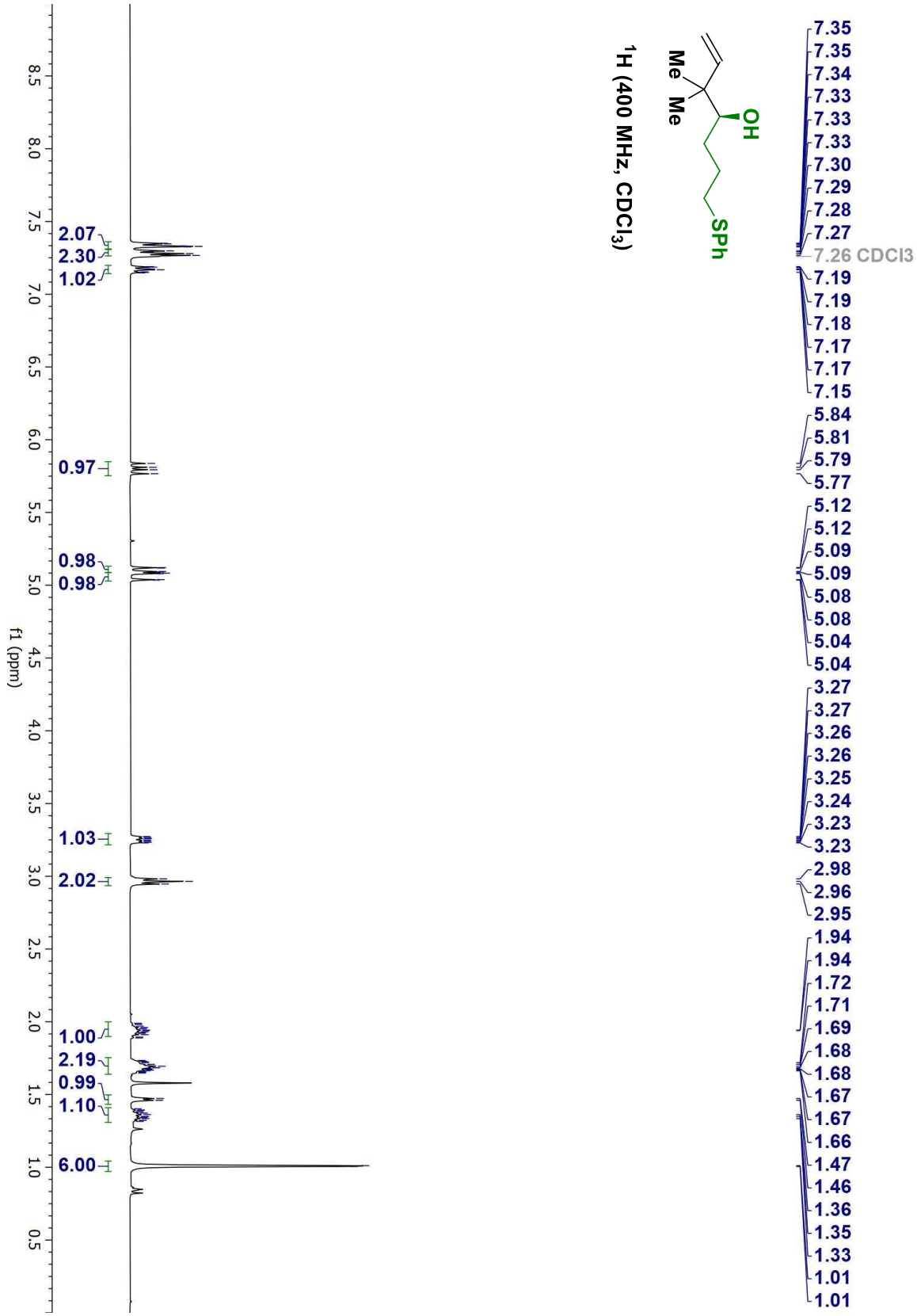
^{13}C NMR (101 MHz, $CDCl_3$): δ 145.3, 136.9, 129.2, 129.0, 125.9, 113.8, 77.9, 41.9, 33.8, 30.5, 26.8, 23.3, 22.0.

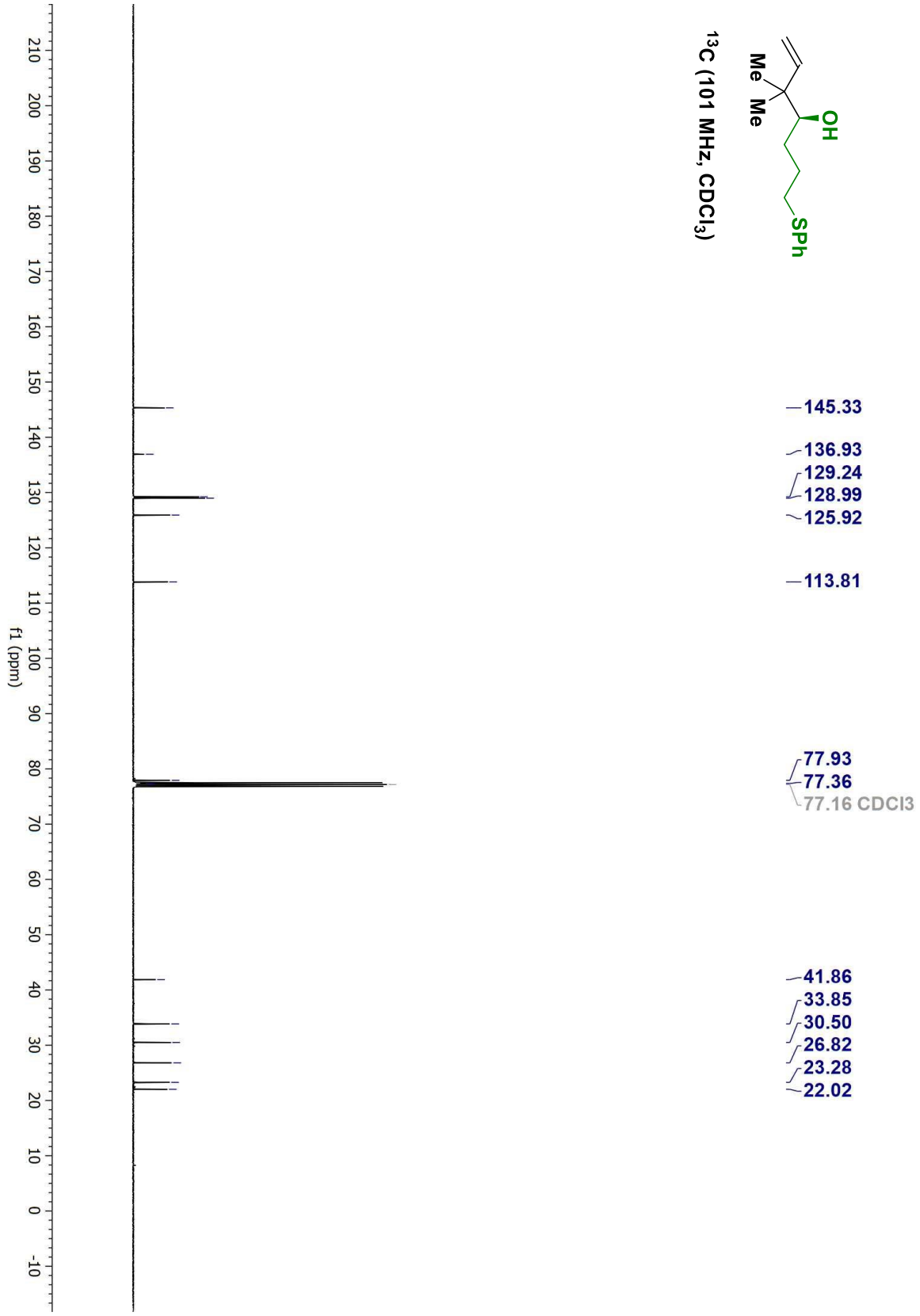
HRMS (Na+, *m/z*) for $C_{15}H_{22}OS$: calcd. = 273.1284; found = 273.1291.

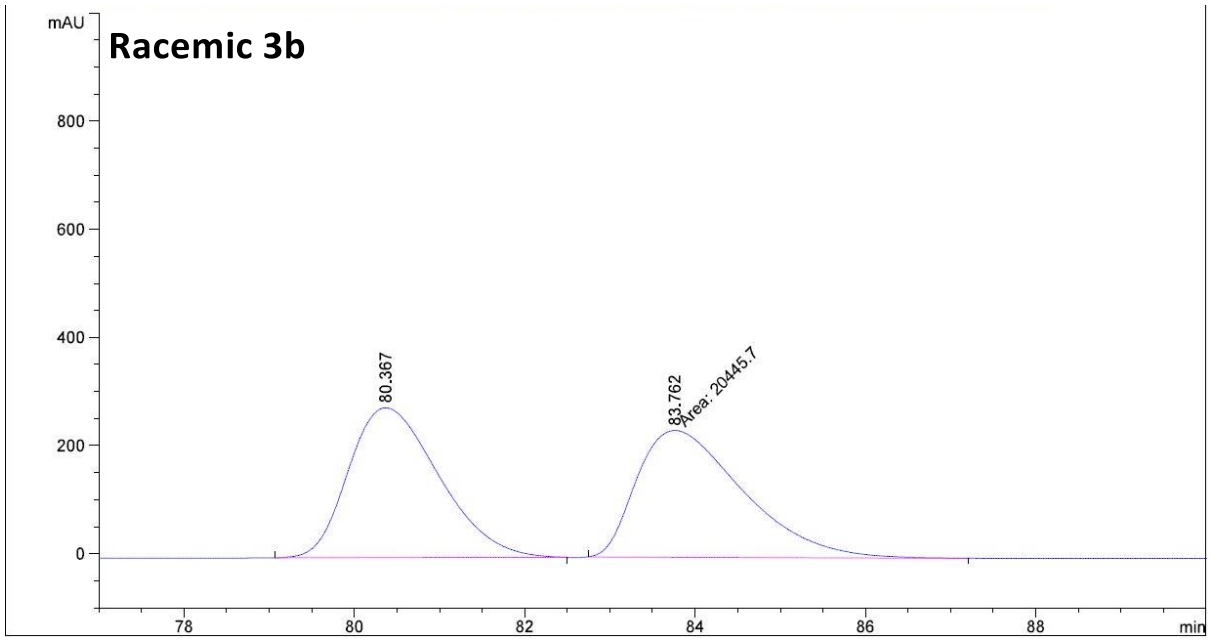
FTIR (neat): 3444, 3077, 2958, 2868, 1639, 1584, 1480, 1285, 1070, 915, 738, 690 cm^{-1}.

HPLC: (Chiralcel columns Amylose 3-1 + Amylose 3-2, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm).

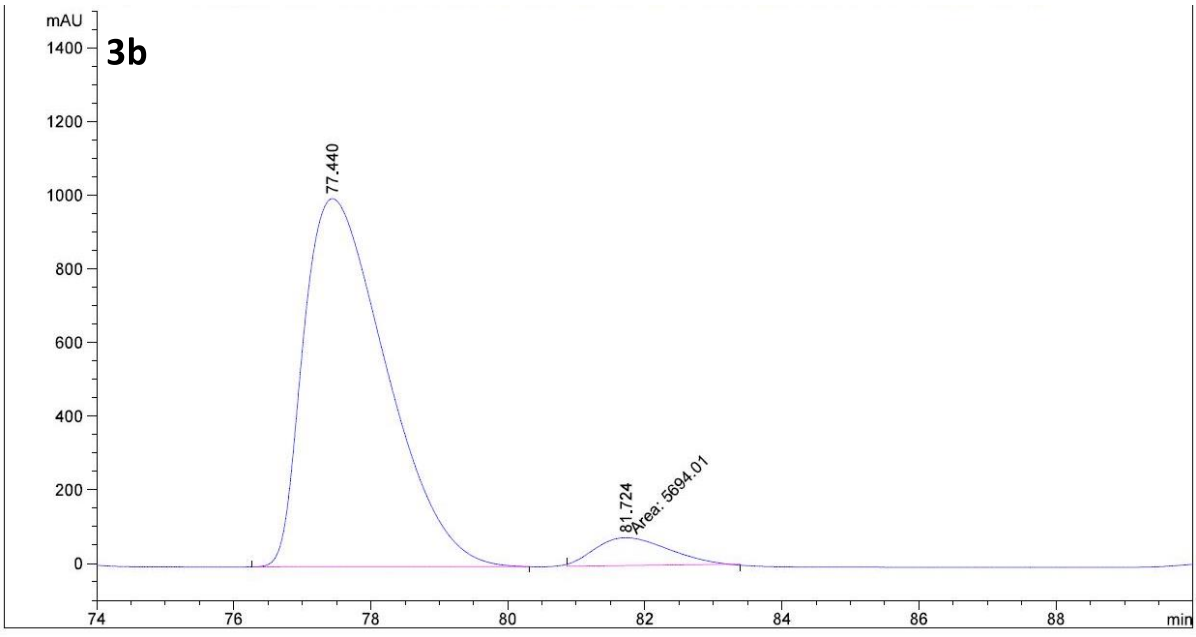
$[\alpha]_D^{24}$ = -2.75 (c = 1.0, $CHCl_3$).


^{1}H (400 MHz, CDCl$_3$)
Me Me
OH
SPh
7.35
7.35
7.34
7.33
7.33
7.33
7.30
7.29
7.28
7.27
7.26 CDCl3
7.19
7.19
7.18
7.17
7.17
7.15
5.84
5.81
5.79
5.77
5.12
5.12
5.09
5.09
5.08
5.08
5.04
5.04
3.27
3.27
3.26
3.26
3.25
3.24
3.23
3.23
2.98
2.96
2.95
1.94
1.94
1.72
1.71
1.69
1.68
1.68
1.67
1.67
1.66
1.47
1.46
1.36
1.35
1.33
1.01
1.01
2.07
2.30
1.02
0.97
0.98
0.98
1.03
2.02
1.00
2.19
0.99
1.10
6.00
f1 (ppm)

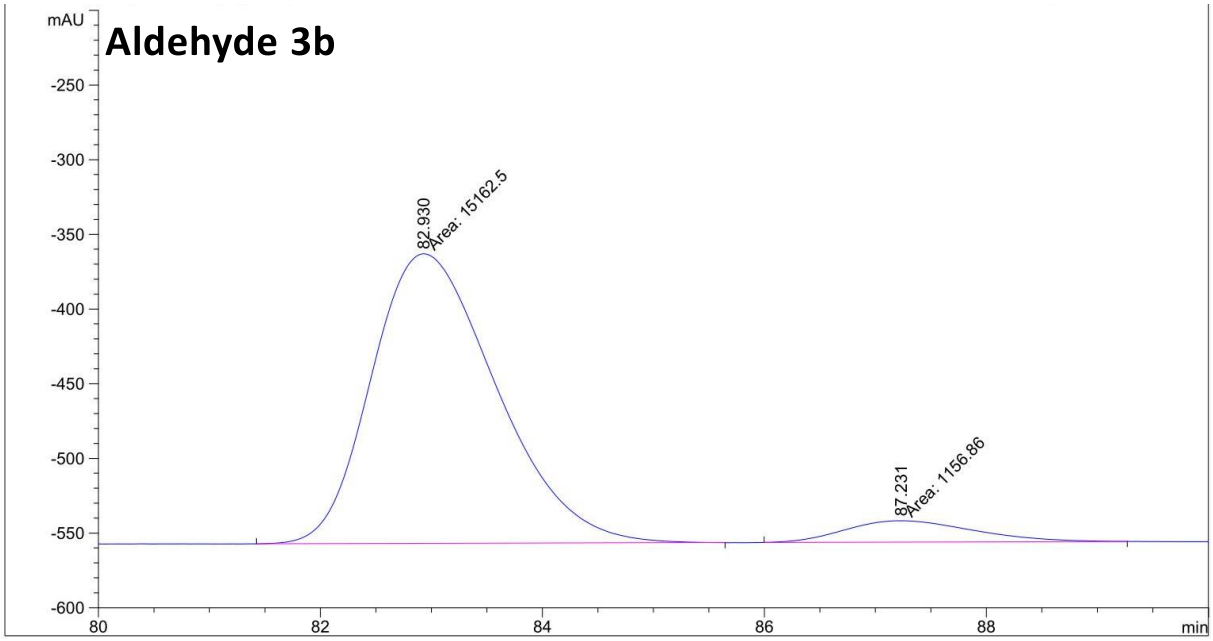

^{13}C (101 MHz, $CDCl_3$)
Me
Me
OH
SPh
145.33
136.93
129.24
128.99
125.92
113.81
77.93
77.36
77.16 CDCl3
41.86
33.85
30.50
26.82
23.28
22.02
f1 (ppm)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	80.367	BB	1.1470	2.04634e4	277.28897	50.0217
2	83.762	MM	1.4503	2.04457e4	234.95982	49.9783

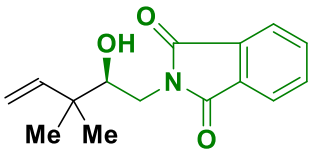


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	77.440	BB	1.2873	8.37597e4	999.86316	93.6347
2	81.724	MM	1.2476	5694.01172	76.06358	6.3653



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	82.930	MM	1.3031	1.51625e4	193.92921	92.9111
2	87.231	MM	1.3438	1156.86389	14.34767	7.0889

(R)-2-(2-hydroxy-3,3-dimethylpent-4-en-1-yl)isoindoline-1,3-dione (3c)



Alcohol **2c** (38.2 mg, 0.2 mmol) was subjected to standard reaction conditions (120 °C, 48 h). Flash column chromatography (SiO_2: 8:92 EtOAc:hexanes) provided the title compound **3c** as a yellow oil in 72% yield (37.3 mg, 0.14 mmol, >20:1 rr, 84% ee).

TLC (SiO_2): R_f = 0.3 (1:2 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, J = 5.4 Hz, 2H), 7.72 (d, J = 5.5 Hz, 2H), 5.94 (dd, J = 17.4, 10.9 Hz, 1H), 5.19 – 5.08 (m, 2H), 3.94 – 3.84 (m, 1H), 3.70 – 3.56 (m, 2H), 2.22 (d, J = 6.0 Hz, 1H), 1.14 (s, 6H).

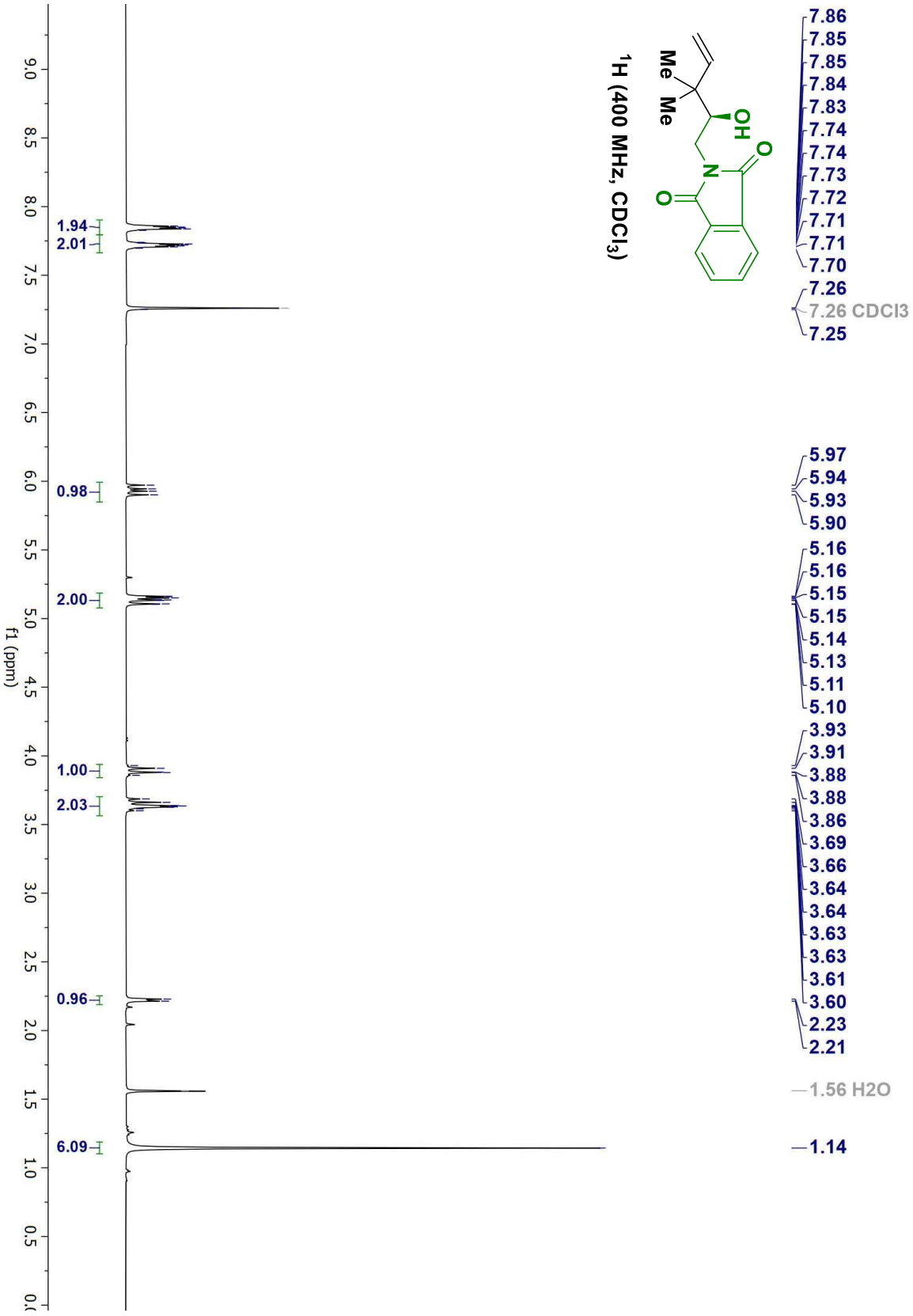
^{13}C NMR (101 MHz, $CDCl_3$): δ 169.1, 143.9, 134.2, 132.2, 123.5, 114.1, 77.4, 76.9, 41.1, 23.4, 22.6.

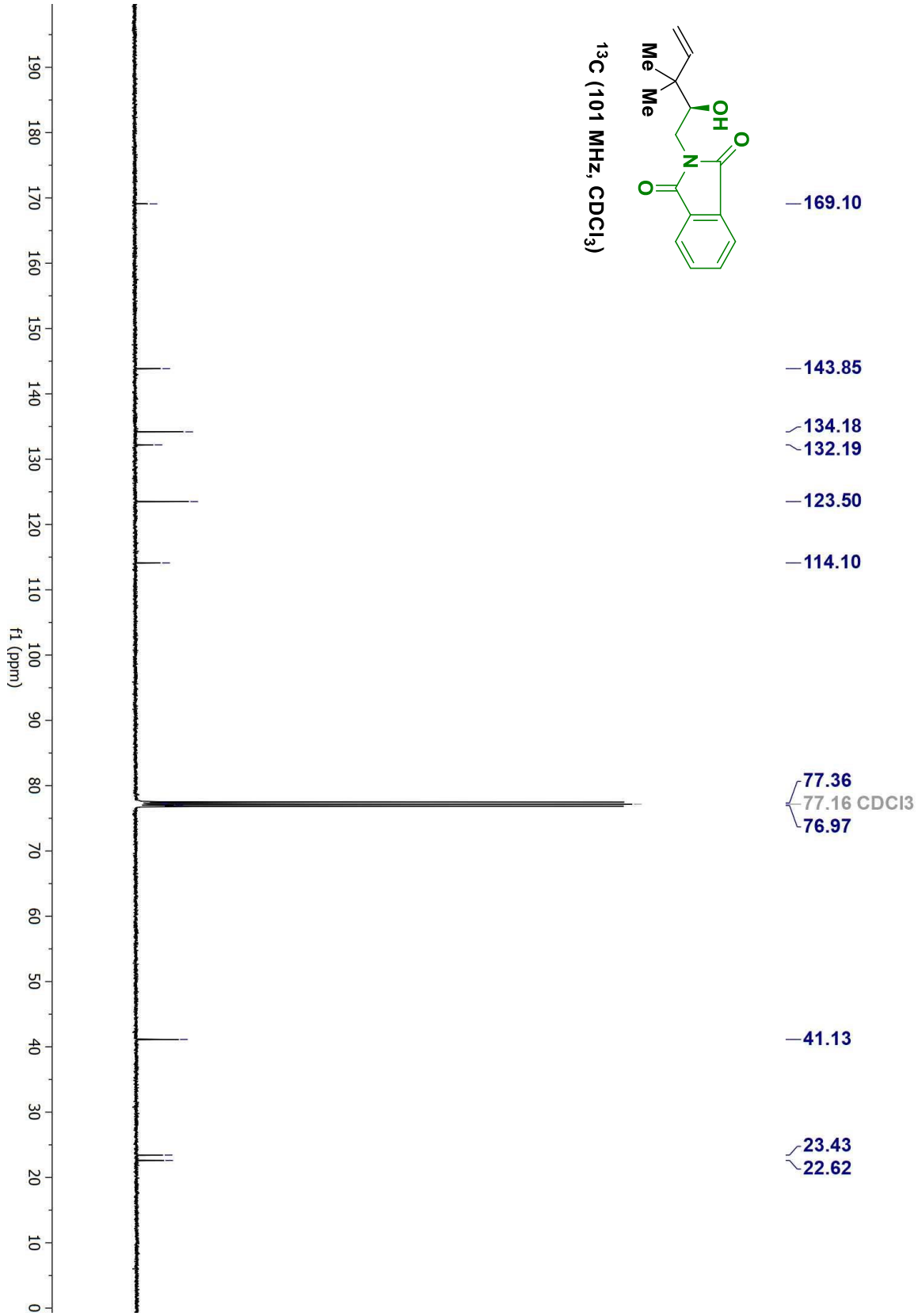
HRMS (Na+, *m/z*) for $C_{15}H_{17}NO_3$: calcd. = 282.1192; found = 282.1194.

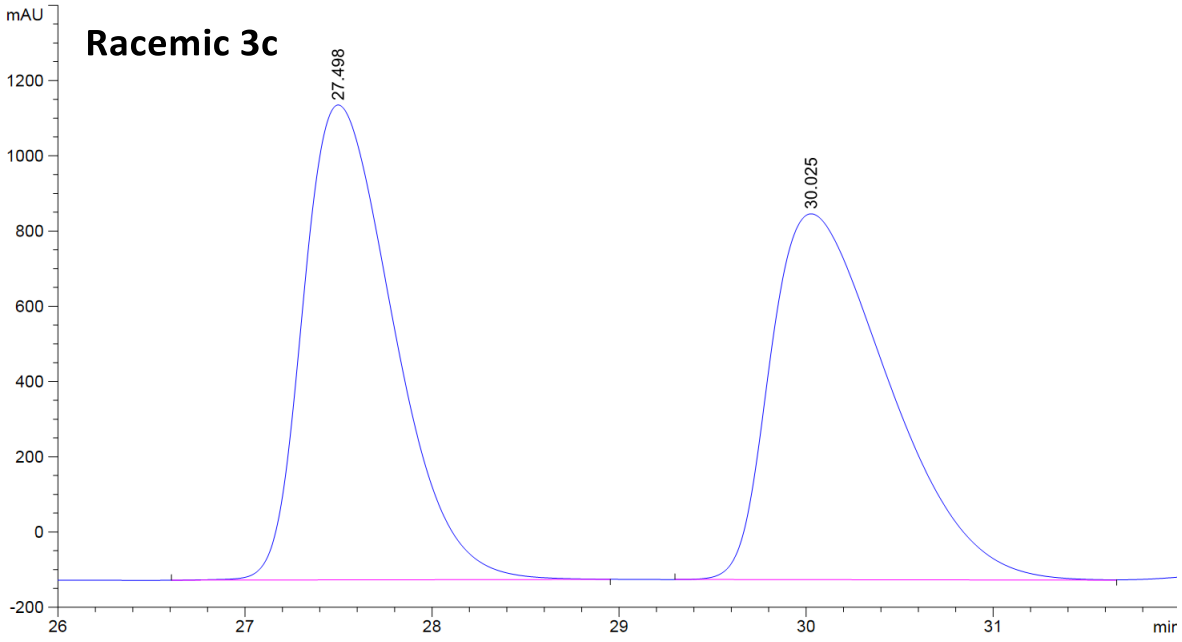
FTIR (neat): 3325, 2967, 2833, 1759, 1624, 1574, 1424, 1294, 1013, 935, 724 cm^{-1}.

HPLC: (Chiralcel columns Cellulose-5, Hexane:2-PrOH = 97:03, 0.5 mL/min, 210 nm).

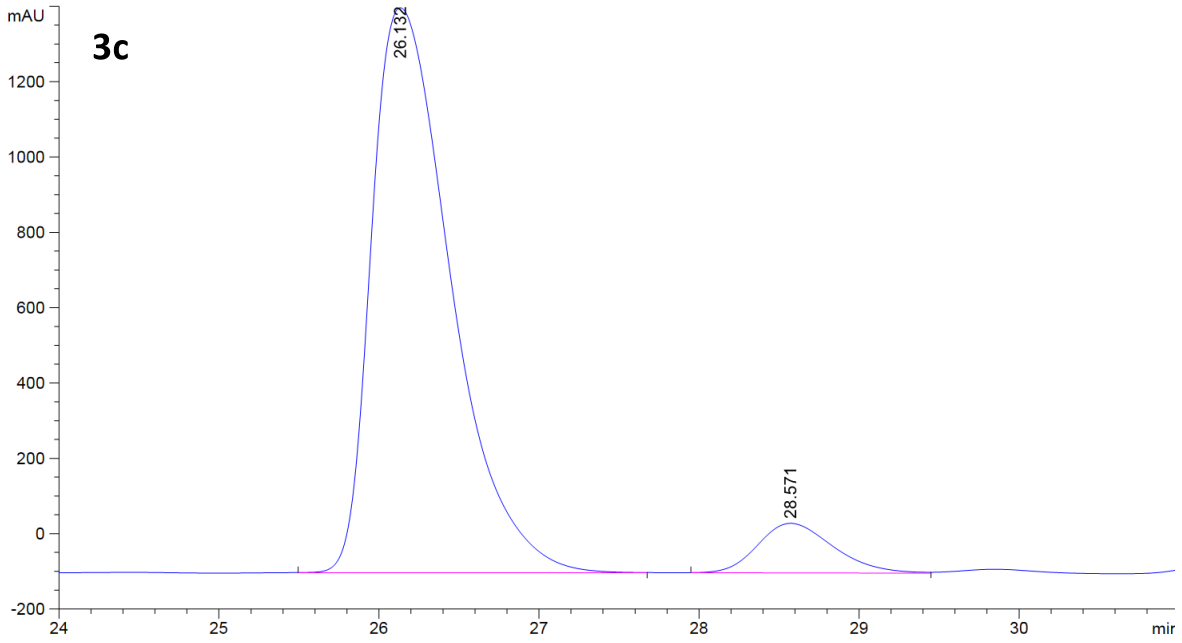
$[\alpha]_D^{24}$ = -8.5 (c = 1.0, $CHCl_3$).


^{1}H (400 MHz, CDCl$_3$)
Me
Me
OH
N
O
O
7.86
7.85
7.85
7.84
7.83
7.74
7.74
7.73
7.72
7.71
7.71
7.70
7.26
7.26 CDCl3
7.25
5.97
5.94
5.93
5.90
5.16
5.16
5.15
5.15
5.14
5.13
5.11
5.10
3.93
3.91
3.88
3.88
3.86
3.69
3.66
3.64
3.64
3.63
3.63
3.61
3.60
2.23
2.21
1.56 H2O
1.14
1.94
2.01
0.98
2.00
1.00
2.03
0.96
6.09
f1 (ppm)


^{13}C (101 MHz, CDCl$_3$)
Me
Me
OH
O
N
O
169.10
143.85
134.18
132.19
123.50
114.10
77.36
77.16 CDCl3
76.97
41.13
23.43
22.62
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

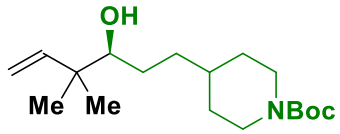


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.498	BB	0.5251	4.23250e4	1262.66516	49.7265
2	30.025	BB	0.6792	4.27906e4	972.75665	50.2735



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.132	BB	0.5361	5.16912e4	1499.88110	92.2561
2	28.571	BB	0.5119	4338.94336	131.84384	7.7439

***Tert*-butyl (*S*)-4-(3-hydroxy-4,4-dimethylhex-5-en-1-yl)piperidine-1-carboxylate (3d)**



Alcohol **2d** (48.6 mg, 0.2 mmol) was subjected to standard reaction conditions (120 °C, 48 h). Flash column chromatography (SiO_2: 3:97 EtOAc:hexanes) provided the title compound **3d** as a yellow oil in 70% yield (43.4 mg, 0.14 mmol, 15:1 rr, 91% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 2:98 Acetone:hexanes).

TLC (SiO_2): R_f = 0.25 (1:4 EtOAc:Hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 5.80 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.09 (dd, *J* = 10.8, 1.4 Hz, 1H), 5.05 (dd, *J* = 17.5, 1.4 Hz, 1H), 4.06 (s, 2H), 3.21 (dd, *J* = 9.0, 4.7 Hz, 1H), 2.66 (s, 2H), 1.68 – 1.60 (m, 2H), 1.55 – 1.51 (m, 2H), 1.45 (s, 9H), 1.26 – 1.20 (m, 3H), 1.14 – 1.02 (m, 2H), 1.00 (s, 6H).

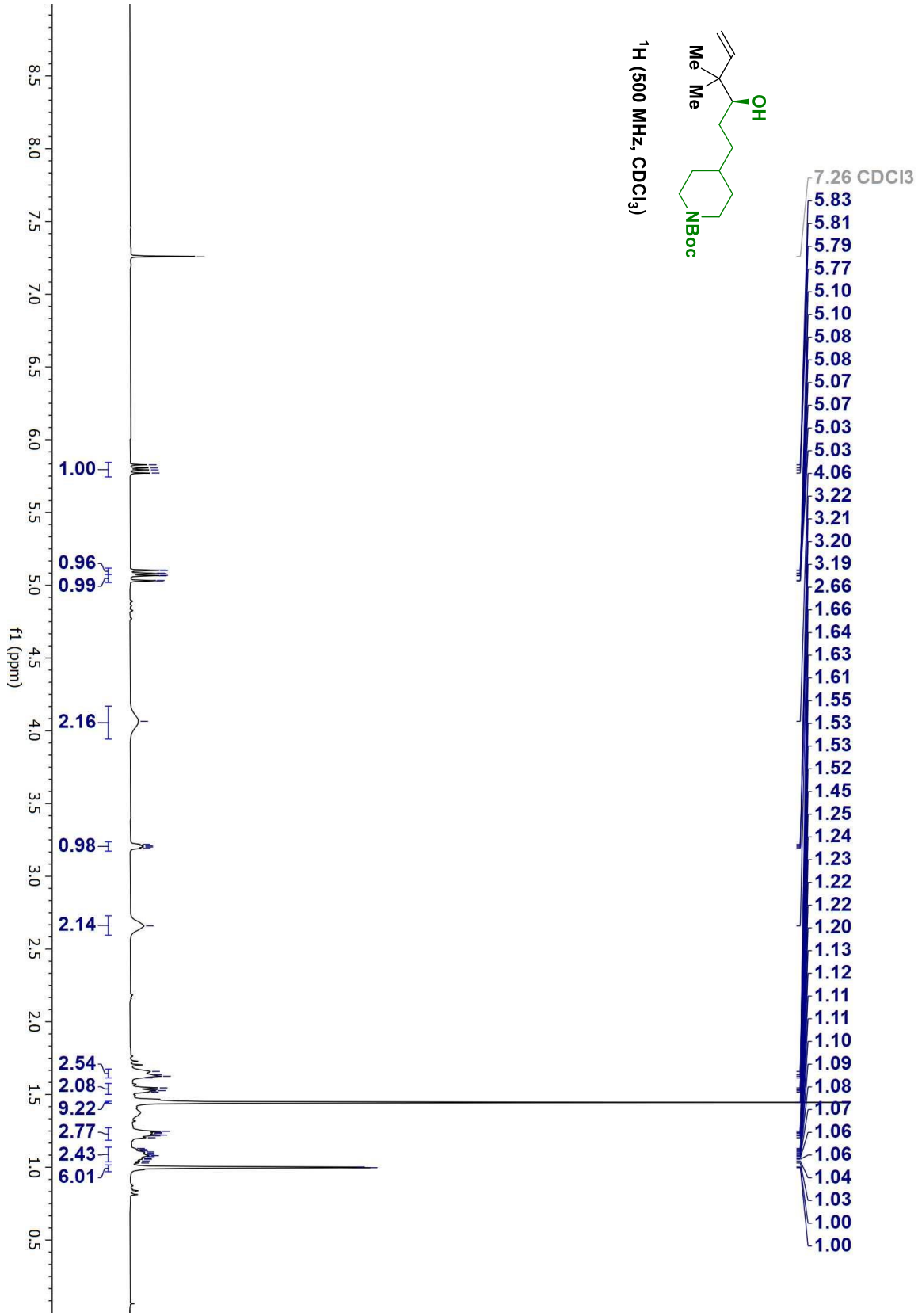
^{13}C NMR (126 MHz, $CDCl_3$): δ 155.1, 145.5, 113.7, 79.3, 78.5, 77.4, 41.9, 36.2, 34.0, 28.6, 28.4, 23.3, 22.1.

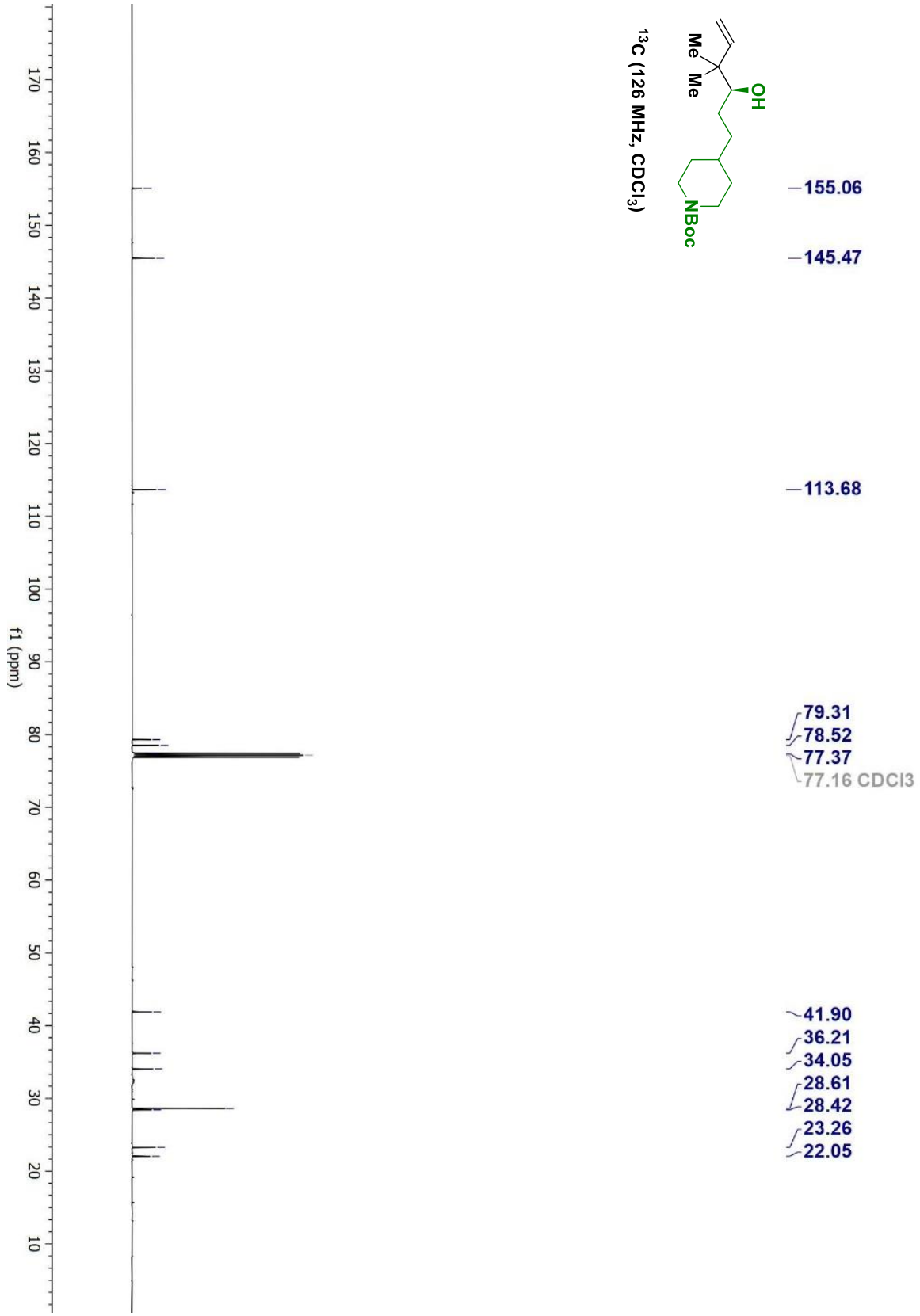
HRMS (Na+, *m/z*) for $C_{18}H_{33}NO_3$: calcd. = 334.2353; found = 334.2344.

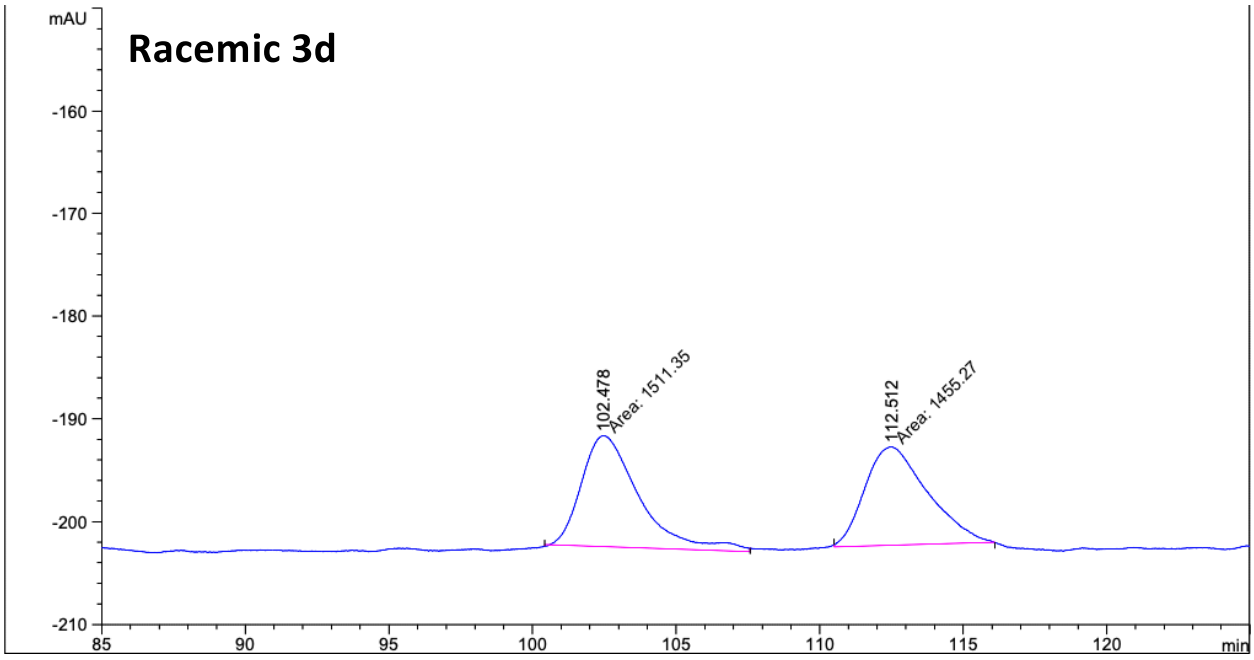
FTIR (neat): 3025, 2973, 2929, 1694, 1469, 1365, 1276, and 1165 cm^{-1}.

HPLC: (Phenomenex LC Columns Cellulose-2 + Cellulose-5, Hexane:2-PrOH = 98:02, 0.5 mL/150min, 254 nm).

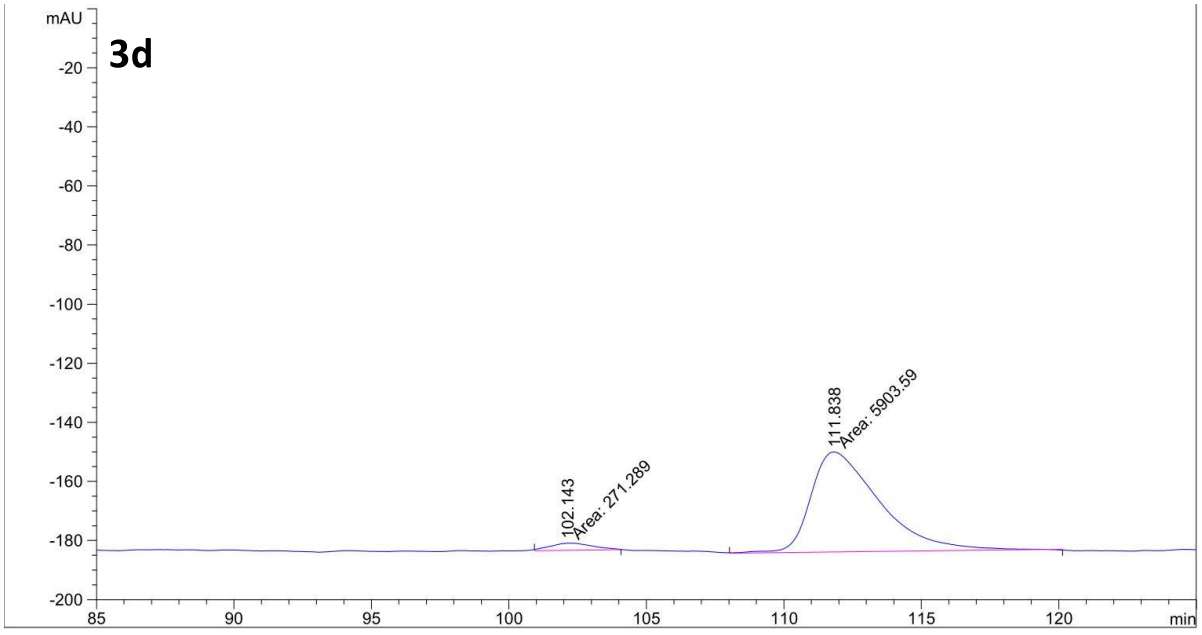
$[\alpha]_D^{24}$ = -4.0 (c = 0.5, $CHCl_3$).


^{1}H (500 MHz, CDCl$_3$)
Me
Me
OH
NBoc
7.26 CDCl3
5.83
5.81
5.79
5.77
5.10
5.10
5.08
5.08
5.07
5.07
5.03
5.03
4.06
3.22
3.21
3.20
3.19
2.66
1.66
1.64
1.63
1.61
1.55
1.53
1.53
1.52
1.45
1.25
1.24
1.23
1.22
1.22
1.20
1.13
1.12
1.11
1.11
1.10
1.09
1.08
1.07
1.06
1.06
1.04
1.03
1.00
1.00
1.00
0.96
0.99
2.16
0.98
2.14
2.54
2.08
9.22
2.77
2.43
6.01
f1 (ppm)


^{13}C (126 MHz, CDCl$_3$)
Me
Me
OH
NBoc
155.06
145.47
113.68
79.31
78.52
77.37
77.16 CDCl3
41.90
36.21
34.05
28.61
28.42
23.26
22.05
f1 (ppm)

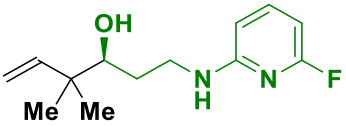


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	102.478	MM	2.3328	1511.34705	10.79779	50.9451
2	112.512	MM	2.5297	1455.27136	9.58785	49.0549



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	102.143	MM	1.8183	271.28867	2.48661	4.3934
2	111.838	MM	2.8994	5903.59375	33.93587	95.6066

(*S*)-1-((6-fluoropyridin-2-yl)amino)-4,4-dimethylhex-5-en-3-ol (3e)



Alcohol **2e** (34.0 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h). Flash column chromatography (SiO_2: 12:88 EtOAc:hexanes) provided the title compound **3e** as a white solid in 72% yield (34.3 mg, 0.14 mmol, 14:1 rr, 85% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 6:94 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.5 (2:3 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.44 (q, J = 8.1 Hz, 1H), 6.19 (dd, J = 8.0, 2.3 Hz, 1H), 6.10 (dd, J = 7.7, 2.2 Hz, 1H), 5.81 (dd, J = 17.5, 10.8 Hz, 1H), 5.10 (dd, J = 10.8, 1.4 Hz, 1H), 5.06 (dd, J = 17.5, 1.4 Hz, 1H), 4.94 (s, 1H), 3.55 (td, J = 14.1, 4.2 Hz, 1H), 3.39 (ddd, J = 11.3, 4.3, 2.1 Hz, 1H), 3.33 (dt, J = 13.0, 5.3 Hz, 1H), 2.36 (d, J = 4.2 Hz, 1H), 1.81 (dddd, J = 14.1, 7.9, 5.9, 1.8 Hz, 1H), 1.52 (ddt, J = 14.1, 11.1, 5.7 Hz, 1H), 1.02 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.5 (d, J = 236.6 Hz), 158.4 (d, J = 16.5 Hz), 145.3, 141.7 (d, J = 8.4 Hz), 113.8, 103.1 (d, J = 4.2 Hz), 95.4 (d, J = 36.4 Hz), 76.5, 41.6, 40.3, 31.2, 23.2, 22.1.

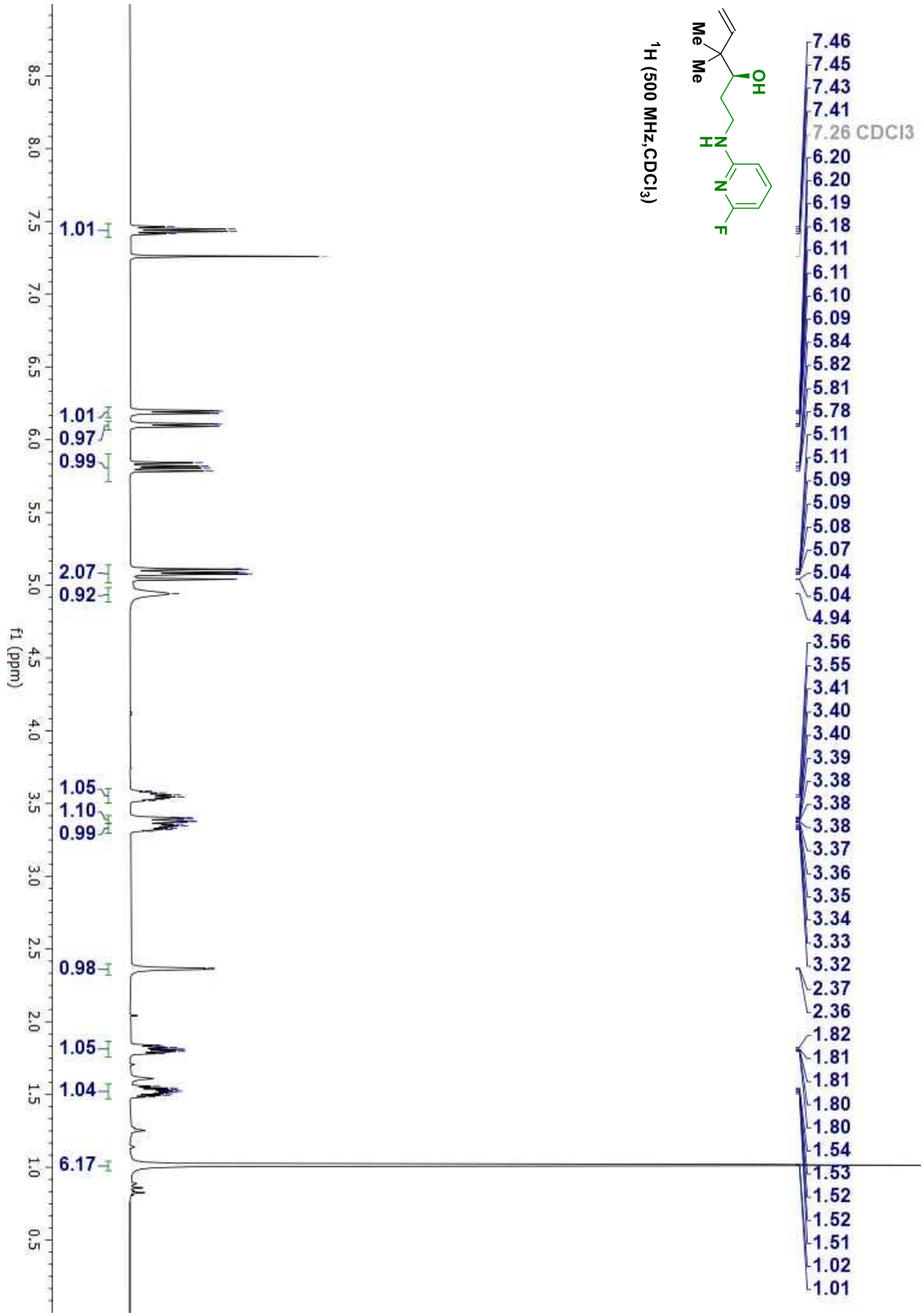
^{19}F NMR (471 MHz, $CDCl_3$): δ -70.01.

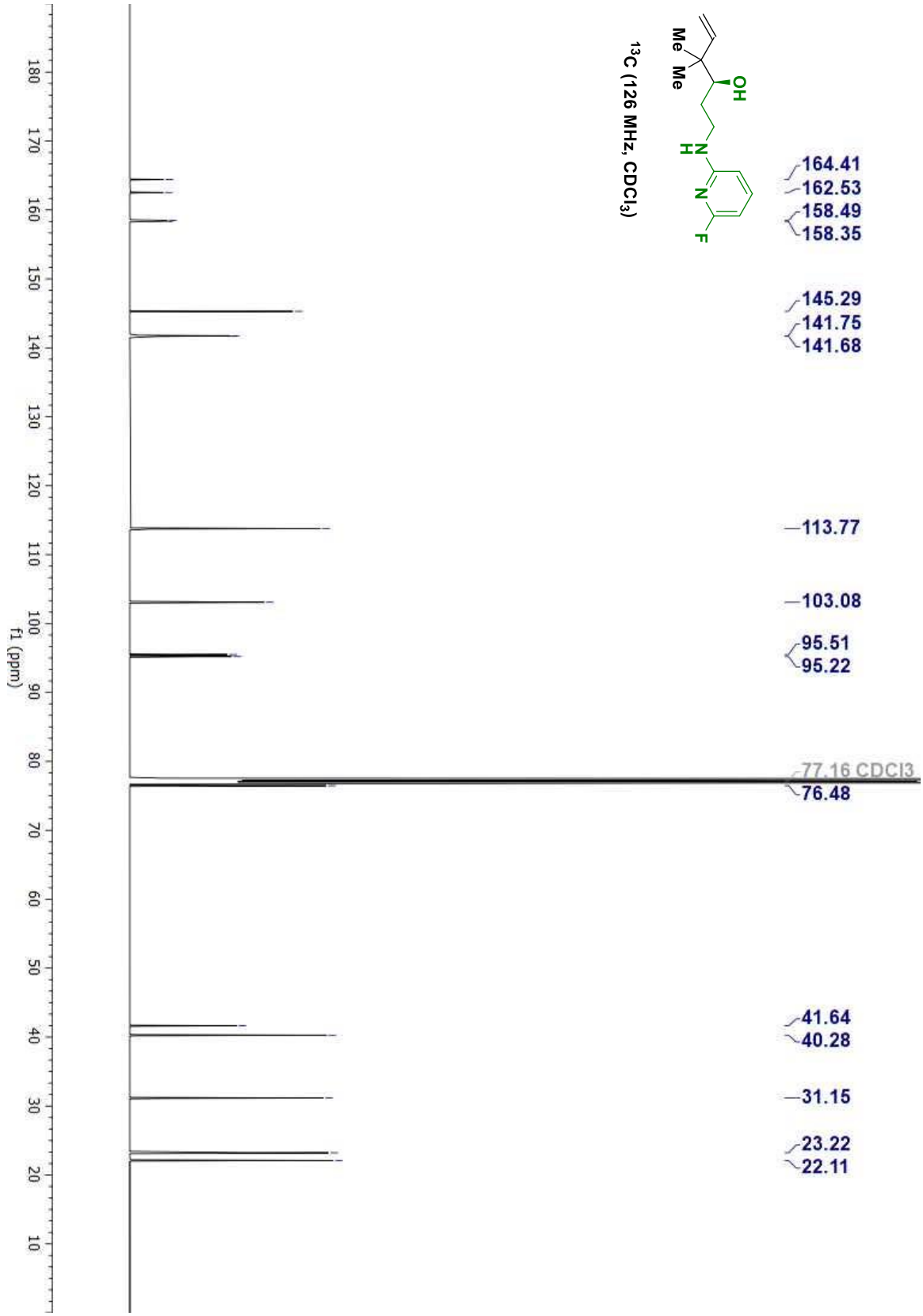
HRMS (Na+, *m/z*) for $C_{13}H_{19}FN_2O$: calcd. = 261.1374; found = 261.1371.

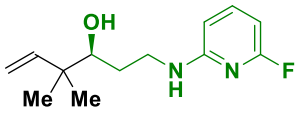
FTIR (neat): 3054, 2957, 1661, 1572, 1510, 1307, 1113, 899, 778 cm^{-1}.

HPLC: (Chiralcel columns Amylose 3-2, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm).

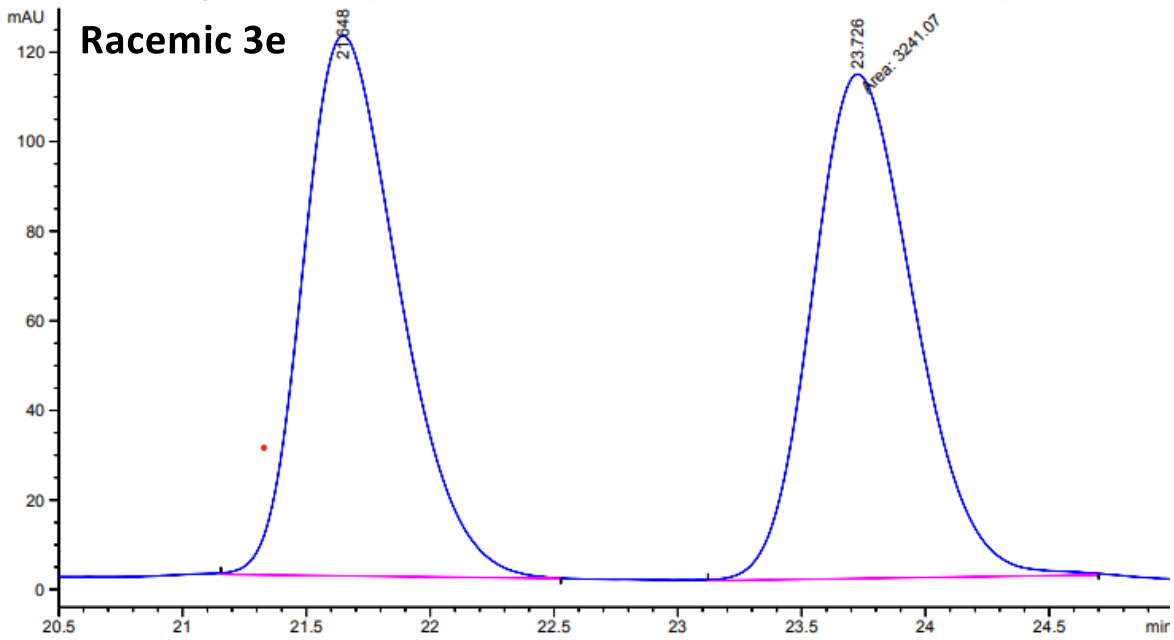
$[\alpha]_D^{24}$ = -14.5 (c = 0.1, $CHCl_3$).


