

Supporting Information

Aldehyde (α -Methoxy)Allylation via 2-Propanol Mediated Reductive Coupling: Halide-Dependent Regio- and Enantioselection from 1 of 24 Fluxional Diastereomeric-at-Ruthenium-SEGPHOS Complexes

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Table of Contents

General Information	S2
Spectroscopy, Spectrometry and Data Collection	S2
Methoxyallene 1 and Known Aldehydes 2a-2k	S3
Products 3a-3k	S4
Deuterium Labelling Studies	S56
Syntheses of Ruthenium-Halide Complexes	S59
Pd-Catalyzed Asymmetric Tsuji-Reduction of Compound 3h	S65
Synthesis of C ₁₂ -C ₁₇ Fragment of Bafilomycin A ₁ 4k	S71
Synthesis of 3i -(3,5-dinitrobenzoate)	S74
Single Crystal Diffraction Data for 3i -(3,5-dinitrobenzoate)	S77
Computational Studies	S79
References	S121

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 which include $\text{Ru}_3(\text{CO})_{12}$, allyl iodide, (*R*)-SEGPHOS, (*S*)-SEGPHOS, *rac*-BINAP, 2-propanol 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 (^1H 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 (101, 126 MHz) spectrometer and were routinely run with broadband decoupling. Deuterium nuclear magnetic resonance (^2H NMR) spectra were recorded in CHCl_3 solution with a Varian Gemini 500 (92 MHz) spectrometer (relaxation delay 2.00s).

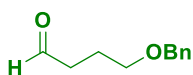
Methoxyallene 1

Methoxyallene **1** was prepared in accordance with the procedure reported in Ref. 1.

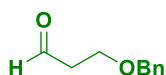


1
Ref. 1

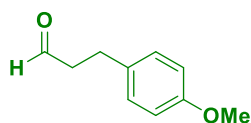
Known Aldehydes 2a-2k



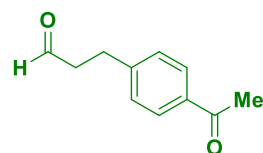
2a
Ref. 2



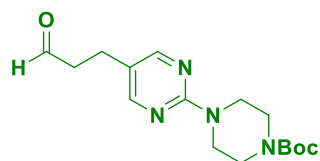
2b
Ref. 3



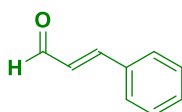
2c
Ref. 4



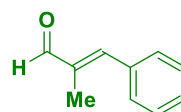
2d
Ref. 4



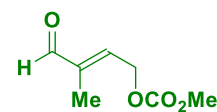
2e
Ref. 5



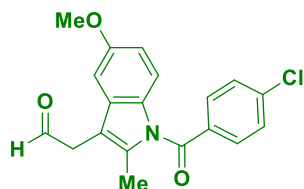
2f
Commercial



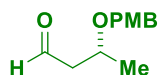
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Commercial



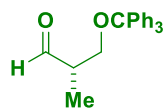
2h
Ref. 6



2i
Ref. 7



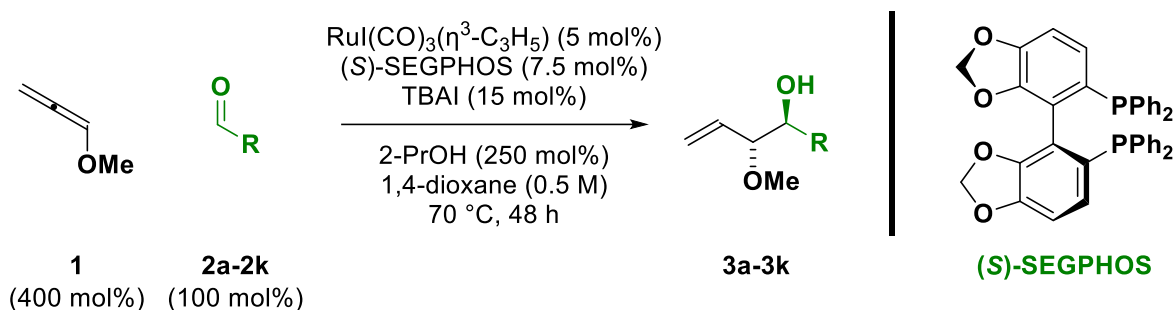
2j
Ref. 8



2k
Ref. 9

Products 3a-3k

General Procedure

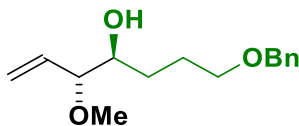


An oven-dried pressure tube equipped with a magnetic stir bar was charged with aldehyde **2a-2k** (0.2 mmol, 100 mol%), $\text{RuI}(\text{CO})_3(\eta^3\text{-C}_3\text{H}_5)$ (3.6 mg, 0.01 mmol, 5 mol%), (**R**)-SEGPHOS (9.2 mg, 0.015 mmol, 7.5 mol%) or (**S**)-SEGPHOS (9.2 mg, 0.015 mmol, 7.5 mol%), and TBAI (11.0 mg, 0.03 mmol, 15 mol%) under an argon atmosphere. 2-propanol (38 μL , 0.5 mmol, 250 mol%), 1,4-dioxane (0.4 mL, 0.5 M), and methoxyallene **1** (72 μL , 0.8 mmol, 400 mol%) were added via syringe. The tube was purged with argon for approximately 15 seconds. The tube was sealed with a PTFE-lined cap, placed in a 70 °C oil bath and allowed to stir for 48 hours. After reaching ambient temperature, the reaction mixture was concentrated *in vacuo* and the residue was subjected to flash column chromatography (SiO_2) under the noted conditions to furnish products **3a-3k**.

Diastereomeric ratios were determined by ^1H NMR of a purified reaction. Enantiomeric excesses were determined by chiral stationary phase HPLC.

Racemic reactions were performed using *rac*-BINAP (9.3 mg, 0.015 mmol, 7.5 mol%) as ligand.

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



Aldehyde **2a** (36.0 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(S)-SEGPHOS** as ligand. Upon flash column chromatography (SiO₂: 2:98 acetone:hexanes), the title compound **3a** was isolated as a yellow oil in 66% yield (32.7 mg, 0.13 mmol, 91% ee, 6:1 dr).

TLC (SiO₂): R_f = 0.5 (3:7 acetone:hexanes).

¹H NMR (400 MHz, C₆D₆): δ 7.28 – 7.20 (m, 4H), 5.67 (ddd, *J* = 17.1, 10.4, 8.0 Hz, 1H), 5.26 (ddd, *J* = 10.4, 1.8, 0.8 Hz, 1H), 5.19 (ddd, *J* = 17.3, 1.8, 0.9 Hz, 1H), 4.41 (s, 2H), 3.59 (dq, *J* = 7.7, 3.7 Hz, 1H), 3.43 – 3.37 (m, 3H), 3.21 (s, 3H), 2.38 (dd, *J* = 4.4, 1.8 Hz, 1H), 1.76 – 1.66 (m, 1H), 1.61 (ddd, *J* = 13.6, 6.9, 2.3 Hz, 1H), 1.57 – 1.50 (m, 1H), 1.35 (dtd, *J* = 14.4, 8.8, 5.6 Hz, 1H).

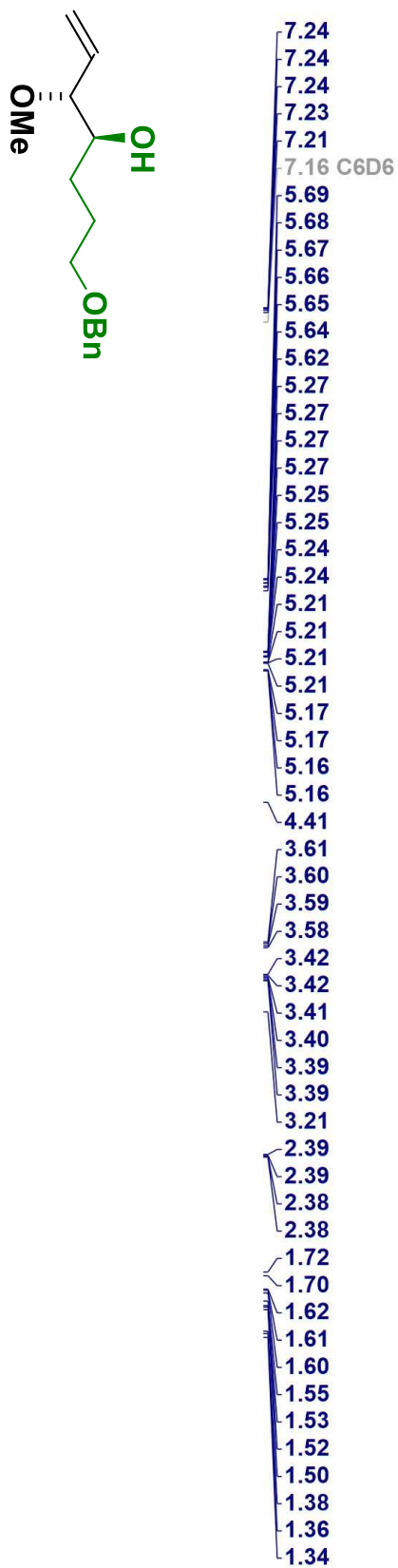
¹³C NMR (101 MHz, C₆D₆): δ 139.4, 135.4, 128.5, 128.2, 127.9, 127.6, 86.6, 73.2, 73.0, 70.6, 56.2, 29.6, 26.7.

HRMS (Na⁺, *m/z*) for C₁₅H₂₂O₃: calcd. = 273.1461; found = 273.1467.

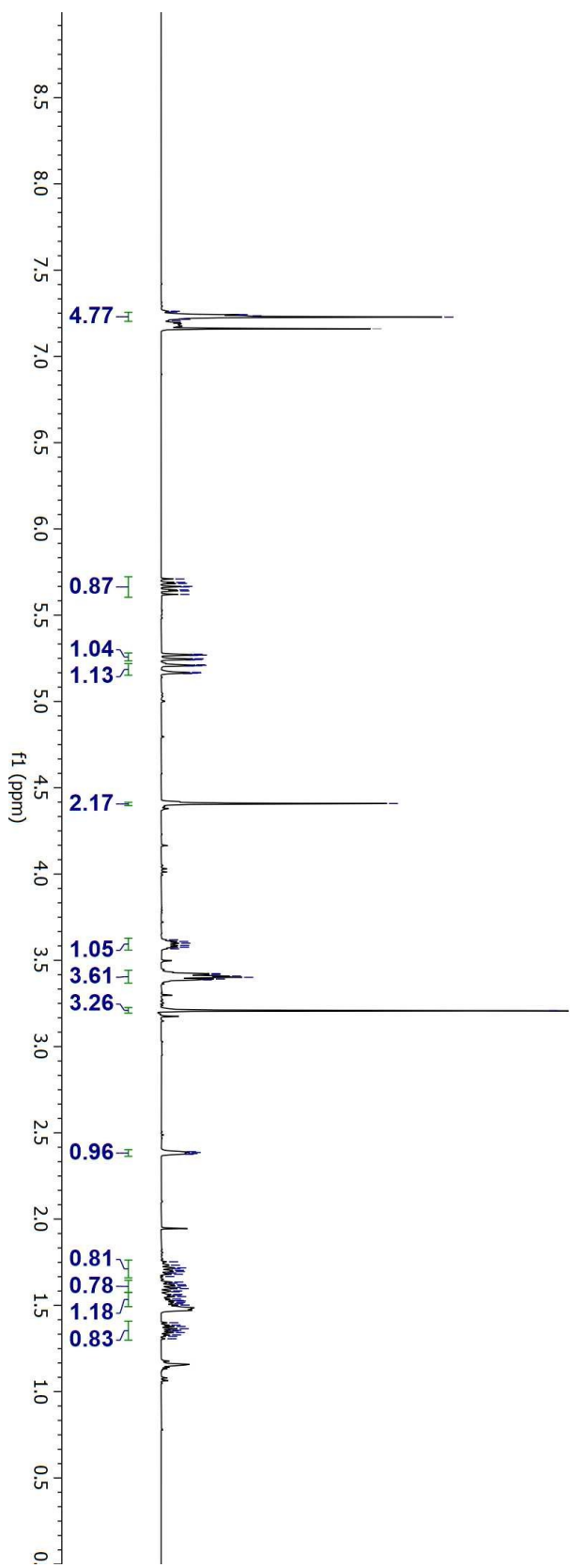
FTIR (neat): 3445, 2926, 2342, 1683, 1448, 1089, 752, 668 cm⁻¹.

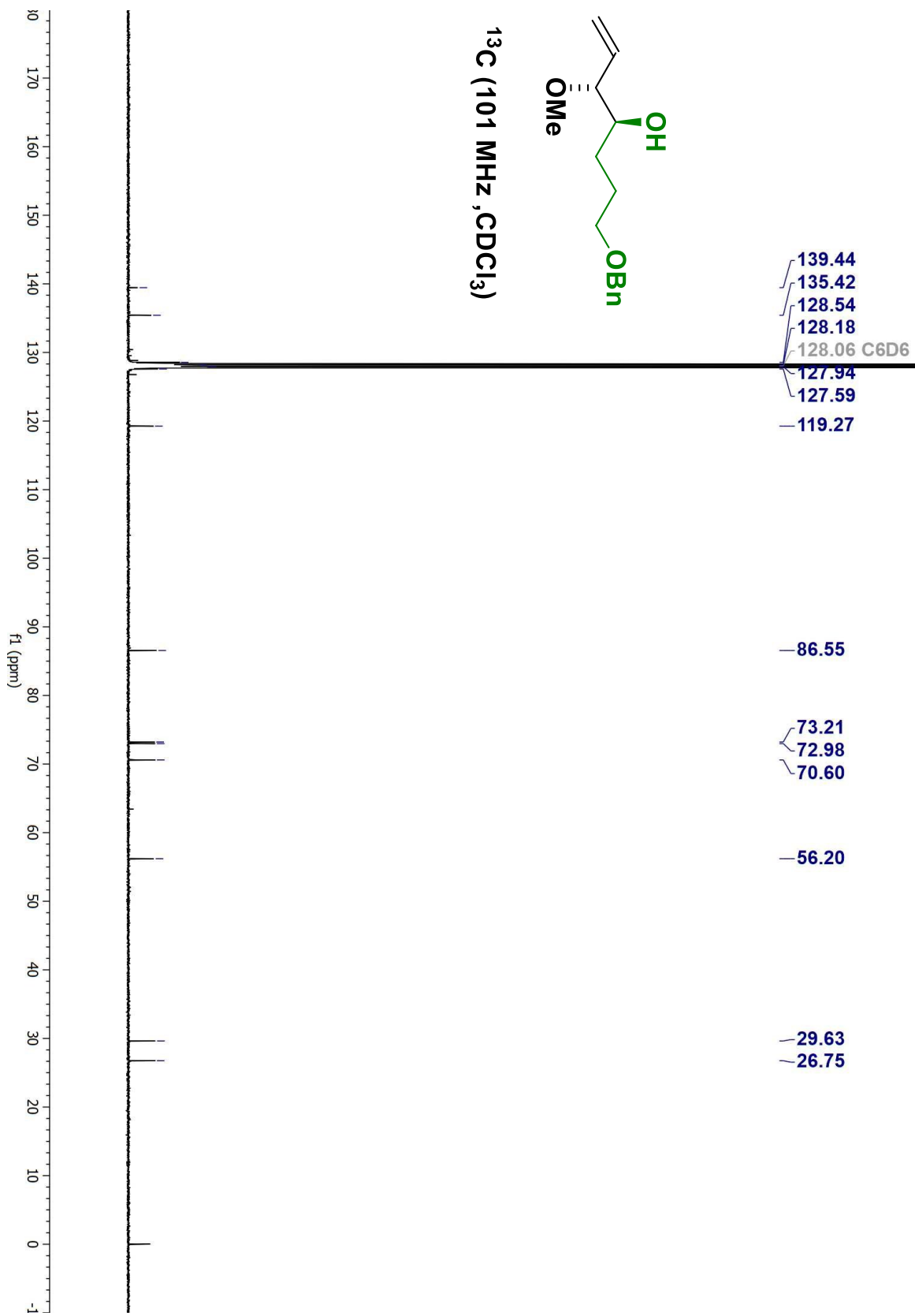
HPLC: Chiralcel column OJ-H, Hexane:2-PrOH = 98:02, 0.5 mL/min, 210 nm.

[α]_D²⁴ = -59.4 (*c* = 0.51, CHCl₃).

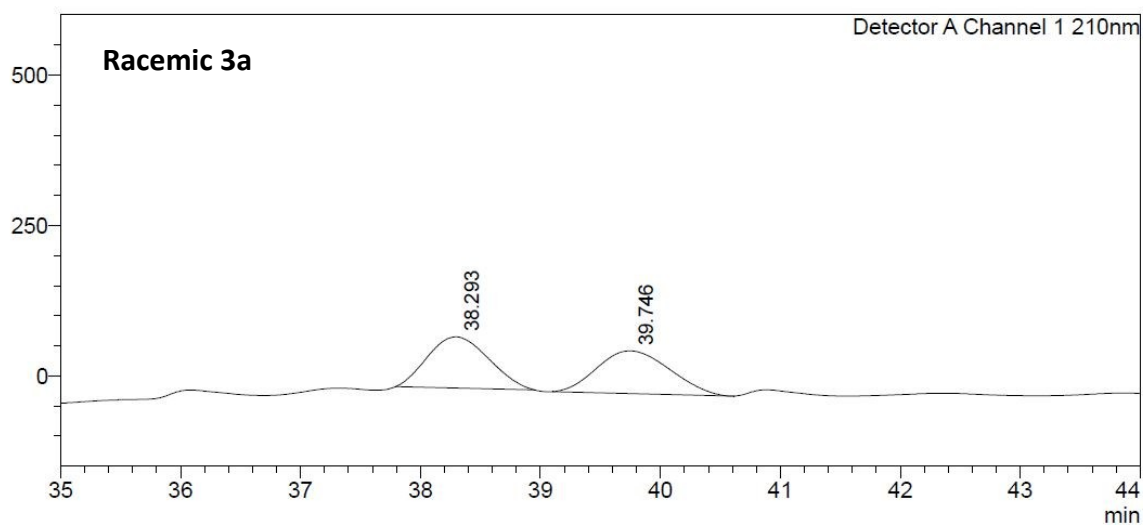


¹H (400 MHz, CDCl₃)



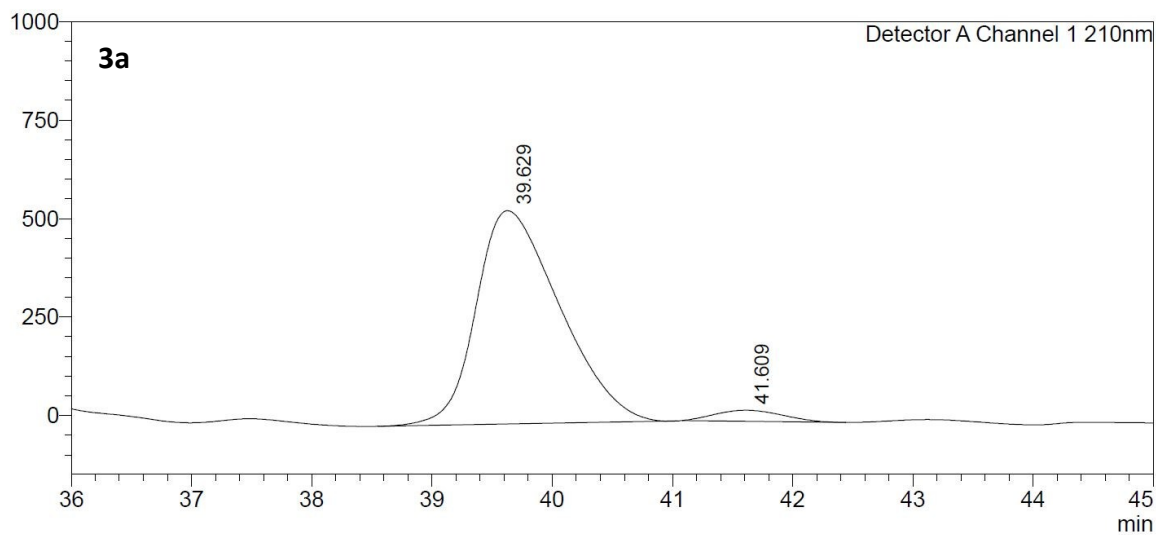


mV



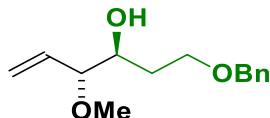
Peak#	Ret. Time	Area	Height	Conc.
1	38.293	3019392	85064	50.331
2	39.746	2979642	70941	49.669
Total		5999034	156006	

mV



Peak#	Ret. Time	Area	Height	Conc.
1	39.629	26192397	541593	96.000
2	41.609	1091297	28014	4.000
Total		27283694	569607	

(3*S*,4*R*)-1-(benzyloxy)-4-methoxyhex-5-en-3-ol (3b)



Aldehyde **2b** (33.2 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(S)-SEGPHOS** as ligand. Upon flash column chromatography (SiO₂:2:98 acetone:hexanes), the title compound **3b** was isolated as a yellow oil in 76% yield (36.0 mg, 0.15 mmol, 86% ee, 4:1 dr).

TLC (SiO₂): R_f = 0.46 (1:2 acetone:hexanes).

¹H NMR (400 MHz, CDCl₃): δ 7.37 – 7.27 (m, 5H), 5.76 (ddd, *J* = 17.3, 10.4, 8.0 Hz, 1H), 5.37 – 5.25 (m, 2H), 4.52 (s, 2H), 3.85 (d, *J* = 12.3 Hz, 1H), 3.72 – 3.60 (m, 3H), 3.50 (dd, *J* = 7.9, 4.5 Hz, 1H), 3.31 (s, 3H), 2.77 (s, 1H).

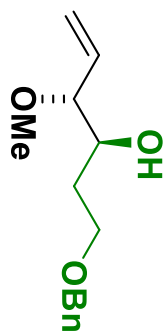
¹³C NMR (101 MHz, CDCl₃): δ 138.3, 134.8, 128.6, 127.8, 119.9, 86.0, 73.4, 72.1, 68.5, 56.7, 32.3, 29.9.

HRMS (Na⁺, *m/z*) for C₁₄H₂₀O₃: calcd. = 259.1305; found = 259.1294.

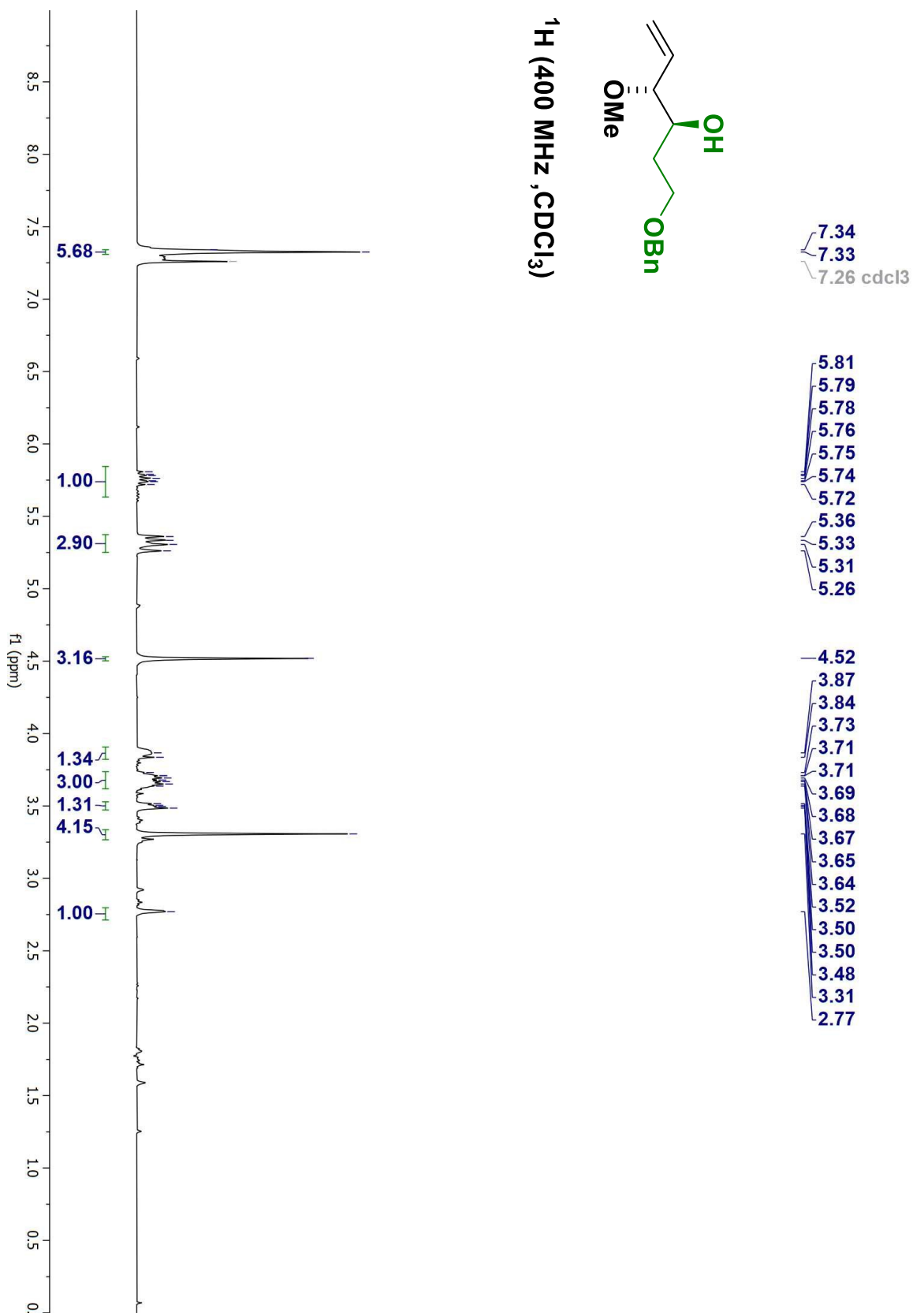
FTIR (neat): 3459, 2927, 2859, 2341, 1688, 1095, 737, 668 cm⁻¹.

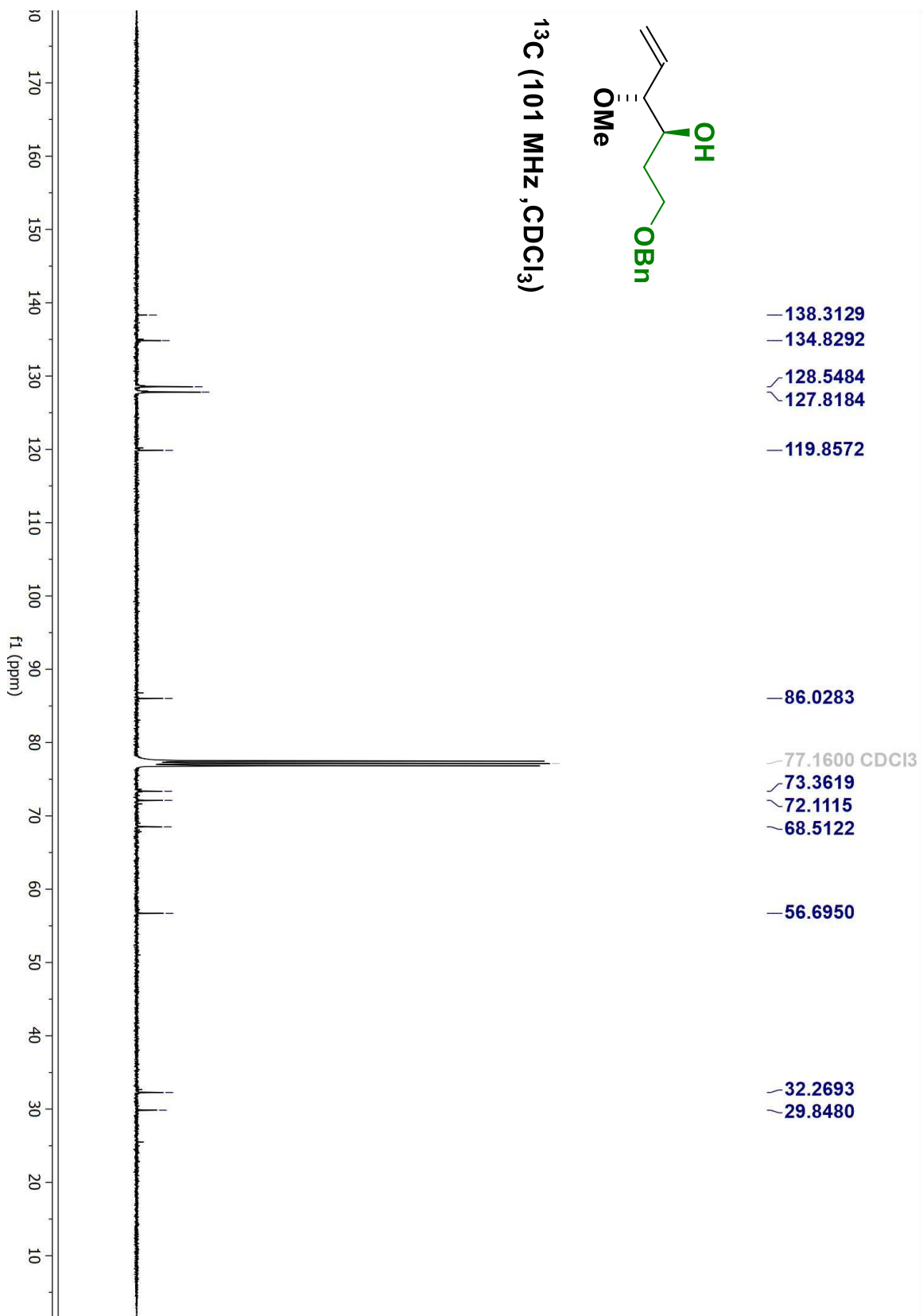
HPLC: Chiralcel column OD-H, Hexane:2-PrOH = 99:01, 0.5 mL/min, 210 nm.

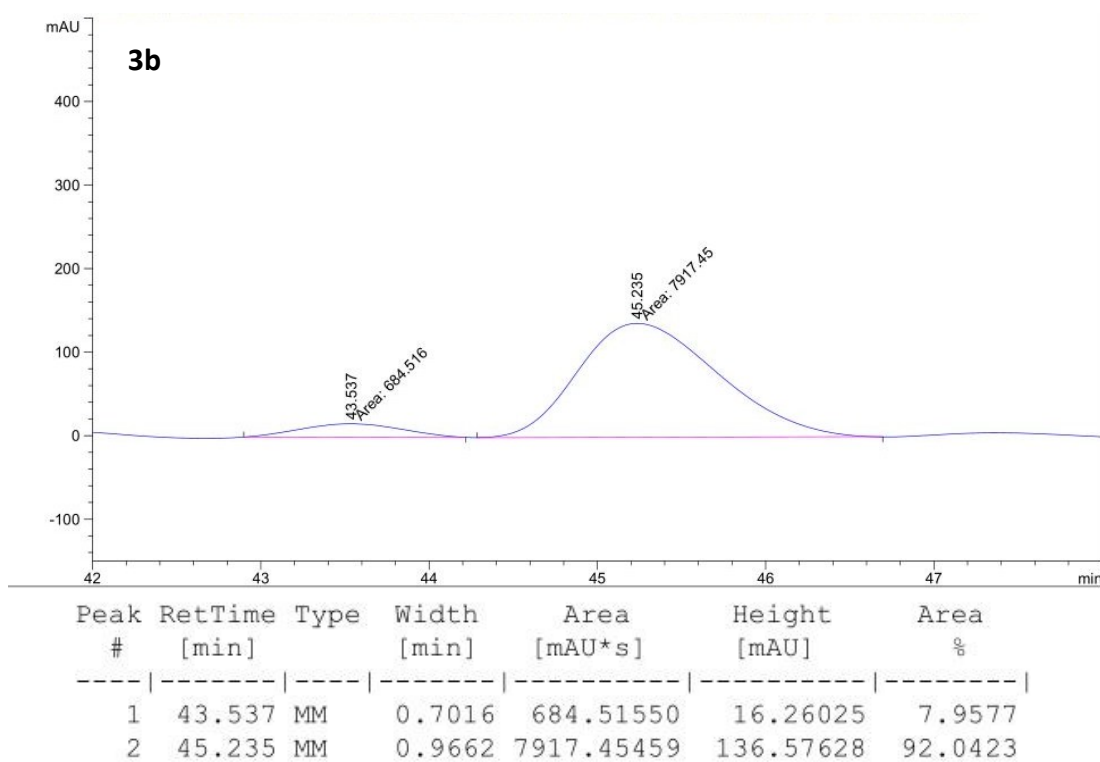
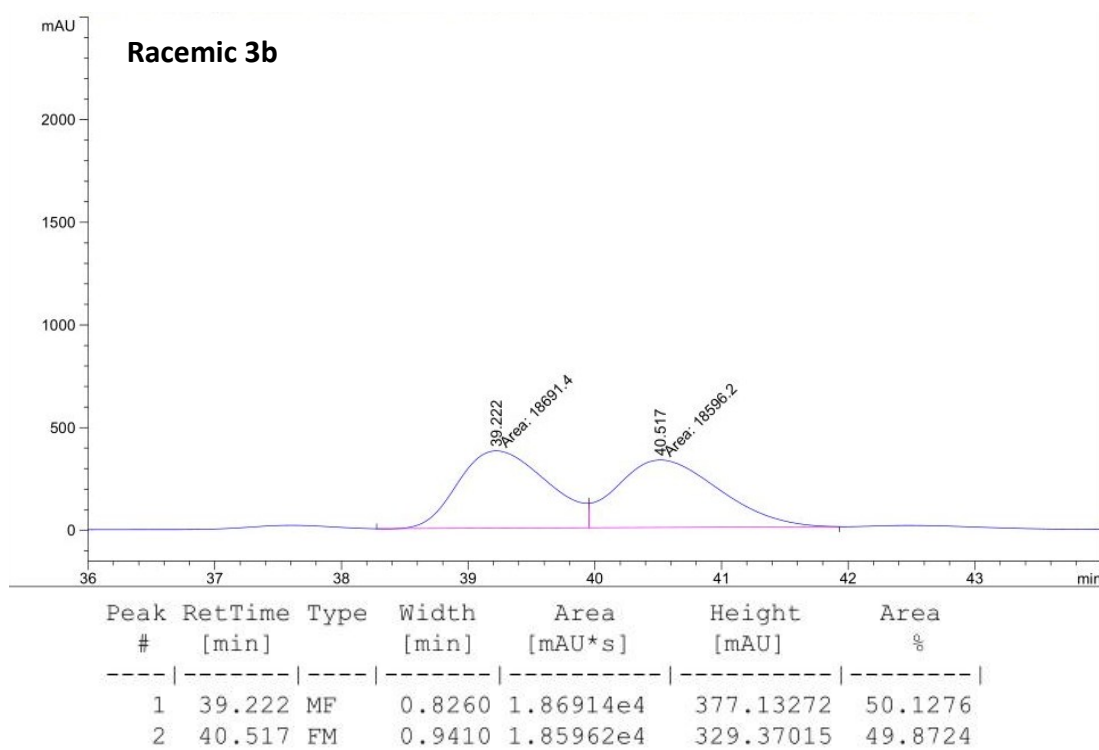
$[\alpha]_D^{24}$ = -19.8 (*c* = 0.51, CHCl₃).



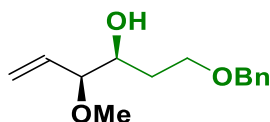
^1H (400 MHz, CDCl_3)







(3*S*,4*R*)-1-(benzyloxy)-4-methoxyhex-5-en-3-ol (syn-3b)



Absolute Stereochemical Assignment of Minor Diastereomer: Aldehyde **2b** (328 mg, 2.0 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(*S*)-SEGPHOS** as ligand. Upon flash column chromatography (SiO₂:4.5:95.5 acetone:hexanes), the title compound **syn-3b** was separated from the major diastereomer as a clear, yellow oil (71.8 mg, 0.3 mmol). The title compound is identical to previously reported material in all respects, including optical rotation.¹⁰

TLC (SiO₂): R_f = 0.22 (1:6.5 acetone:hexanes).

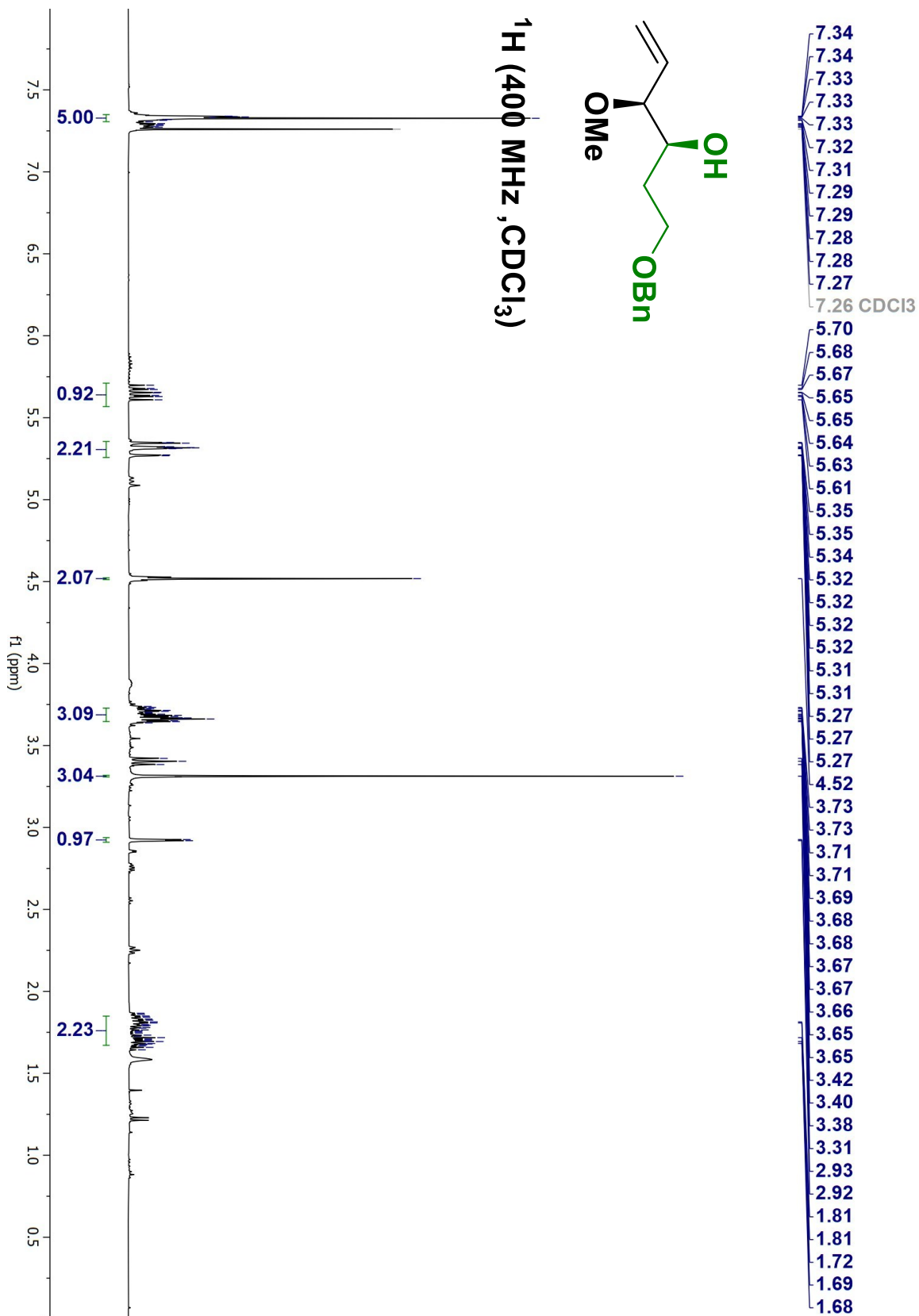
¹H NMR (400 MHz, CDCl₃): δ 7.35 – 7.27 (m, 5H), 5.65 (ddd, J = 17.1, 10.5, 8.0 Hz, 1H), 5.35 – 5.26 (m, 2H), 4.52 (s, 2H), 3.75 – 3.63 (m, 3H), 3.40 (t, J = 7.5 Hz, 1H), 3.31 (s, 3H), 2.92 (d, J = 2.5 Hz, 1H), 1.88 – 1.64 (m, 2H).

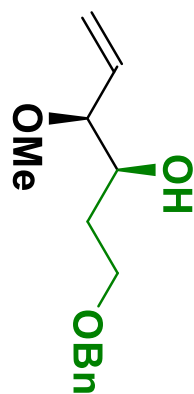
¹³C NMR (126 MHz, CDCl₃): δ 138.45, 134.99, 128.52, 127.81, 127.73, 120.28, 86.79, 73.27, 71.62, 67.84, 56.69, 32.62.

HRMS (Na⁺, *m/z*) for C₁₄H₂₀O₃: calcd. = 259.1305; found = 259.1294.

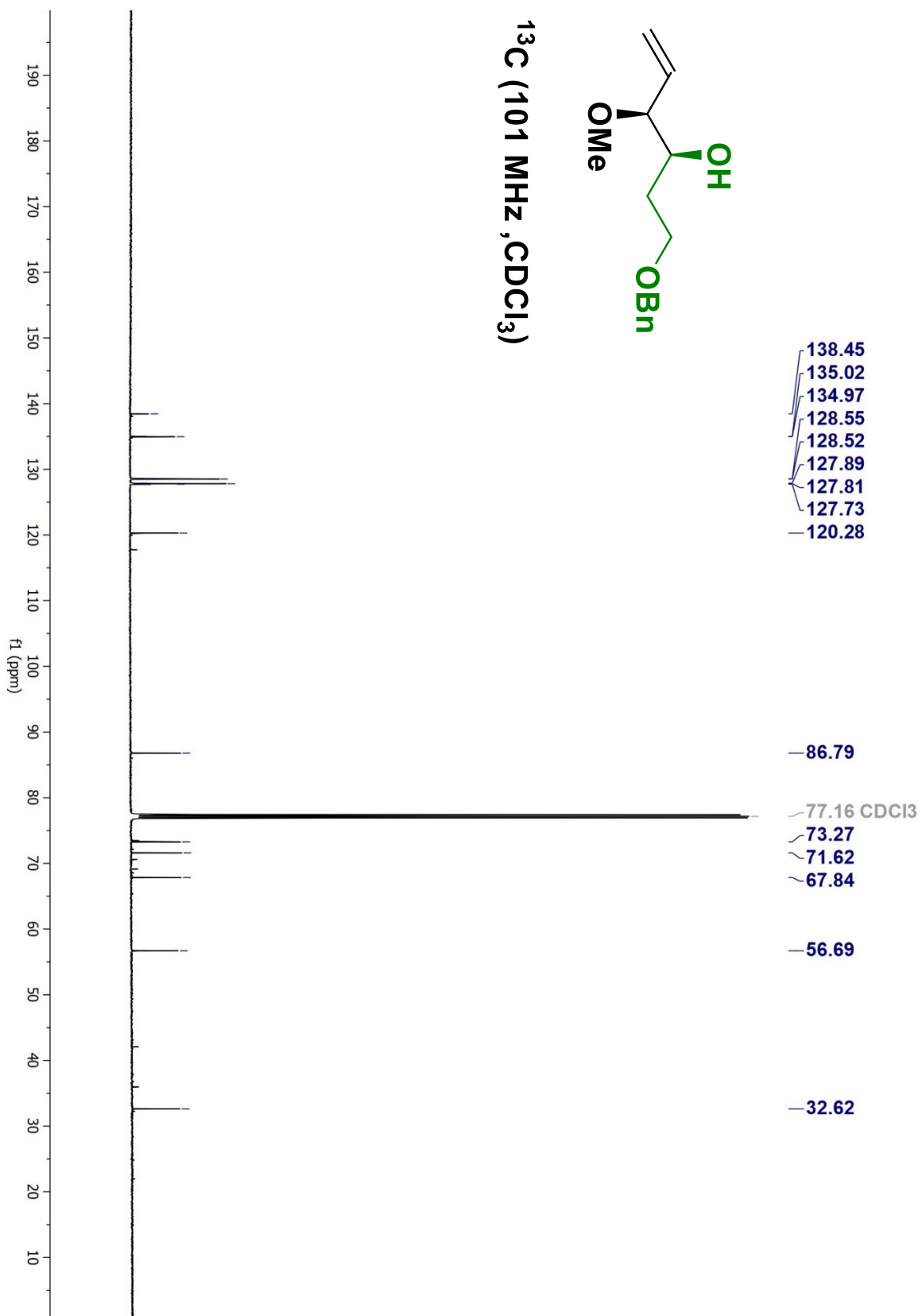
FTIR (neat): 3441, 2858, 1715, 1639, 1495, 1453, 1429, 1361 cm⁻¹.

[α]_D²⁴ = 3.46 (c = 0.26, CHCl₃).

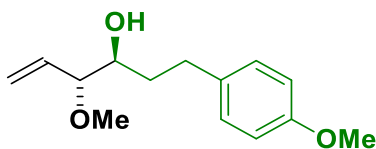




^{13}C (101 MHz, CDCl_3)



(3*S*,4*R*)-4-methoxy-1-(4-methoxyphenyl)hex-5-en-3-ol (3c)



Aldehyde **2c** (32.8 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) in Acetone (0.5 M) with **(S)-SEGPPOS** as ligand. Upon flash column chromatography (SiO₂: 3:97 acetone:petroleum ether), the title compound **3c** was isolated as a brown oil in 76% yield (35.9 mg, 0.15 mmol, 86% ee, 3:1 dr).

TLC (SiO₂): R_f = 0.6 (1:3 acetone:petroleum ether).

¹H NMR (500 MHz, CDCl₃): δ 7.12 (d, *J* = 8.2 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 5.76 (ddd, *J* = 17.9, 10.4, 8.1 Hz, 1H), 5.36 (d, *J* = 10.5 Hz, 1H), 5.28 (d, *J* = 17.3 Hz, 1H), 3.78 (s, 3H), 3.70 (s, 1H), 3.50 (dd, *J* = 8.2, 3.8 Hz, 1H), 3.30 (s, 3H), 2.80 (dt, *J* = 14.6, 7.6 Hz, 1H), 2.60 (dt, *J* = 13.8, 8.3 Hz, 1H), 2.12 (s, 1H), 1.73 – 1.66 (m, 2H).

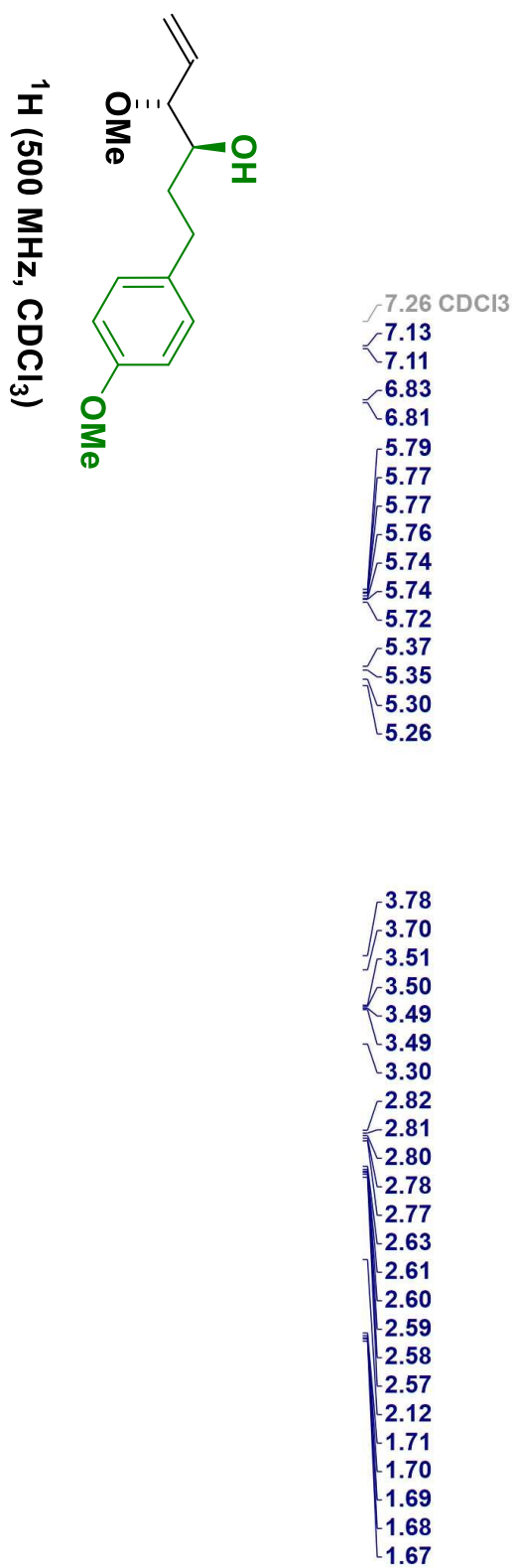
¹³C NMR (126 MHz, CDCl₃): δ 157.9, 134.3, 129.5, 120.3, 113.9, 86.2, 77.4, 72.4, 56.6, 55.4, 34.3, 31.2.

