Supporting Information

Kinetic Resolution of *tert*-alcohols through S_N2' Reaction Catalyzed by Chiral Bisphophoric Acid/Silver(I) Salt-Combined System

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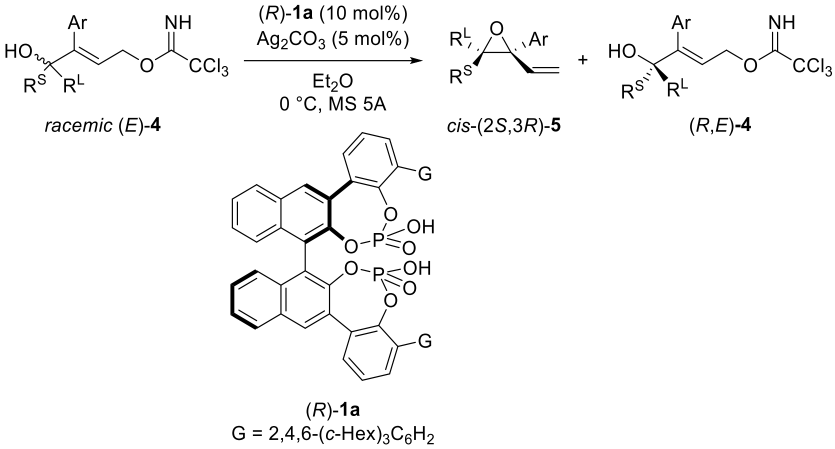
Contents

1. General Information

All reactions were carried out under nitrogen atmosphere in flame-dried glassware. Dichloromethane (CH_2Cl_2) and toluene were supplied from KANTO Chemical Co., Inc. as "Dehydrated solvent system". Other solvents and reagents were purchased from commercial suppliers and used without further purification. Purification of reaction products was carried out by flash column chromatography using silica gel 60 N ((Merck 40-63 μm). Analytical thin layer chromatography (TLC) was performed on Merck precoated TLC plates (silica gel 60 GF 254, 0.25 mm). ^{1}H NMR spectra were recorded on a JEOL ECA-600 (600 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane or solvent resonance as the internal standard ($CDCl_3$: 7.26 ppm, TMS: 0.00 ppm). ^{13}C NMR spectra were recorded on a JEOL ECA-600 (151 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: 77.16 ppm). ^{19}F NMR spectra were recorded on JEOL ECA-600 (565 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from the $C_6H_5CF_3$ (-67.2 ppm) resonance as the external standard. Infrared spectra were recorded on a Jasco FT/IR-4100 spectrometer. Chiral stationary phase HPLC analysis was performed on a Jasco LC-2000 Plus Series system with DACIEL chiral analytical column (4.6 mmΦ* 250 mm length). Optical rotations were measured on a Jasco P-1020 digital polarimeter with a sodium lamp and reported as follows; $[\alpha]^{T\,°C}_{D}$ (*c* = g/100 mL, solvent, % ee). High resolution mass spectra analysis was performed on a Bruker Daltonics solariX 9.4T FT-ICR-MS spectrometer and a JEOL JMS-T100GCV Time-of-Flight Mass Spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University.

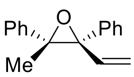
2. Enantioselective Reaction of

Representative procedure for the kinetic resolution of *tert*-alcohols



To a mixture of MS 5Å (40.0 mg), (*R*)-**1a** (12.4 mg, 0.01 mmol, 10 mol%) and Ag_2CO_3 (1.4 mg, 0.005 mmol, 5 mol%) was added Et_2O (0.5 mL). The reaction mixture was stirred at room temperature for 15 min and then cooled at 0 °C. To the reaction mixture was added a solution of racemic (*E*)-**4** (0.1 mmol) in Et_2O (0.5 mL) at the same temperature and the reaction mixture was stirred for 96 h. The reaction mixture was quenched with NEt_3 (10 μL) and directly purified by flash column chromatography (Hexane/EtOAc = 10:1) to give **5** and (*R*,*E*)-**4**. The enantiomeric excess was determined by chiral stationary phase HPLC analysis.

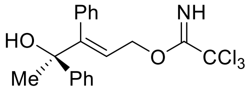
(2*S*,3*R*)-2-methyl-2,3-diphenyl-3-vinyloxirane (5a)



5a

48% yield (11.3 mg); colorless oil; $[\alpha]_D^{26}$ +69.5 (*c* 5.0, $CHCl_3$, 98% ee); R_f = 0.72 (Hexane/EtOAc= 4/1); ^1H NMR (600 MHz, $CDCl_3$): δ 7.15-7.11 (m, 4H), 7.08 (t, *J* = 7.6 Hz, 4H), 7.03-7.00 (m, 2H), 6.30 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.40-5.33 (m, 2H), 1.80 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 140.5, 137.6, 136.3, 127.6, 127.5, 127.5, 126.8, 126.7, 126.4, 118.9, 71.5, 69.5, 20.5; IR (ATR): 2954, 2922, 2868, 2853, 1741, 1459, 1376, 803, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{17}H_{16}NaO$ 259.1093, found: 259.1092; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5/0.5, 1.0 mL/min, 40 °C, 220 nm) 5.7 min (minor), 6.2 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

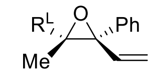
(*R*,*E*)-4-hydroxy-3,4-diphenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4a)



4a

52% yield (20.7 mg); colorless oil; $[\alpha]_D^{25}$ –31.7 (*c* 0.79, $CHCl_3$, 88% ee); R_f = 0.32 (Hexane/EtOAc= 4/1); ^1H NMR (600 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.43-7.41 (m, 2H), 7.32 (td, *J* = 7.6, 1.8 Hz, 2H), 7.26 (tt, *J* = 7.1, 1.8 Hz, 1H), 7.23-7.17 (m, 3H), 6.77-6.75 (m, 2H), 6.28 (t, *J* = 6.9 Hz, 1H), 4.56 (d, *J* = 6.9 Hz, 2H), 2.02 (s, 1H), 1.72 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.7, 152.3, 145.5, 136.5, 129.5, 128.2, 128.1, 127.7, 127.3, 126.0, 120.5, 91.6, 77.05, 67.3, 28.9; IR (ATR): 3338, 2981, 1660, 1298, 1073, 977, 822, 796, 700, 648 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{19}H_{18}Cl_3NNaO_2$ 420.0295, found: 420.0295; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 9.6 min (minor), 11.0 min (major). The absolute configurations were assigned as (*R*) by derivatization.

(2*S*,3*R*)-2-methyl-3-phenyl-2-(4-(trifluoromethyl)phenyl)-3-vinyloxirane (5b)

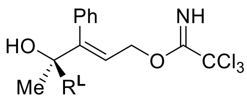


5b

(R^L = 4-$CF_3C_6H_4$)

34% yield (10.3 mg); colorless oil; $[\alpha]_D^{27}$ +136.3 (*c* 0.82, $CHCl_3$, 94% ee); R_f = 0.45 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.33 (d, *J* = 8.2 Hz, 2H), 7.26-7.24 (m, 2H), 7.10-7.07 (m, 4H), 7.04 (tt, *J* = 6.0, 2.4 Hz, 1H), 6.28 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.42-5.33 (m, 2H), 1.79 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 144.6, 137.0, 135.7, 129.0 (q, *J* = 31.9Hz), 127.8, 127.4, 127.2, 126.8, 124.6 (q, *J* = 4.4 Hz), 124.2 (q, *J* = 271.8 Hz), 119.5, 71.7, 69.0, 20.2; IR (ATR): 2954, 2922, 2868, 2853, 1734, 1459, 1376, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{18}H_{15}F_3NaO$ 327.0967, found: 327.0966; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.9:0.1, 1.0 mL/min, 40 °C, 220 nm) 6.1 min (minor), 6.5 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2S,3*R*) by derivatization of **4a** and NOE analysis.

(*R*,*E*)-4-hydroxy-3-phenyl-4-(4-(trifluoromethyl)phenyl)pent-2-en-1-yl 2,2,2-trichloroacetimidate (4b)

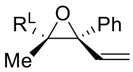


4b

(R^L = 4-$CF_3C_6H_4$)

47% yield (21.9 mg); colorless oil; $[\alpha]_D^{25}$ –17.9 (*c* 1.9, $CHCl_3$, 81% ee); R_f = 0.35 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.23 (s, 1H), 7.56 (q, *J* = 8.9 Hz, 4H), 7.27-7.20 (m, 4H), 6.78-6.76 (m, 2H), 6.27 (t, *J* = 6.5 Hz, 1H), 4.59-4.53 (m, 2H), 2.06 (s, 1H), 1.75 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.7, 151.4, 149.7, 135.9, 129.52 (q, *J* = 33.2 Hz), 129.51, 128.4, 128.1, 126.4, 125.2 (q, *J* = 4.4 Hz), 121.9 (q, *J* = 273.5Hz), 121.5, 91.6, 67.0, 29.2, one carbon was not found due to overlapping; IR (ATR): 3340, 2981, 1661, 1324, 1164, 1123, 1072, 797, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{20}H_{17}Cl_3F_3NNaO_2$ 488.0169, found: 488.0168.; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 8.5 min (minor), 10.1 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

(2*S*,3*R*)-2-(4-chlorophenyl)-2-methyl-3-phenyl-3-vinyloxirane (5c)

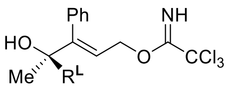


5c

(R^L = 4-ClC_6H_4)

43% yield (11.6 mg); colorless oil; $[\alpha]_D^{26}$ +175.05 (*c* 0.7, $CHCl_3$, 94% ee); R_f = 0.32 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.10-7.09 (m, 4H), 7.07-7.03 (m, 5H), 6.26 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.40-5.31 (m, 2H), 1.76 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 139.1, 137.3, 135.9, 132.5, 127.8, 127.8, 127.7, 127.4, 127.1, 119.3, 71.6, 68.9, 20.3; IR (ATR): 2954, 2922, 2868, 1735, 1460, 1376, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{17}H_{15}ClNaO$ 293.0704, found: 293.0703; HPLC analysis: Chiralpak OD-3 column (Hexane:^{i}PrOH = 99.9/0.1, 1.0 mL/min, 40 °C, 220 nm) 8.4 min (minor), 9.1 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

(*R*,*E*)-4-(4-chlorophenyl)-4-hydroxy-3-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4c)

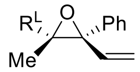


4c

(R^L = 4-ClC_6H_4)

45% yield (19.5 mg); colorless oil; $[\alpha]_D^{25}$ –28.9 (*c* 1.58, $CHCl_3$, 92% ee); R_f = 0.35 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.21 (s, 1H), 7.36 (td, *J* = 5.5, 3.2 Hz, 2H), 7.29 (dt, *J* = 8.9, 2.2 Hz, 2H), 7.25-7.20 (m, 3H), 6.77 (td, *J* = 4.8, 2.7 Hz, 2H), 6.26 (t, *J* = 6.5 Hz, 1H), 4.55 (dd, *J* = 6.9, 1.4 Hz, 2H), 1.99 (s, 1H), 1.71 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.6, 151.8, 144.1, 136.2, 133.2, 129.5, 128.4, 127.9, 127.5, 120.9, 91.5, 76.7, 67.1, 29.1; IR (ATR): 3338, 2978, 1661, 1490, 1300, 1219, 1091, 1013, 978, 771, 703, 649 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{19}H_{17}Cl_4NNaO_2$ 453.9906, found: 453.9905; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 9.8 min (minor), 11.8 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

(2*S*,3*R*)-2-methyl-3-phenyl-2-(p-tolyl)-3-vinyloxirane (5d)

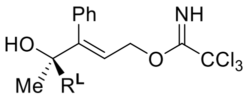


5d

(R^L = 4-MeC_6H_4)

40% yield (10.0 mg); colorless oil; $[\alpha]_D^{27}$ +137.4 (*c* 0.64, $CHCl_3$, 94% ee); R_f = 0.43 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.14-7.08 (m, 4H), 7.05-7.01 (m, 3H), 6.88 (d, *J* = 7.6 Hz, 2H), 6.29 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.38-5.30 (m, 2H), 2.17 (s, 3H), 1.77 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 137.8, 137.5, 136.5, 136.3, 128.3, 127.6, 127.5, 126.7, 126.3, 118.8, 71.6, 69.4, 21.2, 20.6; IR (ATR): 2955, 2924, 2854, 1712, 1446, 812, 771, 700 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{18}H_{18}NaO$ 273.1250, found: 273.1249.; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5/0.5, 1.0 mL/min, 40 °C, 220 nm) 4.6 min (minor), 4.8 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

(*R*,*E*)-4-hydroxy-3-phenyl-4-(p-tolyl)pent-2-en-1-yl 2,2,2-trichloroacetimidate (4d)

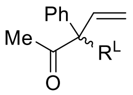


4d

(R^L = 4-MeC_6H_4)

40% yield (16.5 mg); colorless oil; $[\alpha]_D^{25}$ –9.14 (*c* 1.44, $CHCl_3$, 85% ee); R_f = 0.36 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.32-7.30 (m, 2H), 7.24-7.18 (m, 3H), 7.13 (d, *J* = 7.6 Hz, 2H), 6.78-6.77 (m, 2H), 6.28 (t, *J* = 6.9 Hz, 1H), 4.56 (d, *J* = 6.9 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.7, 152.5, 142.5, 136.9, 136.6, 129.5, 128.9, 128.1, 127.7, 125.9, 120.2, 91.6, 76.9, 67.3, 28.8, 21.2; IR (ATR): 3340, 2979, 1660, 1291, 1075, 976, 819, 794, 772, 703, 647 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{20}H_{20}Cl_3NNaO_2$ 434.0452, found: 434.0451.; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 9.5 min (minor), 11.6 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

3-(4-methoxyphenyl)-3-phenylpent-4-en-2-one (6e)

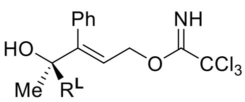


6e

(R^L = 4-$MeOC_6H_4$)

48% yield (12.8 mg); colorless oil; R_f = 0.58 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.33 (t, *J* = 7.6 Hz, 2H), 7.30-7.27 (m, 1H), 7.14-7.12 (m, 2H), 7.06-7.04 (m, 2H), 6.88-6.86 (m, 2H), 6.75 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.39 (d, *J* = 11.7 Hz, 1H), 4.75 (d, *J* = 17.2 Hz, 1H), 3.81 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 206.9, 158.7, 140.8, 140.5, 132.4, 131.1, 129.9, 128.3, 127.3, 118.5, 113.6, 70.1, 55.4, 28.5; IR (ATR): 3085, 3057, 3001, 2954, 2927, 2868, 2836, 1708, 1629, 1608, 1509, 1462, 1445, 1295, 1249, 1182, 1161, 1033, 928, 827 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{18}H_{18}NaO_2$ 289.3298, found: 289.3293; Compound was obtained as *racemic*.

(*R*,*E*)-4-hydroxy-4-(4-methoxyphenyl)-3-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4e)

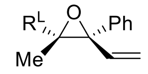


4e

(R^L = 4-$MeOC_6H_4$)

11% yield (4.7 mg); colorless oil; $[\alpha]_D^{25}$ –67.5 (*c* 0.98, $CHCl_3$, 67% ee); R_f = 0.30 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.34 (td, *J* = 5.8, 3.7 Hz, 2H), 7.24-7.18 (m, 3H), 6.85 (td, *J* = 6.0, 3.7 Hz, 2H), 6.77-6.75 (m, 2H), 6.28 (t, *J* = 6.9 Hz, 1H), 4.55 (d, *J* = 6.9 Hz, 2H), 3.82 (s, 3H), 1.95 (s, 1H), 1.69 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.7, 158.8, 152.5, 137.5, 136.7, 129.5, 128.1, 127.7, 127.3, 120.1, 113.5, 91.5, 76.7, 67.3, 55.4, 28.8; IR (ATR): 3337, 2935, 2636, 2310, 1725, 1661, 1249, 1086, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{20}H_{20}Cl_3NNaO_3$ 450.0401, found: 450.0401.; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 14.2 min (major), 17.7 min (minor). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

(2*S*,3*R*)-2-(3-chlorophenyl)-2-methyl-3-phenyl-3-vinyloxirane (5f)

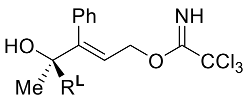


5f

(R^L = 3-ClC_6H_4)

40% yield (10.8 mg); colorless oil; $[\alpha]_D^{27}$ +80.1 (*c* 0.56, $CHCl_3$, 95% ee); R_f = 0.33 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.14 (d, *J* = 1.4 Hz, 1H), 7.11 (d, *J* = 4.1 Hz, 4H), 7.05 (q, *J* = 4.4 Hz, 1H), 7.00-6.98 (m, 3H), 6.26 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.41-5.32 (m, 2H), 1.77 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 142.6, 137.1, 135.8, 133.6, 128.9, 127.7, 127.4, 127.1, 127.0, 126.7, 124.6, 119.4, 71.6, 68.8, 20.2; IR (ATR): 2957, 2923, 2869, 1733, 1459, 1261, 1081, 772 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{17}H_{15}ClNaO$ 293.0704, found: 293.0703.; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.9/0.1, 1.0 mL/min, 40 °C, 220 nm) 9.3 min (minor), 11.8 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

(*R*,*E*)-4-(3-chlorophenyl)-4-hydroxy-3-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4f)

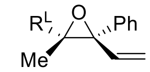


4f

(R^L = 3-ClC_6H_4)

45% yield (19.5 mg); colorless oil; $[\alpha]_D^{21}$ –49.1 (*c* 1.7, $CHCl_3$, 85% ee); R_f = 0.34 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.23 (s, 1H), 7.44 (s, 1H), 7.29 (qd, *J* = 4.4, 2.2 Hz, 1H), 7.26-7.21 (m, 5H), 6.79 (dd, *J* = 8.2, 1.4 Hz, 2H), 6.26 (t, *J* = 6.5 Hz, 1H), 4.57 (q, *J* = 3.4 Hz, 2H), 2.01 (s, 1H), 1.71 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.6, 151.6, 147.7, 136.1, 134.2, 129.5, 129.4, 128.2, 127.9, 127.4, 126.3, 124.2, 121.2, 91.5, 76.7, 67.1, 28.9; IR (ATR): 3339, 2980, 2310, 1725, 1661, 1076, 795, 703 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{19}H_{17}Cl_4NNaO_2$ 453.9906, found: 453.9905.; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 98:2, 1.0 mL/min, 40 °C, 220 nm) 18.5 min (minor), 19.4 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

(2*S*,3*R*)-2-methyl-3-phenyl-2-(m-tolyl)-3-vinyloxirane (5g)

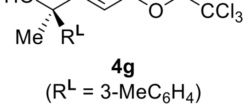


5g

(R^L = 3-MeC_6H_4)

41% yield (10.3 mg); colorless oil; $[\alpha]_D^{27}$ +126.1 (*c* 0.5, $CHCl_3$, 94% ee); R_f = 0.44 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.13-7.07 (m, 4H), 7.03-7.01 (m, 1H), 6.97-6.91 (m, 3H), 6.82 (d, *J* = 7.6 Hz, 1H), 6.29 (dd, *J* = 17.2, 10.3 Hz, 1H), 5.39-5.31 (m, 2H), 2.17 (s, 3H), 1.77 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 140.3, 137.6, 137.1, 136.3, 127.5, 127.5, 127.1, 126.8, 123.5, 118.9, 71.5, 69.5, 21.4, 20.5; IR (ATR): 2953, 2922, 2868, 2852, 1734, 1459, 1376, 772 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{18}H_{18}NaO$ 273.1250, found: 273.1249.; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5/0.5, 1.0 mL/min, 40 °C, 220 nm) 5.2 min (minor), 5.7 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

(*R*,*E*)-4-hydroxy-3-phenyl-4-(m-tolyl)pent-2-en-1-yl 2,2,2-trichloroacetimidate (4g)

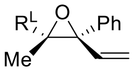


4g

(R^L = 3-MeC_6H_4)

43% yield (17.7 mg); colorless oil; $[\alpha]_D^{25}$ –59.1 (*c* 1.72, $CHCl_3$, 78% ee); R_f = 0.35 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.19 (s, 1H), 7.25 (s, 1H), 7.24-7.17 (m, 5H), 7.09-7.07 (m, 1H), 6.77 (dt, *J* = 8.2, 1.7 Hz, 2H), 6.27 (t, *J* = 6.5 Hz, 1H), 4.56 (dd, *J* = 6.9, 1.4 Hz, 2H), 2.34 (s, 3H), 2.06 (s, 1H), 1.70 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.6, 152.4, 145.4, 137.8, 136.5, 129.5, 128.1, 128.1, 127.7, 126.6, 123.0, 120.4, 91.5, 76.9, 67.3, 28.9, 21.7; IR (ATR): 3341, 2954, 2923, 1661, 1294, 1077, 976, 821, 794, 704, 648 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{20}H_{20}Cl_3NNaO_2$ 434.0452, found: 434.0451.; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 8.7 min (minor), 9.7 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

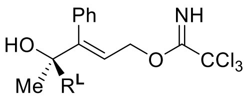
(2*S*,3*R*)-2-(3-methoxyphenyl)-2-methyl-3-phenyl-3-vinyloxirane (5h)



5h
(R^L = 3-$MeOC_6H_4$)

45% yield (10.9 mg); colorless oil; $[\alpha]_D^{27}$ +120.5 (*c* 0.8, $CHCl_3$, 90% ee); R_f = 0.67 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.14-7.12 (m, 2H), 7.10-7.08 (m, 2H), 7.05-6.99 (m, 2H), 6.76-6.75 (m, 1H), 6.66 (q, *J* = 1.4 Hz, 1H), 6.57-6.55 (m, 1H), 6.28 (dd, *J* = 17.2, 10.3 Hz, 1H), 5.39-5.31 (m, 2H), 3.63 (s, 3H), 1.78 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 158.9, 142.1, 137.5, 136.2, 128.6, 127.6, 127.5, 126.9, 119.0, 118.9, 112.7, 111.9, 71.6, 69.3, 55.2, 20.4; IR (ATR): 2954, 2923, 2852, 1734, 1602, 1454, 1287, 1216, 1046, 772, 699 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{18}H_{18}NaO_2$ 289.1199, found: 289.1199; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5:0.5, 1.0 mL/min, 40 °C, 220 nm) 6.8 min (minor), 7.2 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5a**.

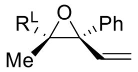
(*R*,*E*)-4-hydroxy-4-(3-methoxyphenyl)-3-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4h)



4h
(R^L = 3-$MeOC_6H_4$)

37% yield (15.9 mg); colorless oil; $[\alpha]_D^{25}$ –10.2 (*c* 1.38, $CHCl_3$, 94% ee); R_f = 0.30 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.26-7.18 (m, 4H), 7.01-6.99 (m, 2H), 6.82-6.78 (m, 3H), 6.27 (t, *J* = 6.5 Hz, 1H), 4.56 (dd, *J* = 6.9, 1.4 Hz, 2H), 3.78 (s, 3H), 2.10 (s, 1H), 1.71 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): 162.6, 159.6, 152.12, 147.3, 136.4, 129.5, 129.2, 128.1, 127.8, 120.5, 118.4, 112.6, 111.8, 91.5, 76.9, 67.2, 55.4, 28.9; IR (ATR): 3338, 2938, 1661, 1598, 1486. 1288, 1252, 1074, 976, 794, 774, 703, 647 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{20}H_{20}Cl_3NNaO_3$ 450.0401, found: 450.0400; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 95/5, 40 °C, 220 nm) 11.4 min (major), 14.2 min (minor). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

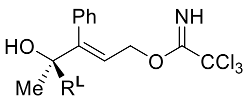
(2*S*,3*R*)-2-(2-chlorophenyl)-2-methyl-3-phenyl-3-vinyloxirane (5i)



5i
(R^L = 2-ClC_6H_4)

37% yield (10.3 mg); colorless oil; $[\alpha]_D^{25}$ +140.2 (*c* 0.1, $CHCl_3$, 94% ee); R_f = 0.32 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.45 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.30-7.28 (m, 2H), 7.10-7.06 (m, 3H), 7.04-6.97 (m, 3H), 6.44 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.48-5.45 (m, 2H), 1.76 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 138.7, 136.9, 134.7, 131.2, 128.9, 128.9, 128.5, 127.2, 127.0, 126.8, 126.3, 119.0, 70.7, 70.1, 19.4; IR (ATR): 2955, 2925, 2854, 1733, 1446, 731, 699 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{17}H_{15}ClNaO$: 293.0704, found: 293.0703.; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5:0.5, 1.0 mL/min, 40 °C, 220 nm) 5.0 min (minor), 5.4 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

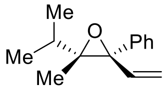
(*S*,*E*)-4-(2-chlorophenyl)-4-hydroxy-3-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4i)



4i
(R^L = 2-ClC_6H_4)

49% yield (20.0 mg); colorless oil; $[\alpha]_D^{25}$ –1.7 (*c* 1.01, $CHCl_3$, 56% ee); R_f = 0.34 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 (s, 1H), 7.50 (dd, *J* = 7.2, 2.4 Hz, 1H), 7.36 (dd, *J* = 7.2, 1.7 Hz, 1H), 7.23 (q, *J* = 3.4 Hz, 3H), 7.21-7.17 (m, 2H), 7.03 (q, *J* = 3.0 Hz, 2H), 6.05 (t, *J* = 6.9 Hz, 1H), 4.56 (d, *J* = 6.9 Hz, 2H), 3.04 (s, 1H), 1.79 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.6, 150.5, 142.2, 136.5, 132.3, 131.3, 129.5, 128.9, 128.4, 128.0, 127.7, 126.9, 122.1, 91.5, 76.9, 67.1, 27.3; IR (ATR): 3340, 2954, 2925, 1661, 1293, 1219, 1078, 796, 702 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{19}H_{17}Cl_4NNaO_2$ 453.9906, found.: 453.9905; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 10.8 min (minor), 12.3 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

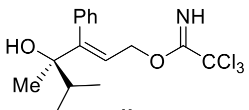
(2*S*,3*R*)-2-isopropyl-2-methyl-3-phenyl-3-vinyloxirane (5j)



5j

32% yield (7.9 mg); colorless oil; $[\alpha]_D^{27}$ +74.4 (*c* 0.1, $CHCl_3$, 92% ee); R_f = 0.72 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.36-7.32 (m, 4H), 7.27-7.25 (m, 2H), 6.18 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.28-5.20 (m, 2H), 1.28 (s, 3H), 1.17-1.12 (m, 1H), 0.96 (d, *J* = 6.9 Hz, 3H), 0.74 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 138.7, 136.7, 128.1, 127.1, 127.1, 117.9, 71.8, 71.3, 31.4, 17.9, 17.8, 11.7; IR (ATR): 2953, 2922, 2868, 2853, 1734, 1460, 1376, 772 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{14}H_{18}NaO$ 225.1250, found: 225.1249.; HPLC analysis: Chiralpak IC-3 column (Hexane = 100, 1.0 mL/min, 40 °C, 220 nm) 10.0 min (minor), 11.6 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

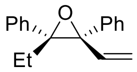
(*R*,*E*)-4-hydroxy-4,5-dimethyl-3-phenylhex-2-en-1-yl 2,2,2-trichloroacetimidate (4j)



4j

52% yield (18.2 mg); colorless oil; $[\alpha]_D^{25}$ +7.5 (*c* 1.69, $CHCl_3$, 50% ee); R_f = 0.34 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 (s, 1H), 7.35-7.29 (m, 3H), 7.16 (q, *J* = 2.7 Hz, 2H), 6.09 (t, *J* = 6.5 Hz, 1H), 4.49 (d, *J* = 6.2 Hz, 2H), 1.79-1.74 (m, 1H), 1.41 (s, 1H), 1.33 (s, 3H), 0.97 (d, *J* = 6.9 Hz, 3H), 0.93 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.6, 152.8, 137.5, 129.4, 128.3, 127.5, 120.5, 91.6, 76.9, 67.3, 33.9, 24.2, 17.1, 17.1; IR (ATR): 3343, 2972, 2876, 1724, 1661, 1370, 1296, 1219, 1075, 977, 772, 707 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{16}H_{20}Cl_3NNaO_2$ 386.0452, found: 386.0452; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 6.6 min (major), 7.1 min (minor). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

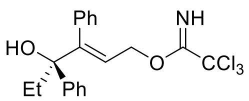
(2*S*,3*R*)-2-ethyl-2,3-diphenyl-3-vinyloxirane (5k)



5k

49% yield (12.3 mg); colorless oil; $[\alpha]_D^{27}$ +15.0 (*c* 0.98, $CHCl_3$, 95% ee); R_f = 0.73 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.12-7.11 (m, 4H), 7.07 (td, *J* = 7.6, 3.7 Hz, 4H), 7.02-6.99 (m, 2H), 6.35 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.39-5.36 (m, 2H), 2.16 (td, *J* = 14.4, 7.1 Hz, 1H), 2.01 (td, *J* = 14.3, 7.1 Hz, 1H), 0.93 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 138.4, 138.0, 135.9, 129.9, 127.5, 127.5, 127.2, 127.2, 126.7, 126.7, 118.6, 73.9, 71.8, 26.0, 9.5; IR (ATR): 2954, 2922, 2852, 1732, 1461, 1376, 1217, 759, 698 cm^{-1}; HRMS(ESI) *m/z*: $[M+Na]^+$ Calcd for $C_{18}H_{18}NaO$ 273.1250, found: 273.1249.; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5/0.5, 1.0 mL/min, 40 °C, 220 nm) 4.6 min (minor), 5.1 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

(*R*,*E*)-4-hydroxy-3,4-diphenylhex-2-en-1-yl 2,2,2-trichloroacetimidate (4k)

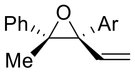


4k

39% yield (16.1 mg); colorless oil; $[\alpha]_D^{25}$ -16.7 (*c* 1.48, $CHCl_3$, 98% ee); R_f = 0.32 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.38-7.36 (m, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.27-7.21 (m, 2H), 7.17 (t, *J* = 7.6 Hz, 2H), 6.71 (d, *J* = 6.9 Hz, 2H), 6.27 (t, *J* = 6.5 Hz, 1H), 4.55 (d, *J* = 6.9 Hz, 2H), 2.06 (td, *J* = 7.9, 6.6 Hz, 2H), 1.91 (d, *J* = 2.1 Hz, 1H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (151

MHz, $CDCl_3$): δ 162.6, 151.4, 144.3, 136.5, 129.5, 128.1, 128.1, 127.7, 127.2, 126.5, 120.8, 91.5, 79.2, 67.3, 32.4, 7.9; IR (ATR): 3340, 2955, 2925, 1661, 1291, 1076, 976, 795, 771, 700, 648 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{20}H_{20}Cl_3NNaO_2$ 434.0452, found: 434.0452.; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 8.1 min (minor), 9.0 min (major). Configuration Assignment: The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

(2*R*,3*S*)-2-(4-methoxyphenyl)-3-methyl-3-phenyl-2-vinyloxirane (5l)

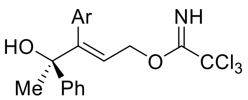


5l

(Ar = 4-MeOC_6H_4)

44% yield (11.7 mg); colorless oil; $[\alpha]_D^{26}$ +266.3 (*c* 0.3, $CHCl_3$, 86% ee); R_f = 0.68 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.14-7.13 (m, 2H), 7.10-7.08 (m, 2H), 7.02 (qd, *J* = 6.0, 4.0 Hz, 3H), 6.61 (td, *J* = 5.8, 3.4 Hz, 2H), 6.27 (dd, *J* = 16.8, 10.7 Hz, 1H), 5.37-5.28 (m, 2H), 3.67 (s, 3H), 1.78 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 158.3, 140.6, 136.6, 129.8, 128.6, 127.6, 126.7, 126.4, 118.7, 113.0, 71.2, 69.4, 55.2, 20.5; IR (ATR): 2956, 2922, 2869, 1741, 1460, 1247, 1026, 804, 769 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{18}H_{18}NaO_2$ 289.1199, found: 289.1198; HPLC analysis Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5/0.5, 1.0 mL/min, 40 °C, 220 nm) 7.2 min (minor), 7.4 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*R*,3*S*) by analogy with compound **5b**.

(*R*,*E*)-4-hydroxy-3-(4-methoxyphenyl)-4-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4l)

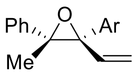


4l

(Ar = 4-MeOC_6H_4)

36% yield (15.4 mg); colorless oil; $[\alpha]_D^{25}$ –29.5 (*c* 1.15, $CHCl_3$, 84% ee); R_f = 0.30 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (s, 1H), 7.43-7.42 (m, 2H), 7.33-7.30 (m, 2H), 7.25-7.27 (m, 1H), 6.72 (td, *J* = 5.5, 3.2 Hz, 2H), 6.68-6.66 (m, 2H), 6.27 (t, *J* = 6.9 Hz, 1H), 4.58 (d, *J* = 6.2 Hz, 2H), 3.76-3.74 (m, 3H), 2.05 (s, 1H), 1.71 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.7, 159.2, 152.0, 145.6, 130.7, 128.5, 128.2, 127.3, 125.9, 120.6, 113.6, 91.6, 67.4, 55.3, 28.9; IR (ATR): 3337, 2935, 2636, 2310, 1725, 1661, 1249, 1086, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{20}H_{20}Cl_3NNaO_3$ 450.0401, found: 450.040; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 12.1 min (minor), 14.7 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

(2*R*,3*S*)-2-(4-chlorophenyl)-3-methyl-3-phenyl-2-vinyloxirane (5m)

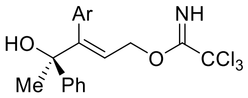


5m

(Ar = 4-ClC_6H_4)

34% yield (13.3 mg); colorless oil; $[\alpha]_D^{26}$ +123.8 (*c* 1.54, $CHCl_3$, 92% ee); R_f = 0.32 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.13-7.08 (m, 4H), 7.06-7.03 (m, 5H), 6.25 (dd, *J* = 17.2, 10.3 Hz, 1H), 5.40 (dd, *J* = 11.0, 1.4 Hz, 1H), 5.31 (dd, *J* = 16.8, 1.7 Hz, 1H), 1.78 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 140.1, 136.3, 135.7, 132.6, 128.9, 127.85, 127.82, 127.0, 126.3, 119.4, 70.9, 69.6, 20.5; IR (ATR): 2958, 2922, 2869, 1741, 1459, 1260, 1092, 1023, 802, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{17}H_{15}ClNaO$ 293.0704, found: 293.0703; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5/0.5, 1.0 mL/min, 40 °C, 220 nm) 4.8 min (major), 5.1 min (minor). Configuration Assignment: The relative and absolute configurations were assigned as (2*R*,3*S*) by analogy with compound **5b**.

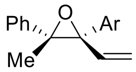
(*R*,*E*)-3-(4-chlorophenyl)-4-hydroxy-4-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4m)



4m
(Ar = 4-ClC$_6$H$_4$)

49% yield (14.7 mg); colorless oil; $[\alpha]_D^{25}$ -7.1 (*c* 3.37, $CHCl_3$, 56% ee); R_f = 0.34 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.22 (s, 1H), 7.40-7.38 (m, 2H), 7.33-7.31 (m, 2H), 7.28-7.26 (m, 1H), 7.16 (dt, *J* = 8.9, 2.1 Hz, 2H), 6.68 (dd, *J* = 8.6, 2.4 Hz, 2H), 6.32 (t, *J* = 6.9 Hz, 1H), 4.54 (d, *J* = 6.9 Hz, 2H), 2.03 (s, 1H), 1.71 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.6, 151.4, 144.9, 135.1, 133.8, 130.9, 128.4, 128.3, 127.5, 125.9, 120.8, 91.5, 76.9, 66.9, 28.7; IR (ATR): 3338, 2983, 1660, 1489, 1090, 829, 768, 701 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{19}H_{17}Cl_4NNaO$ 453.9906, found: 453.9905; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 10.2 min (minor), 11.8 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

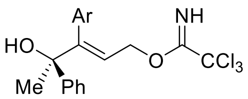
(2*R*,3*S*)-2-([1,1'-biphenyl]-4-yl)-3-methyl-3-phenyl-2-vinyloxirane (5n)



5n
(Ar = 4-PhC$_6$H$_4$)

26% yield (11.9 mg); colorless oil; $[\alpha]_D^{26}$ +164.1 (*c* 1.56, $CHCl_3$, 95% ee); R_f = 0.73 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.47-7.45 (m, 2H), 7.37-7.35 (m, 2H), 7.33-7.31 (m, 2H), 7.29-7.26 (m, 1H), 7.19-7.16 (m, 4H), 7.10-7.07 (m, 2H), 7.01 (dd, *J* = 8.2, 6.2 Hz, 1H), 6.33 (dd, *J* = 16.8, 10.7 Hz, 1H), 5.42-5.36 (m, 2H), 1.80 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 140.7, 140.4, 139.5, 136.7, 136.2, 128.7, 127.8, 127.7, 127.3, 127.0, 126.8, 126.4, 126.3, 119.0, 71.4, 69.6, 20.5; IR (ATR): 3028, 2957, 2924, 2868, 1740, 1487, 1446, 768, 698 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{23}H_{20}NaO$ 335.1406, found: 335.1406; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.9/0.1, 1.0 mL/min, 40 °C, 220 nm) 12.8 min (minor), 13.2 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*R*,3*S*) by analogy with compound **5b**.

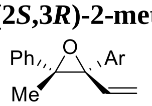
(*R*,*E*)-3-([1,1'-biphenyl]-4-yl)-4-hydroxy-4-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4n)



4n
(Ar = 4-PhC$_6$H$_4$)

71% yield (23.3 mg); colorless oil; $[\alpha]_D^{25}$ –27.2 (*c* 5.6, $CHCl_3$, 36% ee); R_f = 0.33 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.23 (s, 1H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.47-7.46 (m, 2H), 7.43-7.40 (m, 4H), 7.36-7.27 (m, 4H), 6.84-6.82 (m, 2H), 6.32 (t, *J* = 6.9 Hz, 1H), 4.63 (d, *J* = 6.9 Hz, 2H), 2.05 (s, 1H), 1.76 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.7, 152.0, 145.5, 140.5, 140.5, 135.5, 130.0, 128.9, 128.3, 127.5, 127.4, 127.1, 126.7, 126.0, 120.6, 91.5, 67.3, 29.0; IR (ATR, cm^{-1}): 3337, 2983, 1661, 1486, 1300, 1074, 771, 699; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{25}H_{22}Cl_3NNaO_2$ 496.0608, found: 496.0607; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 13.6 min (minor), 15.4 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

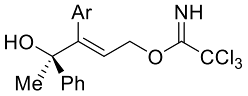
(2*S*,3*R*)-2-methyl-2-phenyl-3-(m-tolyl)-3-vinyloxirane (5p)



5p
(Ar = 3-MeC$_6$H$_4$)

30% yield (7.5 mg); colorless oil; $[\alpha]_D^{26}$ +120.7 (*c* 1.1, $CHCl_3$, 96% ee); R_f = 0.44 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.14-7.13 (m, 2H), 7.09-7.06 (m, 2H), 7.03-7.02 (m, 1H), 6.96-6.93 (m, 2H), 6.88 (d, *J* = 7.9 Hz, 1H), 6.82 (d, *J* = 7.2 Hz, 1H), 6.29 (dd, *J* = 17.2, 10.7 Hz, 1H), 5.38-5.32 (m, 2H), 2.17 (s, 3H), 1.78 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 140.5, 137.5, 137.1, 136.4, 128.2, 127.5, 127.4, 126.7, 126.4, 124.5, 118.7, 71.5, 69.4, 21.4, 20.5; IR (ATR): 2954, 2922, 2868, 2853, 1741, 1460, 1376, 1081, 804, 770 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{18}H_{18}NaO$: 273.1250, found: 273.1249; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.5:0.5, 1.0 mL/min, 40 °C, 220 nm) 4.9 min (minor), 5.1 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

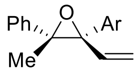
(*R*,*E*)-4-hydroxy-4-phenyl-3-(m-tolyl)pent-2-en-1-yl 2,2,2-trichloroacetimidate (4p)



4p
(Ar = 3-MeC$_6$H$_4$)

63% yield (26.0 mg); colorless oil; $[\alpha]_D^{25}$ –118.9 (*c* 1.35, CHCl$_3$, 56% ee); R$_f$ = 0.35 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, CDCl$_3$): δ 8.20 (s, 1H), 7.43 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.28-7.25 (m, 1H), 7.07-7.02 (m, 2H), 6.59 (s, 1H), 6.52 (d, *J* = 6.9 Hz, 1H), 6.24 (t, *J* = 6.5 Hz, 1H), 4.56 (d, *J* = 7.6 Hz, 2H), 2.21 (s, 3H), 2.03 (s, 1H), 1.72 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$): δ 162.7, 152.5, 145.6, 137.6, 136.3, 130.4, 128.5, 128.2, 127.9, 127.3, 126.5, 126.0, 120.3, 91.7, 76.95, 67.3, 28.9, 21.5; IR (ATR): 3338, 2973, 1607, 1509, 1287, 1244, 1074, 796, 701, 648 cm^{-1}; HRMS(ESI) *m*/*z*: [M+Na]$^+$ Calcd for C$_{20}$H$_{20}$Cl$_3$NNaO$_2$ 434.0452, found: 434.0452; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 8.3 min (minor), 9.5 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

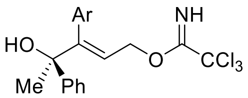
(2*R*,3*S*)-2-(3-chlorophenyl)-3-methyl-3-phenyl-2-vinyloxirane (5q)



5q
(Ar = 3-ClC$_6$H$_4$)

30% yield (8.1 mg); colorless oil; $[\alpha]_D^{25}$ +131.0 (*c* 0.3, CHCl$_3$, 97% ee); R$_f$ = 0.33 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, CDCl$_3$): δ 7.14-7.09 (m, 5H), 7.06-7.03 (m, 1H), 6.99 (qd, *J* = 3.7, 2.1 Hz, 3H), 6.26 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.43-5.33 (m, 2H), 1.77 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$): δ 139.9, 139.7, 135.4, 133.5, 128.9, 127.7, 127.7, 127.1, 127.1, 126.3, 125.6, 119.5, 71.2, 69.7, 20.4; IR (ATR): 2953, 2919, 2868, 2850, 1741, 1460, 1376, 772 cm^{-1}; HRMS(ESI) *m*/*z*: [M+Na]$^+$ Calcd for C$_{17}$H$_{15}$ClNaO 293.0704, found: 293.0703; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.9:0.1, 1.0 mL/min, 40 °C, 220 nm) 11.0 min (minor), 12.0 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*R*,3*S*) by analogy with compound **5b**.

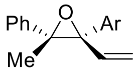
(*R*,*E*)-3-(3-chlorophenyl)-4-hydroxy-4-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4q)



4q
(Ar = 3-ClC$_6$H$_4$)

51% yield (21.7 mg); colorless oil; $[\alpha]_D^{25}$ –76.4 (*c* 2.04, CHCl$_3$, 47% ee); R$_f$ = 0.33 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, CDCl$_3$): δ 8.23 (s, 1H), 7.41-7.39 (m, 2H), 7.35-7.32 (m, 2H), 7.30-7.27 (m, 1H), 7.22-7.20 (m, 1H), 7.11 (t, *J* = 7.9 Hz, 1H), 6.78 (t, *J* = 2.1 Hz, 1H), 6.62-6.61 (m, 1H), 6.30 (t, *J* = 6.9 Hz, 1H), 4.54 (d, *J* = 6.9 Hz, 2H), 2.00 (t, *J* = 2.1 Hz, 1H), 1.72 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$): δ 162.6, 151.3, 144.8, 138.5, 133.9, 129.7, 129.3, 128.4, 127.9, 127.7, 127.5, 125.9, 121.0, 91.5, 76.8, 66.8, 28.7; IR (ATR): 3339, 1662, 1301, 1080, 771, 701, 649 cm^{-1}; HRMS(ESI) *m*/*z*: [M+Na]$^+$ Calcd for C$_{19}$H$_{17}$Cl$_4$NNaO$_2$ 453.9906, found: 453.9905; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 10.3 min (minor), 11.2 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

(2*S*,3*R*)-2-methyl-3-(naphthalen-2-yl)-2-phenyl-3-vinyloxirane (5s)

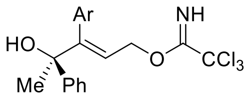


5s
(Ar = 2-naphthyl)

53% yield (13.2 mg); colorless oil; $[\alpha]_D^{25}$ +124.5 (*c* 0.79, CHCl$_3$, 84% ee); R$_f$ = 0.72 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, CDCl$_3$): δ 7.68-7.65 (m, 2H), 7.61 (s, 1H), 7.55 (d, *J* = 8.2 Hz, 1H), 7.38-7.33 (m, 2H), 7.24-7.23 (m, 1H), 7.19-7.17 (m, 2H), 7.02 -6.99 (m, 2H), 6.93-6.90 (m, 1H), 6.36 (dd, *J* = 17.2, 11.0 Hz, 1H), 5.41-5.33 (m, 2H), 1.84 (s, 3H); ^{13}C NMR (151 MHz, CDCl$_3$): δ 140.4, 136.3, 135.2, 132.8, 132.4, 127.9, 127.6, 127.2, 126.8, 126.6, 126.3, 125.9, 125.7, 125.5, 119.3, 71.6, 69.7, 20.6; IR (ATR): 2954, 2922, 2868, 2852, 1741, 1460, 1376, 1219, 772 cm^{-1}; HRMS(ESI) *m*/*z*: [M+Na]$^+$: Calcd for C$_{21}$H$_{18}$NaO 309.1250, found: 309.1249; HPLC analysis:

Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.8:0.2, 1.0 mL/min, 40 °C, 220 nm) 10.4 min (minor), 10.8 min (major). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*R*) by analogy with compound **5b**.

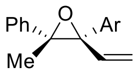
(*R*,*E*)-4-hydroxy-3-(naphthalen-2-yl)-4-phenylpent-2-en-1-yl 2,2,2-trichloroacetimidate (4s)



4s
(Ar = 2-naphthyl)

34% yield (18.8 mg); colorless oil; $[\alpha]_D^{21}$ –23.1 (*c* 3.3, $CHCl_3$, >99% ee); R_f = 0.32 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 (s, 1H), 7.77-7.76 (m, 1H), 7.64 (d, *J* = 8.2 Hz, 2H), 7.46-7.41 (m, 4H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.30-7.27 (m, 1H), 7.25 (d, *J* = 5.5 Hz, 1H), 6.84 (d, *J* = 8.2 Hz, 1H), 6.37 (t, *J* = 6.9 Hz, 1H), 4.58 (d, *J* = 6.9 Hz, 2H), 2.12-2.10 (m, 1H), 1.76 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.6, 152.4, 145.4, 134.1, 132.8, 132.7, 128.7, 128.3, 128.2, 127.7, 127.5, 127.4, 126.3, 126.3, 126.1, 120.8, 91.5, 67.2, 28.9; IR (ATR): 3335, 2981, 1660, 1297, 1073, 820, 796, 700, 648 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{23}H_{20}Cl_3NNaO_2$: 470.0452, found:470.0451; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95/5, 1.0 mL/min, 40 °C, 220 nm) 13.8 min (minor), 15.1 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

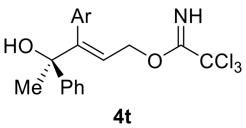
(2*S*,3*S*)-2-methyl-2-phenyl-3-(thiophen-2-yl)-3-vinyloxirane (5t)



5t
(Ar = 2-thiophenyl)

40% yield (9.7 mg); colorless oil; $[\alpha]_D^{26}$ +51.6 (*c* 0.2, $CHCl_3$, 86% ee (major diastereomer), 90% ee (minor diastereomer)); R_f = 0.33 (Hexane/EtOAc= 10/1); ^{1}H NMR (600 MHz, $CDCl_3$) for mixture of diastereomers: δ 7.40-7.35 (m, 4H), 7.32-7.28 (m, 2H), 7.25-7.22 (m, 2H), 7.18 (t, *J* = 7.2 Hz, 2H), 7.13 (tt, *J* = 6.6 Hz, 1.2 Hz, 1H), 7.09-7.05 (m, 2H), 7.00-6.98 (m, 1H), 6.71-6.66 (m, 2H), 6.32 (dd, *J* = 16.8 Hz, 10.2 Hz, 1H), 5.53-5.44 (m, 3H), 5.19-5.11 (m, 2H), 1.74 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) for mixture of diastereomers: δ 141.3, 140.2, 136.0, 135.3, 128.3, 127.8, 127.5, 127.2, 126.8, 126.7, 126.6, 126.5, 126.22, 126.16, 125.1, 124.8, 120.5, 119.0, 71.2, 71.0, 68.3, 22.2, 21.1, some carbon could not be assigned due to presence of diastereomers; IR (ATR): 2955, 2922, 2869, 1741, 1436, 1376, 1219, 772 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{15}H_{16}NaOS$ 265.0658, Found: 265.0657; HPLC analysis: Chiralcel OD-3 column (Hexane:^{i}PrOH = 99.8/0.2, 1.0 mL/min, 40 °C, 220 nm) major diastereomer: 9.8 min (minor), 11.8 min (major), minor diastereomer: 7.8 min (major), 8.8 min (minor). Configuration Assignment: The relative and absolute configurations were assigned as (2*S*,3*S*) by analogy with compound **5b**.

(*R*,*Z*)-4-hydroxy-4-phenyl-3-(thiophen-2-yl)pent-2-en-1-yl 2,2,2-trichloroacetimidate (4t)

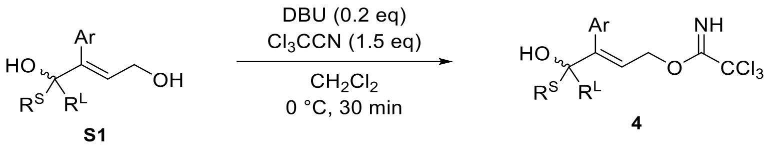


4t
(Ar = 2-thiophenyl)

49% yield (19.8 mg); colorless oil; $[\alpha]_D^{25}$ –6.84 (*c* 1.35, $CHCl_3$, 48% ee); R_f = 0.31 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.29 (s, 1H), 7.49-7.47 (m, 2H), 7.36-7.34 (m, 2H), 7.31-7.28 (m, 1H), 7.20-7.19 (m, 1H), 6.90 (q, *J* = 2.7 Hz, 1H), 6.65 (t, *J* = 2.4 Hz, 1H), 6.40 (t, *J* = 6.5 Hz, 1H), 4.82 (d, *J* = 6.9 Hz, 2H), 2.14 (s, 1H), 1.76 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.7, 145.2, 144.9, 136.2, 129.0, 128.4, 127.6, 126.9, 126.6, 126.03, 123.6, 91.5, 67.3, 29.0; IR (ATR): 3450, 2983, 1719, 1220, 1067, 826, 770, 699 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{17}H_{16}Cl_3NNaO_2S$ 425.9860, found: 425.9859; HPLC analysis: Chiralpak IA-3 column (Hexane:^{i}PrOH = 95:5, 1.0 mL/min, 40 °C, 220 nm) 11.0 min (minor), 12.8 min (major). The absolute configurations were assigned as (*R*) by analogy with compound **4a**.

3. Preparation of Substrates

Allylic substrates **4** were prepared by following the literature procedure.[1]



S1 → **4**

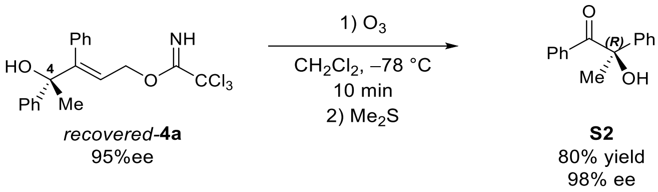
To a solution of **S1** (1.0 eq.) and trichloroacetonitrile (1.5 eq) in CH_2Cl_2 (0.2M) was added DBU (0.2 eq) at 0 °C. The resulting solution was stirred for 30 min at the same temperature. Then the residual crude was concentrated and purified by flash column chromatography on silica gel (Hexane/EtOAc = 20/1) to obtain **4** as a colorless oil.

[1] S. Kayal, J. Kikuchi, M. Shimizu, M. Terada, *ACS Catal.* **2019**, *9*, 6846–6850.

4. Determination of the relative and absolute configuration

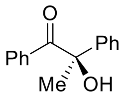
4-1. The absolute configuration of recovered-**4a**

The absolute configuration on C4 position of recovered-**4a** was determined to be *R* by derivatization into the stereochemically known compound **S2**.[2] The stereochemistry of the remaining recovered **4** was assigned by analogy.



To a solution of *recovered*-**4a** (50 mg, 0.125 mmol, 95% ee) in CH_2Cl_2 (2.0 mL) was bubbled with O_3 until the solution turned blue at –78 °C (10 min). To the blue solution was added Me_2S (1.0 mL) and the mixture was slowly warmed to rt. The mixture was concentrated in vacuo to give a residue, which was then washed with H_2O was added and extracted with EtOAc. The combined EtOAc extracts were washed with brine, dried over Na_2SO_4, and concentrated after filtration. The residual crude was purified by silica gel column chromatography (Hexane/EtOAc = 19/1) to give **S2** (22.6 mg, 80% yield).

(*R*)-2-hydroxy-1,2-diphenylpropan-1-one (S2)



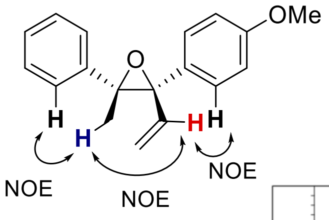
S2

80% yield (22.6 mg); colorless oil; $[\alpha]_D^{26}$ +174.5 (*c* 0.24, EtOH, 98% ee); R_f = 0.42 (Hexane/EtOAc= 4/1); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.69-7.67 (m, 2H), 7.47-7.44 (m, 3H), 7.39 (t, *J* = 7.9 Hz, 2H), 7.34-7.28 (m, 3H), 4.78 (s, 1H), 1.90 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 202.1, 142.5, 133.5, 133.1, 130.3, 129.1, 128.4, 128.3, 126.0, 79.2, 26.2; IR (ATR): 3448, 1673, 1447, 1255, 768, 700 cm^{-1}; HRMS(ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{15}H_{14}NaO_2$ 249.0886, found: 249.0886; HPLC analysis: Chiralpak IC-3 column (Hexane:^{i}PrOH = 98:2, 1.0 mL/min, 40 °C, 220 nm) 13.5 min (major), 14.0 min (minor).

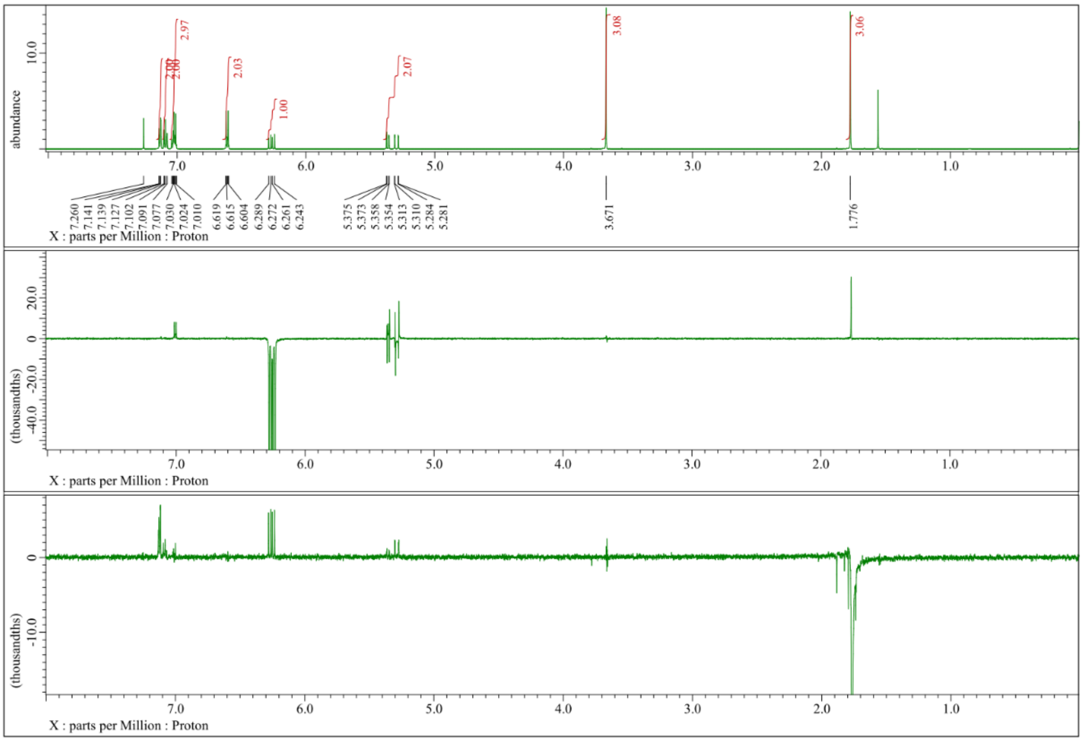
[2] S.-B. D. Sim, M. Wang, Y. Zhao, *ACS Catal*. **2015**, *5*, 3609-3612.

4-2. The absolute configuration of **5a**

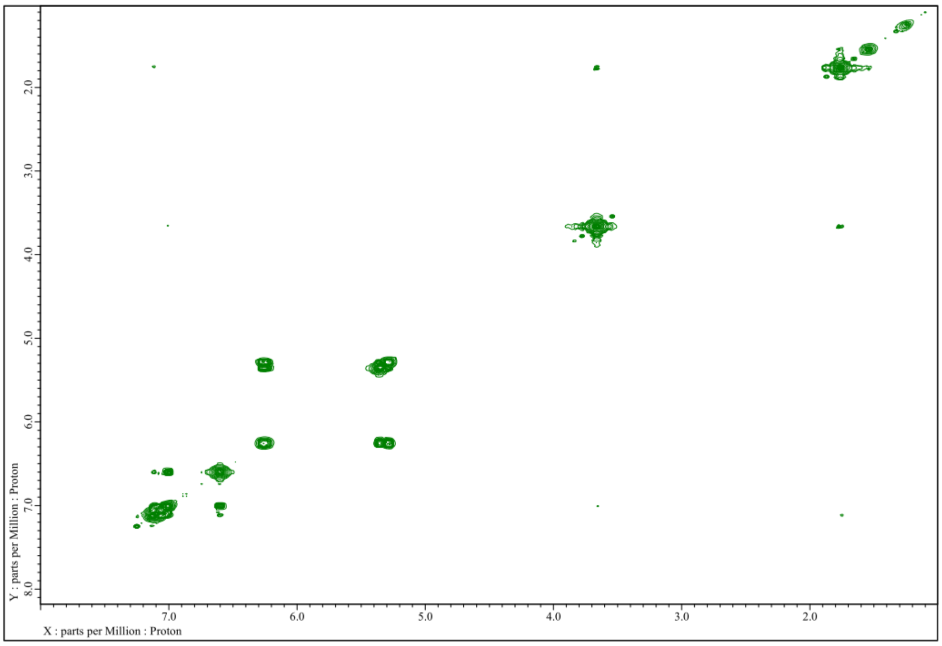
According to the follwoing NOE analysis of **5l** and the absolute configuration of **4a**, the absolute configuration of **5a** was assigned to be (2*S*,3*R*). The stereochemistry of the remaining products **5** was assigned by analogy.



5l

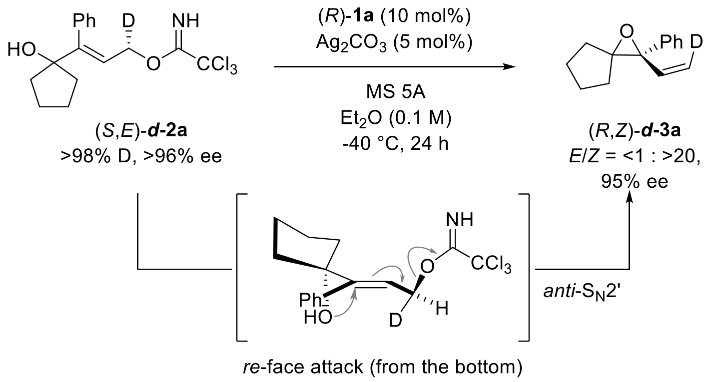


COSY (600 MHz, $CDCl_3$) spectra of **5l**



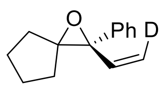
5. Determination of the reaction pathway of the intramolecular S_N2' reaction[3]

To elucidate the mechanism of the present intramolecular S_N2' reaction, enantioenriched (*S*,*E*)-***d*-2a** containing deuterium at the allylic position was employed. In the proposed deuterated substrate study, the stereochemical relationship between the chirality at the deuterated carbon as well as the geometry of starting (*S*,*E*)-***d*-2a** and the geometry of the migrated double bond, in combination with the newly generated stereogenic center, would offer important information of the reaction pathway. As shown in the following scheme, enantioenriched (*R*,*Z*)-***d*-3a** (95% ee) was obtained in good yield with high (*Z*)-selectivity, clearly suggesting that the *anti*-S_N2' pathway is the rational mechanism for the present intramolecular S_N2' reaction.



In an oven and vacuum-dried reaction tube, MS 5Å (40.0 mg), catalyst (*R*)-**1a** (12.4 mg, 0.01 mmol, 10 mol%) and Ag_2CO_3 (1.4 mg, 0.005 mmol, 5 mol%) were taken with 0.5 mL of Et_2O. The reaction mixture was stirred at room temperature for 15 min and then cooled at -40 °C. To the reaction mixture was added a solution of ***d*-2a** (36.3 mg, 0.1 mmol) in Et_2O (0.5 mL) at the same temperature. The reaction mixture was stirred for 24 h. The reaction mixture was quenched with NEt_3 (10 μL) and directly purified by flash column chromatography (Hexane/EtOAc = 10:1) to give ***d*-3a** (14.5 mg) in 72% yield (*E*/*Z* = 1:>20) with 95% ee.

(*R*,*Z*)-2-phenyl-2-(vinyl-2-d)-1-oxaspiro[2.4]heptane (*d*-3a)



***d*-3a**

72% yield (14.5 mg); colorless oil; $[\alpha]^{D}_{26}$ +57.9 (c 0.47, $CHCl_3$, 95% ee); R_f = 0.71 (Hexane/EtOAc= 4/1); ^1H NMR (C_6D_6, 600MHz) δ 7.38 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.20-7.00 (m, 4H), 6.05 (dt, *J* = 10.8, 2.4 Hz, 1H), 5.14 (d, *J* = 10.8 Hz, 1H), 1.92-1.84 (m, 1H), 1.78-1.68 (m, 1H), 1.65-1.55 (m, 1H), 1.54-1.44 (m, 1H), 1.42-1.20 (m, 4H); ^{13}C NMR (C_6D_6, 151MHz) δ 139.4, 137.7, 130.8, 127.3 (4C), 117.8 (t, *J* = 27.5 Hz, 1C), 76.9, 67.8, 31.9, 30.5, 25.4, 25.3; IR (ATR) 2922, 2360, 2309, 1732, 1459, 1218, 772 cm^{-1}; HRMS (FD+) *m*/*z*: [M] Calcd for $C_{14}H_{15}DO$ 201.1264, Found 201.1262; HPLC analysis: Chiralpak OD-3 (Hexane:iPrOH = 99.3/0.7, 1.0 mL/min, 40 °C, 220 nm) 4.2 min (minor), 4.5 min (major).

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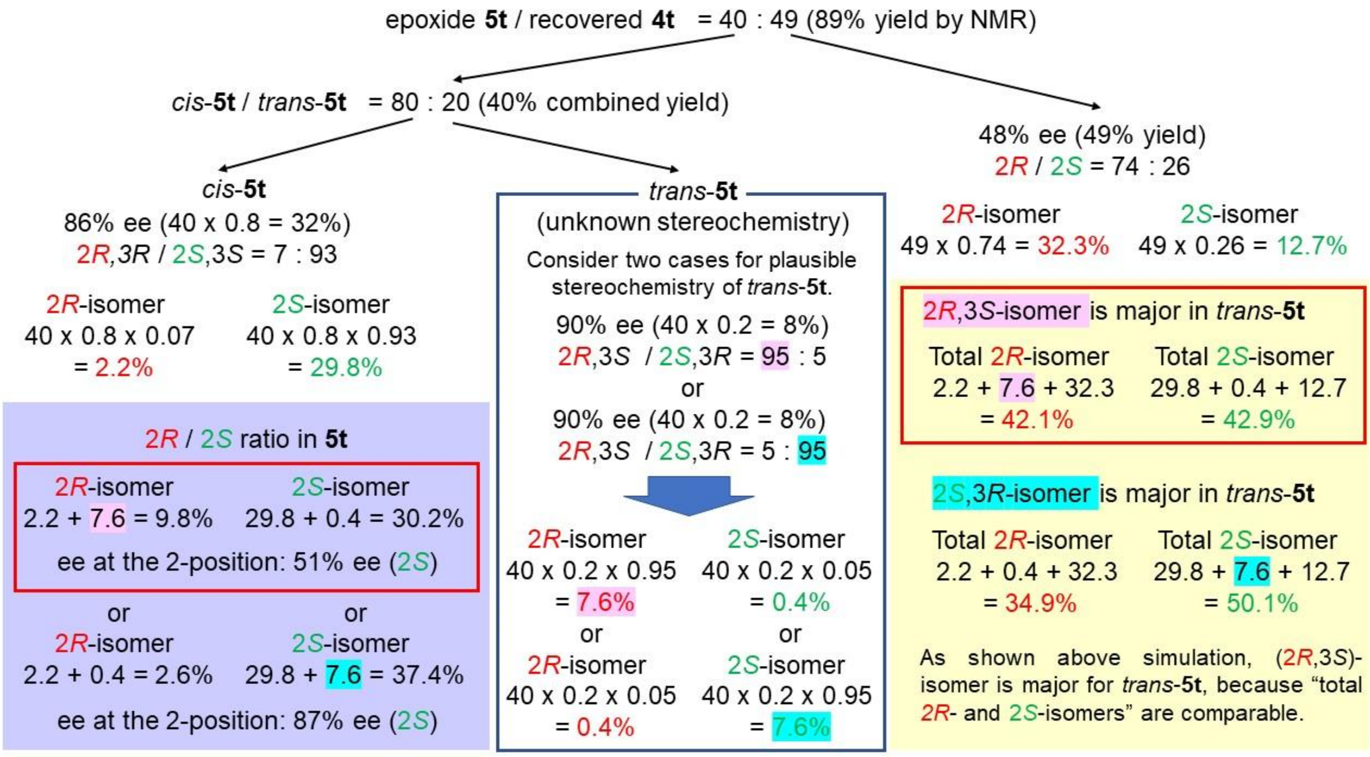
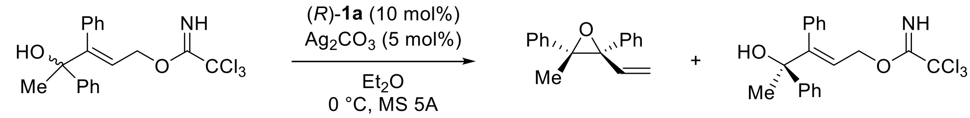
[3] S. Kayal, J. Kikuchi, N. Shinagawa, S. Umemiya, M. Terada, *Tetrahedron* **2021**, *98*, 132412.

6. Stereochemical assignment of *trans*-5t and calculation of conversion *c* in Table 2, entry 19

Absolute stereochemistry of *trans*-**5t** was assigned to be (2*R*,3*S*) based on the distribution of the stereochemical outcomes of *cis*- and *trans*-**5t** and recovered (*Z*)-**4t**, as shown in the following simulation. In this regard, conversion *c* was calculated using 51% ee for $ee_{product}$ averaged at the 2-position of *cis*- and *trans*-**5t**. The calculation process was shown in the following scheme.



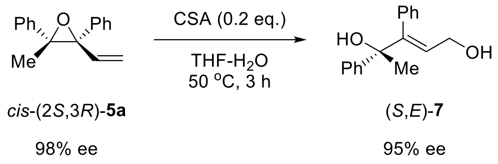
7. Large scale experiment



1.0 mmol of racemic (*E*)-**4a**   *cis*-(2*S*,3*R*)-**5a**   (*R*,*E*)-**4a**

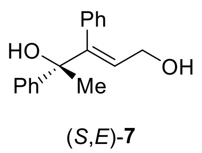
To a mixture of MS 5Å (400 mg), (*R*)-**1a** (124 mg, 0.1 mmol, 10 mol%) and Ag_2CO_3 (14 mg, 0.05 mmol, 5 mol%) was added Et_2O (5.0 mL). The reaction mixture was stirred at room temperature for 15 min and then cooled at 0 °C. To the reaction mixture was added a solution of racemic (*E*)-**4a** (0.40 g, 1.0 mmol) in Et_2O (5.0 mL) at the same temperature and the reaction mixture was stirred for 96 h. The reaction mixture was quenched with NEt_3 (100 μL) and directly purified by flash column chromatography (Hexane/EtOAc = 10:1) to give **5a** (106 mg, 45%) with 98% ee and (*R*,*E*)-**4a** (200 mg, 50%) with 87% ee. The enantiomeric excess was determined by chiral stationary phase HPLC analysis.

8. Derivatization

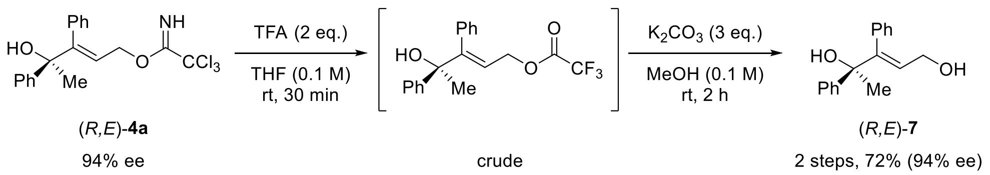


To a solution of cis-(2*S*,3*R*)-**5a** (23.6 mg, 0.1 mmol, 98% ee) in THF (0.8 mL) and H_2O (0.2 mL) was added 10-camphorsulfonic acid (CSA) (4.6 mg, 0.02 mmol). The reaction mixture was stirred at 50 °C for 3 h. The reaction was quenched with aq. $NaHCO_3$ (1 mL) and the aqueous phase was extracted with EtOAc (1 mL) three times. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in *vacuo*. The crude was purified by flash column chromatography (Hexane/EtOAc = 2:1 to 1:1) to give (*S*,*E*)-**7** in 68% yield with 95% ee. The enantiomeric excess was determined by chiral stationary phase HPLC analysis.

(*S*, *E*)-3,4-diphenylpent-2-ene-1,4-diol (7)



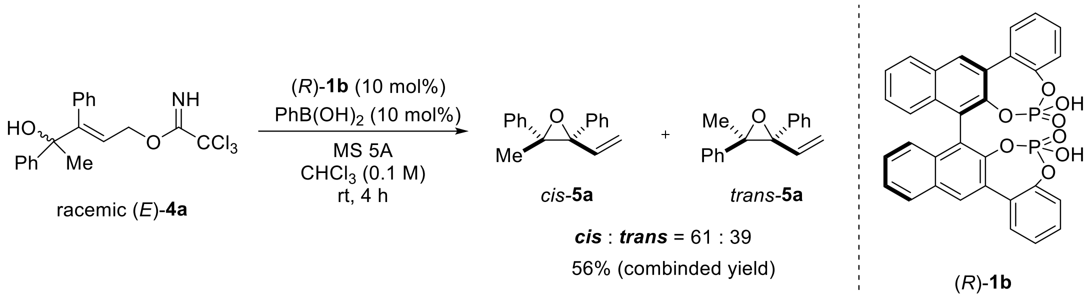
68% yield (17.3 mg); colorless oil; $[\alpha]_D^{25}$ +27.4 (c 0.79, $CHCl_3$, 95% ee); R_f = 0.42 (Hexane/EtOAc= 1/2); ^{1}H NMR ($CDCl_3$, 600MHz) δ 7.42 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 8.4 Hz, 2H), 7.28-7.15 (m, 4H), 6.74 (dd, *J* = 8.4, 1.2 Hz, 2H), 6.14 (t, *J* = 6.6 Hz, 1H), 3.91 (dd, *J* = 6.6, 1.8 Hz, 2H), 1.71 (s, 3H), 1.60 (bs, 2H); ^{13}C NMR ($CDCl_3$, 151MHz) δ 149.2. 145.7, 136.9, 129.5 (2C), 128.0 (2C), 127.9 (2C), 127.4, 127.0, 125.9, 125.8 (2C), 76.8, 60.5, 28.9; IR (ATR): 3224, 1491, 1447, 1302, 1147, 1136, 1089, 1066, 1021, 979, 902 cm^{-1}; HRMS (FD) *m*/*z*: $[M]^+$ Calcd for $C_{17}H_{18}O_2$ 254.1307, found 254.1306; HPLC analysis: Chiralpak IA column (Hexane:^{i}PrOH = 90:10, 0.7 mL/min, 30 °C, 220 nm) 16.1 min (major), 17.8 min (minor).



To a solution of (*R*,*E*)-**4a** (39.8 mg, 0.1 mmol, 94% ee) in THF (1 mL) was added trifluoroacetic acid (TFA) (15 μL, 0.2 mmol) at room temperature. The reaction mixture was stirred at that temperature for 30 min. The reaction was quenched with aq. $NaHCO_3$ (2 mL) and the aqueous phase was extracted with EtOAc (1 mL) three times. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in *vacuo*. To a solution of the crude in MeOH (1 mL) was added potassium carbonate (41 mg, 0.3 mmol) at room temperature. The reaction mixture was stirred at that temperature for 2 h. The reaction was quenched with aq. NH_4Cl (2 mL) and the aqueous phase was extracted with EtOAc (1 mL) three times. The combined organic layers were washed with brine, dried over Na2SO4, filtered and concentrated in vacuo. The crude was purified by flash column chromatography (Hexane/EtOAc = 2:1 to 1:1) to give (*R*,*E*)-**7** in 72% yield with 94% ee. The enantiomeric excess was determined by chiral stationary phase HPLC analysis.

