Supporting Information

Chiral Benzazaborole as Catalyst for Enantioselective Sulfonylation of *cis*-1,2-Diols

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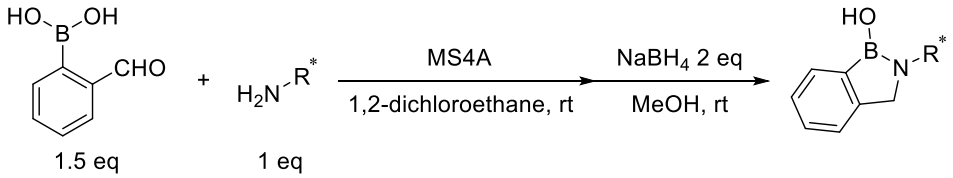
Contents

1. General

Dry solvents were purchased from commercial suppliers and used without further purification. Analytical thin-layer chromatography (TLC) was performed on glass plates coated with 0.25 mm 230-400 mesh silica gel containing a fluorescent indicator (Merck, #1.05715.0009). Silica gel column chromatography was performed on Kanto silica gel 60 (spherical, 100-210 μm). Alumina column chromatography was performed on aluminium oxide 90 active neutral (Merck, #1.01077.1000). Preparative thin-layer chromatography was performed on glass plates coated with 1 mm 230-400 mesh silica gel. IR spectra were recorded on JASCO FT/IR-4100 using ATR. ^{1}H-NMR spectra were recorded on JEOL ECS-400 (400 MHz), ECA-500 (500 MHz), ECX-400 (400 MHz) spectrometers. Chemical shifts of ^{1}H-NMR spectra were reported relative to tetramethyl silane (δ 0). ^{13}C-NMR spectra were recorded on JEOL ECS-400 (100 MHz), ECA-500 (125 MHz), ECX-400 (100 MHz) spectrometers. Chemical shifts of ^{13}C-NMR spectra were reported relative to $CDCl_3$ (δ 77.0). Splitting patterns were reported as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad.

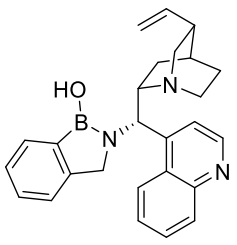
2. Synthesis of chiral Benzazaboroles and boronic acid catalysts

A. 1a, 1b, 1c, 1d and 1e



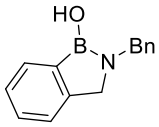
2-Formylphenylboronic acid (1.5 eq), amine (1 eq), 4A molecular sieves and 1,2-dichloroethane (0.35 M) were added to a round-bottom flask containing a stir bar under Ar. After being stirred for appropriate time at room temperature, 4A molecular sieves were removed from the mixture by filtration, and the filtrate in one-necked round-bottom flask was concentrated under reduced pressure. The residue was dissolved in MeOH (0.35 M), and sodium borohydride (2 eq) was added portionwise at 0 °C. After being stirred for 10 minutes at 0 °C, the mixture was further stirred for appropriate time at room temperature. The reaction was quenched by the addition of water at 0 °C, and the aqueous layer was extracted with dichloromethane 5 times. The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. After purification by alumina column chromatography (Chloroform/methanol = 1/0 to 100/1), corresponding catalysts were obtained.

2-((*S*)-quinolin-4-yl((1*S*,2*S*,4*S*,5*R*)-5-vinylquinuclidin-2-yl)methyl)-2,3-dihydro-1*H*-benzo[*c*][1,2]azaborol-1-ol (1a)



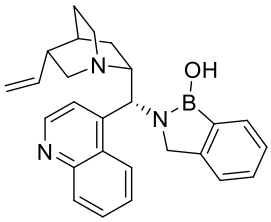
Cinchonidinee-derived amine was used; reaction time: 22 h for Schiff base formation, 4 h for reduction; white solids (72% yield); **^{1}H NMR** (400 MHz, CD_3OD): δ 8.94 (d, *J* = 4.5 Hz, 1H), 8.44 (d, *J* = 7.7 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.86-7.71 (m, 3H), 7.49 (d, *J* = 6.6 Hz, 1H), 7.20-6.96 (m, 2H), 6.86 (br s, 1H), 6.00-5.76 (m, 1H), 5.27-4.95 (m, 3H), 3.88 (br, 2H), 3.59-3.21 (m, 3H), 3.05-2.67 (m, 2H), 2.36 (br s, 1H), 1.62 (br s, 3H), 1.40-1.28 (m, 1H), 0.73 (br s, 1H); **^{13}C NMR** (100 MHz, CD_3OD): δ 150.8, 149.1, 144.9, 142.6, 134.1, 131.2, 130.2, 129.6, 128.6, 128.3, 127.9, 124.8, 121.6, 115.0, 61.3, 56.6, 52.2, 41.9, 40.8, 28.7, 28.4, 26.6; **IR** (neat) 3255, 3060, 3001, 2941, 1593, 1446, 1392, 1360, 1218, 745 cm^{-1}; **HRMS** (ESI+) calcd for $C_{26}H_{29}BN_3O$ $[M + H]^+$ 410.2404: found 410.2394; **$[\alpha]_D^{24}$** = +36.8 (*c* = 1.0, $CHCl_3$).

2-benzyl-2,3-dihydro-1H-benzo[c][1,2]azaborol-1-ol (1b)



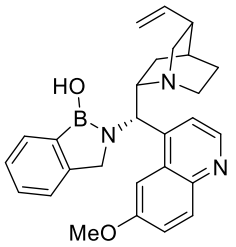
Benzyl amine was used; reaction time: 16 h for Schiff base formation, 3 h for reduction; white solids (56% yield); **^{1}H NMR** (400 MHz, CD_3OD): δ 8.28 (s, 1H), 7.48-7.18 (m, 9H), 4.39 (s, 2H), 3.87 (s, 2H); **^{13}C NMR** (100 MHz, CD_3OD): δ 142.2, 136.1, 131.6, 130.8, 129.9, 129.4, 128.3, 127.6, 124.3, 54.1, 52.2; **IR** (neat) 3240, 3071, 3038, 1452, 1354, 1289, 1218, 1180, 741, 702 cm^{-1}; **HRMS** (ESI+) calcd for $C_{14}H_{17}BNO_2$ $[M + H_3O]^+$ 242.1352: found 242.1347.

2-((*R*)-quinolin-4-yl((1*S*,2*R*,4*S*,5*R*)-5-vinylquinuclidin-2-yl)methyl)-2,3-dihydro-1*H*-benzo[c][1,2]azaborol-1-ol (1c)



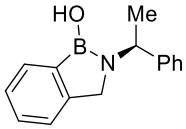
Cinchonine-derived amine was used; reaction time: 14 h for Schiff base formation, 2 h for reduction; white solids (30% yield); **^{1}H NMR** (400 MHz, CD_3OD): δ 8.97 (d, *J* = 4.7 Hz, 1H), 8.64-8.23 (m, 1H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.97-7.69 (m, 3H), 7.60-7.42 (m, 1H), 7.36-6.68 (m, 3H), 5.96-5.76 (m, 1H), 5.32-5.02 (m, 3H), 3.97 (br s, 2H), 3.07 (s, 4H), 2.39 (br s, 1H), 1.66 (br s, 4H), 1.09 (m, 2H); **^{13}C NMR** (100 MHz, CD_3OD): δ 150.9, 149.2, 144.4, 141.2, 134.1, 131.4, 130.3, 129.5, 128.7, 128.1, 127.8, 124.8, 121.6, 115.3, 61.3, 51.8, 40.4, 38.3, 29.0, 27.1, 26.4, 25.9, 12.5; **IR** (neat) 2935, 2865, 1593, 1452, 1387, 1360, 751 cm^{-1}; **HRMS** (ESI+) calcd for $C_{26}H_{29}BN_3O$ $[M + H]^+$ 410.2398: found 410.2404; **$[\alpha]_D^{17}$** = +78.4 (*c* = 0.5, $CHCl_3$).

2-((*S*)-(6-methoxyquinolin-4-yl)((1*S*,2*S*,4*S*,5*R*)-5-vinylquinuclidin-2-yl)methyl)-2,3-dihydro-1*H*-benzo[*c*][1,2]azaborol-1-ol (1d)



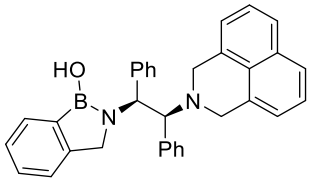
Quinine-derived amine was used; reaction time: 15 h for Schiff base formation, 5 h for reduction; white solids (35% yield);**^{1}H NMR** (400 MHz, CD_3OD): δ 7.61-7.24 (m, 7H), 7.24-7.13 (m, 2H), 7.07 (d, J = 7.0 Hz, 1H), 3.98 (s, 2H), 3.86 (s, 2H); **^{13}C NMR** (100 MHz, CD_3OD): δ 158.7, 146.8, 144.0, 141.4, 132.9, 130.4, 129.5, 126.6, 122.6, 120.4, 113.8, 101.5, 59.9, 55.4, 55.1, 50.4, 48.6, 40.6, 39.5, 27.5, 27.3, 25.4, 11.1; **IR** (neat) 3370, 2484, 2229, 2065, 1473, 1370, 1120, 974 cm^{-1}; **HRMS** (ESI+) calcd for $C_{27}H_{31}BN_3O_2$ $[M + H]^+$ 440.2509: found 440.2505; **$[\alpha]_D^{24}$** = +13.8 (*c* = 1.0, $CHCl_3$).

(*S*)-2-(1-phenylethyl)-2,3-dihydro-1*H*-benzo[*c*][1,2]azaborol-1-ol (1e)



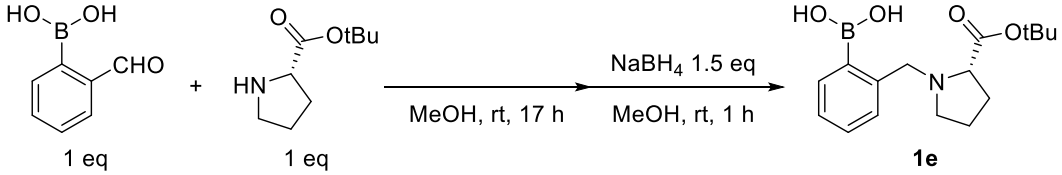
(*S*)-(-)-1-Phenylethylamine was used; reaction time: 20 h for Schiff base formation, 2 h for reduction; white solids (50% yield);**^{1}H NMR** (400 MHz, DMSO-D6): δ 8.23 (s, 1H), 7.69 (d, *J* = 7.0 Hz, 1H), 7.39-7.16 (m, 8H), 4.89 (q, *J* = 7.0 Hz, 1H), 4.00 (d, *J* = 16.6 Hz, 1H), 3.65 (d, *J* = 16.6 Hz, 1H), 1.60 (d, J = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, CD_3OD): δ 141.3, 140.5, 133.0, 130.0, 129.5, 128.6, 127.9, 126.6, 58.9, 53.8, 20.9; **IR** (neat) 3294, 3001, 1446, 1337, 1300, 1218, 1186, 1110, 908, 751, 708 cm^{-1}; **HRMS** (ESI+) calcd for $C_{15}H_{19}BNO_2$ $[M + H_3O]^+$ 256.1503: found 256.1502; **$[\alpha]_D^{24}$** = **–**2.1 (*c* = 1.0, $CHCl_3$).

2-((1*S*,2*S*)-2-(1H-benzo[de]isoquinolin-2(3H)-yl)-1,2-diphenylethyl)-2,3-dihydro-1*H*-benzo[*c*][1,2]azaborol-1-ol (1f)



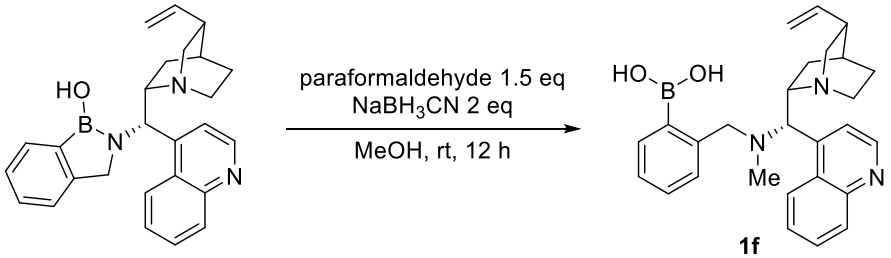
(1*S*,2*S*)-2-(1*H*-benzo[*de*]isoquinolin-2(3*H*)-yl)-1,2-diphenylethan-1-amine was used; reaction time: 16 h for Schiff base formation, 2 h for reduction; white solids (11% yield);**^{1}H NMR** (400 MHz, CD_3OD): δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 7.0 Hz, 2H), 7.40-7.12 (m, 13H), 7.05 (t, *J* = 6.8 Hz, 1H), 6.92 (td, *J* = 6.1, 1.4 Hz, 1H), 6.66 (d, *J* = 7.7 Hz, 1H), 5.22 (d, *J* = 11.8 Hz, 1H), 4.72 (d, *J* = 11.8 Hz, 1H), 4.24 (d, *J* = 13.8 Hz, 2H), 3.93 (s, 2H), 3.85 (d, *J* = 12.5 Hz, 2H); **^{13}C NMR** (100 MHz, CD_3OD): δ 136.4, 135.1, 134.5, 133.7, 132.9, 131.6, 131.3, 129.7, 129.5, 129.2, 129.0, 128.9, 128.3, 128.0, 127.4, 127.0, 126.6, 123.1, 72.5, 60.4, 54.2, 51.4; **IR** (neat) 33358, 3060. 3038, 2935, 2506, 2224, 2077, 1446, 1376, 1110, 968, 751, 702 cm^{-1}; **HRMS** (ESI+) calcd for $C_{33}H_{30}BN_2O$ $[M + H]^+$ 481.2451: found 481.2439; **$[\alpha]_D^{24}$** = +46.5 (*c* = 1.0, $CHCl_3$).

B. (*S*)-(2-((2-(*tert*-butoxycarbonyl)pyrrolidin-1-yl)methyl)phenyl)boronic acid (1g)



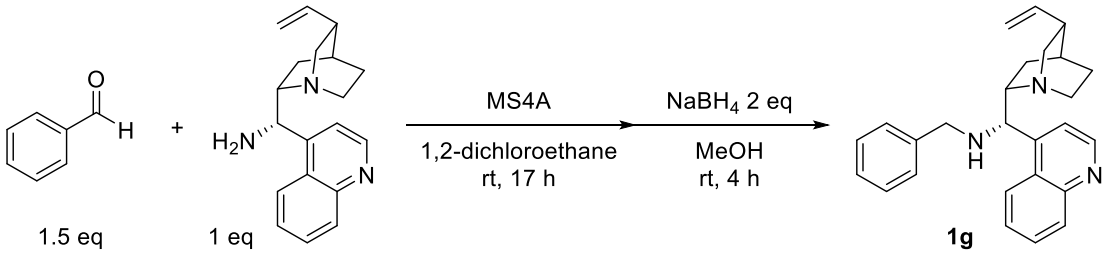
2-Formylphenylboronic acid (1 mmol, 1 eq), L-proline *tert*-butyl ester (1 mmol, 1 eq) and methanol (7.4 ml) were added to a round-bottom flask containing a stir bar under Ar. After being stirred for 17 h at room temperature, sodium borohydride (1.5 mmol, 1.5 eq) was added portionwise at 0 °C. After being stirred for 10 minutes at 0 °C, the mixture was further stirred for 1 h at room temperature. The reaction mixture was concentrated under reduced pressure and directly purified by alumina column chromatography (Chloroform). product was obtained as white solids (51% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.02 (br, 2H), 7.93-7.85 (m, 1H), 7.35-7.29 (m, 2H), 7.23-7.14 (m, 1H), 3.92 (d, *J* = 12.0 Hz, 1H), 3.82 (d, *J* = 12.0 Hz, 1H), 3.33-3.15 (m, 1H), 3.12-2.96 (m, 1H), 2.64-2.51 (m, 1H), 2.22-2.12 (m, 1H), 2.01-1.76 (m, 3H), 1.34 (s, 9H); **^{13}C NMR** (100 MHz, CD_3OD): δ 172.1, 142.1, 142.0, 131.7, 127.6, 126.3, 125.0, 80.8, 64.9, 57.6, 53.3, 28.8, 27.8, 22.5; **IR** (neat) 3341, 3012, 2980, 1730, 1338, 1216, 750 cm^{-1}; **HRMS** (ESI+) calcd for $C_{16}H_{25}O_4NB$ [M + H]$^+$ 306.1871: found 306.1868; **[α]$_D^{24}$** = -50.4 (*c* = 1.0, $CHCl_3$).

C. (2-((methyl((S)-quinolin-4-yl((1*S*,2*S*,4*S*,5*R*)-5-vinylquinuclidin-2-yl)methyl)amino)methyl)phenyl)boronic acid (1h)



1a (0.51 mmol, 1 eq), paraformaldehyde (0.77 mmol, 1.5 eq) and methanol (1.5 ml) was added to a round-bottom /flask containing a stir bar under Ar. The mixture was cooled to 0 °C, and sodium cyanoborohydride (1.02 mmol, 2 eq) was slowly added. After being stirred for 12 h at room temperature, the reaction was quenched by the addition of water at 0 °C. The aqueous layer was extracted with dichloromethane 5 times. The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. After purification by alumina column chromatography (Chloroform and Chloroform/methanol = 1/0 to 100/1), product was obtained as white solids (83% yield). **^{1}H NMR** (400 MHz, CD_3Cl): δ 8.98 (d, J = 3.6 Hz, 1H), 8.16 (d, *J* = 8.3 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 3.6 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.35-7.00 (m, 5H), 5.84-5.51 (m, 1H), 5.21-4.63 (m, 2H), 4.52 (d, *J* = 9.7 Hz, 1H), 3.62 (d, *J* = 13.7 Hz, 1H), 3.35 (d, *J* = 13.7 Hz, 1H), 3.18 (dd, *J* = 13.7, 10.1 Hz, 1H), 3.07-2.56 (m, 4H), 2.21 (br s, 1H), 1.80-1.39 (m, 3H), 1.22-1.01 (m, 1H), 0.91-0.62 (m, 1H); **^{13}C NMR** (100 MHz, CD_3Cl, 50 °C): δ 149.4, 148.8, 142.2, 141.9, 141.3, 135.3, 130.6, 130.3, 129.1, 128.8, 127.1, 126.6, 123.4, 119.9, 114.2, 61.1, 58.5, 58.1, 56.3, 55.8, 40.9, 39.6, 35.8, 28.0, 27.5, 27.2, 17.3; **IR** (neat) 2944, 2865, 1443, 1376, 1346, 905, 725, 647 cm^{-1}; **HRMS** (ESI+) calcd for $C_{27}H_{33}BN_3O_2$ [M + H]$^+$ 442.2666: found 442.2643; **[α]$_D^{25}$** = +13.3 (*c* = 1.0, $CHCl_3$).

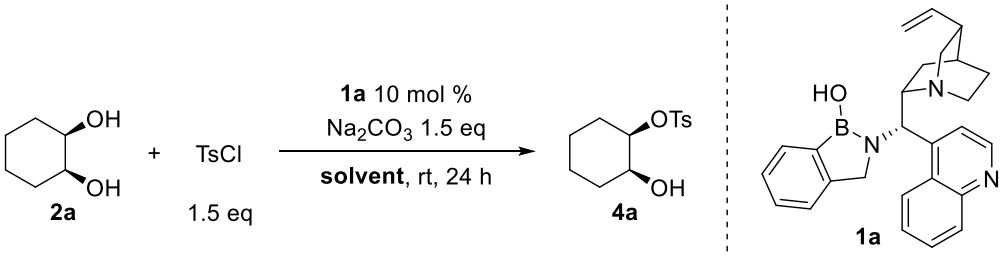
D. (*S*)-N-benzyl-1-(quinolin-4-yl)-1-((1*S*,2*S*,4*S*,5*R*)-5-vinylquinuclidin-2-yl)methanamine (1i)



Benzaldehyde (1.5 eq), chinchonidine-derived amine (1 eq), 4A molecular sieves and 1,2-dichloroethane (0.35 M) were added to a round-bottom flask containing a stir bar under Ar. After being stirred for 17 h at room temperature, 4A molecular sieves were removed from the mixture by filtration, and the filtrate in one-necked round-bottom flask was concentrated under reduced pressure. The residue was dissolved in MeOH (0.35 M), and sodium borohydride (2 eq) was added portionwise at 0 °C. After being stirred for 10 minutes at 0 °C, the mixture was further stirred for 4 h at room temperature. The reaction was quenched by the addition of water at 0 °C, and the aqueous layer was extracted with dichloromethane 5 times. The combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure. After purification by silica gel column chromatography column chromatography (hexane/ethyl acetate = 1/5), product was obtained as colorless oil (66% yield).**^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.98 (d, *J* = 3.6 Hz, 1H), 8.16 (d, *J* = 8.3 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 3.6 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.41-6.92 (m, 5H), 5.97-5.50 (m, 1H), 5.23-4.73 (m, 2H), 4.52 (d, *J* = 9.7 Hz, 1H), 3.62 (d, *J* = 13.7 Hz, 1H), 3.35 (d, *J* = 13.7 Hz, 1H), 3.21-3.15 (m, 1H), 3.10-2.40 (m, 4H), 2.21 (br s, 1H), 1.71-1.36 (m, 3H), 1.22-1.01 (m, 1H), 0.98-0.60 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.5, 148.5, 148.1, 141.6, 140.3, 130.3, 128.8, 128.7, 128.1, 128.0, 126.7, 126.0, 122.5, 119.9, 114.0, 62.4, 55.9, 55.7, 50.8, 40.7, 39.7, 27.9, 27.3, 25.0; **IR** (neat) 2941, 2865, 2250, 2213, 1446, 914, 724, 642 cm^{-1}; **HRMS** (ESI+) calcd for $C_{26}H_{30}N_3$ $[M+H]^+$ 384.2434: found 384.2427; **$[\alpha]_D^{25}$** = +91.5 (*c* = 1.0, $CHCl_3$).

3.Optimization of reaction conditions

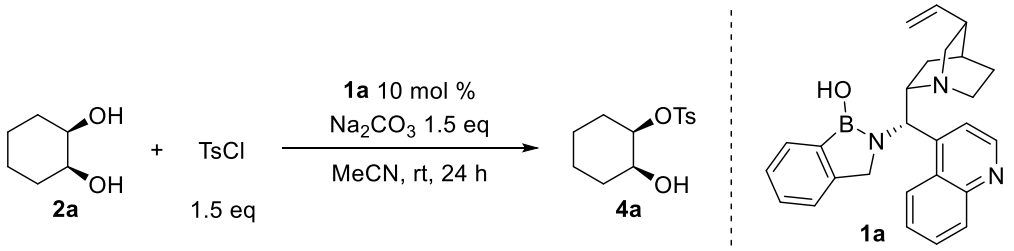
3-1. Screening of solvent



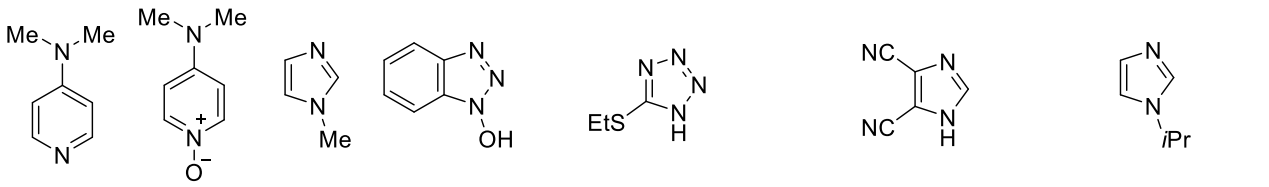
entry	solvent	yield (%)	ee (%)
1	MeCN	45	70
2	$CHCl_3$	13	–12
3	toluene	6	–51
4	THF	11	47
5	DMF	trace	N.D.

cis-1,2-Cyclohexanediol **2a** (0.1 mmol, 1 eq), sodium carbonate (0.15 mmol, 1.5 eq), catalyst **1a** (0.01 mmol, 10 mol %), and tosyl chloride **3a** (0.15 mmol, 1.5 eq) were added to a round-bottom flask containing a stir bar under Ar. To the flask, **solvent** (0.5 ml) was added. After being stirred for 24 h, water was added to the reaction mixture, and then the aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate =2/1) to afford product **4a**. The enantiomeric excesses of the product were determined by chiral stationary phase HPLC using Daicel Chiralcel OJ-H column.

3-2. Screening of nucleophilic co-catalysts

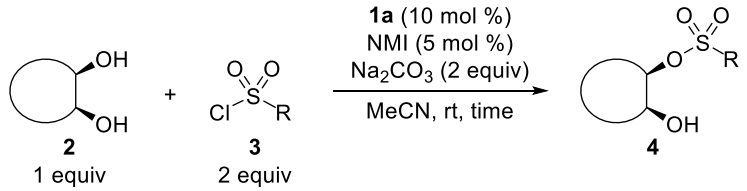


entry	**co-catalyst**	time (h)	yield (%)	ee (%)
1	DMAP	25	44	75
2	DMAP oxide	24	85	79
3	NMI	13	92	83
4	HOBt	13	35	69
5	5-(Ethylthio)-1*H*-tetrazole	18	27	*rac*
6	4,5-Dicyanoimidazole	19	84	72
7	*N*-Isopropylimidazole	16	86	71



cis-1,2-Cyclohexanediol **2a** (0.1 mmol, 1 eq), sodium carbonate (0.2 mmol, 2 eq), catalyst **1a** (0.01 mmol, 10 mol %), **co-catalyst** (0.005 mmol, 5 mol %) and tosyl chloride **3a** (0.2 mmol, 2 eq) were added to a round-bottom flask containing a stir bar under Ar. To the flask, acetonitrile (0.5 ml) was added. After being stirred for appropriate time, water was added to the reaction mixture, and then the aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate =2/1) to afford product **4a**. The enantiomeric excesses of the product were determined by chiral stationary phase HPLC using Daicel Chiralcel OJ-H column.

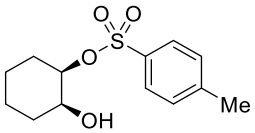
4. General procedure for enantioselective sulfonylation of *cis*-1,2-diols



Diol **2** (0.2 mmol, 1 eq), sodium carbonate (0.4 mmol, 2 eq), catalyst **1a** (0.02 mmol, 10 mol%), and sulfonyl chloride **3** (0.4 mmol, 2 eq) were added to a one-necked round-bottom flask containing a stir bar, under Ar atmosphere. To the flask, 10 mM solution of 1-methylimidazole (NMI) in acetonitrile (1.0 ml, 0.01 mmol, 5 mol%) was added. After stirring for the appropriate length of time at room temperature, water was added to the reaction mixture, and then, the aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate = 3:1 or 2:1) to afford product **4**. The enantiomeric excesses of the products were determined by chiral stationary phase HPLC on Daicel Chiralpak AS-H, AD-3, and Chiralcel OJ-H columns.

5. Analytical data for products of enantioselective sulfonylation of *cis*-1,2-diols

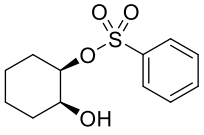
(1*R*,2*S*)-2-hydroxycyclohexyl 4-methylbenzenesulfonate (4a)



Reaction time: 13 h; colorless oil (50.9 mg, 92% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 4.70-4.61 (m, 1H), 3.83 (br, 1H), 2.46 (s, 3H), 2.01 (d, *J* = 5.0, H), 1.95-1.87 (m, 1H), 1.78-1.71 (m, 1H), 1.67-1.47 (m, 4H), 1.34-1.25 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.9, 133.8, 129.9, 127.7, 123.9, 122.4, 80.6, 67.0, 31.4, 28.4, 21.6; **IR** (neat) 3418, 2945, 2870, 1343, 1174, 930, 892, 669 cm^{-1}; **HRMS** (ESI+) calcd for $C_{13}H_{18}O_4NaS$ $[M + Na]^+$ 293.0818: found 293.0812; $[\alpha]_D^{22}$ = +3.4 (*c* = 1.0, $CHCl_3$, 81% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 13.5 min, major enantiomer t_R = 12.1 min, 81% ee.

(1*R*,2*S*)-2-hydroxycyclohexyl benzenesulfonate (4b)

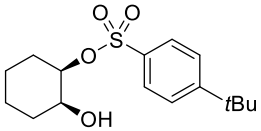


Reaction time: 12 h; colorless oil (25.7 mg, 96% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.3 Hz, 2H), 7.67 (t, *J* = 7.3 Hz, 1H), 7.57 (t, *J* = 7.3 Hz, 2H), 4.69-4.65 (m, 1H), 3.84 (br, 1H), 1.97-1.89 (m, 2H), 1.79-1.72 (m, 1H), 1.68-1.48 (m, 4H), 1.35-1.25 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 137.1, 133.8, 129.3, 127.6, 83.4, 69.1, 30.2, 27.7, 21.6, 20.7; **IR** (neat) 3213, 2945, 2865, 1451, 1355, 1184, 1098, 937, 895 cm^{-1}; **HRMS** (ESI+) calcd for

$C_{12}H_{20}NSO_4$ $[M + NH_4]^+$ 274.1108: found 274.1103; $[\alpha]_D^{23}$ = +3.6 (*c* = 1.0, $CHCl_3$, 84% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 18.2 min, major enantiomer t_R = 15.2 min, 84% ee.

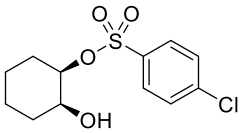
(1*R*,2*S*)-2-hydroxycyclohexyl 4-(*tert*-butyl)benzenesulfonate (4c)



Reaction time: 19 h; colorless oil (54.7 mg, 86% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.8 Hz, 2H), 7.56 (d, *J* = 8.8 Hz, 2H), 4.69-4.65 (m, 1H), 3.85-3.81 (m, 1H), 2.01 (br, 1H), 1.97-1.89 (m, 1H), 1.81-1.73 (m, 1H), 1.68-1.51 (m, 4H), 1.35 (s, 9H), 1.33-1.25 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 157.6, 134.0, 127.4, 126.2, 83.1, 68.9, 35.2, 31.0, 30.2, 27.7, 21.7, 20.7; **IR** (neat) 3555, 2956, 1344, 1189, 943, 900, 761 cm^{-1}; **HRMS** (ESI+) calcd for $C_{16}H_{28}O_4NS$ $[M + NH_4]^+$ 330.1734: found 330.1730; $[\alpha]_D^{23}$ = +4.2 (*c* = 1.0, $CHCl_3$, 77% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AS-H column (hexane:2-propanol = 95:5, 1.0 mL/min, 254 nm); minor enantiomer t_R = 24.7 min, major enantiomer t_R = 20.4 min, 77% ee.

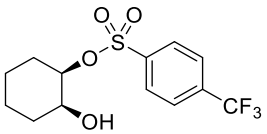
(1R,2S)-2-hydroxycyclohexyl 4-chlorobenzenesulfonate (4d)



Reaction time: 13 h; colorless oil (54.8 mg, 90% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.6 Hz, 2H), 7.54 (d, *J* = 8.8 Hz, 2H), 4.70-4.67 (m, 1H), 3.86-3.84 (m, 1H), 1.98-1.90 (m, 1H), 1.82-1.49 (m, 6H), 1.36-1.25 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 140.3, 135.6, 129.5, 129.1, 83.8, 69.0, 30.2, 27.8, 21.5, 20.8; **IR** (neat) 3534, 2951, 2865, 1350, 1189, 1092, 932, 900 cm^{-1}; **HRMS** (ESI+) calcd for $C_{12}H_{15}O_4ClNaS$ $[M + Na]^+$ 313.0272: found 313.0267; $[\alpha]_D^{23}$ = +1.9 (*c* = 1.0, $CHCl_3$, 80% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 17.1 min, major enantiomer t_R = 11.2 min, 80% ee.

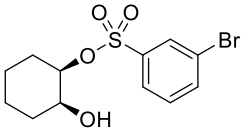
(1*R*,2*S*)-2-hydroxycyclohexyl 4-(trifluoromethyl)benzenesulfonate (4e)



Reaction time: 14 h; colorless oil (53.6 mg, 82% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.08 (d, *J* = 8.2 Hz, 2H), 7.83 (d, *J* = 8.4 Hz, 2H), 4.78-4.75 (m, 1H), 3.88-3.86 (m, 1H), 2.01-1.93 (m, 1H), 1.81-1.71 (m, 1H), 1.68-1.52 (m, 4H), 1.38-1.30 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 140.8, 135.3 (d, *J* = 33.5 Hz), 128.2, 126.4 (d, *J* = 3.8 Hz), 123.0 (d, *J* = 274.0 Hz), 84.3, 69.0, 30.2, 27.9, 21.5, 20.8; **IR** (neat) 3424, 2941, 2870, 1360, 1333, 1170, 1120, 930, 898, 768 cm^{-1}; **HRMS** (ESI+) calcd for $C_{13}H_{15}O_4F_3NaS$ $[M + Na]^+$ 347.0535: found 347.0526; $[\alpha]_D^{22}$ = +1.8 (*c* = 1.0, $CHCl_3$, 78% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 10.1 min, major enantiomer t_R = 7.6 min, 78% ee.