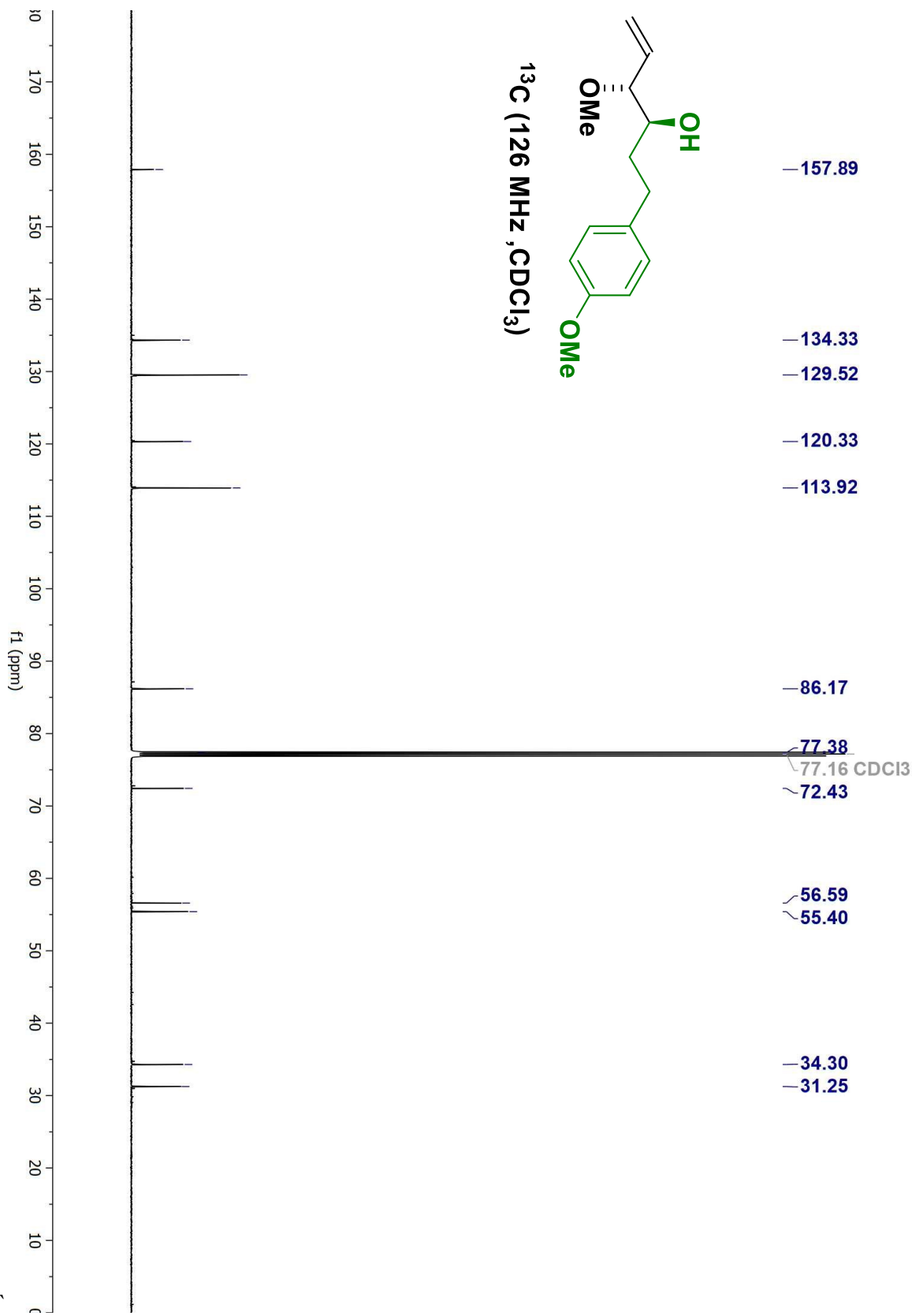
HRMS (Na⁺, *m/z*) for C₁₄H₂₀O₃: calcd. = 259.1305; found = 259.1303.

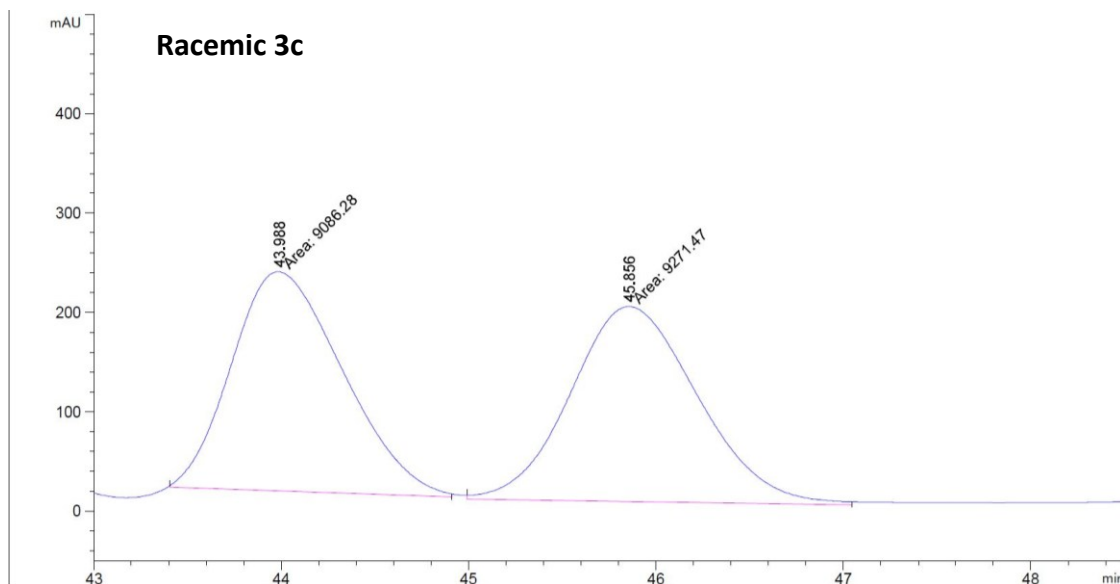
FTIR (neat): 3465, 2933, 2833, 1512, 1454, 1245, 1178, 1036, 931, 519, 418 cm⁻¹.

HPLC: Chiralcel columns 2 x OJ-H, Hexane:2-PrOH = 97:03, 1.0 mL/min, 230 nm.

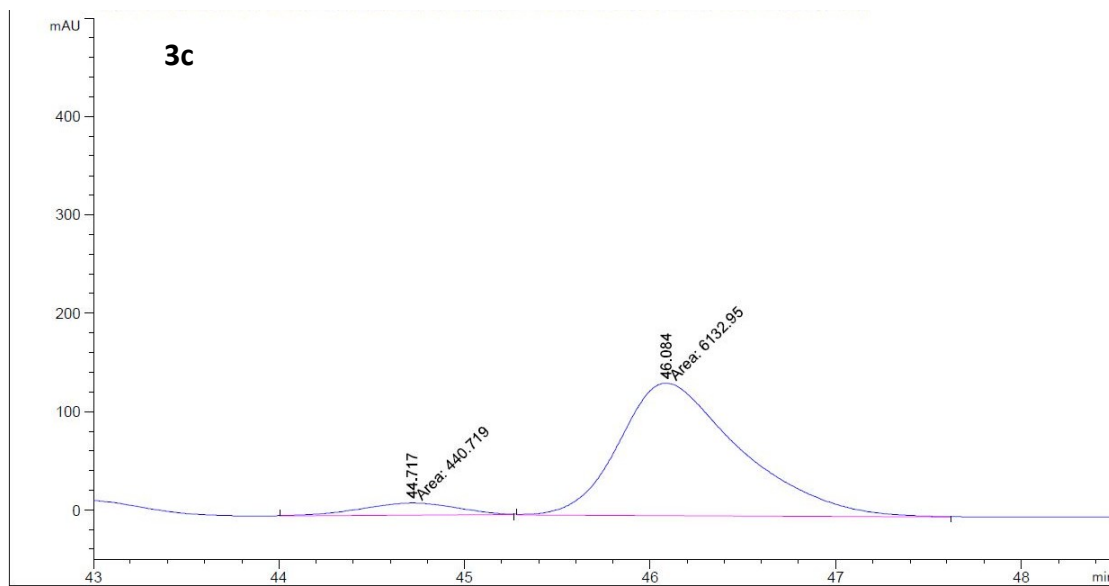
[α]_D²⁴ = -12.2 (*c* = 0.2, CHCl₃).





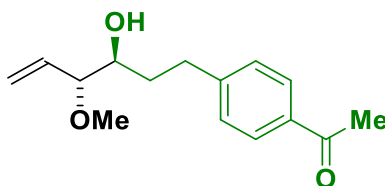


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	43.988	MM	0.6862	9086.27637	220.68233	49.4956
2	45.856	MM	0.7872	9271.47168	196.29604	50.5044



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	44.717	MM	0.5994	440.71866	12.25410	6.7043
2	46.084	MM	0.7580	6132.95166	134.85158	93.2957

1-(4-((3*S*,4*R*)-3-hydroxy-4-methoxyhex-5-en-1-yl)phenyl)ethan-1-one (3d)



Aldehyde **2d** (35.2 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(S)-SEGPHOS** as ligand. Upon flash column chromatography (SiO₂: 10:90 EtOAc:hexanes), the title compound **3d** was isolated as a brown oil in 89% yield (44.4 mg, 0.18 mmol, 84% ee, 3:1 dr).

TLC (SiO₂): R_f = 0.6 (2:3 EtOAc:hexanes).

¹H NMR (500 MHz, CDCl₃): δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 5.78 – 5.70 (m, 1H), 5.37 (dd, *J* = 10.5, 1.7 Hz, 1H), 5.29 (d, *J* = 17.6 Hz, 1H), 3.67 (dd, *J* = 8.5, 4.3 Hz, 1H), 3.50 (dd, *J* = 8.1, 4.0 Hz, 1H), 3.30 (s, 3H), 2.92 (dt, *J* = 14.5, 6.7 Hz, 1H), 2.78 – 2.69 (m, 1H), 2.58 (s, 3H), 2.15 (d, *J* = 4.5 Hz, 1H), 1.79 – 1.70 (m, 2H).

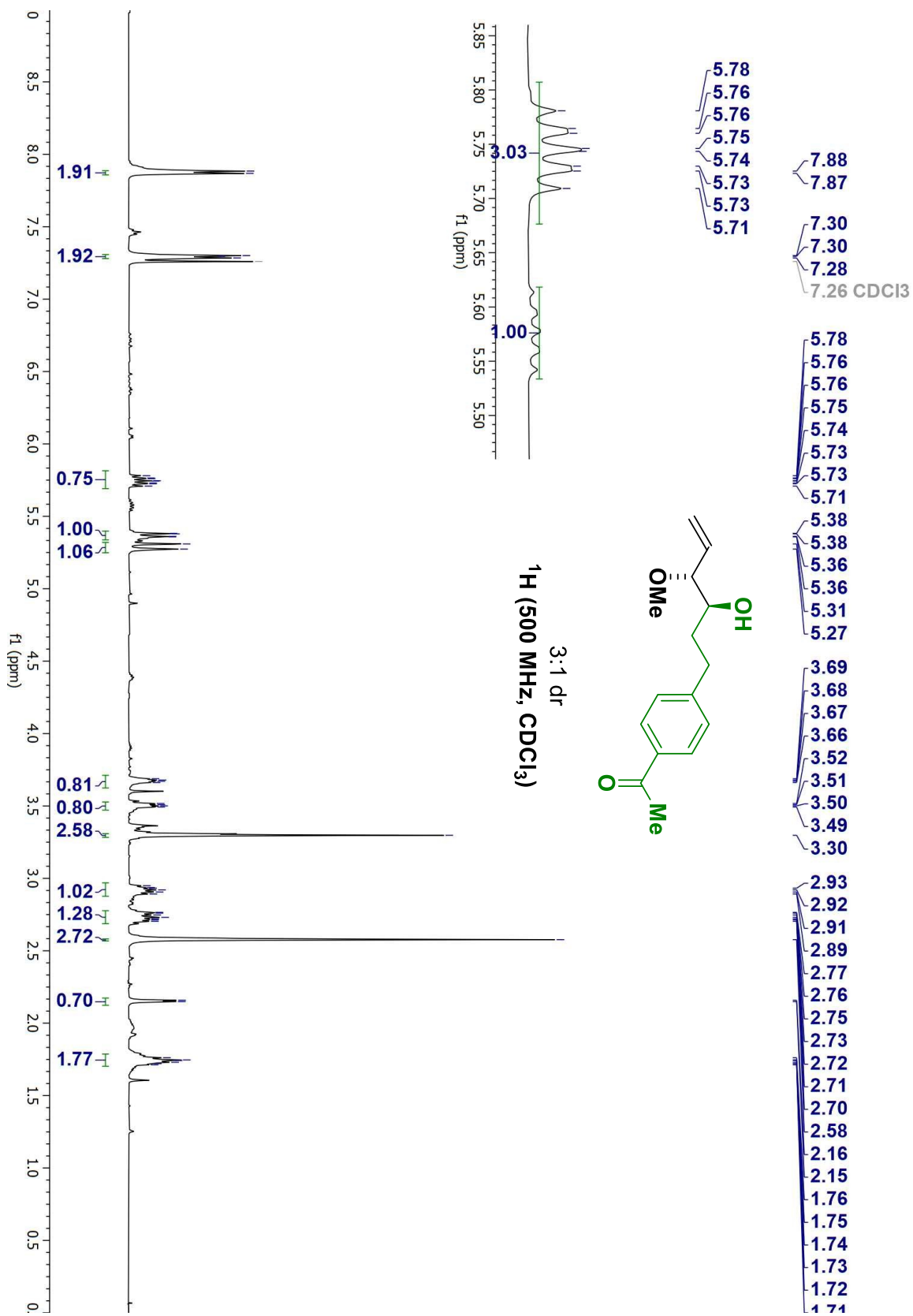
¹³C NMR (126 MHz, CDCl₃): δ 198.0, 148.2, 134.3, 128.9, 128.7, 120.5, 86.1, 77.4, 72.3, 56.6, 33.6, 32.2, 26.7.

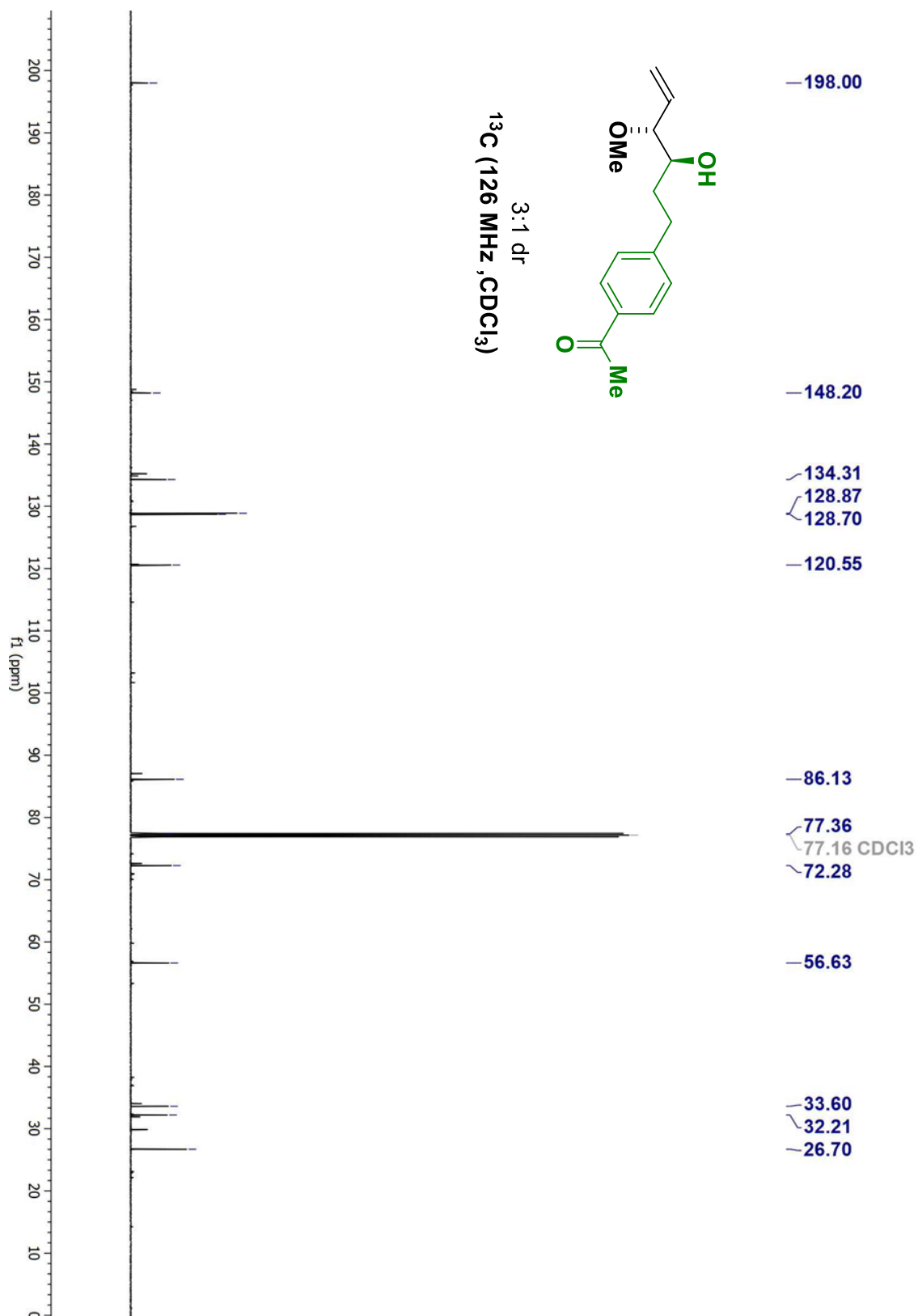
HRMS (Na⁺, *m/z*) for C₁₅H₂₀O₃: calcd. = 271.1305; found = 271.1307.

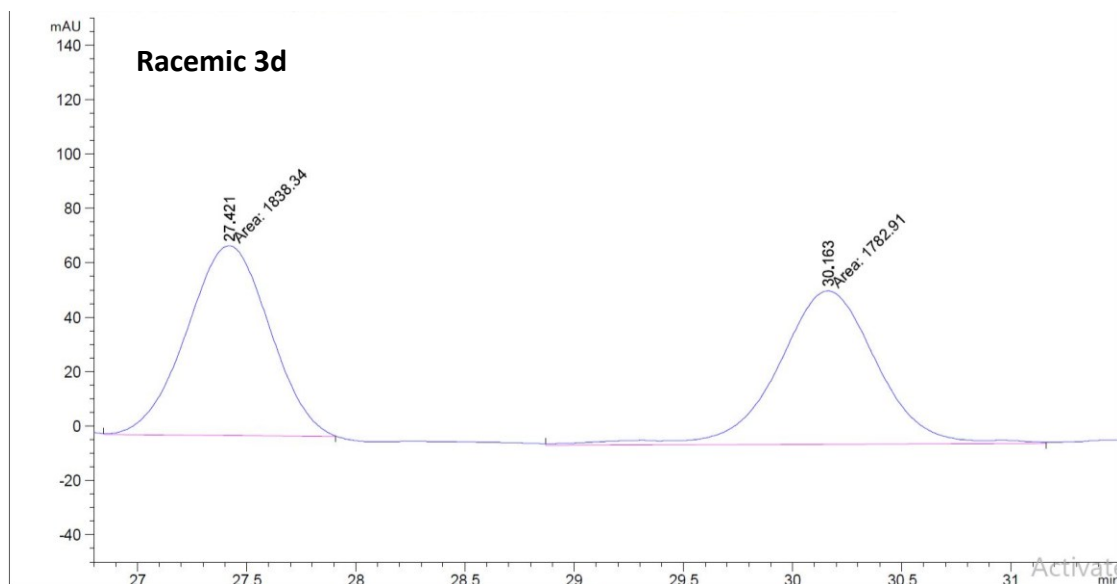
FTIR (neat): 2988, 2869, 1680, 1360, 1269, 1142, 697, 592, 530, 498, 408 cm⁻¹.

HPLC: Chiralcel columns 2 x OJ-H, Hexane:2-PrOH = 90:10, 1.0 mL/min, 254 nm.

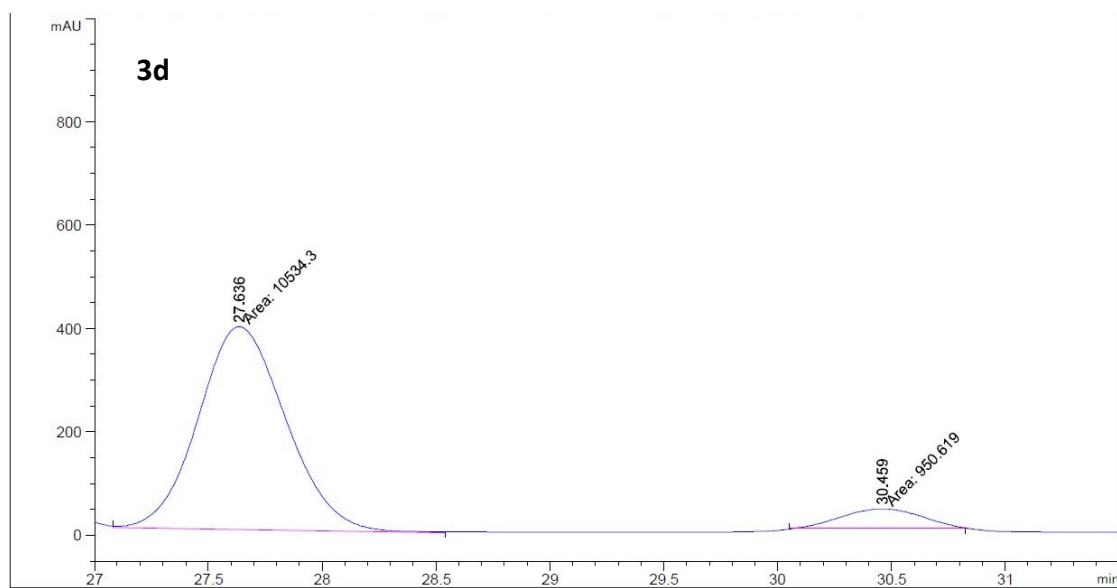
[α]_D²⁴ = -46.8 (*c* = 0.2, CHCl₃).





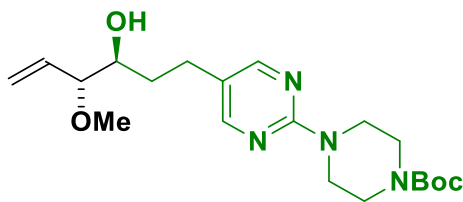


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.421	MM	0.4390	1838.34497	69.79600	50.7655
2	30.163	MM	0.5276	1782.90674	56.32660	49.2345



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.636	MM	0.4469	1.05343e4	392.83246	91.7229
2	30.459	MM	0.4122	950.61865	38.43510	8.2771

tert-butyl 4-(5-((3*S*,4*R*)-3-hydroxy-4-methoxyhex-5-en-1-yl)pyrimidin-2-yl)piperazine-1-carboxylate (3e**)**



Aldehyde **2e** (64.1 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(S)-SEGPHOS** as ligand. Upon flash column chromatography (SiO₂: 8:92 acetone:hexanes), the title compound **3e** was isolated as a brown oil in 60% yield (46.9 mg, 0.12 mmol, 86% ee, 3:1 dr).

TLC (SiO₂): R_f = 0.6 (1:2 acetone:hexanes).

¹H NMR (400 MHz, C₆D₆): δ 8.18 (s, 2H), 5.68 – 5.51 (m, 1H), 5.06 (dd, *J* = 10.4, 2.0 Hz, 1H), 5.01 – 4.91 (m, 1H), 3.77 (dt, *J* = 7.8, 3.0 Hz, 6H), 3.14 (dd, *J* = 8.1, 4.0 Hz, 1H), 3.01 (s, 3H), 2.59 – 2.39 (m, 2H), 2.31 (dtd, *J* = 21.3, 12.4, 7.8 Hz, 2H), 2.12 (d, *J* = 4.4 Hz, 1H), 1.43 (s, 9H).

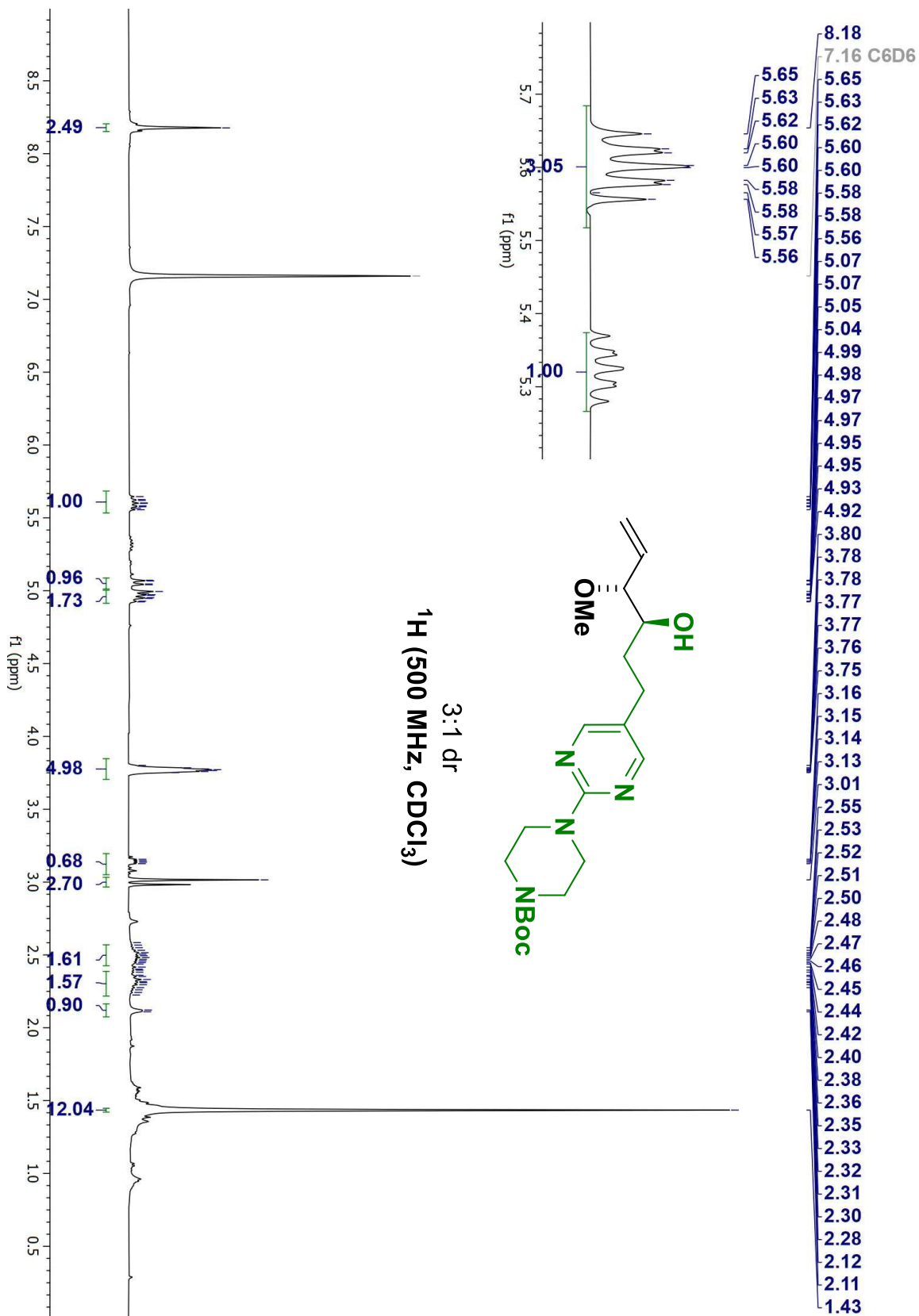
¹³C NMR (101 MHz, C₆D₆): δ 161.4, 158.0, 154.7, 135.1, 127.9, 123.3, 119.7, 86.5, 79.3, 71.8, 56.2, 44.1, 34.0, 28.5, 25.8.

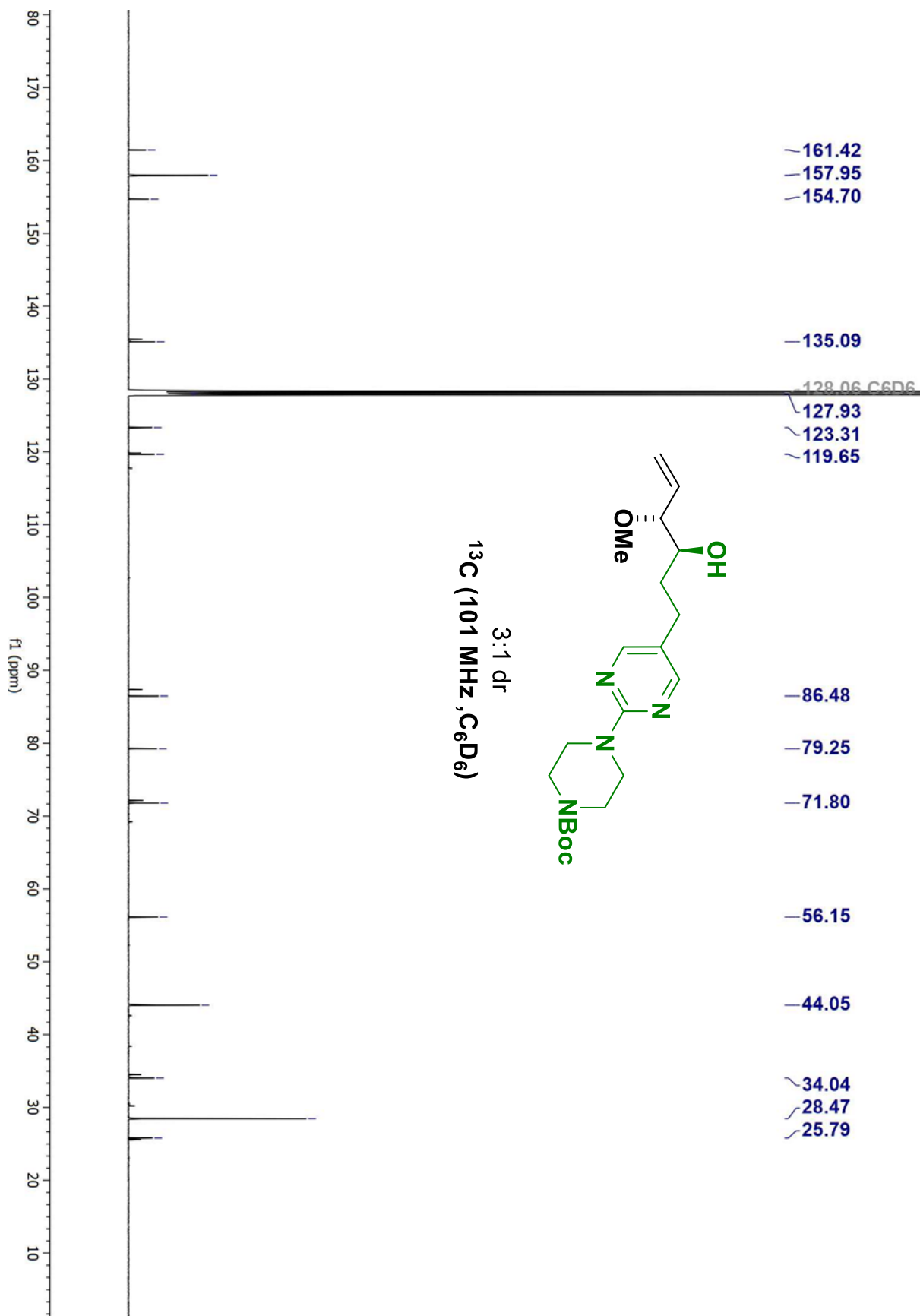
HRMS (H⁺, *m/z*) for C₂₀H₃₂ N₄O₄: calcd. = 393.2496; found = 393.2488.

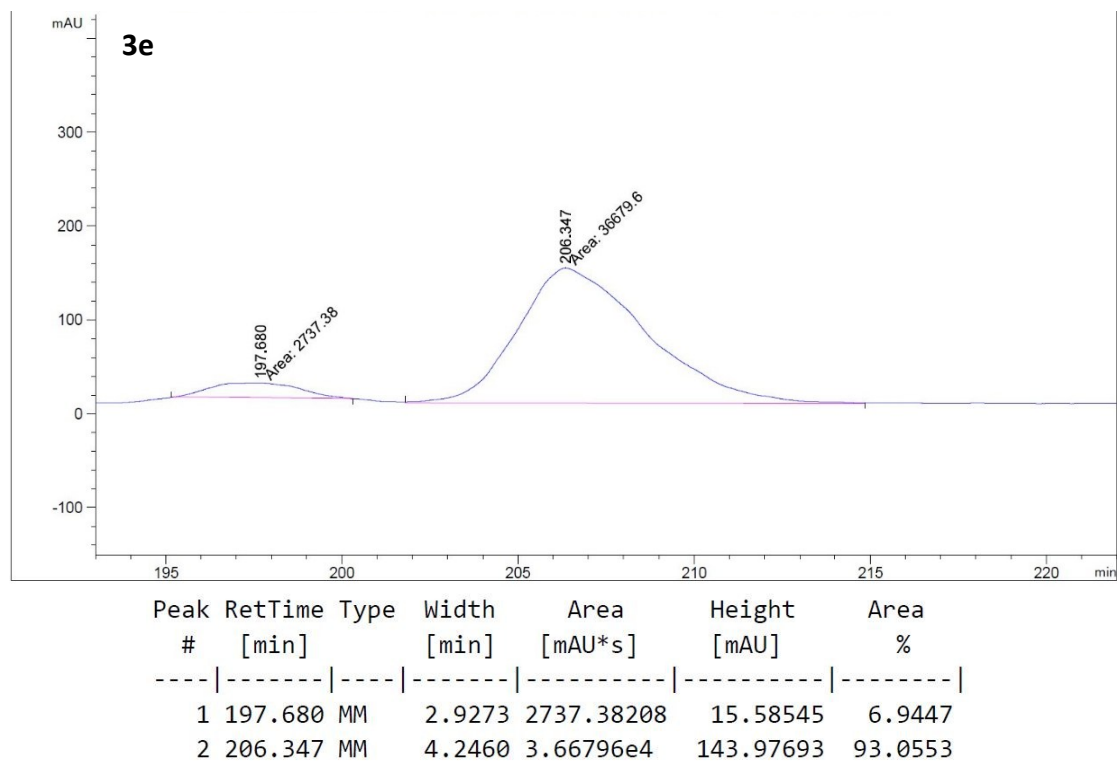
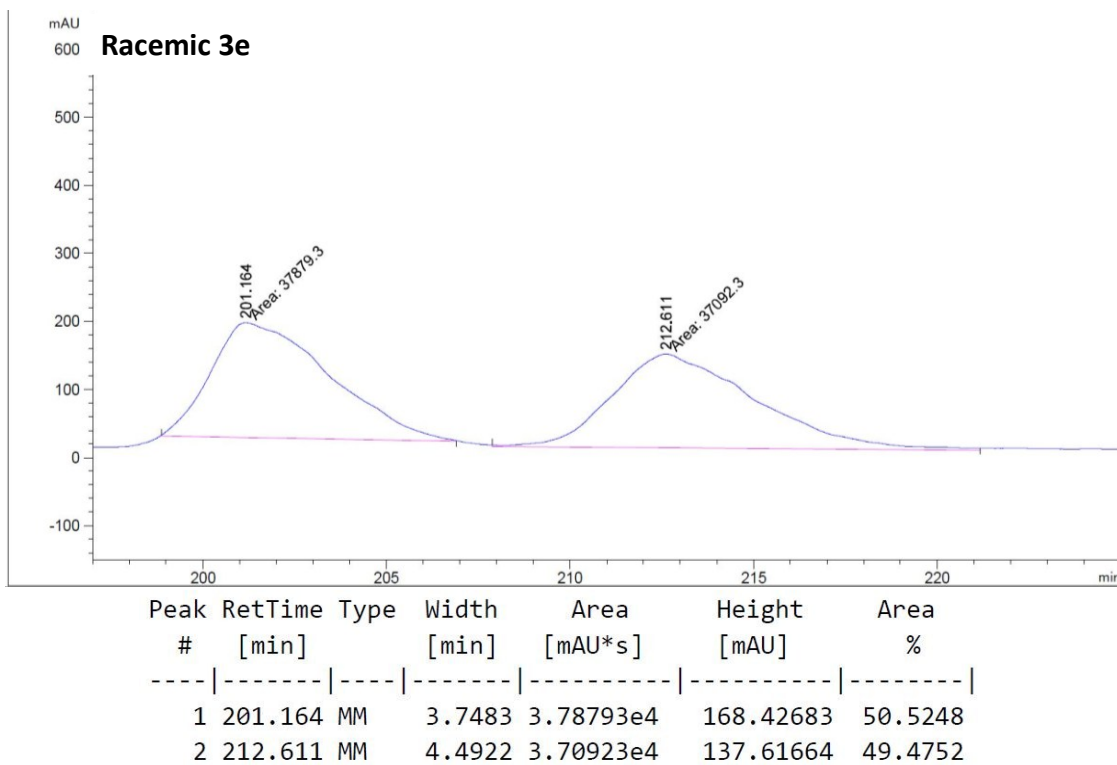
FTIR (neat): 3659, 2980, 2884, 1462, 1382, 1251, 1151, 1073, 955, 818, 415 cm⁻¹.

HPLC: Chiralcel columns 2 x OJ-H, Hexane:2-PrOH = 93:07, 0.5 mL/min, 230 nm.

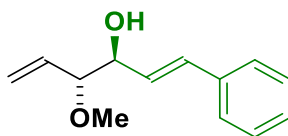
[α]_D²⁴ = 38.8 (c = 0.6, CHCl₃).







(3*S*,4*R*, *E*)-4-methoxy-1-phenylhexa-1,5-dien-3-ol (3f)



Aldehyde **2f** (26.4 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(S)-SEGPPOS** as ligand. Upon flash column chromatography (SiO₂:10:90 EtOAc:hexanes), the title compound **3f** was isolated as a yellow oil in 90% yield (36.7 mg, 0.18 mmol, 84% ee, 2:1 dr).

TLC (SiO₂): R_f = 0.40 (1:2 EtOAc:hexanes).

¹H NMR (400 MHz, CDCl₃): δ 7.39 (d, *J* = 7.9 Hz, 2H), 7.31 (dd, *J* = 7.9, 7.3 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 6.64 (d, *J* = 16.2 Hz, 1H), 6.23 (dd, *J* = 16.2, 6.7 Hz, 1H), 5.77 (ddd, *J* = 17.6, 10.4, 7.9 Hz, 1H), 5.38 (d, *J* = 10.4 Hz, 1H), 5.36 (d, *J* = 17.6 Hz, 1H), 4.38 - 4.34 (m, 1H), 3.72 (dd, *J* = 7.9, 4.1 Hz, 1H), 3.36 (s, 3H), 2.37 (d, *J* = 5.2 Hz, 1H).

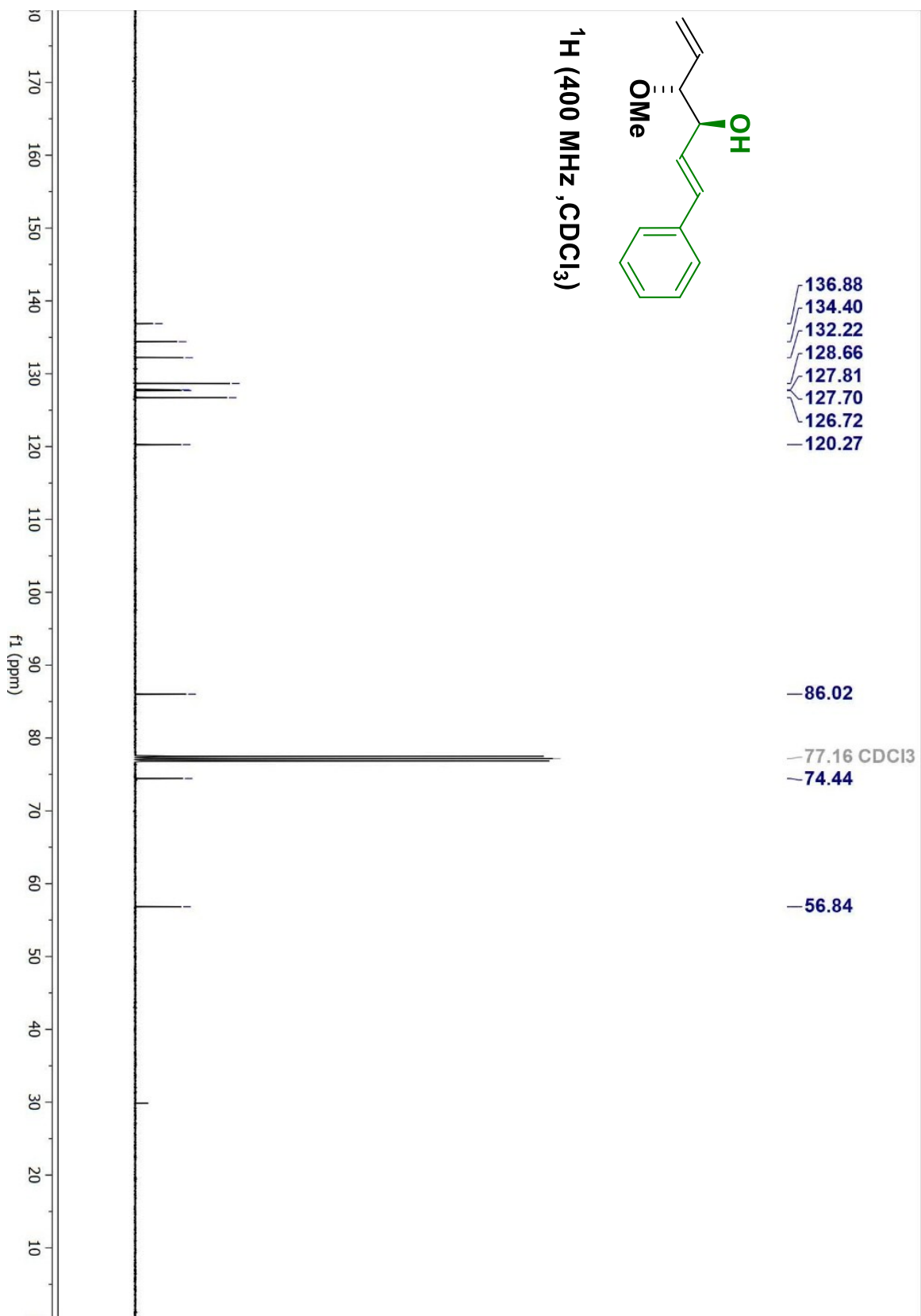
¹³C NMR (101 MHz, CDCl₃): δ 136.9, 134.4, 132.2, 128.7, 127.8, 127.7, 126.7, 120.3, 86.0, 77.2, 74.4, 56.8.

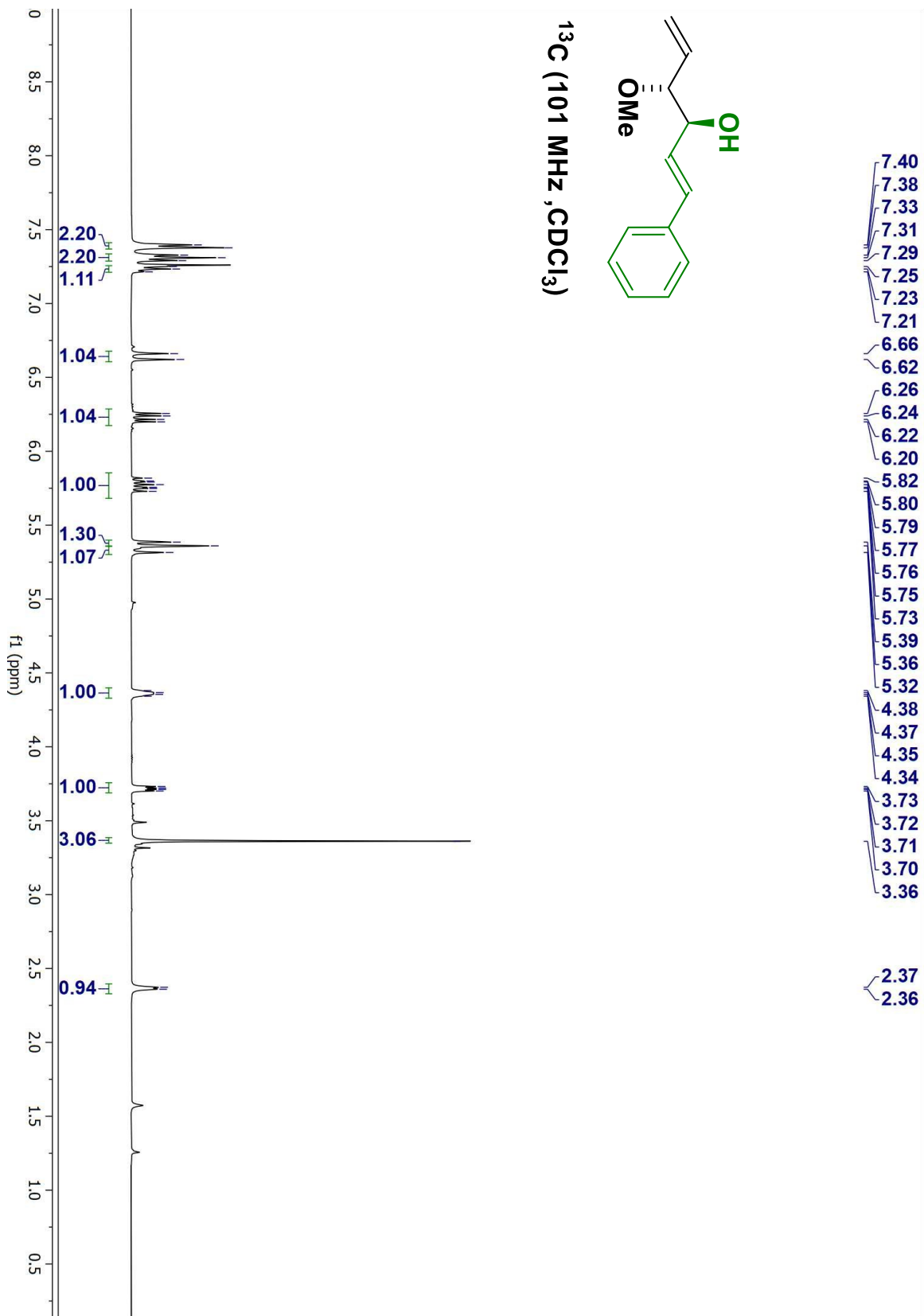
HRMS (Na⁺, *m/z*) for C₁₃H₁₆O₂: calcd. = 227.1043; found = 227.1048.

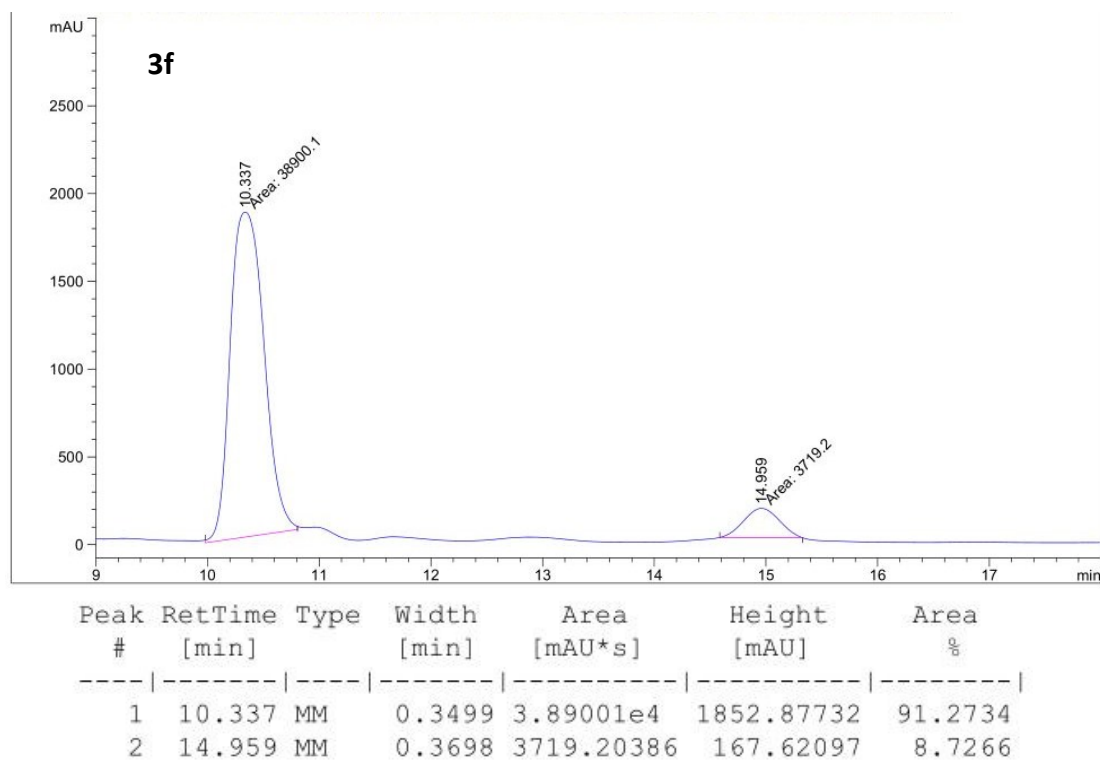
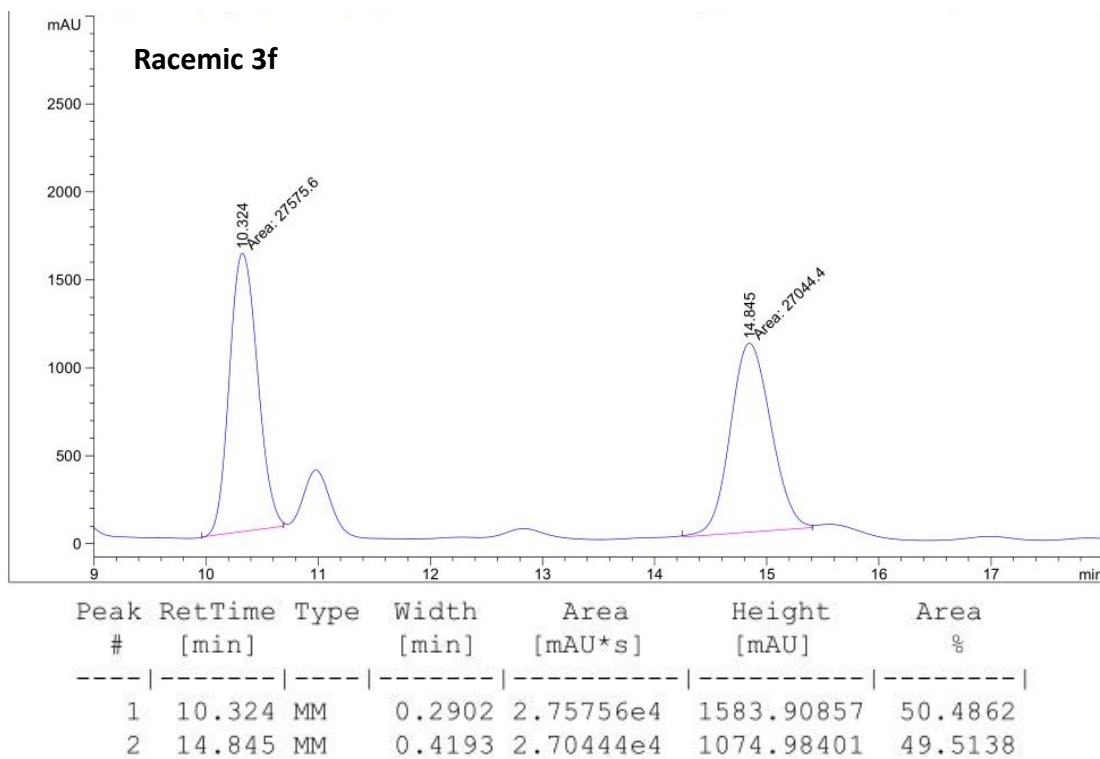
FTIR (neat): 3433, 2928, 1265, 1086, 967, 907, 730 cm⁻¹.