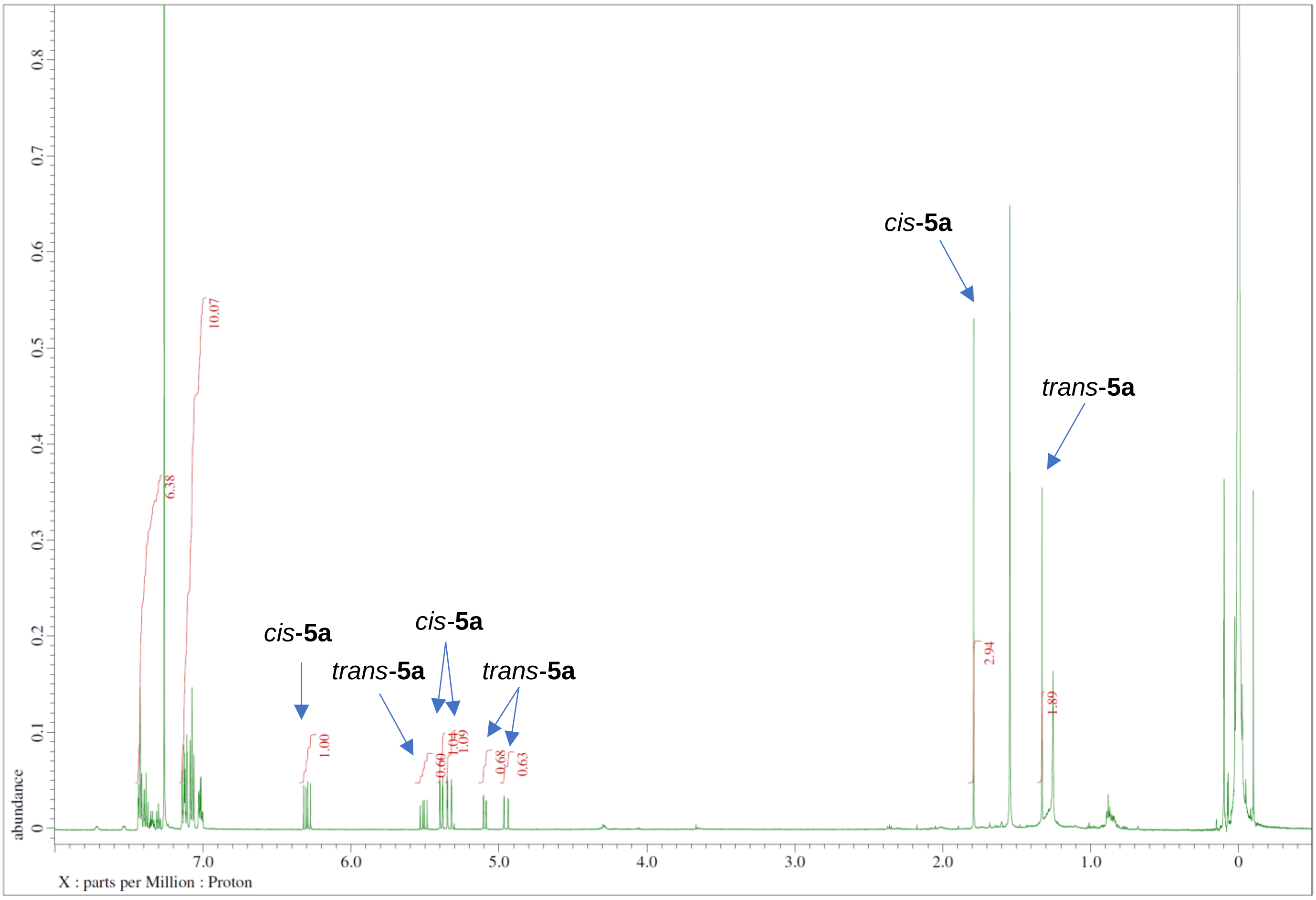
9. Main reaction using catalyst (*R*)-1b

9-1. Reaction of racemic (*E*)-**4a** using (*R*)-**1b**/phenylboronic acid co-catalyst system in chloroform

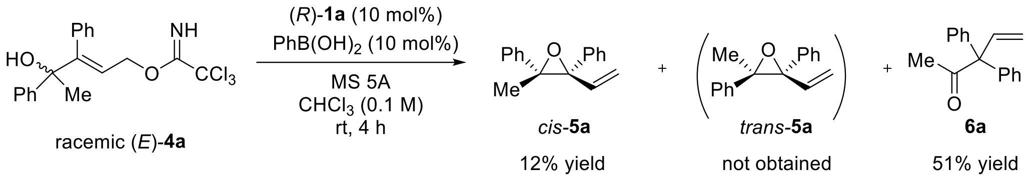


To a mixture of MS 5Å (40.0 mg), (*R*)-**1b** (5.9 mg, 0.01 mmol, 10 mol%) and $PhB(OH)_2$ (1.2 mg, 0.01 mmol, 10 mol%) was added chloroform (0.5 mL). The reaction mixture was stirred at room temperature for 15 min. To the reaction mixture was added a solution of (*E*)-**4a** (39.8 mg, 0.1 mmol) in chloroform (0.5 mL) at the same temperature and the reaction mixture was stirred for 4 h. The reaction mixture was quenched with NEt_3 (10 μL) and directly purified by flash column chromatography (Hexane/EtOAc = 10:1) to give *cis*-**5a** and *trans*-**5a** (dr = 61 : 39) in 56% combined yield.

^1H NMR (600 MHz, $CDCl_3$) spectra of *cis*-**5a** and *trans*-**5a**

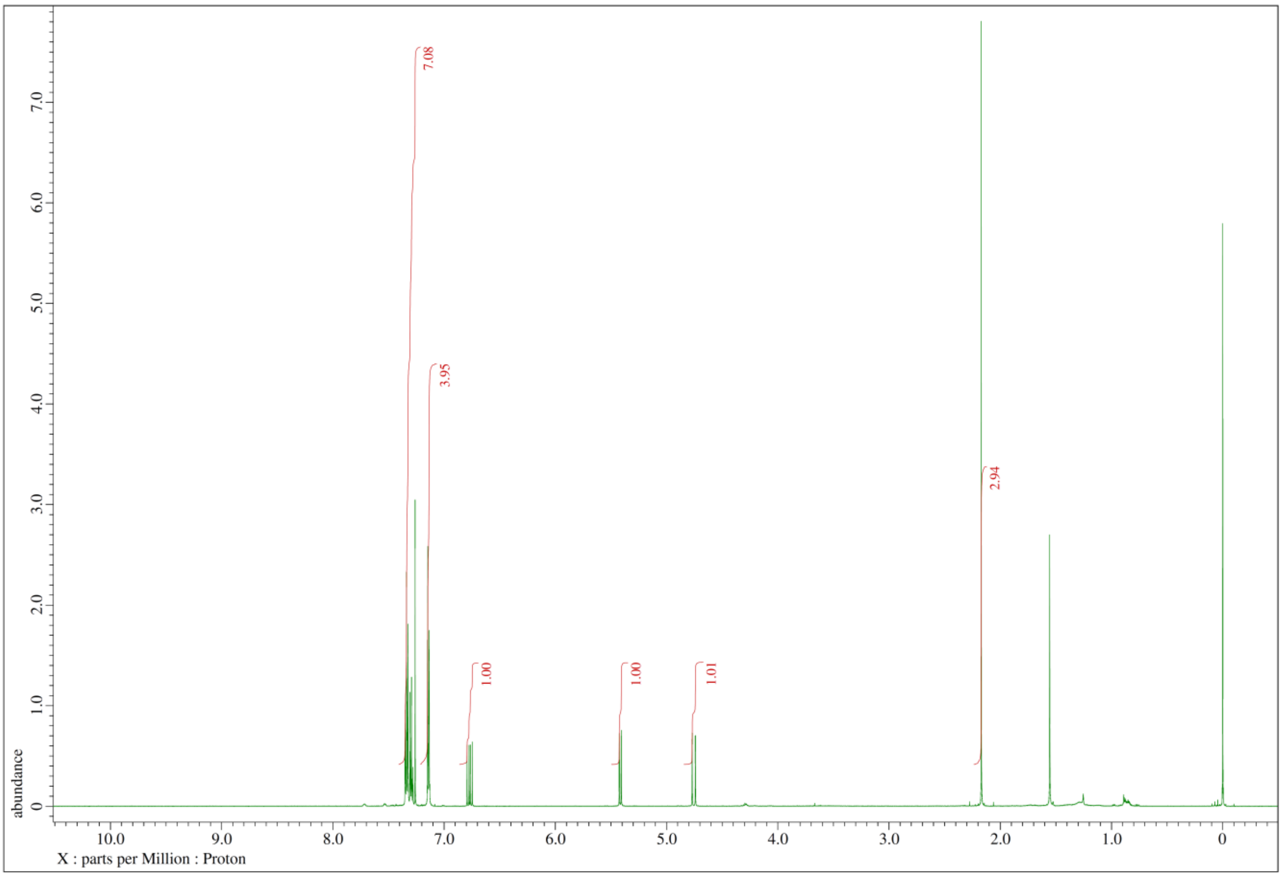


9-2. Reaction of racemic (*E*)-**4a** using (*R*)-**1a**/phenylboronic acid co-catalyst system in chloroform



To a mixture of MS 5Å (40.0 mg), (*R*)-**1a** (12.4 mg, 0.01 mmol, 10 mol%) and $PhB(OH)_2$ (1.2 mg, 0.01 mmol, 10 mol%) was added chloroform (0.5 mL). The reaction mixture was stirred at room temperature for 15 min. To the reaction mixture was added a solution of (*E*)-**4a** (39.8 mg, 0.1 mmol) in chloroform (0.5 mL) at the same temperature and the reaction mixture was stirred for 4 h. The reaction mixture was quenched with NEt_3 (10 μL) and directly purified by flash column chromatography (Hexane/EtOAc = 10:1) to give *cis*-**5a** as a single diastereomer in 12 % yield along with the formation of a significant amount of vinylogous Wagner-Meerwein shift product **6a** in 51% yield.

^{1}H NMR (600 MHz, $CDCl_3$) spectra of rearrangement product **6a**



10. DFT Calculation

To acquire mechanistic insights into the present reaction, we conducted DFT calculation (Gaussian 16 package). The model system of bisphosphoric acid (*R*)-**1b** and substrates (*S*,*E*)-**4a** or (*R*,*E*)-**4a** were employed. Geometries were optimized and characterized using frequency calculations at the B97D/6-31G(d) level. Gibbs free energies (kcal mol^{-1}) in solution phase were calculated using single-point energy calculations at the same level as those for the optimized structures according to the SCRF method based on CPCM (ϵ = 4.335 for diethyl ether).

7.1 Energy profile of the intramolecular S_N2' reaction of (*S*,*E*)-**4a** using (*R*)-**1b**

As illustrated in the Figure S1, the reaction energy profile shows that the present intramolecular S_N2' reaction does not proceed in a synchronous concerted fashion but proceeds in a stepwise pathway, although the energy of the 2nd step is lower than the 1st step.

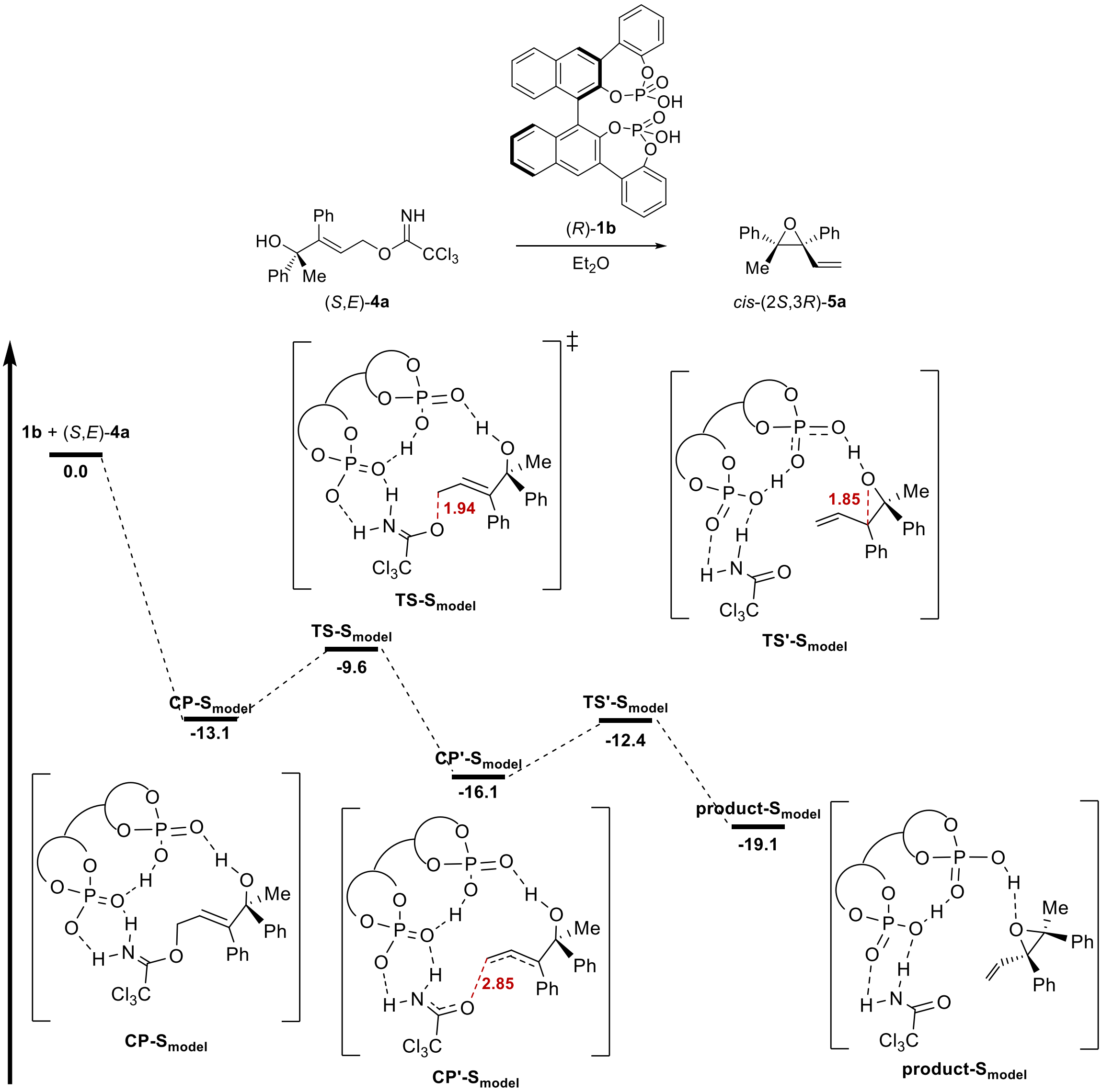
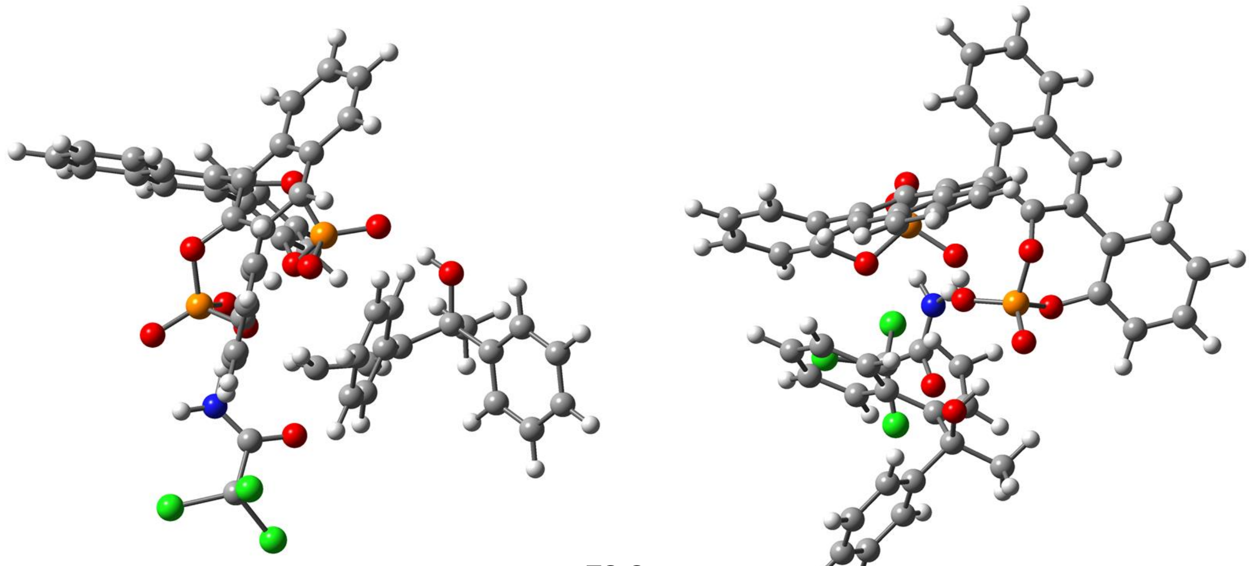
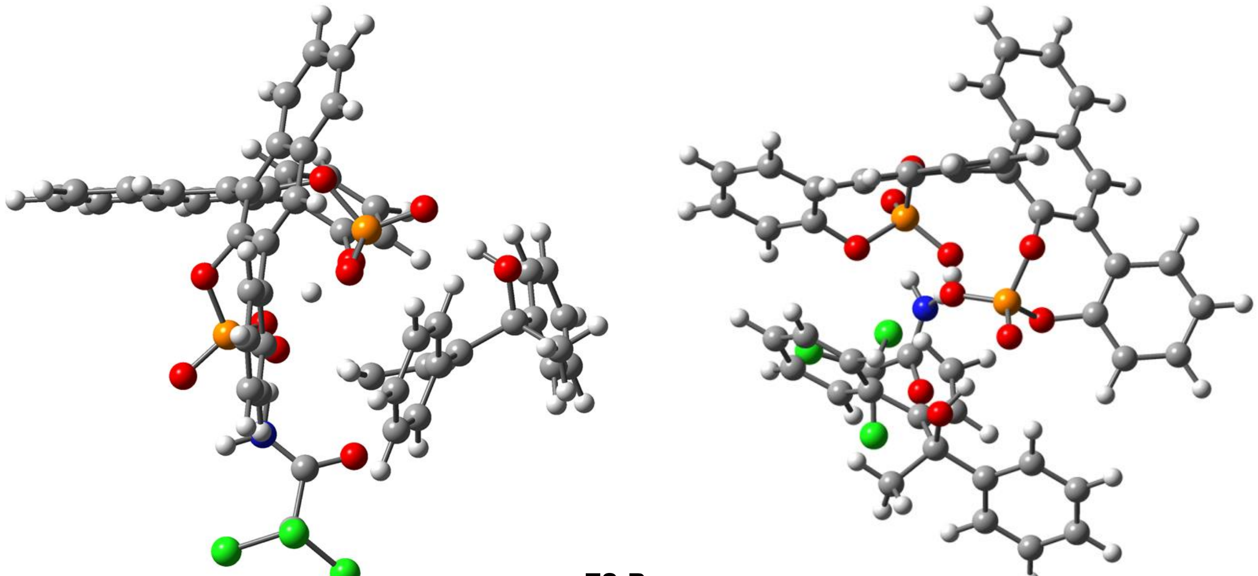


Figure S1. The potential energy for the sum of (*R*)-**1b** and (*S*,*E*)-**4a** was set to zero. Geometries were optimized and characterized using frequency calculations at the B97D/631G(d) level. Gibbs free energies (kcal/mol) in solution phase were calculated using single calculations at the same level as those for the optimized structures according to the SCRF method based on CPCM (ϵ = 4.335 for diethyl ether).

3D structures of the transition states



TS-S$_{model}$
ΔG = 0.7 kcal/mol



TS-R$_{model}$
ΔG = 0.0 kcal/mol

Figure S2. Transition states of intramolecular S$_N$2’ reaction of (*S*,*E*)-**4a** or (*R*,*E*)-**4a** catalyzed by (*R*)-**1b**. Geometries were optimized and characterized using frequency calculations at the B97D/631G(d) level. Gibbs free energies (kcal/mol) in solution phase were calculated using single calculations at the same level as those for the optimized structures according to the SCRF method based on CPCM (ϵ = 4.335 for diethyl ether).

Cartesian coordinates

(S,E)-4a
B97D/6-31g(d);E(RB97D) = -2319.954205 hartree
Zero-point Energy Correction = 0.322777 hartree
Thermal Correction to Energy = 0.347134 hartree
Thermal correction to Enthalpy = 0.348078 hartree
Thermal correction to Gibbs Free Energy = 0.264879 hartree
Sum of electronic and Zero-point Energies = -2319.631428 hartree
Sum of electronic and thermal Energies = -2319.607071 hartree
Sum of electronic and thermal Enthalpies = -2319.606127 hartree
Sum of electronic and thermal Free Energies = -2319.689325 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -2319.961837 hartree
Gibbs Free Energy in ether = -2319.696958 hartree
The number of Imaginary frequencies = 0

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	8	0	3.293136	-0.839389	-2.310657
2	1	0	2.751286	-0.804531	-3.119742
3	6	0	1.286074	-0.057395	-1.192129
4	6	0	1.695586	1.256823	-0.615306
5	6	0	0.882752	1.863668	0.368980
6	6	0	2.901810	1.894679	-0.981059
7	6	0	1.250754	3.082674	0.953649
8	1	0	-0.030512	1.361373	0.685858
9	6	0	3.266114	3.114005	-0.395190
10	1	0	3.546658	1.424478	-1.720588
11	6	0	2.443440	3.715044	0.571333
12	1	0	0.607262	3.531161	1.713522
13	1	0	4.199454	3.595928	-0.694287
14	1	0	2.733967	4.663854	1.027388
15	6	0	0.035027	-0.281833	-1.663156
16	1	0	-0.249806	-1.282679	-1.989802
17	6	0	-1.036655	0.756332	-1.799914
18	1	0	-0.649153	1.782100	-1.765828
19	1	0	-1.621157	0.625704	-2.723128
20	8	0	-1.968878	0.584780	-0.668498
21	6	0	-3.009289	-0.234365	-0.889198
22	6	0	-3.925862	-0.213116	0.383964
23	17	0	-4.594724	1.466598	0.598780
24	17	0	-2.962991	-0.681591	1.847387
25	17	0	-5.315345	-1.366685	0.215969
26	7	0	-3.182766	-0.879139	-1.973877
27	1	0	-4.034288	-1.445124	-1.952606
28	6	0	2.367317	-1.168030	-1.241624
29	6	0	3.152080	-1.210489	0.072498
30	6	0	4.555784	-1.225176	0.105888
31	6	0	2.436188	-1.289623	1.282119
32	6	0	5.231860	-1.310117	1.333895
33	1	0	5.116485	-1.163433	-0.825582
34	6	0	3.110120	-1.375937	2.506564
35	1	0	1.344473	-1.265497	1.259815
36	6	0	4.514354	-1.385617	2.536543
37	1	0	6.324080	-1.314652	1.347271
38	1	0	2.539627	-1.428978	3.436233
39	1	0	5.043063	-1.448237	3.489993
40	6	0	1.814289	-2.586998	-1.510732
41	1	0	1.098281	-2.890746	-0.733329
42	1	0	1.316975	-2.640383	-2.493441
43	1	0	2.660185	-3.288146	-1.510416

(R)-1b
B97D/6-31g(d);E(RB97D) = -2514.837965 hartree
Zero-point Energy Correction = 0.441700 hartree
Thermal Correction to Energy = 0.474622 hartree
Thermal correction to Enthalpy = 0.475566 hartree
Thermal correction to Gibbs Free Energy = 0.378772 hartree
Sum of electronic and Zero-point Energies = -2514.396265 hartree
Sum of electronic and thermal Energies = -2514.363343 hartree
Sum of electronic and thermal Enthalpies = -2514.362398 hartree
Sum of electronic and thermal Free Energies = -2514.459193 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -2514.855996 hartree
Gibbs Free Energy in ether = -2514.477224 hartree
The number of Imaginary frequencies = 0

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	15	0	-1.910725	0.641295	-2.282350
2	15	0	1.702609	-2.050490	-0.899772
3	8	0	-2.377316	1.805651	-3.052087
4	8	0	-0.584512	-0.026226	-2.817025
5	1	0	-0.306968	-0.889275	-2.402008
6	8	0	-2.904846	-0.646360	-2.168448
7	8	0	-1.692573	1.059718	-0.716881
8	8	0	2.280211	-3.425805	-0.320555
9	1	0	1.926013	-4.182426	-0.817689
10	8	0	0.418376	-2.186038	-1.632661
11	8	0	2.823482	-1.374394	-1.835903
12	8	0	1.744249	-1.176998	0.442524
13	6	0	-0.591842	0.172800	1.186104
14	6	0	-1.715780	0.207659	0.373330
15	6	0	-2.923086	-0.482372	0.698520
16	6	0	-2.932815	-1.233494	1.860254
17	1	0	-3.824157	-1.800219	2.114114
18	6	0	-1.823619	-1.297551	2.735126
19	6	0	-1.872489	-2.055577	3.936790
20	1	0	-2.782025	-2.605110	4.167503
21	6	0	-0.798214	-2.088094	4.794446
22	1	0	-0.846690	-2.667465	5.712246
23	6	0	0.373805	-1.358145	4.482495
24	1	0	1.217682	-1.379060	5.166713
25	6	0	0.455565	-0.622694	3.321228
26	1	0	1.359081	-0.066194	3.097122
27	6	0	-0.632526	-0.574702	2.407600
28	6	0	-4.156100	-0.402268	-0.127873
29	6	0	-4.136628	-0.502357	-1.530097
30	6	0	-5.312186	-0.583076	-2.297325
31	6	0	-6.534888	-0.506836	-1.612152
32	1	0	-7.453626	-0.547468	-2.189615
33	6	0	-6.585483	-0.353399	-0.229032
34	1	0	-7.544048	-0.267029	0.274628
35	6	0	-5.406290	-0.306027	0.505937
36	1	0	-5.440114	-0.180683	1.583771
37	6	0	0.642964	0.918408	0.786943
38	6	0	1.764918	0.228555	0.369094
39	6	0	2.978262	0.854562	-0.034088
40	6	0	3.017681	2.235701	-0.000372
41	1	0	3.916730	2.749668	-0.329099
42	6	0	1.913945	3.008258	0.432663
43	6	0	1.980167	4.427613	0.473277
44	1	0	2.897592	4.915098	0.152681
45	6	0	0.908464	5.169678	0.910005
46	1	0	0.968300	6.254034	0.936718
47	6	0	-0.277860	4.519902	1.326932
48	1	0	-1.120884	5.111388	1.672663
49	6	0	-0.376528	3.147279	1.292444
50	1	0	-1.291587	2.660606	1.610014
51	6	0	0.708471	2.349894	0.840175
52	6	0	4.170476	0.073106	-0.450352
53	6	0	4.080889	-1.026711	-1.317908
54	6	0	5.197107	-1.764081	-1.742000
55	6	0	6.451011	-1.359360	-1.257750
56	1	0	7.333658	-1.902109	-1.582128
57	6	0	6.576957	-0.272441	-0.396035
58	1	0	7.557826	0.021856	-0.034292
59	6	0	5.448064	0.435220	0.005445
60	1	0	5.541456	1.268805	0.694578
61	1	0	5.119329	-2.607935	-2.395270
62	1	0	-5.316863	-0.741661	-3.355497

CP-R_{model}
B97D/6-31g(d);E(RB97D) = -4834.844722 hartree
Zero-point Energy Correction = 0.766683 hartree
Thermal Correction to Energy = 0.824459 hartree
Thermal correction to Enthalpy = 0.825403 hartree
Thermal correction to Gibbs Free Energy = 0.671314 hartree
Sum of electronic and Zero-point Energies = -4834.078038 hartree
Sum of electronic and thermal Energies = -4834.020263 hartree
Sum of electronic and thermal Enthalpies = -4834.019319 hartree
Sum of electronic and thermal Free Energies = -4834.173407 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.867098 hartree
Gibbs Free Energy in ether = -4834.195784 hartree
The number of Imaginary frequencies = 0

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	8	0	-2.135447	2.017079	-3.542179
2	1	0	-1.451546	2.303176	-2.888366
3	6	0	-2.943556	0.510256	-1.837492
4	6	0	-2.432910	-0.784368	-2.373470
5	6	0	-3.059665	-1.981416	-1.956746
6	6	0	-1.312483	-0.869295	-3.229713
7	6	0	-2.574687	-3.229601	-2.372056
8	1	0	-3.931667	-1.920879	-1.303527
9	6	0	-0.824437	-2.118949	-3.630942
10	1	0	-0.817987	0.043620	-3.546906
11	6	0	-1.449366	-3.302412	-3.206236
12	1	0	-3.074780	-4.142443	-2.040365
13	1	0	0.064460	-2.169071	-4.262453
14	1	0	-1.051263	-4.271104	-3.512053
15	6	0	-3.011846	0.713649	-0.494104
16	1	0	-3.430804	1.637570	-0.099866
17	6	0	-2.325867	-0.160858	0.476288
18	1	0	-1.639081	-0.868841	0.008311
19	1	0	-1.830903	0.413201	1.267409
20	8	0	-3.330575	-1.064537	1.242925
21	6	0	-2.822293	-1.921620	2.069179
22	6	0	-3.865681	-2.948441	2.606898
23	17	0	-4.136758	-4.120724	1.253072
24	17	0	-5.390832	-2.102824	3.033739
25	17	0	-3.251605	-3.833592	4.060146
26	7	0	-1.561972	-1.990814	2.394333

27	1	0	-1.205188	-2.756624	2.966165
28	6	0	-3.323948	1.627647	-2.850090
29	1	0	-0.775333	-1.397320	1.932535
30	6	0	-3.999030	2.824297	-2.151267
31	6	0	-3.320992	4.045131	-1.984620
32	6	0	-5.298828	2.698788	-1.619112
33	6	0	-3.928543	5.113622	-1.303837
34	1	0	-2.315772	4.164760	-2.383762
35	6	0	-5.907424	3.763134	-0.939864
36	1	0	-5.831219	1.751199	-1.718802
37	6	0	-5.222007	4.978406	-0.777838
38	1	0	-3.384060	6.053652	-1.188442
39	1	0	-6.915335	3.642921	-0.536189
40	1	0	-5.693584	5.810070	-0.249807
41	6	0	-4.247848	1.059635	-3.948707
42	1	0	-4.473806	1.859288	-4.668641
43	1	0	-3.735182	0.237790	-4.466278
44	1	0	-5.188209	0.681479	-3.522833
45	15	0	0.376837	2.094452	-0.687584
46	15	0	1.332836	-2.195819	1.029601
47	8	0	-0.054480	2.896569	-1.866924
48	8	0	0.280825	0.534197	-0.861325
49	1	0	0.426257	-0.022465	0.005544
50	8	0	-0.466911	2.355585	0.708610
51	8	0	1.898957	2.491393	-0.242012
52	8	0	1.220228	-3.236371	2.093691
53	8	0	0.523248	-0.878382	1.238019
54	8	0	0.797651	-2.681150	-0.469393
55	8	0	2.899811	-1.805599	0.708493
56	6	0	3.358547	0.985970	0.948473
57	6	0	2.419755	2.016501	0.970906
58	6	0	2.012910	2.679835	2.170703
59	6	0	2.640184	2.314766	3.356949
60	1	0	2.332736	2.790176	4.290682
61	6	0	3.653466	1.321517	3.392345
62	6	0	4.308917	0.974716	4.610846
63	1	0	4.014374	1.493071	5.526560
64	6	0	5.299031	0.007563	4.631812
65	1	0	5.795502	-0.249747	5.569495
66	6	0	5.674275	-0.651432	3.428956
67	1	0	6.459334	-1.409590	3.450522
68	6	0	5.050349	-0.344001	2.230907
69	1	0	5.338881	-0.854153	1.312949
70	6	0	4.021085	0.639637	2.174529
71	6	0	0.947273	3.711786	2.157765
72	6	0	-0.241119	3.550762	1.408429
73	6	0	-1.257160	4.511458	1.399752
74	6	0	-1.107297	5.672029	2.171849
75	1	0	-1.894330	6.428366	2.167997
76	6	0	0.054759	5.858707	2.938680
77	1	0	0.179502	6.763973	3.535441
78	6	0	1.067421	4.891142	2.924483
79	1	0	1.983646	5.045333	3.497030
80	6	0	3.610309	0.249590	-0.326851
81	6	0	3.237323	-1.090447	-0.442767
82	6	0	3.267294	-1.794695	-1.689400
83	6	0	3.763516	-1.125556	-2.803004
84	1	0	3.769064	-1.633786	-3.769399
85	6	0	4.241871	0.207695	-2.727992
86	6	0	4.781505	0.868179	-3.871120
87	1	0	4.822885	0.322008	-4.816546
88	6	0	5.246055	2.169139	-3.783796
89	1	0	5.658175	2.665888	-4.664253
90	6	0	5.189271	2.860507	-2.542716
91	1	0	5.563273	3.884004	-2.476708
92	6	0	4.660162	2.249910	-1.417298
93	1	0	4.618371	2.786960	-0.470300
94	6	0	4.164331	0.914934	-1.473532
95	6	0	2.758914	-3.181871	-1.815805
96	6	0	1.556677	-3.594347	-1.194340
97	6	0	1.049137	-4.888147	-1.362889
98	6	0	1.734809	-5.804332	-2.171369
99	1	0	1.341136	-6.814295	-2.301290
100	6	0	2.929895	-5.421456	-2.803123
101	1	0	3.475309	-6.132502	-3.426147
102	6	0	3.431836	-4.127333	-2.620660
103	1	0	4.370377	-3.831332	-3.092661
104	1	0	-2.143925	4.339047	0.788958
105	1	0	0.115926	-5.148087	-0.864039

TS-R$_{model}$

B97D/6-31g(d);E(RB97D) = -4834.840011 hartree
Zero-point Energy Correction = 0.765333 hartree
Thermal Correction to Energy = 0.822904 hartree
Thermal correction to Enthalpy = 0.823848 hartree
Thermal correction to Gibbs Free Energy = 0.670080 hartree
Sum of electronic and Zero-point Energies = -4834.074678 hartree
Sum of electronic and thermal Energies = -4834.017107 hartree
Sum of electronic and thermal Enthalpies = -4834.016163 hartree
Sum of electronic and thermal Free Energies = -4834.169931 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.860644 hartree
Gibbs Free Energy in ether = -4834.190564 hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.677191	2.744169	-3.248305
2	1	0	-0.952046	2.856998	-2.578612
3	6	0	-2.788362	1.312683	-1.659256
4	6	0	-2.533941	-0.009973	-2.255349
5	6	0	-3.269447	-1.124494	-1.773035
6	6	0	-1.568544	-0.222034	-3.272838
7	6	0	-3.045065	-2.405112	-2.289168
8	1	0	-4.028224	-0.967937	-1.007105
9	6	0	-1.333540	-1.509698	-3.760862
10	1	0	-0.988775	0.622463	-3.631919
11	6	0	-2.069053	-2.604889	-3.277036
12	1	0	-3.627739	-3.246440	-1.911124
13	1	0	-0.556074	-1.664459	-4.510624
14	1	0	-1.867513	-3.607888	-3.654322
15	6	0	-2.837656	1.470106	-0.277967
16	1	0	-3.139188	2.429425	0.136859
17	6	0	-2.265353	0.531140	0.606958
18	1	0	-1.741616	-0.326532	0.196889
19	1	0	-1.933382	0.888079	1.579921
20	8	0	-3.662205	-0.634535	1.462798
21	6	0	-3.212345	-1.619119	2.103719
22	6	0	-4.240767	-2.766565	2.447355
23	17	0	-4.034733	-4.007986	1.129032
24	17	0	-5.917951	-2.141501	2.445448
25	17	0	-3.886285	-3.524221	4.054796
26	7	0	-1.954122	-1.808707	2.470988
27	1	0	-1.624541	-2.702738	2.833576
28	6	0	-2.928853	2.552628	-2.592676
29	1	0	-1.181650	-1.216864	2.099744
30	6	0	-3.375902	3.809873	-1.821053
31	6	0	-2.465501	4.841932	-1.529216
32	6	0	-4.697928	3.920760	-1.343493
33	6	0	-2.870115	5.958537	-0.779322
34	1	0	-1.438101	4.778025	-1.881047
35	6	0	-5.103015	5.034652	-0.594840
36	1	0	-5.413756	3.120553	-1.539486
37	6	0	-4.187781	6.060322	-0.308532
38	1	0	-2.147957	6.749870	-0.566671
39	1	0	-6.132067	5.099602	-0.234991
40	1	0	-4.500455	6.929384	0.274030
41	6	0	-3.928732	2.237776	-3.728897
42	1	0	-3.999484	3.120142	-4.380549
43	1	0	-3.563048	1.380960	-4.309479
44	1	0	-4.926328	1.999958	-3.333888
45	15	0	0.789510	2.123750	-0.476133
46	15	0	0.829715	-2.325016	0.930166
47	8	0	0.461230	3.101611	-1.556687
48	8	0	0.350973	0.643745	-0.739507
49	1	0	0.410786	-0.007551	0.109583
50	8	0	0.112687	2.451484	0.995795
51	8	0	2.386299	2.168275	-0.138125
52	8	0	0.579879	-3.375889	1.960363
53	8	0	0.367534	-0.873428	1.233021
54	8	0	0.079350	-2.617420	-0.533485
55	8	0	2.416968	-2.303645	0.471443
56	6	0	3.541120	0.274655	0.811554
57	6	0	2.870807	1.483875	0.987354
58	6	0	2.705152	2.112329	2.260348
59	6	0	3.316394	1.518724	3.359257
60	1	0	3.187094	1.964663	4.347539
61	6	0	4.081145	0.329243	3.236231
62	6	0	4.727244	-0.255922	4.365223
63	1	0	4.624606	0.234533	5.336209
64	6	0	5.470001	-1.416502	4.233137
65	1	0	5.960985	-1.856135	5.103522
66	6	0	5.596524	-2.038424	2.960704
67	1	0	6.186970	-2.951217	2.861825
68	6	0	4.973295	-1.500476	1.846617
69	1	0	5.069235	-1.982791	0.874772
70	6	0	4.194840	-0.311606	1.947881
71	6	0	1.890106	3.342867	2.410365
72	6	0	0.645085	3.502224	1.757113
73	6	0	-0.134025	4.654311	1.906422
74	6	0	0.317194	5.684767	2.743028
75	1	0	-0.284795	6.587417	2.862662
76	6	0	1.542636	5.553301	3.416659
77	1	0	1.902563	6.355128	4.063688
78	6	0	2.316506	4.398586	3.244991
79	1	0	3.281681	4.304305	3.745551
80	6	0	3.504378	-0.399343	-0.521447
81	6	0	2.816681	-1.605973	-0.666564
82	6	0	2.572669	-2.205007	-1.944938
83	6	0	3.108027	-1.584515	-3.068458
84	1	0	2.912730	-2.010098	-4.055067
85	6	0	3.886520	-0.402297	-2.974950
86	6	0	4.458574	0.203809	-4.132397
87	1	0	4.285750	-0.264537	-5.104437
88	6	0	5.219674	1.355167	-4.026626
89	1	0	5.654279	1.810694	-4.918545
90	6	0	5.439888	1.944988	-2.751740
91	1	0	6.047003	2.848809	-2.672033
92	6	0	4.888625	1.386113	-1.610226
93	1	0	5.059955	1.844379	-0.636714
94	6	0	4.091603	0.206847	-1.683600
95	6	0	1.761020	-3.438462	-2.082359
96	6	0	0.563109	-3.628191	-1.352730

97	6	0	-0.212447	-4.784392	-1.505961
98	6	0	0.183416	-5.774186	-2.415386
99	1	0	-0.419588	-6.676828	-2.532511
100	6	0	1.359855	-5.604096	-3.164578
101	1	0	1.680209	-6.374049	-3.868740
102	6	0	2.137037	-4.452287	-2.990547
103	1	0	3.066857	-4.329040	-3.548785
104	1	0	-1.078648	4.725595	1.365983
105	1	0	-1.121502	-4.879715	-0.912507

CP'-R$_{model}$

B97D/6-31g(d);E(RB97D) = -4834.843462 hartree
Zero-point Energy Correction = 0.764451 hartree
Thermal Correction to Energy = 0.823457 hartree
Thermal correction to Enthalpy = 0.824401 hartree
Thermal correction to Gibbs Free Energy = 0.668608 hartree
Sum of electronic and Zero-point Energies = -4834.079012 hartree
Sum of electronic and thermal Energies = -4834.020005 hartree
Sum of electronic and thermal Enthalpies = -4834.019061 hartree
Sum of electronic and thermal Free Energies = -4834.174855 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.864393 hartree
Gibbs Free Energy in ether = -4834.195785 hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.887465	2.874819	2.775042
2	1	0	-3.035529	2.067339	2.206345
3	6	0	-1.042802	3.280735	1.208139
4	6	0	0.005793	2.564903	1.894672
5	6	0	1.355015	2.690415	1.424139
6	6	0	-0.230081	1.747908	3.045804
7	6	0	2.396174	2.019382	2.059856
8	1	0	1.578743	3.356000	0.593436
9	6	0	0.818977	1.066285	3.652602
10	1	0	-1.247839	1.623113	3.397476
11	6	0	2.134731	1.192640	3.164656
12	1	0	3.413095	2.128706	1.686061
13	1	0	0.610633	0.407293	4.495821
14	1	0	2.951256	0.645160	3.636951
15	6	0	-0.936600	3.544436	-0.195789
16	1	0	-1.527876	4.364714	-0.602373
17	6	0	-0.287793	2.712455	-1.069370
18	1	0	0.173331	1.788150	-0.734909
19	1	0	-0.307436	2.919280	-2.138758
20	8	0	2.427506	3.143046	-1.729479
21	6	0	3.164891	2.249392	-2.139443
22	6	0	4.740119	2.483343	-2.052027
23	17	0	5.731453	0.961429	-2.172622
24	17	0	5.125323	3.288299	-0.478040
25	17	0	5.168459	3.584391	-3.426215
26	7	0	2.771133	1.125170	-2.767531
27	1	0	3.367620	0.302269	-2.848660
28	6	0	-2.261946	3.869759	1.977086
29	1	0	1.777922	0.906057	-2.717859
30	6	0	-3.297440	4.513507	1.024438
31	6	0	-4.227692	3.687658	0.359437
32	6	0	-3.322830	5.897193	0.767150
33	6	0	-5.163844	4.237556	-0.526677
34	1	0	-4.220320	2.611871	0.527955
35	6	0	-4.260887	6.448021	-0.122149
36	1	0	-2.612703	6.562547	1.258416
37	6	0	-5.186155	5.620204	-0.772540
38	1	0	-5.879646	3.578518	-1.022531
39	1	0	-4.265584	7.525362	-0.300441
40	1	0	-5.917553	6.046921	-1.461882
41	6	0	-1.678349	4.896592	2.984464
42	1	0	-2.516490	5.378373	3.507895
43	1	0	-1.051317	4.357273	3.705451
44	1	0	-1.068590	5.664648	2.487438
45	15	0	-2.185248	-0.033851	0.271585
46	15	0	2.029595	-1.504741	-0.975519
47	8	0	-3.088694	0.714146	1.214563
48	8	0	-0.671363	0.003629	0.458143
49	1	0	0.107393	-0.437585	-0.664177
50	8	0	-2.398030	0.426629	-1.320936
51	8	0	-2.729098	-1.590905	0.222920
52	8	0	3.046050	-1.793979	-2.020958
53	8	0	0.748172	-0.717072	-1.465030
54	8	0	2.535742	-0.540425	0.270706
55	8	0	1.564753	-2.865382	-0.193274
56	6	0	-1.211749	-3.357492	-0.396955
57	6	0	-2.206322	-2.443438	-0.745846
58	6	0	-2.771822	-2.371499	-2.057173
59	6	0	-2.370313	-3.321034	-2.990484
60	1	0	-2.770531	-3.275478	-4.005455
61	6	0	-1.426133	-4.332079	-2.669461
62	6	0	-1.040988	-5.318116	-3.625350
63	1	0	-1.495671	-5.285881	-4.618393
64	6	0	-0.114579	-6.295052	-3.302744
65	1	0	0.172691	-7.044952	-4.042352
66	6	0	0.464635	-6.324179	-2.004486
67	1	0	1.191438	-7.099388	-1.754273
68	6	0	0.118657	-5.375417	-1.056045
69	1	0	0.566612	-5.399623	-0.063037
70	6	0	-0.825865	-4.352053	-1.356668
71	6	0	-3.735240	-1.300645	-2.413667
72	6	0	-3.541855	0.047458	-2.018437
73	6	0	-4.433542	1.057928	-2.400105
74	6	0	-5.547006	0.743051	-3.190706
75	1	0	-6.241829	1.531498	-3.487339
76	6	0	-5.764360	-0.584128	-3.595410
77	1	0	-6.633670	-0.839282	-4.204037
78	6	0	-4.867255	-1.587005	-3.207064
79	1	0	-5.040776	-2.622901	-3.504197
80	6	0	-0.535003	-3.214757	0.926938
81	6	0	0.802787	-2.824350	0.979780
82	6	0	1.459743	-2.462139	2.196711
83	6	0	0.733287	-2.563814	3.379577
84	1	0	1.202917	-2.267948	4.319850
85	6	0	-0.606519	-3.025518	3.402100
86	6	0	-1.328533	-3.151426	4.625972
87	1	0	-0.824070	-2.886733	5.558714
88	6	0	-2.635662	-3.606104	4.632414
89	1	0	-3.180076	-3.700559	5.573988
90	6	0	-3.271559	-3.955923	3.409281
91	1	0	-4.300579	-4.319995	3.420569
92	6	0	-2.600163	-3.834235	2.203905
93	1	0	-3.093740	-4.098365	1.269462
94	6	0	-1.257136	-3.360003	2.159287
95	6	0	2.856259	-1.966808	2.224513
96	6	0	3.362592	-1.058098	1.264295
97	6	0	4.662999	-0.544280	1.348426
98	6	0	5.492950	-0.919669	2.412176
99	1	0	6.505354	-0.517246	2.477389
100	6	0	5.019594	-1.820408	3.381431
101	1	0	5.663271	-2.130746	4.206305
102	6	0	3.723562	-2.338812	3.277000
103	1	0	3.361621	-3.057324	4.014135
104	1	0	-4.232235	2.078863	-2.075633
105	1	0	4.998981	0.152652	0.581780

TS'-R$_{model}$

B97D/6-31g(d);E(RB97D) = -4834.833519 hartree
Zero-point Energy Correction = 0.758745 hartree
Thermal Correction to Energy = 0.817934 hartree
Thermal correction to Enthalpy = 0.818878 hartree
Thermal correction to Gibbs Free Energy = 0.660303 hartree
Sum of electronic and Zero-point Energies = -4834.074773 hartree
Sum of electronic and thermal Energies = -4834.015585 hartree
Sum of electronic and thermal Enthalpies = -4834.014640 hartree
Sum of electronic and thermal Free Energies = -4834.173215 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.853541 hartree
Gibbs Free Energy in ether = -4834.193238 hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.347146	3.064593	1.384964
2	1	0	-2.028619	2.649053	0.547030
3	6	0	0.230811	3.517757	0.482388
4	6	0	1.380302	2.906649	1.194884
5	6	0	2.674756	3.125451	0.667277
6	6	0	1.241485	2.153581	2.382800
7	6	0	3.803806	2.633045	1.334461
8	1	0	2.793793	3.681536	-0.261469
9	6	0	2.374571	1.660097	3.035745
10	1	0	0.244581	1.924489	2.751403
11	6	0	3.658887	1.903514	2.521883
12	1	0	4.791600	2.806539	0.907107
13	1	0	2.257385	1.050354	3.931100
14	1	0	4.533265	1.495627	3.029367
15	6	0	0.109510	3.363350	-0.958589
16	1	0	-0.569353	4.041604	-1.474917
17	6	0	0.747944	2.386429	-1.646967
18	1	0	1.391540	1.657843	-1.161460
19	1	0	0.632246	2.304548	-2.728924
20	8	0	3.643031	1.287784	-2.361537
21	6	0	4.011863	0.123883	-2.451636
22	6	0	5.571647	-0.192906	-2.302729
23	17	0	5.944044	-1.920600	-1.841597
24	17	0	6.282338	0.889978	-1.045461
25	17	0	6.320790	0.163417	-3.917405
26	7	0	3.239669	-0.930575	-2.795906
27	1	0	3.500780	-1.888321	-2.572010
28	6	0	-0.774512	4.380256	1.200830
29	1	0	2.234626	-0.764442	-2.796332
30	6	0	-1.597606	5.354326	0.377647
31	6	0	-2.985157	5.197759	0.234845
32	6	0	-0.956975	6.463112	-0.207493
33	6	0	-3.725842	6.144557	-0.490216
34	1	0	-3.481694	4.332692	0.672092
35	6	0	-1.697146	7.404758	-0.934499
36	1	0	0.124433	6.579452	-0.100815
37	6	0	-3.086411	7.247529	-1.075479
38	1	0	-4.803871	6.013217	-0.600549
39	1	0	-1.191238	8.257577	-1.391368
40	1	0	-3.664654	7.979560	-1.642595
41	6	0	-0.392920	5.003733	2.542929
42	1	0	-1.316957	5.264577	3.079359

43	1	0	0.205276	4.317816	3.154258
44	1	0	0.179828	5.926949	2.368487
45	15	0	-2.265000	0.663033	-0.701079
46	15	0	1.375731	-2.269354	-0.459467
47	8	0	-2.786033	2.047480	-0.288758
48	8	0	-0.814065	0.344837	-0.415562
49	1	0	-0.073628	-0.734903	-1.115562
50	8	0	-2.523799	0.409078	-2.310003
51	8	0	-3.280865	-0.429861	-0.015419
52	8	0	2.287928	-3.299332	-1.016695
53	8	0	0.518108	-1.479161	-1.535697
54	8	0	2.091966	-1.027272	0.363242
55	8	0	0.366675	-2.902713	0.671706
56	6	0	-2.423848	-2.641577	0.423878
57	6	0	-3.117183	-1.764011	-0.406183
58	6	0	-3.734116	-2.165704	-1.630927
59	6	0	-3.696321	-3.515281	-1.963360
60	1	0	-4.140425	-3.846449	-2.904255
61	6	0	-3.067283	-4.473164	-1.124813
62	6	0	-3.053829	-5.858554	-1.463841
63	1	0	-3.542801	-6.172794	-2.388993
64	6	0	-2.437536	-6.784048	-0.639248
65	1	0	-2.432647	-7.841981	-0.908598
66	6	0	-1.809569	-6.357533	0.562928
67	1	0	-1.328568	-7.092253	1.211358
68	6	0	-1.797563	-5.018084	0.916694
69	1	0	-1.312485	-4.696776	1.837629
70	6	0	-2.414640	-4.037742	0.087269
71	6	0	-4.383987	-1.168770	-2.515624
72	6	0	-3.797599	0.090683	-2.792827
73	6	0	-4.414257	1.017623	-3.640669
74	6	0	-5.638056	0.700028	-4.245638
75	1	0	-6.119083	1.423428	-4.906520
76	6	0	-6.239176	-0.544178	-3.996118
77	1	0	-7.195209	-0.796387	-4.458179
78	6	0	-5.617167	-1.459460	-3.138310
79	1	0	-6.091327	-2.418199	-2.921001
80	6	0	-1.690052	-2.105344	1.609024
81	6	0	-0.296148	-2.150674	1.643629
82	6	0	0.469814	-1.560416	2.699318
83	6	0	-0.221132	-0.927037	3.727399
84	1	0	0.343494	-0.446806	4.529046
85	6	0	-1.637182	-0.875996	3.765626
86	6	0	-2.328471	-0.235775	4.836555
87	1	0	-1.740556	0.227252	5.632995
88	6	0	-3.711849	-0.209349	4.870096
89	1	0	-4.232705	0.281279	5.694705
90	6	0	-4.457784	-0.830308	3.830751
91	1	0	-5.548818	-0.816096	3.866200
92	6	0	-3.814683	-1.451195	2.772392
93	1	0	-4.393971	-1.922433	1.979478
94	6	0	-2.391487	-1.483985	2.697457
95	6	0	1.950588	-1.600209	2.721254
96	6	0	2.724657	-1.350395	1.567538
97	6	0	4.121892	-1.327824	1.603254
98	6	0	4.785342	-1.546351	2.817424
99	1	0	5.876327	-1.530753	2.846901
100	6	0	4.044214	-1.792865	3.985357
101	1	0	4.554190	-1.977238	4.932590
102	6	0	2.645534	-1.824333	3.930395
103	1	0	2.065462	-2.039575	4.829451
104	1	0	-3.917360	1.971220	-3.819506
105	1	0	4.669348	-1.123656	0.685424

Product-R_{model}

B97D/6-31g(d);E(RB97D) = -4834.847522 hartree
Zero-point Energy Correction = 0.762498 hartree
Thermal Correction to Energy = 0.822376 hartree
Thermal correction to Enthalpy = 0.823321 hartree
Thermal correction to Gibbs Free Energy = 0.662454 hartree
Sum of electronic and Zero-point Energies = -4834.085024 hartree
Sum of electronic and thermal Energies = -4834.025146 hartree
Sum of electronic and thermal Enthalpies = -4834.024201 hartree
Sum of electronic and thermal Free Energies = -4834.185068 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.865840 hartree
Gibbs Free Energy in ether = -4834.203386 hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.127617	3.231491	1.428720
2	1	0	-2.325051	2.528294	0.630370
3	6	0	0.059970	3.526129	0.575667
4	6	0	1.347177	2.951703	1.098173
5	6	0	2.569010	3.459943	0.619627
6	6	0	1.350148	1.937721	2.073305
7	6	0	3.782510	2.953973	1.104953
8	1	0	2.567730	4.233611	-0.149432
9	6	0	2.565689	1.448920	2.571410
10	1	0	0.402791	1.533525	2.425444
11	6	0	3.782954	1.951179	2.086036
12	1	0	4.722987	3.334460	0.704811
13	1	0	2.563910	0.657095	3.321107
14	1	0	4.725685	1.548710	2.460509
15	6	0	-0.223114	3.439921	-0.889428
16	1	0	-1.154256	3.917217	-1.202716
17	6	0	0.558090	2.837626	-1.799814
18	1	0	1.499800	2.350994	-1.543758
19	1	0	0.261425	2.831169	-2.850882
20	8	0	3.828895	1.589449	-2.109366
21	6	0	4.095822	0.408309	-2.280265
22	6	0	5.620634	-0.051166	-2.140257
23	17	0	5.845217	-1.845302	-1.868348
24	17	0	6.377213	0.825533	-0.756985
25	17	0	6.440450	0.415875	-3.691722
26	7	0	3.237304	-0.548679	-2.699128
27	1	0	3.419892	-1.542271	-2.575859
28	6	0	-0.649913	4.603936	1.366636
29	1	0	2.252010	-0.295558	-2.694233
30	6	0	-1.552219	5.588455	0.670145
31	6	0	-2.940301	5.382402	0.593407
32	6	0	-0.991193	6.747674	0.101397
33	6	0	-3.759158	6.325917	-0.046422
34	1	0	-3.379009	4.485132	1.030161
35	6	0	-1.809158	7.688073	-0.539030
36	1	0	0.088950	6.902101	0.150341
37	6	0	-3.196691	7.479467	-0.613849
38	1	0	-4.836394	6.156581	-0.100991
39	1	0	-1.363909	8.579915	-0.984554
40	1	0	-3.833964	8.211312	-1.114107
41	6	0	-0.063898	5.112877	2.674837
42	1	0	-0.882837	5.364114	3.366875
43	1	0	0.589576	4.360112	3.133003
44	1	0	0.516770	6.028718	2.484923
45	15	0	-2.312755	0.634040	-0.403448
46	15	0	1.346347	-2.213519	-0.579482
47	8	0	-3.012321	1.937161	0.163513
48	8	0	-0.874182	0.440096	-0.034549
49	1	0	-0.021221	-0.533855	-0.947383
50	8	0	-2.484732	0.617471	-2.028538
51	8	0	-3.330999	-0.535557	0.082065
52	8	0	2.214611	-3.149609	-1.335156
53	8	0	0.478296	-1.235242	-1.489810
54	8	0	2.087149	-1.134176	0.413833
55	8	0	0.348611	-3.022997	0.444335
56	6	0	-2.438270	-2.777338	0.211731
57	6	0	-3.131553	-1.803880	-0.500532
58	6	0	-3.710549	-2.025425	-1.786064
59	6	0	-3.645981	-3.312794	-2.307929
60	1	0	-4.058096	-3.508337	-3.299764
61	6	0	-3.023595	-4.374138	-1.599080
62	6	0	-2.981830	-5.696068	-2.133027
63	1	0	-3.447305	-5.880841	-3.103914
64	6	0	-2.366094	-6.721585	-1.436390
65	1	0	-2.338886	-7.729608	-1.854353
66	6	0	-1.766869	-6.464145	-0.172964
67	1	0	-1.285878	-7.278029	0.372541
68	6	0	-1.782400	-5.189505	0.369563
69	1	0	-1.319225	-4.996332	1.336338
70	6	0	-2.400992	-4.109742	-0.323362
71	6	0	-4.330187	-0.912574	-2.544213
72	6	0	-3.738600	0.371061	-2.616089
73	6	0	-4.313603	1.413583	-3.348768
74	6	0	-5.508705	1.189623	-4.046353
75	1	0	-5.960724	2.000955	-4.619301
76	6	0	-6.117583	-0.074885	-4.001675
77	1	0	-7.051296	-0.254559	-4.537078
78	6	0	-5.533753	-1.106255	-3.256120
79	1	0	-6.015086	-2.083961	-3.199134
80	6	0	-1.725269	-2.401780	1.469053
81	6	0	-0.330614	-2.425070	1.507528
82	6	0	0.418797	-1.967326	2.638371
83	6	0	-0.292150	-1.482414	3.732405
84	1	0	0.258338	-1.095515	4.592149
85	6	0	-1.709528	-1.469143	3.767463
86	6	0	-2.419811	-0.993652	4.909405
87	1	0	-1.846093	-0.624718	5.762940
88	6	0	-3.803610	-1.007292	4.938308
89	1	0	-4.338649	-0.643809	5.817733
90	6	0	-4.531489	-1.503401	3.821884
91	1	0	-5.622560	-1.522204	3.853424
92	6	0	-3.870220	-1.961810	2.694015
93	1	0	-4.435437	-2.339608	1.842630
94	6	0	-2.446501	-1.949039	2.624858
95	6	0	1.900317	-2.000876	2.677729
96	6	0	2.695286	-1.613985	1.577315
97	6	0	4.091213	-1.581452	1.643792
98	6	0	4.733086	-1.936541	2.836754
99	1	0	5.822719	-1.910232	2.891813
100	6	0	3.972234	-2.327496	3.951313
101	1	0	4.465481	-2.615932	4.881120
102	6	0	2.575477	-2.362877	3.865342
103	1	0	1.981335	-2.685958	4.721742
104	1	0	-3.809555	2.379828	-3.369727
105	1	0	4.652271	-1.257080	0.769859

CP-S_{model}

B97D/6-31g(d);E(RB97D) = -4834.841664 hartree
Zero-point Energy Correction = 0.766233 hartree
Thermal Correction to Energy = 0.824040 hartree
Thermal correction to Enthalpy = 0.824984 hartree

Thermal correction to Gibbs Free Energy = 0.669815 hartree
Sum of electronic and Zero-point Energies = -4834.075430 hartree
Sum of electronic and thermal Energies = -4834.017624 hartree
Sum of electronic and thermal Enthalpies = -4834.016680 hartree
Sum of electronic and thermal Free Energies = -4834.171849 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.864911 hartree
Gibbs Free Energy in ether = -4834.195096 hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.081060	-3.907321	-0.478717
2	1	0	-1.211142	-3.680893	-0.889840
3	6	0	-2.756021	-1.615423	-0.820121
4	6	0	-2.794401	-1.170948	0.601156
5	6	0	-3.615553	-0.071001	0.938239
6	6	0	-2.041747	-1.792051	1.621617
7	6	0	-3.684136	0.397118	2.257202
8	1	0	-4.214428	0.399161	0.156802
9	6	0	-2.107316	-1.314199	2.935559
10	1	0	-1.397349	-2.628498	1.371291
11	6	0	-2.927394	-0.223053	3.261930
12	1	0	-4.329840	1.244595	2.498239
13	1	0	-1.498265	-1.787092	3.707670
14	1	0	-2.958958	0.151228	4.285884
15	6	0	-2.447829	-0.745696	-1.819694
16	1	0	-2.493909	-1.062242	-2.860889
17	6	0	-1.789773	0.547203	-1.556293
18	1	0	-1.484473	0.665709	-0.515373
19	1	0	-0.957868	0.737851	-2.245053
20	8	0	-2.751629	1.750507	-1.793357
21	6	0	-2.286868	2.924002	-1.511571
22	6	0	-3.381602	4.034904	-1.497630
23	17	0	-4.222378	3.851251	0.096530
24	17	0	-4.528829	3.793197	-2.855581
25	17	0	-2.660011	5.690119	-1.618463
26	7	0	-1.048786	3.186075	-1.193954
27	1	0	-0.777583	4.117325	-0.877856
28	6	0	-3.078483	-3.102752	-1.111110
29	1	0	-0.290299	2.432314	-1.004246
30	15	0	1.022638	-1.824477	-1.366920
31	15	0	1.047660	2.251794	1.018938
32	8	0	0.438023	-3.184890	-1.530578
33	8	0	0.381221	-0.928974	-0.245990
34	1	0	0.635400	0.082722	-0.285863
35	8	0	0.942647	-0.847233	-2.701272
36	8	0	2.633641	-1.905000	-1.102562
37	8	0	1.076352	3.743014	1.040447
38	8	0	0.857084	1.557804	-0.366325
39	8	0	-0.205867	1.585252	1.890801
40	8	0	2.356482	1.591985	1.769871
41	6	0	3.804092	-0.161035	0.093289
42	6	0	3.393644	-0.725697	-1.113581
43	6	0	3.765856	-0.199983	-2.389228
44	6	0	4.657038	0.866979	-2.417460
45	1	0	4.939120	1.301950	-3.378417
46	6	0	5.188947	1.426342	-1.226573
47	6	0	6.130133	2.497340	-1.266872
48	1	0	6.441858	2.880334	-2.241564
49	6	0	6.640399	3.035732	-0.098230
50	1	0	7.361449	3.854412	-0.139763
51	6	0	6.227349	2.520274	1.160887
52	1	0	6.637226	2.944689	2.079280
53	6	0	5.306394	1.488037	1.233729
54	1	0	4.991285	1.098881	2.201033
55	6	0	4.754956	0.915446	0.051372
56	6	0	3.197753	-0.752525	-3.642281
57	6	0	1.827840	-1.086941	-3.763518
58	6	0	1.288504	-1.580513	-4.955919
59	6	0	2.116320	-1.742549	-6.075363
60	1	0	1.699071	-2.130656	-7.006135
61	6	0	3.478543	-1.412502	-5.989388
62	1	0	4.131550	-1.544420	-6.853765
63	6	0	4.006519	-0.928907	-4.786086
64	1	0	5.069397	-0.694360	-4.707566
65	6	0	3.197875	-0.629496	1.375611
66	6	0	2.381294	0.236483	2.106460
67	6	0	1.626619	-0.190816	3.245879
68	6	0	1.762430	-1.512357	3.657394
69	1	0	1.175798	-1.866745	4.507388
70	6	0	2.629820	-2.420510	2.998236
71	6	0	2.781443	-3.764264	3.451724
72	1	0	2.206784	-4.087615	4.322989
73	6	0	3.640538	-4.636763	2.806336
74	1	0	3.749907	-5.663361	3.161192
75	6	0	4.386927	-4.194092	1.679925
76	1	0	5.069854	-4.883235	1.179519
77	6	0	4.252784	-2.898365	1.208551
78	1	0	4.825951	-2.566561	0.343544
79	6	0	3.367191	-1.977688	1.840347
80	6	0	0.714260	0.728744	3.966926
81	6	0	-0.147902	1.613914	3.279905
82	6	0	-1.027496	2.461295	3.962698
83	6	0	-1.080827	2.425857	5.362186
84	1	0	-1.766779	3.086122	5.896384
85	6	0	-0.248587	1.543152	6.070965
86	1	0	-0.279455	1.513698	7.161564
87	6	0	0.639765	0.712578	5.376668
88	1	0	1.308019	0.045238	5.923849
89	1	0	-1.670743	3.120476	3.380228
90	1	0	0.226808	-1.826297	-4.988440
91	6	0	-4.441770	-3.426035	-0.486668
92	6	0	-4.595945	-4.437468	0.474749
93	6	0	-5.569978	-2.686606	-0.890573
94	6	0	-5.862594	-4.708066	1.017445
95	1	0	-3.723228	-5.003757	0.795049
96	6	0	-6.833366	-2.954838	-0.348598
97	1	0	-5.449552	-1.885883	-1.624229
98	6	0	-6.984115	-3.970757	0.609704
99	1	0	-5.970039	-5.497095	1.765308
100	1	0	-7.698001	-2.369915	-0.670455
101	1	0	-7.967002	-4.181743	1.036657
102	6	0	-3.109614	-3.455190	-2.616129
103	1	0	-3.877114	-2.882628	-3.158714
104	1	0	-2.123003	-3.266812	-3.067261
105	1	0	-3.339342	-4.525864	-2.704651

TS-S$_{model}$

B97D/6-31g(d);E(RB97D) = -4834.838141 hartree
Zero-point Energy Correction = 0.764903 hartree
Thermal Correction to Energy = 0.822408 hartree
Thermal correction to Enthalpy = 0.823352 hartree
Thermal correction to Gibbs Free Energy = 0.670063 hartree
Sum of electronic and Zero-point Energies = -4834.073237 hartree
Sum of electronic and thermal Energies = -4834.015733 hartree
Sum of electronic and thermal Enthalpies = -4834.014789 hartree
Sum of electronic and thermal Free Energies = -4834.168077 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.859556 hartree
Gibbs Free Energy in ether = -4834.189493 hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.661477	-4.056900	-0.028488
2	1	0	-0.792661	-3.832793	-0.454661
3	6	0	-2.552359	-1.945297	-0.777226
4	6	0	-2.711539	-1.267357	0.521325
5	6	0	-3.529625	-0.109828	0.579432
6	6	0	-2.106352	-1.731567	1.715233
7	6	0	-3.742280	0.553622	1.791972
8	1	0	-4.018441	0.240548	-0.329154
9	6	0	-2.308272	-1.048134	2.916389
10	1	0	-1.459064	-2.601212	1.674629
11	6	0	-3.127441	0.091409	2.964820
12	1	0	-4.383125	1.436212	1.817933
13	1	0	-1.806802	-1.396302	3.820226
14	1	0	-3.263378	0.628178	3.904191
15	6	0	-2.264927	-1.233160	-1.932245
16	1	0	-2.283047	-1.739889	-2.895367
17	6	0	-1.656070	0.046207	-1.882754
18	1	0	-1.406898	0.453069	-0.907530
19	1	0	-0.994030	0.318180	-2.704769
20	8	0	-2.905947	1.476454	-2.286972
21	6	0	-2.478230	2.642757	-2.065843
22	6	0	-3.574791	3.772539	-1.995574
23	17	0	-4.094879	3.816161	-0.252493
24	17	0	-4.965976	3.366163	-3.048226
25	17	0	-2.921509	5.393967	-2.474250
26	7	0	-1.222113	2.986793	-1.834757
27	1	0	-0.971004	3.918570	-1.506786
28	6	0	-2.697391	-3.491345	-0.827612
29	1	0	-0.479325	2.277262	-1.648694
30	15	0	1.273448	-1.950068	-1.133076
31	15	0	0.832897	2.395226	0.544284
32	8	0	0.754505	-3.350300	-1.172081
33	8	0	0.474693	-0.940975	-0.242577
34	1	0	0.684046	0.099158	-0.422157
35	8	0	1.329638	-1.188970	-2.601015
36	8	0	2.840683	-1.924427	-0.671110
37	8	0	0.815340	3.871265	0.329167
38	8	0	0.823910	1.469601	-0.704862
39	8	0	-0.496365	1.828118	1.384718
40	8	0	2.060093	1.941909	1.553304
41	6	0	3.781277	0.037268	0.384721
42	6	0	3.555484	-0.719905	-0.763466
43	6	0	4.072046	-0.366072	-2.047793
44	6	0	4.924389	0.729557	-2.125951
45	1	0	5.313539	1.035416	-3.099150
46	6	0	5.277135	1.483166	-0.976231
47	6	0	6.180236	2.583941	-1.060328
48	1	0	6.605693	2.835176	-2.034846
49	6	0	6.512511	3.314831	0.067203
50	1	0	7.205432	4.155160	-0.007529
51	6	0	5.951758	2.970412	1.327536
52	1	0	6.220841	3.547136	2.214441
53	6	0	5.063059	1.913744	1.440131
54	1	0	4.633764	1.656586	2.407637
55	6	0	4.693788	1.144246	0.299403
56	6	0	3.684103	-1.119851	-3.264108
57	6	0	2.350553	-1.532702	-3.499960
58	6	0	1.983120	-2.214728	-4.664679

59	6	0	2.950776	-2.494146	-5.639454
60	1	0	2.666477	-3.028452	-6.547654
61	6	0	4.280825	-2.091764	-5.437520
62	1	0	5.042101	-2.313201	-6.187463
63	6	0	4.636549	-1.418212	-4.262671
64	1	0	5.673271	-1.124003	-4.090729
65	6	0	3.023010	-0.262599	1.636349
66	6	0	2.090503	0.663743	2.109748
67	6	0	1.214467	0.383487	3.208017
68	6	0	1.339013	-0.847455	3.842969
69	1	0	0.665565	-1.090650	4.667371
70	6	0	2.307296	-1.804618	3.445661
71	6	0	2.439889	-3.052432	4.123714
72	1	0	1.770632	-3.263408	4.961439
73	6	0	3.398099	-3.972198	3.734049
74	1	0	3.491971	-4.924373	4.259822
75	6	0	4.267176	-3.674345	2.648695
76	1	0	5.027345	-4.398933	2.350603
77	6	0	4.156298	-2.475439	1.963461
78	1	0	4.824044	-2.254506	1.131562
79	6	0	3.171726	-1.511716	2.328414
80	6	0	0.199355	1.364092	3.661107
81	6	0	-0.592696	2.093209	2.743957
82	6	0	-1.554442	3.014385	3.175356
83	6	0	-1.771312	3.203376	4.546515
84	1	0	-2.521319	3.921364	4.884135
85	6	0	-1.018727	2.471008	5.480231
86	1	0	-1.177279	2.616180	6.550338
87	6	0	-0.041453	1.570943	5.036520
88	1	0	0.569320	1.025397	5.758174
89	1	0	-2.128483	3.554955	2.423291
90	1	0	0.941668	-2.511612	-4.790774
91	6	0	-4.057562	-3.842403	-0.210916
92	6	0	-4.162643	-4.653279	0.930365
93	6	0	-5.228695	-3.329428	-0.801422
94	6	0	-5.425142	-4.953900	1.465902
95	1	0	-3.257387	-5.044276	1.391337
96	6	0	-6.487865	-3.625395	-0.263849
97	1	0	-5.150439	-2.684543	-1.679955
98	6	0	-6.589870	-4.442124	0.874132
99	1	0	-5.496085	-5.588855	2.351790
100	1	0	-7.386918	-3.217637	-0.730830
101	1	0	-7.569521	-4.674657	1.296794
102	6	0	-2.604503	-4.091587	-2.248336
103	1	0	-3.394781	-3.709949	-2.912326
104	1	0	-1.617254	-3.877395	-2.684984
105	1	0	-2.720733	-5.179719	-2.153735

CP’ -S_{model}

B97D/6-31g(d);E(RB97D) = -4834.843434 hartree
Zero-point Energy Correction = 0.763655 hartree
Thermal Correction to Energy = 0.822731 hartree
Thermal correction to Enthalpy = 0.823675 hartree
Thermal correction to Gibbs Free Energy = 0.665168 hartree
Sum of electronic and Zero-point Energies = -4834.079779 hartree
Sum of electronic and thermal Energies = -4834.020704 hartree
Sum of electronic and thermal Enthalpies = -4834.019759 hartree
Sum of electronic and thermal Free Energies = -4834.178266 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.865041 hartree
Gibbs Free Energy in ether = -4834.199873 hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.602015	-4.287883	0.029483
2	1	0	0.218897	-3.904001	-0.409471
3	6	0	-1.941660	-2.606977	-1.041290
4	6	0	-2.360927	-1.826421	0.098536
5	6	0	-3.274555	-0.741570	-0.098289
6	6	0	-1.970759	-2.146866	1.435549
7	6	0	-3.771776	-0.024931	0.988639
8	1	0	-3.631332	-0.509184	-1.099398
9	6	0	-2.464988	-1.412227	2.505663
10	1	0	-1.237375	-2.932790	1.583669
11	6	0	-3.367194	-0.350974	2.292812
12	1	0	-4.470641	0.793179	0.816306
13	1	0	-2.129006	-1.642558	3.516540
14	1	0	-3.734732	0.229040	3.139650
15	6	0	-1.805900	-2.003820	-2.332264
16	1	0	-1.828975	-2.651933	-3.207452
17	6	0	-1.466973	-0.689382	-2.509793
18	1	0	-1.288568	-0.032208	-1.666041
19	1	0	-1.289105	-0.293457	-3.509332
20	8	0	-3.285984	1.494366	-2.646715
21	6	0	-2.954466	2.604660	-2.237849
22	6	0	-4.103961	3.646681	-1.864431
23	17	0	-3.585082	4.907839	-0.653919
24	17	0	-5.521462	2.757906	-1.188074
25	17	0	-4.573413	4.464738	-3.413225
26	7	0	-1.697525	3.084434	-2.180983
27	1	0	-1.436103	3.889598	-1.614082
28	6	0	-1.674984	-4.133400	-0.887731
29	1	0	-0.941745	2.415636	-2.319537
30	15	0	1.676283	-1.708554	-1.130317
31	15	0	0.321069	2.498992	0.333393
32	8	0	1.441735	-3.191050	-1.271179
33	8	0	0.623853	-0.837901	-0.445220
34	1	0	0.667602	0.546001	-0.717195
35	8	0	1.934116	-0.974944	-2.605228
36	8	0	3.145493	-1.486716	-0.407259
37	8	0	0.178769	3.953807	0.064471
38	8	0	0.618282	1.595394	-0.927843
39	8	0	-1.025064	1.758080	0.955756
40	8	0	1.438710	2.202412	1.495009
41	6	0	3.607969	0.584248	0.738605
42	6	0	3.695260	-0.206792	-0.406360
43	6	0	4.388577	0.211705	-1.585784
44	6	0	5.086452	1.413069	-1.540362
45	1	0	5.605529	1.763429	-2.434890
46	6	0	5.116510	2.216045	-0.369732
47	6	0	5.861463	3.431298	-0.322592
48	1	0	6.421903	3.732726	-1.210819
49	6	0	5.876851	4.209935	0.822016
50	1	0	6.451037	5.138151	0.847343
51	6	0	5.144061	3.799766	1.969183
52	1	0	5.163164	4.414655	2.871082
53	6	0	4.402554	2.629492	1.952016
54	1	0	3.842053	2.321083	2.834040
55	6	0	4.359316	1.807495	0.789007
56	6	0	4.337972	-0.601352	-2.824487
57	6	0	3.134250	-1.194584	-3.281016
58	6	0	3.090554	-1.937270	-4.467170
59	6	0	4.251947	-2.094869	-5.235604
60	1	0	4.216050	-2.675678	-6.159238
61	6	0	5.456121	-1.510874	-4.810276
62	1	0	6.366725	-1.635752	-5.398885
63	6	0	5.492106	-0.778338	-3.617476
64	1	0	6.430005	-0.341650	-3.269471
65	6	0	2.688470	0.179999	1.843817
66	6	0	1.559288	0.952824	2.113434
67	6	0	0.567371	0.573028	3.072121
68	6	0	0.763143	-0.613768	3.771700
69	1	0	0.010929	-0.935581	4.494525
70	6	0	1.907038	-1.426148	3.569346
71	6	0	2.099556	-2.633135	4.304896
72	1	0	1.337776	-2.928490	5.030797
73	6	0	3.228964	-3.408588	4.108473
74	1	0	3.367982	-4.330842	4.675938
75	6	0	4.214995	-3.000803	3.168290
76	1	0	5.107506	-3.612118	3.022441
77	6	0	4.052228	-1.838678	2.432126
78	1	0	4.808648	-1.534537	1.710117
79	6	0	2.894801	-1.023962	2.597853
80	6	0	-0.631766	1.404248	3.328771
81	6	0	-1.363762	2.013449	2.283041
82	6	0	-2.501243	2.791188	2.531424
83	6	0	-2.956386	2.953793	3.846248
84	1	0	-3.842627	3.560062	4.042090
85	6	0	-2.265491	2.339460	4.904708
86	1	0	-2.608400	2.466694	5.933010
87	6	0	-1.115139	1.584357	4.643535
88	1	0	-0.556045	1.135935	5.466482
89	1	0	-3.019926	3.241670	1.686426
90	1	0	2.139868	-2.375745	-4.771401
91	6	0	-2.948490	-4.761139	-0.303551
92	6	0	-2.928335	-5.453533	0.917359
93	6	0	-4.162152	-4.637487	-1.007370
94	6	0	-4.109065	-6.020589	1.422680
95	1	0	-1.989145	-5.551117	1.459374
96	6	0	-5.341571	-5.197030	-0.498774
97	1	0	-4.185107	-4.093335	-1.954690
98	6	0	-5.317835	-5.892421	0.720950
99	1	0	-4.081770	-6.565032	2.369040
100	1	0	-6.276043	-5.089760	-1.053169
101	1	0	-6.234532	-6.330590	1.120546
102	6	0	-1.310230	-4.849992	-2.207545
103	1	0	-2.131163	-4.814605	-2.939774
104	1	0	-0.399185	-4.408621	-2.636131
105	1	0	-1.114921	-5.901523	-1.957511