^{1}H (500 MHz, CDCl$_3$)
Me
Me
OH
H
N
N
F
7.26 CDCl3
f1 (ppm)

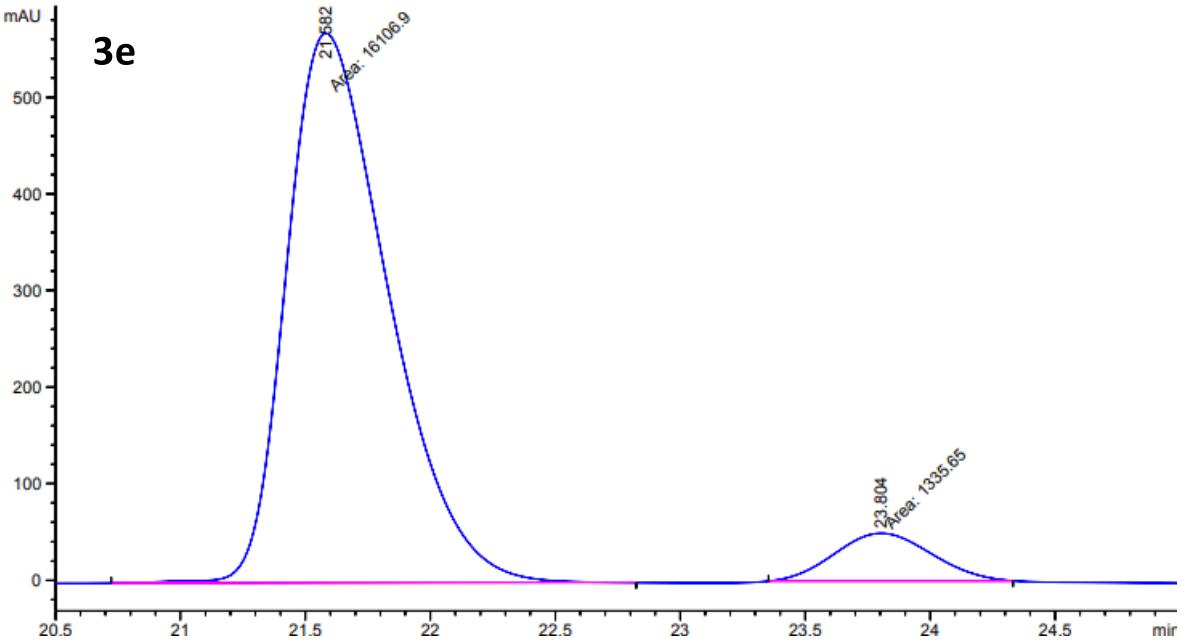

^{13}C (126 MHz, CDCl$_3$)
Me
Me
OH
H
N
N
F
164.41
162.53
158.49
158.35
145.29
141.75
141.68
113.77
103.08
95.51
95.22
77.16 CDCl3
76.48
41.64
40.28
31.15
23.22
22.11
f1 (ppm)



^{19}F (471 MHz,$CDCl_3$)

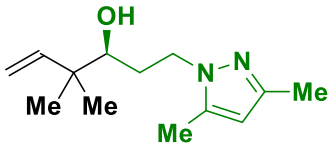


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.648	BB	0.4192	3260.17944	120.67209	50.1470
2	23.726	MM	0.4795	3241.06958	112.64754	49.8530



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.582	MM	0.4717	1.61069e4	569.14410	92.3426
2	23.804	MM	0.4497	1335.65039	49.50010	7.6574

(*S*)-1-(3,5-dimethyl-1H-pyrazol-1-yl)-4,4-dimethylhex-5-en-3-ol (3f)



Alcohol **2f** (30.8 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h). Flash column chromatography (SiO_2: 25:75 EtOAc:hexanes) provided the title compound **3f** as a pale yellow solid in 76% yield (33.8 mg, 0.15 mmol, 16:1 rr, 86% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 10:90 Acetone:cyclohexane).

TLC (SiO_2): R_f = 0.2 (1:2 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 5.90 – 5.79 (m, 1H), 5.78 (s, 1H), 5.12 – 4.94 (m, 2H), 4.21 – 4.04 (m, 2H), 3.24 (dd, J = 10.7, 2.1 Hz, 1H), 2.23 (s, 3H), 2.21 (s, 3H), 2.02 (dddd, J = 14.7, 8.5, 6.6, 1.9 Hz, 1H), 1.65 (ddt, J = 13.8, 11.1, 5.7 Hz, 1H), 1.01 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 145.4, 113.2, 105.1, 89.9, 77.4, 75.8, 46.5, 41.5, 32.0, 22.9, 22.7, 13.5, 11.1.

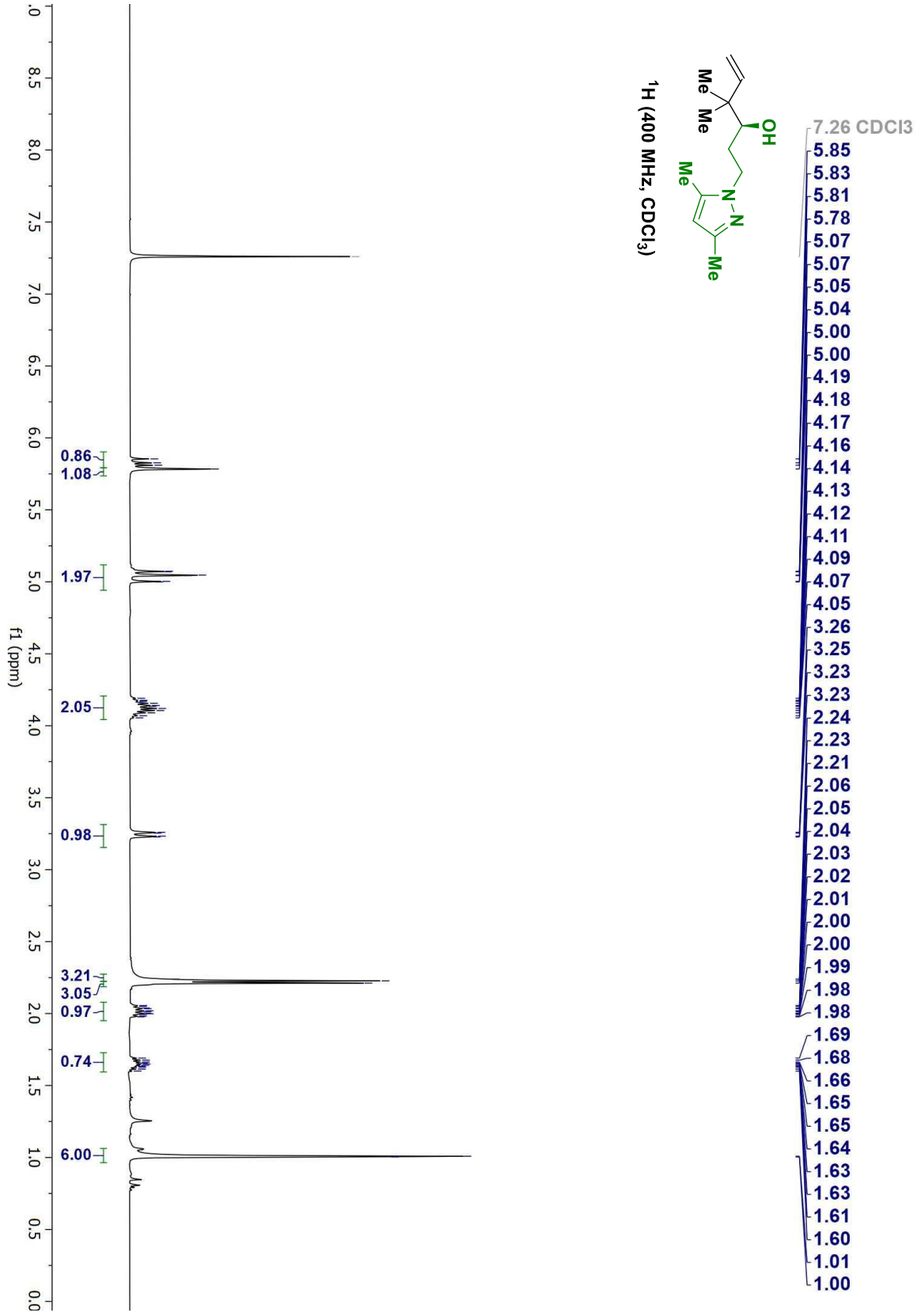
HRMS (H+, *m/z*) for $C_{13}H_{22}N_2O$: calcd. = 228.1703; found = 228.1707

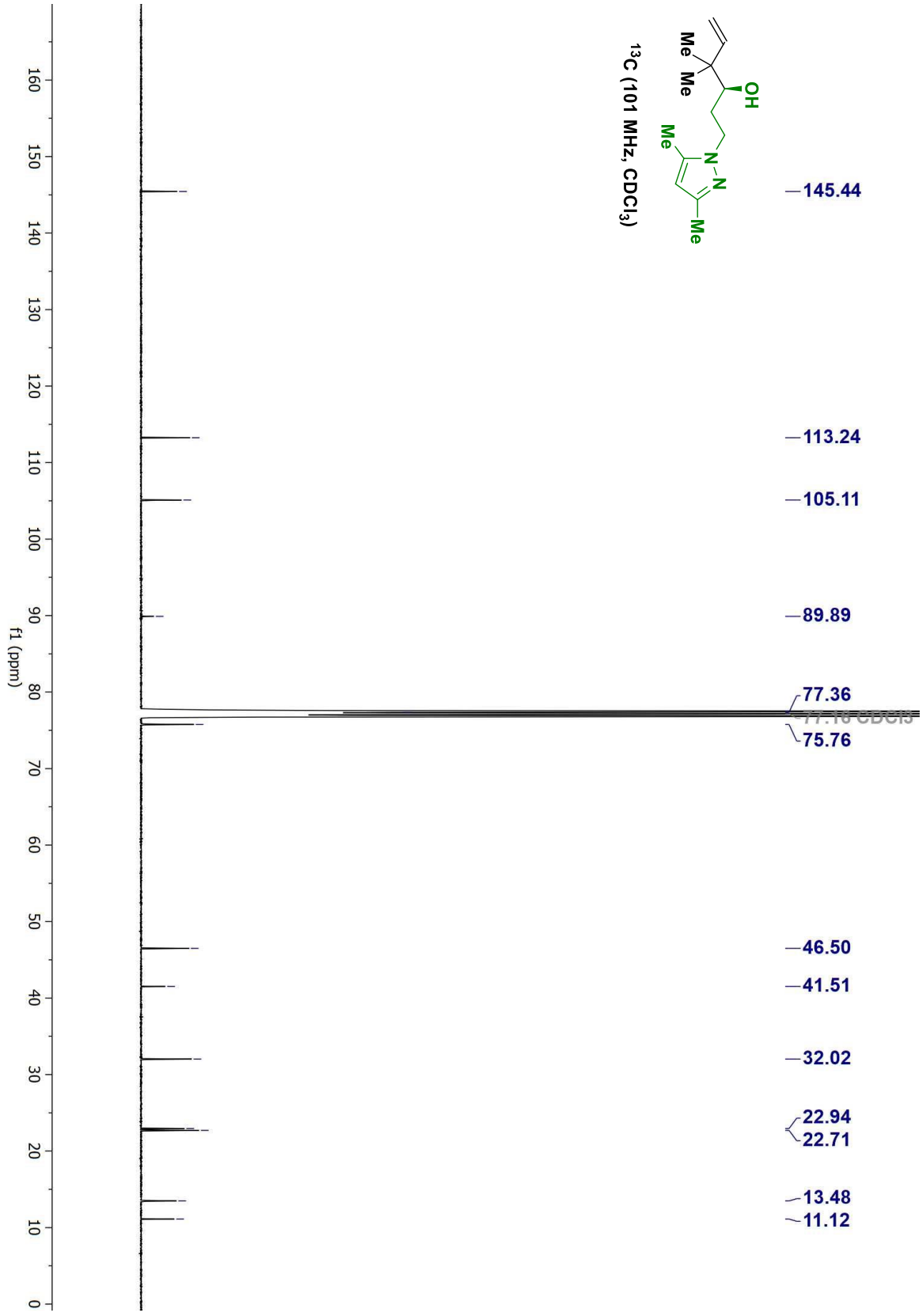
FTIR (neat): 3264, 2928, 2843, 1524, 1424, 1368, 1233 cm^{-1}, 954, 924, 768 cm^{-1}.

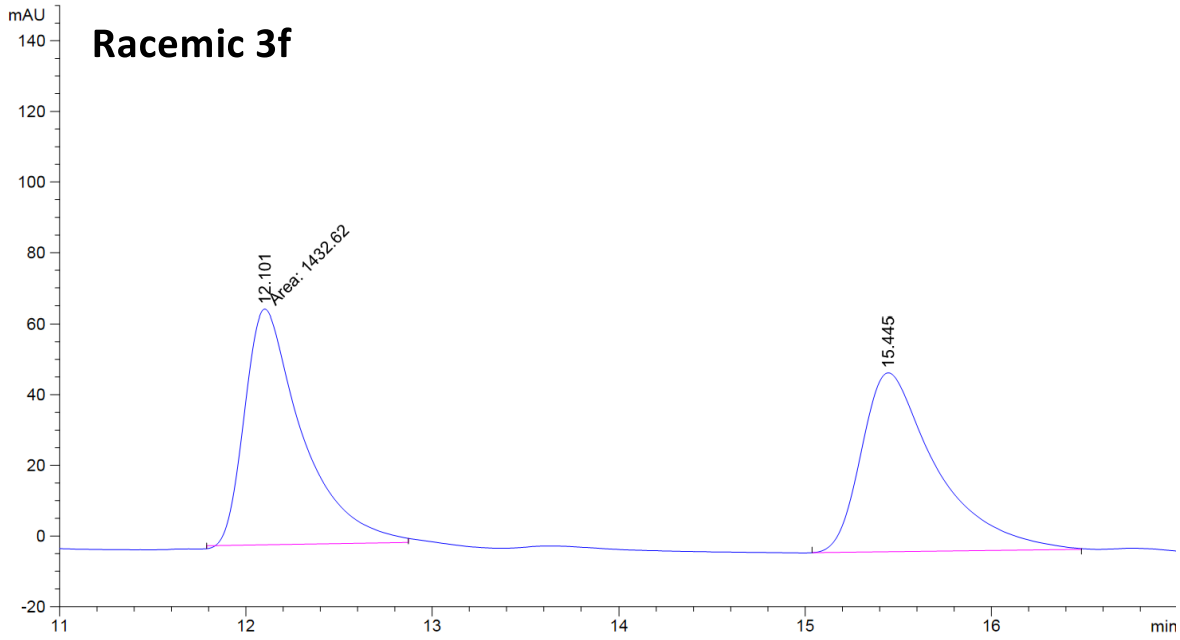
HPLC: (Chiralcel columns Cellulose 5, Hexane:2-PrOH = 96:04, 0.5 mL/min, 210 nm).

$[\alpha]_D^{24}$ = -46.2 (c = 0.1, $CHCl_3$).

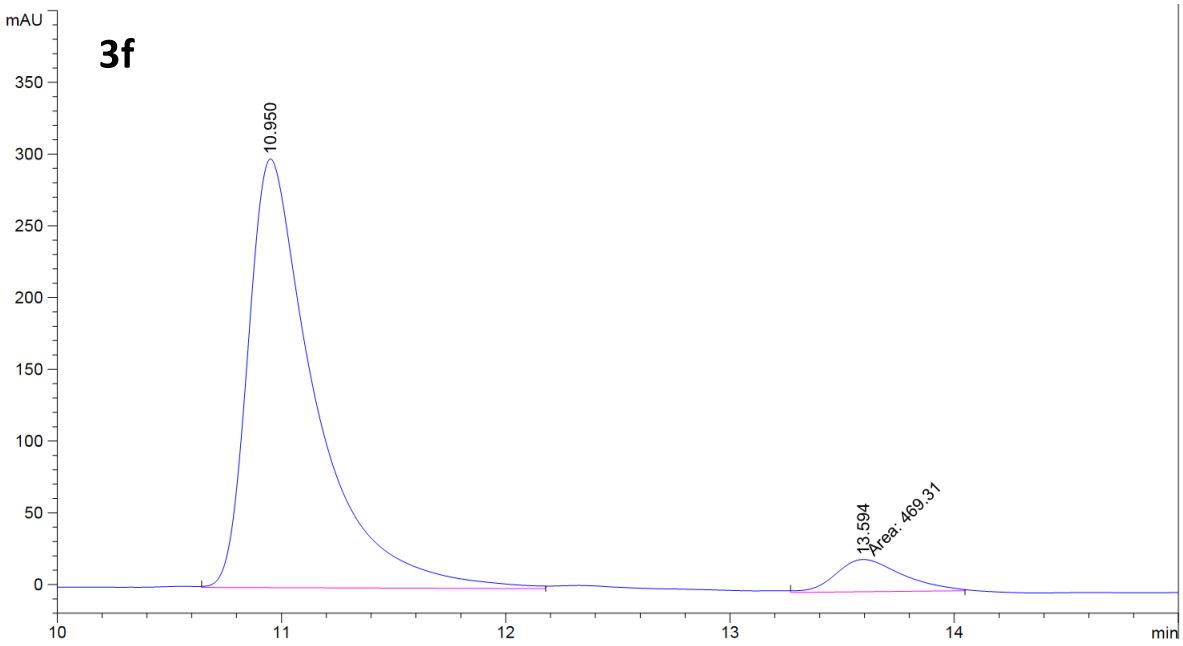
Melting Point: 67-69 °C.


^{1}H (400 MHz, CDCl$_3$)
Me
Me
OH
Me
N
N
Me
7.26 CDCl3
5.85
5.83
5.81
5.78
5.07
5.07
5.05
5.04
5.00
5.00
4.19
4.18
4.17
4.16
4.14
4.13
4.12
4.11
4.09
4.07
4.05
3.26
3.25
3.23
3.23
2.24
2.23
2.21
2.06
2.05
2.04
2.03
2.02
2.01
2.00
2.00
1.99
1.98
1.98
1.69
1.68
1.66
1.65
1.65
1.64
1.63
1.63
1.61
1.60
1.01
1.00
0.86
1.08
1.97
2.05
0.98
3.21
3.05
0.97
0.74
6.00
f1 (ppm)


^{13}C (101 MHz, CDCl$_3$)
Me
Me
OH
Me
N
N
Me
145.44
113.24
105.11
89.89
77.36
77.16 CDCl3
75.76
46.50
41.51
32.02
22.94
22.71
13.48
11.12
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

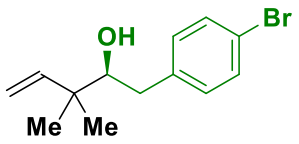


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.101	MM	0.3586	1432.62268	66.57875	50.2468
2	15.445	BB	0.4087	1418.55054	50.66459	49.7532



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.950	BB	0.2991	6227.99707	298.86868	92.9926
2	13.594	MM	0.3460	469.30966	22.60351	7.0074

(*S*)-1-(4-bromophenyl)-3,3-dimethylpent-4-en-2-ol (3g)



Alcohol **2g** (40.2 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h). Flash column chromatography (SiO_2: 1:99 EtOAc:hexanes) provided the title compound **3g** as a clear oil in 70% yield (37.8 mg, 0.14 mmol,12:1 rr, 88% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 1:99 Acetone:pentane).

TLC (SiO_2): R_f = 0.45 (1:9 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (d, J = 8.2 Hz 2H), 7.11 (d, J = 8.2 Hz, 2H), 5.90 (dd, J = 17.5, 10.9 Hz, 1H), 5.24-5.04 (m, 2H), 3.46 (ddd, J = 10.6, 3.9, 2.0 Hz, 1H), 2.82 (dd, J = 13.8, 2.0 Hz, 1H), 2.43 (dd J= 13.8, 10.6 Hz, 1H), 1.51 (d, J = 3.9 Hz, 1H), 1.10 (s, 6H)

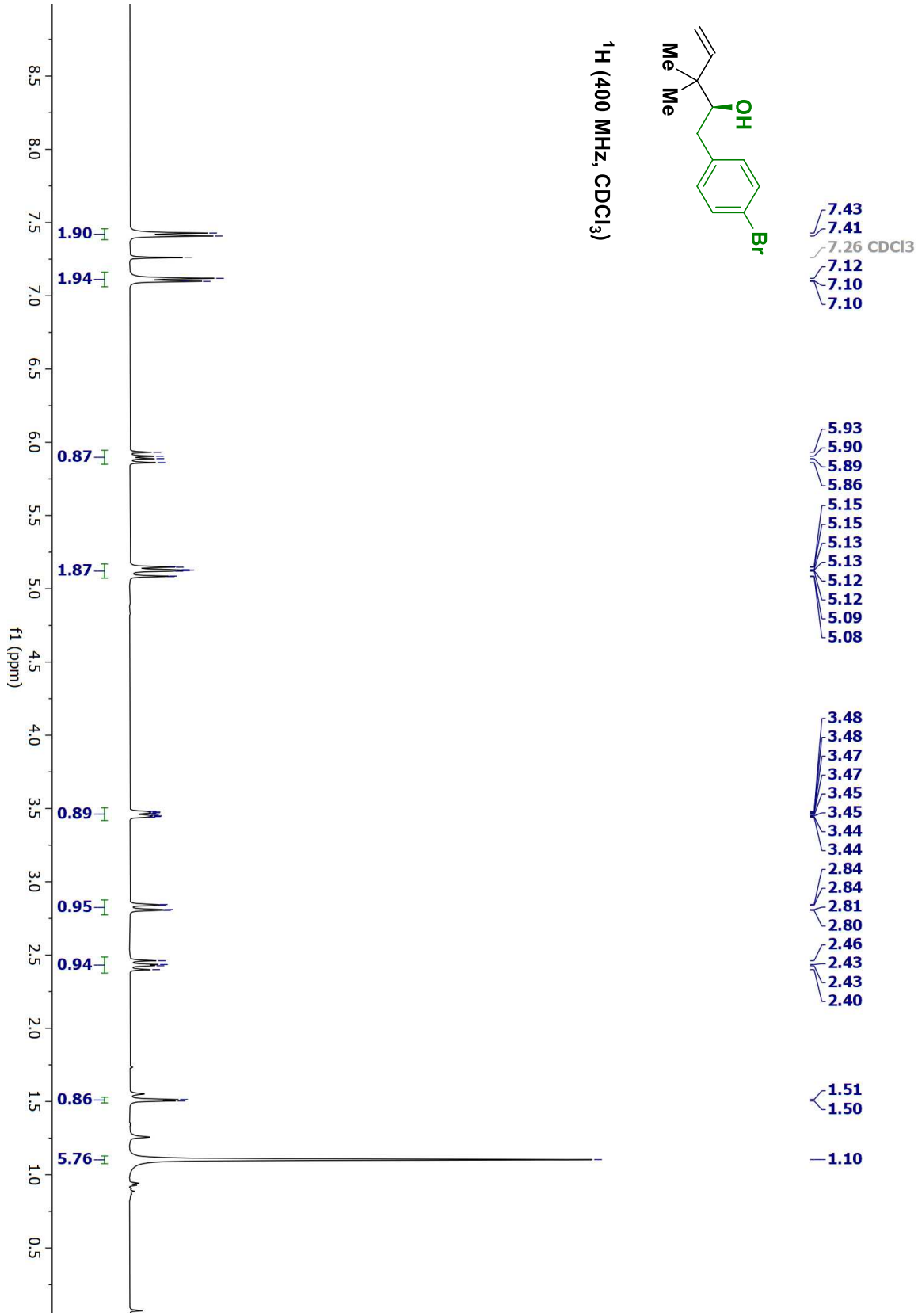
^{13}C NMR (101 MHz, $CDCl_3$): δ 145.1, 139.1, 131.6, 131.2, 120.3, 113.7, 79.3, 41,7, 37.8, 23.0, 22.6.

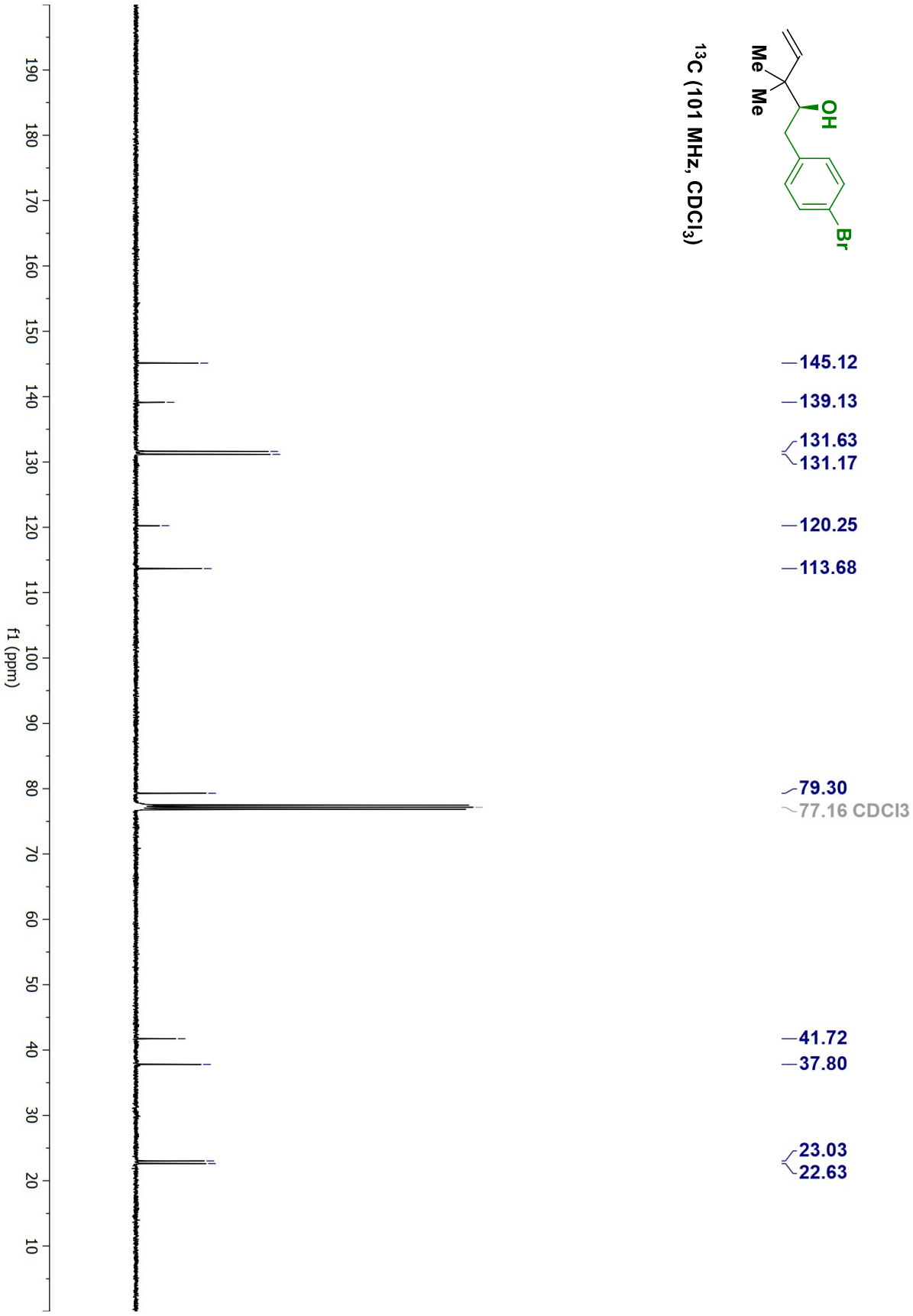
HRMS (Na+, *m/z*) for $C_{13}H_{17}BrO$: calcd. = 291.0263; found = 291.0355.

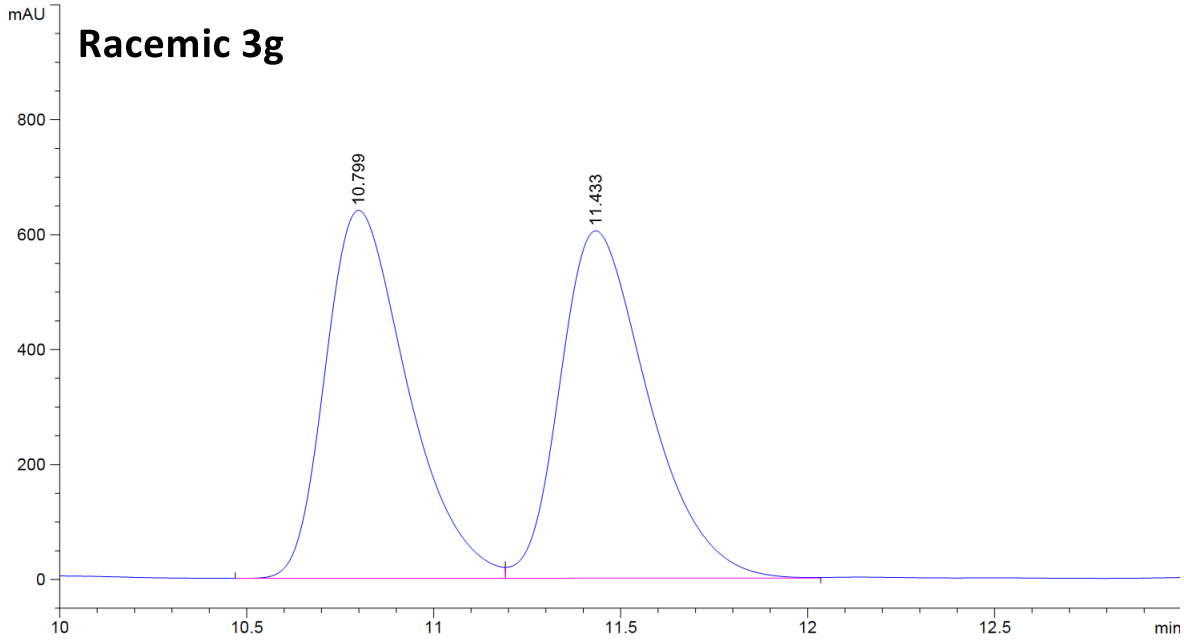
FTIR (neat): 3047, 2965, 2928, 2872, 1711, 1665, 1595, 1526, 1481 cm^{-1}.

HPLC: (Chiralcel columns Chiralcel column Amylose 3, Hexane:2-PrOH = 98:02, 0.5 mL/min, 210 nm).

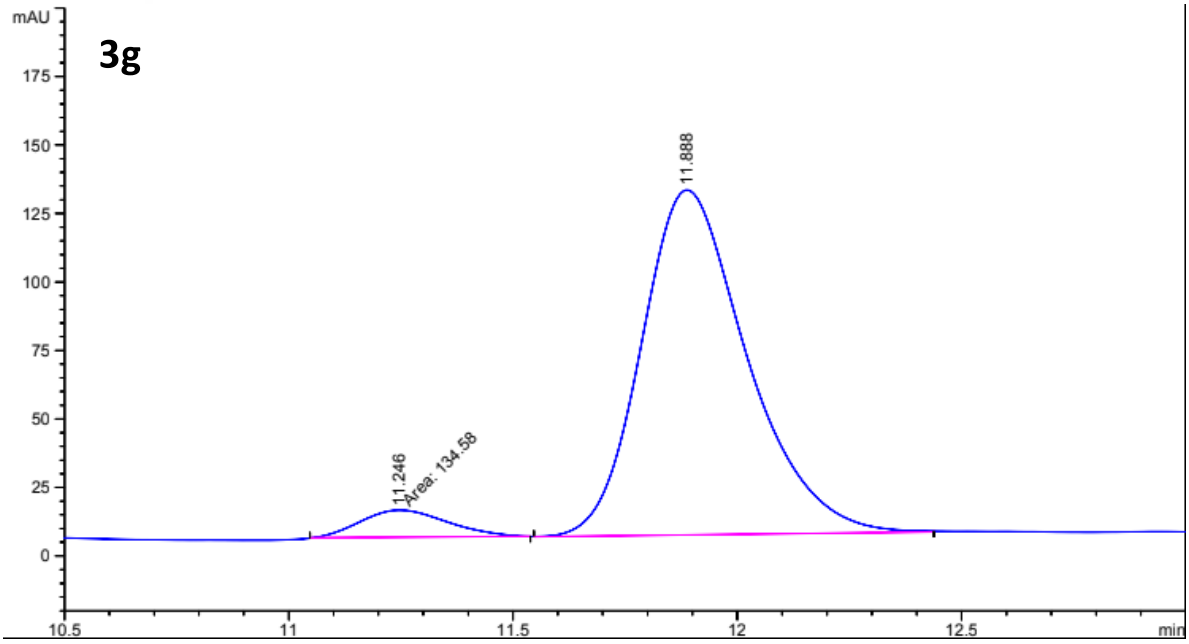
$[\alpha]_D^{24}$ = -18 (c = 0.1, $CHCl_3$).


^{1}H (400 MHz, CDCl$_3$)
Me
Me
OH
Br
7.43
7.41
7.26 CDCl3
7.12
7.10
7.10
5.93
5.90
5.89
5.86
5.15
5.15
5.13
5.13
5.12
5.12
5.09
5.08
3.48
3.48
3.47
3.47
3.45
3.45
3.44
3.44
2.84
2.84
2.81
2.80
2.46
2.43
2.43
2.40
1.51
1.50
1.10
1.90
1.94
0.87
1.87
0.89
0.95
0.94
0.86
5.76
f1 (ppm)


^{13}C (101 MHz, $CDCl_3$)
Me
Me
OH
Br
145.12
139.13
131.63
131.17
120.25
113.68
79.30
77.16 CDCl3
41.72
37.80
23.03
22.63
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

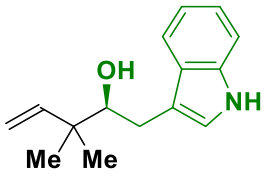


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.799	VV	0.2339	9763.81836	640.45917	49.6333
2	11.433	VB	0.2512	9908.09766	604.66211	50.3667



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.246	MM	0.2254	134.58035	9.95323	6.1261
2	11.888	VB	0.2490	2062.24829	125.95834	93.8739

(*S*)-1-(1H-indol-3-yl)-3,3-dimethylpent-4-en-2-ol (3h)



Alcohol **2h** (32.2 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h). Flash column chromatography (SiO_2: 10:90 EtOAc:hexanes) provided the title compound **3h** as a yellow oil in 82% yield (37.6 mg, 0.16 mmol, 12:1 rr, 92% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 5:95 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.4 (1:3 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (s, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.2 Hz, 1H), 7.21 (t, J = 7.8 Hz, 1H), 7.17 – 7.08 (m, 2H), 6.02 (dd, J = 18.0, 10.4 Hz, 1H), 5.18 – 5.08 (m, 2H), 3.64 (dd, J = 10.8, 2.0 Hz, 1H), 3.08 (dd, J = 14.7, 2.0 Hz, 1H), 2.63 (dd, J = 14.7, 10.8 Hz, 1H), 1.69 (s, 1H), 1.17 (s, 6H).

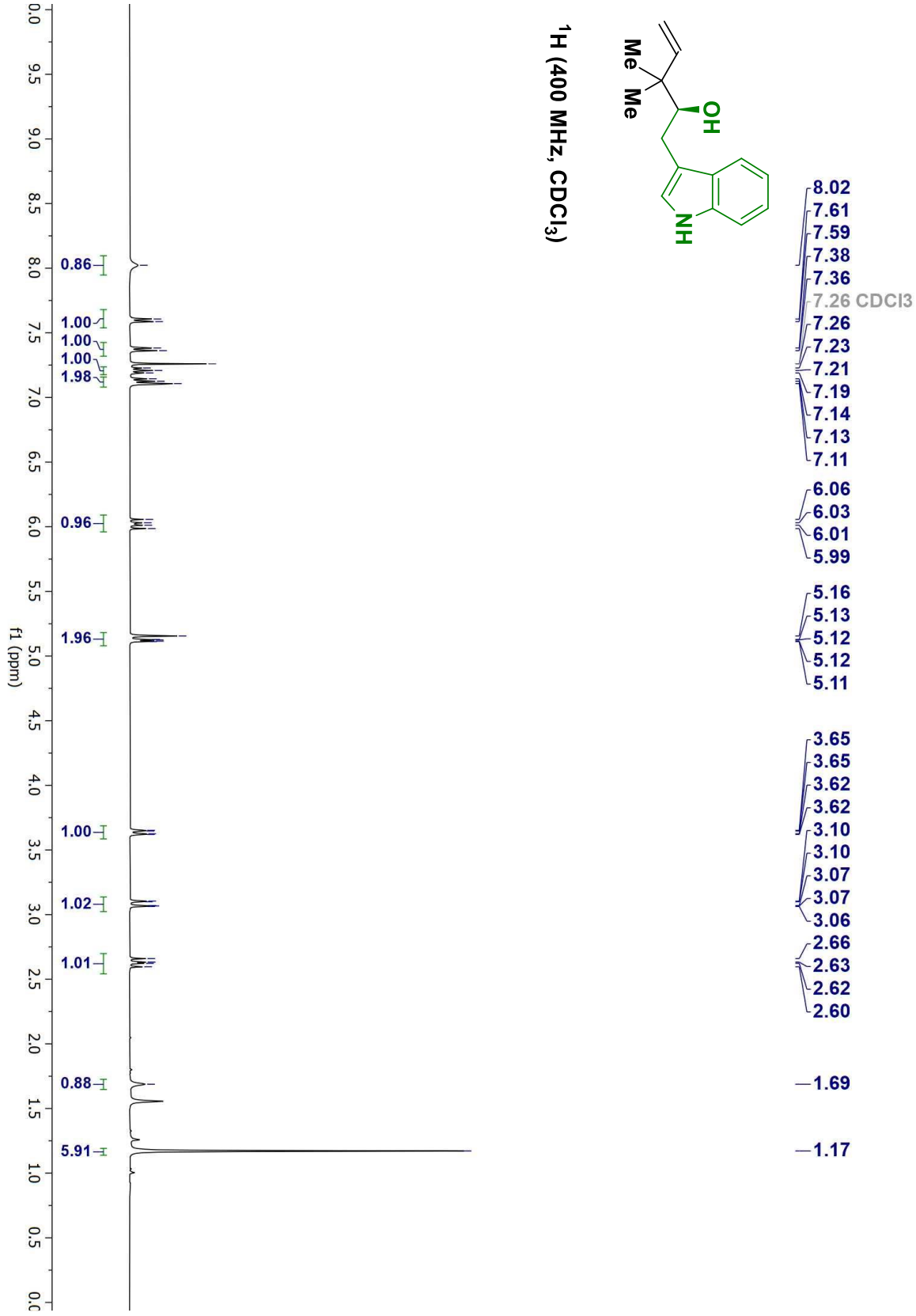
^{13}C NMR (101 MHz, $CDCl_3$): δ 145.5, 136.7, 127.6, 122.8, 122.4, 119.6, 119.0, 113.5, 112.9, 111.4, 77.9, 41.4, 28.2, 23.2, 23.0.

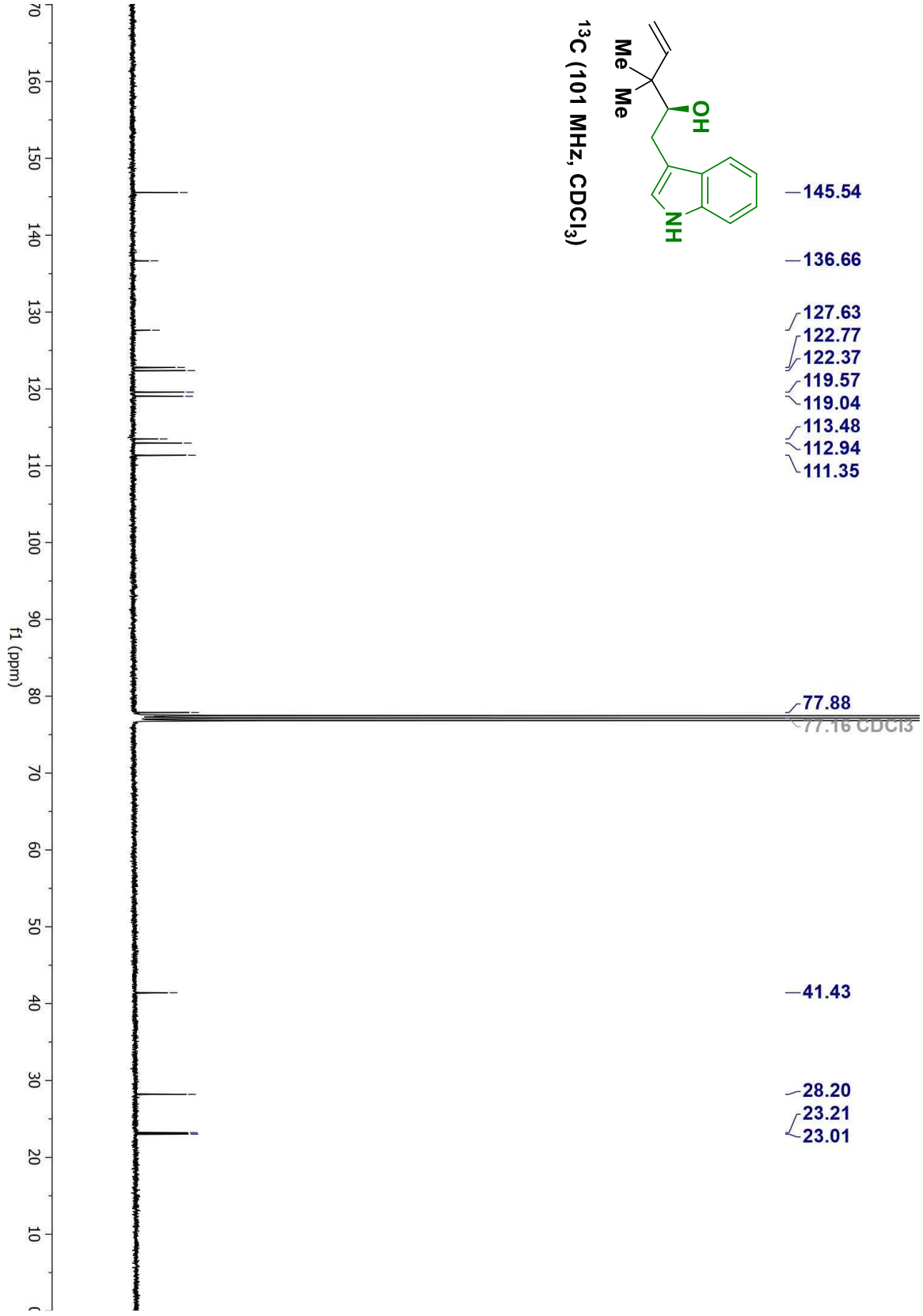
HRMS (Na+, *m/z*) for $C_{15}H_{19}NO$: calcd. = 252.1398; found = 252.1563.

FTIR (neat): 3384, 2927, 2869, 1627, 1442, 1411, 1384, 1233, 1210, 1078, 1015 cm^{-1}.

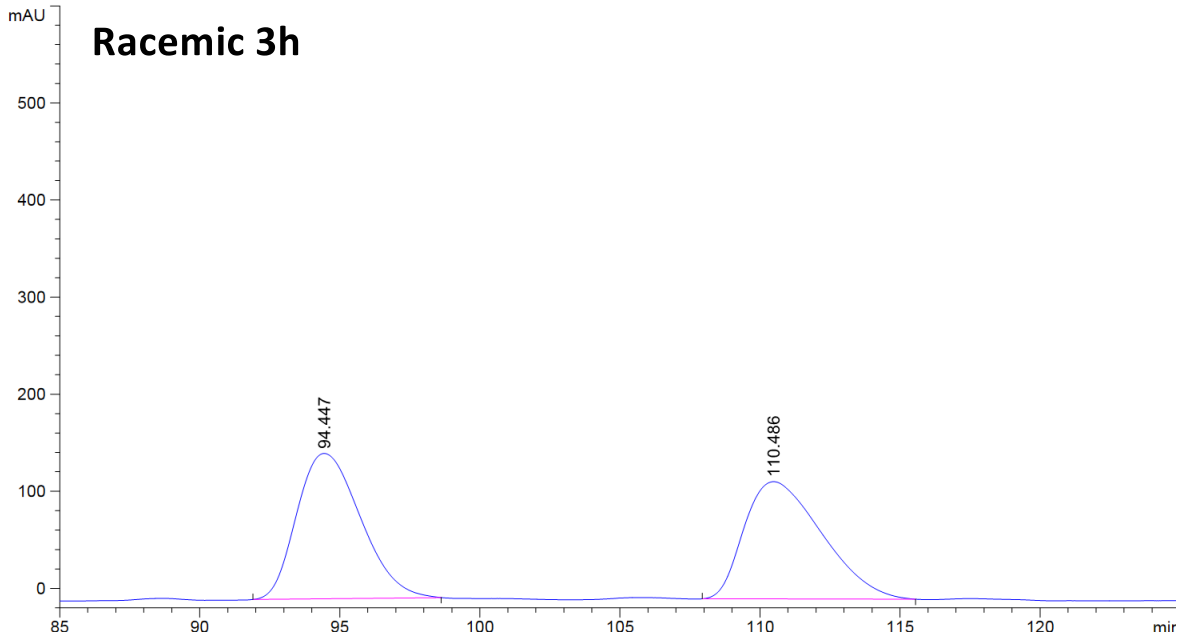
HPLC: (Chiralcel column Amylose 3, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm).

$[\alpha]_D^{24}$ = -34.6 (c = 0.1, $CHCl_3$).


^{1}H (400 MHz, CDCl$_3$)
Me Me
OH
NH
8.02
7.61
7.59
7.38
7.36
7.26 CDCl3
7.26
7.23
7.21
7.19
7.14
7.13
7.11
6.06
6.03
6.01
5.99
5.16
5.13
5.12
5.12
5.11
3.65
3.65
3.62
3.62
3.10
3.10
3.07
3.07
3.06
2.66
2.63
2.62
2.60
1.69
1.17
0.86
1.00
1.00
1.00
1.98
0.96
1.96
1.00
1.02
1.01
0.88
5.91
f1 (ppm)

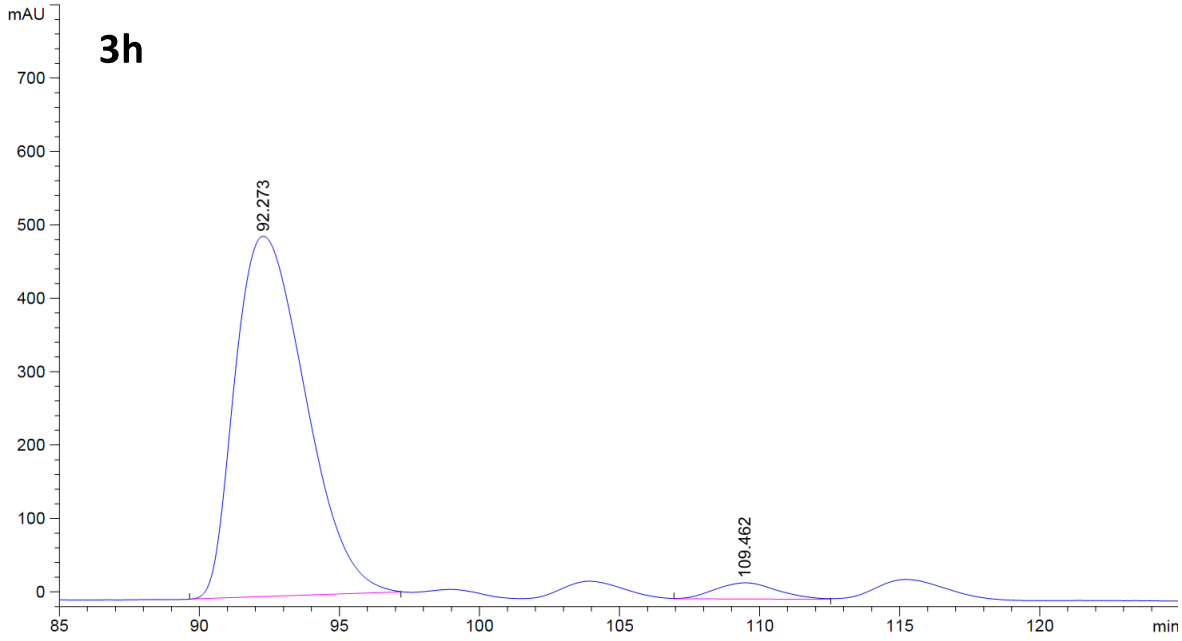

^{13}C (101 MHz, CDCl$_3$)
Me Me
OH
NH
145.54
136.66
127.63
122.77
122.37
119.57
119.04
113.48
112.94
111.35
77.88
77.16 CDCl3
41.43
28.20
23.21
23.01
f1 (ppm)

Racemic 3h



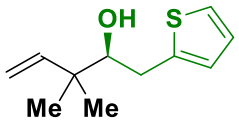
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	94.447	BB	2.0179	2.37865e4	149.84703	50.4603
2	110.486	BB	2.2590	2.33525e4	120.92726	49.5397

3h



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	92.273	BB	2.4088	8.58074e4	491.02670	96.1458
2	109.462	VV	1.8262	3439.77051	22.12077	3.8542

(*S*)-3,3-dimethyl-1-(thiophen-2-yl)pent-4-en-2-ol (3i)



Alcohol **2i** (25.6 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h) with DME (0.5 M) as solvent. Flash column chromatography (SiO_2: 2:98 EtOAc:hexanes) provided the title compound **3i** as a yellow oil in 65% yield (25.5 mg, 0.13 mmol, 12:1 rr, 88% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 1:99 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.5 (1:4 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.17 (d, *J* = 5.2 Hz, 1H), 6.95 (dd, *J* = 5.2, 3.4 Hz, 1H), 6.87 (d, *J* = 3.4 Hz, 1H), 5.91 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.15 – 5.07 (m, 2H), 3.53 (ddd, *J* = 10.6, 3.7, 2.0 Hz, 1H), 3.08 (dd, *J* = 14.8, 2.0 Hz, 1H), 2.74 (dd, *J* = 14.8, 10.6 Hz, 1H), 1.76 (d, *J* = 3.7 Hz, 1H), 1.11 (s, 6H).

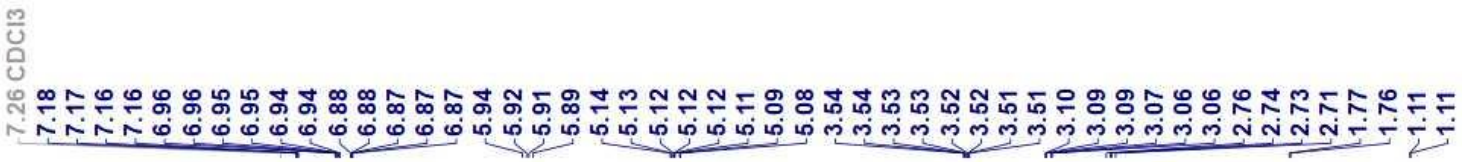
^{13}C NMR (126 MHz, $CDCl_3$): δ 145.0, 142.3, 127.0, 125.8, 124.2, 113.5, 79.3, 41.5, 33.0, 23.0, 22.9.

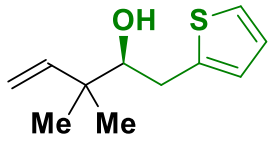
HRMS (Na+, *m/z*) for $C_{11}H_{16}OS$: calcd. = 219.0892; found = 219.0895.

FTIR (neat): 3397, 2960, 2927, 2872, 1945, 1773, 1568, 1444, 1217, 1059, 912, 761, 691, 674 cm^{-1}.

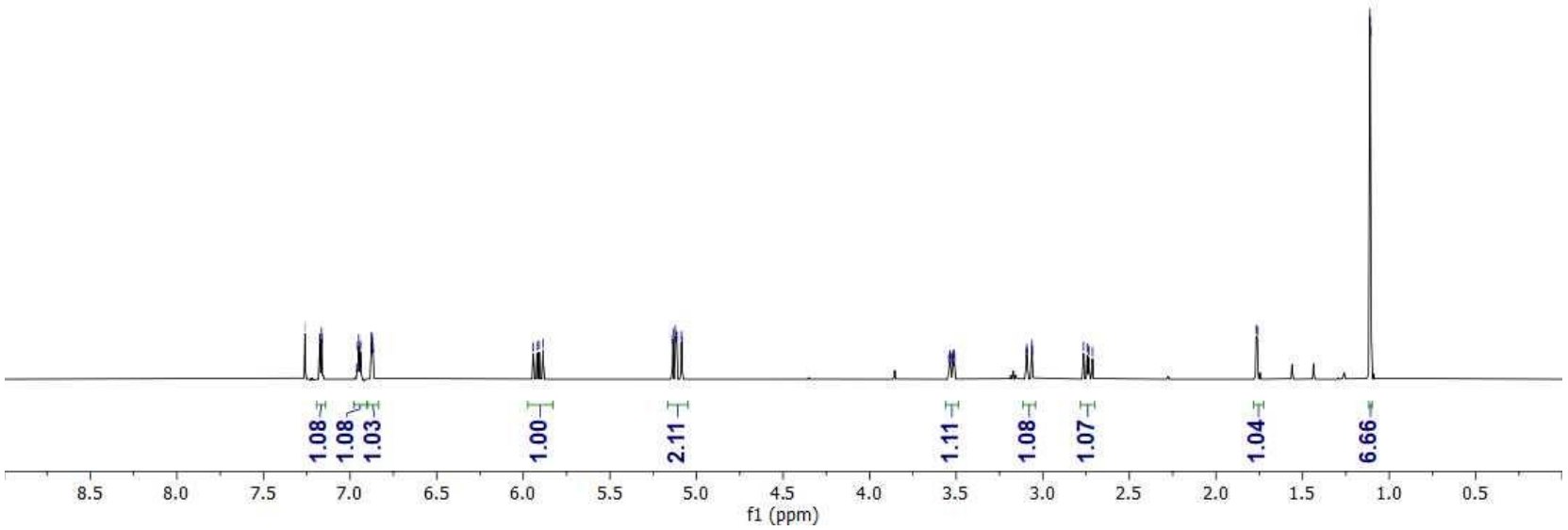
HPLC: (Chiralcel columns Amylose 3, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm).

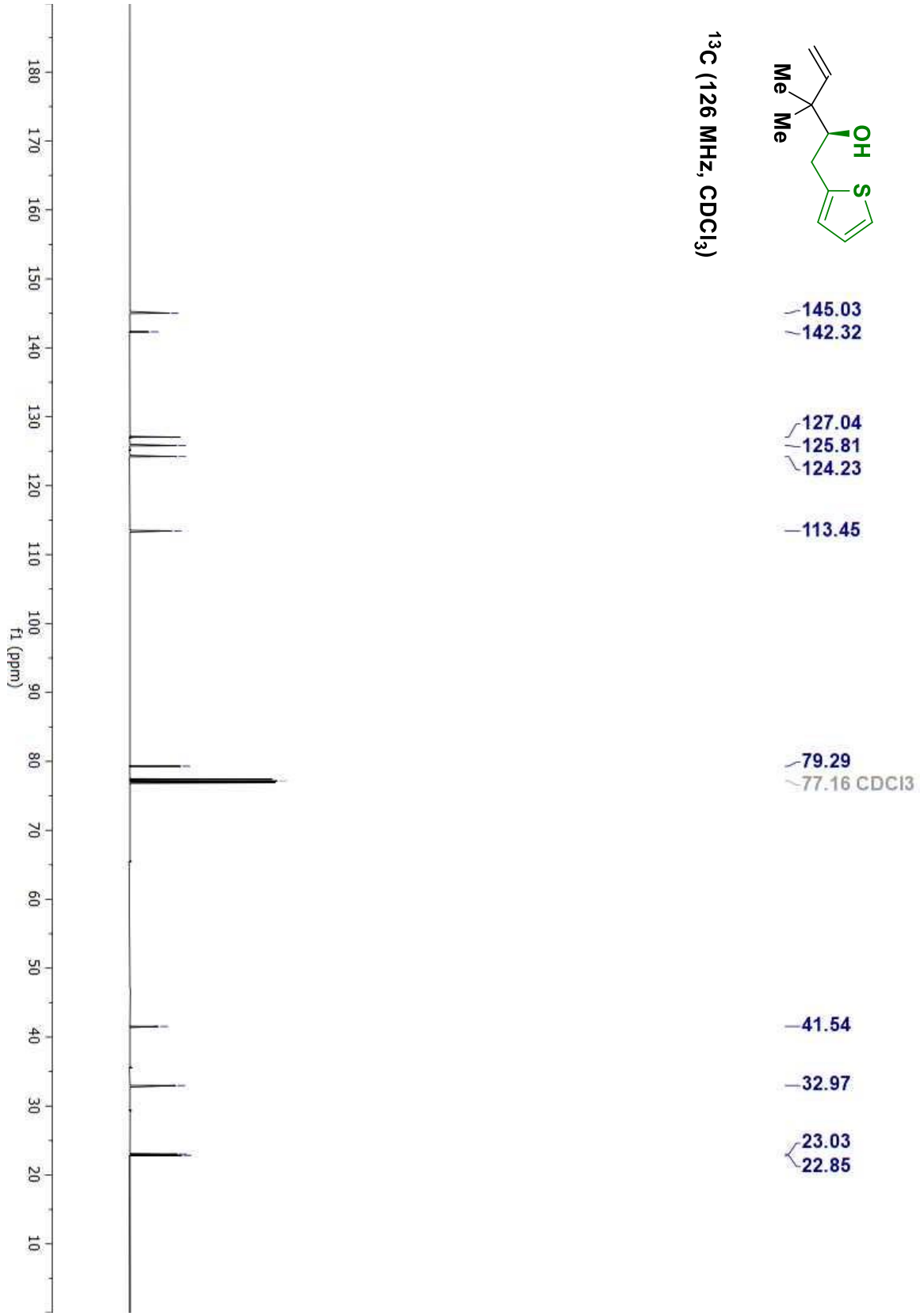
$[\alpha]_D^{24}$ = -44.5 (c = 0.1, $CHCl_3$).

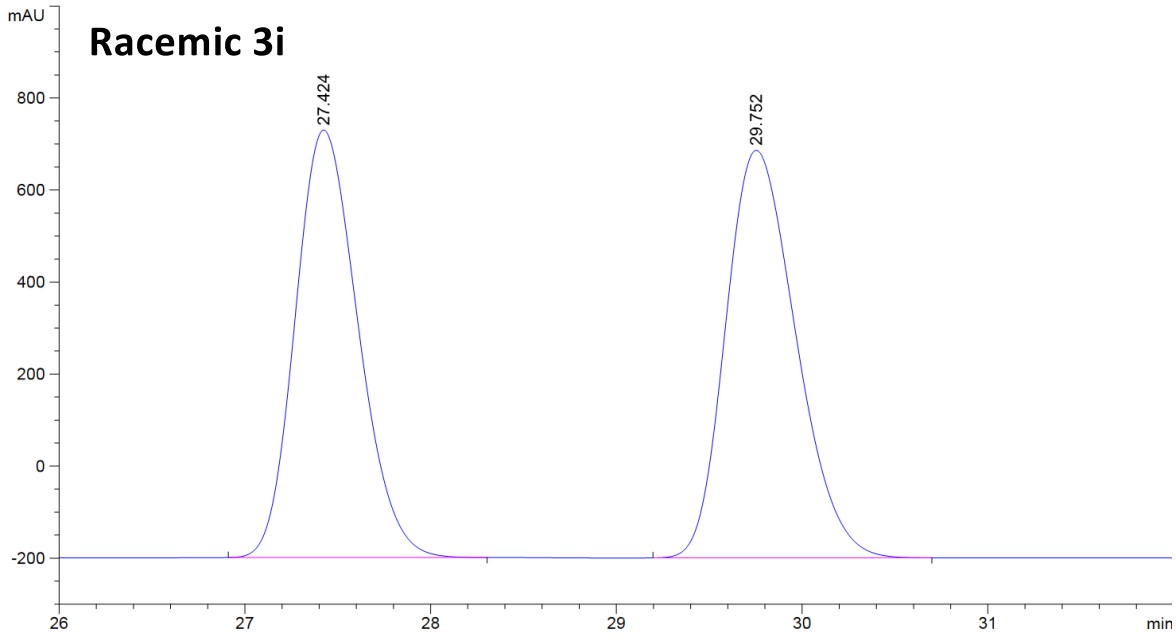




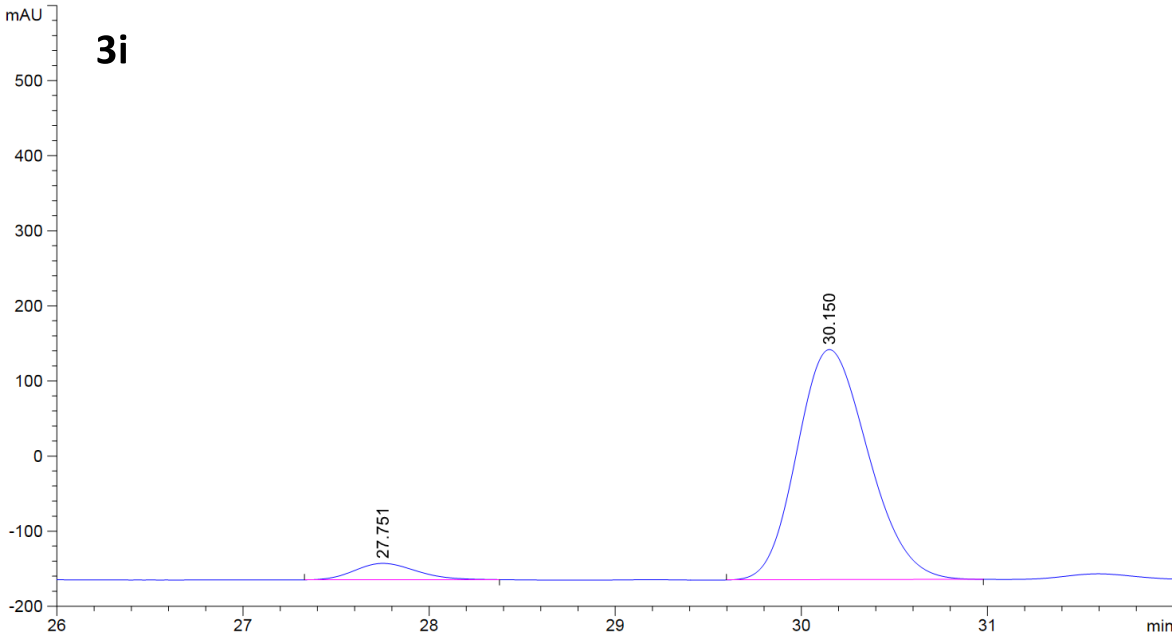
^{1}H (500 MHz, $CDCl_3$)




^{13}C (126 MHz, $CDCl_3$)
Me
Me
OH
S
145.03
142.32
127.04
125.81
124.23
113.45
79.29
77.16 CDCl3
41.54
32.97
23.03
22.85
f1 (ppm)

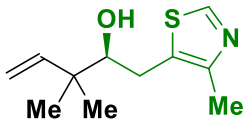


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.424	BB	0.3660	2.18262e4	929.38342	48.3963
2	29.752	BB	0.4124	2.32727e4	886.13647	51.6037



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.751	BB	0.3578	516.09271	21.99064	5.9518
2	30.150	BB	0.4163	8155.11182	306.59778	94.0482

(*S*)-3,3-dimethyl-1-(4-methylthiazol-5-yl)pent-4-en-2-ol (3j)



Alcohol **2j** (28.6 mg, 0.2 mmol) was subjected to standard reaction conditions (120 °C, 48 h). Flash column chromatography (SiO_2: 25:75 EtOAc:hexanes) provided the title compound **3j** as a red oil in 72% yield (30.5 mg, 0.14 mmol, 16:1 rr, 88% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 10:90 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.3 (1:1 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (s, 1H), 5.89 (dd, J = 17.5, 10.8 Hz, 1H), 5.22 – 5.06 (m, 2H), 3.43 (dd, J = 10.5, 1.9 Hz, 1H), 2.99 (dd, J = 15.1, 1.9 Hz, 1H), 2.66 (dd, J = 15.0, 10.5 Hz, 1H), 2.38 (s, 3H), 1.85 (s, 1H), 1.11 (s, 6H).