HPLC: Chiralcel column OD-H, Hexane:2-PrOH = 95:05, 0.5 mL/min, 254 nm.

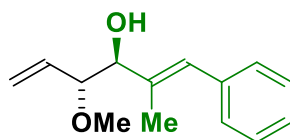
[α]_D²⁴ = -33.3 (c = 0.75, CHCl₃).







(3*S*,4*R*,*E*)-4-methoxy-2-methyl-1-phenylhexa-1,5-dien-3-ol (3g)



Aldehyde **2g** (29.2 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(*S*)-SEGPHOS** as ligand. Upon flash column chromatography (SiO₂: 5:95 Et₂O:hexanes), the title compound **3g** was isolated as a yellow oil in 84% yield (36.6 mg, 0.17 mmol, 93% ee, 4:1 dr).

TLC (SiO₂): R_f = 0.6 (1:3 Et₂O:hexanes).

¹H NMR (400 MHz, CDCl₃): δ 7.35 – 7.27 (m, 4H), 7.21 (t, *J* = 7.2 Hz, 1H), 6.58 (s, 1H), 5.79 (ddd, *J* = 17.8, 10.5, 7.8 Hz, 1H), 5.39 – 5.29 (m, 2H), 4.33 – 4.28 (m, 1H), 3.76 (dd, *J* = 7.9, 4.7 Hz, 1H), 3.36 (s, 3H), 2.44 (d, *J* = 3.2 Hz, 1H), 1.87 (s, 3H).

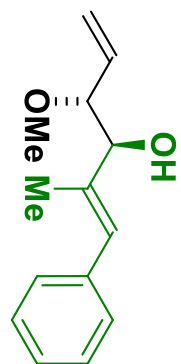
¹³C NMR (101 MHz, CDCl₃): δ 137.8, 136.2, 134.1, 129.2, 128.2, 127.1, 126.5, 119.9, 84.6, 77.9, 56.8, 14.9.

HRMS (Na⁺, *m/z*) for C₁₄H₁₈O₂: calcd. = 241.1199; found = 241.1199.

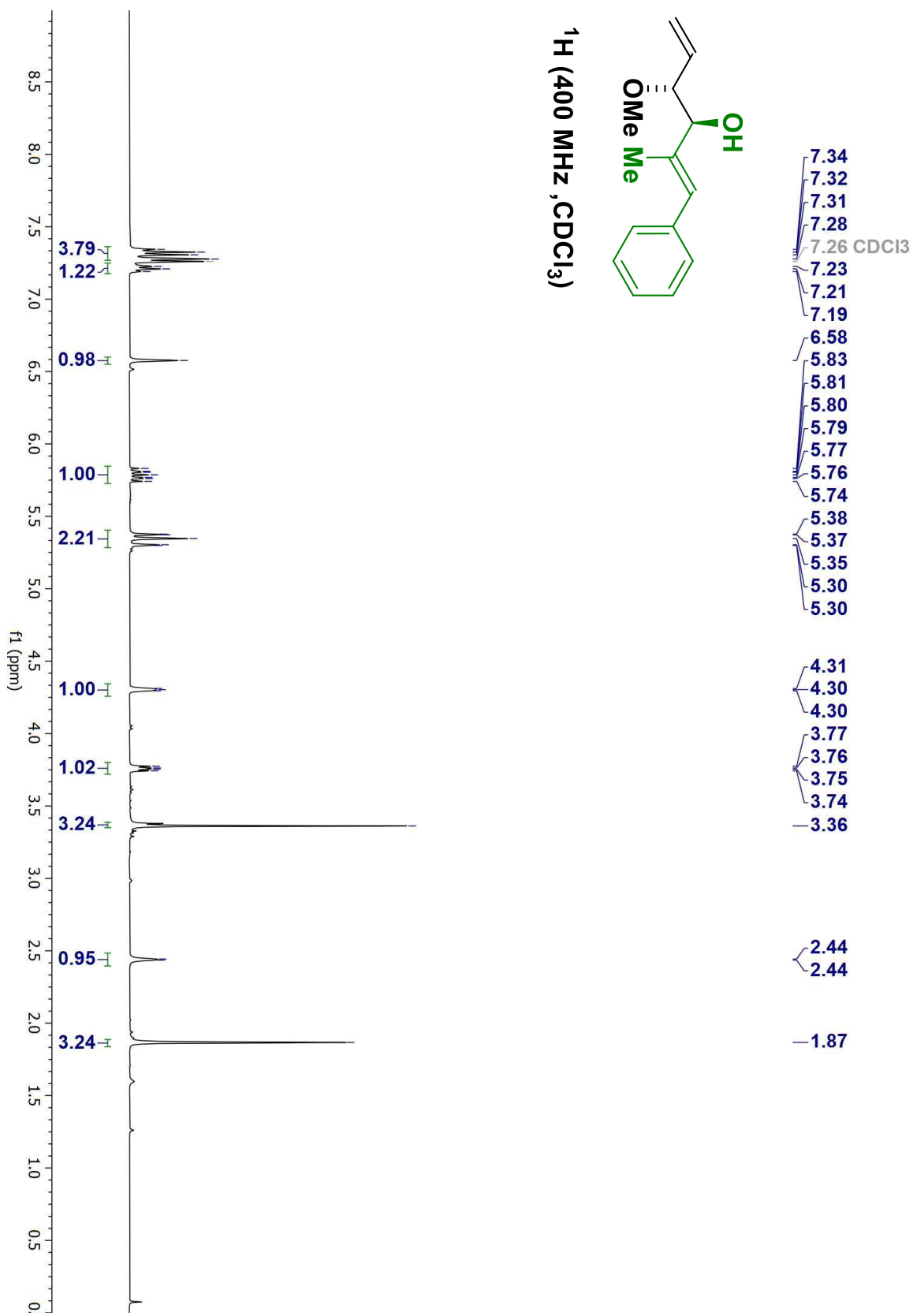
FTIR (neat): 3446, 2931, 2824, 2159, 1690, 1447, 1099, 700 cm⁻¹.

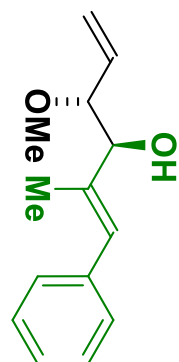
HPLC: Chiralcel column OJ-H, Hexane:2-PrOH = 98:02, 1.0 mL/min, 210 nm.

[α]_D²⁴ = -27.2 (*c* = 0.11, CHCl₃).

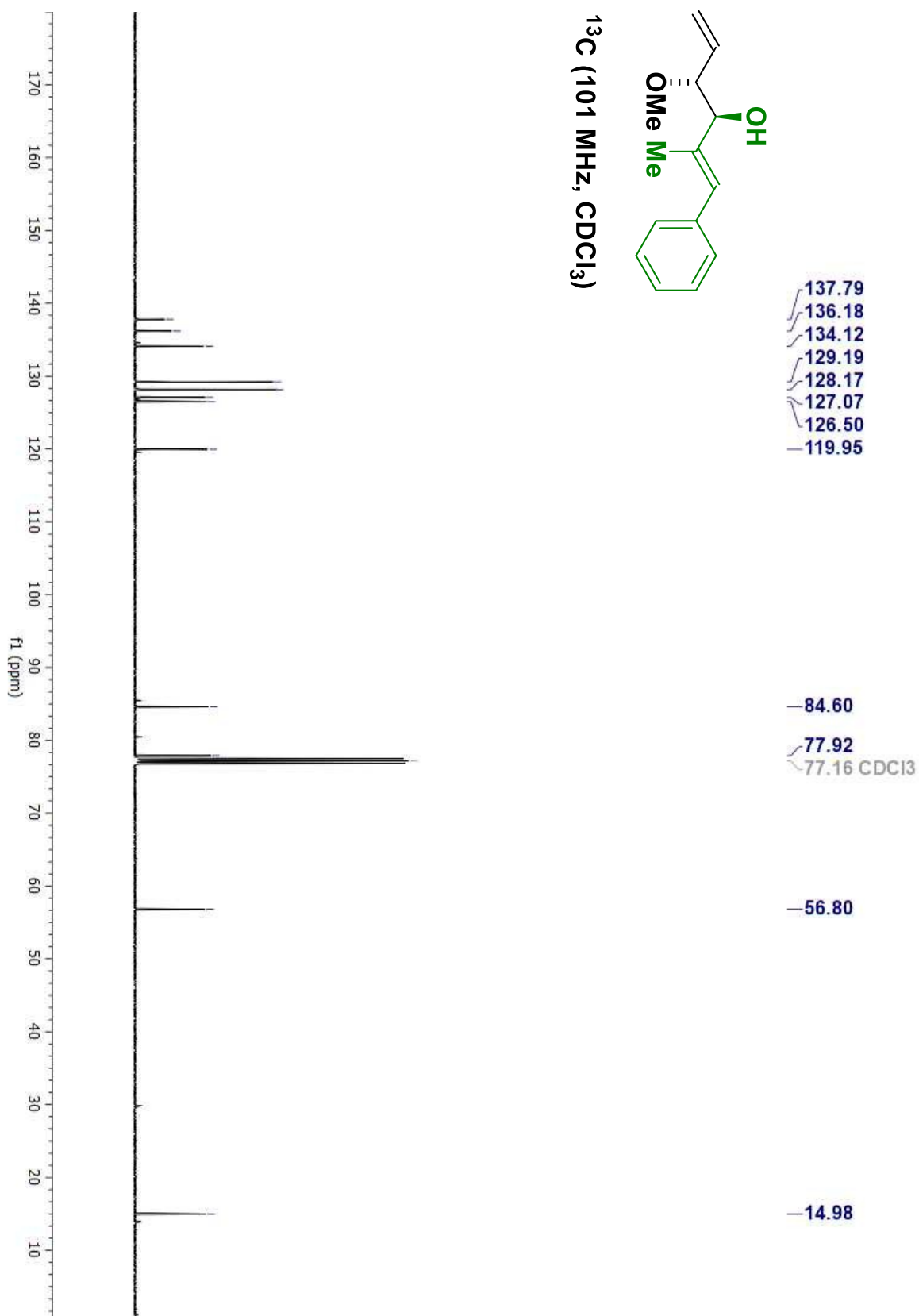


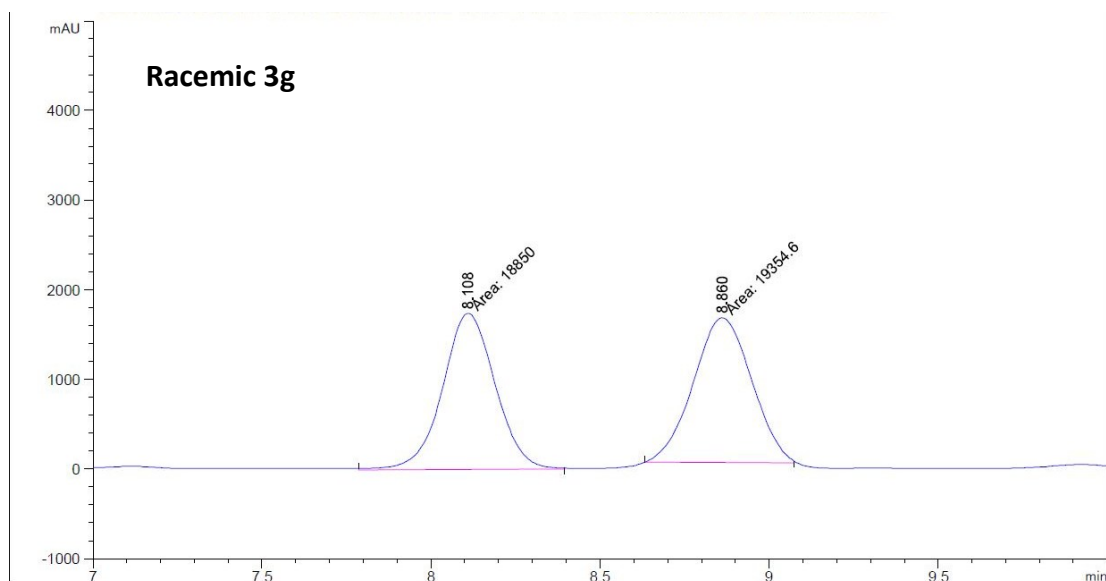
^1H (400 MHz, CDCl_3)



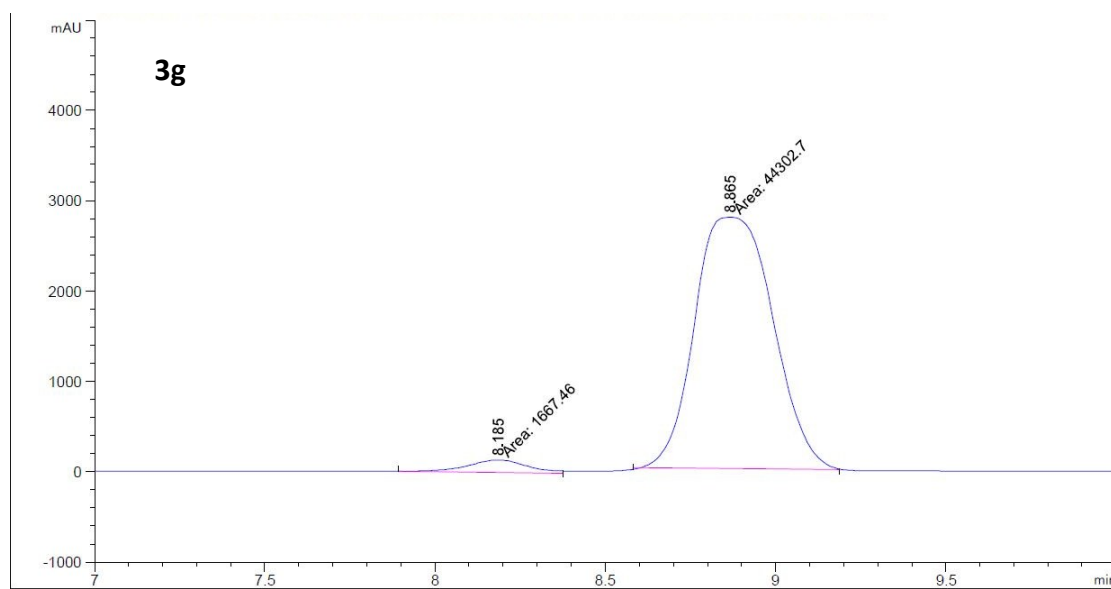


^{13}C (101 MHz, CDCl_3)



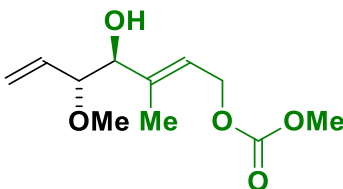


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.108	MM	0.1804	1.88500e4	1741.48718	49.3397
2	8.860	MM	0.1996	1.93546e4	1615.93079	50.6603



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.185	MM	0.2006	1667.45996	138.52988	3.6273
2	8.865	MM	0.2655	4.43027e4	2780.86841	96.3727

(4*S*,5*R*,*E*)-4-hydroxy-5-methoxy-3-methylhepta-2,6-dien-1-yl methyl carbonate (3h)



Aldehyde **2h** (31.6 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(*S*)-SEGPHOS** as ligand. Upon flash column chromatography (SiO₂: 15:85 Et₂O:hexanes), the title compound **3h** was isolated as a yellow oil in 80% yield (35.8 mg, 0.16 mmol, 92% ee, 3:1 dr).

TLC (SiO₂): R_f = 0.5 (2:1 Et₂O:hexanes).

¹H NMR (500 MHz, C₆D₆): δ 5.82 (t, *J* = 6.9 Hz, 1H), 5.62 (ddd, *J* = 17.8, 10.5, 7.8 Hz, 1H), 5.08 – 4.95 (m, 2H), 4.62 (d, *J* = 7.0 Hz, 2H), 4.00 (t, *J* = 3.6 Hz, 1H), 3.40 – 3.29 (m, 4H), 2.98 (s, 3H), 2.04 (t, *J* = 3.1 Hz, 1H), 1.51 (s, 3H).

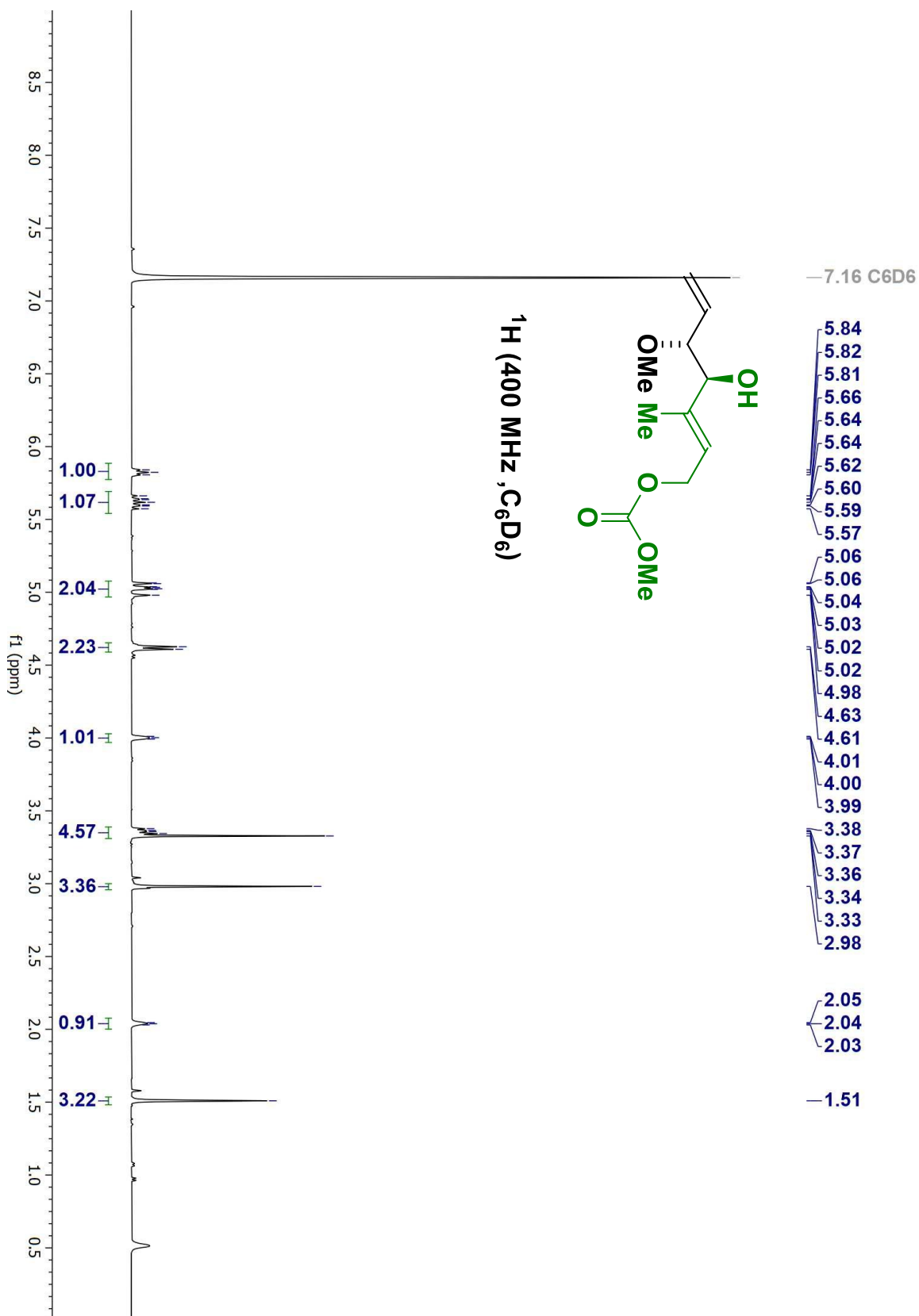
¹³C NMR (101 MHz, CDCl₃): δ 156.3, 140.2, 134.6, 120.9, 119.2, 84.7, 77.1, 64.2, 56.2, 54.2, 13.3.

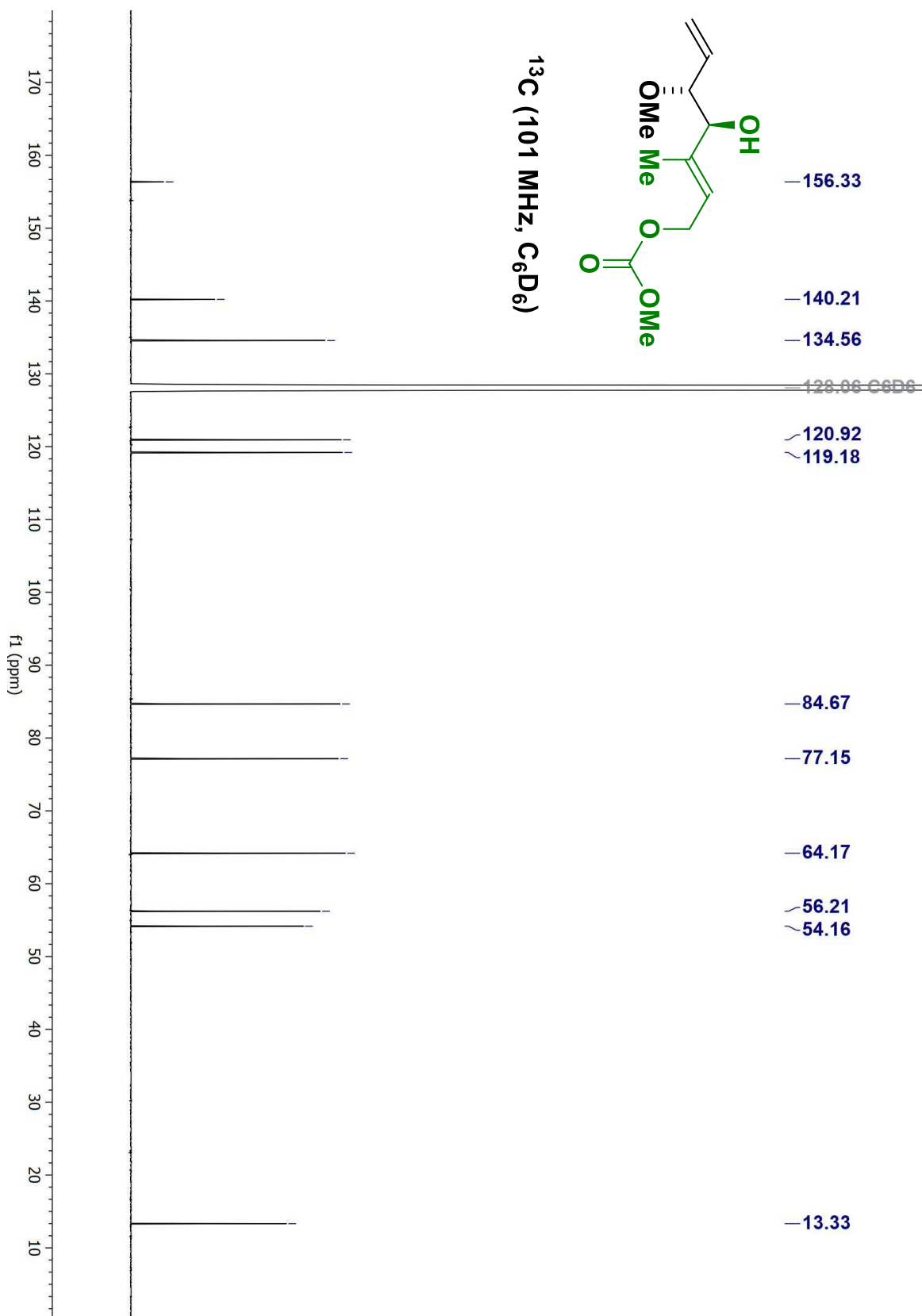
HRMS (Na⁺, *m/z*) for C₁₁H₁₈O₅: calcd. = 253.1046; found = 253.1050.

FTIR (neat): 3480, 2925, 2342, 1748, 1444, 1266, 1096, 938 cm⁻¹.

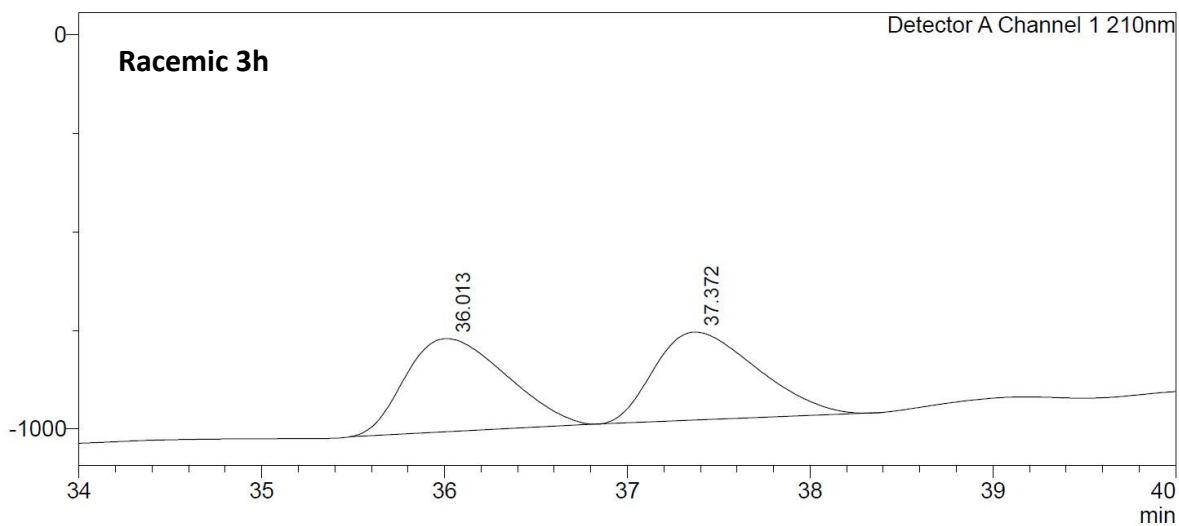
HPLC: Chiralcel column OJ-H, Hexane:2-PrOH = 95:02, 0.5 mL/min, 210 nm.

[α]_D²⁴ = 34.7 (*c* = 0.87, CHCl₃).



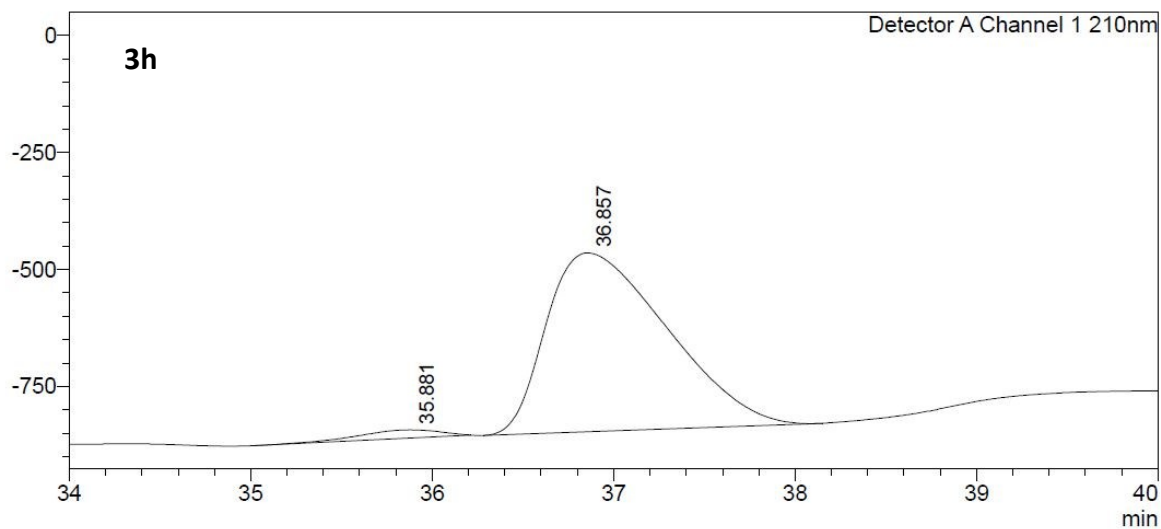


mV



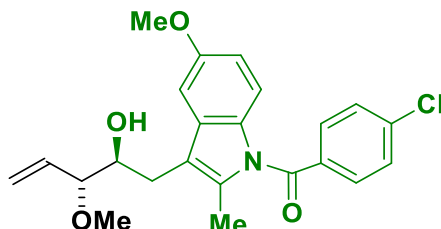
Peak#	Ret. Time	Area	Height	Conc.
1	36.013	9070471	236529	50.977
2	37.372	8722912	223306	49.023
Total		17793383	459836	

mV



Peak#	Ret. Time	Area	Height	Conc.
1	35.881	559187	17386	3.073
2	36.857	17635812	381890	96.927
Total		18194999	399276	

(4-chlorophenyl)(3-((2*S*,3*R*)-2-hydroxy-3-methoxypent-4-en-1-yl)-5-methoxy-2-methyl-1*H*-indol-1-yl)methanone (3i)



Aldehyde **2h** (341.5 mg, 1 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with $\text{RuI}(\text{CO})_3(\eta^3\text{-C}_3\text{H}_5)$ (10 mol%), **(*S*)-SEGPHOS** (15 mol%), and TBAI (20 mol%). Upon flash column chromatography (SiO_2 : 7:93 EtOAc:PhMe) the title compound **3h** was isolated as viscous yellow semi-solid in 55% yield (227.63 mg, 0.55 mmol, 82% ee, 3:1 dr).

TLC (SiO_2): R_f = 0.4 (1:3 EtOAc:PhMe)

^1H NMR (500 MHz, CDCl_3): δ 7.65 (d, J = 8.5 Hz, 2H), 7.46 (d, J = 8.5 Hz, 2H), 6.98 (d, J = 2.5 Hz, 1H), 6.88 (d, J = 9.0 Hz, 1H), 6.65 (dd, J = 9.0, 2.5 Hz, 1H), 5.88 (ddd, J = 17.2, 10.5, 8.1 Hz, 1H), 5.47 (d, J = 10.5 Hz, 1H), 5.38 (d, J = 17.6 Hz, 1H), 3.97 (dt, J = 8.8, 4.4 Hz, 1H), 3.83 (s, 3H), 3.60 (dd, J = 8.1, 4.5 Hz, 1H), 3.35 (s, 3H), 2.90 (dd, J = 14.6, 4.2 Hz, 1H), 2.79 (dd, J = 14.6, 8.6 Hz, 1H), 2.35 (s, 3H), 2.03 (bs, 1H).

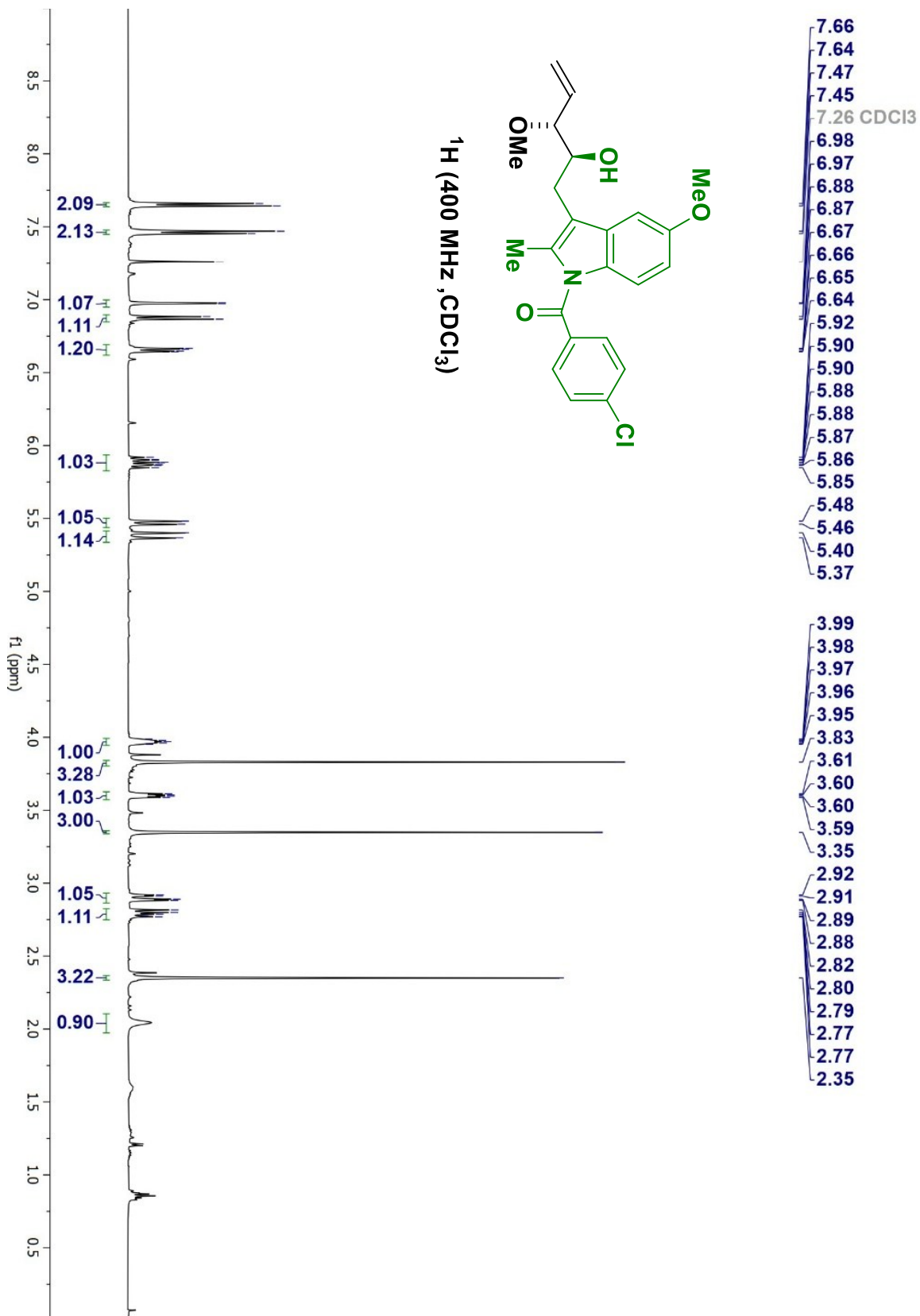
^{13}C NMR (126 MHz, CDCl_3): δ 168.4, 156.0, 139.2, 135.7, 134.7, 134.3, 131.6, 131.3, 129.2, 120.9, 116.4, 115.0, 111.3, 102.0, 85.8, 73.4, 56.7, 55.9, 27.4, 13.8.

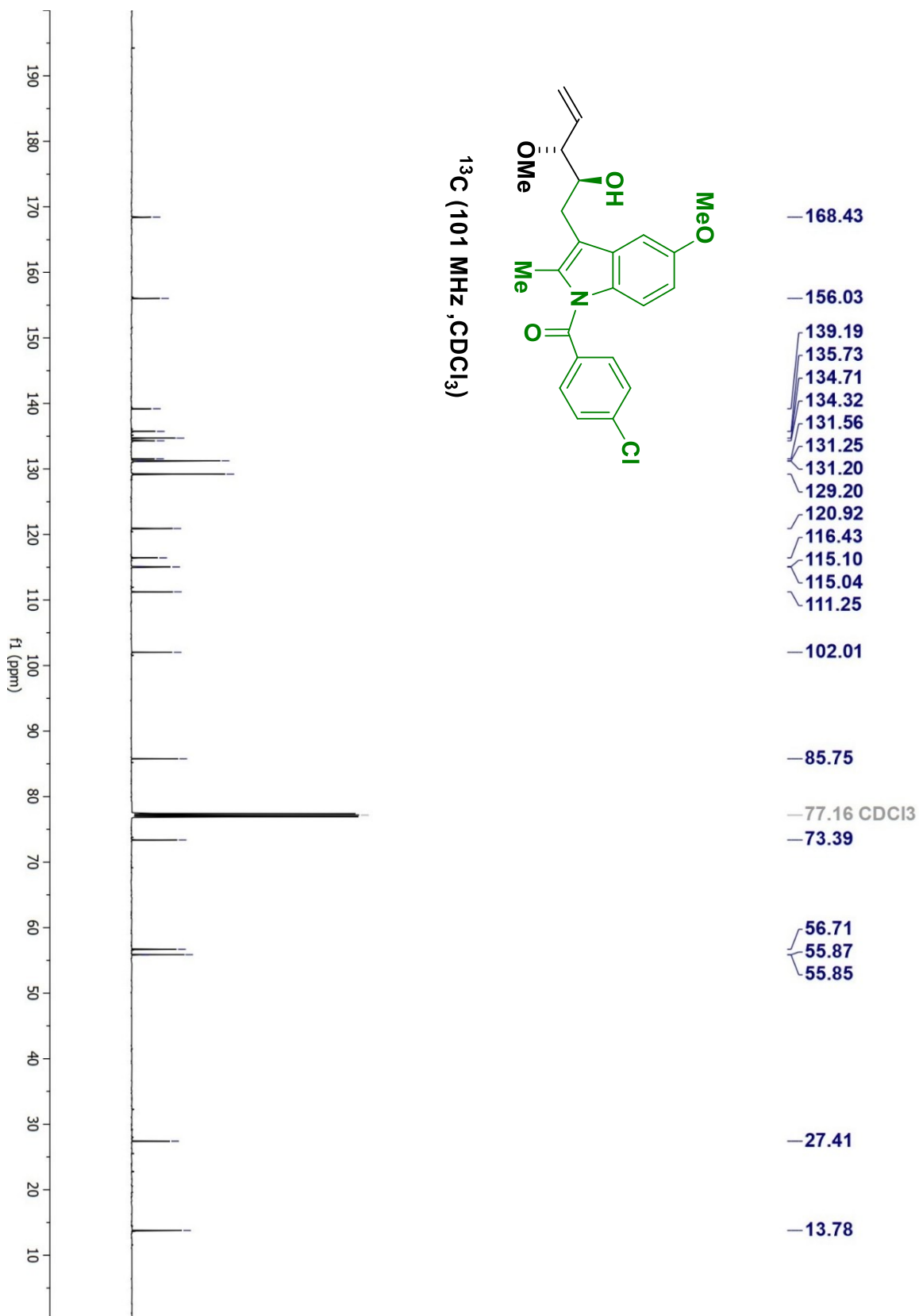
HRMS (Na^+ , m/z) for $\text{C}_{23}\text{H}_{24}\text{ClNO}_4$: calcd. = 436.1286; found = 436.1274.

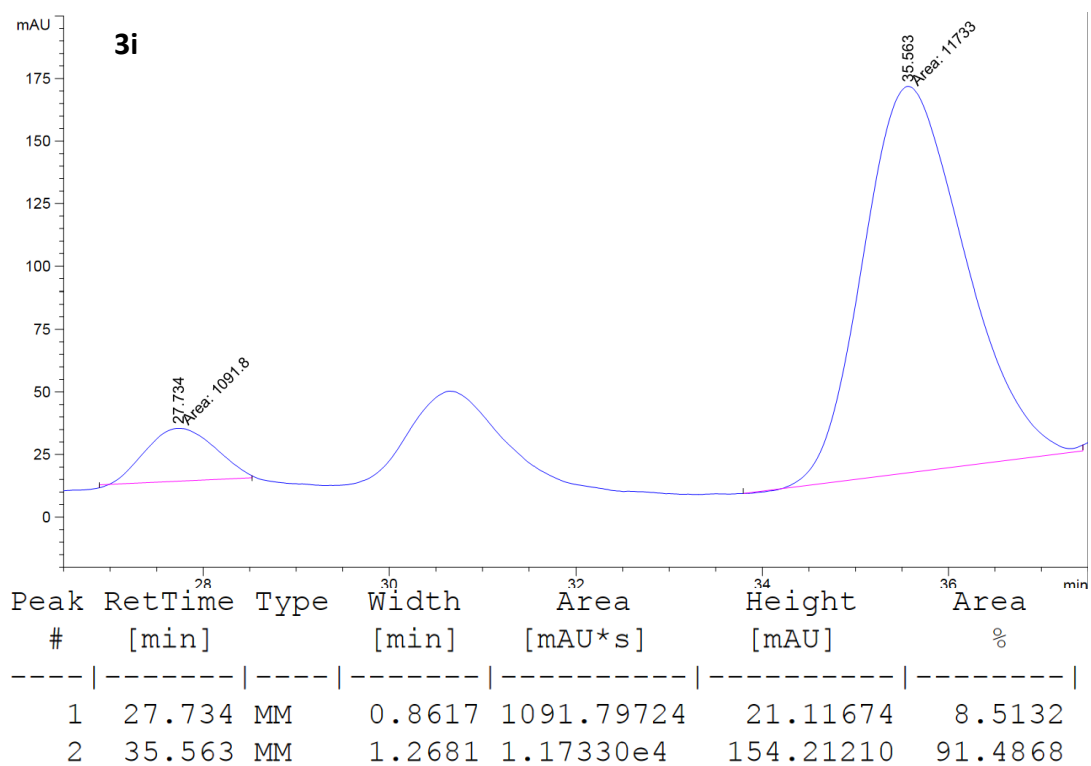
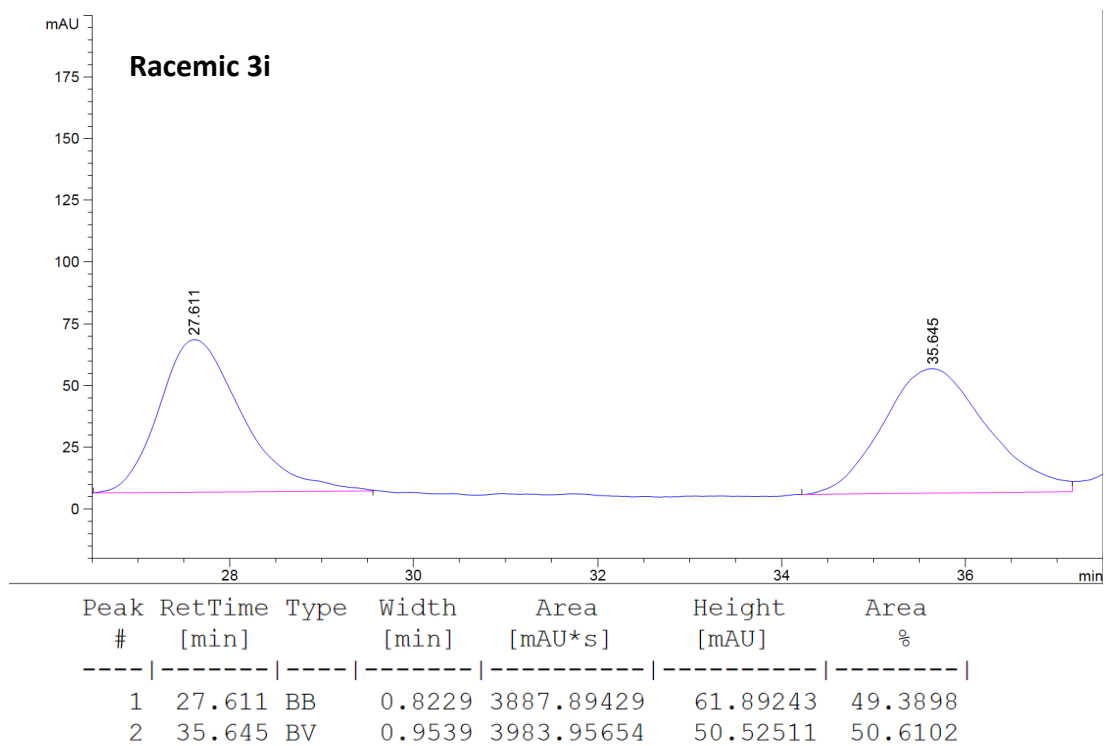
FTIR (neat): 3307, 3031, 2675, 1940, 1738, 1608, 1180 cm^{-1} .

HPLC: Chiralcel column CELLULOSE-5, Hexane:2-PrOH = 90:10, 1.0 mL/min, 210 nm.

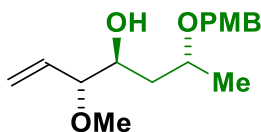
$[\alpha]_D^{24} = 2.3$ (c = 2.26, CHCl_3).







(3*R*,4*S*,6*R*)-3-methoxy-6-((4-methoxybenzyl)oxy)hept-1-en-4-ol (3j)



Aldehyde **2j** (41.7 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with $\text{Ru}(\text{CO})_3(\eta^3\text{-C}_3\text{H}_5)$ (10 mol%), **(*S*)-SEGPHOS** (15 mol%), and TBAI (20 mol%). Upon flash column chromatography (SiO_2 : 3:97 EtOAc:hexanes) the title compound **3j** was isolated as yellow oil in 66% yield (38.7 mg, 0.14 mmol, 3:1 dr).

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

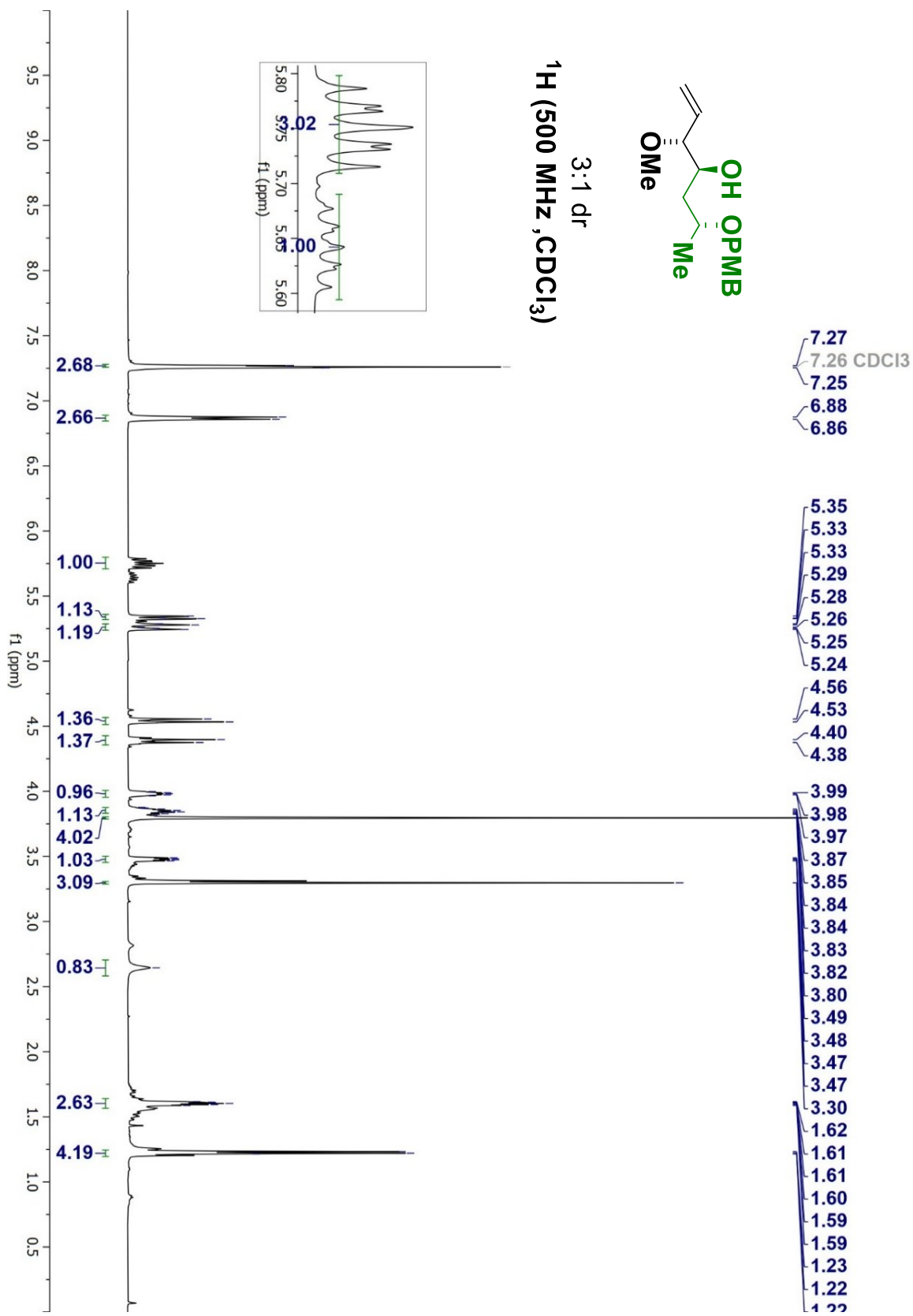
^1H NMR (500 MHz, CDCl_3): δ 7.26 (d, J = 8.6 Hz, 2H), 6.87 (d, J = 8.7 Hz, 2H), 5.34 (d, J = 10.2 Hz, 1H), 5.27 (dd, J = 17.6, 4.4 Hz, 1H), 4.54 (d, J = 11.2 Hz, 1H), 4.39 (d, J = 11.2 Hz, 1H), 3.98 (dt, J = 8.1, 4.1 Hz, 1H), 3.89 – 3.82 (m, 1H), 3.80 (s, 3H), 3.48 (dd, J = 7.8, 4.3 Hz, 1H), 3.30 (s, 3H), 2.64 (s, 1H), 1.63 – 1.58 (m, 2H), 1.23 (d, J = 6.3 Hz, 3H).