TS’ -S_{model}

B97D/6-31g(d);E(RB97D) = -4834.835787 hartree
Zero-point Energy Correction = 0.759004 hartree
Thermal Correction to Energy = 0.818024 hartree
Thermal correction to Enthalpy = 0.818968 hartree
Thermal correction to Gibbs Free Energy = 0.662505 hartree
Sum of electronic and Zero-point Energies = -4834.076782 hartree
Sum of electronic and thermal Energies = -4834.017762 hartree
Sum of electronic and thermal Enthalpies = -4834.016818 hartree
Sum of electronic and thermal Free Energies = -4834.173282 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.856516 hartree
Gibbs Free Energy in ether = -4834.194011 hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.160702	2.936929	-1.134683
2	1	0	-0.666655	2.459768	-1.797342
3	6	0	1.777319	2.377996	-1.840694
4	6	0	2.711177	2.051793	-0.735531

5	6	0	3.936404	1.418365	-1.056044
6	6	0	2.464235	2.419128	0.605319
7	6	0	4.887336	1.164526	-0.058884
8	1	0	4.145176	1.142289	-2.088390
9	6	0	3.409649	2.143519	1.595652
10	1	0	1.512350	2.872250	0.862426
11	6	0	4.623268	1.516170	1.272156
12	1	0	5.828761	0.681400	-0.326020
13	1	0	3.191917	2.396291	2.632681
14	1	0	5.346935	1.290663	2.056130
15	6	0	1.598207	1.423234	-2.927519
16	1	0	1.296007	1.808726	-3.900978
17	6	0	1.707438	0.087249	-2.734637
18	1	0	1.929458	-0.329050	-1.754005
19	1	0	1.552175	-0.626229	-3.543706
20	8	0	2.215956	-3.084905	-2.971858
21	6	0	2.466242	-3.704537	-1.946487
22	6	0	3.998035	-3.813792	-1.510016
23	17	0	4.315154	-4.845221	-0.028962
24	17	0	4.553013	-2.119170	-1.151589
25	17	0	4.935415	-4.494008	-2.891558
26	7	0	1.564917	-4.331494	-1.160562
27	1	0	1.768203	-4.618795	-0.206589
28	6	0	1.105798	3.724187	-1.897898
29	1	0	0.593986	-4.070547	-1.324042
30	15	0	-1.895858	0.517394	-1.798919
31	15	0	0.073996	-2.548738	1.192954
32	8	0	-1.590795	1.875303	-2.455179
33	8	0	-0.721593	-0.230384	-1.210841
34	1	0	-0.719362	-1.589206	-0.653941
35	8	0	-2.663969	-0.484474	-2.849254
36	8	0	-3.065480	0.833198	-0.689225
37	8	0	0.397993	-3.899132	1.717992
38	8	0	-0.632880	-2.532825	-0.221858
39	8	0	1.368148	-1.537752	0.971791
40	8	0	-0.852004	-1.686853	2.246551
41	6	0	-3.235193	-0.491327	1.310169
42	6	0	-3.616199	-0.255162	-0.008653
43	6	0	-4.610345	-1.021437	-0.691038
44	6	0	-5.236868	-2.040995	0.018195
45	1	0	-5.982922	-2.660354	-0.483667
46	6	0	-4.923349	-2.309415	1.376738
47	6	0	-5.589999	-3.343507	2.098585
48	1	0	-6.344446	-3.938281	1.578202
49	6	0	-5.291572	-3.585256	3.428457
50	1	0	-5.807475	-4.379524	3.971373
51	6	0	-4.312523	-2.795791	4.091705
52	1	0	-4.085066	-2.987274	5.142053
53	6	0	-3.640547	-1.789688	3.416740
54	1	0	-2.888996	-1.190927	3.929551
55	6	0	-3.913554	-1.522051	2.044283
56	6	0	-4.986704	-0.710362	-2.092530
57	6	0	-4.037620	-0.399173	-3.097319
58	6	0	-4.425675	-0.111610	-4.411155
59	6	0	-5.782846	-0.134177	-4.758609
60	1	0	-6.083126	0.090981	-5.783536
61	6	0	-6.746881	-0.443893	-3.786060
62	1	0	-7.807023	-0.456642	-4.044859
63	6	0	-6.347128	-0.721476	-2.473692
64	1	0	-7.094078	-0.936136	-1.707542
65	6	0	-2.129222	0.317390	1.905638
66	6	0	-0.923327	-0.293832	2.249375
67	6	0	0.209300	0.444656	2.719641
68	6	0	0.075795	1.819869	2.868348
69	1	0	0.933650	2.403091	3.206106
70	6	0	-1.128870	2.497188	2.557105
71	6	0	-1.235301	3.913600	2.689780
72	1	0	-0.362373	4.470183	3.039863
73	6	0	-2.417145	4.565851	2.381845
74	1	0	-2.491293	5.650342	2.485996
75	6	0	-3.543644	3.817548	1.941757
76	1	0	-4.478759	4.332682	1.714022
77	6	0	-3.466676	2.441765	1.795981
78	1	0	-4.334935	1.879361	1.455473
79	6	0	-2.258177	1.739647	2.077590
80	6	0	1.506702	-0.207454	3.006453
81	6	0	2.058767	-1.172692	2.135660
82	6	0	3.316106	-1.739495	2.365184
83	6	0	4.061648	-1.336702	3.481075
84	1	0	5.042106	-1.780552	3.663030
85	6	0	3.538276	-0.380552	4.367215
86	1	0	4.106491	-0.076709	5.248326
87	6	0	2.273677	0.170376	4.129680
88	1	0	1.851499	0.899360	4.823831
89	1	0	3.693888	-2.482329	1.665936
90	1	0	-3.650994	0.113368	-5.144187
91	6	0	1.698706	4.851678	-1.078345
92	6	0	0.930975	5.477333	-0.082243
93	6	0	3.002532	5.300490	-1.343851
94	6	0	1.471371	6.545874	0.648181
95	1	0	-0.071545	5.105922	0.134854
96	6	0	3.540792	6.369434	-0.613677
97	1	0	3.603026	4.797549	-2.105340
98	6	0	2.775548	6.994652	0.384382
99	1	0	0.873579	7.025557	1.426289
100	1	0	4.558750	6.707591	-0.816952
101	1	0	3.196391	7.823819	0.956601
102	6	0	0.552055	4.243179	-3.228356
103	1	0	1.377154	4.611782	-3.856815
104	1	0	-0.013831	3.470984	-3.764551
105	1	0	-0.122576	5.085247	-3.016398

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product-S_{model}

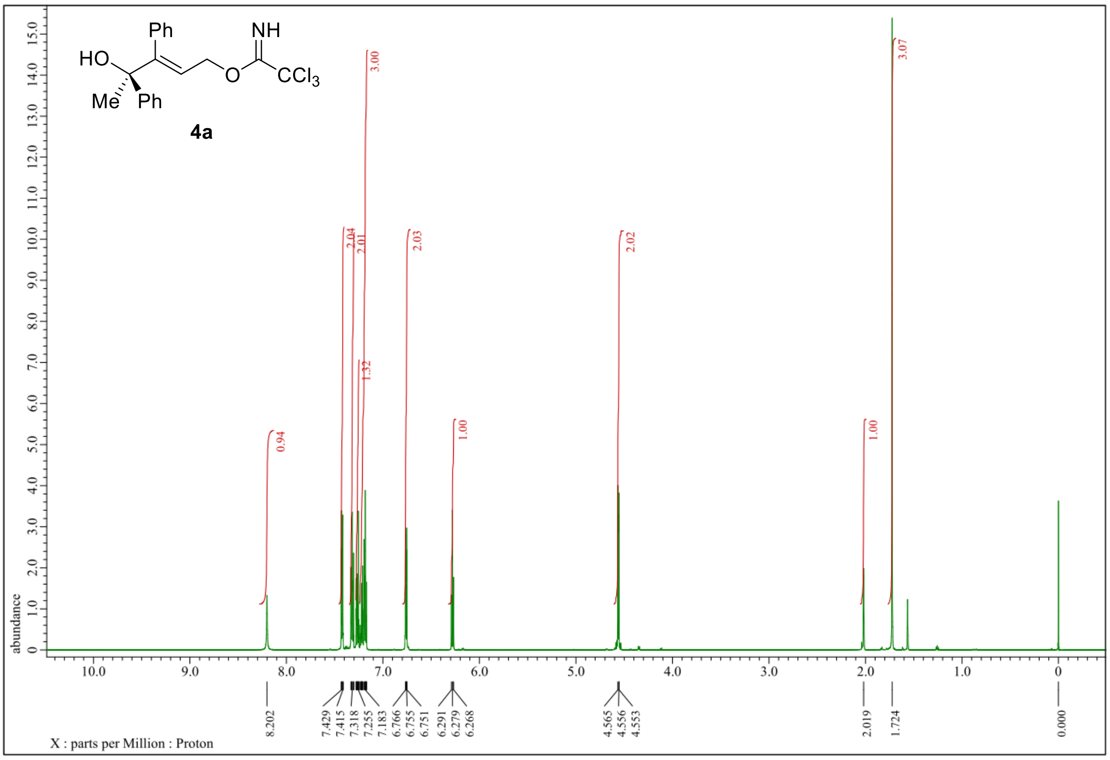
B97D/6-31g(d);E(RB97D) = -4834.848332 hartree
Zero-point Energy Correction = 0.762403 hartree
Thermal Correction to Energy = 0.822321 hartree
Thermal correction to Enthalpy = 0.823265 hartree
Thermal correction to Gibbs Free Energy = 0.663665 hartree
Sum of electronic and Zero-point Energies = -4834.085928 hartree
Sum of electronic and thermal Energies = -4834.026011 hartree
Sum of electronic and thermal Enthalpies = -4834.025066 hartree
Sum of electronic and thermal Free Energies = -4834.184666 hartree
cpcm(ether)/B97D/6-31g(d); E(RB97D) = -4834.868272 hartree
Gibbs Free Energy in ether = -4834.204607 hartree
The number of Imaginary frequencies = 1

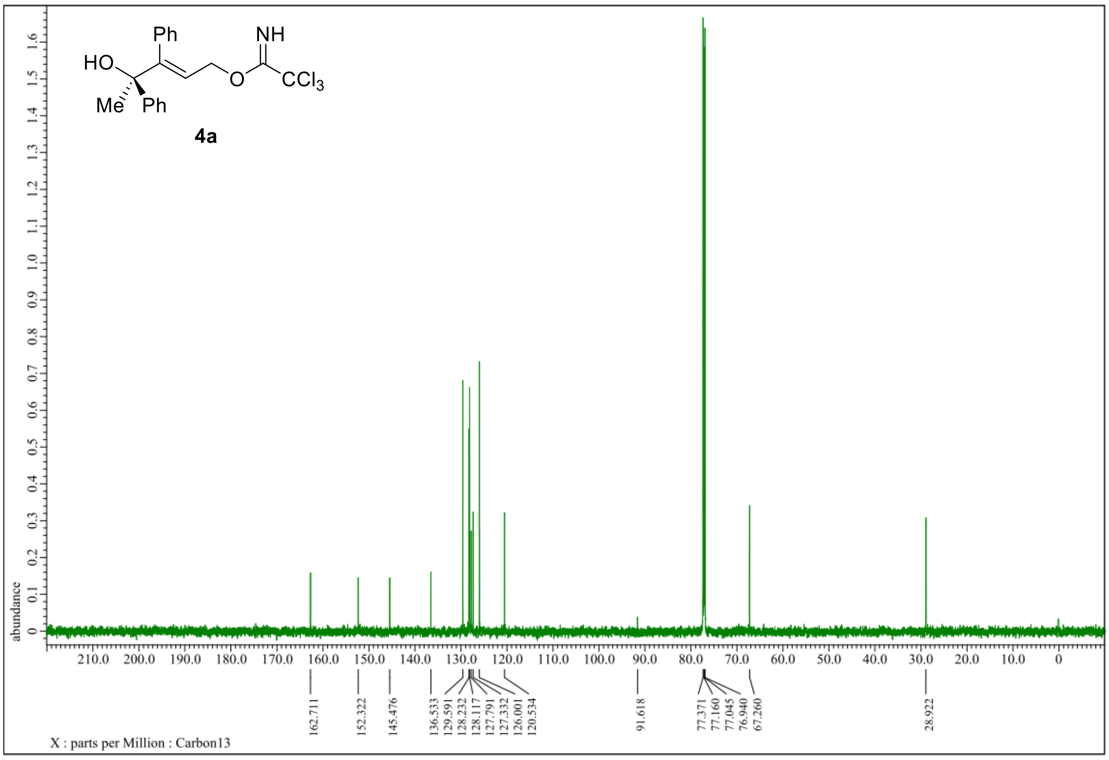
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.774158	2.803614	-1.210962
2	1	0	-0.548912	2.489075	-2.048564
3	6	0	2.009502	2.317267	-1.899769
4	6	0	3.025386	1.682583	-0.986442
5	6	0	4.327078	1.475098	-1.480926
6	6	0	2.729457	1.362094	0.347738
7	6	0	5.327930	0.962985	-0.644752
8	1	0	4.548627	1.707824	-2.523682
9	6	0	3.733636	0.852518	1.184286
10	1	0	1.717725	1.508416	0.720054
11	6	0	5.032664	0.654246	0.693617
12	1	0	6.333578	0.802485	-1.038542
13	1	0	3.501052	0.602295	2.218259
14	1	0	5.807879	0.251808	1.348742
15	6	0	1.749082	1.645930	-3.209387
16	1	0	1.322291	2.258299	-4.005253
17	6	0	1.960183	0.336163	-3.418689
18	1	0	2.356760	-0.322486	-2.647187
19	1	0	1.720170	-0.124309	-4.378550
20	8	0	1.778717	-2.884653	-2.841913
21	6	0	2.014147	-3.656259	-1.923586
22	6	0	3.540033	-3.864261	-1.507904
23	17	0	3.813652	-5.088261	-0.156611
24	17	0	4.180699	-2.265330	-0.970242
25	17	0	4.436230	-4.440142	-2.969913
26	7	0	1.092944	-4.392547	-1.258314
27	1	0	1.281598	-4.810780	-0.352509
28	6	0	1.723203	3.787613	-1.709270
29	1	0	0.130240	-4.094400	-1.399919
30	15	0	-1.783768	0.767256	-1.772370
31	15	0	-0.374212	-2.634625	1.140901
32	8	0	-1.419315	2.145885	-2.460667
33	8	0	-0.633211	0.001407	-1.195449
34	1	0	-0.803637	-1.468209	-0.692257
35	8	0	-2.587734	-0.126706	-2.867512
36	8	0	-2.944836	1.195890	-0.710890
37	8	0	-0.332868	-4.052074	1.573758
38	8	0	-0.970090	-2.400681	-0.313399
39	8	0	1.071068	-1.846033	1.053994
40	8	0	-1.216461	-1.698095	2.202517
41	6	0	-3.372191	-0.160794	1.233051
42	6	0	-3.661728	0.158756	-0.089904
43	6	0	-4.709471	-0.452997	-0.842223
44	6	0	-5.495978	-1.399895	-0.193990
45	1	0	-6.288410	-1.905508	-0.749092
46	6	0	-5.285113	-1.741682	1.167629
47	6	0	-6.113648	-2.698047	1.826173
48	1	0	-6.914835	-3.173690	1.255799
49	6	0	-5.909253	-3.013358	3.158317
50	1	0	-6.548489	-3.747039	3.652926
51	6	0	-4.865809	-2.379553	3.887217
52	1	0	-4.712959	-2.628993	4.938782
53	6	0	-4.037665	-1.453164	3.274705
54	1	0	-3.237353	-0.974050	3.836960
55	6	0	-4.212480	-1.113658	1.902368
56	6	0	-4.965198	-0.074435	-2.253577
57	6	0	-3.930775	0.126923	-3.197620
58	6	0	-4.194334	0.474792	-4.526059
59	6	0	-5.520866	0.627226	-4.951318
60	1	0	-5.728957	0.899001	-5.987482
61	6	0	-6.571983	0.431319	-4.041366
62	1	0	-7.607724	0.555269	-4.361714
63	6	0	-6.291021	0.090650	-2.713170
64	1	0	-7.103607	-0.037085	-1.996228
65	6	0	-2.194416	0.471704	1.898424
66	6	0	-1.096876	-0.309730	2.258845
67	6	0	0.107429	0.252701	2.790144
68	6	0	0.163000	1.630926	2.968479
69	1	0	1.087760	2.082786	3.331944
70	6	0	-0.936206	2.471968	2.662391
71	6	0	-0.868473	3.881936	2.867556
72	1	0	0.054278	4.303121	3.273137
73	6	0	-1.947969	4.694742	2.566323
74	1	0	-1.885995	5.772988	2.725384

75	6	0	-3.145279	4.120548	2.057812
76	1	0	-3.999136	4.762442	1.833021
77	6	0	-3.240005	2.754480	1.845069
78	1	0	-4.162621	2.324252	1.457172
79	6	0	-2.141200	1.890314	2.124818
80	6	0	1.282501	-0.583593	3.122869
81	6	0	1.734506	-1.609082	2.264055
82	6	0	2.891404	-2.344530	2.536802
83	6	0	3.636581	-2.055632	3.687298
84	1	0	4.543094	-2.625066	3.899220
85	6	0	3.211970	-1.042897	4.563474
86	1	0	3.782240	-0.821503	5.467229
87	6	0	2.044756	-0.322650	4.282707
88	1	0	1.700308	0.455630	4.965667
89	1	0	3.202322	-3.115950	1.835689
90	1	0	-3.354588	0.607171	-5.208005
91	6	0	2.449362	4.534133	-0.620126
92	6	0	1.828067	4.767315	0.617965
93	6	0	3.747530	5.019127	-0.853131
94	6	0	2.503666	5.483180	1.616422
95	1	0	0.827473	4.373955	0.798365
96	6	0	4.423441	5.730208	0.148375
97	1	0	4.235059	4.820272	-1.809959
98	6	0	3.801992	5.965033	1.385836
99	1	0	2.015768	5.663578	2.577208
100	1	0	5.436903	6.093382	-0.033635
101	1	0	4.329597	6.516768	2.166544
102	6	0	1.205034	4.683303	-2.826278
103	1	0	2.050490	5.150852	-3.354229
104	1	0	0.586846	4.134299	-3.548450
105	1	0	0.595342	5.487112	-2.385069

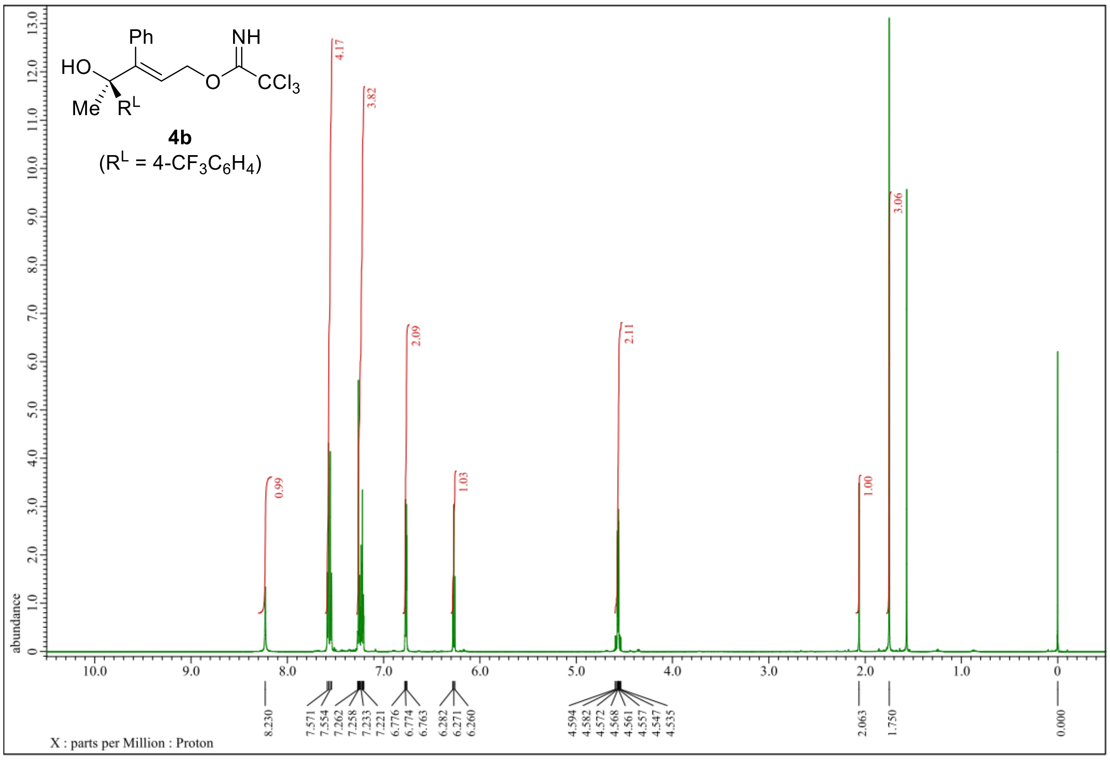
11. NMR Charts

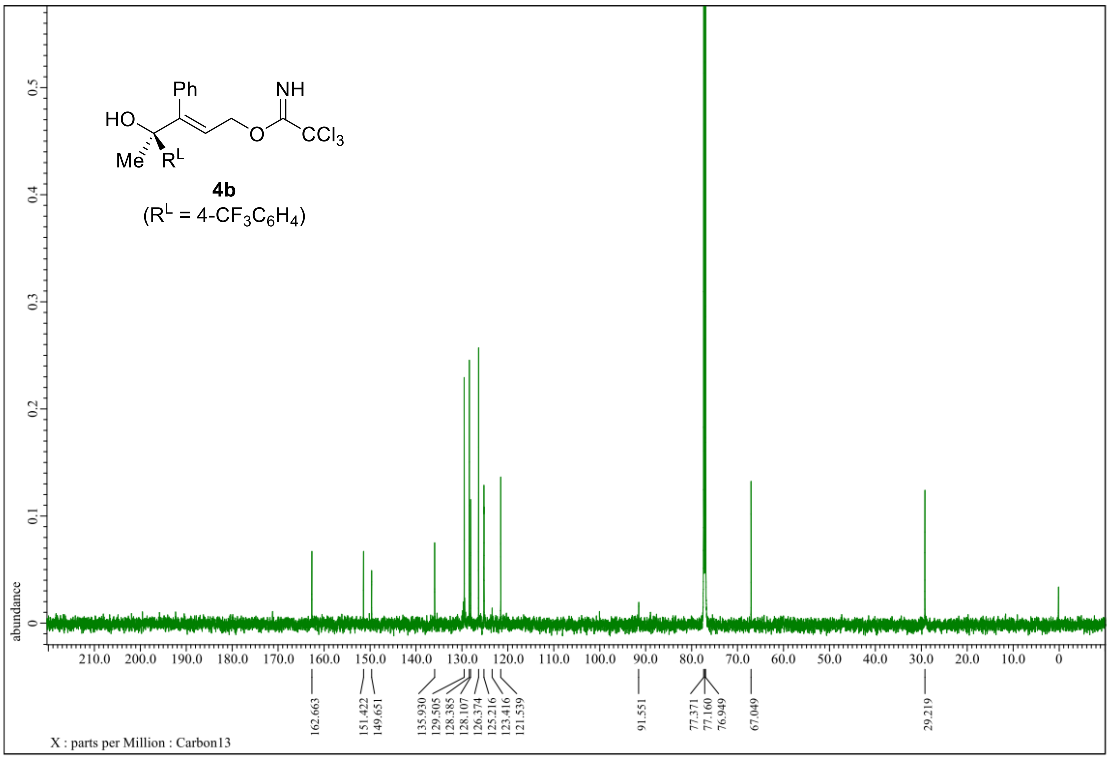
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4a**



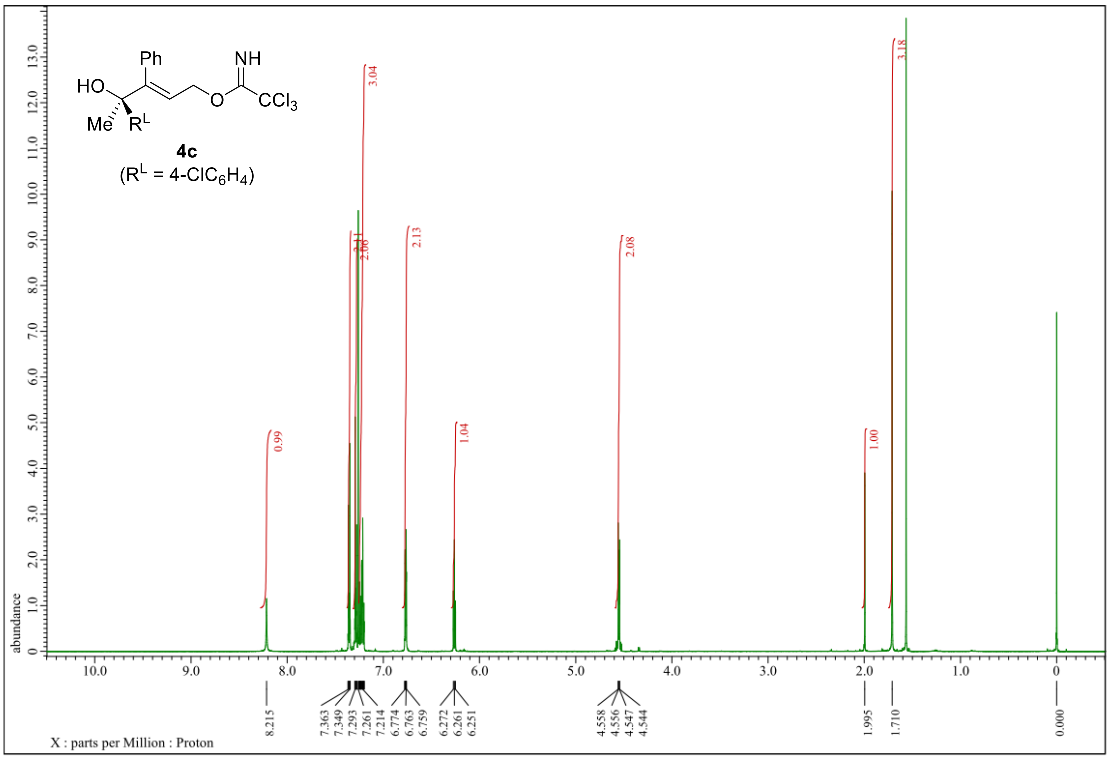


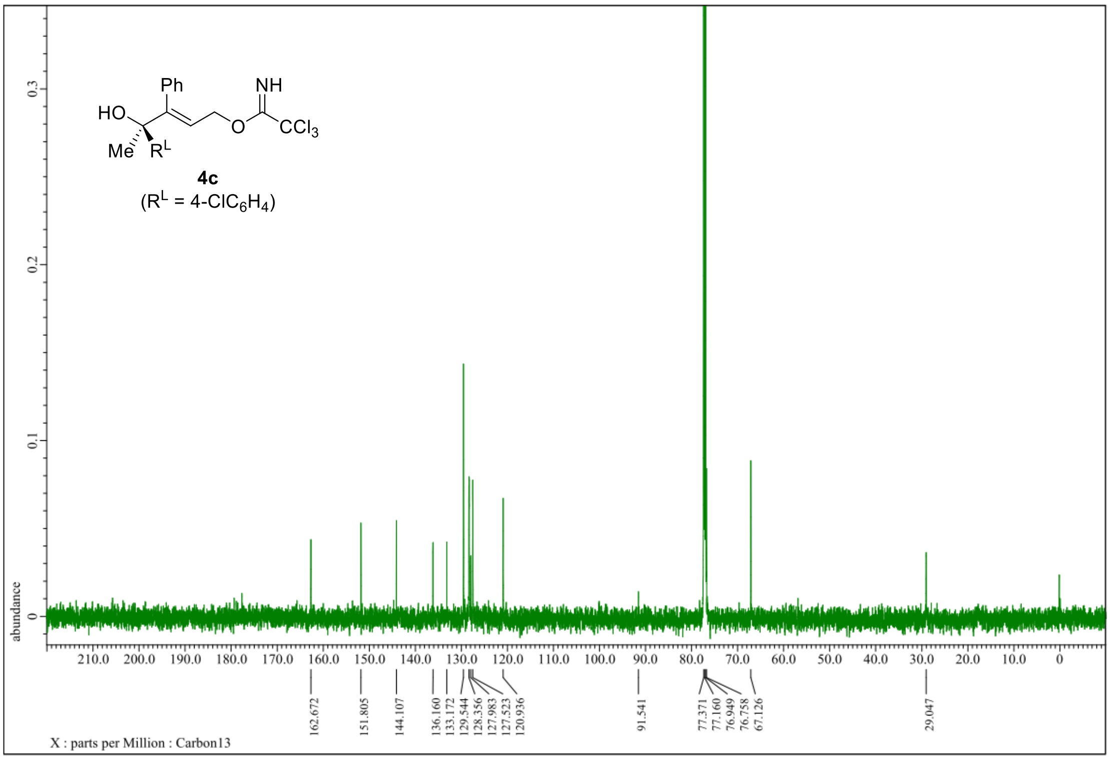
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4b**



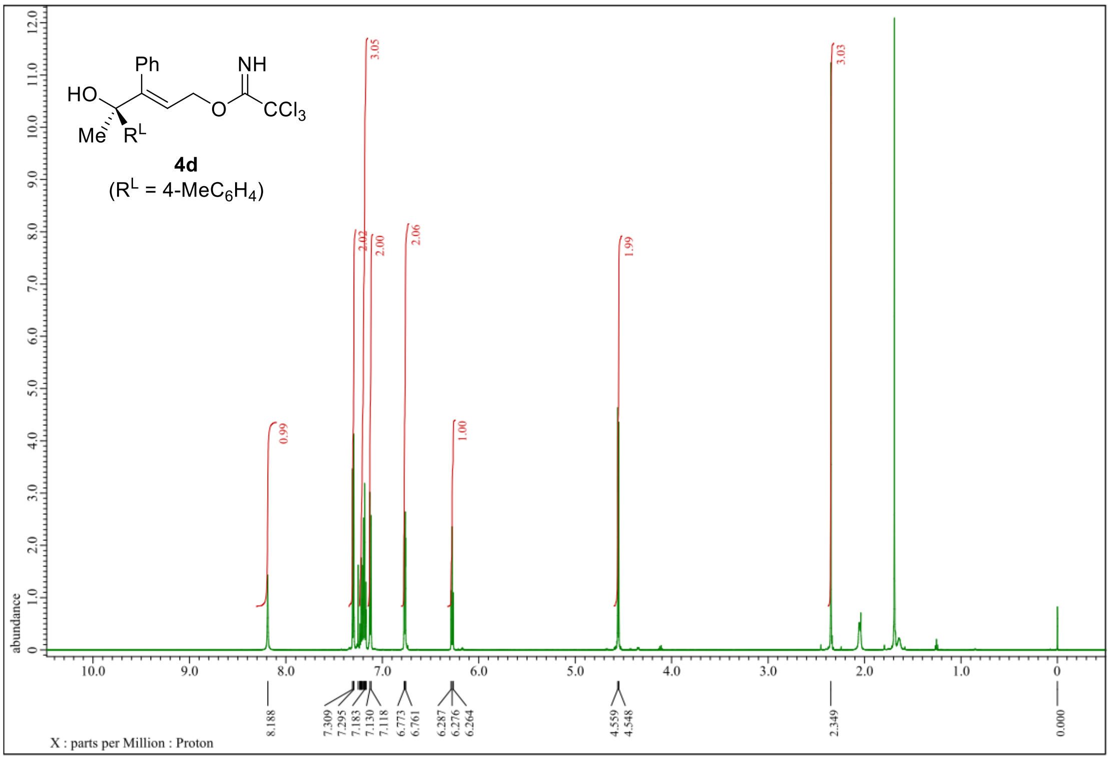


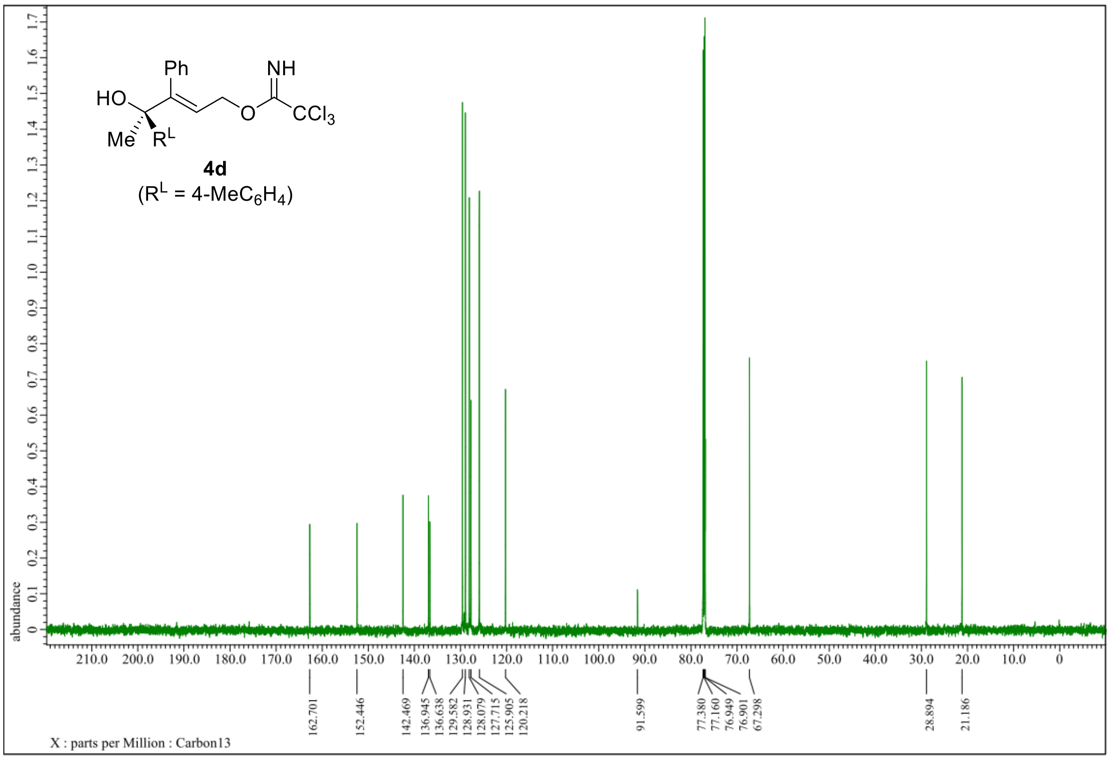
^1H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4c**



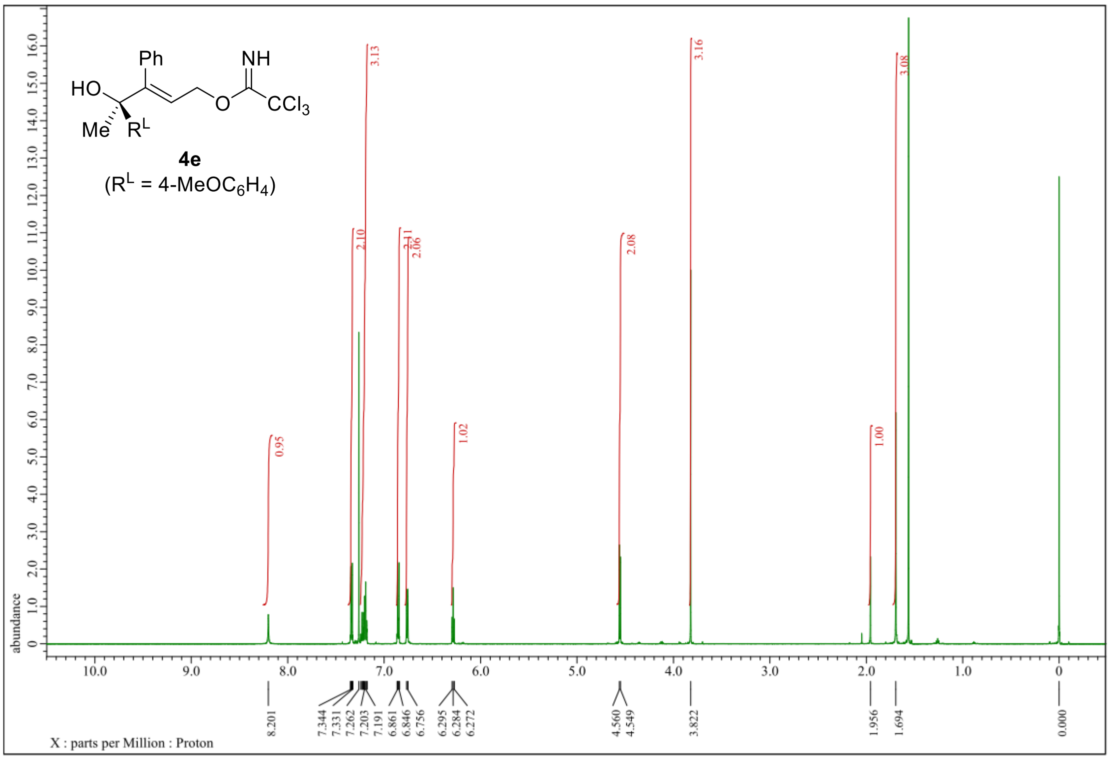


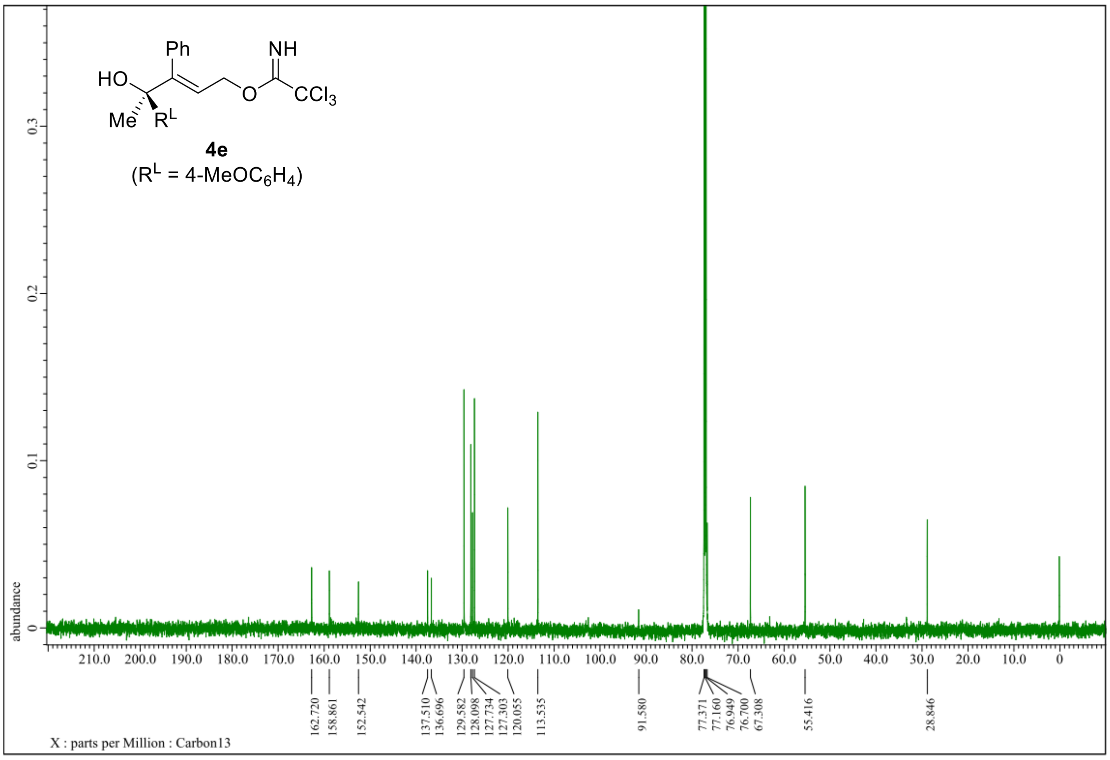
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **4d**



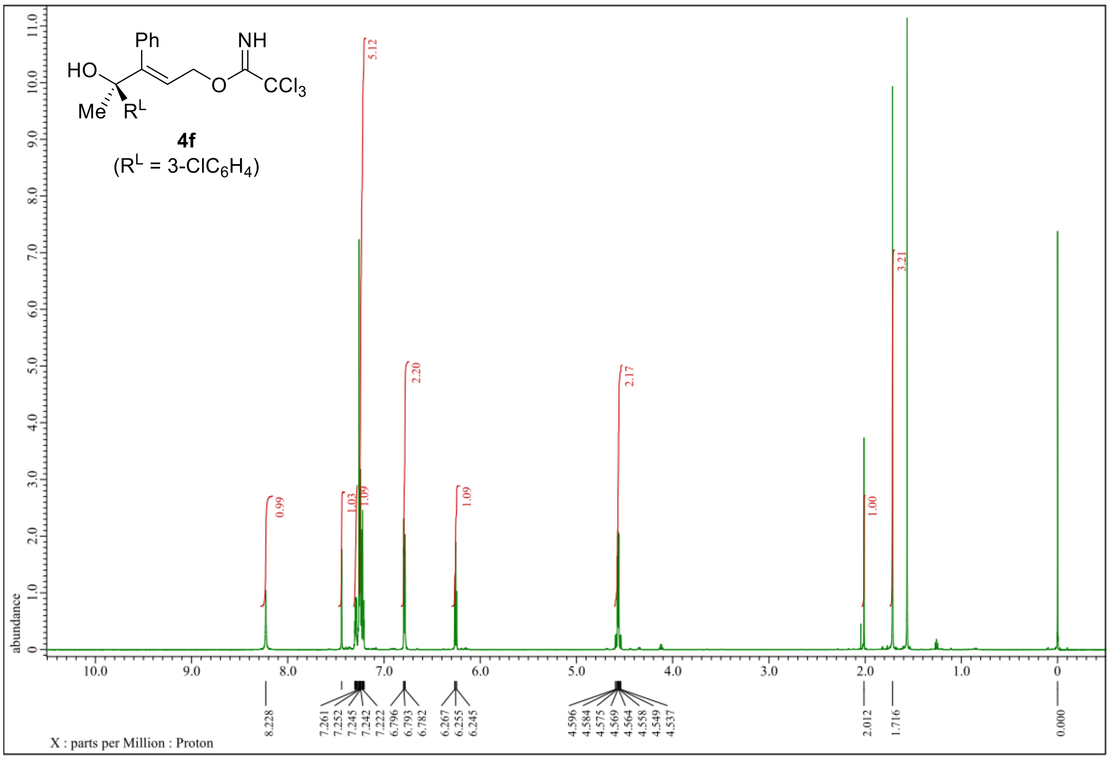


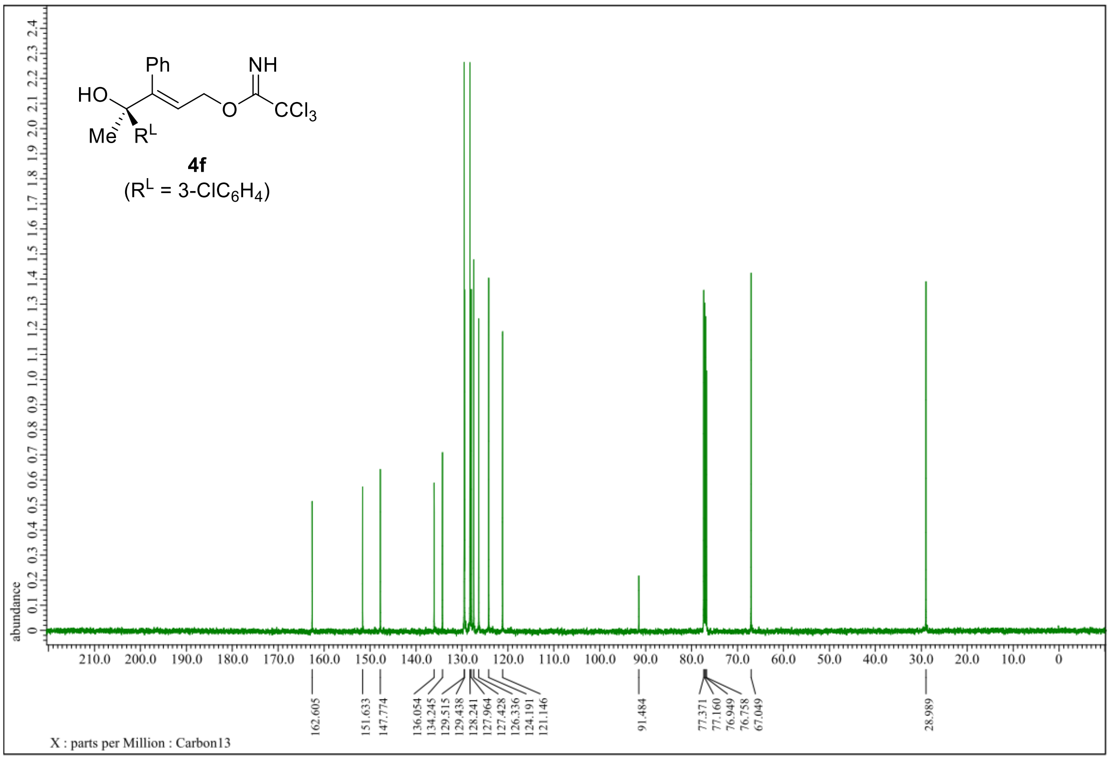
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4e**



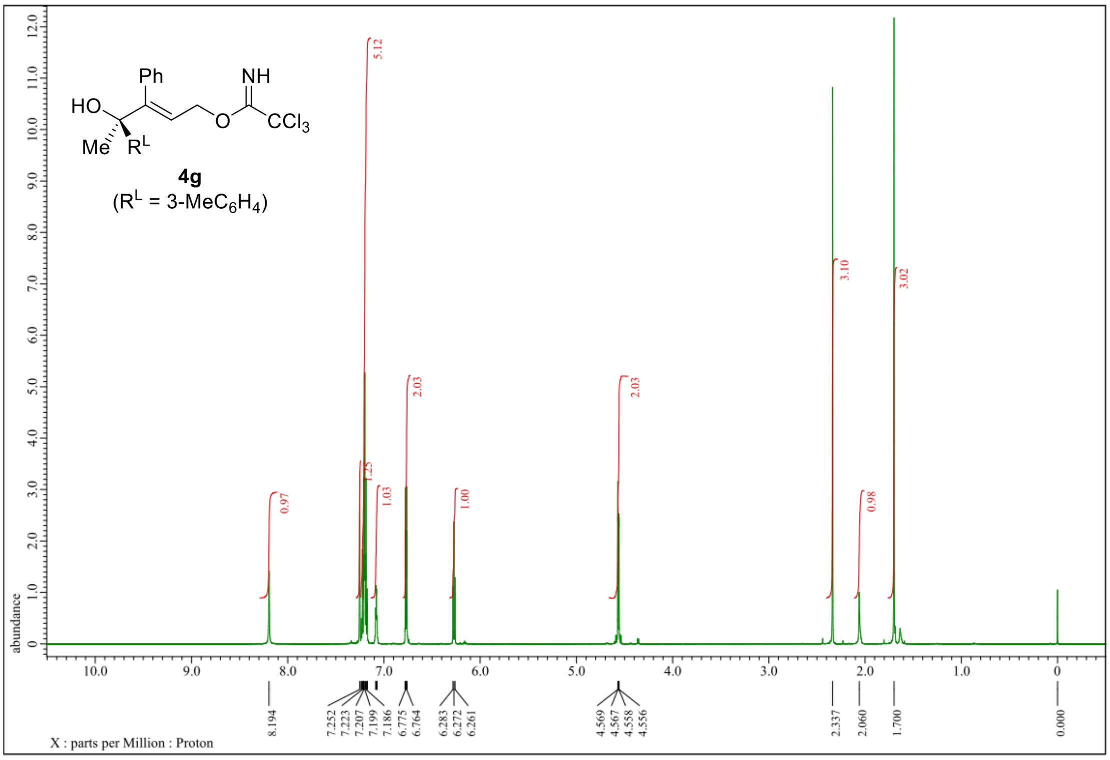


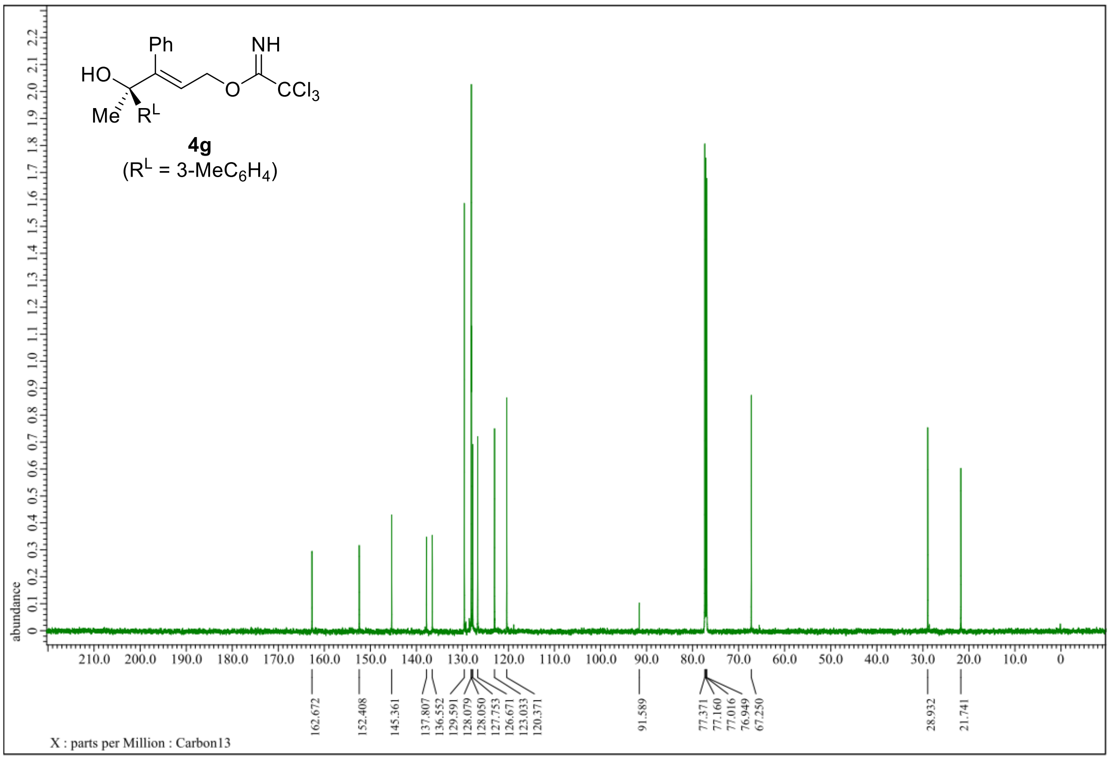
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4f**



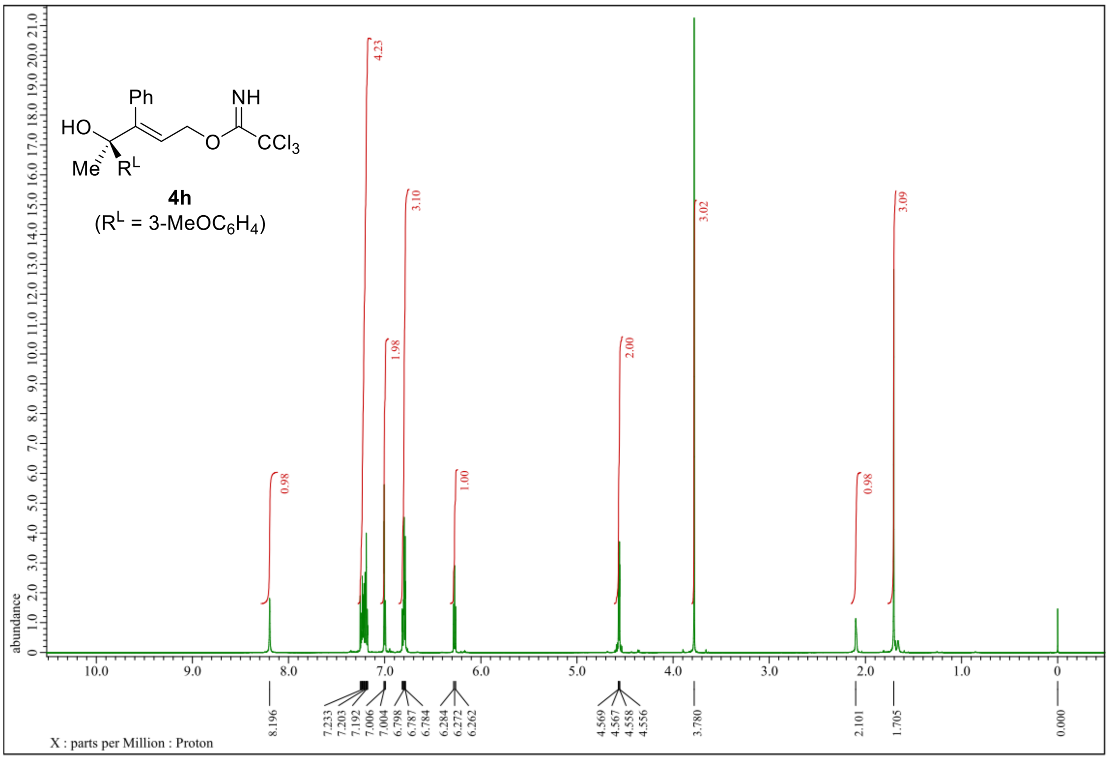


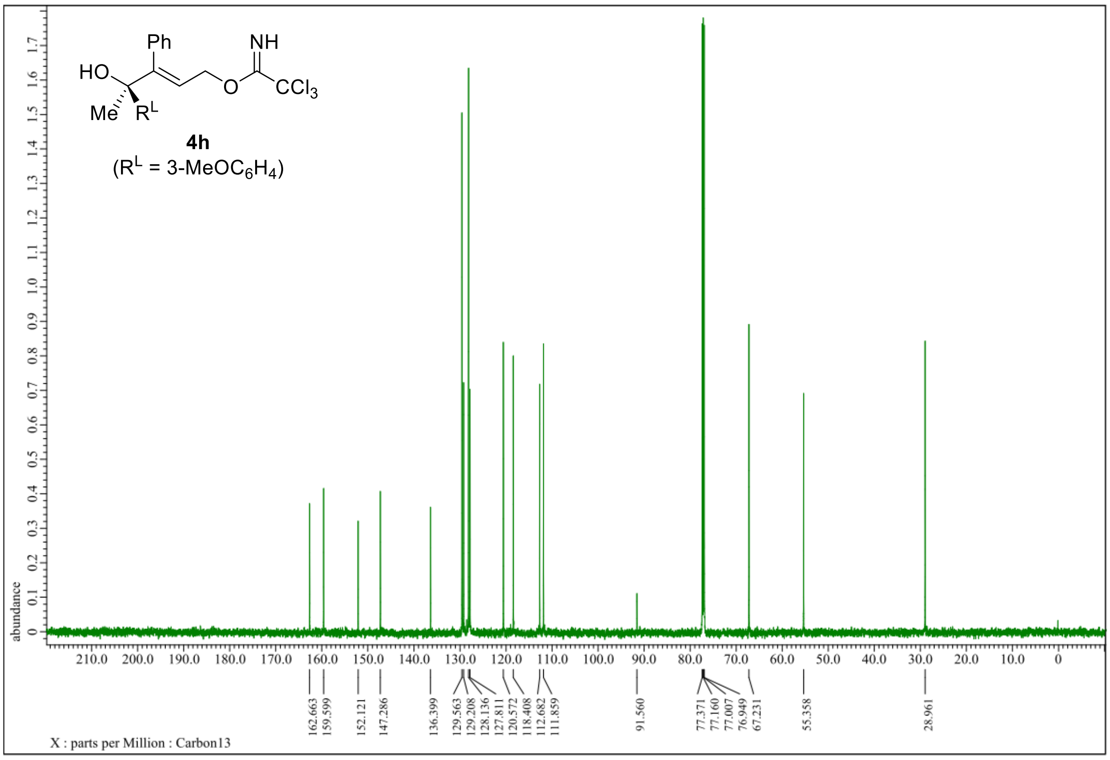
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **4g**



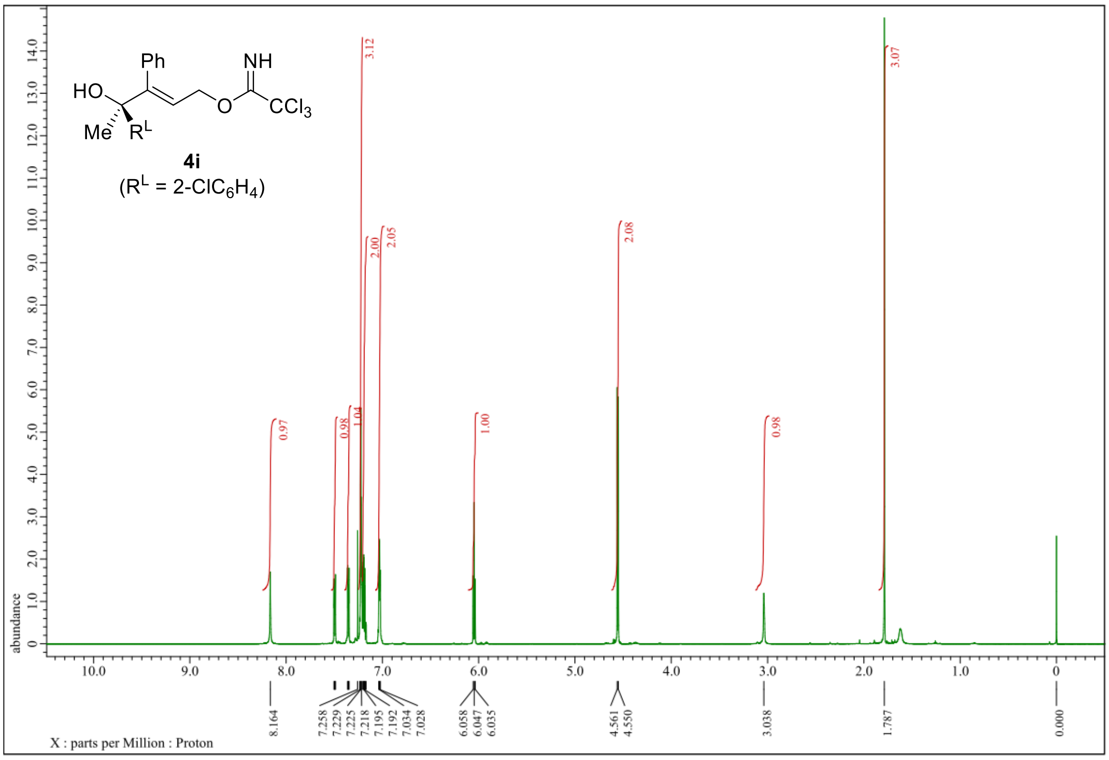


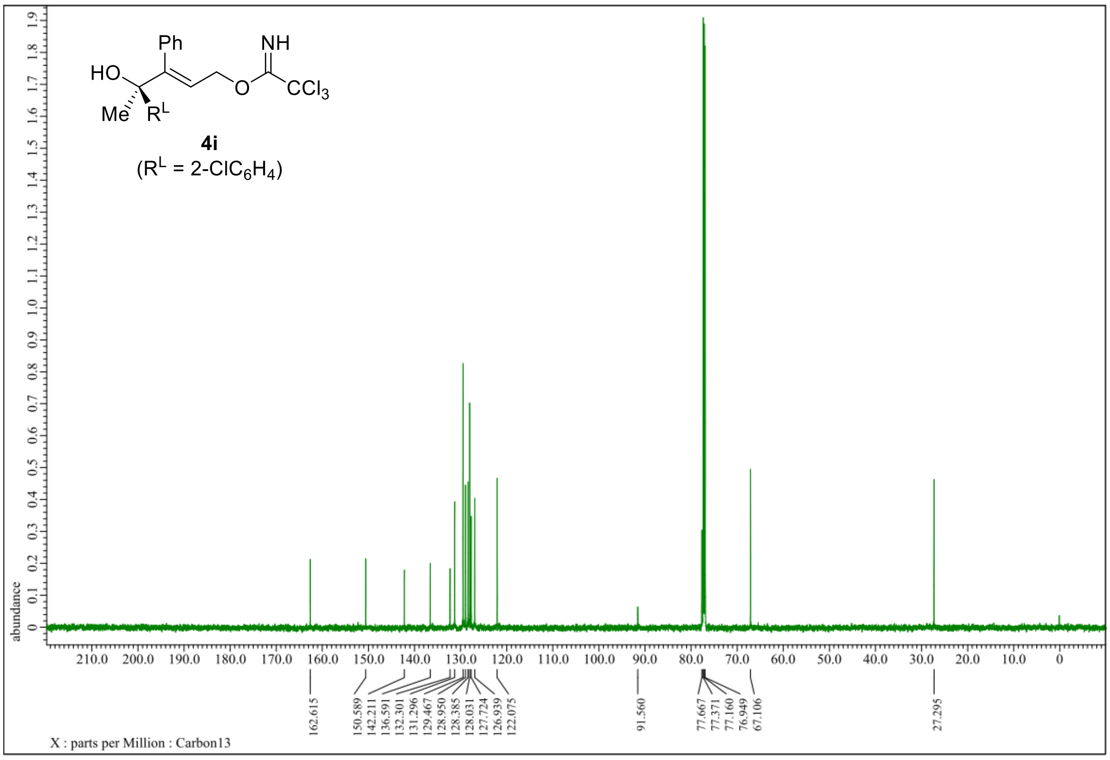
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4h**



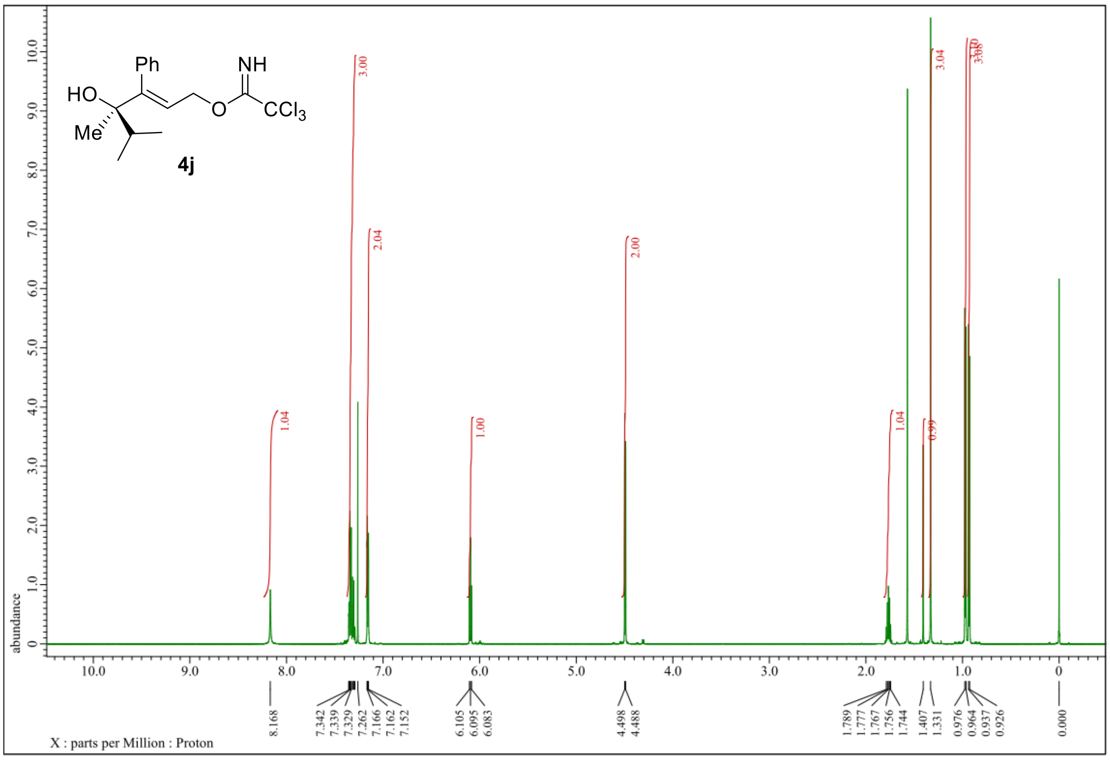


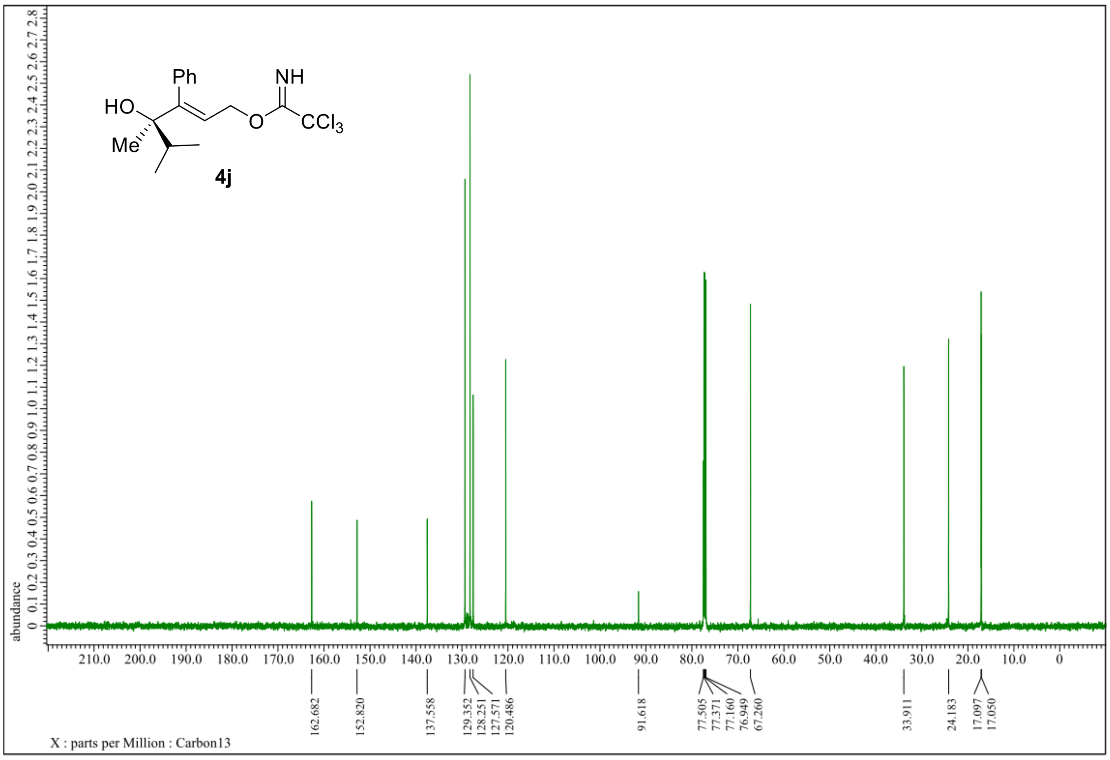
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **4i**



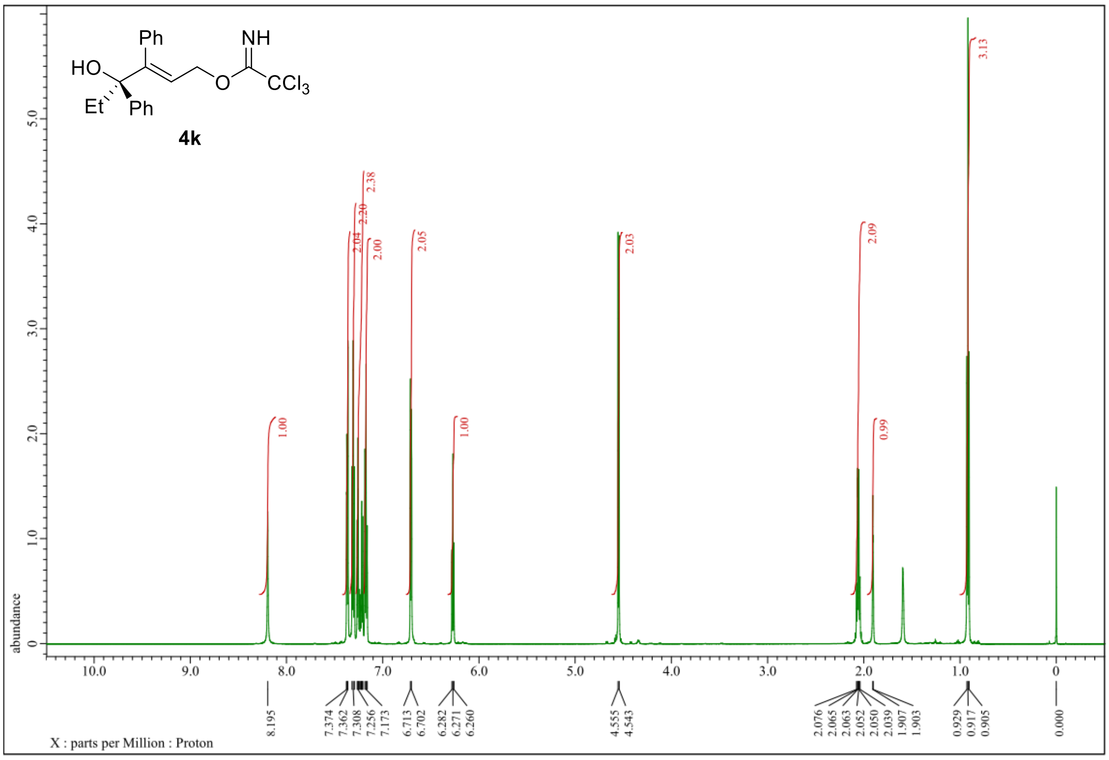


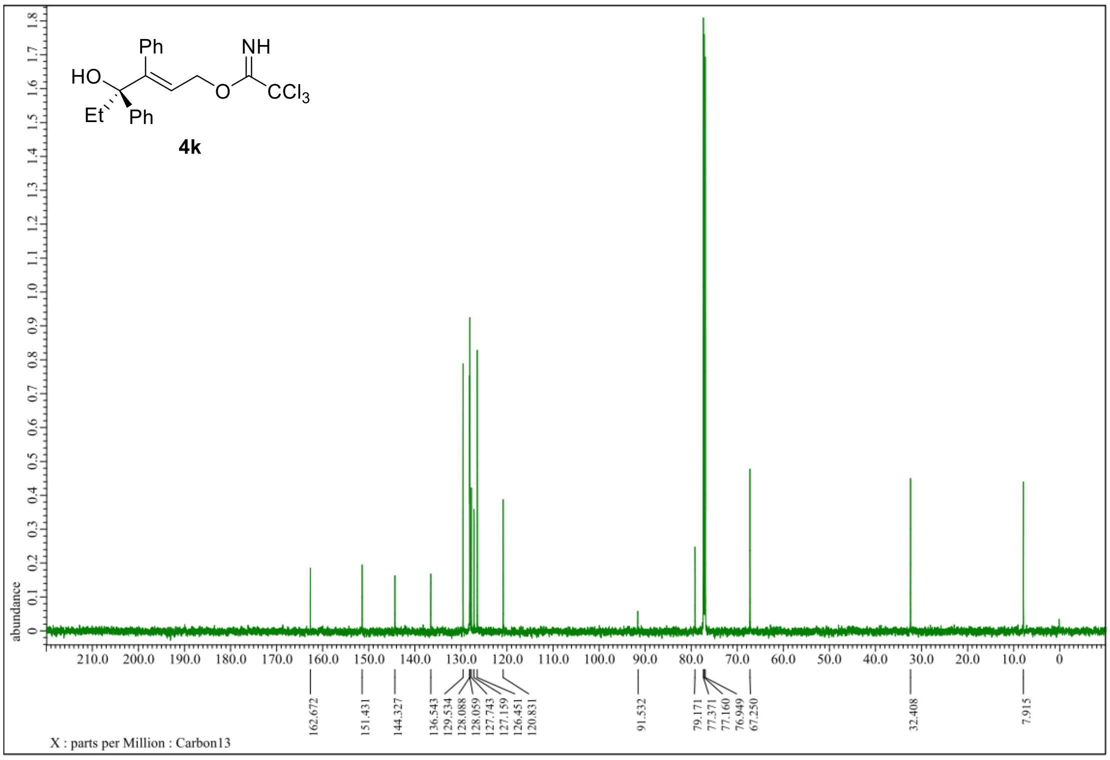
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4j**



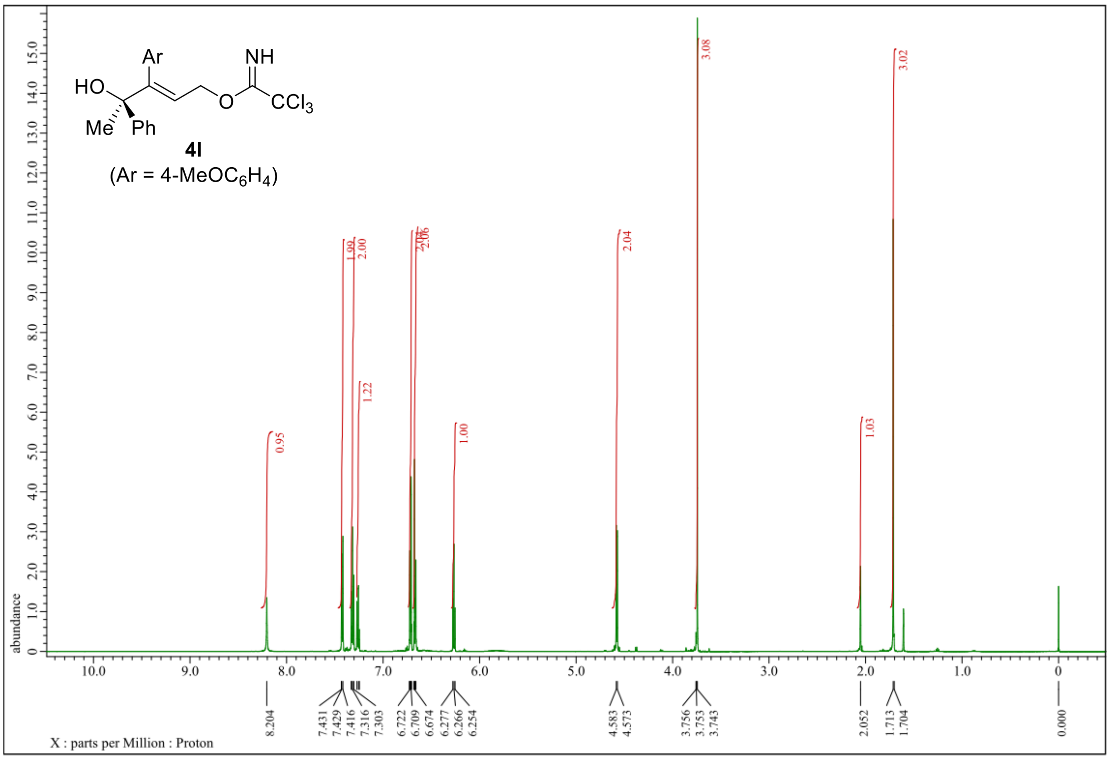


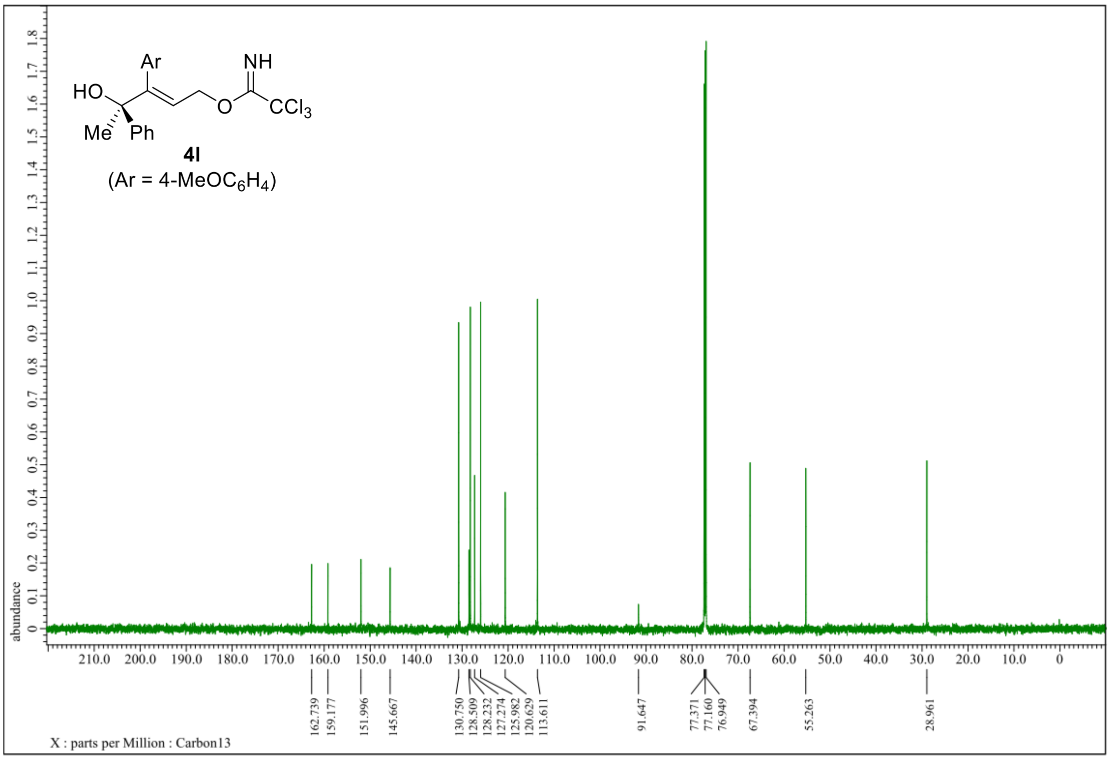
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4k**