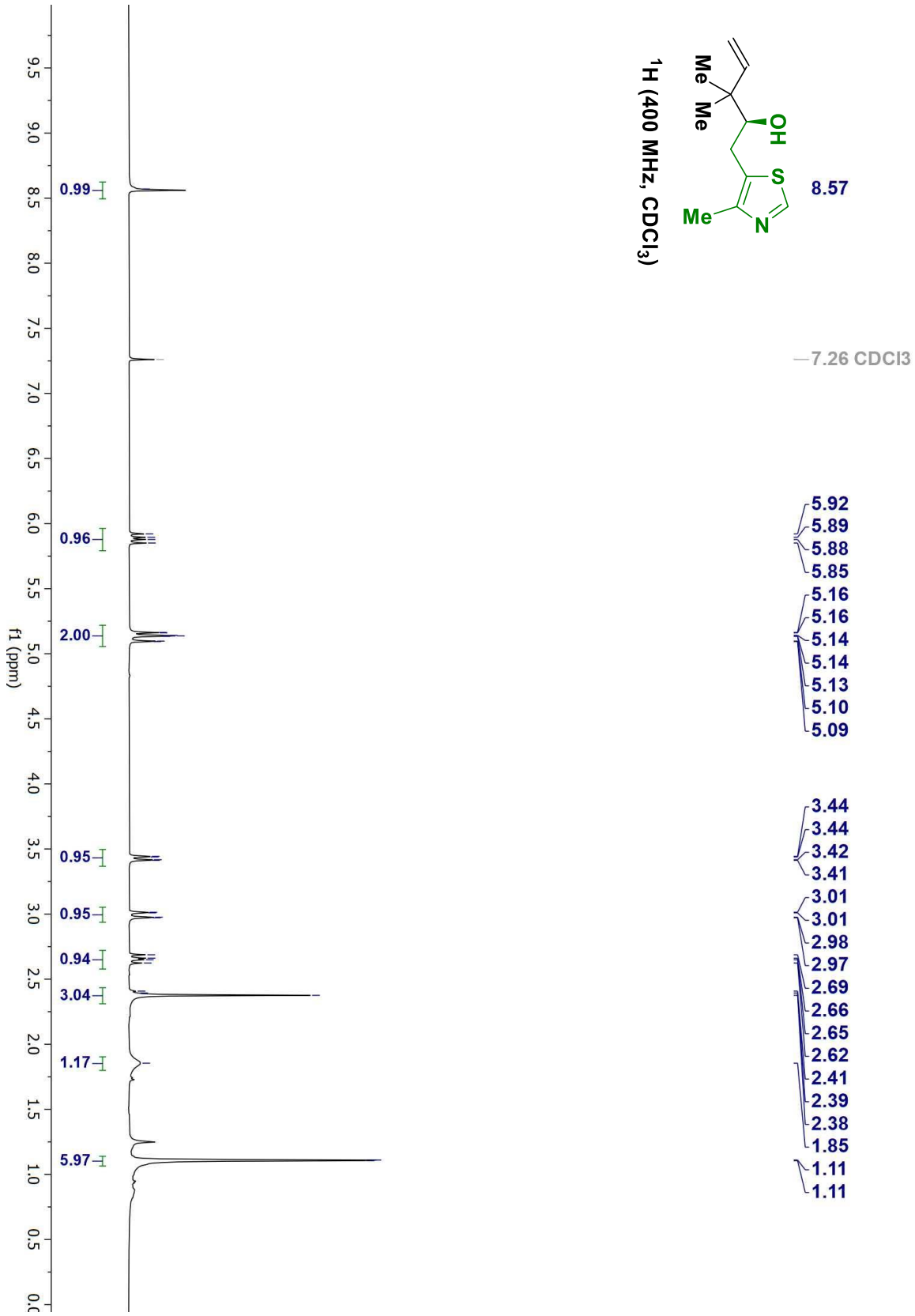
^{13}C NMR (101 MHz, $CDCl_3$): δ 150.0, 149.5, 144.7, 129.1, 114.0, 79.0, 41.7, 29.1, 22.8, 22.7, 15.2.

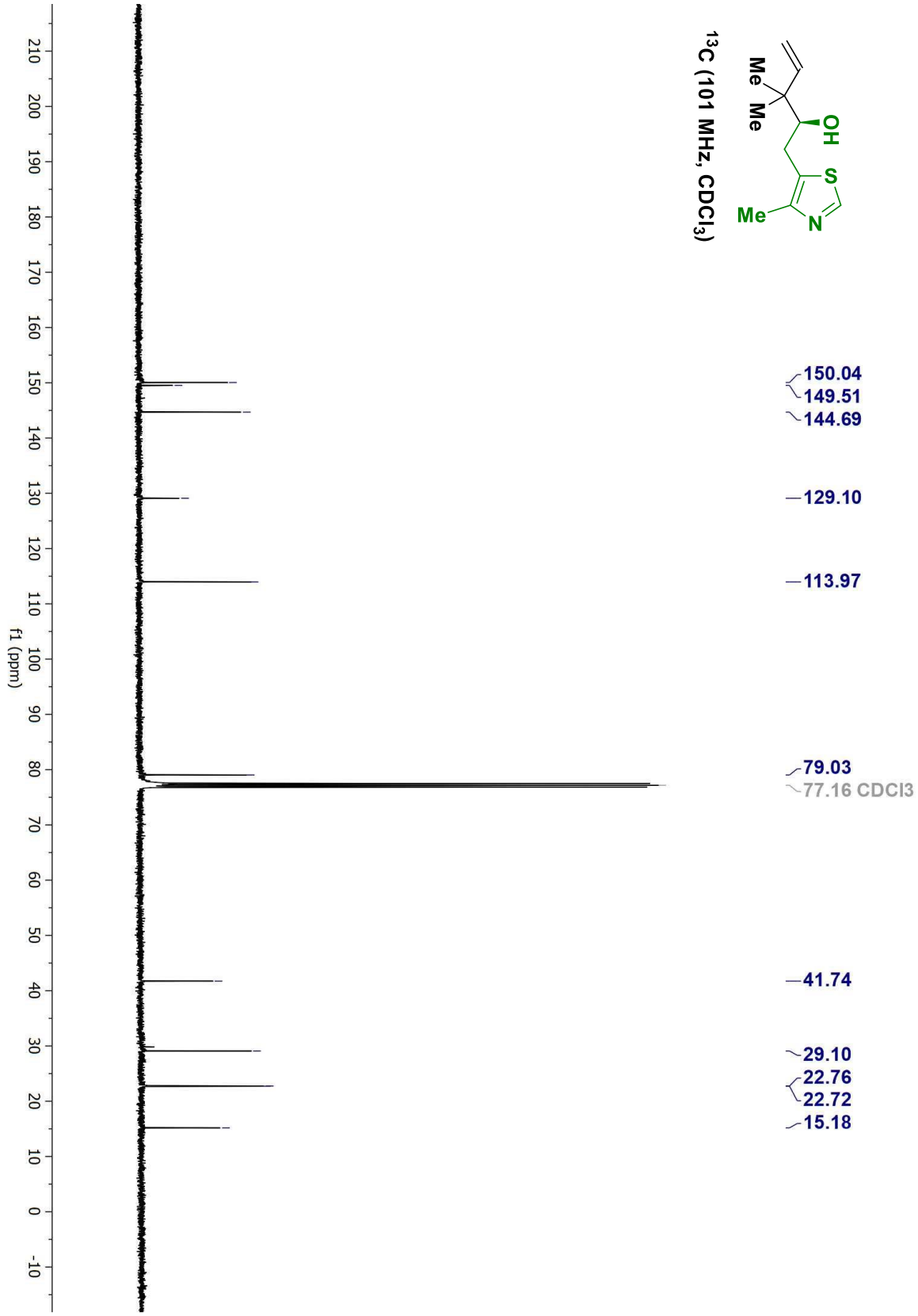
HRMS (Na+, *m/z*) for $C_{11}H_{17}NOS$: calcd. = 234.0898; found = 234.0899.

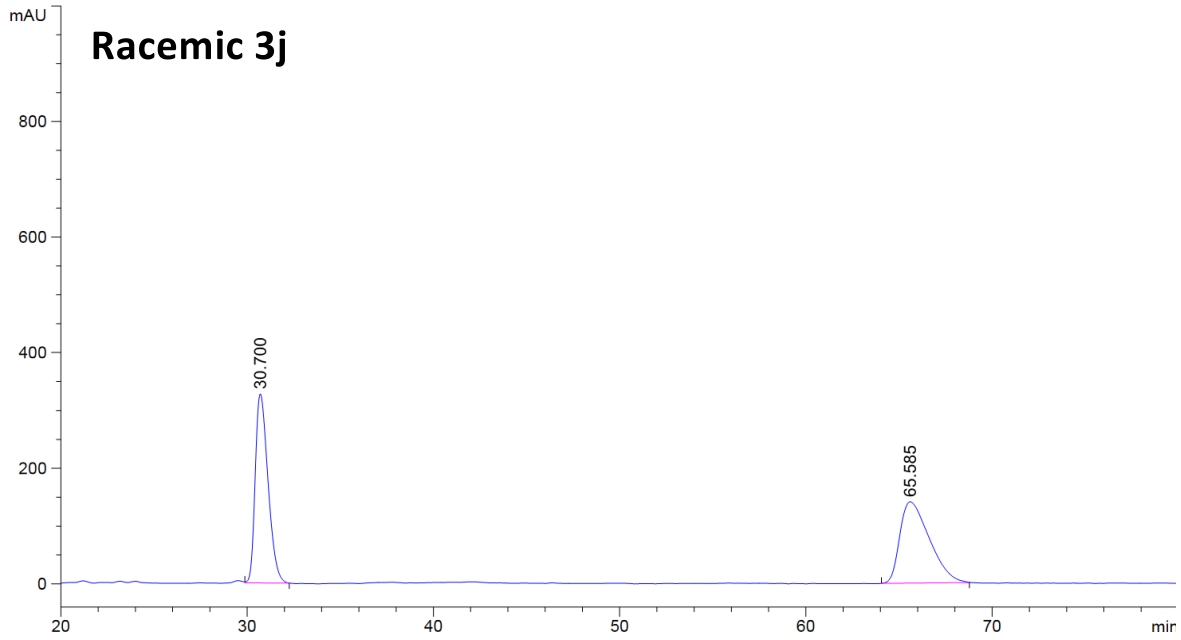
FTIR (neat): 3346, 2926, 2911, 1567, 1429, 1393, 1258, 1023, 734, 693 cm^{-1}.

HPLC: (Chiralcel columns Amylose 3, Hexane:2-PrOH = 97:03, 0.5 mL/min, 210 nm).

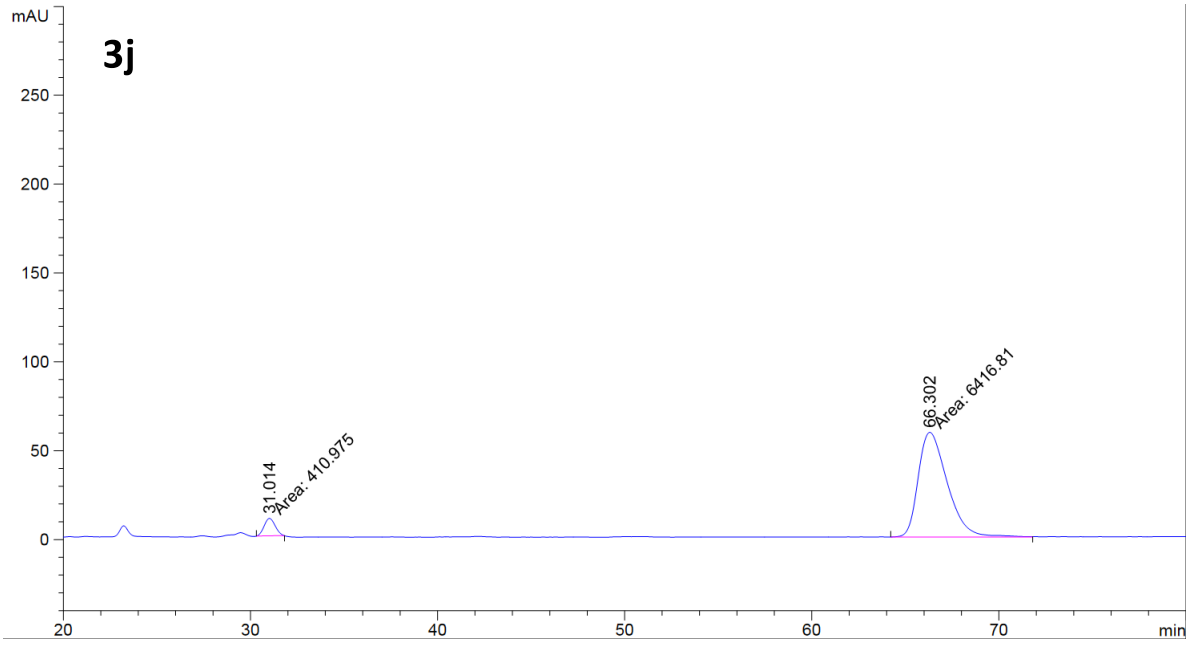
$[\alpha]_D^{24}$ = -36.4 (c = 0.1, $CHCl_3$).


^{1}H (400 MHz, CDCl$_3$)
Me
Me
OH
S
Me
N
8.57
7.26 CDCl3
5.92
5.89
5.88
5.85
5.16
5.16
5.14
5.14
5.13
5.10
5.09
3.44
3.44
3.42
3.41
3.01
3.01
2.98
2.97
2.69
2.66
2.65
2.62
2.41
2.39
2.38
1.85
1.11
1.11
0.99
0.96
2.00
0.95
0.95
0.94
3.04
1.17
5.97
f1 (ppm)


^{13}C (101 MHz, $CDCl_3$)
Me
Me
OH
S
Me
N
150.04
149.51
144.69
129.10
113.97
79.03
77.16 CDCl3
41.74
29.10
22.76
22.72
15.18
f1 (ppm)

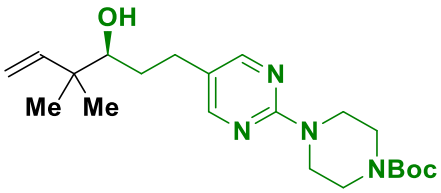


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.700	VB	0.7415	1.56413e4	327.31174	50.1866
2	65.585	BB	1.5796	1.55250e4	140.88731	49.8134



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.014	MM	0.6916	410.97479	9.90449	6.0192
2	66.302	MM	1.8128	6416.81299	58.99518	93.9808

tert-butyl (S)-4-(5-(3-hydroxy-4,4-dimethylhex-5-en-1-yl)pyrimidin-2-yl)piperazine-1-carboxylate (3k)



Alcohol **2k** (64.5 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h) with $RuH_2CO(PPh_3)_3$ (5 mol%), and LiI (10 mol%). Flash column chromatography (SiO_2: 25:75 EtOAc:hexanes) provided the title compound **3k** as a yellow oil in 73% yield (56.7 mg, 0.15 mmol, 12:1 rr, 85% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 10:90 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.4 (1:1 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.18 (s, 2H), 5.75 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.08 (dd, *J* = 10.8, 1.3 Hz, 1H), 5.03 (dd, *J* = 17.5, 1.3 Hz, 1H), 3.75 (t, *J* = 5.2 Hz, 4H), 3.48 (t, *J* = 5.2 Hz, 4H), 3.22 (ddd, *J* = 10.8, 4.8, 1.9 Hz, 1H), 2.70 (ddd, *J* = 14.2, 9.4, 4.8 Hz, 1H), 2.45 (ddd, *J* = 14.2, 9.0, 7.5 Hz, 1H), 1.74 – 1.66 (m, 1H), 1.65 (d, *J* = 4.8 Hz, 1H), 1.56 – 1.49 (m, 1H), 1.47 (s, 9H), 0.97 (s, 6H).

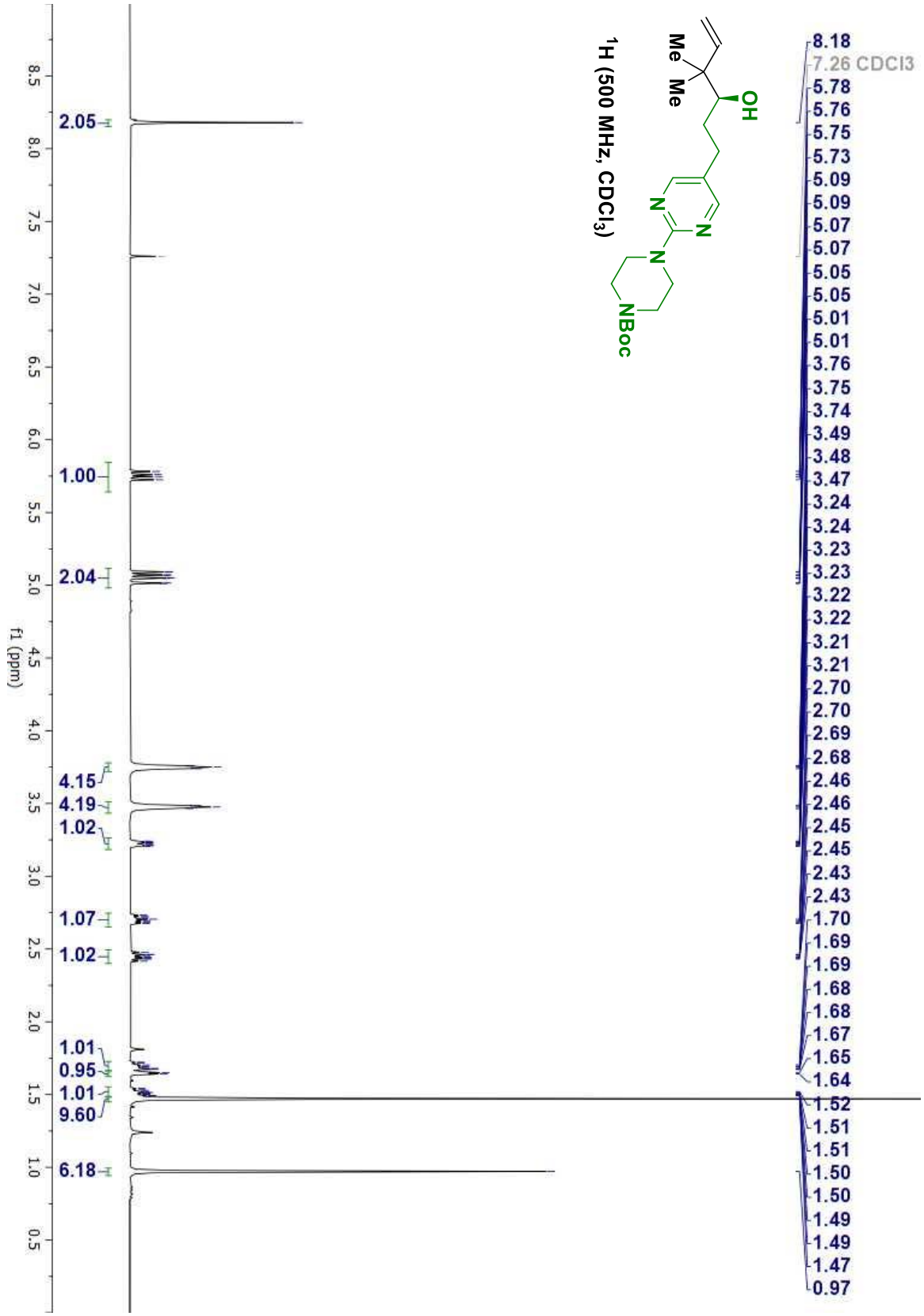
^{13}C NMR (126 MHz, $CDCl_3$): δ 160.9, 157.8, 155.0, 145.2, 123.3, 113.9, 80.0, 43.9, 41.8, 32.9, 28.6, 26.7, 23.2, 21.9.

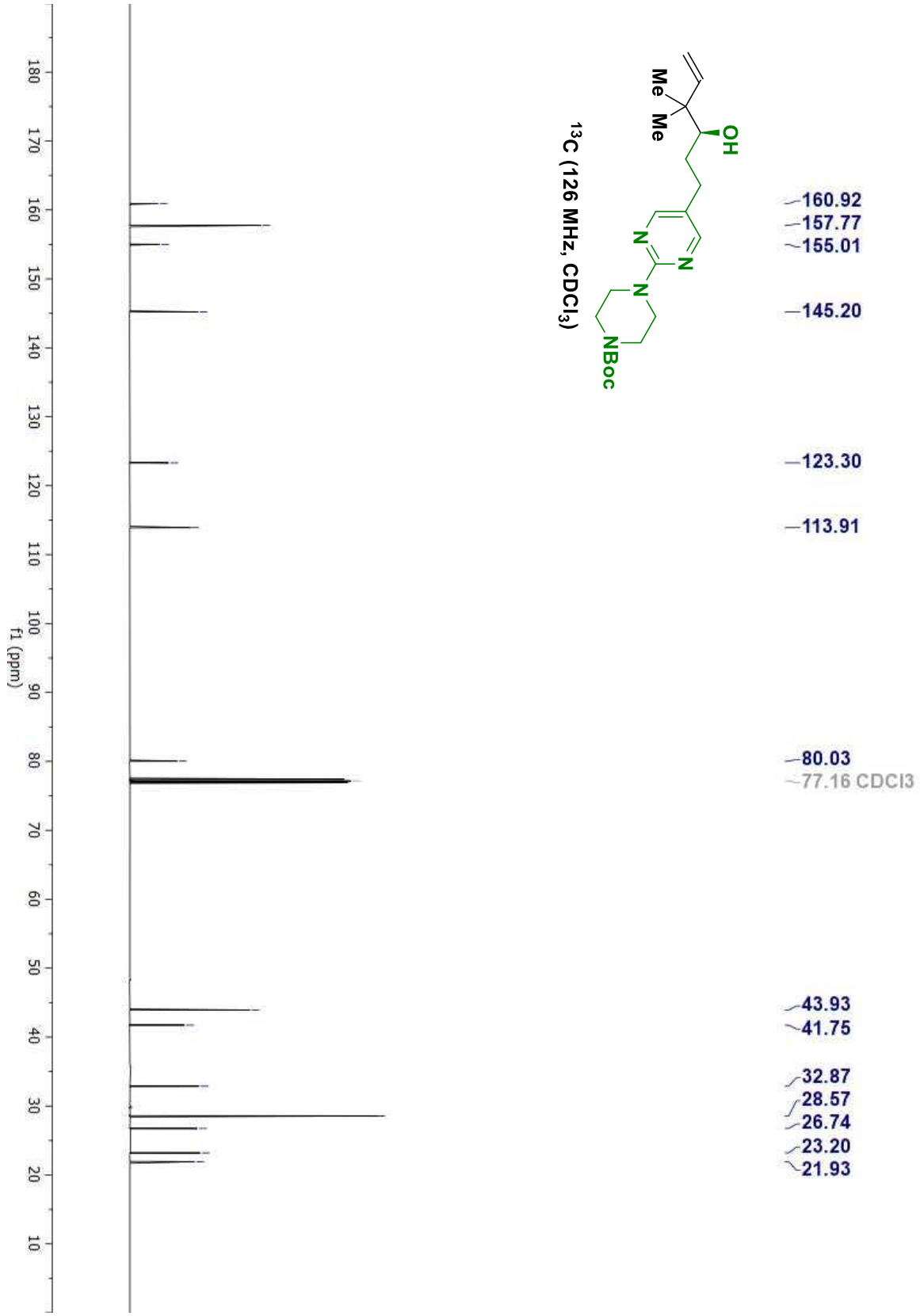
HRMS (H+, *m/z*) for $C_{21}H_{34}N_4O_3$: calcd. = 391.2704; found = 391.2710.

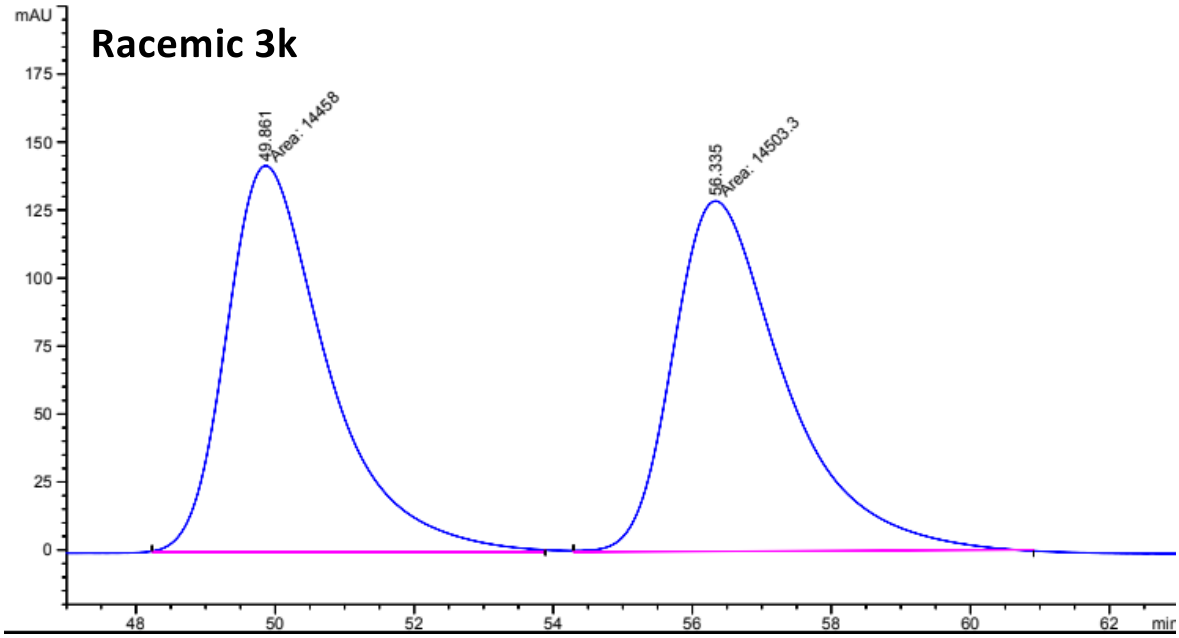
FTIR (neat): 3456, 2972, 2860, 1694, 1493, 1416, 1361, 1243, 1164, 1077, 998, 795 cm^{-1}.

HPLC: (Chiralcel columns AD-H 4, Hexane:2-PrOH = 95:5, 0.5 mL/min, 210 nm).

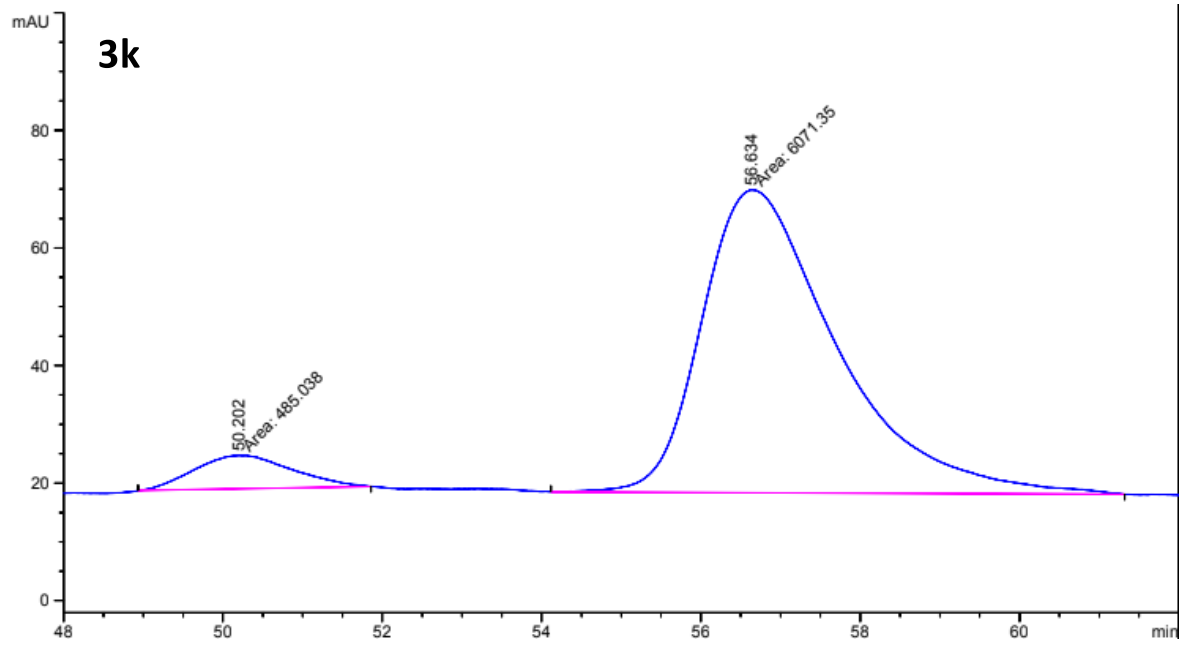
$[\alpha]_D^{24}$ = -10.7 (c = 0.1, $CHCl_3$).


^{1}H (500 MHz, CDCl$_3$)
Me
Me
OH
N
N
N
NBoc
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
2.05
1.00
2.04
4.15
4.19
1.02
1.07
1.02
1.01
0.95
1.01
9.60
6.18
8.18
7.26 CDCl3
5.78
5.76
5.75
5.73
5.09
5.09
5.07
5.07
5.05
5.05
5.01
5.01
3.76
3.75
3.74
3.49
3.48
3.47
3.24
3.24
3.23
3.23
3.22
3.22
3.21
3.21
2.70
2.70
2.69
2.68
2.46
2.46
2.45
2.45
2.43
2.43
1.70
1.69
1.69
1.68
1.68
1.67
1.65
1.64
1.52
1.51
1.51
1.50
1.50
1.49
1.49
1.47
0.97


^{13}C (126 MHz, CDCl$_3$)
Me
Me
OH
N
N
N
NBoc
160.92
157.77
155.01
145.20
123.30
113.91
80.03
77.16 CDCl3
43.93
41.75
32.87
28.57
26.74
23.20
21.93
f1 (ppm)

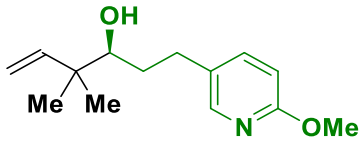


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	49.861	MM	1.6957	1.44580e4	142.10597	49.9219
2	56.335	MM	1.8754	1.45033e4	128.88811	50.0781



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	50.202	MM	1.4209	485.03766	5.68940	7.3979
2	56.634	MM	1.9642	6071.35303	51.51575	92.6021

(*S*)-1-(6-methoxypyridin-3-yl)-4,4-dimethylhex-5-en-3-ol (3l)



Alcohol **2l** (33.4 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h). Flash column chromatography (SiO_2: 10:90 EtOAc:hexanes) provided the title compound **3l** as a yellow oil in 74% yield (37.8 mg, 0.149 mmol, 13:1 rr, 85% ee).

Separation of regioisomers: Flash column chromatography (SiO_2: 5:95 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.32 (1:3 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 8.4 Hz, 1H), 5.77 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.12 – 5.02 (m, 2H), 3.91 (s, 3H), 3.28 – 3.22 (m, 1H), 2.87 – 2.78 (m, 1H), 2.58 – 2.52 (m, 1H), 1.79 – 1.73 (m, 1H), 1.56 – 1.50 (m, 1H), 0.99 (s, 6H).

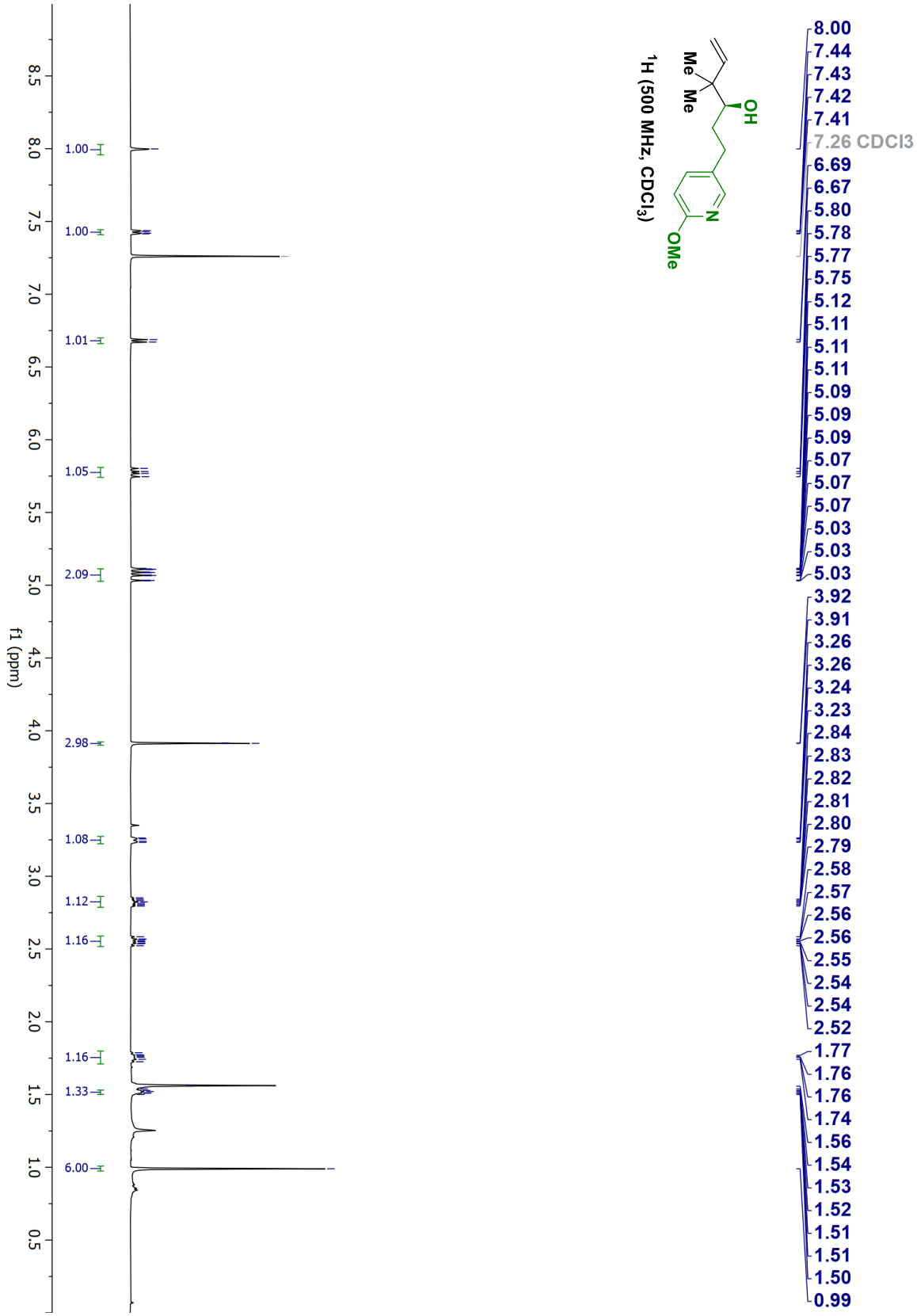
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 146.3, 145.3, 139.2, 130.2, 113.9, 110.5, 53.4, 41.7, 33.1, 29.4, 23.2, 21.9

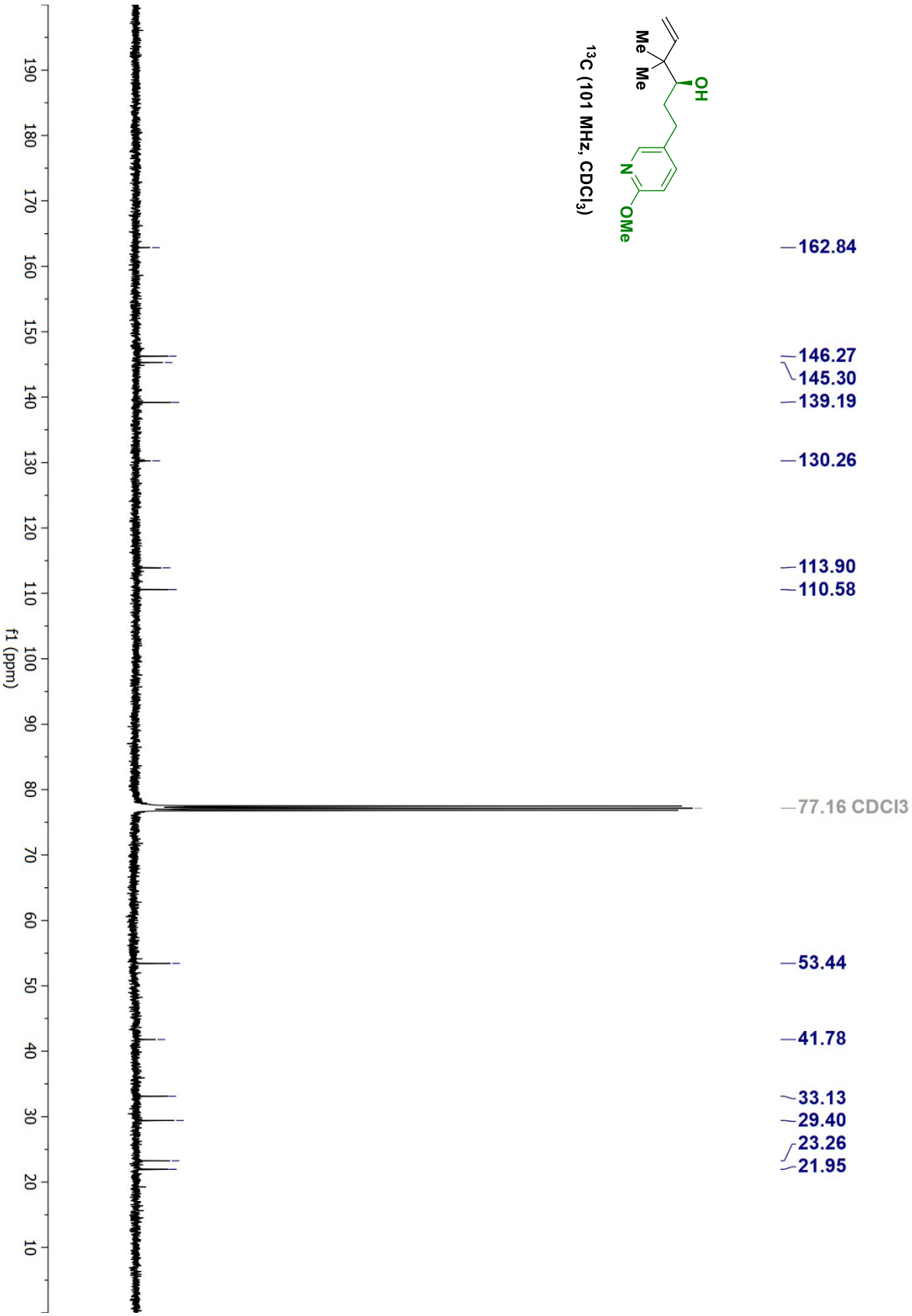
HRMS (Na+, *m/z*) for $C_{14}H_{21}NO_2$: calcd. = 258.1372; found = 258.1449.

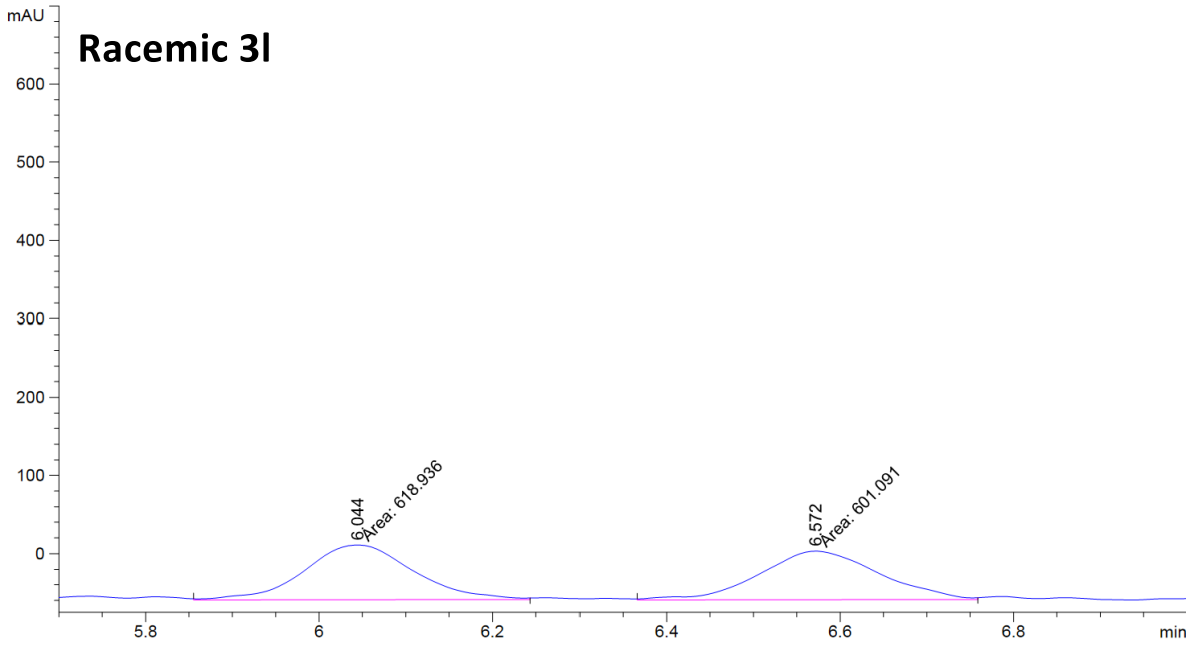
FTIR (neat): 3388, 2948, 2925, 2855, 1736, 1608, 1572, 1492, 1462, 1415, 1390, 1364, 1074, 1028 cm^{-1}.

HPLC: (Phenomenex LC Columns Cellulose-5, Hexane: 2-PrOH = 90:10, 1.0 mL/min, 210 nm).

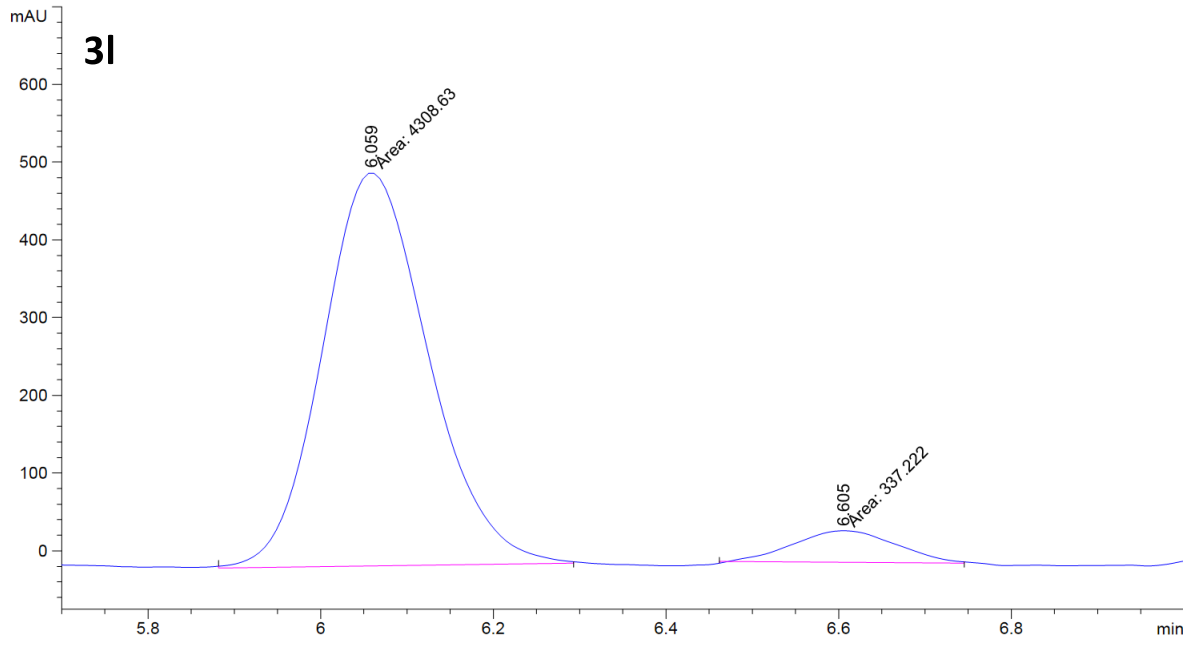
$[\alpha]_D^{24}$ = -19.0 (c = 0.1, $CHCl_3$).


1H (500 MHz, CDCl3)
Me
Me
OH
N
OMe
8.00
7.44
7.43
7.42
7.41
7.26 CDCl3
6.69
6.67
5.80
5.78
5.77
5.75
5.12
5.11
5.11
5.11
5.09
5.09
5.09
5.07
5.07
5.07
5.03
5.03
5.03
3.92
3.91
3.26
3.26
3.24
3.23
2.84
2.83
2.82
2.81
2.80
2.79
2.58
2.57
2.56
2.56
2.55
2.54
2.54
2.52
1.77
1.76
1.76
1.74
1.56
1.54
1.53
1.52
1.51
1.51
1.50
0.99
1.00
1.00
1.01
1.05
2.09
2.98
1.08
1.12
1.16
1.16
1.33
6.00
f1 (ppm)


^{13}C (101 MHz, CDCl$_3$)
Me
Me
OH
N
OMe
162.84
146.27
145.30
139.19
130.26
113.90
110.58
77.16 CDCl3
53.44
41.78
33.13
29.40
23.26
21.95
f1 (ppm)

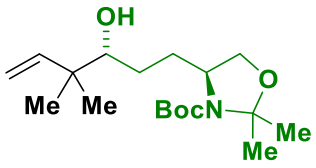


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.044	MM	0.1469	618.93591	70.22833	50.7313
2	6.572	MM	0.1604	601.09106	62.45972	49.2687



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.059	MM	0.1419	4308.63232	506.17874	92.7414
2	6.605	MM	0.1382	337.22168	40.68252	7.2586

tert-butyl (S)-4-((R)-3-hydroxy-4,4-dimethylhex-5-en-1-yl)-2,2-dimethyloxazolidine-3-carboxylate (3m)



Alcohol **2m** (51.9 mg, 0.2 mmol) was subjected to standard reaction conditions (110 °C, 48 h) with **(*S*)-SEGPHOS** as ligand. Flash column chromatography (SiO_2: 3:97 EtOAc:hexanes) provided the title compound **3m** as a yellow oil in 56% yield (36.2mg, 0.11 mmol, 10:1 rr, 6:1 dr).

Separation of regioisomers: Flash column chromatography (SiO_2: 2:98 EtOAc:hexanes).

TLC (SiO_2): R_f = 0.25 (1:4 EtOAc:Hexanes).

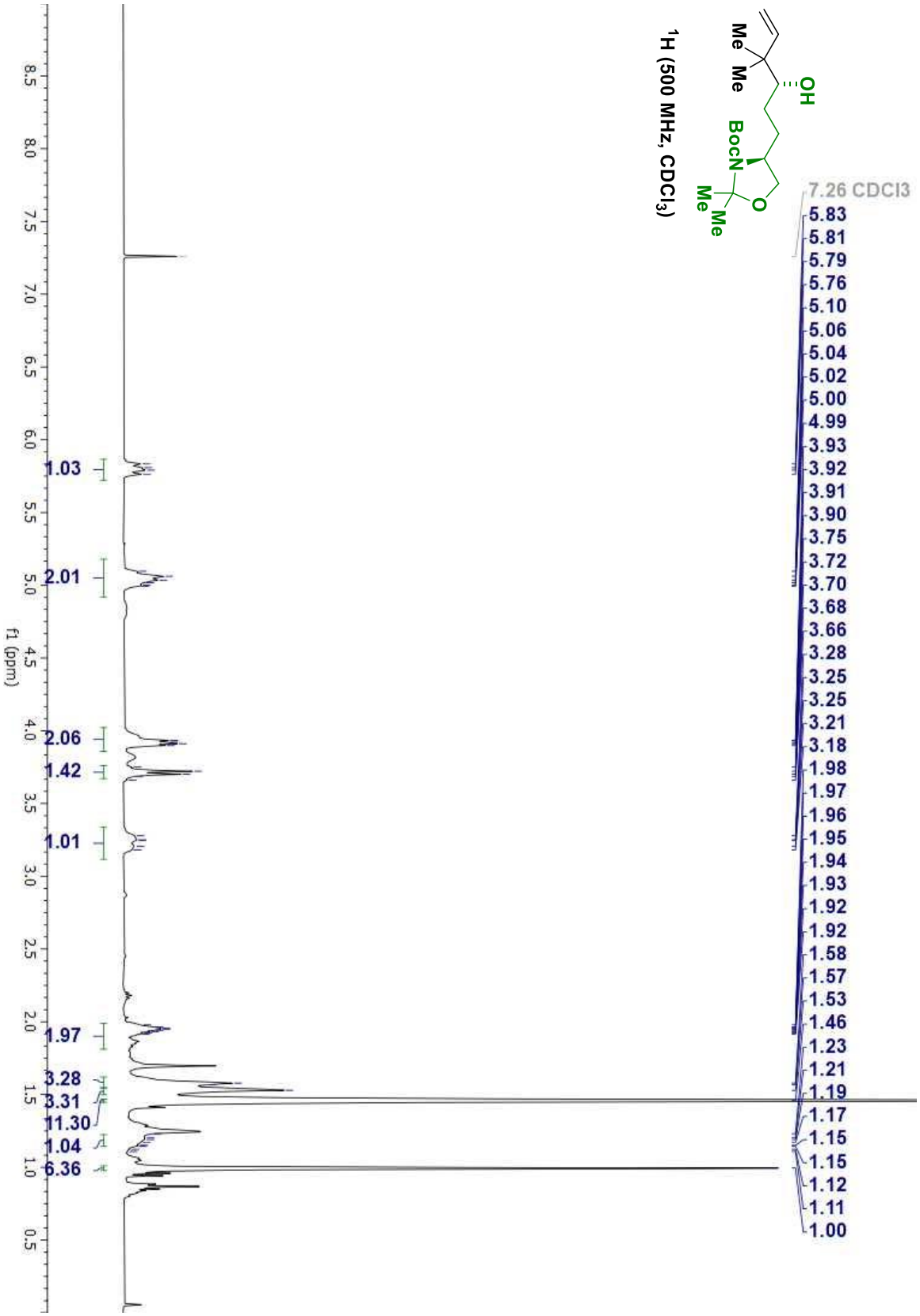
^{1}H NMR (500 MHz, $CDCl_3$) δ: 5.94 – 5.70 (m, 1H), 5.94 – 5.70 (m, 2H), 4.00 – 3.88 (m, 2H), 3.70 (tt, *J* = 19.8, 8.7 Hz, 1H), 3.38 – 3.14 (m, 1H), 2.02 – 1.91 (m, 1H), 1.91 – 1.81 (m, 1H), 1.62 (s, 3H), 1.54 (s, 3H), 1.48 (s, 11H), 1.00 (s, 6H).

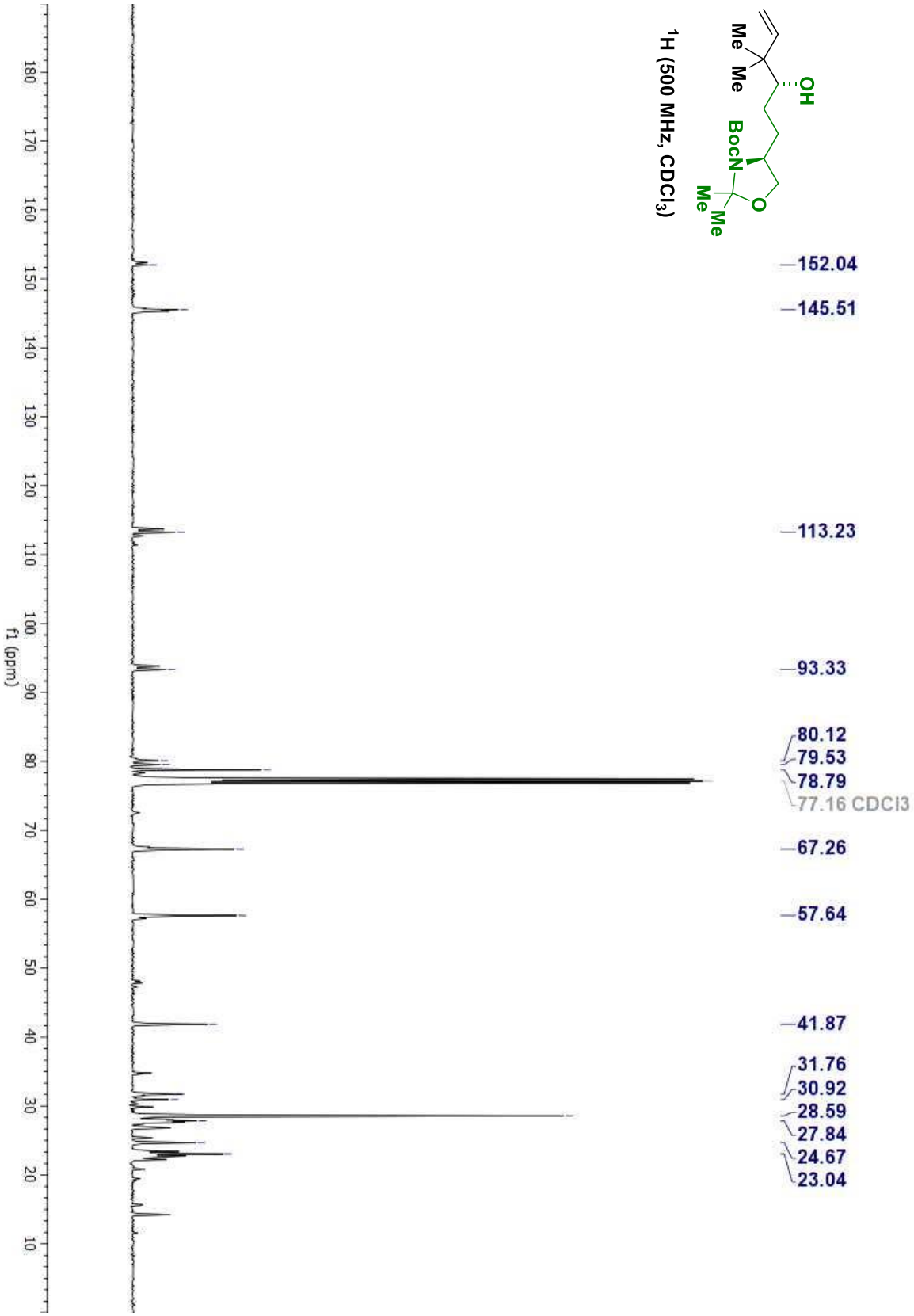
^{13}C NMR (126 MHz, $CDCl_3$) δ: 152.1, 145.3, 113.3, 93.9, 78.8, 78.4, 67.6, 67.3, 57.5, 48.2, 41.9, 29.9, 28.6, 27.9, 26.9, 24.7, 23.4, 23.1.

HRMS (Na+, *m/z*) for $C_{18}H_{33}NO_4$: calcd. = 350.2302; found = 350.2298.

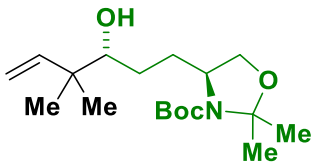
FTIR (neat): 3107, 3011, 2796, 1851, 1769, 1499, 1103, 499,406 cm^{-1}.

$[\alpha]_D^{24}$ = - 40.0 (c = 0.4, $CHCl_3$)


^{1}H (500 MHz, CDCl$_3$)
Me
Me
OH
BocN
Me
Me
O
7.26 CDCl3
5.83
5.81
5.79
5.76
5.10
5.06
5.04
5.02
5.00
4.99
3.93
3.92
3.91
3.90
3.75
3.72
3.70
3.68
3.66
3.28
3.25
3.25
3.21
3.18
1.98
1.97
1.96
1.95
1.94
1.93
1.92
1.92
1.58
1.57
1.53
1.46
1.23
1.21
1.19
1.17
1.15
1.15
1.12
1.11
1.00
1.03
2.01
2.06
1.42
1.01
1.97
3.28
3.31
11.30
1.04
6.36
f1 (ppm)


^{1}H (500 MHz, CDCl$_3$)
Me
Me
OH
BocN
Me
Me
O
152.04
145.51
113.23
93.33
80.12
79.53
78.79
77.16 CDCl3
67.26
57.64
41.87
31.76
30.92
28.59
27.84
24.67
23.04
f1 (ppm)

tert-butyl (S)-4-((S)-3-hydroxy-4,4-dimethylhex-5-en-1-yl)-2,2-dimethyloxazolidine-3-carboxylate (*epi*-3m)



Alcohol **2m** (51.9 mg, 0.2 mmol) was subjected to standard reaction conditions (110 °C, 48 h) with **(*R*)-SEGPHOS** as ligand. Flash column chromatography (SiO_2: 3:97 EtOAc:hexanes) provided the title compound *epi*-**3m** as a yellow oil in 55% yield (36.0 mg, 0.11 mmol,12:1 rr, >20:1 dr).

TLC (SiO_2): R_f = 0.25 (1:4 EtOAc:Hexanes).

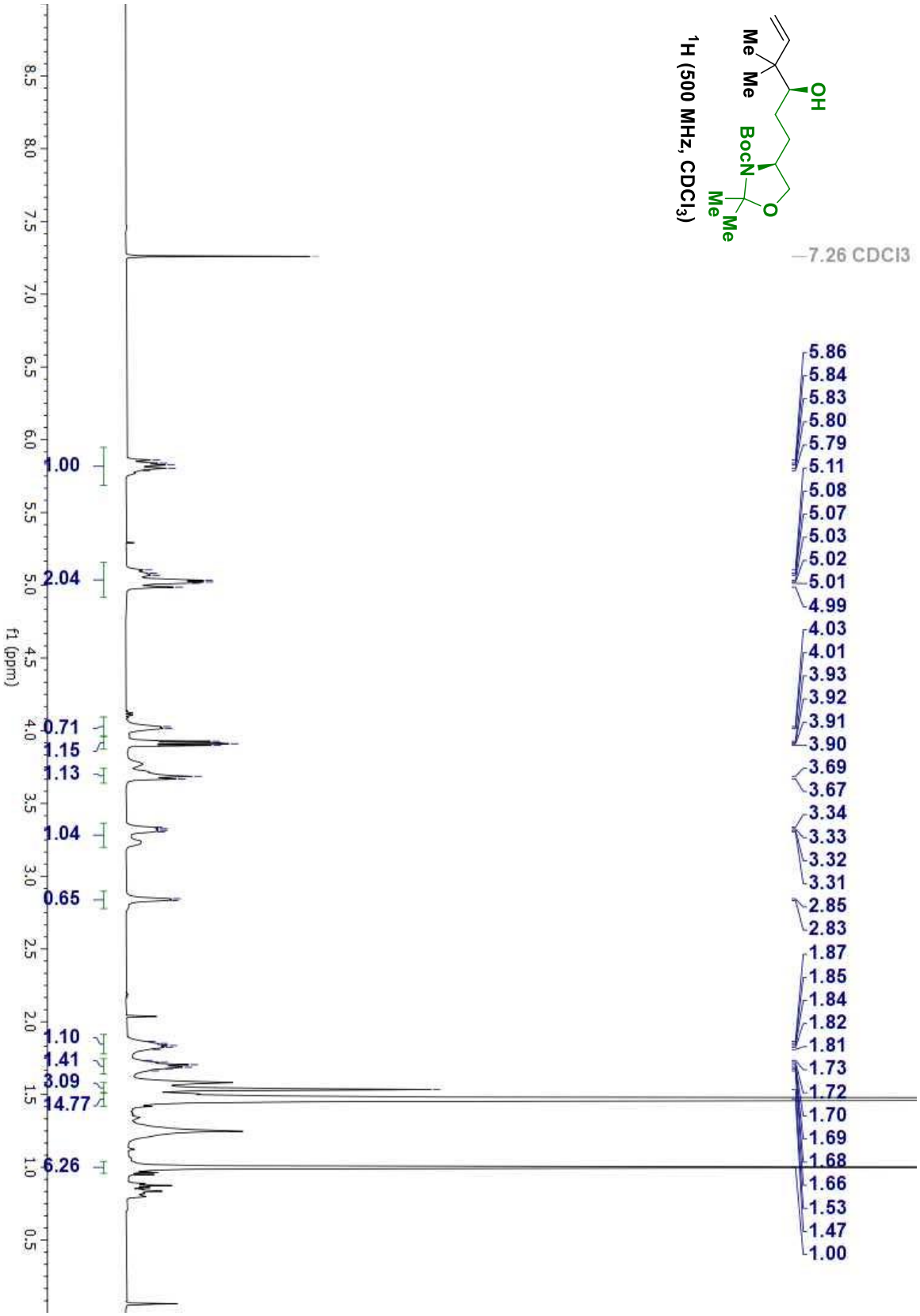
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.82 (m, 1H), 5.15 – 4.95 (m, 2H), 4.07 – 3.87 (m, 2H), 3.70 (tt, *J* = 21.1, 8.8 Hz, 1H), 3.39 – 3.15 (m, 1H), 2.04 – 1.91 (m, 1H), 1.89 – 1.82 (m, 1H), 1.61 (s, 3H), 1.54 (s, 3H), 1.47 (s, 11H), 1.01 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 152.1, 145.3, 113.3, 93.9, 78.8, 78.4, 67.6, 67.3, 57.6, 48.2, 41.9, 29.9, 28.6, 27.9, 26.9, 24.7, 23.4, 23.1.