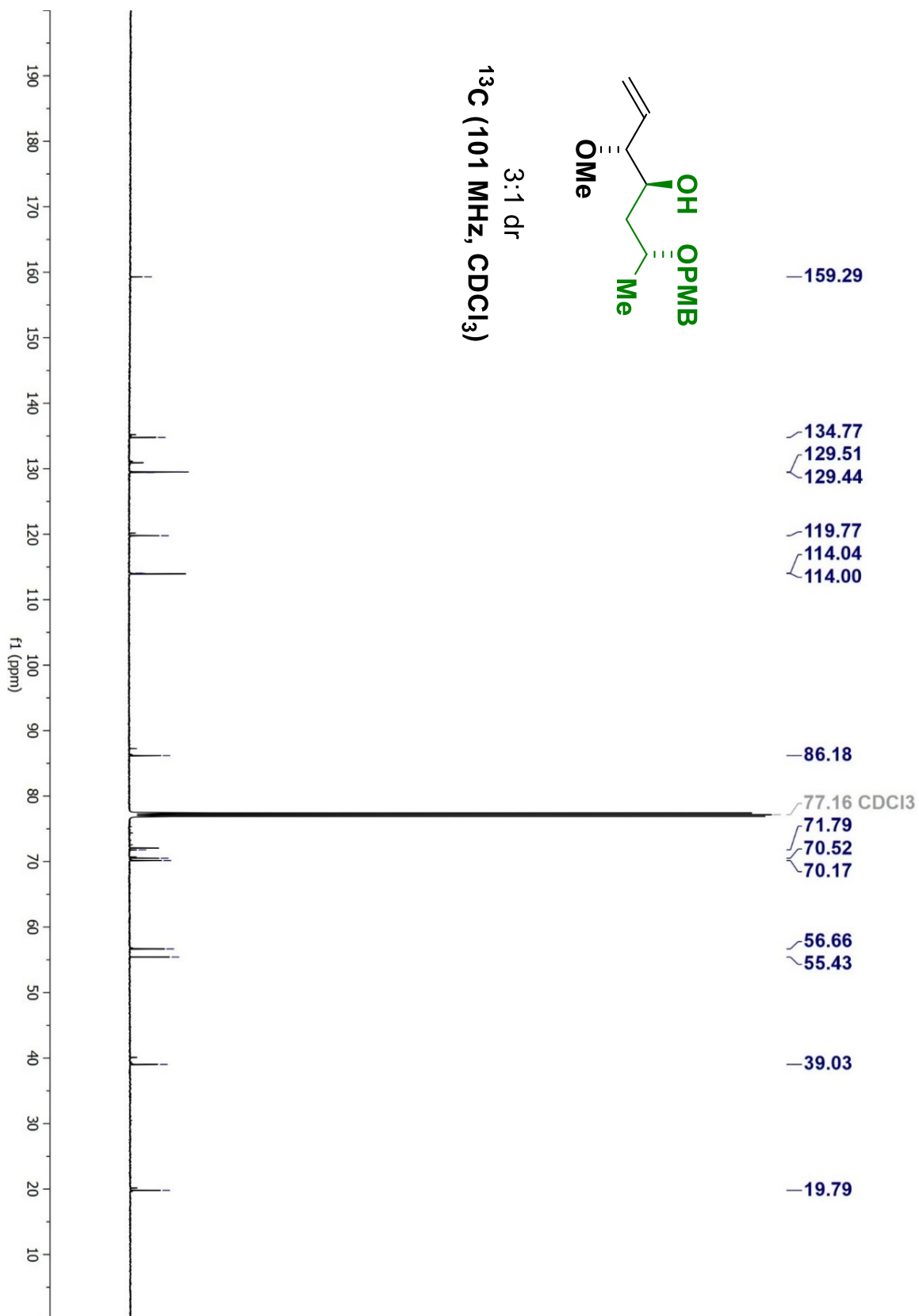
^{13}C NMR (101 MHz, CDCl_3): δ 159.3, 134.8, 129.4, 119.8, 114.02, 86.2, 71.8, 70.5, 70.2, 56.7, 55.4, 39.0, 19.8.

HRMS (Na^+ , m/z) for $\text{C}_{16}\text{H}_{24}\text{O}_4$: calcd. = 303.1567; found = 303.1568

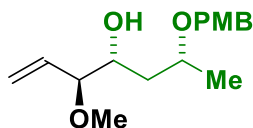
FTIR (neat): 3460, 2931, 2930, 1708, 1611, 1512, 1245, 1070 cm^{-1} .

$[\alpha]_D^{24}$ = -50.4 (c = 1.25, CHCl_3).





(3*S*,4*R*,6*R*)-3-methoxy-6-((4-methoxybenzyl)oxy)hept-1-en-4-ol (*epi*-3j)



Aldehyde **2j** (41.6 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with $\text{RuI}(\text{CO})_3(\eta^3\text{-C}_3\text{H}_5)$ (10 mol%), **(*S*)-SEGPHOS** (15 mol%), and TBAI (20 mol%). Upon flash column chromatography (SiO_2 : 5:95 acetone:hexanes), the title compound ***epi*-3j** was isolated as yellow oil in 69% yield (38.7 mg, 0.14 mmol, 4:1 dr).

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

^1H NMR (400 MHz, CDCl_3): δ 7.25 (d, J = 8.8 Hz, 2H), 6.86 (d, J = 8.6 Hz, 2H), 5.76 (ddd, J = 17.3, 10.4, 7.8 Hz, 1H), 5.33 (d, J = 10.4 Hz, 1H), 5.27 (d, J = 18.1 Hz, 1H), 4.57 (d, J = 11.0 Hz, 1H), 4.35 (d, J = 11.0 Hz, 1H), 3.79 (s, 4H), 3.57 (d, J = 1.8 Hz, 1H), 3.41 (dd, J = 7.8, 4.9 Hz, 1H), 3.30 (s, 3H), 1.73 – 1.66 (m, 2H), 1.24 (d, J = 6.0 Hz, 3H).

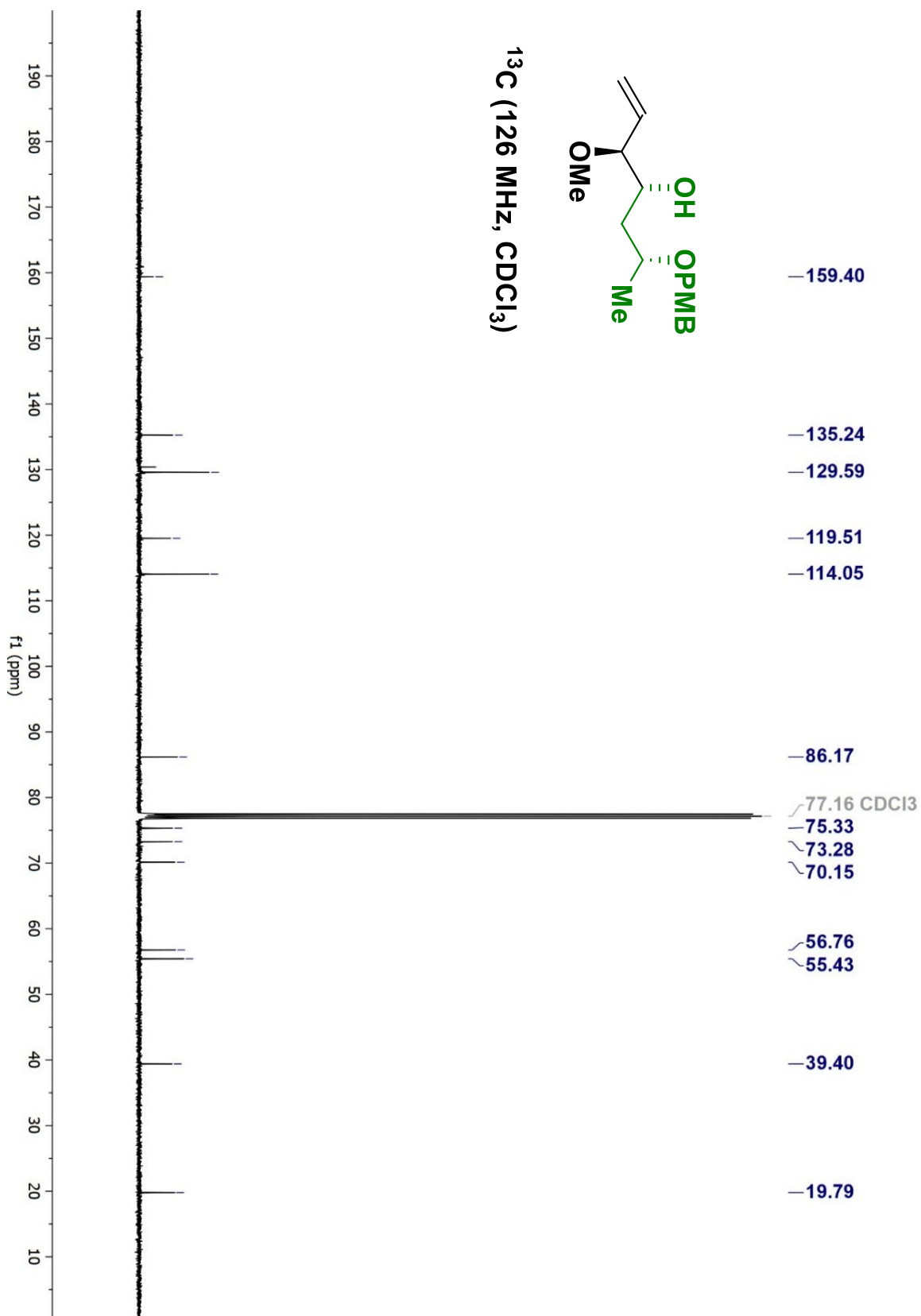
^{13}C NMR (101 MHz, CDCl_3): δ 159.4, 135.0, 130.4, 129.4, 119.5, 113.9, 75.3, 73.3, 70.1, 56.7, 55.4, 39.1, 19.6.

HRMS (Na^+ , m/z) for $\text{C}_{16}\text{H}_{24}\text{O}_4$: calcd. = 303.1567; found = 303.1568.

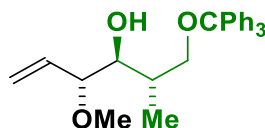
FTIR (neat): 3467, 2970, 2932, 2360, 1612, 1512, 1245, 1084 cm^{-1} .

$[\alpha]_D^{24}$ = -9.6 (c = 1.25, CHCl_3).





(2*S*,3*S*,4*R*)-4-methoxy-2-methyl-1-(trityloxy)hex-5-en-3-ol (3k)



Aldehyde **2k** (66.0 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **RuHCl(CO)(PPh₃)₃** (10 mol%), **(*S*)-SEGPPOS** (10 mol%), and **NaI** (20 mol%). Upon flash column chromatography (SiO₂: 1:6:3 acetone:petroleum ether:CH₂Cl₂), the title compound **3k** was isolated as a yellow oil in 66% yield (53.1 mg, 0.13 mmol, 1.2:1 dr (crude), 1.3:1 (purified)).

TLC (SiO₂): R_f = 0.6 (1:6:3 acetone:petroleum ether: CH₂Cl₂).

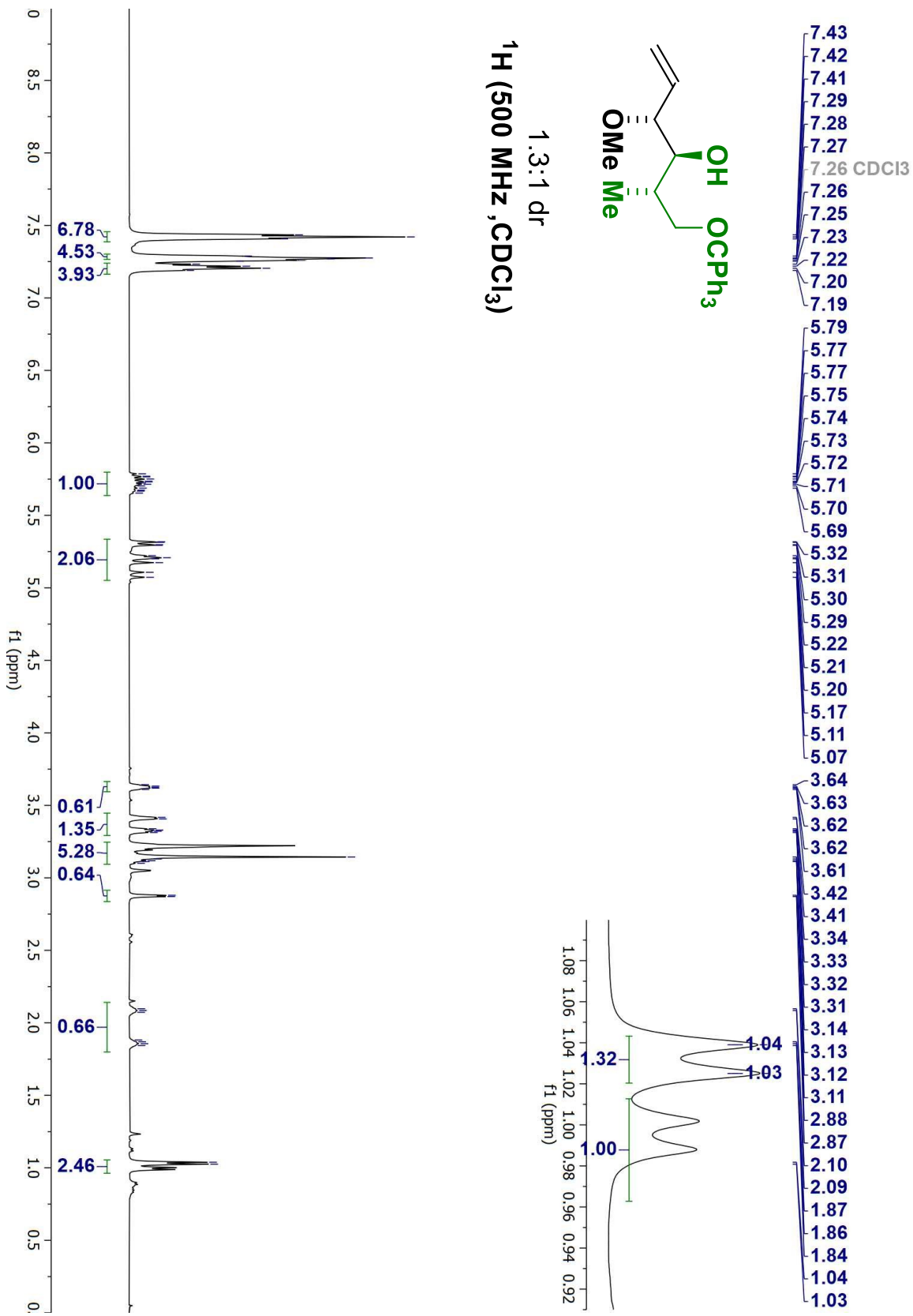
¹H NMR (500 MHz, CDCl₃): δ 7.42 (t, *J* = 6.9 Hz, 7H), 7.27 (dt, *J* = 8.0, 5.0 Hz, 4H), 7.21 (q, *J* = 7.0 Hz, 4H), 5.80 – 5.63 (m, 1H), 5.32 – 5.06 (m, 2H), 3.63 (dt, *J* = 7.6, 4.7 Hz, 1H), 3.43 – 3.29 (m, 1H), 3.17 – 3.09 (m, 5H), 2.88 (d, *J* = 4.3 Hz, 1H), 2.12 – 1.81 (m, 1H), 1.03 (d, *J* = 7.0 Hz, 3H).

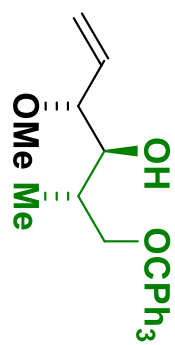
¹³C NMR (126 MHz, CDCl₃): δ 144.1, 134.6, 128.8, 128.0, 127.1, 119.9, 87.0, 84.2, 76.1, 65.9, 56.2, 35.2, 14.5.

HRMS (Na⁺, *m/z*) for C₂₇H₃₀O₃: calcd. = 425.2087; found = 425.2083.

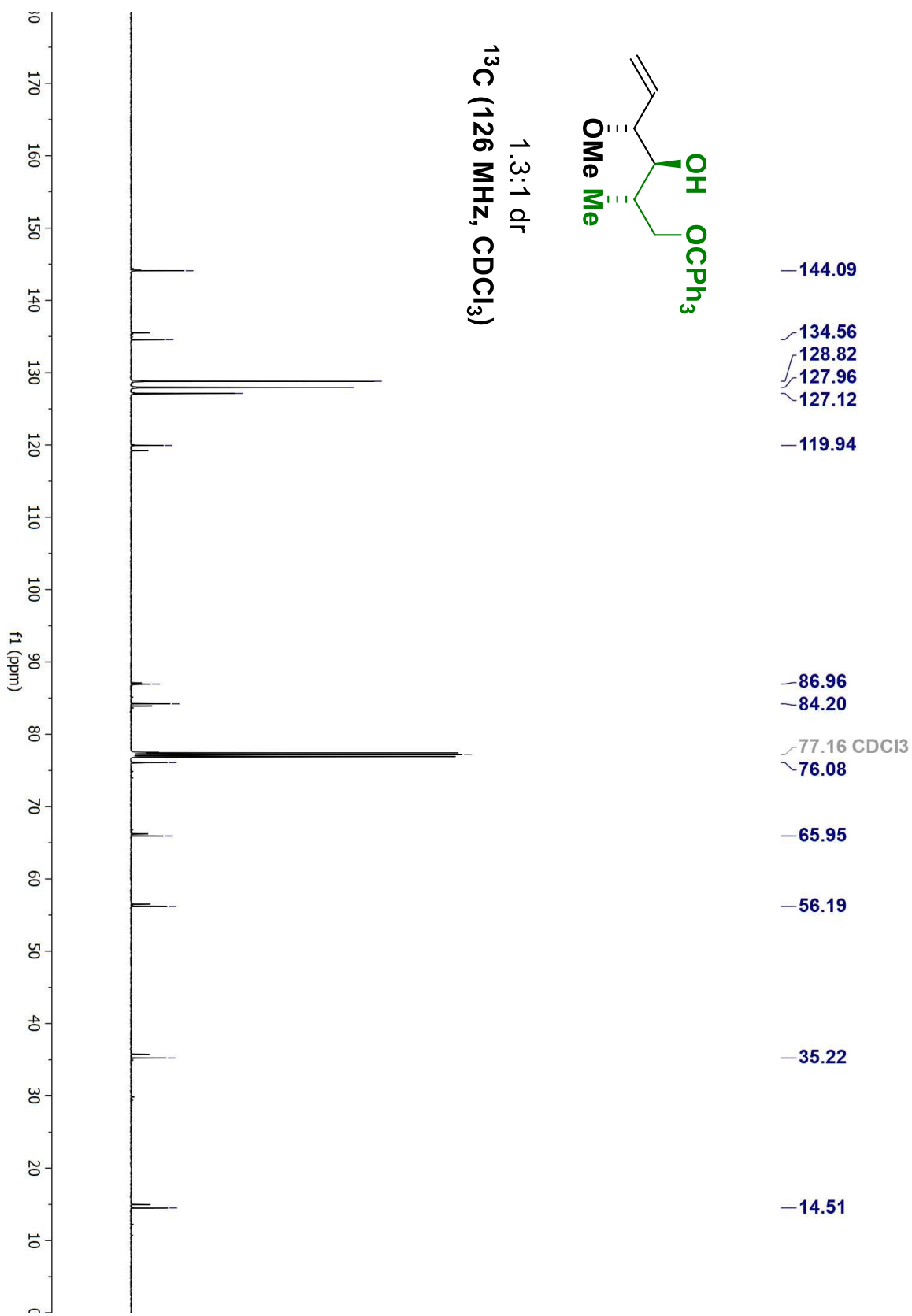
FTIR (neat): 3675, 3057, 2930, 1730, 1448, 1033, 929, 898 cm⁻¹.

[α]_D²⁴ = 4.7 (*c* = 0.26, CHCl₃).

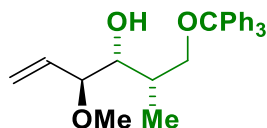




1.3:1 dr
 ^{13}C (126 MHz, CDCl_3)



(2*S*,3*R*,4*S*)-4-methoxy-2-methyl-1-(trityloxy)hex-5-en-3-ol (*epi*-3k)



Aldehyde **2k** (1.32 g, 4.0 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **RuHCl(CO)(PPh₃)₃** (10 mol%), **(*S*)-SEGPHOS** (10 mol%), and **NaI** (20 mol%). Upon flash column chromatography (SiO₂: 1:6:3 acetone:petroleum ether: CH₂Cl₂), the title compound ***epi*-3k** was isolated as a yellow oil in 80% yield (1.28 g, 3.18 mmol, 2.3:1 dr).

TLC (SiO₂): R_f = 0.6 (1:6:3 acetone:petroleum ether: CH₂Cl₂)

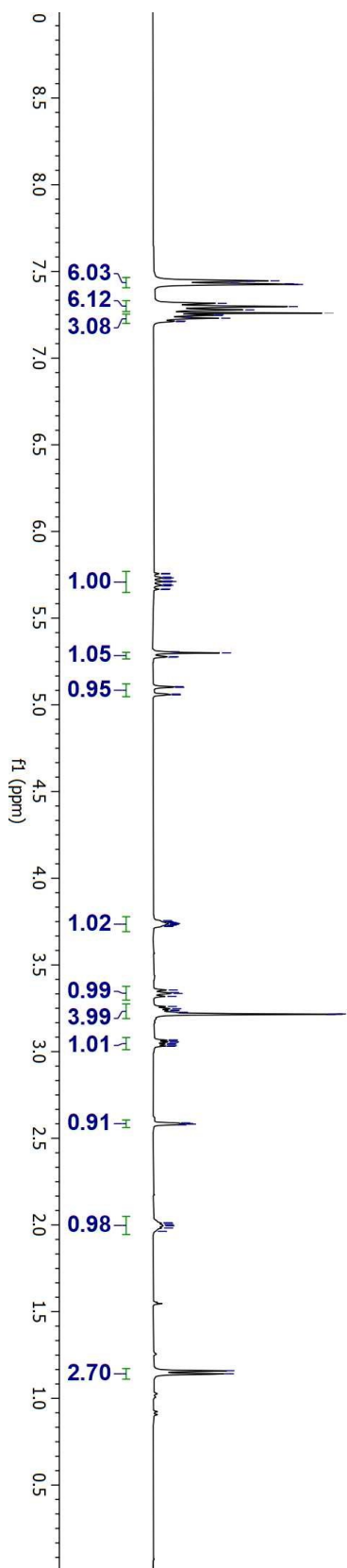
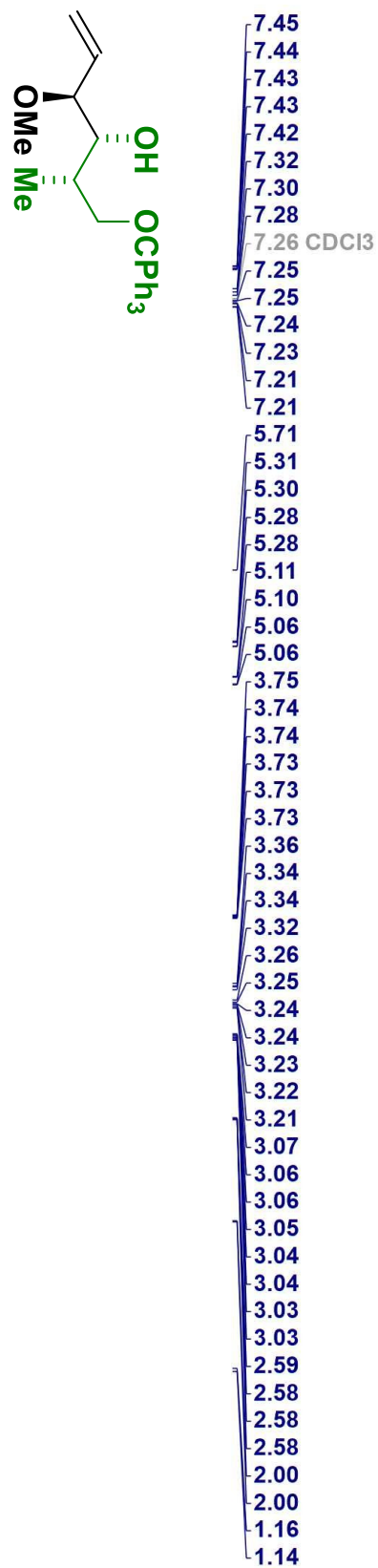
¹H NMR (400 MHz, CDCl₃): δ 7.46 – 7.42 (m, 6H), 7.30 (t, *J* = 7.5 Hz, 6H), 7.25 – 7.20 (m, 3H), 5.77 – 5.65 (m, 1H), 5.30 (d, *J* = 2.5 Hz, 1H), 5.08 (dd, *J* = 17.3, 1.8 Hz, 1H), 3.74 (ddt, *J* = 6.3, 4.8, 2.7 Hz, 1H), 3.34 (dd, *J* = 8.2, 6.3 Hz, 1H), 3.27 – 3.18 (m, 4H), 3.05 (ddd, *J* = 9.0, 4.4, 1.2 Hz, 1H), 2.58 (dd, *J* = 2.8, 1.6 Hz, 1H), 2.05 – 1.94 (m, 1H), 1.15 (d, *J* = 7.1 Hz, 3H).

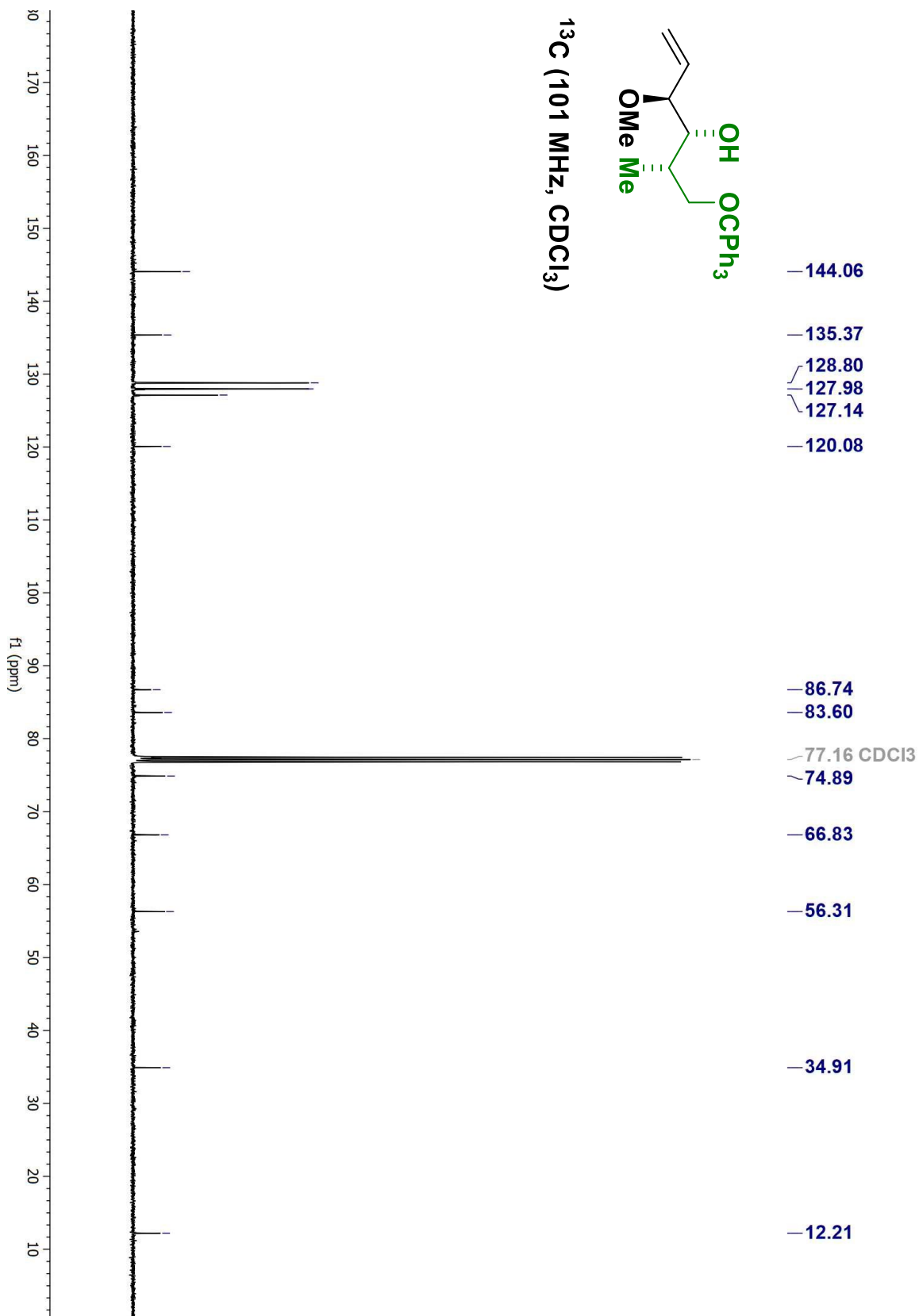
¹³C NMR (101 MHz, CDCl₃): δ 144.1, 135.4, 128.8, 128.0, 127.1, 120.1, 86.7, 83.6, 74.9, 66.8, 56.3, 34.9, 12.2.

HRMS (Na⁺, *m/z*) for C₂₇H₃₀O₃: calcd. = 425.2087; found = 425.2083.

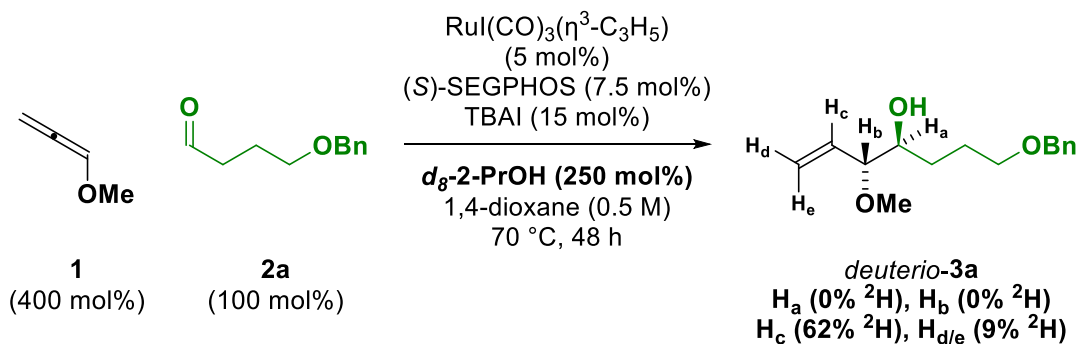
FTIR (neat): 3053, 32984, 2235, 1490, 1448, 1263, 1088, 897 cm⁻¹.

[α]_D²⁴ = -4.7 (*c* = 0.26, CHCl₃).





Deuterium Labeling Studies



Aldehyde **2a** (36.5 mg, 0.2 mmol) was subjected to standard reaction conditions (70 °C, 48 h) with **(S)-SEGPHOS** as ligand and ***d*₈-2-propanol** (250 mol%) as reductant. Upon flash column chromatography (SiO₂: 3:97 acetone:hexanes), the title compound *deuterio-3a* was isolated as a yellow oil in 40% yield (20.0 mg, 0.08 mmol).

¹H NMR (400 MHz, CDCl₃): δ 7.37 – 7.29 (m, 5H), 5.63 (dt, *J* = 17.9, 9.5 Hz, 0.38H), 5.38 – 5.25 (m, 1.91H), 4.50 (s, 2H), 3.53 – 3.46 (m, 4H), 3.35 (dd, *J* = 4.6 Hz, 1H), 3.31 (s, 3H), 1.88 – 1.79 (m, 1H), 1.72 (dt, *J* = 13.6, 7.7 Hz, 2H), 1.46 – 1.35 (m, 1H).

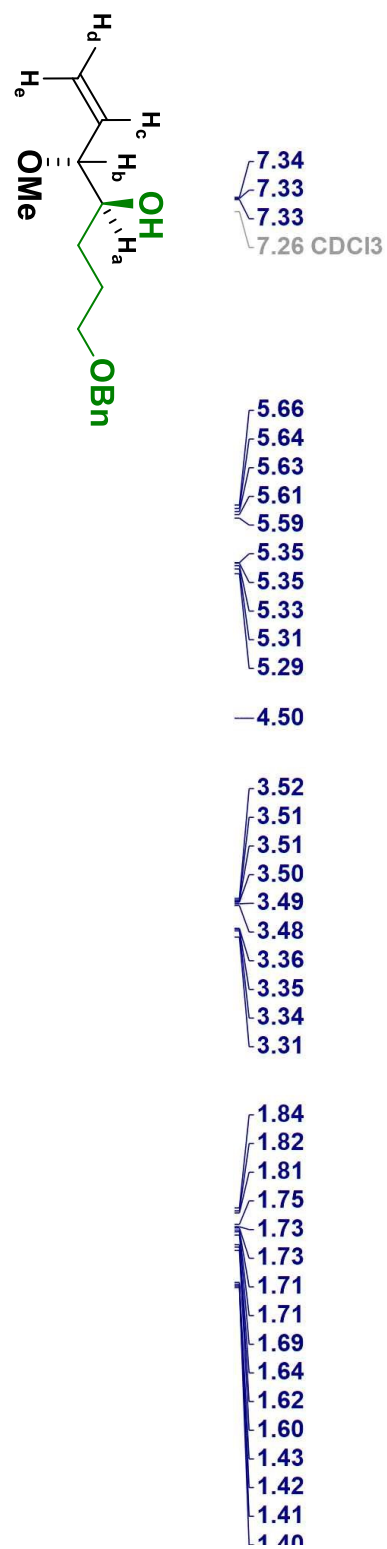
²H NMR (92 MHz, CHCl₃): δ 5.67 (s, 0.62H), 5.36 (s, 0.08H).

HRMS (Na⁺, *m/z*) for C₁₅H₂₂O₃: calcd. = 273.1569; found = 273.1454.

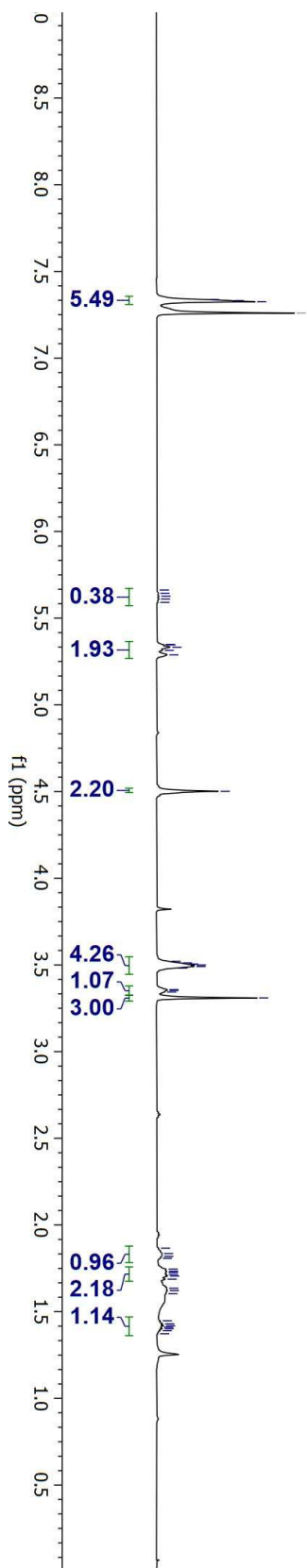
(Na⁺, *m/z*) for C₁₅H₂₁DO₃: calcd. = 250.1632; found = 274.1511.

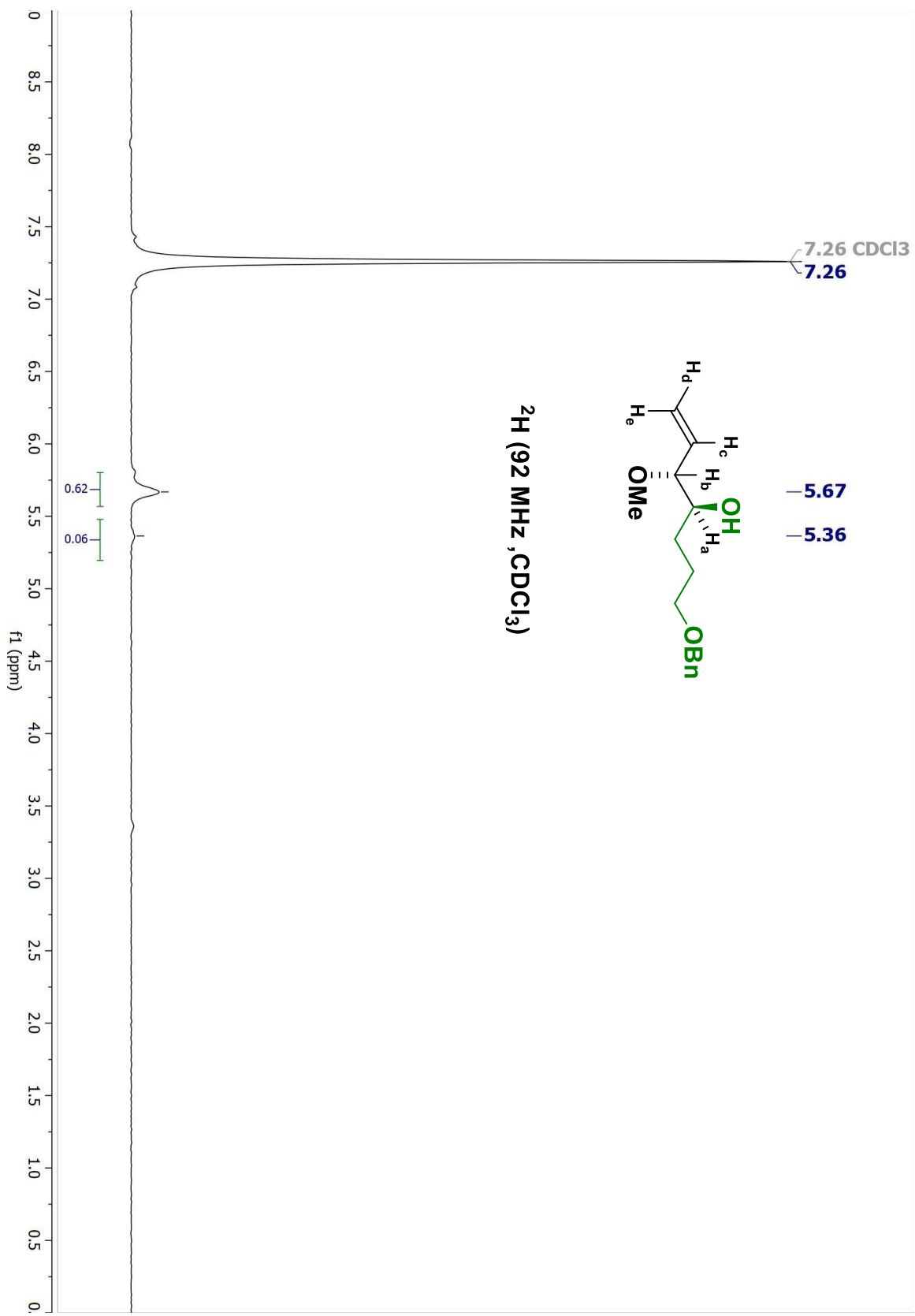
(Na⁺, *m/z*) for C₁₅H₂₀D₂O₃: calcd. = 275.1694; found = 275.1554.

(Na⁺, *m/z*) for C₁₅H₁₉D₃O₃: calcd. = 276.1757; found = 276.1581.

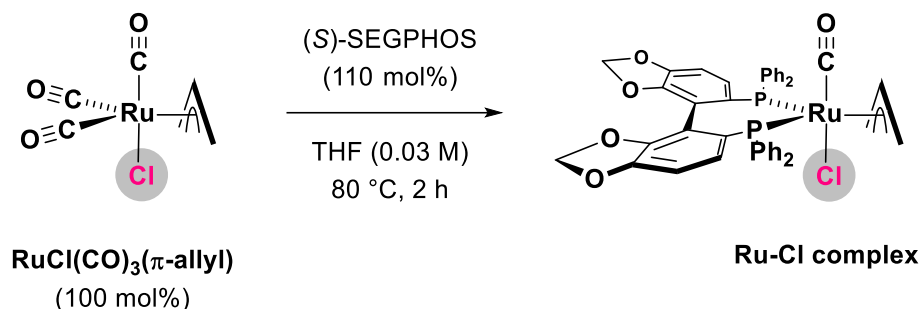


¹H (400 MHz, CDCl₃)





Synthesis of Ruthenium-Chloride Complex

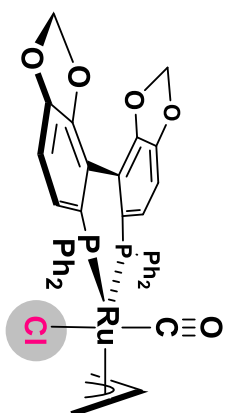


To an oven-dried pressure tube equipped with a magnetic stir bar under an argon atmosphere charged with $\text{RuCl(CO)}_3(\pi\text{-allyl})$ complex (14 mg, 0.06 mmol) and $(S)\text{-SEGPHOS}$ (37 mg, 0.06 mmol) was added THF (2 mL, 0.03 M). The pressure tube was backfilled with argon and sealed with a PTFE lined cap and the reaction mixture was allowed to stir for 2 hours at 80 °C. After cooling to ambient temperature, the reaction mixture was transferred to a 10 mL round-bottomed flask. The solids were filtered through a Buchner funnel and triturated with hexanes (5 mL) and to afford the Ru-Cl complex as an off-white solid in 85% yield (41.6 mg, 0.05 mmol).

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

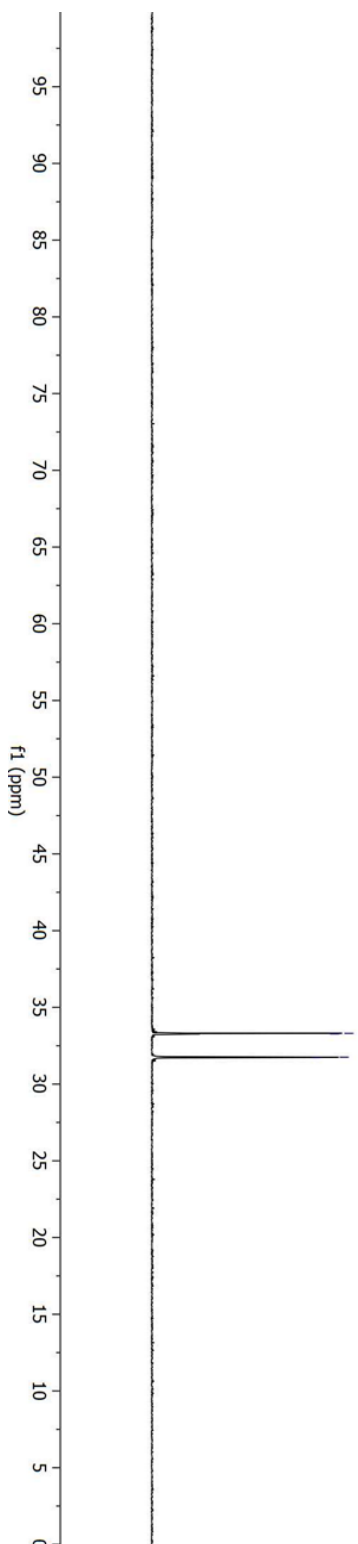
Solid State ^{31}P NMR (162 MHz, 12 kHz, 3.5 ms): δ : 33.3 (broad), 26.7 (broad).

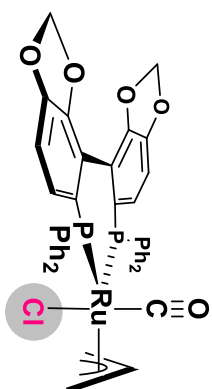
HRMS (Na^+ , m/z): for $\text{C}_{42}\text{H}_{33}\text{ClO}_5\text{P}_2\text{Ru}$ calcd. = 839.0436; found = 839.0458.