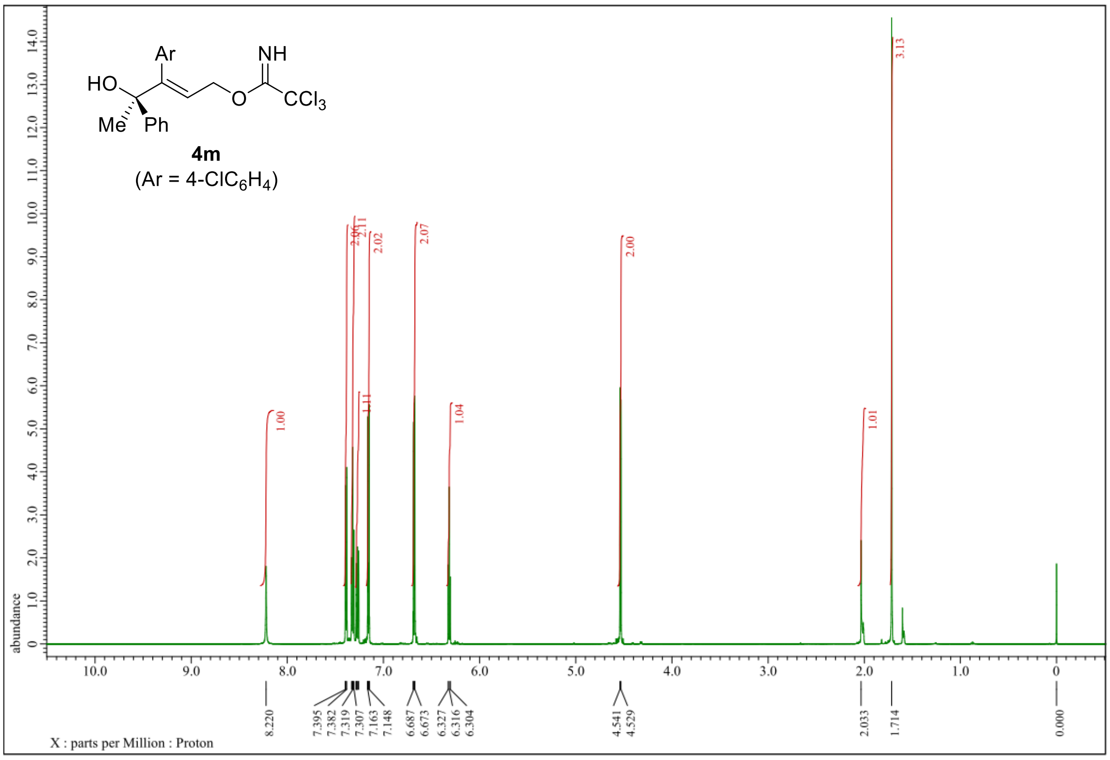


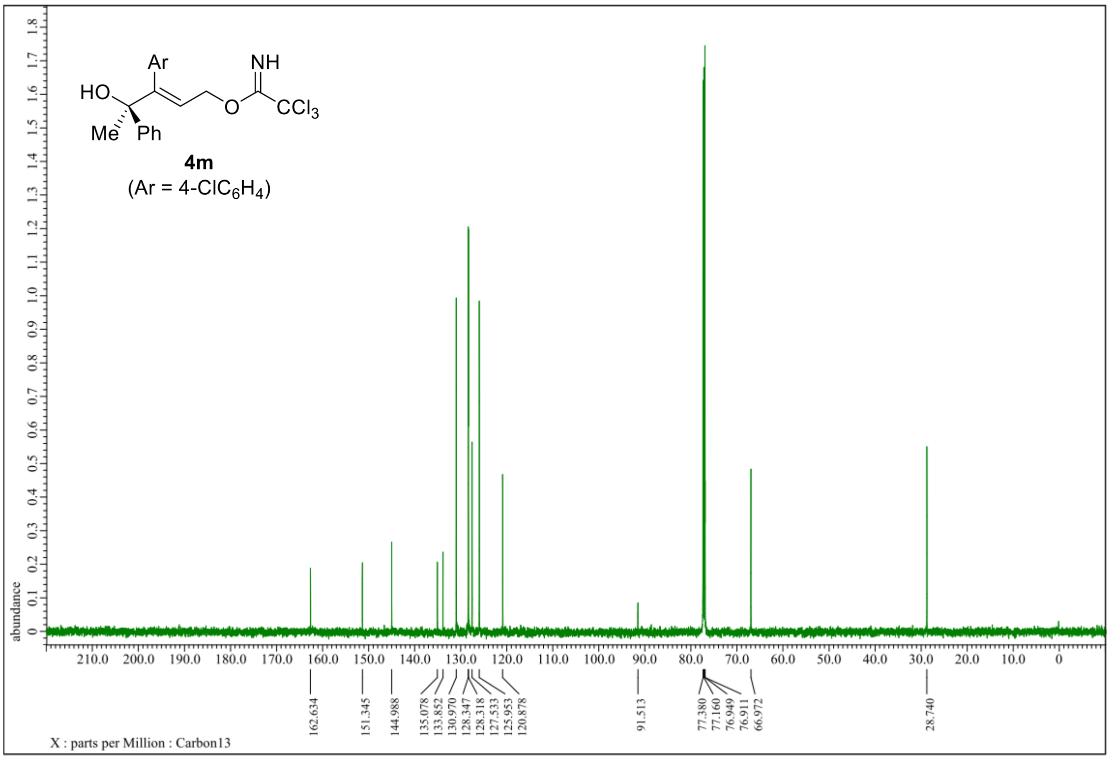
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4l**



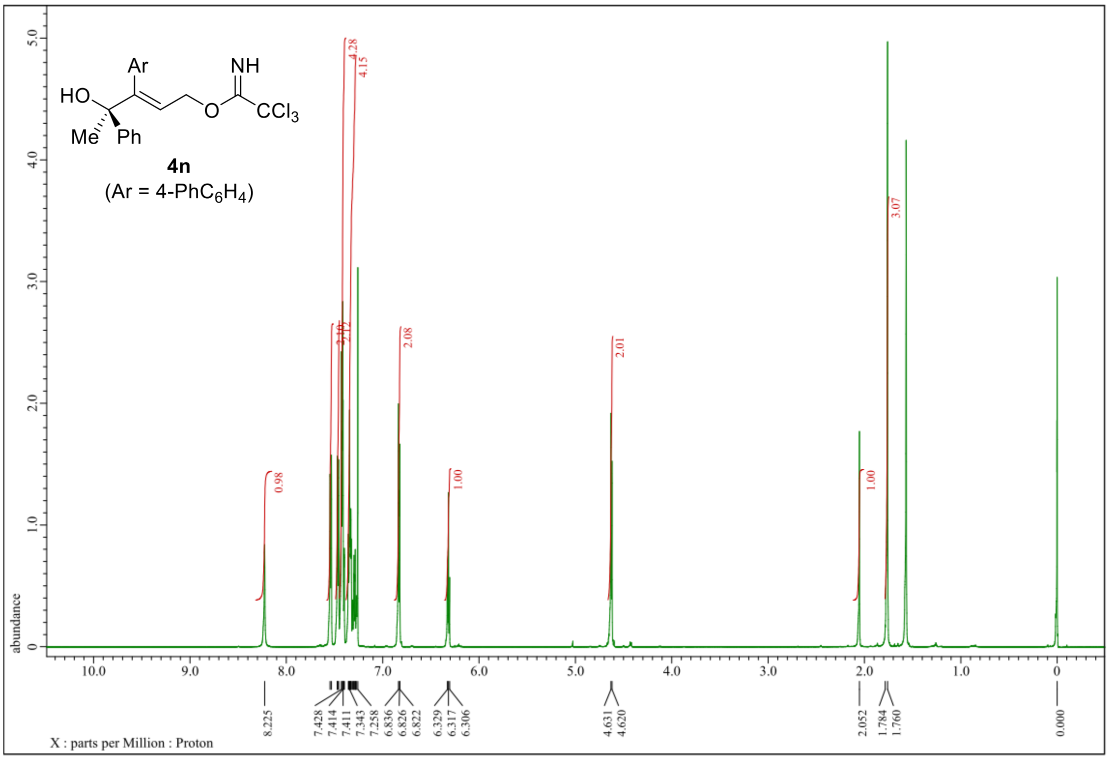


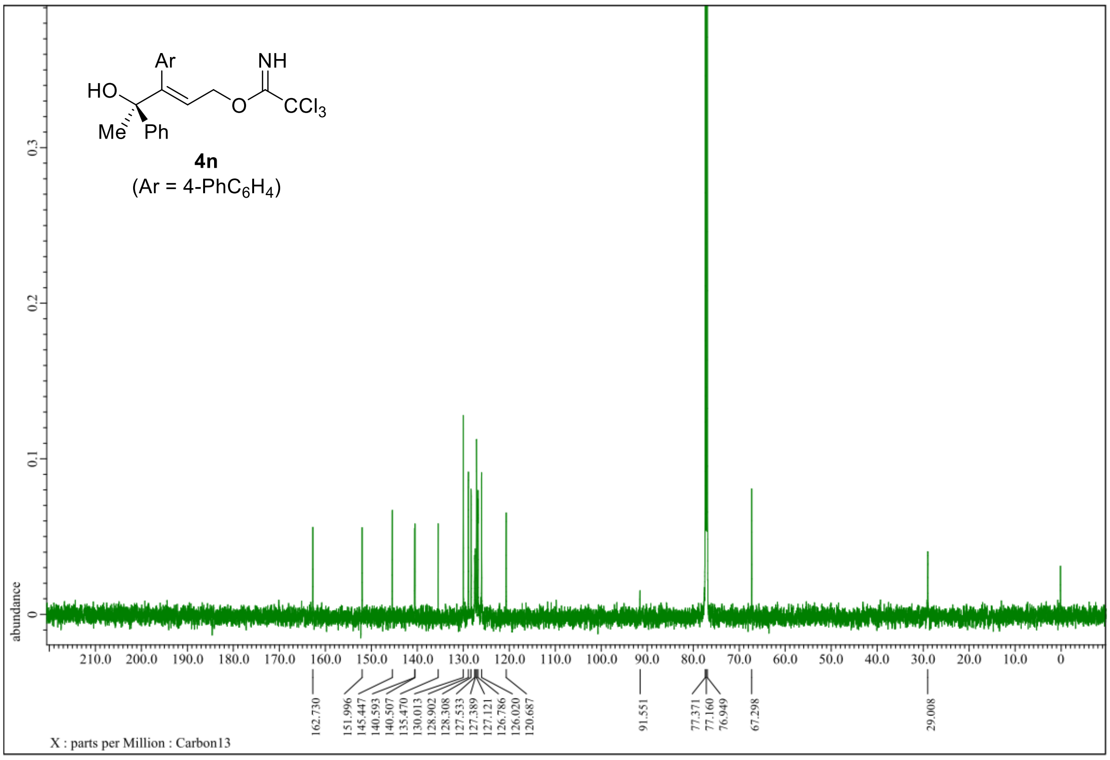
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4m**



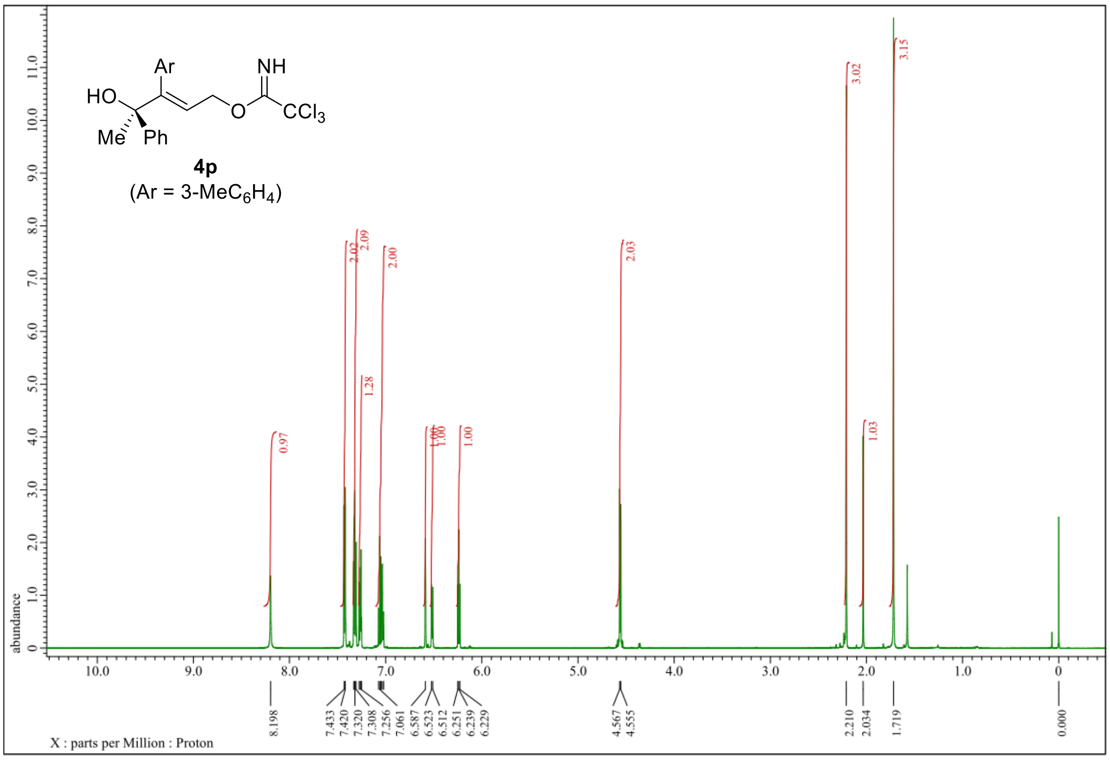


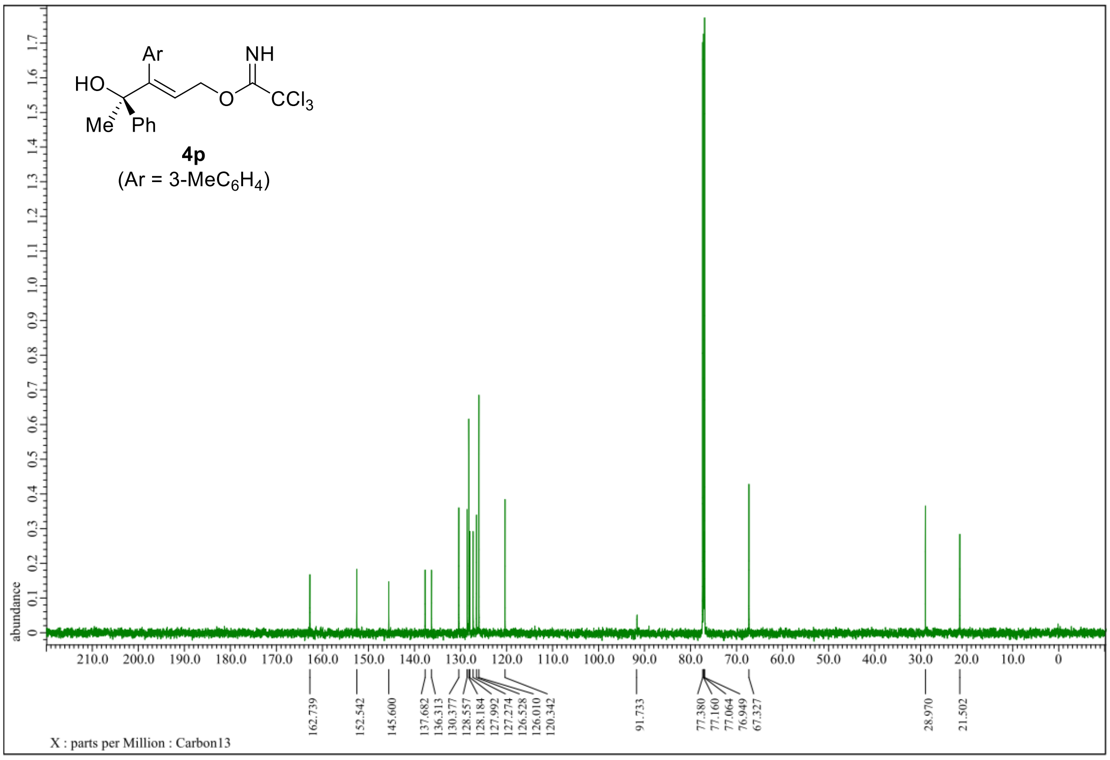
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4n**



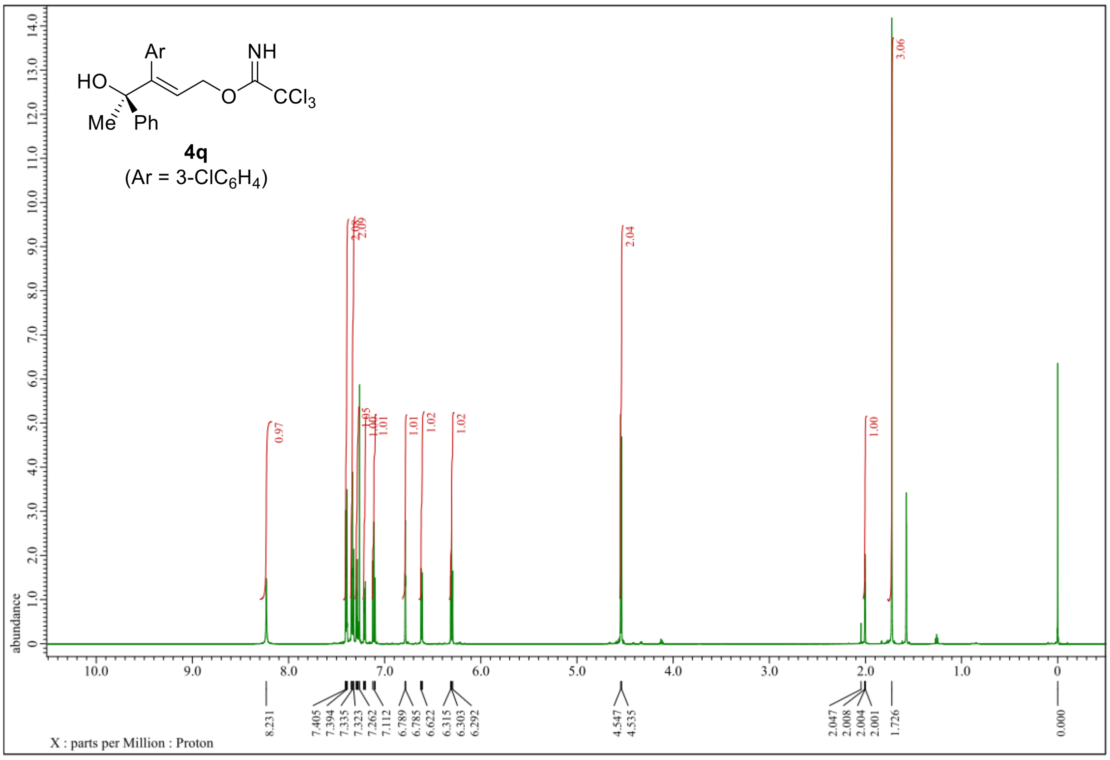


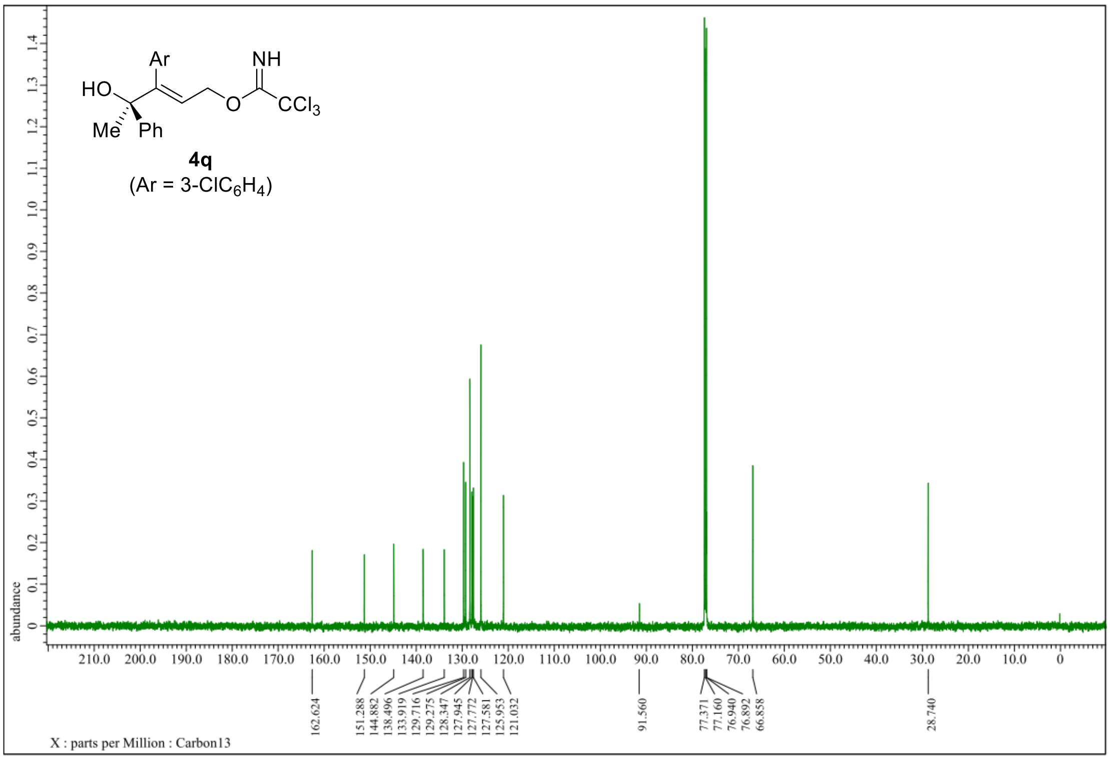
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4p**



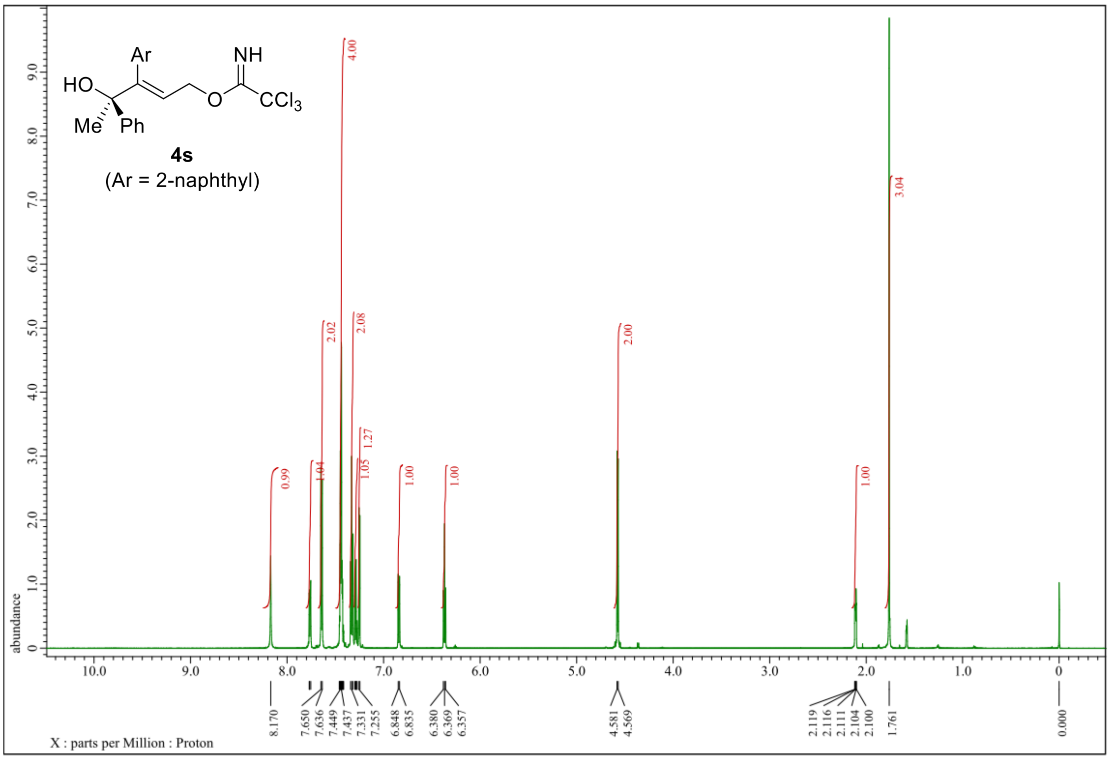


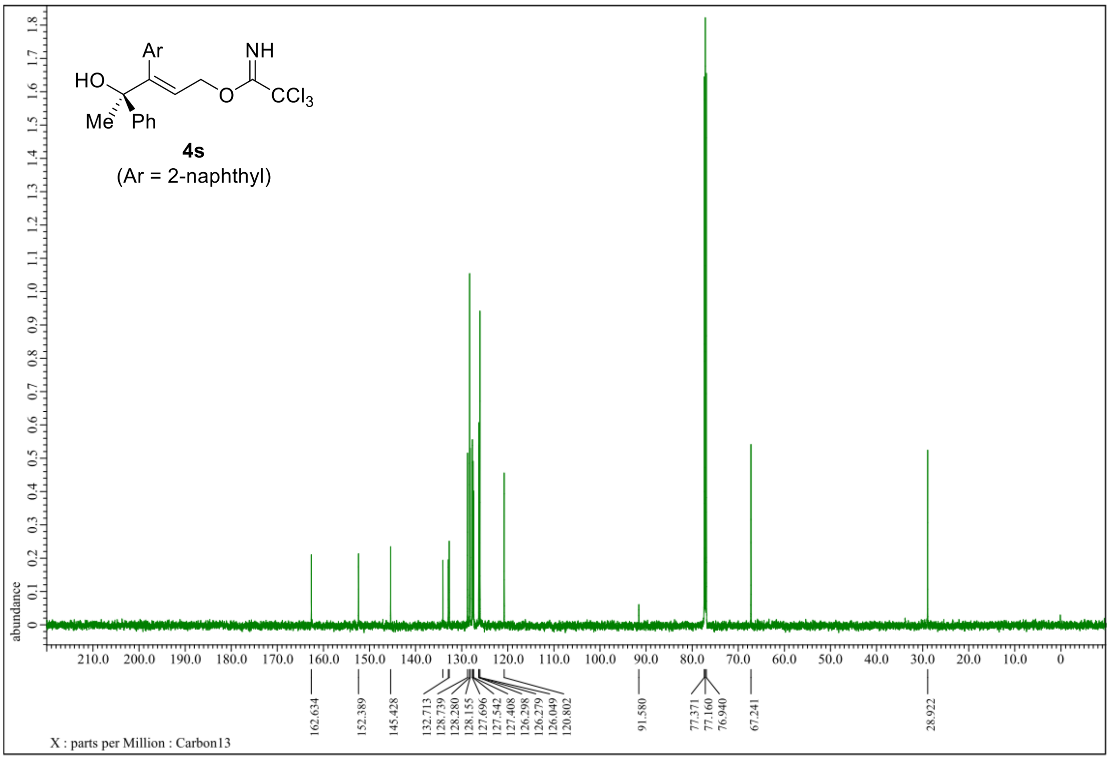
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4q**



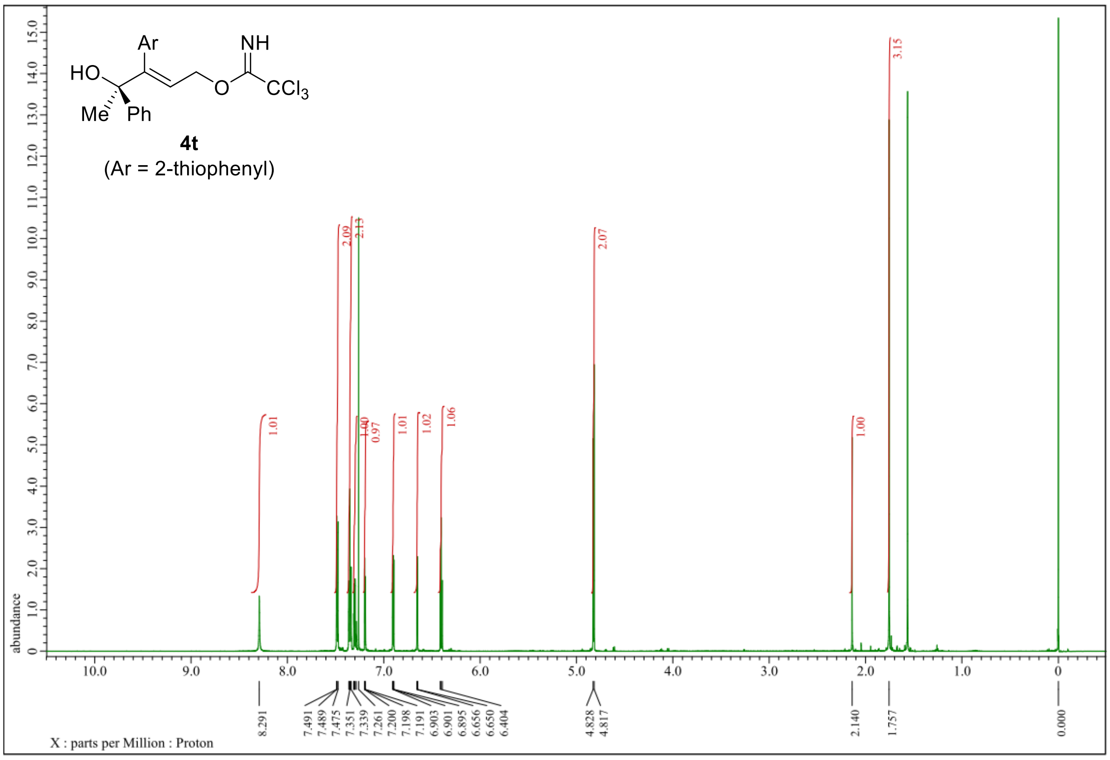


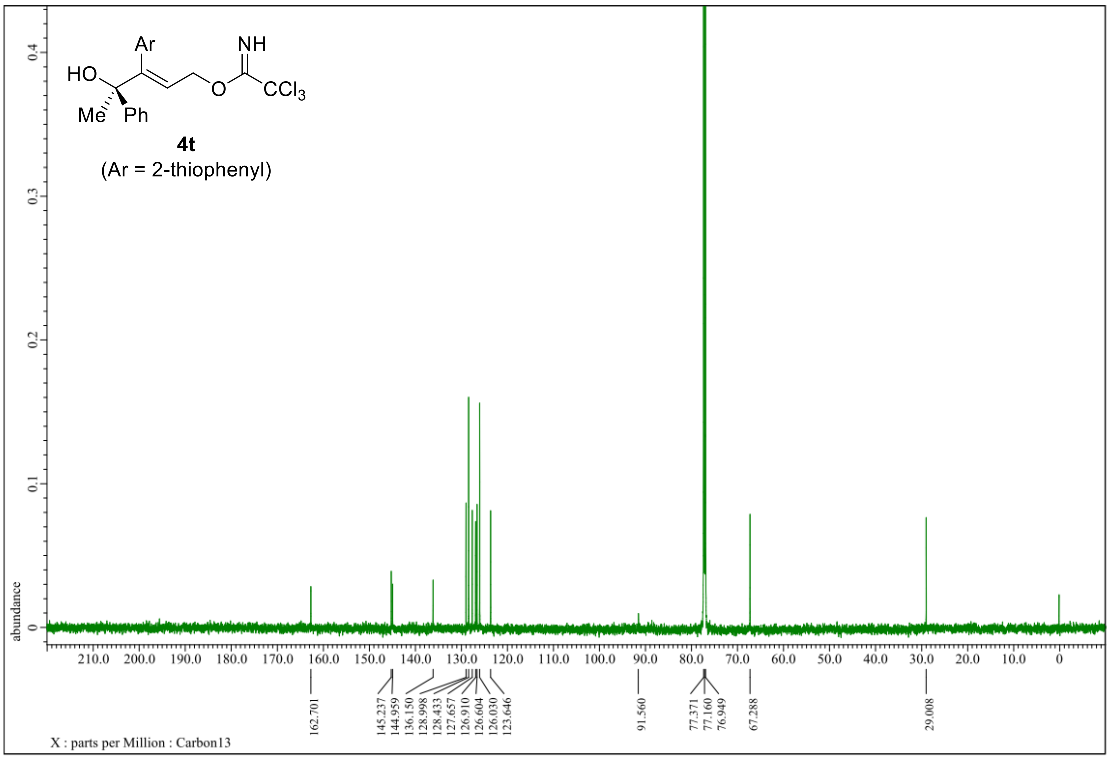
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **4s**



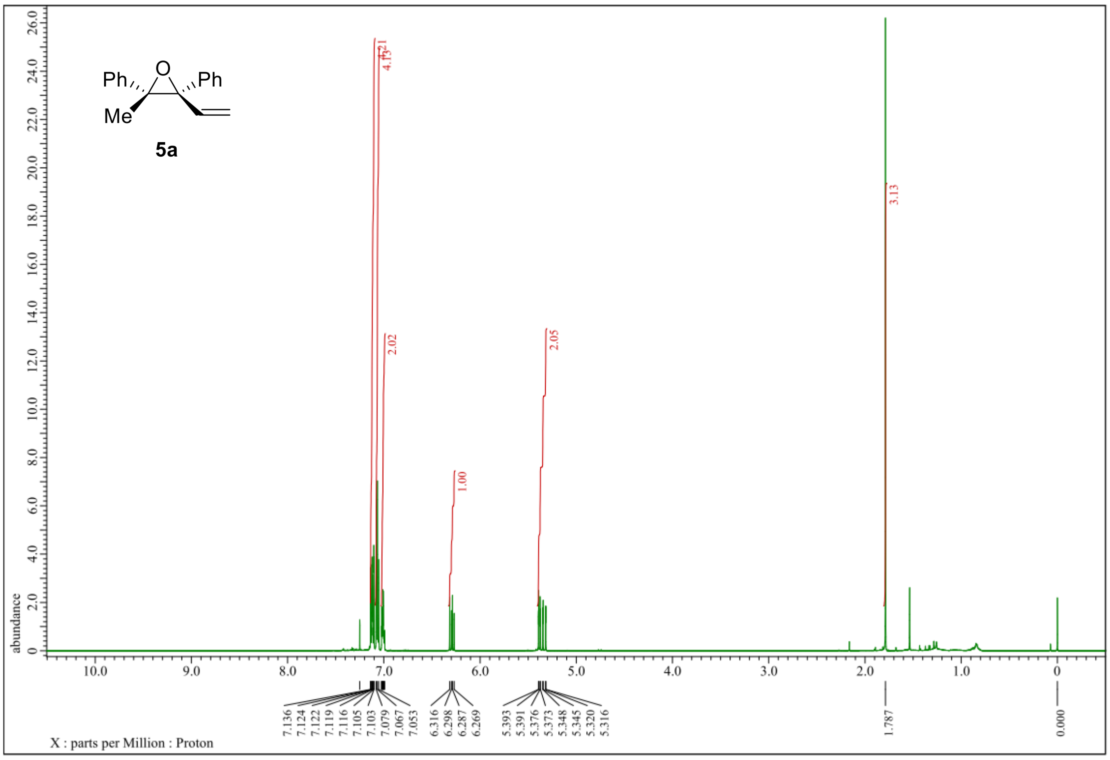


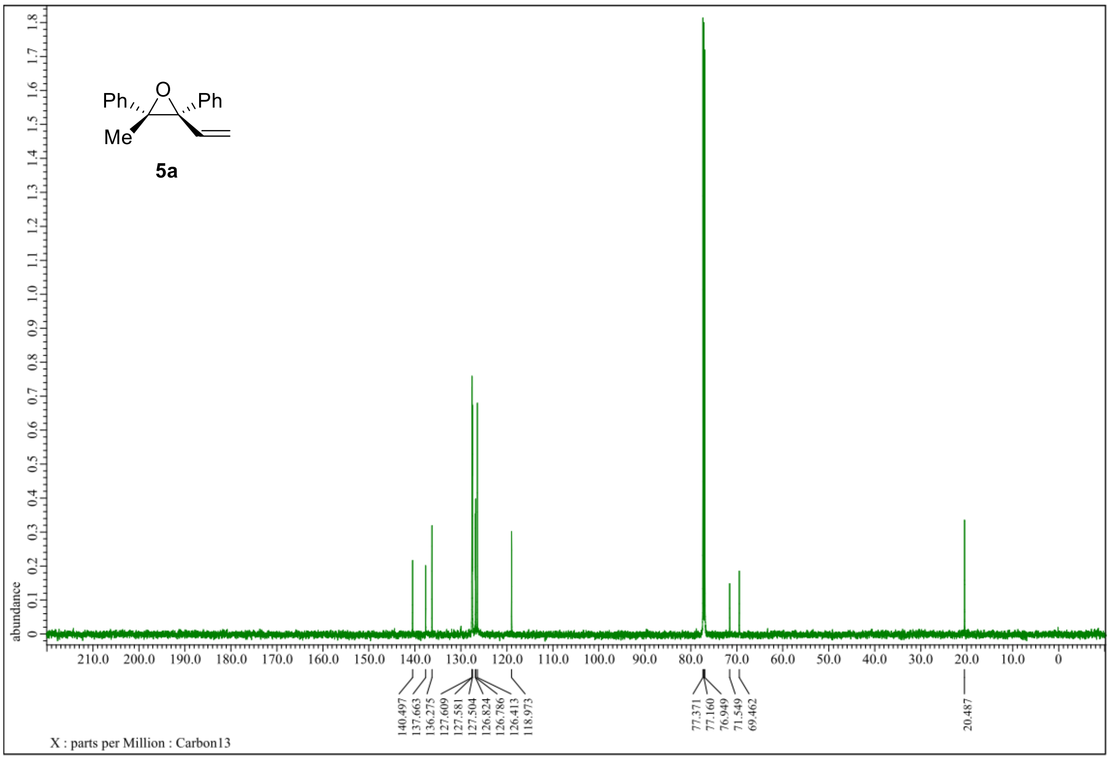
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **4t**



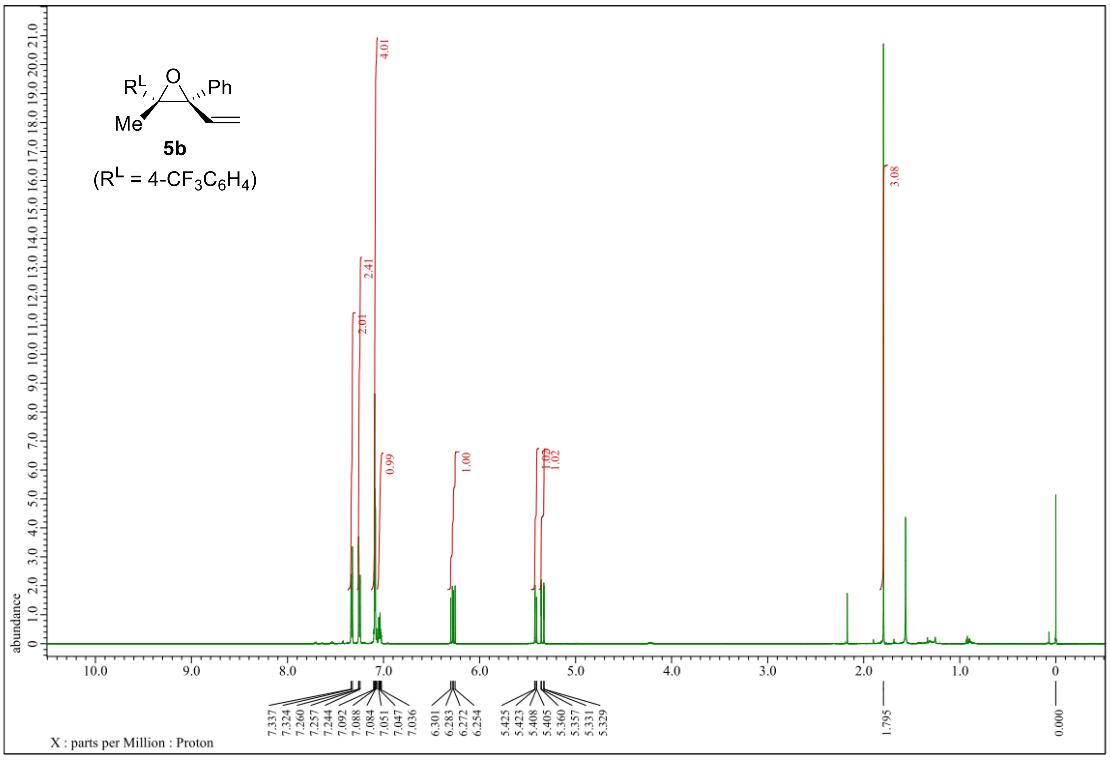


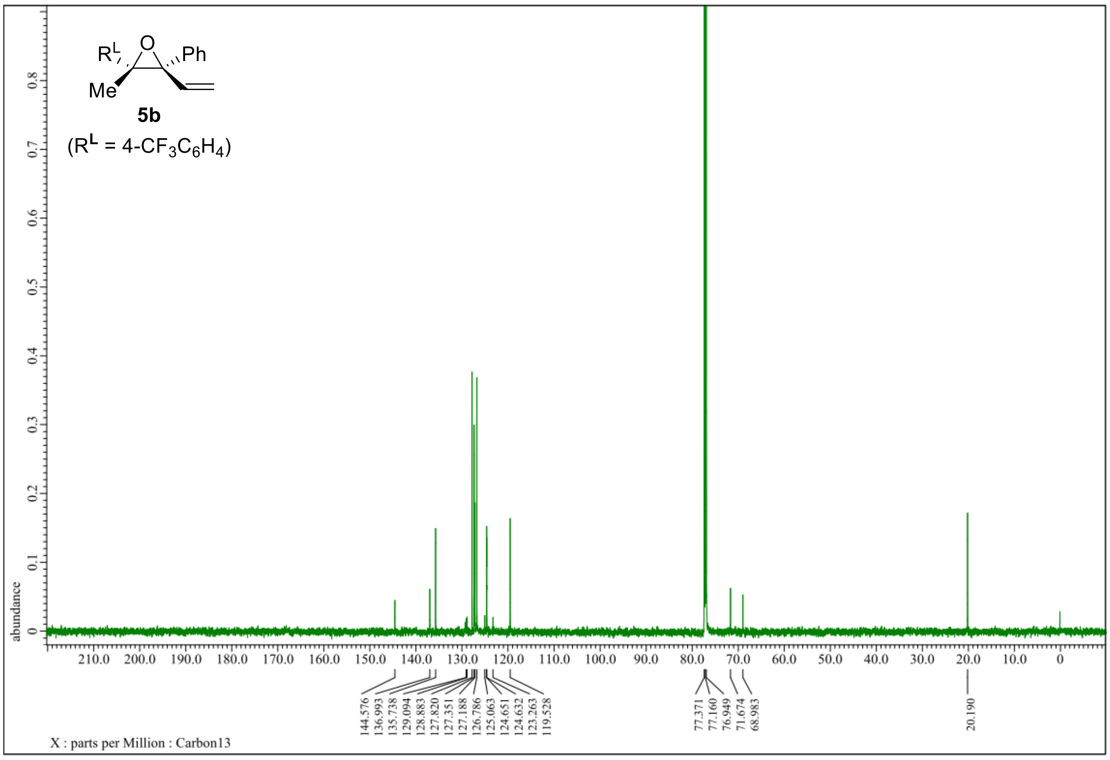
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **5a**



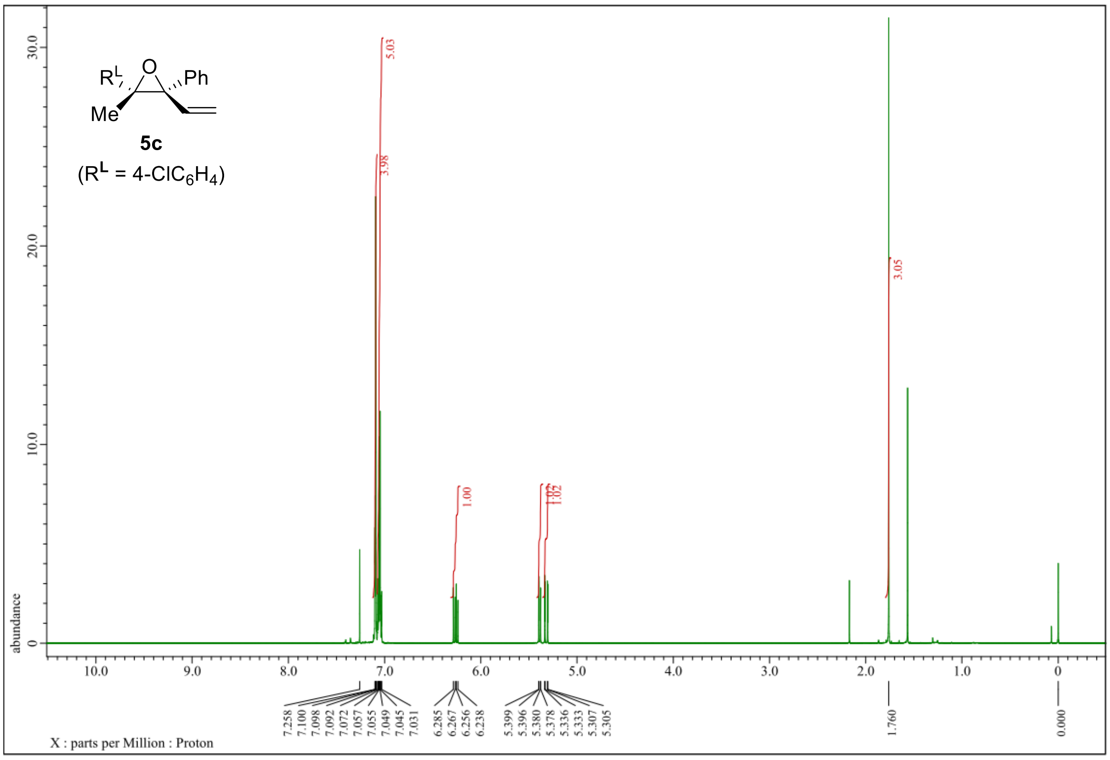


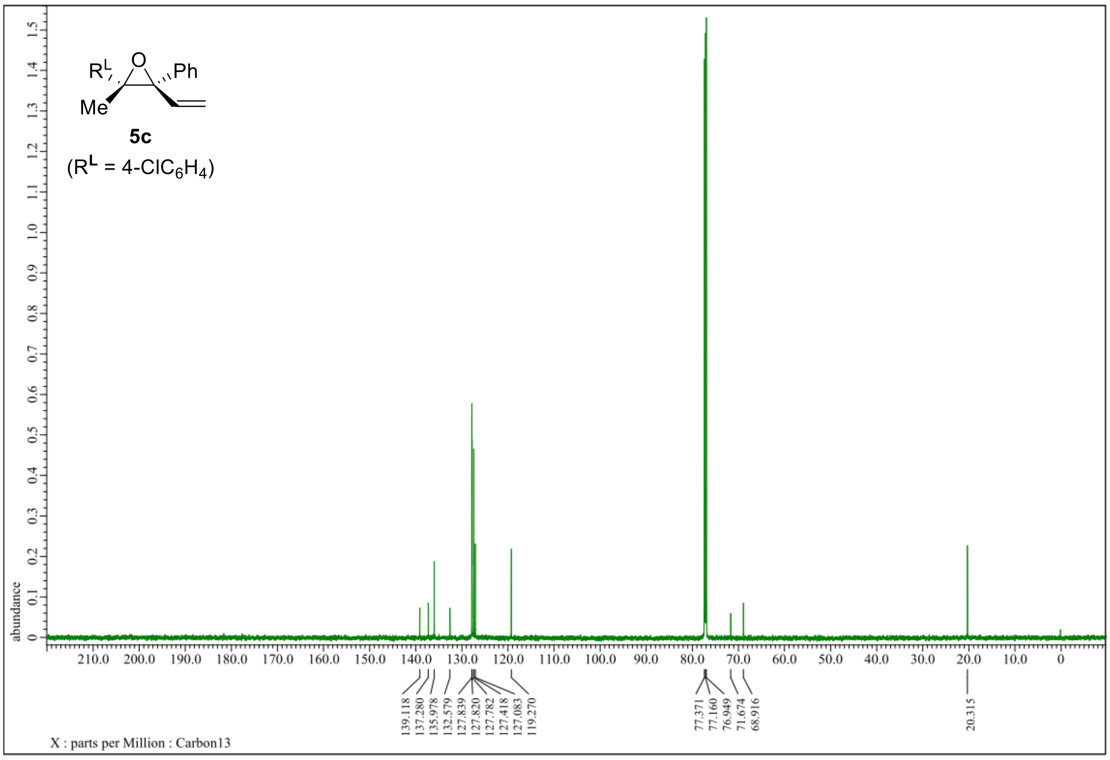
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5b**



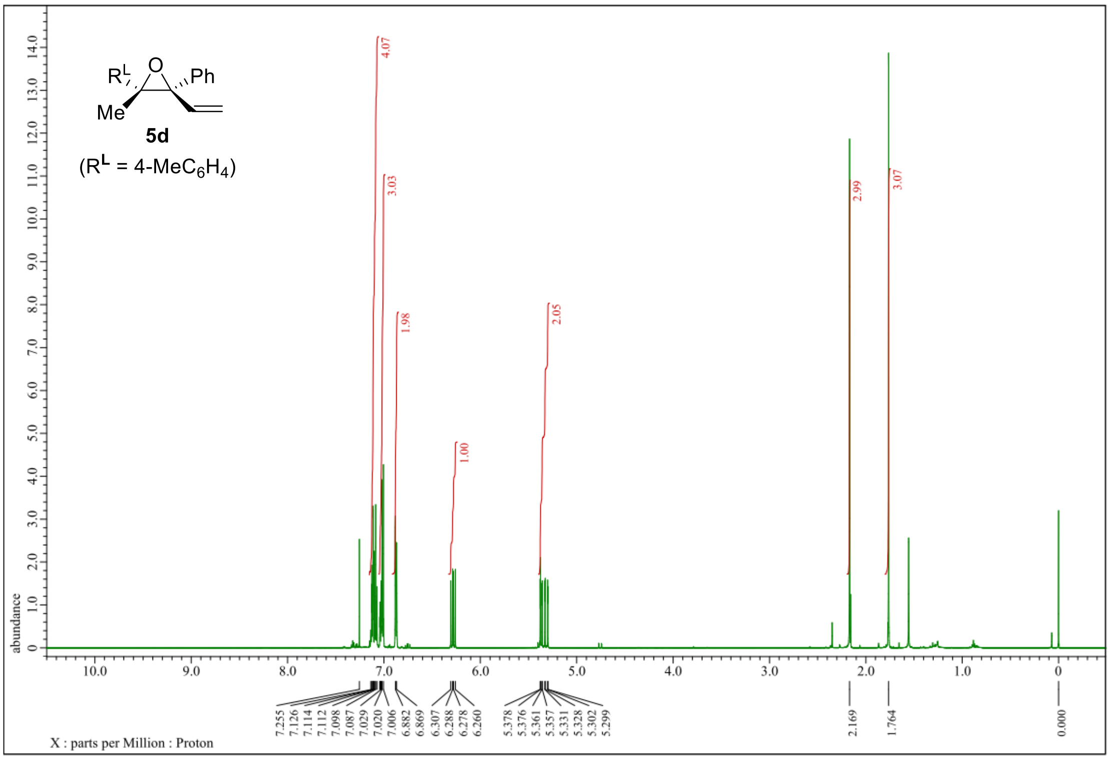


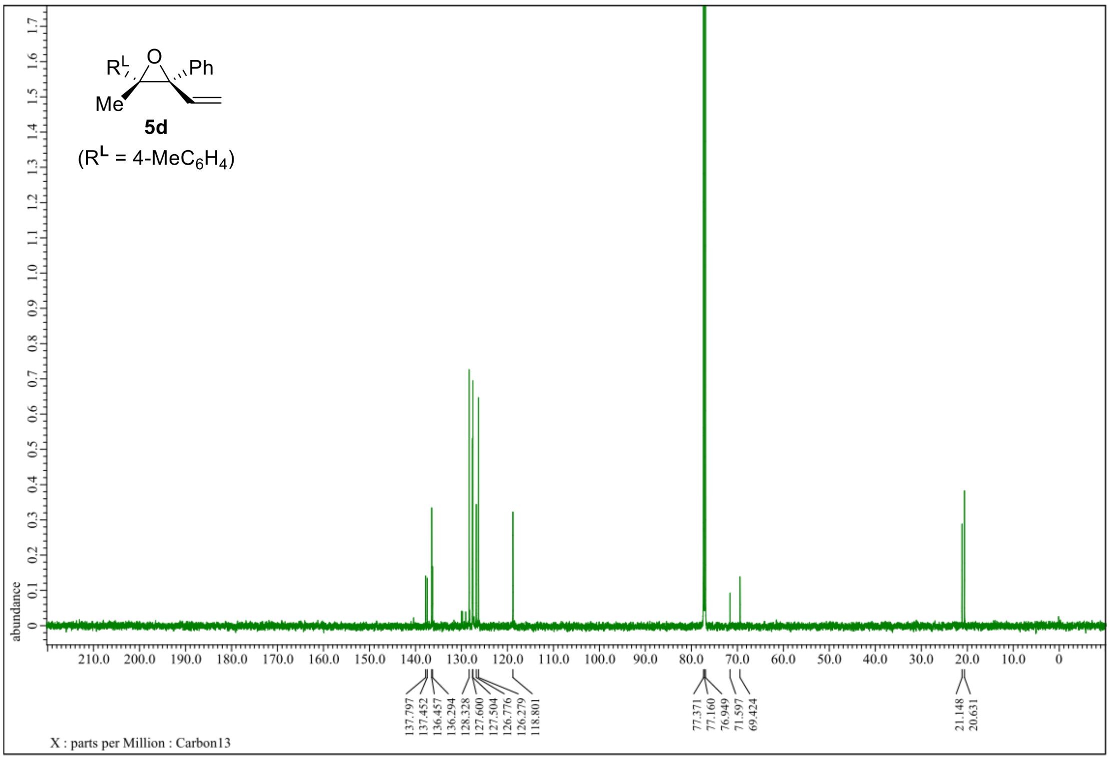
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **5c**



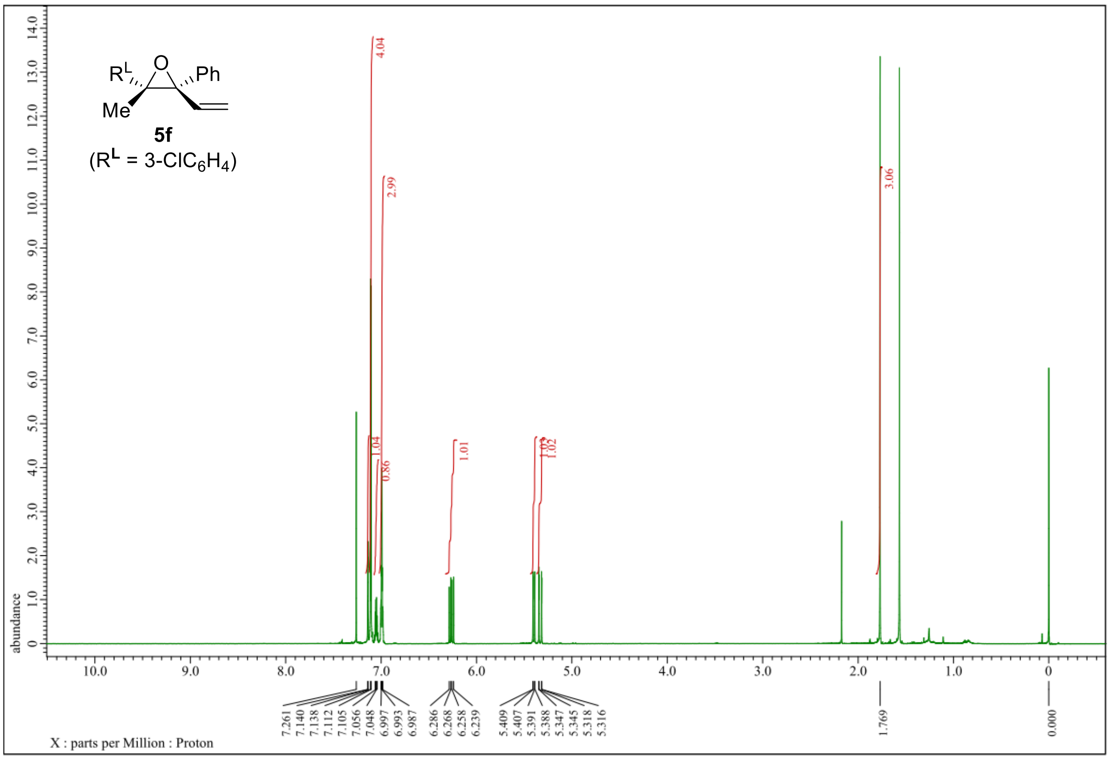


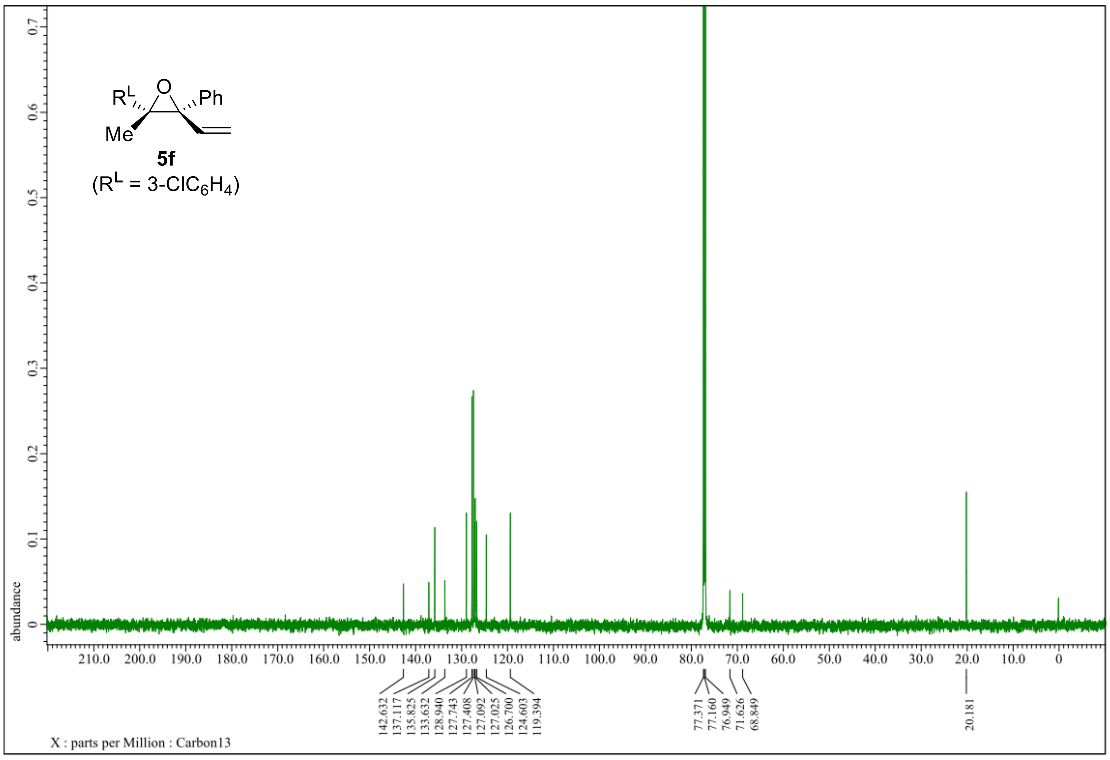
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **5d**



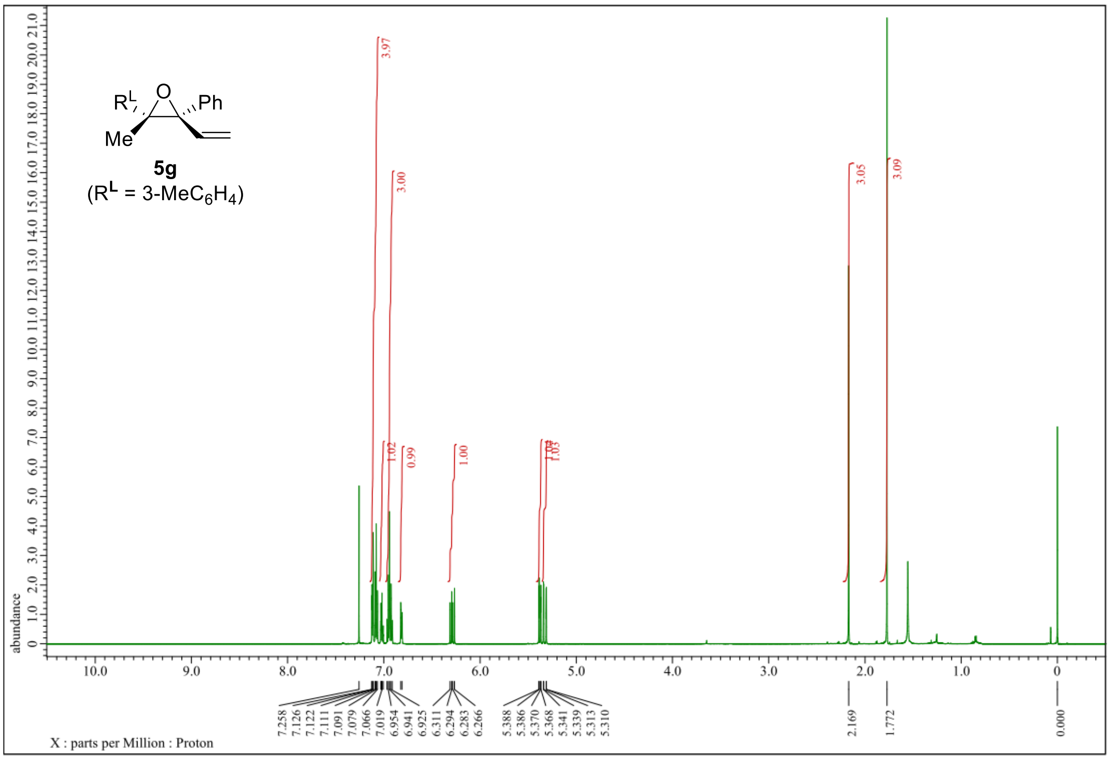


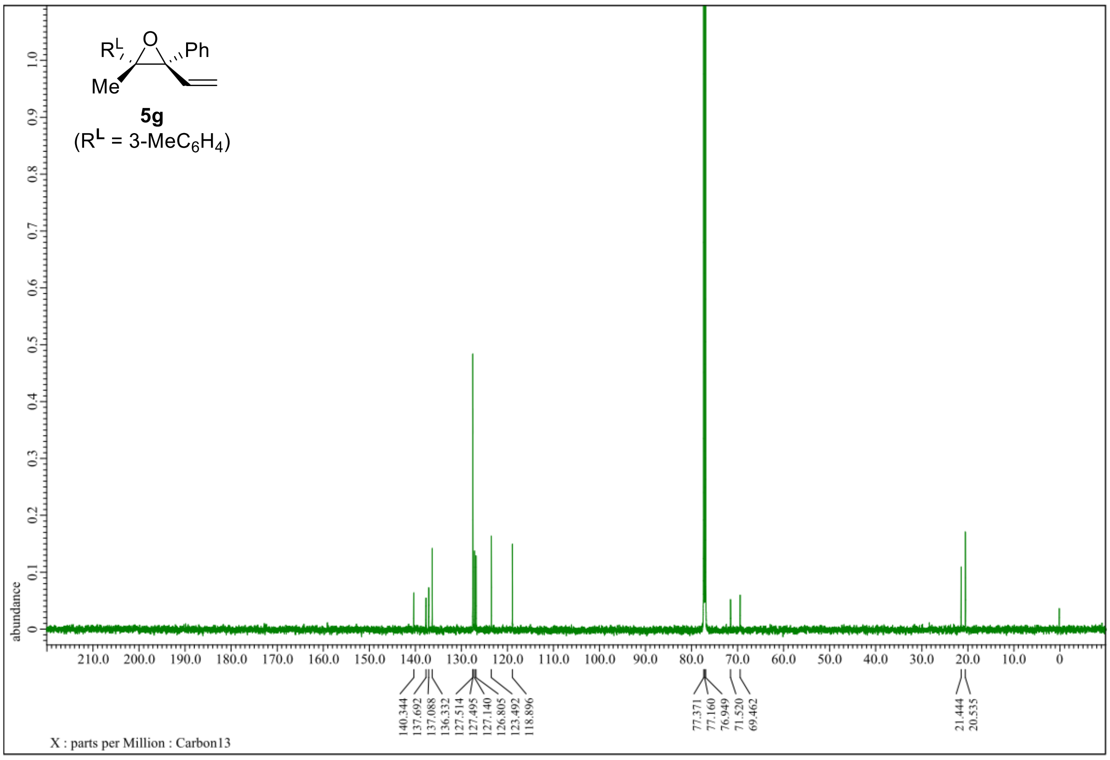
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5f**



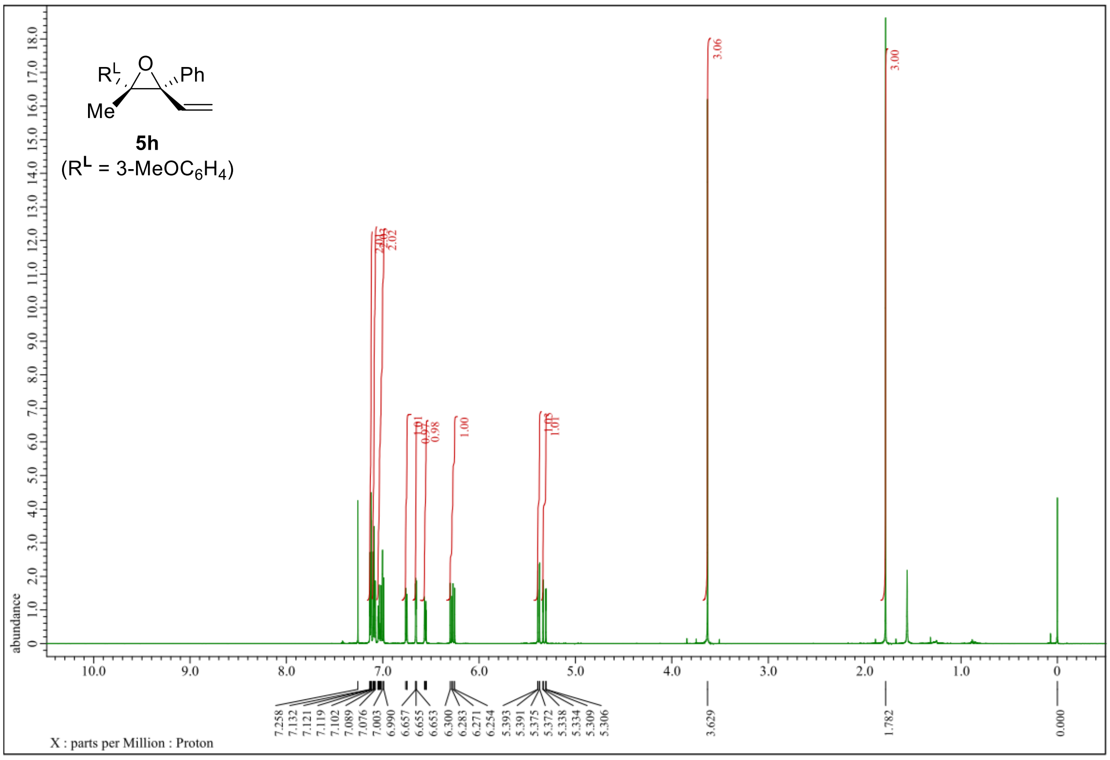


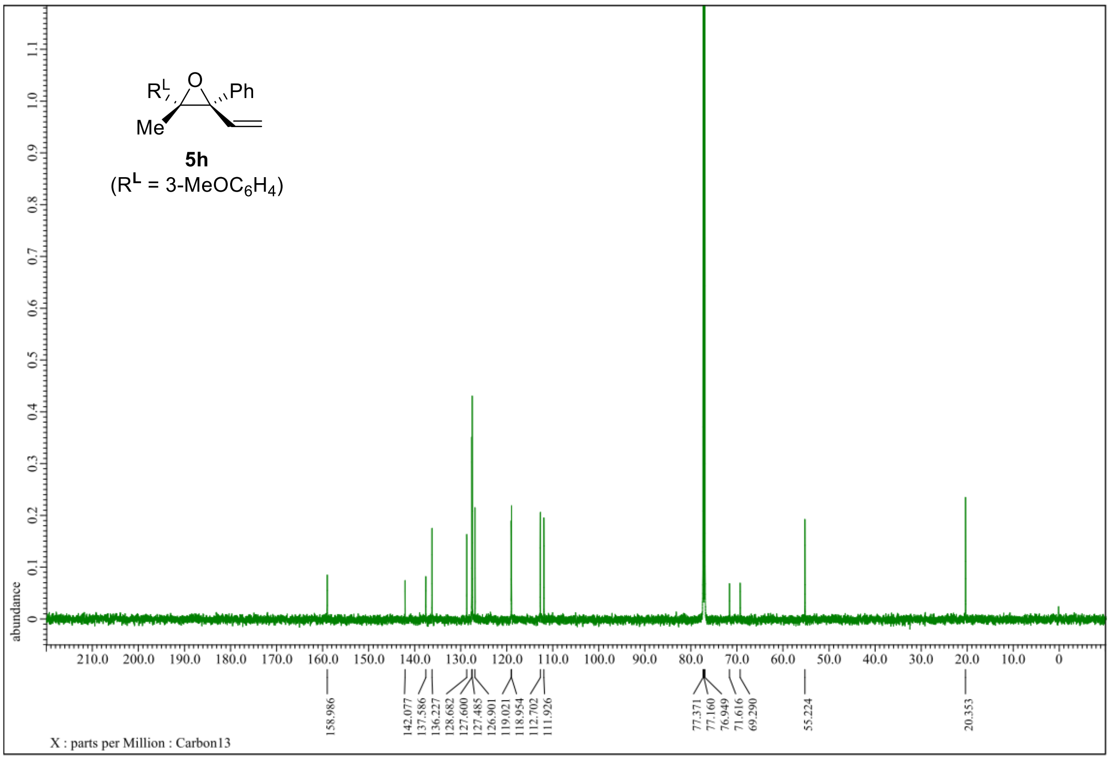
^1H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5g**



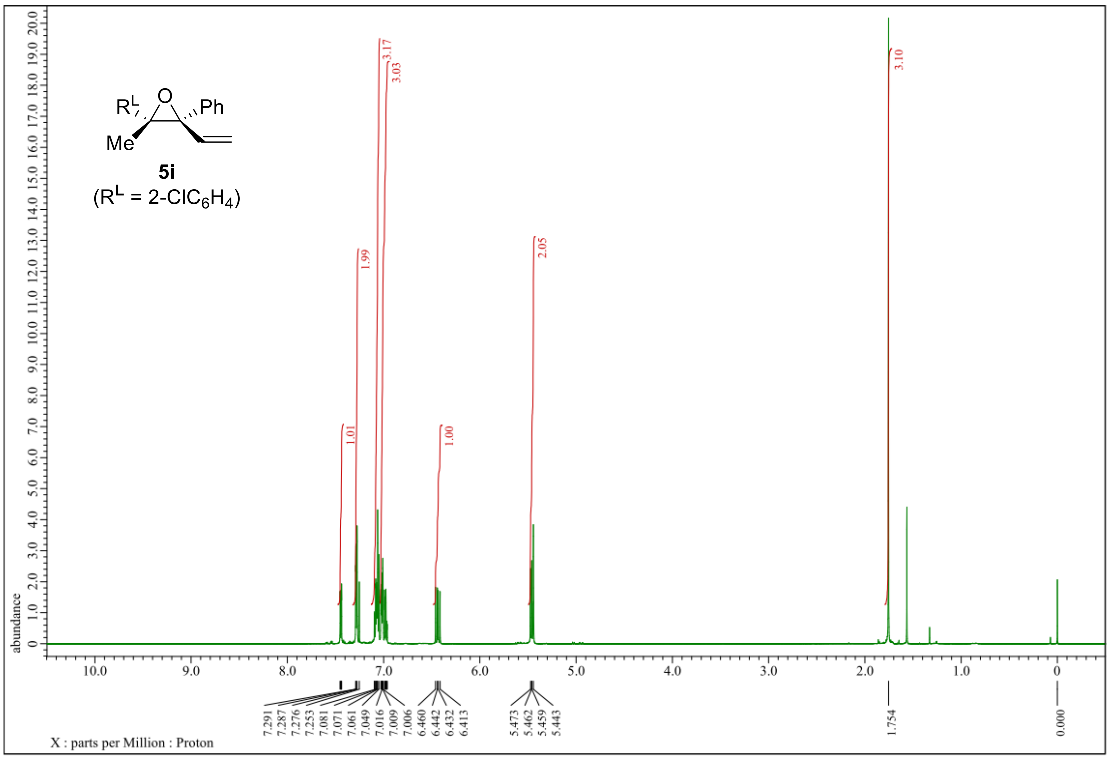


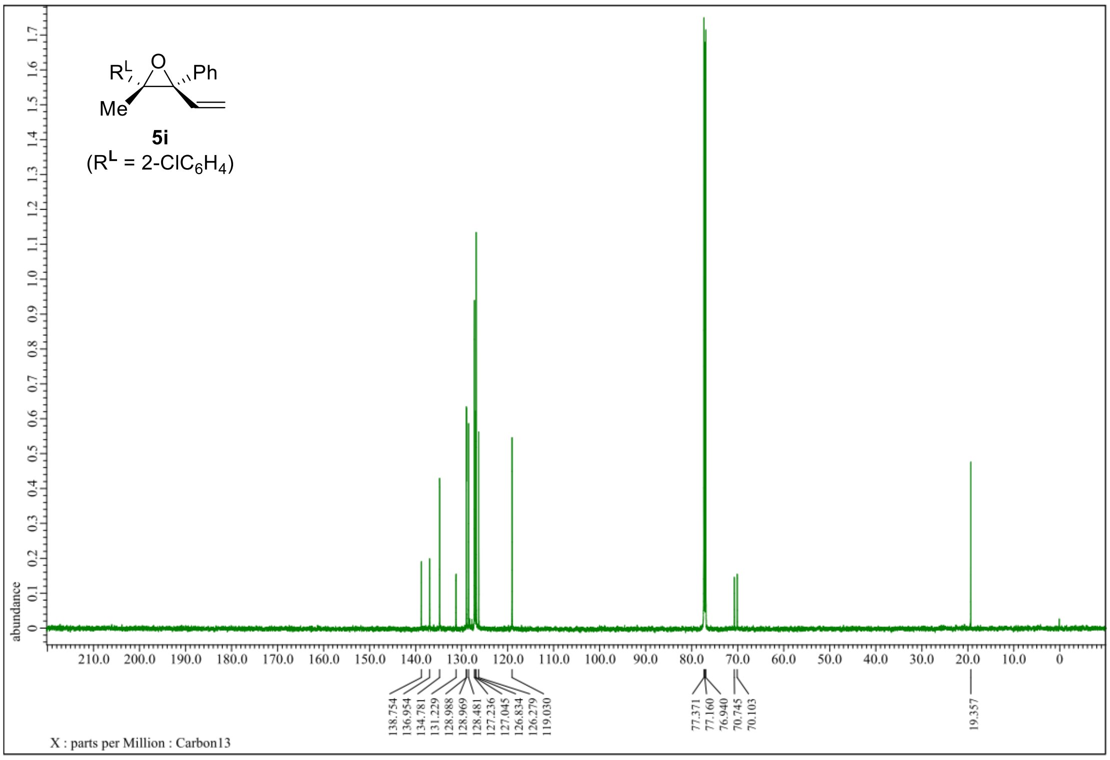
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5h**