HRMS (Na+, *m/z*) for $C_{18}H_{33}NO_4$: calcd. = 350.2302; found = 350.2298.

FTIR (neat): 3273, 3021, 2846, 1892, 1738, 1506, 1178, 536 cm^{-1}.

$[\alpha]_D^{24}$ = + 40.0 (c = 0.4, $CHCl_3$)


^{1}H (500 MHz, CDCl$_3$)
Me
Me
OH
BocN
O
Me
Me
7.26 CDCl3
f1 (ppm)
1.00
2.04
0.71
1.15
1.13
1.04
0.65
1.10
1.41
3.09
14.77
6.26
5.86
5.84
5.83
5.80
5.79
5.11
5.08
5.07
5.03
5.02
5.01
4.99
4.03
4.01
3.93
3.92
3.91
3.90
3.69
3.67
3.34
3.33
3.32
3.31
2.85
2.83
1.87
1.85
1.84
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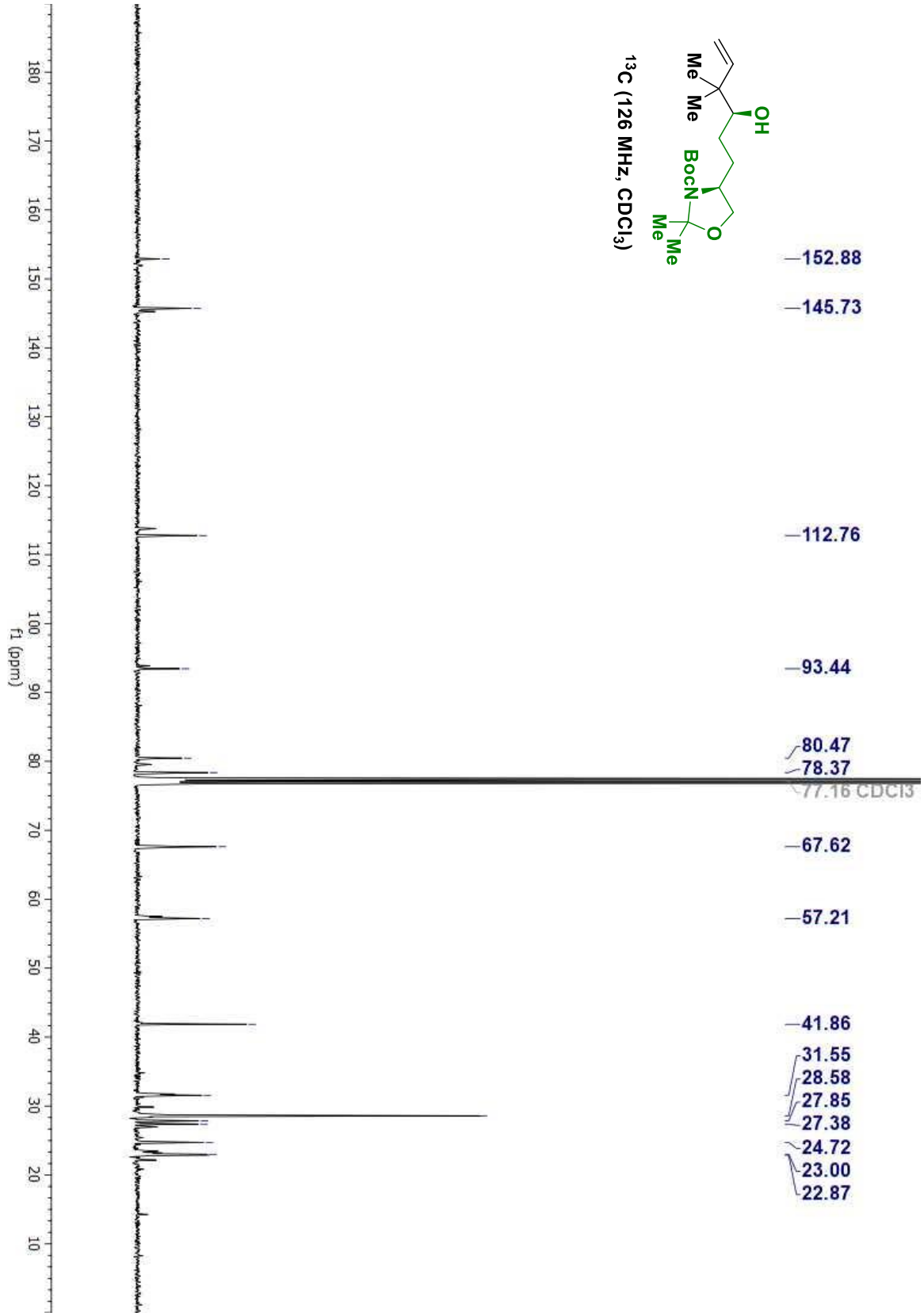
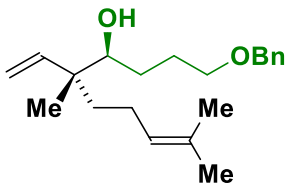
1.70
1.69
1.68
1.66
1.53
1.47
1.00


^{13}C (126 MHz, CDCl$_3$)
Me
Me
OH
BocN
O
Me
Me
152.88
145.73
112.76
93.44
80.47
78.37
77.16 CDCl3
67.62
57.21
41.86
31.55
28.58
27.85
27.38
24.72
23.00
22.87
f1 (ppm)

(4*S*,5*R*)-1-(benzyloxy)-5,9-dimethyl-5-vinyldec-8-en-4-ol (4a)



An oven-dried pressure tube equipped with a magnetic stir bar under an argon atmosphere, charged with alcohol **2a** (36.0 mg, 0.2 mmol, 100 mol%), $RuHCl(CO)(PPh_3)_3$ (14.3 mg, 0.02 mmol, 7.5 mol%), **(*S*)-DM-SEGPHOS** (10.8 mg, 0.02 mmol, 7.5 mol%), LiI (4.0 mg, 0.03 mmol, 15 mol%) and trifluoroethanol (43 μL, 0.6 mmol, 300 mol%), was added MTBE (0.4 mL, 0.5 M) and myrcene **1b** (86 μL, 0.5 mmol, 250 mol%). The tube was sealed with a PTFE lined cap, the reaction vessel was placed in a 115 °C oil bath and was allowed to stir for 48 hours, at which point the reaction vessel was removed from the oil bath and the reaction mixture was allowed to reach ambient temperature. The solvent was removed *in vacuo* and the residue was subjected to flash column chromatography (SiO_2: 8:92 EtOAc:hexanes) to furnish the title compound **4a** as a yellow oil in 56% yield (35.3 mg, 0.11 mmol, 5:1 rr, 86% ee, >20:1 dr).

TLC (SiO_2): R_f = 0.4 (2:3 EtOAc:Hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 – 7.34 (m, 4H), 7.32 – 7.29 (m, 1H), 5.79 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.22 (dd, *J* = 10.9, 1.5 Hz, 1H), 5.11 (t, *J* = 7.2 Hz, 1H), 5.07 (dd, *J* = 17.6, 1.5 Hz, 1H), 4.54 (s, 2H), 3.58 – 3.48 (m, 2H), 3.32 (ddd, *J* = 10.7, 3.7, 1.6 Hz, 1H), 2.02 (d, *J* = 3.7 Hz, 1H), 1.94 (dt, *J* = 12.8, 6.4 Hz, 1H), 1.91 – 1.84 (m, 2H), 1.76 – 1.71 (m, 1H), 1.70 (s, 3H), 1.69 – 1.66 (m, 1H), 1.60 (s, 3H), 1.43 (ddd, *J* = 13.1, 11.6, 5.6 Hz, 1H), 1.39 – 1.27 (m, 2H), 0.99 (s, 3H).

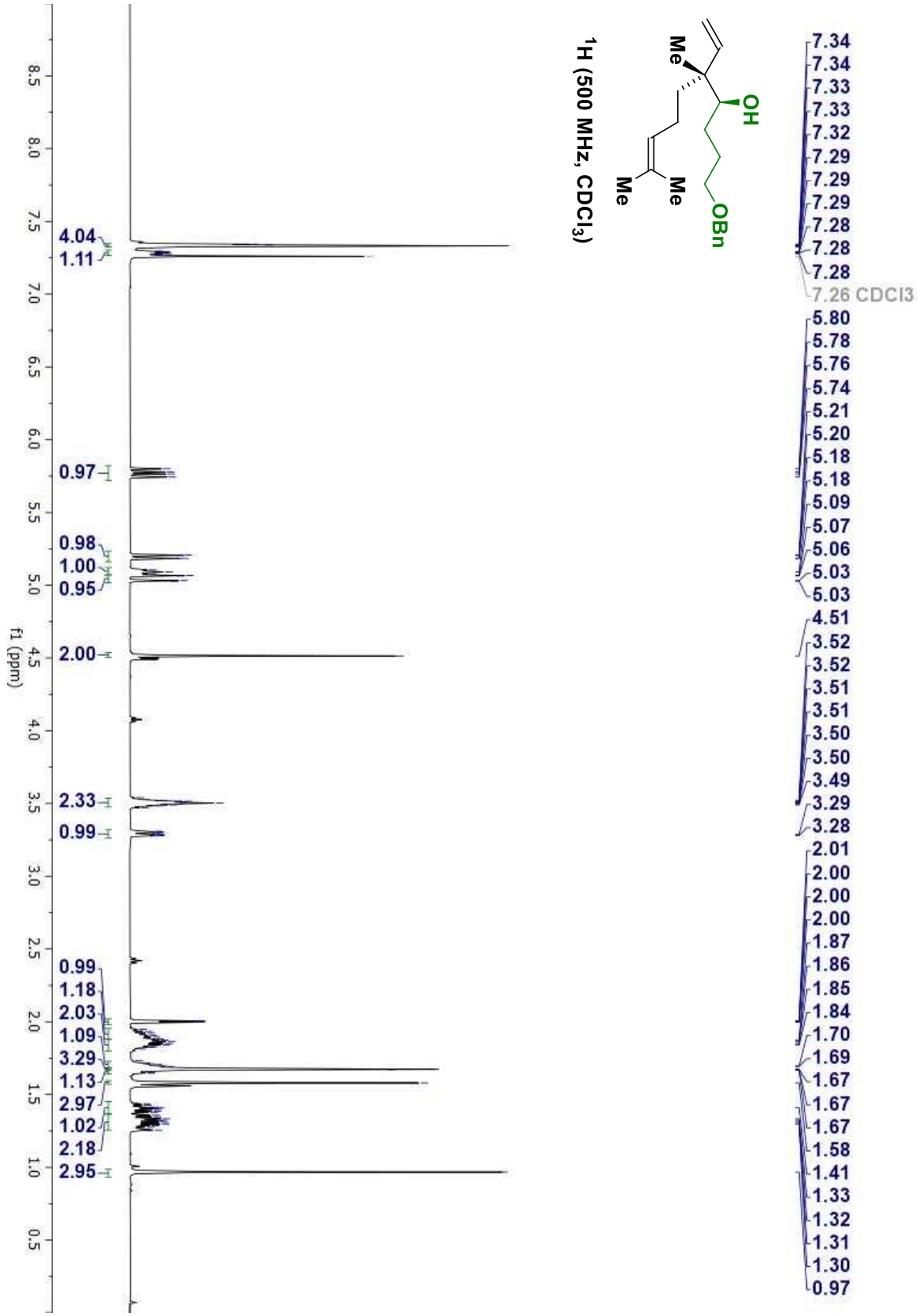
^{13}C NMR (126 MHz, $CDCl_3$): δ 144.4, 138.6, 131.4, 128.5, 127.8, 127.7, 125.0, 115.0, 73.1, 70.6, 45.1, 37.5, 28.1, 27.4, 25.8, 22.9, 17.8, 17.1.

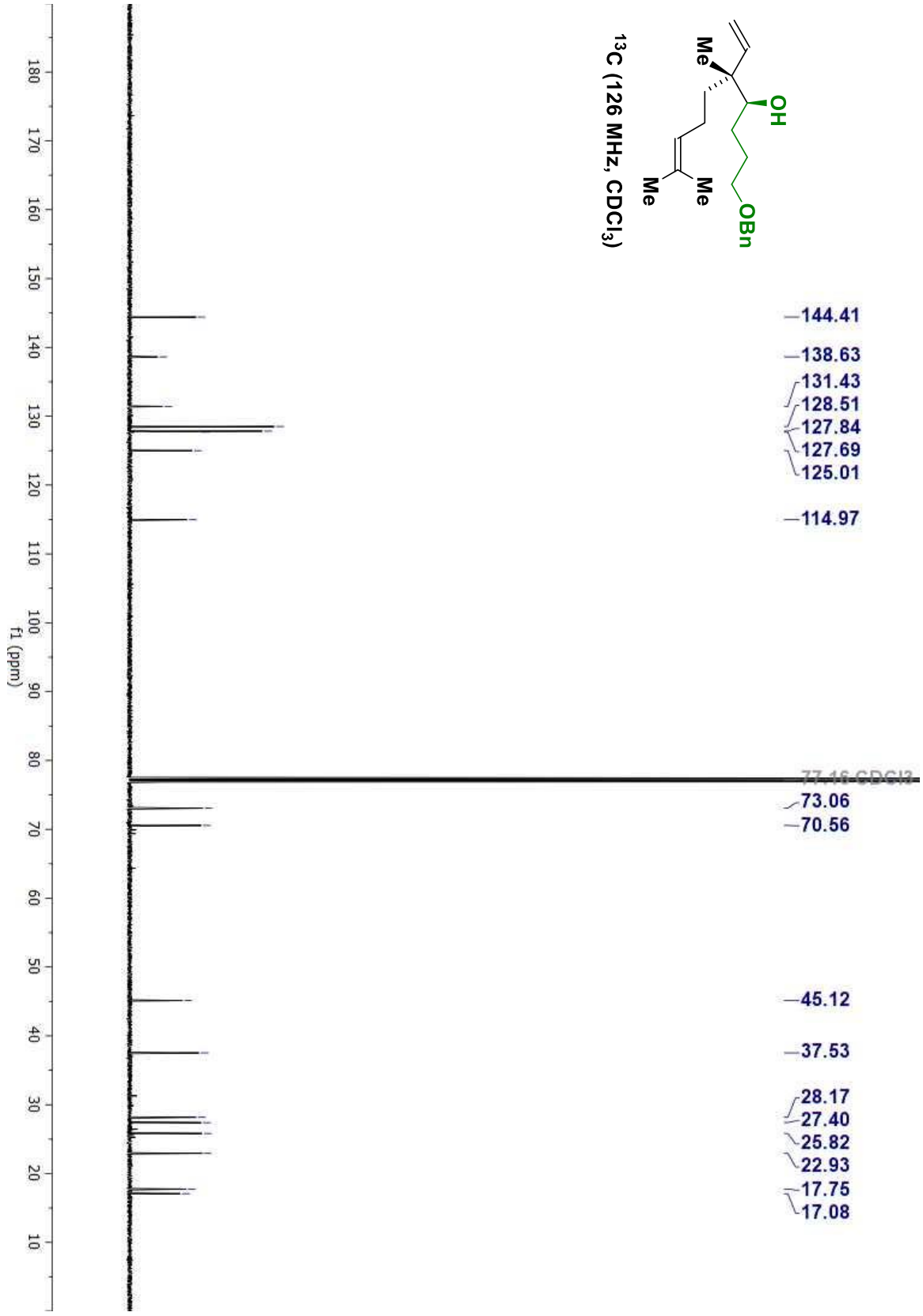
HRMS (H+, *m/z*) for $C_{21}H_{32}O_2$: calcd. = 317.2475; found = 317.2487.

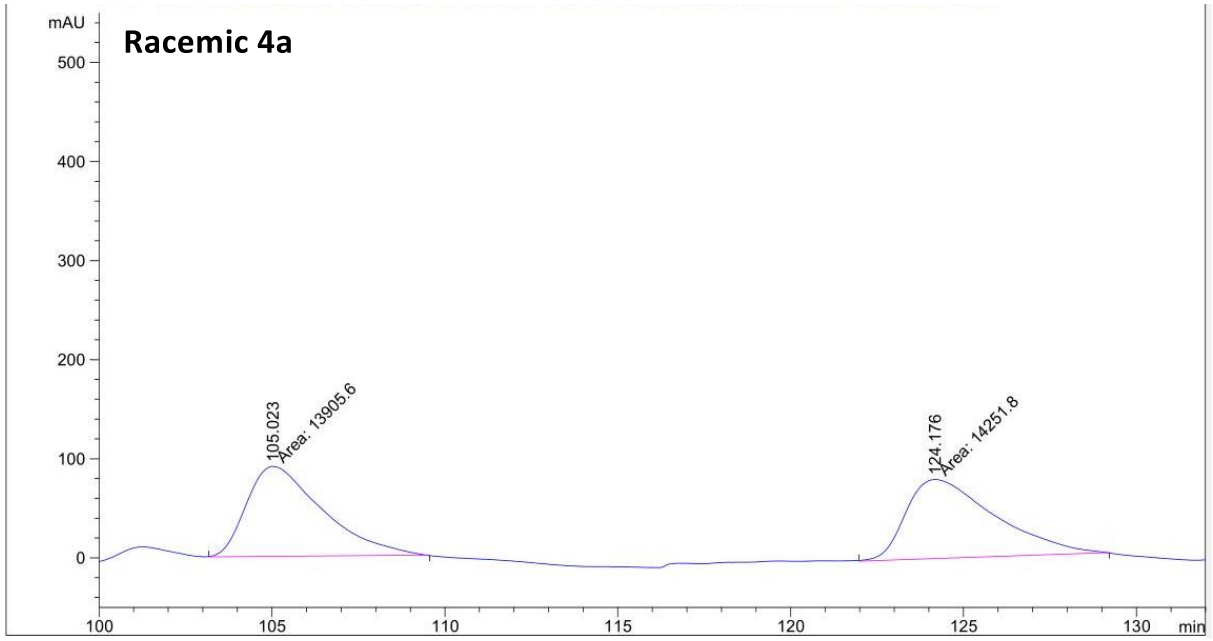
FTIR (neat): 3030, 2962, 2922, 2854, 1733, 1453, 1361, 1097, 910, 734, 696 cm^{-1}.

HPLC: (Phenomenex LC Columns Cellulose-2 + Cellulose-5, Hexane: 2-PrOH = 99:01, 0.5 mL/160min, 210 nm).

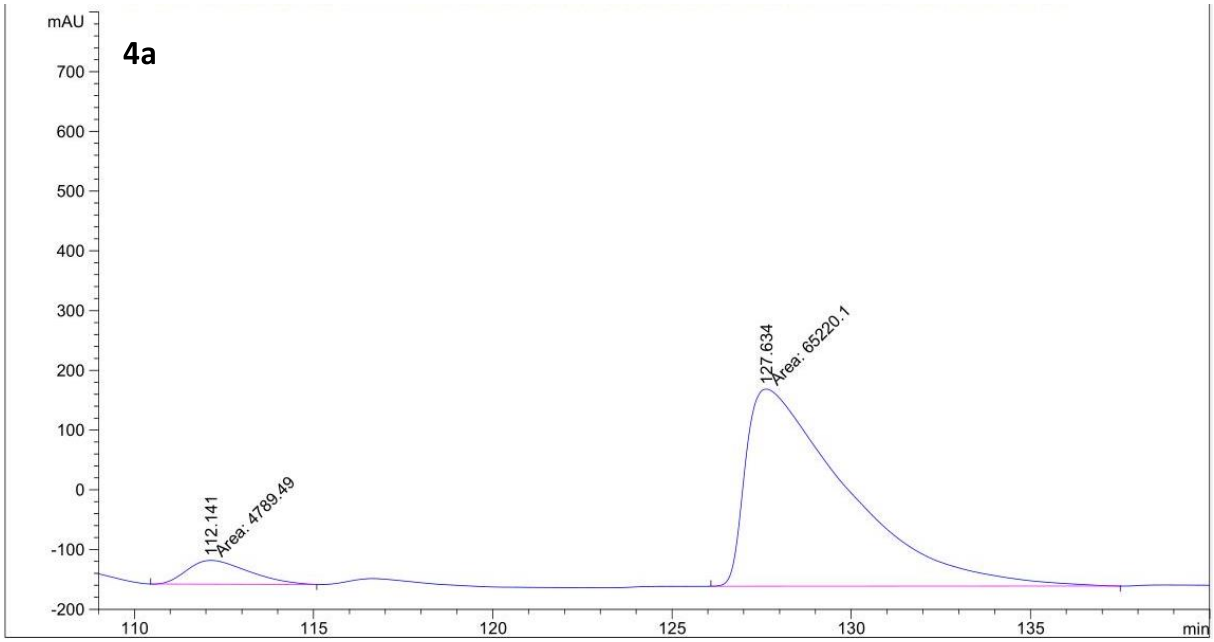
$[\alpha]_D^{24}$ = +28.7 (c = 0.4, $CHCl_3$).


^{1}H (500 MHz, CDCl$_3$)
Me
OH
Me
Me
OBn
7.34
7.34
7.33
7.33
7.32
7.29
7.29
7.29
7.28
7.28
7.28
7.26 CDCl3
5.80
5.78
5.76
5.74
5.21
5.20
5.18
5.18
5.09
5.07
5.06
5.03
5.03
4.51
3.52
3.52
3.51
3.51
3.50
3.50
3.49
3.29
3.28
2.01
2.00
2.00
2.00
1.87
1.86
1.85
1.84
1.70
1.69
1.67
1.67
1.67
1.58
1.41
1.33
1.32
1.31
1.30
0.97
4.04
1.11
0.97
0.98
1.00
0.95
2.00
2.33
0.99
0.99
1.18
2.03
1.09
3.29
1.13
2.97
1.02
2.18
2.95
f1 (ppm)


^{13}C (126 MHz, CDCl$_3$)
Me
OH
Me
Me
OBn
144.41
138.63
131.43
128.51
127.84
127.69
125.01
114.97
77.16 CDCl3
73.06
70.56
45.12
37.53
28.17
27.40
25.82
22.93
17.75
17.08
f1 (ppm)

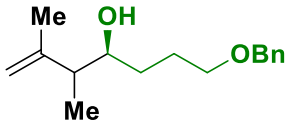


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	105.023	MM	2.5492	1.39056e4	90.91379	49.3852
2	124.176	MM	2.9720	1.42518e4	79.92323	50.6148



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	112.141	MM	1.9922	4789.48779	40.06916	6.8412
2	127.634	MM	3.2932	6.52201e4	330.07645	93.1588

(4*S*)-7-(benzyloxy)-2,3-dimethylhept-1-en-4-ol (*sec*-3a)



Alcohol **2a** (36.0 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h) without KI. Flash column chromatography (SiO_2: 8:92 EtOAc:hexanes) provided the title compound *sec*-**3a** as a yellow oil in 74% yield (37.2 mg, 0.15 mmol, 1:16 rr, 11% ee, 3:1 dr).

TLC (SiO_2): R_f = 0.5 (1:3 EtOAc:hexanes).

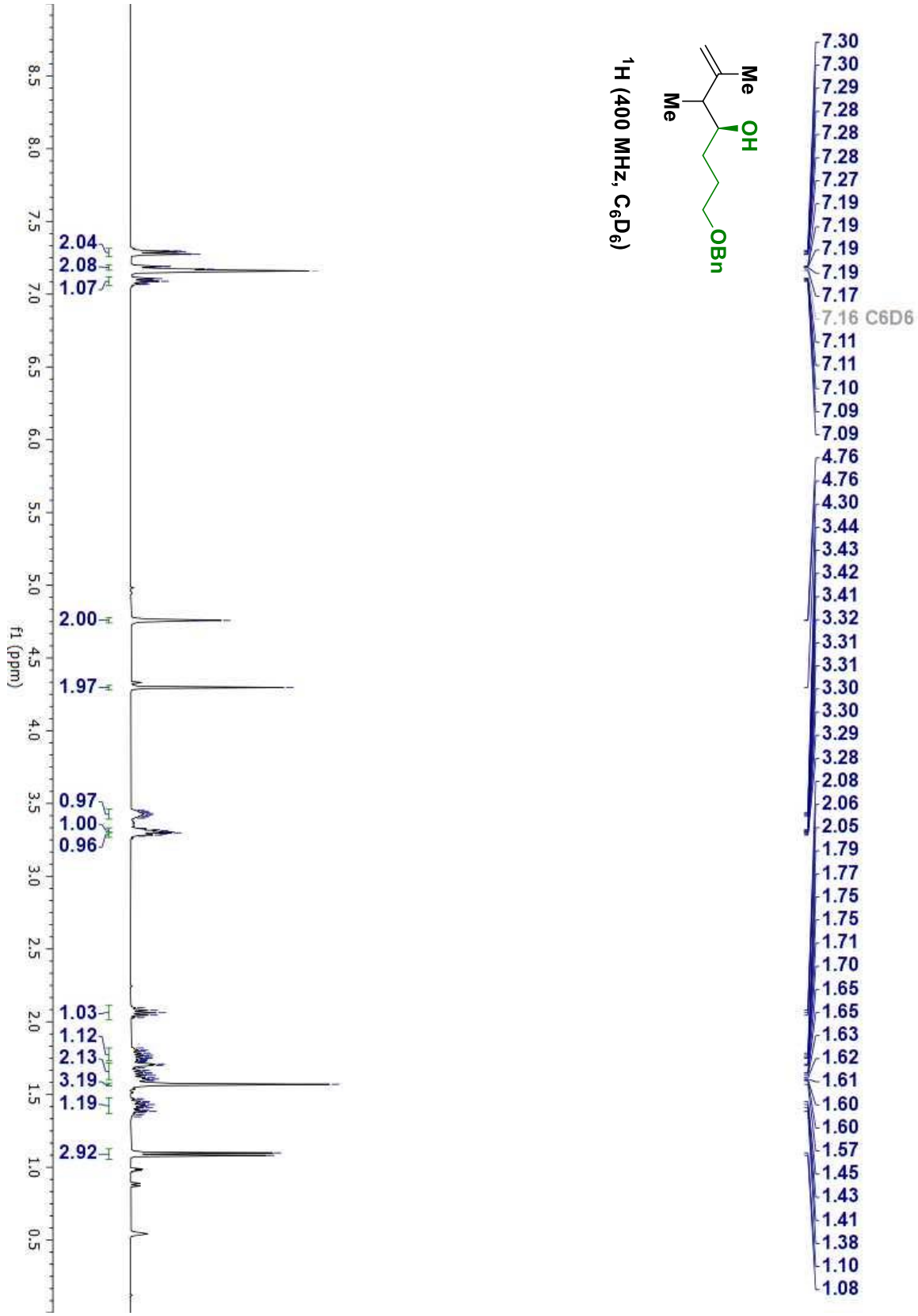
^{1}H NMR (400 MHz, C_6D_6): δ 7.31 – 7.26 (m, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.12 – 7.06 (m, 1H), 4.76 (d, *J* = 1.6 Hz, 2H), 4.30 (s, 2H), 3.43 (ddt, *J* = 9.3, 6.1, 3.3 Hz, 1H), 3.31 (dd, *J* = 4.6, 2.1 Hz, 1H), 3.29 (dt, *J* = 5.8, 2.1 Hz, 1H), 2.06 (p, *J* = 6.8 Hz, 1H), 1.83 – 1.72 (m, 1H), 1.72 – 1.59 (m, 2H), 1.57 (s, 3H), 1.49 – 1.33 (m, 1H), 1.09 (d, *J* = 6.9 Hz, 3H).

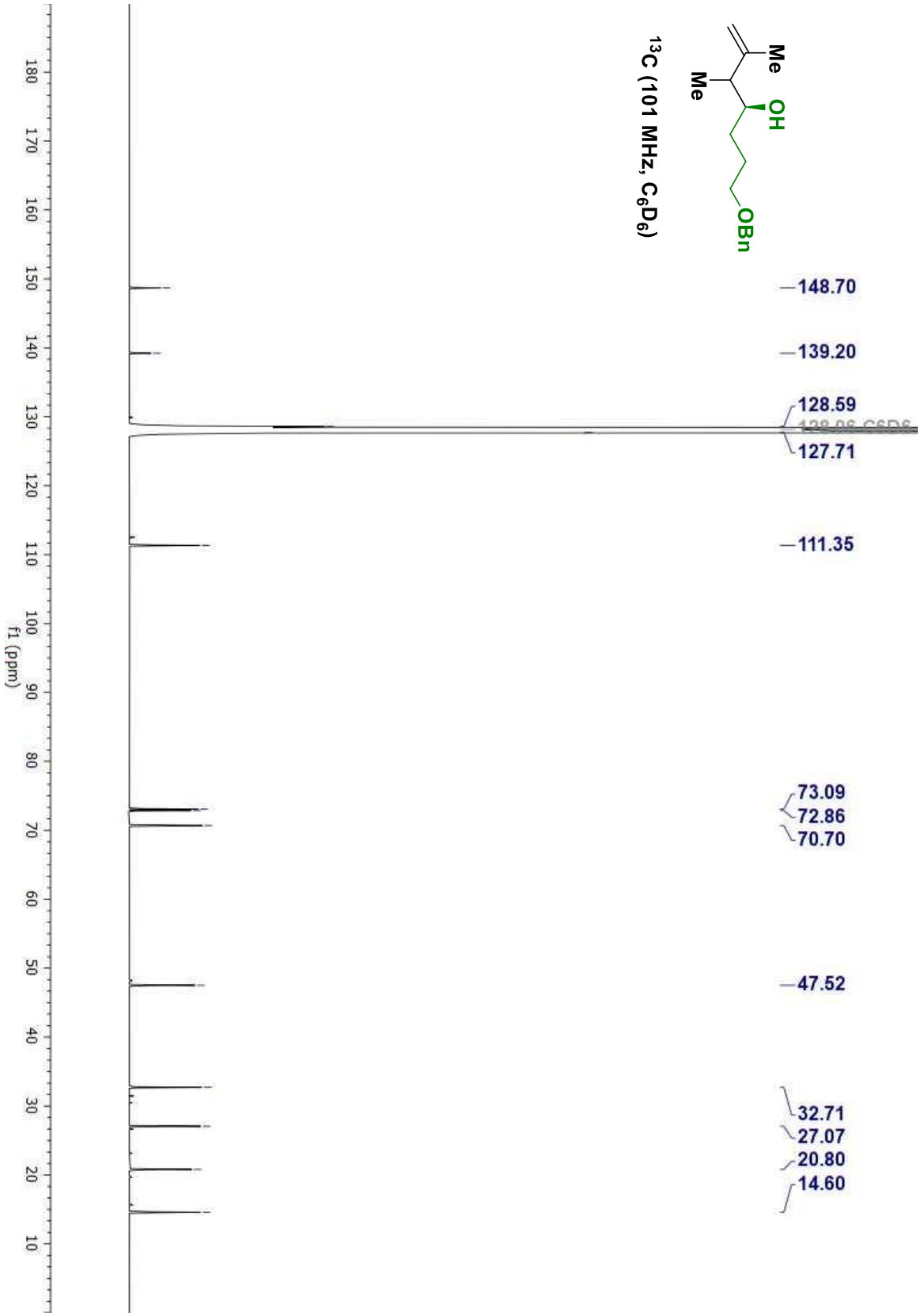
^{13}C NMR (101 MHz, C_6D_6): δ 148.7, 139.2, 128.6, 127.7, 111.4, 73.1, 72.9, 70.7, 47.5, 32.7, 27.1, 20.8, 14.6.

HRMS (Na+, *m/z*) for $C_{16}H_{24}O_2$: calcd. = 271.1669; found = 271.1673.

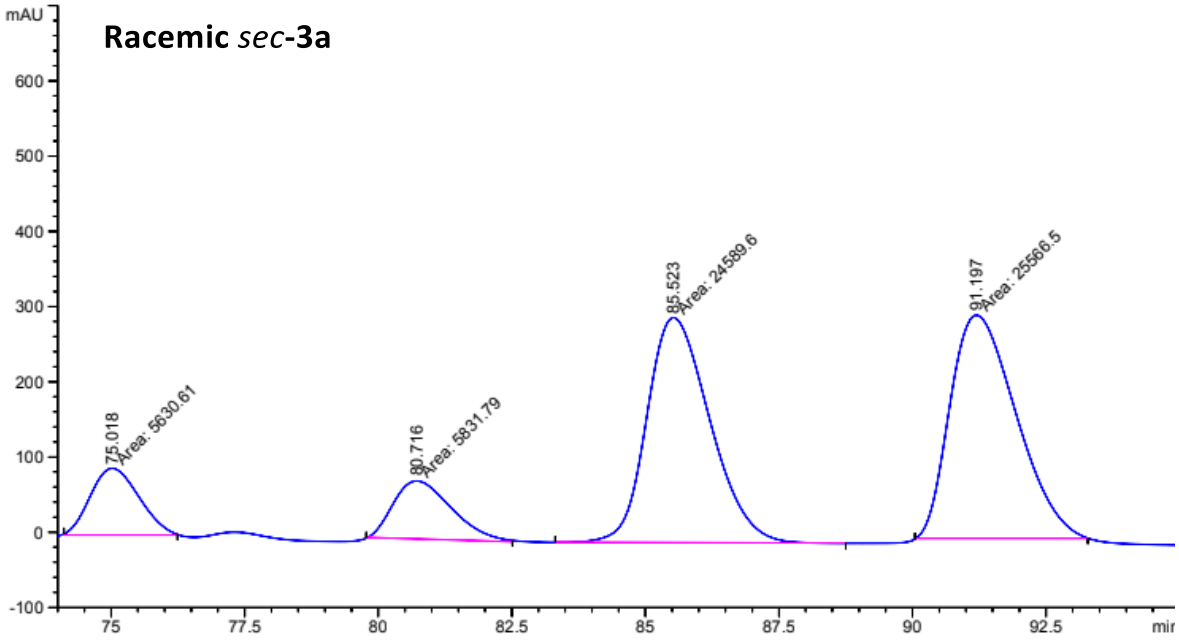
FTIR (neat): 3030, 2919, 2856, 1644, 1453, 1363, 1096, 966, 910, 734, 697 cm^{-1}.

HPLC: (Chiralcel columns Amylose 3-1 + Amylose 3-2, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm).


^{1}H (400 MHz, C_6D_6)
Me
Me
OH
OBn
7.30
7.30
7.29
7.28
7.28
7.28
7.27
7.19
7.19
7.19
7.19
7.17
7.16 C6D6
7.11
7.11
7.10
7.09
7.09
4.76
4.76
4.30
3.44
3.43
3.42
3.41
3.32
3.31
3.31
3.30
3.30
3.29
3.28
2.08
2.06
2.05
1.79
1.77
1.75
1.75
1.71
1.70
1.65
1.65
1.63
1.62
1.61
1.60
1.60
1.57
1.45
1.43
1.41
1.38
1.10
1.08
2.04
2.08
1.07
2.00
1.97
0.97
1.00
0.96
1.03
1.12
2.13
3.19
1.19
2.92
f1 (ppm)

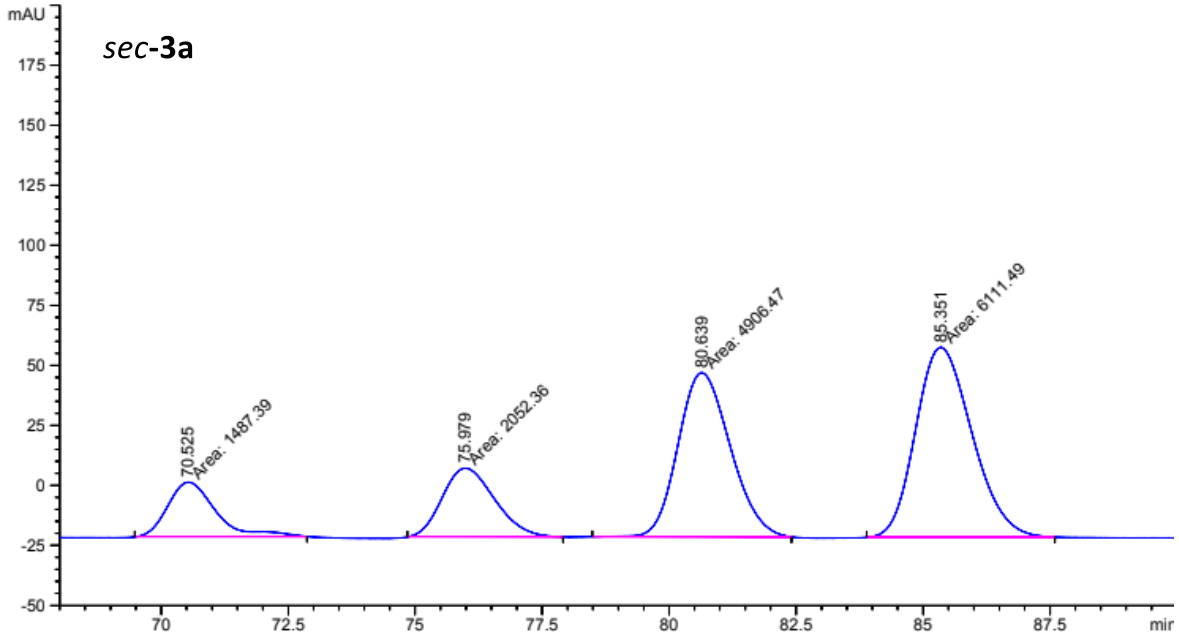

^{13}C (101 MHz, C_6D_6)
Me
Me
OH
OBn
148.70
139.20
128.59
127.71
111.35
73.09
72.86
70.70
47.52
32.71
27.07
20.80
14.60
f1 (ppm)

Racemic *sec*-3a



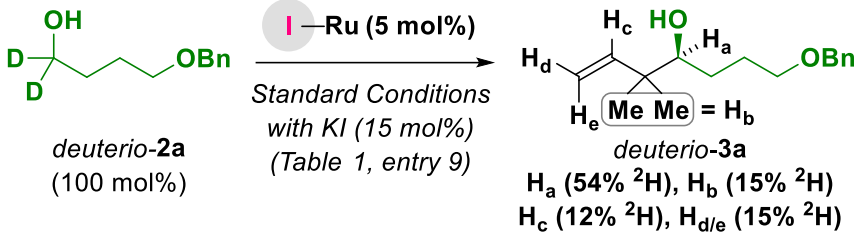
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	75.018	MM	1.0551	5630.60547	88.94267	9.1379
2	80.716	MM	1.2604	5831.79492	77.11305	9.4644
3	85.523	MM	1.3695	2.45896e4	299.26282	39.9062
4	91.197	MM	1.4345	2.55665e4	297.04886	41.4916

***sec*-3a**



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	70.525	MM	1.0953	1487.38940	22.63306	10.2172
2	75.979	MM	1.1953	2052.36035	28.61818	14.0981
3	80.639	MM	1.1954	4906.46826	68.40901	33.7036
4	85.351	MM	1.2882	6111.49170	79.06740	41.9811

Deuterium Labeling Studies

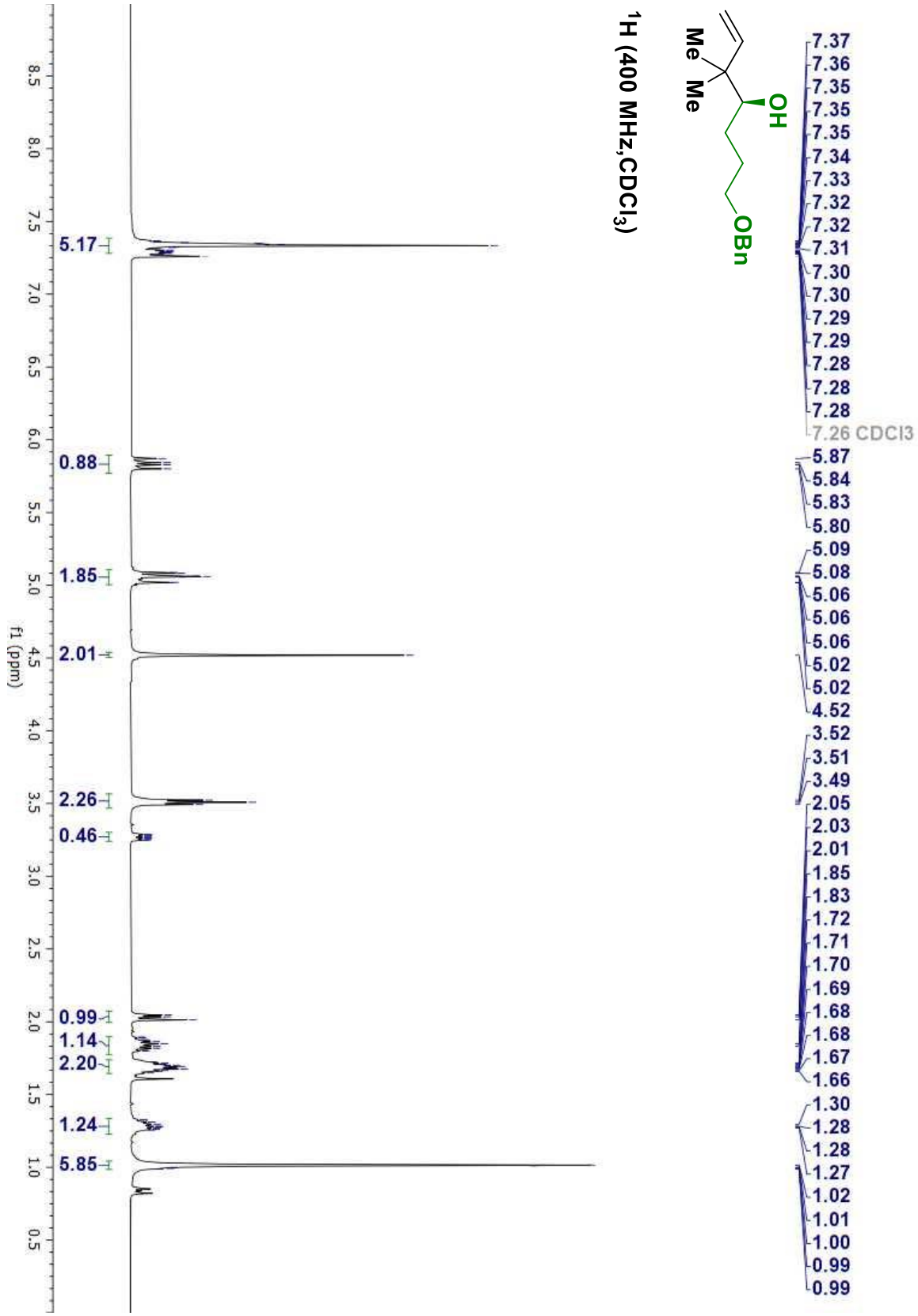


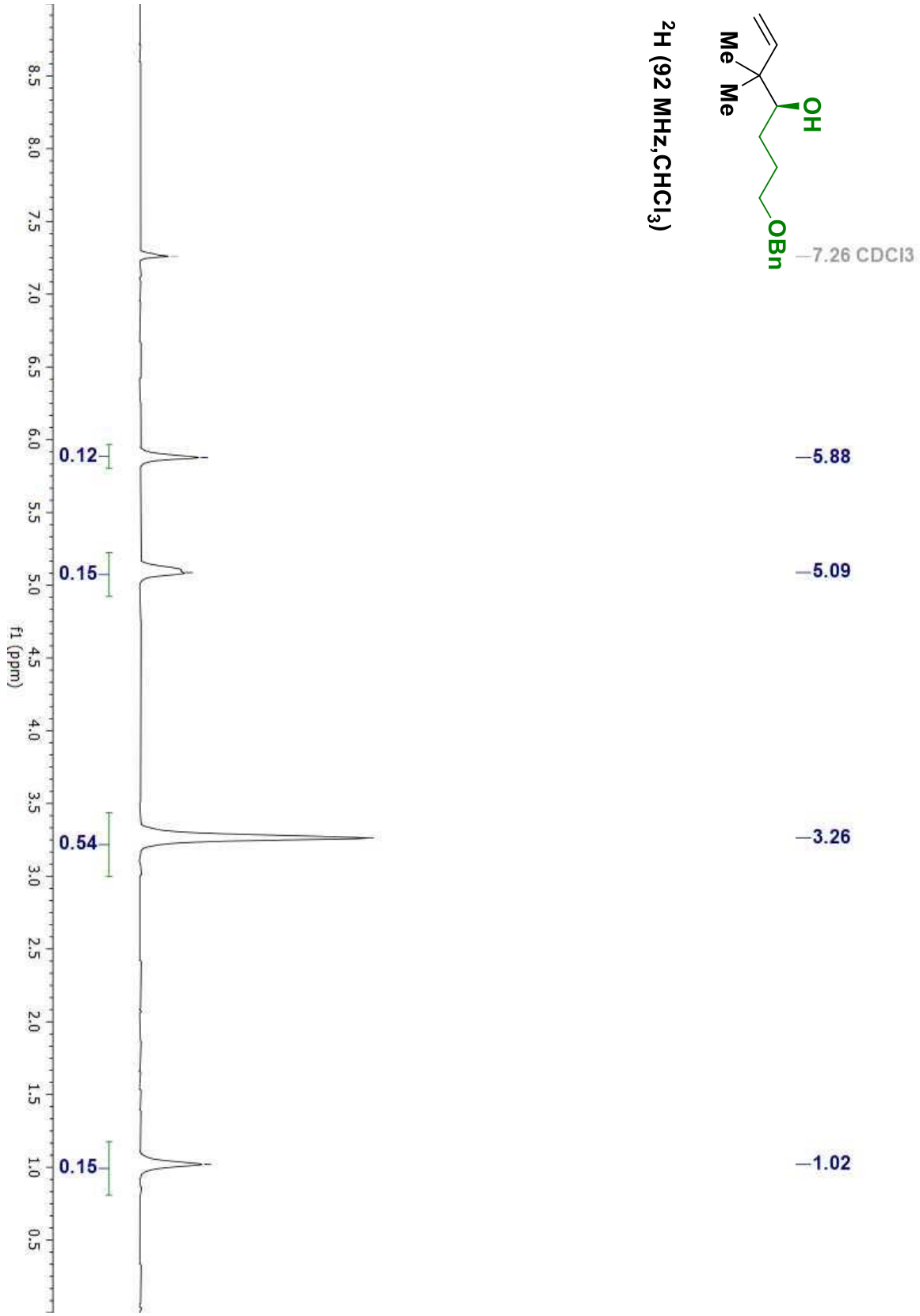
Alcohol *deuterio*-**2a** (36.5 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h). Flash column chromatography (SiO_2: 7:93 EtOAc:hexanes) provided the title compound *deuterio*-**3a** as a yellow oil in 36% yield (18.0 mg, 0.07 mmol).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.27 (m, 5H), 5.84 (dd, *J* = 17.5, 10.8 Hz, 0.88H), 5.10 – 4.99 (m, 1.85H), 4.52 (s, 2H), 3.51 (t, *J* = 6.0 Hz, 2H), 3.27 (ddd, *J* = 10.6, 4.6, 1.7 Hz, 0.46H), 2.07 – 1.99 (m, 1H), 1.92 – 1.78 (m, 1H), 1.69 (ddt, *J* = 12.5, 6.7, 2.6 Hz, 2H), 1.34 – 1.23 (m, 1H), 1.01 (s, 5.85H).

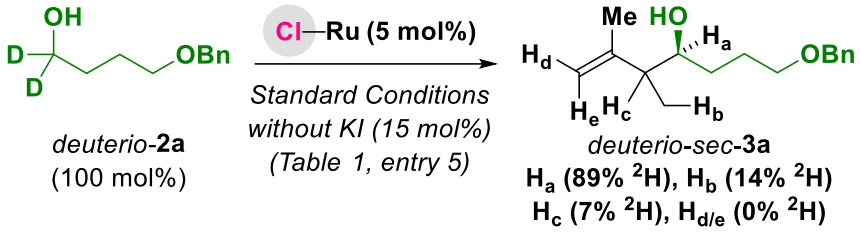
^{2}H NMR (92 MHz, $CHCl_3$): δ 5.88 (s, 0.12H), 5.09 (s, 0.15H), 3.26 (s, 0.54H), 1.02 (s, 0.15H).

HRMS (Na+, *m/z*) for $C_{16}H_{23}DO_2$: calcd. = 249.1832; found = 272.1741.
(Na+, *m/z*) for $C_{16}H_{22}D_2O_2$: calcd. = 250.1902; found = 273.1799.
(Na+, *m/z*) for $C_{16}H_{21}D_3O_2$: calcd. = 251.1965; found = 274.1859.
(Na+, *m/z*) for $C_{16}H_{20}D_4O_2$: calcd. = 252.2027; found = 275.1924.
(Na+, *m/z*) for $C_{16}H_{19}D_5O_2$: calcd. = 253.2090; found = 276.1981.


^{1}H (400 MHz,CDCl$_3$)
Me
Me
OH
OBn
7.37
7.36
7.35
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.28
7.26 CDCl3
5.87
5.84
5.83
5.80
5.09
5.08
5.06
5.06
5.06
5.02
5.02
4.52
3.52
3.51
3.49
2.05
2.03
2.01
1.85
1.83
1.72
1.71
1.70
1.69
1.68
1.68
1.67
1.66
1.30
1.28
1.28
1.27
1.02
1.01
1.00
0.99
0.99
5.17
0.88
1.85
2.01
2.26
0.46
0.99
1.14
2.20
1.24
5.85
f1 (ppm)


^{2}H (92 MHz,CHCl$_3$)
Me
Me
OH
OBn
7.26 CDCl3
5.88
5.09
3.26
1.02
0.12
0.15
0.54
0.15
f1 (ppm)

Deuterium Labeling Study

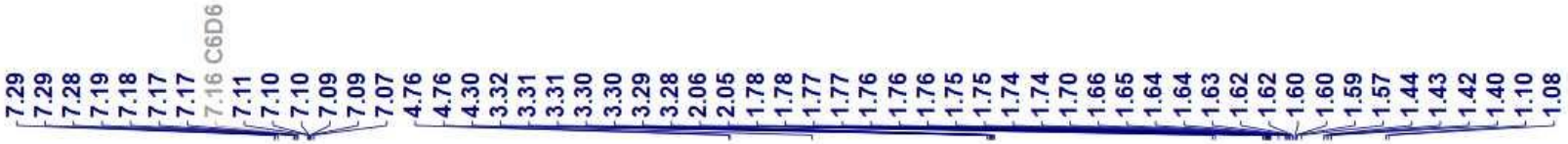


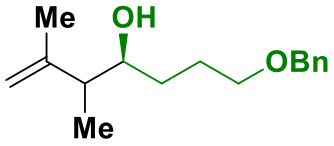
Alcohol *deuterio*-**2a** (36.5 mg, 0.2 mmol) was subjected to standard reaction conditions (115 °C, 48 h) without KI. Flash column chromatography (SiO_2: 7:93 EtOAc:hexanes) provided the title compound *deuterio-sec*-**3a** as a yellow oil in 50% yield (26.0 mg, 0.10 mmol).

^{1}H NMR (400 MHz, C_6D_6): 7.34 – 7.25 (m, 2H), 7.18 (d, *J* = 7.5 Hz, 2H), 7.12 – 7.06 (m, 1H), 4.76 (d, *J* = 1.5 Hz, 2H), 4.30 (s, 2H), 3.42 (m, *J* = 7.8 Hz, 0.11H), 3.31 (dd, *J* = 6.9, 4.4 Hz, 1H), 3.29 (dd, *J* = 6.9, 2.4 Hz, 1H), 2.06 (q, *J* = 6.9 Hz, 0.93H), 1.81 – 1.72 (m, 1H), 1.72 – 1.59 (m, 2H), 1.57 (s, 3H), 1.42 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.09 (d, *J* = 6.9 Hz, 2.86H).

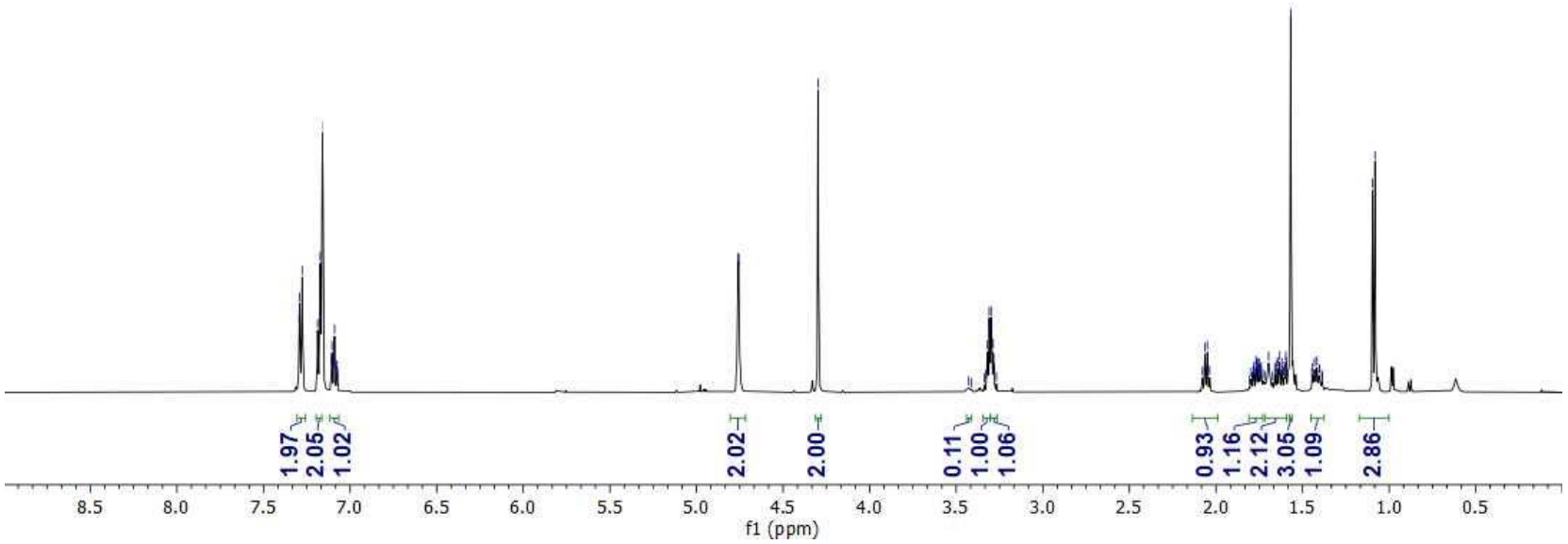
^{2}H NMR (92 MHz, C_6D_6): δ 5.88 (s, 0.12H), 5.09 (s, 0.15H), 3.26 (s, 0.54H), 1.02 (s, 0.15H).

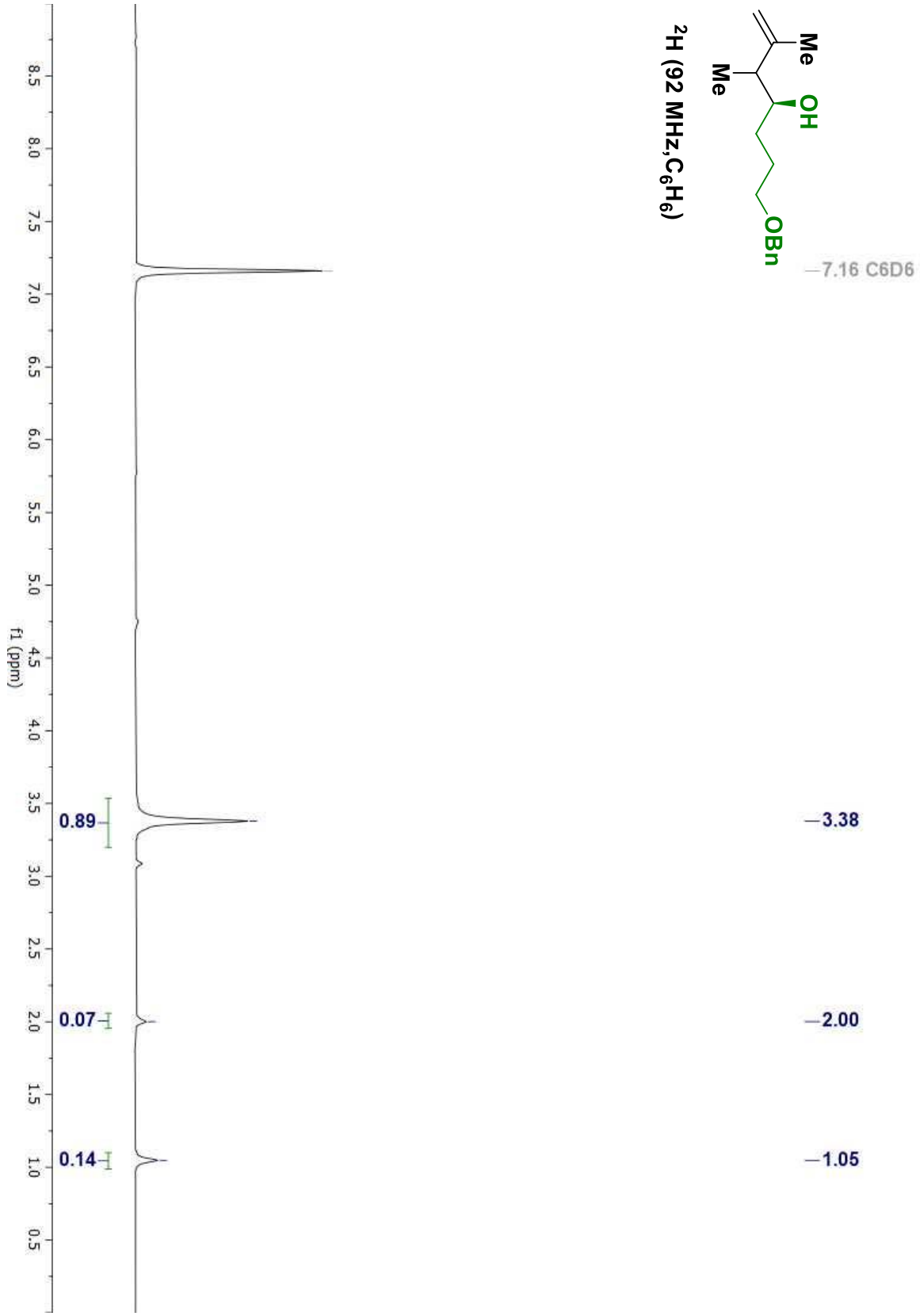
HRMS (Na+, *m/z*) for $C_{16}H_{23}DO_2$: calcd. = 249.1832; found = 272.1730.
(Na+, *m/z*) for $C_{16}H_{22}D_2O_2$: calcd. = 250.1902; found = 273.1782.
(Na+, *m/z*) for $C_{16}H_{21}D_3O_2$: calcd. = 251.1965; found = 274.1836.
(Na+, *m/z*) for $C_{16}H_{20}D_4O_2$: calcd. = 252.2027; found = 275.1869.
(Na+, *m/z*) for $C_{16}H_{19}D_5O_2$: calcd. = 253.2090; found = 276.1879.