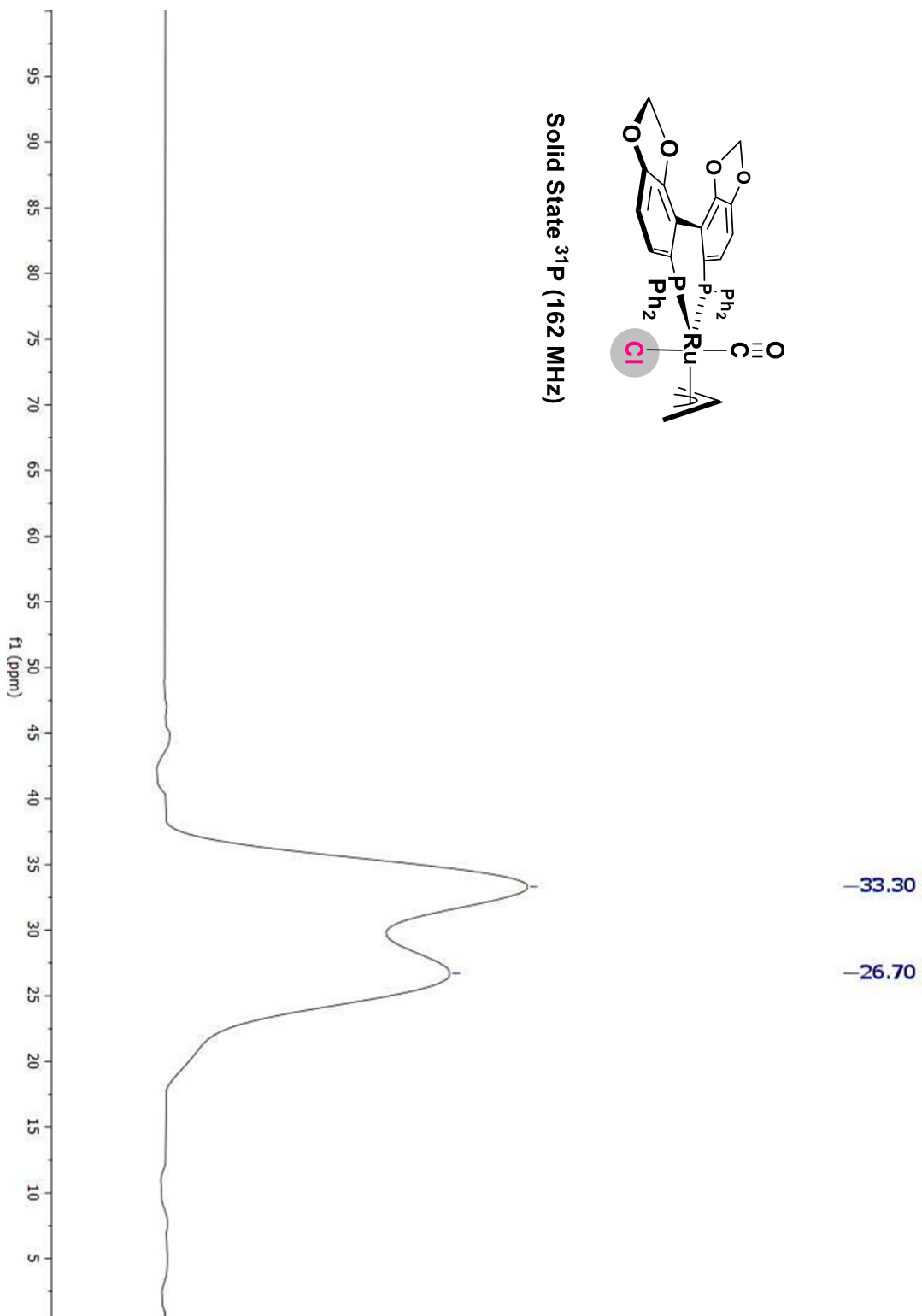
$^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz)

33.30
33.28
31.75
31.73

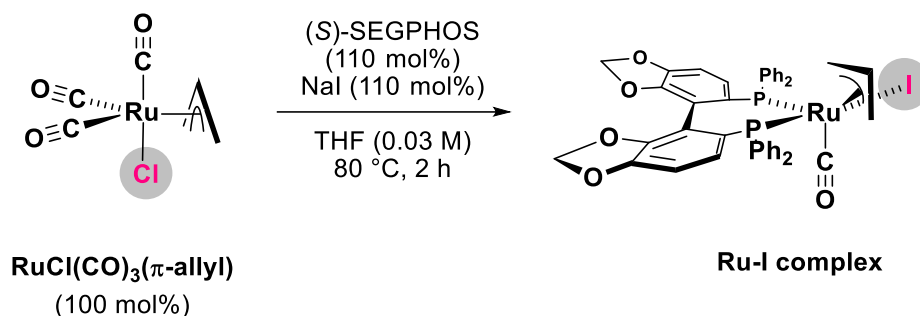




Solid State ^{31}P (162 MHz)



Synthesis of Ruthenium-Iodide Complex

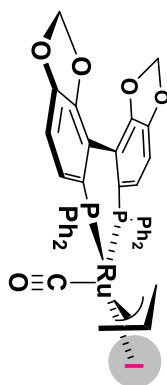


To an oven-dried pressure tube equipped with a magnetic stir bar under an argon atmosphere charged with $\text{RuCl(CO)}_3(\pi\text{-allyl})$ complex (14 mg, 0.06 mmol), (S)-SEGPHOS (37 mg, 0.06 mmol), and NaI (9 mg, 0.06 mmol) was added THF (2 mL, 0.03 M). The pressure tube was backfilled with argon,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

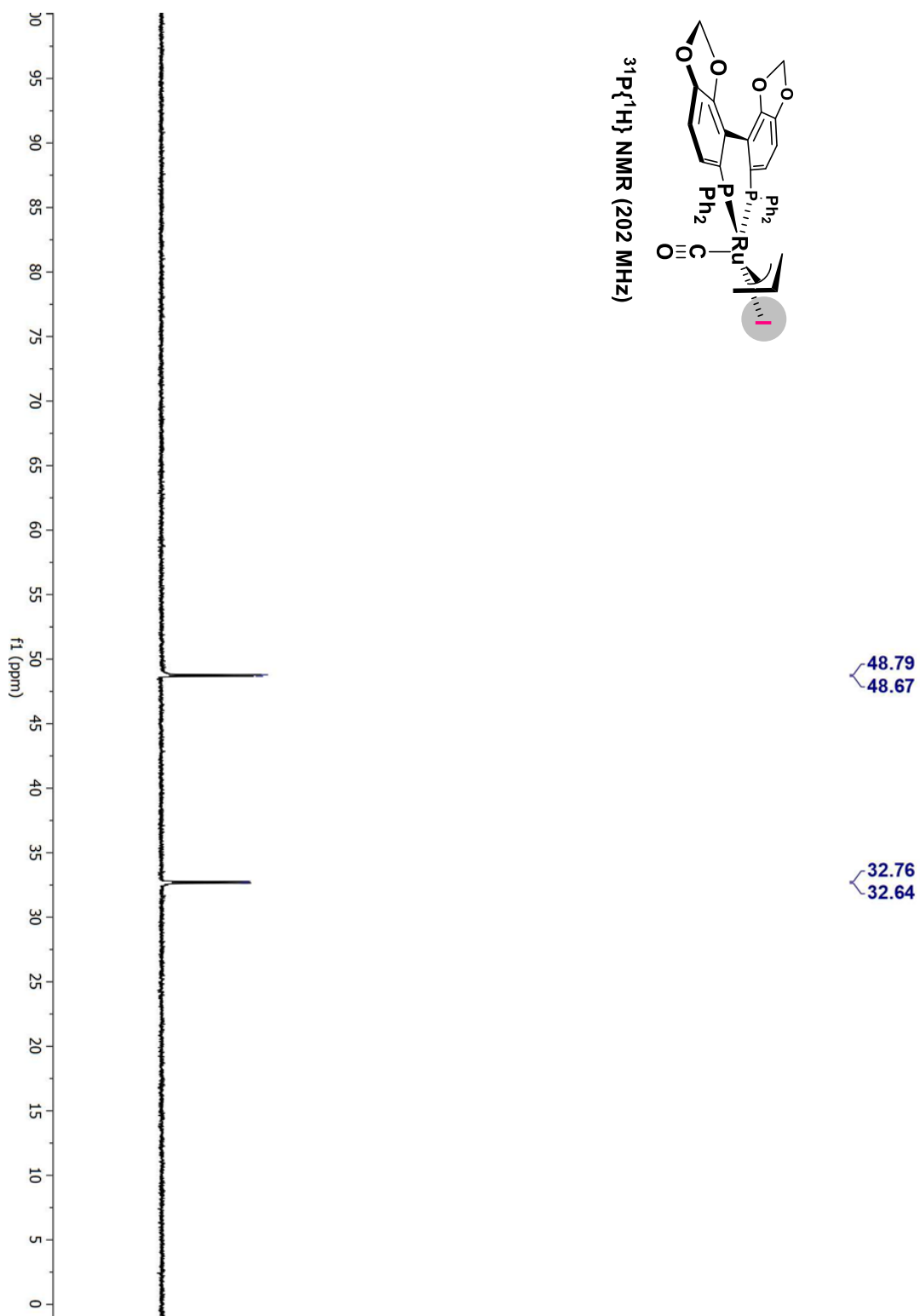
$^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz, C_6D_6): δ : 48.7 (d, $J = 25.1$ Hz), 32.7 (d, $J = 25.2$ Hz).

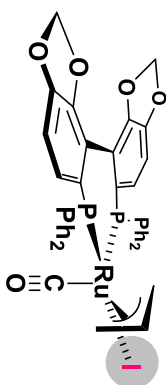
Solid State ^{31}P NMR (162 MHz, 12 kHz, 3.5 ms): δ : 48.6 (broad), 32.0 (broad).

HRMS (K^+ , m/z): for $\text{C}_{42}\text{H}_{33}\text{IO}_5\text{P}_2\text{Ru}$ calcd. = 946.9534; found = 946.9544.

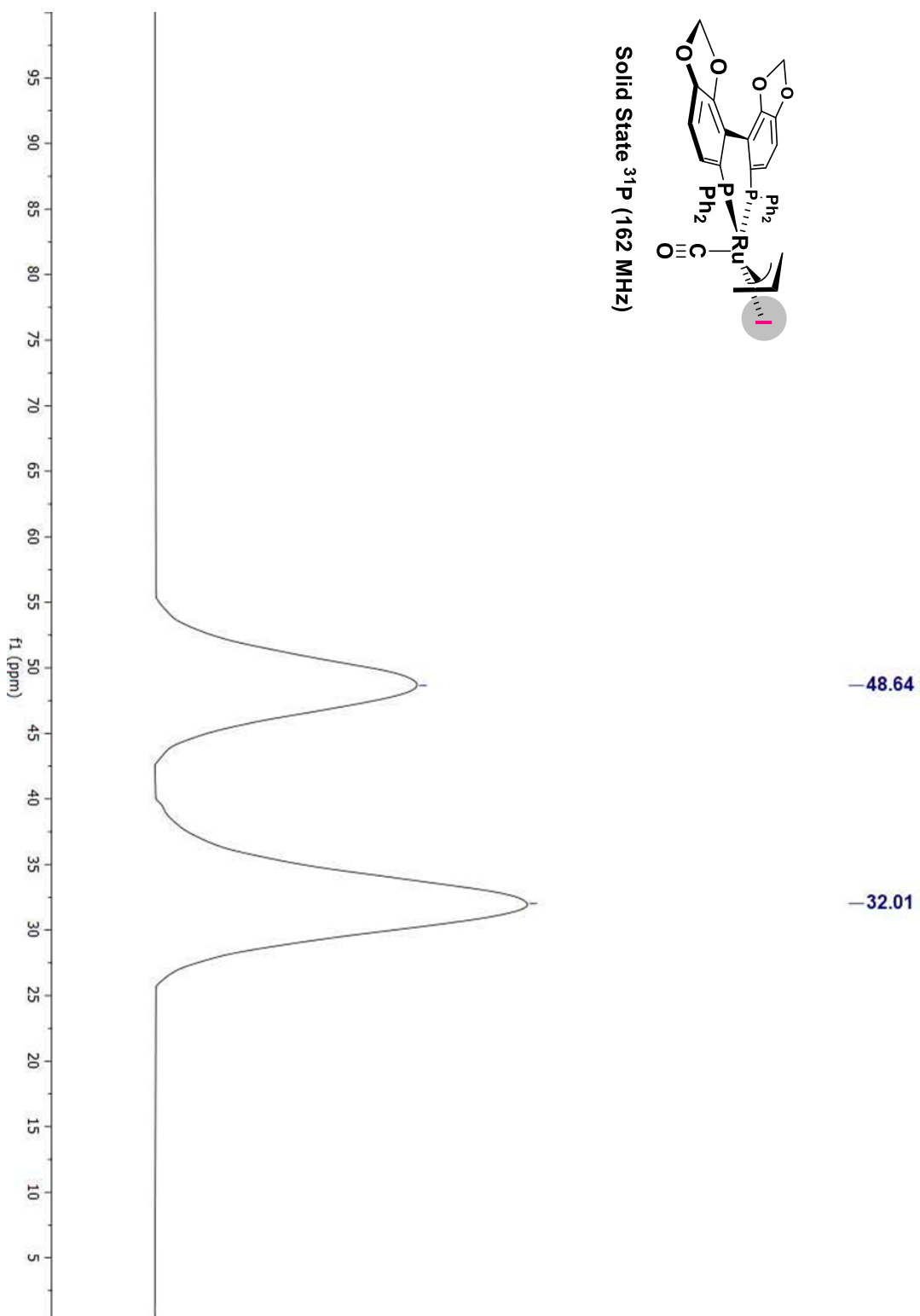


$^3\text{P}\{^1\text{H}\}$ NMR (202 MHz)



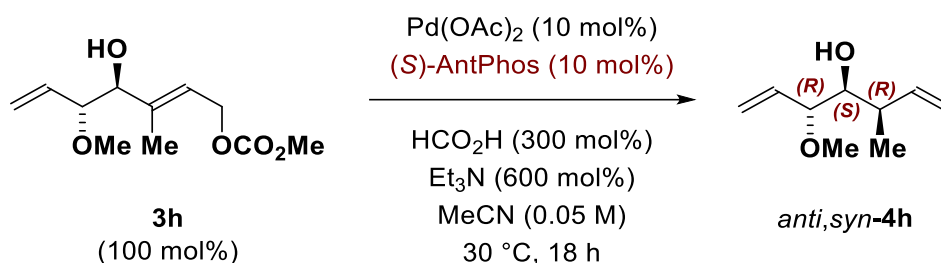


Solid State ^{31}P (162 MHz)



Pd-Catalyzed Asymmetric Tsuji-Reduction of Compound **3h**

(3*S*,4*R*)-4-methoxy-1-(4-methoxyphenyl)hex-5-en-3-ol (*anti*,*syn*-**4h**)



An oven-dried round-bottomed flask equipped with a magnetic stir bar was charged with Pd(OAc)_2 (4.5 mg, 0.02 mmol, 10 mol%) and $(S)\text{-AntPhos}$ (7.4 mg, 0.02 mmol, 10 mol%). Compound **3h** (46 mg, 0.2 mmol, 100 mol%) was added as a solution in MeCN (4.0 mL, 0.05 M) via syringe. Et_3N (171 μL , 1.2 mmol, 600 mol%), and HCO_2H (23.0 μL , 0.6 mmol, 300 mol%) were added via syringe. The reaction mixture was allowed to stir at $30\text{ }^\circ\text{C}$ for 18 hours. The solvent was concentrated *in vacuo* and the residue was subjected to flash chromatography (SiO_2 : 2:98 acetone:hexanes) to furnish the title compound *anti*,*syn*-**4h** in 70% yield (21.6 mg, 0.14 mmol, 4:1 dr) as a yellow oil.

TLC (SiO_2): R_f = 0.6 (1:2 acetone:hexanes).

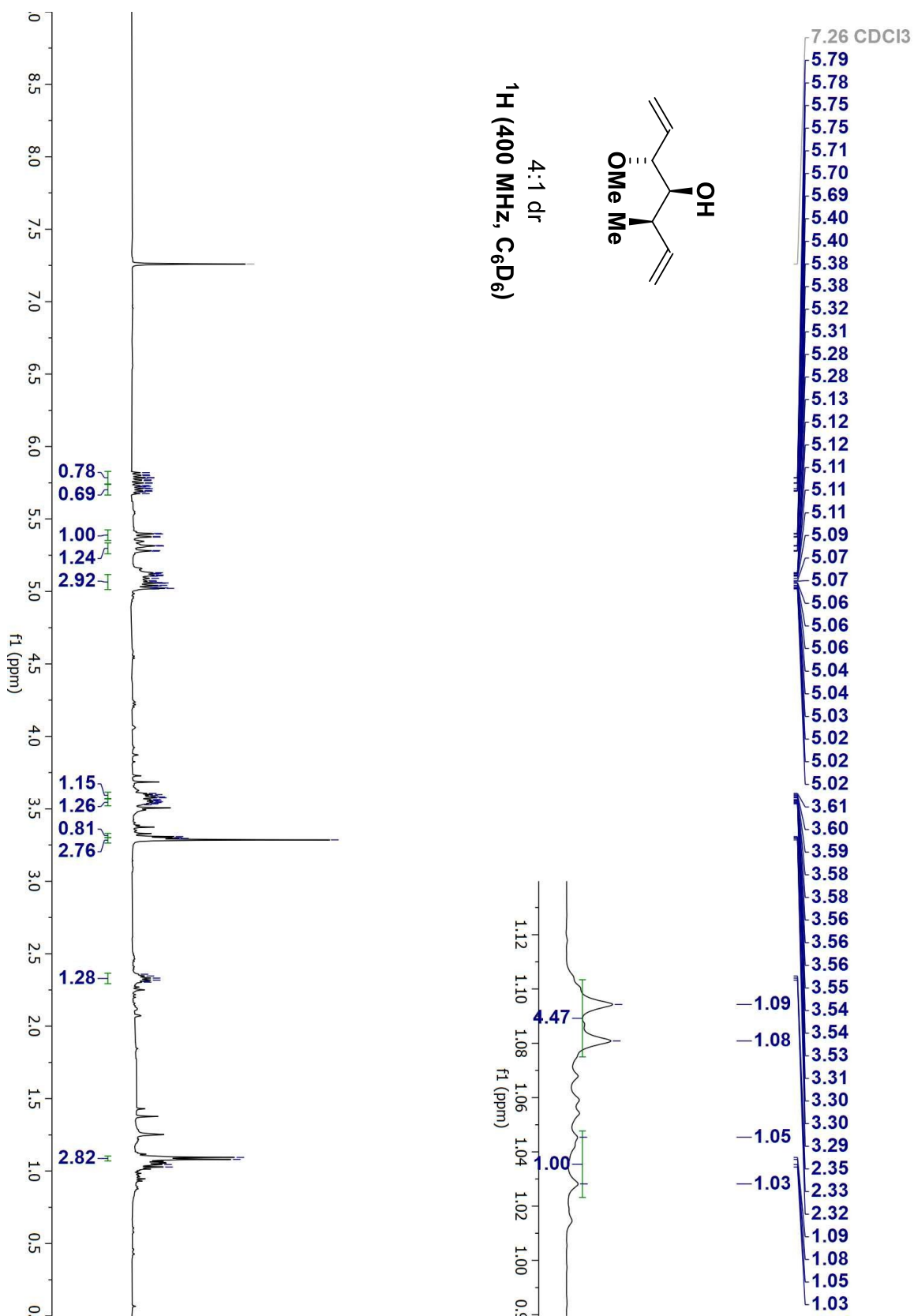
^1H NMR (500 MHz, CDCl_3): δ 5.83 – 5.74 (m, 1H), 5.74 – 5.66 (m, 1H), 5.39 (d, J = 10.5 Hz, 1H), 5.30 (d, J = 15.8 Hz, 1H), 5.13 – 5.01 (m, 2H), 3.61 – 3.57 (m, 1H), 3.55 (ddd, J = 7.4, 4.2, 2.7 Hz, 1H), 3.32 – 3.29 (m, 1H), 3.29 (s, 3H), 2.33 (dt, J = 14.0, 6.5 Hz, 1H), 1.09 (d, J = 6.7 Hz, 3H).

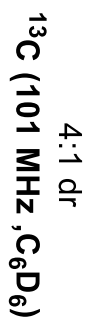
^{13}C NMR (126 MHz, CDCl_3): δ 140.7, 133.7, 120.6, 115.4, 83.9, 75.9, 56.3, 40.0, 15.9.

HRMS (Na^+ , m/z) for $\text{C}_9\text{H}_{16}\text{O}_2$: calcd. = 179.1043; found = 179.1037.

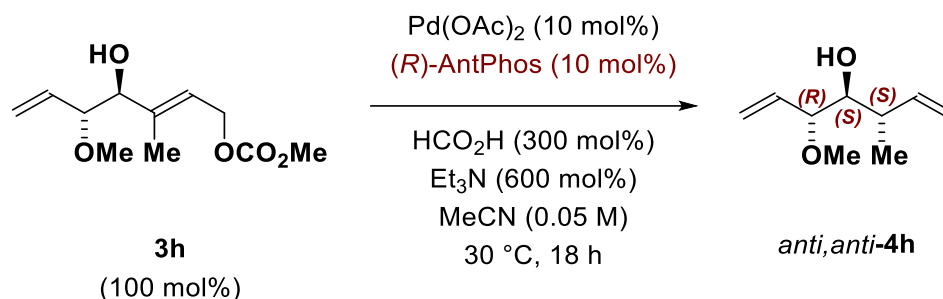
FTIR (neat): 2868, 2346, 2160, 1978, 1637, 1148, 669, 455, 414 cm^{-1} .

$[\alpha]_D^{24}$ = -31.8 (c = 0.11, CHCl_3).





(3*S*,4*R*)-4-methoxy-1-(4-methoxyphenyl)hex-5-en-3-ol (*anti,anti*-4*h*)



An oven-dried round-bottomed flask equipped with a magnetic stir bar was charged with Pd(OAc)_2 (4.5 mg, 0.02 mmol, 10 mol%) and $(R)\text{-AntPhos}$ (7.4 mg, 0.02 mmol, 10 mol%). Compound **3h** (46 mg, 0.2 mmol, 100 mol%) was added as a solution in MeCN (4.0 mL, 0.05 M) via syringe. Et_3N (171 μL , 1.2 mmol, 600 mol%), and HCO_2H (23.0 μL , 0.6 mmol, 300 mol%) were added via syringe. The reaction mixture was allowed to stir at $30\text{ }^\circ\text{C}$ for 18 hours. The solvent was concentrated *in vacuo* and the residue was subjected to flash chromatography (SiO_2 : 2:98 acetone:hexanes) to furnish the title compound *anti,anti*-**4h** in 61% yield (19.2 mg, 0.12 mmol, 6:1 dr) as a yellow oil.

TLC (SiO_2): R_f = 0.6 (1:2 acetone:hexanes).

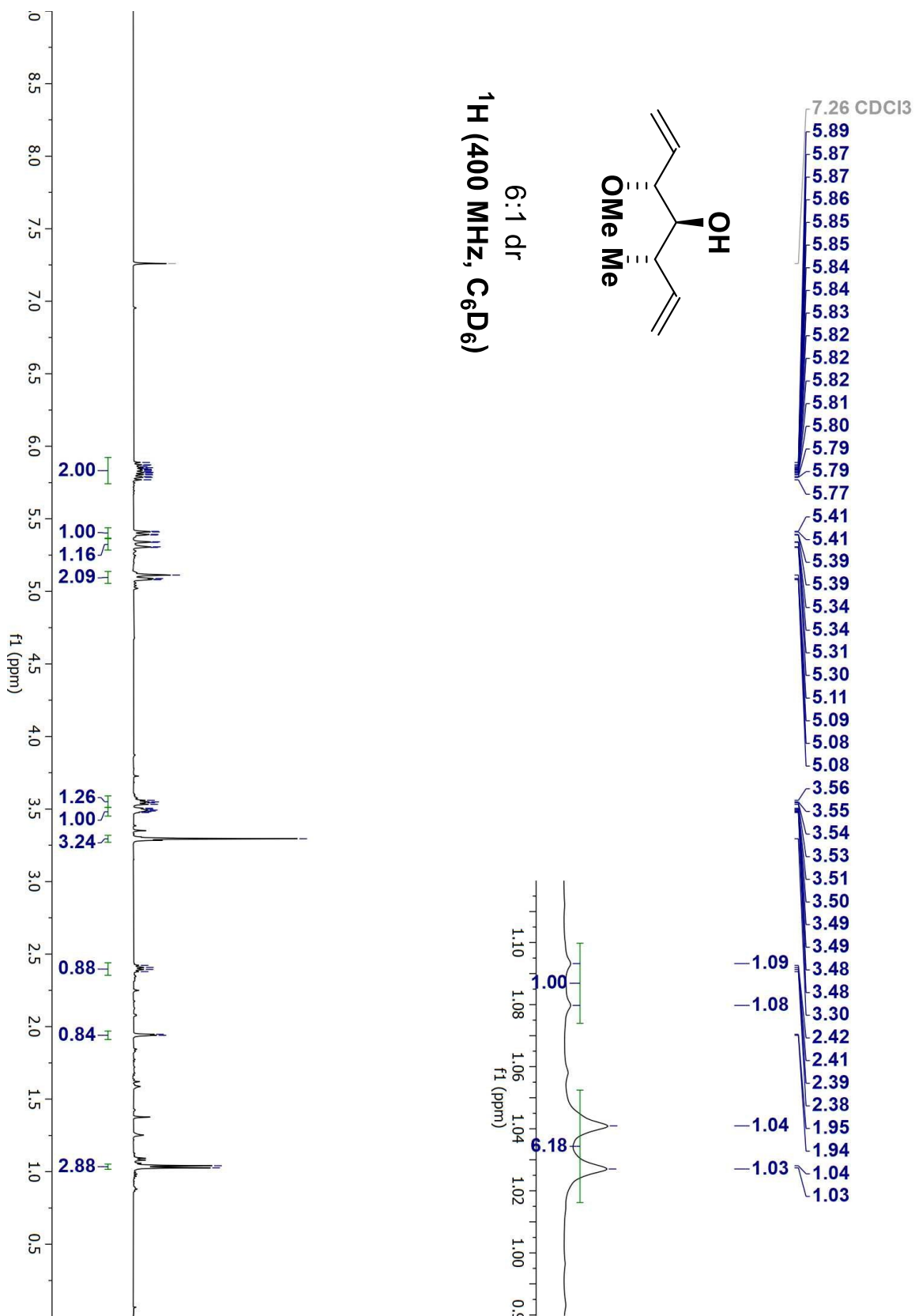
^1H NMR (500 MHz, CDCl_3): δ 5.91 – 5.75 (m, 2H), 5.40 (dd, J = 10.3, 1.8 Hz, 1H), 5.32 (dd, J = 17.3, 1.9 Hz, 1H), 5.13 – 5.06 (m, 2H), 3.55 (dd, J = 8.3, 5.1 Hz, 1H), 3.49 (td, J = 5.8, 3.0 Hz, 1H), 3.30 (s, 3H), 2.40 (q, J = 7.1 Hz, 1H), 1.94 (d, J = 3.3 Hz, 1H), 1.03 (d, J = 7.0 Hz, 3H).

^{13}C NMR (126 MHz, CDCl_3): δ 140.4, 134.6, 120.6, 115.8, 84.2, 76.1, 56.4, 39.8, 16.7.

HRMS (Na^+ , m/z) for $\text{C}_9\text{H}_{16}\text{O}_2$: calcd. = 179.1043; found = 179.1037.

FTIR (neat): 2886, 2369, 2159, 1968, 1654, 1141, 636, 536, 409 cm^{-1} .

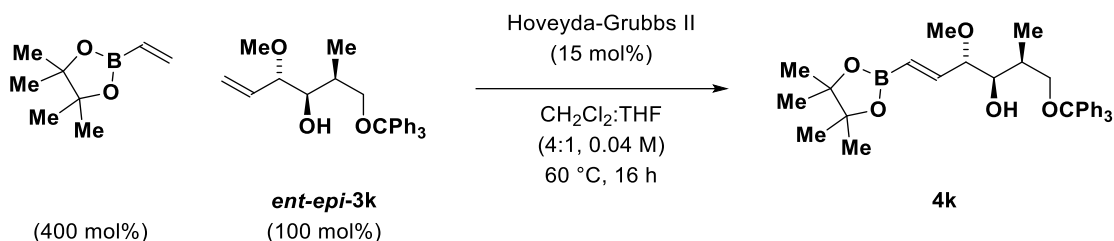
$[\alpha]_D^{24}$ = -17.2 (c = 0.11, CHCl_3).





Synthesis of C₁₂-C₁₇ Fragment of Bafilomycin A₁ (**4k**)

(2*S*,3*R*,4*S*,*E*)-4-methoxy-2-methyl-6-(4,4,5,5-tetraethyl-1,3,2-dioxaborolan-2-yl)-1-(trityloxy)hex-5-en-3-ol (**4k**)



An oven-dried 25 mL round-bottomed flask equipped with a magnetic stir bar was charged with Hoveyda-Grubbs second generation catalyst (10.0 mg, 0.018 mmol, 5 mol%). *Ent-epi-3k* (140 mg, 0.35 mmol, 100 mol%) was added as a solution in CH₂Cl₂:tetrahydrofuran (7.0 mL : 1.75 mL, 0.04 M, 4:1 v/v) followed by vinylboronic acid pinacol ester (209.4 mg, 0.23 mL, 1.36 mmol, 400 mol%) via syringe. The reaction vessel was placed in a 60 °C oil bath and was allowed to stir for 3 hours. A second addition of Hoveyda-Grubbs second generation catalyst (10.0 mg, 0.018 mmol, 5 mol%) was added and the reaction vessel was purged under vacuum and backfilled with argon. The reaction vessel was placed in a 60 °C oil bath and was allowed to stir for 3 hours. A third addition of Hoveyda-Grubbs second generation catalyst (10.0 mg, 0.018 mmol, 5 mol%) was added and the reaction vessel was purged under vacuum and backfilled with argon. The reaction was allowed to stir in a 60 °C oil bath for 16 hours. The reaction mixture was concentrated *in vacuo* and the residue was subjected to flash column chromatography (SiO₂: 2:98 acetone:hexanes) to furnish the title compound **4k** as a yellow oil in 70% yield (129.8 mg, 0.25 mmol).

TLC (SiO₂): R_f = 0.33 (1:4 acetone:hexanes).

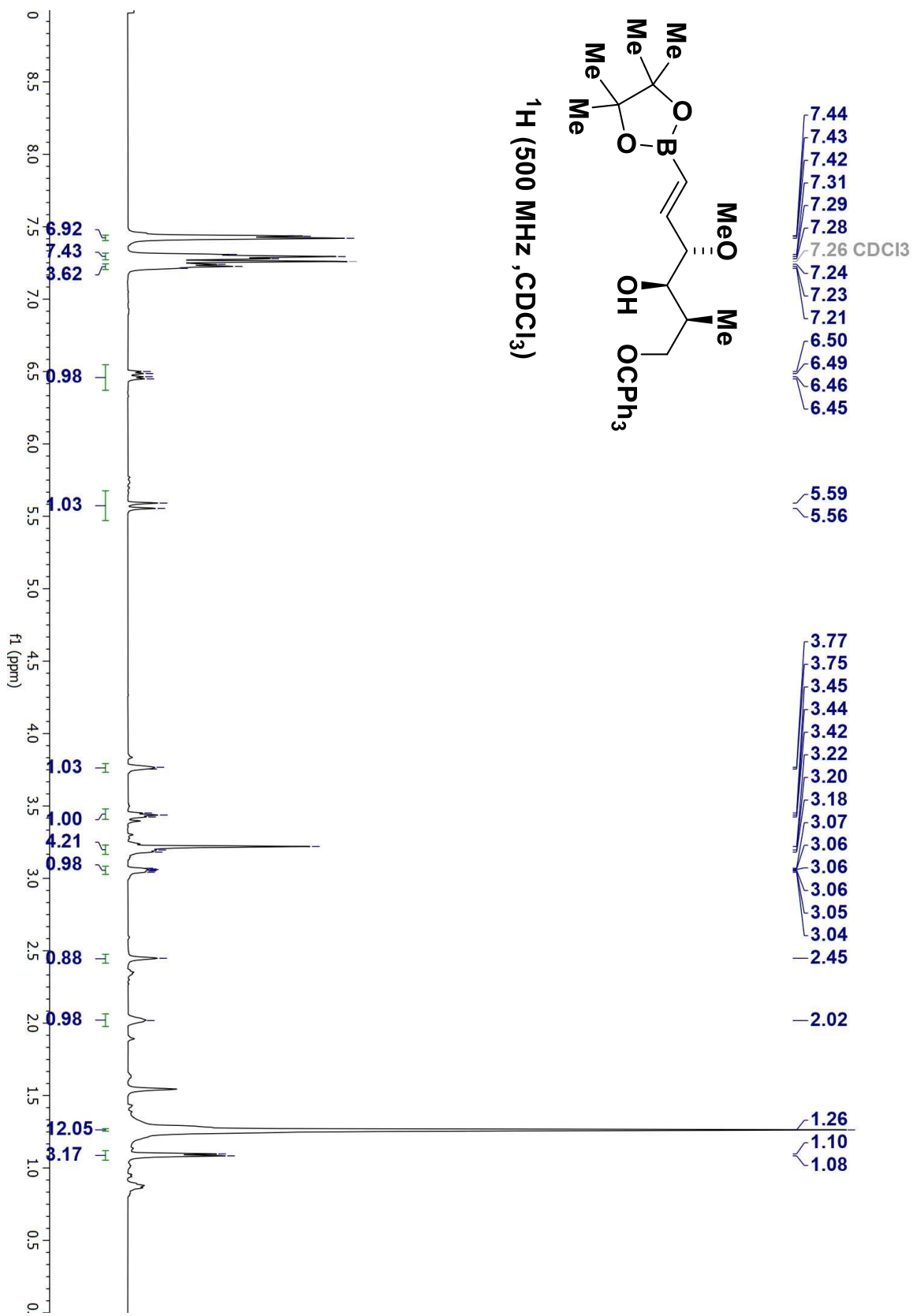
¹H NMR (500 MHz, CDCl₃): δ 7.43 (d, *J* = 7.1 Hz, 6H), 7.29 (t, *J* = 7.5 Hz, 7H), 7.26 – 7.20 (m, 3H), 6.47 (dd, *J* = 18.2, 7.2 Hz, 1H), 5.57 (d, *J* = 18.2 Hz, 1H), 3.76 (d, *J* = 6.1 Hz, 1H), 3.44 (t, *J* = 6.9 Hz, 1H), 3.26–3.17 (m, 4H), 3.09 – 3.01 (m, 1H), 2.45 (s, 1H), 2.02 (s, 1H), 1.26 (s, 12H), 1.09 (d, *J* = 7.0 Hz, 3H).

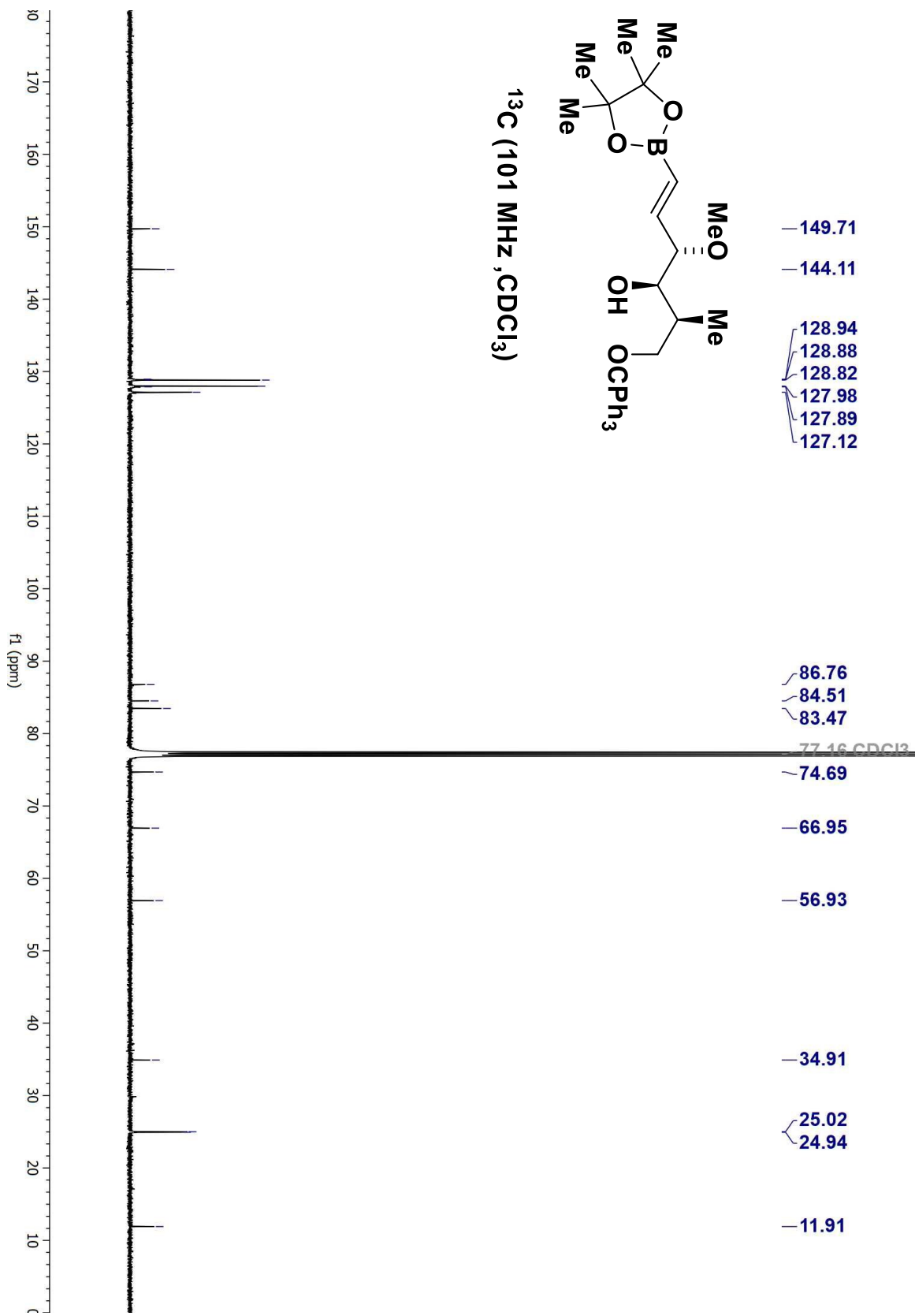
¹³C NMR (101 MHz, CDCl₃): δ 149.71, 144.11, 128.94, 128.88, 128.82, 127.98, 127.89, 127.12, 86.76, 84.51, 83.47, 74.69, 66.95, 56.93, 34.91, 25.02, 24.94, 11.91.

HRMS (K⁺, *m/z*): for C₃₃H₄₁BO₅ calcd. = 566.2715; found = 566.2696.

FTIR (neat): 2979, 2930, 2871, 1639, 1449, 1361, 1327, 1143, 848, 707 cm⁻¹.

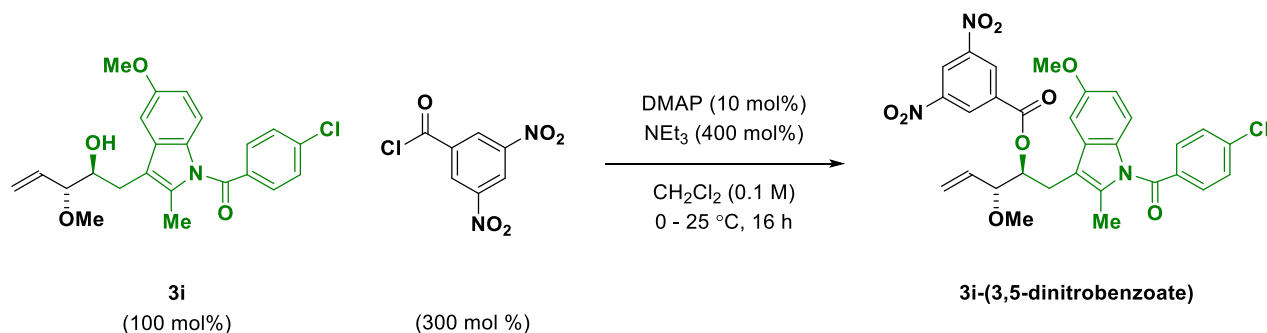
[α]_D²⁴ = 82.7 (*c* = 0.75, CHCl₃).





Synthesis of 3i-(3,5-dinitrobenzoate)

(2*S*,3*R*)-1-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-3-methoxypent-4-en-2-yl 3,5-dinitrobenzoate (3i-(3,5-dinitrobenzoate))



An oven-dried 25 mL round-bottomed flask equipped with a magnetic stir bar was charged **3i** (41.3 mg, 0.1 mmol, 100 mol%) and DMAP (19 mg, 0.1 mmol, 100 mol%). NEt₃ (42 μ L, 0.3 mmol, 300 mol%) and CH₂Cl₂ (1.0 mL, 0.1 M) were added via syringe. The reaction mixture was cooled to 0 °C in an ice bath and 3,5-dinitrobenzoyl chloride (84 mg, 0.3 mmol, 300 mol%) was added in a single portion. The reaction mixture was allowed to stir at 0 °C for 30 minutes, warmed to ambient temperature and stirred for 24 hours. The reaction was diluted with CH₂Cl₂ (4 mL) and H₂O (4 mL). The reaction mixture was transferred to a separatory funnel with the aid of CH₂Cl₂. The layers were separated and the organic layer was washed with saturated NaCl (aq) (5 mL). The organic layer was dried (Na₂SO₄), filtered and concentrated *in vacuo*. The residue was subjected to flash column chromatography (SiO₂: 3:97 acetone: CH₂Cl₂) to furnish the title compound **3i-(3,5-dinitrobenzoate)** as a yellow crystalline solid in 44% yield (27.6 mg, 0.045 mmol).

TLC (SiO₂): R_f = 0.95 (1:9 acetone: CH₂Cl₂).

¹H NMR (500 MHz, CDCl₃): δ 9.16 (s, 1H), 8.96 (s, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.7 Hz, 2H), 7.00 (d, *J* = 2.5 Hz, 1H), 6.77 (d, *J* = 9.1 Hz, 1H), 6.55 (d, *J* = 9.1 Hz, 1H), 5.90 (dt, *J* = 17.8, 9.5 Hz, 1H), 5.54 (q, *J* = 6.2 Hz, 1H), 5.52 – 5.43 (m, 2H), 3.87 (dd, *J* = 7.9, 4.8 Hz, 1H), 3.76 (s, 3H), 3.37 (s, 3H), 3.16 (d, *J* = 6.7 Hz, 2H), 2.38 (s, 3H).

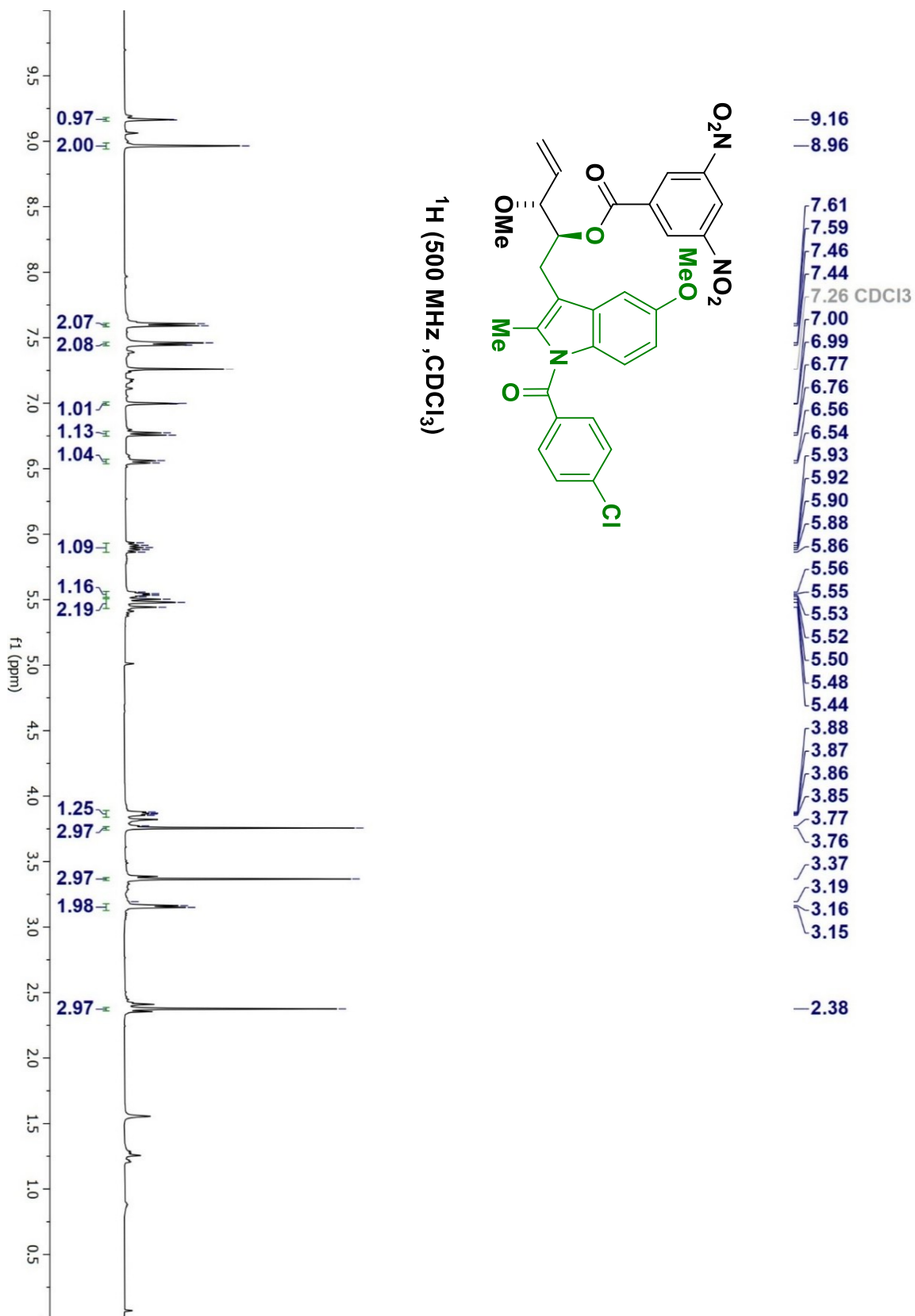
¹³C NMR (101 MHz, CDCl₃): δ 168.3, 161.9, 155.9, 148.5, 139.3, 135.7, 133.8, 131.1, 131.0, 130.9, 129.3, 129.2, 122.2, 121.5, 114.9, 114.5, 110.8, 101.9, 83.2, 77.3, 77.3, 56.9, 55.6, 24.9, 13.5.

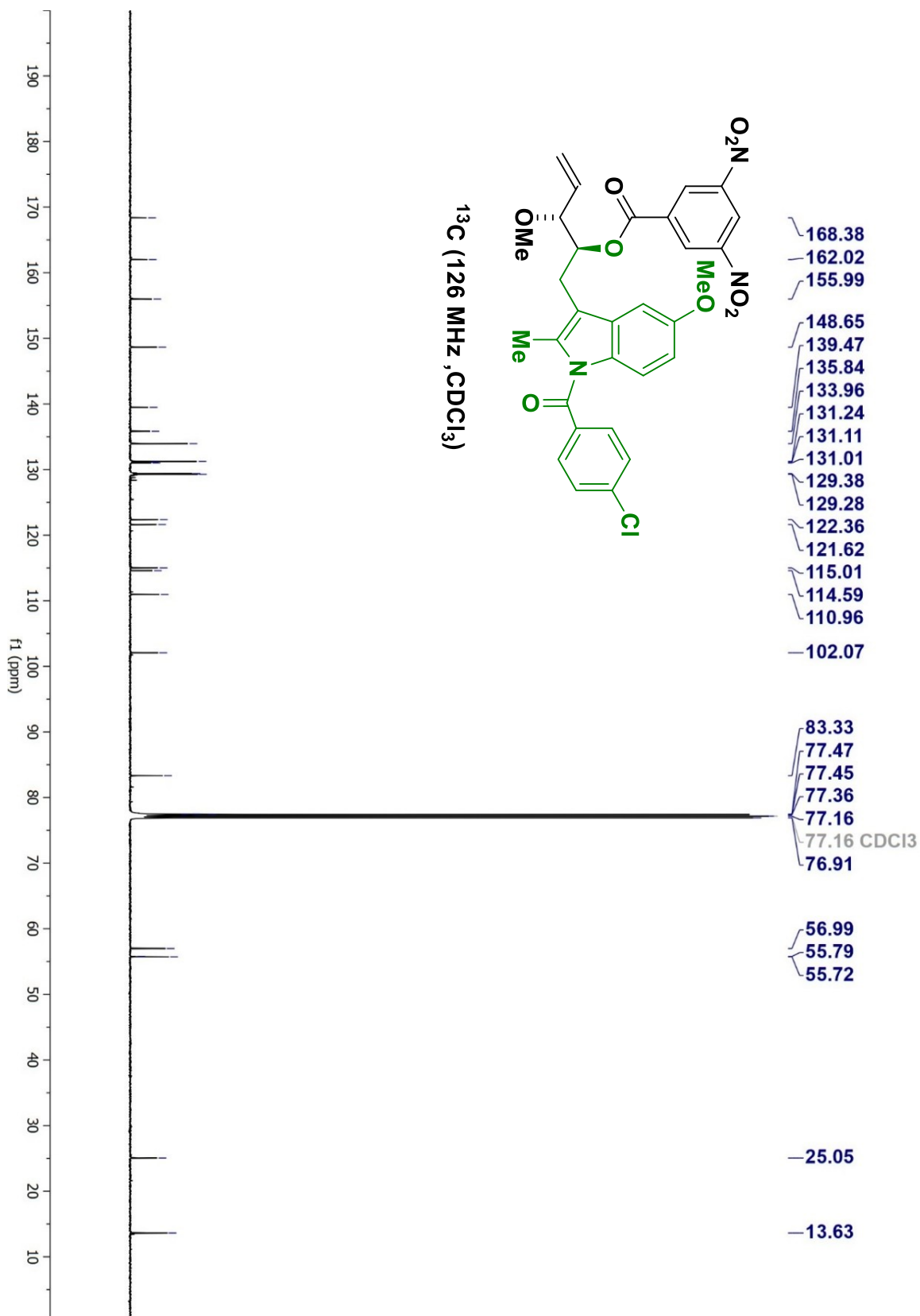
HRMS (Na⁺, *m/z*): for C₃₀H₂₆ClN₃O₉: calcd. = 608.1430; found = 608.1430.

FTIR (neat): 3907, 2980, 2360, 1719, 1682, 1539, 1478 cm⁻¹.

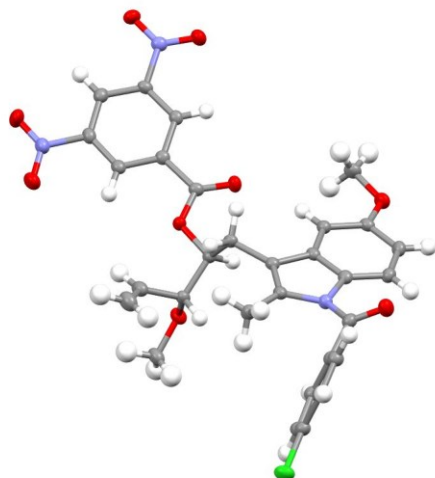
$[\alpha]_D^{24}$ = -47.2 (*c* = 1.25, CHCl₃).

MP: 110 - 111 °C





Single Crystal Diffraction Data for 3i-(3,5-dinitrobenzoate)



Crystals grew as clusters of yellow needles of **3i-(3,5-dinitrobenzoate)** by slow evaporation of n-hexanes into a diethyl ether solution. A suitable crystal 0.239 x 0.015 x 0.015 mm³ was selected and mounted on a suitable support on an XtaLAB Synergy, Single source at home/near, HyPix diffractometer. The crystal was kept at a steady 100.01(10) K during data collection. The structure was solved with the ShelXT¹¹ structure solution program using the Intrinsic Phasing solution method and by using Olex2¹¹ as the graphical interface. The model was refined with version 2018/3 of ShelXL^{11c} using Least Squares minimization.

Table S1. Crystal data and structure refinement for **3i-(3,5-dinitroenzoate)**.