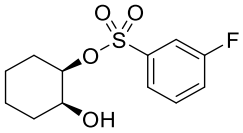
(1*R*,2*S*)-2-hydroxycyclohexyl 3-bromobenzenesulfonate (4f)



Reaction time: 13 h; colorless oil (52.9 mg, 77% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (t, *J* = 1.8 Hz, 1H), 7.89-7.86 (m, 1H), 7.80-7.77 (m, 1H), 7.44 (t, *J* = 7.9 Hz, 1H), 4.73-4.69 (m, 1H), 3.87-3.85 (m, 1H), 1.98-1.92 (m, 1H), 1.79-1.72 (m, 1H), 1.70-1.51 (m, 5H), 1.39-1.30 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 138.9, 136.8, 130.7, 130.5, 126.2, 123.1, 83.9, 69.1, 30.1, 27.9, 21.5, 20.8,; **IR** (neat) 3550, 2940, 2860, 1355, 1178, 927, 900 cm^{-1}; **HRMS** (ESI+) calcd for $C_{12}H_{19}O_4BrS$ $[M + NH_4]^+$ 354.0198: found 354.0187; **$[\alpha]_D^{23}$** = –9.0 (*c* = 0.5, $CHCl_3$, 73% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 27.6 min, major enantiomer t_R = 24.7 min, 73% ee.

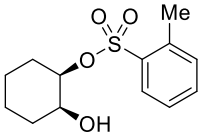
(1*R*,2*S*)-2-hydroxycyclohexyl 3-fluorobenzenesulfonate (4g)



Reaction time: 13 h; colorless oil (52.4 mg, 95% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 7.9 Hz, 1H), 7.65 (td, *J* = 7.9, 2.3 Hz, 1H), 7.67-7.64 (m, 1H), 7.37 (dt, *J* = 3.4, 8.3 Hz, 1H), 4.76-4.69 (m, 1H), 3.87-3.85 (m, 1H), 2.10-1.91 (m, 2H), 1.81-1.72 (m, 1H), 1.70-1.50 (m, 4H), 1.37-1.24 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 162.2 (d, *J* = 253.9 Hz), 139.0, 131.1, 123.4, 121.0 (d, *J* = 21.1 Hz), 115.0 (d, *J* = 24.9 Hz), 84.0, 68.9, 30.1, 27.8, 21.5, 20.7; **IR** (neat) 3588, 3020, 2940, 1365, 1220, 1173, 921, 755 cm^{-1}; **HRMS** (ESI+) calcd for $C_{12}H_{19}O_4NFS$ $[M + NH_4]^+$ 292.1013: found 292.1013; **$[\alpha]_D^{23}$** = +1.3 (*c* = 1.0, $CHCl_3$, 82% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AD-3 column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 19.9 min, major enantiomer t_R = 15.6 min, 82% ee.

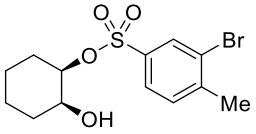
(1*R*,2*S*)-2-hydroxycyclohexyl 2-methylbenzenesulfonate (4h)



Reaction time: 14 h; colorless oil (54.1 mg, 95% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.37-7.30 (m, 2H), 4.65-4.61 (m, 1H), 3.89 (br, 1H), 2.69 (s, 3H), 2.00 (d, *J* = 4.8 Hz, 1H), 1.94-1.86 (m, 1H), 1.81-1.74 (m, 1H), 1.67-1.46 (m, 4H), 1.36-1.26 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 138.2, 135.3, 133.7, 132.5, 129.5, 126.1, 83.1, 68.9, 30.2, 27.5, 27.8, 20.6, 20.2; **IR** (neat) 3533, 2946, 2870, 1452, 1337, 1180, 925, 892 cm^{-1}; **HRMS** (ESI+) calcd for $C_{16}H_{19}N_3NaO_2$ $[M + Na]^+$ 308.1369: found 308.1362; **$[\alpha]_D^{24}$** = +7.6 (*c* = 1.0, $CHCl_3$, 84% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 0.5 mL/min, 254 nm); minor enantiomer t_R = 22.0 min, major enantiomer t_R = 20.2 min, 84% ee.

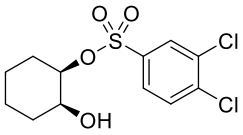
(1*R*,2*S*)-2-hydroxycyclohexyl 3-bromo-4-methylbenzenesulfonate (4i)



eaction time: 13 h; colorless oil (56.2 mg, 80% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 2.0 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H) 7.60 (dd, *J* = 2.3, 8.4 Hz, 1H), 4.7-4.65 (m, 1H), 3.86-3.84 (m, 1H), 2.49 (s, 3H), 2.05-1.90 (m, 2H), 1.81-1.72 (m, 1H), 1.68-1.50(m, 4H), 1.36-1.25 (m, 2H) ; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 139.7, 136.1, 133.3, 131.3, 129.4, 126.2, 83.7, 68.9, 30.2, 27.8, 23.0, 21.6, 20.7; **IR** (neat) 3463, 2941, 2865, 1354, 1174, 925, 898, 757 cm^{-1}; **HRMS** (ESI+) calcd for $C_{13}H_{17}BrO_4NaS$ $[M + Na]^+$ 372.9903: found 372.9895; $\mathbf{[\alpha]_D^{22}}$ = +2.6 (*c* = 1.0, $CHCl_3$, 80% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AD-3 column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 15.8 min, major enantiomer t_R = 12.9 min, 80% ee.

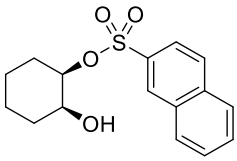
(1*R*,2*S*)-2-hydroxycyclohexyl 3,4-dichlorobenzenesulfonate (4j)



Reaction time: 13 h; colorless oil (55.7 mg, 84% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 2.3 Hz, 1H), 7.77 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 4.75-4.68 (m, 1H), 3.88-3.85 (m, 1H), 2.05-1.95 (m, 2H), 1.81-1.52 (m, 5H), 1.39-1.24 (m, 1H) ; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 136.7, 136.9, 133.8, 131.3, 129.6, 126.6, 84.3, 69.0, 30.3, 27.9, 21.5, 20.8; **IR** (neat) 3430, 2935, 2859, 1365, 1174, 925 cm^{-1}; **HRMS** (ESI+) calcd for $C_{12}H_{14}O_4Cl_2NaS$ $[M + Na]^+$ 346.9882: found 346.9874; $\mathbf{[\alpha]_D^{22}}$ = +0.4 (*c* = 1.0, $CHCl_3$, 77% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AD-3 column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 14.3 min, major enantiomer t_R = 12.1 min, 77% ee.

(1*R*,2*S*)-2-hydroxycyclohexyl naphthalene-2-sulfonate (4k)

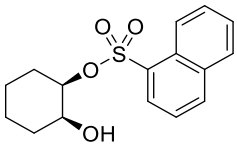


Reaction time: 14 h; white solids (52.5 mg, 85% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.52 (d, *J* = 1.6 Hz, 1H), 8.00 (dd, *J* = 8.4, 2.7 Hz, 2H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.89 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.71-7.63 (m, 2H), 4.72-4.67 (m, 1H), 3.89-3.84 (m, 1H). 1.98-1.90 (m, 1H), 1.87 (br, 1H), 1.79-1.72 (m, 1H), 1.68-1.48 (m, 4H), 1.34-1.25 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 135.2, 133.8, 131.9, 129.7, 129.4, 128.0, 127.8, 83.5, 69.0, 30.2, 27.8, 21.7, 20,7; **IR** (neat) 3523, 2940, 2865, 1350, 1173, 664 cm^{-1}; **HRMS** (ESI+) calcd for $C_{16}H_{22}O_4NS$ $[M + NH_4]^+$ 324.0264:

found 324.1260; $[\alpha]_D^{23}$ = +0.4 (*c* = 1.0, $CHCl_3$, 84% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 28.4 min, major enantiomer t_R = 19.3 min, 84% ee.

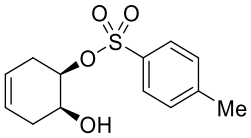
(1*R*,2*S*)-2-hydroxycyclohexyl naphthalene-1-sulfonate (4l)



Reaction time: 13 h; white solids (54.6 mg, 89% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.64 (dd, *J* = 8.6, 0.9 Hz, 1H), 8.31 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.97 (d, *J* = 8.3 Hz, 1H), 7.73 (dt, *J* = 7.9, 1.4 Hz, 1H), 7.64 (dt, *J* = 7.5, 1.1 Hz, 1H), 7.58 (t, *J* = 7.9 Hz, 1H), 4.65-4.61 (m, 1H), 3.73-3.71 (m, 1H), 1.93-1.79 (m, 2H), 1.74-1.49 (m, 4H), 1.45-1.37 (m, 1H), 1.30-1.17 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 135.3, 134.1, 132.2, 130.0, 129.0, 128.7, 128.3, 127.2, 124.6, 124.1, 83.8, 69.0, 30.2, 27.7, 21.6, 20.8; **IR** (neat) 3397, 2935, 1343, 1170, 757 cm^{-1}; **HRMS** (ESI+) calcd for $C_{16}H_{18}O_4NaS$ $[M + Na]^+$ 329.0818: found 329.0813; $[\alpha]_D^{22}$ = +10.0 (*c* = 1.0, $CHCl_3$, 76% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AS-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 27.7 min, major enantiomer t_R = 24.9 min, 76% ee.

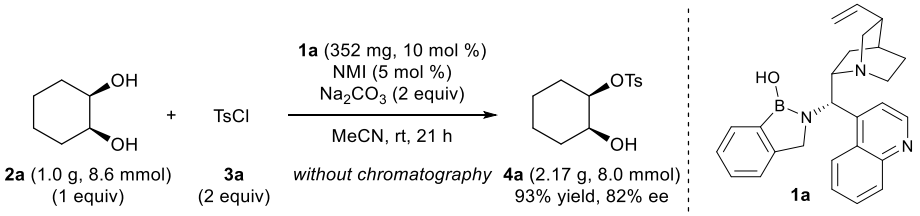
(1*R*,6*S*)-6-hydroxycyclohex-3-en-1-yl benzenesulfonate (4m)



Reaction time: 14 h; colorless oil (27.7 mg, 92% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 5.60-5.51 (m, 1H), 5.51-5.46 (m, 1H), 4.78-4.75 (m, 1H), 4.05-4.03 (m, 1H), 2.46 (s, 3H), 2.44-2.64 (m, 1H), 2.30-2.22 (m, 2H), 2.09 (d, *J* = 5.7 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.9, 133.9, 129.9, 127.7, 123.9, 122.4, 80.6, 67.1, 31.5, 28.5, 21.7; **IR** (neat) 3517, 3038, 2919, 1604, 1354, 1180, 914, 881, 745, 669 cm^{-1}; **HRMS** (ESI+) calcd for $C_{13}H_{16}O_4NaS$ $[M + Na]^+$ 291.0662: found 291.0656; $[\alpha]_D^{22}$ = +7.8 (*c* = 1.0, $CHCl_3$, 76% ee).

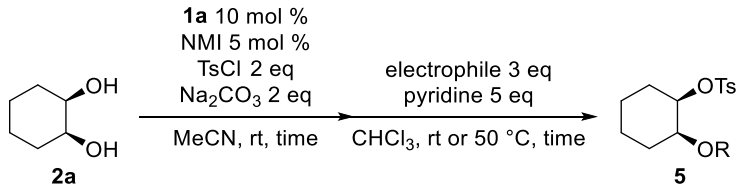
Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 254 nm); minor enantiomer t_R = 18.0 min, major enantiomer t_R = 20.4 min, 76% ee.

6. Gram scale synthesis of 4a.



Diol **2a** (1.0 g, 8.6 mmol, 1 eq), sodium carbonate (17.2 mmol, 2 eq), catalyst **1a** (352 mg, 0.86 mmol, 10 mol %), and sulfonyl chloride **3a** (17.2 mmol, 2 eq) were added to a round-bottom flask containing a stir bar, under Ar atmosphere. To the flask, acetonitrile (43 ml) and NMI (0.43 mmol, 5 mol %) were added. After stirring for 21 h at room temperature, water (30 ml) and ethyl acetate (30 ml) were added. After stirring for 10 min, separated organic layer was washed with 10% HCl aq (30ml × 2), saturated $NaHCO_3$ aq (30ml × 2), water (30ml × 2) and brine (30 ml), and then dried over Na_2SO_4. Removal of the solvent under reduced pressure afforded product **4a** (2.17 g, 93% yield, 82 % ee). The enantiomeric excesses of the products were determined by chiral stationary phase HPLC on Daicel Chiralcel OJ-H column.

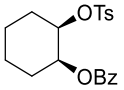
7. General procedure for enantioselective sequential dual protection of *cis*-1,2-diols



Diol **2** (0.1 mmol, 1 eq), sodium carbonate (0.2 mmol, 2 eq), catalyst **1a** (0.01 mmol, 10 mol %) and sulfonyl chloride **3** (0.2 mmol, 2 eq) were added to a round-bottom flask containing a stir bar under Ar. To the flask, 10 mM solution of 1-methylimidazole (NMI) in acetonitrile (0.5 ml, 0.005 mmol, 5 mol %) was added. After being stirred for appropriate time at room temperature, solvent was removed under reduced pressure. To the residue, Choloroform (0.1 ml) and pyridine (0.5 mmol, 5 eq) were added. The mixture was cooled to 0 ℃, and additional electrophile (0.3 mmol, 3 eq) was slowly added. After being stirred for appropriate time at roon temperature or 50 ℃, water was added to the reaction flask, and separated aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica-gel column chromatography to afford sequentially protected product **5**. The enantiomeric excesses of the products were determined by chiral stationary phase HPLC using Chiralpak AD-3 column.

8. Analytical data for products of enantioselective sequential dual protection of *cis*-1,2-diols

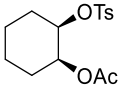
(1*S*,2*R*)-2-(tosyloxy)cyclohexyl benzoate (5a)



Reaction time: 15 h for tosylation, 8 h for acylation (at room temperature); white solids (30.0 mg, 80% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.89 (d, *J* = 7.3 Hz, 1H), 7.71 (d, *J* = 7.3 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 4.97 (td, *J* = 9.7, 3.0 Hz, 1H), 4.87-4.85 (m, 1H), 2.26 (s, *J* = 3H), 2.14-2.09 (m, 1H), 2.03-1.95 (m, 1H), 1.77-1.69 (m, 4H), 1.53-1.36 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 165.4, 144.3, 133.9, 132.9, 129.8, 129.6, 128.1, 127.5, 79.1, 71.8, 29.2, 26.7, 22.3, 21.5, 20.2; **IR** (neat) 2935, 2870, 2359, 2337, 1718, 1360, 173, 1174, 1110, 898 cm^{-1}; **HRMS** (ESI+) calcd for $C_{20}H_{22}O_5SNa$ $[M + Na]^+$ 397.1080: found 390.1078; **$[\alpha]_D^{22}$** = +5.4 (*c* = 1.0, $CHCl_3$, 80% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AD-3 column (hexane:2-propanol = 99:1, 1.0 mL/min, 254 nm); minor enantiomer t_R = 46.2 min, major enantiomer t_R = 65.7 min, 80% ee.

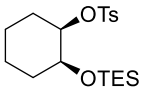
(1*S*,2*R*)-2-(tosyloxy)cyclohexyl acetate (5b)



Reaction time: 19 h for tosylation, 17 h for acylation (at room temperature); white solids (25.9 mg, 79% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.2 Hz, 2 H), 7.34 (d, *J* = 8.2 Hz, 2 H), 4.75-4.71 (m, 2 H), 2.44 (s, 3H), 1.90 (s, 3H), 1.93-1.79 (m, 2H), 1.73-1.52 (m, 4H), 1.44-1.25 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.3, 144.5, 134.3, 129.7, 127.8, 78.9, 71.2, 29.1, 26.5, 22.3, 21.6, 20.9, 20.1; **IR** (neat) 2952, 2865, 1739, 1360, 1240, 1180, 1028, 935, 898, 751 cm^{-1}; **HRMS** (ESI+) calcd for $C_{15}H_{24}O_5NS$ $[M + NH_4]^+$ 330.1370: found 330.1366; **$[\alpha]_D^{22}$** = **–** 24.3 (*c* = 1.0, $CHCl_3$, 79% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AD-3 column (hexane:2-propanol = 99:1, 1.0 mL/min, 254 nm); minor enantiomer t_R = 39.6 min, major enantiomer t_R = 63.4 min, 79% ee.

(1*R*,2*S*)-2-((triethylsilyl)oxy)cyclohexyl 4-methylbenzenesulfonate (5c)

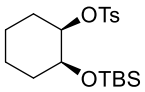


Reaction time: 15 h for tosylation, 4 h for silylation (at 50 °C); white solids (34.4 mg, 84% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.4 Hz, 2 H), 7.31 (d, *J* = 8.6 Hz, 2 H), 4.47-4.43 (m, 1H), 3.89-3.87 (m, 1H), 2.44 (s, 3H), 2.05-1.96 (m, 1H), 1.74-1.59 (m, 3H), 1.51-1.39 (m, 2H), 1.32-1.21 (m, 2H), 0.90 (t, *J* = 7.9 Hz, 9H), 0.52 (q, *J* = 8.2 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.2, 1340.8, 129.5, 127.7, 83.1, 69.4, 31.9, 27.5, 22.6, 21.6, 20.2, 6.8, 4.8; **IR** (neat) 2951, 2875, 1360, 1170, 903, 729 cm^{-1}; **HRMS** (ESI+) calcd for $C_{19}H_{32}O_4SSiNa$ $[M + Na]^+$ 407.1683: found 407.1682; **$[\alpha]_D^{22}$** = +13.2 (*c* = 1.0, $CHCl_3$, 81% ee).

Enantiomeric excess was determined after deprotection of silyl moiety (see section 8 for details) by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:1, 1.0 mL/min, 254 nm); minor enantiomer t_R = 13.5 min, major

enantiomer t_R = 12.1 min 81% ee.

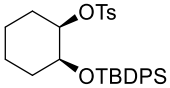
(1*R*,2*S*)-2-((tert-butyldimethylsilyl)oxy)cyclohexyl 4-methylbenzenesulfonate (5d)



Reaction time: 16 h for tosylation, 26 h for silylation (at 50 °C); white solids (27.1 mg, 76% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.2 Hz, 2 H), 7.29 (d, *J* = 8.2 Hz, 2 H), 4.40-4.37 (m, 1H), 3.94-3.93 (m, 1H), 2.42 (s, 3H), 1.96-1.87 (m, 1H), 1.68-1.37 (m, 4H), 1.27-1.18(m, 1H), 1.27-1.18 (m, 2H), 0.84 (s, 9H), 0.0 (s); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.2, 134.8, 129.6, 127.6, 83.1, 69.2, 32.2, 26.9, 25.7, 23.3, 21.6, 19.4, 18.1, -4.9, -5.0; **IR** (neat) 2941, 2886, 2853, 1370, 1174, 941, 914, 729 cm^{-1}; **HRMS** (ESI+) calcd for $C_{19}H_{32}O_4SSiNa$ $[M + Na]^+$ 407.1683: found 407.1681; **$[\alpha]_D^{22}$** = +22.1 (*c* = 1.0, $CHCl_3$, 81% ee).

Enantiomeric excess was determined after deprotection of silyl moiety (see section 8 for details) by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:1, 1.0 mL/min, 254 nm); minor enantiomer t_R = 13.5 min, major enantiomer t_R = 12.1 min 81% ee.

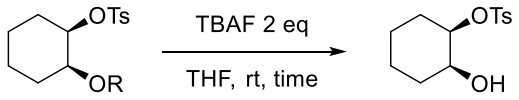
(1*R*,2*S*)-2-((*tert*-butyldiphenylsilyl)oxy)cyclohexyl 4-methylbenzenesulfonate (5e)



Reaction time: 16 h for tosylation, 50 h for silylation (at 50 °C); white solids (36.6 mg, 74% yield); **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.70-7.61 (m, 4H), 7.60-7.55 (m, 2H), 7.45-7.29 (m, 6H), 7.20 (d, *J* = 8.0 Hz, 2H), 4.44 (d, *J* = 7.7 Hz, 1H), 3.81 (d, *J* = 2.9 Hz, 1H), 2.40 (s, 3H), 2.19-2.05 (m, 1H), 1.79-1.45 (m, 4H), 1.36-1.11 (m, 3H), 1.04 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 140.0, 136.1, 135.8, 134.7, 134.2, 133.4, 139.5, 127.6, 127.5, 82.8, 70.6, 31.1, 27.9, 26.9, 22.4, 21.6, 20.4, 19.3; **IR** (neat) 2941, 2853, 1354, 1180, 757 cm^{-1}; **HRMS** (ESI+) calcd for $C_{29}H_{36}O_4SSiNa$ $[M+ Na]^+$ 531.1996: found 531.1993; **$[\alpha]_D^{22}$** = +2.6 (*c* = 1.0, $CHCl_3$, 81% ee).

Enantiomeric excess was determined by HPLC with a Chiralpak AD-3 column (hexane:2-propanol = 99:1, 1.0 mL/min, 254 nm); minor enantiomer t_R = 39.6 min, major enantiomer t_R = 74.6 min, 81% ee.

9. Determination of ee of dual protection products



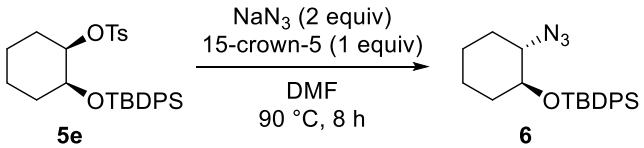
5 **4a**

entry	**5**	R	time (h)	yield (%)	ee (%)
1	**5c**	TES	2	85	81
2	**5d**	TBS	4	84	81

Dual protection product **5** (1 eq), and THF (0.2 M) were added to a round-bottom flask containing a stir bar under Ar. To the flask, tetrabutylammonium fluoride solution (1 mol/L, 2 eq) was added at 0 °C. After being stirred for appropriate time at room temperature, water was added to the reaction mixture, and then the aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate = 2/1) to afford product **4a**. The enantiomeric excesses of the products were determined by chiral stationary phase HPLC using Daicel Chiralcel OJ-H column.

10. Transformation of the products

10-1. Azidation of 5f



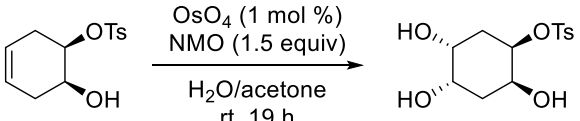
5e
81% ee

6
71% yield, 81% ee

5e (0.038 mmol, 1 eq), 15-crown-5 (0.038 mmol, 1 eq) and DMF (0.1 ml) were added to a round-bottom flask containing a stir bar. To this flask, sodium azide (0.076 mmol, 2 eq) was added. After being stirred for 8 h at 90°C, the mixture was cooled to rt. Water was added to the reaction mixture, and separated aqueous layer was extracted with ethyl acetate in 3 times. The combined organic layers were washed with water and brine, and dried over Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica-gel column chromatography (hexane/ chloroform = 5/1) to afford product **6** as colorless oil (10.1 mg, 71% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79-7.63 (m, 4H), 7.47-7.33 (m, 6H), 3.61-3.45 (m, 1H), 3.37-3.19 (m, 1H), 2.10-1.91 (m, 1H), 1.71-1.46 (m, 4H), 1.39-1.19 (m, 3H), 1.08 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 165.7, 133.1, 129.8, 129.7, 128.4, 124.0, 123.5, 72.6, 59.6, 30.3, 30.1; **IR** (neat) 3077, 3060, 2935, 2865, 2098, 1267, 1104, 702 cm^{-1}; **HRMS** (ESI+) calcd for $C_{13}H_{13}N_3NaO_2$ $[M + Na]^+$ 402.1972: found 402.1968; $[\alpha]_D^{22}$ = +0.9 (*c* = 0.5, $CHCl_3$, 81% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column (hexane, 0.5 mL/min, 220 nm); major enantiomer tr = 11.1 min, minor enantiomer tr = 10.4 min, 81% ee.

10-2. Dihydroxylation of (1*R*,6*S*)-6-hydroxycyclohex-3-en-1-yl benzenesulfonate 4m



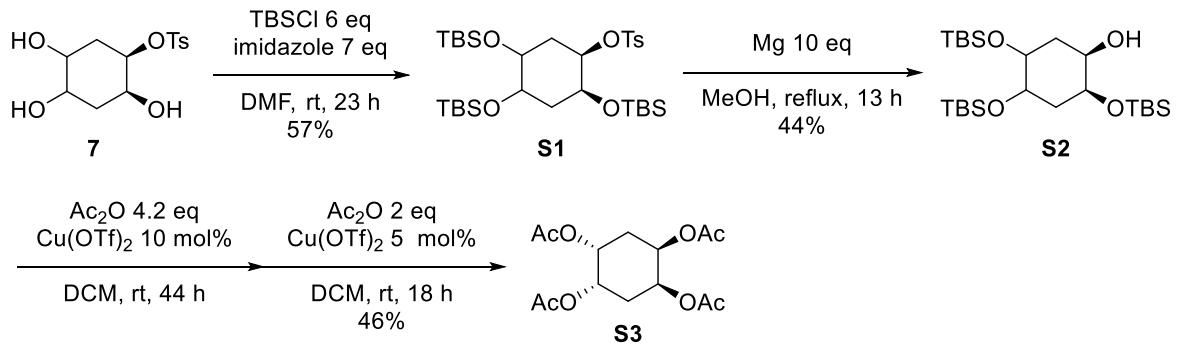
4m
76% ee

7
89% yield, dr = 5:1, 76% ee

4m (0.11 mmol, 1eq), 4-Methylmorpholine *N*-Oxide (50% in water, 0.17 mmol, 1.5 eq) and water/acetone (1/3, 0.60 ml) were added to a round-bottom flask containing a stir bar. To this flask, osmium tetroxide (4% in water, 0.011mmol, 1 mol %) was added. After being stirred for 19 h, the reaction mixture was directly purified by silica-gel column chromatography (ethyl acetate as eluent) to afford product **6** as white solid (30.6 mg, 89% yield). The diastereomeric ratio of the products was determined by ^{1}H NMR spectroscopy. Diastereomers were separated by further silica-gel column chromatography (chloroform/methanol = 20/1). Spectra of major diastereomer; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.81 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 4.91-4.76 (m, 1H), 4.30-3.89 (m, 3H), 2.46 (s, 3H), 2.15-2.00 (m, 1H), 2.00-1.69 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 145.1, 133.4, 130.0, 127.7, 80.1, 68.1, 66.8, 33.1, 30.9, 21.6; **IR** (neat) 3403, 2359, 2337, 1349, 1174, 898 cm^{-1}; **HRMS** (ESI+) calcd for $C_{13}H_{18}NaO_6S$ $[M + Na]^+$ 325.0716: found 325.0715; $[\alpha]_D^{22}$ = +16.4 (*c* = 0.25, $CHCl_3$).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 90:10, 1.0 mL/min, 220 nm) ; major enantiomer tr = 37.3 min, minor enantiomer tr = 43.2 min, 76% ee.

11. Determination of relative stereochemistry of 7

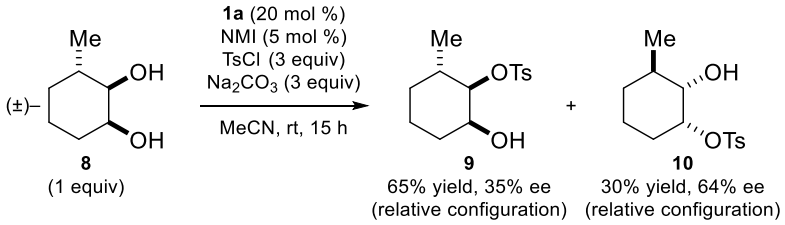


7 (0.16 mmol, 1 eq), imidazole (1.28 mmol, 8 eq) and DMF (0.5 ml) were added to a round-bottom flask containing a stir bar under Ar. To this flask, TBSCl (0.96 mmol, 6 eq) was added. After being stirred for 24 h at room temperature, water was added to the reaction flask, and separated aqueous layer was extracted with dichloromethane 4 times. The combined organic layers were dried over Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica-gel column chromatography (hexane/ethyl acetate = 3/1) to afford product **S1**. (57% yield).

S1 (0.084 mmol, 1 eq), magnesium (0.84 mmol, 10 eq) and methanol (1.4 ml) were added to a round-bottom flask containing a stir bar under Ar. After being stirred for 3 h at room temperature, the resulting suspension was heated to reflux for 13 h. The resulting reaction mixture was purified by silica-gel column chromatography (hexane/ethyl acetate = 20/1 to hexane/chloroform = 5/1) to afford product **S2**. (57% yield).

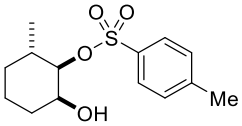
S2 (0.0367 mmol, 1 eq), $Cu(OTf)_2$ (0.004 mmol, 10 mol %) and dichloromethane (0.2 ml) were added to a round-bottom flask containing a stir bar under Ar. To this flask, acetic anhydride (0.15 mmol, 4.2 eq) was added. After being stirred for 44 h at room temperature, water was added to the reaction flask, and separated aqueous layer was extracted with dichloromethane. The combined organic layers were washed with saturated $NaHCO_3$aq and dried over Na_2SO_4. the residue contained some partially acetylated compounds. This mixture was further stirred with $Cu(OTf)_2$ (0.002 mmol, 5 mol %) , dichloromethane (0.5 ml) and acetic anhydride (0.073 mmol, 2 eq) for 18 h. Water was added to the reaction flask, and separated aqueous layer was extracted with dichloromethane. The combined organic layers were washed with saturated $NaHCO_3$aq and dried over Na_2SO_4. The residue was purified by silica-gel column chromatography (hexane/ethyl acetate = 20/1 to 5/1 to 1/1) to afford product **S3**. (46% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 5.30 (s, 4H), 2.06 (s, 16H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.2, 67.8, 29.1, 21.0. ^{1}H and ^{13}C NMR were identical to those reported in the literature.[1]

12. Kinetic resolution of 3-methylcyclohexane-1,2-diol 8



Diol **8** (0.1 mmol, 1 eq), sodium carbonate (0.3 mmol, 1 eq), catalyst **1a** (0.02 mmol, 20 mol%), and sulfonyl chloride **3** (0.3 mmol, 3 eq) were added to a round-bottom flask containing a stir bar, under Ar atmosphere. To the flask, 10 mM solution of 1-methylimidazole (NMI) in acetonitrile (0.5 ml, 0.005 mmol, 5 mol%) was added. After stirring for 15 h at room temperature, solvent was removed under reduced pressure, and them the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate = 3:1 to 1:1) to afford mixture of **9** and **10**. Regioisomers were separated by preparative TLC on silica gel (hexane/ether = 1:1). The enantiomeric excesses of the products were determined by chiral stationary phase HPLC on Chiralcel OJ-H column.

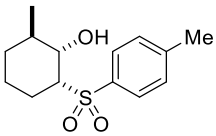
(1*R*,2*S*,6*S*)-2-hydroxy-6-methylcyclohexyl 4-methylbenzenesulfonate (9)



Colorless oil (18.4 mg, 65% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.82 (dd, *J* = 6.5, 1.8 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 4.20 (dd, *J* = 10.3, 2.7 Hz, 1H), 4.12 (d, *J* = 2.5 Hz, 1H), 2.46 (s, 3H), 2.12-1.96 (m, 2H), 1.97-1.82 (m, 1H), 1.78-1.67 (m, 1H), 1.67-1.60 (m, 1H), 1.53-1.33 (m, 2H), 1.13-0.90 (m, 1H), 0.76 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.9, 134.0, 129.8, 127.7, 89.6, 68.0, 32.8, 31.0, 30.9, 21.7, 18.6, 18.0; **IR** (neat) 3537, 2935, 1712, 1457, 1354, 1278, 1180, 914 cm^{-1}; **HRMS** (ESI+) calcd for $C_{14}H_{20}O_4NaS$ $[M + Na]^+$ 307.0975: found 307.0972; **$[\alpha]_D^{20}$** = +13.5 (*c* = 0.5, $CHCl_3$, 35% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 95:5, 1.0 mL/min, 254 nm); minor enantiomer t_R = 17.9 min, major enantiomer t_R = 14.1 min, 35% ee.

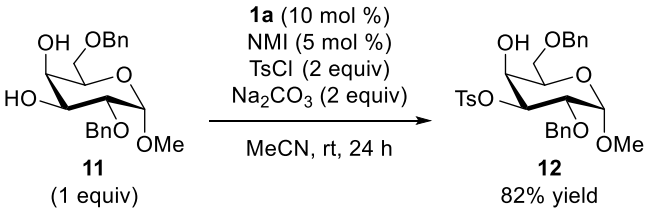
(1*S*,2*R*,6*R*)-2-methyl-6-tosylcyclohexan-1-ol (10)



Colorless oil (8.6 mg, 30% yield); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.83 (d, J = 8.1 Hz, 2H), 7.35 (d, J = 8.1 Hz, 2H), 4.83 (s, 1H), 3.27-3.04 (m, 1H), 2.45 (s, 3H), 2.08-1.90 (m, 1H), 1.89-1.31 (m, 6H), 1.10-0.90 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.8, 134.0, 129.9, 127.7, 82.6, 75.7, 34.3, 32.1, 29.9, 21.7, 19.2, 18.0; **IR** (neat) 3538, 2935, 1723, 1349, 11174, 903 cm^{-1}; **HRMS** (ESI+) calcd for $C_{14}H_{20}O_4NaS$ $[M + Na]^+$ 307.0975: found 307.0972; **$[\alpha]_D^{20}$** = -1.2 (*c* = 0.2, $CHCl_3$, 71% ee).

Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (hexane:2-propanol = 95:5, 1.0 mL/min, 254 nm); minor enantiomer t_R = 22.0 min, major enantiomer t_R = 24.1 min, 64% ee

13. Regioselective sulfonylation of protected methyl α-D-galactopyranoside 11



Protected methyl α-D-galactopyranoside **11** (0.1 mmol, 1 eq), sodium carbonate (0.2 mmol, 2 eq), catalyst **1a** (0.01 mmol, 10 mol%), and sulfonyl chloride **3** (0.2 mmol, 2 eq) were added to a round-bottom flask containing a stir bar, under Ar atmosphere. To the flask, 10 mM solution of 1-methylimidazole (NMI) in acetonitrile (0.5 ml, 0.005 mmol, 5 mol%) was added. After stirring for the 24 h at room temperature, water was added to the reaction mixture, and then, the aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate = 5:1 to 1:1) to afford product **12** (43.1 mg, 82% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.14-7.36 (m, 12H), 4.86 (dd, J = 10.0, 3.2 Hz, 1H), 4.60 (d, *J* = 3.7 Hz, 1H), 4.56 (s, 2H), 4.41 (d, *J* = 12.0 Hz, 1H), 4.35 (s, 1H), 4.32 (d, *J* = 12.0 Hz, 1H), 3.88-3.93 (m, 2H), 3.74-3.67 (m, 2H), 3.33 (s, 3H), 2.82-2.86 (m, 1H), 2.39 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.8, 137.7, 137.5, 133.7, 129.7, 128.5, 128.3, 127.9, 127.87, 127.85, 127.7, 98.5, 80.7, 73.7, 73.2, 73.1, 69.9, 69.7, 67.8, 55.4, 21.7; **IR** (neat) 3489, 2924, 2870, 1454, 1145, 813, 669 cm^{-1}; $C_{28}H_{32}O_8NaS$ $[M + Na]^+$ 551.1710: found 551.1702; **$[\alpha]_D$** ^{19}= +68.0 (*c* = 1.0, $CHCl_3$).

14. Mechanistic Studies

14-1. Determination of the structure of 1a as benzazaborole

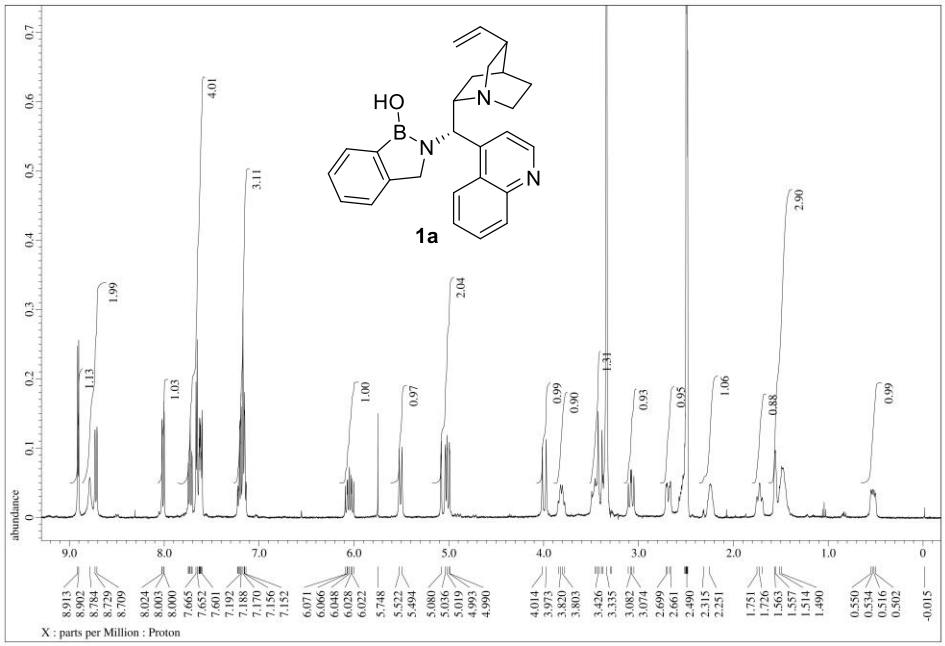
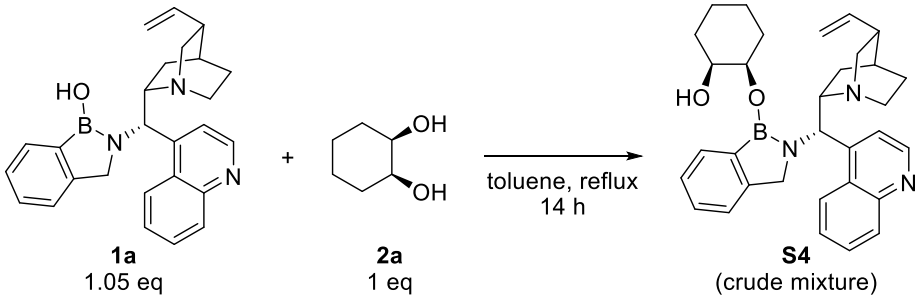


Chart-a (^{1}H NMR spectrum of **1a** in DMSO-d_6)

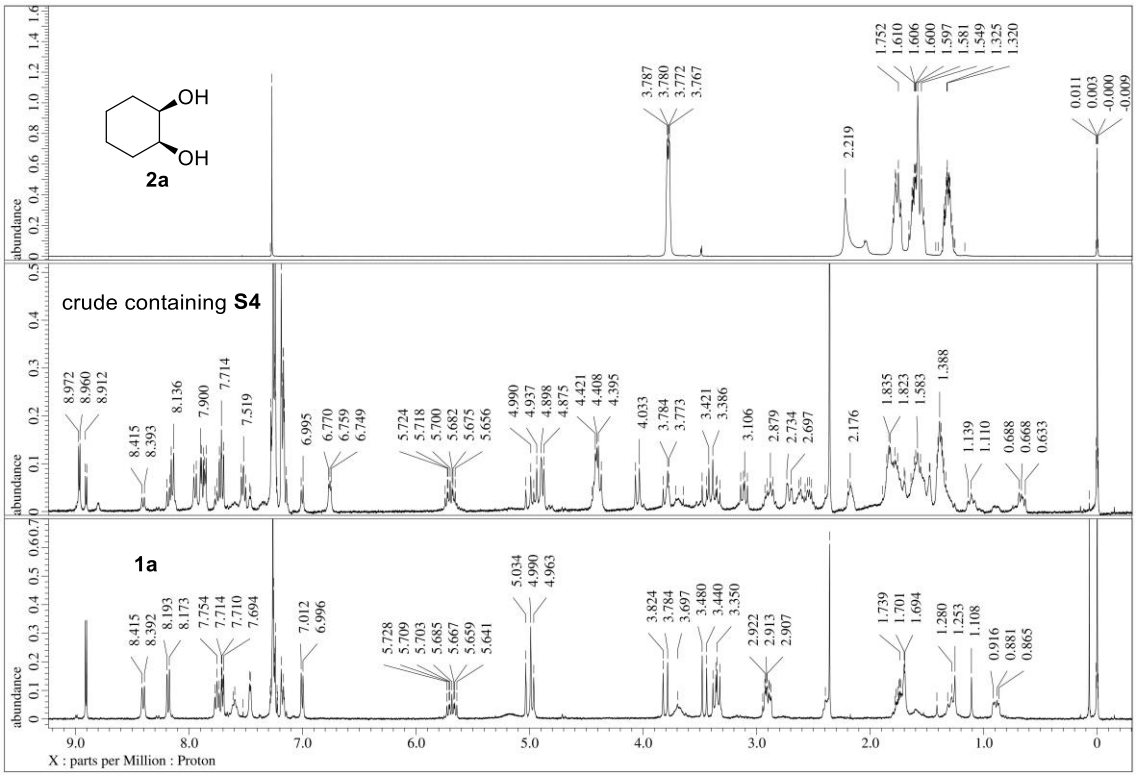
The integral value of OH group bound to the boron atom (broad singlet at 8.78 ppm) is 1H. Moreover, the chemical shift is close to that of previously reported benzazaborole compound.[2] ESI-MS analysis also support the structure of **1a** as benzazaborole (HRMS calcd for $C_{26}H_{29}BN_3O$ $[M + H]^+$ 410.2404: found 410.2394). These observations indicate that **1a** is a benzazaborole derivative, and is not a boronic acid compound.

14-2. Formation of intermediate S4

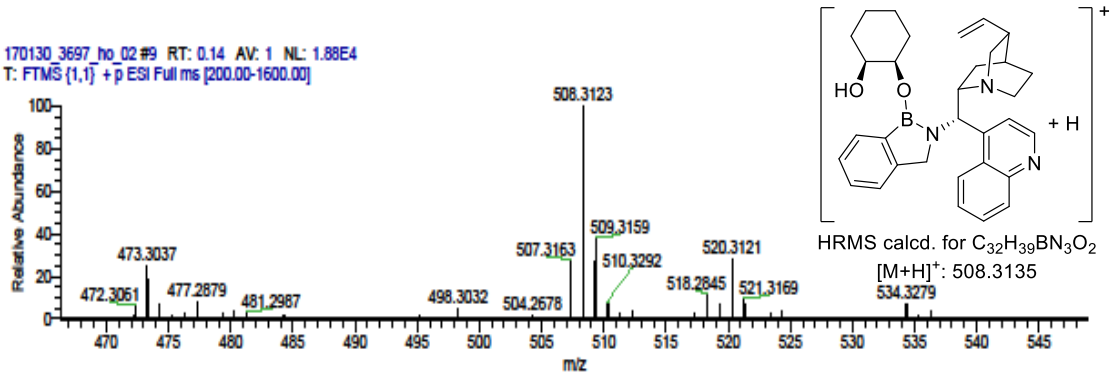


1a (0.053 mmol, 1.05eq), *cis*-1,2-cyclohexanediol **2a** (0.05 mmol, 1 eq) and toluene (0.5 ml) were added to a round-bottom flask containing a stir bar. After being stirred for 14 h at 100°C, solvent was removed under reduced pressure. Resulting crude mixture contained **S4**. Formation of the **S4** was confirmed by ^{1}H-NMR (**Chart-b**).

Chart-b

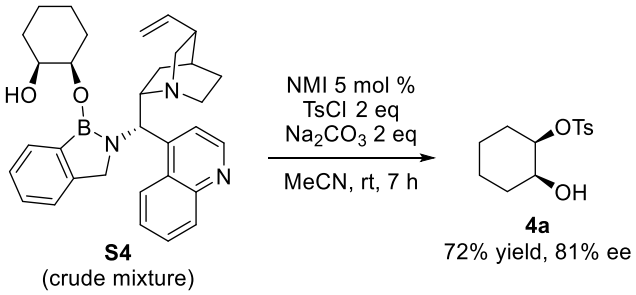


ESI-MS analysis



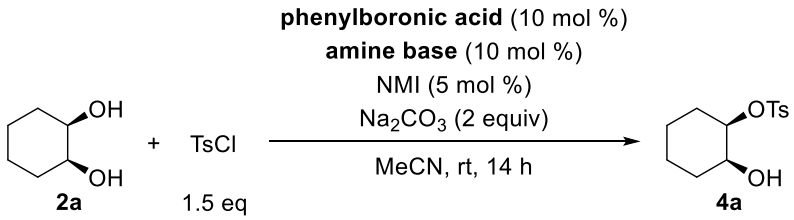
ESI-MS analysis of the catalyst-substrate mixture solution suggested formation of intermediate **S4** when mixing **1a** with **2a** in acetonitrile. An ion peak at *m/z* = 508.3123 was attributed to **S4**.

14-3. Sulfonylataion from intermediate S4



To the crude mixture including **S4** in a round-bottom flask containing a stir bar, sodium carbonate (0.1 mmol, 2 eq), NMI (0.0025 mmol, 5 mol %) and tosyl chloride **3a** (0.1 mmol, 2 eq) were added. To the flask, acetonitrile (0.5 ml) was added. After being stirred for 7 h, water was added, and then the separated aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate =2/1) to afford product **4a** in 72% yield with 81% ee.

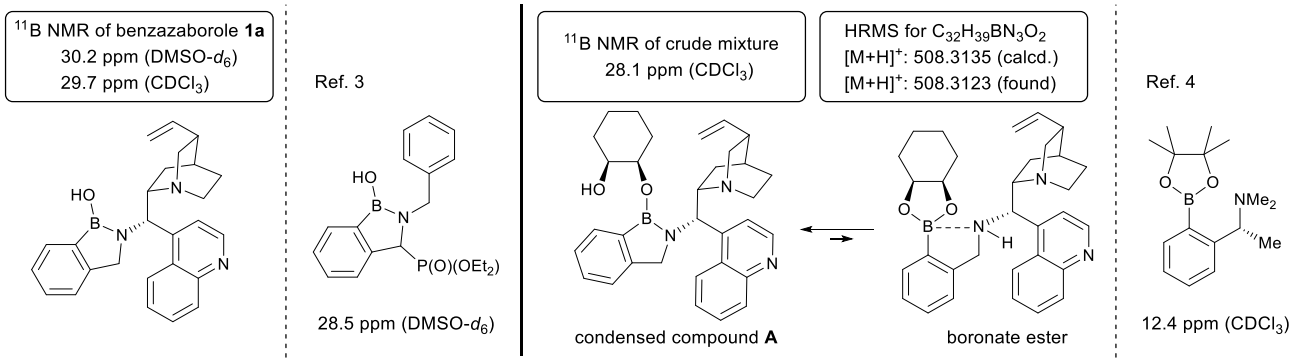
14-4. Reactions catalyzed by phenylboronic acid with external amine bases



entry	**amine base**	yield (%)
1	diethylamine	trace
2	triethylamine	17%

Diol **2a** (0.1 mmol, 1 eq), sodium carbonate (0.2 mmol, 2 eq), **phenylboronic acid** (0.01 mmol, 10 mol %) and tosyl chloride **3a** (0.2 mmol, 2 eq) were added to a round-bottom flask containing a stir bar under Ar. To the flask, 10 mM solution of 1-methylimidazole (NMI) in acetonitrile (1.0 ml, 0.01 mmol, 5 mol %) and **amine base** (0.01 mmol, 10 mol %) were added. After being stirred for 14 h at room temperature, water was added to the reaction mixture, and then the aqueous layer was extracted with ethyl acetate 3 times. The combined organic layers were washed with water and brine, and then dried over Na_2SO_4. After removal of the solvent under reduced pressure, the resulting residue was purified by silica-gel column chromatography (hexane/ethyl acetate = 2/1) to afford product **4**.

14-5. ^{11}B NMR study



^{11}B NMR of benzazaborole **1a** was examined. Chemical shift of **1a** was 30.2 ppm in DMSO-d_6 (or 29.7 ppm in $CDCl_3$), and the value was similar to that of benzazaborole derivative reported by Młynarz *et al.* (28.5 ppm in DMSO-d_6).[3]

^{11}B NMR study of crude mixture was also investigated. While clear ^{1}H NMR chart was obtained in $CDCl_3$, ^{1}H NMR chart in DMSO-d_6 became messy. In general, ^{11}B NMR of 2-aminomethyl phenyl bononate ester has a peak between 10 and 20 (for example, 12.4 ppm in $CDCl_3$).[4] Compared to this value, observed chemical shift of crude mixture in $CDCl_3$ was 28.1 ppm in ^{11}B NMR. This result suggests that the intermediate exists as a not boronate ester but benzazaborole derivative.

15. Reference

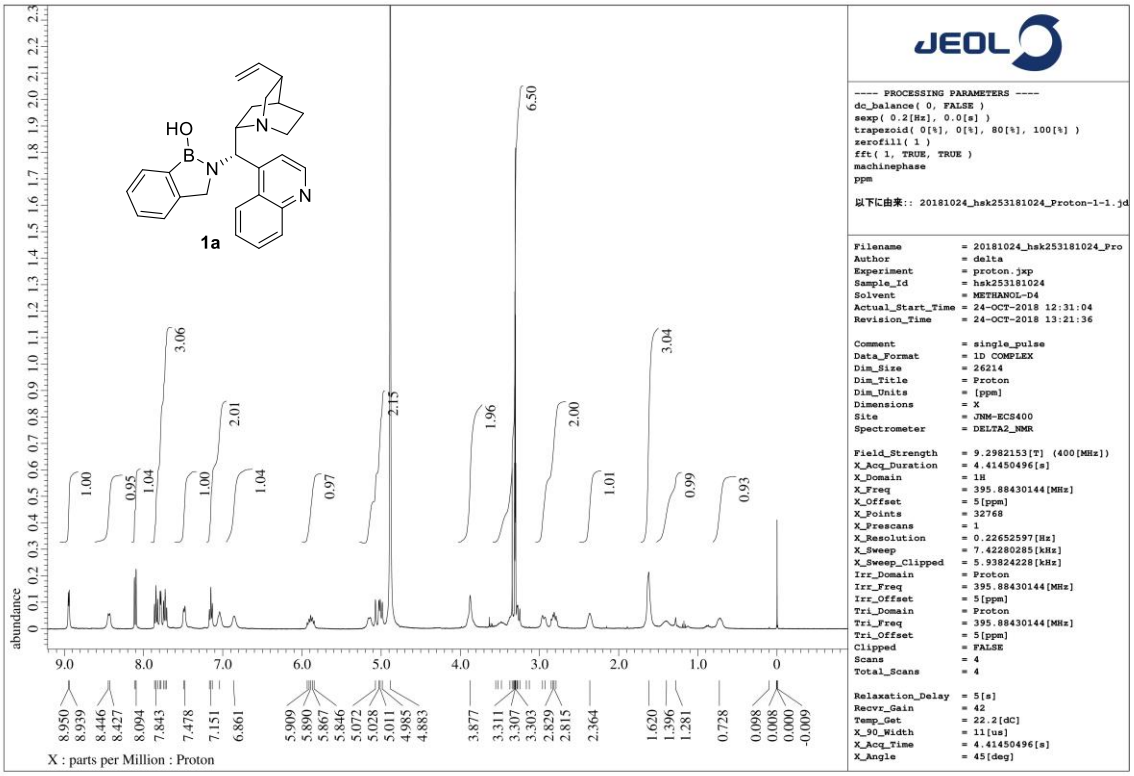
[1] T. Tschamber, F. Backenstrass, H. Fritz, J. Streith, *Helv. Chim. Acta* **1992**, *75*, 1052.

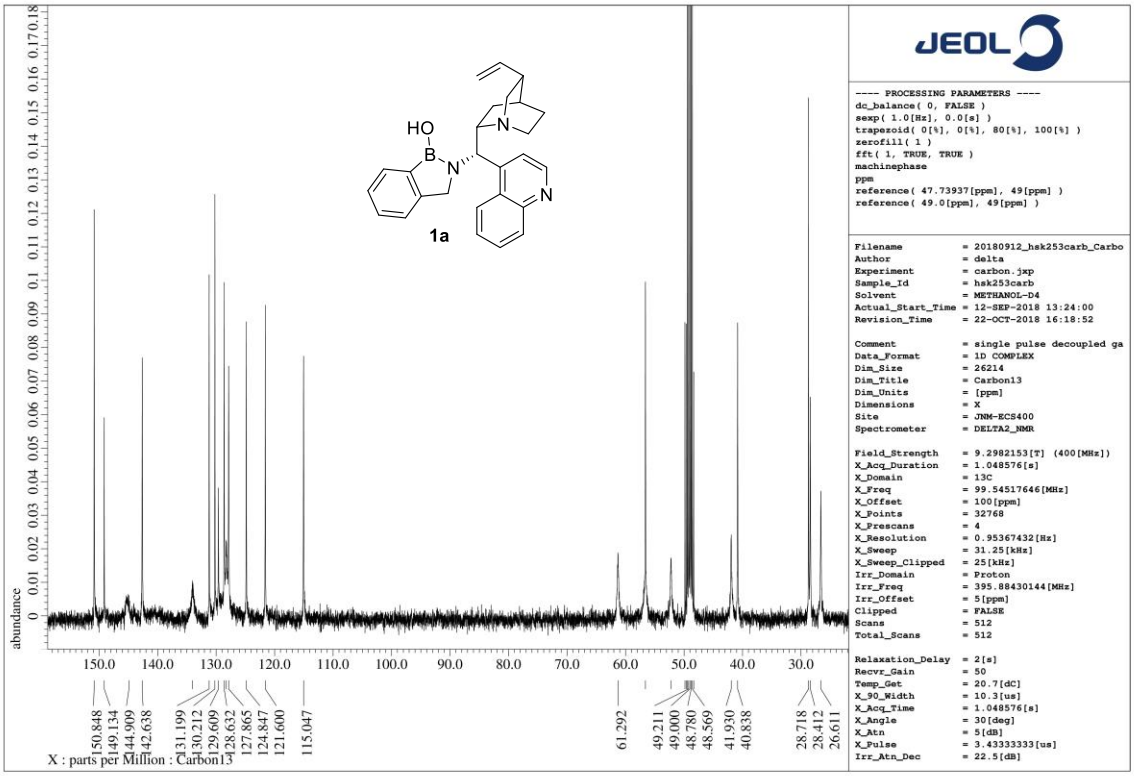
[2] R. Zhang, Y.-D. Zhang, L.-X. Wang, C.-H. Ge, Z.-Y. Ma, J.-P. Miao, X.-D. Zhang, *Inorg. Chem. Commun.* **2016**, *74*, 52.

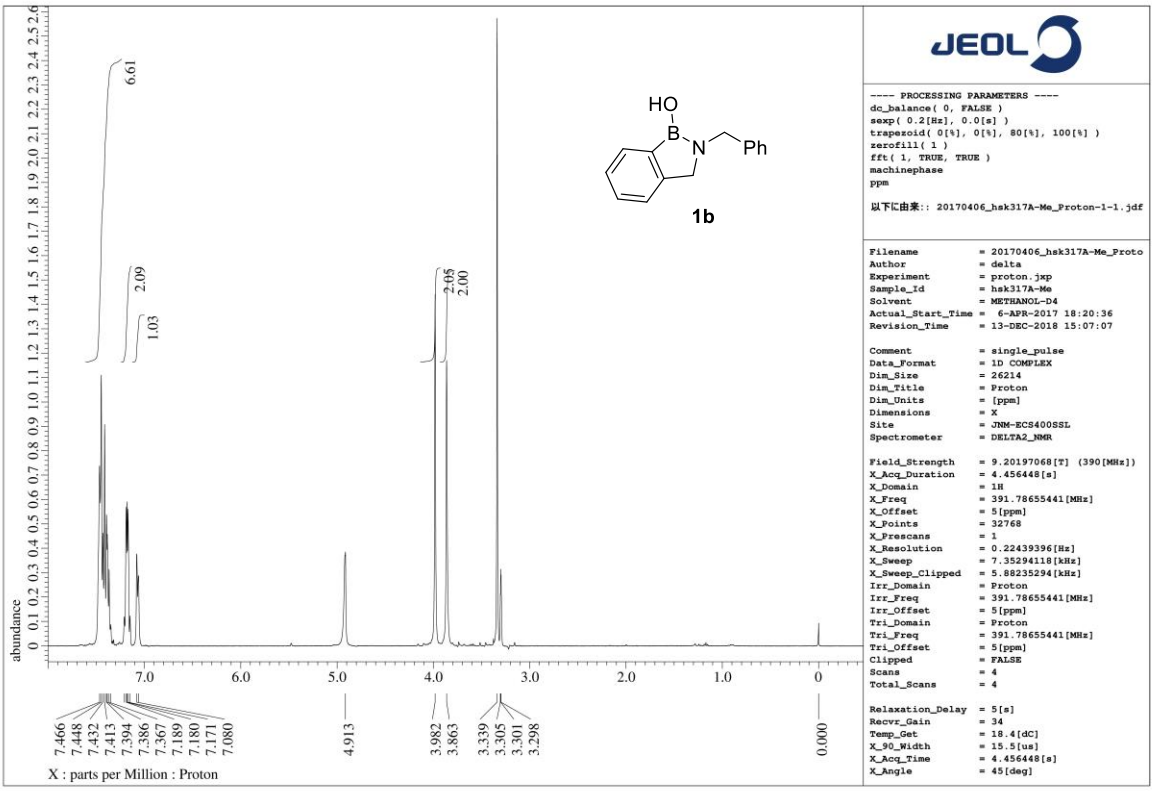
[3] A. Rydzewska, K. S´lepokura, T. Lis, P. Kafarski, P Młynarz, *Tetrahedron Lett.* **2009**, *50*, 132.

[4] S. Aichhorn, R. Bigler, E. L. Myers, V. K. Aggarwal, *J. Am. Chem. Soc.* **2017**, *139*, 9519.

16. ^{1}H-NMR and ^{13}C-NMR spectra



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7.367
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3.305
3.301
3.298
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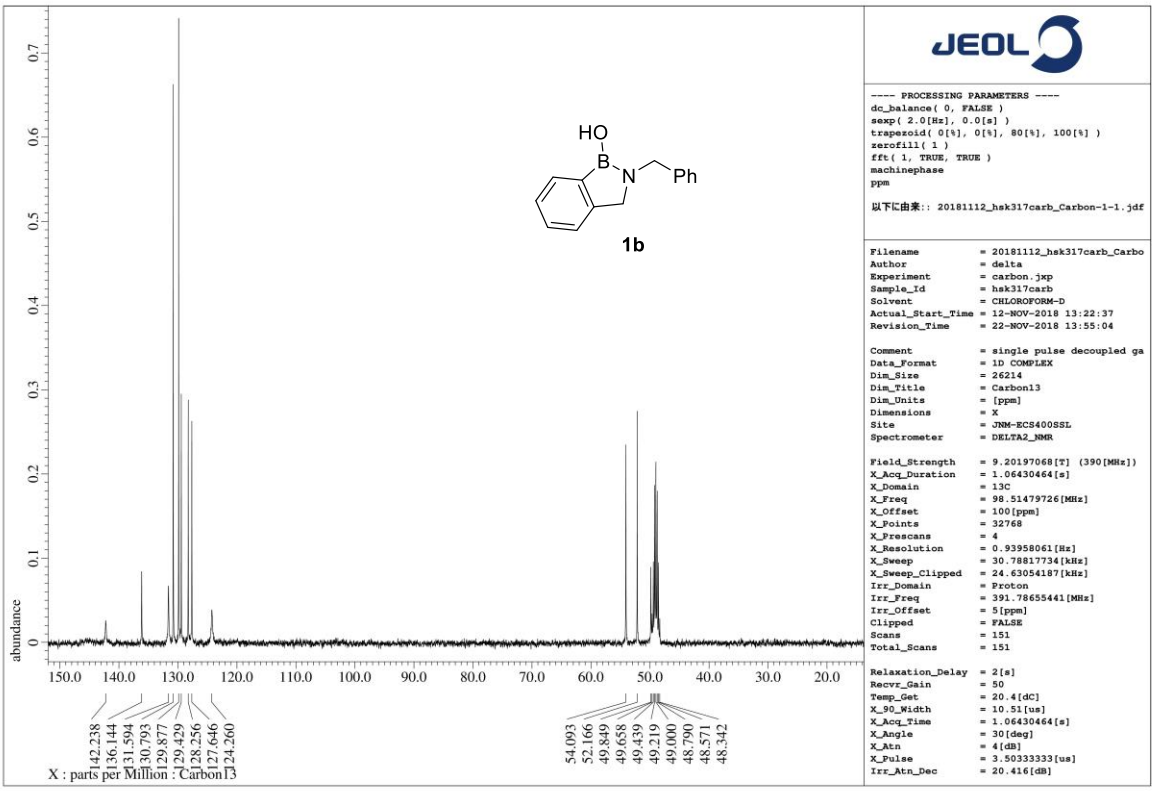
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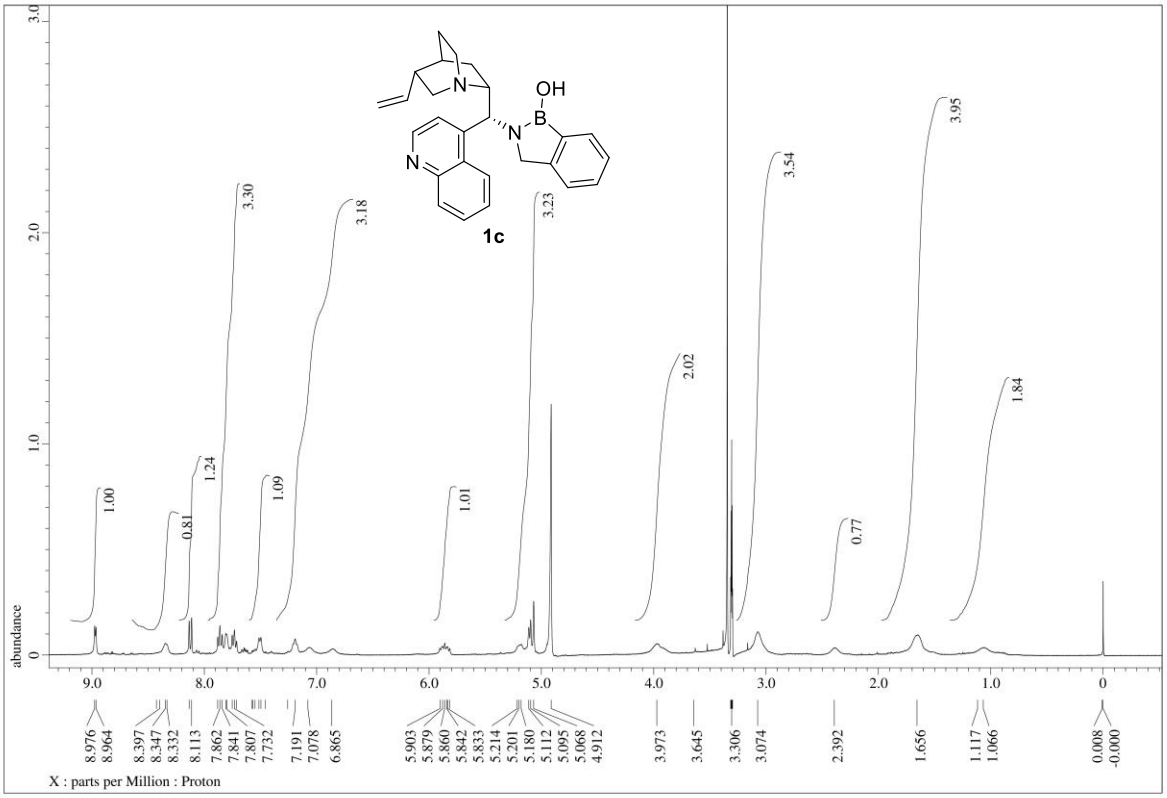
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3.23
2.02
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8.976
8.964
8.397
8.347
8.332
8.113
7.862
7.841
7.807
7.732
7.191
7.078
6.865
5.903
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5.860
5.842
5.833
5.214
5.201
5.180
5.112
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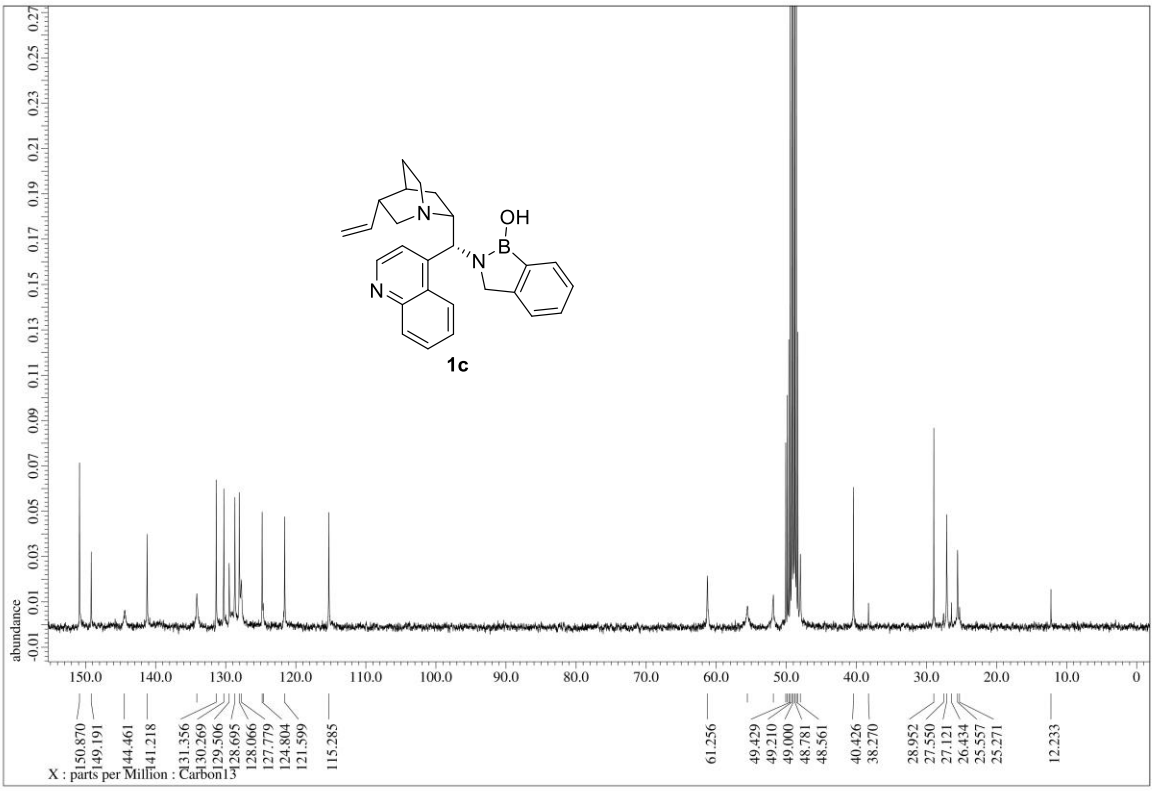
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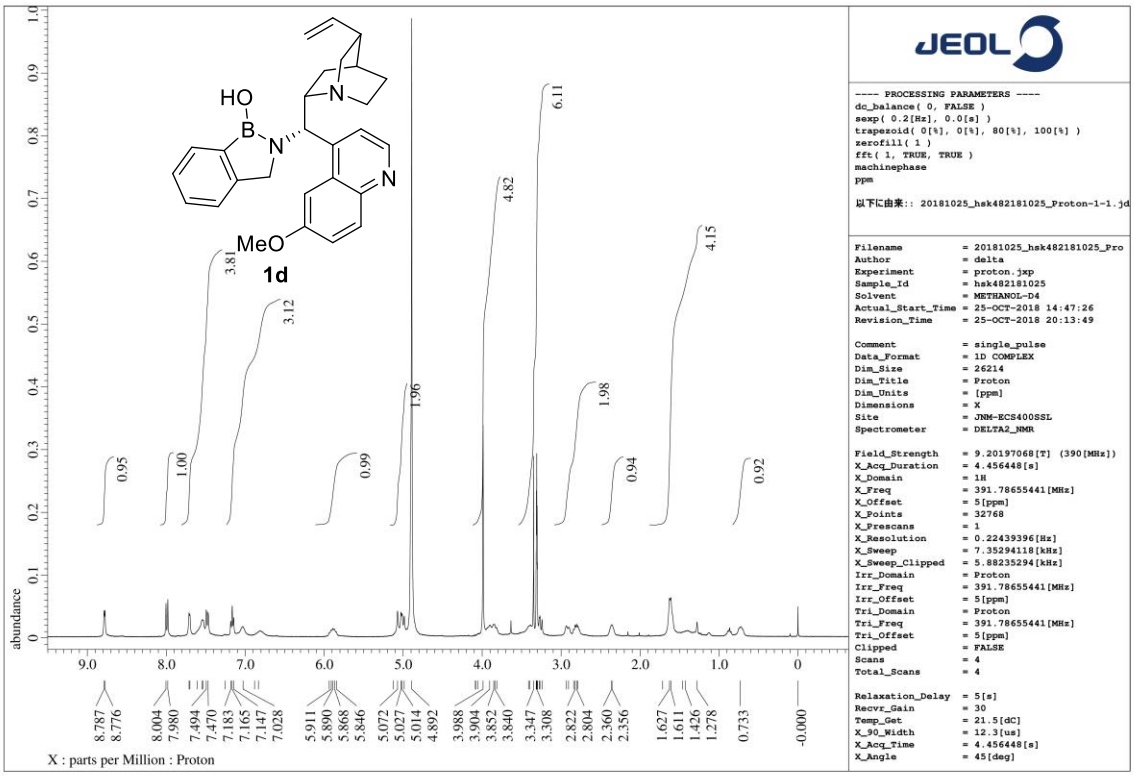