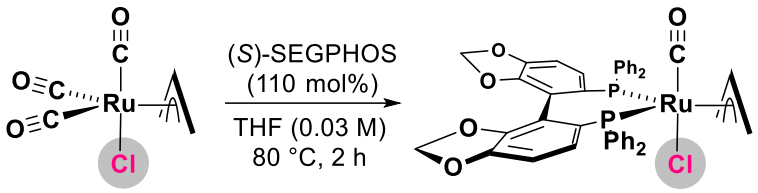


^{1}H (400 MHz,C_6D_6)




^{2}H (92 MHz,C_6H_6)
Me
OH
Me
OBn
7.16 C6D6
f1 (ppm)
0.89
0.07
0.14
3.38
2.00
1.05

Ruthenium Chloride Complex



$RuCl(CO)_3(\pi\text{-allyl})$
(100 mol%)

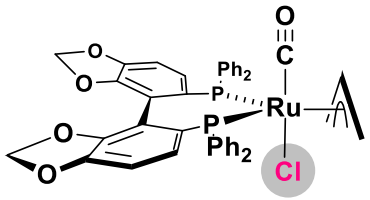
Ru-Cl complex

To a dried pressure tube equipped with a magnetic stir bar under an argon atmosphere charged with $RuCl(CO)_3(\pi$-allyl) complex (14 mg, 0.06 mmol) and (*S*)-SEGPHOS (37 mg, 0.06 mmol) was added THF (2 mL, 0.03 M). The pressure tube was backfilled with argon, sealed with a PTFE lined cap. The reaction vessel was placed in an oil bath at 80 °C and the reaction mixture was allowed to allowed to stir for 2 hours. The reaction vessel was removed from the oil bath and the reaction mixture was allowed to reach ambient temperature. The pressure tube was opened and the reaction mixture was transferred to a 10 mL round bottom flask with the aid of THF. The solution was triturated with hexanes (5 mL) and filtered through a Hirsch funnel to afford the Ru-Cl complex as an off-white solid in 85% yield (41.6 mg, 0.05 mmol).

$^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6): δ 33.3 (d, J = 4.1 Hz), 31.7 (d, J = 4.1 Hz).

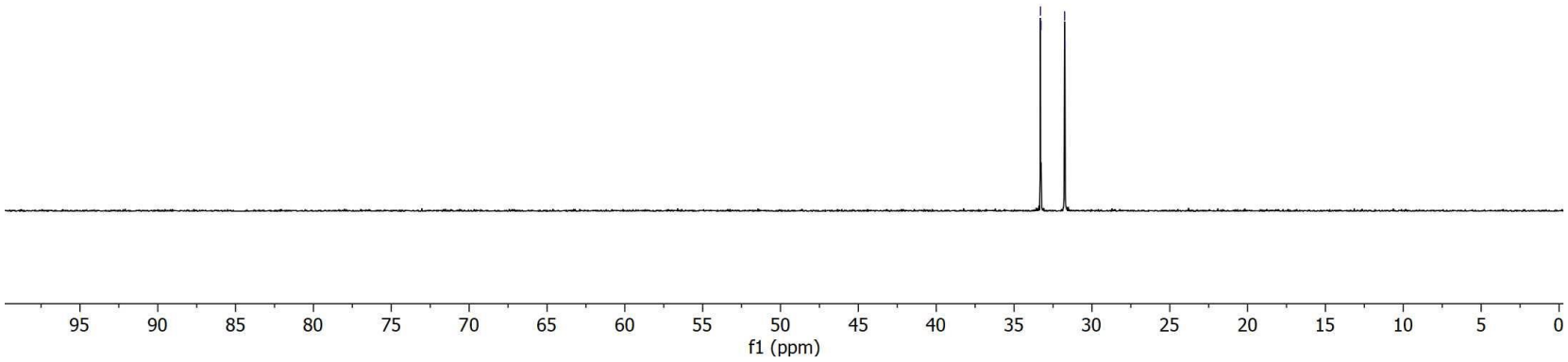
Solid State ^{31}P NMR (162 MHz, 12 kHz, 3.5 ms): δ 33.3 (broad), 26.7 (broad).

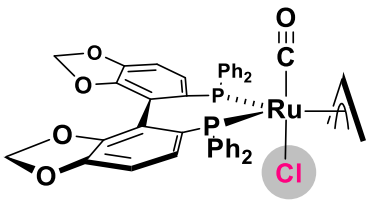
HRMS (Na+, *m/z*) for $C_{42}H_{33}ClO_5P_2Ru$: calcd. = 839.0436; found = 839.0458.



$^{31}P\{^{1}H\}$ NMR (202 MHz)

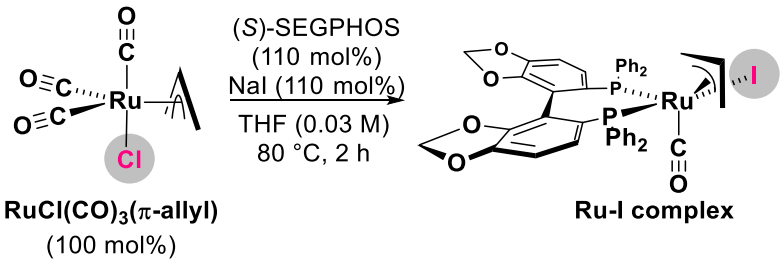
33.30
33.28
31.75
31.73





Solid State ^{31}P (162 MHz)

Ruthenium Iodide Complex

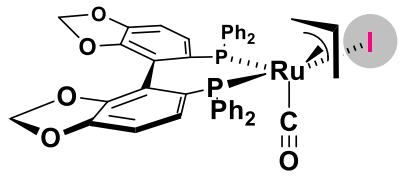


To a dried pressure tube equipped with a magnetic stir bar under an argon atmosphere charged with $RuCl(CO)_3(\pi\text{-allyl})$ complex (14 mg, 0.06 mmol), (*S*)-SEGPHOS (37 mg, 0.06 mmol), and NaI (9 mg, 0.06 mmol), was added THF (2 mL, 0.03 M). The pressure tube was backfilled with argon, sealed with a PTFE lined cap. The reaction vessel was placed in an oil bath at 80 °C and the reaction mixture was allowed to allowed to stir for 2 hours. The reaction vessel was removed from the oil bath and the reaction mixture was allowed to reach ambient temperature. The pressure tube was opened, and the reaction solution was transferred to a 10 mL round bottom flask with the aid of THF. The solution was triturated with hexanes (5 mL) and filtered through a Hirsch funnel to afford the Ru-I complex as a yellow solid in 82% Yield (44.8 mg, 0.05 mmol).

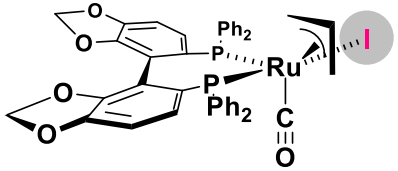
$^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6): δ 48.7 (d, J = 25.1 Hz), 32.7 (d, J = 25.2 Hz).

Solid State ^{31}P NMR (162 MHz, 12 kHz, 3.5 ms): δ 48.6 (broad), 32.0 (broad).

HRMS (K+, *m/z*) for $C_{42}H_{33}IO_5P_2Ru$: calcd. = 946.9534; found = 946.9544.

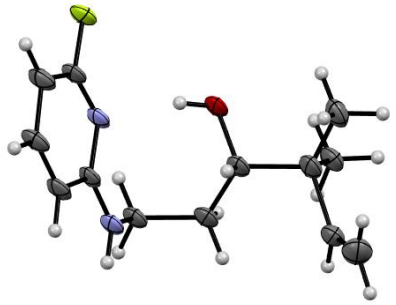


$^{31}P\{^{1}H\}$ NMR (202 MHz)



Solid State ^{31}P (162 MHz)

Single Crystal Diffraction Data for Coupling Product 3e



Crystals grew as clusters of colorless needles by vapor diffusion of n-pentane into a diethyl ether solution. The data crystal was cut from a longer crystal and had approximate dimensions; 0.28 x 0.081 x 0.075 mm. The data were collected on a Rigaku Oxford Diffraction HyPix6000E Synergy-S diffractometer using a μ-focus Cu Kα radiation source (λ = 1.54184Å) with collimating mirror monochromators. A total of 3612 frames of data were collected using ω-scans with a scan range of 0.5° and a counting time of 7 seconds per frame for frames collected with a detector offset of +/- 48.0° and 31 seconds per frame with frames collected with a detector offset of 104.5°. The data were collected at 100 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table S1. Data collection, unit cell refinement and data reduction were performed using Rigaku Oxford Diffraction's CrysAlisPro V 1.171.41.123a. The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares on F2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2018/3. Structure analysis was aided by use of the programs PLATON and OLEX2. The hydrogen atoms on the carbon atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom. The hydrogen atoms on O1 and N2 were observed in a ΔF map and refined with isotropic displacement parameters. A cylindrical void along 0,0,z contained highly disordered solvent molecules that could not be adequately modeled. The scattering due to these solvent molecules was accounted for using Bypass as utilized in OLEX2. The vinyl group atoms were disordered about two orientations with occupancies close to 50% each. The absolute structure was determined using the method of Flack and confirmed using the Hooft y-parameter method, which resulted in a Hooft y-parameter of -0.01(4).

Table S1. Crystal data and structure refinement for **3e**.

Empirical formula	C_{13} H_{19} F N_2 O	
Formula weight	238.30	
Temperature	100.0(5) K	
Wavelength	1.54184 Å	
Crystal system	hexagonal	
Space group	P 65	
Unit cell dimensions	a = 19.3391(6) Å	α= 90°.
	b = 19.3391(6) Å	β= 90°.
	c = 6.43042(13) Å	γ = 120°.
Volume	2082.76(13) $Å^3$	
Z	6	
Density (calculated)	1.140 g/m^3	
Absorption coefficient	0.671 mm^{-1}	
F(000)	768	
Crystal size	0.28 x 0.081 x 0.075 mm^3	
Theta range for data collection	2.638 to 76.224°	
Index ranges	-24<=h<=22, -24<=k<=17, -8<=l<=7	
Reflections collected	25998	
Independent reflections	2860 [R(int) = 0.0299]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.685	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2860 / 1 / 183	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0332, wR2 = 0.0948	
R indices (all data)	R1 = 0.0385, wR2 = 0.0981	
Absolute structure parameter	-0.02(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.149 and -0.115 $e.Å^{-3}$	

Figure S1. View of **3e** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level.

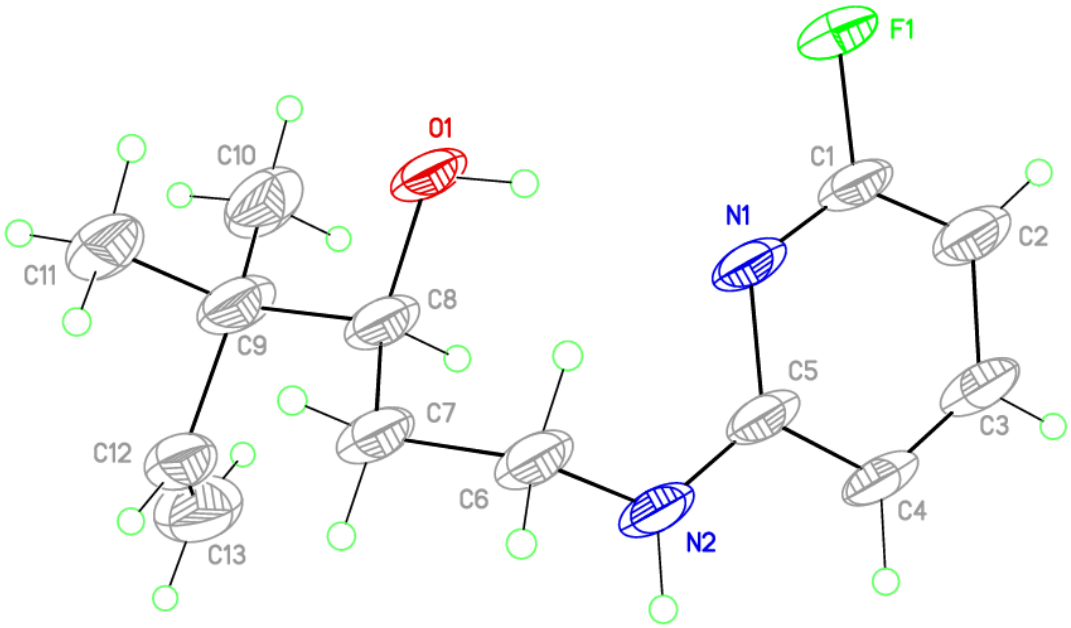
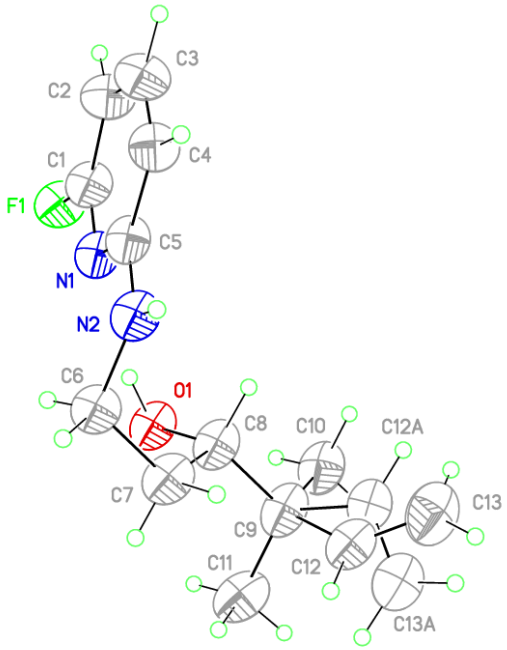
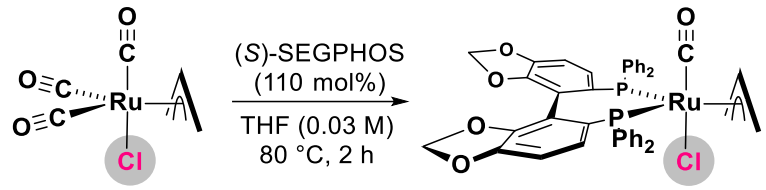


Figure S2. View of **3e** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. The lower occupancy C atoms of the disordered vinyl group are labeled C12A and C13A.



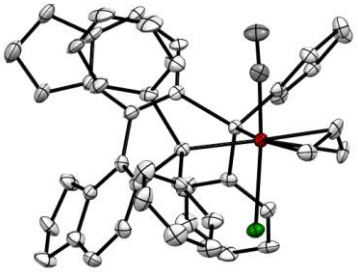
Single Crystal Diffraction Data for Ruthenium Complexes

Ruthenium Chloride Complex



$RuCl(CO)_3(\pi\text{-allyl})$
(100 mol%)

Ru-Cl complex

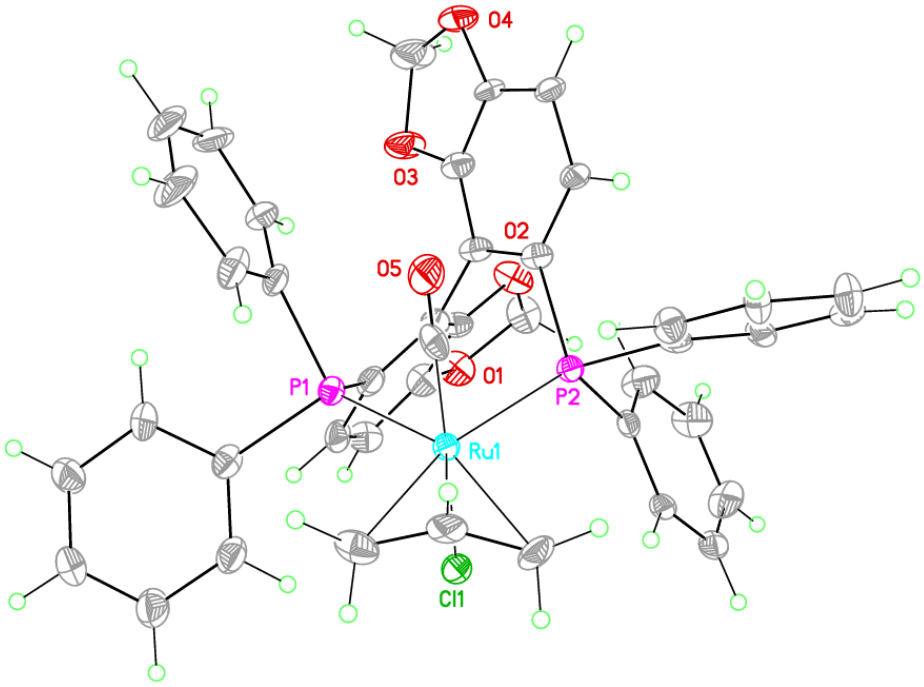


To a dried pressure tube equipped with a magnetic stir bar under an argon atmosphere, charged with $RuCl(CO)_3(\pi\text{-allyl})$ complex (14 mg, 0.06 mmol) and (*S*)-SEGPHOS (37 mg, 0.06 mmol), was added THF (2 mL, 0.03 M). The pressure tube was backfilled with argon and sealed with a PTFE lined cap and the reaction mixture was allowed to stir for 2 hours at 80 °C. The reaction mixture was directly subjected to an individual recrystallization apparatus under a bed of argon. Crystals grew as pale yellow needles by vapor diffusion of *n*-pentane into a THF solution. The data crystal was cut from a larger crystal and had approximate dimensions; 0.16 x 0.051 x 0.036 mm. The data were collected on an Agilent Technologies SuperNova Dual Source diffractometer using a μ-focus Cu Kα radiation source (λ = 1.5418Å) with collimating mirror monochromators. A total of 2962 frames of data were collected using ω-scans with a scan range of 0.5° and a counting time of 8 seconds per frame for frames collected with a detector offset of +/- 48.6° and 32 seconds per frame with frames collected with a detector offset of 107.8°. The data were collected at 100 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table S2. Data collection, unit cell refinement and data reduction were performed using Rigaku Oxford Diffraction's CrysAlisPro V 1.171.40.71a. The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2018/3. Structure analysis was aided by use of the programs PLATON and OLEX2. The hydrogen atoms on the carbon atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The absolute configuration was assigned knowing the configuration of the starting diphosphorus ligand and was corroborated using the method of Flack.

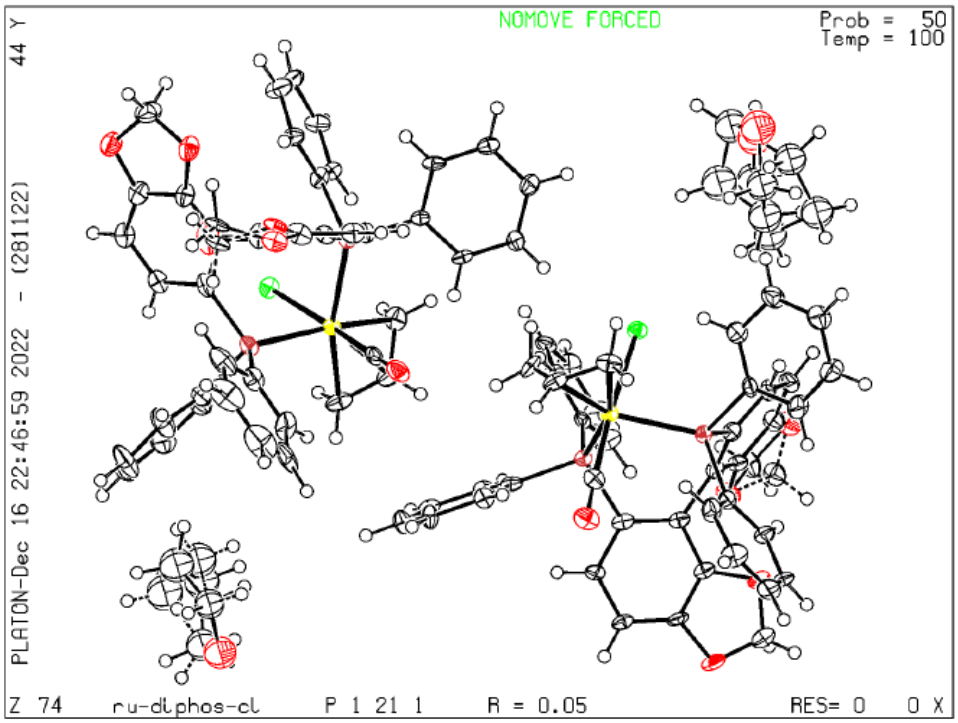
Table S2. Crystal data and structure refinement for **Ru-Cl** complex.

Empirical formula	$C_{46}\ H_{41}\ Cl\ O_6\ P_2\ Ru$	
Formula weight	888.25	
Temperature	100.0(3) K	
Wavelength	1.54184 Å	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 10.4482(2) Å	α= 90°.
	b = 36.6441(4) Å	β= 116.757(2)°.
	c = 11.5633(2) Å	γ = 90°.
Volume	3953.13(13) $Å^3$	
Z	4	
Density (calculated)	1.492 g/m^3	
Absorption coefficient	5.007 mm^{-1}	
F(000)	1824	
Crystal size	0.156 x 0.051 x 0.036 mm^3	
Theta range for data collection	2.411 to 77.036°	
Index ranges	-13<=h<=12, -45<=k<=37, -14<=l<=14	
Reflections collected	38582	
Independent reflections	10931 [R(int) = 0.0591]	
Completeness to theta = 67.684°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.61981	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10931 / 1045 / 1026	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1367	
R indices (all data)	R1 = 0.0543, wR2 = 0.1372	
Absolute structure parameter	0.083(9)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.433 and -1.318 $e.Å^{-3}$	

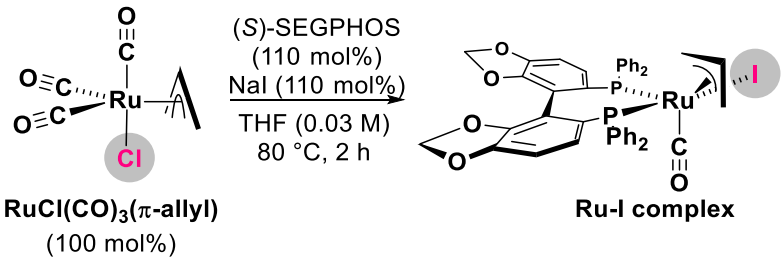
Figure S3. View of the Ru-Cl complex 1 in **1** showing the heteroatom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.



View of the Ru-Cl complex in Xtal3, showing two molecules of the complex in the asymmetric unit.

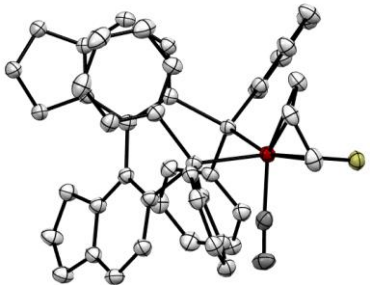


Ruthenium Iodide Complex



$RuCl(CO)_3(\pi$-allyl)
(100 mol%)

Ru-I complex

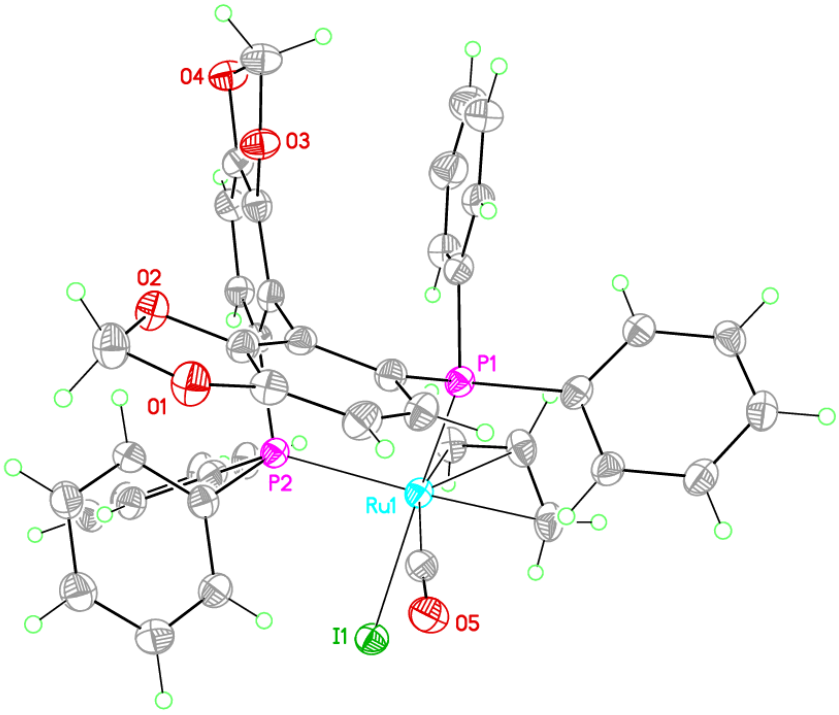


To a dried pressure tube equipped with a magnetic stir bar under an argon atmosphere, charged with $RuCl(CO)_3(\pi$-allyl) complex (14 mg, 0.06 mmol), (*S*)-SEGPHOS (37 mg, 0.06 mmol), and NaI (9 mg, 0.06 mmol), was added THF (2 mL, 0.03 M). The pressure tube was backfilled with argon and sealed with a PTFE lined cap and the reaction mixture was allowed to stir for 2 hours at 80 °C. The reaction mixture was directly subjected to an individual recrystallization apparatus under a bed of argon. Crystals grew as long yellow needles by vapor diffusion of *n*-pentane into a THF solution. The data crystal was cut from a longer crystal and had approximate dimensions; 0.20 x 0.13 x 0.11 mm. The data were collected on a Rigaku Oxford Diffraction HyPix6000E Synergy-S diffractometer using a μ-focus Cu Kα radiation source (λ = 1.54184Å) with collimating mirror monochromators. A total of 2173 frames of data were collected using ω-scans with a scan range of 0.5° and a counting time of 2 seconds per frame for frames collected with a detector offset of +/- 48.3° and 9 seconds per frame with frames collected with a detector offset of -106.0 and 110.1°. The data were collected at 100 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table S3. Data collection, unit cell refinement and data reduction were performed using Rigaku Oxford Diffraction's CrysAlisPro V 1.171.42.25a. The structure was solved by direct methods using SHELXT and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2018/3. Structure analysis was aided by use of the programs PLATON and OLEX2. The hydrogen atoms on the carbon atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom. The absolute structure was determined using the method of Flack and confirmed using the Hooft y-parameter method, which resulted in a Hooft y-parameter of -0.012(1).

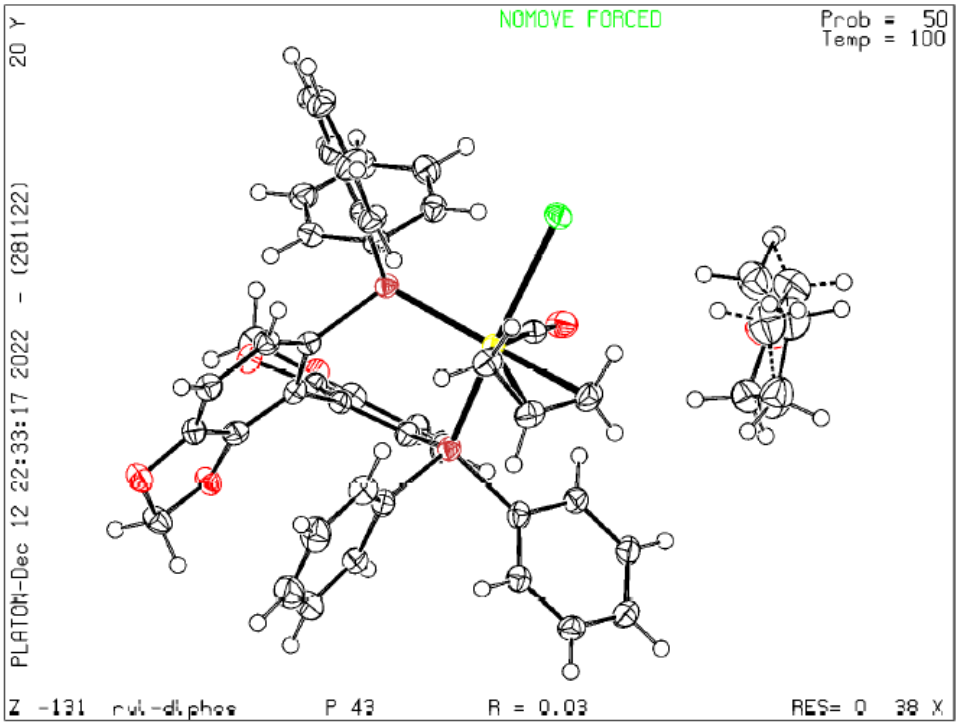
Table S3. Crystal data and structure refinement for **Ru-I** complex.

Empirical formula	$C_{46}\ H_{41}\ I\ O_6\ P_2\ Ru$	
Formula weight	979.70	
Temperature	100.0(1) K	
Wavelength	1.54184 Å	
Crystal system	tetragonal	
Space group	P 43	
Unit cell dimensions	a = 17.94215(7) Å	α= 90°.
	b = 17.94215(7) Å	β= 90°.
	c = 12.33385(8) Å	γ = 90°.
Volume	3970.52(4) $Å^3$	
Z	4	
Density (calculated)	1.639 g/m^3	
Absorption coefficient	10.472 mm^{-1}	
F(000)	1968	
Crystal size	0.201 x 0.129 x 0.109 mm^3	
Theta range for data collection	2.463 to 79.016°	
Index ranges	-19<=h<=22, -22<=k<=22, -15<=l<=15	
Reflections collected	29899	
Independent reflections	8172 [R(int) = 0.0344]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.544 and 0.262	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8172 / 66 / 540	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0251, wR2 = 0.0681	
R indices (all data)	R1 = 0.0251, wR2 = 0.0682	
Absolute structure parameter	-0.003(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.582 and -0.491 $e.Å^{-3}$	

Figure S4. View of the Ru-I complex 1 in **1** showing the heteroatom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.



View of the Ru-I complex in Xtal3, showing a single molecule in the asymmetric unit.



DFT Calculations.

DFT calculations were conducted using the *Gaussian16*[6] program package. Geometry optimization and analytical vibrational frequency analysis were performed via the restricted Kohn-Sham DFT using the long-range corrected (LC) hybrid density functional with empirical dispersion corrections (ωB97X-D).[7] Pople's 6-311G(d,p) basis set for C, H, O, P and I atoms[8,9] and the SDD with the effective core potential for the Ru atom[10] were used for the Gaussian basis functions (5d type polarization functions). The solvent effect of THF were estimated by the polarizable continuum model with integral equation formalism (IEF-PCM)[11] for the gas-phase optimized structures. For the IEF-PCM calculations, the Def2-TZVPP basis set[12] was used for basis functions (ωB97X-D(PCM)/Def2-TZVPP//ωB97X-D/(SDD, 6-311G(d,p))). The Gibbs free energy at 393 K was estimated by the PCM total energy and the gas-phase thermal free energy term.

Structures of iodide-bound π-allyl complex [RuI(CO)(η^3-C_3H_5)((*S*)-SEGPHOS)], **K**–**N**, and chloride-bound π-allyl complex [RuCl(CO)(η^3-C_3H_5)((*S*)-SEGPHOS)], **K'**–**N'**, are shown in Figures S5. The corresponding iodide-bound π-prenyl complex [RuI(CO)(η^3-$CH_2CHC(CH_3)_2$)((*S*)-SEGPHOS)], **B** and **O**–**U**, and chloride-bound π-prenyl complex [RuCl(CO)(η^3-$CH_2CHC(CH_3)_2$)((*S*)-SEGPHOS)], **B'** and **O'**–**U'**, are shown Figures S6.

For the six-membered cyclic transition state structures for the attack of π-prenyl ligand by acetaldehyde, 36 structures were examined (Figure S7). Among these structures, which include both *cis*- and *trans*-p-allyl species, two transition state structures from the lowest energy structure are **TS2B** and **TS1B**. In these *cis*- p-allyl species, the hydrogen atom in aldehyde is directed to the iodide ligand (the distances between the hydrogen atom and the iodide atom are 2.99 and 2.93 Å in **TS2B**, and **TS1B**, respectively), as suggested by our previous study.[13] The reaction pathways via **TS1B** (*tert*-prenylation pathway) and via **TS2B** (*sec*-prenylation pathway) are shown in Figure 4. Structures are shown in Figures S8 and S9.

Table S4. Total Electronic Energy (*E*) and Gibbs Free Energy (*G*) in THF at 333K (au)

	E (ωB97X-D/(SDD, 6-311G (d,p)))	*thermal free term (393K)*	*E* (ωB97X-D(PCM)/Def2-TZVPP//ωB97X-D/(SDD, 6-311G(d,p)))	*G*
K	−9693.709404	0.529931	−3072.136118	−3071.606187
L	−9693.700638	0.530859	−3072.125888	−3071.595029
M	−9693.702402	0.528228	−3072.127615	−3071.599387
N	−9693.701186	0.528977	−3072.125591	−3071.596614
K′	−3234.233118	0.532118	−3234.557126	−3234.025008
L′	−3234.223762	0.532857	−3234.546447	−3234.013590
M′	−3234.233691	0.529312	−3234.554793	−3234.025481
N′	−3234.231120	0.529854	−3234.551784	−3234.021930
B	−9772.322854	0.580106	−3150.757744	−3150.177638
O	−9772.324121	0.581442	−3150.758027	−3150.176585
P	−9772.318517	0.582837	−3150.750196	−3150.167359
Q	−9772.325545	0.580450	−3150.760873	−3150.180423
R	−9772.328684	0.581862	−3150.760104	−3150.178242
S	−9772.325528	0.580230	−3150.757537	−3150.177307
T	−9772.326736	0.580674	−3150.757485	−3150.176811
U	−9772.321964	0.581304	−3150.753675	−3150.172371
B′	−3312.846693	0.582890	−3313.179090	−3312.596200
O′	−3312.849828	0.583570	−3313.180704	−3312.597134
P′	−3312.843786	0.585989	−3313.172582	−3312.586593
Q′	−3312.850478	0.580966	−3313.182481	−3312.601515
R′	−3312.860454	0.584850	−3313.187682	−3312.602832
S′	−3312.858644	0.584457	−3313.186392	−3312.601935
T′	−3312.858608	0.583325	−3313.185546	−3312.602221
U′	−3312.857280	0.585118	−3313.183682	−3312.598564
A	−9576.973176	0.463931	−2955.393363	−2954.929432
isoprene	−195.290464	0.073830	−195.318009	−195.244179
ethanal	−153.820932	0.021003	−153.848911	−153.827908
C	−9926.149153	0.622470	−3304.606067	−3303.983597
TS1A	−9926.144318	0.626132	−3304.601059	−3303.974927
D	−9926.164489	0.629264	−3304.618039	−3303.988775
TS1B	−9926.157885	0.632595	−3304.610019	−3303.977424
E	−9926.186506	0.638511	−3304.637560	−3303.999049
F	−9772.312489	0.580933	−3150.744663	−3150.163730
G	−9772.306923	0.575815	−3150.743299	−3150.167484
H	−9926.140784	0.623752	−3304.599414	−3303.975662
TS2A	−9926.140269	0.625967	−3304.597523	−3303.971556
I	−9926.163395	0.629812	−3304.616177	−3303.986365

TS2B	−9926.160079	0.633091	−3304.611816	−3303.978725
J	−9926.185046	0.636295	−3304.636991	−3304.000696

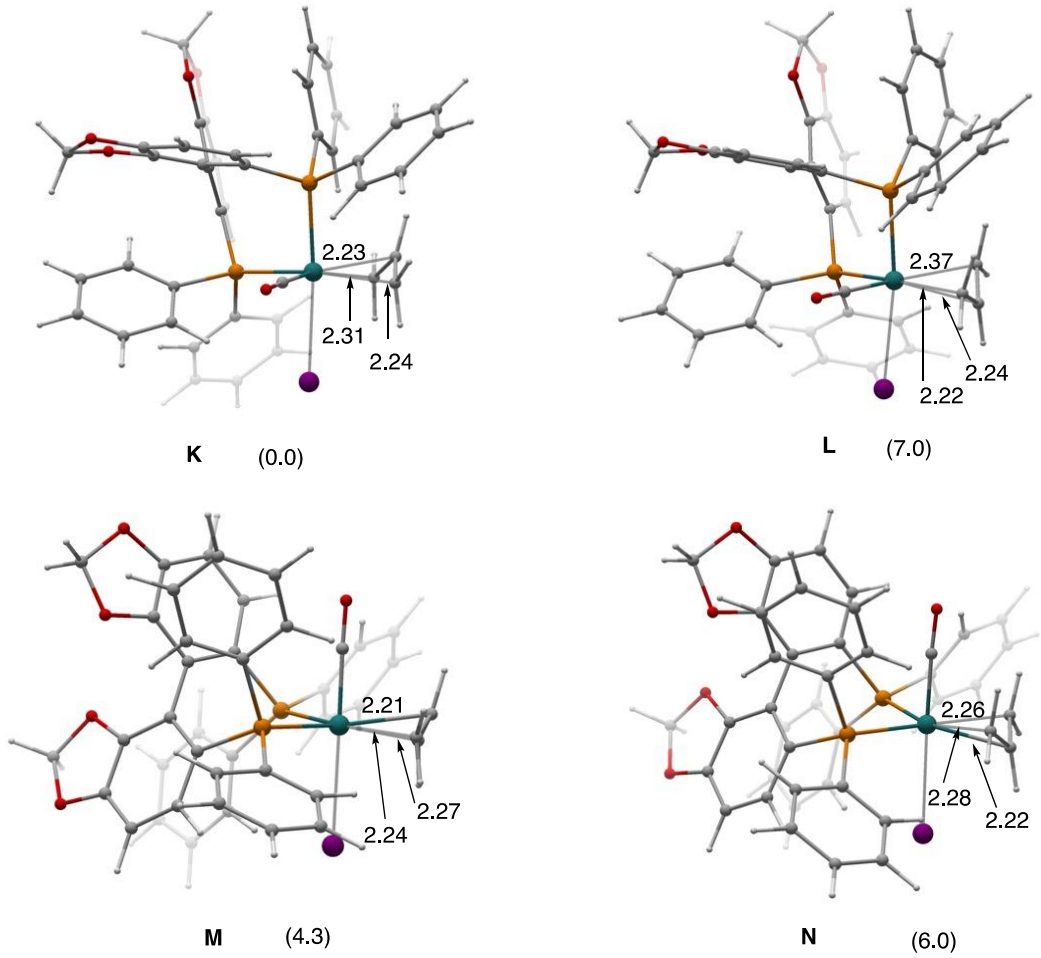


Figure S5. Structures of iodide-bound π-allyl complex [RuI(CO)(η^3-C_3H_5)((*S*)-SEGPHOS)], **K**–**N**, and chloride-bound π-allyl complex [RuCl(CO)(η^3-C_3H_5)((*S*)-SEGPHOS)], **K'**–**N'**. The bond lengths are given in Å. The relative Gibbs free energies at 393 K are given in parentheses (kcal/mol).

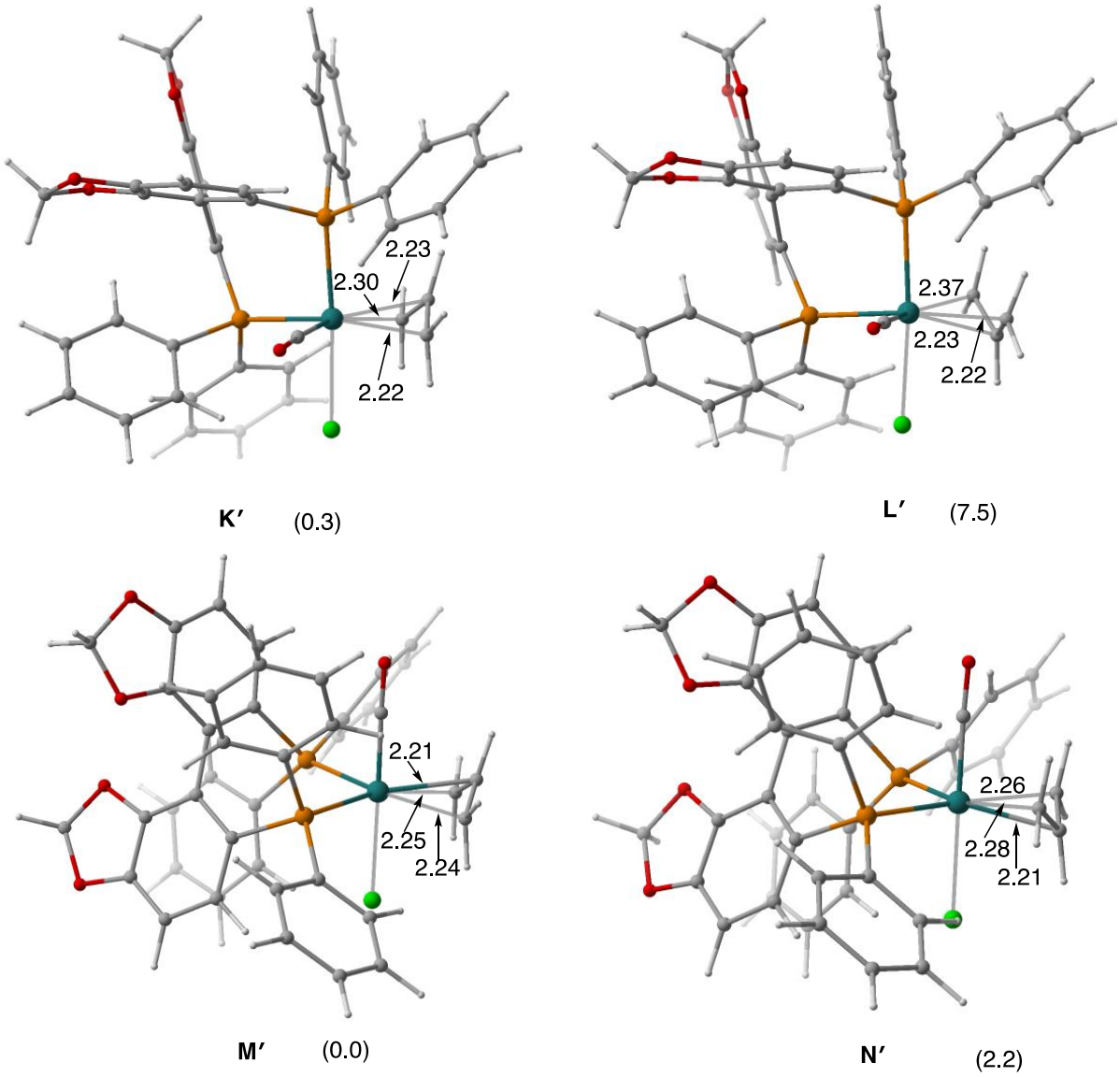


Figure S5. *(Continued.)*

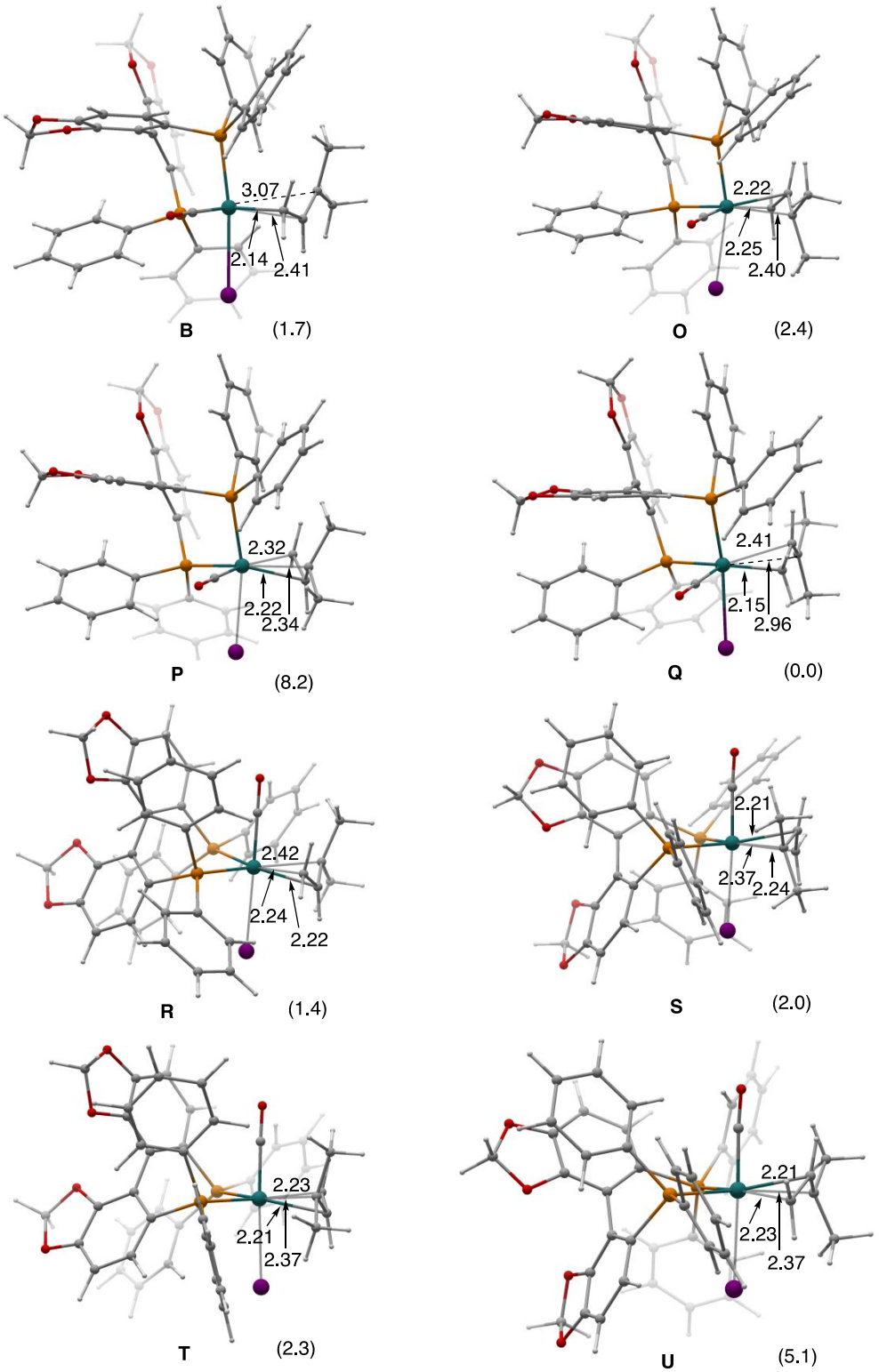


Figure S6. Structures of iodide-bound π-prenyl complex [RuI(CO)(η^3-$CH_2CHC(CH_3)_2$)((*S*)-SEGPHOS)], **B** and **O**–**U**, and of chloride-bound π-prenyl complex [RuCl(CO)(η^3-$CH_2CHC(CH_3)_2$)((*S*)-SEGPHOS)], **B'** and **O'**–**U'**. The bond lengths are given in Å. The relative Gibbs free energies at 393 K are given in parentheses (kcal/mol).

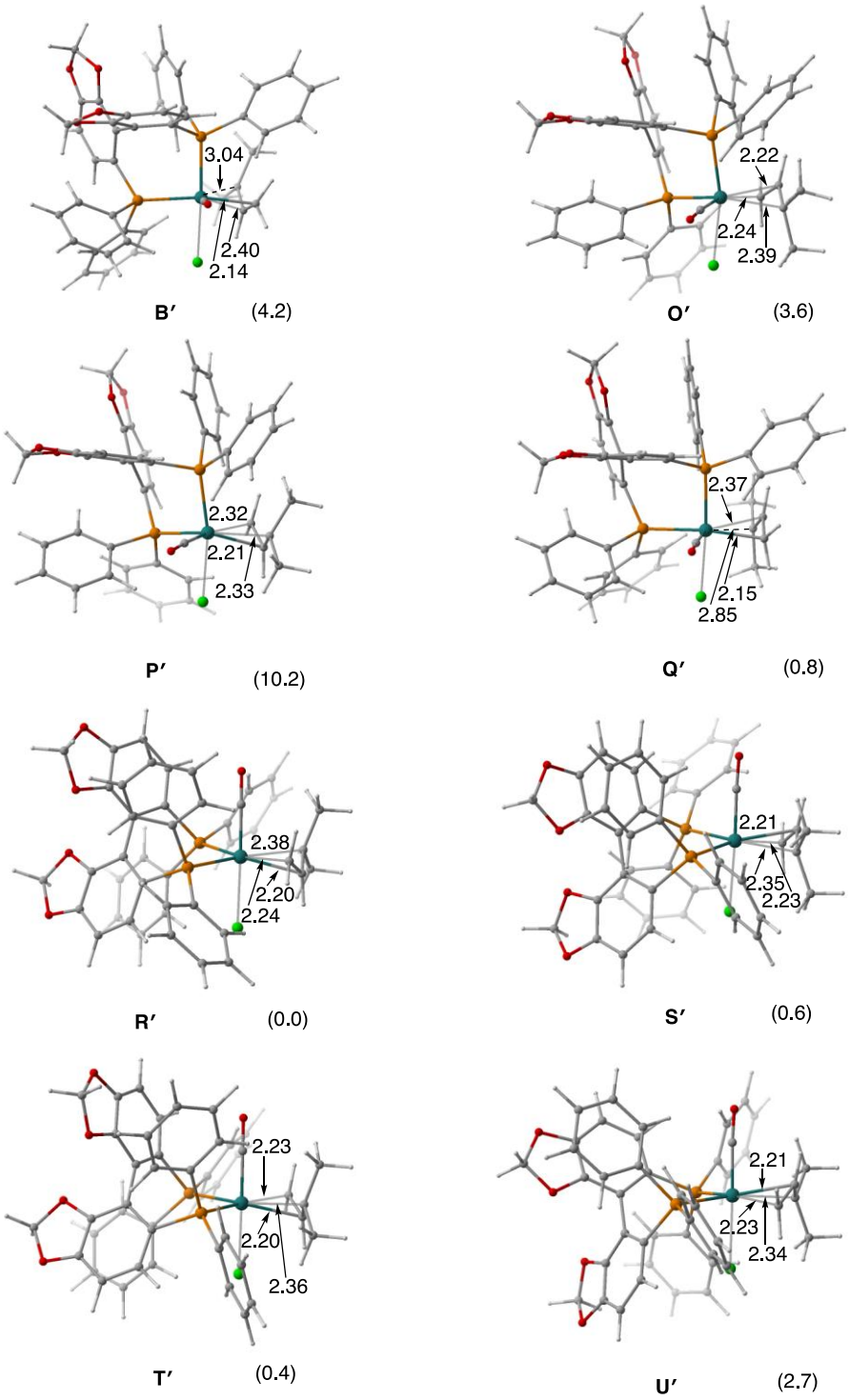


Figure S6. (*Continued.*)

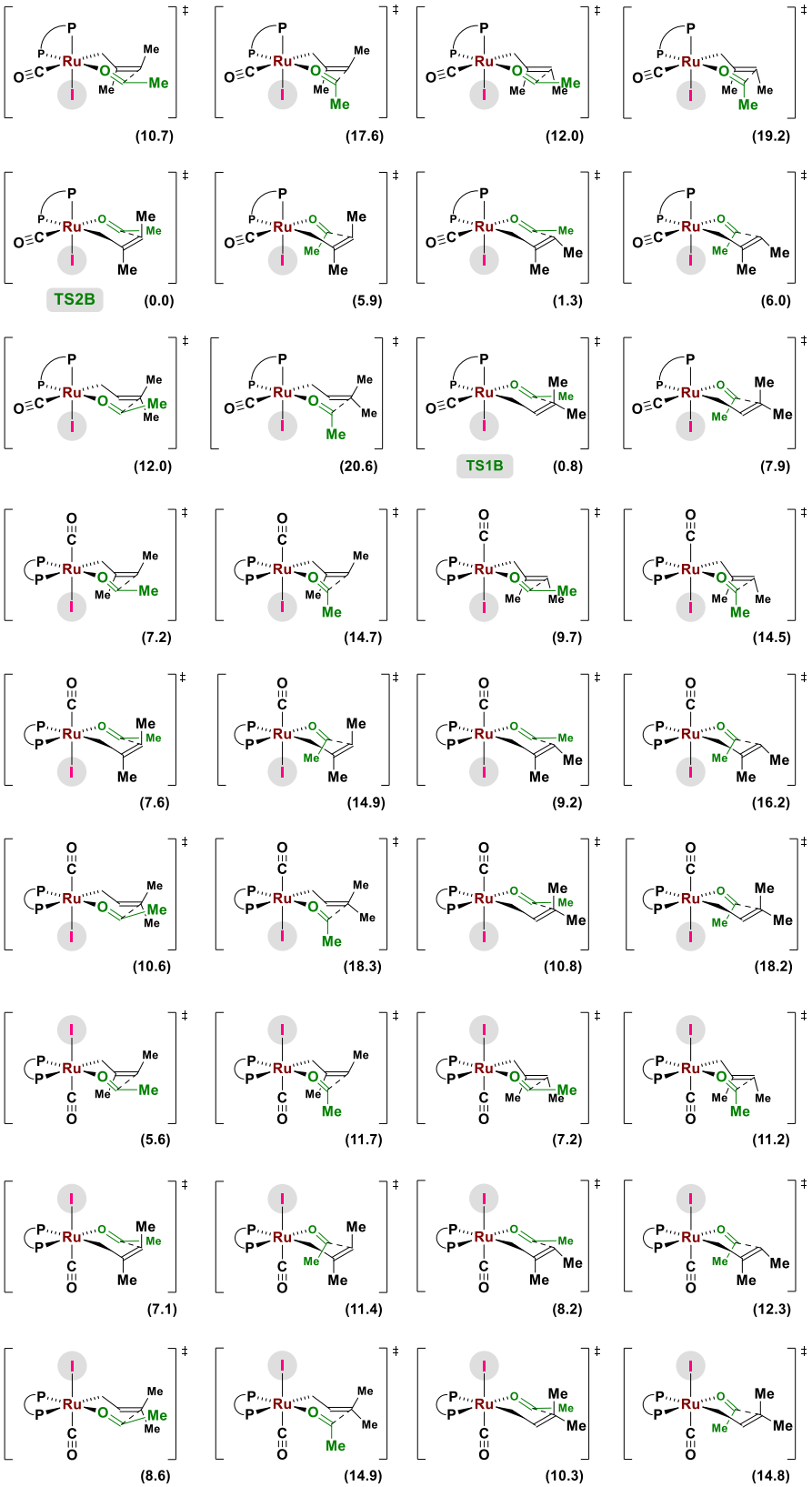


Figure S7. Examined transition structures. The relative Gibbs free energies at 393 K are given in parentheses (kcal/mol).

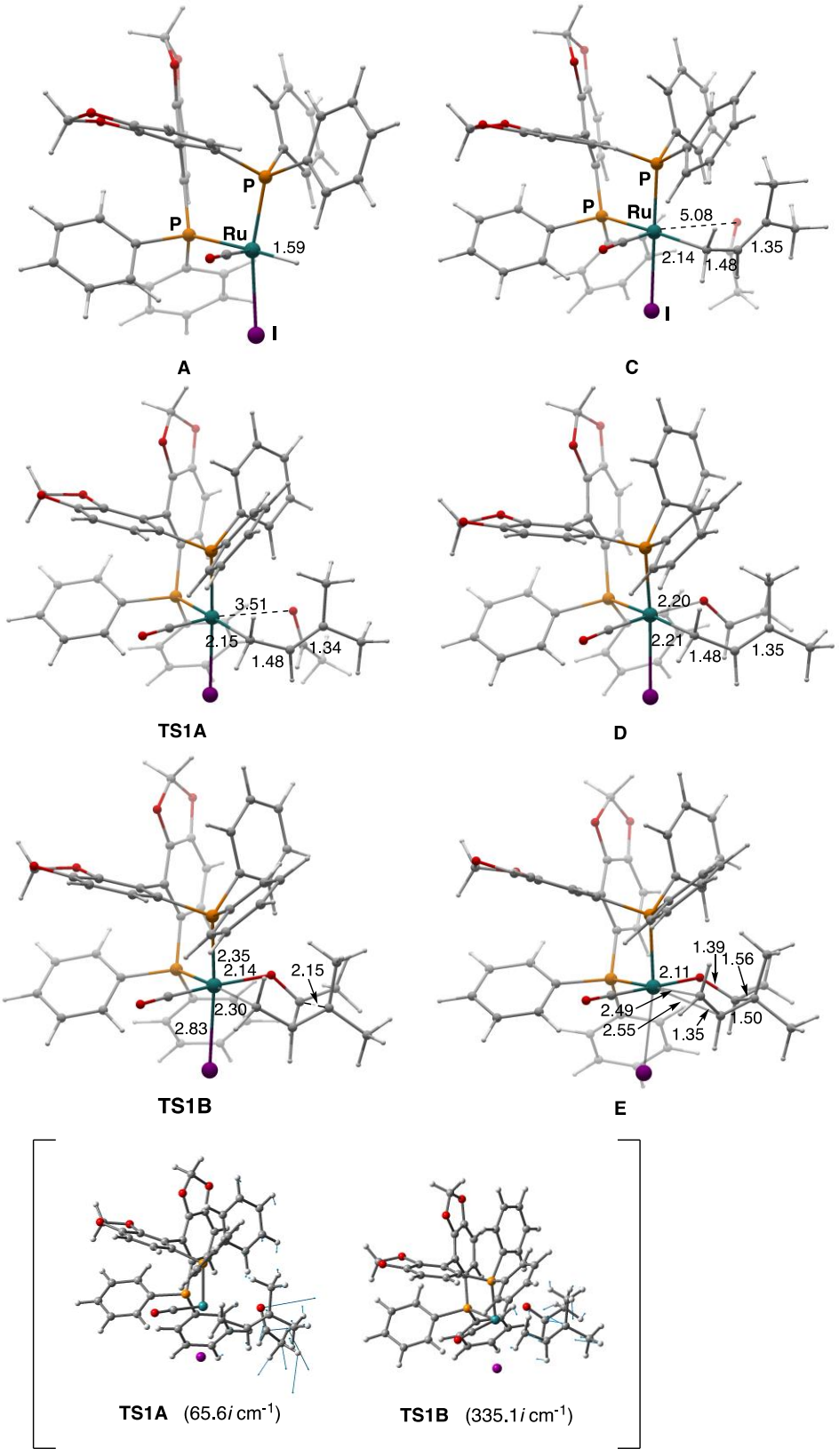


Figure S8. Structures along the *tert*-prenylation pathway. The bond lengths are given in Å.

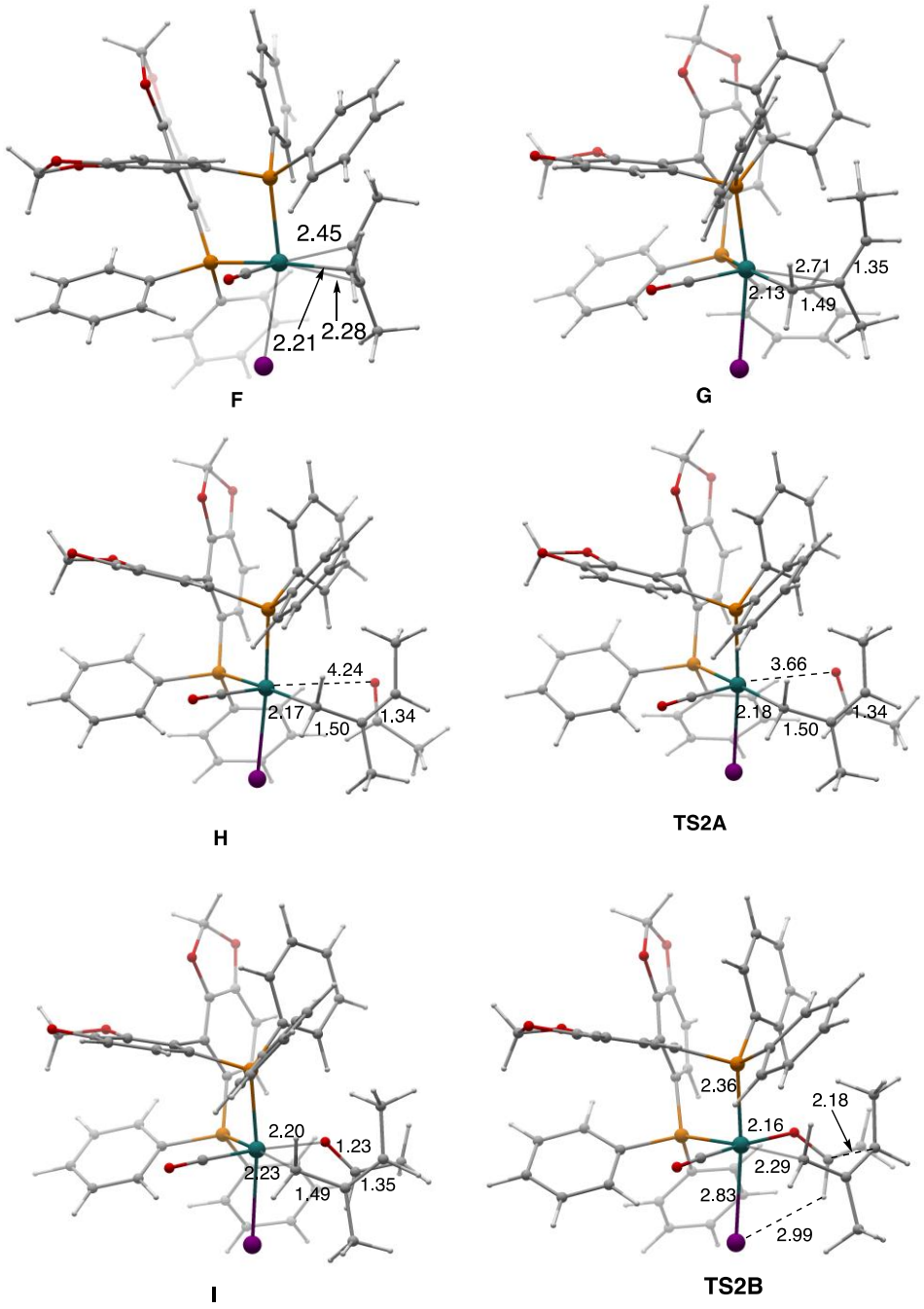
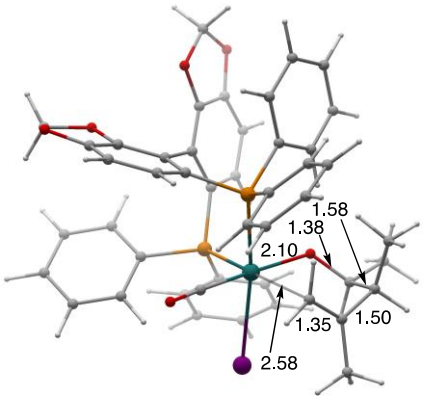
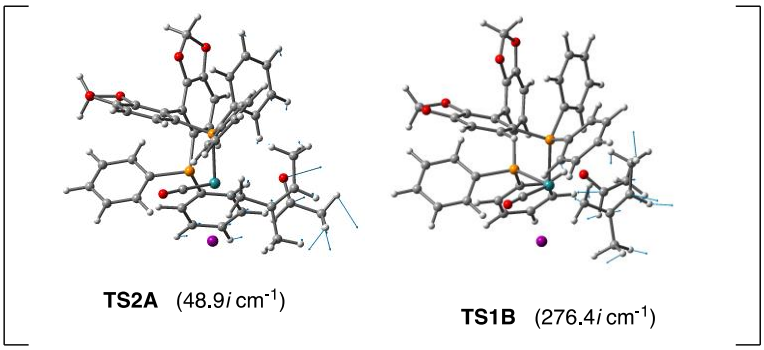


Figure S9. Structures along the *sec*-prenylation pathway. The bond lengths are given in Å.