Empirical formula	C ₃₀ H ₂₆ ClN ₃ O ₉	
Formula weight	607.99	
Temperature	108(12) K	
Wavelength	1.54184 Å	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 19.4548(2) Å	a = 90°.
	b = 6.9773(1) Å	b = 91.642(10)°.
	c = 20.5536(2) Å	g = 90°.
Volume	2788.84(6) Å ³	
Z	4	
Density (calculated)	1.448 Mg/m ³	
Absorption coefficient	1.751 mm ⁻¹	
F(000)	1264.0	
Crystal size	0.239 x 0.015 x 0.015 mm ³	
Radiation	Cu Kα (λ = 1.54184)	
Theta range for data collection	2.338 to 76.872°.	
Index ranges	-24 ≤ h ≤ 24, -8 ≤ k ≤ 6, -25 ≤ l ≤ 25	
Reflections collected	28844	
Independent reflections	9490	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.5870	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9490 / 1 / 781	
Goodness-of-fit on F2	1.061	
Final R indices [I > 2σ(I)]	R1 = 0.0400, wR2 = 0.1040	
R indices (all data)	R1 = 0.0402, wR2 = 0.1039	
Absolute structure parameter	0.031(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.400 and -0.330 e.Å ⁻³	
Flack Parameter	0.031(7)	

Computational Studies

The computational investigation primarily aimed to elucidate the origins of the enantioselectivity of a nucleophilic attack of an electron-rich allylic system on an aldehyde. The workflow was divided into two phases: the generation of diastereomeric complexes involving the catalyst, ligands, and substrates, and the addition exhibiting diastereo- and enantioselectivity.

To investigate these processes, each complex geometry underwent an initial conformational exploration via metadynamics using GFN2-xTB¹² as implemented in CREST¹³ (version 3.0.2), employing APLB¹⁴ for implicit dioxane solvation. The resulting conformational ensemble was subsequently clustered based on dihedral angles through *k*-means clustering combined with PCA. The resulting reduced ensemble underwent refinement via ORCA (version 6.1.0)¹⁵ using a multilevel approach through the Ensemble Analyzer¹⁶ automation scheme: high-energy conformers were eliminated through single-point calculations at PBE¹⁷-D4¹⁸/def2-SV(P)¹⁹ [CPCM(dioxane)]²⁰, the retained structures were geometrically optimized at r²SCAN-3c²¹ [CPCM(dioxane)], and the final electronic energies were computed via ω B97X-D4rev^{22,23}/def2-QZVPP [CPCM (dioxane)] calculations.

Consequently, the Gibbs free energy was determined as:

$$G = E_{\omega\text{B97X-D4rev}} + G_{\text{therm}, r^2\text{SCAN-3c}} \quad (\text{eq 1})$$

where $E_{\omega\text{B97X-D4rev}}$ represents the final electronic energy at ω B97X-D4rev/def2-QZVPP [CPCM(dioxane)] and $G_{\text{therm}, r^2\text{SCAN-3c}}$ denotes the thermal correction calculated at the r²SCAN-3c level under standard pressure, standard concentration (1M) and at the reaction temperature (343K).

Evaluation of the diastereomeric complexes

Six different complexes can be generated, each existing as a pair of diastereomers due to the desymmetrizing effect of the enantiopure phosphinic ligand. These twelve possible structures are shown in Figure S1. For the following discussion, to differentiate these diastereomeric complexes, the bottom row will be addressed as A', B', etc. The computed population of these complexes is reported in Table S1. The average free energy was calculated as:

$$G_{\text{av}} = \sum_i p_i G_i \quad (\text{eq 2})$$

$$p_i = \frac{g_i \exp(-\Delta G_i/RT)}{\sum_j g_j \exp(-\Delta G_j/RT)} \quad (\text{eq 3})$$

where g_i is the degeneracy of the conformer, R is the gas constant, and T is the absolute temperature. Figure S2 shows the best conformer for the D complex. As previously reported in the literature,²⁴ an important interaction between the aldehydic hydrogen atom and the iodine can be highlighted.

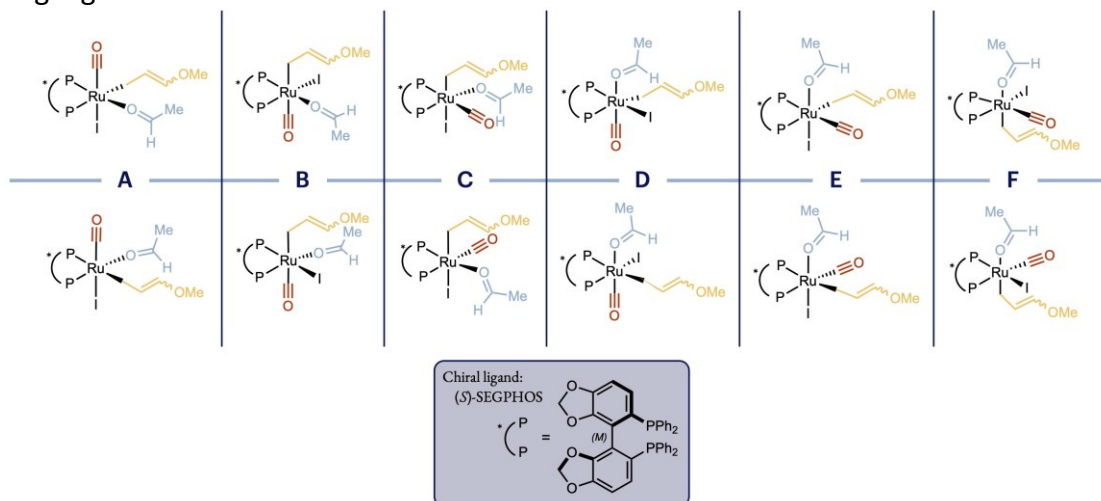


Figure S1: The twelve possible diastereoisomeric complexes

Table S2: Boltzmann population of the various conformers. The number of conformers refers to the final ensemble after the optimization process. ΔG_{av} values are considered against the most stable complex and evaluated at $\omega\text{B97X-D4rev/def2-QZVPP}$ [CPCM(Dioxane)]// $\text{r}^2\text{SCAN-3c}$ [CPCM(Dioxane)] at 343K.

Complex	<i>Trans</i> isomer			<i>Cis</i> isomer		
	# Conf.	ΔG_{av} [kcal mol ⁻¹]	Population (%)	# Conf.	ΔG_{av} [kcal mol ⁻¹]	Population (%)
A	12	3.40	0.28	8	3.85	0.15
A'	13	2.73	0.72	13	2.33	1.28
B	7	6.42	0	9	6.97	0
B'	4	9.70	0	7	7.17	0
C	9	7.13	0	10	7.25	0
C'	11	7.09	0	13	7.19	0
D	5	0.56	15.83	4	0.75	12.15
D'	4	0.00	35.40	3	0.12	29.69
E	8	16.87	0	6	15.89	0
E'	8	13.05	0	9	16.72	0
F	1	1.45	4.5	10	10.68	0
F'	11	8.53	0	9	8.29	0

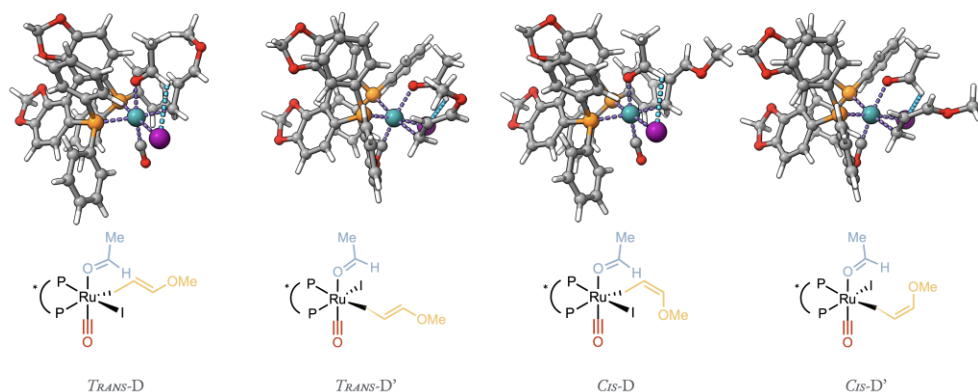


Figure S2: Best conformer for D and D' for both the trans and cis complex. in blue, in purple, in orange, in red, in gray, and in white. The dashed blue bond is the interaction.

Enantioselective Addition

TS Optimization

The transition state (TS) localization has been conducted only starting from the populated D complexes. The TS is a Zimmerman-Traxler-*like* transition state²⁵ - so a constrained 6-membered ring with the coordination of a metal atom. To compare with experimental data, the aldehyde was modified to match the experimentally used aldehyde.

The presence of the CH-I interaction reduces the number of transition states from sixteen to eight (four for *trans* and four for *cis* isomers): the rotation of the face of the aldehyde is very high in energy due to the loss of this interaction. To ensure the identification of the global minimum for each reacting approach, every located TS was subjected to an extensive conformational search. The generated ensembles were then screened and fully optimized using Ensemble Analyzer, in order to rigorously define the best TS structure.

These TS have been optimized following the same protocol used for the complexes. The diastereomeric ratio (d.r.) and the enantiomeric excess (*ee*%) are calculated as:

$$\text{d.r.} = \frac{p_{\text{anti}}}{p_{\text{syn}}} = \frac{p_{\text{RS}} + p_{\text{SR}}}{p_{\text{RR}} + p_{\text{SS}}} \quad (\text{eq 4})$$

$$ee_{\%, \text{ anti}} = \frac{p_{\text{RS}} - p_{\text{SR}}}{p_{\text{RS}} + p_{\text{SR}}} \times 100 \quad (\text{eq 5})$$

$$ee_{\%, \text{ syn}} = \frac{p_{\text{RR}} - p_{\text{SS}}}{p_{\text{RR}} + p_{\text{SS}}} \times 100 \quad (\text{eq 6})$$

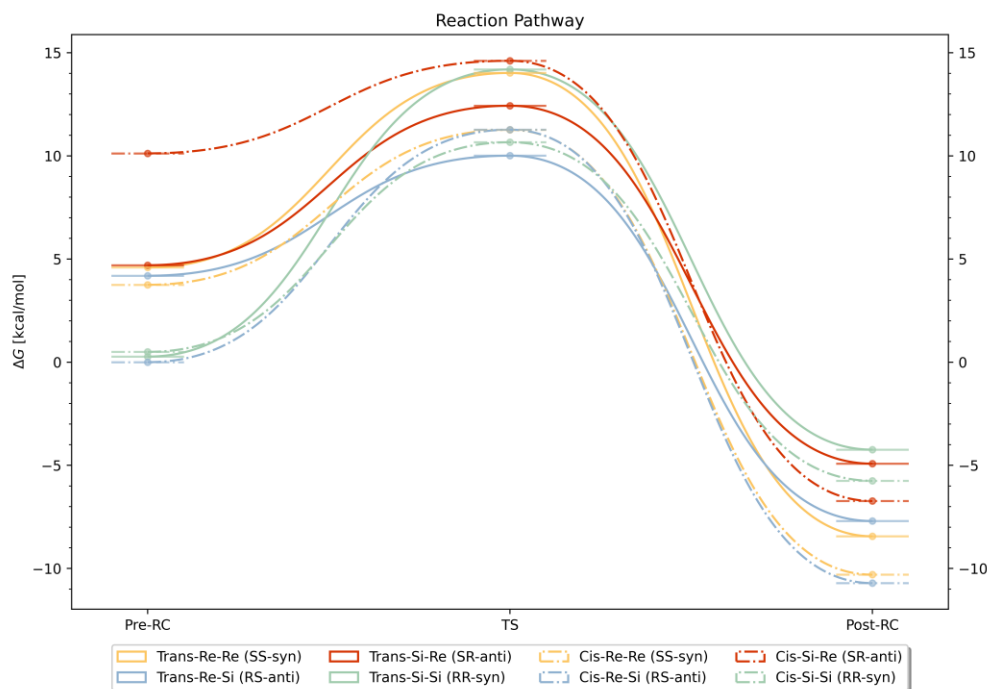
where p_i is the Boltzmann population calculated on the $\Delta\Delta G^\ddagger$.

Table S3 shows the reaction profile of these four diastereomeric approaches. Post-reaction complex (RC) has been optimized from the geometry resulting from the displacement along the imaginary frequency of the TS. On the other hand, the Pre-RC is the best conformer from previous conformational analysis.

From these data, the calculated d.r. is 2.16 to 1 in favour to the *anti* product which is in good agreement with the experimental results (4 to 1 towards the *anti* product). Furthermore, the calculated *ee*_% of the *anti* product is 95.0% toward the configuration compared to the 86% experimental value in favour of the same product.

Table S3: Relative energies in kcal mol⁻¹ for the addition reaction on the D complexes at ω B97X-D4rev/def2-QZVPP [CPCM]//r²SCAN-3c level at 343K.

Complex	Aldehyde	Allyl	Final Conf.	Pre-RC	TS	Post-RC	$\Delta\Delta G^\ddagger$	Pop TS [%]
<i>Trans</i> -D'	Re	Re	SS (<i>syn</i>)	4.59	14.02	-8.44	4.01	0.16
<i>Trans</i> -D'	Re	Si	RS (<i>anti</i>)	4.19	10.01	-7.70	0.00	57.57
<i>Trans</i> -D	Si	Re	SR (<i>anti</i>)	4.70	12.43	-4.92	2.42	1.65
<i>Trans</i> -D	Si	Si	RR (<i>syn</i>)	0.27	14.19	-4.24	4.17	0.13
<i>Cis</i> -D'	Re	Re	SS (<i>syn</i>)	3.75	11.26	-10.3	1.25	9.16
<i>Cis</i> -D'	Re	Si	RS (<i>anti</i>)	0.00	11.27	-10.71	1.26	9.09
<i>Cis</i> -D	Si	Re	SR (<i>anti</i>)	10.12	14.61	-6.73	4.60	0.07
<i>Cis</i> -D	Si	Si	RR (<i>syn</i>)	0.50	10.66	-5.75	0.65	22.17



Rationalization for Calculation

The characterization of non-covalent interactions in the four most relevant transition states was achieved through NCI analysis, employing the NCIPLOT software package (version 4.2).²⁶ Figure S3 displays the identified interactions, rendered according to standard visualization colors: blue isosurfaces denote stabilizing associations (e.g., hydrogen bonds), green areas correspond to weak Van der Waals interactions, and red surfaces highlight destabilizing steric clashes; the darker the color, the stronger the interaction.

From these maps, it is possible to observe that the CH-I interaction and a CH₂-Ph dispersive interaction are conserved across all the key transition states. Furthermore, a strongly directional hydrogen bond between the carbonyl oxygen of the aldehyde and the *ortho*-hydrogen atom of the catalyst's phenyl ring is present in the *Trans-Re-Si*, *Trans-Si-Re*, and *Cis-Re-Re* transition states. Conversely, in the *Cis-Si-Si* TS, the aldehyde lacks this strong hydrogen bond, interacting primarily via a weaker dispersive Van der Waals force.

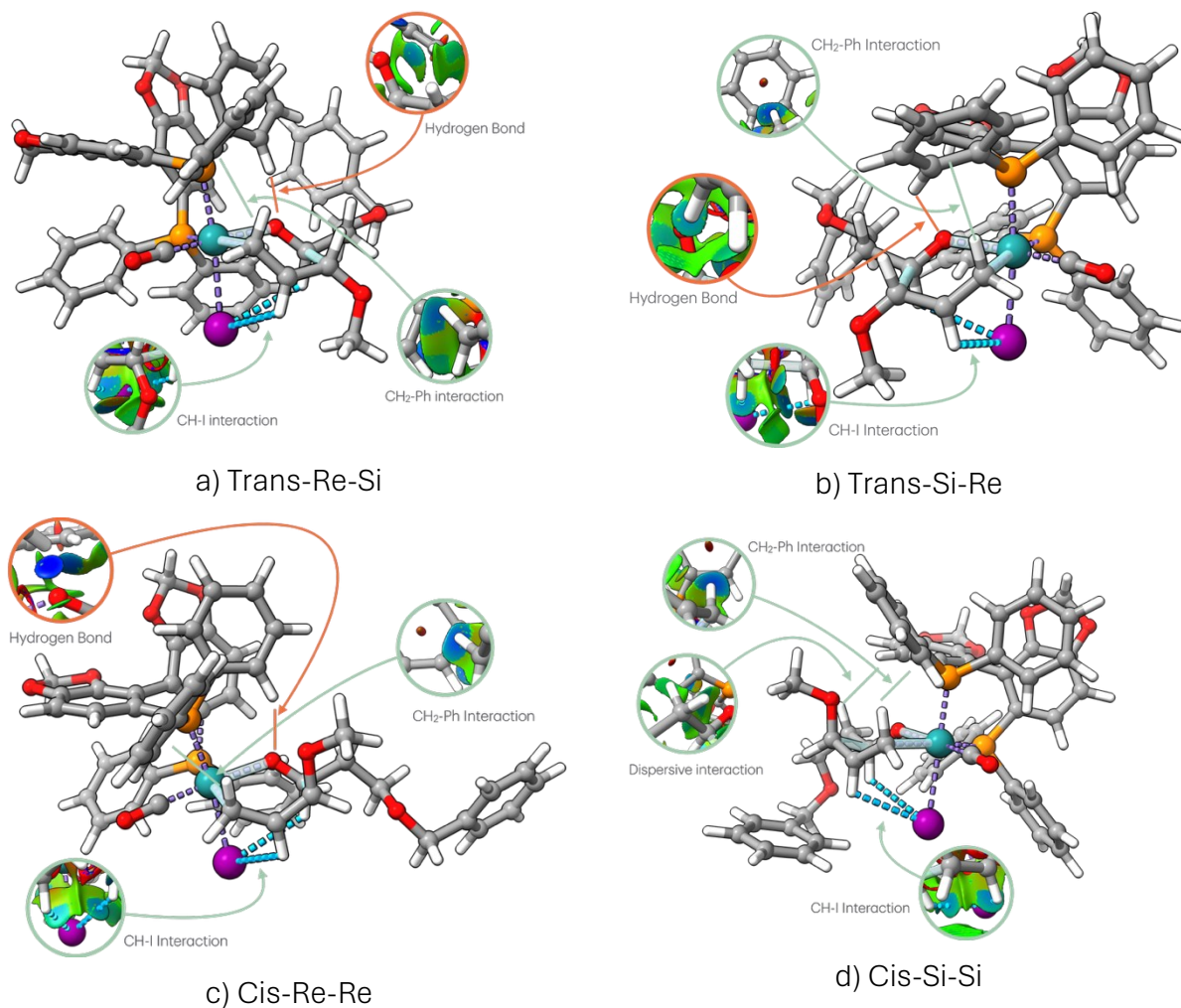


Figure S3: Selected NCI surfaces on TS geometries. Blue areas indicate strong attractive interactions (e.g., Hydrogen Bonds), while green areas denote Van der Waals or dispersive interactions.

Moreover, steric effects were examined by estimating the free space surrounding the metal centre in the TS through the buried volume ($\%V_{\text{bur}}$) method, a standard tool in ligand-steric assessments. A spherical region with a radius of 6 Å was centred on the ruthenium atom, and the volume occupied by nearby atoms was removed from this sphere to determine $\%V_{\text{bur}}$. The sphere was then divided into quadrants to quantify how this percentage of space is spatially distributed. These calculations were carried out with the SEQCrow²⁷ toolkit inside ChimeraX.²⁸

The buried volume is obtained from these maps, and the reported values correspond to the percentage of buried volume in the four front quadrants of the sphere. As can be seen, there is a significant difference between the two quadrants in which the reaction takes place.

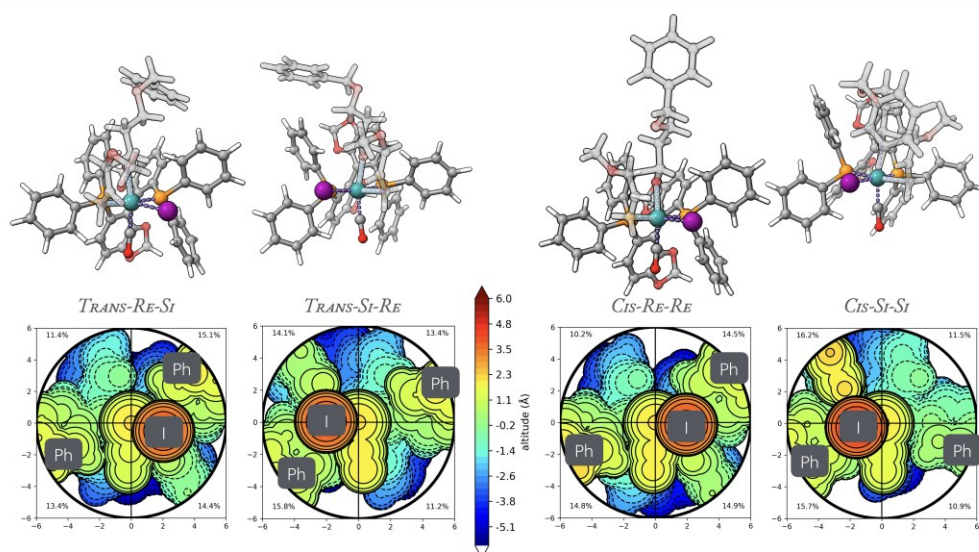


Figure S4: Distance maps of the populated TS geometries. On top the geometry with the same orientation used to create the map. The fading atoms are the reagents which have been excluded for this type of analysis.

Table S4: Buried volume percentage of the TS geometries. In blue the sector in which the aldehyde and the allylic moiety are reacting. NE: north-east, NW: north-west, SW: southwest, SE: south-east

Complex	NE	NW	SW	SE
<i>Trans</i> -Re-Si	15.1	11.4	13.4	14.4
<i>Trans</i> -Si-Re	13.4	14.1	15.8	11.2
<i>Cis</i> -Re-Re	14.5	10.2	14.8	14.9
<i>Cis</i> -Si-Si	11.5	16.2	15.7	10.9

Computational Geometries

Pre - Cis Re Re

Ru	1.7802	1.5129	0.4212
C	3.5782	2.6755	-0.2601
P	0.3229	3.2729	0.0136
I	3.6750	-0.4593	1.1967
P	0.0057	-0.0143	0.9969
O	1.6895	0.7597	-1.5920
C	2.0353	2.2161	2.0743
O	2.2726	2.6796	3.1162
C	-1.6809	0.3557	0.3419
C	0.3260	-1.7274	0.3925
C	-0.3640	-0.2991	2.7803
C	1.1143	4.9299	-0.2236
C	-0.9158	3.2764	-1.3522
C	-0.7527	3.4910	1.5004
C	2.0826	5.3778	0.6867
C	2.7194	6.5990	0.5041
C	2.4281	7.3821	-0.6101
C	1.4991	6.9297	-1.5397
C	0.8453	5.7142	-1.3490
C	-2.0182	4.1351	-1.2676
C	-2.9495	4.1858	-2.2972
C	-2.7912	3.3803	-3.4237
C	-1.6916	2.5330	-3.5160
C	-0.7528	2.4813	-2.4873
C	0.6413	-0.1499	3.7380
C	0.3766	-0.4043	5.0807
C	-0.8922	-0.8158	5.4786
C	-1.8935	-0.9847	4.5249
C	-1.6327	-0.7293	3.1830
C	0.5820	-2.7738	1.2819
C	0.9331	-4.0344	0.8059

C	1.0337	-4.2693	-0.5612
C	0.7732	-3.2338	-1.4559
C	0.4285	-1.9732	-0.9826
C	-2.3449	-0.5020	-0.5363
C	-3.6144	-0.2191	-1.0610
C	-4.2069	0.9452	-0.6385
C	-3.5778	1.7869	0.2678
C	-2.3116	1.5553	0.7671
C	-1.7812	2.5380	1.7467
C	-2.4351	2.6541	2.9571
C	-2.1256	3.6237	3.9035
C	-1.1629	4.5724	3.6660
C	-0.4830	4.4817	2.4427
O	-3.5034	1.9132	3.3932
C	-3.6343	2.2470	4.7854
O	-2.9683	3.5098	4.9769
O	-5.4095	1.4801	-1.0147
C	-5.6258	2.5890	-0.1206
O	-4.3662	2.8800	0.5093
C	2.5563	0.0969	-2.1853
H	3.4033	-0.3364	-1.6378
C	2.3344	-0.3122	-3.6132
C	4.3015	2.0678	-1.3679
C	4.0387	2.2875	-2.6740
O	2.9947	3.0881	-3.0466
C	3.0675	3.5832	-4.3864
H	2.3647	4.7625	1.5358
H	3.4602	6.9279	1.2272
H	2.9345	8.3317	-0.7583
H	1.2766	7.5223	-2.4228
H	0.1280	5.3806	-2.0906
H	-2.1545	4.7583	-0.3875
H	-3.8040	4.8521	-2.2161
H	-3.5244	3.4140	-4.2248

H	-1.5620	1.9025	-4.3915
H	0.1007	1.8170	-2.5575
H	1.6405	0.1402	3.4326
H	1.1684	-0.2816	5.8140
H	-1.0986	-1.0119	6.5273
H	-2.8841	-1.3162	4.8247
H	-2.4225	-0.8612	2.4494
H	0.5218	-2.6075	2.3525
H	1.1352	-4.8339	1.5130
H	1.3115	-5.2532	-0.9286
H	0.8380	-3.4065	-2.5271
H	0.2222	-1.1751	-1.6867
H	-1.8853	-1.4404	-0.8184
H	-4.1030	-0.8945	-1.7550
H	-0.9361	5.3549	4.3818
H	0.2809	5.2215	2.2403
H	-4.6922	2.3517	5.0363
H	-3.1305	1.4767	5.3896
H	-5.9550	3.4592	-0.6950
H	-6.3575	2.2985	0.6475
H	2.2929	0.5825	-4.2483
H	1.3379	-0.7719	-3.6784
H	5.1028	1.3621	-1.1602
H	4.6196	1.8433	-3.4807
H	3.8705	4.3255	-4.4824
H	3.2419	2.7680	-5.1020
H	2.1055	4.0550	-4.5985
H	3.2110	3.6606	-0.5394
H	4.2089	2.7382	0.6294
C	3.3736	-1.2926	-4.1170
O	4.6183	-0.6060	-4.2181
C	5.7112	-1.4815	-4.5195
C	5.5911	-2.1095	-5.8859
C	5.4709	-3.4907	-6.0348
C	5.3393	-4.0585	-7.3009
C	5.3191	-3.2448	-8.4293

C	5.4330	-1.8617	-8.2883
C	5.5695	-1.2990	-7.0248
H	3.0723	-1.7012	-5.0936
H	3.4684	-2.1384	-3.4123
H	6.6046	-0.8499	-4.4625
H	5.7894	-2.2641	-3.7485
H	5.4794	-4.1264	-5.1521
H	5.2486	-5.1362	-7.4046
H	5.2158	-3.6848	-9.4172
H	5.4213	-1.2235	-9.1676
H	5.6587	-0.2208	-6.9130

TS - Cis Re Re

Ru	1.8347	1.5170	0.5038
C	3.6534	2.8137	-0.1973
P	0.3426	3.2510	0.0935
I	3.7794	-0.4124	1.3086
P	0.1322	-0.0066	1.1063
O	1.7560	0.8318	-1.4916
C	2.0772	2.2193	2.1683
O	2.3085	2.6929	3.2067
C	-1.5066	0.3033	0.3209
C	0.4927	-1.7613	0.6509
C	-0.3114	-0.1822	2.8835
C	1.1394	4.9112	-0.0926
C	-0.8541	3.2690	-1.3093
C	-0.7982	3.4403	1.5333
C	2.0267	5.3815	0.8867
C	2.6800	6.5971	0.7286
C	2.4884	7.3525	-0.4260
C	1.6438	6.8760	-1.4215
C	0.9727	5.6659	-1.2575
C	-1.9103	4.1881	-1.2776
C	-2.8199	4.2455	-2.3258
C	-2.6907	3.3811	-3.4119

C	-1.6392	2.4710	-3.4476	H	3.3561	6.9442	1.5047
C	-0.7166	2.4160	-2.4046	H	3.0081	8.2978	-0.5536
C	0.6763	-0.0566	3.8628	H	1.5021	7.4441	-2.3365
C	0.3674	-0.2713	5.2026	H	0.3251	5.3113	-2.0518
C	-0.9263	-0.6251	5.5755	H	-2.0272	4.8532	-0.4257
C	-1.9083	-0.7771	4.5995	H	-3.6352	4.9631	-2.2906
C	-1.6044	-0.5584	3.2602	H	-3.4093	3.4187	-4.2261
C	0.5003	-2.7798	1.6066	H	-1.5339	1.7935	-4.2907
C	0.8373	-4.0819	1.2439	H	0.1044	1.7076	-2.4262
C	1.1637	-4.3854	-0.0731	H	1.6958	0.1800	3.5780
C	1.1507	-3.3758	-1.0329	H	1.1450	-0.1667	5.9537
C	0.8262	-2.0746	-0.6717	H	-1.1658	-0.7932	6.6220
C	-2.0225	-0.5625	-0.6431	H	-2.9162	-1.0730	4.8785
C	-3.2378	-0.3272	-1.3011	H	-2.3776	-0.6823	2.5083
C	-3.9303	0.7977	-0.9269	H	0.2583	-2.5649	2.6418
C	-3.4484	1.6496	0.0569	H	0.8481	-4.8599	2.0019
C	-2.2337	1.4682	0.6882	H	1.4298	-5.4015	-0.3505
C	-1.8332	2.4775	1.7006	H	1.4022	-3.5986	-2.0665
C	-2.6026	2.6080	2.8397	H	0.8307	-1.2899	-1.4179
C	-2.3926	3.5981	3.7916	H	-1.4797	-1.4642	-0.8966
C	-1.4137	4.5472	3.6341	H	-3.6107	-1.0058	-2.0604
C	-0.6214	4.4457	2.4814	H	-1.2615	5.3423	4.3557
O	-3.6958	1.8588	3.1899	H	0.1445	5.1965	2.3353
C	-3.9819	2.2340	4.5489	H	-5.0610	2.3498	4.6742
O	-3.3332	3.4986	4.7813	H	-3.5565	1.4807	5.2288
O	-5.1125	1.2741	-1.4207	H	-5.6656	3.2682	-1.2344
C	-5.4538	2.4052	-0.5951	H	-6.3097	2.1443	0.0428
O	-4.3136	2.6935	0.2336	H	2.2606	0.6926	-4.2186
C	2.7231	0.2970	-2.1439	H	1.4206	-0.6683	-3.5049
H	3.4679	-0.3034	-1.6030	H	5.0688	1.3242	-0.8632
C	2.3992	-0.1679	-3.5520	H	4.6102	1.4955	-3.2393
C	4.3201	2.0482	-1.1773	H	4.2472	4.0365	-4.2641
C	3.9622	1.9784	-2.5102	H	3.5720	2.5588	-5.0127
O	3.0435	2.8785	-3.0090	H	2.5023	3.9466	-4.6525
C	3.3692	3.3777	-4.3083	H	3.1958	3.7234	-0.5716
H	2.2376	4.7881	1.7704	H	4.2039	2.9359	0.7341

C	3.3932	-1.1546	-4.1299
O	4.6177	-0.4791	-4.4193
C	5.6434	-1.3661	-4.8751
C	5.3245	-1.9903	-6.2118
C	5.2504	-3.3747	-6.3606
C	4.9471	-3.9396	-7.5983
C	4.7063	-3.1204	-8.6967
C	4.7720	-1.7343	-8.5543
C	5.0808	-1.1741	-7.3203
H	2.9837	-1.6080	-5.0460
H	3.5824	-1.9685	-3.4069
H	6.5444	-0.7465	-4.9479
H	5.8243	-2.1523	-4.1249
H	5.4305	-4.0158	-5.5004
H	4.8937	-5.0198	-7.7021
H	4.4677	-3.5582	-9.6619
H	4.5869	-1.0912	-9.4103
H	5.1314	-0.0936	-7.2072

Post - Cis Re Re

Ru	2.0183	1.3552	0.5650
C	3.7670	2.9459	-0.2787
P	0.4985	3.0954	0.1615
I	3.8891	-0.6302	1.5724
P	0.2940	-0.0586	1.2901
O	1.6872	0.4014	-1.2589
C	2.3754	2.1178	2.2061
O	2.6700	2.6065	3.2195
C	-1.2585	0.1804	0.3292
C	0.5916	-1.8788	1.1121
C	-0.2167	0.0361	3.0522
C	1.2773	4.7766	0.0546
C	-0.6194	3.1351	-1.3005
C	-0.7307	3.2580	1.5347
C	2.0974	5.2599	1.0845

C	2.7419	6.4850	0.9656
C	2.6075	7.2414	-0.1959
C	1.8262	6.7561	-1.2377
C	1.1650	5.5358	-1.1152
C	-1.6656	4.0667	-1.3262
C	-2.4955	4.1494	-2.4362
C	-2.3007	3.2931	-3.5204
C	-1.2626	2.3677	-3.4927
C	-0.4134	2.2905	-2.3902
C	0.7654	0.1510	4.0390
C	0.4110	0.1443	5.3842
C	-0.9238	0.0124	5.7569
C	-1.9016	-0.1395	4.7777
C	-1.5502	-0.1363	3.4321
C	0.1537	-2.7699	2.0950
C	0.3511	-4.1403	1.9370
C	0.9775	-4.6345	0.7984
C	1.4136	-3.7486	-0.1841
C	1.2308	-2.3810	-0.0256
C	-1.5840	-0.7392	-0.6683
C	-2.7196	-0.6066	-1.4774
C	-3.5277	0.4754	-1.2284
C	-3.2286	1.3909	-0.2298
C	-2.0921	1.3120	0.5515
C	-1.8442	2.3727	1.5528
C	-2.7682	2.5787	2.5583
C	-2.6069	3.5338	3.5529
C	-1.5206	4.3733	3.5720
C	-0.5962	4.2259	2.5283
O	-3.8999	1.8468	2.8012
C	-4.5841	2.5481	3.8544
O	-3.6286	3.4404	4.4578
O	-4.6902	0.8258	-1.8536
C	-5.0983	2.0759	-1.2632
O	-4.1932	2.3592	-0.1813
C	2.7875	0.0856	-2.0557

H	3.4491	-0.6650	-1.5705
C	2.2941	-0.5047	-3.3831
C	4.1145	1.7761	-0.8680
C	3.6653	1.3439	-2.2261
O	2.9193	2.3436	-2.9083
C	3.7461	3.2659	-3.6089
H	2.2686	4.6731	1.9796
H	3.3651	6.8398	1.7816
H	3.1200	8.1944	-0.2914
H	1.7273	7.3240	-2.1584
H	0.5734	5.1740	-1.9484
H	-1.8309	4.7278	-0.4790
H	-3.2987	4.8814	-2.4528
H	-2.9576	3.3520	-4.3844
H	-1.1084	1.6964	-4.3333
H	0.3965	1.5677	-2.3466
H	1.8120	0.2159	3.7608
H	1.1845	0.2392	6.1406
H	-1.1995	0.0139	6.8078
H	-2.9436	-0.2669	5.0581
H	-2.3190	-0.2768	2.6795
H	-0.3331	-2.4092	2.9942
H	0.0136	-4.8195	2.7148
H	1.1314	-5.7035	0.6796
H	1.9134	-4.1211	-1.0741
H	1.5779	-1.6788	-0.7742
H	-0.9434	-1.5966	-0.8323
H	-2.9470	-1.3265	-2.2558
H	-1.3861	5.1225	4.3443
H	0.2310	4.9220	2.4984
H	-5.4080	3.1361	3.4237
H	-4.9343	1.8314	4.6013
H	-5.0251	2.8710	-2.0165
H	-6.1150	1.9753	-0.8678
H	1.7375	0.2573	-3.9427
H	1.5826	-1.3021	-3.1313

H	4.8246	1.1133	-0.3809
H	4.5547	1.0648	-2.8165
H	4.4515	3.7764	-2.9361
H	4.3137	2.7584	-4.4029
H	3.0825	4.0105	-4.0577
H	3.2034	3.6811	-0.8370
H	4.2432	3.2672	0.6423
C	3.3710	-1.1017	-4.2690
O	4.1024	-0.0478	-4.9087
C	5.2108	-0.5305	-5.6650
C	4.7996	-1.3618	-6.8576
C	5.3186	-2.6405	-7.0553
C	4.9379	-3.3976	-8.1622
C	4.0242	-2.8827	-9.0763
C	3.4941	-1.6073	-8.8804
C	3.8813	-0.8516	-7.7799
H	2.9160	-1.7512	-5.0329
H	4.0658	-1.7225	-3.6743
H	5.7452	0.3677	-5.9983
H	5.8899	-1.1138	-5.0214
H	6.0245	-3.0490	-6.3353
H	5.3498	-4.3927	-8.3051
H	3.7224	-3.4721	-9.9375
H	2.7795	-1.2014	-9.5913
H	3.4656	0.1407	-7.6225

Pre - Cis Re Si

Ru	4.4219	-3.4146	-0.7873
C	6.0275	-4.7224	-1.5915
P	5.8416	-1.5852	-0.6631
I	2.8213	-5.7397	-0.6643
P	2.4766	-2.1016	-0.1537
O	3.8120	-3.1392	-2.8514
C	4.9636	-3.8461	0.8887
O	5.3388	-4.1831	1.9381

C	2.5548	-0.3155	-0.6182	O	3.2954	1.5705	2.7200
C	0.8639	-2.6476	-0.8816	C	3.6276	1.9909	4.0555
C	2.0551	-2.0337	1.6370	O	4.7079	1.1564	4.5134
C	7.6465	-2.0025	-0.7025	O	3.0272	3.6515	-1.6433
C	5.7741	-0.1665	-1.8409	C	3.9627	4.0283	-0.6148
C	5.5988	-0.7030	0.9451	O	4.3709	2.8251	0.0598
C	8.4946	-1.4831	-1.6868	C	3.7356	-4.0651	-3.6693
C	9.8303	-1.8714	-1.7536	H	3.8766	-5.1050	-3.3517
C	10.3441	-2.7846	-0.8400	C	3.2848	-3.8257	-5.0676
C	9.5060	-3.3244	0.1316	C	6.4707	-4.3392	-2.9372
C	8.1686	-2.9502	0.1899	C	6.3610	-5.0530	-4.0735
C	6.4943	0.9983	-1.5498	O	5.7957	-6.3027	-4.1055
C	6.4554	2.0797	-2.4209	C	6.0002	-7.0106	-5.3297
C	5.6862	2.0171	-3.5823	H	8.1171	-0.7754	-2.4166
C	4.9664	0.8628	-3.8719	H	10.4678	-1.4557	-2.5289
C	5.0150	-0.2285	-3.0077	H	11.3868	-3.0848	-0.8915
C	2.2588	-3.1648	2.4321	H	9.8864	-4.0545	0.8400
C	1.8989	-3.1523	3.7758	H	7.5311	-3.4172	0.9332
C	1.3302	-2.0126	4.3384	H	7.0780	1.0629	-0.6348
C	1.1049	-0.8907	3.5449	H	7.0180	2.9791	-2.1858
C	1.4581	-0.9024	2.1996	H	5.6433	2.8705	-4.2536
C	0.7345	-2.7956	-2.2686	H	4.3474	0.8127	-4.7644
C	-0.4503	-3.2591	-2.8266	H	4.4384	-1.1195	-3.2188
C	-1.5257	-3.5982	-2.0092	H	2.6746	-4.0670	1.9955
C	-1.4060	-3.4580	-0.6314	H	2.0645	-4.0382	4.3820
C	-0.2224	-2.9841	-0.0701	H	1.0561	-2.0017	5.3897
C	1.7281	0.2095	-1.6128	H	0.6485	-0.0015	3.9712
C	1.8060	1.5424	-2.0403	H	1.2750	-0.0233	1.5895
C	2.7266	2.3376	-1.4052	H	1.5633	-2.5426	-2.9194
C	3.5351	1.8409	-0.3938	H	-0.5296	-3.3656	-3.9052
C	3.5164	0.5212	0.0140	H	-2.4478	-3.9733	-2.4443
C	4.4549	0.1313	1.0968	H	-2.2352	-3.7228	0.0186
C	4.2980	0.7213	2.3360	H	-0.1498	-2.8912	1.0081
C	5.1508	0.4870	3.4056	H	0.9791	-0.4201	-2.0775
C	6.2541	-0.3199	3.2788	H	1.1688	1.9159	-2.8340
C	6.4650	-0.8988	2.0192	H	6.9352	-0.4972	4.1038

H	7.3506	-1.5072	1.8932
H	3.9612	3.0382	4.0334
H	2.7598	1.8498	4.7072
H	4.8365	4.5001	-1.0755
H	3.4650	4.6959	0.1028
H	3.8470	-4.4847	-5.7408
H	2.2394	-4.1780	-5.1135
H	6.9391	-3.3633	-3.0653
H	6.7281	-4.6770	-5.0296
H	7.0659	-7.2239	-5.4862
H	5.4499	-7.9493	-5.2438
H	5.6150	-6.4400	-6.1863
H	6.8592	-4.6344	-0.8897
H	5.6474	-5.7460	-1.5639
C	3.3553	-2.3757	-5.5016
O	2.7090	-2.2690	-6.7670
C	2.5710	-0.9183	-7.1896
C	1.5603	-0.1261	-6.3866
C	1.6457	1.2666	-6.3406
C	0.6816	2.0130	-5.6690
C	-0.3668	1.3714	-5.0131
C	-0.4426	-0.0193	-5.0325
C	0.5107	-0.7625	-5.7226
H	4.4051	-2.0451	-5.5801
H	2.8569	-1.7326	-4.7612
H	3.5471	-0.4046	-7.1701
H	2.2474	-0.9714	-8.2368
H	2.4683	1.7724	-6.8427
H	0.7554	3.0970	-5.6480
H	-1.1160	1.9518	-4.4816
H	-1.2483	-0.5289	-4.5108
H	0.4470	-1.8471	-5.7494

TS - Cis Re Si

Ru	4.4192	-3.4510	-0.8784
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C	6.1205	-4.8177	-1.7175
P	5.8498	-1.6292	-0.6456
I	2.8542	-5.8062	-0.8124
P	2.5196	-2.1992	-0.2042
O	3.8297	-3.0262	-2.8846
C	4.9433	-3.9717	0.7889
O	5.3001	-4.3622	1.8251
C	2.6202	-0.4317	-0.7230
C	0.8751	-2.7263	-0.8783
C	2.1448	-2.1182	1.5926
C	7.6467	-2.0907	-0.6099
C	5.8855	-0.2047	-1.8151
C	5.5574	-0.7508	0.9548
C	8.5367	-1.5916	-1.5676
C	9.8685	-1.9993	-1.5843
C	10.3380	-2.9094	-0.6447
C	9.4588	-3.4280	0.3018
C	8.1253	-3.0359	0.3097
C	6.5781	0.9577	-1.4552
C	6.6377	2.0333	-2.3319
C	5.9983	1.9650	-3.5693
C	5.3127	0.8097	-3.9293
C	5.2616	-0.2772	-3.0591
C	2.3043	-3.2663	2.3730
C	1.9597	-3.2507	3.7207
C	1.4485	-2.0925	4.3002
C	1.2618	-0.9548	3.5196
C	1.5997	-0.9689	2.1706
C	0.7351	-3.0123	-2.2411
C	-0.4923	-3.4003	-2.7627
C	-1.6006	-3.5259	-1.9287
C	-1.4689	-3.2527	-0.5719
C	-0.2413	-2.8525	-0.0478
C	1.8644	0.0200	-1.8058
C	1.9531	1.3277	-2.3010
C	2.8008	2.1784	-1.6361

C	3.5418	1.7547	-0.5427	H	-0.5785	-3.6183	-3.8240
C	3.5258	0.4548	-0.0746	H	-2.5580	-3.8421	-2.3333
C	4.4319	0.1160	1.0491	H	-2.3232	-3.3539	0.0914
C	4.2642	0.7587	2.2599	H	-0.1639	-2.6506	1.0148
C	5.0833	0.5364	3.3586	H	1.1690	-0.6510	-2.2951
C	6.1591	-0.3138	3.2922	H	1.3731	1.6423	-3.1617
C	6.3873	-0.9398	2.0582	H	6.8092	-0.4865	4.1427
O	3.2675	1.6351	2.5961	H	7.2604	-1.5731	1.9749
C	3.6104	2.1230	3.9056	H	4.0153	3.1419	3.8187
O	4.6268	1.2504	4.4328	H	2.7283	2.0838	4.5507
O	3.0900	3.4846	-1.9206	H	4.8637	4.3725	-1.3032
C	3.9616	3.9324	-0.8652	H	3.4234	4.6470	-0.2271
O	4.3247	2.7789	-0.0852	H	3.6315	-4.3286	-5.8630
C	3.8013	-3.9561	-3.7612	H	2.1398	-3.8909	-5.0477
H	3.6842	-4.9924	-3.4249	H	6.8080	-3.2749	-3.0448
C	3.2145	-3.6489	-5.1115	H	6.0762	-4.1865	-5.1218
C	6.3277	-4.2543	-2.9962	H	7.2550	-6.8971	-4.3263
C	5.7983	-4.6935	-4.1935	H	5.9201	-7.8262	-5.0790
O	5.3635	-6.0067	-4.3551	H	6.6489	-6.4427	-5.9491
C	6.3611	-6.8332	-4.9620	H	6.9067	-4.6224	-0.9953
H	8.1973	-0.8810	-2.3131	H	5.7371	-5.8360	-1.6952
H	10.5379	-1.5990	-2.3405	C	3.3611	-2.2003	-5.5282
H	11.3778	-3.2232	-0.6562	O	2.6527	-2.0266	-6.7568
H	9.8040	-4.1547	1.0314	C	2.4470	-0.6620	-7.0823
H	7.4582	-3.4901	1.0341	C	1.3656	0.0118	-6.2606
H	7.0646	1.0236	-0.4852	C	1.2485	1.4038	-6.2874
H	7.1783	2.9311	-2.0442	C	0.2192	2.0414	-5.6018
H	6.0335	2.8131	-4.2477	C	-0.6928	1.2947	-4.8573
H	4.8037	0.7536	-4.8883	C	-0.5676	-0.0911	-4.8084
H	4.7149	-1.1743	-3.3243	C	0.4500	-0.7293	-5.5138
H	2.6719	-4.1832	1.9235	H	4.4240	-1.9350	-5.6667
H	2.0909	-4.1494	4.3163	H	2.9471	-1.5416	-4.7500
H	1.1864	-2.0801	5.3545	H	3.3888	-0.0934	-6.9938
H	0.8468	-0.0514	3.9579	H	2.1567	-0.6475	-8.1409
H	1.4386	-0.0801	1.5688	H	1.9641	1.9929	-6.8582
H	1.5961	-2.9304	-2.8922	H	0.1353	3.1242	-5.6383

H	-1.4897	1.7917	-4.3113
H	-1.2642	-0.6821	-4.2193
H	0.5365	-1.8119	-5.4891

Post - Cis Re Si

Ru	4.3677	-3.5050	-0.9123
C	5.9404	-5.2932	-1.7356
P	5.8272	-1.7134	-0.6366
I	2.6462	-5.8386	-0.7416
P	2.5267	-2.2230	-0.2208
O	3.6680	-3.0649	-2.8303
C	4.8467	-4.0578	0.7851
O	5.1465	-4.4683	1.8298
C	2.6877	-0.4786	-0.7810
C	0.8565	-2.6866	-0.8774
C	2.1808	-2.1302	1.5802
C	7.6064	-2.2383	-0.5365
C	5.9100	-0.3317	-1.8442
C	5.5338	-0.8119	0.9436
C	8.5764	-1.6744	-1.3742
C	9.8928	-2.1271	-1.3437
C	10.2673	-3.1488	-0.4783
C	9.3098	-3.7248	0.3512
C	7.9916	-3.2829	0.3157
C	6.6038	0.8408	-1.5197
C	6.6877	1.8745	-2.4435
C	6.0722	1.7523	-3.6894
C	5.3788	0.5896	-4.0085
C	5.2993	-0.4563	-3.0911
C	2.2322	-3.3026	2.3389
C	1.8969	-3.2785	3.6884
C	1.5004	-2.0882	4.2919
C	1.4165	-0.9246	3.5324
C	1.7467	-0.9459	2.1815
C	0.7121	-3.2263	-2.1587

C	-0.5514	-3.5122	-2.6618
C	-1.6869	-3.2727	-1.8923
C	-1.5487	-2.7410	-0.6146
C	-0.2851	-2.4470	-0.1068
C	1.9696	-0.0791	-1.9087
C	2.0663	1.2082	-2.4508
C	2.8827	2.0909	-1.7874
C	3.5924	1.7169	-0.6546
C	3.5704	0.4357	-0.1385
C	4.4615	0.1209	1.0008
C	4.3236	0.8077	2.1907
C	5.1173	0.5621	3.3039
C	6.1314	-0.3642	3.2771
C	6.3345	-1.0341	2.0627
O	3.3667	1.7359	2.5020
C	3.7439	2.2506	3.7920
O	4.6898	1.3237	4.3564
O	3.1759	3.3846	-2.1162
C	4.0133	3.8807	-1.0548
O	4.3633	2.7603	-0.2218
C	3.9502	-4.0501	-3.7818
H	3.6222	-5.0547	-3.4474
C	3.2098	-3.7529	-5.0914
C	6.1486	-4.2569	-2.5920
C	5.4767	-4.1553	-3.9498
O	5.7412	-5.3069	-4.7527
C	7.1066	-5.4196	-5.1374
H	8.3097	-0.8877	-2.0704
H	10.6250	-1.6767	-2.0077
H	11.2947	-3.5006	-0.4562
H	9.5824	-4.5302	1.0270
H	7.2697	-3.7669	0.9622
H	7.0706	0.9477	-0.5436
H	7.2283	2.7816	-2.1870
H	6.1289	2.5678	-4.4054
H	4.8827	0.4957	-4.9710