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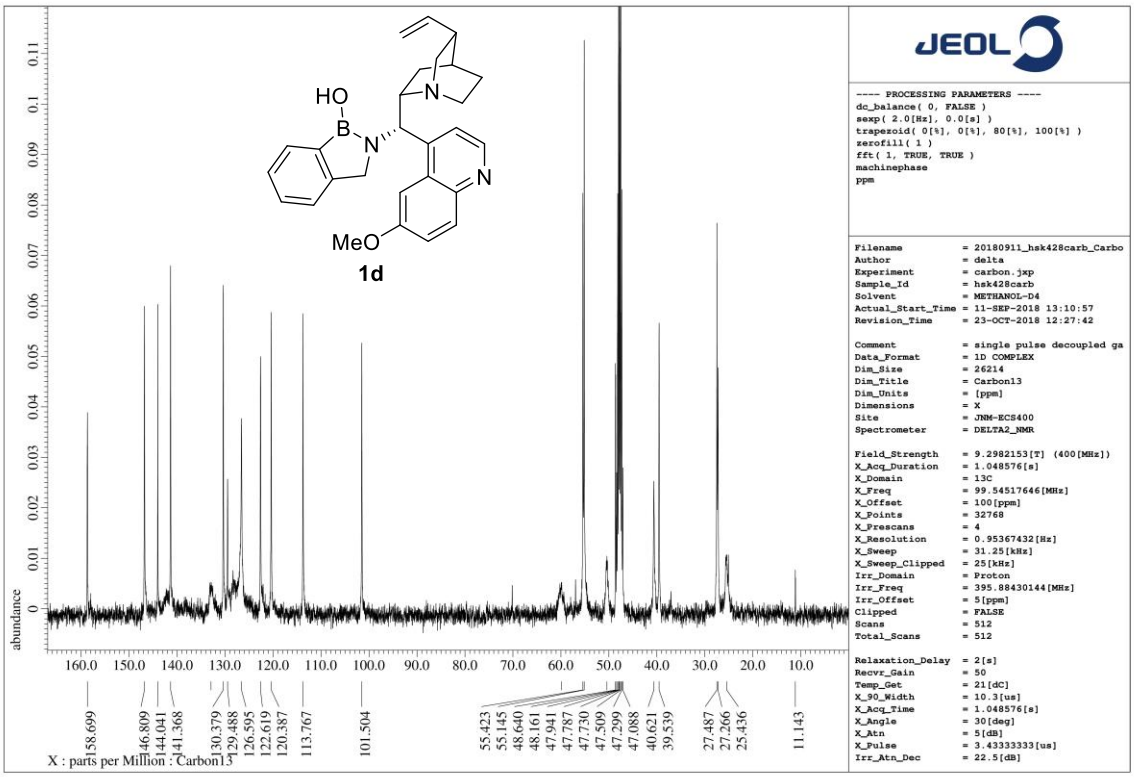


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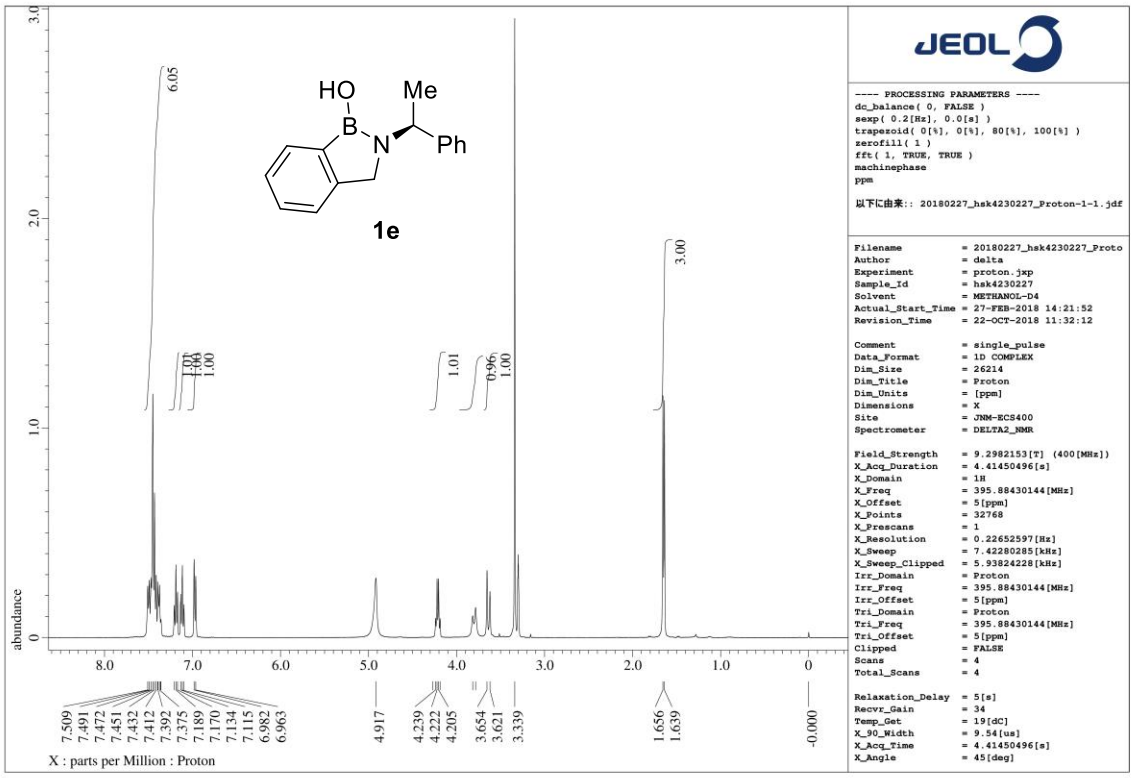
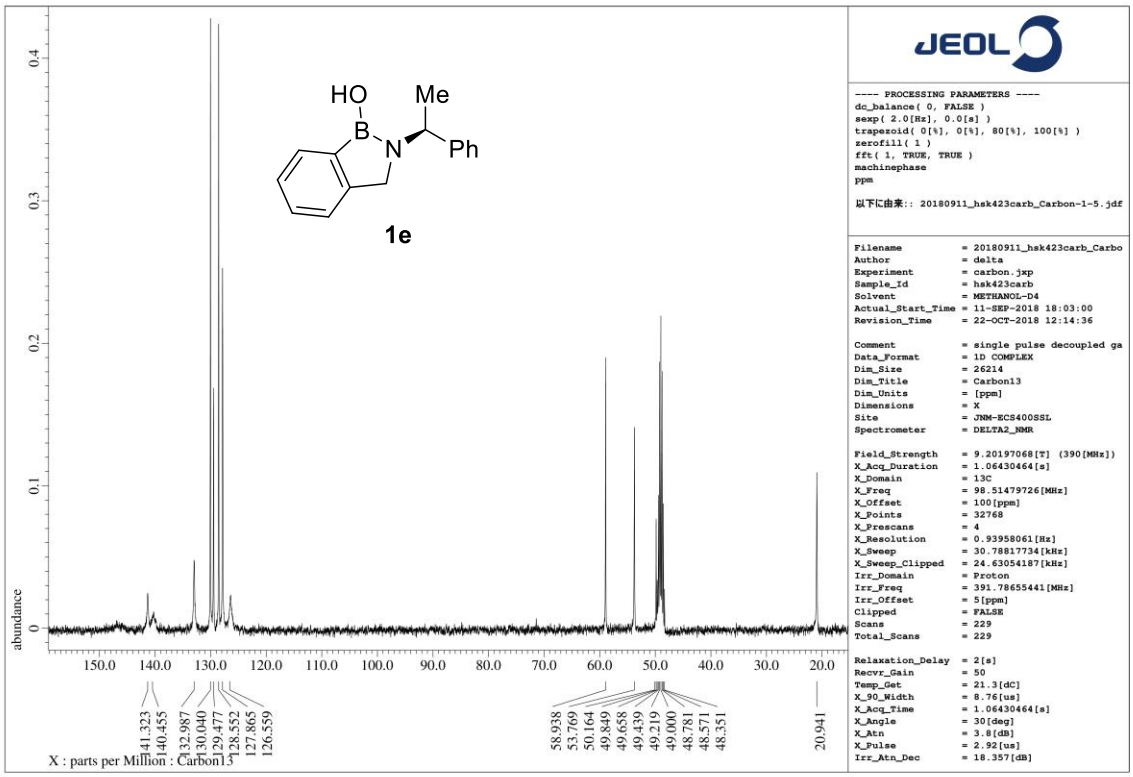
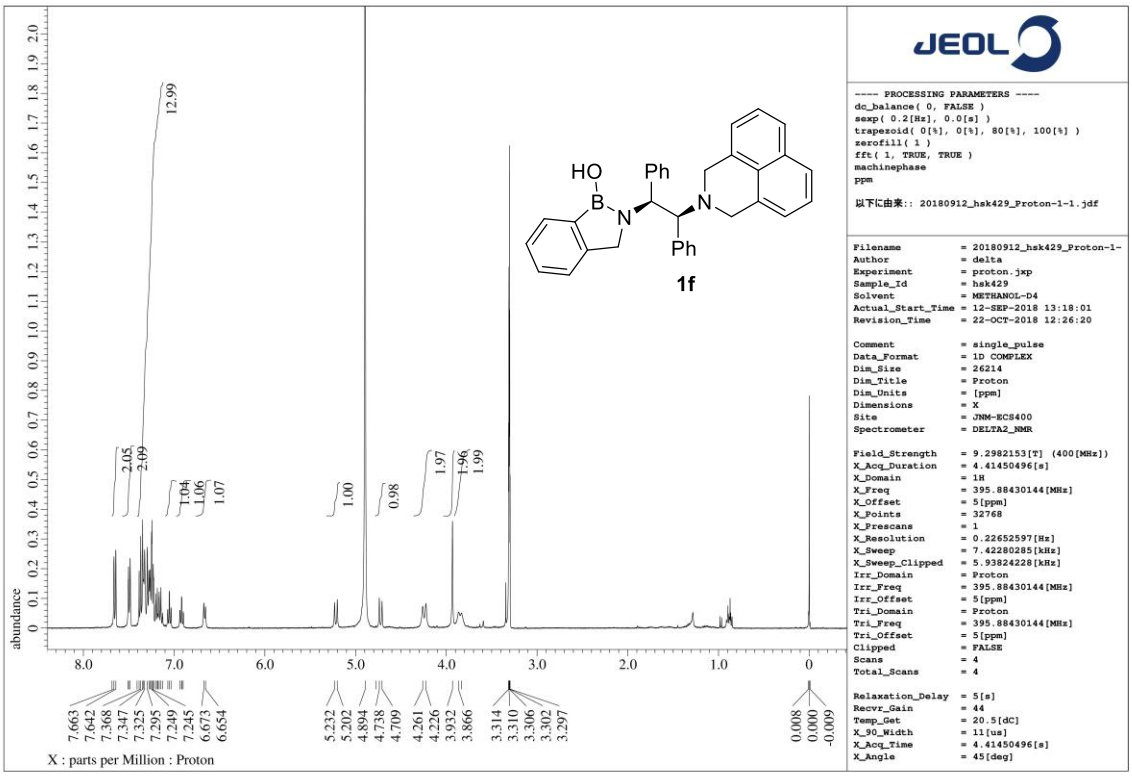
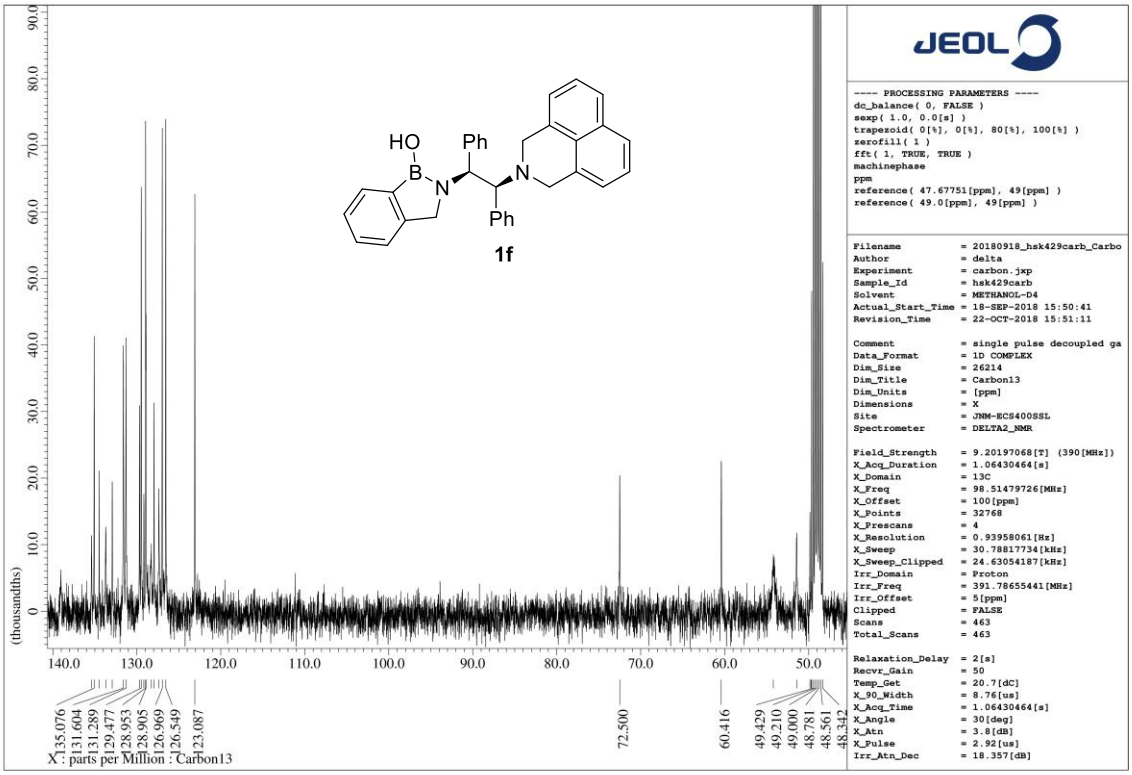
X_Sweep_Clipped     = 25[kHz]
Irr_Domain          = Proton
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 512
Total_Scans         = 512