J



TS2A (48.9*i* cm^{-1})

TS1B (276.4*i* cm^{-1})

Figure S9. (*Continued*).

Cartesian coordinates of stationary points at the ωB97X-D/(SDD, 6-311G(d,p)) level of theory are given below:

K (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.188194	1.383254	-0.075258
2	53	0	4.001460	1.134959	0.278430
3	15	0	-1.127827	1.560740	0.004784
4	15	0	1.142028	-0.999915	-0.320110
5	8	0	-2.941010	-2.403711	4.022934
6	8	0	-2.405287	-3.155566	1.926597
7	8	0	-4.029435	-1.997234	-0.614917
8	8	0	-3.954106	-2.908027	-2.726959
9	8	0	1.199946	1.567203	2.937307
10	6	0	-1.819267	0.416552	1.266407
11	6	0	-2.188036	0.861282	2.529161
12	1	0	-2.184218	1.919266	2.748891
13	6	0	-2.576308	-0.015373	3.549623
14	1	0	-2.862525	0.344363	4.528685
15	6	0	-2.576292	-1.349747	3.244857
16	6	0	-2.563664	-3.557567	3.280413
17	1	0	-3.353516	-4.304412	3.345295
18	1	0	-1.606089	-3.934723	3.659576
19	6	0	-2.239138	-1.804394	1.977108
20	6	0	-1.847205	-0.969300	0.957528
21	6	0	-1.631717	-1.551962	-0.396794
22	6	0	-2.742151	-2.030782	-1.053241
23	6	0	-4.811984	-2.611617	-1.629406
24	1	0	-5.243175	-3.540447	-1.242961
25	1	0	-5.588142	-1.916312	-1.957344
26	6	0	-2.697473	-2.584024	-2.322344
27	6	0	-1.513199	-2.727238	-2.993446
28	1	0	-1.468197	-3.168547	-3.980178
29	6	0	-0.362044	-2.268961	-2.340674
30	1	0	0.586549	-2.387355	-2.845564
31	6	0	-0.395819	-1.681625	-1.080565
32	6	0	1.185137	1.446525	1.796704
33	6	0	1.676135	2.028717	-2.240949
34	1	0	1.180200	1.658566	-3.131523
35	1	0	2.755601	1.940809	-2.241119
36	6	0	1.055734	3.064495	-1.528705
37	6	0	1.583842	3.569540	-0.322633
38	1	0	0.041327	3.345201	-1.806866
39	1	0	0.985023	4.287595	0.225875
40	1	0	2.654983	3.658317	-0.195435
41	6	0	-2.218457	1.199454	-1.429443
42	6	0	-3.602837	1.145273	-1.248603
43	6	0	-1.685368	0.939836	-2.686407
44	6	0	-4.435694	0.846371	-2.315767
45	1	0	-4.027142	1.321267	-0.266141

46	6	0	-2.519753	0.628886	-3.753340
47	1	0	-0.612094	0.934844	-2.814720
48	6	0	-3.894896	0.582845	-3.570555
49	1	0	-5.509024	0.810209	-2.165428
50	1	0	-2.091218	0.407444	-4.723763
51	1	0	-4.545085	0.333020	-4.401115
52	6	0	-1.682352	3.255828	0.486273
53	6	0	-1.170792	3.849265	1.646265
54	6	0	-2.506627	4.021883	-0.339141
55	6	0	-1.512750	5.147859	1.992333
56	1	0	-0.482673	3.308185	2.282060
57	6	0	-2.833987	5.330528	-0.000277
58	1	0	-2.896611	3.607762	-1.259753
59	6	0	-2.347946	5.894340	1.169444
60	1	0	-1.108708	5.581458	2.899735
61	1	0	-3.471485	5.907608	-0.660243
62	1	0	-2.606002	6.913355	1.433814
63	6	0	1.267478	-2.036129	1.200119
64	6	0	0.665852	-3.295045	1.259875
65	6	0	2.049646	-1.611126	2.273007
66	6	0	0.828490	-4.101484	2.377963
67	1	0	0.064299	-3.651587	0.432901
68	6	0	2.203730	-2.415478	3.394946
69	1	0	2.571265	-0.664480	2.223965
70	6	0	1.591344	-3.660540	3.452997
71	1	0	0.361311	-5.080095	2.402804
72	1	0	2.813239	-2.066443	4.220179
73	1	0	1.717493	-4.289833	4.327182
74	6	0	2.464231	-1.731390	-1.373960
75	6	0	2.747998	-1.143456	-2.607265
76	6	0	3.200495	-2.844631	-0.975611
77	6	0	3.732145	-1.664511	-3.432352
78	1	0	2.200147	-0.264002	-2.915231
79	6	0	4.196625	-3.359298	-1.797803
80	1	0	3.017686	-3.309071	-0.015462
81	6	0	4.463414	-2.775142	-3.027154
82	1	0	3.940945	-1.190749	-4.384732
83	1	0	4.770008	-4.217688	-1.466853
84	1	0	5.244767	-3.175203	-3.663341

L (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.274442	1.369866	-0.094386
2	53	0	4.054120	0.956735	0.312531
3	15	0	-1.060213	1.624503	-0.065178
4	15	0	1.107373	-1.023756	-0.311596
5	8	0	-2.977801	-2.147901	4.102176
6	8	0	-2.481374	-2.988515	2.030443

7	8	0	-4.082148	-1.941072	-0.511256
8	8	0	-4.038522	-2.976516	-2.566203
9	8	0	1.213869	1.587027	2.907561
10	6	0	-1.781705	0.537650	1.238706
11	6	0	-2.131488	1.035679	2.487172
12	1	0	-2.095895	2.099205	2.671406
13	6	0	-2.542640	0.209847	3.540371
14	1	0	-2.812290	0.614900	4.506347
15	6	0	-2.585773	-1.133851	3.285266
16	6	0	-2.639345	-3.337749	3.398511
17	1	0	-3.449305	-4.059053	3.495851
18	1	0	-1.689331	-3.728235	3.783534
19	6	0	-2.271884	-1.642266	2.032538
20	6	0	-1.860922	-0.857343	0.980453
21	6	0	-1.677274	-1.504349	-0.348595
22	6	0	-2.801928	-2.000619	-0.966707
23	6	0	-4.895804	-2.504603	-1.530532
24	1	0	-5.463129	-3.342906	-1.119322
25	1	0	-5.556897	-1.731956	-1.934367
26	6	0	-2.776614	-2.627382	-2.202081
27	6	0	-1.602685	-2.818320	-2.879929
28	1	0	-1.575436	-3.313815	-3.841285
29	6	0	-0.438780	-2.336016	-2.268307
30	1	0	0.502240	-2.482915	-2.780722
31	6	0	-0.452240	-1.687327	-1.038279
32	6	0	1.247276	1.439540	1.770346
33	6	0	1.623903	3.554896	-0.298225
34	1	0	2.369133	3.987743	0.360881
35	1	0	0.674724	4.075311	-0.318250
36	6	0	2.087946	2.926362	-1.477372
37	6	0	1.222987	2.217709	-2.307809
38	1	0	3.154148	2.802812	-1.620447
39	1	0	0.204970	2.569589	-2.425237
40	1	0	1.628240	1.700137	-3.170223
41	6	0	-2.176444	1.208466	-1.475357
42	6	0	-3.557290	1.263059	-1.263125
43	6	0	-1.700352	0.783542	-2.711642
44	6	0	-4.439904	0.926521	-2.277780
45	1	0	-3.943443	1.558763	-0.293848
46	6	0	-2.585447	0.435461	-3.724680
47	1	0	-0.636416	0.676141	-2.868841
48	6	0	-3.955004	0.511585	-3.513815
49	1	0	-5.508121	0.981029	-2.099198
50	1	0	-2.198888	0.087169	-4.675208
51	1	0	-4.643111	0.236941	-4.305289
52	6	0	-1.604825	3.338342	0.354191
53	6	0	-2.386202	4.099321	-0.514819
54	6	0	-1.102585	3.954323	1.507117
55	6	0	-2.690584	5.424969	-0.220706
56	1	0	-2.758683	3.669531	-1.435333
57	6	0	-1.421449	5.268743	1.808080
58	1	0	-0.427365	3.420029	2.163379
59	6	0	-2.221498	6.009767	0.945016

60	1	0	-3.295549	5.998335	-0.913704
61	1	0	-1.024881	5.720847	2.709701
62	1	0	-2.461182	7.041722	1.174129
63	6	0	1.218136	-2.045903	1.223356
64	6	0	0.564203	-3.277443	1.311870
65	6	0	2.019865	-1.634606	2.287250
66	6	0	0.700388	-4.070585	2.443154
67	1	0	-0.061593	-3.622710	0.498309
68	6	0	2.146569	-2.424111	3.422805
69	1	0	2.574928	-0.708576	2.223641
70	6	0	1.486337	-3.642834	3.506316
71	1	0	0.190908	-5.027119	2.488113
72	1	0	2.771897	-2.083454	4.239693
73	1	0	1.591223	-4.260754	4.391368
74	6	0	2.374844	-1.809642	-1.391304
75	6	0	2.812293	-1.114060	-2.517003
76	6	0	2.883801	-3.082929	-1.144014
77	6	0	3.720620	-1.686334	-3.394849
78	1	0	2.451972	-0.108621	-2.687296
79	6	0	3.803802	-3.651684	-2.016784
80	1	0	2.577508	-3.634758	-0.264455
81	6	0	4.219386	-2.959302	-3.146026
82	1	0	4.055415	-1.128461	-4.261828
83	1	0	4.200373	-4.638508	-1.806648
84	1	0	4.940279	-3.403897	-3.822851

M (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.645475	-1.683466	-0.860384
2	53	0	1.307495	-2.763459	1.736983
3	15	0	1.751668	0.290931	-0.126074
4	15	0	-1.559939	-0.869482	-0.317160
5	8	0	-2.233102	3.104916	1.932236
6	8	0	-1.467600	2.956695	4.097052
7	8	0	-0.773907	4.321771	-0.595297
8	8	0	-1.935604	4.634987	-2.546909
9	8	0	0.186959	-0.513005	-3.567639
10	6	0	0.800232	1.161695	1.182910
11	6	0	-0.429113	1.811258	0.891407
12	6	0	-1.066907	2.402371	1.959282
13	6	0	-0.607809	2.315442	3.262614
14	6	0	0.544132	1.641361	3.569491
15	1	0	0.894713	1.546764	4.588291
16	6	0	1.243591	1.074610	2.498843
17	1	0	2.155702	0.534981	2.714440
18	6	0	-2.548104	3.405516	3.285429
19	1	0	-3.459450	2.871644	3.570492
20	1	0	-2.660681	4.486308	3.398701

21	6	0	-1.112690	1.896047	-0.429933
22	6	0	-1.765847	0.807947	-1.070057
23	6	0	-2.497657	1.020288	-2.230569
24	1	0	-3.017159	0.194904	-2.695922
25	6	0	-2.616468	2.282975	-2.825994
26	1	0	-3.183211	2.430260	-3.735487
27	6	0	-1.987837	3.321014	-2.193730
28	6	0	-1.276399	3.127378	-1.019477
29	6	0	0.360898	-0.940720	-2.513624
30	6	0	2.310936	-2.993078	-1.595721
31	6	0	1.077999	-3.447315	-2.125679
32	1	0	0.881454	-3.284449	-3.183403
33	6	0	0.000166	-3.814296	-1.308063
34	1	0	0.169419	-4.308435	-0.361095
35	1	0	-0.960322	-3.997412	-1.775219
36	6	0	-1.383167	5.303963	-1.421399
37	1	0	-0.628228	6.014414	-1.757352
38	1	0	-2.184817	5.800884	-0.861081
39	1	0	3.051272	-2.613965	-2.292744
40	1	0	2.708535	-3.479300	-0.713379
41	6	0	-2.828960	-1.939082	-1.126972
42	6	0	-3.796065	-2.601916	-0.372244
43	6	0	-2.753987	-2.212902	-2.497568
44	6	0	-4.677086	-3.495179	-0.973622
45	1	0	-3.864804	-2.435382	0.694924
46	6	0	-3.645849	-3.087383	-3.099429
47	1	0	-1.986095	-1.754091	-3.107531
48	6	0	-4.613088	-3.733964	-2.337658
49	1	0	-5.415128	-4.004874	-0.364919
50	1	0	-3.574116	-3.274539	-4.164802
51	1	0	-5.303344	-4.426691	-2.805194
52	6	0	-2.362089	-0.540431	1.310463
53	6	0	-1.815365	-0.962649	2.516075
54	6	0	-3.573396	0.160742	1.316982
55	6	0	-2.466050	-0.686447	3.714612
56	1	0	-0.875088	-1.496715	2.525873
57	6	0	-4.227682	0.419090	2.510399
58	1	0	-4.004319	0.508996	0.384891
59	6	0	-3.671723	-0.001673	3.716015
60	1	0	-2.019660	-1.011337	4.647217
61	1	0	-5.170112	0.955731	2.500180
62	1	0	-4.179219	0.206827	4.651659
63	6	0	2.075490	1.577824	-1.406416
64	6	0	1.900003	2.939930	-1.177871
65	6	0	2.643239	1.163682	-2.611382
66	6	0	2.242540	3.866976	-2.154044
67	1	0	1.486243	3.290693	-0.241303
68	6	0	2.995759	2.089527	-3.582038
69	1	0	2.818013	0.108282	-2.789830
70	6	0	2.786864	3.445308	-3.359409
71	1	0	2.088714	4.923279	-1.963255
72	1	0	3.430226	1.750344	-4.515262
73	1	0	3.053870	4.169344	-4.120860

74	6	0	3.469074	0.222530	0.540111
75	6	0	4.071504	1.388378	1.023371
76	6	0	4.219723	-0.944337	0.466437
77	6	0	5.391803	1.375732	1.443059
78	1	0	3.506974	2.312506	1.073346
79	6	0	5.548100	-0.954609	0.878944
80	1	0	3.761330	-1.850328	0.101256
81	6	0	6.134731	0.201164	1.370945
82	1	0	5.844151	2.285257	1.821688
83	1	0	6.117706	-1.874900	0.821318
84	1	0	7.168702	0.191578	1.697233

N (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.593285	-1.671406	-0.874032
2	53	0	0.915058	-2.939427	1.681225
3	15	0	1.786495	0.217145	-0.071284
4	15	0	-1.569230	-0.780839	-0.324686
5	8	0	-2.082688	3.272405	1.841434
6	8	0	-1.345119	3.174246	4.017662
7	8	0	-0.510184	4.356152	-0.667838
8	8	0	-1.661993	4.710469	-2.618034
9	8	0	0.204156	-0.491226	-3.588106
10	6	0	0.869069	1.173545	1.199160
11	6	0	-0.325139	1.868732	0.867544
12	6	0	-0.947839	2.523527	1.906568
13	6	0	-0.504697	2.466890	3.217719
14	6	0	0.614569	1.757633	3.562542
15	1	0	0.952618	1.690179	4.587794
16	6	0	1.297240	1.118261	2.521454
17	1	0	2.185278	0.550894	2.765948
18	6	0	-2.414573	3.607051	3.182495
19	1	0	-3.331638	3.082778	3.467926
20	1	0	-2.523671	4.690166	3.268285
21	6	0	-0.987601	1.956758	-0.466066
22	6	0	-1.702364	0.898210	-1.091669
23	6	0	-2.431236	1.139286	-2.248109
24	1	0	-3.003939	0.341017	-2.697276
25	6	0	-2.482808	2.399188	-2.859136
26	1	0	-3.050876	2.567987	-3.764065
27	6	0	-1.786454	3.405813	-2.248097
28	6	0	-1.079629	3.186135	-1.075553
29	6	0	0.360623	-0.909203	-2.529243
30	6	0	-0.110859	-3.575069	-1.869605
31	6	0	1.244535	-3.694365	-1.512335
32	1	0	1.482192	-4.323381	-0.663982
33	6	0	2.246062	-2.808682	-1.955737
34	1	0	2.247764	-2.449569	-2.980188
35	1	0	3.231943	-2.897303	-1.514196
36	6	0	-1.068607	5.360856	-1.502711

37	1	0	-0.277411	6.024989	-1.849799
38	1	0	-1.839234	5.907123	-0.944789
39	1	0	-0.393033	-3.311502	-2.883170
40	1	0	-0.832671	-4.188182	-1.341152
41	6	0	-2.872407	-1.827990	-1.104429
42	6	0	-3.783008	-2.524715	-0.309786
43	6	0	-2.872714	-2.067946	-2.482493
44	6	0	-4.685117	-3.416152	-0.880295
45	1	0	-3.789050	-2.385040	0.763630
46	6	0	-3.786309	-2.941364	-3.052375
47	1	0	-2.145022	-1.586797	-3.123820
48	6	0	-4.698271	-3.619833	-2.251842
49	1	0	-5.378408	-3.952337	-0.242458
50	1	0	-3.774030	-3.103215	-4.124198
51	1	0	-5.405413	-4.311204	-2.695616
52	6	0	-2.370926	-0.380822	1.292870
53	6	0	-1.813782	-0.688047	2.527868
54	6	0	-3.599673	0.288512	1.248137
55	6	0	-2.477254	-0.344560	3.701712
56	1	0	-0.855956	-1.185272	2.579904
57	6	0	-4.264651	0.618591	2.417632
58	1	0	-4.038865	0.553477	0.292715
59	6	0	-3.703726	0.299853	3.651827
60	1	0	-2.023165	-0.584055	4.656183
61	1	0	-5.220290	1.128550	2.365883
62	1	0	-4.221987	0.558324	4.568987
63	6	0	2.238164	1.467739	-1.347560
64	6	0	2.118839	2.840095	-1.145651
65	6	0	2.820407	1.007303	-2.529138
66	6	0	2.537107	3.734196	-2.123604
67	1	0	1.689787	3.224588	-0.229319
68	6	0	3.248560	1.899768	-3.500414
69	1	0	2.944621	-0.058221	-2.687688
70	6	0	3.099655	3.267729	-3.303569
71	1	0	2.426620	4.799474	-1.954005
72	1	0	3.694447	1.525581	-4.414707
73	1	0	3.425699	3.965843	-4.066248
74	6	0	3.463223	0.003908	0.665665
75	6	0	4.204515	1.131290	1.035245
76	6	0	4.037826	-1.254786	0.799623
77	6	0	5.487961	0.995645	1.538923
78	1	0	3.777871	2.122048	0.927794
79	6	0	5.329111	-1.390193	1.299888
80	1	0	3.465894	-2.134143	0.540687
81	6	0	6.054803	-0.268744	1.670961
82	1	0	6.049655	1.877898	1.824112
83	1	0	5.759281	-2.379518	1.404728
84	1	0	7.060265	-0.374904	2.062734

B (NIMAG=0)

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	44	0	1.384312	1.003685	0.398758
2	53	0	3.996712	0.032519	0.885240
3	15	0	-0.852336	1.672405	0.294510
4	15	0	0.862293	-1.256660	-0.343968
5	8	0	-3.522447	-2.465309	3.608838
6	8	0	-3.051576	-2.982912	1.429492
7	8	0	-4.359343	-1.192572	-0.978112
8	8	0	-4.329572	-1.877238	-3.168398
9	8	0	1.048605	0.679040	3.330607
10	6	0	-1.846555	0.493732	1.309212
11	6	0	-2.187578	0.806767	2.618940
12	1	0	-2.001395	1.802153	2.996861
13	6	0	-2.758334	-0.125152	3.494449
14	1	0	-3.013083	0.135744	4.512709
15	6	0	-2.966366	-1.383681	2.999124
16	6	0	-3.291928	-3.545919	2.711581
17	1	0	-4.178539	-4.176375	2.669201
18	1	0	-2.402443	-4.102355	3.032731
19	6	0	-2.665099	-1.700337	1.681274
20	6	0	-2.103306	-0.807865	0.798941
21	6	0	-1.935635	-1.247253	-0.614708
22	6	0	-3.075448	-1.437427	-1.360265
23	6	0	-5.170242	-1.678327	-2.037362
24	1	0	-5.618364	-2.635264	-1.743216
25	1	0	-5.931692	-0.937005	-2.279832
26	6	0	-3.058646	-1.855951	-2.681615
27	6	0	-1.884171	-2.145479	-3.323004
28	1	0	-1.865026	-2.477991	-4.352370
29	6	0	-0.708142	-1.975992	-2.582713
30	1	0	0.232878	-2.206292	-3.063206
31	6	0	-0.710639	-1.529233	-1.265176
32	6	0	1.165410	0.764607	2.188825
33	6	0	2.198398	2.974827	0.605850
34	1	0	3.013201	3.018865	1.323721
35	1	0	1.476359	3.772562	0.757998
36	6	0	2.623747	2.721750	-0.759254
37	6	0	1.920118	2.963640	-1.902056
38	6	0	2.467743	2.540573	-3.237417
39	1	0	3.344053	1.898271	-3.132818
40	1	0	1.712124	2.011624	-3.830991
41	1	0	2.755390	3.422343	-3.822313
42	6	0	0.779512	3.939272	-1.973371
43	1	0	0.003961	3.627246	-2.675159
44	1	0	0.319576	4.133894	-1.006940
45	1	0	1.177813	4.892500	-2.343326
46	1	0	3.576431	2.216967	-0.882790
47	6	0	-1.804341	1.659600	-1.278306
48	6	0	-3.191203	1.822116	-1.260386
49	6	0	-1.168402	1.400432	-2.487653
50	6	0	-3.920739	1.759406	-2.438594
51	1	0	-3.705914	1.970958	-0.317461

52	6	0	-1.899038	1.324817	-3.665761
53	1	0	-0.098609	1.225243	-2.497101
54	6	0	-3.275218	1.510751	-3.644387
55	1	0	-4.996795	1.888666	-2.411631
56	1	0	-1.393294	1.102606	-4.598247
57	1	0	-3.846780	1.442450	-4.562775
58	6	0	-1.228308	3.332573	1.013082
59	6	0	-2.014903	4.285177	0.364266
60	6	0	-0.632585	3.681776	2.229966
61	6	0	-2.223710	5.538212	0.929111
62	1	0	-2.455690	4.067128	-0.599319
63	6	0	-0.853962	4.926502	2.800536
64	1	0	0.027036	2.986276	2.732898
65	6	0	-1.653158	5.859998	2.151928
66	1	0	-2.832950	6.264607	0.403453
67	1	0	-0.384187	5.170695	3.746162
68	1	0	-1.817357	6.837200	2.591403
69	6	0	0.731277	-2.598288	0.914511
70	6	0	-0.031754	-3.740066	0.654974
71	6	0	1.415696	-2.506981	2.125592
72	6	0	-0.109176	-4.764408	1.588586
73	1	0	-0.576993	-3.830663	-0.276511
74	6	0	1.328319	-3.528165	3.063182
75	1	0	2.041555	-1.650357	2.333223
76	6	0	0.566289	-4.658579	2.798883
77	1	0	-0.702156	-5.645185	1.367496
78	1	0	1.865374	-3.436743	3.999950
79	1	0	0.503983	-5.457272	3.530021
80	6	0	2.095536	-1.893977	-1.542917
81	6	0	2.541701	-1.007771	-2.522733
82	6	0	2.590109	-3.193632	-1.524942
83	6	0	3.451032	-1.416111	-3.484787
84	1	0	2.184057	0.016054	-2.514843
85	6	0	3.514992	-3.599842	-2.481169
86	1	0	2.270555	-3.888716	-0.758014
87	6	0	3.942408	-2.717330	-3.463538
88	1	0	3.791224	-0.714809	-4.238561
89	1	0	3.906812	-4.610161	-2.451126
90	1	0	4.666564	-3.037357	-4.204116

O (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.497663	0.932514	-0.118647
2	53	0	3.990616	-0.378787	0.448178
3	15	0	-0.708376	1.703430	0.045307
4	15	0	0.734555	-1.334404	-0.320376
5	8	0	-3.614059	-1.814321	3.867274
6	8	0	-3.373142	-2.530161	1.698589
7	8	0	-4.503733	-0.947458	-0.759340

8	8	0	-4.614509	-1.750649	-2.912525
9	8	0	1.774552	1.439429	2.850198
10	6	0	-1.654383	0.697266	1.273921
11	6	0	-1.835297	1.125767	2.583228
12	1	0	-1.495476	2.104525	2.883699
13	6	0	-2.471879	0.343358	3.554061
14	1	0	-2.602071	0.695630	4.568392
15	6	0	-2.932107	-0.881433	3.152441
16	6	0	-3.726755	-2.946334	3.010580
17	1	0	-4.758662	-3.298478	3.011178
18	1	0	-3.029644	-3.722297	3.344589
19	6	0	-2.780769	-1.313577	1.844429
20	6	0	-2.137214	-0.577271	0.876789
21	6	0	-2.074584	-1.130318	-0.501077
22	6	0	-3.257069	-1.285453	-1.186374
23	6	0	-5.394299	-1.323015	-1.800329
24	1	0	-6.025045	-2.150070	-1.458003
25	1	0	-5.993166	-0.457706	-2.092680
26	6	0	-3.325466	-1.774055	-2.480055
27	6	0	-2.200498	-2.180215	-3.145839
28	1	0	-2.246816	-2.575928	-4.151696
29	6	0	-0.985243	-2.061300	-2.459745
30	1	0	-0.092650	-2.409962	-2.958151
31	6	0	-0.896226	-1.541897	-1.172950
32	6	0	1.631936	1.205836	1.733467
33	6	0	2.030706	1.143584	-2.292856
34	1	0	1.376550	0.841620	-3.102933
35	1	0	3.032923	0.734903	-2.357124
36	6	0	1.827783	2.423898	-1.730715
37	6	0	2.644729	2.959204	-0.718442
38	6	0	2.259827	4.286587	-0.104346
39	1	0	1.217302	4.546209	-0.272618
40	1	0	2.447279	4.293636	0.971934
41	1	0	2.878408	5.079144	-0.541683
42	6	0	4.146957	2.789473	-0.744600
43	1	0	4.565142	2.741812	0.262172
44	1	0	4.480139	1.904944	-1.278929
45	1	0	4.567677	3.673148	-1.241885
46	1	0	0.915398	2.962062	-1.981567
47	6	0	-1.899280	1.702553	-1.360514
48	6	0	-3.245986	1.986737	-1.118077
49	6	0	-1.491954	1.410864	-2.656451
50	6	0	-4.161370	1.983523	-2.158493
51	1	0	-3.580157	2.197977	-0.108302
52	6	0	-2.411772	1.395655	-3.698474
53	1	0	-0.460702	1.152514	-2.844252
54	6	0	-3.746903	1.682635	-3.452309
55	1	0	-5.203148	2.206508	-1.956521
56	1	0	-2.083449	1.146007	-4.700636
57	1	0	-4.465227	1.664744	-4.263963
58	6	0	-0.878549	3.454330	0.619862
59	6	0	-1.459690	4.425658	-0.198883
60	6	0	-0.306510	3.869710	1.826981

61	6	0	-1.486237	5.761101	0.186325
62	1	0	-1.885689	4.153668	-1.155067
63	6	0	-0.353838	5.198229	2.221115
64	1	0	0.218711	3.169224	2.459819
65	6	0	-0.942896	6.151946	1.401053
66	1	0	-1.934460	6.495656	-0.472908
67	1	0	0.095231	5.489550	3.163565
68	1	0	-0.966493	7.192977	1.702006
69	6	0	0.406726	-2.322149	1.201981
70	6	0	-0.360073	-3.487845	1.120128
71	6	0	0.943152	-1.952233	2.430641
72	6	0	-0.586479	-4.261706	2.247827
73	1	0	-0.783808	-3.792185	0.169931
74	6	0	0.697994	-2.716423	3.565617
75	1	0	1.572785	-1.078543	2.505809
76	6	0	-0.066409	-3.871465	3.477886
77	1	0	-1.174409	-5.169364	2.165062
78	1	0	1.117800	-2.408960	4.516112
79	1	0	-0.248704	-4.472333	4.362245
80	6	0	1.830044	-2.473935	-1.276791
81	6	0	2.237956	-2.124630	-2.565378
82	6	0	2.312410	-3.659651	-0.726226
83	6	0	3.085812	-2.945744	-3.292667
84	1	0	1.901729	-1.196203	-3.002917
85	6	0	3.169868	-4.477957	-1.451278
86	1	0	2.049941	-3.941567	0.284206
87	6	0	3.557174	-4.128128	-2.736139
88	1	0	3.390492	-2.651457	-4.290576
89	1	0	3.545380	-5.388118	-0.997809
90	1	0	4.231436	-4.765372	-3.296935

P (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.571614	0.867263	-0.208026
2	53	0	4.094420	-0.354745	0.404980
3	15	0	-0.631792	1.731668	-0.077948
4	15	0	0.730632	-1.396511	-0.276034
5	8	0	-3.631890	-1.388657	4.017316
6	8	0	-3.435448	-2.284316	1.913055
7	8	0	-4.518773	-0.918244	-0.633779
8	8	0	-4.669001	-1.841369	-2.736046
9	8	0	1.729929	1.290093	2.775604
10	6	0	-1.568854	0.816931	1.233733
11	6	0	-1.711714	1.348270	2.509799
12	1	0	-1.313252	2.326095	2.734333
13	6	0	-2.377794	0.674372	3.539662
14	1	0	-2.477811	1.105570	4.526540

15	6	0	-2.906632	-0.549369	3.231138
16	6	0	-3.784624	-2.582315	3.258615
17	1	0	-4.824894	-2.905748	3.297562
18	1	0	-3.104231	-3.347040	3.649505
19	6	0	-2.785859	-1.087405	1.959713
20	6	0	-2.115042	-0.459487	0.935050
21	6	0	-2.087601	-1.111847	-0.400125
22	6	0	-3.282382	-1.293734	-1.058104
23	6	0	-5.427359	-1.322640	-1.647551
24	1	0	-6.084133	-2.105835	-1.255669
25	1	0	-5.997690	-0.455186	-1.987972
26	6	0	-3.374115	-1.852664	-2.322046
27	6	0	-2.262618	-2.292500	-2.990448
28	1	0	-2.328973	-2.726748	-3.979116
29	6	0	-1.036046	-2.152144	-2.330126
30	1	0	-0.145712	-2.513491	-2.827409
31	6	0	-0.927563	-1.582165	-1.065944
32	6	0	1.650155	1.098440	1.645674
33	6	0	2.526630	2.916732	-0.829463
34	6	0	2.830914	1.870346	-1.732760
35	6	0	1.834672	1.237335	-2.486916
36	1	0	3.820086	1.430022	-1.708411
37	1	0	0.984719	1.822914	-2.805982
38	1	0	2.113771	0.448532	-3.173589
39	6	0	1.633541	4.037745	-1.330416
40	1	0	0.753358	3.699508	-1.877278
41	1	0	1.304955	4.691857	-0.524691
42	1	0	2.230103	4.650171	-2.018635
43	6	0	3.627561	3.443016	0.066410
44	1	0	4.195554	4.228686	-0.448744
45	1	0	3.199247	3.893843	0.966579
46	1	0	4.317787	2.657352	0.373926
47	6	0	-1.890678	1.670294	-1.429104
48	6	0	-3.210475	2.030905	-1.136754
49	6	0	-1.589304	1.213935	-2.708005
50	6	0	-4.191276	1.974887	-2.114310
51	1	0	-3.475705	2.341932	-0.132514
52	6	0	-2.574835	1.149002	-3.686139
53	1	0	-0.598480	0.847195	-2.927221
54	6	0	-3.874628	1.537192	-3.396159
55	1	0	-5.207875	2.261650	-1.869253
56	1	0	-2.324955	0.772640	-4.671178
57	1	0	-4.642311	1.482122	-4.159648
58	6	0	-0.757649	3.497107	0.475334
59	6	0	-1.497815	4.449759	-0.225163
60	6	0	0.002423	3.930518	1.566713
61	6	0	-1.495099	5.784290	0.163434
62	1	0	-2.061701	4.170614	-1.104076
63	6	0	-0.007475	5.259145	1.965235
64	1	0	0.633708	3.242197	2.108346
65	6	0	-0.757051	6.194717	1.263410
66	1	0	-2.069592	6.504708	-0.407603
67	1	0	0.590121	5.562972	2.816907

68	1	0	-0.754824	7.235922	1.564770
69	6	0	0.463198	-2.297470	1.316324
70	6	0	-0.507192	-3.297330	1.425245
71	6	0	1.282466	-2.040166	2.413449
72	6	0	-0.651361	-4.019288	2.601248
73	1	0	-1.168430	-3.509717	0.593819
74	6	0	1.124797	-2.750591	3.596990
75	1	0	2.068459	-1.301761	2.344556
76	6	0	0.159283	-3.742603	3.695640
77	1	0	-1.399493	-4.802726	2.657239
78	1	0	1.769777	-2.528890	4.439113
79	1	0	0.043602	-4.302574	4.617020
80	6	0	1.704843	-2.643998	-1.235723
81	6	0	2.585423	-2.223089	-2.228760
82	6	0	1.537219	-4.014692	-1.031761
83	6	0	3.262890	-3.142151	-3.018732
84	1	0	2.768019	-1.168537	-2.361243
85	6	0	2.219001	-4.935592	-1.815669
86	1	0	0.880318	-4.378573	-0.253348
87	6	0	3.079005	-4.502853	-2.816881
88	1	0	3.950540	-2.789526	-3.778738
89	1	0	2.079921	-5.995743	-1.636659
90	1	0	3.613700	-5.222994	-3.426007

Q (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.371226	0.959085	0.388108
2	53	0	3.928672	-0.089232	0.967686
3	15	0	-0.835663	1.703166	0.299138
4	15	0	0.774246	-1.293040	-0.301010
5	8	0	-3.867464	-2.281490	3.477858
6	8	0	-3.313275	-2.818201	1.321846
7	8	0	-4.417426	-0.930292	-1.100909
8	8	0	-4.348927	-1.590506	-3.304872
9	8	0	1.010954	0.702923	3.327520
10	6	0	-1.917165	0.586983	1.285949
11	6	0	-2.305772	0.914456	2.578435
12	1	0	-2.095573	1.899451	2.969030
13	6	0	-2.969372	0.011080	3.417764
14	1	0	-3.264670	0.282305	4.422292
15	6	0	-3.219374	-1.232542	2.904438
16	6	0	-3.666606	-3.369856	2.582436
17	1	0	-4.593408	-3.932752	2.483469
18	1	0	-2.840792	-3.992695	2.947849
19	6	0	-2.868842	-1.561274	1.601716
20	6	0	-2.217303	-0.696590	0.754408
21	6	0	-2.016075	-1.124566	-0.658921
22	6	0	-3.135867	-1.221949	-1.451763
23	6	0	-5.200800	-1.098225	-2.274541

24	1	0	-5.992930	-1.825174	-2.080541
25	1	0	-5.610428	-0.130066	-2.577898
26	6	0	-3.096540	-1.623555	-2.777355
27	6	0	-1.920749	-1.987310	-3.376306
28	1	0	-1.885198	-2.314620	-4.406897
29	6	0	-0.764628	-1.907918	-2.589709
30	1	0	0.175819	-2.194509	-3.039922
31	6	0	-0.786207	-1.479933	-1.266589
32	6	0	1.145867	0.762353	2.186093
33	6	0	2.562156	2.398592	-1.908919
34	6	0	1.861902	2.952876	-0.869443
35	6	0	2.197665	2.936810	0.536248
36	1	0	0.906002	3.403882	-1.133613
37	1	0	3.247586	2.872420	0.804894
38	1	0	1.658913	3.663016	1.136422
39	6	0	4.019335	2.041055	-1.852905
40	1	0	4.451920	2.178495	-0.866395
41	1	0	4.205892	1.003225	-2.145184
42	1	0	4.555948	2.681229	-2.563473
43	6	0	2.008691	2.471455	-3.310409
44	1	0	2.653189	3.112760	-3.922020
45	1	0	1.998586	1.491755	-3.803028
46	1	0	0.999966	2.883872	-3.341281
47	6	0	-1.768365	1.795121	-1.279126
48	6	0	-3.128741	2.111975	-1.277483
49	6	0	-1.140660	1.491850	-2.480341
50	6	0	-3.837061	2.148729	-2.469012
51	1	0	-3.635177	2.318704	-0.340945
52	6	0	-1.852325	1.516161	-3.673193
53	1	0	-0.100114	1.195611	-2.470886
54	6	0	-3.200061	1.848934	-3.669791
55	1	0	-4.890564	2.405968	-2.460134
56	1	0	-1.354613	1.259067	-4.600955
57	1	0	-3.758118	1.863926	-4.599042
58	6	0	-1.065026	3.396845	0.995038
59	6	0	-0.596785	3.680425	2.283730
60	6	0	-1.567011	4.448799	0.228186
61	6	0	-0.681803	4.962044	2.805775
62	1	0	-0.136061	2.905548	2.882992
63	6	0	-1.634741	5.737772	0.746519
64	1	0	-1.903694	4.275558	-0.785589
65	6	0	-1.204574	5.996772	2.038791
66	1	0	-0.318149	5.154164	3.808482
67	1	0	-2.024470	6.539750	0.130109
68	1	0	-1.260254	7.001085	2.442742
69	6	0	0.522499	-2.584346	0.989960
70	6	0	-0.312914	-3.677532	0.746378
71	6	0	1.202841	-2.512682	2.204597
72	6	0	-0.467672	-4.672999	1.701366
73	1	0	-0.852999	-3.752273	-0.189586
74	6	0	1.037974	-3.504289	3.163258
75	1	0	1.886477	-1.697264	2.397252
76	6	0	0.202495	-4.585652	2.916102

77	1	0	-1.114863	-5.517904	1.492290
78	1	0	1.572787	-3.429413	4.102782
79	1	0	0.079869	-5.361748	3.663713
80	6	0	1.999502	-2.063078	-1.430378
81	6	0	2.402486	-3.391236	-1.336454
82	6	0	2.540153	-1.257897	-2.431891
83	6	0	3.328695	-3.904227	-2.238445
84	1	0	2.010170	-4.026767	-0.552066
85	6	0	3.451507	-1.771652	-3.340328
86	1	0	2.251417	-0.214132	-2.479710
87	6	0	3.850217	-3.100644	-3.242715
88	1	0	3.647287	-4.936480	-2.148496
89	1	0	3.866065	-1.130878	-4.110631
90	1	0	4.575267	-3.503716	-3.940641

R (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.201374	1.257783	-0.605995
2	53	0	1.877976	1.895997	2.126102
3	15	0	-1.091850	1.476420	-0.054538
4	15	0	1.283364	-1.124181	-0.142191
5	8	0	-2.357309	-3.421674	1.451012
6	8	0	-2.882676	-2.833195	3.611864
7	8	0	-3.729509	-2.322954	-1.194184
8	8	0	-3.301053	-3.495375	-3.114526
9	8	0	0.561534	0.436640	-3.403122
10	6	0	-1.716907	0.178255	1.080358
11	6	0	-1.774293	-1.177811	0.663089
12	6	0	-2.212267	-2.078840	1.607519
13	6	0	-2.528915	-1.725838	2.909172
14	6	0	-2.438981	-0.428841	3.338440
15	1	0	-2.663121	-0.149988	4.359226
16	6	0	-2.031266	0.518226	2.391958
17	1	0	-1.947201	1.549828	2.706112
18	6	0	-2.702899	-3.937574	2.729084
19	1	0	-1.885326	-4.564663	3.096563
20	1	0	-3.639114	-4.495020	2.653250
21	6	0	-1.399914	-1.745640	-0.665065
22	6	0	-0.064762	-1.946535	-1.113020
23	6	0	0.176361	-2.706218	-2.249511
24	1	0	1.191425	-2.901088	-2.560199
25	6	0	-0.851315	-3.266650	-3.018563
26	1	0	-0.642132	-3.861365	-3.897590
27	6	0	-2.130481	-3.034018	-2.594720
28	6	0	-2.386936	-2.310924	-1.438847
29	6	0	0.799808	0.763603	-2.326796
30	6	0	3.422363	1.721514	-1.453060
31	6	0	2.731490	2.831729	-0.942164
32	1	0	3.056280	3.212986	0.017656

33	6	0	1.495848	3.313451	-1.434006
34	1	0	1.285215	3.293608	-2.498955
35	1	0	1.048749	4.156397	-0.921190
36	6	0	-4.318512	-2.819251	-2.388052
37	1	0	-4.690949	-1.978016	-2.985867
38	1	0	-5.111729	-3.521126	-2.134340
39	6	0	3.562548	1.534161	-2.948947
40	1	0	3.617041	0.484506	-3.235822
41	1	0	2.767636	2.009814	-3.522901
42	1	0	4.509775	1.994202	-3.256724
43	6	0	4.610492	1.208489	-0.673878
44	1	0	4.799298	0.156795	-0.897415
45	1	0	5.513436	1.765148	-0.956979
46	1	0	4.460982	1.309503	0.401835
47	6	0	1.074415	-2.101755	1.418657
48	6	0	1.057963	-3.496221	1.293397
49	6	0	0.900862	-1.537790	2.676102
50	6	0	0.899075	-4.303472	2.407683
51	1	0	1.168691	-3.954935	0.317215
52	6	0	0.731013	-2.349545	3.793630
53	1	0	0.885444	-0.464000	2.789042
54	6	0	0.737970	-3.729821	3.666296
55	1	0	0.897432	-5.381755	2.292990
56	1	0	0.588673	-1.889944	4.764763
57	1	0	0.613482	-4.359461	4.540765
58	6	0	2.870753	-1.830157	-0.751676
59	6	0	3.818001	-2.301887	0.158776
60	6	0	3.222589	-1.761690	-2.101758
61	6	0	5.069845	-2.721297	-0.275113
62	1	0	3.585618	-2.336521	1.215784
63	6	0	4.464710	-2.201282	-2.537066
64	1	0	2.532788	-1.345519	-2.824838
65	6	0	5.393835	-2.685117	-1.624185
66	1	0	5.792873	-3.076897	0.449875
67	1	0	4.711425	-2.147480	-3.591440
68	1	0	6.368000	-3.019359	-1.961970
69	6	0	-2.264628	1.426091	-1.477290
70	6	0	-3.487741	0.761153	-1.424484
71	6	0	-1.964898	2.196990	-2.600545
72	6	0	-4.382306	0.848925	-2.484234
73	1	0	-3.752269	0.169468	-0.557258
74	6	0	-2.857180	2.283491	-3.659118
75	1	0	-1.029101	2.742087	-2.643339
76	6	0	-4.068843	1.605216	-3.605724
77	1	0	-5.335316	0.334693	-2.421970
78	1	0	-2.605351	2.883013	-4.526198
79	1	0	-4.767955	1.673179	-4.431568
80	6	0	-1.711254	3.042309	0.709172
81	6	0	-3.088894	3.233207	0.864392
82	6	0	-0.846759	4.058440	1.100993
83	6	0	-3.583163	4.410184	1.403091
84	1	0	-3.784144	2.458879	0.563020
85	6	0	-1.343222	5.242765	1.636417

86	1	0	0.220479	3.915087	1.021080
87	6	0	-2.709286	5.422053	1.788608
88	1	0	-4.653292	4.539676	1.518301
89	1	0	-0.651587	6.019772	1.940917
90	1	0	-3.095861	6.344621	2.207081

S (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.783664	-1.589477	-0.637259
2	53	0	0.816244	-1.930896	2.232598
3	15	0	1.623600	0.631099	-0.192907
4	15	0	-1.524518	-0.991960	-0.515989
5	8	0	-2.482771	2.624531	2.403380
6	8	0	-1.397798	2.853474	4.402415
7	8	0	-1.168625	4.261250	-0.043385
8	8	0	-2.156686	4.713368	-2.071754
9	8	0	0.739516	-1.152340	-3.584674
10	6	0	0.799630	1.416507	1.253193
11	6	0	-0.579498	1.730984	1.126025
12	6	0	-1.194177	2.189977	2.266828
13	6	0	-0.532676	2.352172	3.476270
14	6	0	0.808017	2.108362	3.595165
15	1	0	1.334625	2.263788	4.526939
16	6	0	1.459971	1.628660	2.453868
17	1	0	2.513549	1.403157	2.531970
18	6	0	-2.680062	2.714665	3.807398
19	1	0	-3.148971	1.789289	4.166786
20	1	0	-3.282384	3.593311	4.031691
21	6	0	-1.314482	1.821489	-0.170719
22	6	0	-1.801202	0.766588	-0.988692
23	6	0	-2.399805	1.058278	-2.211180
24	1	0	-2.751445	0.249554	-2.837026
25	6	0	-2.569448	2.366306	-2.680465
26	1	0	-3.023973	2.570160	-3.640699
27	6	0	-2.128999	3.371819	-1.863417
28	6	0	-1.533005	3.097006	-0.643443
29	6	0	0.743363	-1.282649	-2.437122
30	6	0	2.782639	-2.840332	-0.849021
31	6	0	1.647078	-3.467784	-1.416378
32	1	0	1.589151	-3.514699	-2.502620
33	6	0	0.487764	-3.809469	-0.689901
34	1	0	0.559846	-4.112563	0.346637
35	1	0	-0.349579	-4.230247	-1.234751
36	6	0	-1.543787	5.305789	-0.929422
37	1	0	-0.649662	5.851036	-1.243420
38	1	0	-2.262655	5.962513	-0.432263
39	6	0	3.393427	-3.382806	0.422017
40	1	0	3.876085	-2.601469	1.007820
41	1	0	2.677137	-3.888632	1.063682

42	1	0	4.171492	-4.102689	0.134264
43	6	0	3.830360	-2.301507	-1.800800
44	1	0	4.389200	-1.487405	-1.334091
45	1	0	4.555331	-3.086425	-2.052372
46	1	0	3.398621	-1.924743	-2.730536
47	6	0	-2.539289	-1.227096	0.994445
48	6	0	-3.369911	-0.237443	1.508226
49	6	0	-2.558539	-2.500541	1.564758
50	6	0	-4.193987	-0.511111	2.595512
51	1	0	-3.390226	0.750002	1.066827
52	6	0	-3.386354	-2.773715	2.641404
53	1	0	-1.916395	-3.278253	1.168471
54	6	0	-4.202692	-1.776435	3.164596
55	1	0	-4.842211	0.267401	2.983322
56	1	0	-3.385255	-3.764222	3.080875
57	1	0	-4.846104	-1.989436	4.010943
58	6	0	-2.632838	-1.891333	-1.699612
59	6	0	-4.021656	-1.765797	-1.577945
60	6	0	-2.128262	-2.692889	-2.719660
61	6	0	-4.873107	-2.414648	-2.458319
62	1	0	-4.441985	-1.157367	-0.786146
63	6	0	-2.981177	-3.346664	-3.603235
64	1	0	-1.062373	-2.820591	-2.832918
65	6	0	-4.354780	-3.208404	-3.476268
66	1	0	-5.945594	-2.304007	-2.345810
67	1	0	-2.564048	-3.966577	-4.388512
68	1	0	-5.020876	-3.719562	-4.162123
69	6	0	1.490201	2.061746	-1.364240
70	6	0	1.865349	3.321902	-0.883660
71	6	0	1.027115	1.959345	-2.670825
72	6	0	1.786120	4.442488	-1.694208
73	1	0	2.214859	3.427105	0.136923
74	6	0	0.933866	3.086640	-3.481160
75	1	0	0.708390	1.012392	-3.072060
76	6	0	1.313366	4.329249	-2.998338
77	1	0	2.088139	5.408034	-1.303488
78	1	0	0.553222	2.985438	-4.490795
79	1	0	1.238890	5.206521	-3.631176
80	6	0	3.437091	0.648006	0.130830
81	6	0	4.315774	1.234197	-0.783353
82	6	0	3.970619	-0.052122	1.216109
83	6	0	5.690742	1.137846	-0.605644
84	1	0	3.935224	1.763460	-1.647449
85	6	0	5.344087	-0.131746	1.399474
86	1	0	3.308049	-0.562437	1.906031
87	6	0	6.210089	0.461835	0.489559
88	1	0	6.354883	1.594656	-1.330527
89	1	0	5.735240	-0.676106	2.251583
90	1	0	7.282766	0.390543	0.629418

T (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.318308	-1.031396	-0.692775
2	53	0	1.719240	-2.378481	1.835171
3	15	0	1.256460	1.180693	0.244422
4	15	0	-1.035067	-1.432597	-0.419268
5	8	0	-3.847635	1.696538	1.399807
6	8	0	-3.530119	2.068886	3.646533
7	8	0	-2.581245	3.549693	-0.916986
8	8	0	-3.483943	3.315419	-3.007587
9	8	0	0.575767	-0.125252	-3.432572
10	6	0	-0.178443	1.495998	1.349198
11	6	0	-1.488168	1.450840	0.798325
12	6	0	-2.517895	1.681620	1.681049
13	6	0	-2.327632	1.910684	3.034955
14	6	0	-1.073434	1.950399	3.580899
15	1	0	-0.917288	2.131113	4.635972
16	6	0	-0.000035	1.745658	2.703717
17	1	0	1.001513	1.792891	3.108179
18	6	0	-4.516298	1.822854	2.647073
19	1	0	-5.035492	0.886521	2.873340
20	1	0	-5.204743	2.668963	2.604172
21	6	0	-1.884055	1.213235	-0.623003
22	6	0	-1.930306	-0.056785	-1.261905
23	6	0	-2.538943	-0.195146	-2.500481
24	1	0	-2.598963	-1.170819	-2.961247
25	6	0	-3.090526	0.890810	-3.193353
26	1	0	-3.564295	0.767660	-4.157994
27	6	0	-3.000972	2.113742	-2.586984
28	6	0	-2.434688	2.258021	-1.327051
29	6	0	0.886344	-0.423894	-2.364798
30	6	0	1.872316	-2.908148	-1.772241
31	6	0	3.024763	-2.359280	-1.166709
32	1	0	3.368792	-2.843010	-0.261862
33	6	0	3.566834	-1.087371	-1.436431
34	1	0	1.676158	-2.770812	-2.830894
35	1	0	1.491529	-3.838849	-1.365236
36	6	0	-2.960493	4.262693	-2.084757
37	1	0	-2.073344	4.741656	-2.519041
38	1	0	-3.733066	4.986870	-1.830843
39	6	0	4.633394	-0.577030	-0.493502
40	1	0	5.623386	-0.920579	-0.820164
41	1	0	4.656118	0.515885	-0.479120
42	1	0	4.465259	-0.920639	0.528058
43	6	0	3.770848	-0.611985	-2.860432
44	1	0	4.767164	-0.935748	-3.185890
45	1	0	3.049152	-1.020307	-3.567051
46	1	0	3.759331	0.477633	-2.938048
47	6	0	-1.466680	-2.999230	-1.284940
48	6	0	-1.895727	-4.106036	-0.552540
49	6	0	-1.201613	-3.162064	-2.648434
50	6	0	-2.085798	-5.335091	-1.174372

51	1	0	-2.071762	-4.019510	0.512197
52	6	0	-1.412004	-4.382955	-3.270828
53	1	0	-0.804261	-2.340680	-3.231508
54	6	0	-1.857359	-5.475444	-2.535071
55	1	0	-2.411542	-6.184668	-0.585292
56	1	0	-1.210364	-4.484341	-4.331149
57	1	0	-2.010850	-6.433075	-3.019282
58	6	0	-2.120821	-1.544303	1.078240
59	6	0	-1.673938	-1.415723	2.387590
60	6	0	-3.490949	-1.707116	0.843989
61	6	0	-2.573509	-1.474160	3.446600
62	1	0	-0.624950	-1.258690	2.587697
63	6	0	-4.385846	-1.775009	1.899872
64	1	0	-3.862385	-1.780113	-0.172209
65	6	0	-3.926555	-1.663704	3.209119
66	1	0	-2.205863	-1.365046	4.460227
67	1	0	-5.442653	-1.911829	1.699520
68	1	0	-4.623725	-1.718455	4.038334
69	6	0	1.092146	2.600585	-0.923063
70	6	0	0.470415	3.785599	-0.525441
71	6	0	1.708477	2.556071	-2.171068
72	6	0	0.454059	4.889465	-1.366794
73	1	0	-0.005727	3.851223	0.444708
74	6	0	1.686985	3.656474	-3.017732
75	1	0	2.222630	1.659147	-2.483522
76	6	0	1.056803	4.827609	-2.617736
77	1	0	-0.030892	5.802285	-1.038733
78	1	0	2.166189	3.596360	-3.987985
79	1	0	1.041818	5.690389	-3.274404
80	6	0	2.737153	1.736616	1.198014
81	6	0	3.191376	0.977771	2.279530
82	6	0	3.476602	2.857367	0.812760
83	6	0	4.345688	1.333954	2.961651
84	1	0	2.655288	0.085752	2.577277
85	6	0	4.639485	3.204767	1.490633
86	1	0	3.159286	3.467039	-0.022663
87	6	0	5.077965	2.446551	2.566856
88	1	0	4.677902	0.726215	3.795554
89	1	0	5.201871	4.074785	1.170884
90	1	0	5.986228	2.718512	3.092781

U (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.958229	1.486670	-0.595189
2	53	0	1.009263	1.684666	2.295658
3	15	0	-1.410537	1.205003	-0.346037
4	15	0	1.483842	-0.867585	-0.442243
5	8	0	-1.308043	-3.135448	2.561790
6	8	0	-2.144400	-2.161583	4.452152

7	8	0	-3.362028	-2.931648	0.021475
8	8	0	-3.178021	-4.313875	-1.805702
9	8	0	0.646271	1.538729	-3.556294
10	6	0	-1.866024	0.202410	1.119486
11	6	0	-1.447929	-1.153586	1.113515
12	6	0	-1.579589	-1.821421	2.306351
13	6	0	-2.113076	-1.239126	3.449583
14	6	0	-2.597447	0.040029	3.441255
15	1	0	-3.046574	0.484289	4.319056
16	6	0	-2.447571	0.757137	2.248326
17	1	0	-2.770149	1.788858	2.230904
18	6	0	-1.337548	-3.231006	3.978540
19	1	0	-0.317274	-3.119065	4.368775
20	1	0	-1.785851	-4.179884	4.267595
21	6	0	-1.121600	-1.952015	-0.106425
22	6	0	0.083697	-1.996957	-0.857787
23	6	0	0.189092	-2.870054	-1.936934
24	1	0	1.116633	-2.924073	-2.488181
25	6	0	-0.858227	-3.700941	-2.352521
26	1	0	-0.752945	-4.365558	-3.199589
27	6	0	-2.018527	-3.629301	-1.631065
28	6	0	-2.127974	-2.790254	-0.533972
29	6	0	0.762282	1.456060	-2.409620
30	6	0	1.007038	3.717593	-0.547677
31	6	0	2.137970	3.243069	-1.246748
32	1	0	2.132005	3.354846	-2.329020
33	6	0	3.139374	2.411008	-0.693832
34	1	0	1.065702	3.963005	0.504843
35	1	0	0.259212	4.266269	-1.110200
36	6	0	-4.092184	-3.782479	-0.849009
37	1	0	-4.857653	-3.197380	-1.369104
38	1	0	-4.528866	-4.600595	-0.274088
39	6	0	4.110127	1.770833	-1.664008
40	1	0	4.968932	2.432624	-1.834551
41	1	0	4.499824	0.830048	-1.266666
42	1	0	3.649277	1.550312	-2.628432
43	6	0	3.799925	2.782383	0.615132
44	1	0	4.687360	3.383703	0.376683
45	1	0	3.157307	3.362632	1.271034
46	1	0	4.142371	1.911939	1.177004
47	6	0	-2.471548	0.344616	-1.595562
48	6	0	-3.824794	0.170956	-1.285324
49	6	0	-1.984828	-0.198553	-2.779208
50	6	0	-4.668199	-0.509017	-2.149558
51	1	0	-4.217743	0.563073	-0.354000
52	6	0	-2.826443	-0.892464	-3.641392
53	1	0	-0.938474	-0.125237	-3.027896
54	6	0	-4.169541	-1.046330	-3.332592
55	1	0	-5.715811	-0.626027	-1.894694
56	1	0	-2.421561	-1.322721	-4.549813
57	1	0	-4.824883	-1.588375	-4.005201
58	6	0	-2.257197	2.833083	-0.198041
59	6	0	-3.108043	3.298166	-1.201613

60	6	0	-1.930709	3.690715	0.857702
61	6	0	-3.641819	4.580833	-1.137092
62	1	0	-3.357309	2.667713	-2.045729
63	6	0	-2.478501	4.962869	0.926602
64	1	0	-1.222952	3.370112	1.614566
65	6	0	-3.337723	5.412898	-0.069700
66	1	0	-4.298023	4.925403	-1.928305
67	1	0	-2.218722	5.609184	1.757241
68	1	0	-3.758304	6.410844	-0.018267
69	6	0	2.128220	-1.593750	1.113744
70	6	0	1.669026	-2.808785	1.612816
71	6	0	3.177075	-0.943766	1.764548
72	6	0	2.236836	-3.353271	2.760076
73	1	0	0.864688	-3.338244	1.120158
74	6	0	3.754288	-1.494729	2.897269
75	1	0	3.539123	0.000267	1.379279
76	6	0	3.278595	-2.699661	3.403323
77	1	0	1.867274	-4.299526	3.139936
78	1	0	4.563625	-0.973621	3.394942
79	1	0	3.721559	-3.126602	4.296234
80	6	0	2.800532	-1.402190	-1.630145
81	6	0	3.926408	-2.115483	-1.219017
82	6	0	2.692073	-1.060615	-2.981024
83	6	0	4.925393	-2.451085	-2.127461
84	1	0	4.037523	-2.412544	-0.184763
85	6	0	3.679692	-1.407557	-3.889779
86	1	0	1.824871	-0.525679	-3.341295
87	6	0	4.809113	-2.096538	-3.462941
88	1	0	5.796354	-2.996447	-1.782114
89	1	0	3.568894	-1.129811	-4.931742
90	1	0	5.589467	-2.357546	-4.168671

A (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.159622	1.539966	0.211808
2	53	0	3.847247	1.811149	0.199959
3	15	0	-1.104708	1.659185	-0.162464
4	15	0	1.233082	-0.915948	-0.116209
5	8	0	-3.276100	-2.164853	3.794955
6	8	0	-2.449275	-3.046653	1.851057
7	8	0	-3.823473	-2.202067	-0.968585
8	8	0	-3.441967	-3.286252	-2.945801
9	8	0	0.664789	1.744898	3.106324
10	6	0	-1.552937	1.270279	-1.894202
11	6	0	-0.614225	1.582656	-2.877207
12	1	0	0.324983	2.056658	-2.601010
13	6	0	-0.873436	1.301820	-4.212160
14	1	0	-0.136140	1.546933	-4.967684
15	6	0	-2.073056	0.701745	-4.573066