H	4.7276	-1.3572	-3.3034
H	2.5071	-4.2431	1.8716
H	1.9444	-4.1967	4.2665
H	1.2447	-2.0705	5.3477
H	1.0866	0.0054	3.9872
H	1.6537	-0.0374	1.5958
H	1.6043	-3.4115	-2.7460
H	-0.6448	-3.9360	-3.6582
H	-2.6735	-3.5053	-2.2838
H	-2.4254	-2.5570	-0.0001
H	-0.2035	-2.0421	0.8961
H	1.3055	-0.7810	-2.3988
H	1.5188	1.4829	-3.3460
H	6.7524	-0.5615	4.1438
H	7.1613	-1.7309	2.0037
H	4.2275	3.2302	3.6641
H	2.8613	2.3060	4.4343
H	4.9237	4.3120	-1.4838
H	3.4510	4.6137	-0.4600
H	3.5902	-4.4141	-5.8796
H	2.1477	-3.9961	-4.9535
H	6.9679	-3.5722	-2.3967
H	5.8638	-3.2580	-4.4628
H	7.7610	-5.5864	-4.2689
H	7.1793	-6.2795	-5.8079
H	7.4452	-4.5167	-5.6691
H	6.5861	-5.4366	-0.8741
H	5.2642	-6.1036	-1.9860
C	3.3009	-2.3041	-5.5325
O	2.4895	-2.1533	-6.7057
C	2.2412	-0.7996	-7.0329
C	1.1839	-0.1343	-6.1726
C	0.9845	1.2452	-6.2768
C	-0.0259	1.8725	-5.5548
C	-0.8381	1.1295	-4.6989
C	-0.6320	-0.2418	-4.5762

C	0.3678	-0.8713	-5.3150
H	4.3383	-2.0113	-5.7709
H	2.9382	-1.6440	-4.7317
H	3.1736	-0.2089	-6.9941
H	1.9016	-0.7971	-8.0774
H	1.6205	1.8318	-6.9377
H	-0.1741	2.9447	-5.6523
H	-1.6205	1.6188	-4.1256
H	-1.2484	-0.8303	-3.9011
H	0.5185	-1.9435	-5.2277

Pre - Cis Si Re

Ru	0.6490	1.5677	-0.3193
C	-0.6380	0.3541	-1.7259
P	0.0576	0.2855	1.5345
I	0.9969	3.2820	-2.5673
P	2.1611	2.9430	0.9351
O	2.1749	0.1359	-0.8814
C	-0.8175	2.5678	0.0089
O	-1.8004	3.1736	0.1623
C	2.9059	2.1684	2.4328
C	3.6382	3.4908	-0.0275
C	1.5499	4.5476	1.6025
C	-1.4116	-0.8134	1.2968
C	1.2132	-0.8475	2.4257
C	-0.4299	1.4142	2.9164
C	-2.6093	-0.2834	0.7946
C	-3.7049	-1.1037	0.5548
C	-3.6158	-2.4754	0.7771
C	-2.4194	-3.0177	1.2321
C	-1.3256	-2.1949	1.4900
C	0.8282	-1.3203	3.6867
C	1.6592	-2.1747	4.3997
C	2.8908	-2.5555	3.8698
C	3.2761	-2.0886	2.6175

C	2.4391	-1.2431	1.8920	H	-4.4691	-3.1180	0.5797
C	0.5928	5.2781	0.8942	H	-2.3293	-4.0891	1.3881
C	0.1784	6.5243	1.3549	H	-0.4000	-2.6425	1.8346
C	0.7225	7.0572	2.5202	H	-0.1214	-1.0106	4.1156
C	1.6943	6.3430	3.2170	H	1.3470	-2.5367	5.3756
C	2.1074	5.0954	2.7621	H	3.5471	-3.2131	4.4334
C	4.4312	2.5289	-0.6624	H	4.2370	-2.3772	2.2004
C	5.5177	2.9078	-1.4405	H	2.7386	-0.8755	0.9182
C	5.8182	4.2574	-1.6130	H	0.1887	4.8886	-0.0342
C	5.0314	5.2196	-0.9901	H	-0.5691	7.0794	0.7955
C	3.9500	4.8412	-0.1977	H	0.3982	8.0305	2.8785
C	4.2684	1.8784	2.5040	H	2.1387	6.7589	4.1175
C	4.8500	1.2389	3.6082	H	2.8660	4.5481	3.3132
C	4.0107	0.9274	4.6490	H	4.1912	1.4770	-0.5445
C	2.6599	1.2416	4.6079	H	6.1286	2.1484	-1.9215
C	2.0519	1.8349	3.5191	H	6.6596	4.5548	-2.2325
C	0.5955	2.1116	3.6170	H	5.2527	6.2750	-1.1221
C	0.1679	3.0151	4.5699	H	3.3433	5.6073	0.2733
C	-1.1723	3.2615	4.8419	H	4.9189	2.1638	1.6867
C	-2.1714	2.5802	4.1933	H	5.9101	1.0113	3.6372
C	-1.7680	1.6505	3.2243	H	-3.2195	2.7423	4.4193
O	0.9510	3.7487	5.4235	H	-2.5436	1.0968	2.7119
C	0.0508	4.6891	6.0346	H	0.2755	4.7664	7.1010
O	-1.2809	4.1694	5.8608	H	0.1309	5.6560	5.5152
O	4.3106	0.2969	5.8239	H	2.8366	-0.7549	6.8440
C	3.0891	0.2808	6.5898	H	3.2126	0.9052	7.4841
O	2.0508	0.8350	5.7621	H	2.7625	1.2183	-3.2412
C	2.6701	-0.4276	-1.8724	H	4.2827	0.5426	-2.7061
H	2.9573	-1.4915	-1.7577	H	0.3288	0.1788	-3.6913
C	3.2713	0.2676	-3.0518	H	1.0292	-2.1207	-3.5181
C	0.0898	-0.3422	-2.7702	H	1.8031	-3.7900	-1.8515
C	0.5391	-1.6155	-2.6875	H	0.5131	-4.1701	-0.6742
O	0.3076	-2.3553	-1.5601	H	0.1707	-4.2519	-2.4273
C	0.7261	-3.7178	-1.6451	H	-1.2967	1.1133	-2.1531
H	-2.6873	0.7739	0.5606	H	-1.1963	-0.3425	-1.1056
H	-4.6239	-0.6683	0.1732	C	3.4630	-0.5890	-4.3042

O	2.3414	-0.6352	-5.1838
C	2.0120	0.6256	-5.7984
C	3.1790	1.2732	-6.4974
C	3.7647	0.6649	-7.6114
C	4.8607	1.2478	-8.2375
C	5.3831	2.4488	-7.7574
C	4.8047	3.0613	-6.6496
C	3.7087	2.4734	-6.0211
H	3.6489	-1.6335	-4.0210
H	4.3474	-0.2301	-4.8493
H	1.2201	0.3769	-6.5133
H	1.5949	1.3244	-5.0580
H	3.3562	-0.2721	-7.9837
H	5.3062	0.7703	-9.1060
H	6.2370	2.9058	-8.2497
H	5.2059	3.9979	-6.2721
H	3.2563	2.9491	-5.1525

TS - Cis Si Re

Ru	0.6520	1.6033	-0.3510
C	-0.6587	0.3337	-1.7801
P	0.0334	0.3320	1.5065
I	0.9887	3.2923	-2.6295
P	2.1069	2.9865	0.9019
O	2.1959	0.2114	-0.8370
C	-0.8181	2.6194	-0.0532
O	-1.8022	3.2285	0.0775
C	2.8782	2.1633	2.3576
C	3.5688	3.6054	-0.0438
C	1.4628	4.5572	1.6097
C	-1.4694	-0.7200	1.2578
C	1.1535	-0.8482	2.3795
C	-0.4271	1.4506	2.9059
C	-2.6536	-0.1519	0.7654
C	-3.7734	-0.9380	0.5236

C	-3.7239	-2.3133	0.7366
C	-2.5426	-2.8930	1.1843
C	-1.4241	-2.1045	1.4433
C	0.7643	-1.3157	3.6412
C	1.5624	-2.2195	4.3304
C	2.7659	-2.6538	3.7768
C	3.1547	-2.1911	2.5238
C	2.3496	-1.2972	1.8201
C	0.5408	5.3136	0.8821
C	0.1177	6.5505	1.3588
C	0.6202	7.0489	2.5575
C	1.5603	6.3103	3.2720
C	1.9818	5.0712	2.8015
C	4.3047	2.6998	-0.8131
C	5.3952	3.1270	-1.5592
C	5.7582	4.4722	-1.5587
C	5.0285	5.3796	-0.7988
C	3.9404	4.9512	-0.0410
C	4.2338	1.8350	2.3547
C	4.8495	1.1551	3.4150
C	4.0524	0.8413	4.4880
C	2.7083	1.1850	4.5173
C	2.0648	1.8171	3.4716
C	0.6161	2.1032	3.6228
C	0.2138	2.9688	4.6210
C	-1.1193	3.2236	4.9174
C	-2.1362	2.5933	4.2452
C	-1.7583	1.6984	3.2341
O	1.0177	3.6585	5.4906
C	0.1378	4.5663	6.1774
O	-1.2050	4.0878	5.9749
O	4.3959	0.1894	5.6382
C	3.1947	0.1207	6.4331
O	2.1467	0.7720	5.6929
C	2.5930	-0.4453	-1.8559
H	3.0440	-1.4340	-1.6361

C	3.2334	0.2210	-3.0501
C	0.1643	-0.3280	-2.7262
C	0.8252	-1.5119	-2.4902
O	0.5018	-2.2154	-1.3538
C	1.1040	-3.5050	-1.2569
H	-2.7026	0.9086	0.5395
H	-4.6808	-0.4730	0.1494
H	-4.5964	-2.9293	0.5380
H	-2.4831	-3.9676	1.3328
H	-0.5112	-2.5810	1.7820
H	-0.1634	-0.9673	4.0880
H	1.2461	-2.5801	5.3055
H	3.3965	-3.3513	4.3216
H	4.0936	-2.5220	2.0883
H	2.6455	-0.9285	0.8444
H	0.1735	4.9525	-0.0730
H	-0.6023	7.1267	0.7849
H	0.2900	8.0157	2.9275
H	1.9772	6.7026	4.1958
H	2.7206	4.5078	3.3630
H	4.0059	1.6576	-0.8282
H	5.9554	2.4105	-2.1541
H	6.6025	4.8108	-2.1527
H	5.2990	6.4317	-0.7961
H	3.3795	5.6770	0.5380
H	4.8498	2.1188	1.5102
H	5.9031	0.8994	3.3880
H	-3.1792	2.7656	4.4867
H	-2.5486	1.1780	2.7094
H	0.3702	4.5579	7.2453
H	0.2335	5.5688	5.7351
H	2.9275	-0.9311	6.5921
H	3.3546	0.6519	7.3791
H	2.7272	1.1625	-3.2848
H	4.2380	0.5065	-2.6963
H	0.4027	0.1579	-3.6662

H	1.2870	-2.0708	-3.3027
H	2.1993	-3.4366	-1.2079
H	0.7342	-3.9516	-0.3313
H	0.8181	-4.1373	-2.1085
H	-1.2943	1.1025	-2.2174
H	-1.1824	-0.3422	-1.1120
C	3.4505	-0.6591	-4.2779
O	2.3383	-0.7360	-5.1735
C	2.0138	0.5051	-5.8283
C	3.1892	1.1421	-6.5234
C	3.7975	0.5101	-7.6116
C	4.9002	1.0847	-8.2337
C	5.4065	2.3010	-7.7753
C	4.8055	2.9370	-6.6931
C	3.7028	2.3575	-6.0686
H	3.6446	-1.6964	-3.9732
H	4.3371	-0.3050	-4.8224
H	1.2367	0.2330	-6.5510
H	1.5798	1.2243	-5.1173
H	3.4017	-0.4390	-7.9667
H	5.3637	0.5887	-9.0821
H	6.2658	2.7513	-8.2644
H	5.1943	3.8854	-6.3324
H	3.2332	2.8510	-5.2192

Post - Cis Si Re

Ru	0.6632	1.6775	-0.4662
C	-0.9360	0.3484	-1.9084
P	0.0207	0.4198	1.4010
I	1.0376	3.5250	-2.7092
P	2.0231	3.0696	0.8459
O	2.4416	0.5932	-0.7624
C	-0.8594	2.6958	-0.2479
O	-1.8496	3.2976	-0.1588
C	2.8512	2.1821	2.2282

C	3.4529	3.8527	-0.0277	C	0.3155	3.9482	6.6302
C	1.2444	4.5435	1.6184	O	-1.0243	3.9588	6.1029
C	-1.5317	-0.5701	1.1805	O	4.6323	0.1219	5.3158
C	1.1216	-0.7937	2.2455	C	3.4715	-0.0796	6.1469
C	-0.3842	1.5259	2.8353	O	2.3855	0.6556	5.5557
C	-2.7103	0.0425	0.7310	C	2.5869	-0.3820	-1.7545
C	-3.8692	-0.6986	0.5342	H	3.1971	-1.2205	-1.3538
C	-3.8691	-2.0733	0.7548	C	3.3647	0.1638	-2.9670
C	-2.6966	-2.6973	1.1652	C	0.2945	0.1521	-2.4411
C	-1.5384	-1.9537	1.3774	C	1.2125	-0.9751	-2.1199
C	0.7190	-1.3149	3.4819	O	0.6596	-1.7408	-1.0503
C	1.5130	-2.2478	4.1364	C	1.1761	-3.0622	-0.9781
C	2.7254	-2.6496	3.5766	H	-2.7276	1.1006	0.4949
C	3.1334	-2.1177	2.3573	H	-4.7699	-0.1976	0.1911
C	2.3326	-1.1963	1.6862	H	-4.7725	-2.6543	0.5930
C	0.3734	5.3263	0.8559	H	-2.6747	-3.7723	1.3204
C	-0.1599	6.4972	1.3841	H	-0.6356	-2.4652	1.6890
C	0.1768	6.9026	2.6728	H	-0.2158	-0.9918	3.9333
C	1.0712	6.1441	3.4227	H	1.1876	-2.6556	5.0898
C	1.6101	4.9749	2.8958	H	3.3506	-3.3731	4.0936
C	4.1320	3.1479	-1.0238	H	4.0855	-2.4140	1.9252
C	5.2349	3.7110	-1.6534	H	2.6391	-0.7435	0.7484
C	5.6655	4.9889	-1.3046	H	0.1325	5.0402	-0.1631
C	4.9887	5.6965	-0.3164	H	-0.8379	7.0942	0.7813
C	3.8874	5.1331	0.3245	H	-0.2459	7.8142	3.0858
C	4.2049	1.8655	2.1098	H	1.3596	6.4634	4.4204
C	4.9040	1.1568	3.0953	H	2.3253	4.4067	3.4808
C	4.1917	0.7947	4.2122	H	3.7739	2.1589	-1.2882
C	2.8480	1.1125	4.3525	H	5.7495	3.1526	-2.4310
C	2.1224	1.7735	3.3802	H	6.5213	5.4339	-1.8049
C	0.6865	2.0381	3.6211	H	5.3117	6.6965	-0.0412
C	0.3270	2.7977	4.7177	H	3.3708	5.7047	1.0878
C	-0.9877	3.1239	5.0197	H	4.7492	2.1791	1.2273
C	-2.0316	2.6694	4.2528	H	5.9544	0.9132	2.9794
C	-1.6996	1.8480	3.1661	H	-3.0628	2.9179	4.4780
O	1.1699	3.4195	5.6009	H	-2.5184	1.4351	2.5928

H	0.3546	3.2879	7.5093
H	0.6210	4.9705	6.8670
H	3.2201	-1.1483	6.1621
H	3.6713	0.3125	7.1497
H	2.8919	1.0874	-3.3233
H	4.3516	0.4638	-2.5898
H	0.6314	0.8061	-3.2393
H	1.3053	-1.6029	-3.0238
H	2.2472	-3.0773	-0.7306
H	0.6288	-3.5741	-0.1821
H	1.0217	-3.5995	-1.9262
H	-1.5823	1.1243	-2.3081
H	-1.3662	-0.3852	-1.2416
C	3.5994	-0.8137	-4.1137
O	2.4815	-0.9865	-4.9994
C	2.1513	0.1741	-5.7775
C	3.3102	0.7010	-6.5848
C	3.8818	-0.0811	-7.5924
C	4.9667	0.3919	-8.3219
C	5.4922	1.6559	-8.0532
C	4.9283	2.4408	-7.0518
C	3.8435	1.9626	-6.3191
H	3.8032	-1.8198	-3.7236
H	4.4785	-0.4995	-4.6948
H	1.3438	-0.1621	-6.4375
H	1.7539	0.9823	-5.1458
H	3.4714	-1.0671	-7.7987
H	5.4018	-0.2216	-9.1063
H	6.3381	2.0267	-8.6253
H	5.3335	3.4260	-6.8374
H	3.4045	2.5724	-5.5313

Pre - Cis Si Si

Ru	1.2252	-1.8715	0.0781
C	1.5893	-3.9579	-0.6563

P	1.1175	0.5159	0.5567
I	3.9960	-1.9013	0.7509
P	-1.0096	-1.9418	-0.4190
O	1.5852	-1.2635	-1.9527
C	0.9686	-2.6049	1.7161
O	0.8582	-3.1637	2.7342
C	-1.2979	-0.7750	-1.7915
C	-1.7901	-3.5516	-0.8921
C	-2.2829	-1.4795	0.8458
C	2.0466	1.0772	2.0467
C	1.8635	1.5800	-0.7561
C	-0.5376	1.3080	0.8208
C	2.0622	0.2717	3.1877
C	2.7151	0.6932	4.3406
C	3.3736	1.9199	4.3618
C	3.3671	2.7255	3.2269
C	2.7028	2.3109	2.0758
C	1.1712	2.6391	-1.3448
C	1.7691	3.4064	-2.3427
C	3.0718	3.1375	-2.7495
C	3.7801	2.1016	-2.1429
C	3.1810	1.3260	-1.1576
C	-1.9593	-1.2234	2.1757
C	-2.9607	-0.9371	3.1006
C	-4.2928	-0.9049	2.7040
C	-4.6232	-1.1641	1.3745
C	-3.6262	-1.4539	0.4523
C	-1.5549	-4.6207	-0.0186
C	-2.1806	-5.8456	-0.2129
C	-3.0511	-6.0234	-1.2857
C	-3.3010	-4.9629	-2.1501
C	-2.6806	-3.7309	-1.9532
C	-1.1323	-1.2090	-3.1080
C	-1.2197	-0.3379	-4.1993
C	-1.4789	0.9814	-3.9100
C	-1.6102	1.4304	-2.6030

C	-1.4802	0.6031	-1.5020	H	-3.5365	-6.9825	-1.4422
C	-1.5839	1.2003	-0.1445	H	-3.9900	-5.0867	-2.9810
C	-2.7929	1.7657	0.2096	H	-2.9142	-2.9104	-2.6233
C	-3.0219	2.3884	1.4283	H	-0.8878	-2.2488	-3.2959
C	-2.0259	2.5155	2.3632	H	-1.0798	-0.6845	-5.2178
C	-0.7828	1.9609	2.0302	H	-2.1890	3.0095	3.3148
O	-3.9324	1.7962	-0.5487	H	0.0132	2.0400	2.7603
C	-4.9590	2.3301	0.3073	H	-5.4701	3.1501	-0.2066
O	-4.3114	2.8384	1.4902	H	-5.6499	1.5245	0.5909
O	-1.5710	2.0382	-4.7768	H	-1.4678	4.0383	-4.2273
C	-2.0347	3.1392	-3.9734	H	-3.1161	3.2713	-4.1285
O	-1.7916	2.7909	-2.5996	H	1.7191	-1.2891	-4.5326
C	2.6259	-1.3311	-2.6162	H	2.5080	0.2075	-4.0427
H	3.5789	-1.6145	-2.1482	H	3.6317	-4.0954	-1.4597
C	2.6175	-0.8884	-4.0469	H	3.1073	-4.1955	-3.7917
C	2.5785	-4.0494	-1.7238	H	1.0640	-5.4282	-5.0041
C	2.3216	-4.0661	-3.0463	H	-0.1386	-4.1167	-5.1761
O	1.0441	-3.9467	-3.5303	H	1.5824	-3.8026	-5.5483
C	0.8904	-4.3500	-4.8926	H	1.9370	-4.4985	0.2277
H	1.5724	-0.6955	3.1762	H	0.6285	-4.3516	-0.9840
H	2.7219	0.0523	5.2175	C	3.8703	-1.2765	-4.8056
H	3.8953	2.2439	5.2581	O	4.9783	-0.6187	-4.1933
H	3.8810	3.6827	3.2336	C	6.2362	-1.2082	-4.5477
H	2.7001	2.9520	1.1995	C	6.3876	-2.6018	-3.9885
H	0.1678	2.8870	-1.0196	C	6.5887	-3.6999	-4.8248
H	1.2126	4.2261	-2.7895	C	6.6865	-4.9854	-4.2944
H	3.5384	3.7376	-3.5259	C	6.5767	-5.1815	-2.9209
H	4.8013	1.8866	-2.4435	C	6.3734	-4.0884	-2.0791
H	3.7435	0.5231	-0.6870	C	6.2806	-2.8073	-2.6101
H	-0.9230	-1.2234	2.4931	H	4.0099	-2.3672	-4.7715
H	-2.6921	-0.7325	4.1331	H	3.7885	-0.9783	-5.8636
H	-5.0726	-0.6818	3.4270	H	6.3588	-1.2208	-5.6428
H	-5.6620	-1.1492	1.0559	H	6.9925	-0.5378	-4.1247
H	-3.8961	-1.6567	-0.5804	H	6.6635	-3.5486	-5.8998
H	-0.8779	-4.4938	0.8228	H	6.8407	-5.8339	-4.9555
H	-1.9833	-6.6632	0.4743	H	6.6459	-6.1830	-2.5056

H	6.2791	-4.2312	-1.0059
H	6.1062	-1.9617	-1.9486

TS - Cis Si Si

Ru	1.2522	-1.7893	0.0712
C	1.6350	-4.0355	-0.5370
P	1.0946	0.5357	0.5393
I	4.0236	-1.6976	0.7550
P	-0.9801	-1.8788	-0.4789
O	1.5825	-1.3672	-1.9546
C	1.0058	-2.4542	1.7528
O	0.9173	-2.9939	2.7828
C	-1.2556	-0.6558	-1.8043
C	-1.7187	-3.4824	-1.0317
C	-2.2952	-1.5009	0.7702
C	2.0788	1.1131	1.9884
C	1.7277	1.6247	-0.8104
C	-0.5683	1.2751	0.8915
C	2.0348	0.3875	3.1825
C	2.7469	0.8164	4.2955
C	3.5266	1.9686	4.2254
C	3.5774	2.6935	3.0395
C	2.8527	2.2734	1.9265
C	1.0619	2.7959	-1.1782
C	1.5779	3.6144	-2.1801
C	2.7712	3.2807	-2.8122
C	3.4558	2.1295	-2.4273
C	2.9381	1.3061	-1.4346
C	-2.0182	-1.2853	2.1175
C	-3.0540	-1.0603	3.0209
C	-4.3745	-1.0511	2.5854
C	-4.6582	-1.2724	1.2383
C	-3.6267	-1.5003	0.3372
C	-1.5757	-4.5496	-0.1353
C	-2.1756	-5.7755	-0.3916

C	-2.9306	-5.9551	-1.5488
C	-3.0932	-4.8951	-2.4338
C	-2.4974	-3.6617	-2.1762
C	-1.0189	-1.0069	-3.1348
C	-1.1102	-0.0790	-4.1779
C	-1.4457	1.2083	-3.8281
C	-1.6425	1.5781	-2.5048
C	-1.5090	0.6952	-1.4495
C	-1.6257	1.2141	-0.0646
C	-2.8320	1.7551	0.3308
C	-3.0461	2.3157	1.5826
C	-2.0377	2.4010	2.5093
C	-0.7969	1.8682	2.1336
O	-3.9804	1.8223	-0.4105
C	-4.9976	2.3041	0.4864
O	-4.3345	2.7594	1.6829
O	-1.5495	2.3074	-4.6384
C	-2.0718	3.3489	-3.7924
O	-1.8736	2.9286	-2.4318
C	2.6160	-1.6766	-2.6556
H	3.6057	-1.6949	-2.1814
C	2.5842	-1.1822	-4.0893
C	2.6381	-3.9719	-1.5191
C	2.4348	-3.7189	-2.8684
O	1.1562	-3.8364	-3.3913
C	1.1114	-4.4948	-4.6567
H	1.4447	-0.5199	3.2484
H	2.7038	0.2389	5.2144
H	4.0956	2.2963	5.0909
H	4.1851	3.5915	2.9737
H	2.9024	2.8504	1.0087
H	0.1392	3.0809	-0.6849
H	1.0434	4.5186	-2.4586
H	3.1722	3.9182	-3.5955
H	4.3928	1.8603	-2.9064
H	3.4835	0.4177	-1.1318

H	-0.9925	-1.2645	2.4654
H	-2.8218	-0.8852	4.0675
H	-5.1812	-0.8760	3.2919
H	-5.6871	-1.2752	0.8889
H	-3.8595	-1.6756	-0.7098
H	-0.9943	-4.4178	0.7749
H	-2.0520	-6.5916	0.3144
H	-3.3971	-6.9147	-1.7531
H	-3.6958	-5.0194	-3.3293
H	-2.6672	-2.8403	-2.8633
H	-0.7066	-2.0183	-3.3688
H	-0.9073	-0.3576	-5.2063
H	-2.1885	2.8508	3.4845
H	0.0107	1.9225	2.8529
H	-5.5233	3.1438	0.0219
H	-5.6768	1.4792	0.7420
H	-1.5180	4.2739	-3.9720
H	-3.1491	3.4654	-3.9837
H	1.7038	-1.5955	-4.5965
H	2.4290	-0.0946	-4.0355
H	3.6783	-3.9376	-1.2056
H	3.2550	-3.9053	-3.5641
H	1.4236	-5.5444	-4.5664
H	0.0736	-4.4528	-4.9968
H	1.7549	-3.9920	-5.3936
H	1.9512	-4.4616	0.4132
H	0.6657	-4.3724	-0.8891
C	3.8371	-1.4676	-4.8893
O	4.9383	-0.8005	-4.2656
C	6.2005	-1.3936	-4.5893
C	6.3511	-2.7626	-3.9705
C	6.5150	-3.9017	-4.7589
C	6.6053	-5.1632	-4.1719
C	6.5291	-5.2932	-2.7884
C	6.3658	-4.1586	-1.9937
C	6.2766	-2.9022	-2.5815

H	4.0311	-2.5490	-4.9366
H	3.7233	-1.1069	-5.9250
H	6.3328	-1.4518	-5.6819
H	6.9525	-0.7050	-4.1883
H	6.5668	-3.8011	-5.8411
H	6.7296	-6.0438	-4.7962
H	6.5959	-6.2751	-2.3283
H	6.3041	-4.2510	-0.9125
H	6.1341	-2.0229	-1.9572

Post - Cis Si Si

Ru	1.4236	-1.6802	-0.0419
C	1.6619	-4.1223	-0.5066
P	1.1218	0.5998	0.5111
I	4.2007	-1.3096	0.6696
P	-0.8210	-1.8263	-0.6302
O	1.6896	-1.0846	-2.0048
C	1.2416	-2.3551	1.6681
O	1.2014	-2.8988	2.6977
C	-1.1313	-0.5383	-1.8808
C	-1.5373	-3.4162	-1.2641
C	-2.1599	-1.5713	0.6282
C	2.0878	1.1641	1.9785
C	1.6693	1.7715	-0.8016
C	-0.5753	1.2262	0.9192
C	2.0135	0.4503	3.1787
C	2.7244	0.8708	4.2951
C	3.5301	2.0051	4.2251
C	3.6069	2.7200	3.0351
C	2.8858	2.3073	1.9171
C	0.9953	2.9784	-1.0026
C	1.4509	3.8887	-1.9531
C	2.5906	3.6079	-2.6995
C	3.2806	2.4170	-2.4829
C	2.8231	1.5007	-1.5429

C	-1.9126	-1.4597	1.9932	H	4.2347	3.6039	2.9680
C	-2.9704	-1.3438	2.8925	H	2.9630	2.8734	0.9950
C	-4.2830	-1.3420	2.4346	H	0.1107	3.2174	-0.4219
C	-4.5369	-1.4597	1.0684	H	0.9110	4.8197	-2.1024
C	-3.4840	-1.5781	0.1715	H	2.9447	4.3166	-3.4432
C	-1.5367	-4.4769	-0.3471	H	4.1769	2.1906	-3.0536
C	-2.1243	-5.6934	-0.6662	H	3.3647	0.5774	-1.3785
C	-2.7351	-5.8695	-1.9066	H	-0.8947	-1.4385	2.3624
C	-2.7645	-4.8141	-2.8104	H	-2.7610	-1.2490	3.9542
C	-2.1742	-3.5915	-2.4924	H	-5.1065	-1.2522	3.1376
C	-0.8330	-0.7901	-3.2214	H	-5.5592	-1.4674	0.7002
C	-0.9574	0.1931	-4.2083	H	-3.6925	-1.6743	-0.8908
C	-1.3797	1.4345	-3.7918	H	-1.0786	-4.3470	0.6318
C	-1.6311	1.7095	-2.4557	H	-2.1101	-6.5026	0.0582
C	-1.4734	0.7698	-1.4545	H	-3.1959	-6.8203	-2.1591
C	-1.6250	1.1961	-0.0452	H	-3.2568	-4.9322	-3.7717
C	-2.8501	1.6712	0.3740	H	-2.2408	-2.7772	-3.2036
C	-3.0892	2.1411	1.6582	H	-0.4395	-1.7598	-3.5008
C	-2.0877	2.1999	2.5947	H	-0.7029	-0.0067	-5.2435
C	-0.8283	1.7330	2.1946	H	-2.2564	2.5832	3.5950
O	-3.9963	1.7452	-0.3687	H	-0.0266	1.7777	2.9202
C	-5.0330	2.1415	0.5472	H	-5.5745	2.9982	0.1343
O	-4.3918	2.5311	1.7794	H	-5.6941	1.2859	0.7401
O	-1.5221	2.5747	-4.5360	H	-1.5717	4.4924	-3.7409
C	-2.1020	3.5417	-3.6402	H	-3.1759	3.6399	-3.8587
O	-1.9327	3.0390	-2.3035	H	1.6633	-1.4536	-4.6738
C	2.6774	-1.6765	-2.7797	H	2.5676	-0.0326	-4.1426
H	3.6974	-1.4870	-2.3911	H	3.6581	-3.5259	-0.8919
C	2.6013	-1.1273	-4.2100	H	3.3232	-3.6965	-3.2803
C	2.6499	-3.6134	-1.2849	H	1.4232	-5.6261	-2.8880
C	2.5045	-3.2157	-2.7131	H	0.1732	-5.1114	-4.0534
O	1.2425	-3.5706	-3.2701	H	1.9007	-5.1017	-4.5285
C	1.1927	-4.9251	-3.7036	H	1.8941	-4.5309	0.4721
H	1.3983	-0.4396	3.2511	H	0.7107	-4.3821	-0.9492
H	2.6569	0.3022	5.2180	C	3.7566	-1.5478	-5.0964
H	4.0971	2.3268	5.0940	O	4.9714	-0.9772	-4.5913

C	6.1291	-1.7607	-4.8942
C	6.1577	-3.0390	-4.0914
C	6.0360	-4.2867	-4.7037
C	5.9972	-5.4519	-3.9387
C	6.0836	-5.3762	-2.5517
C	6.2111	-4.1330	-1.9323
C	6.2443	-2.9732	-2.6974
H	3.8371	-2.6452	-5.1247
H	3.5986	-1.2030	-6.1317
H	6.1788	-1.9843	-5.9725
H	6.9844	-1.1266	-4.6355
H	5.9645	-4.3464	-5.7879
H	5.8969	-6.4176	-4.4268
H	6.0530	-6.2823	-1.9528
H	6.2773	-4.0645	-0.8496
H	6.3218	-2.0046	-2.2087

Pre - Trans Re Re

Ru	3.9988	-2.3021	-0.7069
C	5.3886	-4.0412	-0.7598
P	5.5279	-0.9685	0.4078
I	2.0415	-4.0541	-1.7862
P	2.4151	-0.4877	-1.0204
O	4.7022	-1.8744	-2.7086
C	3.4293	-2.8668	0.9213
O	3.0864	-3.2985	1.9473
C	3.1256	1.2160	-1.0257
C	1.4903	-0.5626	-2.6190
C	1.0408	-0.3012	0.1934
C	6.9202	-1.8757	1.2257
C	6.4332	0.4202	-0.3982
C	4.6702	-0.0919	1.7906
C	8.2559	-1.5695	0.9431
C	9.2903	-2.3099	1.5097
C	9.0103	-3.3660	2.3696

C	7.6852	-3.6889	2.6481
C	6.6506	-2.9613	2.0714
C	7.0437	1.3881	0.4081
C	7.7495	2.4363	-0.1684
C	7.8503	2.5323	-1.5553
C	7.2519	1.5679	-2.3592
C	6.5480	0.5108	-1.7851
C	0.5350	-1.4197	0.8594
C	-0.5392	-1.2895	1.7352
C	-1.1229	-0.0439	1.9478
C	-0.6347	1.0717	1.2708
C	0.4408	0.9455	0.3985
C	2.1865	-0.5386	-3.8347
C	1.5126	-0.6822	-5.0417
C	0.1320	-0.8678	-5.0566
C	-0.5666	-0.8952	-3.8548
C	0.1049	-0.7416	-2.6445
C	3.0999	2.0261	-2.1613
C	3.6742	3.3051	-2.1959
C	4.2462	3.7516	-1.0304
C	4.2438	2.9739	0.1190
C	3.7270	1.6944	0.1693
C	3.7977	0.9880	1.4748
C	3.0786	1.5111	2.5312
C	3.1683	1.0278	3.8310
C	4.0276	0.0085	4.1574
C	4.7758	-0.5404	3.1059
O	2.2400	2.5955	2.5026
C	1.5683	2.5741	3.7736
O	2.3734	1.7734	4.6598
O	4.9019	4.9296	-0.7956
C	5.1250	4.9640	0.6273
O	4.8862	3.6376	1.1293
C	4.7925	-2.7470	-3.5843
H	4.3856	-3.7500	-3.4079
C	5.3163	-2.4399	-4.9452

C	6.5810	-3.8121	-1.5796	H	8.6868	-5.9829	-3.9220
C	6.8371	-4.4312	-2.7458	H	7.4764	-5.3772	-5.1010
O	7.9164	-4.0807	-3.5212	H	9.1184	-4.6673	-5.0538
C	8.3150	-5.0950	-4.4503	H	4.7980	-4.8835	-1.1335
H	8.5004	-0.7549	0.2703	H	5.6696	-4.2404	0.2756
H	10.3195	-2.0565	1.2716	C	4.5974	-3.2666	-6.0021
H	9.8183	-3.9415	2.8123	O	4.9869	-4.6246	-5.8119
H	7.4500	-4.5202	3.3065	C	4.1386	-5.5509	-6.5026
H	5.6273	-3.2539	2.2832	C	4.2119	-5.3920	-8.0002
H	6.9564	1.3269	1.4899	C	3.0962	-4.9947	-8.7363
H	8.2167	3.1838	0.4670	C	3.1815	-4.8274	-10.1174
H	8.3938	3.3582	-2.0060	C	4.3892	-5.0496	-10.7717
H	7.3267	1.6372	-3.4409	C	5.5113	-5.4415	-10.0416
H	6.0746	-0.2336	-2.4150	C	5.4217	-5.6126	-8.6652
H	0.9615	-2.3998	0.6766	H	4.8649	-2.9166	-7.0104
H	-0.9203	-2.1678	2.2482	H	3.5037	-3.1690	-5.8875
H	-1.9612	0.0565	2.6319	H	4.4961	-6.5413	-6.2004
H	-1.0926	2.0460	1.4199	H	3.0995	-5.4345	-6.1571
H	0.8148	1.8215	-0.1233	H	2.1535	-4.8159	-8.2237
H	3.2619	-0.4026	-3.8393	H	2.3049	-4.5205	-10.6811
H	2.0706	-0.6512	-5.9740	H	4.4582	-4.9195	-11.8480
H	-0.3941	-0.9898	-5.9992	H	6.4550	-5.6193	-10.5499
H	-1.6429	-1.0424	-3.8522	H	6.2957	-5.9178	-8.0940
H	-0.4583	-0.7772	-1.7179				
H	2.6023	1.6755	-3.0565	TS - Trans Re Re			
H	3.6559	3.9094	-3.0963				
H	4.1316	-0.3535	5.1743	Ru	3.8589	-2.4491	-0.7574
H	5.4644	-1.3397	3.3474	C	5.3578	-4.2295	-0.8696
H	1.4987	3.5917	4.1650	P	5.3430	-1.1157	0.4289
H	0.5826	2.0992	3.6529	I	1.9864	-4.2984	-1.8486
H	6.1630	5.2463	0.8245	P	2.2720	-0.7026	-0.9670
H	4.4115	5.6614	1.0900	O	4.5455	-1.8959	-2.6799
H	5.2285	-1.3660	-5.1455	C	3.2421	-3.0800	0.8425
H	6.3883	-2.6938	-4.9611	O	2.8500	-3.5386	1.8376
H	7.2984	-3.0566	-1.2527	C	3.0823	0.9460	-1.1316
H	6.2102	-5.2311	-3.1441	C	1.1419	-0.6998	-2.4373

C	1.0503	-0.5077	0.3921	O	2.4776	2.1884	4.4848
C	6.6378	-2.0685	1.3613	O	5.1076	4.5164	-1.4940
C	6.3752	0.1891	-0.3649	C	5.3554	4.7676	-0.0978
C	4.4798	-0.1389	1.7387	O	4.9633	3.5888	0.6282
C	8.0012	-1.7963	1.1980	C	4.8390	-2.8048	-3.5411
C	8.9630	-2.5545	1.8610	H	4.3437	-3.7804	-3.4432
C	8.5837	-3.5949	2.7012	C	5.1319	-2.3524	-4.9532
C	7.2318	-3.8841	2.8620	C	6.4508	-3.6955	-1.5860
C	6.2701	-3.1382	2.1896	C	6.6489	-3.7647	-2.9568
C	6.9858	1.1587	0.4405	O	7.7179	-3.0506	-3.4806
C	7.8045	2.1257	-0.1277	C	8.4960	-3.7933	-4.4244
C	8.0175	2.1407	-1.5054	H	8.3257	-0.9967	0.5418
C	7.4189	1.1744	-2.3065	H	10.0147	-2.3269	1.7121
C	6.6038	0.1957	-1.7409	H	9.3353	-4.1840	3.2191
C	0.4287	-1.6555	0.8922	H	6.9179	-4.7024	3.5037
C	-0.5498	-1.5506	1.8749	H	5.2273	-3.4060	2.3171
C	-0.9191	-0.3011	2.3666	H	6.8149	1.1607	1.5140
C	-0.3218	0.8463	1.8525	H	8.2733	2.8727	0.5072
C	0.6515	0.7451	0.8634	H	8.6504	2.9038	-1.9503
C	1.5663	-1.2327	-3.6574	H	7.5808	1.1785	-3.3808
C	0.7463	-1.1734	-4.7787	H	6.1252	-0.5481	-2.3683
C	-0.5163	-0.5937	-4.6936	H	0.6938	-2.6328	0.4999
C	-0.9506	-0.0702	-3.4798	H	-1.0226	-2.4508	2.2566
C	-0.1272	-0.1191	-2.3579	H	-1.6774	-0.2218	3.1406
C	3.1585	1.5324	-2.3961	H	-0.6156	1.8275	2.2155
C	3.8264	2.7409	-2.6325	H	1.0939	1.6485	0.4567
C	4.3841	3.3570	-1.5390	H	2.5408	-1.6974	-3.7229
C	4.3013	2.7990	-0.2714	H	1.0934	-1.5950	-5.7182
C	3.7096	1.5756	-0.0197	H	-1.1618	-0.5565	-5.5668
C	3.7746	1.0379	1.3595	H	-1.9370	0.3778	-3.3992
C	3.1930	1.7511	2.3893	H	-0.4861	0.2928	-1.4205
C	3.2080	1.3267	3.7114	H	2.6822	1.0434	-3.2378
C	3.8501	0.1731	4.0885	H	3.8924	3.1665	-3.6278
C	4.5033	-0.5398	3.0731	H	3.8664	-0.1660	5.1184
O	2.4560	2.9016	2.2832	H	5.0611	-1.4216	3.3614
C	2.2196	3.3232	3.6384	H	2.9196	4.1330	3.8931

H	1.1761	3.6290	3.7477
H	6.4245	4.9479	0.0529
H	4.7430	5.6182	0.2333
H	4.6568	-1.3728	-5.0956
H	6.2103	-2.2021	-5.0965
H	7.1337	-3.0348	-1.0489
H	6.3396	-4.6332	-3.5371
H	9.0127	-4.6288	-3.9318
H	7.8646	-4.1834	-5.2342
H	9.2344	-3.1014	-4.8363
H	4.7886	-5.0201	-1.3568
H	5.5535	-4.4207	0.1819
C	4.5932	-3.3260	-5.9839
O	5.3532	-4.5334	-5.8959
C	4.7539	-5.6203	-6.6083
C	4.6754	-5.3720	-8.0943
C	3.4465	-5.3421	-8.7523
C	3.3821	-5.0973	-10.1230
C	4.5498	-4.8709	-10.8448
C	5.7826	-4.8919	-10.1923
C	5.8441	-5.1428	-8.8265
H	4.6636	-2.8988	-6.9961
H	3.5292	-3.5441	-5.7813
H	5.3919	-6.4859	-6.3966
H	3.7486	-5.8230	-6.2062
H	2.5330	-5.5107	-8.1861
H	2.4188	-5.0786	-10.6251
H	4.5022	-4.6779	-11.9128
H	6.6968	-4.7174	-10.7530
H	6.8042	-5.1580	-8.3155

Post - Trans Re Re

Ru	3.4913	-2.4489	-0.7299
C	4.4656	-4.7470	-0.8528
P	5.2151	-1.1960	0.2076

I	1.1595	-4.0387	-1.4669
P	2.0614	-0.5829	-0.7877
O	3.8978	-2.0199	-2.7295
C	3.0261	-2.9617	0.9841
O	2.7443	-3.3632	2.0378
C	2.9626	0.9961	-1.0800
C	0.7817	-0.5440	-2.1225
C	1.0312	-0.2620	0.7009
C	6.5470	-2.2424	0.9627
C	6.1886	0.0300	-0.7535
C	4.6054	-0.1615	1.6085
C	7.8856	-2.0912	0.5827
C	8.8647	-2.9490	1.0774
C	8.5280	-3.9698	1.9594
C	7.1980	-4.1363	2.3356
C	6.2156	-3.2900	1.8340
C	7.0243	0.9241	-0.0716
C	7.7888	1.8395	-0.7828
C	7.7151	1.8781	-2.1753
C	6.8814	0.9924	-2.8501
C	6.1184	0.0631	-2.1455
C	0.3960	-1.3329	1.3347
C	-0.4515	-1.1055	2.4140
C	-0.6799	0.1912	2.8662
C	-0.0746	1.2638	2.2177
C	0.7699	1.0402	1.1353
C	1.0758	-1.0498	-3.3918
C	0.1368	-0.9670	-4.4125
C	-1.1106	-0.3938	-4.1766
C	-1.4102	0.1022	-2.9123
C	-0.4689	0.0328	-1.8876
C	2.9023	1.5795	-2.3461
C	3.5863	2.7585	-2.6690
C	4.3116	3.3431	-1.6600
C	4.3684	2.7863	-0.3901
C	3.7477	1.5982	-0.0570

C	3.9463	1.0629	1.3088	H	-2.3827	0.5437	-2.7136
C	3.5451	1.8151	2.3956	H	-0.7258	0.4209	-0.9079
C	3.6961	1.3908	3.7091	H	2.3021	1.1154	-3.1193
C	4.3023	0.1969	4.0147	H	3.5421	3.1830	-3.6658
C	4.7699	-0.5627	2.9331	H	4.4255	-0.1400	5.0380
O	2.8813	3.0121	2.3703	H	5.2946	-1.4826	3.1575
C	2.8214	3.4437	3.7419	H	3.5773	4.2249	3.9097
O	3.1298	2.2999	4.5599	H	1.8104	3.7917	3.9699
O	5.0802	4.4702	-1.7127	H	6.6842	4.7053	-0.4128
C	5.5897	4.6682	-0.3791	H	5.1593	5.5865	0.0414
O	5.1751	3.5413	0.4144	H	3.4009	-2.2233	-5.2228
C	4.2359	-3.1425	-3.4925	H	5.1533	-2.0350	-5.1119
H	3.4634	-3.9356	-3.4091	H	6.2700	-3.6487	-0.8829
C	4.3315	-2.7472	-4.9710	H	5.6955	-4.7334	-3.4547
C	5.4224	-3.9986	-1.4633	H	8.1039	-4.0388	-2.2573
C	5.5308	-3.7682	-2.9457	H	7.8903	-4.3542	-4.0080
O	6.6279	-2.8976	-3.2196	H	8.6433	-2.8282	-3.4514
C	7.8750	-3.5748	-3.2309	H	3.7063	-5.2713	-1.4225
H	8.1713	-1.3158	-0.1190	H	4.5685	-5.0242	0.1922
H	9.8957	-2.8167	0.7619	C	4.4765	-3.9021	-5.9441
H	9.2935	-4.6380	2.3433	O	5.8055	-4.4341	-5.8752
H	6.9162	-4.9358	3.0148	C	5.9902	-5.5526	-6.7376
H	5.1857	-3.4650	2.1228	C	5.9419	-5.1881	-8.2036
H	7.0724	0.9086	1.0146	C	5.1709	-5.9244	-9.1019
H	8.4389	2.5275	-0.2490	C	5.1460	-5.5909	-10.4550
H	8.3070	2.6012	-2.7304	C	5.8859	-4.5076	-10.9186
H	6.8167	1.0231	-3.9344	C	6.6524	-3.7609	-10.0239
H	5.4579	-0.6315	-2.6581	C	6.6821	-4.1008	-8.6764
H	0.5388	-2.3450	0.9700	H	4.2707	-3.5562	-6.9691
H	-0.9357	-1.9482	2.8988	H	3.7498	-4.7008	-5.7085
H	-1.3375	0.3659	3.7133	H	6.9799	-5.9531	-6.4837
H	-0.2620	2.2819	2.5476	H	5.2424	-6.3342	-6.5233
H	1.2187	1.8866	0.6261	H	4.5816	-6.7641	-8.7395
H	2.0472	-1.5084	-3.5506	H	4.5405	-6.1725	-11.1446
H	0.3777	-1.3666	-5.3938	H	5.8636	-4.2418	-11.9718
H	-1.8481	-0.3400	-4.9727	H	7.2300	-2.9124	-10.3807

H 7.2731 -3.5167 -7.9752

Pre - Trans Re Si

Ru 1.7817 0.9065 0.7689

C 3.7022 2.0323 1.1610

P 0.7305 2.8629 0.1049

I 2.9683 -1.4423 1.8810

P -0.1206 -0.4527 0.1959

O 2.7818 0.6774 -1.1182

C 1.2393 1.2716 2.4606

O 0.9745 1.5302 3.5649

C -1.2342 0.2199 -1.1136

C 0.2992 -2.1259 -0.4606

C -1.3301 -0.8799 1.5202

C 1.6151 4.4108 0.5979

C 0.2833 3.2249 -1.6487

C -0.9217 2.9884 0.9203

C 2.0119 4.5885 1.9309

C 2.7354 5.7107 2.3139

C 3.1069 6.6625 1.3674

C 2.7528 6.4772 0.0361

C 2.0122 5.3611 -0.3477

C -0.5818 4.2948 -1.9108

C -0.9536 4.5918 -3.2159

C -0.4753 3.8187 -4.2728

C 0.3841 2.7554 -4.0165

C 0.7668 2.4602 -2.7100

C -0.8919 -1.0660 2.8334

C -1.7874 -1.4589 3.8239

C -3.1261 -1.6790 3.5119

C -3.5637 -1.5162 2.1996

C -2.6723 -1.1200 1.2085

C 1.1916 -2.2255 -1.5337

C 1.5615 -3.4677 -2.0343

C 1.0603 -4.6322 -1.4569

C 0.1811 -4.5413 -0.3834

C -0.2014 -3.2967 0.1116

C -1.3520 -0.3963 -2.3597

C -2.1612 0.1158 -3.3837

C -2.8656 1.2584 -3.0978

C -2.7826 1.8659 -1.8534

C -1.9678 1.4056 -0.8378

C -1.9796 2.1668 0.4376

C -3.1588 2.2202 1.1549

C -3.3280 3.0053 2.2888

C -2.3260 3.8215 2.7515

C -1.1180 3.7939 2.0404

O -4.3377 1.5877 0.8552

C -5.1632 1.7740 2.0180

O -4.6101 2.8824 2.7525

O -3.6877 1.9817 -3.9178

C -4.2793 2.9922 -3.0776

O -3.5581 2.9926 -1.8331

C 3.8299 0.0504 -1.3684

H 4.1659 -0.7524 -0.6976

C 4.4677 0.1934 -2.7184

C 4.9168 1.2746 0.8911

C 5.6770 1.4559 -0.2153

O 6.8328 0.8073 -0.5428

C 7.2513 -0.2311 0.3474

H 1.7756 3.8384 2.6788

H 3.0240 5.8305 3.3542

H 3.6820 7.5347 1.6654

H 3.0536 7.2017 -0.7155

H 1.7535 5.2355 -1.3934

H -0.9754 4.8888 -1.0896

H -1.6264 5.4235 -3.4067

H -0.7765 4.0434 -5.2925

H 0.7535 2.1405 -4.8329

H 1.4312 1.6274 -2.5147

H 0.1557 -0.9319 3.0807

H	-1.4321	-1.5967	4.8410
H	-3.8237	-1.9860	4.2864
H	-4.6031	-1.7025	1.9421
H	-3.0247	-0.9977	0.1891
H	1.5888	-1.3213	-1.9817
H	2.2514	-3.5287	-2.8713
H	1.3587	-5.6042	-1.8393
H	-0.2102	-5.4429	0.0793
H	-0.8823	-3.2468	0.9546
H	-0.8123	-1.3142	-2.5582
H	-2.2225	-0.3695	-4.3507
H	-2.4585	4.4612	3.6170
H	-0.3204	4.4392	2.3850
H	-6.1816	2.0163	1.7054
H	-5.1179	0.8691	2.6426
H	-4.1742	3.9695	-3.5585
H	-5.3315	2.7366	-2.8877
H	5.5186	-0.1092	-2.6702
H	4.4021	1.2356	-3.0499
H	5.1927	0.5063	1.6070
H	5.4660	2.2429	-0.9363
H	6.4759	-1.0028	0.4467
H	8.1514	-0.6628	-0.0931
H	7.4816	0.1748	1.3410
H	3.6519	2.9360	0.5507
H	3.6451	2.3032	2.2180
C	3.7195	-0.6876	-3.7167
O	4.3424	-0.5463	-4.9866
C	3.7475	-1.3968	-5.9770
C	2.3127	-1.0326	-6.2672
C	1.2642	-1.8538	-5.8510
C	-0.0594	-1.4914	-6.0911
C	-0.3456	-0.2996	-6.7504
C	0.6960	0.5277	-7.1685
C	2.0162	0.1640	-6.9259
H	2.6645	-0.3731	-3.7667