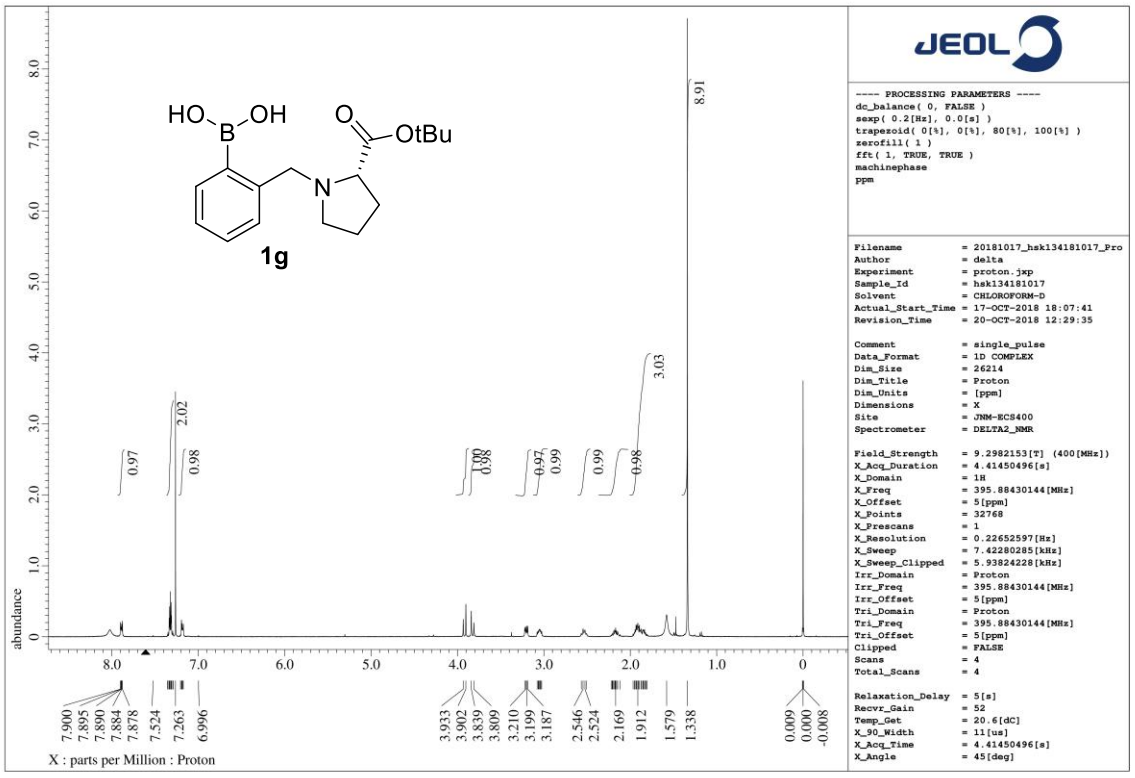
Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 21[dC]
X_90_Width          = 10.3[us]
X_Acq_Time          = 1.048576[s]
X_Angle             = 30[deg]
X_Atn               = 5[dB]
X_Pulse             = 3.43333333[us]
Irr_Atn_Dec         = 22.5[dB]
```

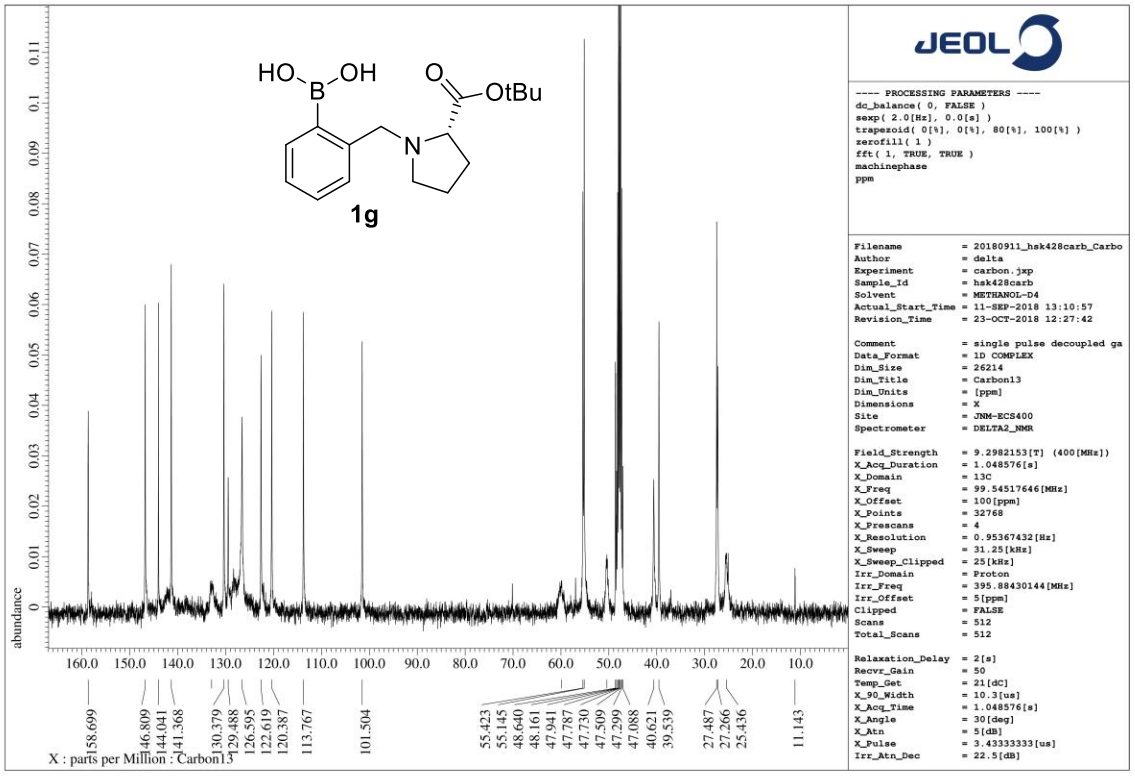

HO
Me
B
N
Ph
1e
6.05
1.01
1.04
1.00
1.01
0.96
1.00
3.00
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.509
7.491
7.472
7.451
7.432
7.412
7.392
7.375
7.189
7.170
7.134
7.115
6.982
6.963
4.917
4.239
4.222
4.205
3.654
3.621
3.339
1.656
1.639
-0.000
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
traperoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180227_hsk4230227_Proton-1-1.jdf
Filename = 20180227_hsk4230227_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = hsk4230227
Solvent = METHANOL-D4
Actual_Start_Time = 27-FEB-2018 14:21:52
Revision_Time = 22-OCT-2018 11:32:12
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 19[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

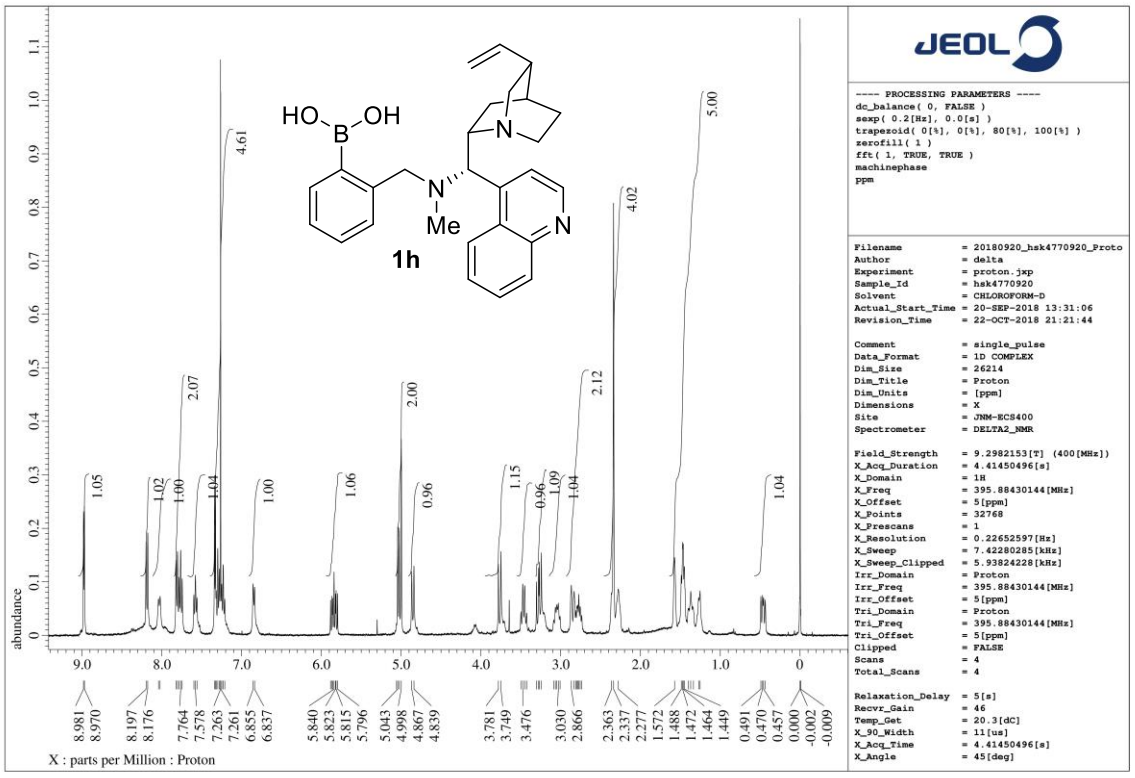

HO
Me
B
N
Ph
1e
abundance
0.4
0.3
0.2
0.1
0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
141.323
140.455
132.987
130.040
129.477
128.552
127.865
126.559
58.938
53.769
50.164
49.849
49.658
49.439
49.219
49.000
48.781
48.571
48.351
20.941
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
traperoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180911_hsk423carb_Carbon-1-5.jdf
Filename = 20180911_hsk423carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk423carb
Solvent = METHANOL-D4
Actual_Start_Time = 11-SEP-2018 18:03:00
Revision_Time = 22-OCT-2018 12:14:36
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 229
Total_Scans = 229
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 8.76[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 3.8[dB]
X_Pulse = 2.92[us]
Irr_Atn_Dec = 18.357[dB]

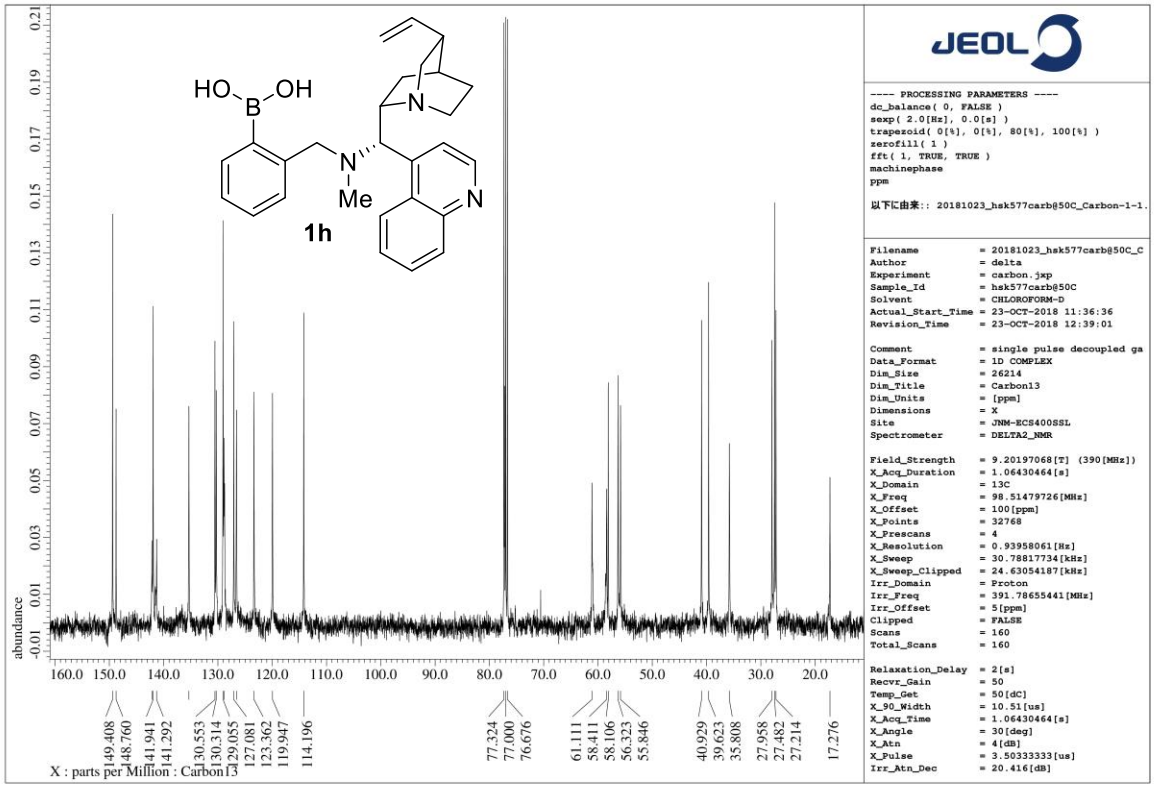

12.99
2.05
2.09
1.04
1.06
1.07
1.00
0.98
1.97
1.96
1.99
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.663
7.642
7.368
7.347
7.325
7.295
7.249
7.245
6.673
6.654
5.232
5.202
4.894
4.738
4.709
4.261
4.226
3.932
3.866
3.314
3.310
3.306
3.302
3.297
0.008
0.000
-0.009
X : parts per Million : Proton
HO
B
N
Ph
Ph
N
1f
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180912_hsk429_Proton-1-1.jdf
Filename = 20180912_hsk429_Proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = hsk429
Solvent = METHANOL-D4
Actual_Start_Time = 12-SEP-2018 13:18:01
Revision_Time = 22-OCT-2018 12:26:20
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 20.5[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

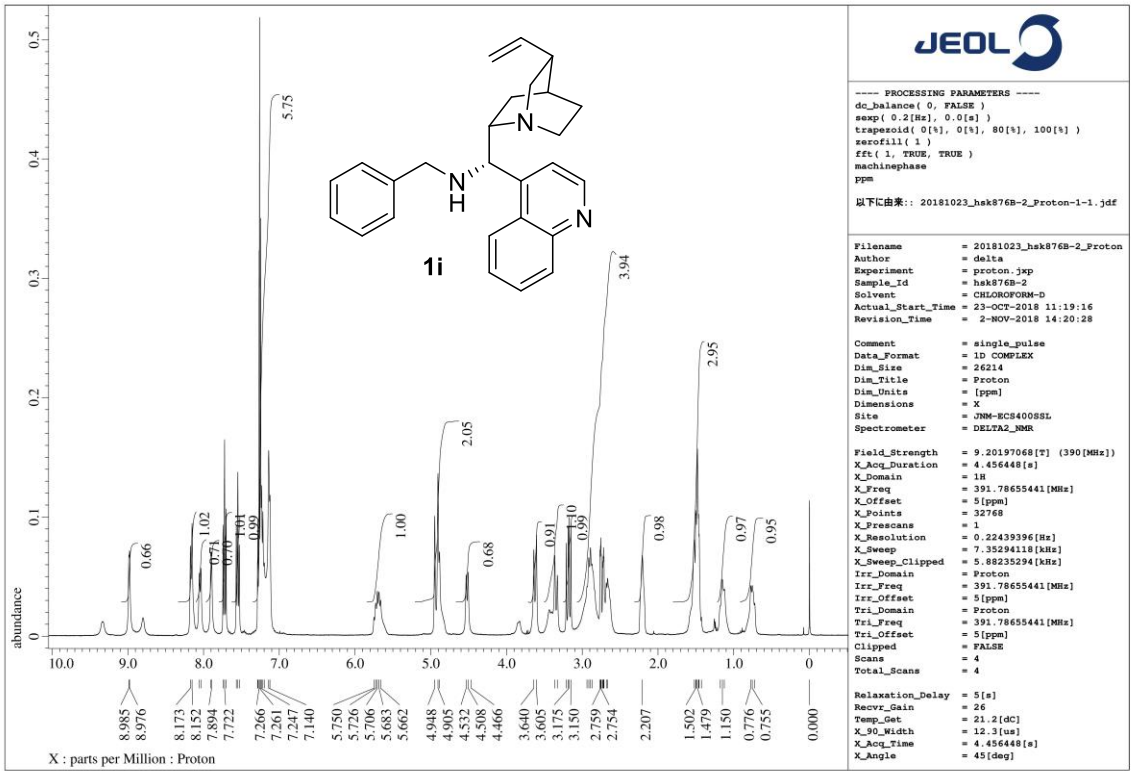

(thousandths)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
135.076
131.604
131.289
129.477
128.953
128.905
126.969
126.549
123.087
72.500
60.416
49.429
49.210
49.000
48.781
48.561
48.342
X : parts per Million : Carbon13
HO
B
N
Ph
Ph
N
1f
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(1.0, 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(47.67751[ppm], 49[ppm])
reference(49.0[ppm], 49[ppm])
Filename = 20180918_hsk429carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk429carb
Solvent = METHANOL-D4
Actual_Start_Time = 18-SEP-2018 15:50:41
Revision_Time = 22-OCT-2018 15:51:11
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 463
Total_Scans = 463
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.7[dC]
X_90_Width = 8.76[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 3.8[dB]
X_Pulse = 2.92[us]
Irr_Atn_Dec = 18.357[dB]

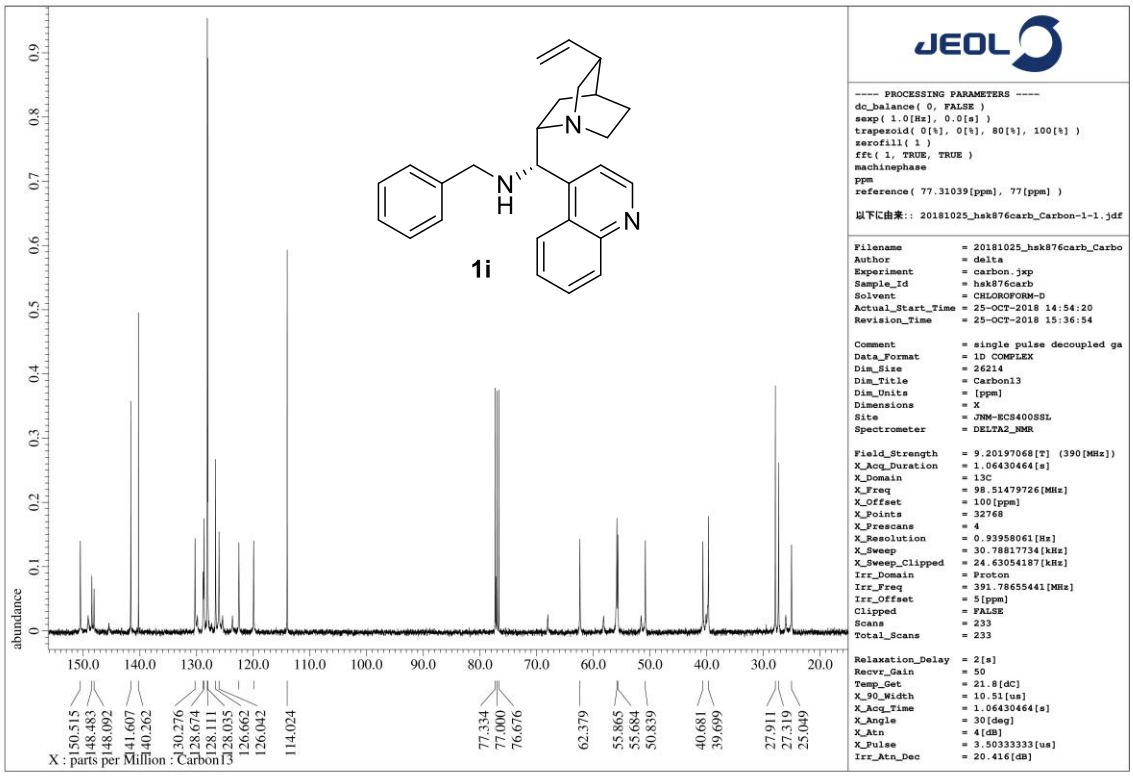

HO
B
OH
O
OtBu
N
1g
8.91
3.03
2.02
0.97
0.98
1.00
0.98
0.97
0.99
0.99
0.98
abundance
X : parts per Million : Proton
7.900
7.895
7.890
7.884
7.878
7.524
7.263
6.996
3.933
3.902
3.839
3.809
3.210
3.199
3.187
2.546
2.524
2.169
1.912
1.579
1.338
0.009
0.000
-0.008
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20181017_hsk134181017_Pro
Author = delta
Experiment = proton.jxp
Sample_Id = hsk134181017
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-OCT-2018 18:07:41
Revision_Time = 20-OCT-2018 12:29:35
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 52
Temp_Get = 20.6[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

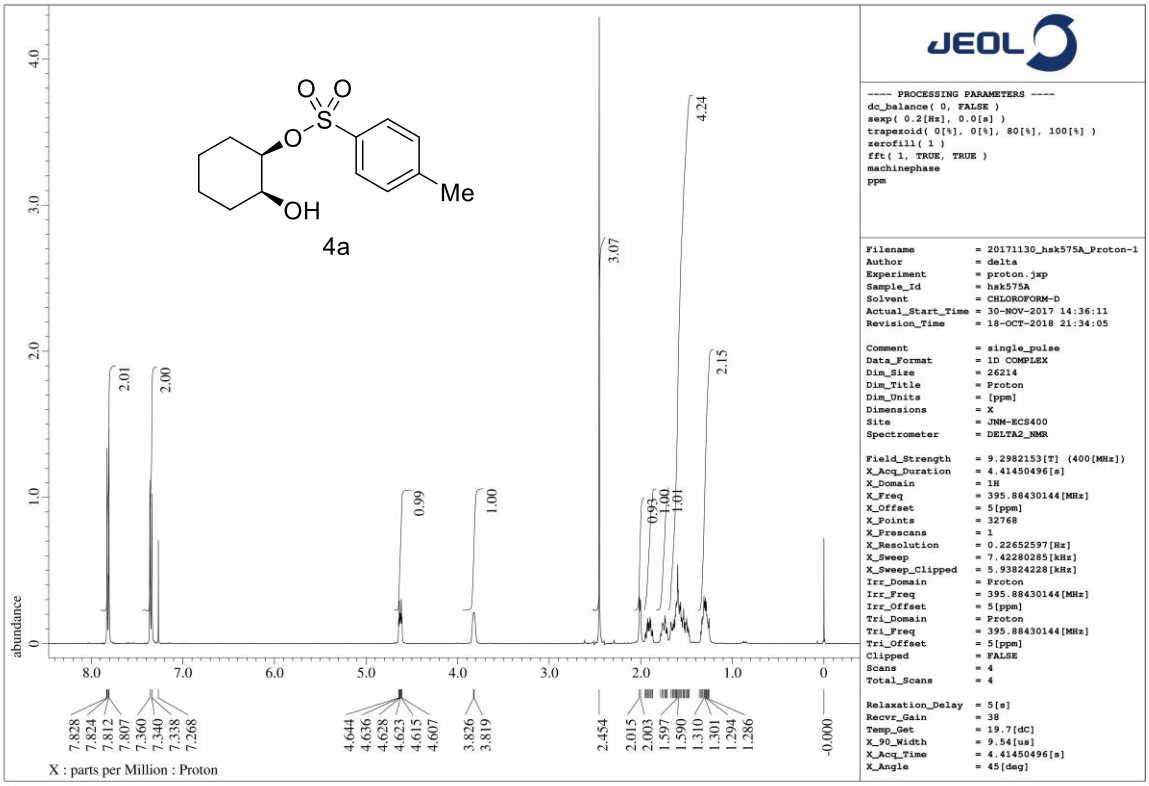

HO
B
OH
O
OtBu
N
1g
abundance
X : parts per Million : Carbon13
158.699
146.809
144.041
141.368
130.379
129.488
126.595
122.619
120.387
113.767
101.504
55.423
55.145
48.640
48.161
47.941
47.787
47.730
47.509
47.299
47.088
40.621
39.539
27.487
27.266
25.436
11.143
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180911_hsk428carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk428carb
Solvent = METHANOL-D4
Actual_Start_Time = 11-SEP-2018 13:10:57
Revision_Time = 23-OCT-2018 12:27:42
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 5[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.5[dB]

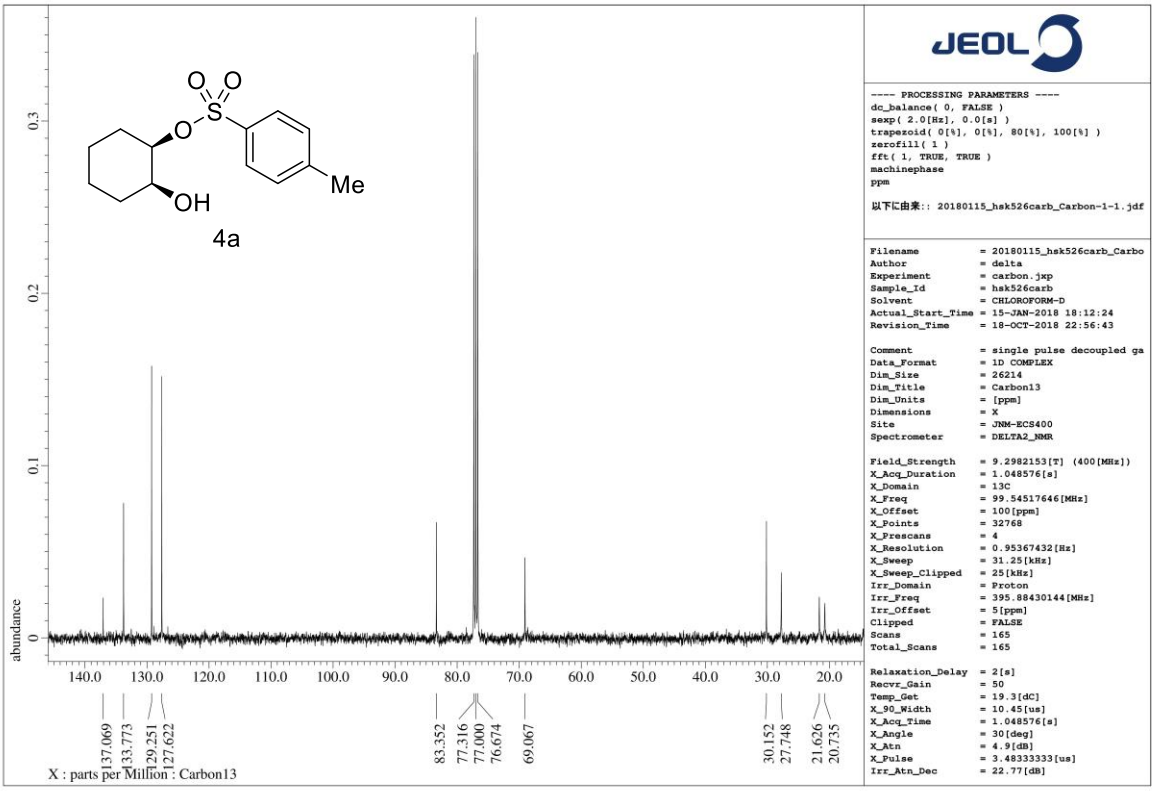

HO
B
OH
N
Me
N
1h
4.61
2.07
2.00
2.12
4.02
5.00
1.05
1.02
1.00
1.04
1.00
1.06
0.96
1.15
0.96
1.09
1.04
1.04
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.981
8.970
8.197
8.176
7.764
7.578
7.263
7.261
6.855
6.837
5.840
5.823
5.815
5.796
5.043
4.998
4.867
4.839
3.781
3.749
3.476
3.030
2.866
2.363
2.337
2.277
1.572
1.488
1.472
1.464
1.449
0.491
0.470
0.457
0.000
-0.002
-0.009
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180920_hsk4770920_Proto
Author = delta
Experiment = proton.jxp
Sample_Id = hsk4770920
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-SEP-2018 13:31:06
Revision_Time = 22-OCT-2018 21:21:44
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 20.3[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

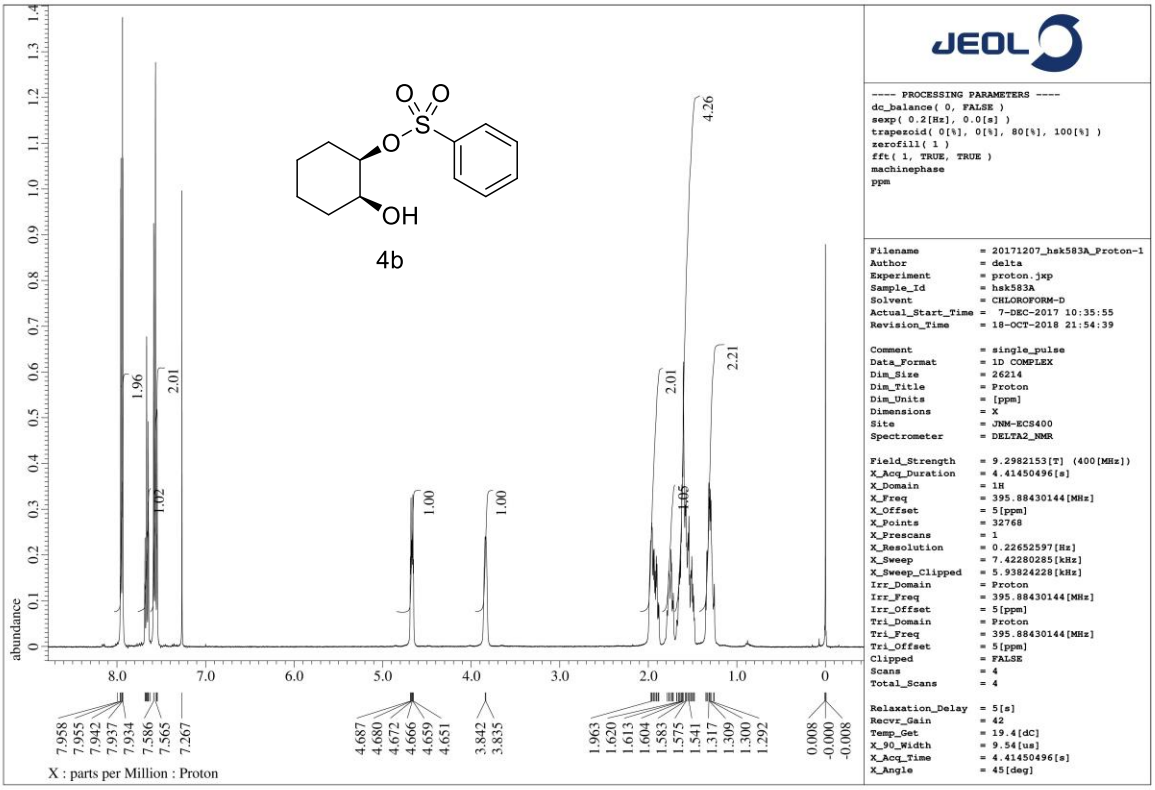

HO
B
OH
N
Me
N
1h
abundance
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
149.408
148.760
141.941
141.292
130.553
130.314
129.055
127.081
123.362
119.947
114.196
77.324
77.000
76.676
61.111
58.411
58.106
56.323
55.846
40.929
39.623
35.808
27.958
27.482
27.214
17.276
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20181023_hsk577carb@50C_Carbon-1-1.
Filename = 20181023_hsk577carb@50C_C
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk577carb@50C
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-OCT-2018 11:36:36
Revision_Time = 23-OCT-2018 12:39:01
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 160
Total_Scans = 160
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 50[dC]
X_90_Width = 10.51[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4[dB]
X_Pulse = 3.50333333[us]
Irr_Atn_Dec = 20.416[dB]

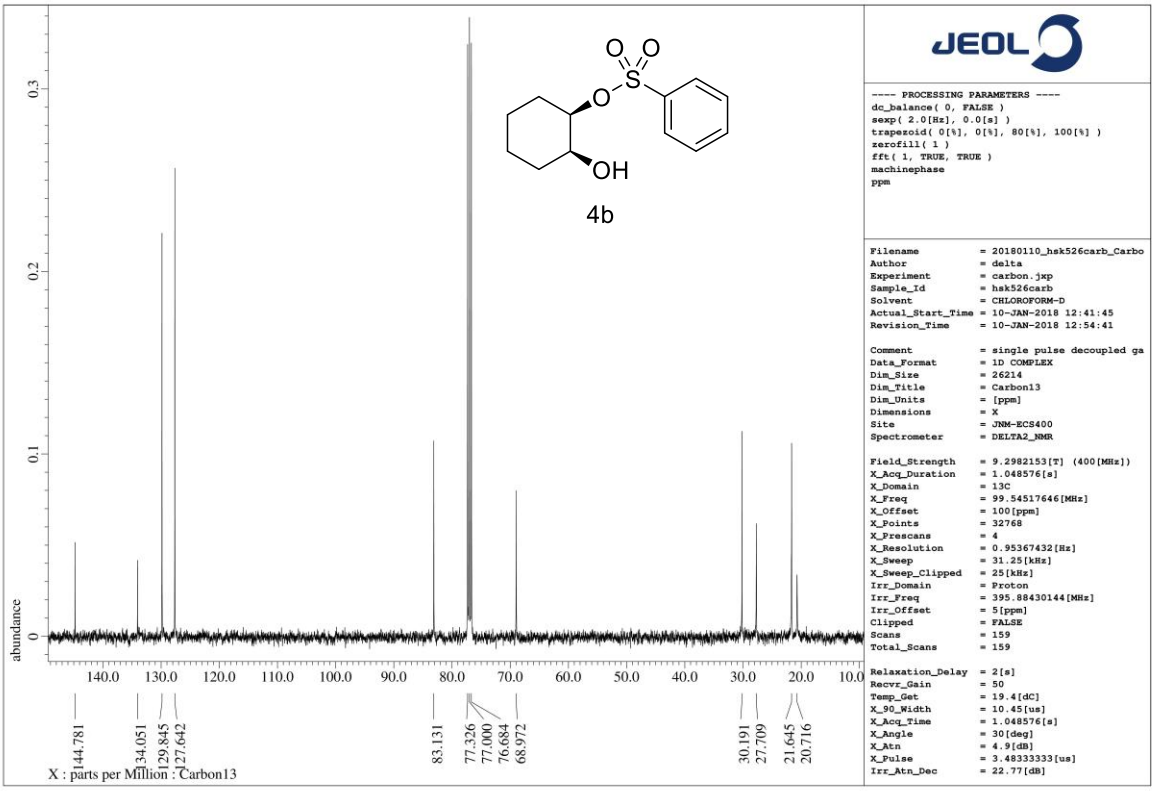

1i
X : parts per Million : Proton
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20181023_hsk876B-2_Proton-1-1.jdf
Filename = 20181023_hsk876B-2_Proton
Author = delta
Experiment = proton.jxp
Sample_Id = hsk876B-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-OCT-2018 11:19:16
Revision_Time = 2-NOV-2018 14:20:28
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 4.456448[s]
X_Domain = 1H
X_Freq = 391.78655441[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22439396[Hz]
X_Sweep = 7.35294118[kHz]
X_Sweep_Clipped = 5.88235294[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 391.78655441[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 26
Temp_Get = 21.2[dC]
X_90_Width = 12.3[us]
X_Acq_Time = 4.456448[s]
X_Angle = 45[deg]

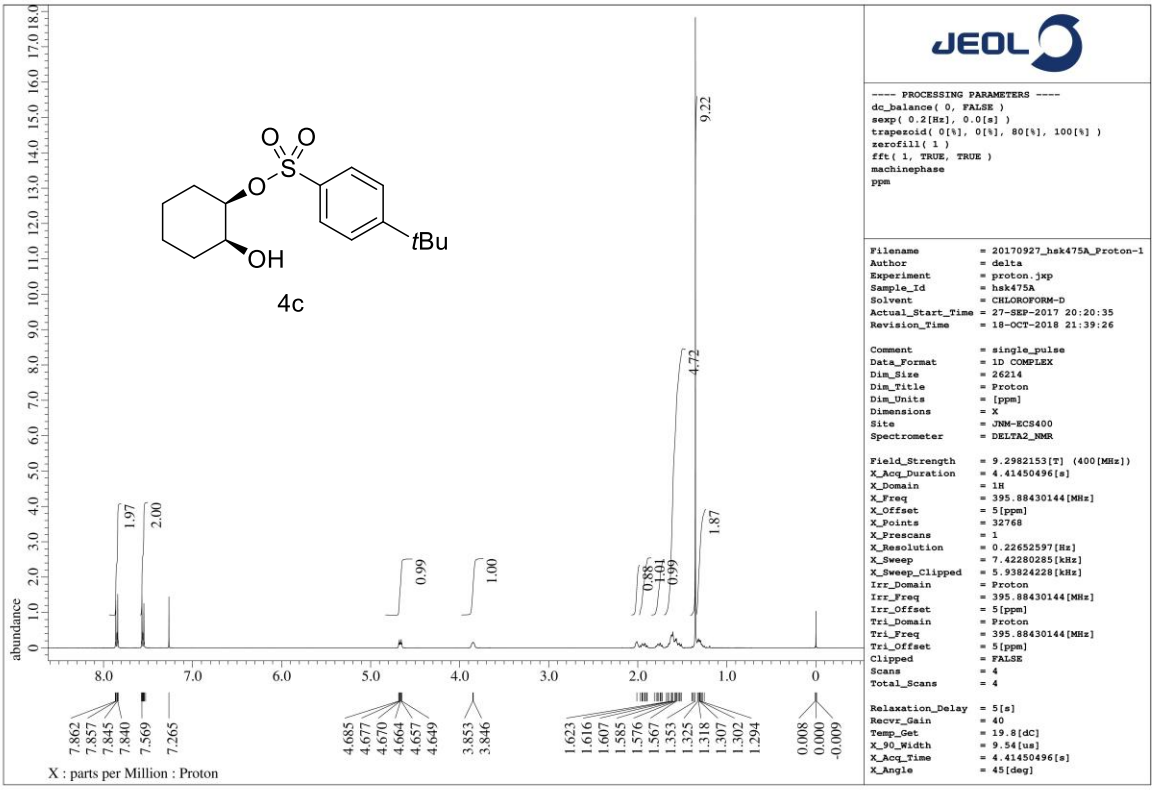

1i