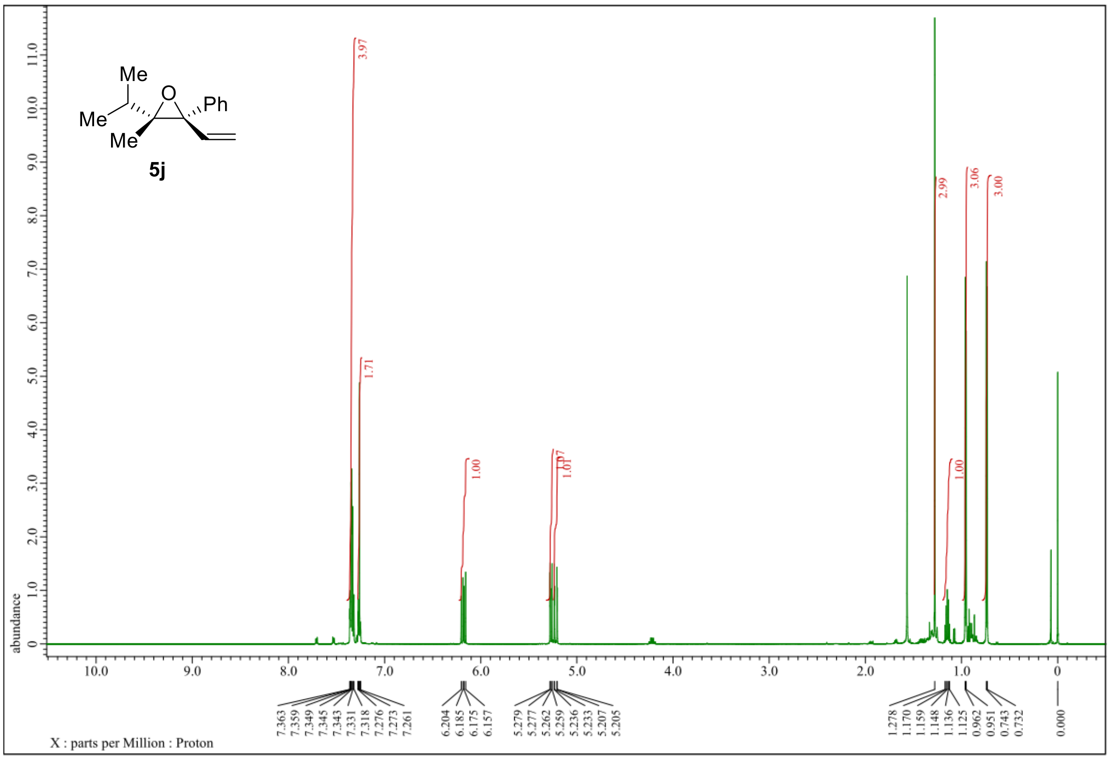


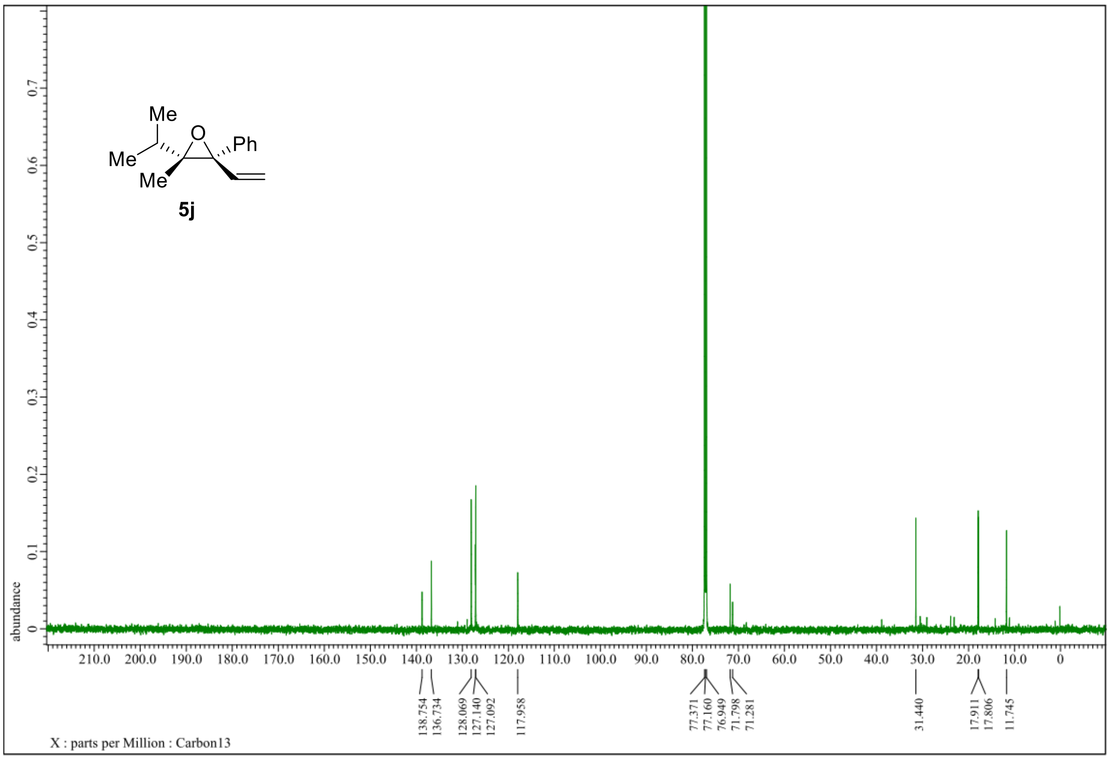
^1H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5i**



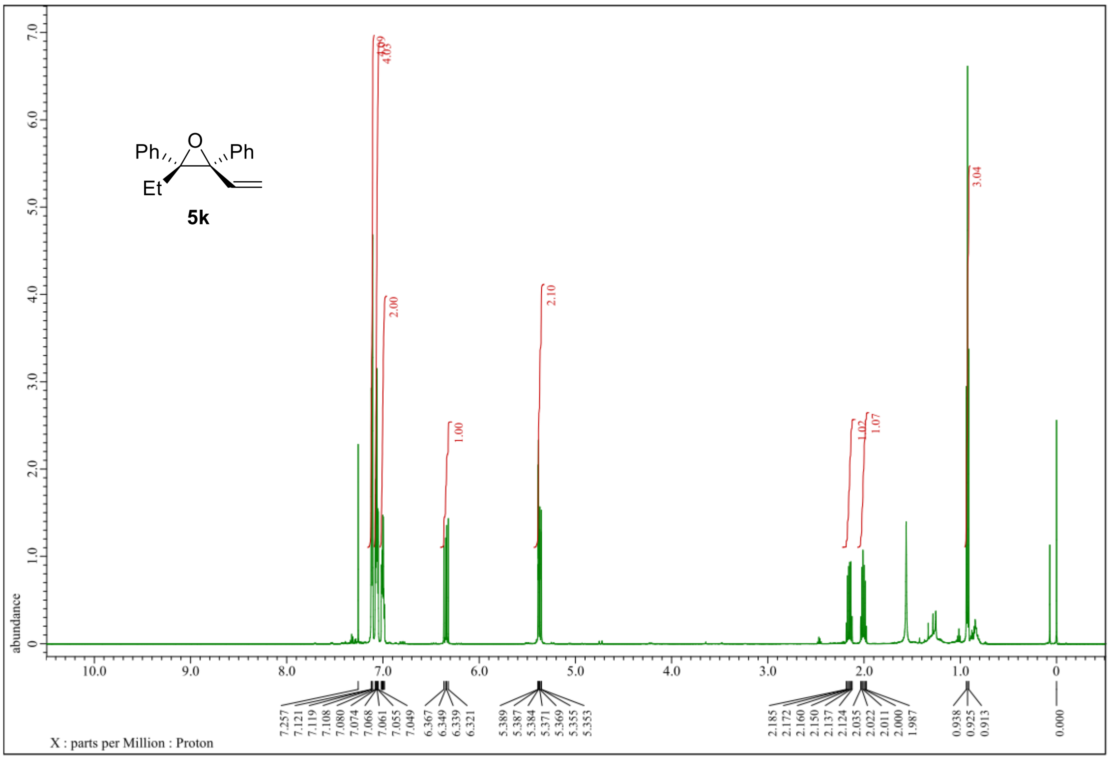


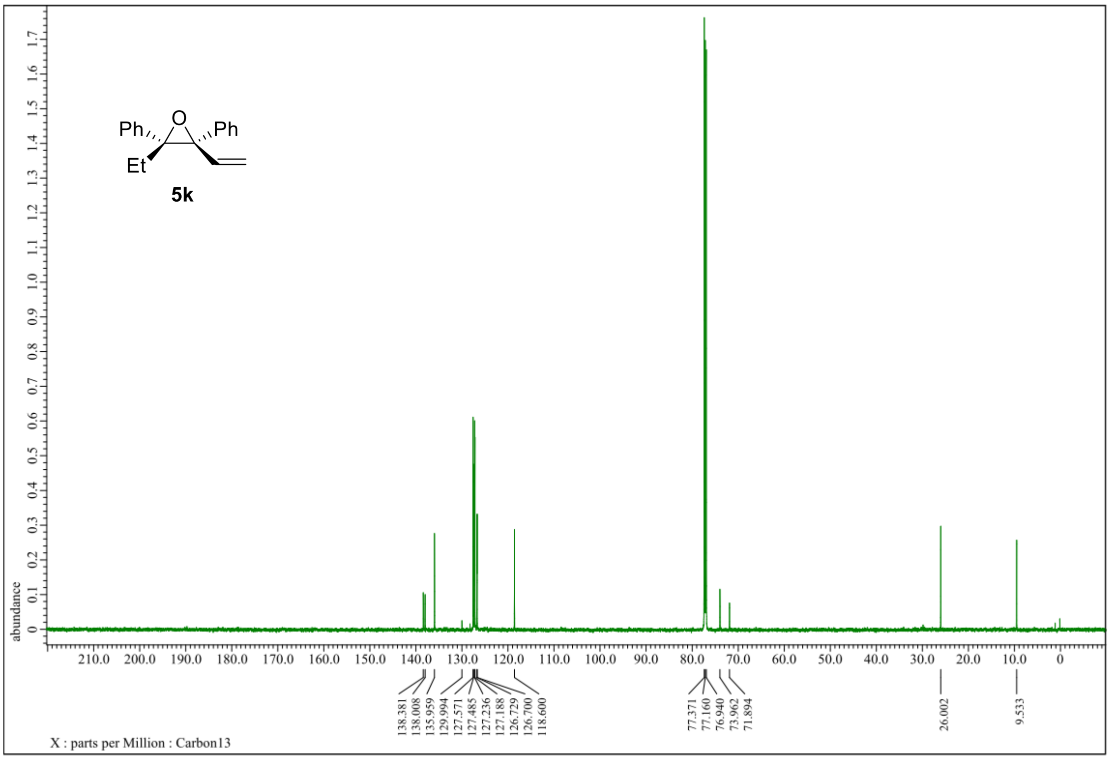
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **5j**



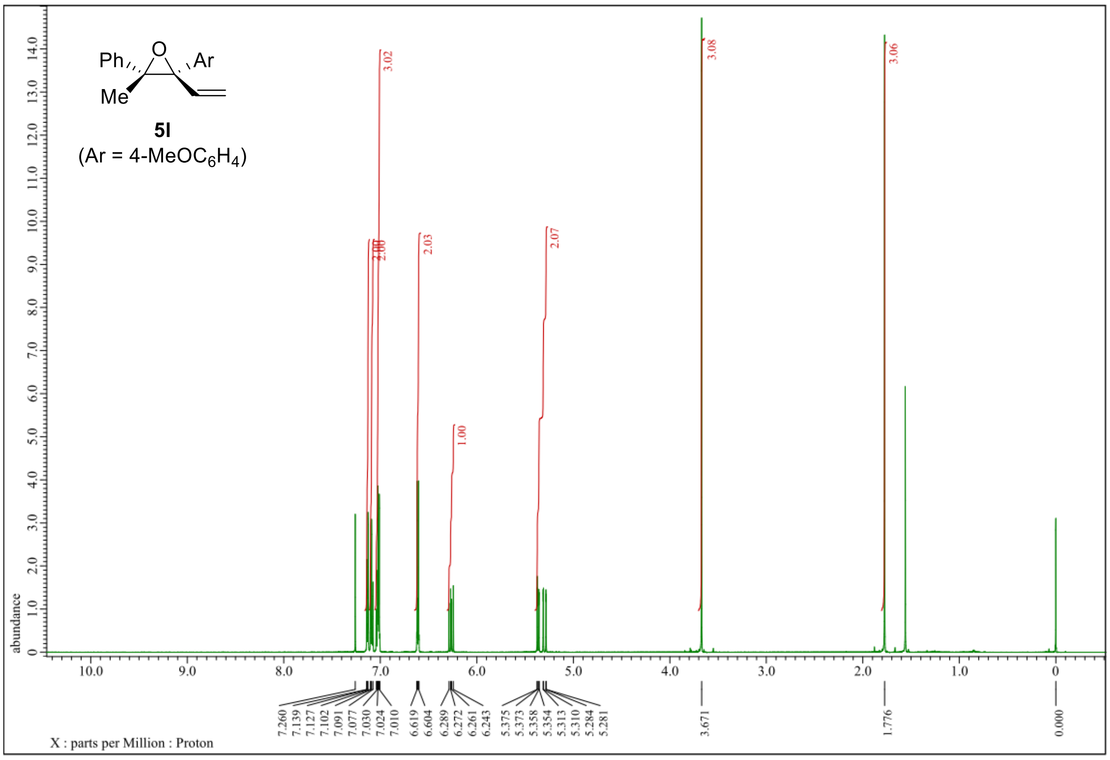


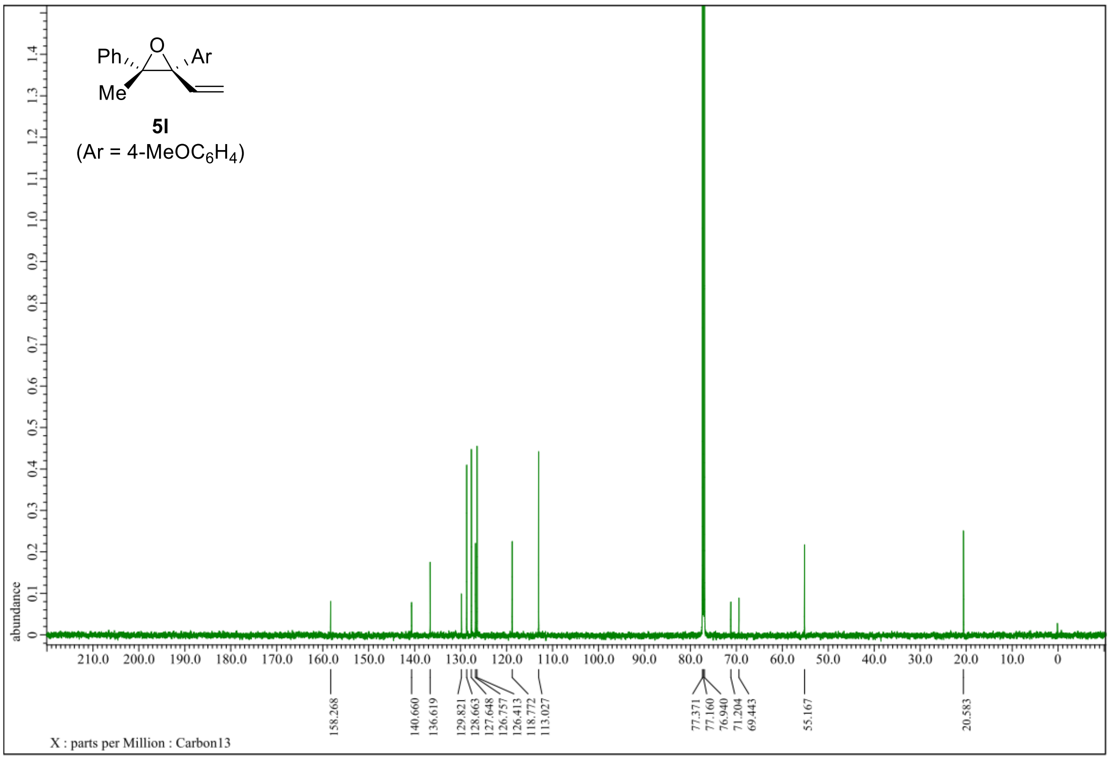
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **5k**



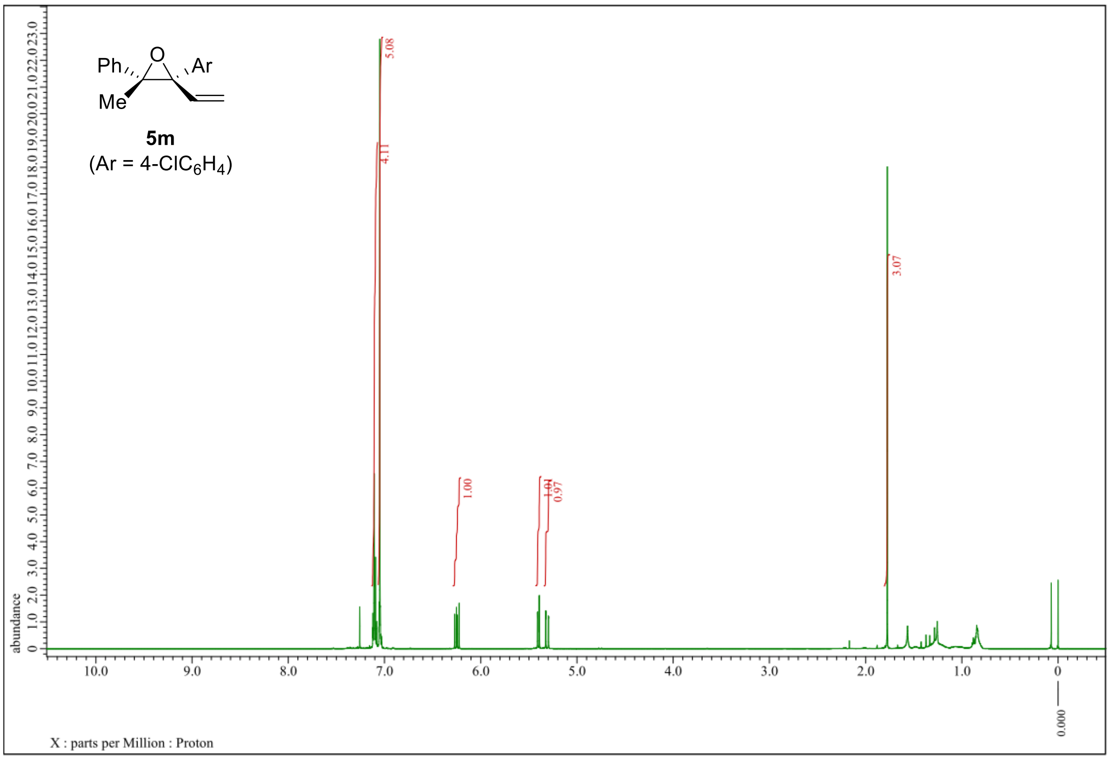


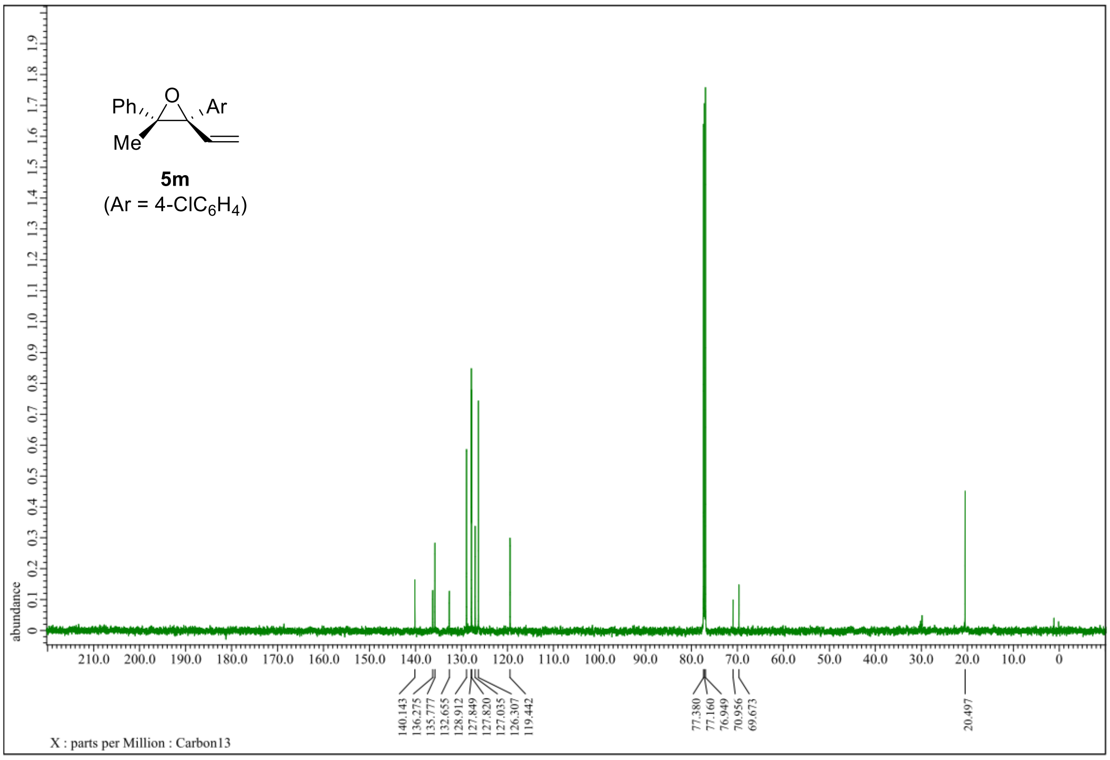
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5l**



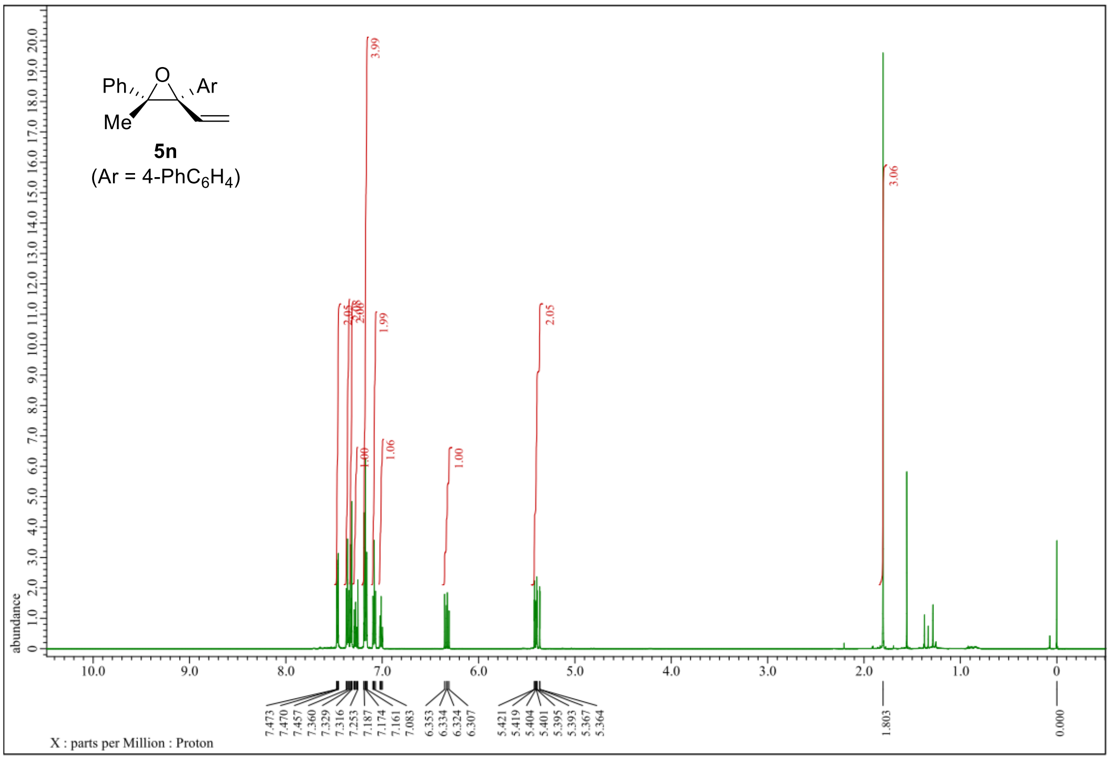


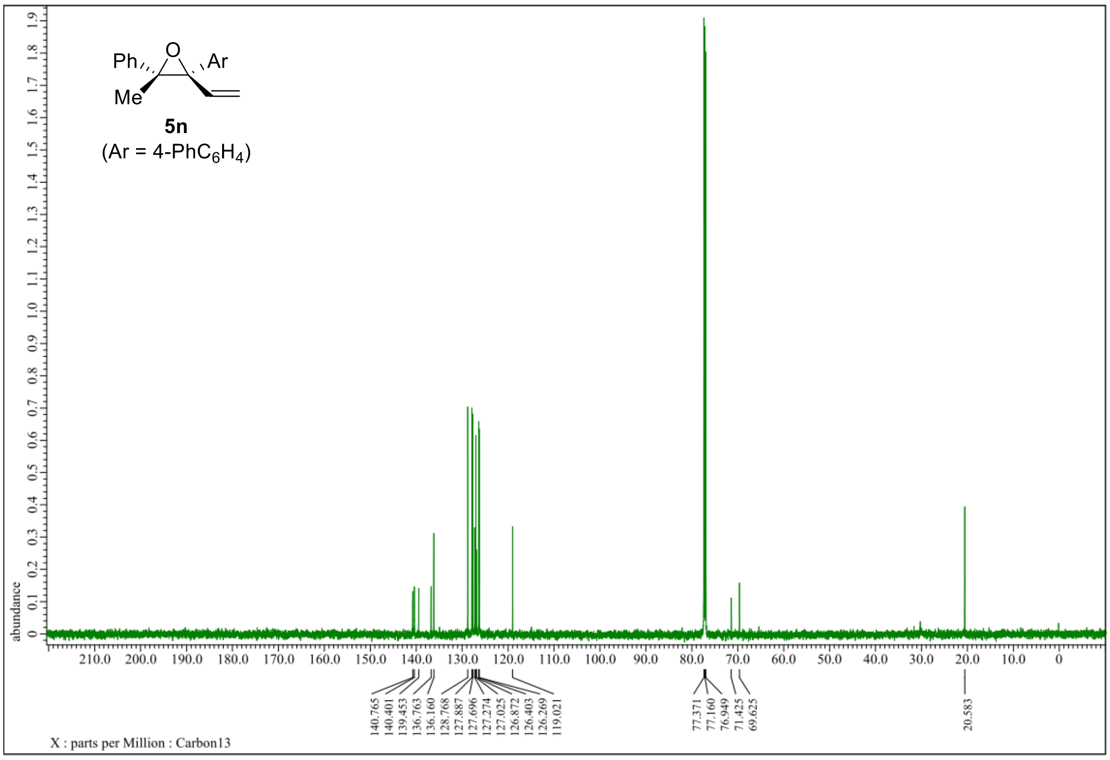
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5m**



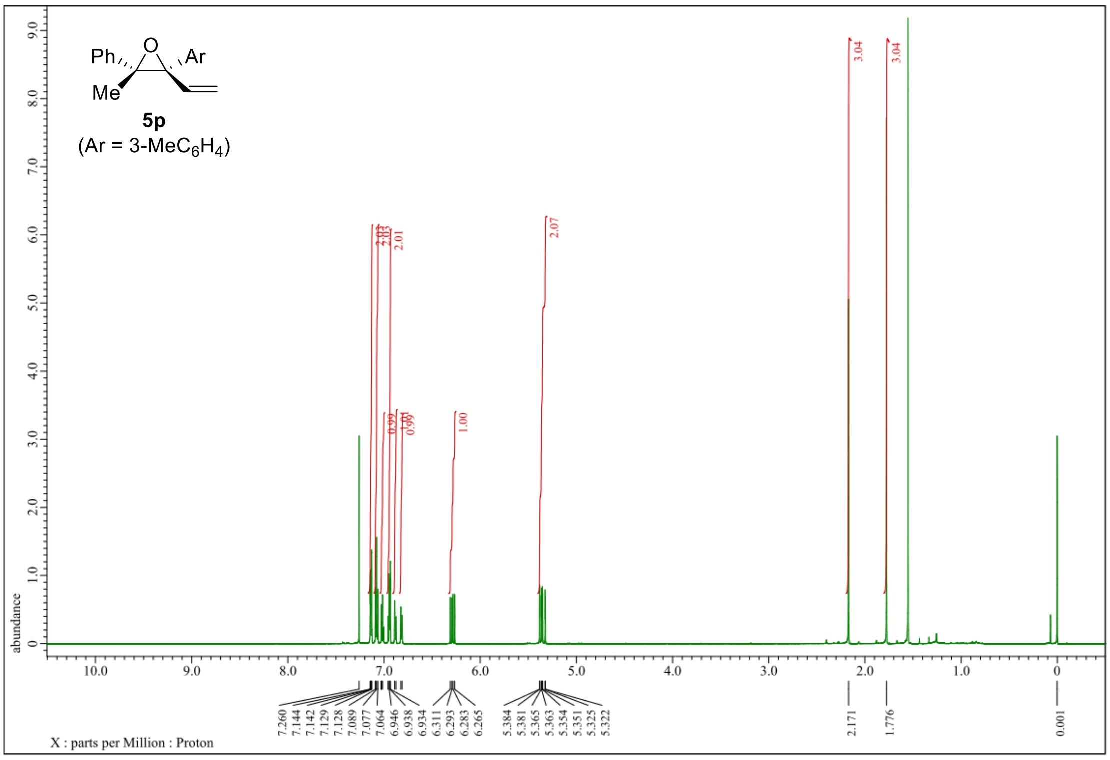


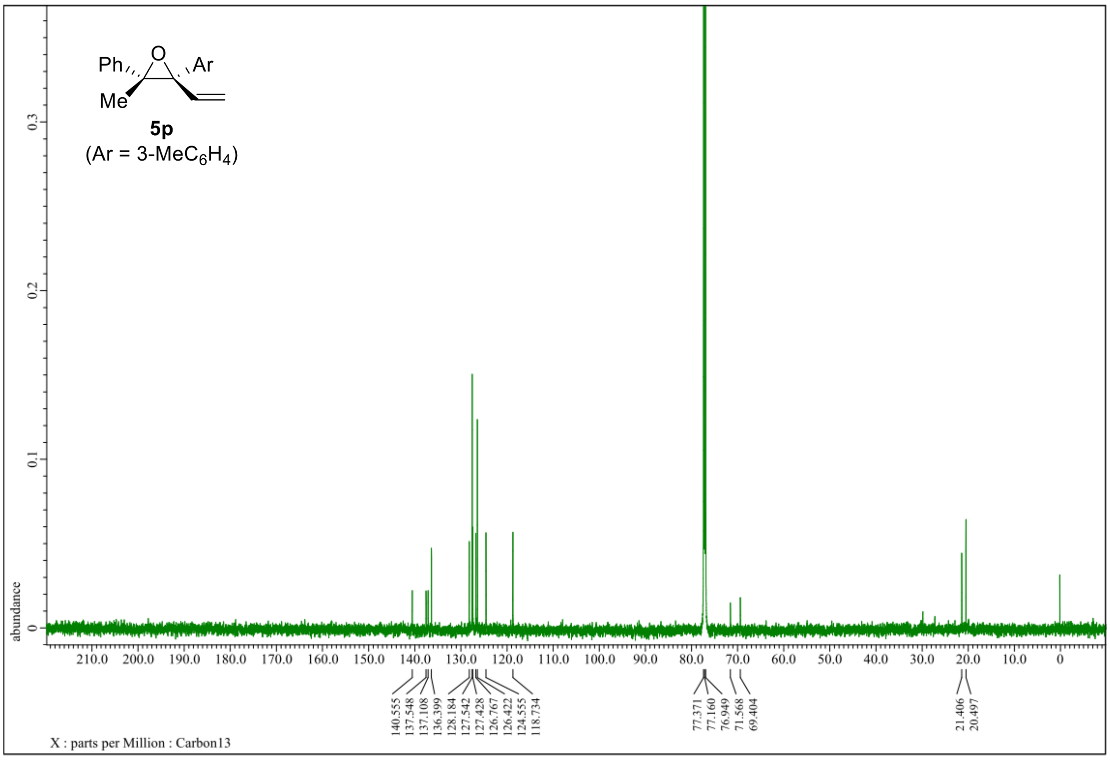
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **5n**



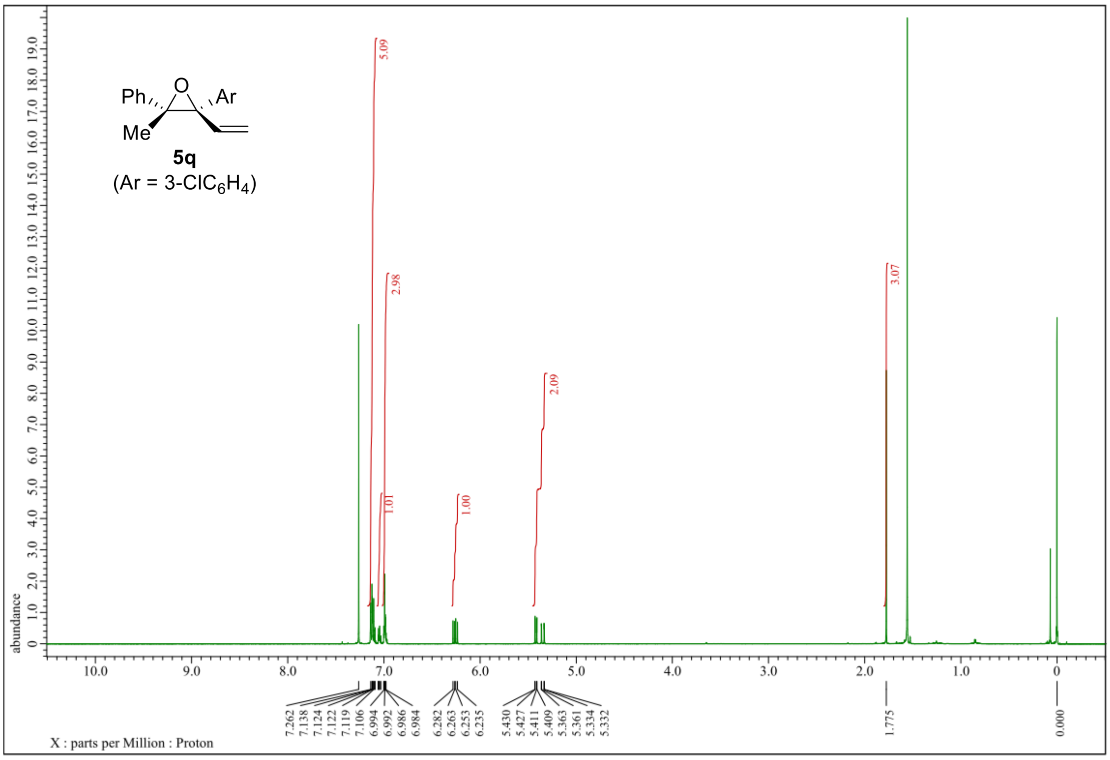


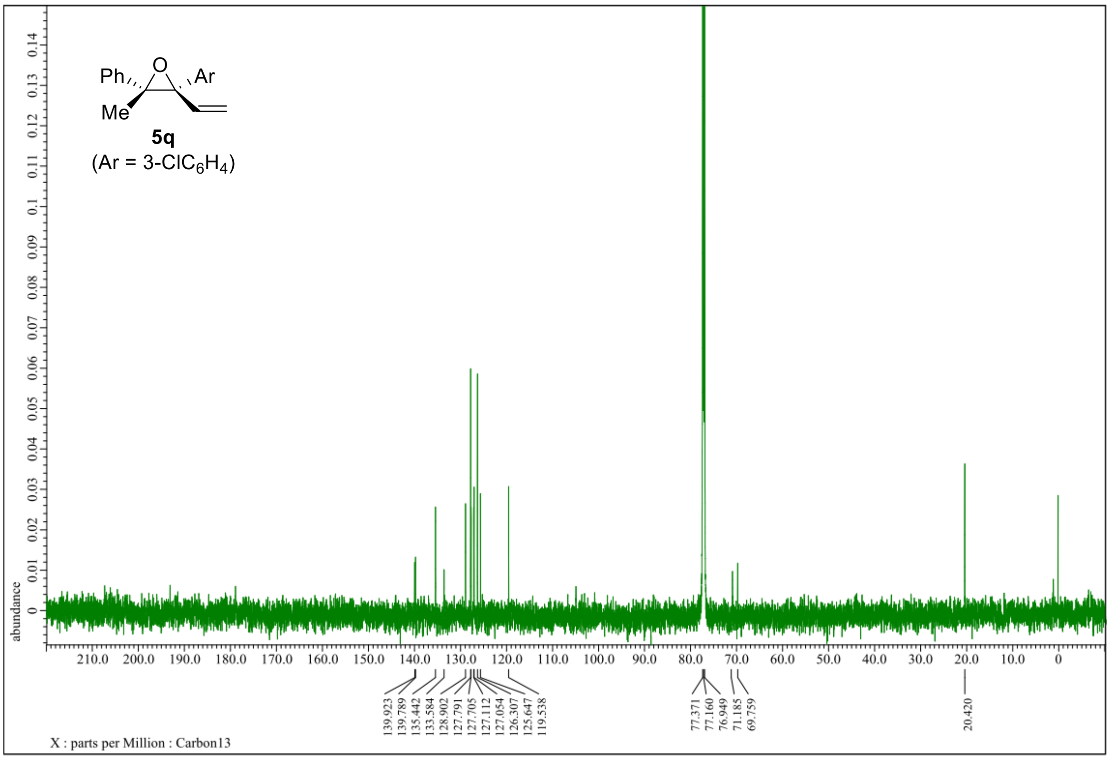
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5p**



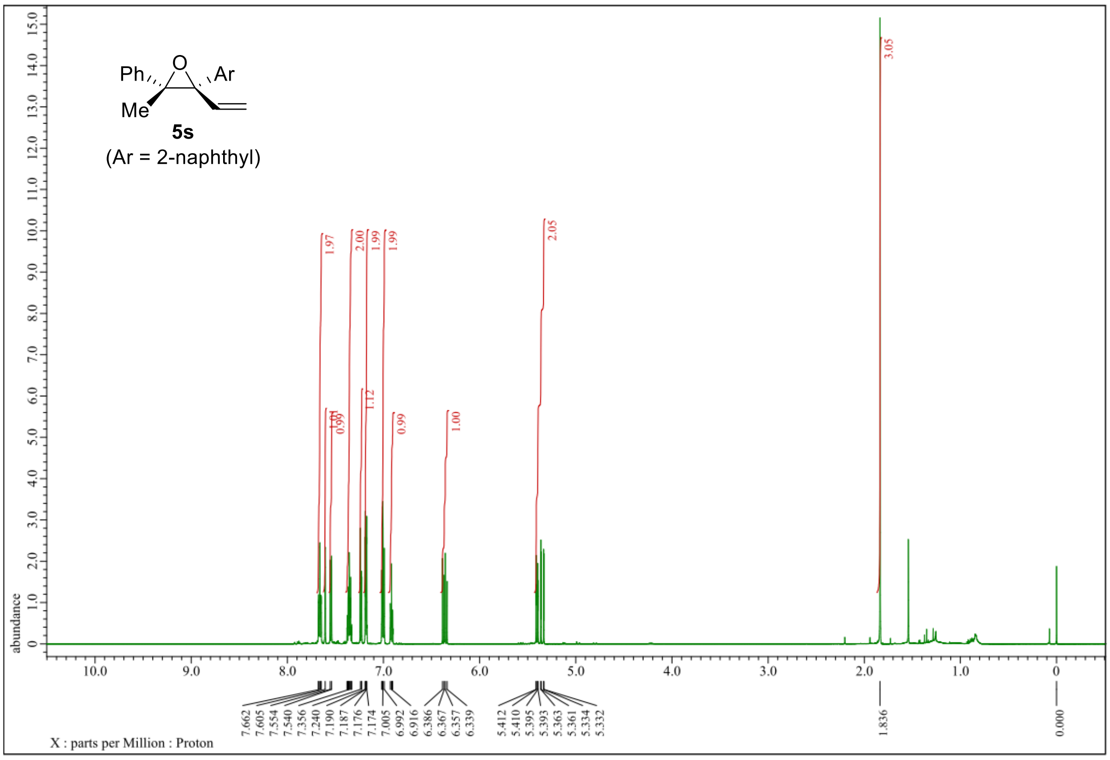


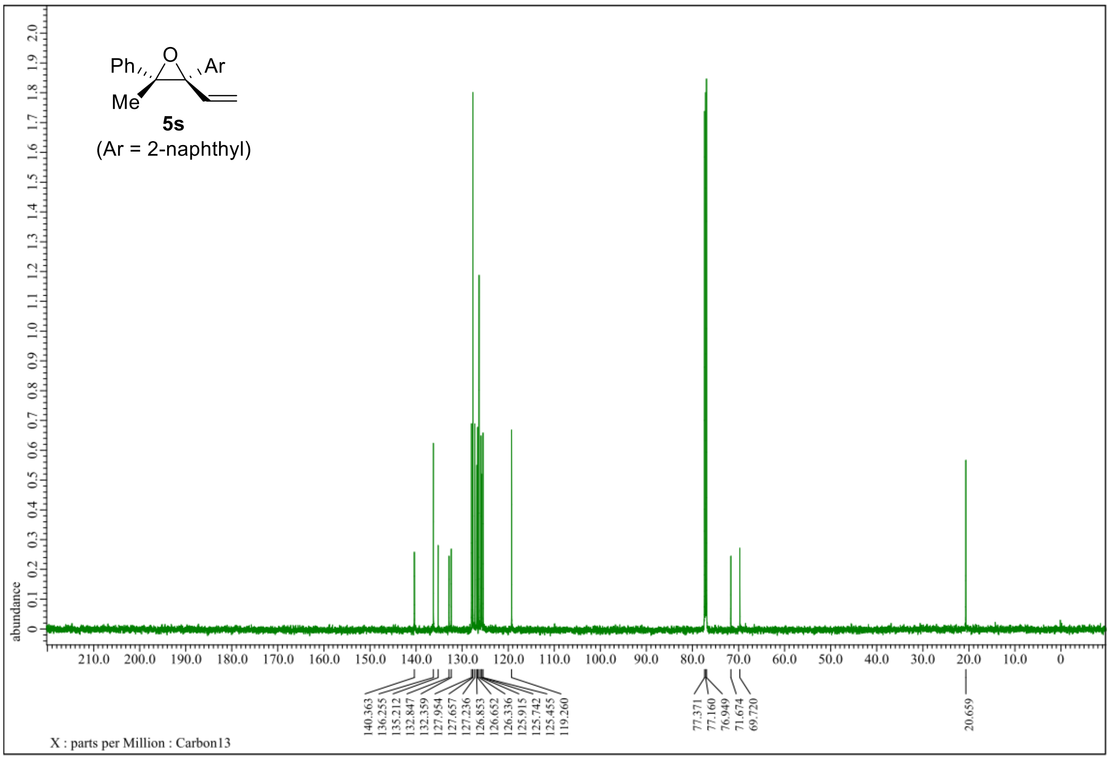
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5q**



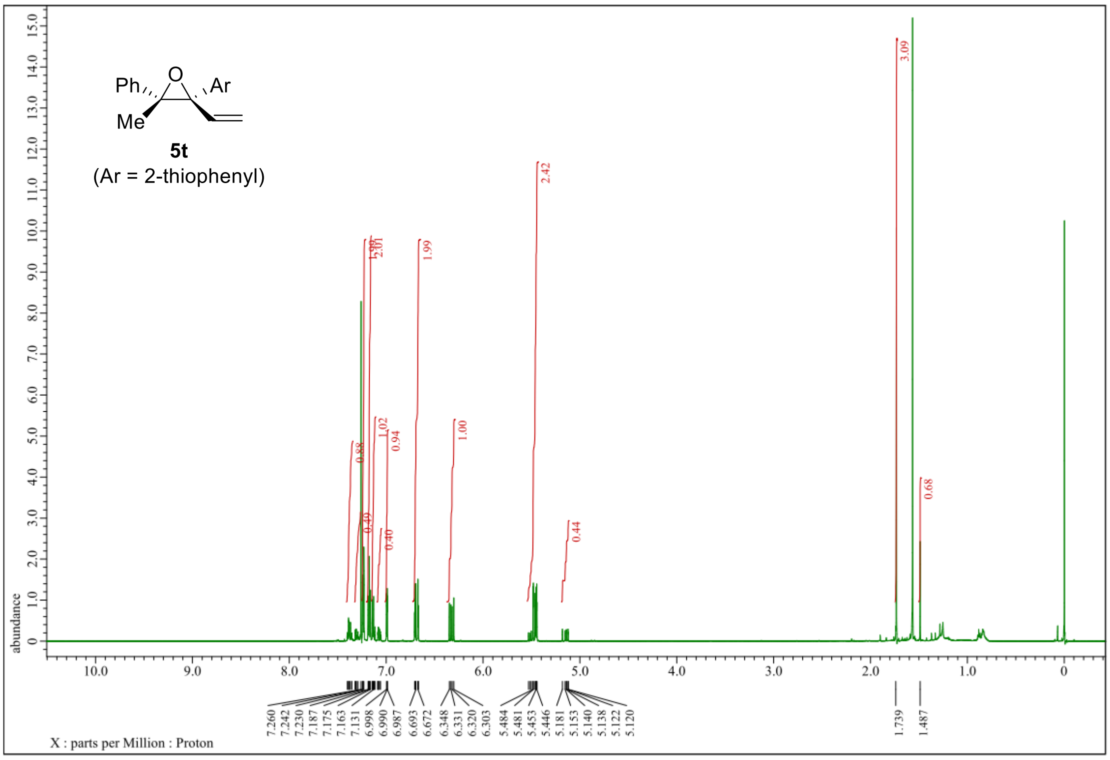


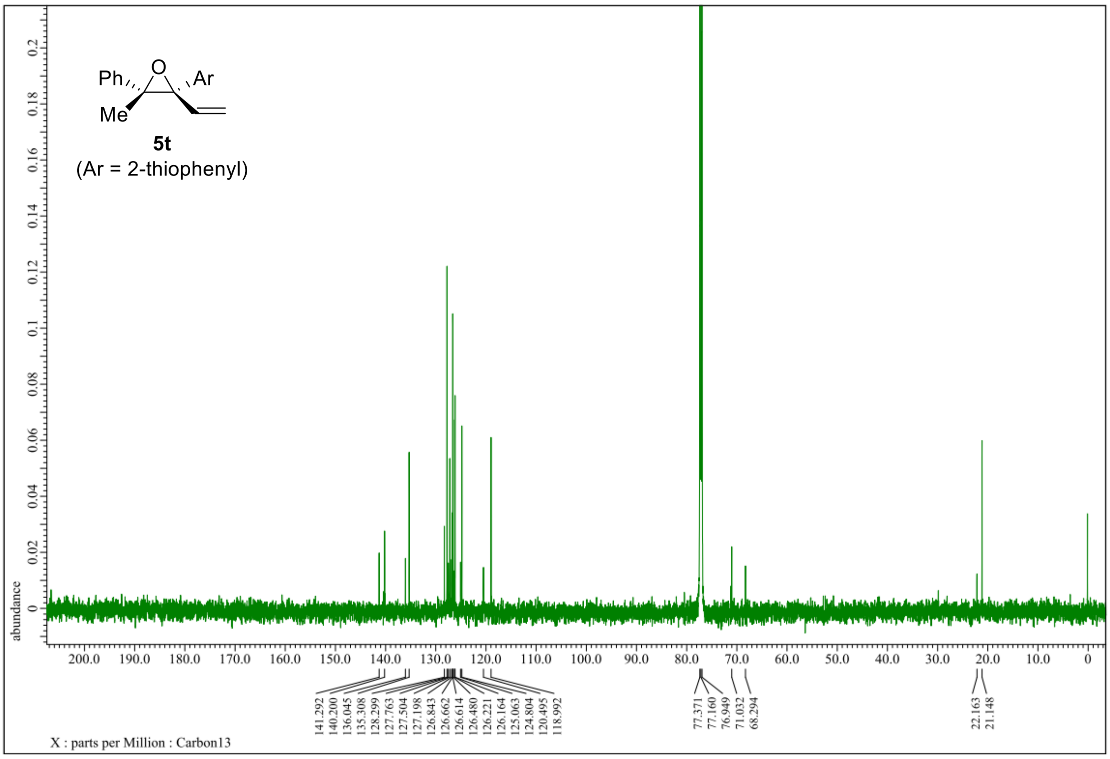
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **5s**



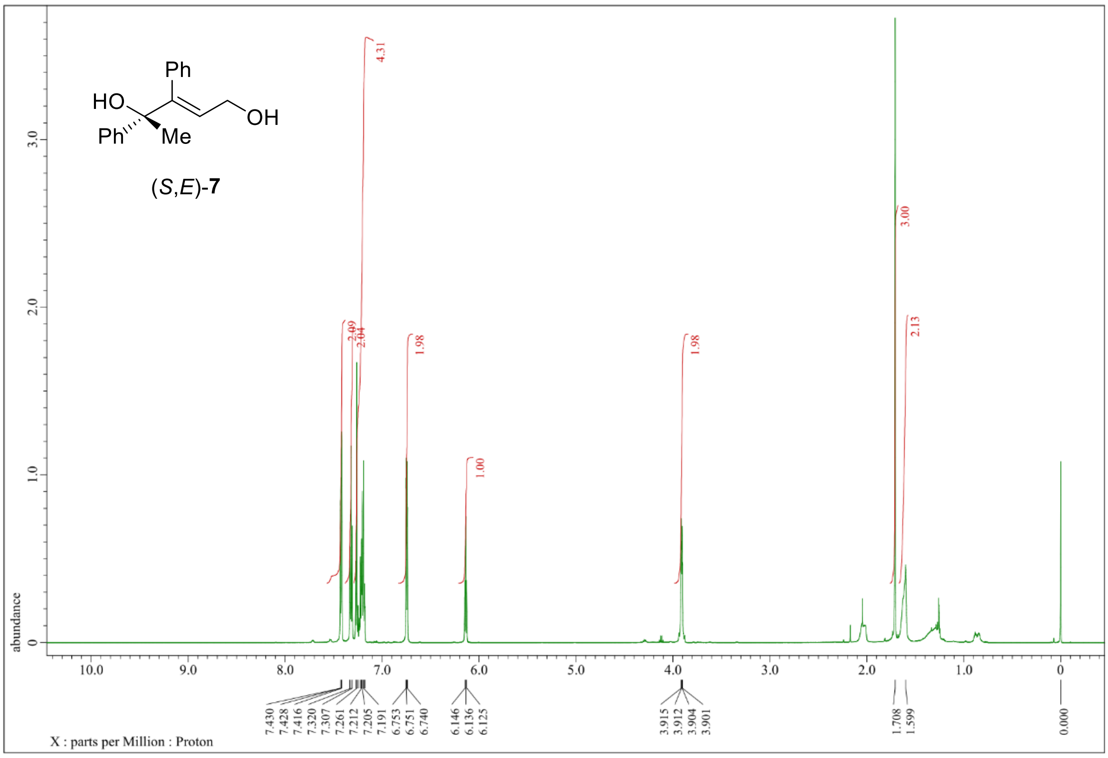


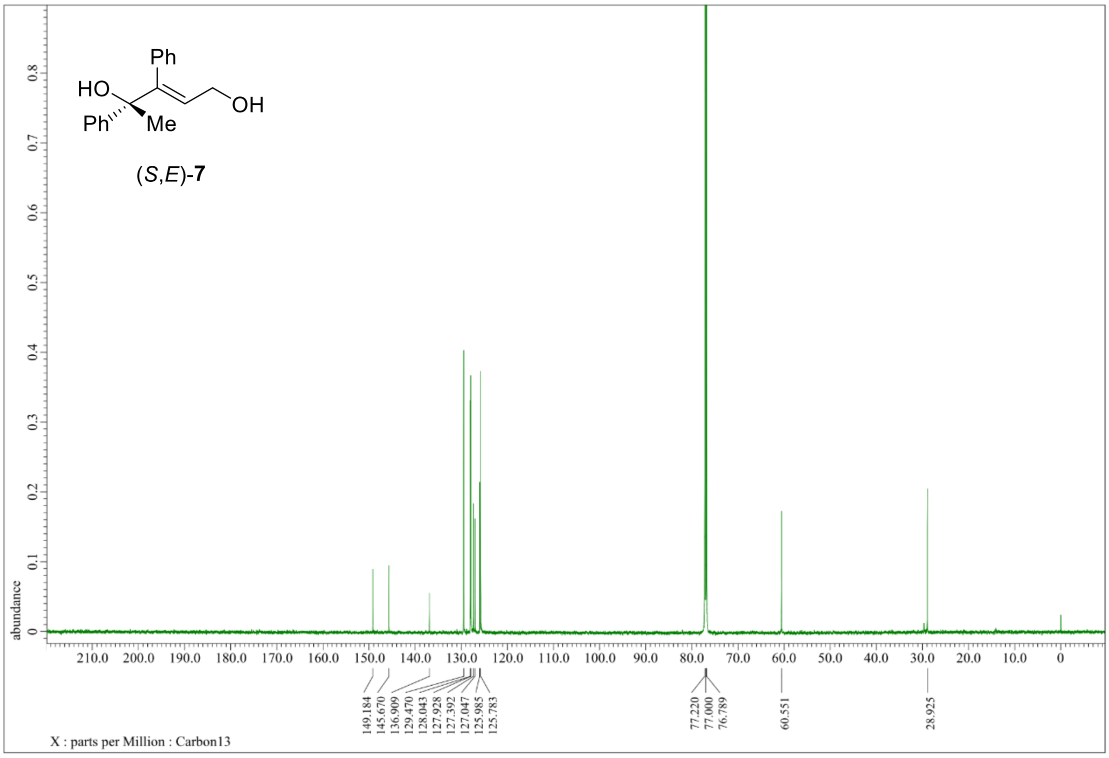
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **5t**



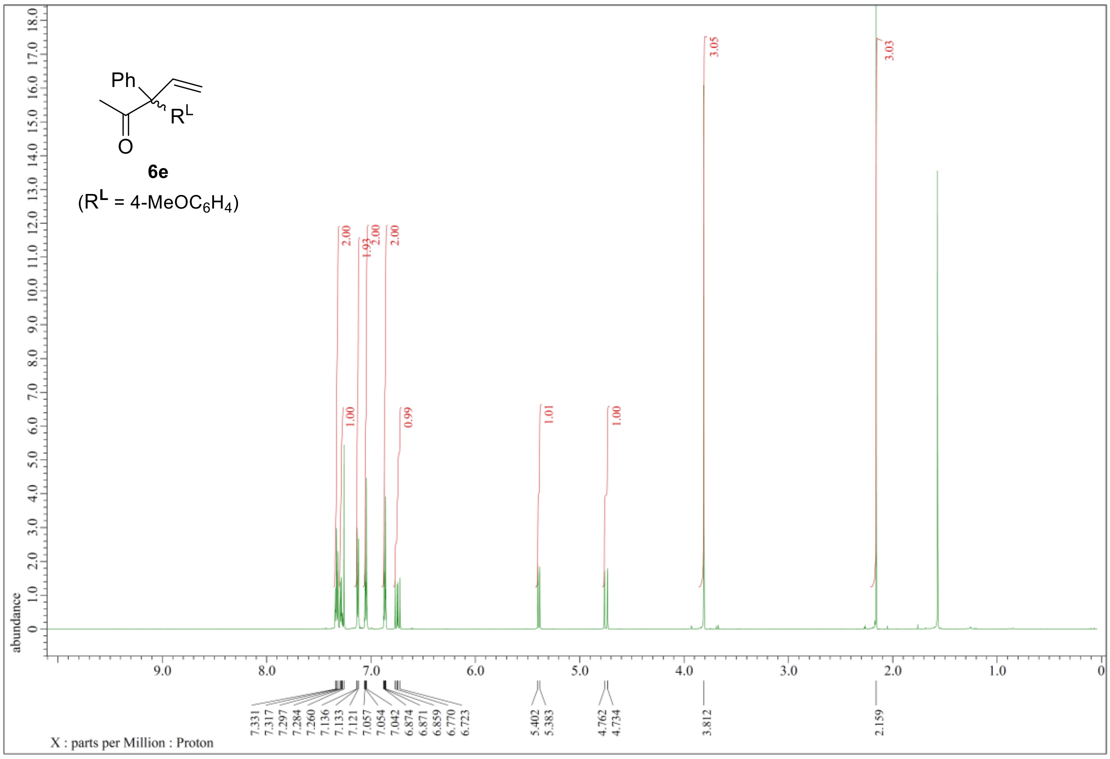


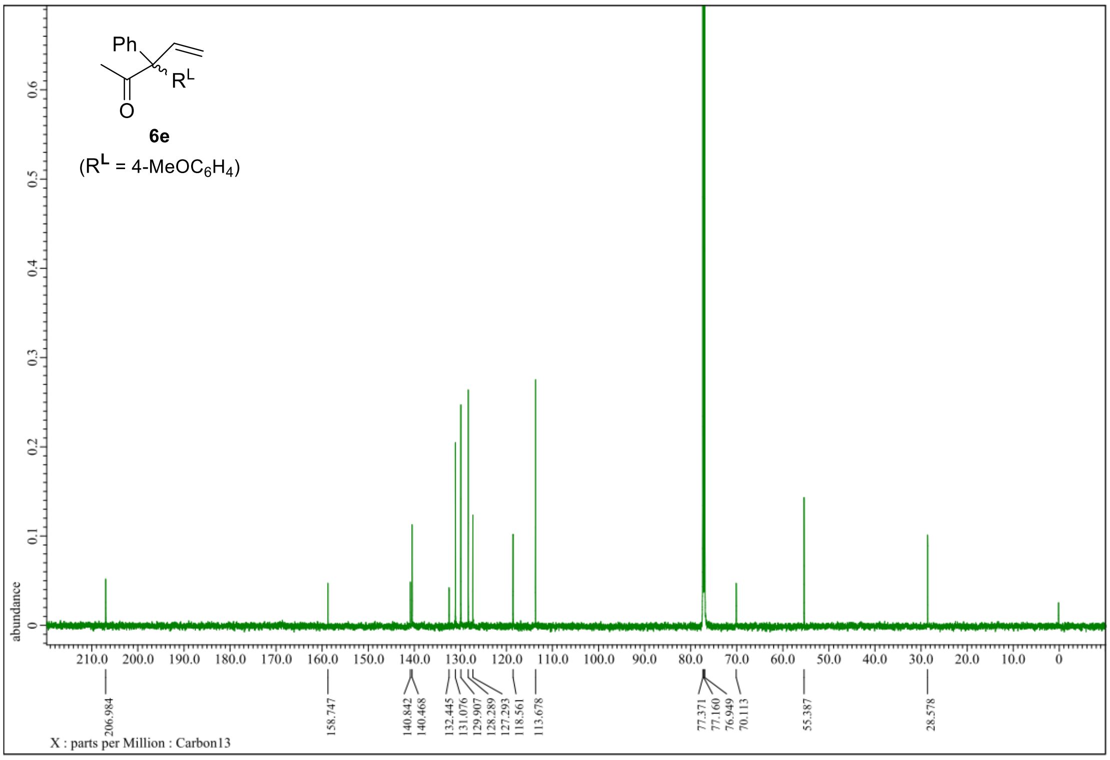
[1]H NMR (600 MHz, $CDCl_3$) and [13]C NMR (151 MHz, $CDCl_3$) spectra of **7**



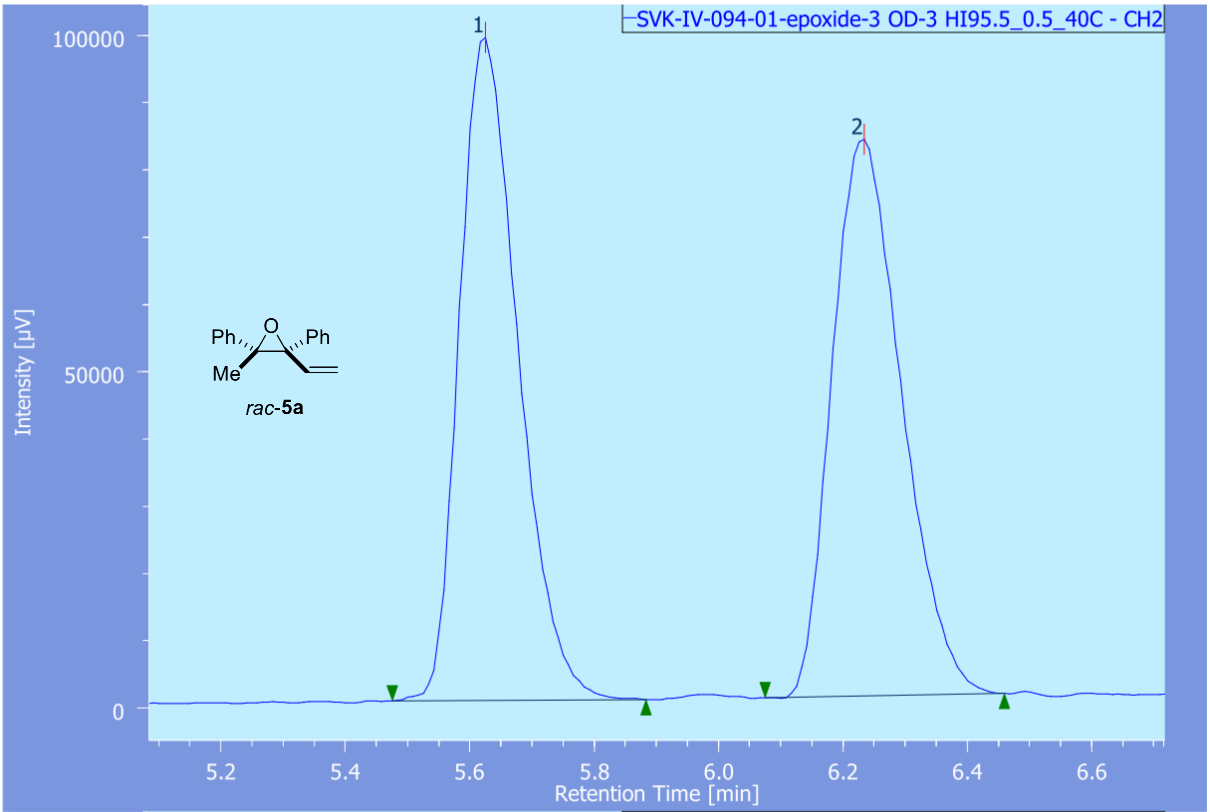


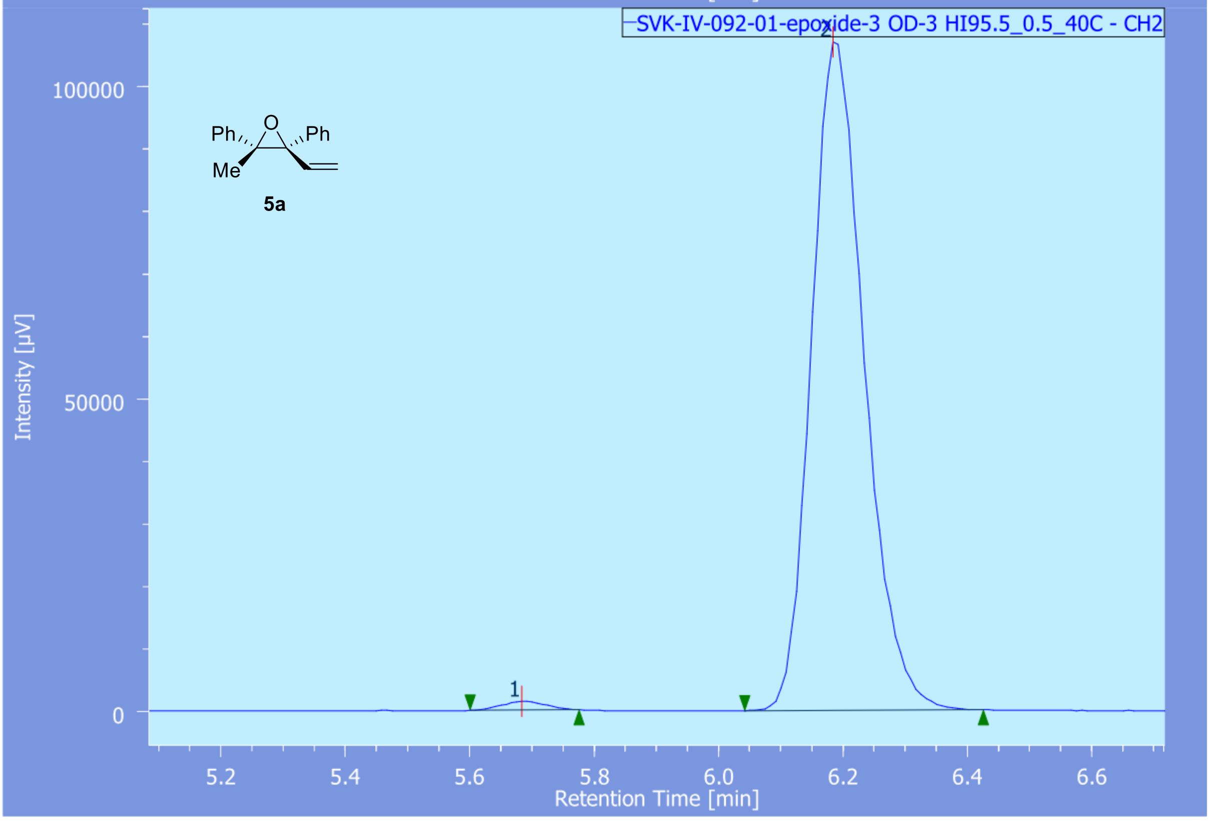
^{1}H NMR (600 MHz, $CDCl_3$) and ^{13}C NMR (151 MHz, $CDCl_3$) spectra of **6e**



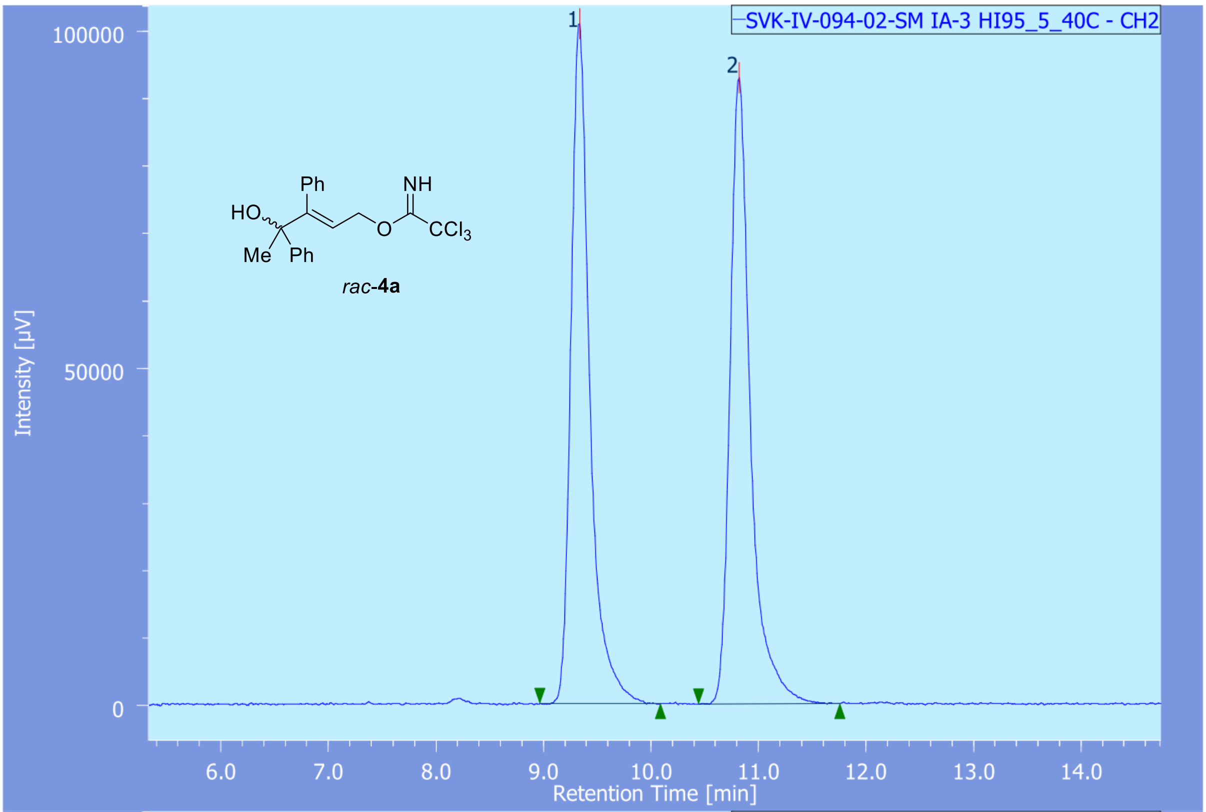


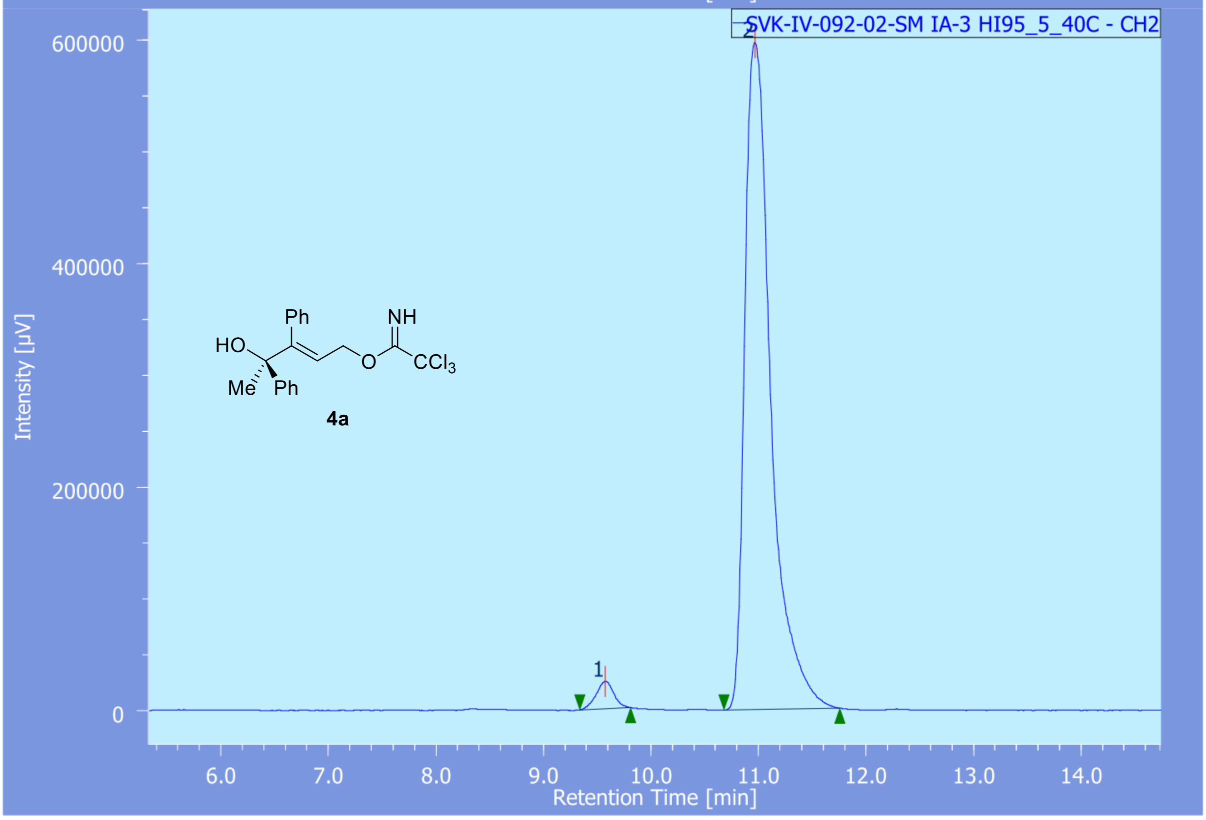
12. HPLC Charts



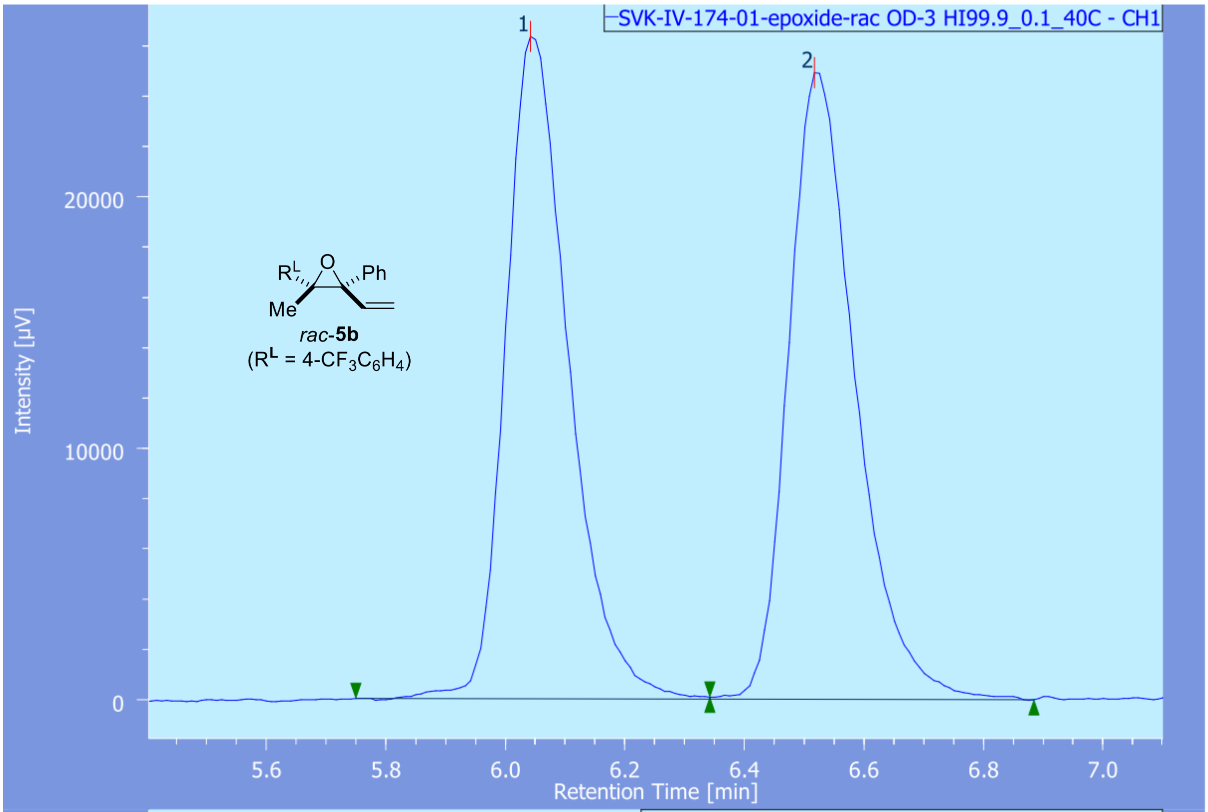


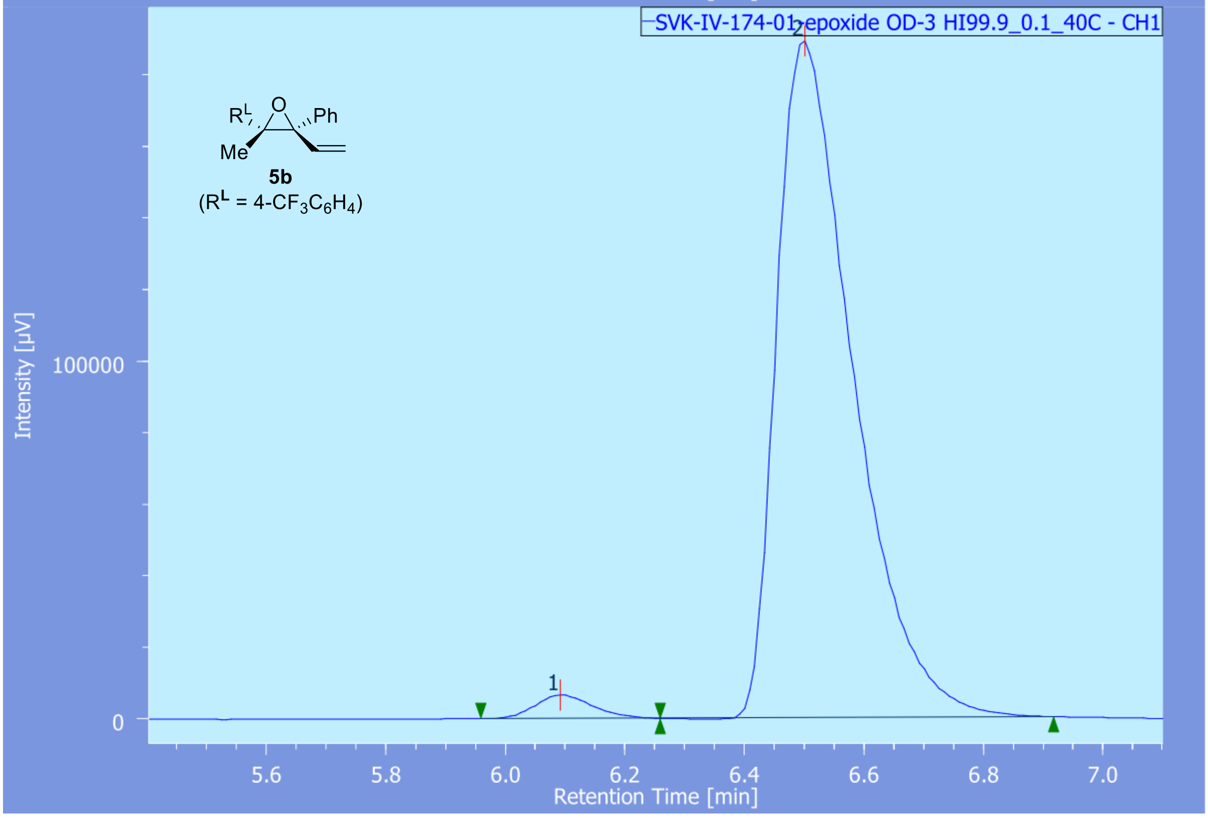
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5a**	5.6	6.2	50.1	49.9
(2*S*,3*R*)-**5a**	5.7	6.2	1.0	99.0