16	1	0	-2.272748	0.470502	-5.613056
17	6	0	-3.015224	0.392536	-3.599172
18	1	0	-3.947043	-0.086639	-3.877073
19	6	0	-2.759092	0.679135	-2.265543
20	1	0	-3.485997	0.402614	-1.509117
21	6	0	-1.978575	3.248523	0.139768
22	6	0	-3.309763	3.406014	-0.256569
23	1	0	-3.824703	2.605147	-0.773383
24	6	0	-3.986103	4.587173	0.005511
25	1	0	-5.017104	4.698080	-0.310340
26	6	0	-3.342354	5.626392	0.669951
27	1	0	-3.871515	6.550348	0.874179
28	6	0	-2.021382	5.477838	1.066152
29	1	0	-1.511435	6.283902	1.580769
30	6	0	-1.339846	4.294533	0.800764
31	1	0	-0.305282	4.186069	1.100409
32	6	0	-2.003645	0.491503	0.935952
33	6	0	-2.540158	1.009924	2.111312
34	1	0	-2.590141	2.082720	2.244849
35	6	0	-2.999483	0.198192	3.154320
36	1	0	-3.410096	0.618864	4.062122
37	6	0	-2.888455	-1.153914	2.971442
38	6	0	-2.722086	-3.339569	3.214832
39	1	0	-3.447386	-4.149419	3.272915
40	1	0	-1.783040	-3.587917	3.725227
41	6	0	-2.374347	-1.685568	1.796699
42	6	0	-1.909334	-0.913991	0.757596
43	6	0	-1.490466	-1.603533	-0.492547
44	6	0	-2.480549	-2.219799	-1.221952
45	6	0	-4.370234	-3.145442	-1.877422
46	1	0	-4.490824	-4.111416	-1.370130
47	1	0	-5.316606	-2.772039	-2.264215
48	6	0	-2.253890	-2.868386	-2.424549
49	6	0	-0.994993	-2.958385	-2.954566
50	1	0	-0.806809	-3.452211	-3.898403
51	6	0	0.039280	-2.376350	-2.213016
52	1	0	1.045278	-2.462273	-2.599117
53	6	0	-0.175817	-1.707358	-1.010293
54	6	0	1.333019	-1.884763	1.437258
55	6	0	2.104109	-1.376470	2.483804
56	1	0	2.607511	-0.422894	2.370278
57	6	0	2.244882	-2.096121	3.662465
58	1	0	2.843731	-1.689378	4.468773
59	6	0	1.619858	-3.329112	3.806487
60	1	0	1.729964	-3.889587	4.728172
61	6	0	0.859831	-3.844342	2.763296
62	1	0	0.382178	-4.813174	2.862306
63	6	0	0.717206	-3.127625	1.581631
64	1	0	0.118272	-3.536826	0.777221
65	6	0	2.669831	-1.523979	-1.079539
66	6	0	3.410674	-2.641364	-0.705316
67	1	0	3.161671	-3.183065	0.199271
68	6	0	4.482368	-3.062957	-1.484562

69	1	0	5.059616	-3.927971	-1.178576
70	6	0	4.815120	-2.378239	-2.644920
71	1	0	5.653616	-2.706441	-3.248647
72	6	0	4.079455	-1.260794	-3.024123
73	1	0	4.344421	-0.710369	-3.919233
74	6	0	3.020653	-0.831458	-2.239681
75	1	0	2.467262	0.056019	-2.528640
76	6	0	0.840259	1.653809	1.972290
77	1	0	1.230931	3.129905	0.264490

isoprene (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.973737	0.006331	-0.000146
2	1	0	2.931402	-0.500892	-0.000100
3	1	0	1.996146	1.090942	-0.000496
4	6	0	0.832969	-0.680768	0.000176
5	6	0	-0.517701	-0.100267	0.000025
6	6	0	-0.653194	1.397559	0.000102
7	1	0	-0.171647	1.832321	-0.881288
8	1	0	-1.702127	1.696573	0.000506
9	1	0	-0.170795	1.832284	0.881038
10	6	0	-1.583791	-0.904390	-0.000143
11	1	0	-2.594145	-0.510153	-0.000263
12	1	0	-1.475142	-1.984101	-0.000079
13	1	0	0.874190	-1.767763	0.000595

ethanal (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.228601	-0.276650	-0.000000
2	6	0	-0.235444	0.396846	0.000002
3	1	0	-0.307676	1.506806	-0.000012
4	6	0	1.165697	-0.147251	0.000000
5	1	0	1.702009	0.222746	-0.879528
6	1	0	1.702027	0.222840	0.879483
7	1	0	1.150930	-1.236758	0.000048

C (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.193036	0.331983	-1.029991
2	53	0	-3.172102	-1.480731	-1.735901
3	15	0	0.452225	1.824502	-0.342163

4	15	0	-0.006172	-1.562922	0.110350
5	8	0	5.445851	-0.678741	-2.351478
6	8	0	4.617469	-1.449914	-0.361287
7	8	0	4.356802	0.598254	2.132050
8	8	0	4.046681	-0.183687	4.260183
9	8	0	0.044286	0.266452	-3.700551
10	6	0	0.484000	2.039115	1.474405
11	6	0	-0.668017	1.713883	2.189149
12	1	0	-1.561908	1.379679	1.669995
13	6	0	-0.695599	1.813876	3.573802
14	1	0	-1.599470	1.534845	4.102674
15	6	0	0.435969	2.246518	4.253236
16	1	0	0.425354	2.315685	5.335047
17	6	0	1.588567	2.578776	3.548571
18	1	0	2.475977	2.902906	4.080254
19	6	0	1.614843	2.475085	2.164872
20	1	0	2.529518	2.695640	1.624028
21	6	0	0.458201	3.543046	-1.001070
22	6	0	0.749751	4.646341	-0.200099
23	1	0	0.969695	4.515928	0.851555
24	6	0	0.729182	5.929423	-0.731947
25	1	0	0.949015	6.776528	-0.092403
26	6	0	0.420357	6.127787	-2.070801
27	1	0	0.398453	7.130303	-2.482525
28	6	0	0.132998	5.035050	-2.879351
29	1	0	-0.114834	5.177587	-3.924675
30	6	0	0.147391	3.753325	-2.347440
31	1	0	-0.093153	2.913199	-2.987859
32	6	0	2.116434	1.208874	-0.850646
33	6	0	2.666779	1.694674	-2.033995
34	1	0	2.214470	2.541817	-2.527834
35	6	0	3.792863	1.127012	-2.638536
36	1	0	4.199097	1.521092	-3.560162
37	6	0	4.346128	0.044305	-2.009887
38	6	0	5.430961	-1.798567	-1.473113
39	1	0	6.443775	-2.003520	-1.130317
40	1	0	4.986284	-2.658632	-1.989321
41	6	0	3.832413	-0.429807	-0.812528
42	6	0	2.724680	0.107331	-0.197353
43	6	0	2.362334	-0.431427	1.138056
44	6	0	3.241517	-0.189508	2.166963
45	6	0	5.017565	0.338620	3.361233
46	1	0	5.804351	-0.409790	3.200443
47	1	0	5.420578	1.267570	3.760831
48	6	0	3.053061	-0.656188	3.456319
49	6	0	1.970056	-1.429702	3.775984
50	1	0	1.811784	-1.805410	4.777930
51	6	0	1.070580	-1.708662	2.740934
52	1	0	0.228767	-2.342696	2.973837
53	6	0	1.229133	-1.219479	1.446512
54	6	0	0.968268	-2.651287	-1.008111
55	6	0	0.568042	-2.818899	-2.333479
56	1	0	-0.308424	-2.304034	-2.704723

57	6	0	1.268311	-3.672540	-3.176499
58	1	0	0.945852	-3.788885	-4.204465
59	6	0	2.369710	-4.373553	-2.702909
60	1	0	2.914418	-5.041056	-3.361514
61	6	0	2.763726	-4.224390	-1.377956
62	1	0	3.613187	-4.779167	-0.994476
63	6	0	2.068278	-3.368954	-0.534444
64	1	0	2.390722	-3.256013	0.493324
65	6	0	-1.128853	-2.747601	0.947684
66	6	0	-1.257907	-4.074257	0.550205
67	1	0	-0.666673	-4.458994	-0.271353
68	6	0	-2.163440	-4.910637	1.193830
69	1	0	-2.264892	-5.939091	0.866837
70	6	0	-2.935859	-4.434730	2.243695
71	1	0	-3.638322	-5.091145	2.744644
72	6	0	-2.806913	-3.110698	2.649671
73	1	0	-3.400476	-2.722546	3.469747
74	6	0	-1.917424	-2.271915	1.995717
75	1	0	-1.820164	-1.242972	2.325045
76	6	0	-0.418352	0.270927	-2.644621
77	6	0	-2.524370	1.840282	-1.749813
78	1	0	-3.039191	1.475517	-2.639180
79	1	0	-2.046228	2.789028	-1.981144
80	6	0	-3.472573	1.951055	-0.619200
81	6	0	-3.533486	2.897713	0.338046
82	6	0	-4.598079	2.865664	1.399240
83	1	0	-5.306401	2.049465	1.244869
84	1	0	-4.159284	2.757161	2.398056
85	1	0	-5.165048	3.803155	1.400863
86	6	0	-2.617333	4.083625	0.421381
87	1	0	-1.941286	3.998034	1.280711
88	1	0	-2.010989	4.213694	-0.472162
89	1	0	-3.200711	4.998300	0.571103
90	1	0	-4.232703	1.173256	-0.585081
91	8	0	-3.820661	0.092234	3.311500
92	6	0	-4.206564	-0.207182	2.207095
93	1	0	-3.602498	0.040110	1.313697
94	6	0	-5.478088	-0.934208	1.905779
95	1	0	-6.079451	-0.341727	1.209333
96	1	0	-5.224603	-1.861626	1.382080
97	1	0	-6.039249	-1.140893	2.817030

TS1A (NIMAG=1, 65.6*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.303778	0.404226	-0.814866
2	53	0	-3.445053	-1.246085	-1.440593
3	15	0	0.538873	1.787584	-0.371921
4	15	0	-0.161037	-1.610054	0.159313
5	8	0	5.282960	-1.089836	-2.512911

6	8	0	4.478669	-1.735507	-0.465964
7	8	0	4.367677	0.419807	1.928792
8	8	0	4.066107	-0.210007	4.113068
9	8	0	-0.362665	0.236943	-3.595150
10	6	0	0.948707	2.141767	1.374838
11	6	0	0.017685	1.835982	2.362040
12	1	0	-0.944841	1.411547	2.098306
13	6	0	0.325217	2.054673	3.700041
14	1	0	-0.401609	1.797477	4.461612
15	6	0	1.556997	2.587542	4.054390
16	1	0	1.799469	2.749337	5.098585
17	6	0	2.487311	2.902622	3.068834
18	1	0	3.452921	3.313346	3.341737
19	6	0	2.188760	2.674162	1.734569
20	1	0	2.932450	2.879501	0.972223
21	6	0	0.559224	3.455872	-1.165623
22	6	0	0.860840	4.618232	-0.456234
23	1	0	1.094011	4.570345	0.598991
24	6	0	0.839060	5.858754	-1.083360
25	1	0	1.070697	6.749127	-0.510112
26	6	0	0.516315	5.958857	-2.428461
27	1	0	0.497832	6.927081	-2.915575
28	6	0	0.200302	4.810159	-3.143578
29	1	0	-0.072828	4.874238	-4.190345
30	6	0	0.210966	3.573682	-2.515726
31	1	0	-0.070350	2.698007	-3.087039
32	6	0	2.080332	1.002651	-1.017016
33	6	0	2.602480	1.398724	-2.243749
34	1	0	2.174818	2.245043	-2.760388
35	6	0	3.680666	0.749183	-2.854155
36	1	0	4.072406	1.075639	-3.807985
37	6	0	4.215861	-0.314872	-2.180262
38	6	0	5.281608	-2.149021	-1.563080
39	1	0	6.299370	-2.327843	-1.218344
40	1	0	4.838910	-3.042369	-2.019424
41	6	0	3.720811	-0.708314	-0.946429
42	6	0	2.654321	-0.096828	-0.327439
43	6	0	2.301303	-0.558107	1.043589
44	6	0	3.213191	-0.296340	2.039540
45	6	0	5.025552	0.266401	3.177423
46	1	0	5.832511	-0.469980	3.075049
47	1	0	5.404612	1.232890	3.508668
48	6	0	3.036023	-0.681217	3.357802
49	6	0	1.941736	-1.407782	3.741246
50	1	0	1.799477	-1.727740	4.764771
51	6	0	1.012112	-1.716062	2.741638
52	1	0	0.160499	-2.316074	3.023741
53	6	0	1.152779	-1.297939	1.421832
54	6	0	0.741775	-2.653794	-1.059472
55	6	0	0.266264	-2.767935	-2.364565
56	1	0	-0.614188	-2.219879	-2.672009
57	6	0	0.889710	-3.618968	-3.269062
58	1	0	0.510046	-3.691174	-4.281435

59	6	0	1.982918	-4.378150	-2.873885
60	1	0	2.465180	-5.046530	-3.578589
61	6	0	2.445821	-4.289126	-1.565614
62	1	0	3.283496	-4.896467	-1.239926
63	6	0	1.831460	-3.431708	-0.664055
64	1	0	2.204577	-3.368533	0.350889
65	6	0	-1.226731	-2.882770	0.964480
66	6	0	-1.358999	-4.166806	0.439206
67	1	0	-0.807058	-4.457705	-0.444707
68	6	0	-2.214744	-5.087664	1.032233
69	1	0	-2.311984	-6.077591	0.601448
70	6	0	-2.941196	-4.744879	2.162584
71	1	0	-3.605152	-5.466217	2.625440
72	6	0	-2.814601	-3.466943	2.693892
73	1	0	-3.374327	-3.186358	3.579255
74	6	0	-1.975851	-2.540358	2.091885
75	1	0	-1.906219	-1.543236	2.506096
76	6	0	-0.705385	0.276994	-2.494557
77	6	0	-2.514554	2.052435	-1.484563
78	1	0	-2.967444	1.791547	-2.443111
79	1	0	-1.933728	2.961447	-1.623126
80	6	0	-3.583973	2.246989	-0.477599
81	6	0	-3.596252	3.079224	0.574978
82	6	0	-4.796414	3.179806	1.476890
83	1	0	-5.604202	2.515927	1.158784
84	1	0	-4.529872	2.935677	2.513406
85	1	0	-5.189230	4.203129	1.489378
86	6	0	-2.461673	3.985582	0.951487
87	1	0	-2.064434	3.718673	1.938013
88	1	0	-1.641872	3.950257	0.237154
89	1	0	-2.803602	5.025093	1.017938
90	1	0	-4.473071	1.639562	-0.636170
91	8	0	-2.871677	0.415330	2.324350
92	6	0	-4.013382	0.109120	2.069649
93	1	0	-4.432133	0.324900	1.075521
94	6	0	-4.925602	-0.589569	3.025199
95	1	0	-5.840081	-0.001348	3.149157
96	1	0	-5.216483	-1.546204	2.579116
97	1	0	-4.443128	-0.750346	3.989513

D (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.359793	0.000384	-0.592269
2	53	0	-3.138123	-2.128362	-1.116826
3	15	0	0.149401	1.792402	-0.424120
4	15	0	0.198129	-1.610997	0.378059
5	8	0	4.946766	-0.442305	-3.117528
6	8	0	4.551048	-1.046438	-0.945271
7	8	0	4.424613	1.363280	1.319132

8	8	0	4.537166	0.912481	3.570991
9	8	0	-0.581329	-0.234209	-3.449681
10	6	0	0.781464	2.428737	1.180328
11	6	0	0.197548	2.050325	2.385971
12	1	0	-0.659632	1.389975	2.377330
13	6	0	0.730105	2.500148	3.589192
14	1	0	0.282871	2.183817	4.524773
15	6	0	1.835544	3.339491	3.596390
16	1	0	2.253282	3.681507	4.536456
17	6	0	2.410426	3.735388	2.393128
18	1	0	3.271934	4.393996	2.389773
19	6	0	1.892411	3.276072	1.192222
20	1	0	2.365781	3.559385	0.258513
21	6	0	-0.359142	3.345831	-1.279442
22	6	0	-0.441140	4.564508	-0.606977
23	1	0	-0.153748	4.635355	0.433778
24	6	0	-0.907998	5.703239	-1.254900
25	1	0	-0.966634	6.639127	-0.710954
26	6	0	-1.299007	5.642609	-2.583953
27	1	0	-1.661517	6.531082	-3.088282
28	6	0	-1.242252	4.429106	-3.259531
29	1	0	-1.570565	4.360452	-4.290030
30	6	0	-0.792859	3.290373	-2.609309
31	1	0	-0.812098	2.345772	-3.139043
32	6	0	1.720995	1.289783	-1.254692
33	6	0	2.013010	1.690758	-2.552117
34	1	0	1.398942	2.436980	-3.034107
35	6	0	3.082457	1.161324	-3.285595
36	1	0	3.291412	1.485666	-4.296078
37	6	0	3.842630	0.209697	-2.662441
38	6	0	5.202410	-1.447164	-2.142498
39	1	0	6.274538	-1.514954	-1.965312
40	1	0	4.777798	-2.400330	-2.482051
41	6	0	3.589640	-0.169245	-1.351141
42	6	0	2.548806	0.334090	-0.607792
43	6	0	2.481173	-0.045194	0.830658
44	6	0	3.448132	0.477748	1.657257
45	6	0	5.212620	1.542301	2.487134
46	1	0	6.190102	1.068827	2.342273
47	1	0	5.312031	2.608716	2.696348
48	6	0	3.523951	0.198855	3.011561
49	6	0	2.656153	-0.678505	3.603806
50	1	0	2.721868	-0.921185	4.656044
51	6	0	1.677782	-1.247089	2.779313
52	1	0	1.005040	-1.964995	3.224334
53	6	0	1.556748	-0.935754	1.428672
54	6	0	1.143611	-2.712885	-0.752466
55	6	0	0.622777	-3.049671	-2.001073
56	1	0	-0.338192	-2.661935	-2.311663
57	6	0	1.313593	-3.915152	-2.840211
58	1	0	0.895818	-4.164725	-3.808456
59	6	0	2.525446	-4.460650	-2.436974
60	1	0	3.061593	-5.139319	-3.091380

61	6	0	3.043242	-4.141150	-1.186602
62	1	0	3.984161	-4.569512	-0.858800
63	6	0	2.358283	-3.271440	-0.349692
64	1	0	2.777125	-3.020738	0.617439
65	6	0	-0.634562	-2.815905	1.493258
66	6	0	-0.731936	-4.164796	1.160722
67	1	0	-0.259640	-4.539885	0.261807
68	6	0	-1.454296	-5.039501	1.963895
69	1	0	-1.528566	-6.083307	1.681740
70	6	0	-2.084921	-4.581795	3.110937
71	1	0	-2.650047	-5.265665	3.733867
72	6	0	-1.988873	-3.238282	3.455334
73	1	0	-2.469335	-2.871932	4.356471
74	6	0	-1.277163	-2.362627	2.649299
75	1	0	-1.210494	-1.318187	2.926465
76	6	0	-0.845737	-0.164045	-2.331422
77	6	0	-2.986996	1.310044	-1.310175
78	1	0	-3.227985	0.952683	-2.313600
79	1	0	-2.603389	2.323389	-1.395823
80	6	0	-4.229471	1.331210	-0.513682
81	6	0	-4.509177	2.195646	0.480446
82	6	0	-5.874179	2.267032	1.109088
83	1	0	-6.499845	1.421444	0.812618
84	1	0	-5.820762	2.295814	2.204205
85	1	0	-6.389424	3.186528	0.805916
86	6	0	-3.500528	3.223848	0.922902
87	1	0	-2.508691	2.774477	1.041194
88	1	0	-3.394127	4.028560	0.185893
89	1	0	-3.783970	3.681205	1.875253
90	1	0	-4.993173	0.602687	-0.780815
91	8	0	-2.191373	0.305632	1.420261
92	6	0	-3.322330	0.000796	1.785527
93	1	0	-3.948563	-0.632859	1.150437
94	6	0	-3.798357	0.326242	3.158453
95	1	0	-4.867035	0.542503	3.156189
96	1	0	-3.648737	-0.566984	3.776951
97	1	0	-3.234994	1.158184	3.582808

TS1B (NIMAG=1, 335.1*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.355334	0.068677	-0.603545
2	53	0	-3.297235	-1.940312	-1.067562
3	15	0	0.287592	1.746545	-0.490456
4	15	0	0.063944	-1.609967	0.348546
5	8	0	5.118750	-0.724254	-2.909627
6	8	0	4.586161	-1.276336	-0.751178
7	8	0	4.444255	1.090334	1.465250
8	8	0	4.368276	0.709017	3.734246
9	8	0	-0.600503	-0.332481	-3.459716

10	6	0	0.923154	2.429618	1.092183
11	6	0	0.296813	2.146426	2.302990
12	1	0	-0.590730	1.524954	2.305829
13	6	0	0.824076	2.646426	3.488960
14	1	0	0.342840	2.406466	4.430329
15	6	0	1.963301	3.438998	3.472573
16	1	0	2.372556	3.823193	4.400216
17	6	0	2.581604	3.736733	2.261779
18	1	0	3.467997	4.361327	2.239432
19	6	0	2.071216	3.226614	1.078377
20	1	0	2.573986	3.436473	0.140524
21	6	0	-0.132020	3.279389	-1.427873
22	6	0	-0.202539	4.522583	-0.800396
23	1	0	0.053930	4.621813	0.246214
24	6	0	-0.617672	5.649415	-1.502689
25	1	0	-0.669480	6.604908	-0.993297
26	6	0	-0.965448	5.552482	-2.841253
27	1	0	-1.286871	6.431729	-3.387770
28	6	0	-0.918063	4.314768	-3.472998
29	1	0	-1.211579	4.219217	-4.511877
30	6	0	-0.521365	3.188553	-2.769593
31	1	0	-0.548776	2.227394	-3.267836
32	6	0	1.844792	1.128429	-1.264033
33	6	0	2.210520	1.486067	-2.555408
34	1	0	1.646851	2.240019	-3.084409
35	6	0	3.301451	0.909781	-3.217990
36	1	0	3.572046	1.201692	-4.223736
37	6	0	4.006695	-0.039214	-2.529360
38	6	0	5.310079	-1.704806	-1.896418
39	1	0	6.368964	-1.769978	-1.650623
40	1	0	4.906187	-2.664900	-2.240645
41	6	0	3.674187	-0.381604	-1.226239
42	6	0	2.607029	0.164333	-0.552849
43	6	0	2.431235	-0.177646	0.885243
44	6	0	3.374740	0.304229	1.762521
45	6	0	5.101024	1.354939	2.697189
46	1	0	6.115618	0.948164	2.661767
47	1	0	5.107663	2.432685	2.879461
48	6	0	3.334043	0.070813	3.126999
49	6	0	2.355995	-0.707235	3.685142
50	1	0	2.325105	-0.906586	4.747954
51	6	0	1.396333	-1.233168	2.811943
52	1	0	0.628900	-1.867441	3.231064
53	6	0	1.403917	-0.977737	1.444874
54	6	0	0.986259	-2.734079	-0.775253
55	6	0	0.416849	-3.124404	-1.986881
56	1	0	-0.554774	-2.746910	-2.278239
57	6	0	1.071331	-4.031982	-2.809741
58	1	0	0.617120	-4.322376	-3.749749
59	6	0	2.293050	-4.569469	-2.425384
60	1	0	2.800544	-5.281410	-3.066985
61	6	0	2.855196	-4.201411	-1.208450
62	1	0	3.799559	-4.629589	-0.890187

63	6	0	2.206867	-3.288997	-0.387375
64	1	0	2.658318	-3.006467	0.555707
65	6	0	-0.824657	-2.803718	1.430008
66	6	0	-0.767647	-4.178985	1.221336
67	1	0	-0.167570	-4.588871	0.419234
68	6	0	-1.501588	-5.040946	2.028729
69	1	0	-1.457786	-6.108549	1.846208
70	6	0	-2.292475	-4.541612	3.052735
71	1	0	-2.868495	-5.216752	3.675395
72	6	0	-2.348729	-3.169474	3.270523
73	1	0	-2.968171	-2.768263	4.065211
74	6	0	-1.625877	-2.308584	2.460746
75	1	0	-1.681085	-1.239666	2.614607
76	6	0	-0.857710	-0.208855	-2.344976
77	6	0	-2.922645	1.564361	-1.366419
78	1	0	-3.117063	1.205381	-2.375024
79	1	0	-2.447765	2.538554	-1.357548
80	6	0	-4.067853	1.485865	-0.529676
81	6	0	-4.265204	2.165991	0.659906
82	6	0	-5.672691	2.236648	1.210392
83	1	0	-6.196213	1.282665	1.097170
84	1	0	-5.681136	2.513723	2.267402
85	1	0	-6.253835	2.998580	0.679085
86	6	0	-3.336868	3.299120	1.021198
87	1	0	-2.294267	2.970888	0.989937
88	1	0	-3.439887	4.133251	0.317883
89	1	0	-3.545784	3.681035	2.024076
90	1	0	-4.829665	0.759071	-0.804433
91	8	0	-2.113526	0.580342	1.333382
92	6	0	-3.334448	0.516455	1.684470
93	1	0	-3.971098	-0.250918	1.235848
94	6	0	-3.634976	0.850049	3.123058
95	1	0	-4.704321	0.895380	3.324267
96	1	0	-3.216160	0.046612	3.739705
97	1	0	-3.155570	1.785649	3.418706

E (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.434938	0.329857	-0.561471
2	53	0	-3.605442	-1.463513	-1.023213
3	15	0	0.527867	1.682990	-0.519116
4	15	0	-0.274166	-1.552646	0.289295
5	8	0	5.025590	-1.483520	-2.788911
6	8	0	4.370869	-1.913751	-0.633048
7	8	0	4.483387	0.340060	1.564733
8	8	0	4.223077	0.039731	3.831933
9	8	0	-0.911555	-0.125961	-3.485576
10	6	0	1.300449	2.291807	1.030810
11	6	0	0.665516	2.126129	2.258719

12	1	0	-0.293352	1.612603	2.282882
13	6	0	1.284205	2.580437	3.418860
14	1	0	0.794312	2.433906	4.374949
15	6	0	2.523034	3.202940	3.359091
16	1	0	3.000663	3.553344	4.267514
17	6	0	3.156713	3.370153	2.130303
18	1	0	4.125044	3.855645	2.075580
19	6	0	2.553997	2.908072	0.971096
20	1	0	3.062004	3.018422	0.019033
21	6	0	0.384721	3.238087	-1.507126
22	6	0	0.500149	4.488507	-0.899911
23	1	0	0.747385	4.564861	0.150651
24	6	0	0.281047	5.654523	-1.626464
25	1	0	0.370088	6.614219	-1.130533
26	6	0	-0.051593	5.591652	-2.970751
27	1	0	-0.219946	6.501058	-3.536005
28	6	0	-0.184548	4.350982	-3.584463
29	1	0	-0.464749	4.284961	-4.629377
30	6	0	0.017060	3.188425	-2.857512
31	1	0	-0.150526	2.237664	-3.347029
32	6	0	1.947869	0.781629	-1.285000
33	6	0	2.378820	1.047583	-2.579021
34	1	0	1.930719	1.850256	-3.143800
35	6	0	3.407990	0.326493	-3.195946
36	1	0	3.731638	0.551160	-4.203273
37	6	0	3.990673	-0.667074	-2.457166
38	6	0	5.109680	-2.431816	-1.731295
39	1	0	6.151655	-2.556580	-1.438333
40	1	0	4.659692	-3.376534	-2.057916
41	6	0	3.589475	-0.927936	-1.155815
42	6	0	2.573222	-0.244736	-0.529501
43	6	0	2.292706	-0.533278	0.901066
44	6	0	3.268498	-0.217068	1.817506
45	6	0	5.097013	0.550085	2.829182
46	1	0	6.045631	0.008652	2.865738
47	1	0	5.239470	1.622686	2.988320
48	6	0	3.114151	-0.398464	3.181791
49	6	0	1.971345	-0.943405	3.702917
50	1	0	1.844520	-1.088404	4.767307
51	6	0	0.972154	-1.300696	2.790955
52	1	0	0.068204	-1.746056	3.179886
53	6	0	1.105752	-1.108108	1.420832
54	6	0	0.520119	-2.720842	-0.884181
55	6	0	-0.086569	-3.001750	-2.107061
56	1	0	-1.004119	-2.502480	-2.388098
57	6	0	0.452811	-3.960413	-2.955583
58	1	0	-0.028872	-4.162505	-3.904957
59	6	0	1.589970	-4.664206	-2.582413
60	1	0	2.005033	-5.417880	-3.242363
61	6	0	2.182187	-4.410832	-1.350500
62	1	0	3.053626	-4.974601	-1.035754
63	6	0	1.652997	-3.444670	-0.506854
64	1	0	2.126278	-3.257769	0.449102

65	6	0	-1.292246	-2.700110	1.310670
66	6	0	-1.234051	-4.080526	1.132221
67	1	0	-0.599121	-4.516239	0.372453
68	6	0	-2.016602	-4.919679	1.917562
69	1	0	-1.971018	-5.991243	1.759831
70	6	0	-2.856636	-4.392047	2.886923
71	1	0	-3.469344	-5.049978	3.493121
72	6	0	-2.916482	-3.014943	3.068071
73	1	0	-3.579506	-2.590050	3.813404
74	6	0	-2.145789	-2.173809	2.281946
75	1	0	-2.192437	-1.097386	2.385771
76	6	0	-1.094211	0.013276	-2.359876
77	6	0	-2.673774	2.310089	-1.437249
78	1	0	-2.890420	1.992624	-2.450822
79	1	0	-2.014083	3.156129	-1.320872
80	6	0	-3.450051	1.886444	-0.414048
81	6	0	-3.469229	2.403494	0.998368
82	6	0	-4.917029	2.828930	1.295746
83	1	0	-5.600022	1.977103	1.227594
84	1	0	-4.994768	3.250391	2.300993
85	1	0	-5.253402	3.592036	0.587884
86	6	0	-2.523069	3.583848	1.208778
87	1	0	-1.484507	3.293788	1.047195
88	1	0	-2.762415	4.405668	0.527329
89	1	0	-2.605179	3.966599	2.228639
90	1	0	-4.230725	1.166874	-0.632391
91	8	0	-1.817221	0.707160	1.473989
92	6	0	-3.064266	1.168820	1.867246
93	1	0	-3.845882	0.407987	1.679117
94	6	0	-3.041012	1.445694	3.369423
95	1	0	-4.008232	1.794686	3.741394
96	1	0	-2.790995	0.523329	3.899998
97	1	0	-2.278347	2.188500	3.619105

F (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.427424	1.088692	0.119728
2	53	0	3.922264	-0.136598	0.782953
3	15	0	-0.836484	1.739192	0.097857
4	15	0	0.833486	-1.206986	-0.380235
5	8	0	-3.313141	-2.086009	3.912214
6	8	0	-2.974914	-2.782212	1.756531
7	8	0	-4.415634	-1.303951	-0.653574
8	8	0	-4.518675	-2.227612	-2.758406
9	8	0	1.232577	1.128403	3.117533
10	6	0	-1.745962	0.655298	1.287389
11	6	0	-2.004952	1.075223	2.585678
12	1	0	-1.793415	2.095180	2.872106
13	6	0	-2.530947	0.224058	3.565426

14	1	0	-2.723640	0.569853	4.572003
15	6	0	-2.782293	-1.066371	3.186009
16	6	0	-3.171914	-3.238116	3.087138
17	1	0	-4.084637	-3.830386	3.134576
18	1	0	-2.291440	-3.808676	3.406309
19	6	0	-2.563783	-1.490576	1.882604
20	6	0	-2.049478	-0.678522	0.898697
21	6	0	-1.972241	-1.238187	-0.479762
22	6	0	-3.156227	-1.523938	-1.118471
23	6	0	-5.296973	-1.657695	-1.709739
24	1	0	-6.015951	-2.396508	-1.349517
25	1	0	-5.797546	-0.757707	-2.080891
26	6	0	-3.219499	-2.084508	-2.384326
27	6	0	-2.085431	-2.417632	-3.074943
28	1	0	-2.130139	-2.867700	-4.057799
29	6	0	-0.864343	-2.139649	-2.447512
30	1	0	0.046433	-2.399577	-2.969302
31	6	0	-0.787900	-1.557026	-1.187891
32	6	0	1.294857	1.029618	1.974897
33	6	0	2.242779	3.138390	0.229402
34	1	0	2.989959	3.339547	0.991564
35	1	0	1.408830	3.829219	0.236564
36	6	0	2.710556	2.606543	-1.002823
37	6	0	1.779043	2.270174	-2.000226
38	1	0	2.221907	1.748026	-2.847742
39	6	0	4.176168	2.433191	-1.294233
40	1	0	4.378820	1.527569	-1.867776
41	1	0	4.463144	3.298046	-1.905670
42	1	0	4.790626	2.423866	-0.397087
43	6	0	0.753550	3.303082	-2.432726
44	1	0	1.285884	4.108461	-2.953987
45	1	0	0.013207	2.914158	-3.127874
46	1	0	0.223214	3.766217	-1.601328
47	6	0	-1.959417	1.585144	-1.355797
48	6	0	-3.324113	1.830611	-1.187862
49	6	0	-1.501642	1.133331	-2.588392
50	6	0	-4.203417	1.671714	-2.249208
51	1	0	-3.704743	2.133028	-0.218523
52	6	0	-2.382293	0.959495	-3.647106
53	1	0	-0.455754	0.879185	-2.702250
54	6	0	-3.733185	1.237614	-3.483410
55	1	0	-5.258551	1.877491	-2.106848
56	1	0	-2.012978	0.588711	-4.595953
57	1	0	-4.420163	1.100054	-4.310814
58	6	0	-1.154184	3.466506	0.678581
59	6	0	-1.889028	4.389337	-0.067359
60	6	0	-0.544549	3.907646	1.858671
61	6	0	-2.040957	5.699932	0.371008
62	1	0	-2.337464	4.098934	-1.008147
63	6	0	-0.710084	5.210670	2.303997
64	1	0	0.087479	3.240784	2.430378
65	6	0	-1.463141	6.112595	1.562379
66	1	0	-2.612184	6.398780	-0.229295

67	1	0	-0.231875	5.523702	3.224823
68	1	0	-1.584096	7.134147	1.904061
69	6	0	0.688919	-2.437233	0.997899
70	6	0	0.022956	-3.645406	0.766624
71	6	0	1.226409	-2.205126	2.261037
72	6	0	-0.092238	-4.596356	1.769862
73	1	0	-0.415685	-3.847247	-0.203103
74	6	0	1.095020	-3.149131	3.272259
75	1	0	1.778078	-1.300168	2.460816
76	6	0	0.439997	-4.348648	3.030078
77	1	0	-0.606800	-5.528734	1.565758
78	1	0	1.519738	-2.944073	4.247925
79	1	0	0.349385	-5.089990	3.816774
80	6	0	2.010248	-2.001577	-1.548405
81	6	0	2.581633	-3.250552	-1.325326
82	6	0	2.353551	-1.294545	-2.700791
83	6	0	3.477155	-3.784055	-2.245291
84	1	0	2.352422	-3.803452	-0.423423
85	6	0	3.236956	-1.832097	-3.624074
86	1	0	1.933167	-0.309208	-2.861470
87	6	0	3.804031	-3.081153	-3.396155
88	1	0	3.927815	-4.750879	-2.052245
89	1	0	3.494980	-1.269459	-4.514260
90	1	0	4.506744	-3.498467	-4.108449

G (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.450357	0.885311	-0.318518
2	53	0	-3.938125	-0.304638	-0.877478
3	15	0	0.746951	1.713262	-0.269808
4	15	0	-0.729581	-1.343693	0.385730
5	8	0	3.511437	-2.286332	-3.678241
6	8	0	3.191616	-2.812778	-1.472909
7	8	0	4.476687	-0.945645	0.915089
8	8	0	4.534184	-1.586692	3.116510
9	8	0	-1.205525	0.727600	-3.255560
10	6	0	1.729482	1.764221	1.282525
11	6	0	1.108184	1.581868	2.514065
12	1	0	0.034054	1.438609	2.555981
13	6	0	1.855301	1.574043	3.684607
14	1	0	1.360466	1.417013	4.635944
15	6	0	3.231285	1.753850	3.634393
16	1	0	3.815008	1.740247	4.547566
17	6	0	3.861086	1.929493	2.407760
18	1	0	4.936871	2.054513	2.358946
19	6	0	3.116502	1.922175	1.237564
20	1	0	3.620810	2.005023	0.281078
21	6	0	1.027788	3.375711	-1.027337
22	6	0	1.931385	4.308507	-0.515592

23	1	0	2.508142	4.085168	0.371294
24	6	0	2.079080	5.554653	-1.110714
25	1	0	2.780632	6.266074	-0.690153
26	6	0	1.329104	5.891949	-2.229077
27	1	0	1.444090	6.865938	-2.690816
28	6	0	0.419575	4.977126	-2.742416
29	1	0	-0.184649	5.230339	-3.605720
30	6	0	0.263541	3.735682	-2.141064
31	1	0	-0.472404	3.051819	-2.541404
32	6	0	1.766779	0.578126	-1.310379
33	6	0	2.010066	0.898003	-2.640408
34	1	0	1.728440	1.872546	-3.015344
35	6	0	2.594006	-0.003053	-3.539526
36	1	0	2.769688	0.261823	-4.573347
37	6	0	2.918552	-1.237699	-3.046394
38	6	0	3.406303	-3.370832	-2.761970
39	1	0	4.337620	-3.934914	-2.761147
40	1	0	2.544814	-3.993794	-3.032299
41	6	0	2.711664	-1.560205	-1.711722
42	6	0	2.138121	-0.698855	-0.806838
43	6	0	2.050967	-1.140970	0.612409
44	6	0	3.217519	-1.257414	1.329890
45	6	0	5.335050	-1.382126	1.958675
46	1	0	5.807084	-2.329160	1.669104
47	1	0	6.076879	-0.610798	2.164265
48	6	0	3.253247	-1.648740	2.659658
49	6	0	2.112201	-1.987495	3.336790
50	1	0	2.136700	-2.294223	4.373967
51	6	0	0.911758	-1.906042	2.621181
52	1	0	-0.003782	-2.181846	3.126695
53	6	0	0.862258	-1.488743	1.295457
54	6	0	-0.529566	-2.699346	-0.840565
55	6	0	-1.121068	-2.612099	-2.099247
56	1	0	-1.726601	-1.754867	-2.357504
57	6	0	-0.960136	-3.637552	-3.022606
58	1	0	-1.425077	-3.553067	-3.997756
59	6	0	-0.216930	-4.764093	-2.695125
60	1	0	-0.099739	-5.566987	-3.414906
61	6	0	0.373076	-4.860682	-1.439560
62	1	0	0.956323	-5.735644	-1.174787
63	6	0	0.224876	-3.831405	-0.520705
64	1	0	0.707834	-3.906164	0.446626
65	6	0	-1.922845	-1.979044	1.623970
66	6	0	-2.394906	-3.286898	1.635396
67	1	0	-2.061664	-3.992083	0.883571
68	6	0	-3.317278	-3.687162	2.596188
69	1	0	-3.690684	-4.704788	2.588289
70	6	0	-3.768405	-2.788139	3.552300
71	1	0	-4.493486	-3.101838	4.294576
72	6	0	-3.300754	-1.478159	3.545070
73	1	0	-3.661716	-0.763994	4.276207
74	6	0	-2.389017	-1.076590	2.582221
75	1	0	-2.053565	-0.042371	2.566024

76	6	0	-1.297382	0.775740	-2.107291
77	6	0	-2.448491	2.765458	-0.278108
78	1	0	-3.383441	2.726558	-0.835676
79	1	0	-1.850849	3.609863	-0.618004
80	6	0	-2.674195	2.765294	1.193540
81	6	0	-1.832108	3.356108	2.074496
82	1	0	-2.088139	3.273281	3.130388
83	6	0	-3.954714	2.176359	1.752675
84	1	0	-4.012503	2.331229	2.833053
85	1	0	-4.808740	2.682437	1.291871
86	1	0	-4.081976	1.115850	1.541106
87	6	0	-0.710041	4.300433	1.784832
88	1	0	-0.945961	5.271275	2.235478
89	1	0	0.236676	3.976398	2.225473
90	1	0	-0.554067	4.461175	0.720419

H (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.321323	0.242208	-0.776334
2	53	0	-3.217395	-1.690997	-1.337798
3	15	0	0.391293	1.806372	-0.398018
4	15	0	0.035254	-1.597518	0.221715
5	8	0	5.203631	-0.751175	-2.770296
6	8	0	4.581877	-1.402296	-0.663833
7	8	0	4.450301	0.830208	1.734431
8	8	0	4.294446	0.233138	3.942952
9	8	0	-0.421887	0.085921	-3.570207
10	6	0	0.825633	2.199225	1.334490
11	6	0	-0.018184	1.781521	2.358397
12	1	0	-0.937931	1.247596	2.141469
13	6	0	0.309324	2.036988	3.683973
14	1	0	-0.357238	1.697667	4.467794
15	6	0	1.480969	2.715140	3.991033
16	1	0	1.741734	2.908013	5.025446
17	6	0	2.328702	3.136824	2.971259
18	1	0	3.248359	3.659855	3.208133
19	6	0	2.006742	2.875377	1.648383
20	1	0	2.688710	3.170042	0.858043
21	6	0	0.210100	3.460425	-1.196222
22	6	0	0.400168	4.654510	-0.501358
23	1	0	0.671794	4.641164	0.545826
24	6	0	0.217651	5.879160	-1.133059
25	1	0	0.364994	6.794875	-0.572066
26	6	0	-0.157134	5.930765	-2.467531
27	1	0	-0.300252	6.886712	-2.958160
28	6	0	-0.366074	4.748243	-3.166502
29	1	0	-0.680074	4.772995	-4.203418
30	6	0	-0.196554	3.526090	-2.533423
31	1	0	-0.400345	2.618954	-3.088811

32	6	0	1.970583	1.157273	-1.101607
33	6	0	2.390308	1.567903	-2.362302
34	1	0	1.872422	2.371224	-2.865081
35	6	0	3.472131	0.982177	-3.029295
36	1	0	3.781319	1.317562	-4.009977
37	6	0	4.115168	-0.035998	-2.379185
38	6	0	5.316547	-1.798986	-1.813798
39	1	0	6.363373	-1.932890	-1.545354
40	1	0	4.875257	-2.714718	-2.226022
41	6	0	3.728280	-0.436539	-1.108775
42	6	0	2.666954	0.117327	-0.431042
43	6	0	2.433758	-0.334218	0.967119
44	6	0	3.366201	0.023968	1.911665
45	6	0	5.172280	0.759309	2.955181
46	1	0	6.029209	0.085176	2.832254
47	1	0	5.488262	1.760047	3.248171
48	6	0	3.275244	-0.339119	3.245507
49	6	0	2.254766	-1.131421	3.698032
50	1	0	2.179246	-1.425871	4.736169
51	6	0	1.305238	-1.532526	2.751672
52	1	0	0.500451	-2.170478	3.086524
53	6	0	1.363268	-1.142512	1.417061
54	6	0	0.943333	-2.696357	-0.939267
55	6	0	0.453856	-2.913625	-2.226446
56	1	0	-0.457110	-2.429005	-2.551140
57	6	0	1.111307	-3.779854	-3.090910
58	1	0	0.719994	-3.934619	-4.089490
59	6	0	2.256316	-4.446655	-2.675183
60	1	0	2.765825	-5.125911	-3.349763
61	6	0	2.739997	-4.248070	-1.386814
62	1	0	3.625064	-4.775352	-1.047636
63	6	0	2.090098	-3.376492	-0.523975
64	1	0	2.482142	-3.221785	0.473917
65	6	0	-0.970643	-2.774540	1.202949
66	6	0	-0.995163	-4.143172	0.957982
67	1	0	-0.385763	-4.569093	0.170439
68	6	0	-1.823481	-4.969910	1.709518
69	1	0	-1.846157	-6.033748	1.502635
70	6	0	-2.622728	-4.438875	2.711853
71	1	0	-3.268618	-5.087144	3.293217
72	6	0	-2.596076	-3.071020	2.963413
73	1	0	-3.214204	-2.643592	3.745303
74	6	0	-1.781384	-2.244170	2.206672
75	1	0	-1.775698	-1.177956	2.410021
76	6	0	-0.749306	0.135056	-2.466114
77	6	0	-2.745121	1.750777	-1.401260
78	1	0	-3.154430	1.453854	-2.369462
79	1	0	-2.232179	2.700564	-1.544005
80	6	0	-3.886044	1.960136	-0.445933
81	6	0	-3.826785	2.736003	0.649732
82	1	0	-4.748602	2.875280	1.212943
83	6	0	-5.219653	1.362988	-0.825712
84	1	0	-6.019642	1.725439	-0.174371

85	1	0	-5.473880	1.636865	-1.854484
86	1	0	-5.199290	0.271679	-0.793102
87	6	0	-2.660415	3.504601	1.175388
88	1	0	-2.891690	4.574810	1.218514
89	1	0	-2.408259	3.188910	2.193295
90	1	0	-1.775025	3.387517	0.554548
91	8	0	-3.037529	0.589015	3.085732
92	6	0	-4.002048	0.240861	2.443628
93	1	0	-3.879424	-0.351941	1.516979
94	6	0	-5.418015	0.505502	2.852126
95	1	0	-5.985971	0.882933	1.999452
96	1	0	-5.873211	-0.448469	3.140858
97	1	0	-5.458619	1.202674	3.688777

TS2A (NIMAG=1, 48.9*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.376517	0.216267	-0.673027
2	53	0	-3.301027	-1.707341	-1.164253
3	15	0	0.349910	1.795677	-0.384759
4	15	0	0.043083	-1.629655	0.217587
5	8	0	5.194816	-0.635828	-2.837203
6	8	0	4.614719	-1.307996	-0.724336
7	8	0	4.450818	0.863415	1.664253
8	8	0	4.319437	0.279157	3.880144
9	8	0	-0.604221	0.069046	-3.503722
10	6	0	0.886326	2.237695	1.308304
11	6	0	0.130356	1.823653	2.399650
12	1	0	-0.783451	1.258526	2.255862
13	6	0	0.551030	2.119262	3.690801
14	1	0	-0.040516	1.779748	4.532801
15	6	0	1.722553	2.834875	3.895791
16	1	0	2.053885	3.058024	4.903582
17	6	0	2.479248	3.255503	2.806454
18	1	0	3.397807	3.810415	2.961374
19	6	0	2.068553	2.951706	1.517867
20	1	0	2.680322	3.247456	0.672510
21	6	0	0.110010	3.434945	-1.200598
22	6	0	0.261997	4.639944	-0.515358
23	1	0	0.547306	4.644078	0.528136
24	6	0	0.025509	5.853208	-1.151578
25	1	0	0.144591	6.776928	-0.597034
26	6	0	-0.366517	5.882986	-2.481457
27	1	0	-0.551311	6.829841	-2.975781
28	6	0	-0.540001	4.688889	-3.170527
29	1	0	-0.868724	4.695038	-4.203155
30	6	0	-0.317370	3.478083	-2.532620
31	1	0	-0.499023	2.561810	-3.080274
32	6	0	1.909041	1.155032	-1.141936
33	6	0	2.297469	1.572609	-2.410134

34	1	0	1.749115	2.358025	-2.908349
35	6	0	3.391397	1.022643	-3.087602
36	1	0	3.676840	1.363963	-4.073434
37	6	0	4.081882	0.035965	-2.437908
38	6	0	5.368443	-1.668501	-1.873853
39	1	0	6.421866	-1.741240	-1.606649
40	1	0	4.980600	-2.610258	-2.280371
41	6	0	3.722391	-0.374683	-1.163119
42	6	0	2.646497	0.139723	-0.476660
43	6	0	2.436836	-0.320677	0.923281
44	6	0	3.373598	0.053107	1.858216
45	6	0	5.172242	0.836575	2.887230
46	1	0	6.060323	0.203391	2.771451
47	1	0	5.440317	1.854228	3.171737
48	6	0	3.298875	-0.304078	3.194584
49	6	0	2.292391	-1.106322	3.660654
50	1	0	2.230134	-1.395503	4.701170
51	6	0	1.342002	-1.528409	2.724226
52	1	0	0.549579	-2.177311	3.068320
53	6	0	1.384907	-1.148103	1.386481
54	6	0	0.953784	-2.643226	-1.016829
55	6	0	0.396335	-2.872130	-2.273860
56	1	0	-0.556772	-2.431702	-2.535082
57	6	0	1.039421	-3.697033	-3.188226
58	1	0	0.595146	-3.860210	-4.163026
59	6	0	2.236719	-4.314320	-2.851161
60	1	0	2.734672	-4.962424	-3.563840
61	6	0	2.786422	-4.108579	-1.590748
62	1	0	3.709469	-4.603942	-1.309385
63	6	0	2.151253	-3.276756	-0.679110
64	1	0	2.592622	-3.120421	0.297647
65	6	0	-0.860890	-2.916730	1.167343
66	6	0	-0.752500	-4.276864	0.893737
67	1	0	-0.107971	-4.628241	0.098031
68	6	0	-1.491085	-5.197845	1.629044
69	1	0	-1.408227	-6.253895	1.398641
70	6	0	-2.333799	-4.770975	2.645081
71	1	0	-2.909885	-5.492366	3.213620
72	6	0	-2.442412	-3.412902	2.923925
73	1	0	-3.101907	-3.067350	3.712406
74	6	0	-1.718340	-2.492599	2.182775
75	1	0	-1.824095	-1.434293	2.390365
76	6	0	-0.880159	0.110916	-2.385350
77	6	0	-2.819406	1.730096	-1.279841
78	1	0	-3.227788	1.419607	-2.244817
79	1	0	-2.297387	2.671112	-1.443276
80	6	0	-3.972401	1.991897	-0.351143
81	6	0	-3.906058	2.779898	0.733572
82	1	0	-4.831471	2.969965	1.275419
83	6	0	-5.313684	1.435043	-0.759587
84	1	0	-6.100962	1.718243	-0.054934
85	1	0	-5.591257	1.816363	-1.748092
86	1	0	-5.284311	0.346555	-0.843278

87	6	0	-2.700535	3.465542	1.285934
88	1	0	-2.869457	4.543553	1.381818
89	1	0	-2.455878	3.084113	2.283790
90	1	0	-1.826974	3.325512	0.652523
91	8	0	-2.792405	0.472816	2.693869
92	6	0	-3.924335	0.247782	2.323882
93	1	0	-4.102220	-0.348341	1.411194
94	6	0	-5.144413	0.669801	3.081042
95	1	0	-5.885496	1.079770	2.391759
96	1	0	-5.587224	-0.222839	3.537484
97	1	0	-4.892788	1.392287	3.857275

I (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.424764	0.241229	-0.473166
2	53	0	-3.410525	-1.703057	-0.964402
3	15	0	0.333184	1.803433	-0.338913
4	15	0	-0.022166	-1.598060	0.335571
5	8	0	4.664020	-0.924493	-3.361530
6	8	0	4.316454	-1.542895	-1.184424
7	8	0	4.614063	0.733435	1.156906
8	8	0	4.769697	0.179039	3.382177
9	8	0	-0.876742	0.061811	-3.387372
10	6	0	1.133994	2.274512	1.247415
11	6	0	0.572313	1.917433	2.470052
12	1	0	-0.361933	1.371151	2.488323
13	6	0	1.223234	2.238091	3.655935
14	1	0	0.789440	1.938168	4.603117
15	6	0	2.428343	2.926406	3.630239
16	1	0	2.937145	3.167881	4.556509
17	6	0	2.986601	3.296943	2.411362
18	1	0	3.927776	3.834746	2.382233
19	6	0	2.348498	2.964939	1.226371
20	1	0	2.805953	3.224850	0.278023
21	6	0	0.020639	3.446927	-1.119227
22	6	0	0.187540	4.641936	-0.420386
23	1	0	0.545823	4.633099	0.600342
24	6	0	-0.122246	5.861248	-1.012811
25	1	0	0.011819	6.776808	-0.448055
26	6	0	-0.603917	5.906940	-2.312481
27	1	0	-0.844495	6.858136	-2.773410
28	6	0	-0.795074	4.722036	-3.012954
29	1	0	-1.195370	4.739568	-4.019874
30	6	0	-0.500369	3.505250	-2.417196
31	1	0	-0.706765	2.594624	-2.965796
32	6	0	1.773165	1.119258	-1.275597
33	6	0	2.037592	1.518135	-2.579982
34	1	0	1.492718	2.345475	-3.009451
35	6	0	2.993270	0.887651	-3.386464

36	1	0	3.181623	1.213540	-4.400493
37	6	0	3.671202	-0.161883	-2.828865
38	6	0	4.856324	-1.978327	-2.424207
39	1	0	5.922081	-2.168486	-2.307353
40	1	0	4.311397	-2.868817	-2.761523
41	6	0	3.447187	-0.546101	-1.514350
42	6	0	2.514461	0.052965	-0.701083
43	6	0	2.470241	-0.370351	0.725054
44	6	0	3.540293	-0.022019	1.515553
45	6	0	5.480639	0.737168	2.282047
46	1	0	6.360131	0.120069	2.065517
47	1	0	5.761356	1.764429	2.519087
48	6	0	3.640254	-0.363706	2.853872
49	6	0	2.684141	-1.130943	3.462834
50	1	0	2.763533	-1.420371	4.502225
51	6	0	1.596210	-1.522367	2.673318
52	1	0	0.848637	-2.153862	3.129838
53	6	0	1.458766	-1.146105	1.340944
54	6	0	0.736293	-2.742996	-0.889946
55	6	0	0.150948	-2.928663	-2.140946
56	1	0	-0.753016	-2.396389	-2.402739
57	6	0	0.700479	-3.826759	-3.047835
58	1	0	0.234271	-3.956785	-4.017385
59	6	0	1.831713	-4.557547	-2.709564
60	1	0	2.255897	-5.262574	-3.416191
61	6	0	2.411916	-4.389192	-1.456936
62	1	0	3.290230	-4.961835	-1.179706
63	6	0	1.870479	-3.485641	-0.553929
64	1	0	2.337594	-3.354815	0.414760
65	6	0	-0.926870	-2.757405	1.444074
66	6	0	-1.155297	-4.082279	1.081255
67	1	0	-0.756399	-4.469605	0.152475
68	6	0	-1.918417	-4.914067	1.892328
69	1	0	-2.096037	-5.938744	1.586968
70	6	0	-2.459468	-4.436724	3.076554
71	1	0	-3.057420	-5.086722	3.705115
72	6	0	-2.232105	-3.117112	3.450561
73	1	0	-2.643543	-2.735758	4.379077
74	6	0	-1.478822	-2.283773	2.637756
75	1	0	-1.312049	-1.256727	2.935842
76	6	0	-1.051022	0.105078	-2.250174
77	6	0	-2.909026	1.801829	-1.039149
78	1	0	-3.299742	1.496923	-2.012648
79	1	0	-2.353548	2.726651	-1.175456
80	6	0	-4.053115	2.084830	-0.132784
81	6	0	-3.949504	2.873377	0.957489
82	1	0	-4.853591	3.087613	1.523859
83	6	0	-5.400132	1.527001	-0.511510
84	1	0	-6.159134	1.743922	0.245294
85	1	0	-5.726487	1.968379	-1.459173
86	1	0	-5.349844	0.447796	-0.672674
87	6	0	-2.698824	3.582467	1.378830
88	1	0	-2.467777	4.419265	0.709156

89	1	0	-2.783330	3.982472	2.392602
90	1	0	-1.833886	2.913547	1.351666
91	8	0	-2.100932	0.525540	1.598710
92	6	0	-3.265120	0.443183	1.980969
93	1	0	-4.021311	-0.011491	1.334393
94	6	0	-3.634271	0.755090	3.390823
95	1	0	-4.631838	1.192898	3.437906
96	1	0	-3.658350	-0.191969	3.943880
97	1	0	-2.900654	1.420401	3.847178

TS2B (NIMAG=1, 276.4*i* cm^{-1})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.417629	0.248613	-0.479455
2	53	0	-3.461869	-1.655346	-0.906485
3	15	0	0.380140	1.768161	-0.386021
4	15	0	-0.076482	-1.592221	0.317846
5	8	0	4.790939	-1.006761	-3.246625
6	8	0	4.370582	-1.599697	-1.074397
7	8	0	4.596070	0.648472	1.243607
8	8	0	4.641525	0.155543	3.491293
9	8	0	-0.882108	-0.030091	-3.395838
10	6	0	1.175833	2.285956	1.187750
11	6	0	0.606919	1.971292	2.419063
12	1	0	-0.329436	1.426795	2.447621
13	6	0	1.252717	2.336858	3.594984
14	1	0	0.814105	2.071043	4.550084
15	6	0	2.456476	3.026537	3.550307
16	1	0	2.958709	3.304939	4.469928
17	6	0	3.021264	3.352994	2.321315
18	1	0	3.960103	3.894133	2.277281
19	6	0	2.390449	2.975791	1.146005
20	1	0	2.850929	3.204020	0.190898
21	6	0	0.074247	3.389132	-1.215551
22	6	0	0.203716	4.599284	-0.535108
23	1	0	0.540808	4.614394	0.492916
24	6	0	-0.115074	5.801706	-1.157237
25	1	0	-0.010614	6.729800	-0.606888
26	6	0	-0.566472	5.814745	-2.468288
27	1	0	-0.812841	6.752800	-2.952491
28	6	0	-0.720018	4.613639	-3.150950
29	1	0	-1.096362	4.605850	-4.167237
30	6	0	-0.418048	3.413806	-2.525978
31	1	0	-0.599996	2.489356	-3.059907
32	6	0	1.820081	1.047933	-1.291446
33	6	0	2.121197	1.425606	-2.594053
34	1	0	1.588925	2.245043	-3.053278
35	6	0	3.105761	0.787060	-3.358115
36	1	0	3.325468	1.096270	-4.371066
37	6	0	3.774415	-0.245514	-2.759047

38	6	0	4.967281	-2.041558	-2.285732
39	1	0	6.031259	-2.208299	-2.124287
40	1	0	4.454670	-2.947846	-2.631093
41	6	0	3.508765	-0.611726	-1.447351
42	6	0	2.544368	-0.006962	-0.675981
43	6	0	2.440106	-0.404607	0.754178
44	6	0	3.484472	-0.059892	1.579996
45	6	0	5.379538	0.744530	2.424858
46	1	0	6.316494	0.196385	2.284591
47	1	0	5.562307	1.797158	2.652829
48	6	0	3.516596	-0.361704	2.931198
49	6	0	2.510524	-1.076562	3.522986
50	1	0	2.534300	-1.328572	4.574760
51	6	0	1.446481	-1.463966	2.699752
52	1	0	0.654250	-2.048391	3.144234
53	6	0	1.382624	-1.135461	1.349813
54	6	0	0.688251	-2.731582	-0.907099
55	6	0	0.059160	-2.975936	-2.126789
56	1	0	-0.872621	-2.481764	-2.366716
57	6	0	0.600134	-3.885675	-3.026629
58	1	0	0.100304	-4.060666	-3.972051
59	6	0	1.765653	-4.571966	-2.711829
60	1	0	2.183430	-5.285991	-3.413110
61	6	0	2.386586	-4.349134	-1.488030
62	1	0	3.288273	-4.891512	-1.225053
63	6	0	1.853381	-3.433653	-0.591657
64	1	0	2.351398	-3.264157	0.355125
65	6	0	-0.987168	-2.761076	1.410605
66	6	0	-1.055435	-4.124728	1.138893
67	1	0	-0.550921	-4.537927	0.275062
68	6	0	-1.795471	-4.967861	1.960268
69	1	0	-1.850326	-6.025123	1.727437
70	6	0	-2.468011	-4.461460	3.062278
71	1	0	-3.048924	-5.120801	3.697224
72	6	0	-2.399174	-3.101382	3.342878
73	1	0	-2.924700	-2.694899	4.200160
74	6	0	-1.670769	-2.257567	2.519667
75	1	0	-1.634300	-1.196251	2.725940
76	6	0	-1.052750	0.043413	-2.259896
77	6	0	-2.885576	1.900801	-1.075407
78	1	0	-3.229243	1.629562	-2.073573
79	1	0	-2.273537	2.796027	-1.108190
80	6	0	-3.988199	2.066738	-0.158016
81	6	0	-3.848684	2.683336	1.067542
82	1	0	-4.762684	2.858478	1.630138
83	6	0	-5.339418	1.535532	-0.540069
84	1	0	-6.004361	1.440167	0.322276
85	1	0	-5.797311	2.240932	-1.242554
86	1	0	-5.259904	0.571902	-1.043288
87	6	0	-2.668487	3.542295	1.416521
88	1	0	-2.601822	4.411923	0.753644
89	1	0	-2.729194	3.906880	2.444646
90	1	0	-1.735717	2.983855	1.310928

91	8	0	-2.039850	0.670206	1.542305
92	6	0	-3.245405	0.763408	1.911485
93	1	0	-4.002531	0.168361	1.394514
94	6	0	-3.512131	1.046167	3.365389
95	1	0	-4.549590	1.335336	3.536787
96	1	0	-3.319842	0.123061	3.925153
97	1	0	-2.840561	1.820130	3.741354

J (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.412948	0.321632	-0.463965
2	53	0	-3.601798	-1.418827	-0.875742
3	15	0	0.522040	1.702847	-0.441817
4	15	0	-0.227658	-1.554960	0.278128
5	8	0	4.906923	-1.321047	-3.081663
6	8	0	4.363124	-1.860472	-0.920728
7	8	0	4.585506	0.321333	1.373029
8	8	0	4.442324	-0.059622	3.638427
9	8	0	-0.970375	-0.064064	-3.406135
10	6	0	1.338412	2.259265	1.103519
11	6	0	0.730997	2.053934	2.339660
12	1	0	-0.235544	1.554716	2.369912
13	6	0	1.380152	2.464992	3.499560
14	1	0	0.912823	2.288508	4.461854
15	6	0	2.619489	3.085744	3.431358
16	1	0	3.120618	3.401941	4.339611
17	6	0	3.222397	3.297701	2.194035
18	1	0	4.188846	3.786256	2.132831
19	6	0	2.590484	2.877327	1.034461
20	1	0	3.074578	3.020305	0.074274
21	6	0	0.300015	3.293158	-1.354999
22	6	0	0.452091	4.523013	-0.714669
23	1	0	0.771682	4.564750	0.318237
24	6	0	0.177939	5.710733	-1.384839
25	1	0	0.297198	6.654318	-0.864895
26	6	0	-0.248253	5.689614	-2.703854
27	1	0	-0.460615	6.616110	-3.224868
28	6	0	-0.417983	4.469508	-3.348720
29	1	0	-0.769874	4.436771	-4.373319
30	6	0	-0.160073	3.284784	-2.677675
31	1	0	-0.350361	2.348629	-3.186998
32	6	0	1.918477	0.866023	-1.310966
33	6	0	2.284474	1.200750	-2.608644
34	1	0	1.805731	2.029909	-3.107240
35	6	0	3.279812	0.511934	-3.312037
36	1	0	3.554319	0.787724	-4.321263
37	6	0	3.892934	-0.520991	-2.656334
38	6	0	5.027017	-2.330561	-2.086435
39	1	0	6.080072	-2.493968	-1.860769