X : parts per Million : Carbon13
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(1.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(77.31039[ppm], 77[ppm])
以下に由来:: 20181025_hsk876carb_Carbon-1-1.jdf
Filename = 20181025_hsk876carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk876carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-OCT-2018 14:54:20
Revision_Time = 25-OCT-2018 15:36:54
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 233
Total_Scans = 233
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.8[dC]
X_90_Width = 10.51[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4[dB]
X_Pulse = 3.50333333[us]
Irr_Atn_Dec = 20.416[dB]

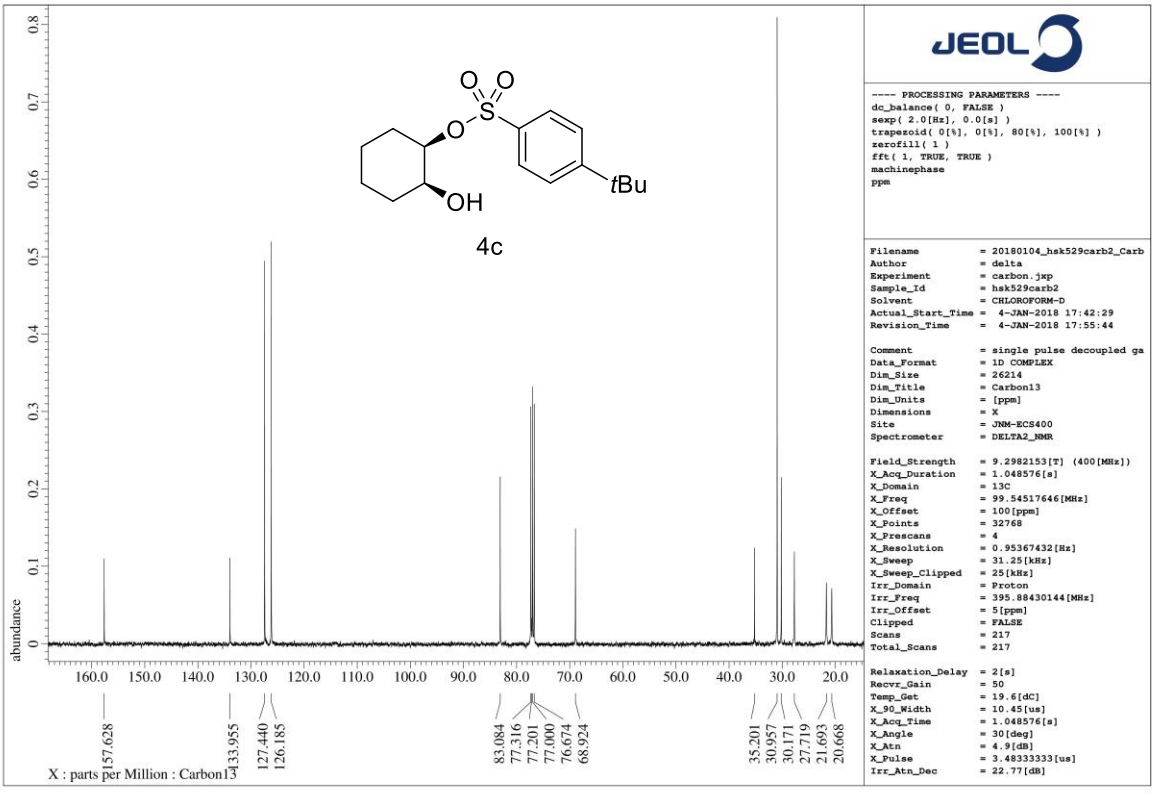

4a
Me
OH
4.24
3.07
2.15
2.01
2.00
0.99
1.00
0.93
1.00
1.01
abundance
X : parts per Million : Proton
7.828
7.824
7.812
7.807
7.360
7.340
7.338
7.268
4.644
4.636
4.628
4.623
4.615
4.607
3.826
3.819
2.454
2.015
2.003
1.597
1.590
1.310
1.301
1.294
1.286
-0.000
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20171130_hsk575A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk575A
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-NOV-2017 14:36:11
Revision_Time = 18-OCT-2018 21:34:05
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 19.7[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

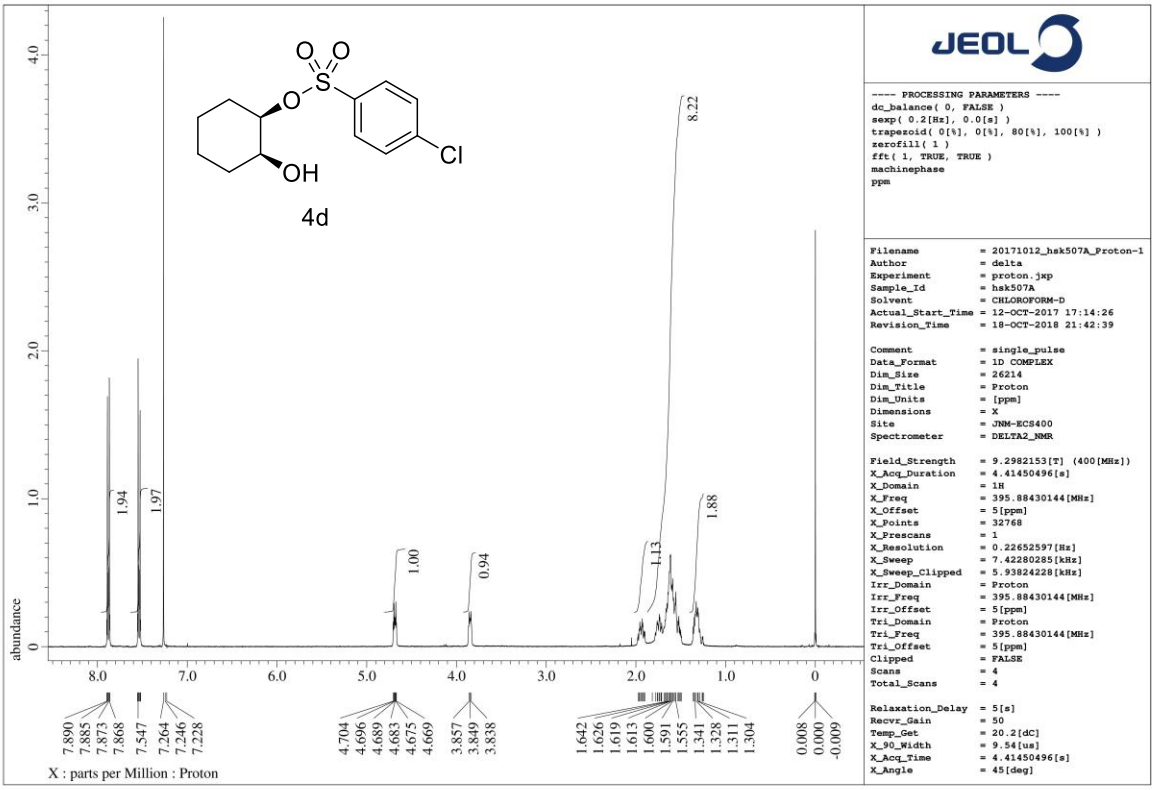

4a
Me
OH
abundance
X : parts per Million : Carbon13
137.069
133.773
129.251
127.622
83.352
77.316
77.000
76.674
69.067
30.152
27.748
21.626
20.735
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180115_hsk526carb_Carbon-1-1.jdf
Filename = 20180115_hsk526carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk526carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JAN-2018 18:12:24
Revision_Time = 18-OCT-2018 22:56:43
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 165
Total_Scans = 165
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.3[dC]
X_90_Width = 10.45[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.48333333[us]
Irr_Atn_Dec = 22.77[dB]

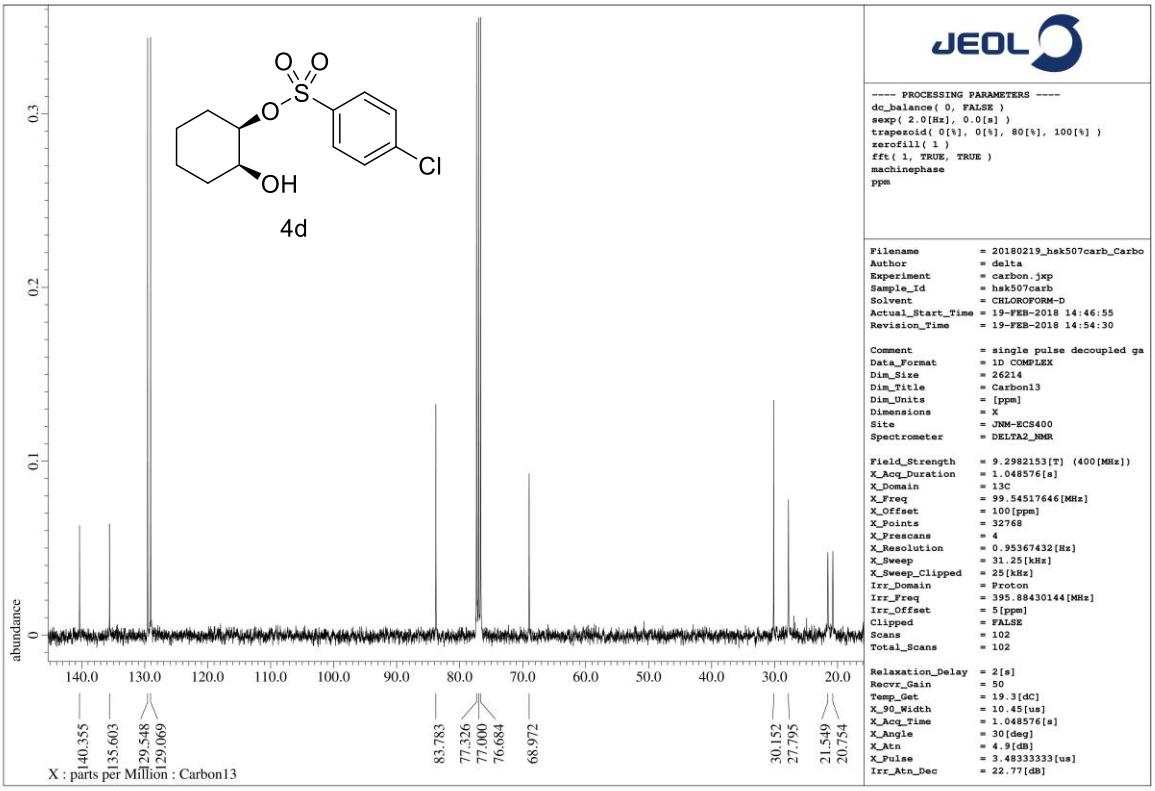

4b
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20171207_hsk583A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk583A
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-DEC-2017 10:35:55
Revision_Time = 18-OCT-2018 21:54:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 19.4[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

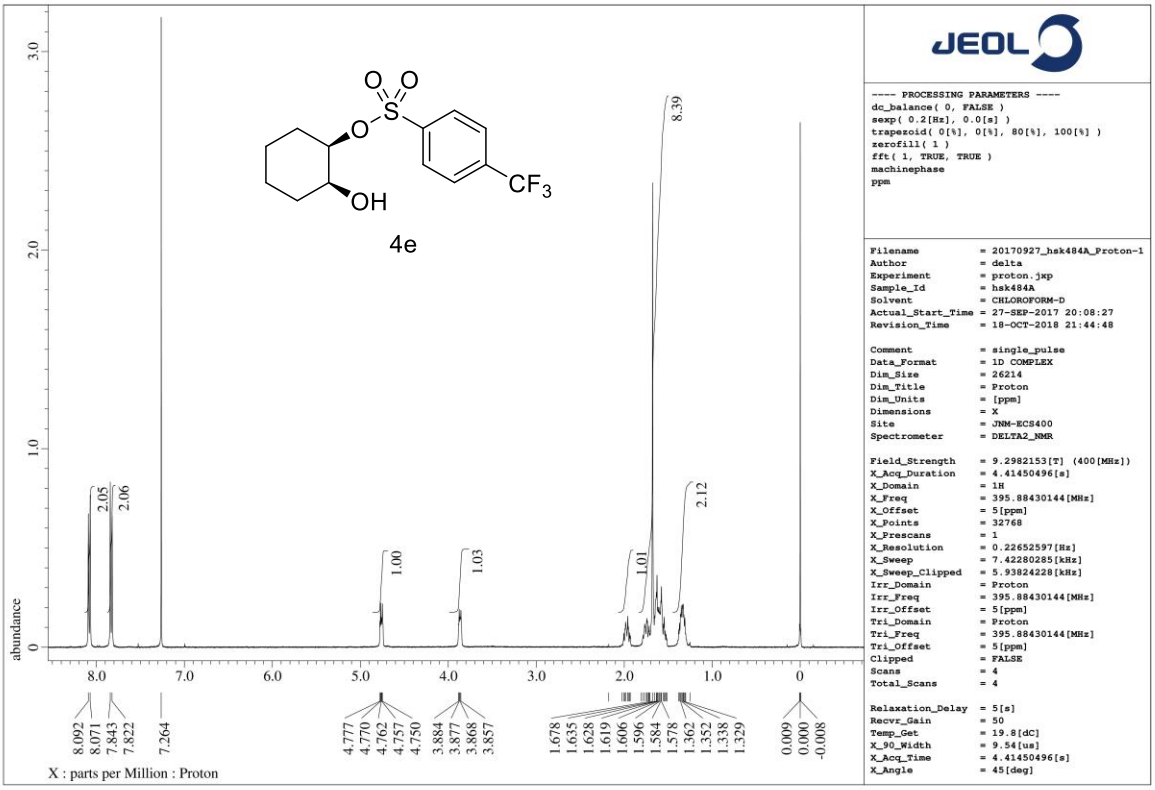

4b
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180110_hsk526carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk526carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-JAN-2018 12:41:45
Revision_Time = 10-JAN-2018 12:54:41
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 159
Total_Scans = 159
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.4[dC]
X_90_Width = 10.45[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.48333333[us]
Irr_Atn_Dec = 22.77[dB]

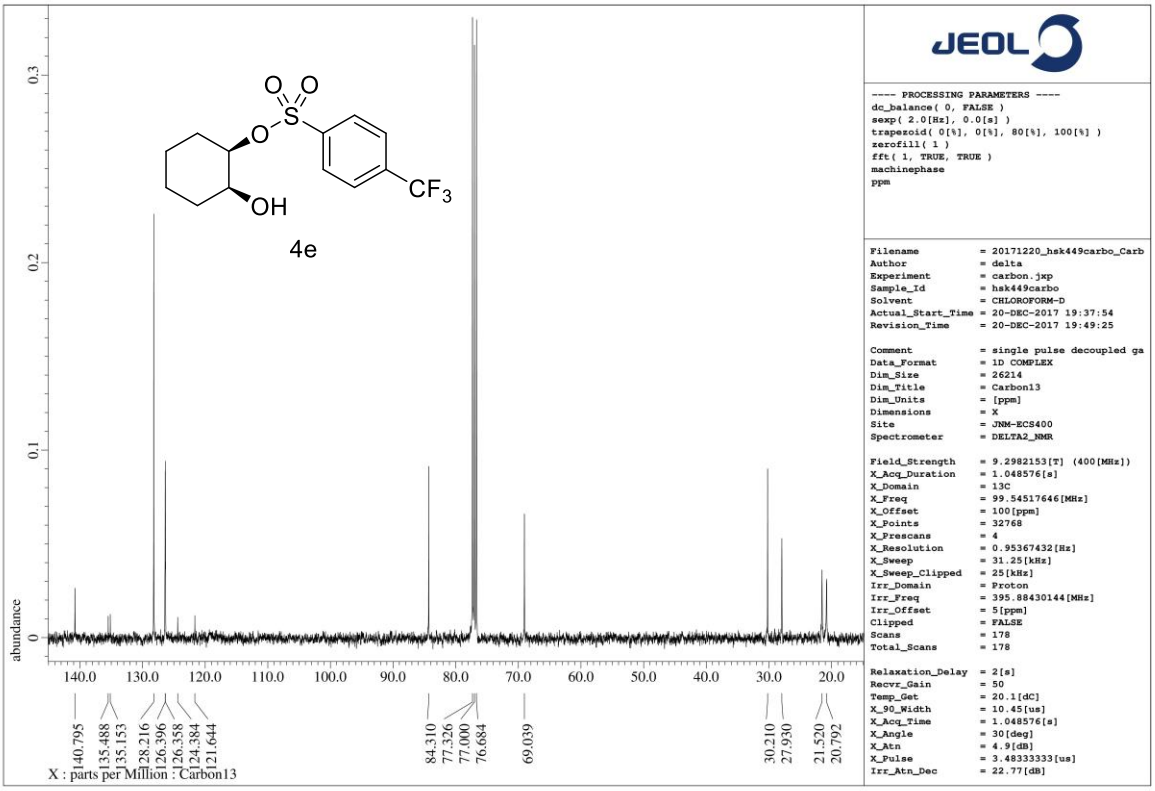

4c
tBu
OH
9.22
4.72
1.97
2.00
0.99
1.00
0.88
1.01
0.99
1.87
abundance
X : parts per Million : Proton
7.862
7.857
7.845
7.840
7.569
7.265
4.685
4.677
4.670
4.664
4.657
4.649
3.853
3.846
1.623
1.616
1.607
1.585
1.576
1.567
1.353
1.325
1.318
1.307
1.302
1.294
0.008
0.000
-0.009
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20170927_hsk475A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk475A
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-SEP-2017 20:20:35
Revision_Time = 18-OCT-2018 21:39:26
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 19.8[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

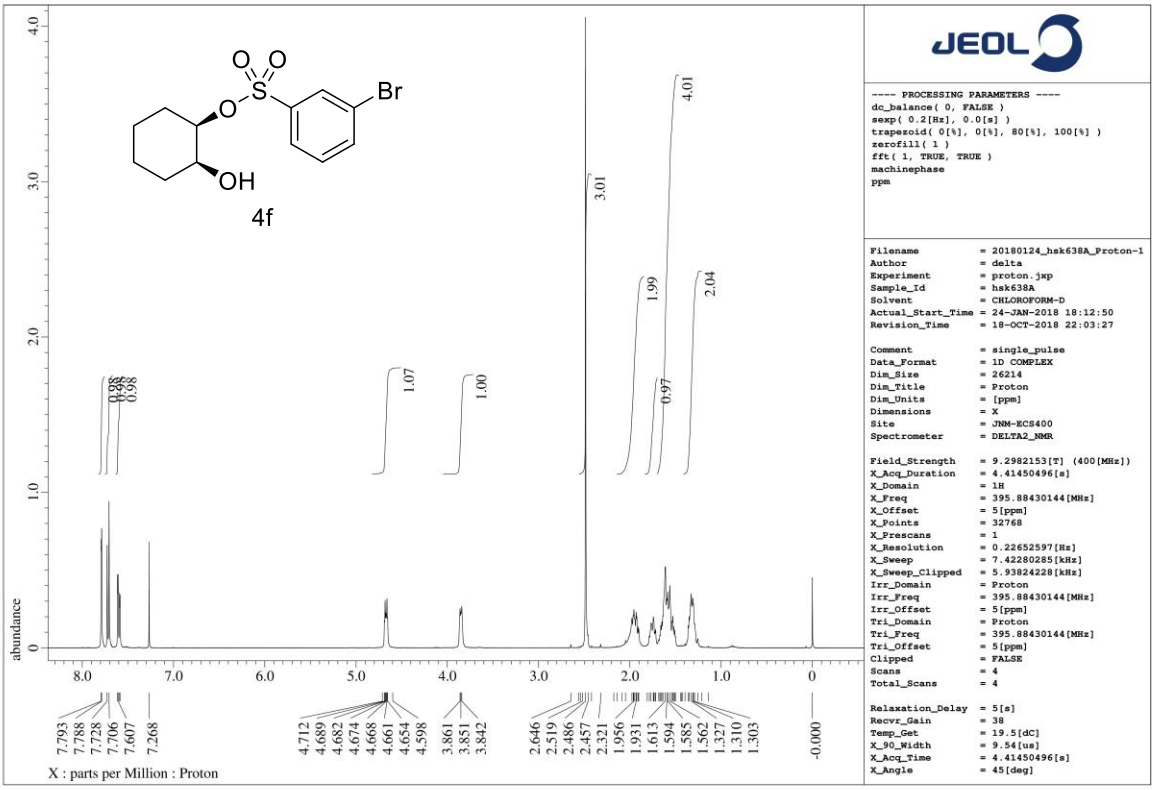

4c
tBu
OH
abundance
X : parts per Million : Carbon13
157.628
133.955
127.440
126.185
83.084
77.316
77.201
77.000
76.674
68.924
35.201
30.957
30.171
27.719
21.693
20.668
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180104_hsk529carb2_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk529carb2
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-JAN-2018 17:42:29
Revision_Time = 4-JAN-2018 17:55:44
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 217
Total_Scans = 217
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.6[dC]
X_90_Width = 10.45[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.48333333[us]
Irr_Atn_Dec = 22.77[dB]

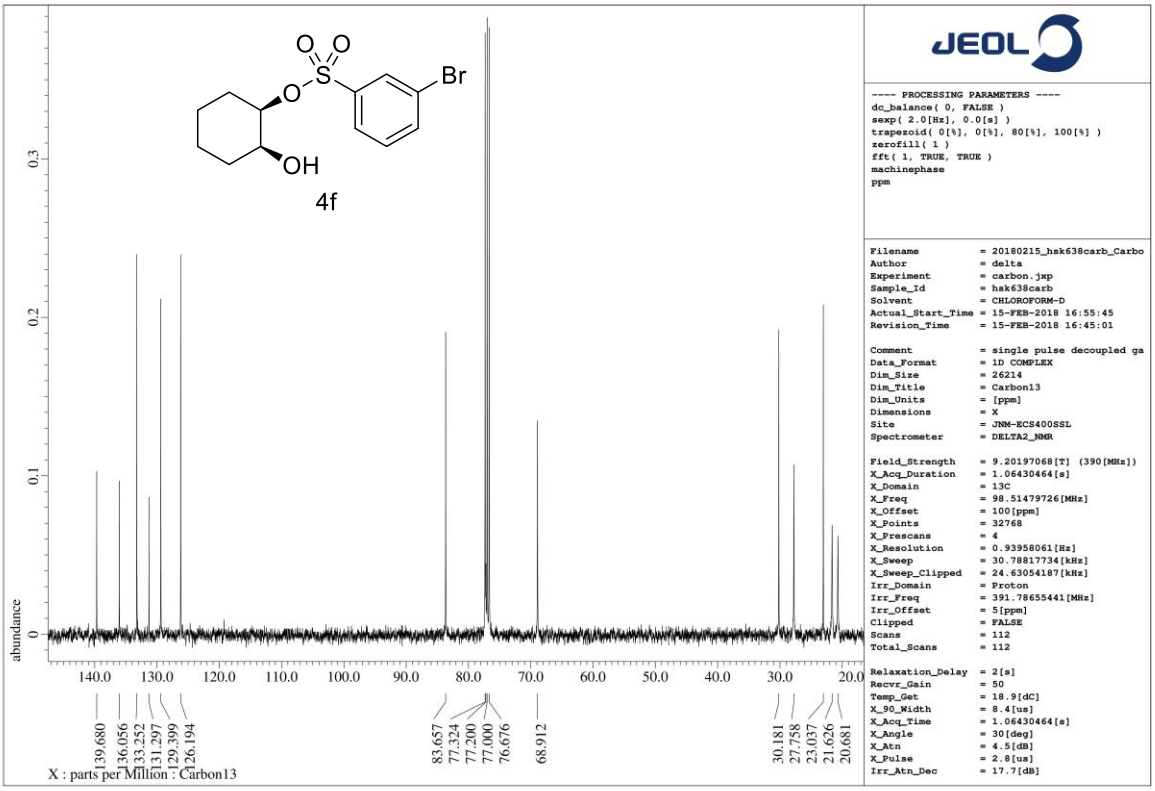

4d
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20171012_hsk507A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk507A
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-OCT-2017 17:14:26
Revision_Time = 18-OCT-2018 21:42:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 20.2[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

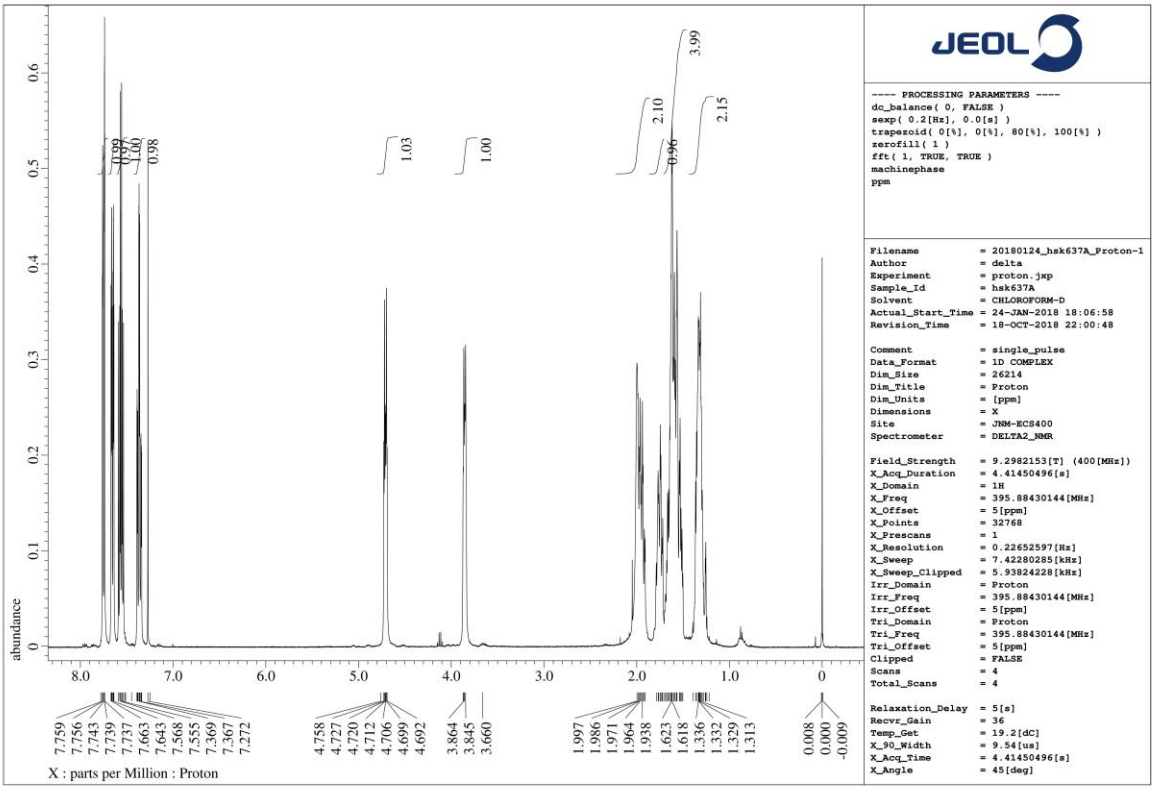

4d
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180219_hsk507carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk507carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2018 14:46:55
Revision_Time = 19-FEB-2018 14:54:30
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 102
Total_Scans = 102
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.3[dC]
X_90_Width = 10.45[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.48333333[us]
Irr_Atn_Dec = 22.77[dB]

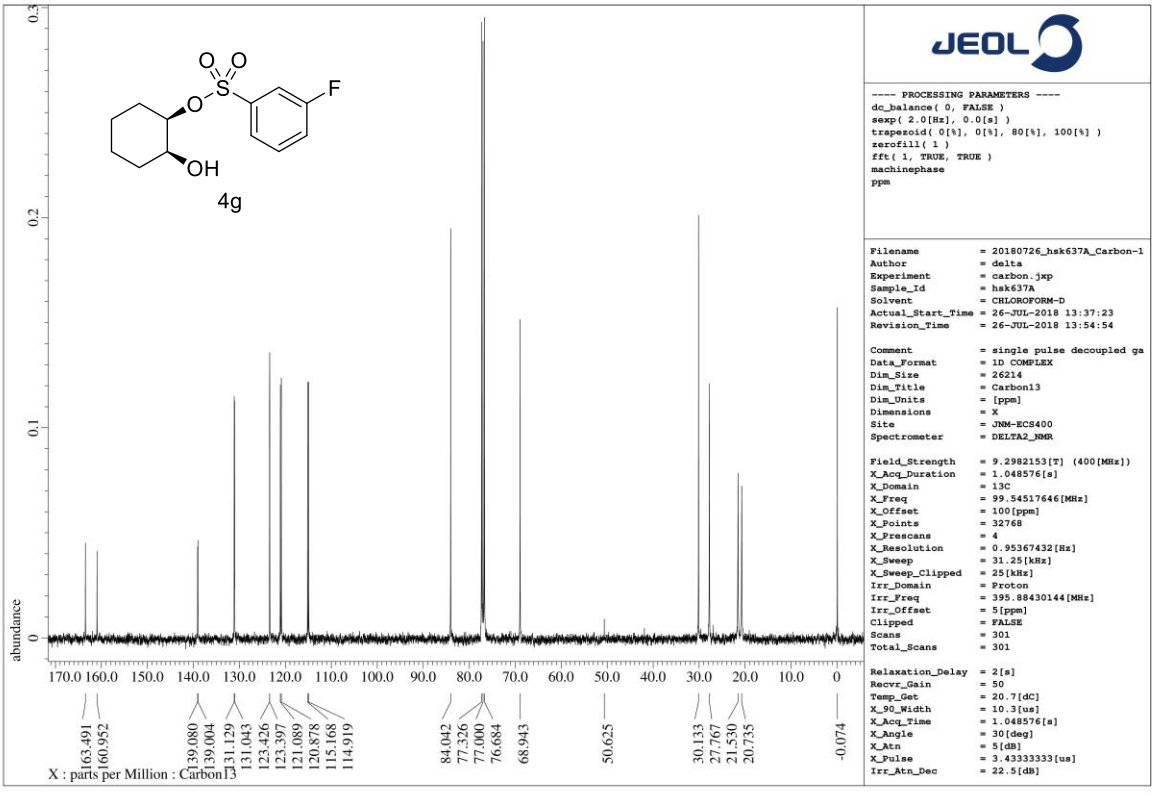

4e
abundance
X : parts per Million : Proton
8.092
8.071
7.843
7.822
7.264
4.777
4.770
4.762
4.757
4.750
3.884
3.877
3.868
3.857
1.678
1.635
1.628
1.619
1.606
1.596
1.584
1.578
1.362
1.352
1.338
1.329
0.009
0.000
-0.008
2.05
2.06
1.00
1.03
1.01
8.39
2.12
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20170927_hsk484A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk484A
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-SEP-2017 20:08:27
Revision_Time = 18-OCT-2018 21:44:48
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 19.8[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

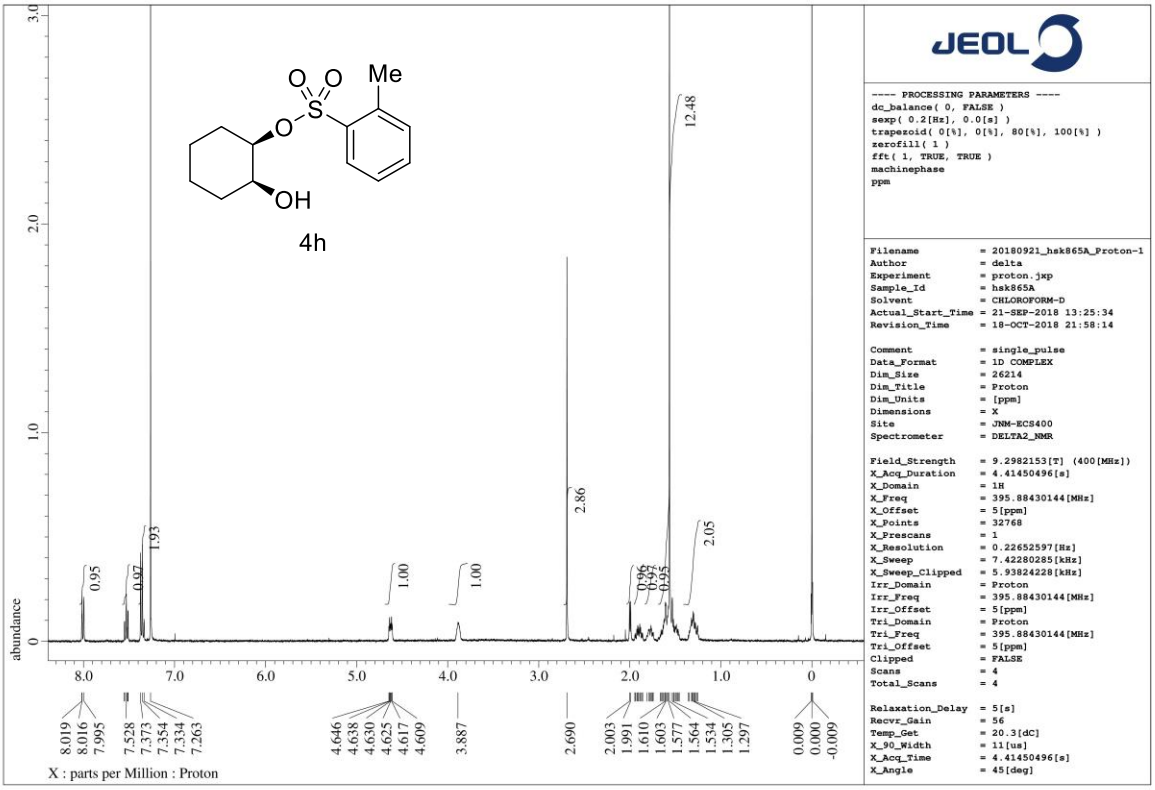

4e
abundance
X : parts per Million : Carbon13
140.795
135.488
135.153
128.216
126.396
126.358
124.384
121.644
84.310
77.326
77.000
76.684
69.039
30.210
27.930
21.520
20.792
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20171220_hsk449carbo_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk449carbo
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-DEC-2017 19:37:54
Revision_Time = 20-DEC-2017 19:49:25
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 178
Total_Scans = 178
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.1[dC]
X_90_Width = 10.45[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.48333333[us]
Irr_Atn_Dec = 22.77[dB]

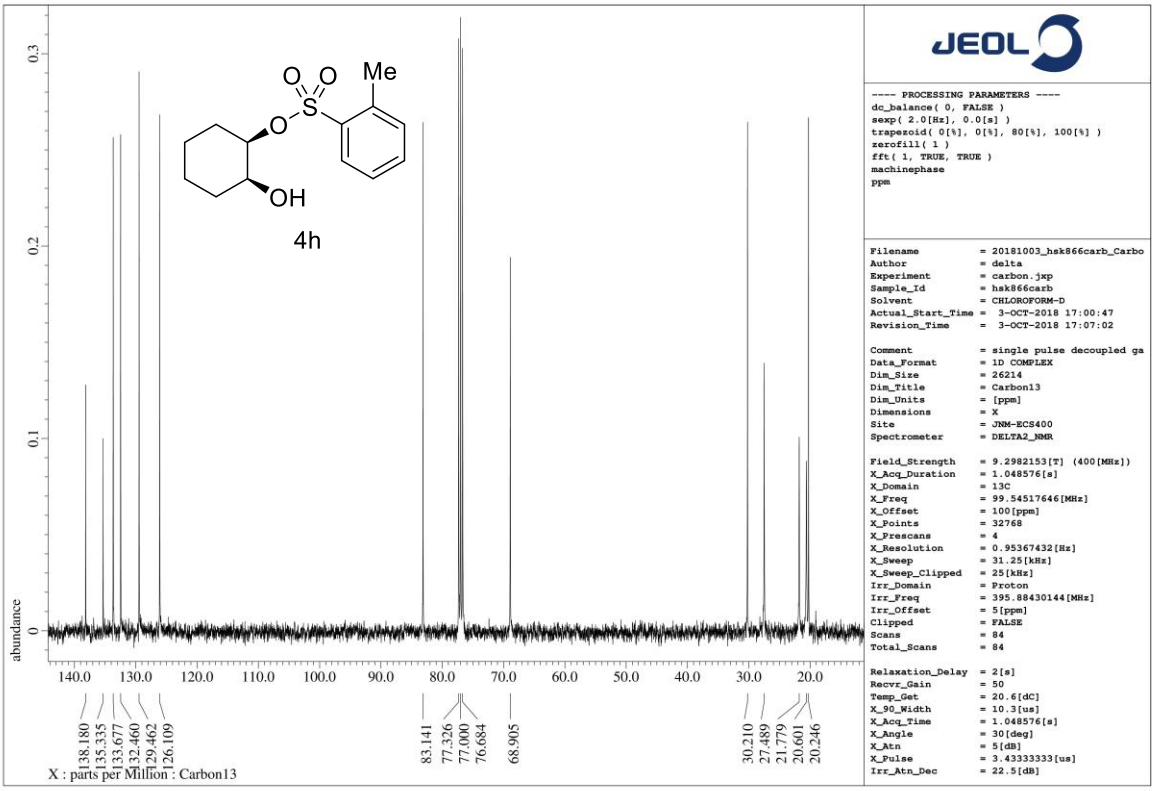

4f
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180124_hsk638A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk638A
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-JAN-2018 18:12:50
Revision_Time = 18-OCT-2018 22:03:27
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 19.5[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

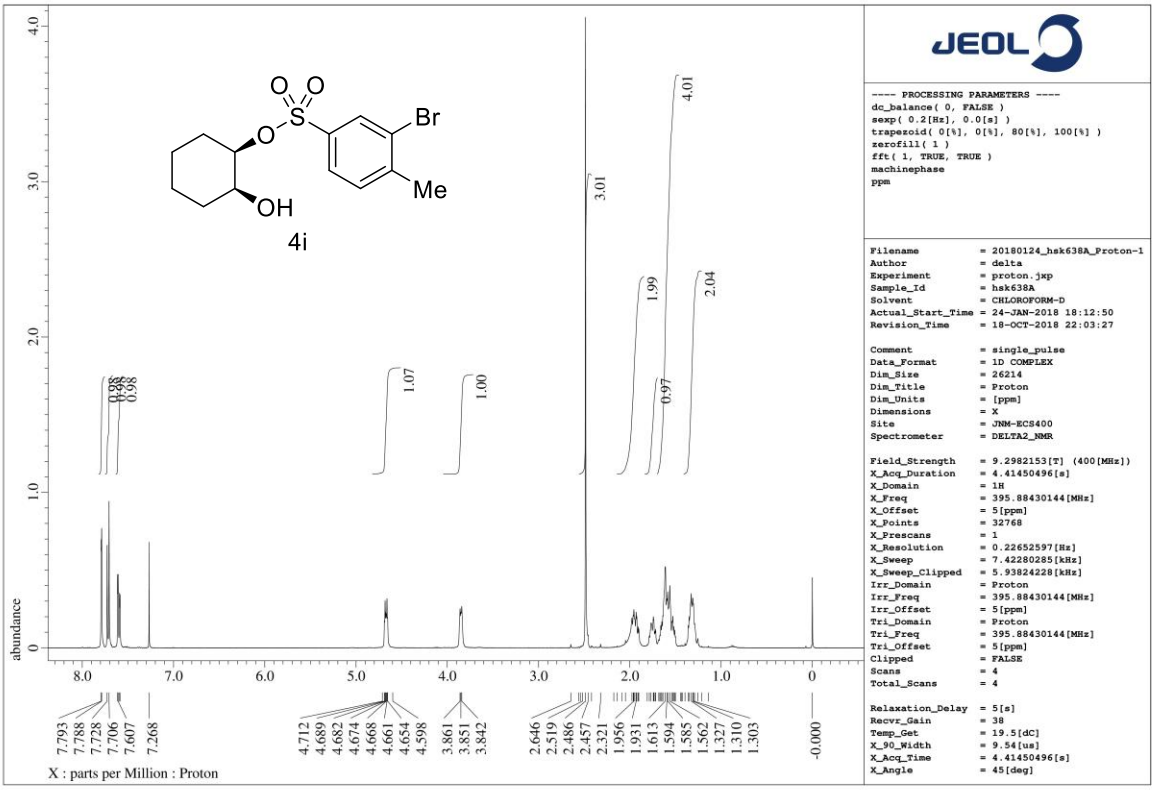

4f
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180215_hsk638carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk638carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-FEB-2018 16:55:45
Revision_Time = 15-FEB-2018 16:45:01
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 112
Total_Scans = 112
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 18.9[dC]