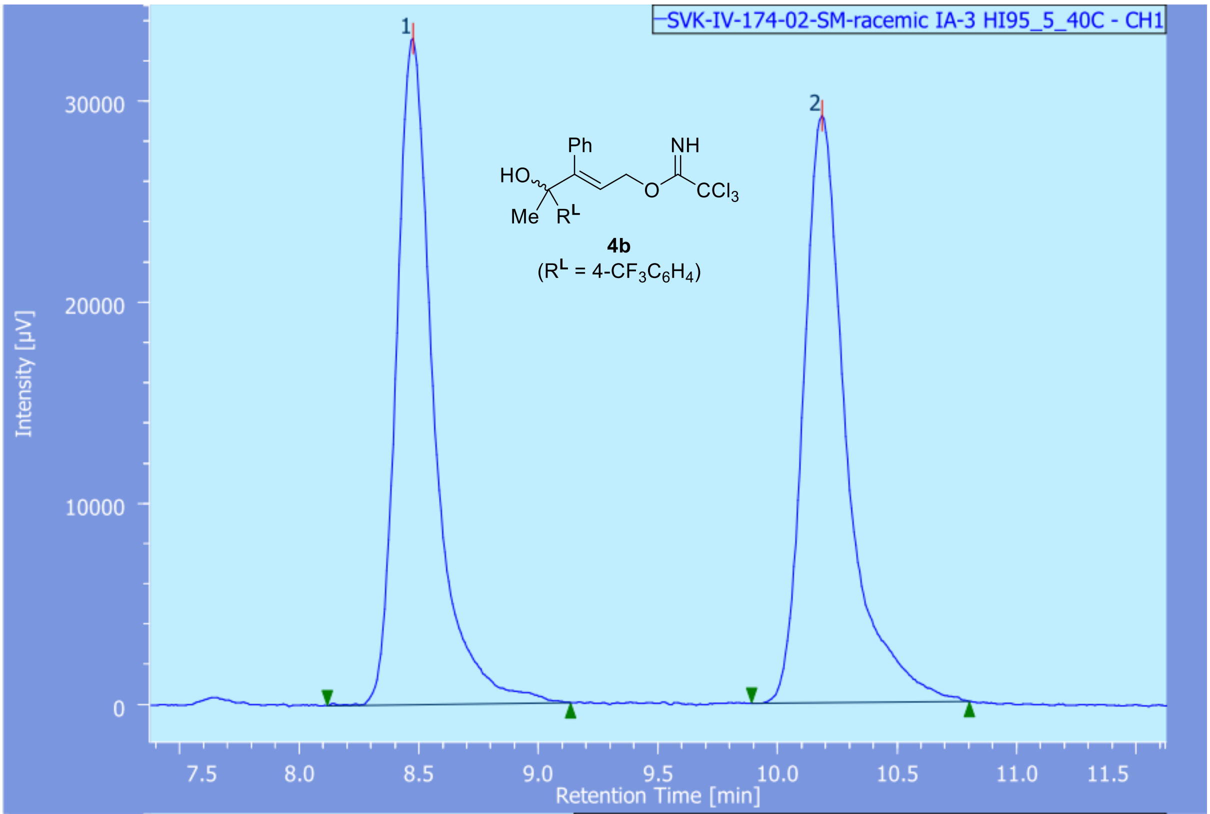


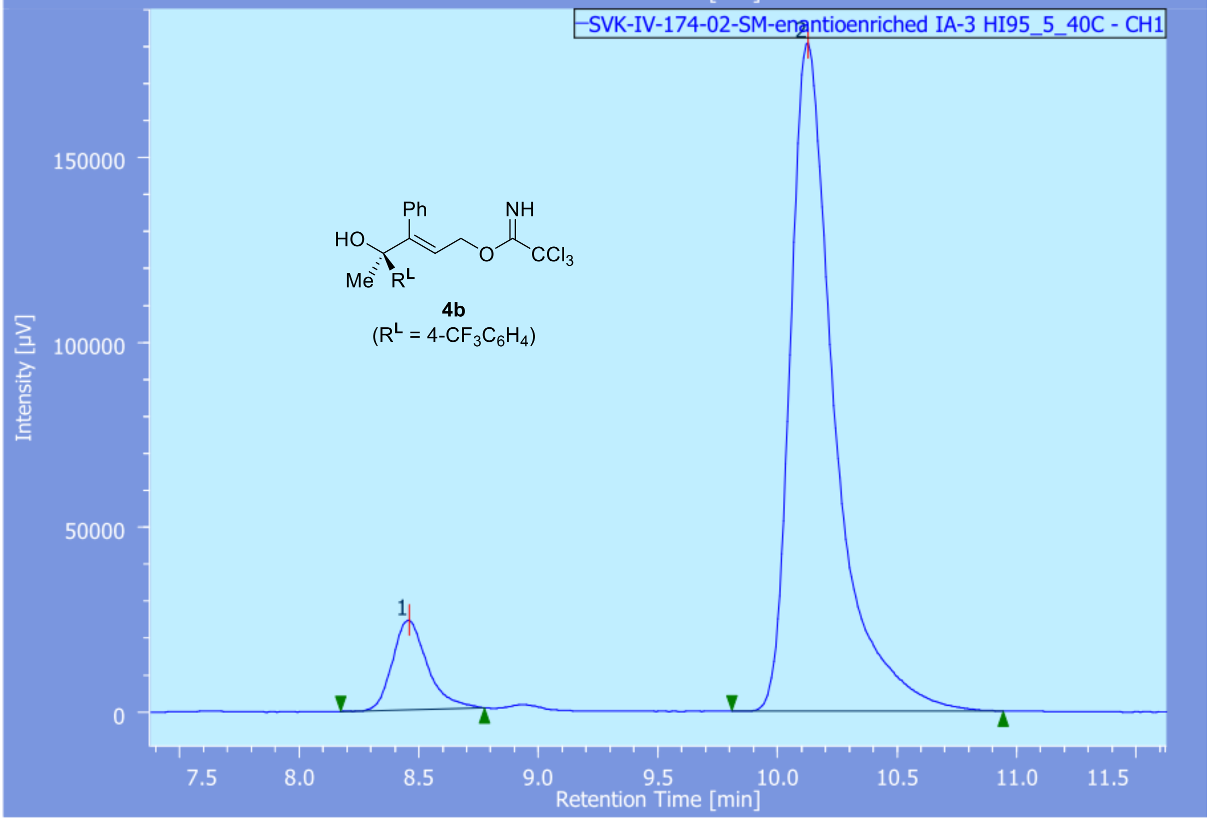
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4a**	9.3	10.8	50.1	49.9
(*R*,*E*)-**4a**	9.6	11.0	2.7	97.3



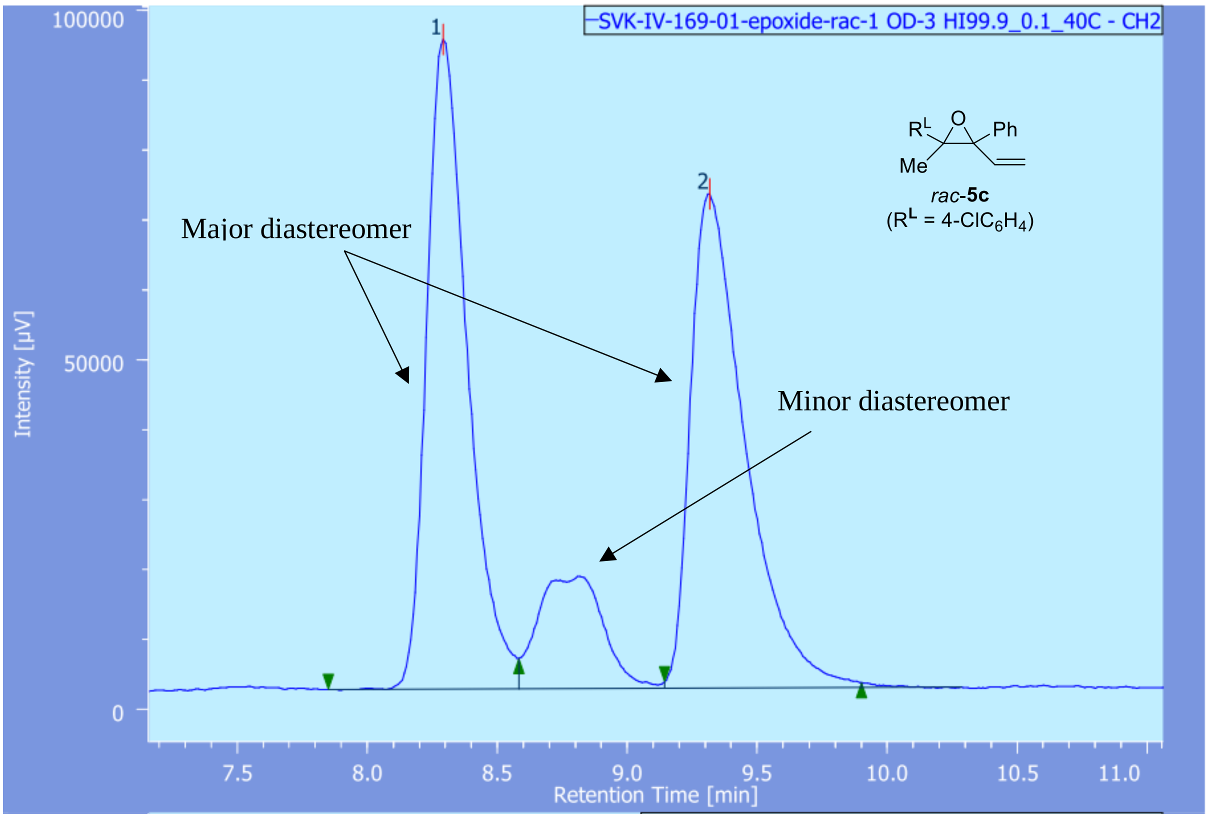


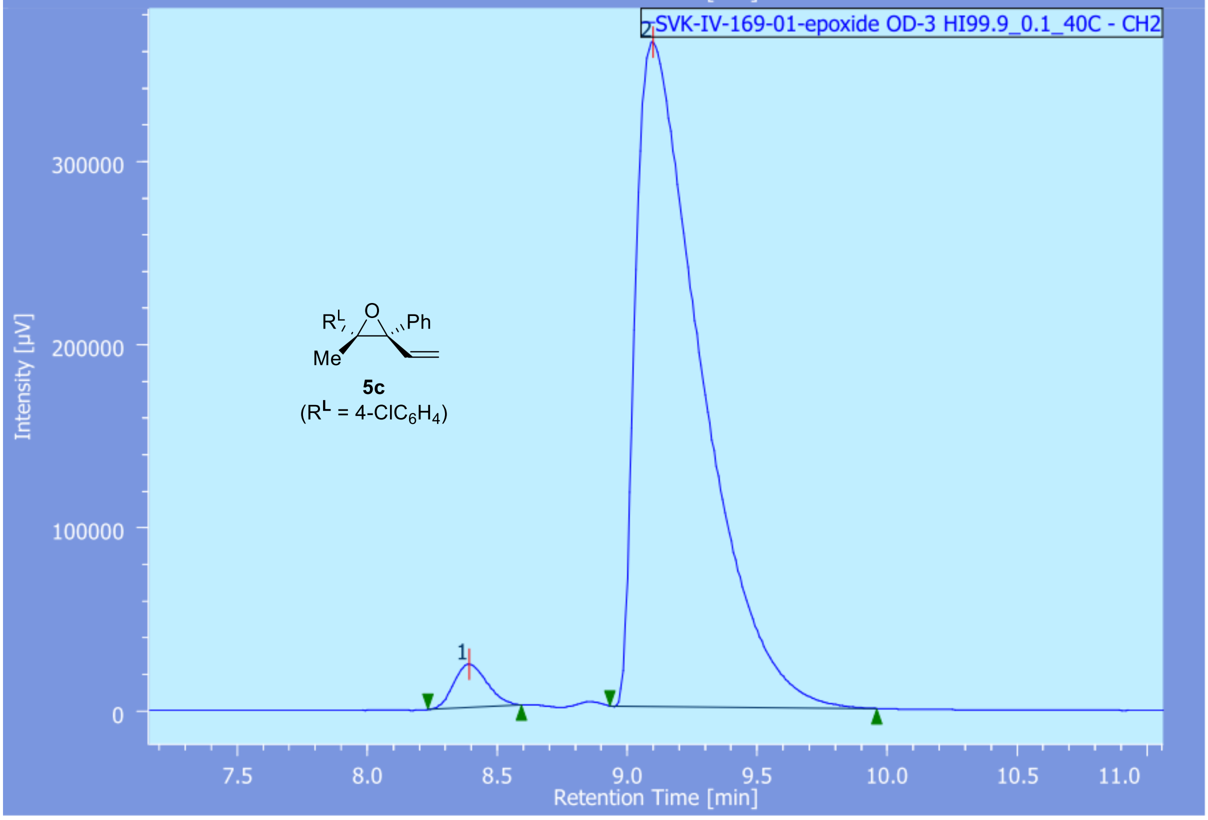
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5b**	6.0	6.5	50.0	50.0
(2*S*,3*R*)-**5b**	6.1	6.5	2.8	97.2



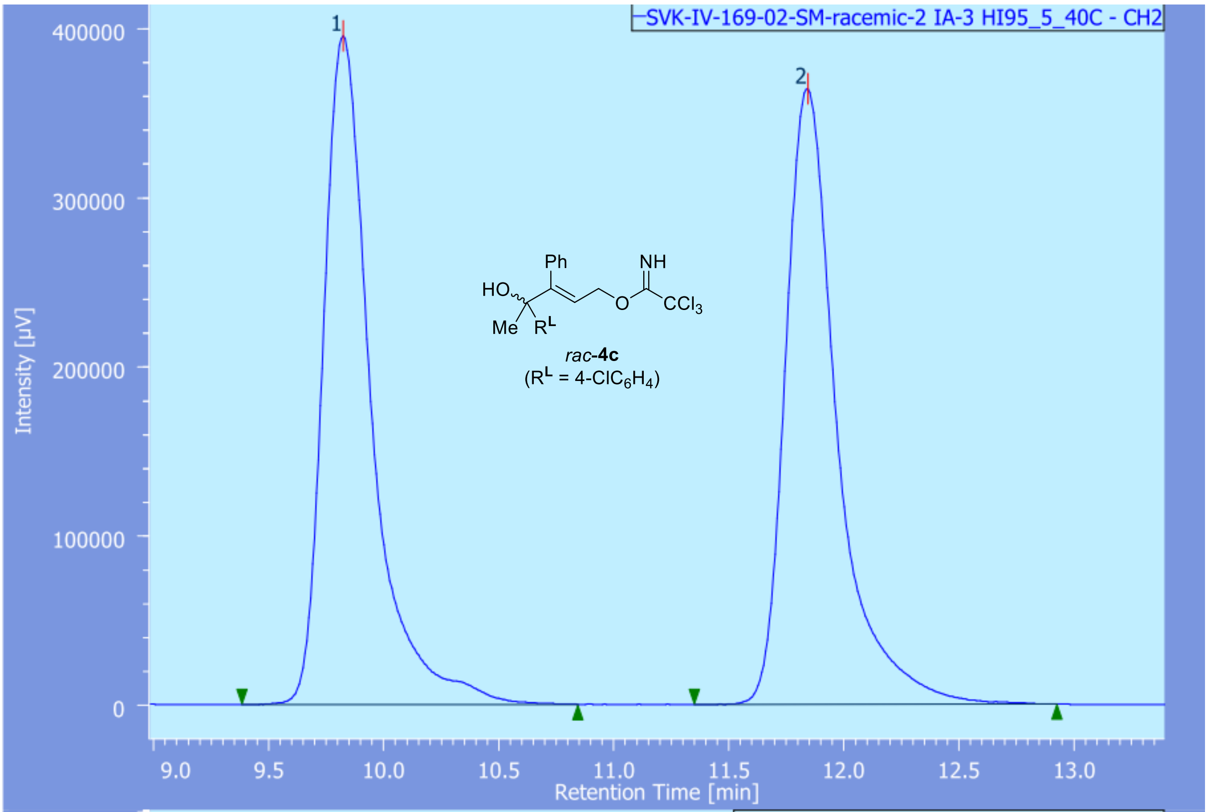


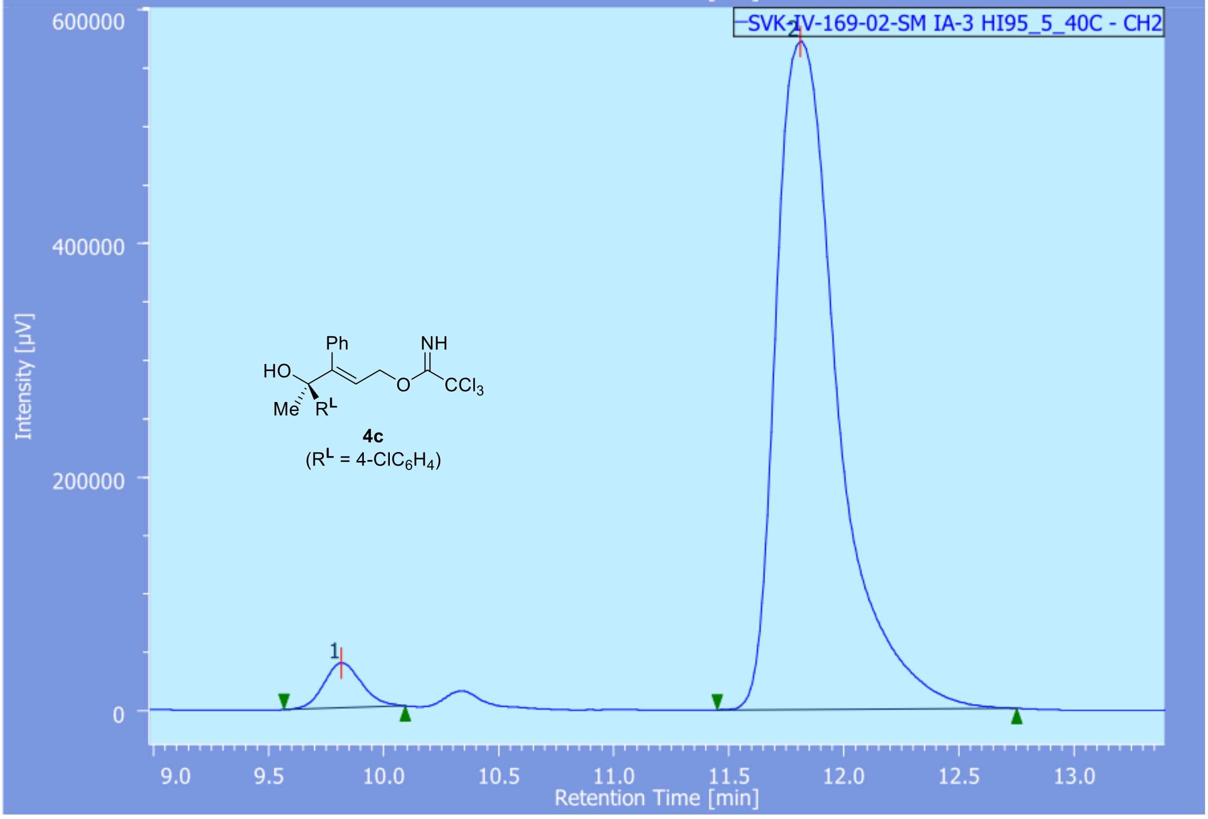
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4b**	8.5	10.2	49.6	50.4
(*R*,*E*)-**4b**	8.5	10.1	9.5	90.5



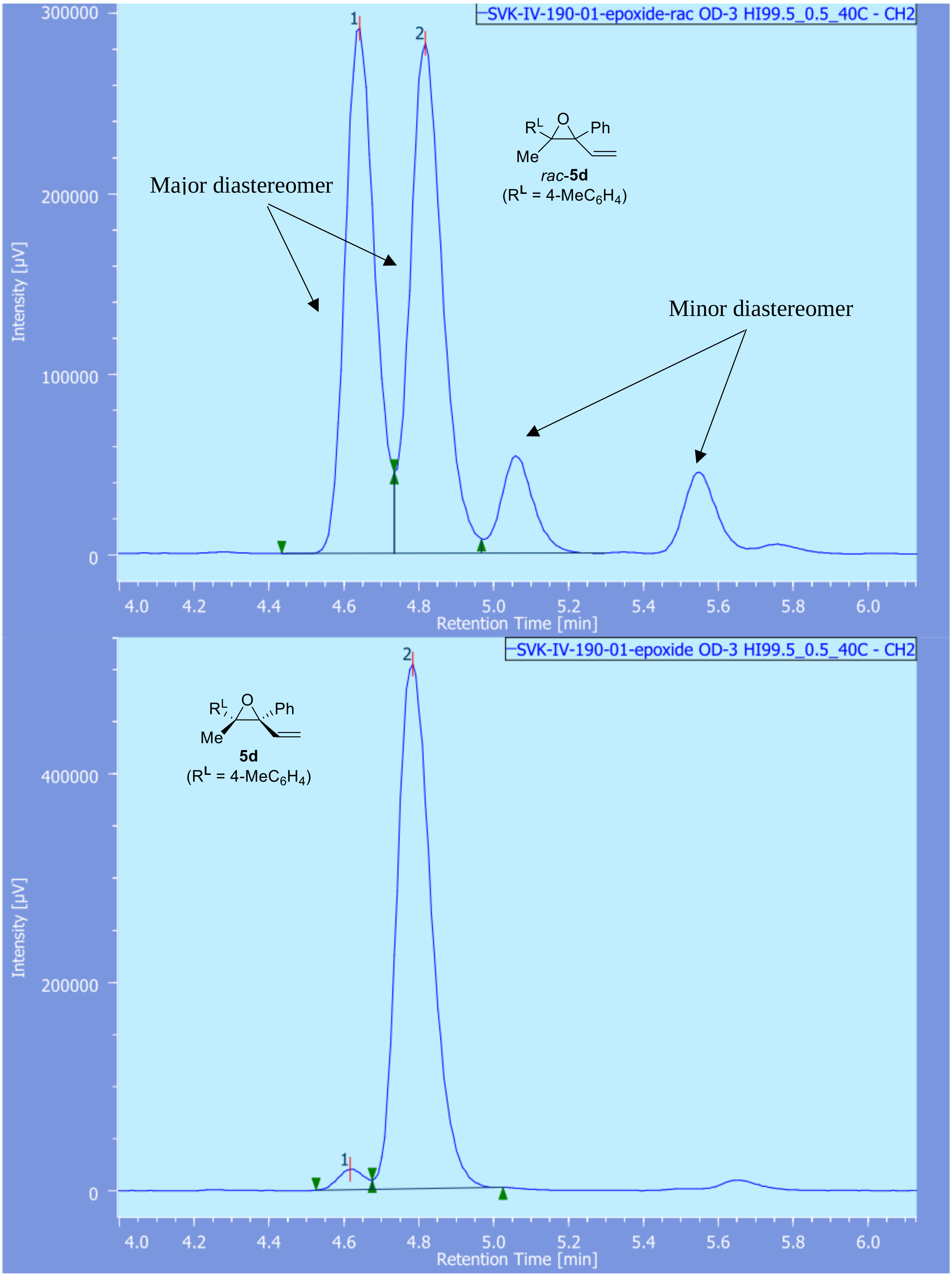


	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5c**	8.3	9.3	49.6	50.4
(2*S*,3*R*)-**5c**	8.4	9.1	3.2	96.8

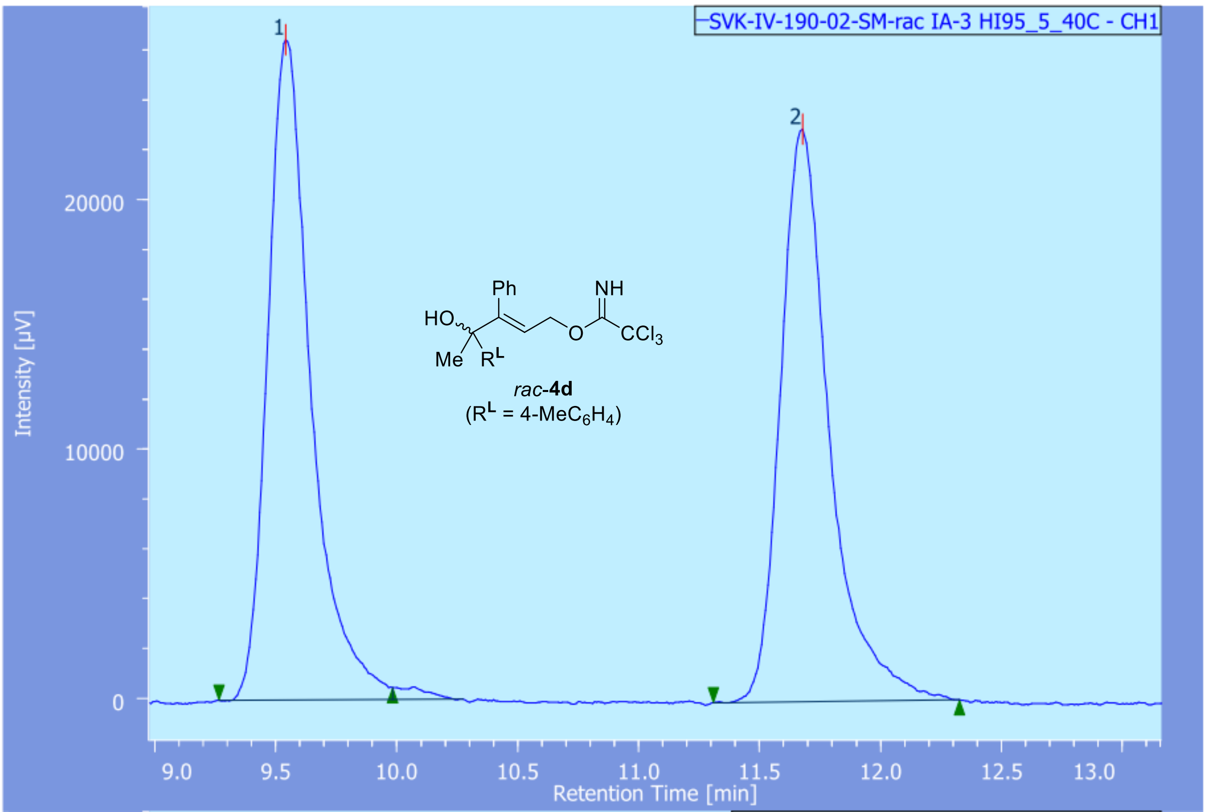


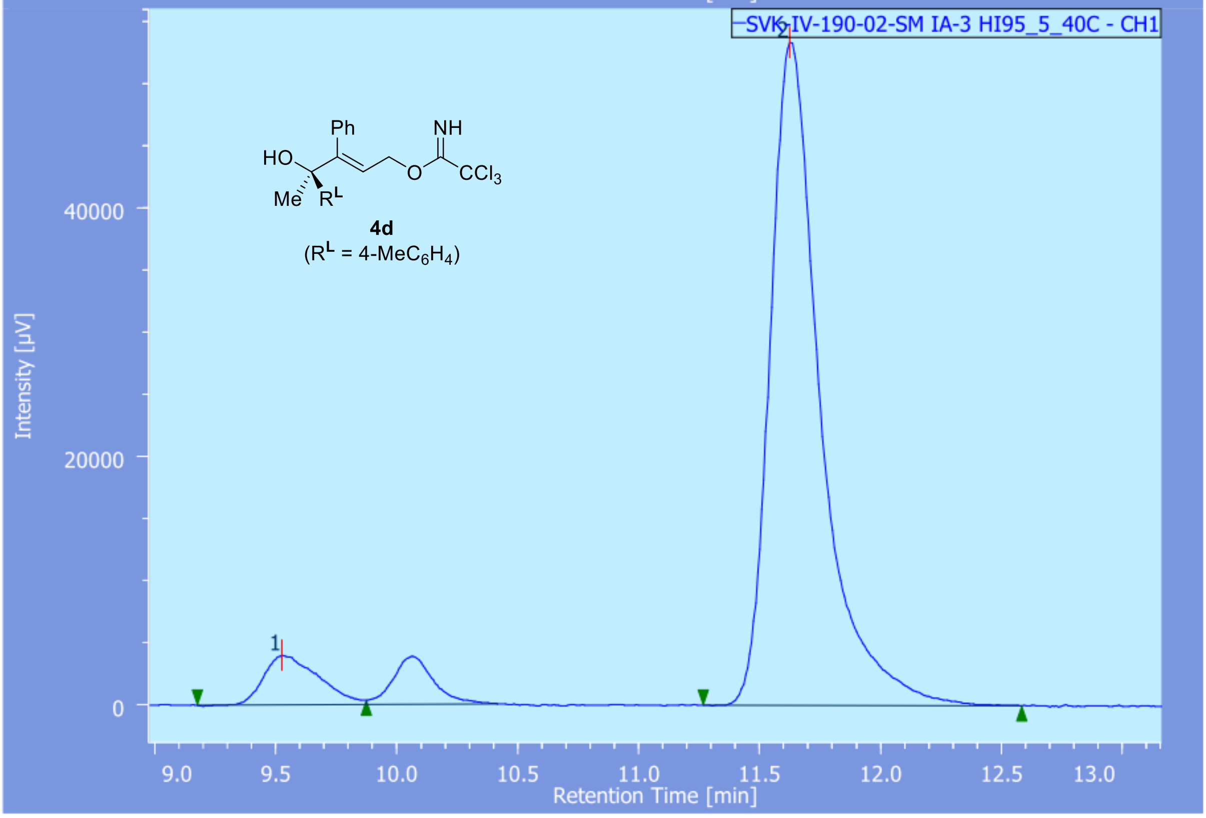


	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4c**	9.8	11.8	50.0	50.0
(*R*,*E*)-**4c**	9.8	11.8	3.9	96.1

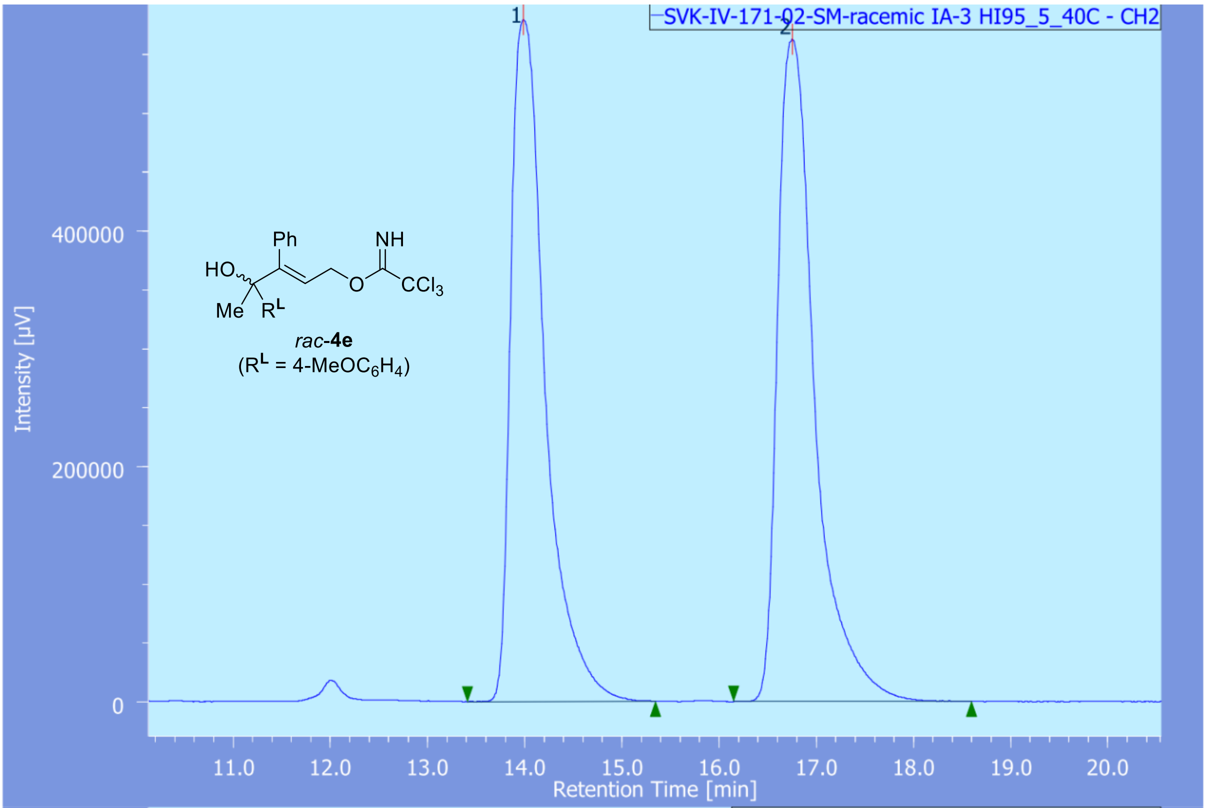


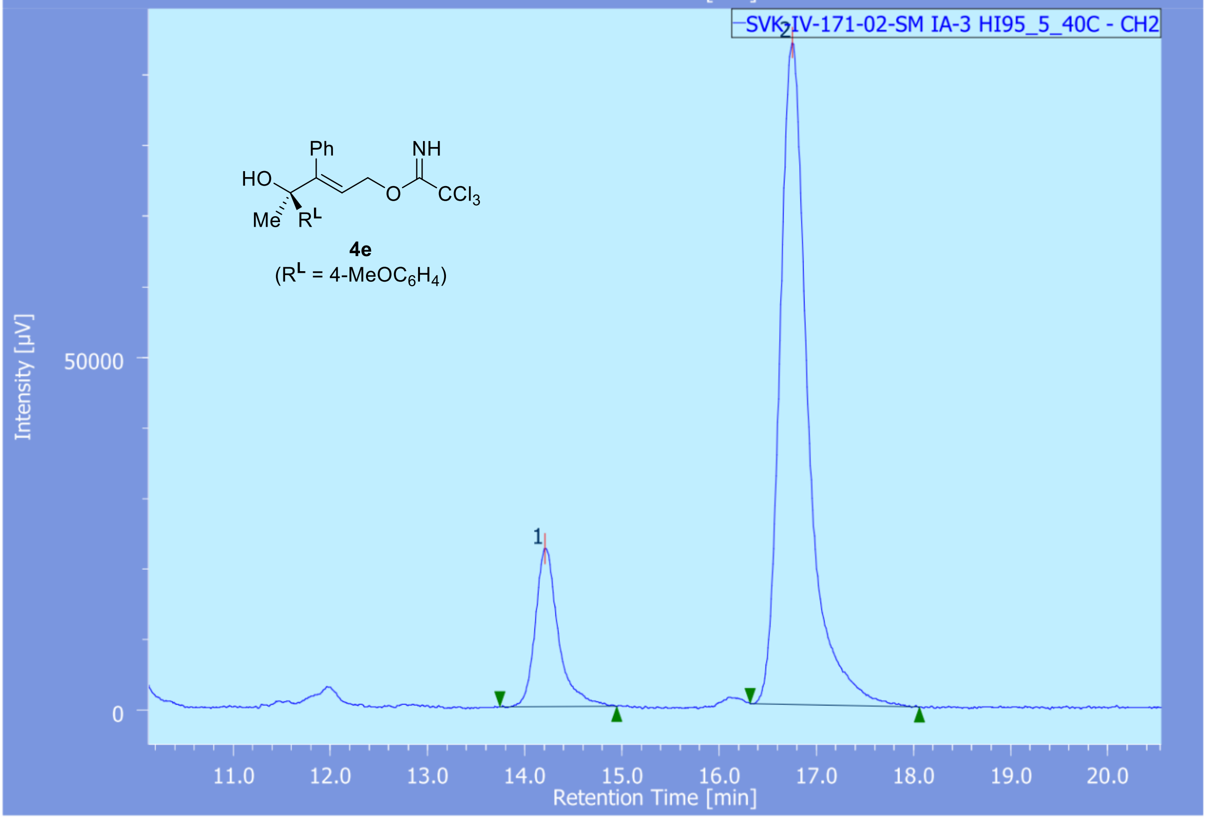
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5d**	4.6	4.8	49.2	50.8
(2*S*,3*R*)-**5d**	4.6	4.8	2.9	97.1



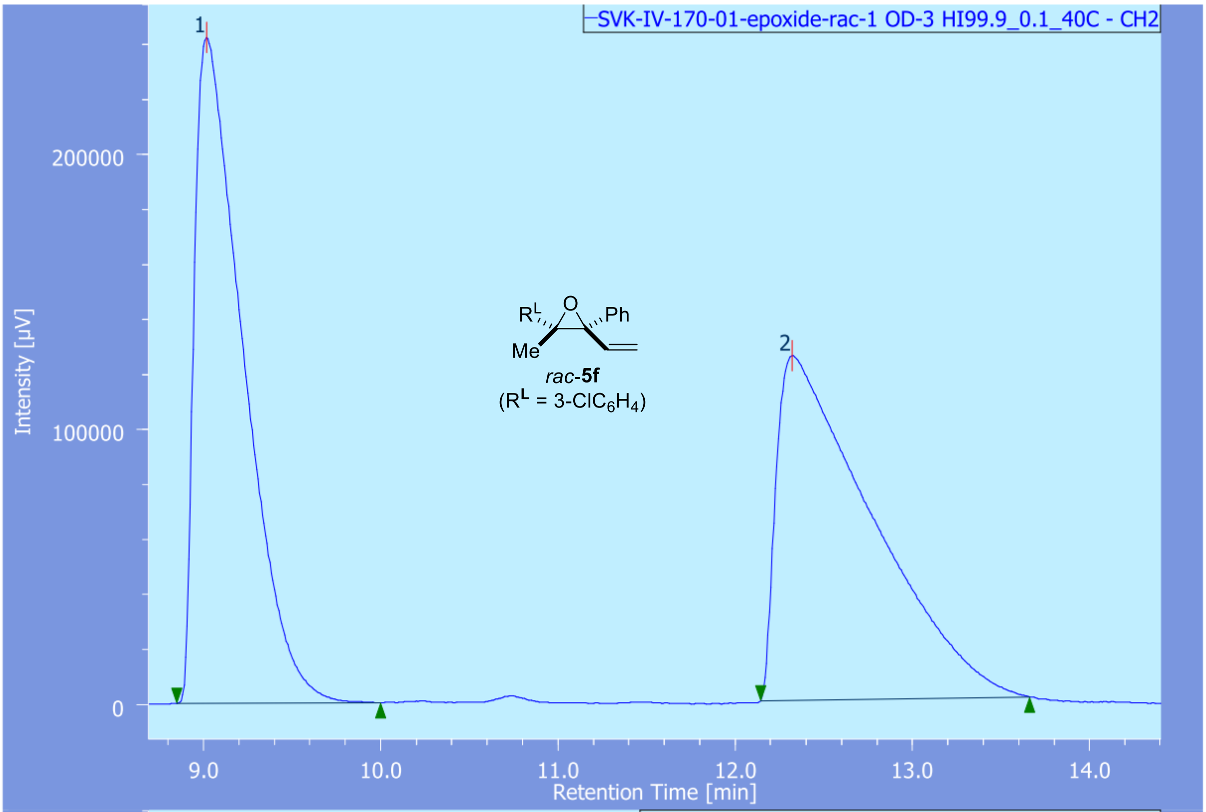


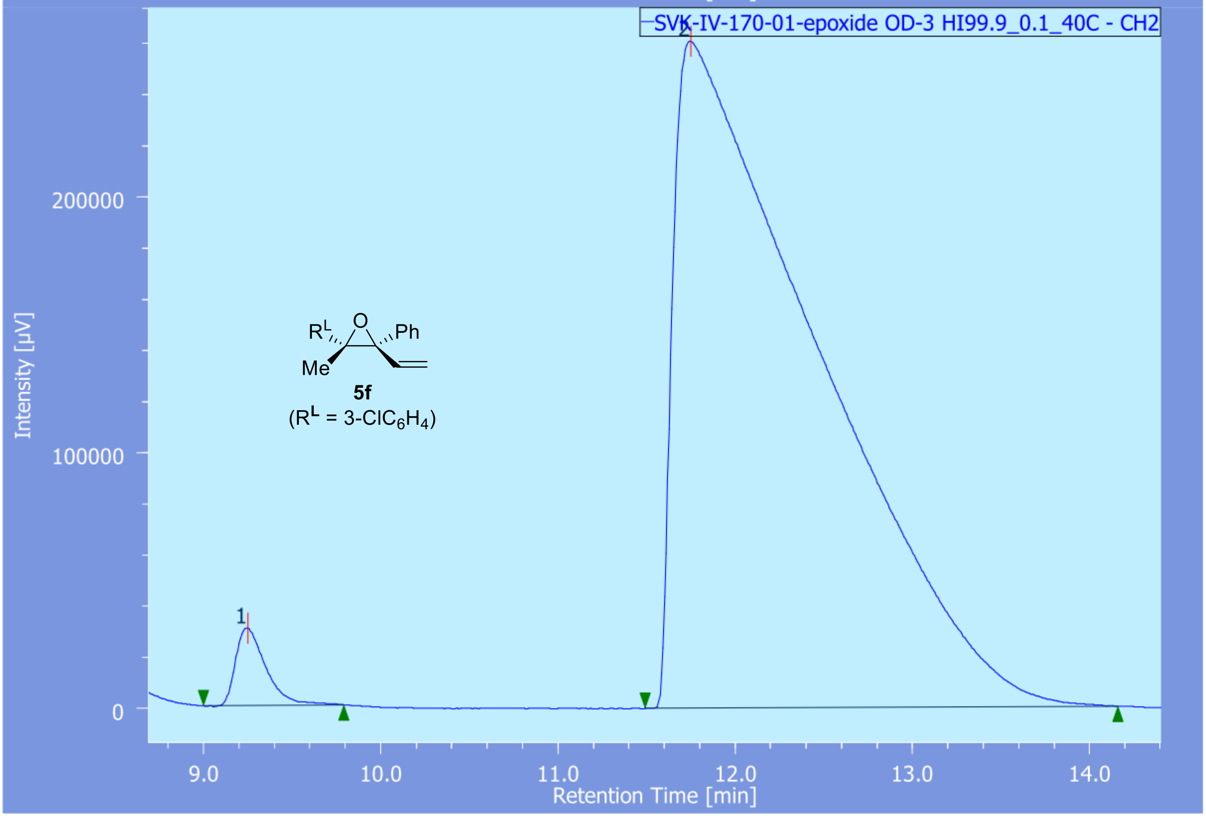
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4d**	9.5	11.7	50.3	49.7
(*R*,*E*)-**4d**	9.5	11.6	7.5	92.5



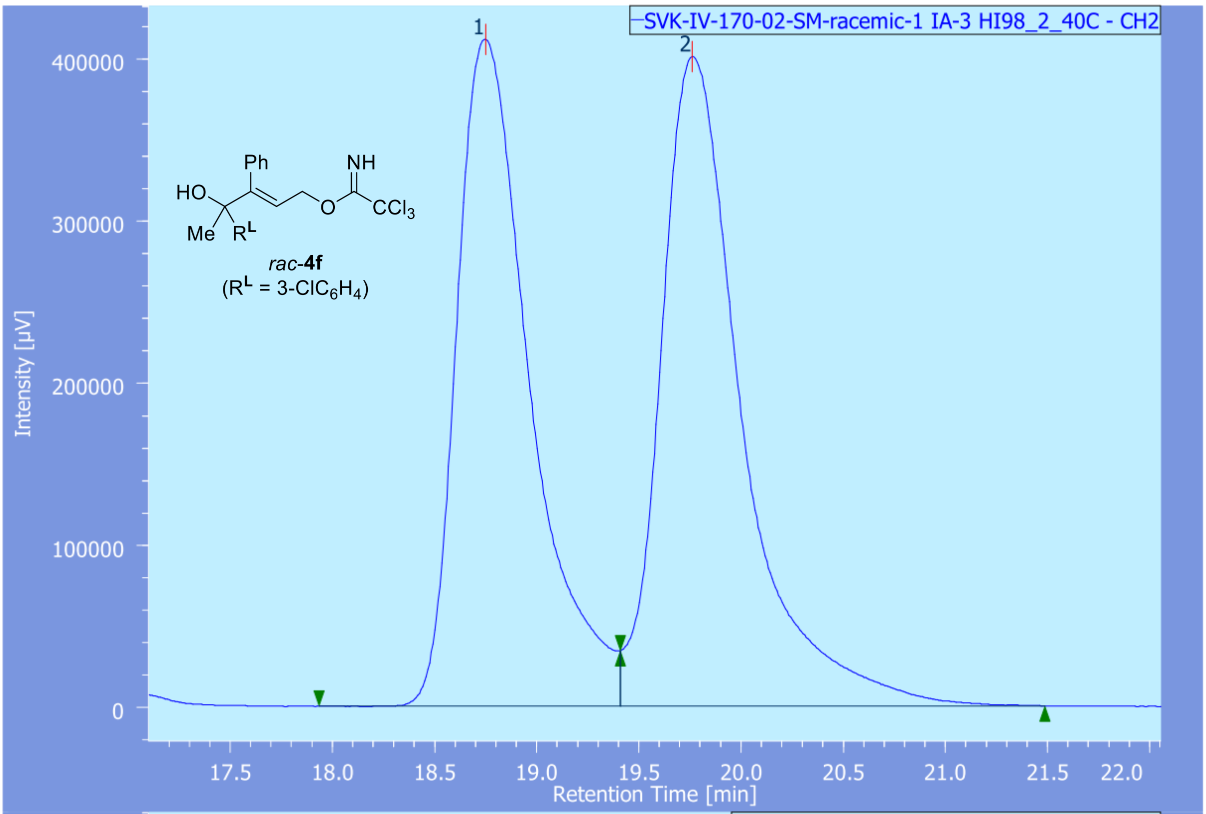


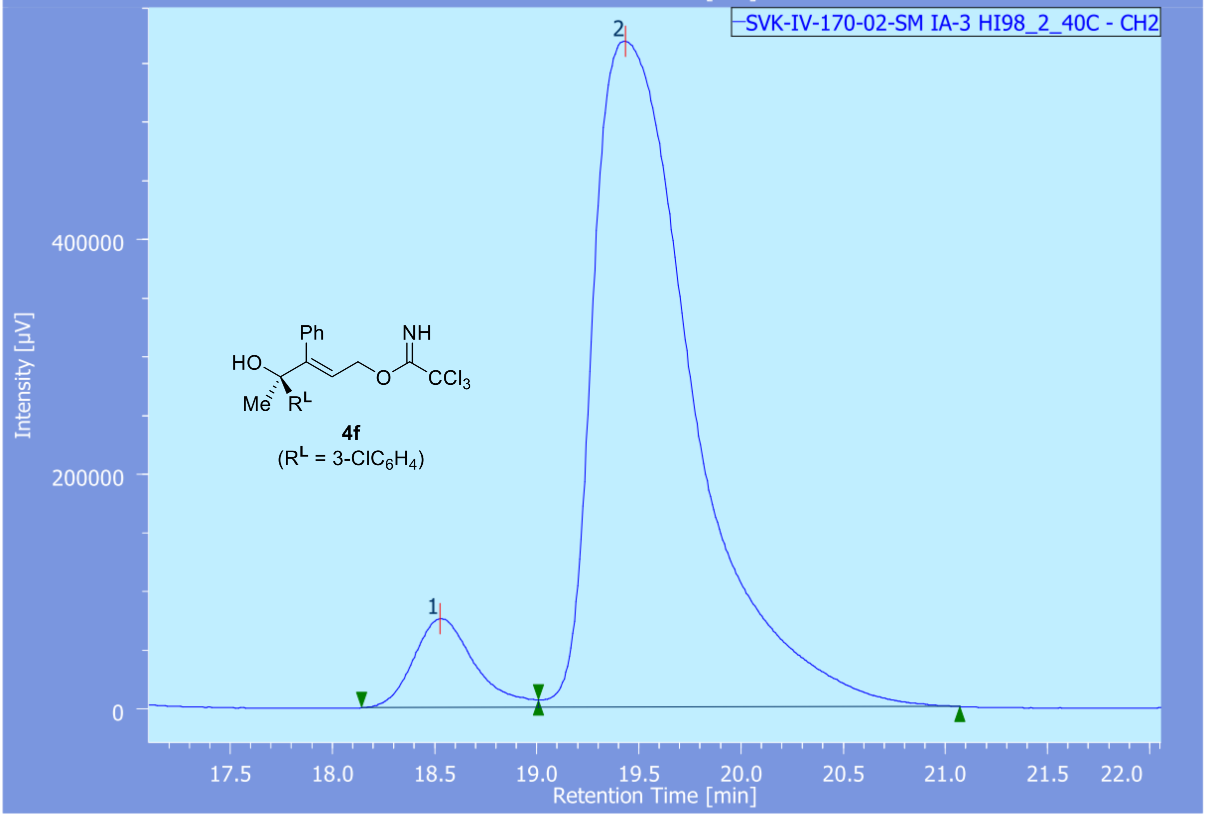
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4e**	14.0	16.8	49.6	50.4
(*R*,*E*)-**4e**	14.2	16.8	16.5	83.5



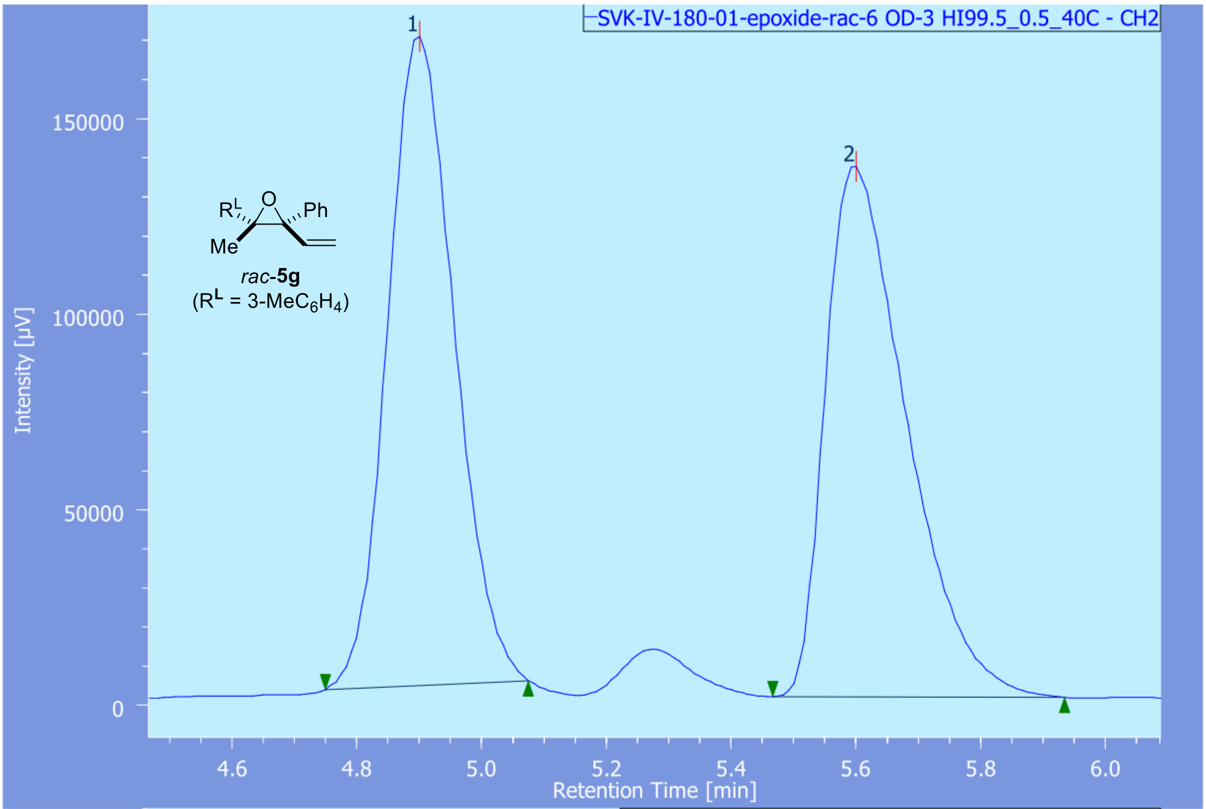


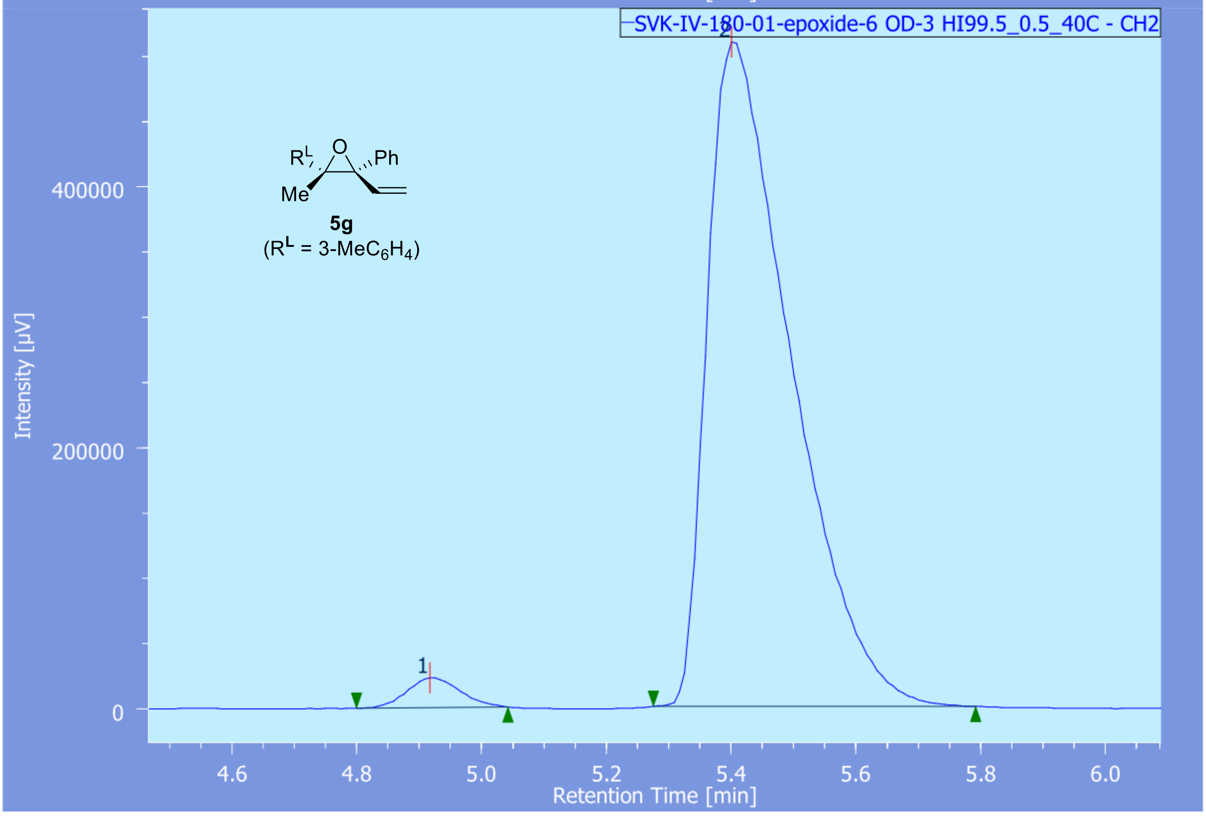
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5f**	9.0	12.3	49.6	50.4
(2*S*,3*R*)-**5f**	9.3	11.8	2.4	97.6



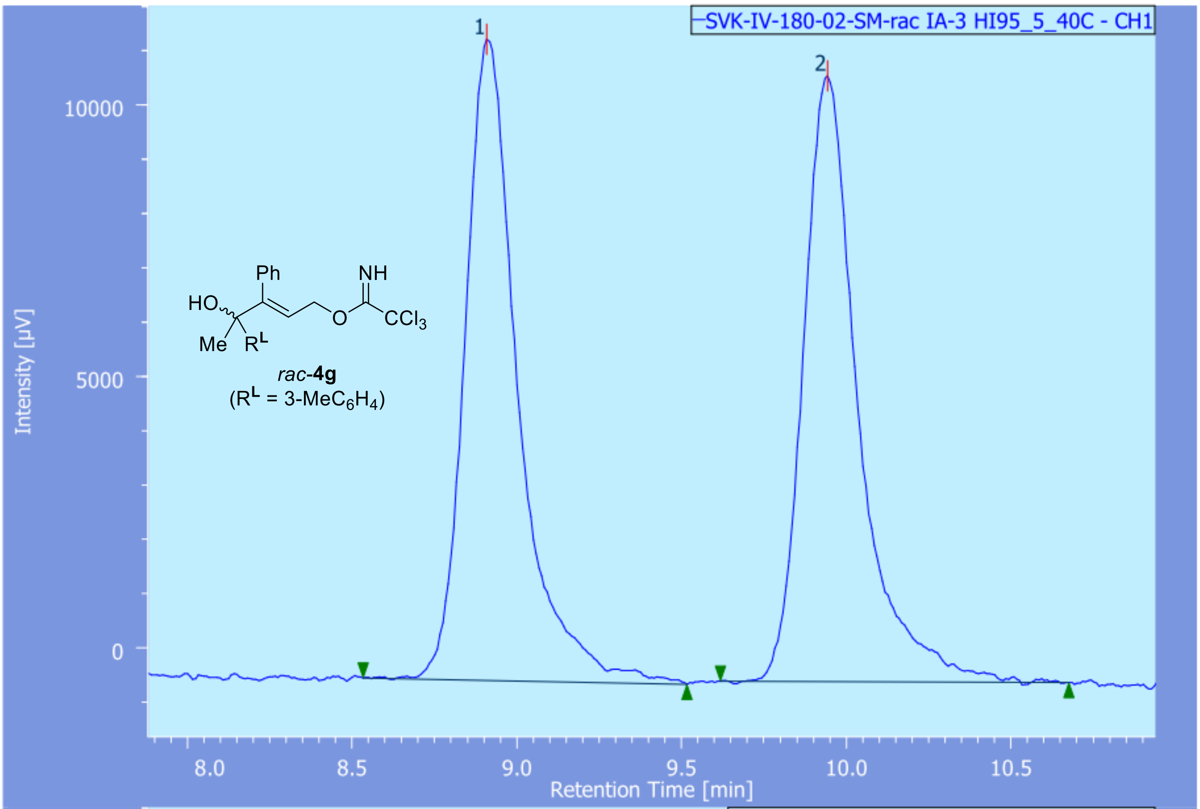


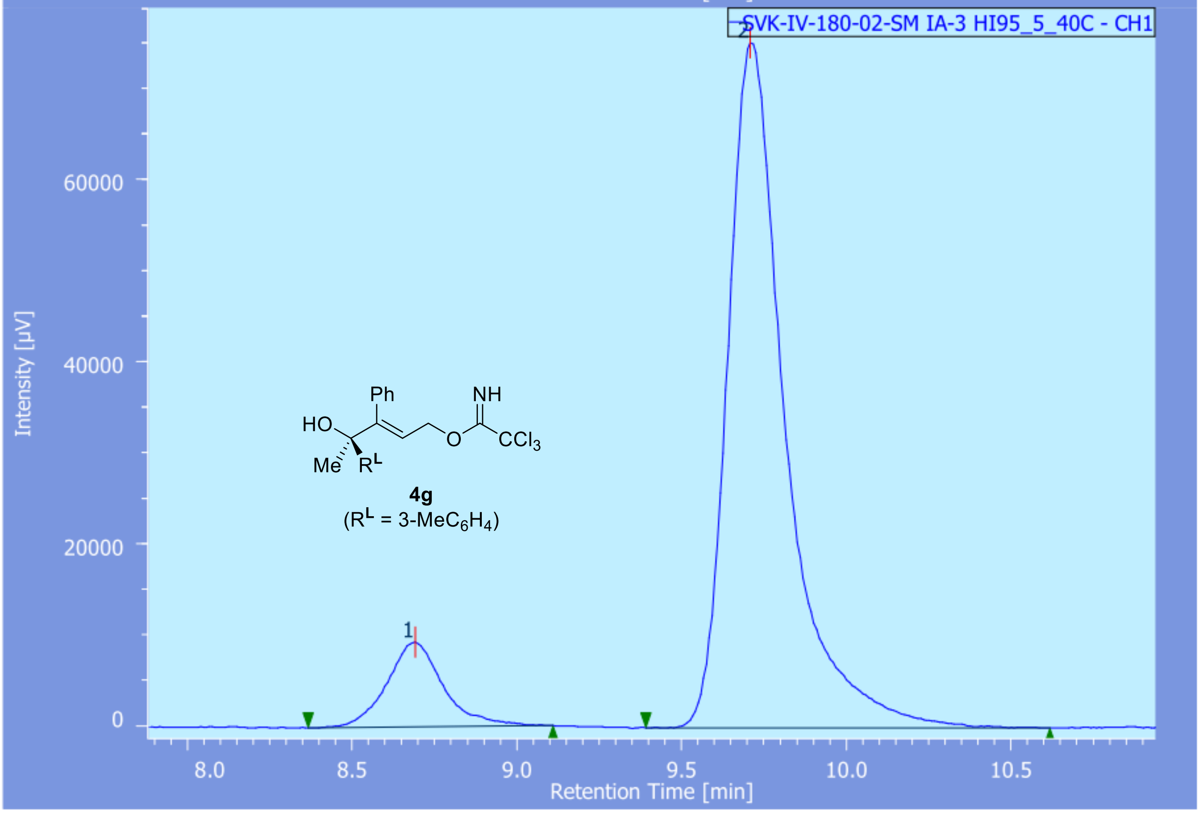
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4f**	18.8	19.8	49.2	50.8
(*R*,*E*)-**4f**	18.5	19.4	7.5	92.5



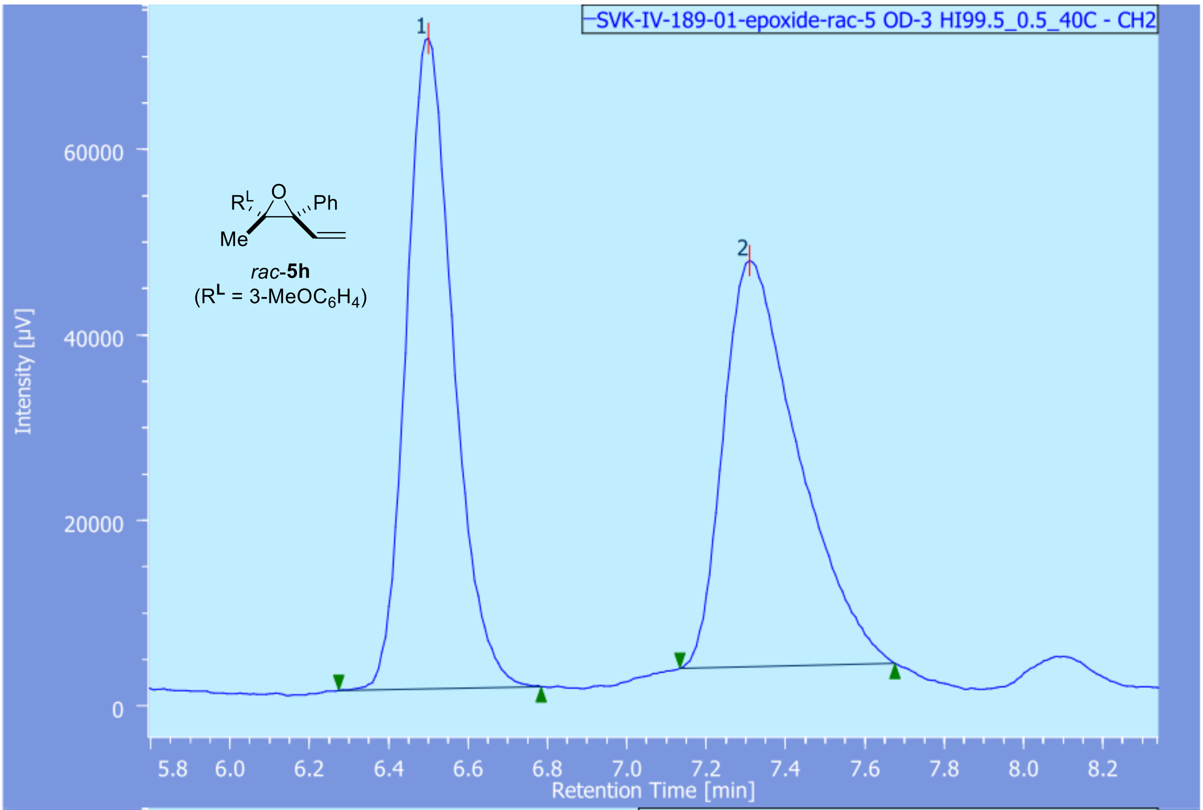


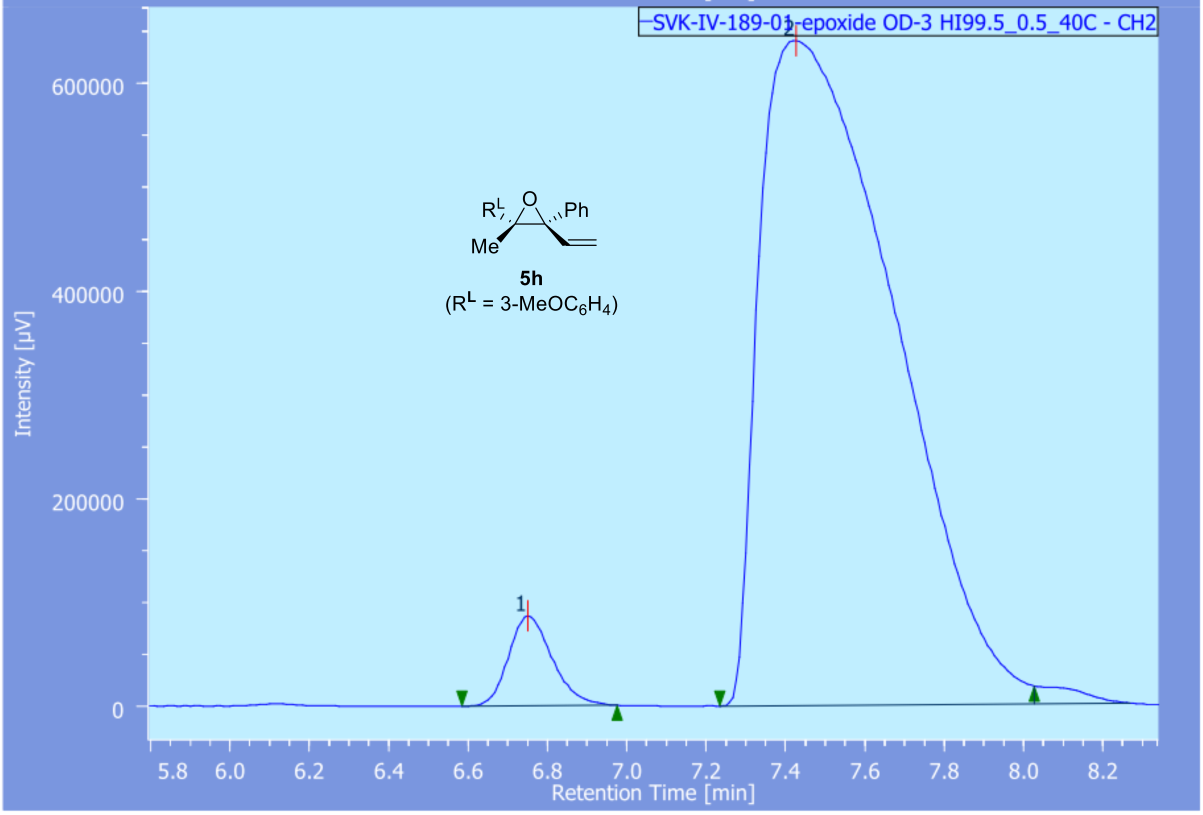
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5g**	4.9	5.6	50.1	49.9
(2*S*,3*R*)-**5g**	4.9	5.4	2.8	97.2



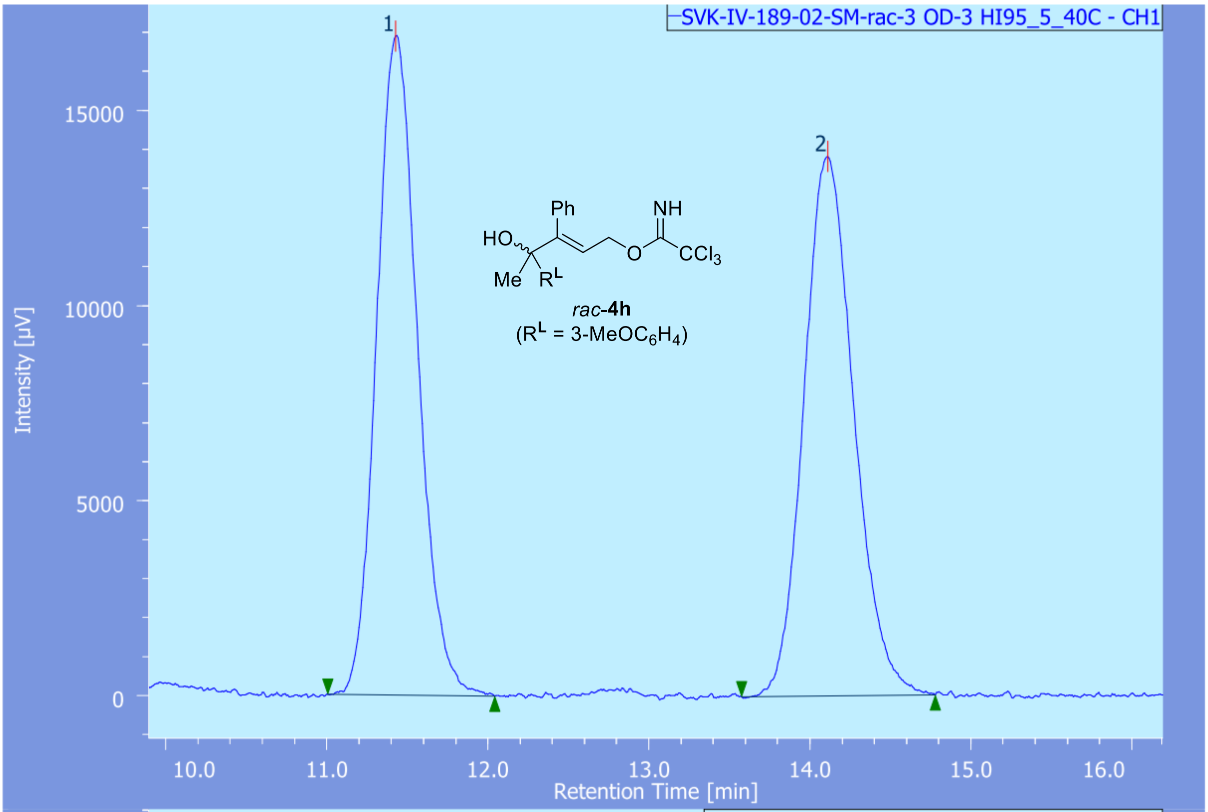


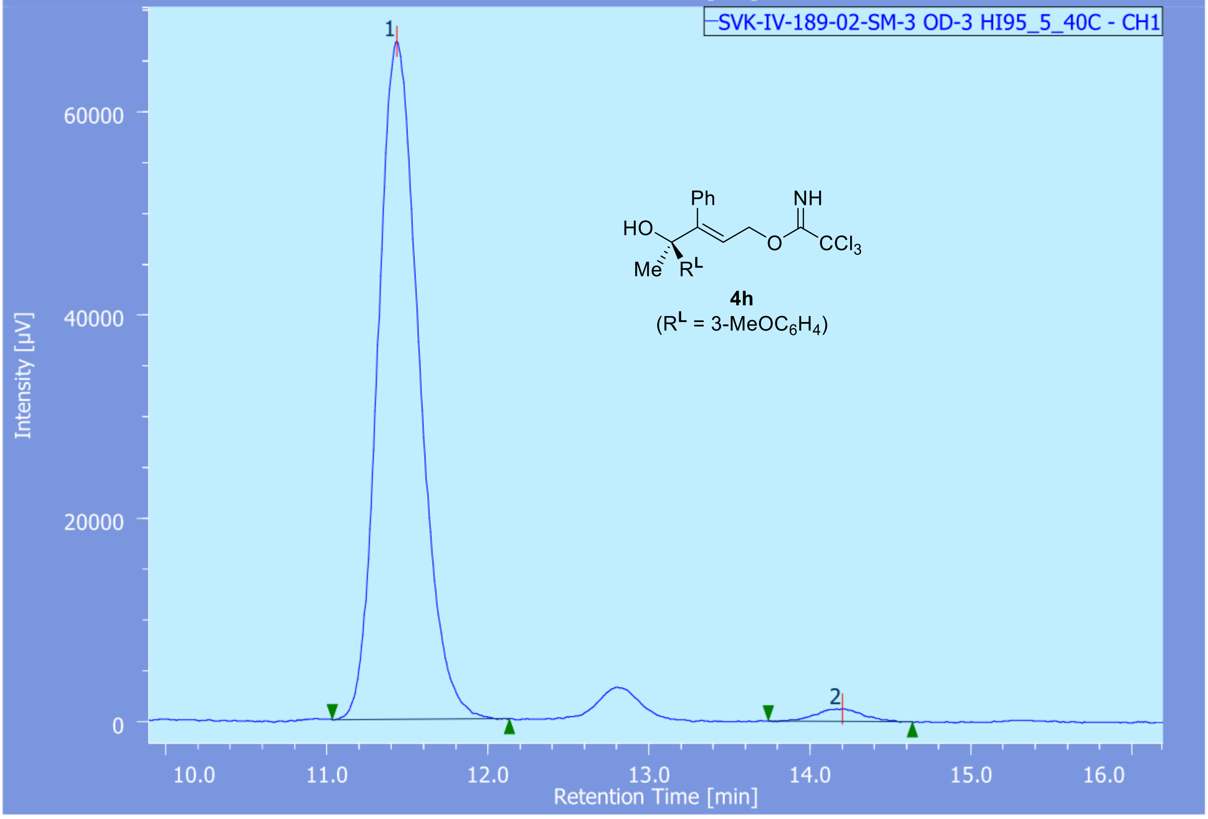
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4g**	8.9	9.9	50.4	49.6
(*R*,*E*)-**4g**	8.7	9.7	10.8	89.2