40	1	0	4.535544	-3.245137	-2.439144
41	6	0	3.557531	-0.849360	-1.351130
42	6	0	2.577427	-0.197023	-0.640352
43	6	0	2.370086	-0.545413	0.789594
44	6	0	3.388824	-0.254565	1.666784
45	6	0	5.259961	0.494931	2.611889
46	1	0	6.214390	-0.036485	2.582185
47	1	0	5.399635	1.562947	2.801189
48	6	0	3.304785	-0.483530	3.030233
49	6	0	2.193529	-1.055891	3.588372
50	1	0	2.121365	-1.239456	4.651899
51	6	0	1.151726	-1.388179	2.715554
52	1	0	0.271526	-1.853493	3.134461
53	6	0	1.213013	-1.145042	1.347839
54	6	0	0.492366	-2.706151	-0.958372
55	6	0	-0.198956	-2.986239	-2.136134
56	1	0	-1.140685	-2.495983	-2.345253
57	6	0	0.290269	-3.930557	-3.029441
58	1	0	-0.256951	-4.132579	-3.942631
59	6	0	1.462517	-4.619500	-2.747483
60	1	0	1.838988	-5.361277	-3.443124
61	6	0	2.140749	-4.366025	-1.561111
62	1	0	3.042332	-4.917274	-1.317065
63	6	0	1.660363	-3.415176	-0.671632
64	1	0	2.200347	-3.229027	0.248273
65	6	0	-1.194986	-2.705504	1.340654
66	6	0	-1.124091	-4.086959	1.180052
67	1	0	-0.512982	-4.524680	0.401692
68	6	0	-1.862883	-4.923217	2.009857
69	1	0	-1.810274	-5.996606	1.867443
70	6	0	-2.668596	-4.390248	3.005410
71	1	0	-3.247194	-5.046207	3.646278
72	6	0	-2.738736	-3.011194	3.169146
73	1	0	-3.375428	-2.583490	3.935658
74	6	0	-2.012763	-2.173452	2.338237
75	1	0	-2.068732	-1.095800	2.429740
76	6	0	-1.112864	0.042876	-2.270243
77	6	0	-2.820195	2.384843	-1.116184
78	1	0	-3.048761	2.199762	-2.160312
79	1	0	-1.981905	3.026838	-0.904408
80	6	0	-3.766437	2.183926	-0.168920
81	6	0	-3.534268	2.483753	1.280008
82	1	0	-4.506222	2.745023	1.715990
83	6	0	-5.135052	1.692446	-0.518118
84	1	0	-5.483990	0.934192	0.186353
85	1	0	-5.816725	2.549326	-0.448002
86	1	0	-5.183964	1.280189	-1.524462
87	6	0	-2.544557	3.616251	1.539510
88	1	0	-2.797400	4.504384	0.954671
89	1	0	-2.544742	3.895943	2.595118
90	1	0	-1.528845	3.311754	1.282616
91	8	0	-1.828304	0.769040	1.540673
92	6	0	-3.083347	1.142411	1.971550

93	1	0	-3.843765	0.387244	1.705792
94	6	0	-3.083453	1.284129	3.494494
95	1	0	-4.051338	1.635148	3.865840
96	1	0	-2.872538	0.316651	3.957248
97	1	0	-2.307555	1.982873	3.818993

Cartesian coordinates of stationary points at the ωB97X-D/(SDD, 6-311G(d,p)) level of theory are given below:

K' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.007100	-2.116204	0.091850
2	17	0	-1.897830	-3.688466	0.452826
3	15	0	1.740659	-0.584726	-0.008299
4	15	0	-1.694278	-0.466872	-0.213115
5	8	0	0.353495	3.703681	3.845333
6	8	0	-0.692389	3.703523	1.808008
7	8	0	1.141413	3.942055	-0.841499
8	8	0	0.311745	4.424955	-2.933675
9	8	0	0.153146	-2.009453	3.105069
10	6	0	1.464472	0.787325	1.185090
11	6	0	2.118597	0.826279	2.409512
12	1	0	2.897317	0.108695	2.625021
13	6	0	1.812187	1.772026	3.395524
14	1	0	2.331578	1.792282	4.344066
15	6	0	0.822109	2.668555	3.097623
16	6	0	-0.793146	4.172220	3.145949
17	1	0	-0.799358	5.261100	3.147737
18	1	0	-1.695040	3.753558	3.608978
19	6	0	0.181675	2.658901	1.865936
20	6	0	0.458980	1.742496	0.878700
21	6	0	-0.185057	1.920144	-0.454137
22	6	0	0.205881	3.016978	-1.187948
23	6	0	1.230340	4.849595	-1.931452
24	1	0	0.959023	5.852730	-1.591212
25	1	0	2.244466	4.825891	-2.339495
26	6	0	-0.295562	3.311627	-2.445045
27	6	0	-1.258998	2.532497	-3.026464
28	1	0	-1.663611	2.762113	-4.003154
29	6	0	-1.690364	1.418844	-2.295929
30	1	0	-2.455911	0.792619	-2.732811
31	6	0	-1.174937	1.093415	-1.045341
32	6	0	0.077421	-1.993753	1.961809
33	6	0	0.101291	-3.116688	-1.980263
34	1	0	0.203925	-2.608719	-2.932975
35	1	0	-0.747158	-3.784915	-1.887329
36	6	0	1.267386	-3.374637	-1.245068
37	6	0	1.229770	-3.973066	0.030330
38	1	0	2.198328	-2.915858	-1.573532
39	1	0	2.159666	-4.038448	0.583606
40	1	0	0.488899	-4.732356	0.249829
41	6	0	2.152130	0.355736	-1.531766
42	6	0	3.083812	1.395418	-1.474152
43	6	0	1.511357	0.081066	-2.734292
44	6	0	3.376330	2.135502	-2.609325

45	1	0	3.568465	1.635641	-0.534046
46	6	0	1.794608	0.832480	-3.868659
47	1	0	0.755667	-0.691966	-2.765751
48	6	0	2.727726	1.858293	-3.809004
49	1	0	4.105751	2.936223	-2.555421
50	1	0	1.272753	0.623851	-4.795244
51	1	0	2.943891	2.447999	-4.692551
52	6	0	3.368753	-1.328040	0.446516
53	6	0	3.482289	-2.045196	1.643084
54	6	0	4.464794	-1.302879	-0.416544
55	6	0	4.669017	-2.675765	1.985526
56	1	0	2.635183	-2.130265	2.311658
57	6	0	5.648624	-1.950960	-0.080367
58	1	0	4.402942	-0.784225	-1.364442
59	6	0	5.758582	-2.630088	1.123635
60	1	0	4.734326	-3.218414	2.921454
61	1	0	6.485309	-1.922848	-0.768987
62	1	0	6.682675	-3.132516	1.385426
63	6	0	-2.506435	0.152361	1.318564
64	6	0	-2.896454	1.483977	1.459991
65	6	0	-2.828083	-0.761617	2.323364
66	6	0	-3.574946	1.899441	2.599133
67	1	0	-2.672861	2.205571	0.684169
68	6	0	-3.503026	-0.341785	3.461613
69	1	0	-2.576079	-1.809062	2.200277
70	6	0	-3.874265	0.989565	3.605458
71	1	0	-3.882349	2.935834	2.689828
72	1	0	-3.743673	-1.062444	4.234449
73	1	0	-4.404462	1.314132	4.494011
74	6	0	-3.155625	-0.974699	-1.210973
75	6	0	-2.961758	-1.735812	-2.362781
76	6	0	-4.450503	-0.588747	-0.868847
77	6	0	-4.034981	-2.092689	-3.165276
78	1	0	-1.963434	-2.054769	-2.624995
79	6	0	-5.527221	-0.954745	-1.668035
80	1	0	-4.630705	-0.008955	0.027450
81	6	0	-5.323334	-1.703987	-2.818201
82	1	0	-3.865603	-2.689521	-4.054236
83	1	0	-6.529501	-0.655184	-1.383477
84	1	0	-6.165318	-1.992532	-3.437322

L’ (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.042069	-2.155592	0.090797
2	17	0	-1.856307	-3.715154	0.527680
3	15	0	1.757122	-0.573450	-0.051378
4	15	0	-1.672954	-0.506658	-0.208809
5	8	0	0.317597	3.629192	3.892671

6	8	0	-0.746506	3.643590	1.865280
7	8	0	1.005803	4.002728	-0.775251
8	8	0	0.120475	4.513722	-2.837008
9	8	0	0.254548	-2.008339	3.091750
10	6	0	1.457724	0.777658	1.169472
11	6	0	2.123998	0.813169	2.387633
12	1	0	2.921103	0.111551	2.584718
13	6	0	1.810944	1.736027	3.392970
14	1	0	2.341843	1.750185	4.335224
15	6	0	0.799686	2.616963	3.122552
16	6	0	-0.845917	4.084482	3.212485
17	1	0	-0.876753	5.172685	3.235019
18	1	0	-1.733905	3.636300	3.675004
19	6	0	0.148111	2.615264	1.897084
20	6	0	0.432714	1.721923	0.890524
21	6	0	-0.232566	1.917244	-0.428877
22	6	0	0.106770	3.047852	-1.136679
23	6	0	1.083803	4.910733	-1.865285
24	1	0	0.850737	5.918708	-1.514629
25	1	0	2.083455	4.860192	-2.307437
26	6	0	-0.427405	3.358399	-2.376695
27	6	0	-1.362925	2.554860	-2.970967
28	1	0	-1.786411	2.793937	-3.937360
29	6	0	-1.738913	1.404074	-2.267900
30	1	0	-2.477784	0.753442	-2.715744
31	6	0	-1.199987	1.071807	-1.029211
32	6	0	0.131135	-2.020415	1.952601
33	6	0	1.434060	-3.887624	0.006511
34	1	0	1.266218	-4.670318	0.738641
35	1	0	2.454975	-3.533338	-0.061352
36	6	0	0.627723	-3.906058	-1.154402
37	6	0	0.652755	-2.868435	-2.083702
38	1	0	-0.199942	-4.604445	-1.192223
39	1	0	1.587491	-2.354637	-2.276889
40	1	0	-0.035054	-2.893303	-2.921738
41	6	0	2.110313	0.433829	-1.556064
42	6	0	3.056245	1.458968	-1.462268
43	6	0	1.425345	0.254830	-2.753723
44	6	0	3.328615	2.268145	-2.554450
45	1	0	3.572867	1.632920	-0.524722
46	6	0	1.689857	1.074377	-3.844367
47	1	0	0.650339	-0.495999	-2.820957
48	6	0	2.644239	2.077502	-3.750526
49	1	0	4.071076	3.053833	-2.468022
50	1	0	1.133749	0.935578	-4.764019
51	1	0	2.846736	2.716853	-4.602332
52	6	0	3.424670	-1.249706	0.359942
53	6	0	4.487545	-1.210748	-0.541596
54	6	0	3.595619	-1.952825	1.558804
55	6	0	5.699688	-1.822910	-0.237125
56	1	0	4.379370	-0.710708	-1.495086
57	6	0	4.808756	-2.546042	1.869193
58	1	0	2.766662	-2.070279	2.245846

59	6	0	5.868927	-2.480115	0.971410
60	1	0	6.510655	-1.784319	-0.955353
61	1	0	4.918185	-3.079504	2.806225
62	1	0	6.814427	-2.954335	1.208198
63	6	0	-2.508306	0.094025	1.321626
64	6	0	-2.920275	1.419326	1.465069
65	6	0	-2.813186	-0.823387	2.328587
66	6	0	-3.606532	1.823706	2.603630
67	1	0	-2.704650	2.147513	0.693238
68	6	0	-3.494035	-0.414173	3.467115
69	1	0	-2.541080	-1.865807	2.209362
70	6	0	-3.889749	0.909969	3.610670
71	1	0	-3.929634	2.855378	2.693829
72	1	0	-3.719902	-1.138515	4.241021
73	1	0	-4.425091	1.225679	4.499335
74	6	0	-3.114281	-1.041503	-1.219002
75	6	0	-2.945633	-2.032603	-2.182098
76	6	0	-4.366064	-0.442491	-1.073844
77	6	0	-4.000460	-2.403224	-3.005266
78	1	0	-1.990549	-2.531854	-2.264227
79	6	0	-5.422600	-0.817390	-1.892910
80	1	0	-4.523043	0.316413	-0.316803
81	6	0	-5.240698	-1.794564	-2.863993
82	1	0	-3.856398	-3.182943	-3.744351
83	1	0	-6.391699	-0.348104	-1.766733
84	1	0	-6.067923	-2.090157	-3.499610

M' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.174729	-2.173434	0.024750
2	17	0	-0.376140	-2.339606	-2.484344
3	15	0	-1.803740	-0.455263	-0.162003
4	15	0	1.696936	-0.672263	-0.010646
5	8	0	1.202548	3.842184	-0.917671
6	8	0	0.497686	4.178678	-3.082313
7	8	0	-0.535562	3.763884	1.719748
8	8	0	0.474027	3.748478	3.776662
9	8	0	-0.099196	-1.956389	2.999507
10	6	0	-1.146319	1.013297	-1.049564
11	6	0	-0.150285	1.846323	-0.472743
12	6	0	0.286100	2.892696	-1.254316
13	6	0	-0.137638	3.098060	-2.556494
14	6	0	-1.055273	2.270945	-3.147059
15	1	0	-1.373742	2.413020	-4.170910
16	6	0	-1.558704	1.229482	-2.360379
17	1	0	-2.286142	0.561997	-2.802068
18	6	0	1.400771	4.634810	-2.080859
19	1	0	2.427475	4.505062	-2.435197

20	1	0	1.184100	5.680059	-1.846985
21	6	0	0.482445	1.697450	0.868584
22	6	0	1.413556	0.681016	1.215130
23	6	0	2.041388	0.702713	2.453364
24	1	0	2.767191	-0.059510	2.699323
25	6	0	1.790852	1.697471	3.407685
26	1	0	2.281371	1.695577	4.371770
27	6	0	0.902172	2.676067	3.054029
28	6	0	0.285677	2.678386	1.811911
29	6	0	-0.134708	-2.018619	1.849899
30	6	0	-1.417263	-4.031431	0.004578
31	6	0	-0.127360	-4.329537	0.504636
32	1	0	-0.023177	-4.548259	1.565447
33	6	0	1.037963	-4.052864	-0.227456
34	1	0	1.041485	-4.141587	-1.306673
35	1	0	1.995880	-4.162413	0.267663
36	6	0	-0.221846	4.567945	2.847767
37	1	0	-1.143100	4.929916	3.303058
38	1	0	0.425988	5.395725	2.532791
39	1	0	-2.266713	-4.156209	0.667495
40	1	0	-1.613275	-4.193121	-1.048156
41	6	0	3.229371	-1.534189	0.554041
42	6	0	4.372373	-1.580677	-0.243102
43	6	0	3.221527	-2.266621	1.746885
44	6	0	5.483404	-2.319937	0.150931
45	1	0	4.402859	-1.048825	-1.185030
46	6	0	4.336097	-2.987033	2.147970
47	1	0	2.336697	-2.289426	2.370393
48	6	0	5.474106	-3.016983	1.349070
49	1	0	6.357832	-2.347555	-0.489154
50	1	0	4.308927	-3.537936	3.081232
51	1	0	6.341890	-3.589375	1.656229
52	6	0	2.330983	0.324270	-1.421771
53	6	0	1.912273	0.102576	-2.729870
54	6	0	3.266150	1.331473	-1.159671
55	6	0	2.416764	0.887206	-3.762621
56	1	0	1.180997	-0.668546	-2.936734
57	6	0	3.779332	2.096857	-2.194293
58	1	0	3.589423	1.520760	-0.141930
59	6	0	3.349046	1.880183	-3.500793
60	1	0	2.071503	0.716275	-4.775683
61	1	0	4.510914	2.868334	-1.979574
62	1	0	3.741206	2.486405	-4.310159
63	6	0	-2.490886	0.203446	1.413257
64	6	0	-2.686603	1.560760	1.654553
65	6	0	-2.926198	-0.720945	2.363264
66	6	0	-3.268716	1.987601	2.841653
67	1	0	-2.381803	2.297726	0.922750
68	6	0	-3.518575	-0.295817	3.543065
69	1	0	-2.804026	-1.782329	2.176321
70	6	0	-3.682998	1.062109	3.789676
71	1	0	-3.403805	3.048956	3.017811
72	1	0	-3.846364	-1.026545	4.273306

73	1	0	-4.136752	1.395721	4.716058
74	6	0	-3.399487	-0.784055	-1.027796
75	6	0	-4.416855	0.175042	-0.978367
76	6	0	-3.627986	-1.975061	-1.708411
77	6	0	-5.633794	-0.055738	-1.599484
78	1	0	-4.261487	1.108022	-0.449437
79	6	0	-4.852471	-2.207648	-2.327007
80	1	0	-2.837455	-2.705314	-1.783483
81	6	0	-5.855910	-1.252192	-2.274299
82	1	0	-6.412145	0.697446	-1.552726
83	1	0	-5.012775	-3.139720	-2.856661
84	1	0	-6.809335	-1.434781	-2.757525

N' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.242620	-2.149997	-0.047917
2	17	0	0.322038	-2.366042	2.456396
3	15	0	1.806558	-0.386750	0.180097
4	15	0	-1.675194	-0.722829	0.013618
5	8	0	-1.316813	3.823868	0.889443
6	8	0	-0.611644	4.219071	3.043324
7	8	0	0.435780	3.767368	-1.732272
8	8	0	-0.576060	3.720279	-3.787863
9	8	0	0.145816	-1.964863	-3.023714
10	6	0	1.118054	1.071312	1.057126
11	6	0	0.094102	1.862992	0.470479
12	6	0	-0.371910	2.907272	1.237277
13	6	0	0.053060	3.148723	2.533370
14	6	0	1.001203	2.363009	3.131976
15	1	0	1.322855	2.535457	4.150190
16	6	0	1.532550	1.323504	2.360379
17	1	0	2.286236	0.689123	2.807283
18	6	0	-1.549005	4.614719	2.047371
19	1	0	-2.563536	4.430047	2.412866
20	1	0	-1.393429	5.667890	1.802582
21	6	0	-0.530934	1.680803	-0.871274
22	6	0	-1.435833	0.638662	-1.214105
23	6	0	-2.067852	0.643214	-2.450174
24	1	0	-2.777625	-0.135098	-2.691596
25	6	0	-1.844259	1.641097	-3.408110
26	1	0	-2.339240	1.625755	-4.369797
27	6	0	-0.976139	2.639984	-3.061036
28	6	0	-0.357372	2.660959	-1.820154
29	6	0	0.193355	-2.006294	-1.874942
30	6	0	-0.844173	-4.116899	-0.315968
31	6	0	0.451998	-4.335955	0.183189
32	1	0	0.536111	-4.580729	1.235364
33	6	0	1.626805	-3.906991	-0.465682

34	1	0	1.719421	-3.981337	-1.544827
35	1	0	2.563847	-3.993505	0.072207
36	6	0	0.104212	4.558615	-2.864342
37	1	0	1.017487	4.936576	-3.322881
38	1	0	-0.559682	5.374861	-2.552938
39	1	0	-1.056271	-4.211302	-1.375681
40	1	0	-1.683363	-4.324763	0.338496
41	6	0	-3.183725	-1.638682	-0.526608
42	6	0	-4.290456	-1.761311	0.313346
43	6	0	-3.188819	-2.337924	-1.738541
44	6	0	-5.379980	-2.542384	-0.057992
45	1	0	-4.308125	-1.255883	1.270146
46	6	0	-4.283278	-3.100386	-2.116183
47	1	0	-2.329422	-2.301749	-2.395958
48	6	0	-5.385581	-3.205970	-1.275237
49	1	0	-6.226012	-2.628818	0.614244
50	1	0	-4.267534	-3.624862	-3.064784
51	1	0	-6.237185	-3.810861	-1.564976
52	6	0	-2.335789	0.270919	1.418320
53	6	0	-1.884677	0.117668	2.725279
54	6	0	-3.328094	1.217899	1.141153
55	6	0	-2.416167	0.906555	3.741052
56	1	0	-1.111611	-0.606886	2.944296
57	6	0	-3.866503	1.988354	2.158950
58	1	0	-3.677813	1.355944	0.123914
59	6	0	-3.406348	1.837361	3.464467
60	1	0	-2.046406	0.787696	4.752926
61	1	0	-4.641518	2.712294	1.931678
62	1	0	-3.820039	2.446101	4.261210
63	6	0	2.507004	0.290014	-1.380539
64	6	0	2.670765	1.652693	-1.615413
65	6	0	2.973657	-0.620527	-2.329465
66	6	0	3.254827	2.097895	-2.795010
67	1	0	2.336617	2.378540	-0.885164
68	6	0	3.567164	-0.176424	-3.501651
69	1	0	2.877235	-1.685143	-2.146870
70	6	0	3.701347	1.186188	-3.741663
71	1	0	3.365166	3.162863	-2.966549
72	1	0	3.920065	-0.896120	-4.231170
73	1	0	4.156274	1.534066	-4.662209
74	6	0	3.383864	-0.721890	1.075264
75	6	0	4.427944	0.206391	1.010265
76	6	0	3.567173	-1.896342	1.799671
77	6	0	5.628571	-0.037425	1.658796
78	1	0	4.307236	1.123611	0.445706
79	6	0	4.774408	-2.140455	2.446554
80	1	0	2.753138	-2.602337	1.887291
81	6	0	5.805580	-1.215323	2.377537
82	1	0	6.429279	0.690968	1.598681
83	1	0	4.900388	-3.057601	3.010530
84	1	0	6.745950	-1.408000	2.881972

B′ (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.861061	-1.631458	-0.839621
2	17	0	0.201708	-3.719583	-1.651520
3	15	0	-1.715489	0.448080	-0.239078
4	15	0	1.356714	-1.119087	0.001038
5	8	0	2.075199	4.198068	-2.851590
6	8	0	2.703224	3.263424	-0.859148
7	8	0	0.866095	3.806488	1.790863
8	8	0	1.613117	3.344015	3.911159
9	8	0	-0.529062	-0.624797	-3.612584
10	6	0	-0.653050	1.754632	-0.996431
11	6	0	-1.035414	2.370392	-2.181611
12	1	0	-2.023075	2.190941	-2.582516
13	6	0	-0.184937	3.217536	-2.902271
14	1	0	-0.499392	3.685784	-3.825151
15	6	0	1.066158	3.413672	-2.384142
16	6	0	3.200440	3.855527	-2.051144
17	1	0	3.756142	4.757970	-1.801972
18	1	0	3.817810	3.123475	-2.586932
19	6	0	1.449902	2.833047	-1.182965
20	6	0	0.637639	1.997420	-0.452541
21	6	0	1.133021	1.546420	0.879318
22	6	0	1.239265	2.498804	1.866160
23	6	0	1.301886	4.397177	3.006055
24	1	0	2.202351	4.994515	2.817984
25	1	0	0.497927	5.004534	3.422077
26	6	0	1.694990	2.221791	3.145456
27	6	0	2.110060	0.965689	3.498177
28	1	0	2.470856	0.744277	4.493803
29	6	0	2.029338	-0.020884	2.508687
30	1	0	2.354450	-1.021056	2.760711
31	6	0	1.547536	0.238082	1.229112
32	6	0	-0.625882	-0.985774	-2.525323
33	6	0	-2.726835	-2.572391	-1.294354
34	1	0	-2.660535	-3.199424	-2.179673
35	1	0	-3.601080	-1.926974	-1.306402
36	6	0	-2.429732	-3.267553	-0.054904
37	6	0	-2.732069	-2.862748	1.212153
38	6	0	-2.257492	-3.654736	2.399983
39	1	0	-1.548471	-4.433522	2.113460
40	1	0	-1.787177	-3.009670	3.151948
41	1	0	-3.109955	-4.133949	2.896010
42	6	0	-3.807284	-1.859171	1.520483
43	1	0	-3.546553	-1.211001	2.359572
44	1	0	-4.069572	-1.237819	0.666943
45	1	0	-4.709278	-2.410523	1.814437
46	1	0	-1.817924	-4.159826	-0.143790

47	6	0	-1.745275	1.002379	1.513305
48	6	0	-2.021933	2.334643	1.826746
49	6	0	-1.402913	0.122889	2.535249
50	6	0	-1.987755	2.767600	3.144316
51	1	0	-2.236552	3.043216	1.034225
52	6	0	-1.355524	0.558255	3.852686
53	1	0	-1.141292	-0.899978	2.288342
54	6	0	-1.653975	1.879392	4.160223
55	1	0	-2.205817	3.804231	3.375081
56	1	0	-1.068061	-0.132544	4.636798
57	1	0	-1.607796	2.221607	5.187639
58	6	0	-3.414913	0.832857	-0.851818
59	6	0	-4.416855	1.376820	-0.047668
60	6	0	-3.733914	0.491256	-2.170445
61	6	0	-5.692041	1.598433	-0.555045
62	1	0	-4.219183	1.612244	0.989609
63	6	0	-5.002079	0.726868	-2.680728
64	1	0	-2.993005	0.019509	-2.803854
65	6	0	-5.986719	1.283674	-1.873675
66	1	0	-6.457122	2.015289	0.089984
67	1	0	-5.223089	0.457185	-3.706882
68	1	0	-6.981460	1.457586	-2.267746
69	6	0	2.633309	-0.672952	-1.247599
70	6	0	3.651560	0.235423	-0.954061
71	6	0	2.616512	-1.295039	-2.497143
72	6	0	4.626227	0.528525	-1.899784
73	1	0	3.685157	0.726000	0.010749
74	6	0	3.590164	-0.995796	-3.440726
75	1	0	1.855617	-2.032891	-2.722357
76	6	0	4.594743	-0.081758	-3.147533
77	1	0	5.415121	1.231355	-1.653854
78	1	0	3.561710	-1.484497	-4.407637
79	1	0	5.354831	0.147925	-3.886225
80	6	0	2.115846	-2.533745	0.886018
81	6	0	1.283017	-3.313748	1.685523
82	6	0	3.473946	-2.831782	0.822098
83	6	0	1.798605	-4.362424	2.431038
84	1	0	0.220061	-3.103258	1.705336
85	6	0	3.989907	-3.891792	1.559277
86	1	0	4.131249	-2.244872	0.191386
87	6	0	3.156871	-4.653952	2.367796
88	1	0	1.138308	-4.963169	3.046564
89	1	0	5.046935	-4.124186	1.496212
90	1	0	3.562479	-5.481681	2.938598

O' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-1.179818	1.602321	0.036753

2	17	0	-0.368485	3.926954	0.551137
3	15	0	-1.595524	-0.691328	0.016747
4	15	0	1.174985	1.288825	-0.209685
5	8	0	2.306957	-3.191884	3.749723
6	8	0	3.029344	-2.611797	1.652616
7	8	0	1.668672	-3.904876	-0.918346
8	8	0	2.561188	-3.762132	-3.035562
9	8	0	-1.598772	1.582886	3.031141
10	6	0	-0.470139	-1.558338	1.200160
11	6	0	-0.897513	-1.952769	2.462305
12	1	0	-1.935705	-1.850616	2.737144
13	6	0	-0.034729	-2.506659	3.415572
14	1	0	-0.389096	-2.809175	4.391738
15	6	0	1.275053	-2.652680	3.047525
16	6	0	3.466366	-2.928639	2.967093
17	1	0	4.091190	-3.820396	2.934507
18	1	0	3.998540	-2.067856	3.388673
19	6	0	1.710915	-2.293286	1.781288
20	6	0	0.887906	-1.739229	0.828328
21	6	0	1.454540	-1.496695	-0.525551
22	6	0	1.812720	-2.598103	-1.267841
23	6	0	2.148615	-4.667915	-2.016500
24	1	0	3.004825	-5.267619	-1.694851
25	1	0	1.340891	-5.296995	-2.400071
26	6	0	2.355710	-2.513636	-2.538831
27	6	0	2.613109	-1.302039	-3.121411
28	1	0	3.054230	-1.226922	-4.106422
29	6	0	2.279505	-0.162763	-2.378185
30	1	0	2.500144	0.801947	-2.811355
31	6	0	1.700025	-0.231830	-1.115857
32	6	0	-1.396713	1.538349	1.901585
33	6	0	-1.537699	2.287539	-2.069685
34	1	0	-1.199582	1.765348	-2.957454
35	1	0	-1.244111	3.330689	-2.023934
36	6	0	-2.762619	1.873547	-1.501470
37	6	0	-3.352704	2.500736	-0.389364
38	6	0	-4.605241	1.887472	0.196225
39	1	0	-4.739254	0.845494	-0.086547
40	1	0	-4.607367	1.952298	1.286872
41	1	0	-5.479183	2.446525	-0.158532
42	6	0	-3.347056	4.003813	-0.221881
43	1	0	-3.271430	4.289133	0.828990
44	1	0	-2.538337	4.500318	-0.748315
45	1	0	-4.302539	4.382351	-0.607119
46	1	0	-3.189480	0.927991	-1.833172
47	6	0	-1.373715	-1.745080	-1.475813
48	6	0	-1.449265	-3.135433	-1.358830
49	6	0	-1.097533	-1.182435	-2.715831
50	6	0	-1.260247	-3.942257	-2.469823
51	1	0	-1.643180	-3.586651	-0.391919
52	6	0	-0.893664	-1.991595	-3.827414
53	1	0	-0.997622	-0.110093	-2.798518
54	6	0	-0.975982	-3.371731	-3.707067

55	1	0	-1.325561	-5.019932	-2.367694
56	1	0	-0.657672	-1.540830	-4.784268
57	1	0	-0.812024	-4.003418	-4.572705
58	6	0	-3.300349	-1.175945	0.538784
59	6	0	-4.167177	-1.829638	-0.339011
60	6	0	-3.799386	-0.774480	1.782463
61	6	0	-5.483076	-2.093594	0.024492
62	1	0	-3.827789	-2.129074	-1.321833
63	6	0	-5.103625	-1.061596	2.154631
64	1	0	-3.186434	-0.198621	2.462108
65	6	0	-5.952994	-1.721595	1.275416
66	1	0	-6.139656	-2.593257	-0.678578
67	1	0	-5.462869	-0.742961	3.126308
68	1	0	-6.977567	-1.932121	1.559724
69	6	0	2.205385	1.159519	1.311582
70	6	0	3.438288	0.504938	1.278995
71	6	0	1.805930	1.795672	2.484732
72	6	0	4.245663	0.470956	2.406967
73	1	0	3.770305	0.016218	0.370762
74	6	0	2.609594	1.748632	3.617405
75	1	0	0.885208	2.362556	2.504052
76	6	0	3.828417	1.083900	3.583309
77	1	0	5.205334	-0.032715	2.362843
78	1	0	2.282981	2.244943	4.523752
79	1	0	4.457776	1.054722	4.466072
80	6	0	2.043987	2.637203	-1.121384
81	6	0	1.623477	2.995115	-2.403362
82	6	0	3.096712	3.343999	-0.544582
83	6	0	2.248873	4.018746	-3.098556
84	1	0	0.797249	2.472105	-2.862966
85	6	0	3.717436	4.376570	-1.237463
86	1	0	3.429272	3.111100	0.457969
87	6	0	3.299783	4.716285	-2.515422
88	1	0	1.904779	4.279583	-4.093040
89	1	0	4.526753	4.922129	-0.765740
90	1	0	3.782707	5.525239	-3.051797

P' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	1.072504	-1.747946	-0.040718
2	17	0	0.293166	-4.056519	0.612005
3	15	0	1.650572	0.537612	-0.072777
4	15	0	-1.270595	-1.254659	-0.194237
5	8	0	-1.851877	3.299578	3.880137
6	8	0	-2.729565	2.819877	1.816536
7	8	0	-1.480729	3.984058	-0.804218
8	8	0	-2.403386	3.911765	-2.911171
9	8	0	1.401214	-1.665984	2.958921

10	6	0	0.624279	1.432923	1.185731
11	6	0	1.143220	1.751435	2.434798
12	1	0	2.175526	1.530333	2.660951
13	6	0	0.384682	2.371948	3.434185
14	1	0	0.808496	2.612227	4.399880
15	6	0	-0.914843	2.666794	3.124144
16	6	0	-3.066825	3.174225	3.151374
17	1	0	-3.588834	4.130605	3.149460
18	1	0	-3.673211	2.376845	3.596240
19	6	0	-1.442950	2.372998	1.876422
20	6	0	-0.726501	1.749558	0.880658
21	6	0	-1.370893	1.562877	-0.446784
22	6	0	-1.695791	2.690652	-1.165770
23	6	0	-1.977323	4.783438	-1.868001
24	1	0	-2.830222	5.370755	-1.513879
25	1	0	-1.176095	5.425821	-2.241309
26	6	0	-2.252590	2.648351	-2.433129
27	6	0	-2.539590	1.457992	-3.046610
28	1	0	-2.965782	1.419050	-4.040221
29	6	0	-2.249438	0.293917	-2.325358
30	1	0	-2.480374	-0.658728	-2.782891
31	6	0	-1.687056	0.320967	-1.052950
32	6	0	1.257093	-1.658356	1.821183
33	6	0	3.200771	-2.534308	-0.587544
34	6	0	2.195693	-2.993494	-1.473975
35	6	0	1.469769	-2.126645	-2.297839
36	1	0	1.830338	-4.006813	-1.351205
37	1	0	1.960433	-1.242492	-2.679485
38	1	0	0.695134	-2.527840	-2.939533
39	6	0	4.240982	-1.574054	-1.133114
40	1	0	3.827888	-0.773164	-1.746944
41	1	0	4.838914	-1.123514	-0.342493
42	1	0	4.927825	-2.150935	-1.765812
43	6	0	3.798064	-3.527969	0.386477
44	1	0	4.622584	-4.080252	-0.083722
45	1	0	4.214208	-3.004623	1.252557
46	1	0	3.053874	-4.241198	0.742387
47	6	0	1.429069	1.687864	-1.500148
48	6	0	1.618924	3.058966	-1.297310
49	6	0	1.014658	1.246839	-2.752471
50	6	0	1.436967	3.958218	-2.336061
51	1	0	1.895774	3.426339	-0.315400
52	6	0	0.823634	2.149598	-3.792170
53	1	0	0.780239	0.204220	-2.903239
54	6	0	1.041959	3.504515	-3.590499
55	1	0	1.593085	5.016958	-2.161212
56	1	0	0.482727	1.789633	-4.755808
57	1	0	0.888629	4.207203	-4.401673
58	6	0	3.386132	0.912052	0.455524
59	6	0	4.245560	1.706701	-0.302584
60	6	0	3.902721	0.286983	1.595400
61	6	0	5.570778	1.887563	0.076554
62	1	0	3.900744	2.171784	-1.215800

63	6	0	5.219382	0.482360	1.984877
64	1	0	3.290295	-0.382075	2.182259
65	6	0	6.061737	1.284256	1.224601
66	1	0	6.220524	2.499979	-0.538179
67	1	0	5.590039	-0.012218	2.875258
68	1	0	7.095203	1.426195	1.519135
69	6	0	-2.230568	-1.116374	1.375932
70	6	0	-3.308694	-0.239855	1.507812
71	6	0	-1.930107	-1.980879	2.428518
72	6	0	-4.063910	-0.221492	2.672714
73	1	0	-3.559016	0.445240	0.706717
74	6	0	-2.679688	-1.951019	3.597420
75	1	0	-1.127414	-2.700526	2.324866
76	6	0	-3.747216	-1.071973	3.724659
77	1	0	-4.908587	0.454744	2.750777
78	1	0	-2.429214	-2.626810	4.406830
79	1	0	-4.335415	-1.056091	4.635521
80	6	0	-2.324997	-2.461913	-1.114663
81	6	0	-1.758229	-3.478507	-1.877339
82	6	0	-3.717735	-2.347686	-1.078014
83	6	0	-2.560709	-4.349072	-2.606108
84	1	0	-0.688884	-3.619199	-1.870322
85	6	0	-4.518924	-3.215667	-1.804256
86	1	0	-4.186849	-1.575942	-0.480526
87	6	0	-3.941099	-4.218074	-2.575515
88	1	0	-2.099562	-5.141116	-3.184798
89	1	0	-5.597250	-3.111900	-1.762490
90	1	0	-4.567075	-4.900604	-3.139448

Q' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.675457	-1.699116	-0.763644
2	17	0	0.630991	-3.645456	-1.562999
3	15	0	-1.777878	0.270459	-0.224762
4	15	0	1.469965	-0.890698	0.003463
5	8	0	1.421245	4.503626	-2.874351
6	8	0	2.201079	3.638844	-0.903479
7	8	0	0.310493	3.946817	1.741175
8	8	0	1.136952	3.617233	3.863146
9	8	0	-0.515762	-0.733394	-3.575256
10	6	0	-0.930102	1.706528	-1.006614
11	6	0	-1.412387	2.279795	-2.176158
12	1	0	-2.378467	1.984504	-2.559154
13	6	0	-0.692324	3.238639	-2.899320
14	1	0	-1.083376	3.675356	-3.808298
15	6	0	0.533099	3.588478	-2.401114
16	6	0	2.594008	4.311594	-2.091534
17	1	0	3.020622	5.279724	-1.834446

18	1	0	3.300834	3.681807	-2.646106
19	6	0	1.010765	3.050997	-1.213350
20	6	0	0.325225	2.112509	-0.478539
21	6	0	0.878894	1.735132	0.853610
22	6	0	0.839186	2.696565	1.837060
23	6	0	0.401102	4.516957	3.039437
24	1	0	0.930863	5.469967	2.980303
25	1	0	-0.605285	4.641443	3.451437
26	6	0	1.340889	2.501458	3.113784
27	6	0	1.948969	1.327274	3.467392
28	1	0	2.356470	1.173487	4.457721
29	6	0	2.010106	0.331854	2.484537
30	1	0	2.484258	-0.605398	2.741341
31	6	0	1.485140	0.503601	1.207624
32	6	0	-0.542114	-1.076178	-2.478752
33	6	0	-1.763400	-3.523442	1.142197
34	6	0	-2.512199	-2.797866	0.246324
35	6	0	-2.442678	-2.847493	-1.189730
36	1	0	-3.166743	-2.040685	0.676296
37	1	0	-2.120882	-3.772024	-1.659216
38	1	0	-3.262424	-2.362264	-1.708568
39	6	0	-1.112337	-4.839589	0.819278
40	1	0	-1.169191	-5.092938	-0.234834
41	1	0	-0.054270	-4.861956	1.093213
42	1	0	-1.620057	-5.619610	1.400104
43	6	0	-1.939998	-3.278099	2.621051
44	1	0	-2.464456	-4.130104	3.069156
45	1	0	-0.982063	-3.199431	3.148145
46	1	0	-2.521750	-2.379462	2.829139
47	6	0	-1.921384	0.848283	1.511245
48	6	0	-2.463883	2.103550	1.796336
49	6	0	-1.425113	0.068877	2.548593
50	6	0	-2.530601	2.552964	3.106457
51	1	0	-2.822344	2.734089	0.989890
52	6	0	-1.478738	0.524263	3.860048
53	1	0	-0.957915	-0.879549	2.317864
54	6	0	-2.035486	1.764435	4.141199
55	1	0	-2.963996	3.523853	3.320297
56	1	0	-1.070687	-0.085565	4.657565
57	1	0	-2.074405	2.123083	5.163505
58	6	0	-3.523087	0.326479	-0.820361
59	6	0	-3.789669	0.058693	-2.168259
60	6	0	-4.602757	0.498764	0.046186
61	6	0	-5.092252	0.019310	-2.642040
62	1	0	-2.977706	-0.143205	-2.855991
63	6	0	-5.909513	0.440736	-0.426671
64	1	0	-4.435432	0.671473	1.101427
65	6	0	-6.158556	0.212794	-1.771579
66	1	0	-5.272584	-0.182822	-3.691448
67	1	0	-6.733034	0.572822	0.265747
68	1	0	-7.177362	0.170660	-2.139283
69	6	0	2.633150	-0.285355	-1.288262
70	6	0	3.513599	0.768106	-1.038243

71	6	0	2.684125	-0.936769	-2.521770
72	6	0	4.416025	1.175765	-2.012786
73	1	0	3.495618	1.280905	-0.084665
74	6	0	3.585349	-0.523796	-3.494026
75	1	0	2.036263	-1.784927	-2.710234
76	6	0	4.450176	0.534945	-3.245134
77	1	0	5.099352	1.991181	-1.800682
78	1	0	3.611250	-1.037363	-4.448050
79	1	0	5.154248	0.853628	-4.005968
80	6	0	2.468560	-2.155648	0.878984
81	6	0	3.841466	-2.299973	0.702006
82	6	0	1.808488	-2.984909	1.782933
83	6	0	4.540793	-3.258474	1.427379
84	1	0	4.368968	-1.673854	-0.007471
85	6	0	2.506073	-3.932183	2.515879
86	1	0	0.735290	-2.887034	1.894724
87	6	0	3.878152	-4.071650	2.336851
88	1	0	5.608210	-3.371195	1.275162
89	1	0	1.976956	-4.573437	3.212077
90	1	0	4.426599	-4.820273	2.897340

R’ (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.730717	-1.863946	-0.026219
2	17	0	0.798541	-1.951458	-2.547820
3	15	0	-1.499260	-1.095305	-0.228240
4	15	0	1.696636	0.347322	-0.043442
5	8	0	-0.873038	4.123876	-0.715704
6	8	0	-1.727393	4.223012	-2.849380
7	8	0	-2.365116	3.083378	1.882806
8	8	0	-1.399843	3.547153	3.908372
9	8	0	0.723566	-1.629622	2.947638
10	6	0	-1.648069	0.544671	-1.034219
11	6	0	-1.141421	1.709379	-0.399164
12	6	0	-1.259197	2.881285	-1.111970
13	6	0	-1.774782	2.942805	-2.396540
14	6	0	-2.229259	1.821846	-3.037958
15	1	0	-2.617353	1.861698	-4.046827
16	6	0	-2.162241	0.619925	-2.323864
17	1	0	-2.516038	-0.282035	-2.805082
18	6	0	-1.084173	4.981111	-1.828985
19	1	0	-0.117655	5.336242	-2.198627
20	1	0	-1.732064	5.808288	-1.530407
21	6	0	-0.490344	1.804684	0.939882
22	6	0	0.836740	1.381287	1.229023
23	6	0	1.419243	1.709279	2.445695
24	1	0	2.440745	1.423177	2.646673
25	6	0	0.742847	2.428507	3.439348

26	1	0	1.216025	2.680376	4.378917
27	6	0	-0.540652	2.806174	3.155981
28	6	0	-1.125871	2.513999	1.932470
29	6	0	0.714320	-1.727778	1.800706
30	6	0	2.636728	-3.273867	0.207024
31	6	0	1.511614	-3.896811	-0.363959
32	1	0	1.534639	-4.052288	-1.436157
33	6	0	0.253843	-4.036039	0.263099
34	1	0	0.183571	-4.232796	1.328495
35	1	0	-0.551239	-4.469518	-0.318489
36	6	0	-2.639461	3.493870	3.215076
37	1	0	-3.290676	2.753838	3.696418
38	1	0	-3.091192	4.484966	3.201453
39	6	0	3.025039	-3.569702	1.640179
40	1	0	3.527249	-2.727504	2.115758
41	1	0	2.181652	-3.866885	2.263872
42	1	0	3.740054	-4.401997	1.635029
43	6	0	3.820446	-3.001076	-0.692495
44	1	0	4.431380	-2.187865	-0.293769
45	1	0	4.464366	-3.888420	-0.753369
46	1	0	3.500191	-2.729776	-1.699798
47	6	0	1.749131	1.589100	-1.410160
48	6	0	2.184466	2.880506	-1.091077
49	6	0	1.369190	1.303673	-2.717383
50	6	0	2.250030	3.861760	-2.066797
51	1	0	2.469057	3.121492	-0.072837
52	6	0	1.422031	2.296830	-3.690983
53	1	0	1.022863	0.311217	-2.970485
54	6	0	1.863986	3.572033	-3.372916
55	1	0	2.596942	4.855658	-1.805773
56	1	0	1.110542	2.063765	-4.702641
57	1	0	1.907238	4.340763	-4.136931
58	6	0	3.470097	0.304688	0.449607
59	6	0	4.468875	0.669775	-0.454072
60	6	0	3.851957	-0.242084	1.677712
61	6	0	5.811058	0.512504	-0.127971
62	1	0	4.204868	1.069556	-1.424803
63	6	0	5.191646	-0.379098	2.010711
64	1	0	3.101320	-0.582734	2.379913
65	6	0	6.178015	-0.002370	1.107083
66	1	0	6.570365	0.794442	-0.848351
67	1	0	5.463274	-0.798687	2.972813
68	1	0	7.225072	-0.119889	1.361587
69	6	0	-2.455625	-0.921359	1.334617
70	6	0	-3.325941	0.140406	1.573304
71	6	0	-2.391423	-1.963265	2.259894
72	6	0	-4.102507	0.166698	2.725402
73	1	0	-3.404138	0.952825	0.861608
74	6	0	-3.164924	-1.935431	3.411238
75	1	0	-1.738540	-2.808151	2.073051
76	6	0	-4.021229	-0.867128	3.649133
77	1	0	-4.785685	0.992874	2.890319
78	1	0	-3.098884	-2.750432	4.122601

79	1	0	-4.627690	-0.845305	4.547553
80	6	0	-2.697118	-2.139793	-1.173485
81	6	0	-4.071634	-1.917988	-1.038810
82	6	0	-2.260760	-3.152483	-2.024764
83	6	0	-4.984778	-2.692525	-1.738220
84	1	0	-4.438249	-1.139607	-0.380938
85	6	0	-3.178719	-3.930014	-2.722968
86	1	0	-1.201362	-3.310240	-2.170696
87	6	0	-4.540063	-3.704713	-2.581525
88	1	0	-6.046385	-2.507011	-1.620196
89	1	0	-2.819702	-4.711009	-3.383498
90	1	0	-5.254034	-4.312872	-3.125801

S' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.769931	1.860336	-0.100178
2	17	0	-0.775947	1.613372	2.396494
3	15	0	-1.697486	-0.356497	0.005423
4	15	0	1.489881	1.121787	-0.168424
5	8	0	2.426607	-3.103082	1.779444
6	8	0	1.496064	-3.628538	3.804302
7	8	0	0.880198	-4.076049	-0.846076
8	8	0	1.705661	-4.099711	-2.993954
9	8	0	-0.823705	2.032344	-3.075717
10	6	0	-0.799187	-1.413199	1.220958
11	6	0	0.522702	-1.818587	0.898205
12	6	0	1.181227	-2.546419	1.862098
13	6	0	0.616508	-2.876500	3.084222
14	6	0	-0.667359	-2.520143	3.395843
15	1	0	-1.121443	-2.794719	4.338373
16	6	0	-1.362083	-1.777102	2.435848
17	1	0	-2.373777	-1.480259	2.667550
18	6	0	2.727709	-3.515207	3.105705
19	1	0	3.349220	-2.751396	3.589982
20	1	0	3.220997	-4.485796	3.078543
21	6	0	1.156433	-1.677000	-0.444179
22	6	0	1.653976	-0.489156	-1.041284
23	6	0	2.158533	-0.520224	-2.337575
24	1	0	2.522675	0.393218	-2.788799
25	6	0	2.217774	-1.695682	-3.096387
26	1	0	2.599313	-1.699408	-4.108629
27	6	0	1.770118	-2.839118	-2.491438
28	6	0	1.270430	-2.822766	-1.199263
29	6	0	-0.794828	1.929338	-1.924993
30	6	0	-2.679871	3.221592	0.082471
31	6	0	-1.536582	3.907139	-0.394887
32	1	0	-1.522473	4.198967	-1.443825
33	6	0	-0.326225	4.000893	0.323302

34	1	0	-0.335281	4.032974	1.406215
35	1	0	0.514224	4.495796	-0.149229
36	6	0	1.161539	-4.913208	-1.958268
37	1	0	0.232789	-5.369632	-2.310176
38	1	0	1.896457	-5.668969	-1.666594
39	6	0	-3.178412	3.480729	1.485278
40	1	0	-3.748262	2.636852	1.870559
41	1	0	-2.384958	3.700668	2.193830
42	1	0	-3.860248	4.340660	1.440861
43	6	0	-3.807473	2.965188	-0.894671
44	1	0	-4.362650	2.067743	-0.609818
45	1	0	-4.519631	3.800651	-0.888107
46	1	0	-3.448227	2.829425	-1.917384
47	6	0	2.479632	0.922053	1.361491
48	6	0	3.370629	-0.133557	1.542187
49	6	0	2.426352	1.941430	2.311644
50	6	0	4.189935	-0.173860	2.664253
51	1	0	3.432994	-0.930976	0.812159
52	6	0	3.244961	1.898504	3.430567
53	1	0	1.731220	2.760688	2.182704
54	6	0	4.127138	0.839885	3.611305
55	1	0	4.889012	-0.994171	2.786864
56	1	0	3.186395	2.691247	4.167147
57	1	0	4.765874	0.807704	4.486985
58	6	0	2.652168	2.198045	-1.128579
59	6	0	4.032837	1.989225	-1.045893
60	6	0	2.184373	3.211222	-1.961971
61	6	0	4.913660	2.767869	-1.781079
62	1	0	4.426761	1.214805	-0.399267
63	6	0	3.066347	3.992806	-2.700641
64	1	0	1.124465	3.402194	-2.040392
65	6	0	4.432813	3.773191	-2.612824
66	1	0	5.980143	2.590743	-1.700739
67	1	0	2.678221	4.775602	-3.342178
68	1	0	5.122004	4.383834	-3.185124
69	6	0	-1.743503	-1.548690	-1.407350
70	6	0	-2.126851	-2.867387	-1.139201
71	6	0	-1.405748	-1.202946	-2.711082
72	6	0	-2.175734	-3.809979	-2.153425
73	1	0	-2.380406	-3.159122	-0.126376
74	6	0	-1.439704	-2.152789	-3.726982
75	1	0	-1.091644	-0.200834	-2.952299
76	6	0	-1.825184	-3.456201	-3.452927
77	1	0	-2.480148	-4.825764	-1.926238
78	1	0	-1.155559	-1.866942	-4.732977
79	1	0	-1.850771	-4.195072	-4.246157
80	6	0	-3.470572	-0.358760	0.502624
81	6	0	-4.462230	-0.754470	-0.398244
82	6	0	-3.859097	0.163911	1.739411
83	6	0	-5.806569	-0.651019	-0.061541
84	1	0	-4.194255	-1.140633	-1.373390
85	6	0	-5.202612	0.246812	2.079000
86	1	0	-3.104797	0.536413	2.422946

87	6	0	-6.181595	-0.159722	1.181135
88	1	0	-6.560440	-0.958569	-0.777349
89	1	0	-5.482097	0.649526	3.046119
90	1	0	-7.230379	-0.085444	1.445480

T' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.816817	1.815568	0.014578
2	17	0	0.738509	2.138058	-2.485854
3	15	0	1.664383	-0.405183	-0.307632
4	15	0	-1.488450	1.158139	-0.001382
5	8	0	-2.776225	-3.209721	-0.667350
6	8	0	-2.381421	-3.972159	-2.801677
7	8	0	-0.826851	-3.706609	1.849850
8	8	0	-1.679442	-3.284443	3.932839
9	8	0	0.624801	1.573603	2.977966
10	6	0	0.468031	-1.540089	-1.122310
11	6	0	-0.731293	-1.881933	-0.440575
12	6	0	-1.586930	-2.723624	-1.113594
13	6	0	-1.348216	-3.188149	-2.397199
14	6	0	-0.205382	-2.856142	-3.072684
15	1	0	-0.011044	-3.216964	-4.073780
16	6	0	0.703359	-2.028294	-2.401120
17	1	0	1.623296	-1.771713	-2.907257
18	6	0	-3.341887	-3.935484	-1.749823
19	1	0	-4.240362	-3.418839	-2.100074
20	1	0	-3.561933	-4.954956	-1.425495
21	6	0	-1.159719	-1.455434	0.924867
22	6	0	-1.701716	-0.181263	1.249119
23	6	0	-2.262555	0.043212	2.497959
24	1	0	-2.696079	1.006957	2.724636
25	6	0	-2.295959	-0.940416	3.495380
26	1	0	-2.739284	-0.752361	4.464007
27	6	0	-1.742761	-2.151282	3.180595
28	6	0	-1.211389	-2.400568	1.921970
29	6	0	0.734737	1.640124	1.832631
30	6	0	0.517679	4.000634	0.368033
31	6	0	1.782110	3.783609	-0.220496
32	1	0	1.851860	3.990324	-1.281589
33	6	0	2.827310	3.014896	0.329141
34	1	0	0.413298	4.164484	1.435852
35	1	0	-0.233880	4.496272	-0.236813
36	6	0	-0.849472	-4.170215	3.192035
37	1	0	0.168540	-4.141278	3.601172
38	1	0	-1.272881	-5.173175	3.220438
39	6	0	3.996548	2.695331	-0.574247
40	1	0	4.746447	3.495254	-0.520097
41	1	0	4.488080	1.766962	-0.270911

42	1	0	3.681348	2.583229	-1.612195
43	6	0	3.229505	3.156467	1.782648
44	1	0	4.023662	3.910404	1.848619
45	1	0	2.414923	3.482417	2.429078
46	1	0	3.644228	2.229840	2.187561
47	6	0	-2.562015	2.556561	0.537855
48	6	0	-3.548447	3.070607	-0.303435
49	6	0	-2.307488	3.214970	1.745908
50	6	0	-4.276663	4.197414	0.064058
51	1	0	-3.749570	2.601495	-1.257949
52	6	0	-3.047306	4.326055	2.119544
53	1	0	-1.516575	2.871414	2.400615
54	6	0	-4.036902	4.822539	1.278181
55	1	0	-5.033511	4.584415	-0.608640
56	1	0	-2.838959	4.813865	3.064980
57	1	0	-4.608081	5.698154	1.564829
58	6	0	-2.489652	0.430763	-1.370759
59	6	0	-2.035901	0.336661	-2.682483
60	6	0	-3.753772	-0.073793	-1.046164
61	6	0	-2.834121	-0.258110	-3.654340
62	1	0	-1.058053	0.719958	-2.939253
63	6	0	-4.552584	-0.649473	-2.021205
64	1	0	-4.112690	-0.022601	-0.024104
65	6	0	-4.090570	-0.748350	-3.330633
66	1	0	-2.462807	-0.337453	-4.669529
67	1	0	-5.533733	-1.028254	-1.756174
68	1	0	-4.709794	-1.207817	-4.093449
69	6	0	2.129804	-1.384609	1.181177
70	6	0	2.041266	-2.777391	1.183858
71	6	0	2.707924	-0.746787	2.276541
72	6	0	2.505654	-3.509602	2.267806
73	1	0	1.607450	-3.295160	0.337469
74	6	0	3.166271	-1.477226	3.364926
75	1	0	2.815427	0.328906	2.276821
76	6	0	3.063998	-2.862387	3.364022
77	1	0	2.433961	-4.591600	2.250708
78	1	0	3.605732	-0.961599	4.210850
79	1	0	3.424900	-3.435762	4.210679
80	6	0	3.219381	-0.566335	-1.291990
81	6	0	3.295501	-0.003321	-2.569770
82	6	0	4.359166	-1.175482	-0.762009
83	6	0	4.474873	-0.061109	-3.298493
84	1	0	2.436022	0.509906	-2.982190
85	6	0	5.542236	-1.219425	-1.490735
86	1	0	4.341182	-1.616761	0.225485
87	6	0	5.604544	-0.665386	-2.761211
88	1	0	4.510267	0.383933	-4.286418
89	1	0	6.416657	-1.691939	-1.057600
90	1	0	6.528278	-0.700624	-3.327884

U' (NIMAG=0)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.775946	-1.839676	-0.064045
2	17	0	-0.590390	-1.581725	2.438343
3	15	0	1.515971	-1.139482	0.032117
4	15	0	-1.659904	0.392206	-0.259079
5	8	0	0.775273	3.739994	1.797167
6	8	0	1.665267	3.369594	3.872070
7	8	0	2.754351	3.211838	-0.755856
8	8	0	2.299304	3.976520	-2.878005
9	8	0	-0.753663	-2.286860	-3.007079
10	6	0	1.742289	0.234128	1.231135
11	6	0	1.168502	1.487254	0.895096
12	6	0	1.201470	2.445675	1.879856
13	6	0	1.758664	2.228788	3.132026
14	6	0	2.360940	1.041546	3.450184
15	1	0	2.820629	0.877786	4.415495
16	6	0	2.333535	0.042606	2.470813
17	1	0	2.772373	-0.915299	2.710889
18	6	0	0.772356	4.199913	3.140747
19	1	0	-0.240025	4.098966	3.553513
20	1	0	1.126932	5.228948	3.171076
21	6	0	0.713318	1.891935	-0.467102
22	6	0	-0.502837	1.546210	-1.113802
23	6	0	-0.780657	2.047726	-2.380102
24	1	0	-1.722523	1.810265	-2.853611
25	6	0	0.107180	2.877442	-3.077785
26	1	0	-0.123248	3.250476	-4.066780
27	6	0	1.275091	3.198796	-2.441163
28	6	0	1.550528	2.731109	-1.166194
29	6	0	-0.754633	-2.065394	-1.871905
30	6	0	-0.439240	-3.990823	0.397683
31	6	0	-1.687335	-3.846360	-0.241764
32	1	0	-1.750934	-4.182075	-1.275292
33	6	0	-2.758742	-3.051932	0.233960
34	1	0	-0.366498	-3.988885	1.477892
35	1	0	0.339442	-4.537236	-0.123184
36	6	0	3.277196	3.964141	-1.840774
37	1	0	4.186832	3.481749	-2.210033
38	1	0	3.469117	4.988395	-1.512252
39	6	0	-3.904497	-2.822237	-0.729523
40	1	0	-4.636875	-3.635299	-0.643901
41	1	0	-4.428044	-1.890012	-0.505246
42	1	0	-3.570323	-2.771126	-1.767436
43	6	0	-3.230731	-3.138276	1.667687
44	1	0	-3.998871	-3.920870	1.723520
45	1	0	-2.438119	-3.373158	2.371782
46	1	0	-3.699514	-2.204879	1.988303
47	6	0	2.453045	-0.432481	-1.394031
48	6	0	3.724630	0.095422	-1.146929
49	6	0	1.937395	-0.359965	-2.683570

50	6	0	4.463130	0.668656	-2.169990
51	1	0	4.133588	0.066220	-0.143205
52	6	0	2.670796	0.230160	-3.707087
53	1	0	0.950215	-0.733958	-2.902599
54	6	0	3.934458	0.743423	-3.455054
55	1	0	5.450005	1.066646	-1.960590
56	1	0	2.243814	0.293510	-4.701121
57	1	0	4.504686	1.203799	-4.254220
58	6	0	2.623949	-2.515305	0.556739
59	6	0	3.610796	-3.014337	-0.294805
60	6	0	2.391740	-3.169342	1.771925
61	6	0	4.364397	-4.124832	0.070084
62	1	0	3.796998	-2.546717	-1.253186
63	6	0	3.156562	-4.266970	2.137884
64	1	0	1.590570	-2.828803	2.418271
65	6	0	4.147161	-4.748763	1.289673
66	1	0	5.123920	-4.499052	-0.607086
67	1	0	2.965861	-4.755204	3.086911
68	1	0	4.738605	-5.611579	1.574765
69	6	0	-2.164430	1.393586	1.196228
70	6	0	-2.110190	2.787474	1.147797
71	6	0	-2.738891	0.774336	2.305028
72	6	0	-2.613279	3.546360	2.195836
73	1	0	-1.672273	3.287921	0.293260
74	6	0	-3.239046	1.535481	3.353456
75	1	0	-2.770835	-0.303948	2.359619
76	6	0	-3.176956	2.922273	3.302539
77	1	0	-2.566147	4.628534	2.142378
78	1	0	-3.671689	1.038906	4.214161
79	1	0	-3.568809	3.515504	4.121594
80	6	0	-3.205837	0.476779	-1.269233
81	6	0	-4.392086	0.991844	-0.745530
82	6	0	-3.231838	-0.067148	-2.557071
83	6	0	-5.569410	0.955402	-1.485387
84	1	0	-4.410902	1.418584	0.248636
85	6	0	-4.401660	-0.087167	-3.301042
86	1	0	-2.335272	-0.486349	-2.992940
87	6	0	-5.579693	0.418233	-2.763928
88	1	0	-6.480989	1.352903	-1.053778
89	1	0	-4.393234	-0.512397	-4.298163
90	1	0	-6.498305	0.391038	-3.338849

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