X_90_Width = 8.4[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.5[dB]
X_Pulse = 2.8[us]
Irr_Atn_Dec = 17.7[dB]

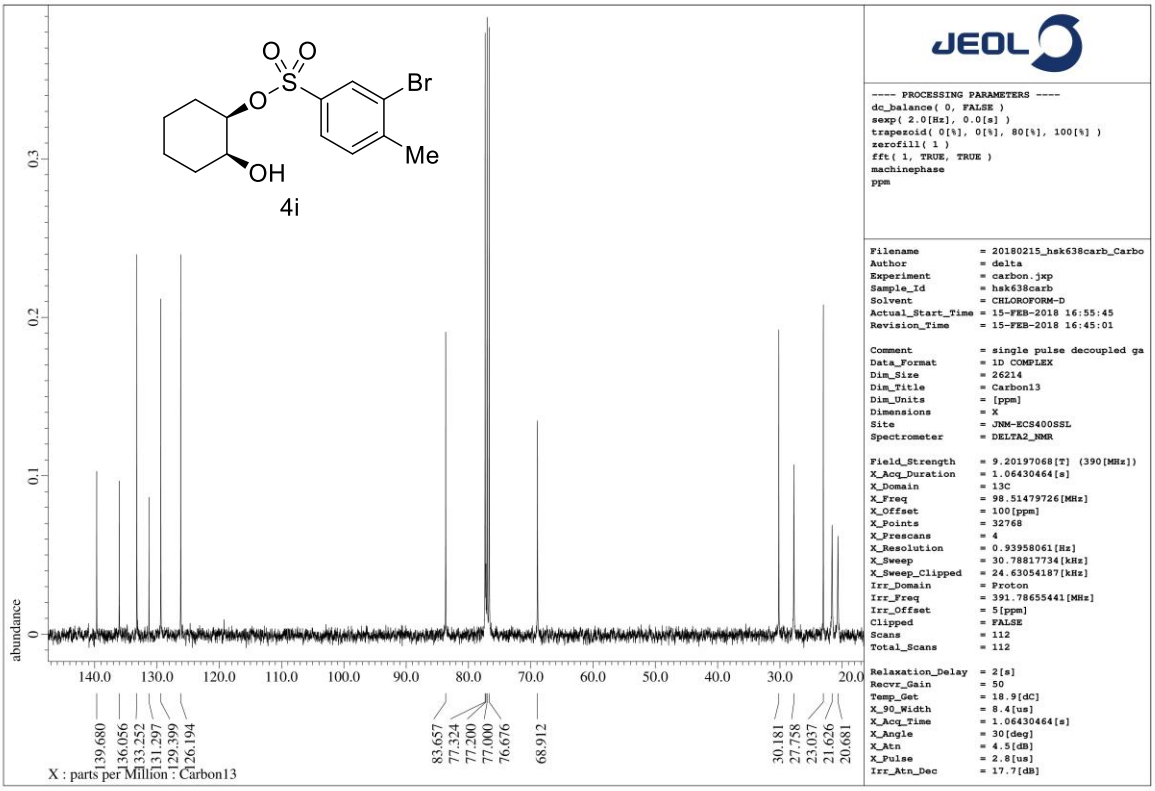

JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180124_hsk637A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk637A
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-JAN-2018 18:06:58
Revision_Time = 18-OCT-2018 22:00:48
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 19.2[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]
abundance
X : parts per Million : Proton

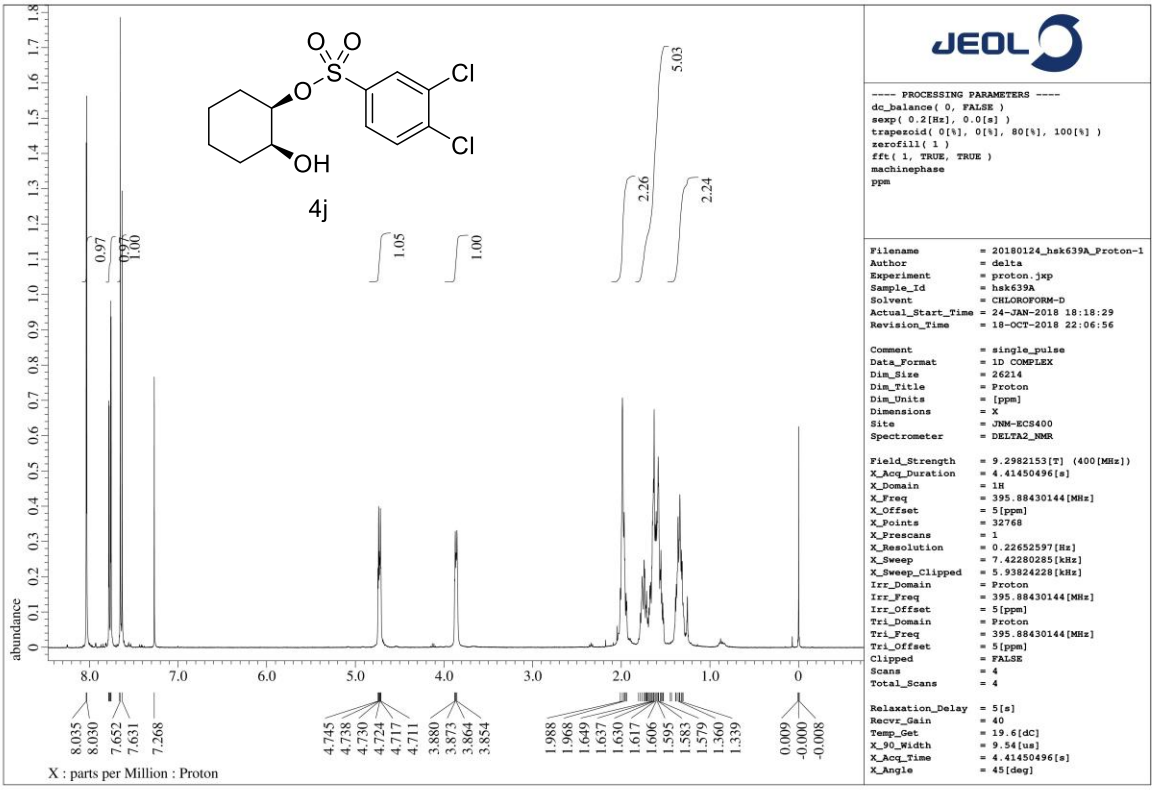

JEOL
4g
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180726_hsk637A_Carbon-1
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk637A
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JUL-2018 13:37:23
Revision_Time = 26-JUL-2018 13:54:54
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 301
Total_Scans = 301
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.7[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 5[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.5[dB]
abundance
X : parts per Million : Carbon13

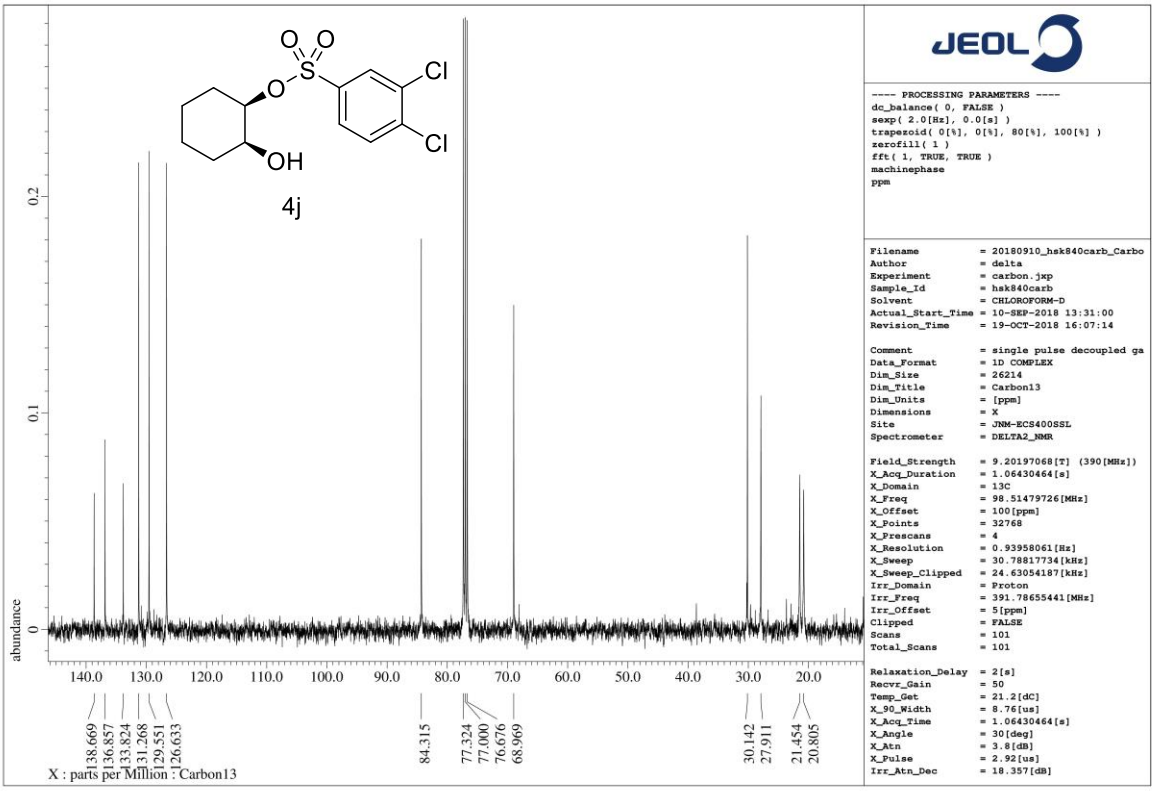

4h
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180921_hsk865A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk865A
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-SEP-2018 13:25:34
Revision_Time = 18-OCT-2018 21:58:14
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 20.3[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

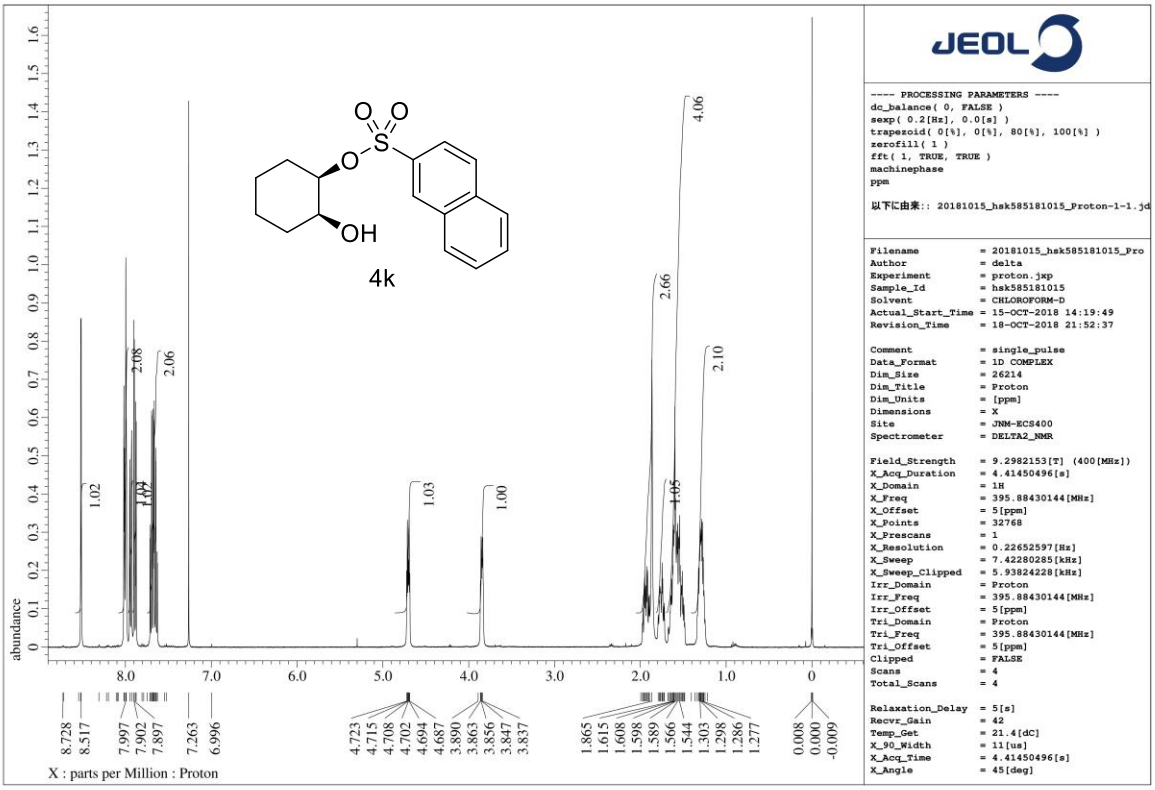

4h
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20181003_hsk866carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk866carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-OCT-2018 17:00:47
Revision_Time = 3-OCT-2018 17:07:02
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 84
Total_Scans = 84
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.6[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 5[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.5[dB]

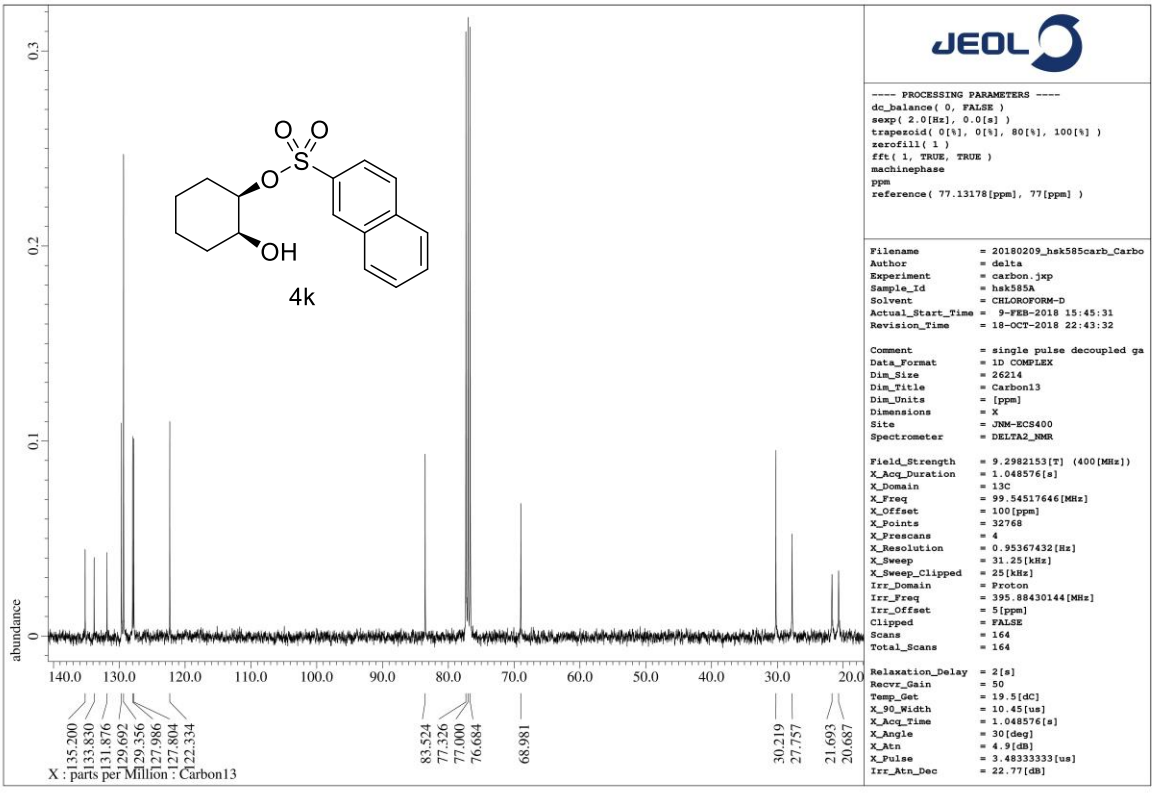

4i
Br
Me
OH
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180124_hsk638A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk638A
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-JAN-2018 18:12:50
Revision_Time = 18-OCT-2018 22:03:27
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 19.5[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

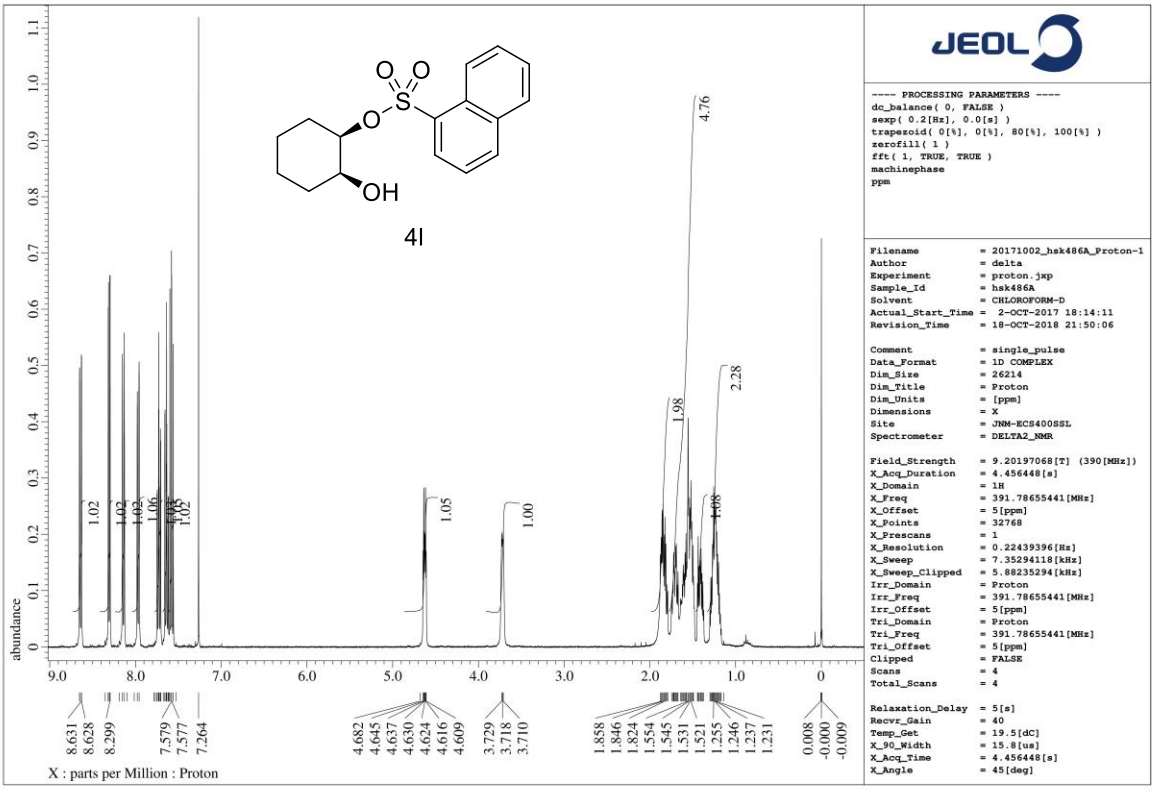

4i
Br
Me
OH
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180215_hsk638carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk638carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-FEB-2018 16:55:45
Revision_Time = 15-FEB-2018 16:45:01
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 112
Total_Scans = 112
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 18.9[dC]
X_90_Width = 8.4[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.5[dB]
X_Pulse = 2.8[us]
Irr_Atn_Dec = 17.7[dB]

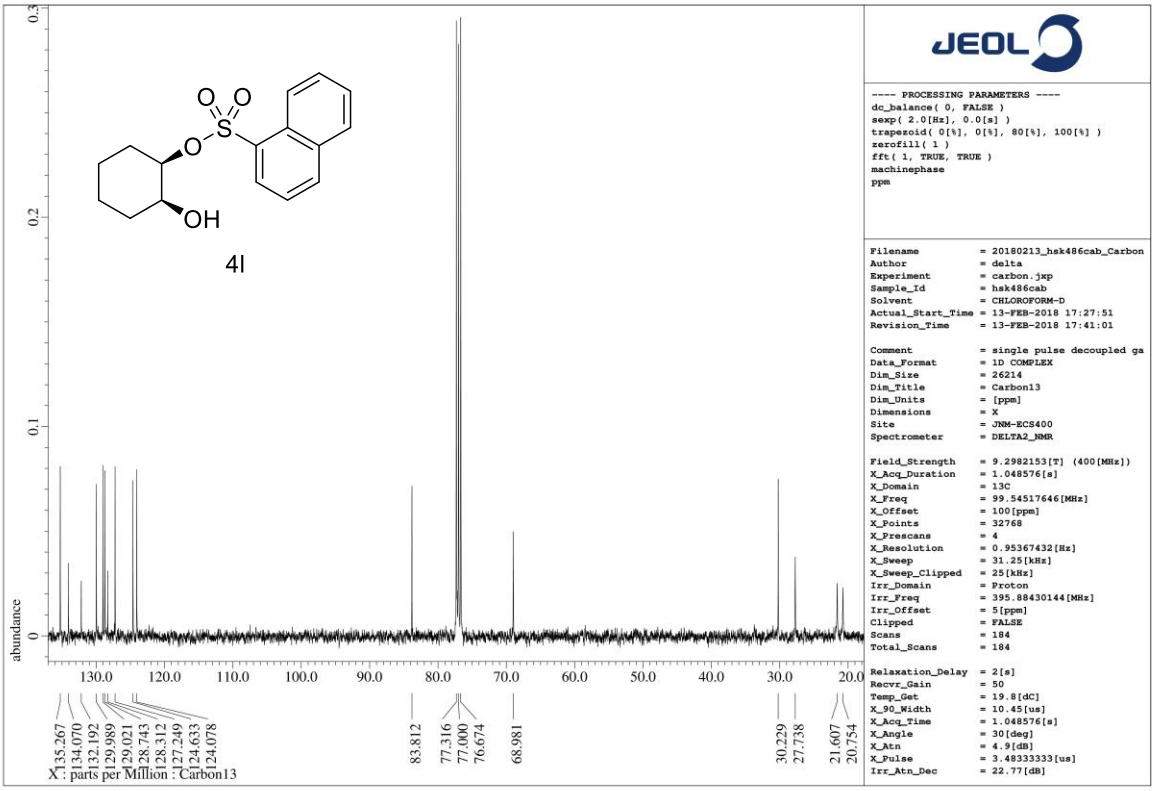

4j
abundance
X : parts per Million : Proton
8.035
8.030
7.652
7.631
7.268
4.745
4.738
4.730
4.724
4.717
4.711
3.880
3.873
3.864
3.854
1.988
1.968
1.649
1.637
1.630
1.617
1.606
1.595
1.583
1.579
1.360
1.339
0.009
-0.000
-0.008
0.97
0.97
1.00
1.05
1.00
2.26
5.03
2.24
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180124_hsk639A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk639A
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-JAN-2018 18:18:29
Revision_Time = 18-OCT-2018 22:06:56
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 19.6[dC]
X_90_Width = 9.54[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

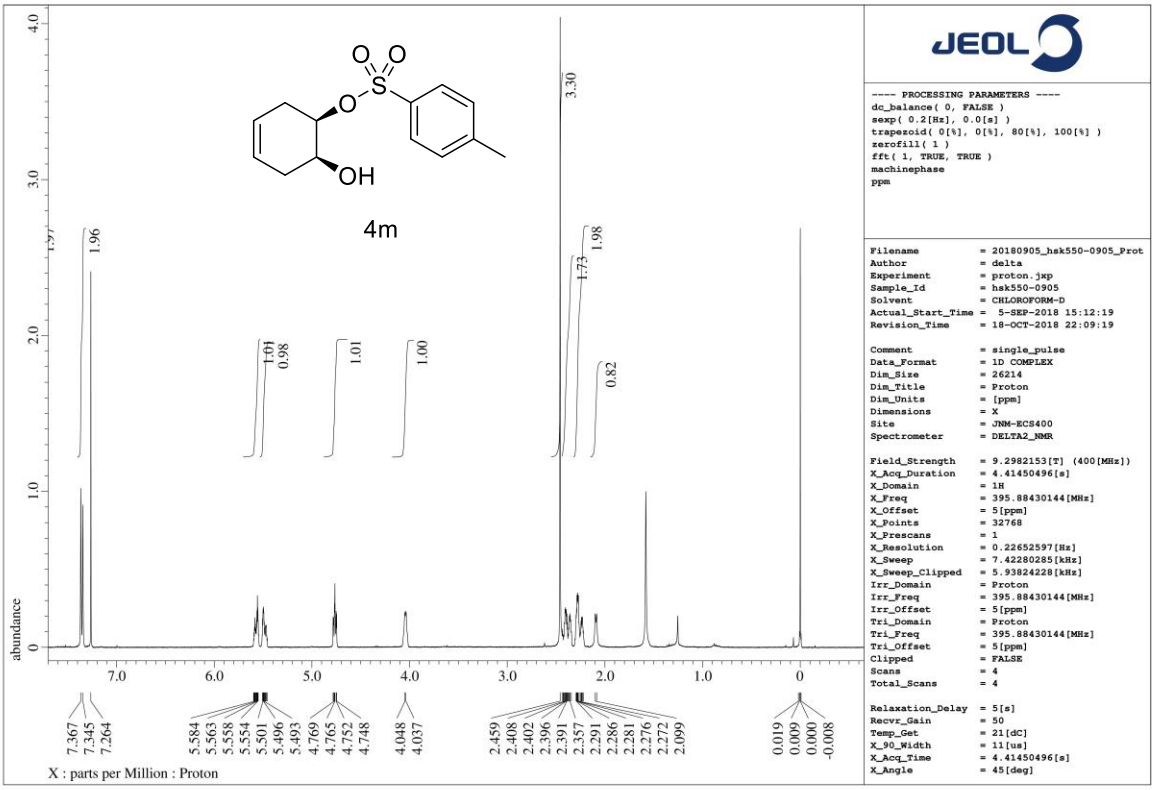

4j
abundance
X : parts per Million : Carbon13
138.669
136.857
133.824
131.268
129.551
126.633
84.315
77.324
77.000
76.676
68.969
30.142
27.911
21.454
20.805
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180910_hsk840carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk840carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-SEP-2018 13:31:00
Revision_Time = 19-OCT-2018 16:07:14
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 101
Total_Scans = 101
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.2[dC]
X_90_Width = 8.76[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 3.8[dB]
X_Pulse = 2.92[us]
Irr_Atn_Dec = 18.357[dB]

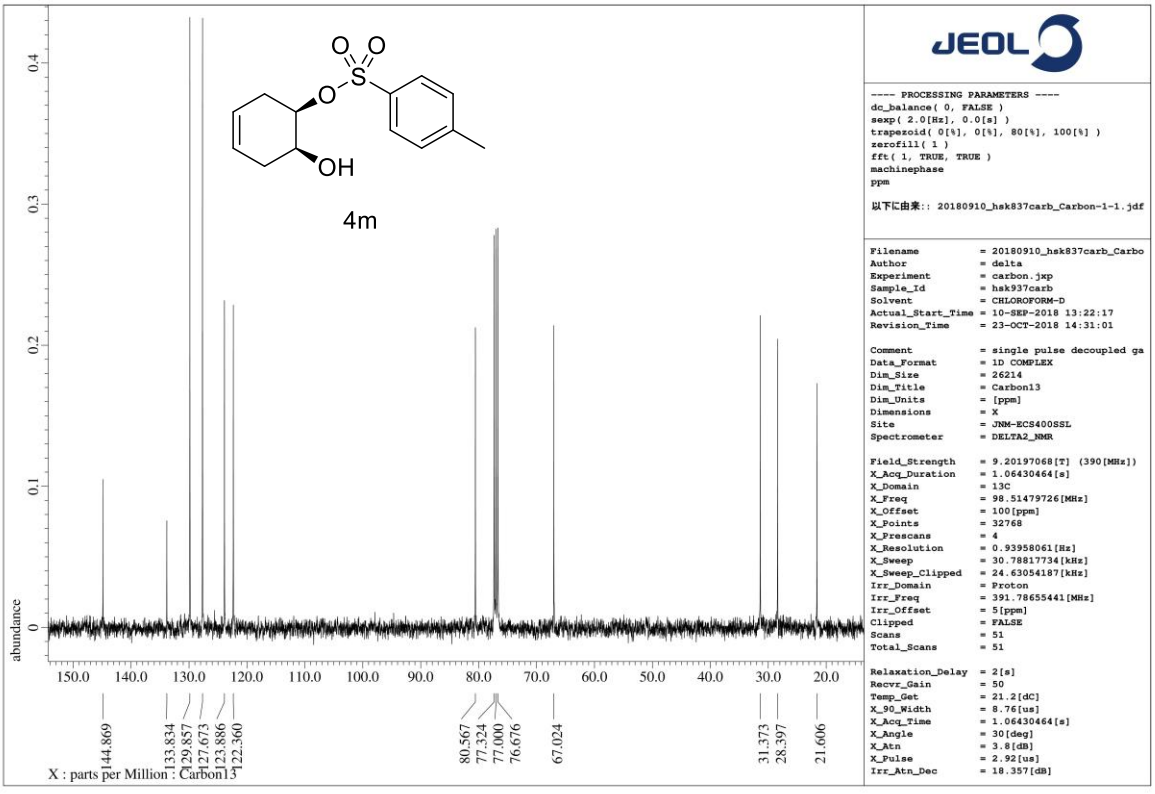

4k
abundance
X : parts per Million : Proton
8.728
8.517
7.997
7.902
7.897
7.263
6.996
4.723
4.715
4.708
4.702
4.694
4.687
3.890
3.863
3.856
3.847
3.837
1.865
1.615
1.608
1.598
1.589
1.566
1.544
1.303
1.298
1.286
1.277
0.008
0.000
-0.009
1.02
2.08
2.06
1.03
1.00
2.66
4.06
2.10
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20181015_hsk585181015_Proton-1-1.jd
Filename = 20181015_hsk585181015_Pro
Author = delta
Experiment = proton.jxp
Sample_Id = hsk585181015
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-OCT-2018 14:19:49
Revision_Time = 18-OCT-2018 21:52:37
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 21.4[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

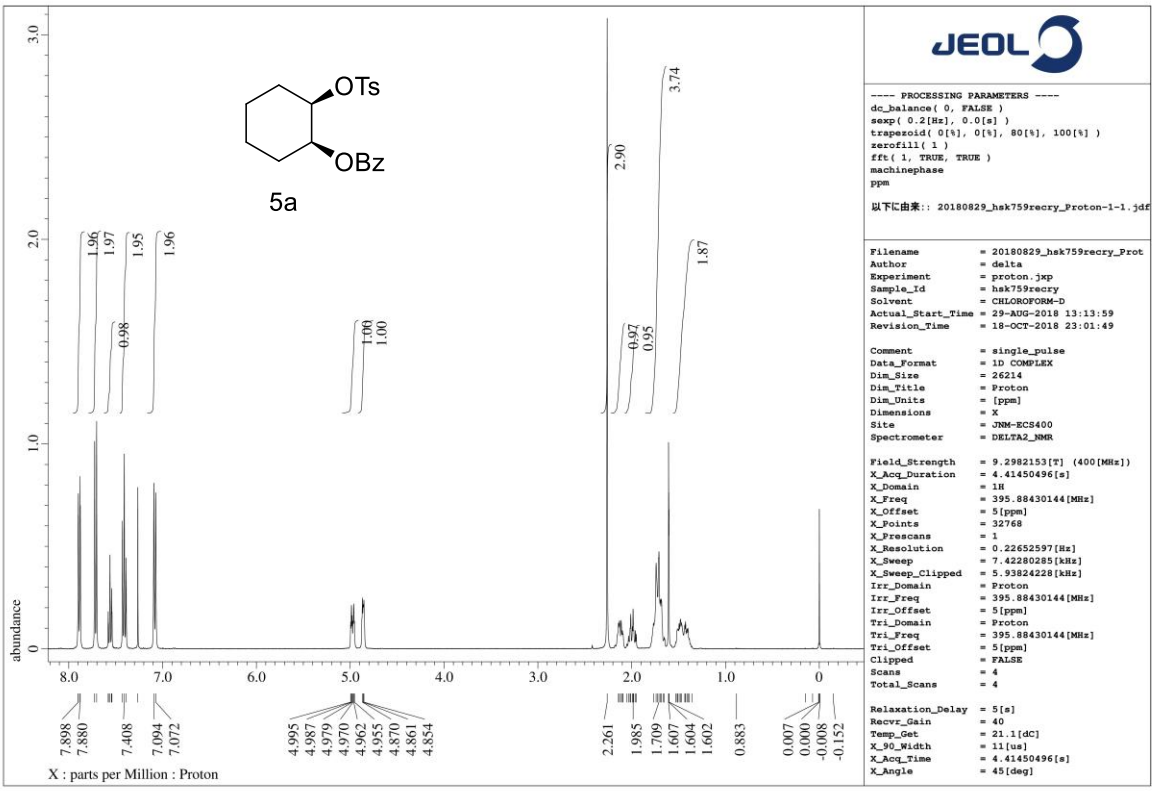

4k
abundance
X : parts per Million : Carbon13
135.200
133.830
131.876
129.692
129.356
127.986
127.804
122.334
83.524
77.326
77.000
76.684
68.981
30.219
27.757
21.693
20.687
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(77.13178[ppm], 77[ppm])
Filename = 20180209_hsk585carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk585A
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-FEB-2018 15:45:31
Revision_Time = 18-OCT-2018 22:43:32
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 164
Total_Scans = 164
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.5[dC]
X_90_Width = 10.45[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.48333333[us]
Irr_Atn_Dec = 22.77[dB]

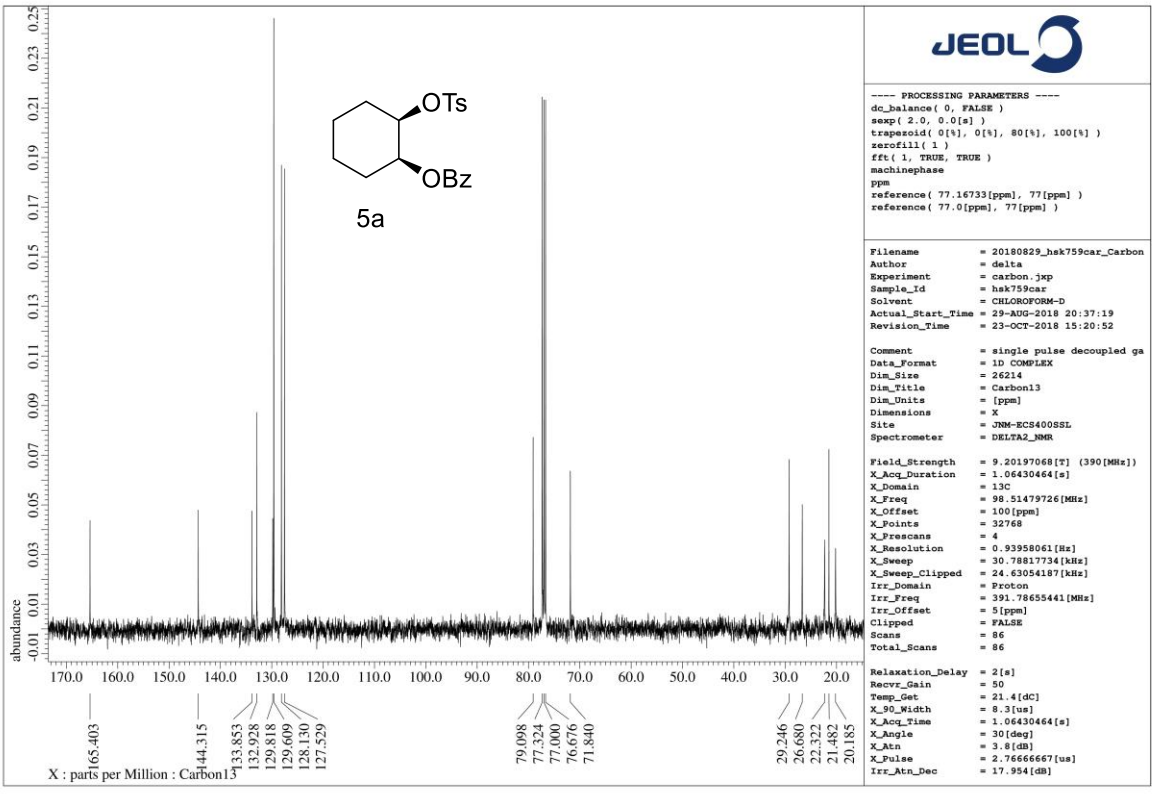

4l
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20171002_hsk486A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk486A
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-OCT-2017 18:14:11
Revision_Time = 18-OCT-2018 21:50:06
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 4.456448[s]
X_Domain = 1H
X_Freq = 391.78655441[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22439396[Hz]
X_Sweep = 7.35294118[kHz]
X_Sweep_Clipped = 5.88235294[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 391.78655441[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 19.5[dC]
X_90_Width = 15.8[us]
X_Acq_Time = 4.456448[s]
X_Angle = 45[deg]

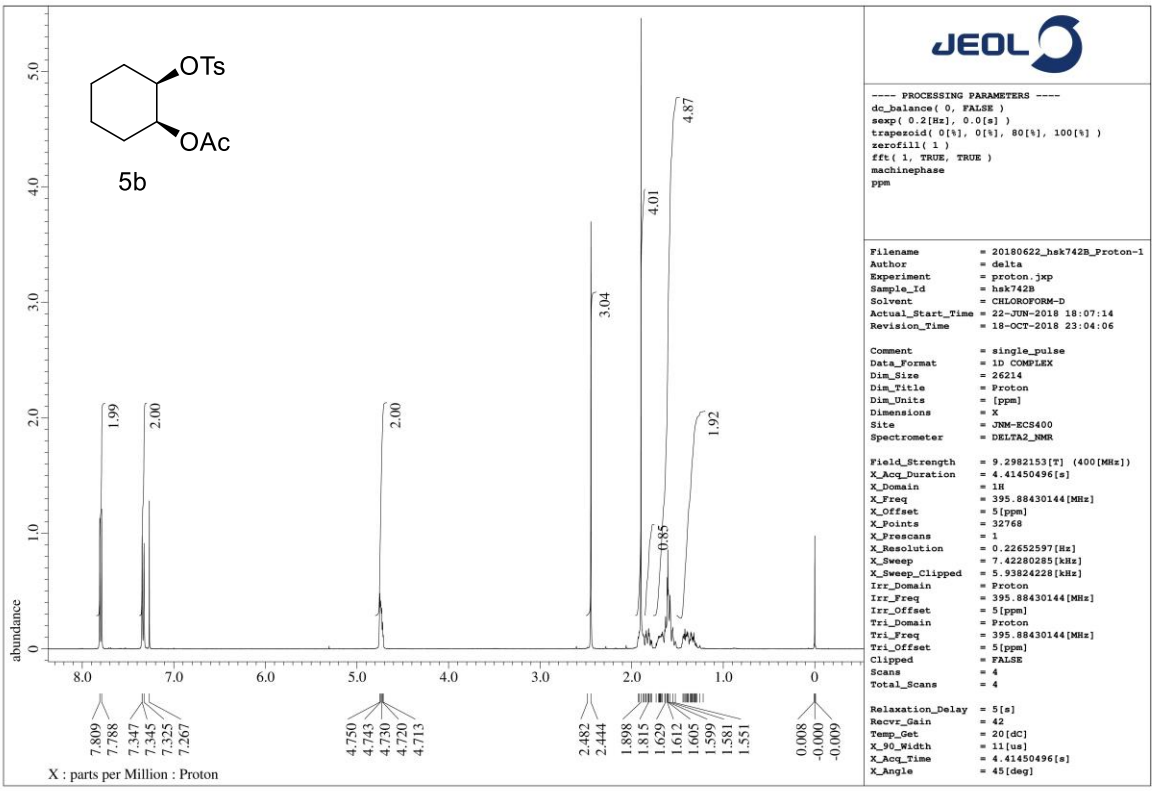

4l
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180213_hsk486cab_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk486cab
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-FEB-2018 17:27:51
Revision_Time = 13-FEB-2018 17:41:01
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 184
Total_Scans = 184
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.8[dC]
X_90_Width = 10.45[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.48333333[us]
Irr_Atn_Dec = 22.77[dB]

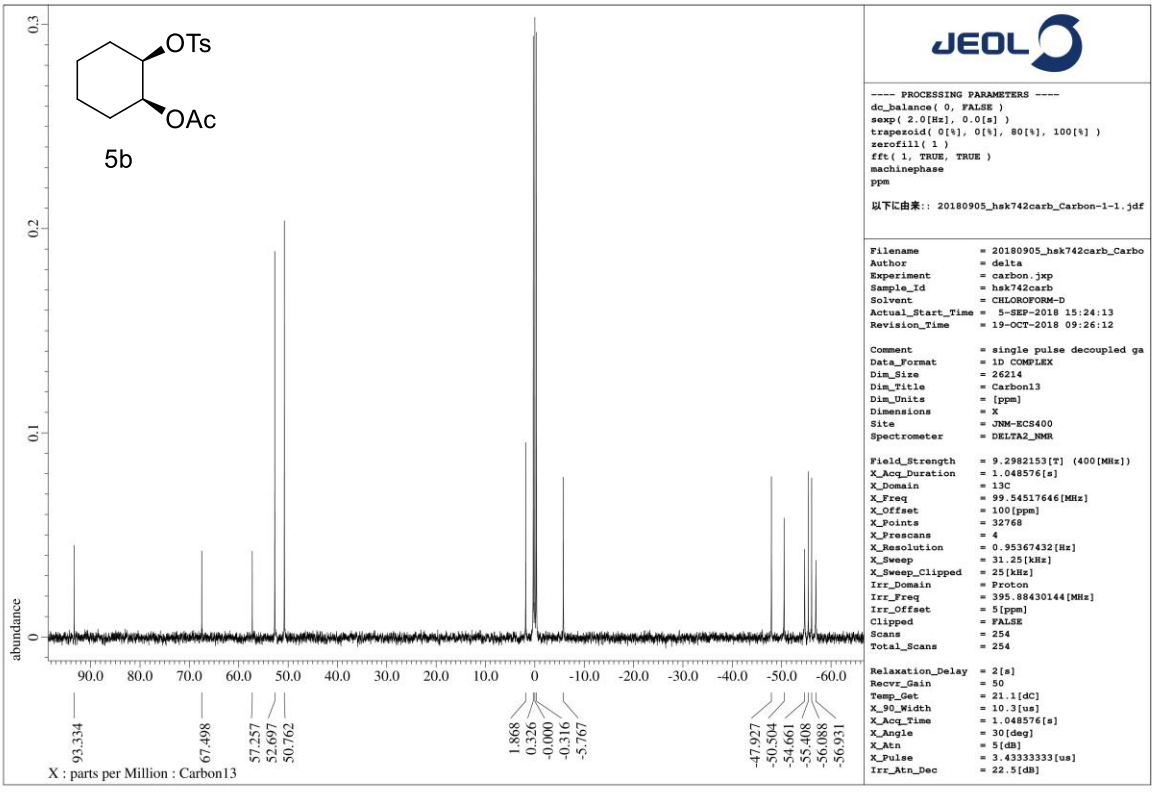

4m
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180905_hsk550-0905_Prot
Author = delta
Experiment = proton.jxp
Sample_Id = hsk550-0905
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2018 15:12:19
Revision_Time = 18-OCT-2018 22:09:19
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 21[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