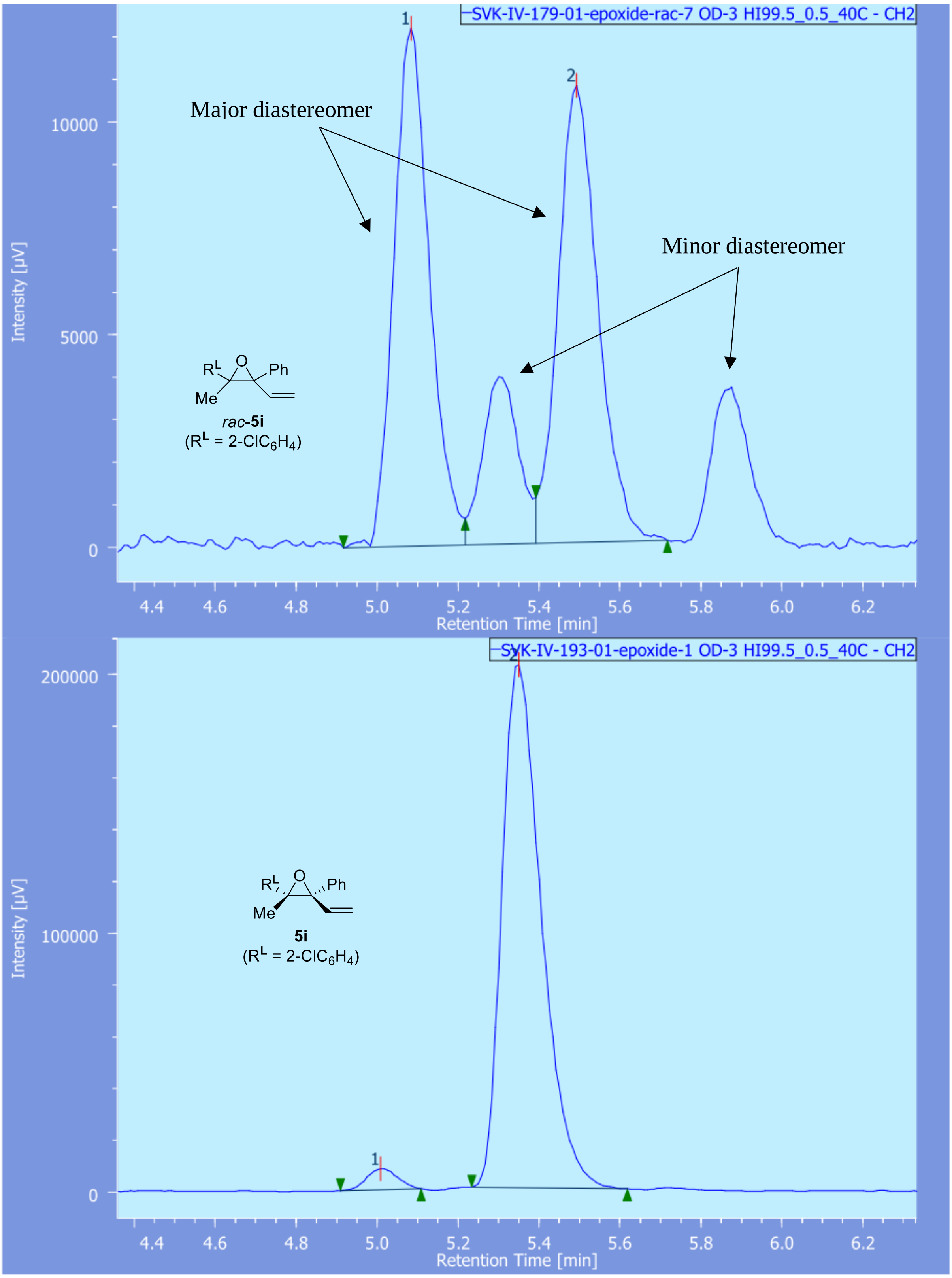


	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5h**	6.5	7.3	50.2	49.8
(2*S*,3*R*)-**5h**	6.8	7.4	4.2	95.8

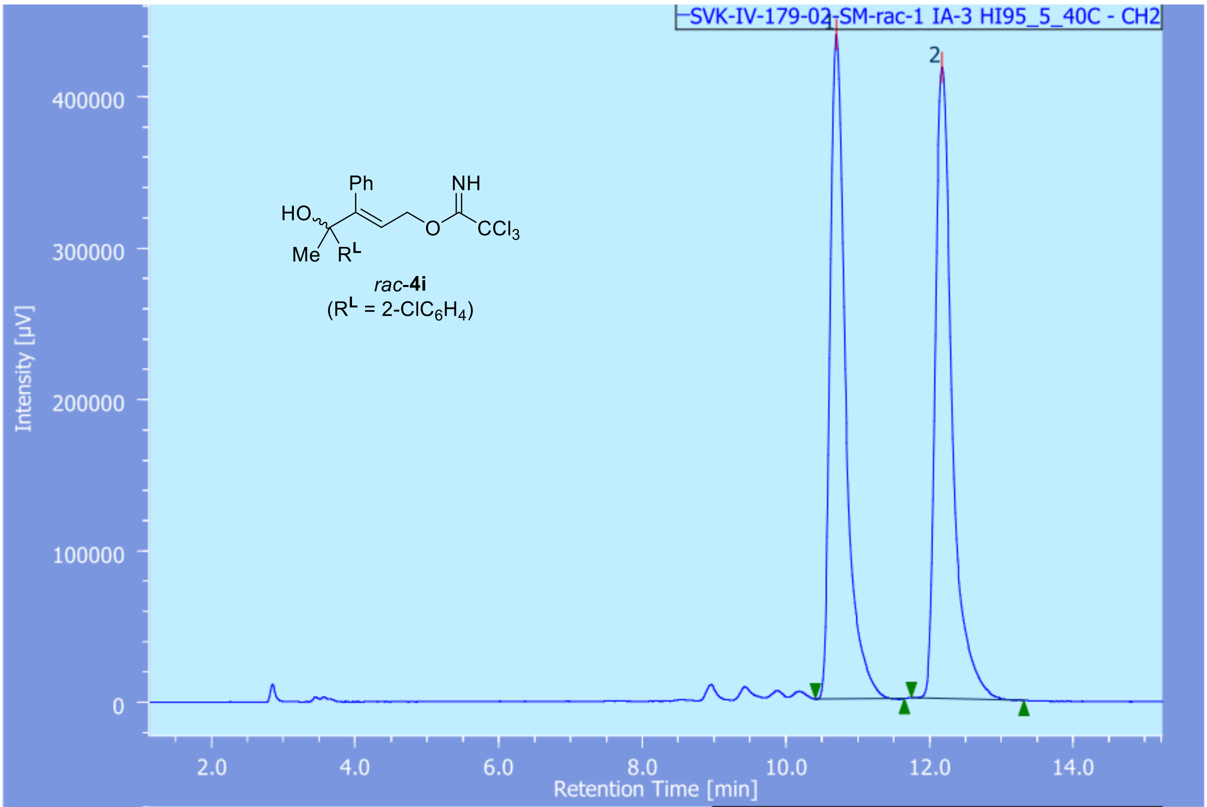


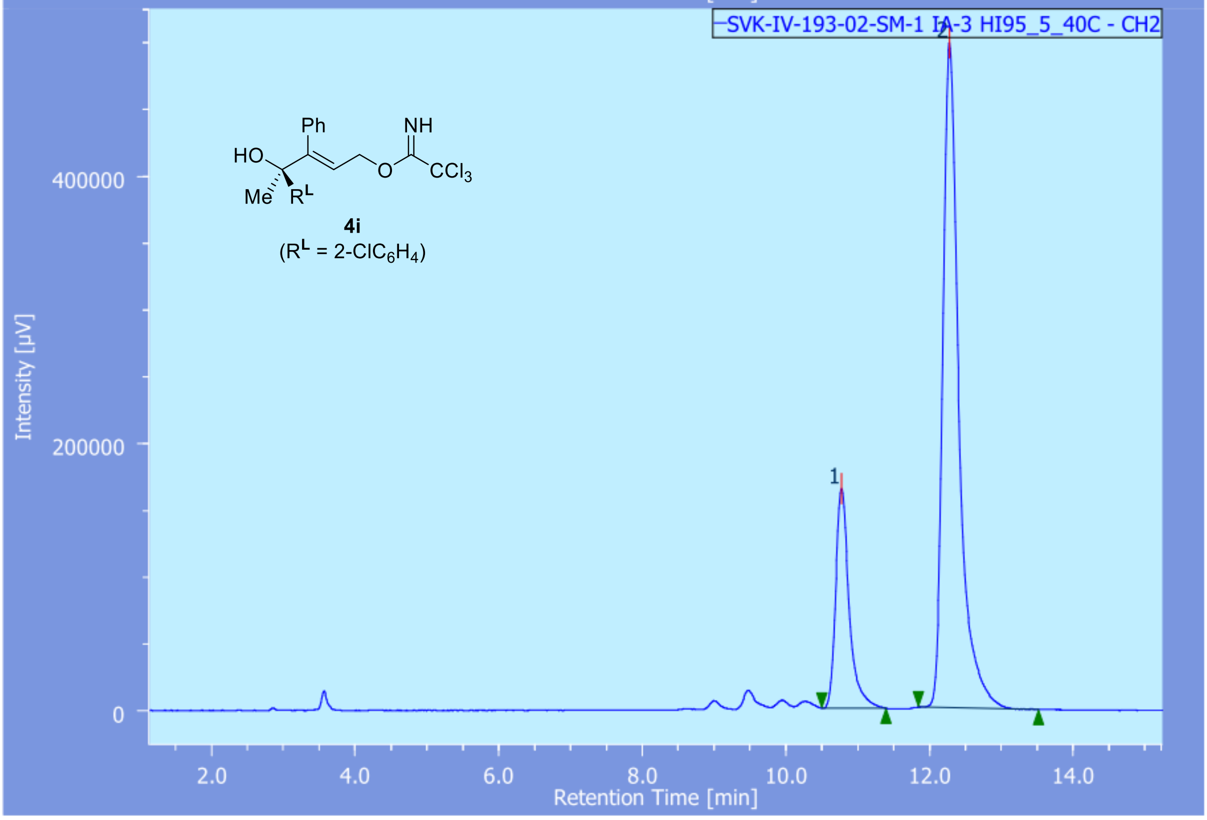


	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4h**	11.4	14.1	49.9	50.1
(*R*,*E*)-**4h**	11.4	14.2	97.9	2.1

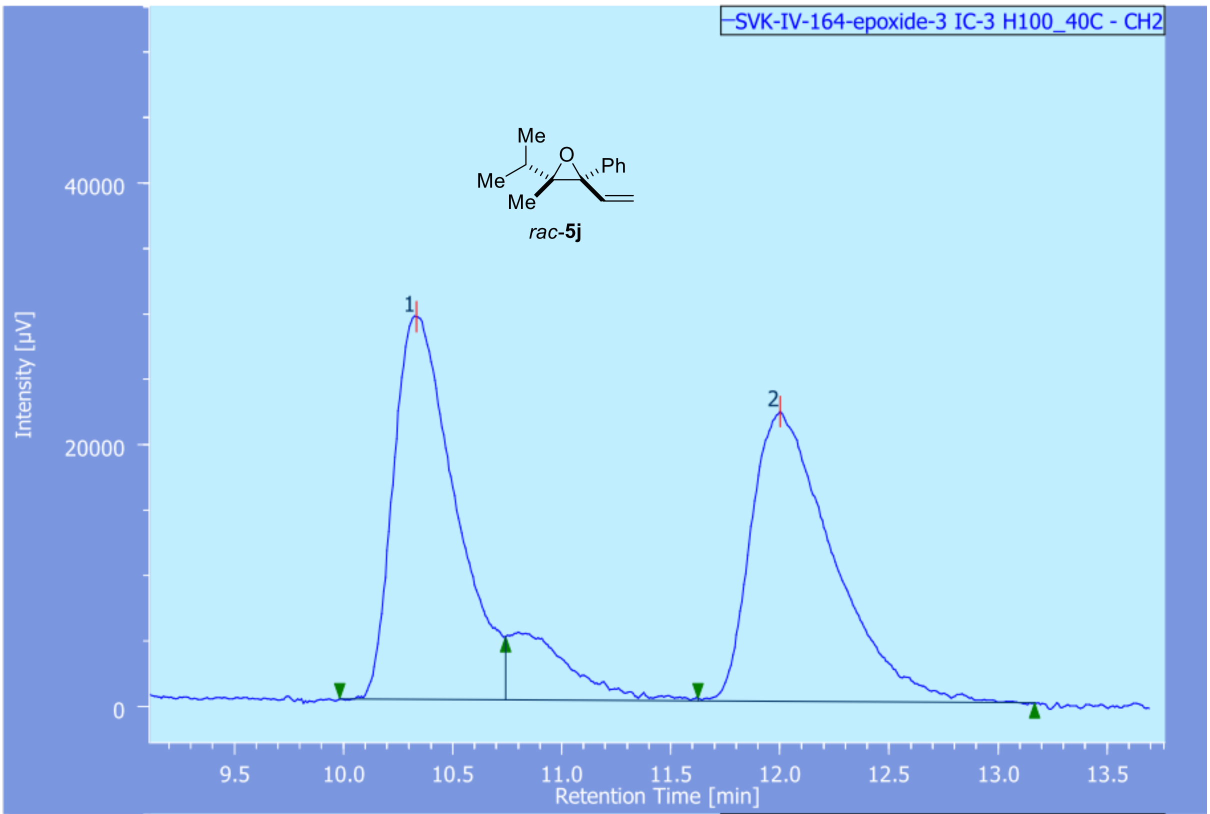


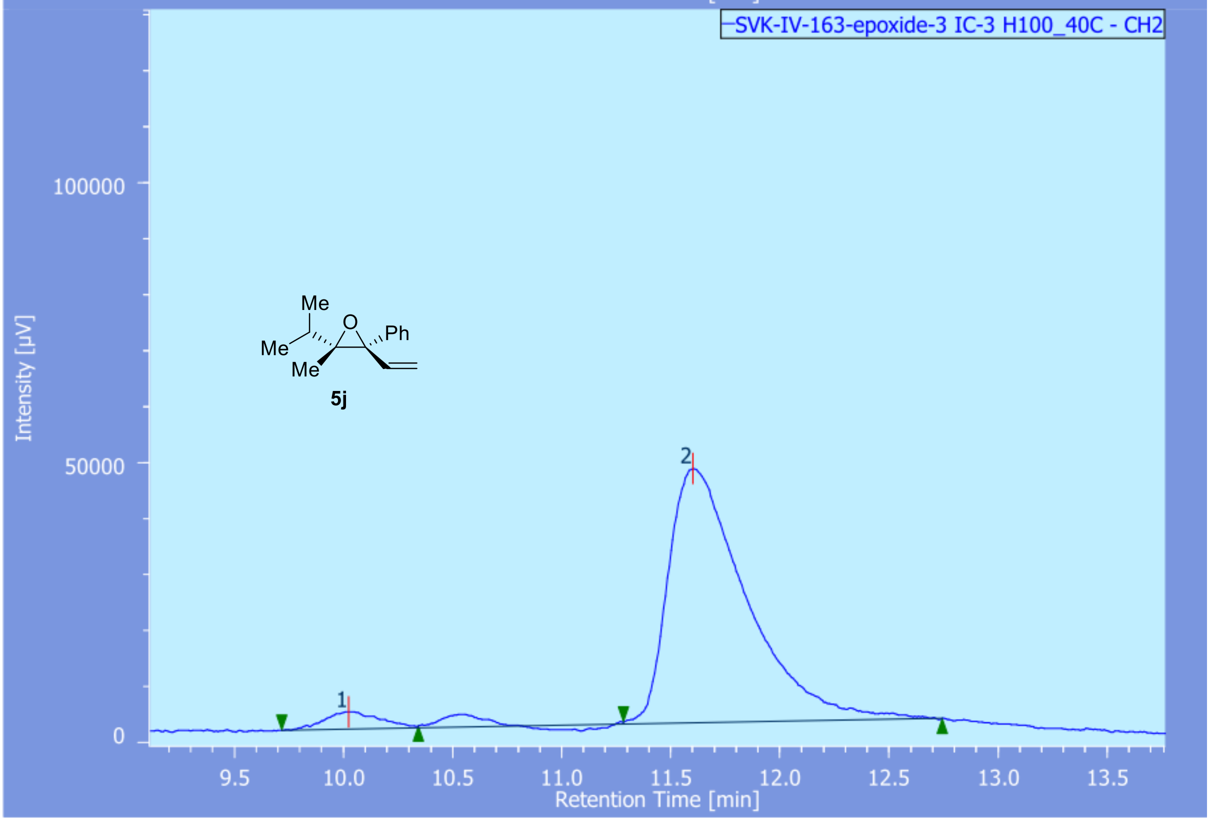
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5i**	5.1	5.5	50.2	49.8
(2*S*,3*R*)-**5i**	5.0	5.4	3.1	96.9



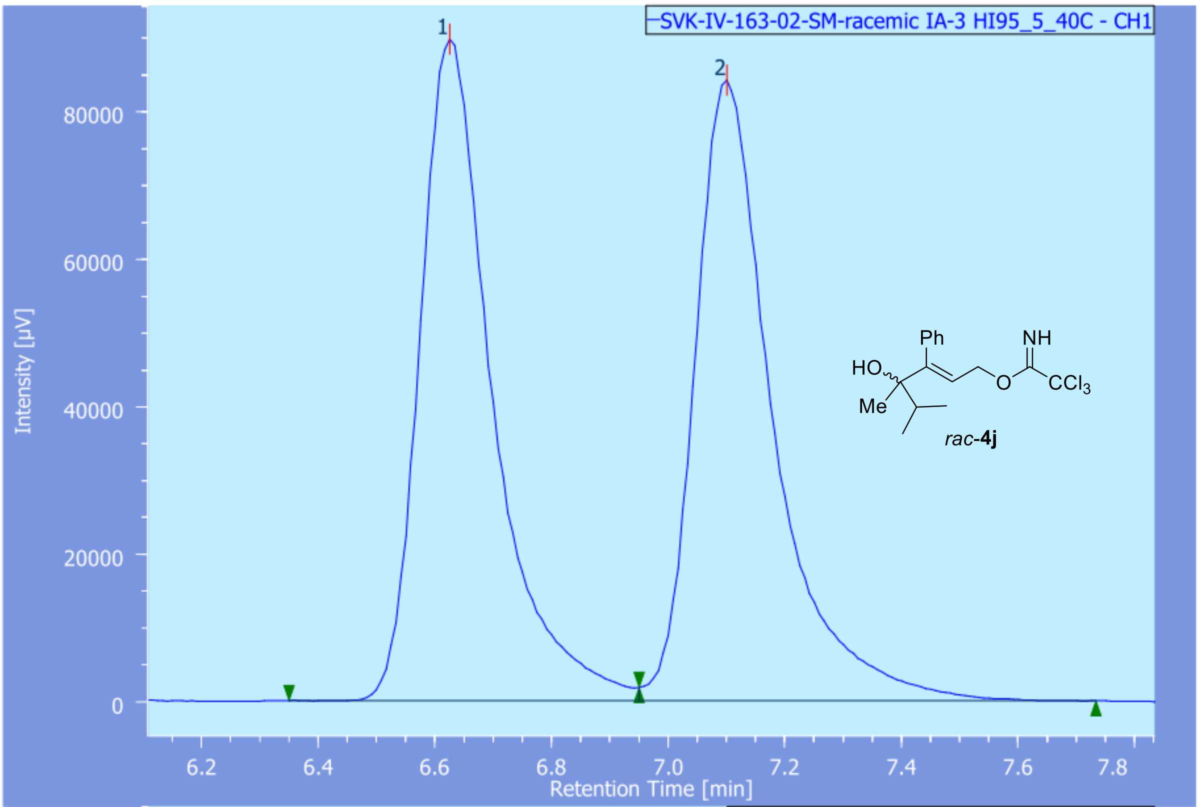


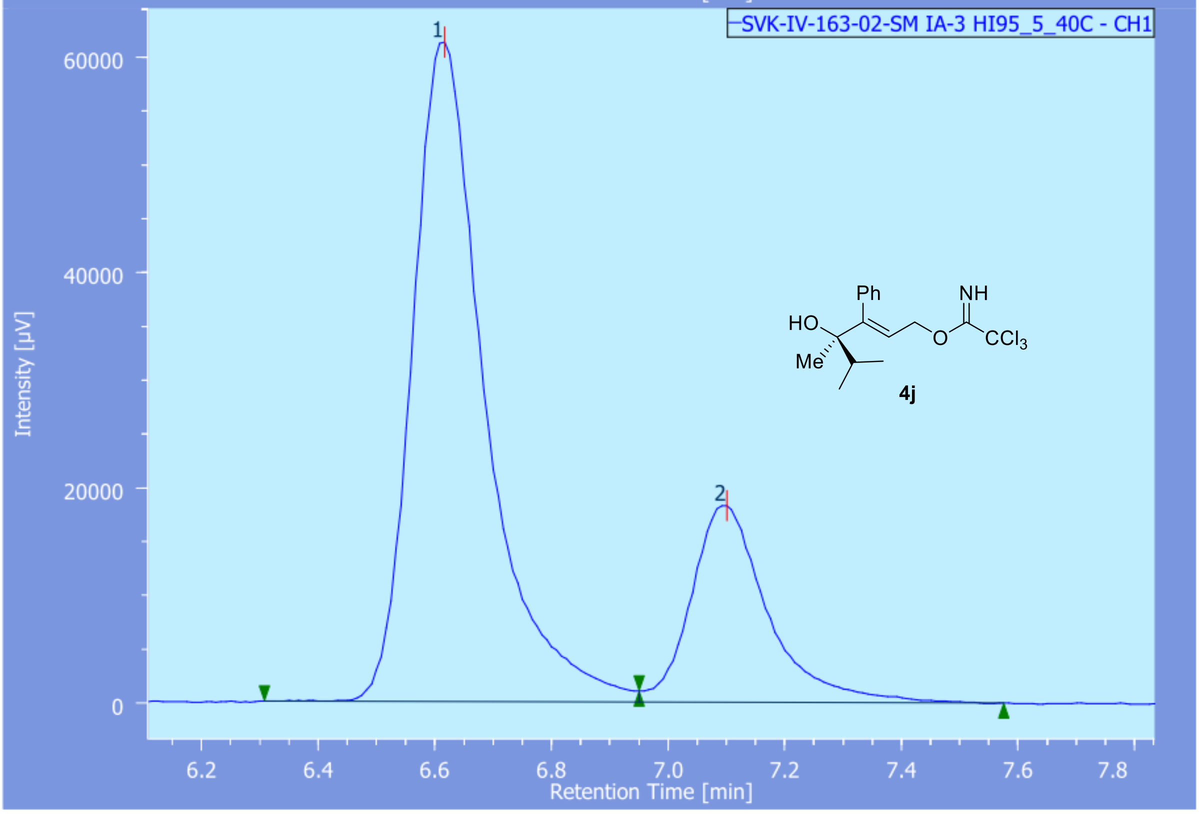
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4i**	10.7	12.2	49.6	50.4
(*R*,*E*)-**4i**	10.8	12.3	21.8	78.2



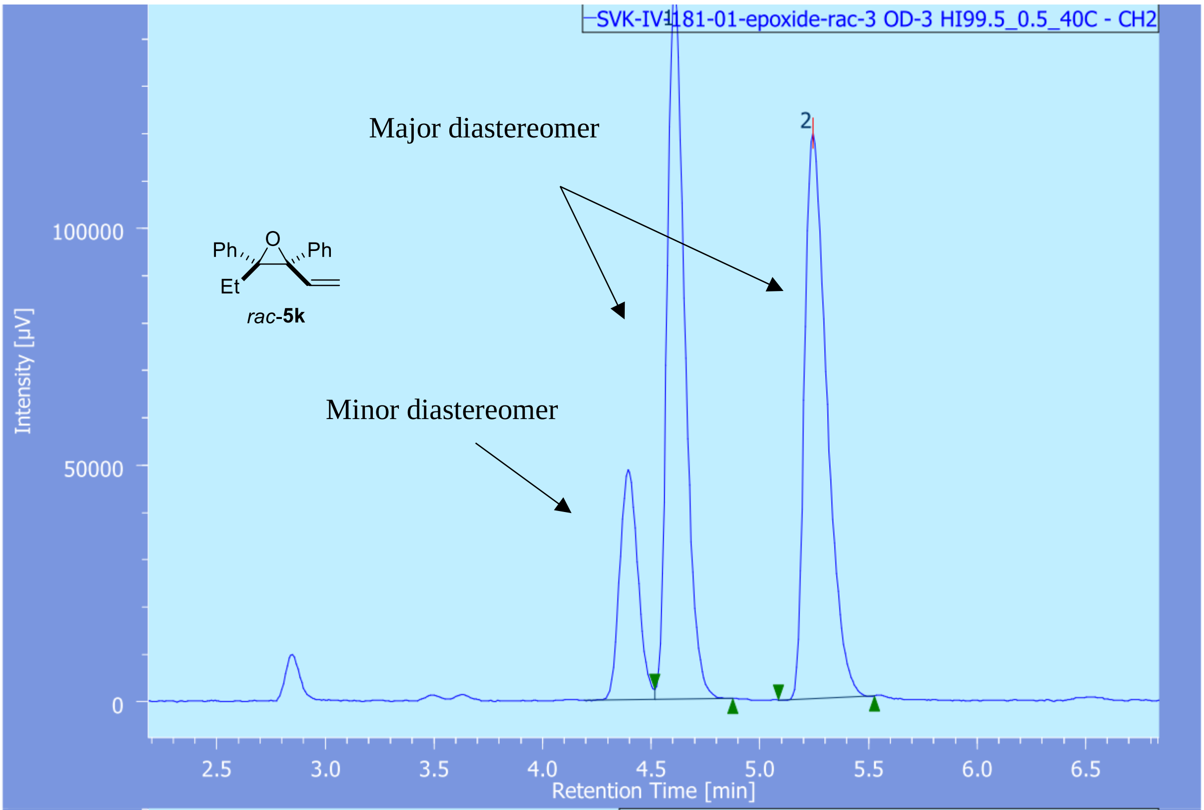


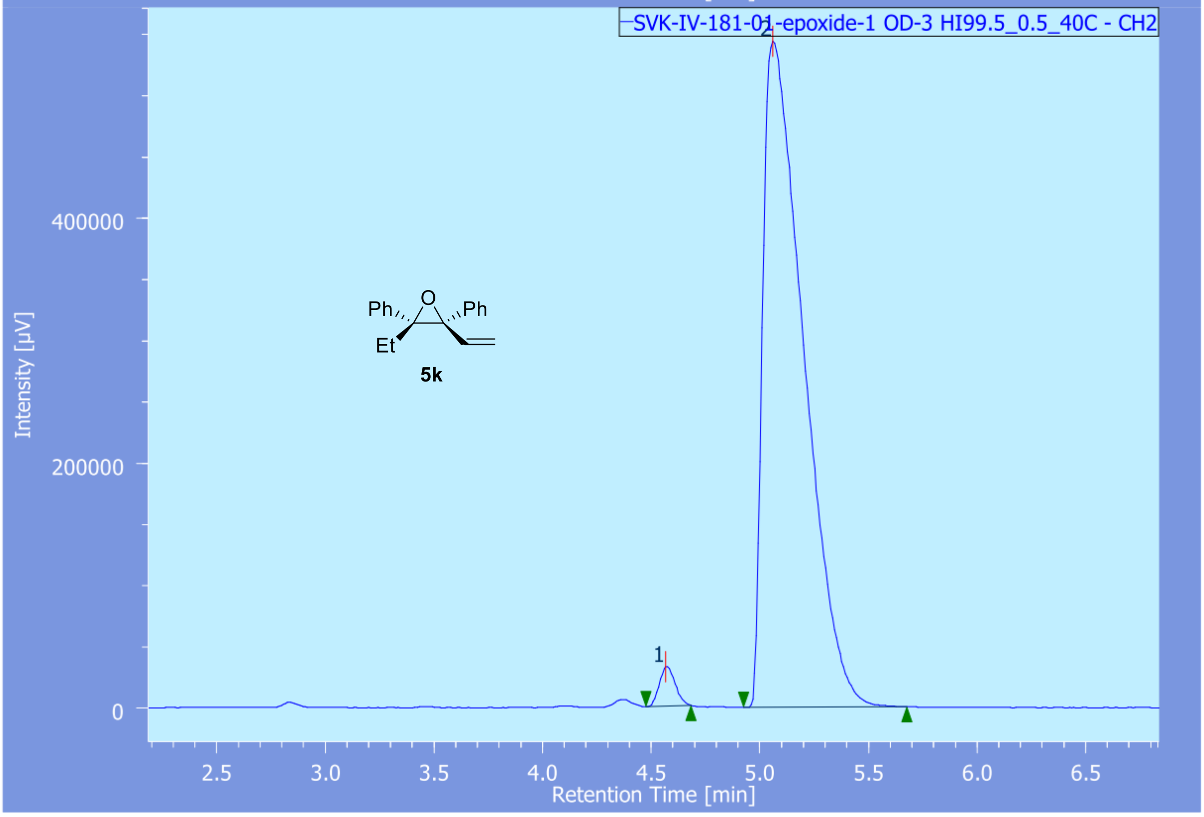
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5j**	10.3	12.0	49.9	50.1
(2*S*,3*R*)-**5j**	10.0	11.6	4.6	95.4



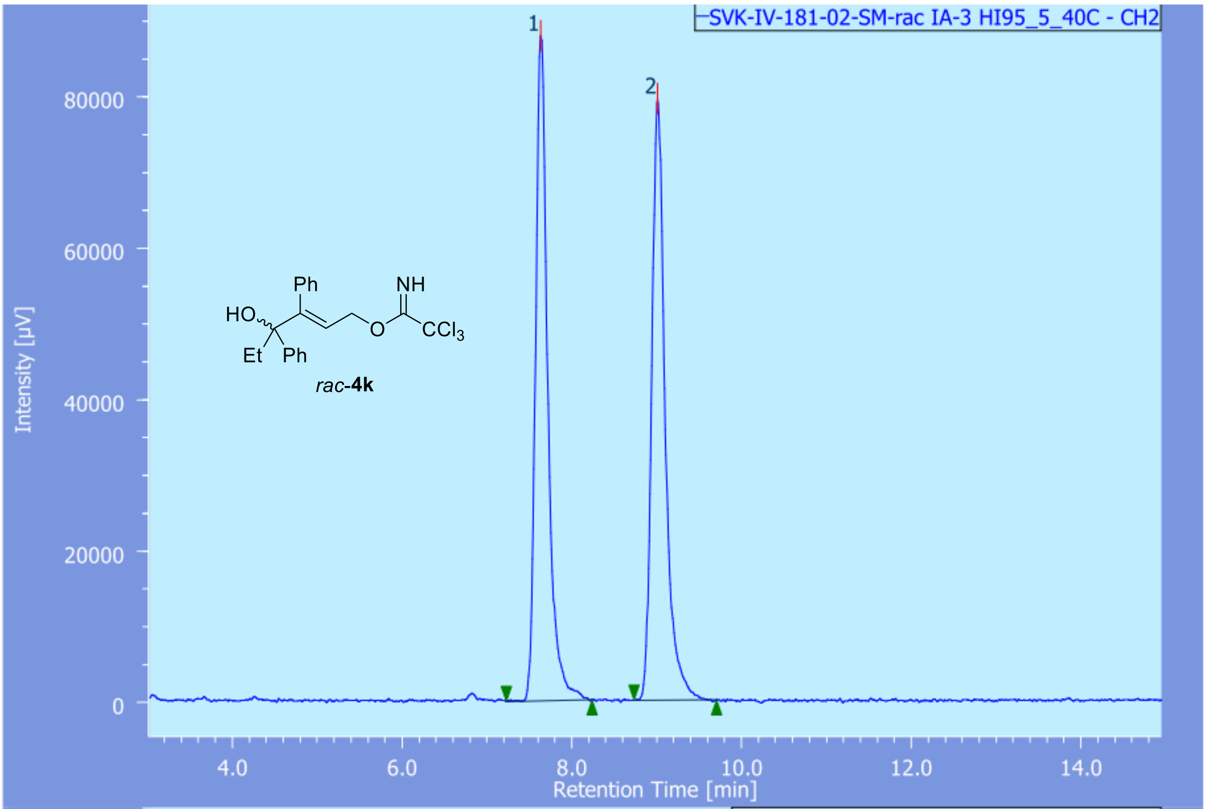


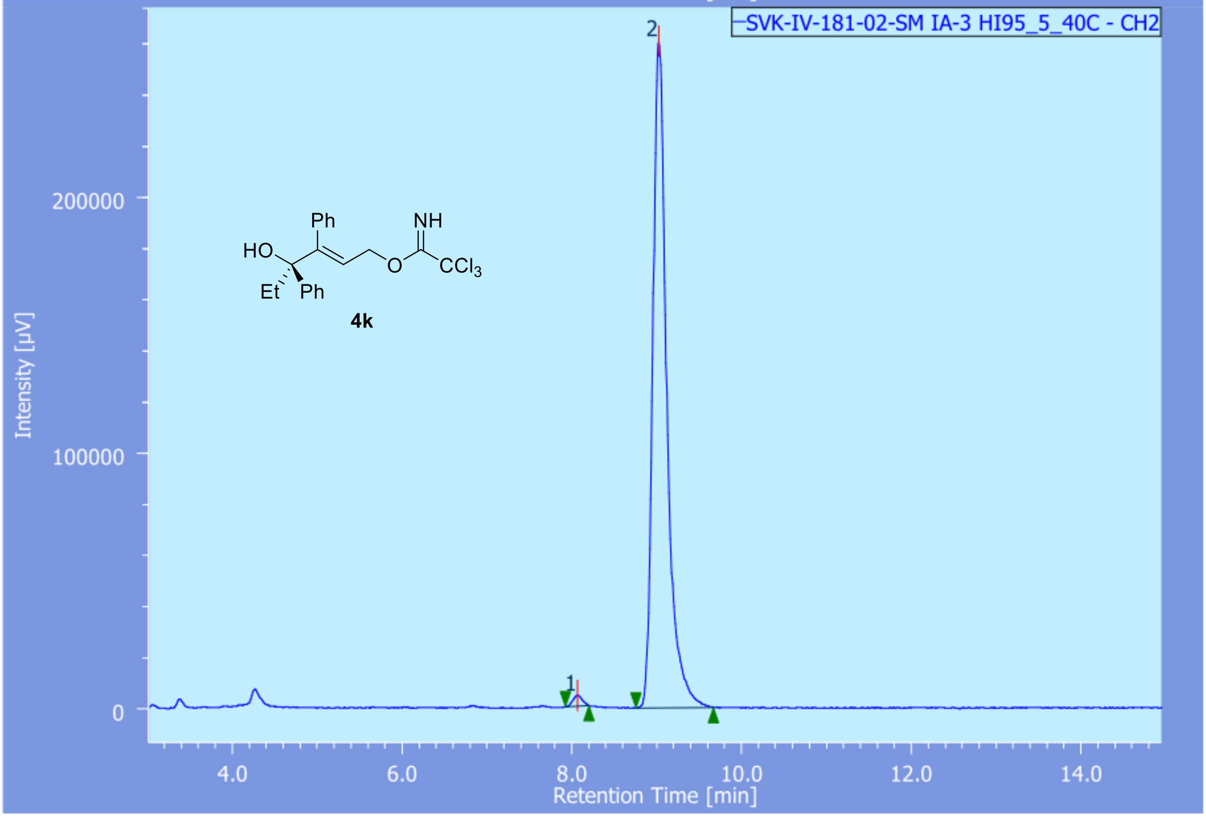
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4j**	6.6	7.1	49.6	50.4
(*R*,*E*)-**4j**	6.6	7.1	76.1	23.9



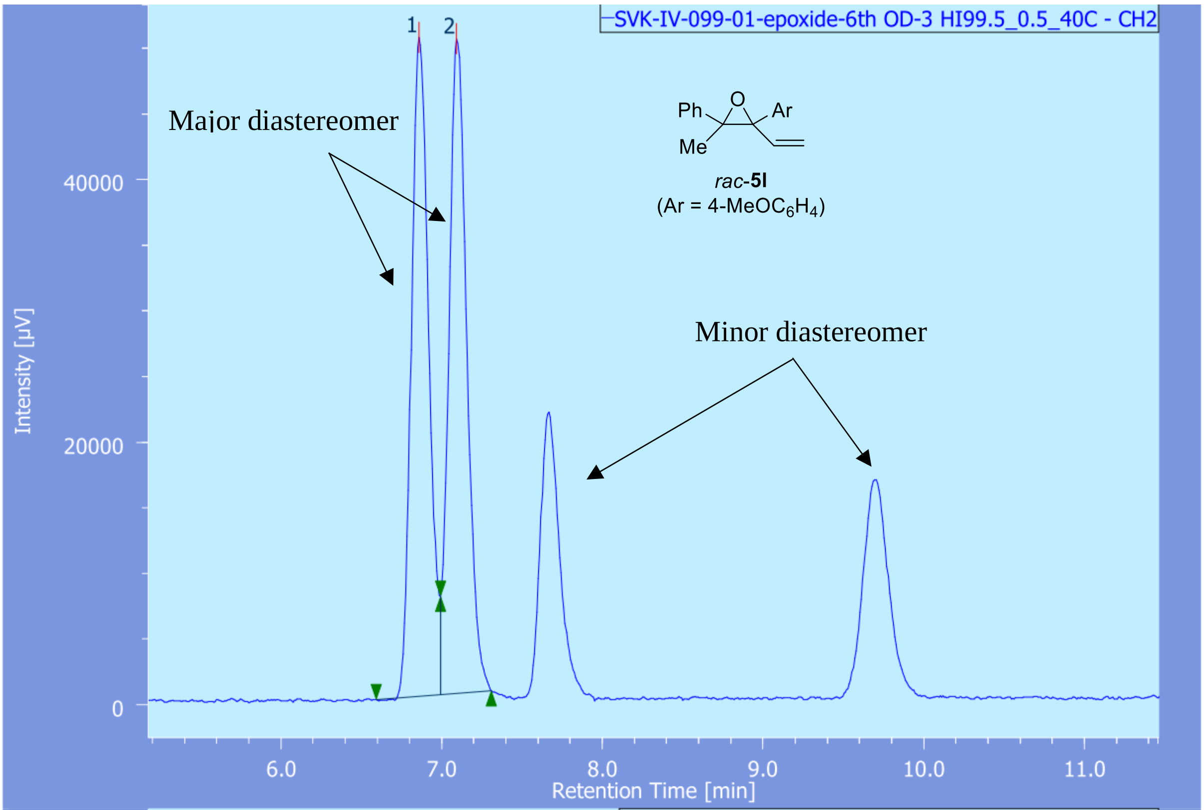


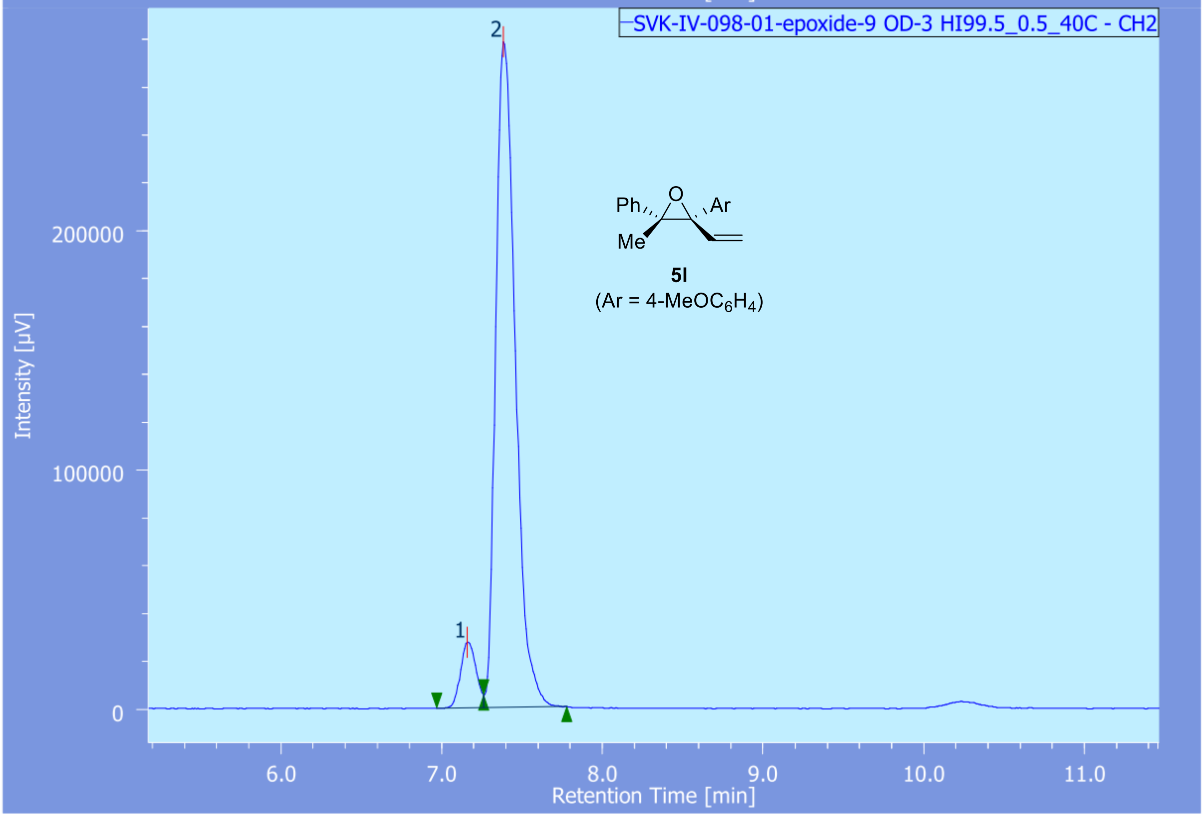
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5k**	4.6	5.2	49.9	50.1
(2*S*,3*R*)-**5k**	4.6	5.1	2.3	97.7



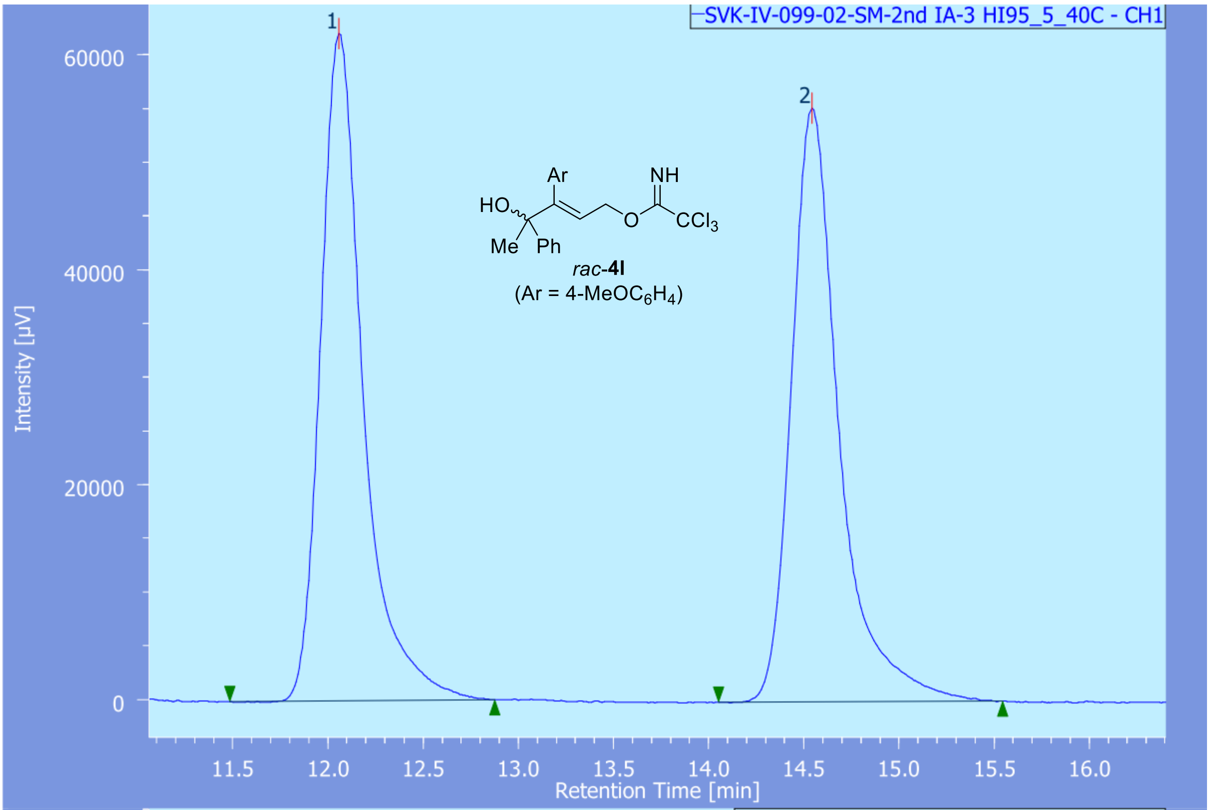


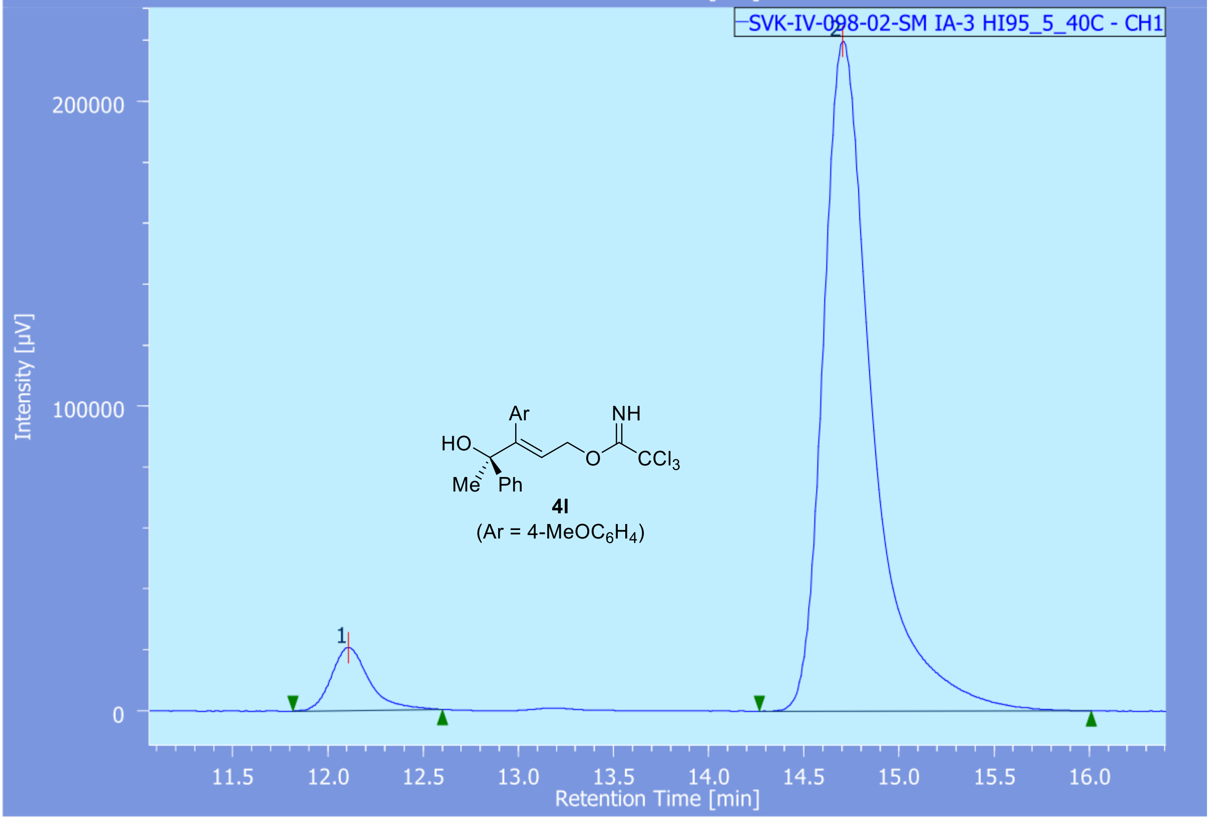
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4k**	7.6	9.0	50.2	49.8
(*R*,*E*)-**4k**	8.1	9.0	1.1	98.9



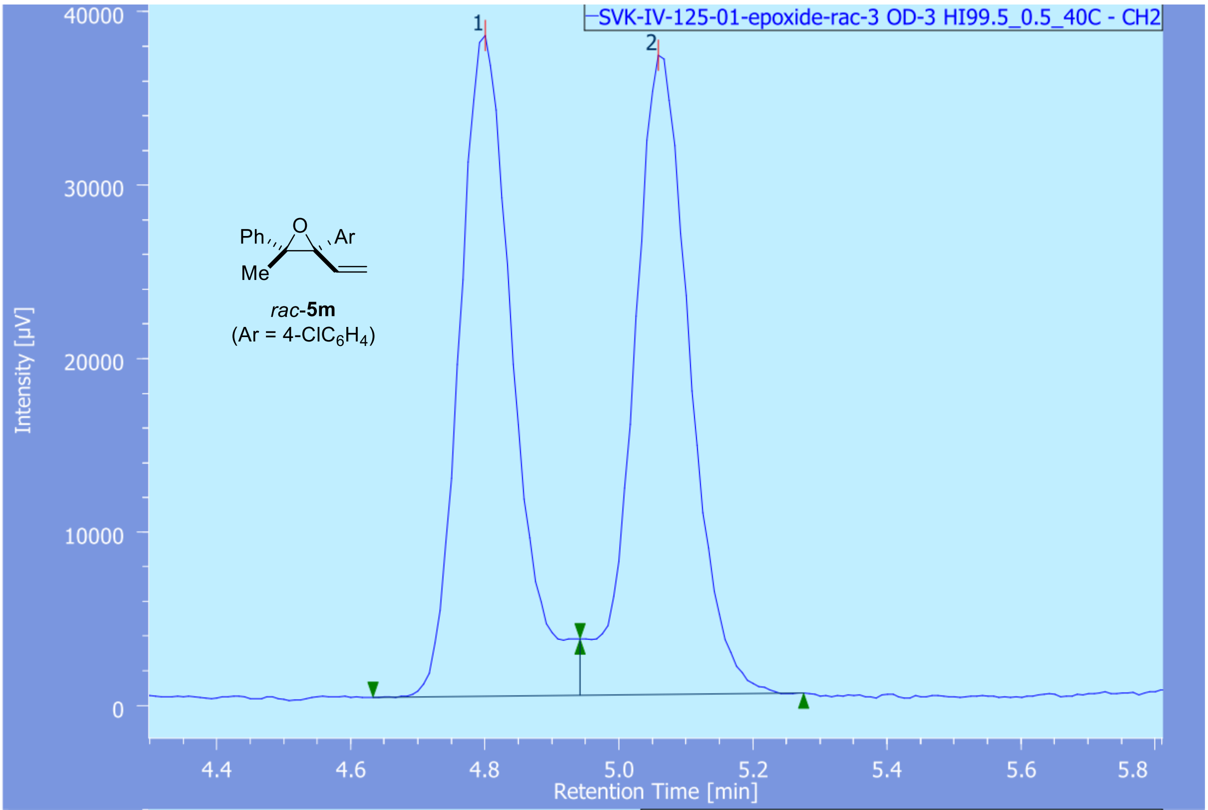


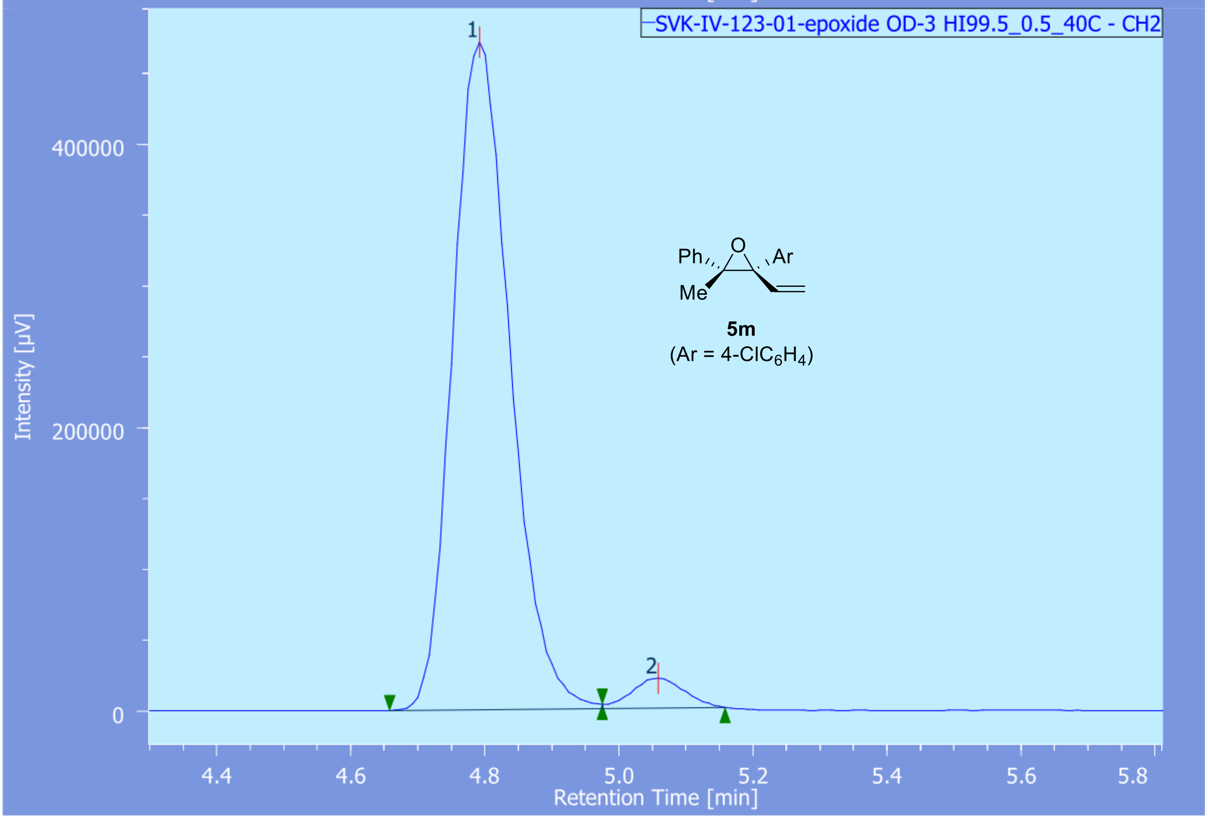
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5l**	6.9	7.1	49.6	50.4
(2*S*,3*R*)-**5l**	7.2	7.4	7.2	92.8



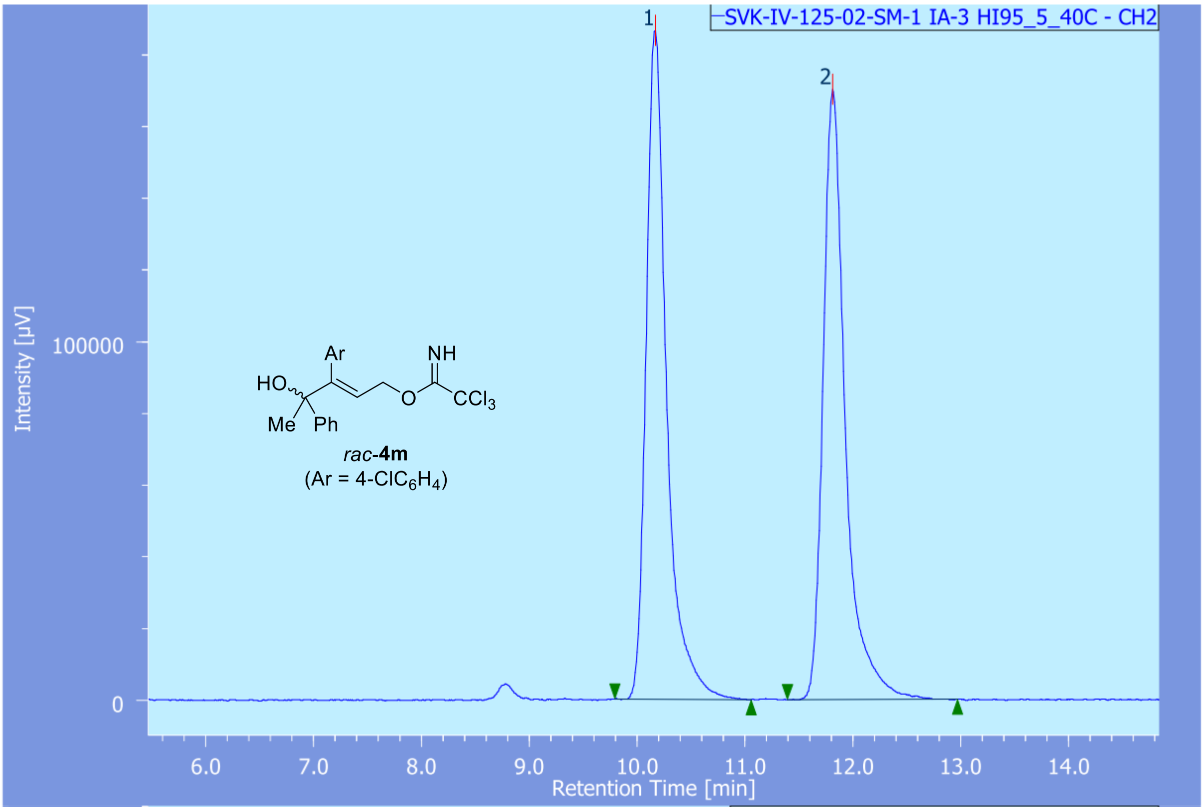


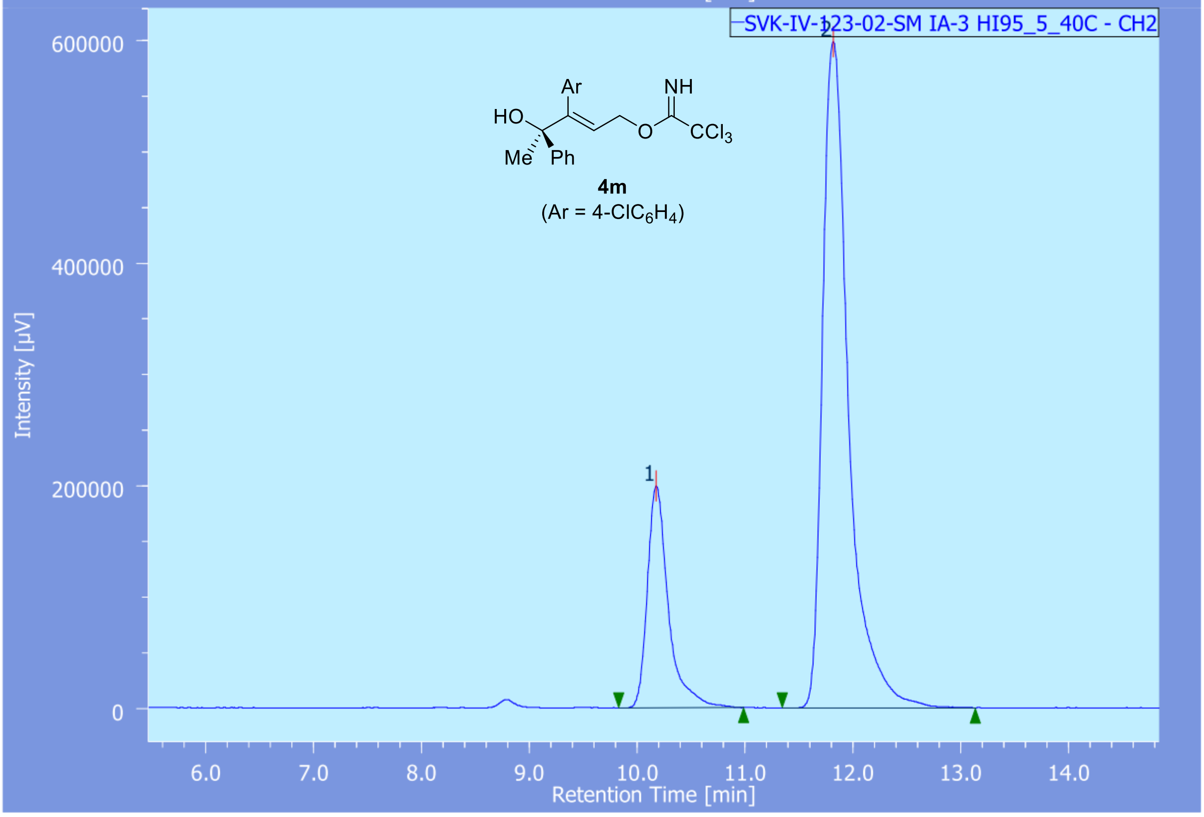
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4l**	12.1	14.5	50.0	50.0
(*R*,*E*)-**4l**	12.1	14.7	6.7	93.3



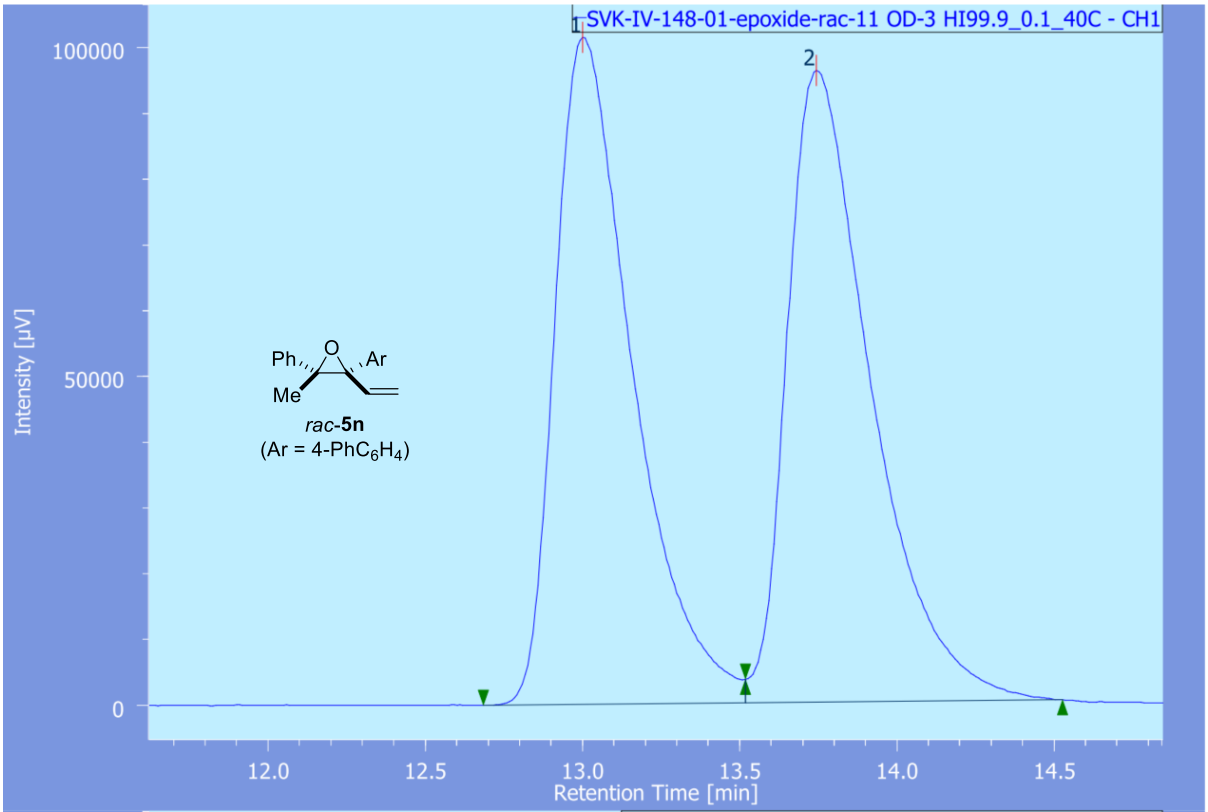


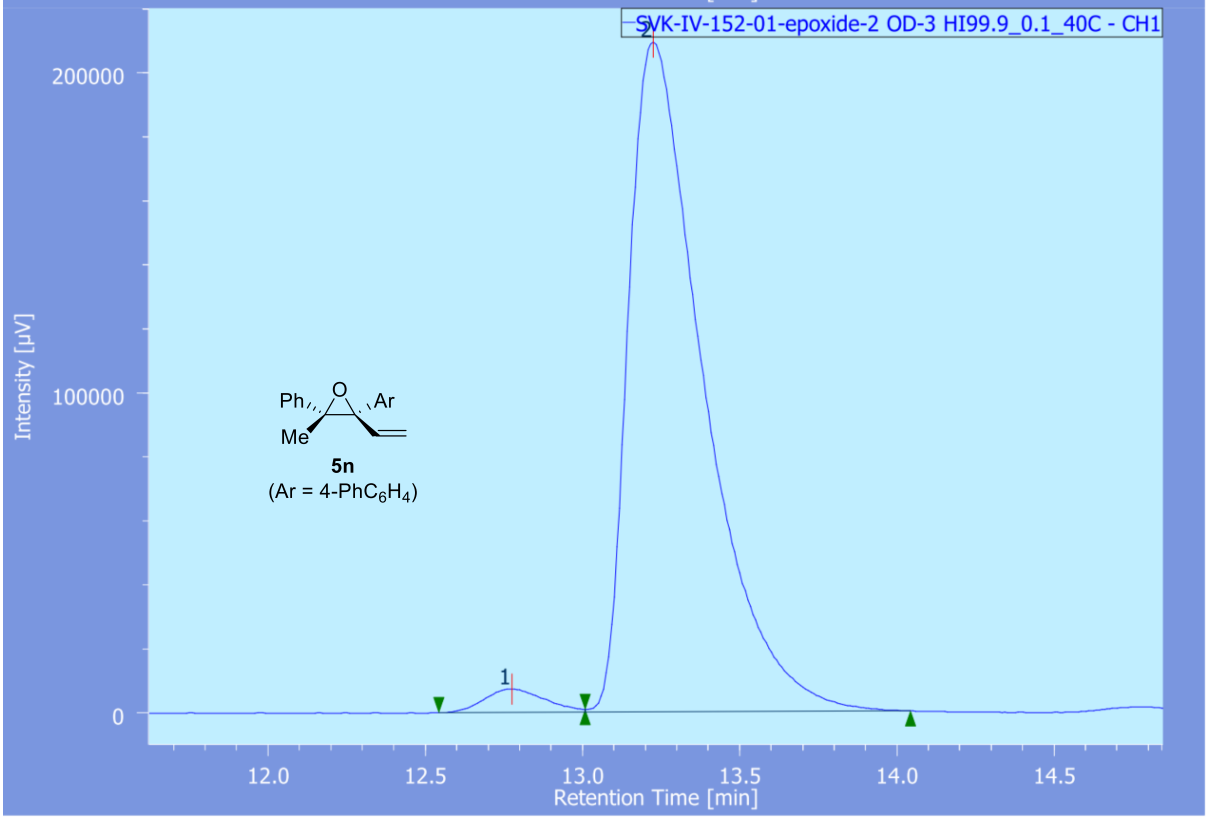
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5m**	4.8	5.1	49.7	50.3
(2*S*,3*R*)-**5m**	4.8	5.1	96.1	3.9



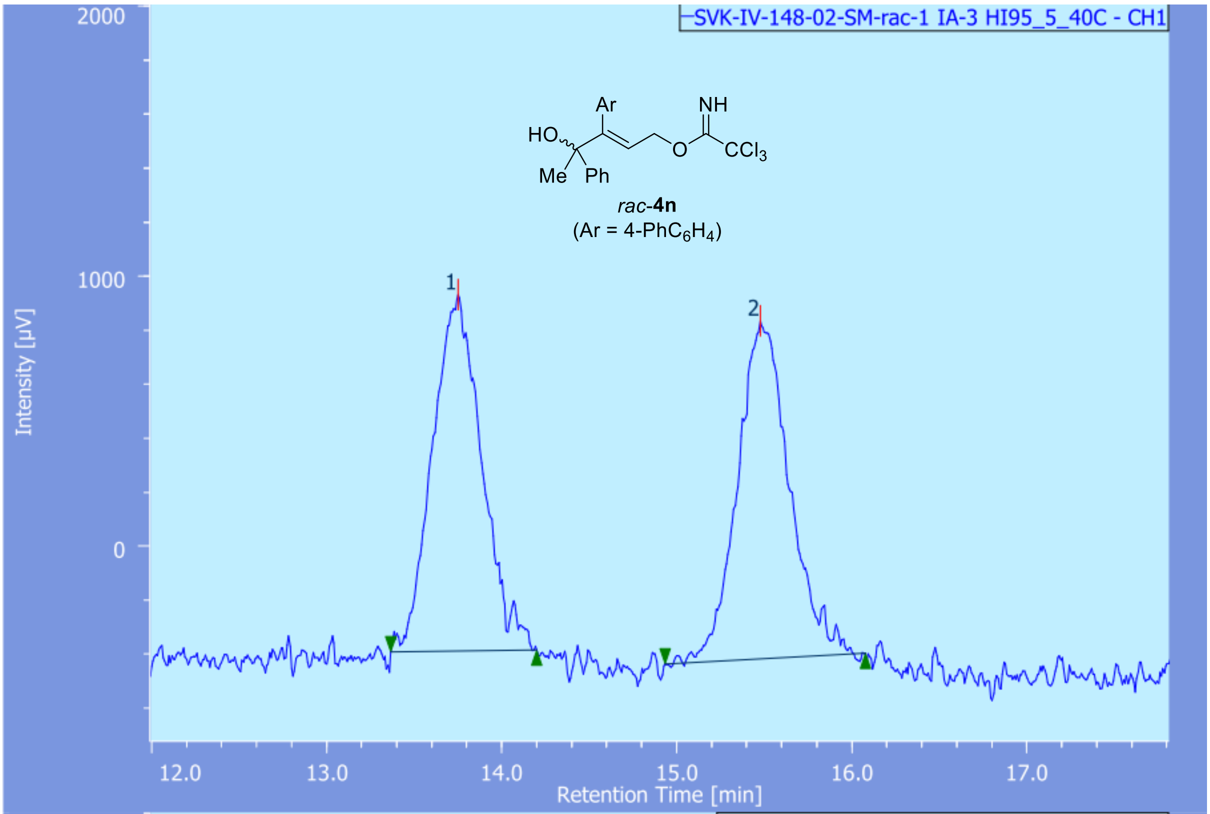


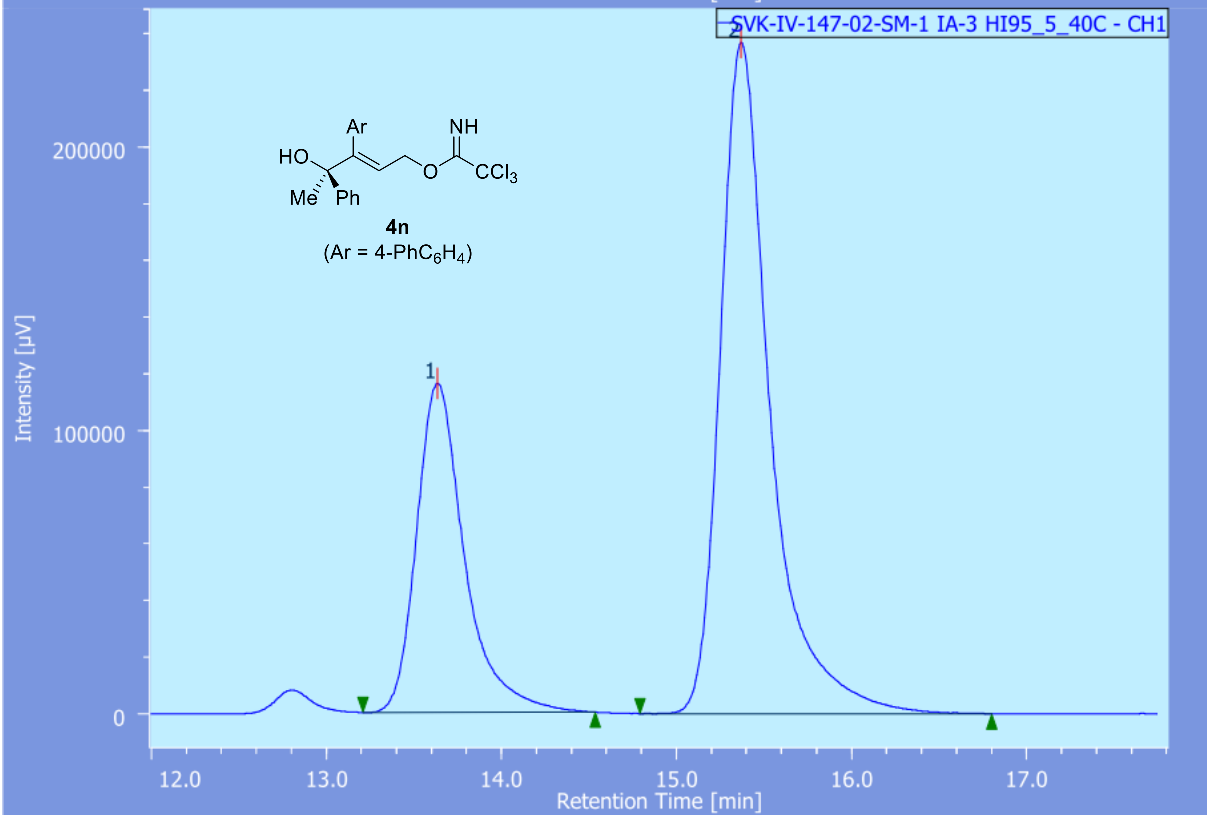
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4m**	10.2	11.8	50.3	49.7
(*R*,*E*)-**4m**	10.2	11.8	21.2	78.8