H	3.7465	-1.7444	-3.3978
H	4.3669	-1.2677	-6.8705
H	3.8118	-2.4486	-5.6541
H	1.4853	-2.7856	-5.3346
H	-0.8653	-2.1427	-5.7633
H	-1.3764	-0.0147	-6.9426
H	0.4764	1.4566	-7.6881
H	2.8288	0.8108	-7.2491

TS - Trans Re Si

Ru	1.8017	0.9176	0.7629
C	3.7638	2.1292	1.2179
P	0.7281	2.8726	0.1046
I	3.0237	-1.4444	1.8723
P	-0.0714	-0.4269	0.2070
O	2.8463	0.7876	-1.0659
C	1.2262	1.2507	2.4561
O	0.9543	1.4960	3.5626
C	-1.1889	0.2340	-1.1006
C	0.3608	-2.0899	-0.4627
C	-1.2625	-0.8665	1.5433
C	1.6084	4.4210	0.5969
C	0.2958	3.2116	-1.6538
C	-0.9228	2.9941	0.9205
C	1.9872	4.6147	1.9331
C	2.7019	5.7440	2.3124
C	3.0812	6.6868	1.3591
C	2.7442	6.4853	0.0254
C	2.0125	5.3620	-0.3553
C	-0.5736	4.2727	-1.9371
C	-0.9340	4.5489	-3.2503
C	-0.4368	3.7658	-4.2916
C	0.4281	2.7123	-4.0123
C	0.7969	2.4347	-2.6980
C	-0.7988	-1.1194	2.8371

C	-1.6803	-1.5296	3.8329	H	1.7665	5.2241	-1.4025
C	-3.0324	-1.6996	3.5461	H	-0.9788	4.8764	-1.1286
C	-3.4961	-1.4715	2.2530	H	-1.6125	5.3713	-3.4599
C	-2.6176	-1.0602	1.2559	H	-0.7277	3.9758	-5.3175
C	1.3346	-2.1725	-1.4627	H	0.8129	2.0913	-4.8172
C	1.6846	-3.4023	-2.0068	H	1.4660	1.6105	-2.4800
C	1.0792	-4.5692	-1.5438	H	0.2574	-1.0217	3.0648
C	0.1172	-4.4942	-0.5417	H	-1.3049	-1.7197	4.8344
C	-0.2464	-3.2605	-0.0045	H	-3.7200	-2.0176	4.3250
C	-1.2844	-0.3914	-2.3445	H	-4.5462	-1.6170	2.0145
C	-2.1052	0.0932	-3.3722	H	-2.9926	-0.8913	0.2517
C	-2.8364	1.2215	-3.0955	H	1.8129	-1.2635	-1.8109
C	-2.7716	1.8402	-1.8549	H	2.4385	-3.4527	-2.7874
C	-1.9522	1.4024	-0.8330	H	1.3604	-5.5324	-1.9604
C	-1.9790	2.1719	0.4355	H	-0.3565	-5.3987	-0.1706
C	-3.1650	2.2327	1.1423	H	-0.9980	-3.2226	0.7771
C	-3.3410	3.0269	2.2693	H	-0.7127	-1.2908	-2.5398
C	-2.3399	3.8435	2.7346	H	-2.1521	-0.3986	-4.3366
C	-1.1259	3.8083	2.0336	H	-2.4779	4.4922	3.5928
O	-4.3398	1.5987	0.8392	H	-0.3331	4.4581	2.3799
C	-5.1896	1.8104	1.9831	H	-6.1938	2.0756	1.6452
O	-4.6248	2.9114	2.7245	H	-5.1810	0.9097	2.6134
O	-3.6690	1.9193	-3.9233	H	-4.1718	3.9093	-3.5884
C	-4.2782	2.9365	-3.0998	H	-5.3292	2.6749	-2.9183
O	-3.5673	2.9507	-1.8461	H	5.5622	0.0940	-2.7517
C	3.9760	0.2237	-1.3080	H	4.3890	1.4053	-3.0463
H	4.2201	-0.7157	-0.7886	H	5.1856	0.5978	1.6941
C	4.5020	0.3640	-2.7203	H	5.4039	2.1126	-0.9832
C	4.8791	1.3105	0.9348	H	6.1721	-1.1533	0.5378
C	5.4879	1.2607	-0.3115	H	7.8357	-1.0091	-0.1090
O	6.6403	0.5543	-0.5869	H	7.3363	-0.0280	1.2999
C	7.0069	-0.4653	0.3478	H	3.6591	3.0066	0.5855
H	1.7448	3.8724	2.6870	H	3.6207	2.3389	2.2763
H	2.9758	5.8778	3.3550	C	3.7299	-0.5423	-3.6683
H	3.6483	7.5651	1.6544	O	4.3052	-0.4127	-4.9677
H	3.0506	7.2030	-0.7305	C	3.7236	-1.3191	-5.9149

C	2.2772	-1.0065	-6.2072
C	1.2563	-1.8487	-5.7644
C	-0.0782	-1.5406	-6.0214
C	-0.4031	-0.3813	-6.7209
C	0.6108	0.4684	-7.1625
C	1.9421	0.1570	-6.9063
H	2.6660	-0.2565	-3.6895
H	3.7958	-1.5932	-3.3373
H	4.3285	-1.2118	-6.8215
H	3.8183	-2.3539	-5.5485
H	1.5087	-2.7539	-5.2161
H	-0.8630	-2.2075	-5.6738
H	-1.4428	-0.1393	-6.9248
H	0.3612	1.3727	-7.7114
H	2.7332	0.8186	-7.2524

Post - Trans Re Si

Ru	2.0955	0.9562	0.8142
C	3.9312	2.6641	1.0099
P	0.8105	2.8558	0.2880
I	3.4222	-1.3521	1.9888
P	0.2535	-0.4495	0.4037
O	2.6331	0.5052	-1.1676
C	1.7306	1.2590	2.5932
O	1.5825	1.4486	3.7312
C	-0.7055	0.1136	-1.0622
C	0.6302	-2.2083	-0.0280
C	-0.9805	-0.6904	1.7415
C	1.4567	4.4483	0.9966
C	0.4772	3.3555	-1.4513
C	-0.9079	2.7566	0.9606
C	1.7379	4.5638	2.3651
C	2.2646	5.7388	2.8880
C	2.5474	6.8160	2.0528
C	2.3018	6.7025	0.6898

C	1.7607	5.5312	0.1644
C	-0.5085	4.3165	-1.7108
C	-0.7308	4.7499	-3.0111
C	0.0182	4.2224	-4.0632
C	0.9960	3.2677	-3.8045
C	1.2322	2.8341	-2.5014
C	-0.5367	-0.8763	3.0527
C	-1.4475	-1.1575	4.0665
C	-2.8054	-1.2655	3.7796
C	-3.2474	-1.1176	2.4675
C	-2.3393	-0.8408	1.4515
C	1.7166	-2.4994	-0.8565
C	1.9837	-3.8081	-1.2355
C	1.1788	-4.8482	-0.7764
C	0.1026	-4.5660	0.0575
C	-0.1767	-3.2523	0.4297
C	-0.5024	-0.5314	-2.2822
C	-1.1316	-0.1305	-3.4663
C	-1.9952	0.9332	-3.3705
C	-2.2312	1.5715	-2.1612
C	-1.5874	1.2281	-0.9879
C	-1.8729	2.0007	0.2402
C	-3.1613	2.0330	0.7352
C	-3.5051	2.6836	1.9128
C	-2.5765	3.3815	2.6456
C	-1.2734	3.4209	2.1304
O	-4.2502	1.3635	0.2440
C	-5.3645	1.8326	1.0238
O	-4.8211	2.4536	2.2042
O	-2.7421	1.5102	-4.3584
C	-3.4368	2.6119	-3.7417
O	-3.1423	2.5764	-2.3332
C	3.9654	0.1939	-1.4541
H	4.2576	-0.7744	-0.9988
C	4.1816	0.1239	-2.9692
C	4.5649	1.5396	0.5924

C	4.8781	1.2854	-0.8559
O	6.2849	1.0566	-1.0212
C	6.7667	-0.2230	-0.6026
H	1.5664	3.7334	3.0395
H	2.4652	5.8035	3.9536
H	2.9673	7.7309	2.4611
H	2.5340	7.5265	0.0212
H	1.5908	5.4680	-0.9040
H	-1.1015	4.7265	-0.8971
H	-1.4927	5.5006	-3.2036
H	-0.1610	4.5594	-5.0809
H	1.5817	2.8517	-4.6190
H	1.9693	2.0639	-2.2847
H	0.5223	-0.8341	3.2829
H	-1.0893	-1.2963	5.0823
H	-3.5153	-1.4789	4.5738
H	-4.3019	-1.2243	2.2284
H	-2.6916	-0.7514	0.4291
H	2.3400	-1.6806	-1.1927
H	2.8345	-4.0177	-1.8781
H	1.3944	-5.8742	-1.0615
H	-0.5270	-5.3694	0.4292
H	-1.0184	-3.0589	1.0853
H	0.1597	-1.3866	-2.3317
H	-0.9451	-0.6390	-4.4053
H	-2.8351	3.8886	3.5684
H	-0.5465	4.0193	2.6631
H	-5.9235	2.5820	0.4444
H	-5.9887	0.9839	1.3142
H	-3.0670	3.5543	-4.1663
H	-4.5156	2.4890	-3.8889
H	5.2379	-0.0939	-3.1731
H	3.9621	1.1093	-3.4045
H	5.0040	0.8678	1.3229
H	4.6851	2.2085	-1.4209
H	6.5122	-1.0110	-1.3243

H	7.8549	-0.1332	-0.5478
H	6.3841	-0.5165	0.3838
H	3.6698	3.4398	0.2976
H	3.8763	2.9250	2.0618
C	3.3210	-0.9223	-3.6461
O	3.7009	-0.9894	-5.0263
C	2.8439	-1.8233	-5.7875
C	1.5344	-1.1693	-6.1788
C	0.4451	-1.9592	-6.5534
C	-0.7333	-1.3724	-7.0076
C	-0.8433	0.0151	-7.0724
C	0.2317	0.8075	-6.6778
C	1.4152	0.2193	-6.2394
H	2.2543	-0.6657	-3.5540
H	3.4758	-1.9130	-3.1847
H	3.4012	-2.0740	-6.7003
H	2.6434	-2.7692	-5.2559
H	0.5225	-3.0434	-6.4964
H	-1.5713	-1.9995	-7.3000
H	-1.7658	0.4752	-7.4143
H	0.1469	1.8905	-6.7105
H	2.2612	0.8315	-5.9399

Pre - Trans Si Re

Ru	0.9500	-2.5935	0.8685
C	0.7664	-4.8407	0.7047
P	1.5315	-0.2591	1.0504
I	3.5087	-3.1799	1.9625
P	-1.1026	-2.1242	-0.1040
O	1.6038	-2.6919	-1.1694
C	0.2562	-2.8550	2.5229
O	-0.1615	-3.1512	3.5703
C	-0.8964	-1.0386	-1.5892
C	-2.0291	-3.5937	-0.7262
C	-2.4312	-1.2184	0.7976

C	2.4410	0.2342	2.5818	O	-0.1370	1.5323	-4.7248
C	2.6608	0.3920	-0.2581	C	0.3275	2.6536	-3.9462
C	0.1523	0.9634	1.0410	O	-0.0964	2.4266	-2.5928
C	2.0538	-0.3000	3.8141	C	2.5780	-3.2782	-1.6624
C	2.6875	0.0949	4.9861	H	3.4175	-3.5897	-1.0255
C	3.7289	1.0187	4.9414	C	2.6799	-3.3977	-3.1533
C	4.1230	1.5514	3.7184	C	1.8577	-5.4926	-0.0300
C	3.4793	1.1675	2.5442	C	1.8023	-5.9350	-1.3039
C	2.4738	1.6456	-0.8462	O	2.7880	-6.5775	-2.0021
C	3.3865	2.1284	-1.7807	C	4.0207	-6.7934	-1.3133
C	4.5053	1.3762	-2.1257	H	1.2564	-1.0328	3.8641
C	4.7102	0.1381	-1.5228	H	2.3751	-0.3334	5.9342
C	3.7926	-0.3557	-0.6017	H	4.2338	1.3173	5.8559
C	-2.3513	-0.9146	2.1547	H	4.9366	2.2698	3.6722
C	-3.3873	-0.2265	2.7818	H	3.7976	1.5950	1.5988
C	-4.5100	0.1616	2.0590	H	1.6217	2.2572	-0.5694
C	-4.5952	-0.1385	0.7005	H	3.2303	3.1077	-2.2259
C	-3.5619	-0.8210	0.0724	H	5.2137	1.7515	-2.8588
C	-3.2549	-3.9833	-0.1791	H	5.5897	-0.4498	-1.7724
C	-3.8808	-5.1519	-0.6080	H	3.9728	-1.3113	-0.1168
C	-3.2949	-5.9463	-1.5875	H	-1.4704	-1.1835	2.7239
C	-2.0589	-5.5829	-2.1171	H	-3.3066	0.0140	3.8379
C	-1.4249	-4.4288	-1.6750	H	-5.3148	0.7019	2.5498
C	-0.9770	-1.5420	-2.8868	H	-5.4665	0.1645	0.1264
C	-0.7273	-0.7625	-4.0243	H	-3.6291	-1.0403	-0.9903
C	-0.3813	0.5478	-3.8041	H	-3.7293	-3.3804	0.5879
C	-0.3371	1.0770	-2.5210	H	-4.8325	-5.4385	-0.1697
C	-0.5834	0.3348	-1.3808	H	-3.7883	-6.8535	-1.9244
C	-0.7013	1.0634	-0.0904	H	-1.5773	-6.2102	-2.8622
C	-1.7433	1.9651	0.0145	H	-0.4351	-4.1829	-2.0482
C	-1.9968	2.7106	1.1568	H	-1.2613	-2.5722	-3.0491
C	-1.1850	2.6254	2.2604	H	-0.8085	-1.1782	-5.0230
C	-0.1007	1.7416	2.1722	H	-1.3720	3.2042	3.1584
O	-2.7095	2.2077	-0.9233	H	0.5606	1.6663	3.0268
C	-3.5249	3.2631	-0.3835	H	-3.3364	4.1904	-0.9425
O	-3.1361	3.4481	0.9916	H	-4.5774	2.9654	-0.4251

H	1.4272	2.6840	-3.9823	P	-1.1242	-2.0794	-0.1292
H	-0.1298	3.5716	-4.3223	O	1.4411	-2.7938	-1.2804
H	3.5094	-4.0562	-3.4283	C	0.4813	-2.6871	2.4819
H	1.7464	-3.8221	-3.5428	O	0.1855	-2.9852	3.5699
H	2.7902	-5.6083	0.5155	C	-0.9456	-0.9456	-1.5750
H	0.9049	-5.8730	-1.9124	C	-2.0038	-3.5705	-0.7771
H	4.6781	-7.3016	-2.0206	C	-2.4777	-1.2643	0.8157
H	4.4744	-5.8426	-1.0014	C	2.4283	0.2751	2.5049
H	3.8690	-7.4221	-0.4262	C	2.4065	0.7045	-0.3270
H	0.7991	-5.1706	1.7464	C	-0.0042	0.9670	1.1296
H	-0.2142	-5.0705	0.2887	C	1.9606	-0.1172	3.7641
C	2.8668	-2.0103	-3.7695	C	2.6938	0.1617	4.9108
O	2.8593	-2.1676	-5.1875	C	3.9147	0.8253	4.8168
C	2.7248	-0.9307	-5.8771	C	4.3892	1.2130	3.5687
C	3.9145	-0.0056	-5.7502	C	3.6513	0.9431	2.4189
C	5.2048	-0.5048	-5.5674	C	2.3321	2.0974	-0.4435
C	6.2909	0.3627	-5.4922	C	3.1139	2.7661	-1.3776
C	6.1016	1.7380	-5.6129	C	3.9730	2.0514	-2.2092
C	4.8166	2.2418	-5.7998	C	4.0511	0.6665	-2.0980
C	3.7300	1.3737	-5.8580	C	3.2730	-0.0063	-1.1587
H	3.8090	-1.5570	-3.4314	C	-2.4337	-1.0952	2.1974
H	2.0422	-1.3513	-3.4534	C	-3.4979	-0.4920	2.8642
H	2.5809	-1.2027	-6.9308	C	-4.6129	-0.0576	2.1562
H	1.8174	-0.4034	-5.5398	C	-4.6643	-0.2288	0.7738
H	5.3518	-1.5782	-5.4805	C	-3.6036	-0.8267	0.1065
H	7.2905	-0.0368	-5.3441	C	-3.2164	-3.9965	-0.2255
H	6.9509	2.4132	-5.5580	C	-3.8207	-5.1717	-0.6671
H	4.6597	3.3132	-5.8915	C	-3.2270	-5.9387	-1.6632
H	2.7251	1.7682	-5.9973	C	-2.0061	-5.5375	-2.2002
TS - Trans Si Re				C	-1.3941	-4.3748	-1.7497
				C	-0.9491	-1.4183	-2.8857
				C	-0.6528	-0.6041	-3.9875
Ru	1.0014	-2.4667	0.7535	C	-0.3429	0.7056	-3.7155
C	0.7822	-4.8093	0.7075	C	-0.3866	1.2054	-2.4195
P	1.4514	-0.1552	0.9968	C	-0.6784	0.4287	-1.3162
I	3.7088	-2.8498	1.5270	C	-0.8475	1.1019	-0.0037

C	-1.9154	1.9652	0.1332	H	-0.4174	-4.0976	-2.1308
C	-2.2025	2.6389	1.3124	H	-1.1946	-2.4521	-3.0849
C	-1.3984	2.5201	2.4189	H	-0.6654	-0.9964	-4.9988
C	-0.2835	1.6786	2.2957	H	-1.6091	3.0488	3.3422
O	-2.8814	2.2275	-0.7995	H	0.3837	1.5975	3.1445
C	-3.7003	3.2619	-0.2252	H	-3.4691	4.2204	-0.7120
O	-3.3653	3.3458	1.1736	H	-4.7547	2.9906	-0.3297
O	-0.0550	1.7162	-4.5935	H	1.4544	2.8461	-3.7121
C	0.3545	2.8180	-3.7575	H	-0.0753	3.7454	-4.1423
O	-0.1636	2.5582	-2.4432	H	3.0744	-4.3613	-3.6425
C	2.3789	-3.4979	-1.7960	H	1.3699	-3.8377	-3.6604
H	3.3590	-3.5219	-1.2975	H	2.7867	-5.5400	0.6755
C	2.3774	-3.5884	-3.3040	H	1.1799	-5.6195	-1.9526
C	1.9129	-5.3648	0.0551	H	5.0568	-6.7551	-1.7806
C	2.0539	-5.5424	-1.3112	H	4.6259	-5.4270	-0.6593
O	3.1188	-6.1891	-1.9053	H	4.1102	-7.1025	-0.3042
C	4.2889	-6.3725	-1.1056	H	0.7560	-5.0445	1.7703
H	1.0174	-0.6437	3.8600	H	-0.1754	-4.9583	0.2186
H	2.3126	-0.1510	5.8787	C	2.7770	-2.2380	-3.8848
H	4.4945	1.0326	5.7117	O	2.7231	-2.3345	-5.3095
H	5.3449	1.7221	3.4815	C	2.8105	-1.0662	-5.9470
H	4.0473	1.2396	1.4537	C	4.1479	-0.3804	-5.7826
H	1.6656	2.6622	0.2018	C	5.3277	-1.1215	-5.6911
H	3.0505	3.8483	-1.4550	C	6.5541	-0.4788	-5.5548
H	4.5841	2.5692	-2.9429	C	6.6176	0.9134	-5.5245
H	4.7212	0.1106	-2.7482	C	5.4455	1.6579	-5.6255
H	3.3472	-1.0833	-1.0574	C	4.2173	1.0123	-5.7419
H	-1.5653	-1.4143	2.7602	H	3.7916	-1.9647	-3.5538
H	-3.4467	-0.3567	3.9407	H	2.0852	-1.4555	-3.5351
H	-5.4392	0.4173	2.6778	H	2.6218	-1.2624	-7.0105
H	-5.5307	0.1092	0.2120	H	2.0123	-0.3978	-5.5811
H	-3.6446	-0.9464	-0.9732	H	5.2752	-2.2070	-5.7153
H	-3.6982	-3.4177	0.5550	H	7.4649	-1.0657	-5.4739
H	-4.7619	-5.4848	-0.2243	H	7.5760	1.4142	-5.4204
H	-3.7034	-6.8517	-2.0087	H	5.4865	2.7437	-5.6007
H	-1.5181	-6.1397	-2.9617	H	3.2994	1.5950	-5.7951

Post - Trans Si Re

Ru	1.0676	-2.4985	0.7551
C	0.2929	-4.8886	0.9274
P	1.5050	-0.2006	0.9966
I	3.8213	-2.7508	1.5198
P	-1.0127	-2.0263	-0.2631
O	1.5080	-2.7750	-1.2820
C	0.5713	-2.6065	2.5200
O	0.2794	-2.8461	3.6230
C	-0.7734	-0.7799	-1.6050
C	-1.8639	-3.4588	-1.0675
C	-2.4253	-1.2955	0.6654
C	2.5670	0.2617	2.4435
C	2.3538	0.6599	-0.3865
C	0.0260	0.8769	1.2367
C	2.2140	-0.1315	3.7392
C	3.0118	0.2057	4.8257
C	4.1848	0.9309	4.6365
C	4.5485	1.3164	3.3514
C	3.7471	0.9868	2.2619
C	2.3240	2.0589	-0.4373
C	3.0412	2.7356	-1.4152
C	3.7825	2.0225	-2.3558
C	3.8100	0.6321	-2.3092
C	3.1026	-0.0522	-1.3229
C	-2.4767	-1.2790	2.0568
C	-3.5888	-0.7538	2.7119
C	-4.6595	-0.2511	1.9812
C	-4.6183	-0.2768	0.5880
C	-3.5089	-0.7938	-0.0671
C	-3.0903	-3.9249	-0.5789
C	-3.6831	-5.0601	-1.1262
C	-3.0656	-5.7476	-2.1655
C	-1.8353	-5.3040	-2.6426

C	-1.2353	-4.1788	-2.0903
C	-0.6768	-1.1511	-2.9447
C	-0.4317	-0.2302	-3.9715
C	-0.2812	1.0829	-3.5989
C	-0.4034	1.4753	-2.2733
C	-0.6366	0.5887	-1.2403
C	-0.8221	1.1281	0.1257
C	-1.8941	1.9670	0.3542
C	-2.1861	2.5040	1.6004
C	-1.3830	2.2657	2.6884
C	-0.2625	1.4517	2.4743
O	-2.8605	2.3246	-0.5440
C	-3.6985	3.2713	0.1423
O	-3.3487	3.2185	1.5399
O	-0.0772	2.1768	-4.3935
C	0.1682	3.2638	-3.4781
O	-0.2925	2.8379	-2.1840
C	2.3939	-3.8033	-1.6215
H	3.4018	-3.5991	-1.2153
C	2.4972	-3.9461	-3.1427
C	1.5634	-4.9965	0.4548
C	1.9020	-5.1397	-1.0042
O	2.7797	-6.2552	-1.2096
C	4.1486	-6.0637	-0.8447
H	1.3161	-0.7099	3.9168
H	2.7169	-0.1111	5.8219
H	4.8142	1.1855	5.4845
H	5.4687	1.8693	3.1860
H	4.0667	1.2780	1.2682
H	1.7464	2.6194	0.2926
H	3.0216	3.8219	-1.4403
H	4.3413	2.5474	-3.1255
H	4.3842	0.0788	-3.0470
H	3.1028	-1.1364	-1.2866
H	-1.6479	-1.6610	2.6393
H	-3.6106	-0.7358	3.7977

H	-5.5242	0.1612	2.4938
H	-5.4511	0.1116	0.0082
H	-3.4787	-0.8002	-1.1536
H	-3.5897	-3.4128	0.2359
H	-4.6337	-5.4062	-0.7306
H	-3.5325	-6.6311	-2.5913
H	-1.3278	-5.8436	-3.4377
H	-0.2490	-3.8727	-2.4154
H	-0.8043	-2.1842	-3.2316
H	-0.3706	-0.5458	-5.0072
H	-1.5966	2.6876	3.6644
H	0.4045	1.2926	3.3111
H	-3.4985	4.2809	-0.2437
H	-4.7470	2.9837	0.0206
H	1.2500	3.4561	-3.4319
H	-0.4010	4.1412	-3.7955
H	3.2389	-4.7194	-3.3817
H	1.5379	-4.2888	-3.5561
H	2.3746	-5.1485	1.1599
H	0.9904	-5.4285	-1.5396
H	4.5977	-7.0604	-0.8251
H	4.6851	-5.4480	-1.5797
H	4.2603	-5.5996	0.1434
H	0.0909	-5.0012	1.9878
H	-0.5589	-4.9449	0.2612
C	2.8862	-2.6483	-3.8180
O	3.0168	-2.9029	-5.2238
C	2.9649	-1.7259	-6.0140
C	4.1283	-0.7819	-5.8086
C	5.4028	-1.2711	-5.5155
C	6.4707	-0.3958	-5.3429
C	6.2808	0.9786	-5.4784
C	5.0140	1.4716	-5.7795
C	3.9421	0.5956	-5.9305
H	3.8382	-2.2709	-3.4095
H	2.1182	-1.8798	-3.6440

H	2.9520	-2.0737	-7.0555
H	2.0236	-1.1802	-5.8308
H	5.5472	-2.3432	-5.4097
H	7.4558	-0.7868	-5.1034
H	7.1159	1.6608	-5.3460
H	4.8564	2.5420	-5.8833
H	2.9474	0.9864	-6.1373

Pre - Trans Si Si

Ru	0.3048	0.8354	-0.3993
C	0.3314	1.9260	-2.3410
P	0.5851	-0.5813	1.5790
I	0.0343	-1.5118	-1.9732
P	0.5227	2.7569	0.8286
O	2.4614	0.7235	-0.5197
C	-1.4973	0.9972	-0.5006
O	-2.6441	1.1245	-0.6707
C	2.1736	2.6794	1.6060
C	0.3631	4.3961	-0.0138
C	-0.6292	3.1600	2.2219
C	-0.5894	-1.9971	1.7067
C	2.2171	-1.4383	1.7565
C	0.4136	0.2094	3.2418
C	-1.9332	-1.7954	1.3787
C	-2.8518	-2.8319	1.4925
C	-2.4360	-4.0906	1.9204
C	-1.0989	-4.3011	2.2416
C	-0.1794	-3.2597	2.1414
C	2.8567	-1.5416	2.9950
C	4.0576	-2.2371	3.1143
C	4.6358	-2.8368	1.9998
C	3.9958	-2.7515	0.7652
C	2.7944	-2.0623	0.6448
C	-1.7846	2.4271	2.4794
C	-2.6529	2.8200	3.4956

C	-2.3737	3.9471	4.2601	H	2.4167	-1.0889	3.8771
C	-1.2202	4.6873	4.0030	H	4.5334	-2.3170	4.0883
C	-0.3560	4.2997	2.9878	H	5.5737	-3.3775	2.0936
C	-0.8204	4.5856	-0.7386	H	4.4295	-3.2217	-0.1127
C	-1.0908	5.8040	-1.3490	H	2.2898	-2.0270	-0.3167
C	-0.1854	6.8566	-1.2400	H	-2.0039	1.5343	1.9048
C	0.9762	6.6883	-0.4936	H	-3.5474	2.2350	3.6899
C	1.2478	5.4694	0.1237	H	-3.0525	4.2512	5.0520
C	3.2928	3.1507	0.9170	H	-0.9978	5.5745	4.5896
C	4.5985	2.9593	1.3830	H	0.5380	4.8860	2.7927
C	4.7319	2.2492	2.5520	H	-1.5498	3.7827	-0.8069
C	3.6292	1.7431	3.2290	H	-2.0132	5.9302	-1.9084
C	2.3298	1.9049	2.7873	H	-0.3925	7.8076	-1.7222
C	1.2234	1.3272	3.5961	H	1.6760	7.5115	-0.3798
C	0.9817	1.8807	4.8364	H	2.1411	5.3748	0.7310
C	0.0020	1.4174	5.7037	H	3.1643	3.6526	-0.0351
C	-0.7776	0.3332	5.3872	H	5.4574	3.3408	0.8415
C	-0.5476	-0.2592	4.1374	H	-1.5377	-0.0452	6.0620
O	1.6329	2.9463	5.3953	H	-1.1565	-1.1129	3.8638
C	0.9264	3.2445	6.6140	H	1.6386	3.2910	7.4439
O	-0.0066	2.1697	6.8452	H	0.3721	4.1845	6.4909
O	5.8768	1.9587	3.2439	H	5.7263	-0.0053	3.9072
C	5.4704	1.0088	4.2486	H	5.9419	1.2618	5.2011
O	4.0424	1.1188	4.3779	H	4.8835	1.5109	-1.4328
C	3.1290	0.3374	-1.4812	H	4.9856	0.0014	-0.5259
H	2.6415	-0.1463	-2.3395	H	1.9176	3.4381	-2.0935
C	4.6208	0.4445	-1.4632	H	2.2230	1.2858	-4.2772
C	1.6122	2.5608	-2.6676	H	4.1622	1.5279	-5.4800
C	2.4543	2.1289	-3.6208	H	3.5493	3.1652	-5.8608
O	3.6821	2.7171	-3.8230	H	5.1886	2.9612	-5.1714
C	4.1648	2.5810	-5.1639	H	0.0526	1.1832	-3.0935
H	-2.2674	-0.8262	1.0250	H	-0.4527	2.6831	-2.2861
H	-3.8915	-2.6578	1.2309	C	5.2538	-0.2130	-2.6696
H	-3.1510	-4.9051	1.9964	O	4.9316	-1.6026	-2.6222
H	-0.7641	-5.2807	2.5710	C	5.2121	-2.2741	-3.8555
H	0.8598	-3.4392	2.3982	C	4.3328	-1.7949	-4.9862

C	4.8796	-1.3577	-6.1922
C	4.0539	-0.9026	-7.2196
C	2.6741	-0.8664	-7.0399
C	2.1217	-1.2956	-5.8331
C	2.9460	-1.7636	-4.8163
H	6.3466	-0.0730	-2.6663
H	4.8565	0.2406	-3.5901
H	6.2741	-2.1533	-4.1241
H	5.0292	-3.3349	-3.6497
H	5.9592	-1.3686	-6.3278
H	4.4907	-0.5652	-8.1557
H	2.0298	-0.5031	-7.8357
H	1.0461	-1.2680	-5.6794
H	2.5074	-2.0915	-3.8764

TS - Trans Si Si

Ru	0.4013	0.5937	-0.3969
C	0.4234	1.4813	-2.5780
P	0.6145	-0.6445	1.6276
I	0.1057	-1.8983	-1.7610
P	0.5920	2.6040	0.7023
O	2.4961	0.5427	-0.5137
C	-1.4186	0.7133	-0.5246
O	-2.5618	0.8061	-0.7321
C	2.2321	2.5927	1.4946
C	0.4265	4.1652	-0.2721
C	-0.5767	3.1139	2.0449
C	-0.5674	-2.0470	1.8182
C	2.2439	-1.4795	1.8916
C	0.4128	0.2574	3.2272
C	-1.9239	-1.8419	1.5492
C	-2.8386	-2.8763	1.7012
C	-2.4077	-4.1363	2.1101
C	-1.0592	-4.3487	2.3750
C	-0.1421	-3.3096	2.2358

C	2.7990	-1.5710	3.1712
C	3.9838	-2.2738	3.3771
C	4.6241	-2.8967	2.3106
C	4.0660	-2.8225	1.0362
C	2.8850	-2.1194	0.8269
C	-1.7685	2.4428	2.3022
C	-2.6497	2.9219	3.2693
C	-2.3466	4.0749	3.9842
C	-1.1564	4.7541	3.7261
C	-0.2794	4.2808	2.7594
C	-0.7219	4.2687	-1.0662
C	-0.9820	5.4283	-1.7862
C	-0.1015	6.5052	-1.7178
C	1.0243	6.4220	-0.9047
C	1.2858	5.2632	-0.1776
C	3.3572	3.0131	0.7840
C	4.6574	2.8357	1.2702
C	4.7765	2.1877	2.4766
C	3.6658	1.7309	3.1756
C	2.3721	1.8845	2.7179
C	1.2476	1.3685	3.5416
C	0.9963	1.9903	4.7468
C	-0.0133	1.5974	5.6152
C	-0.8149	0.5183	5.3382
C	-0.5761	-0.1430	4.1256
O	1.6557	3.0735	5.2579
C	0.9539	3.4350	6.4621
O	-0.0333	2.4131	6.7103
O	5.9148	1.9186	3.1885
C	5.4923	1.0187	4.2314
O	4.0669	1.1634	4.3579
C	3.1211	0.2038	-1.5846
H	2.6312	-0.5121	-2.2592
C	4.6234	0.0981	-1.4708
C	1.6381	2.1855	-2.6376
C	2.8727	1.6797	-3.0325

O	3.9712	2.5379	-2.9329
C	4.3585	3.0774	-4.1985
H	-2.2740	-0.8718	1.2148
H	-3.8882	-2.6993	1.4853
H	-3.1204	-4.9494	2.2157
H	-0.7119	-5.3290	2.6889
H	0.9066	-3.4935	2.4445
H	2.3091	-1.0996	4.0164
H	4.3990	-2.3378	4.3795
H	5.5484	-3.4448	2.4718
H	4.5494	-3.3125	0.1954
H	2.4498	-2.0819	-0.1660
H	-2.0086	1.5324	1.7657
H	-3.5727	2.3836	3.4649
H	-3.0345	4.4463	4.7386
H	-0.9137	5.6602	4.2745
H	0.6461	4.8172	2.5671
H	-1.4286	3.4440	-1.1094
H	-1.8765	5.4899	-2.3992
H	-0.2999	7.4099	-2.2852
H	1.7046	7.2655	-0.8266
H	2.1543	5.2302	0.4712
H	3.2401	3.4520	-0.2008
H	5.5233	3.1725	0.7107
H	-1.5979	0.1948	6.0152
H	-1.1985	-0.9969	3.8868
H	1.6603	3.4669	7.2982
H	0.4479	4.3975	6.3121
H	5.7256	-0.0141	3.9314
H	5.9709	1.3007	5.1720
H	5.0401	1.0756	-1.2054
H	4.8277	-0.5769	-0.6271
H	1.6666	3.1811	-2.1922
H	2.9297	0.9577	-3.8522
H	4.5722	2.2746	-4.9203
H	3.5659	3.7193	-4.6097

H	5.2629	3.6688	-4.0333
H	0.3410	0.5842	-3.1886
H	-0.4678	2.1031	-2.5790
C	5.3021	-0.4304	-2.7159
O	4.8531	-1.7712	-2.9435
C	4.9840	-2.1763	-4.3105
C	4.0006	-1.4527	-5.1982
C	4.4258	-0.5789	-6.1989
C	3.4980	0.1307	-6.9608
C	2.1359	-0.0264	-6.7225
C	1.7033	-0.8997	-5.7244
C	2.6303	-1.6088	-4.9694
H	6.3973	-0.4242	-2.5911
H	5.0626	0.2045	-3.5800
H	6.0144	-2.0138	-4.6663
H	4.7842	-3.2535	-4.3125
H	5.4910	-0.4470	-6.3780
H	3.8407	0.8119	-7.7351
H	1.4116	0.5303	-7.3106
H	0.6420	-1.0262	-5.5281
H	2.2879	-2.2715	-4.1780

Post - Trans Si Si

Ru	0.5420	0.3756	-0.4030
C	0.2390	0.8019	-2.8528
P	0.6785	-0.6810	1.7125
I	0.3395	-2.3160	-1.4475
P	0.7826	2.4498	0.6091
O	2.6051	0.2950	-0.5148
C	-1.3037	0.4487	-0.5027
O	-2.4469	0.5022	-0.7206
C	2.3701	2.4089	1.4986
C	0.7425	3.9740	-0.4373
C	-0.4342	3.0971	1.8482
C	-0.5013	-2.0826	1.9312

C	2.2986	-1.4539	2.1374	C	5.3833	1.0234	4.5962
C	0.3558	0.3273	3.2312	O	3.9601	1.2327	4.6144
C	-1.8649	-1.8882	1.6894	C	3.1286	0.0758	-1.7871
C	-2.7662	-2.9328	1.8491	H	2.6941	-0.8250	-2.2615
C	-2.3166	-4.1908	2.2438	C	4.6447	-0.1238	-1.6803
C	-0.9625	-4.3897	2.4881	C	1.3016	1.5966	-2.5654
C	-0.0577	-3.3418	2.3381	C	2.7474	1.2356	-2.7372
C	2.6791	-1.5602	3.4799	O	3.5689	2.3775	-2.4661
C	3.8429	-2.2380	3.8295	C	3.5340	3.3369	-3.5148
C	4.6373	-2.8178	2.8444	H	-2.2350	-0.9182	1.3776
C	4.2545	-2.7256	1.5089	H	-3.8213	-2.7637	1.6543
C	3.0912	-2.0500	1.1535	H	-3.0194	-5.0115	2.3563
C	-1.6880	2.5296	2.0543	H	-0.5996	-5.3677	2.7909
C	-2.5911	3.1222	2.9346	H	0.9965	-3.5188	2.5217
C	-2.2467	4.2830	3.6171	H	2.0674	-1.1203	4.2608
C	-0.9920	4.8559	3.4135	H	4.1220	-2.3153	4.8770
C	-0.0949	4.2726	2.5292	H	5.5470	-3.3464	3.1170
C	-0.3902	4.1173	-1.2502	H	4.8623	-3.1829	0.7331
C	-0.5700	5.2617	-2.0155	H	2.7951	-1.9812	0.1149
C	0.3785	6.2827	-1.9772	H	-1.9632	1.6130	1.5475
C	1.4942	6.1545	-1.1574	H	-3.5639	2.6643	3.0900
C	1.6758	5.0092	-0.3834	H	-2.9504	4.7406	4.3067
C	3.5529	2.6975	0.8168	H	-0.7115	5.7626	3.9423
C	4.8103	2.5278	1.4065	H	0.8808	4.7270	2.3789
C	4.8272	2.0247	2.6862	H	-1.1345	3.3234	-1.2861
C	3.6582	1.6911	3.3568	H	-1.4515	5.3558	-2.6430
C	2.4045	1.8372	2.7966	H	0.2424	7.1767	-2.5789
C	1.2126	1.4136	3.5671	H	2.2311	6.9513	-1.1106
C	0.9047	2.0951	4.7253	H	2.5402	4.9387	0.2676
C	-0.1906	1.7898	5.5222	H	3.5106	3.0070	-0.2213
C	-1.0210	0.7385	5.2229	H	5.7235	2.7551	0.8675
C	-0.7164	0.0096	4.0653	H	-1.8741	0.4848	5.8426
O	1.5404	3.2028	5.2133	H	-1.3497	-0.8349	3.8259
C	0.9148	3.4819	6.4785	H	1.5895	3.1817	7.2928
O	-0.2894	2.6910	6.5433	H	0.6540	4.5428	6.5284
O	5.9076	1.7897	3.4946	H	5.5892	-0.0434	4.4217

H	5.8159	1.3872	5.5312	C	4.1617	0.1037	-6.3605
H	5.0890	0.7702	-1.2284	C	3.1271	0.8555	-6.9171
H	4.8246	-0.9583	-0.9915	C	1.8038	0.4807	-6.7060
H	1.1243	2.6358	-2.3166	C	1.5176	-0.6490	-5.9391
H	2.9152	0.9115	-3.7801	C	2.5502	-1.3918	-5.3793
H	3.8565	2.8897	-4.4687	H	6.4275	-0.4137	-2.8780
H	2.5286	3.7651	-3.6535	H	5.0882	0.3831	-3.7311
H	4.2220	4.1410	-3.2393	H	5.9684	-1.4831	-5.2762
H	0.3698	-0.1876	-3.2742	H	4.8703	-2.8762	-5.1157
H	-0.7615	1.2233	-2.8860	H	5.1964	0.3986	-6.5232
C	5.3318	-0.4040	-3.0015	H	3.3561	1.7346	-7.5135
O	4.9030	-1.6841	-3.4861	H	0.9958	1.0639	-7.1390
C	4.9809	-1.8059	-4.9079	H	0.4862	-0.9493	-5.7755
C	3.8835	-1.0226	-5.5863	H	2.3247	-2.2584	-4.7618

References

- 1) Anderson, K.R.; Atkinson, S. L.G.; Fujiwara, T.; Giles, M. E.; Matsumoto, T.; Merifield, E.; Singleton, J. T.; Saito, T.; Sotoguchi, T.; Tornos, J. A.; Way, E. L. Routes for the Synthesis of (2S)-2-Methyltetrahydropyran-4-one from Simple Optically Pure Building Blocks. *Org. Process Res. Dev.* **2010**, *14*, 58-71.
- 2) Packard, G. K.; Hu, Y.; Vescovi, A.; Rychnovsky, S. D. Synthesis of Rimocidinolide Methyl Ester, the Aglycone of (+)-Rimocidin. *Angew. Chem. Int. Ed.* **2004**, *43*, 2822-2826.
- 3) Mans, D. M.; Pearson, W. H. Total Synthesis of (+)-Cocaine via Desymmetrization of a *meso*-Dialdehyde. *Org. Lett.* **2004**, *6*, 3305-3308.
- 4) Brito, G. A.; Jung, W. -O.; Yoo, M. Krische, M. J. Enantioselective Iridium-Catalyzed Allylation of Acetylenic Ketones via 2-Propanol-Mediated Reductive Coupling of Allyl Acetate: C14-C23 of Pladienolide D. *Angew. Chem. Int. Ed.* **2019**, *58*, 18803-18807.
- 5) Xiang, M.; Pfaffinger, D. E.; Ortiz, E.; Brito, G. A.; Krische, M. J. Enantioselective Ruthenium-BINAP-Catalyzed Carbonyl Reductive Coupling of Alkoxyallenes: Convergent Construction of *syn-sec,tert*-Diols via (Z)- σ -Allylmetal Intermediates. *J. Am. Chem. Soc.* **2021**, *143*, 8849-8854.
- 6) Schempp, T. T.; Krische, M. J. Total Synthesis of the Acetyl CoA Carboxylase Inhibitor Soraphen A: Asymmetric Tsuji Reduction Enables Successive Olefin Metathesis. *J. Am. Chem. Soc.* **2022**, *144*, 1016-1022.
- 7) Cao, H. -Q.; Liu, H. -N.; Liu, Z.-Y.; Qiao, B.; Zhang, F. -G.; Ma, J. -A. Silver-Promoted Direct Phosphorylation of Bulky C(sp²)-H Bond to Build Fully Substituted β -Phosphonodehydroamino Acids. *Org. Lett.* **2020**, *22*, 6414-6419.
- 8) Andrus, M. B.; Shih, T. -L. Synthesis of Tuckolide, a New Cholesterol Biosynthesis Inhibitor. *J. Org. Chem.* **1996**, *61*, 8780-8785.
- 9) Kawabata, T.; Kimura, Y.; Ito, Y.; Terashima, S.; Sasaki, A.; Sunagawa, M. A Novel and Efficient Synthesis of the Key Intermediate of 1 β -methylcarbapenem antibiotics from (S)-methyl 3-hydroxy-2-methylpropionate. *Tetrahedron Letters*. **1986**, *27*, 6241-6244.
- 10) Canova, S.; Bellosta, V.; Mignani, S.; Bigot, A.; Cossy, J. Rearrangement of Homoallylic Alcohols Induced by DAST. *Org. Lett.* **2006**, *8*, 10, 2091-2094.
- 11) (a) Sheldrick, G. M. ShelXT-Integrated Space-Group and Crystal-Structure Determination. *Acta Cryst.* **2015**, *A71*, 3-8. (b) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. Olex2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Cryst.* **2009**, *42*, 339-341. (c) Sheldrick, G. M. Crystal Structure Refinement with ShelXL. *Acta Cryst.* **2015**, *C71*, 3-8.
- 12) Bannwarth, C.; Ehlert, S.; Grimme, S. GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.* **2019**, *15*, 1652-1671.
- 13) Pracht, P.; Grimme, S.; Bannwarth, C.; Bohle, F.; Ehlert, S.; Feldmann, G.; Gorges, J.; Müller, M.; Neudecker, T.; Plett, C.; Spicher, S.; Steinbach, P.; Wesolowski, P. A.; Zeller, F. CREST—A program for the exploration of low-energy molecular chemical space. *The Journal of Chemical Physics* **2024**, *160*, 114110.

- 14) Ehlert, S.; Stahn, M.; Spicher, S.; Grimme, S. Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. *J. Chem. Theory Comput.* **2021**, *17*, 4250–4261.
- 15) Neese, F. Software Update: The ORCA Program System—Version 6.0. *WIREs Comput Mol Sci.* **2025**, *15*, e70019.
- 16) Pellegrini, A.; Righi, P.; Mazzanti, A.; Mancinelli, M. Ensemble Analyzer: An OpenSource Python Framework for Automated Conformer Ensemble Refinement, 2026.
- 17) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.
- 18) Caldeweyher, E.; Mewes, J.-M.; Ehlert, S.; Grimme, S. Extension and evaluation of the D4 London-dispersion model for periodic systems. *Phys. Chem. Chem. Phys.* **2020**, *22*, 8499–8512.
- 19) Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
- 20) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B.* **2009**, *113*, 6378–6396.
- 21) Grimme, S.; Hansen, A.; Ehlert, S.; Mewes, J.-M. r²SCAN-3c: A "Swiss army knife" composite electronic-structure method. *J. Chem. Phys.* **2021**, *154*, 064103.
- 22) Mardirossian, N.; Head-Gordon, M. ω B97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. *Phys. Chem. Chem. Phys.* **2014**, *16*, 9904–9924.
- 23) Müller, M.; Hansen, A.; Grimme, S. ω B97X-3c: A composite range-separated hybrid DFT method with a molecule-optimized polarized valence double- ζ basis set. *J. Chem. Phys.* **2023**, *158*, 014103.
- 24) Ortiz, E.; Shezaf, J. Z.; Chang, Y.-H.; Gonçalves, T. P.; Huang, K.-W.; Krische, M. J. Understanding Halide Counterion Effects in Enantioselective Ruthenium-Catalyzed Carbonyl (α -Aryl)allylation: Alkynes as Latent Allenes and Trifluoroethanol-Enhanced Turnover in The Conversion of Ethanol to Higher Alcohols via Hydrogen Auto-transfer. *J. Am. Chem. Soc.* **2021**, *143*, 16709–16717.
- 25) Zimmerman, H. E.; Traxler, M. D. The stereochemistry of the Ivanov and Reformatsky reactions. *J. Am. Chem. Soc.* **1957**, *79*, 1920–1923.
- 26) Contreras-García, J.; Johnson, E. R.; Keinan, S.; Chaudret, R.; Piquemal, J.-P.; Beratan, D. N.; Yang, W. NCIPLOT: a program for plotting non-covalent interaction regions. *J. Chem. Theory Comput.* **2011**, *7*, 625–632.
- 27) Schaefer, A. J.; Ingman, V. M.; Wheeler, S. E. SEQCROW: A ChimeraX bundle to facilitate quantum chemical applications to complex molecular systems. *J. Comput. Chem.* **2021**, *42*, 1750–1754.

- 28) Pettersen, E. F.; Goddard, T. D.; Huang, C. C.; Couch, G. S.; Greenblatt, D. M.; Meng, E. C.; Ferrin, T. E. UCSF Chimera--a visualization system for exploratory research and analysis. *J. Comput. Chem.* **2004**, 25, 1605–1612.