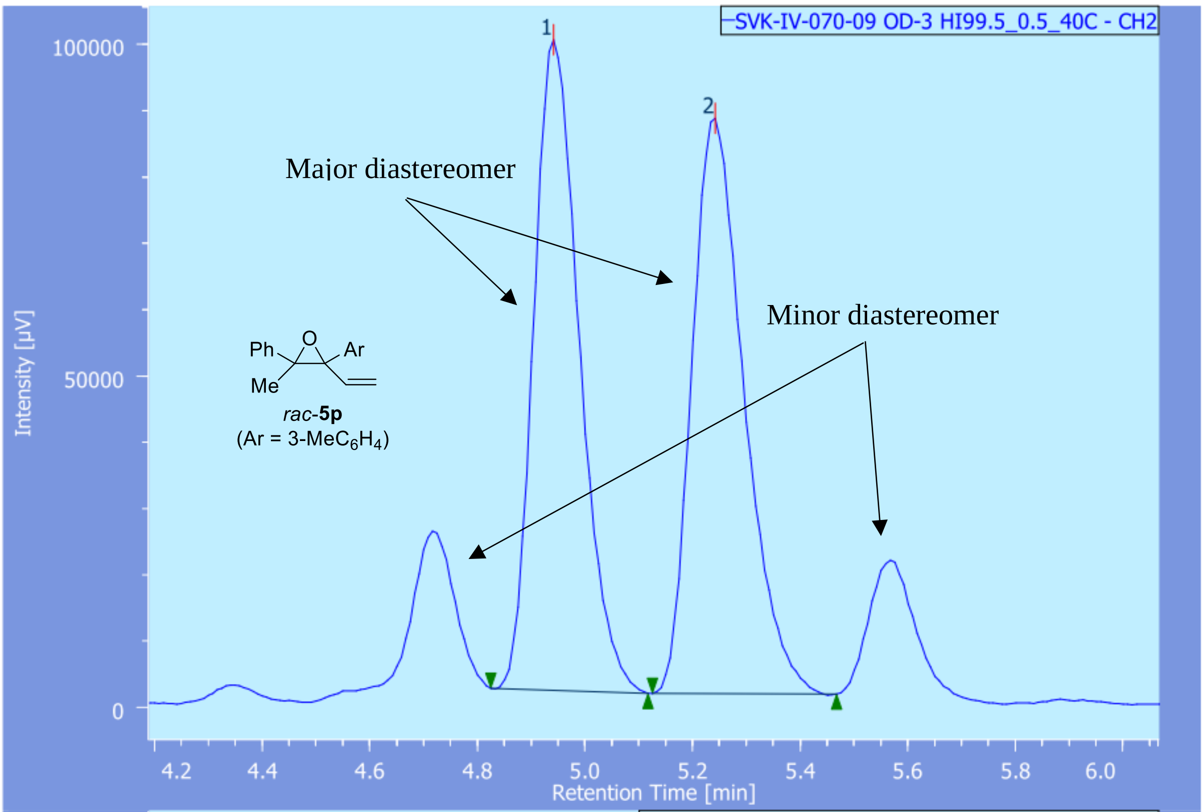


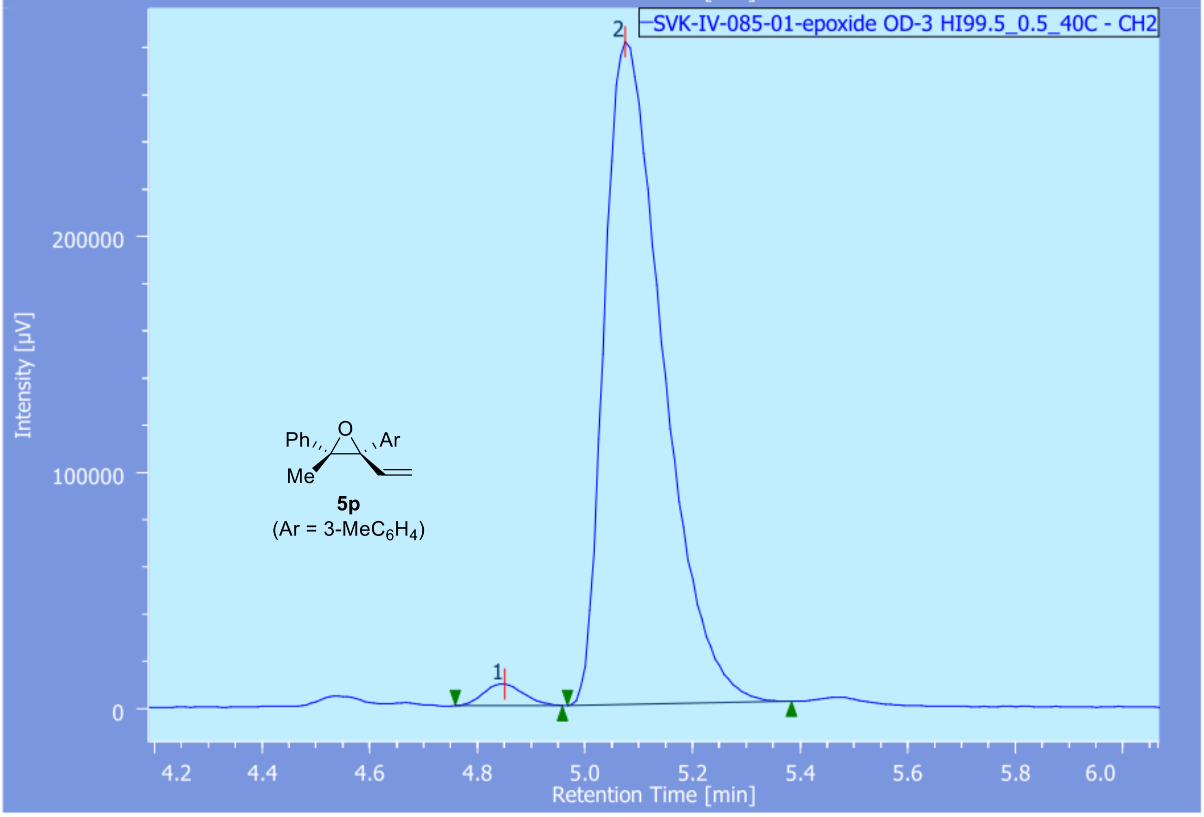
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5n**	13.0	13.7	49.6	50.4
(2*S*,3*R*)-**5n**	12.8	13.2	2.7	97.3



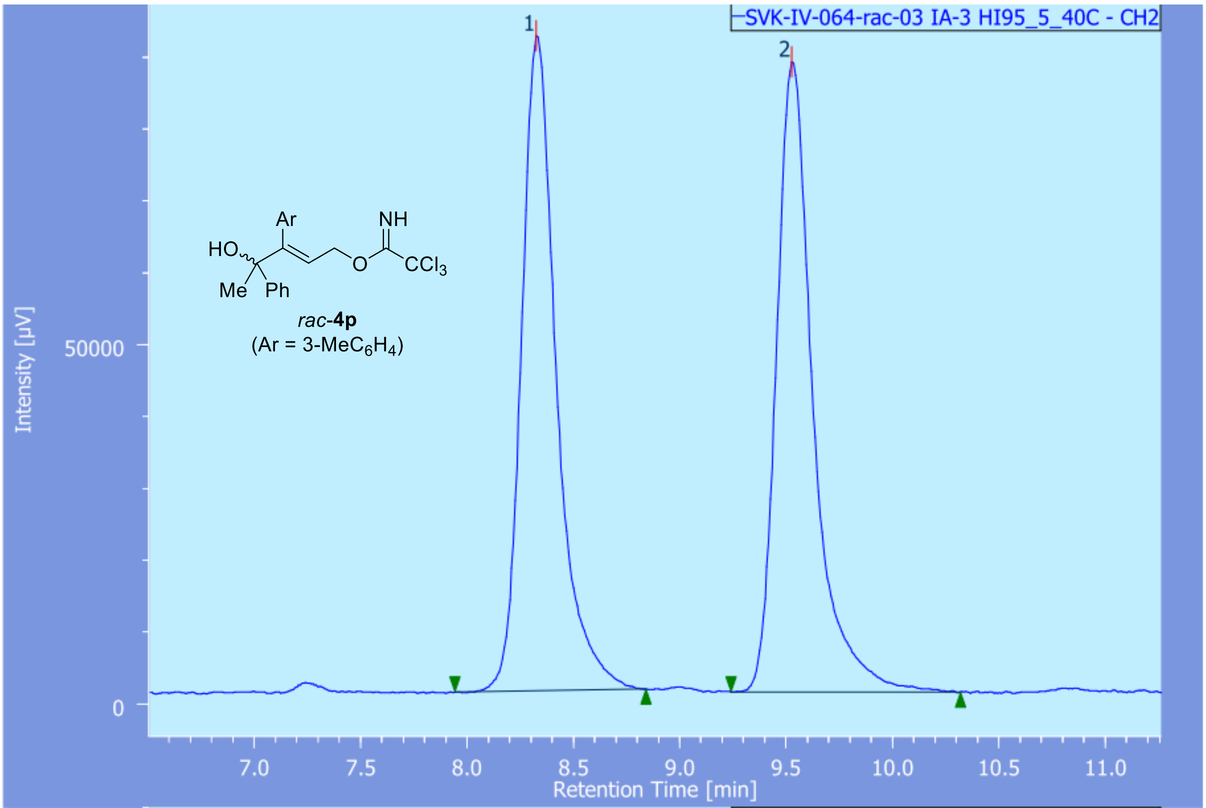


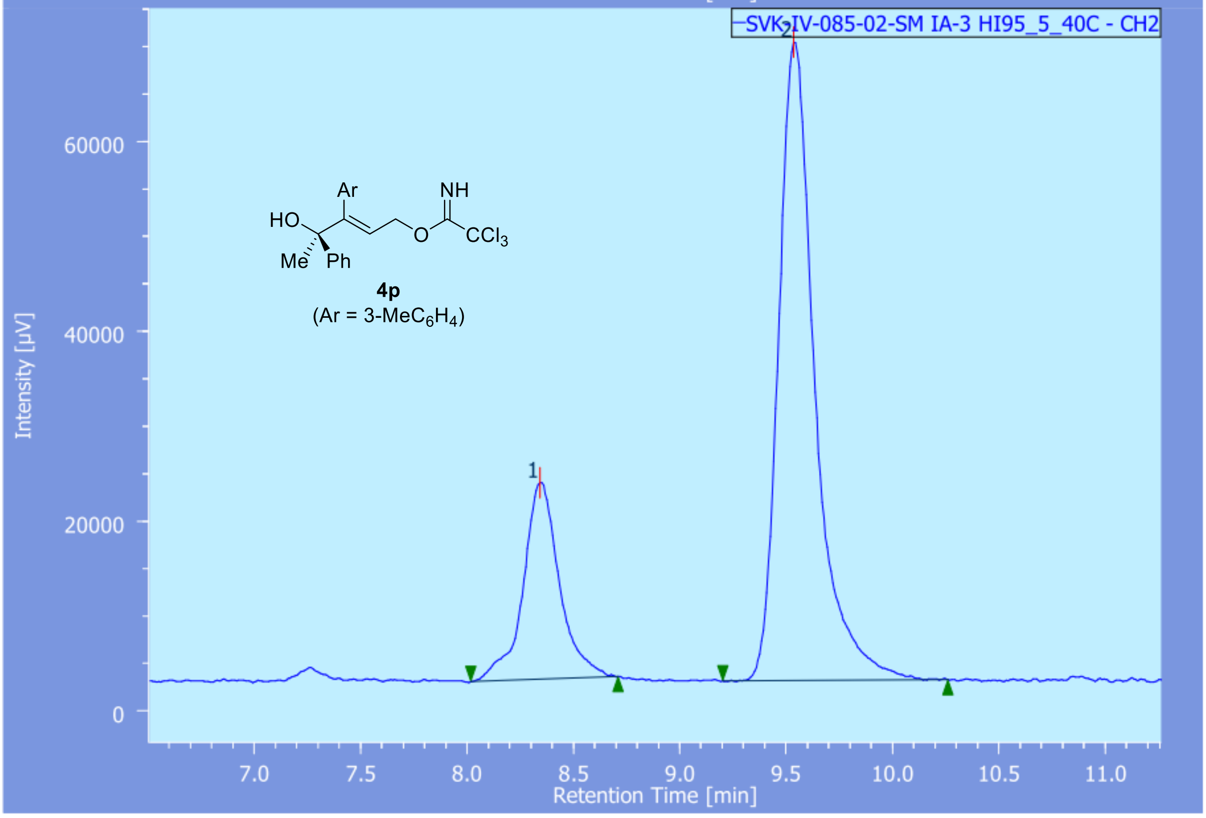
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4n**	13.8	15.5	50.1	49.9
(*R*,*E*)-**4n**	13.6	15.4	31.9	68.1



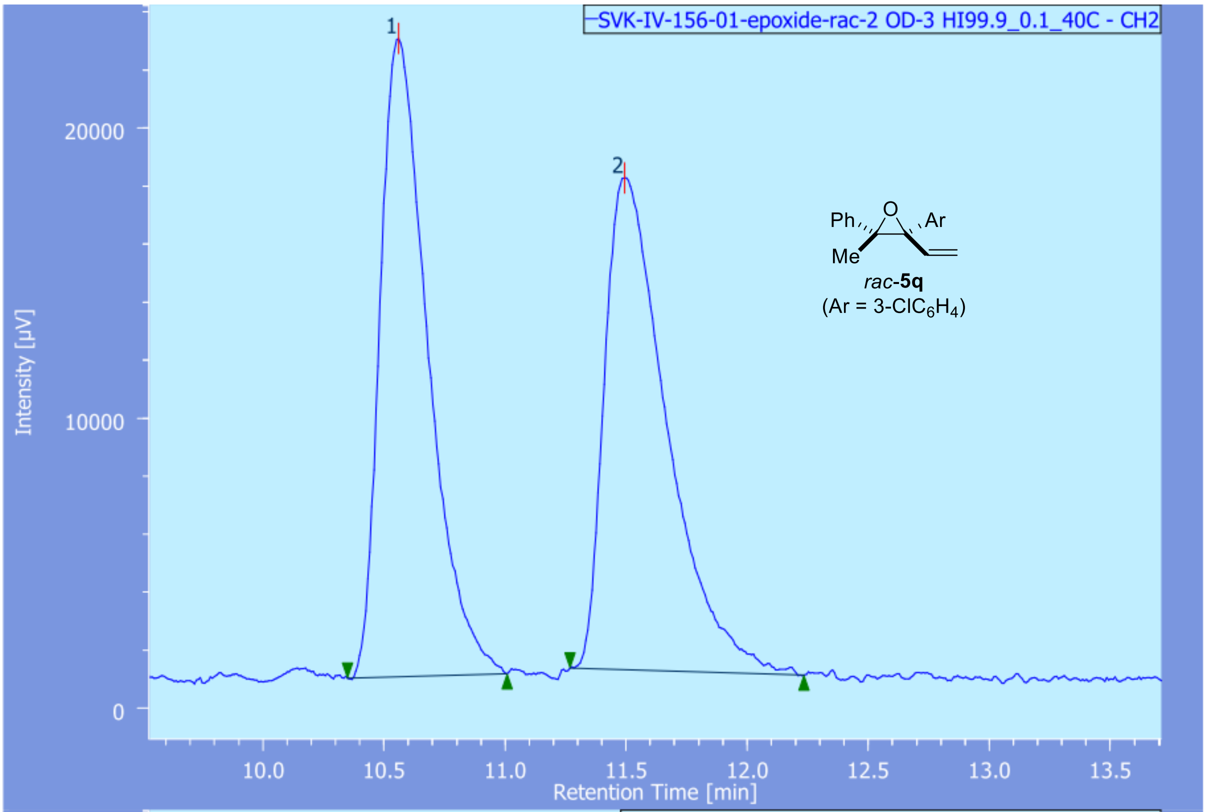


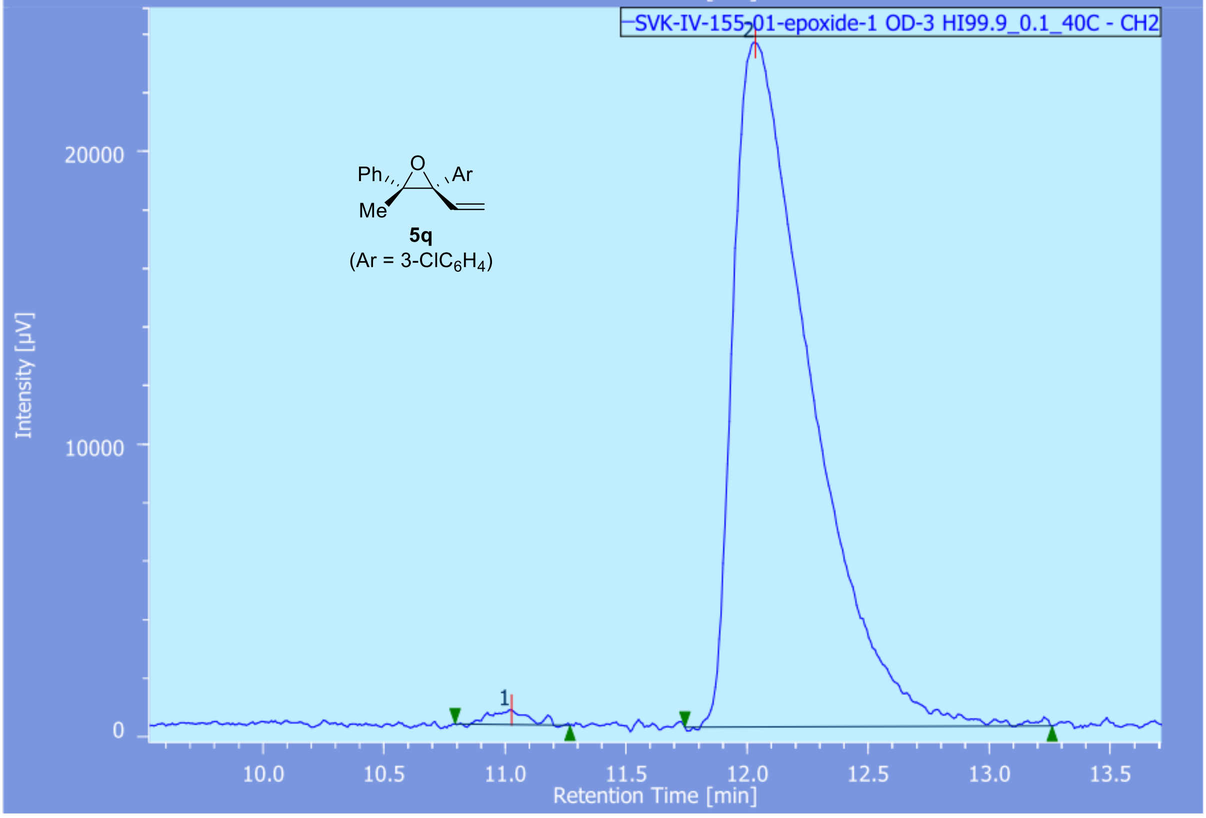
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5p**	4.9	5.2	49.8	50.2
(2*S*,3*R*)-**5p**	4.9	5.1	2.2	97.8



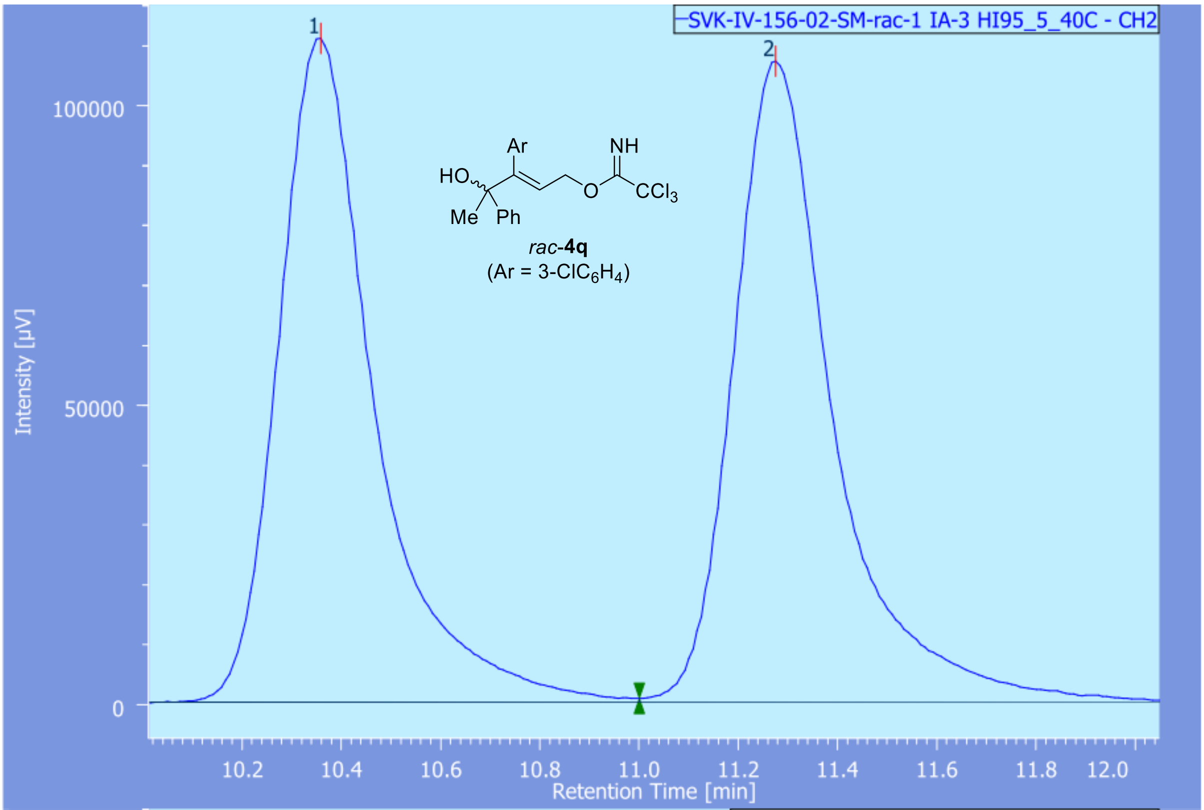


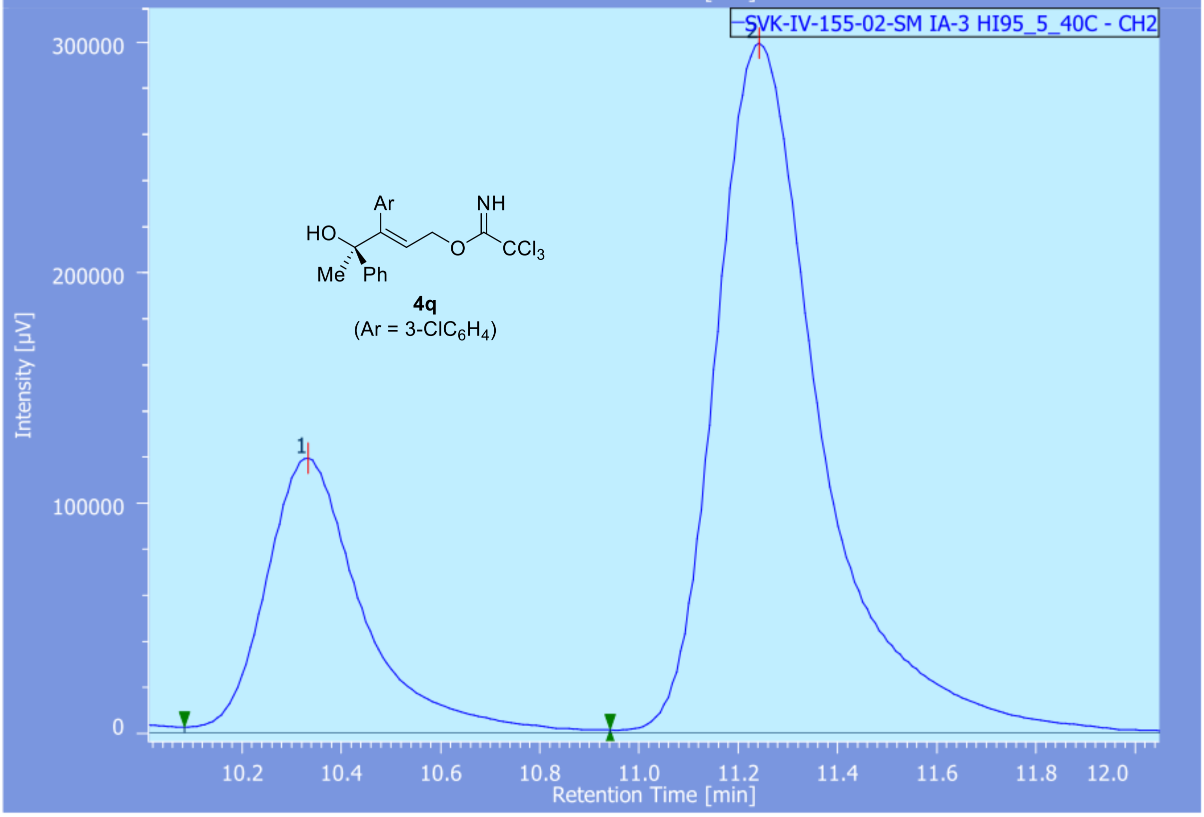
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4p**	8.3	9.5	50.0	50.0
(*R*,*E*)-**4p**	8.3	9.5	23.7	76.3



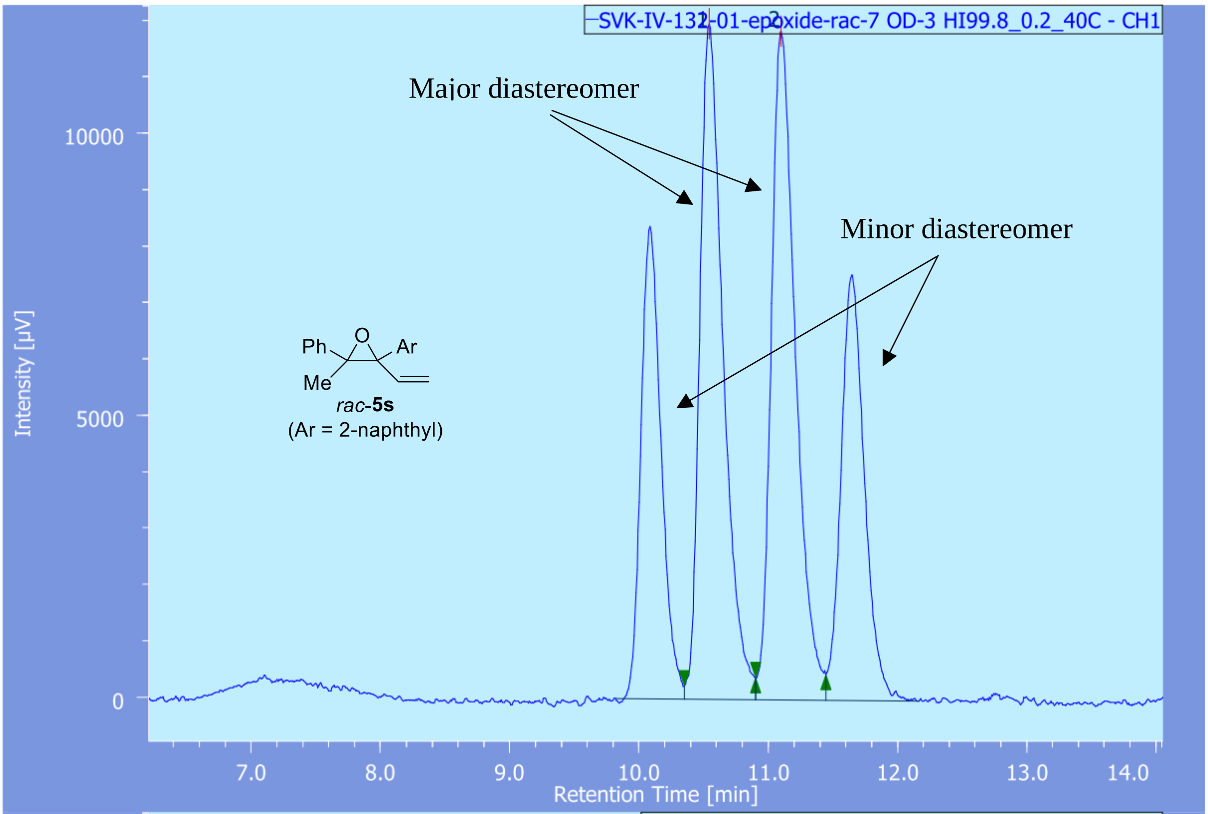


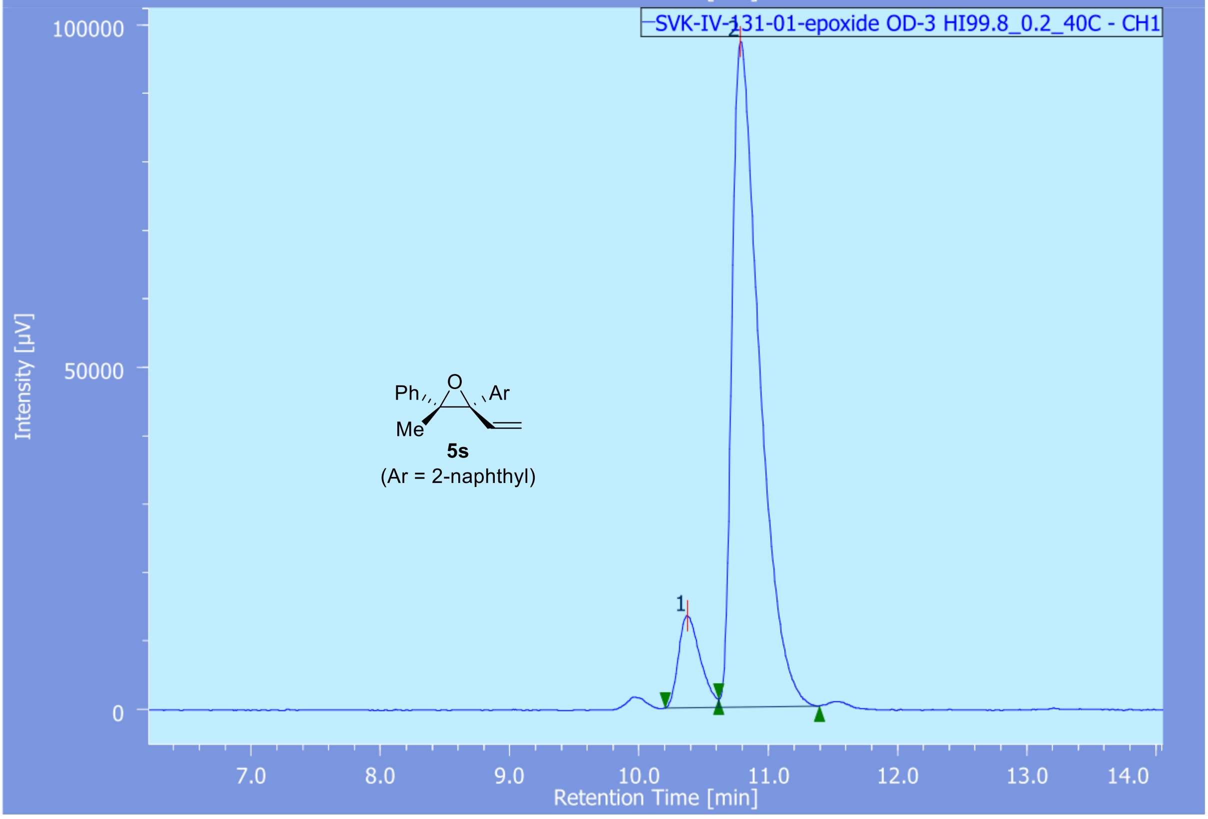
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5q**	10.6	11.5	49.7	50.3
(2*S*,3*R*)-**5q**	11.0	12.0	1.0	99.0



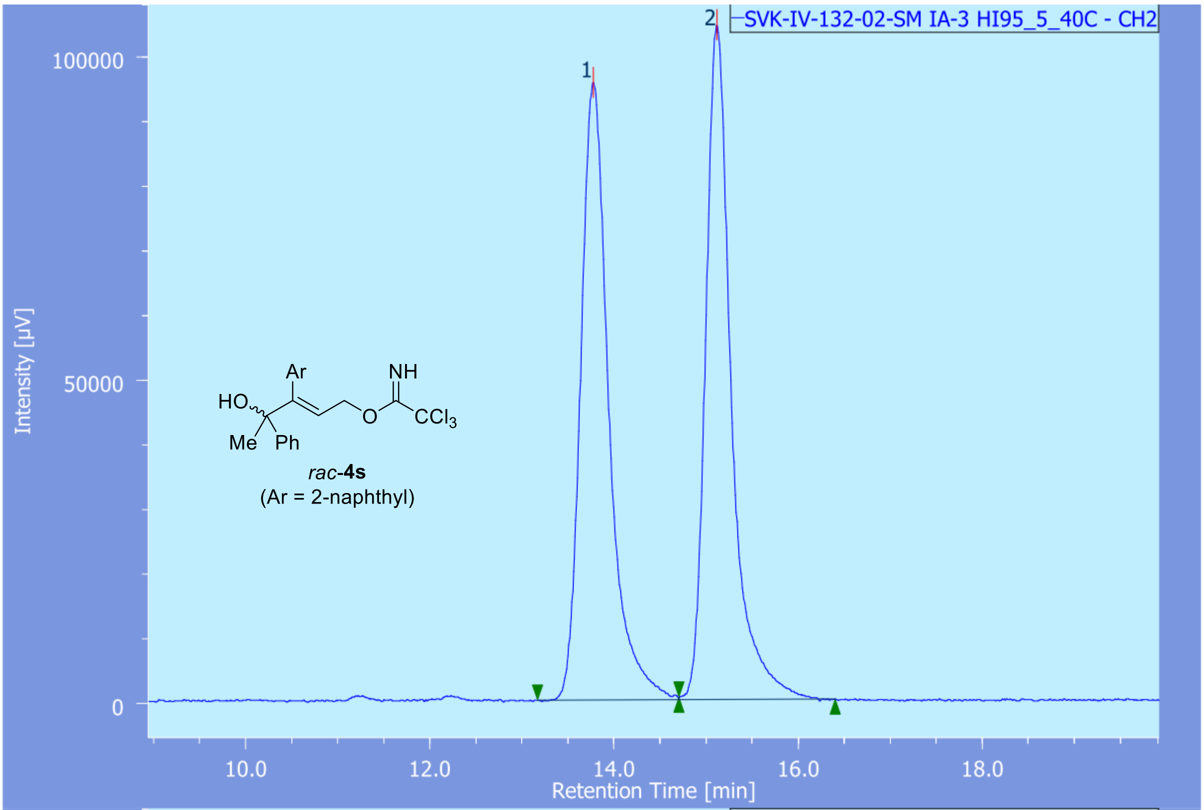


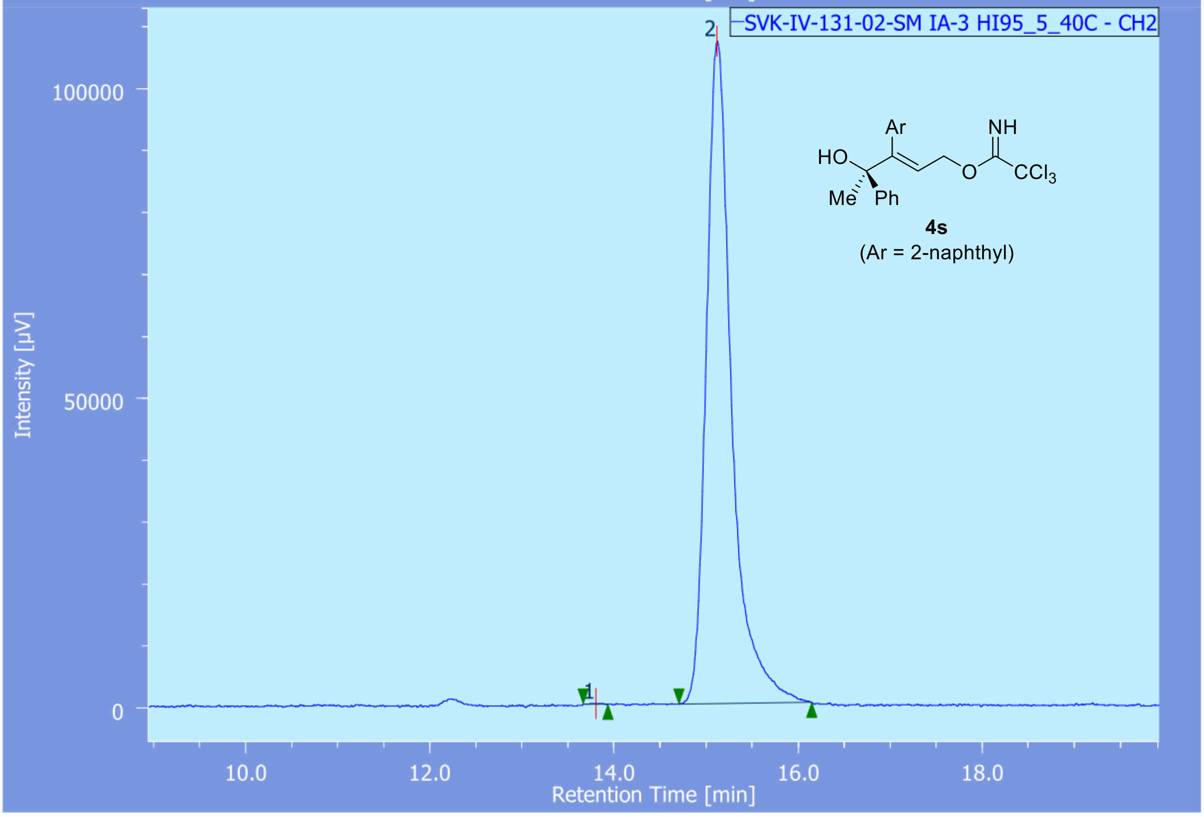
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4q**	10.4	11.3	49.9	50.1
(*R*,*E*)-**4q**	10.3	11.2	26.7	73.3



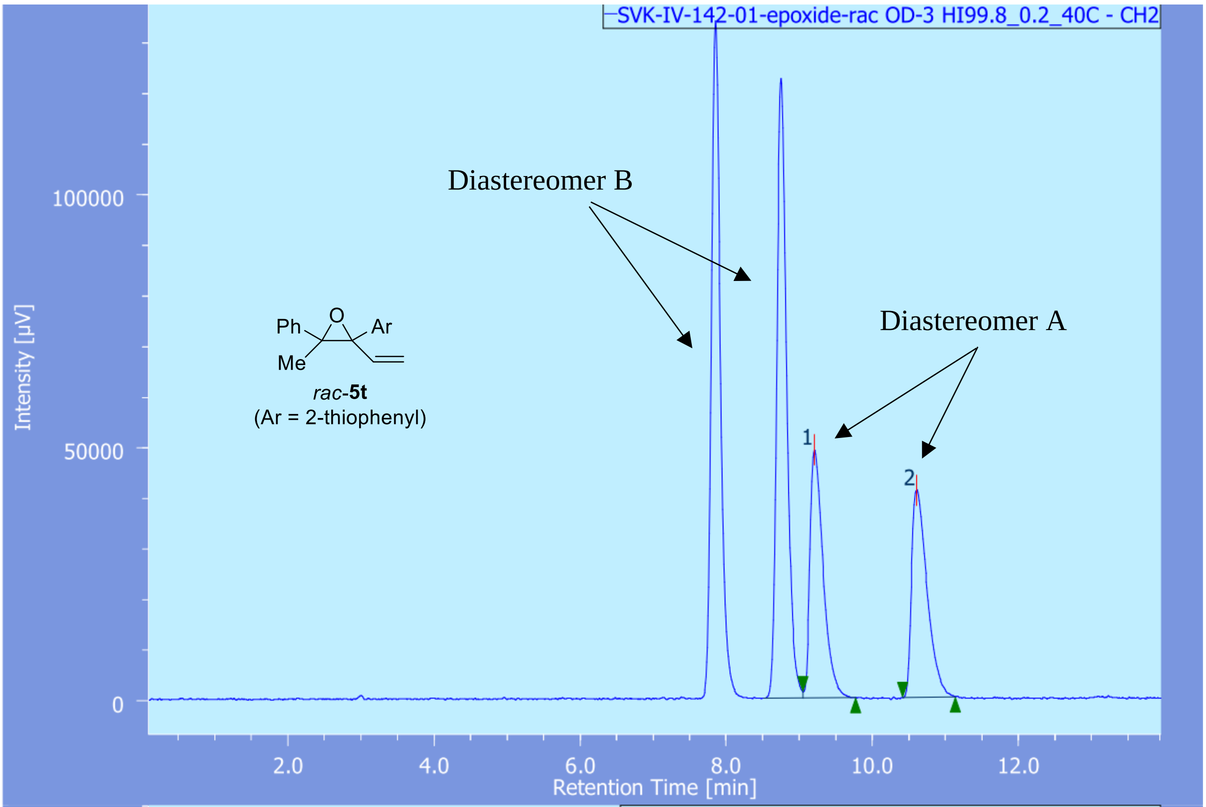


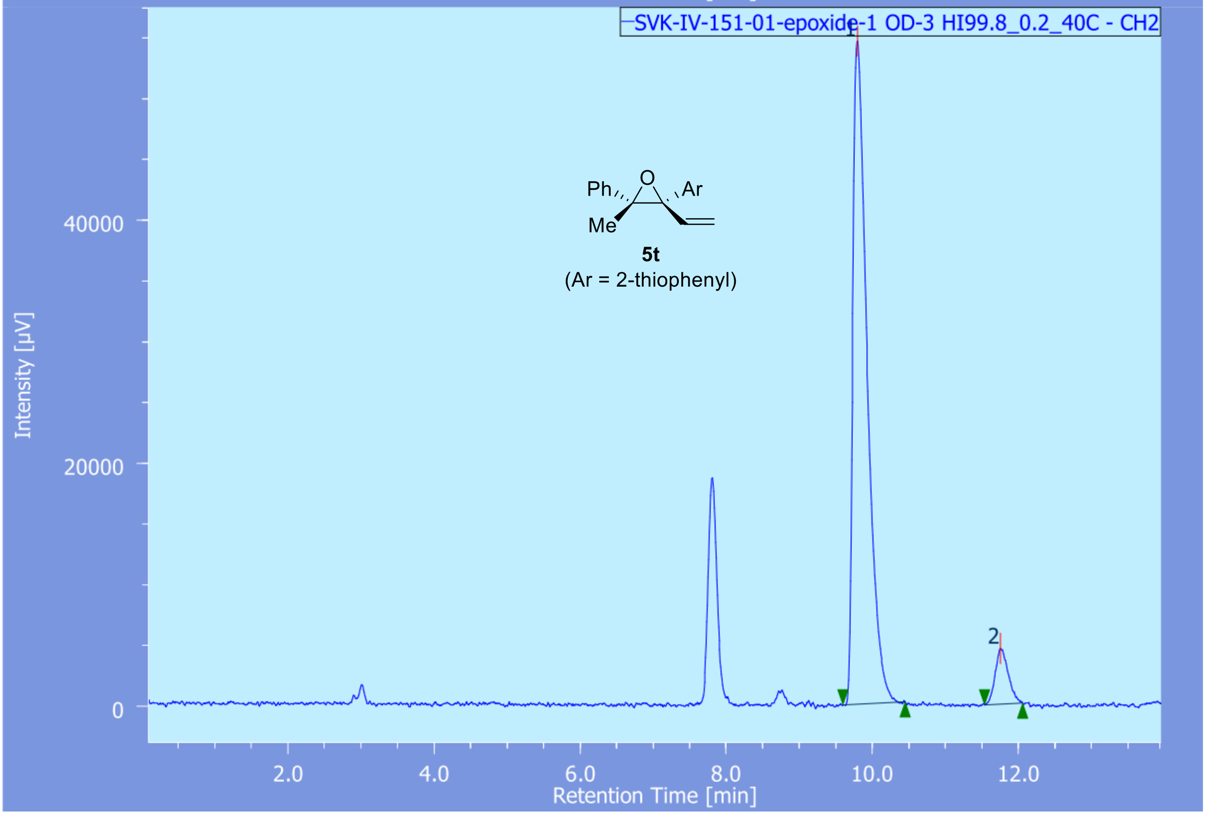
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5s**	10.5	11.1	49.6	50.4
(2*S*,3*R*)-**5s**	10.4	10.8	9.9	90.1



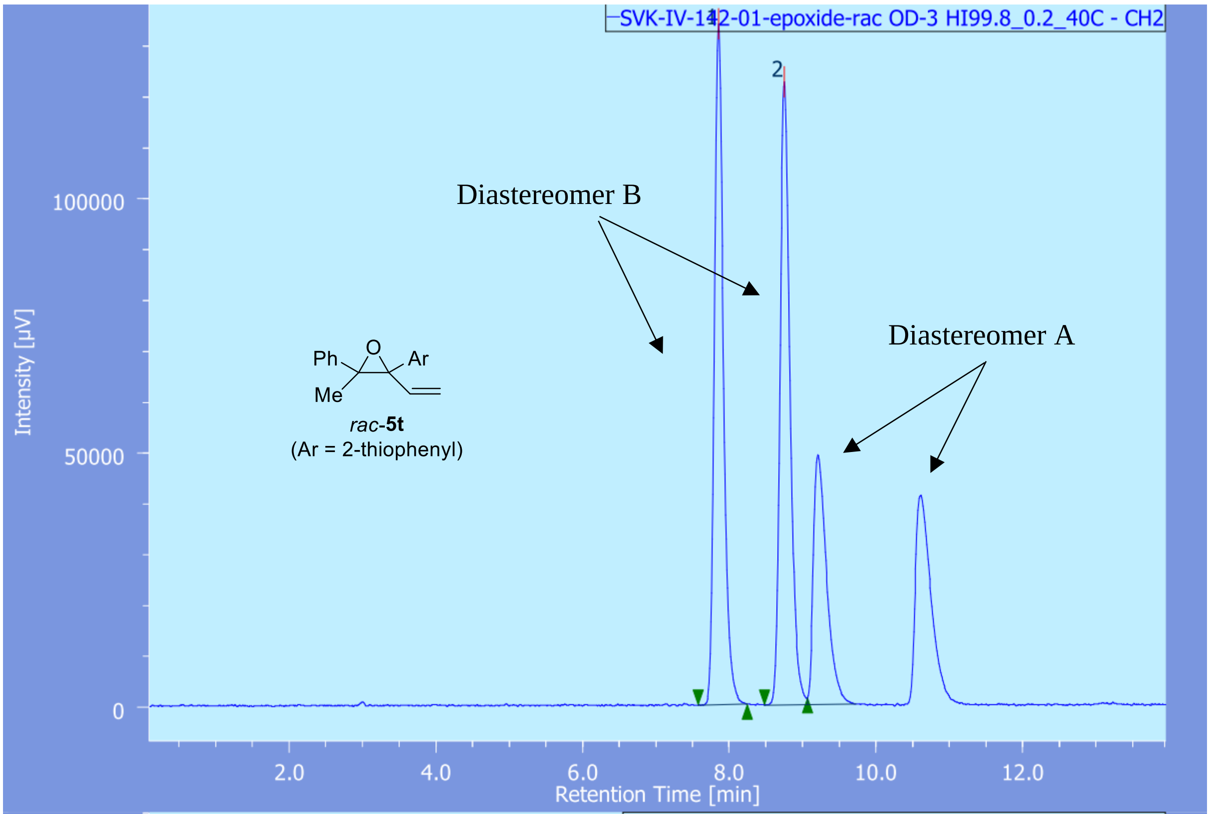


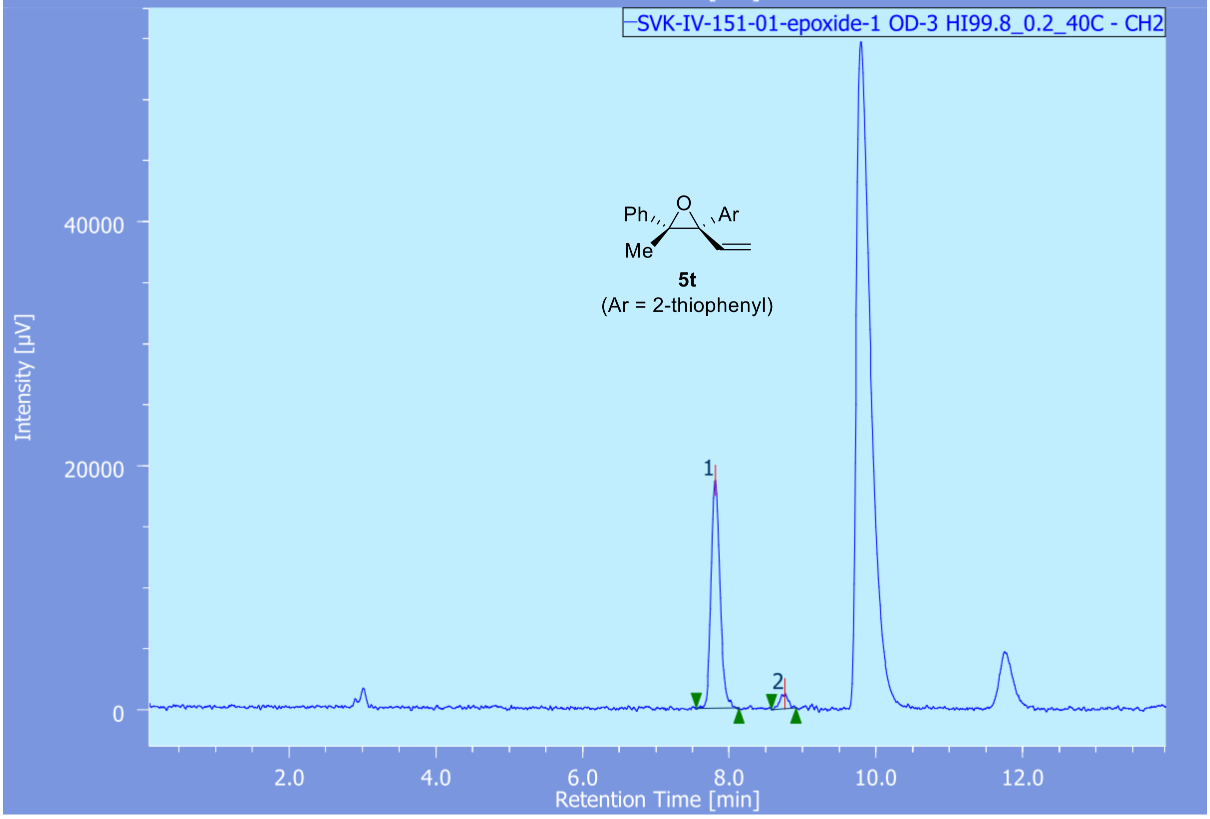
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4s**	13.8	15.1	50.0	50.0
(*R*,*E*)-**4s**	13.8	15.1	0.1	99.9



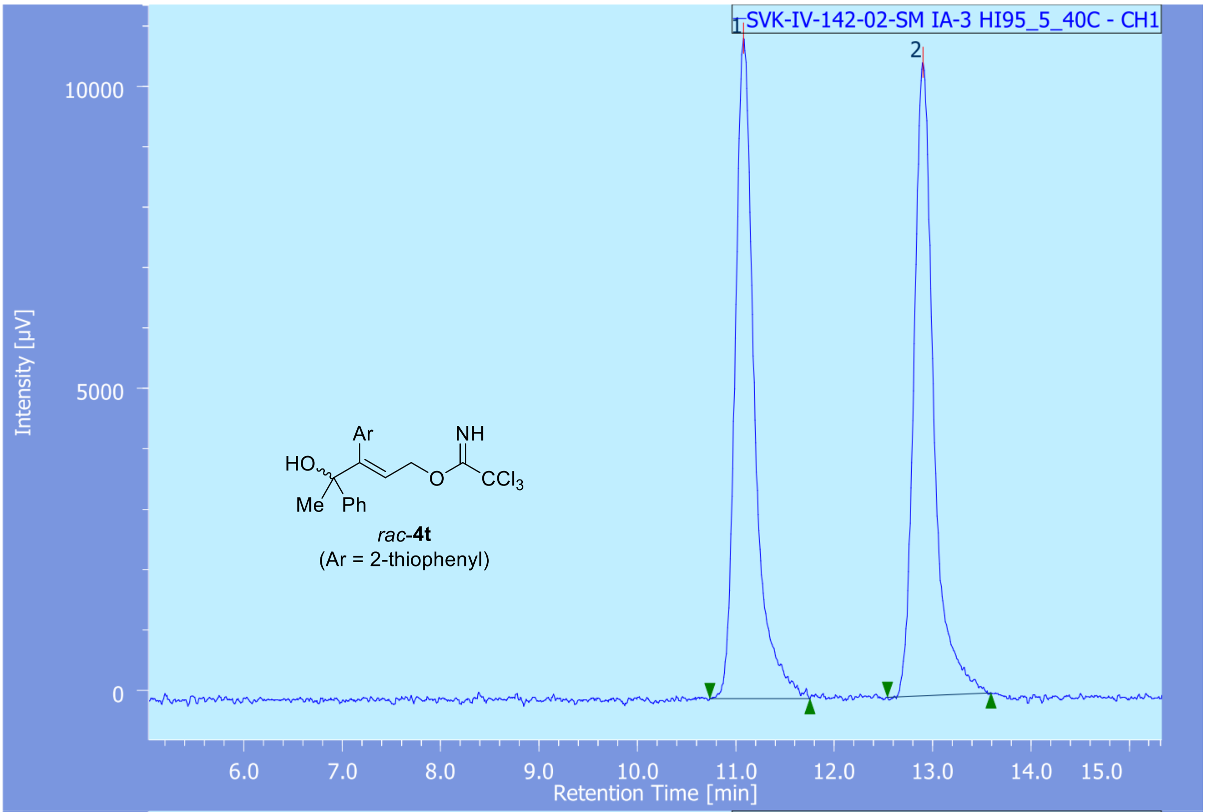


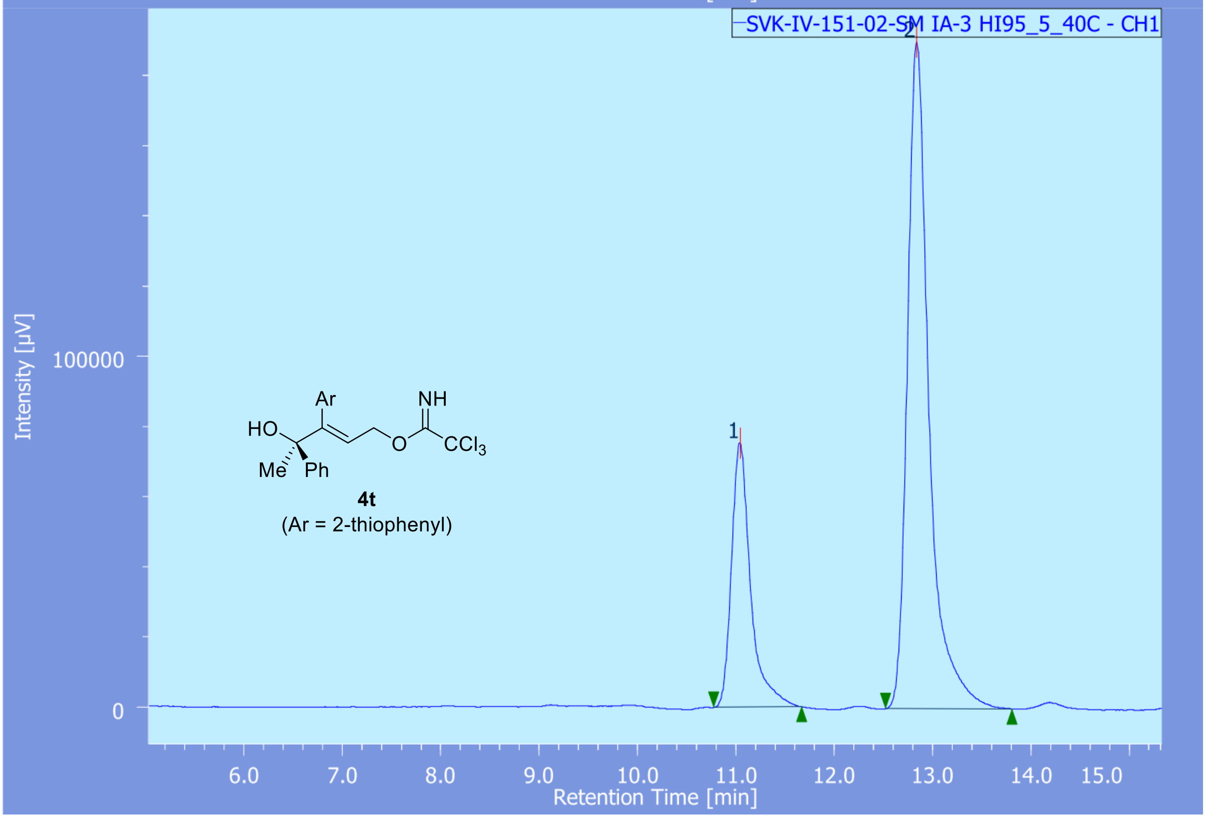
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
***rac*-5t major**	9.2	10.6	50.5	49.5
(2*S*,3*S*)-**5t**	9.8	11.8	92.9	7.1



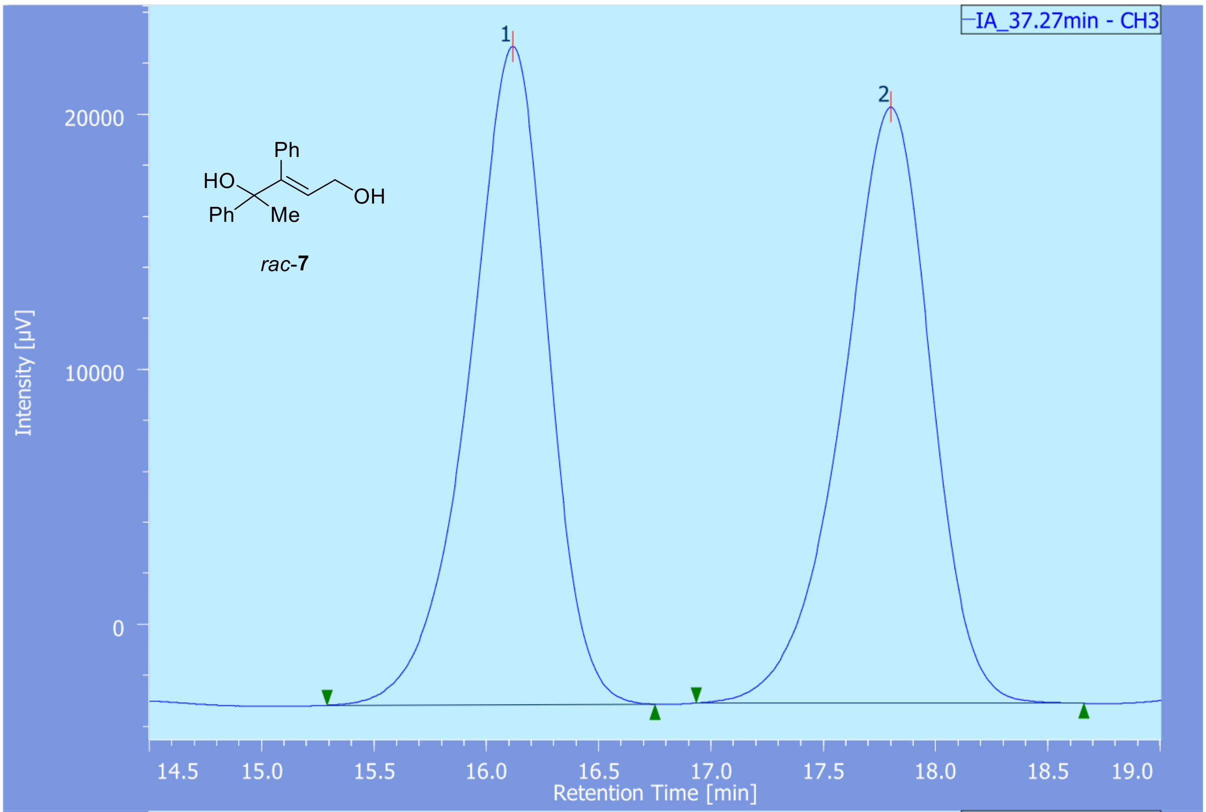


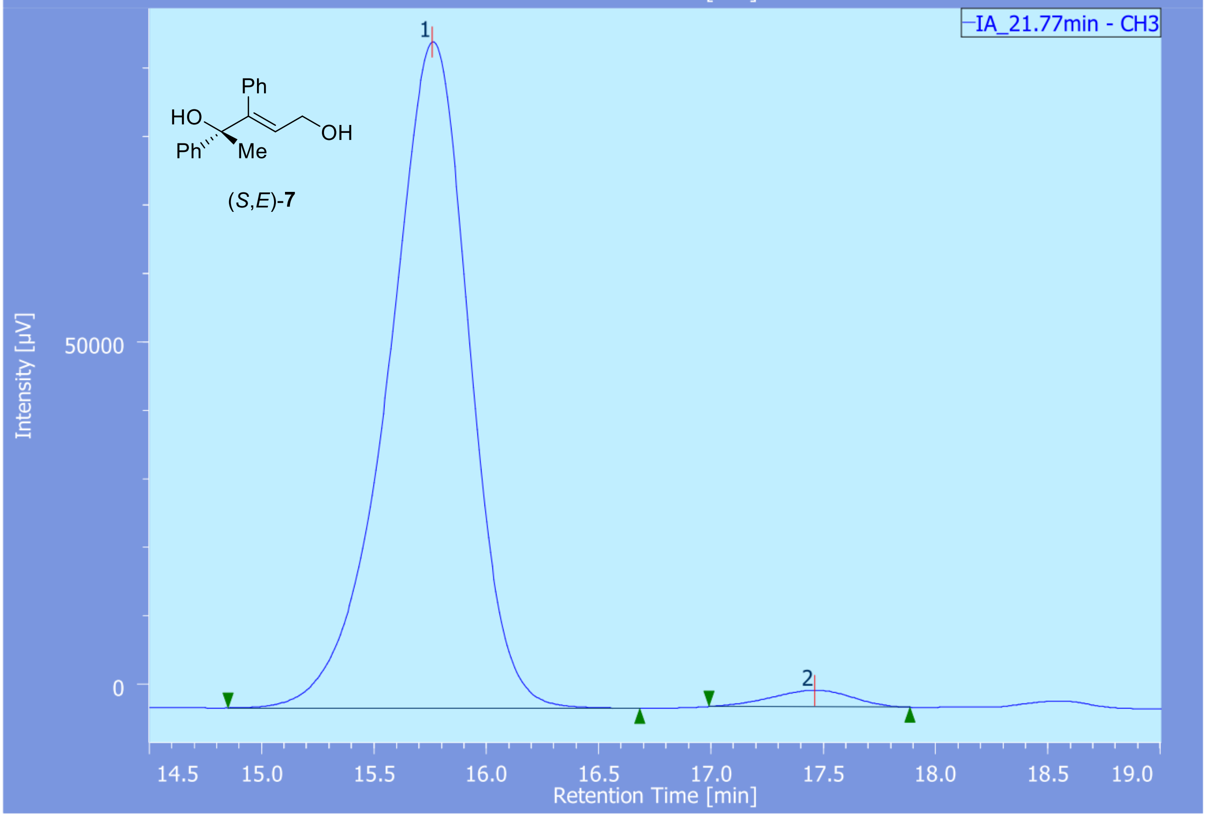
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**5t minor**	7.9	8.8	49.9	50.1
(2*S*,3*S*)-**5t**	7.8	8.8	94.0	6.0



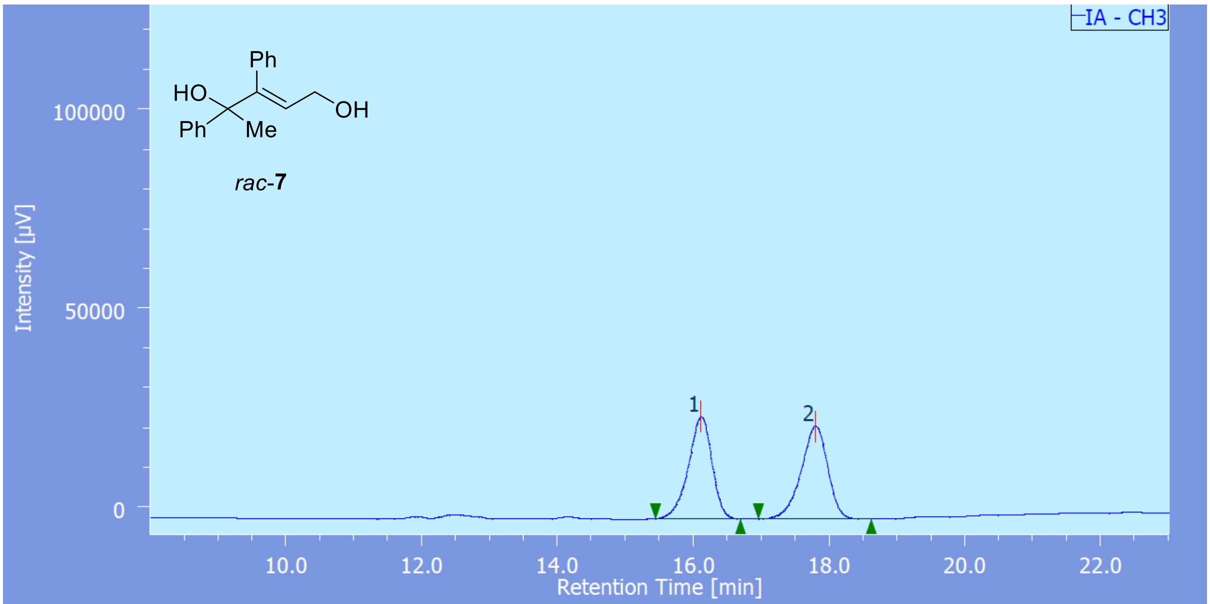


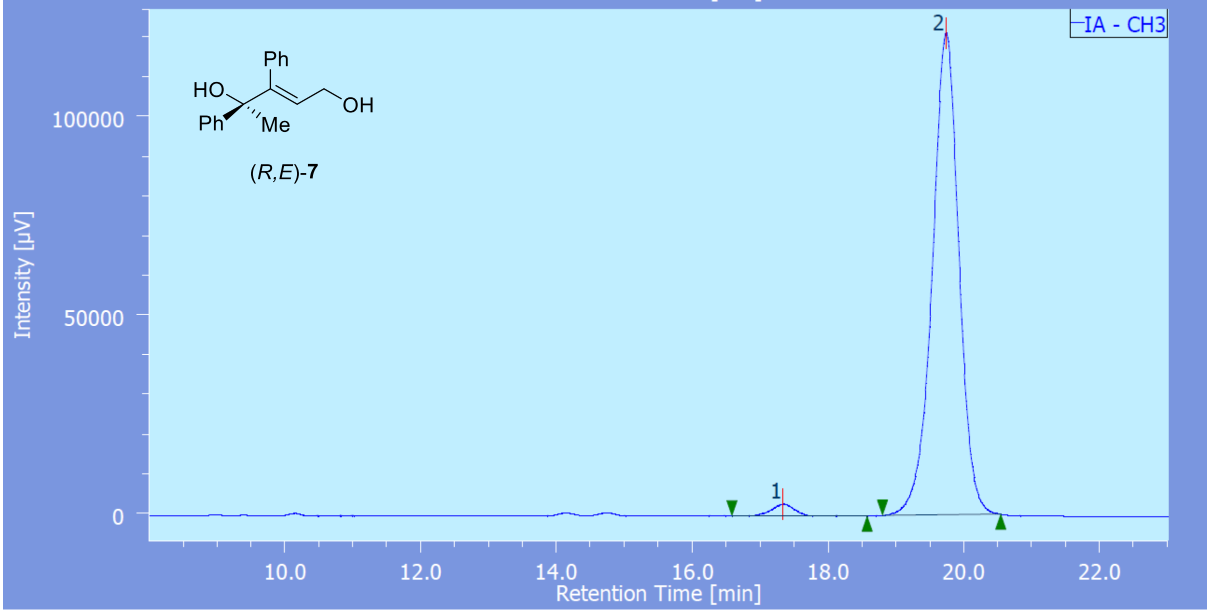
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**4t**	11.1	12.9	50.4	49.6
(*R*,*Z*)-**4t**	11.0	12.8	26.0	74.0



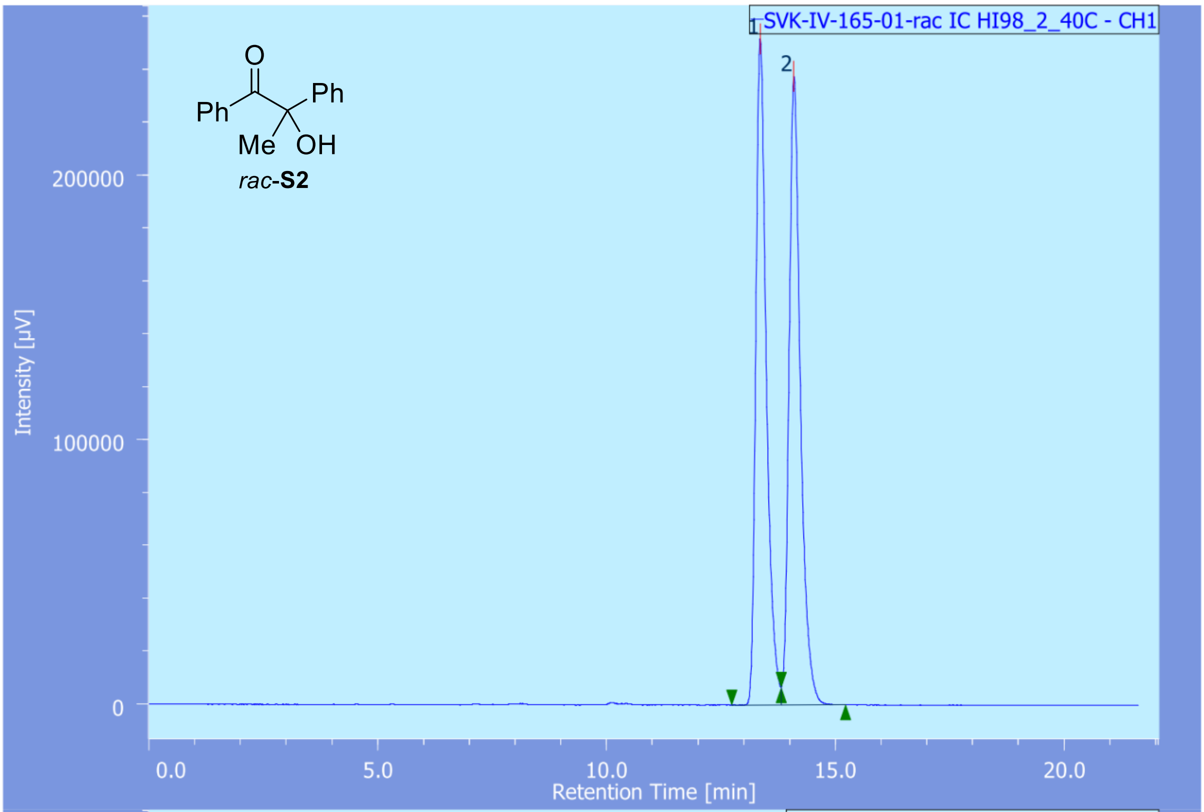


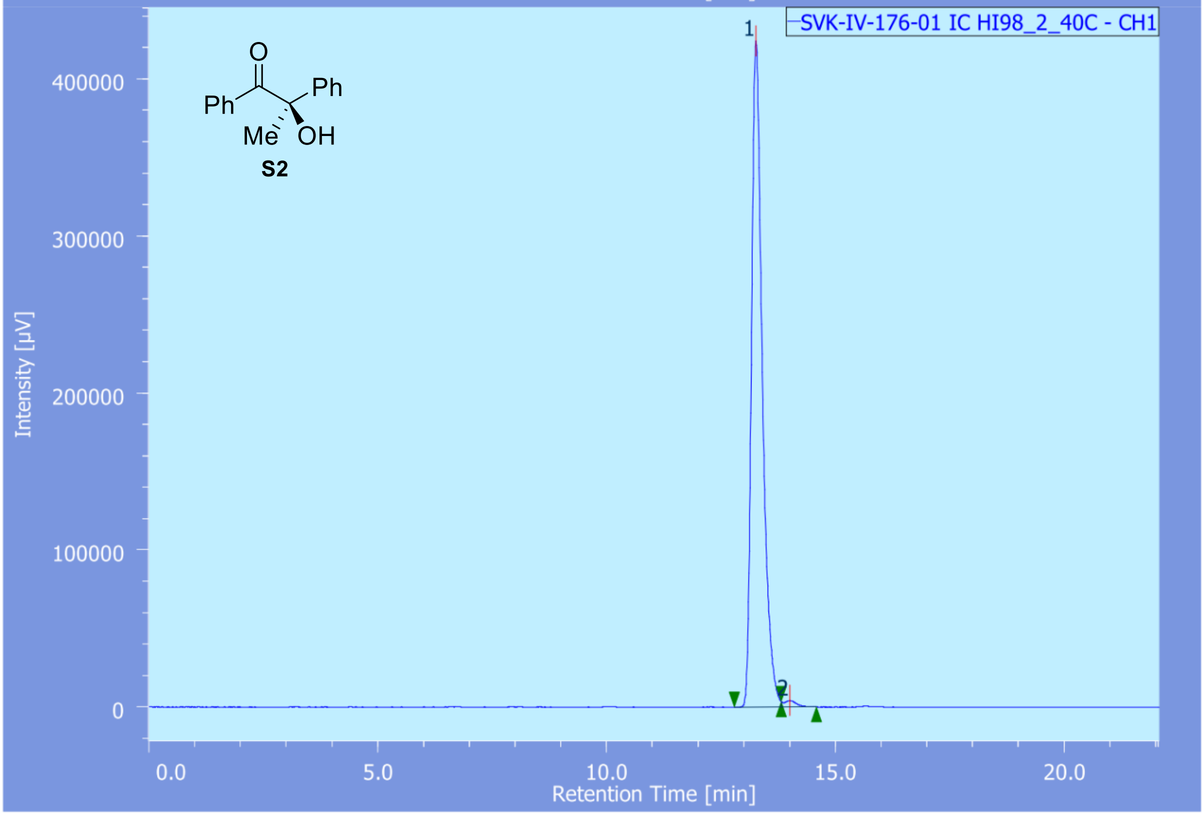
	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**7**	16.1	17.8	49.7	50.3
(*S*,*E*)-**7**	15.8	17.5	97.6	2.4





	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**7**	16.1	17.8	49.7	50.3
(*R*,*E*)-**7**	17.3	19.7	97.2	2.8





	Retention time (1)	Retention time (2)	% Area (1)	% Area (2)
rac-**S2**	13.4	14.1	49.7	50.3
(*R*)-**S2**	13.3	14.0	98.9	1.1

13. Reference

Complete Reference of Gaussian 16 (Ref. 22)

Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.