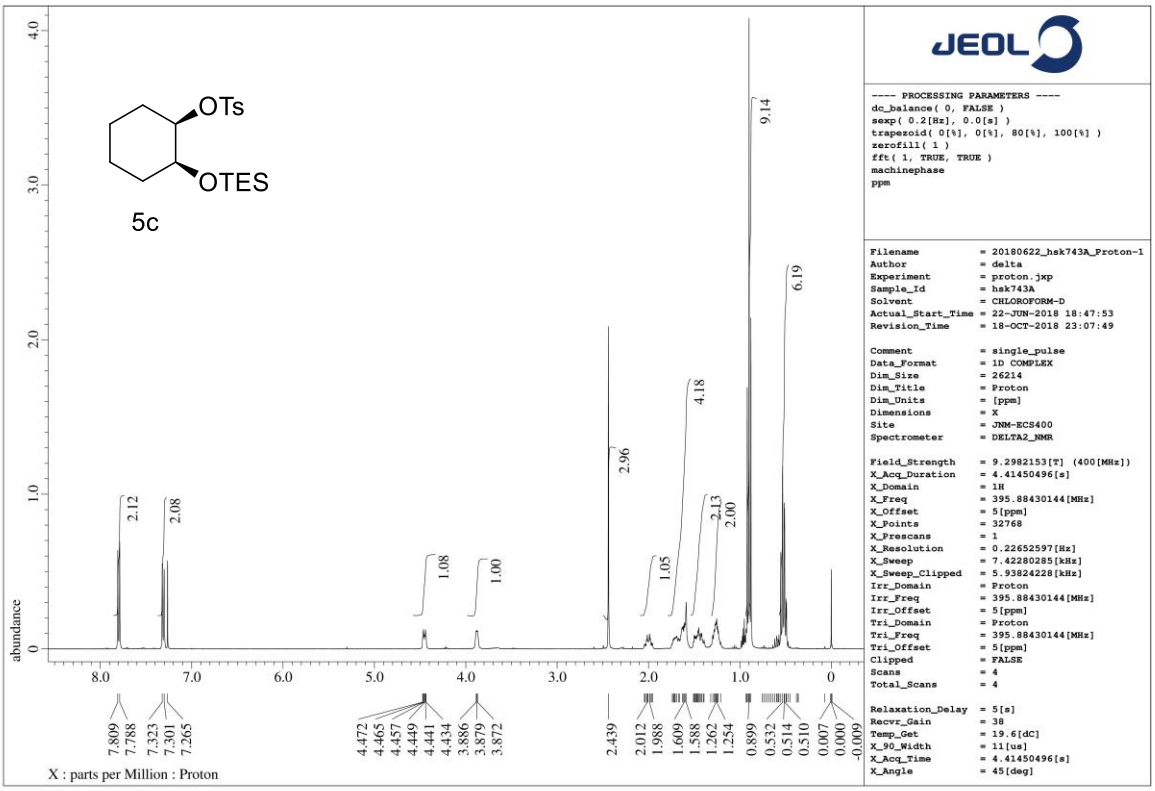

4m
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180910_hsk837carb_Carbon-1-1.jdf
Filename = 20180910_hsk837carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk937carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-SEP-2018 13:22:17
Revision_Time = 23-OCT-2018 14:31:01
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 51
Total_Scans = 51
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.2[dC]
X_90_Width = 8.76[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 3.8[dB]
X_Pulse = 2.92[us]
Irr_Atn_Dec = 18.357[dB]

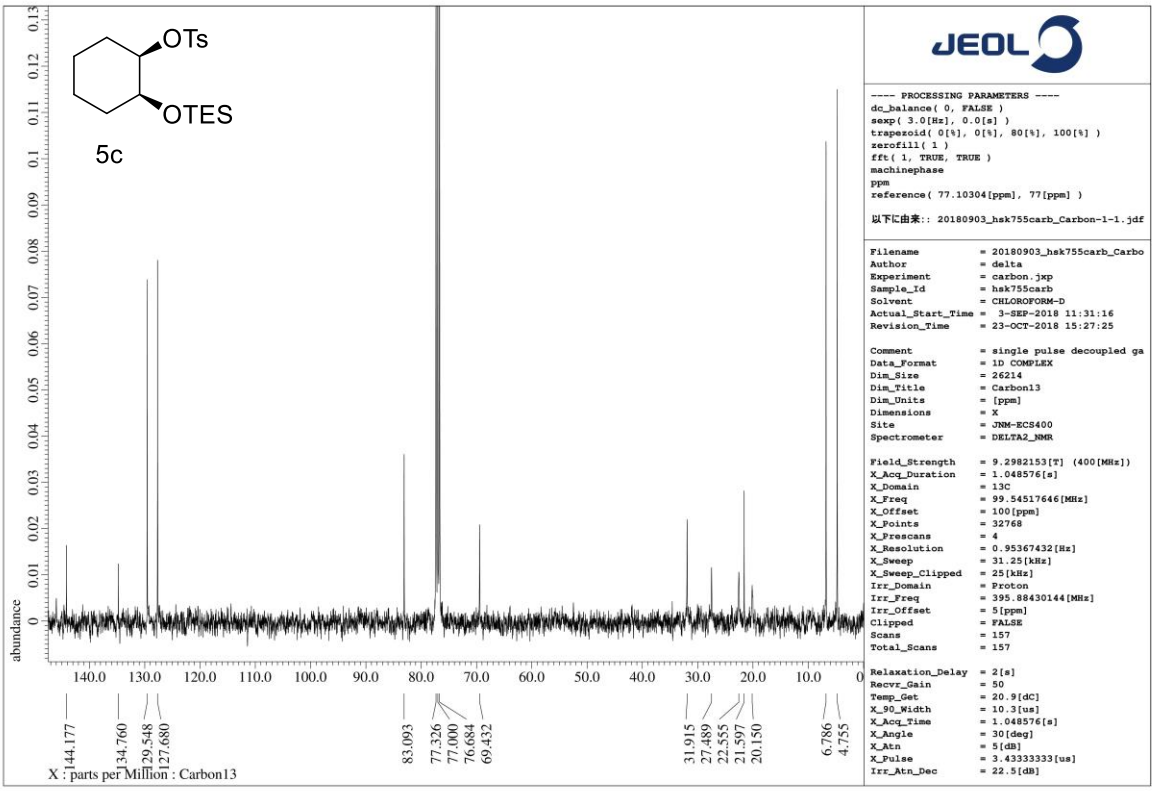

OTs
OBz
5a
X : parts per Million : Proton
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180829_hsk759recry_Proton-1-1.jdf
Filename = 20180829_hsk759recry_Prot
Author = delta
Experiment = proton.jxp
Sample_Id = hsk759recry
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2018 13:13:59
Revision_Time = 18-OCT-2018 23:01:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 21.1[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

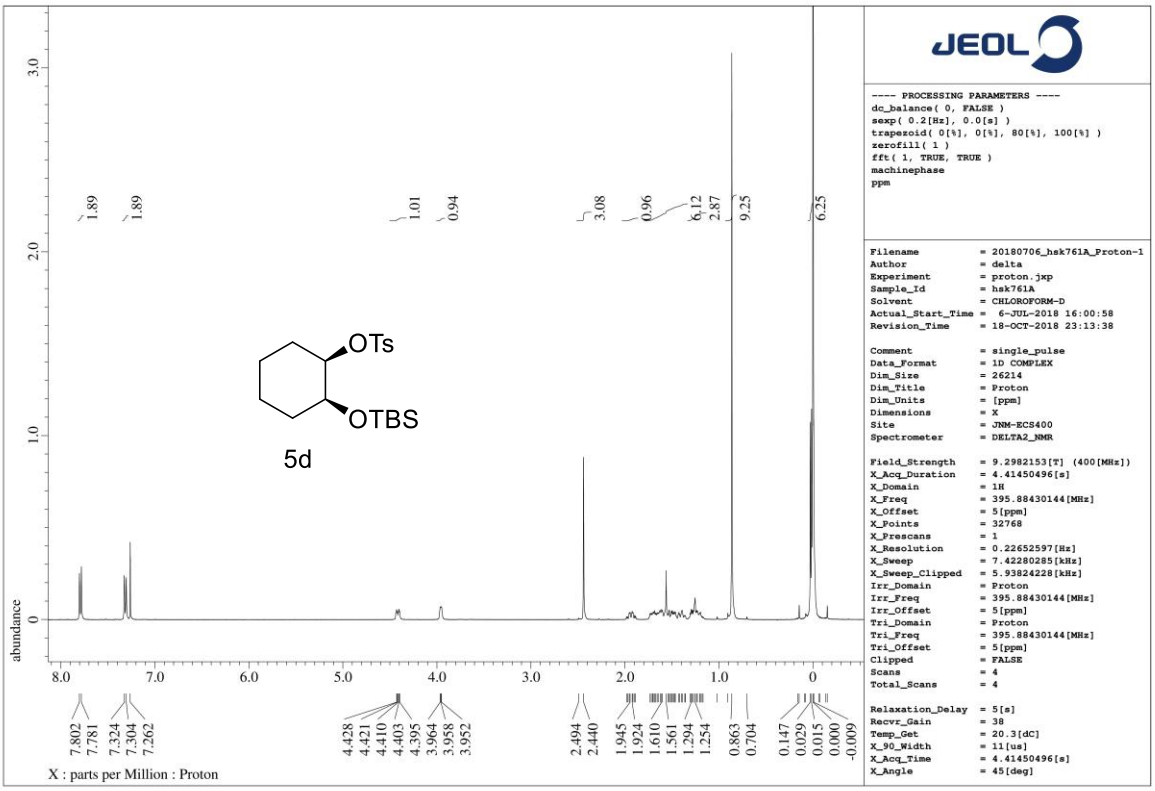

OTs
OBz
5a
X : parts per Million : Carbon13
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0, 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(77.16733[ppm], 77[ppm])
reference(77.0[ppm], 77[ppm])
Filename = 20180829_hsk759car_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk759car
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2018 20:37:19
Revision_Time = 23-OCT-2018 15:20:52
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 86
Total_Scans = 86
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 8.3[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 3.8[dB]
X_Pulse = 2.76666667[us]
Irr_Atn_Dec = 17.954[dB]

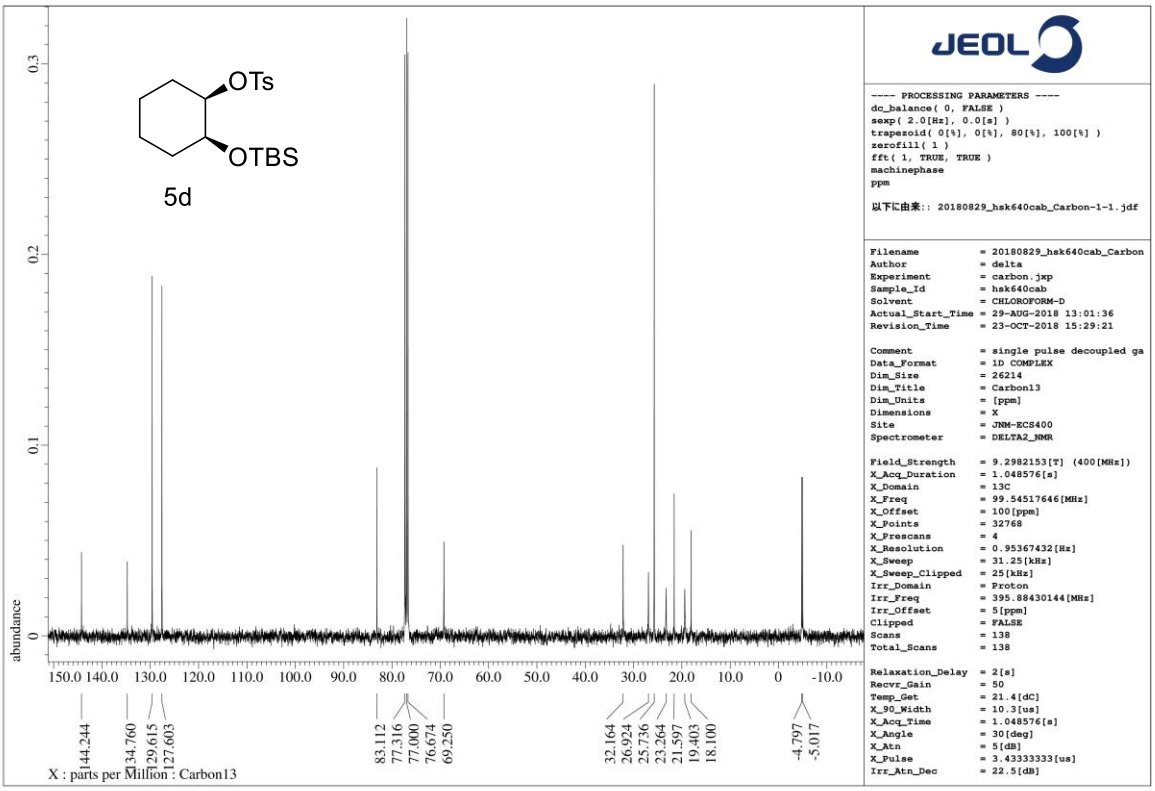

OTs
OAc
5b
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180622_hsk742B_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk742B
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JUN-2018 18:07:14
Revision_Time = 18-OCT-2018 23:04:06
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 20[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

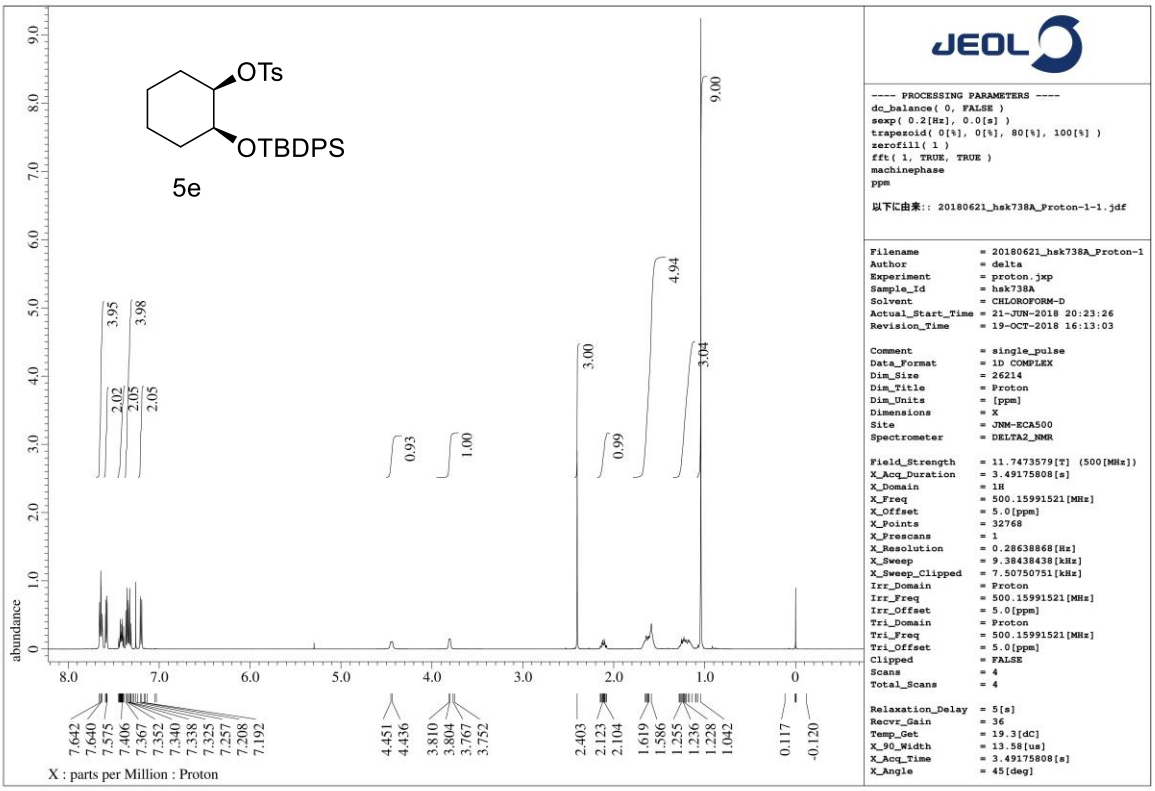

OTs
OAc
5b
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180905_hsk742carb_Carbon-1-1.jdf
Filename = 20180905_hsk742carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk742carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2018 15:24:13
Revision_Time = 19-OCT-2018 09:26:12
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 254
Total_Scans = 254
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.1[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 5[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.5[dB]

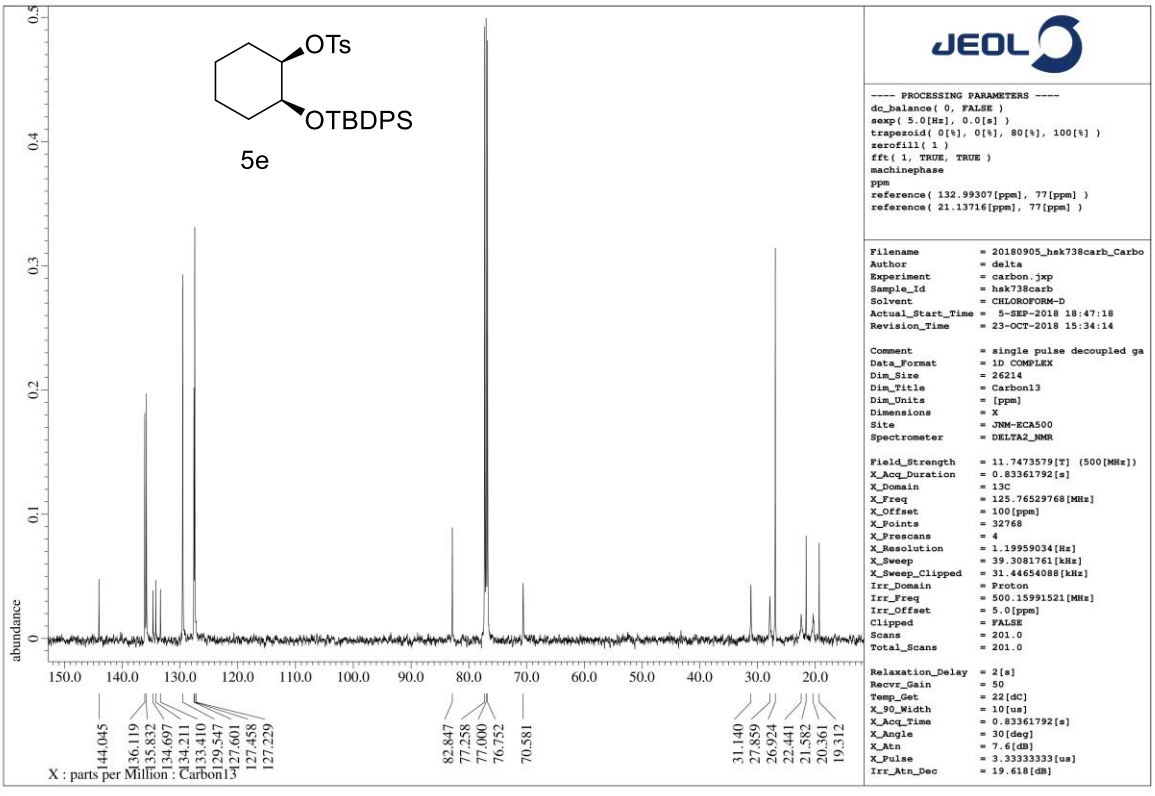

OTs
OTES
5c
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180622_hsk743A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk743A
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JUN-2018 18:47:53
Revision_Time = 18-OCT-2018 23:07:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 19.6[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

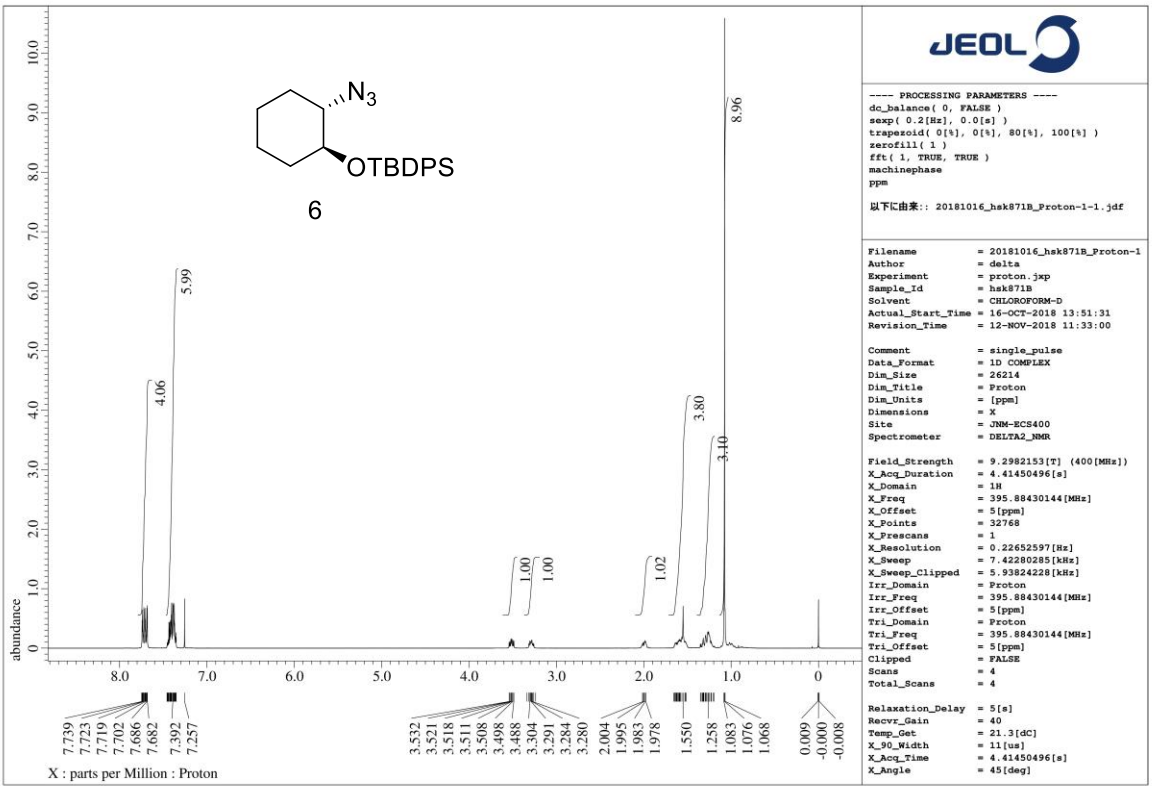

OTs
OTES
5c
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(3.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(77.10304[ppm], 77[ppm])
以下に由来:: 20180903_hsk755carb_Carbon-1-1.jdf
Filename = 20180903_hsk755carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk755carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-SEP-2018 11:31:16
Revision_Time = 23-OCT-2018 15:27:25
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 157
Total_Scans = 157
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.9[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 5[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.5[dB]


OTs
OTBS
5d
1.89
1.89
1.01
0.94
3.08
0.96
6.12
2.87
9.25
6.25
7.802
7.781
7.324
7.304
7.262
4.428
4.421
4.410
4.403
4.395
3.964
3.958
3.952
2.494
2.440
1.945
1.924
1.610
1.561
1.294
1.254
0.863
0.704
0.147
0.029
0.015
0.000
-0.009
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180706_hsk761A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk761A
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-JUL-2018 16:00:58
Revision_Time = 18-OCT-2018 23:13:38
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 20.3[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]


OTs
OTBS
5d
144.244
134.760
129.615
127.603
83.112
77.316
77.000
76.674
69.250
32.164
26.924
25.736
23.264
21.597
19.403
18.100
-4.797
-5.017
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180829_hsk640cab_Carbon-1-1.jdf
Filename = 20180829_hsk640cab_Carbon
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk640cab
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2018 13:01:36
Revision_Time = 23-OCT-2018 15:29:21
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 138
Total_Scans = 138
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 10.3[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 5[dB]
X_Pulse = 3.43333333[us]
Irr_Atn_Dec = 22.5[dB]


OTs
OTBDPS
5e
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20180621_hsk738A_Proton-1-1.jdf
Filename = 20180621_hsk738A_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk738A
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-JUN-2018 20:23:26
Revision_Time = 19-OCT-2018 16:13:03
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 3.49175808[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.28638868[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 19.3[dC]
X_90_Width = 13.58[us]
X_Acq_Time = 3.49175808[s]
X_Angle = 45[deg]


OTs
OTBDPS
5e
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(5.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
reference(132.99307[ppm], 77[ppm])
reference(21.13716[ppm], 77[ppm])
Filename = 20180905_hsk738carb_Carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk738carb
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2018 18:47:18
Revision_Time = 23-OCT-2018 15:34:14
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 201.0
Total_Scans = 201.0
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22[dC]
X_90_Width = 10[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 7.6[dB]
X_Pulse = 3.33333333[us]
Irr_Atn_Dec = 19.618[dB]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

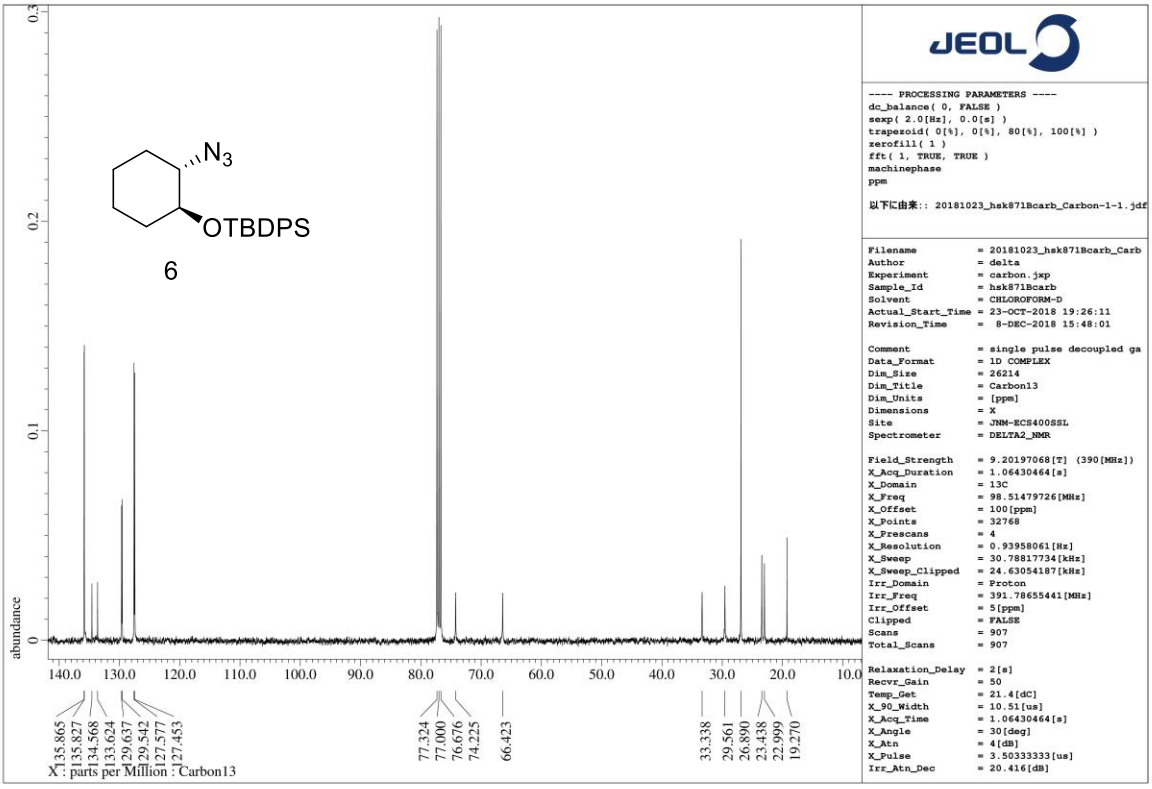
以下に由来:: 20181016_hsk871B_Proton-1-1.jdf

Filename           = 20181016_hsk871B_Proton-1
Author             = delta
Experiment         = proton.jxp
Sample_Id          = hsk871B
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 16-OCT-2018 13:51:31
Revision_Time      = 12-NOV-2018 11:33:00

Comment            = single_pulse
Data_Format        = 1D COMPLEX
Dim_Size           = 26214
Dim_Title          = Proton
Dim_Units          = [ppm]
Dimensions         = X
Site               = JNM-ECS400
Spectrometer       = DELTA2_NMR

Field_Strength     = 9.2982153[T] (400[MHz])
X_Acq_Duration     = 4.41450496[s]
X_Domain           = 1H
X_Freq             = 395.88430144[MHz]
X_Offset           = 5[ppm]
X_Points           = 32768
X_Prescans         = 1
X_Resolution       = 0.22652597[Hz]
X_Sweep            = 7.42280285[kHz]
X_Sweep_Clipped    = 5.93824228[kHz]
Irr_Domain         = Proton
Irr_Freq           = 395.88430144[MHz]
Irr_Offset         = 5[ppm]
Tri_Domain         = Proton
Tri_Freq           = 395.88430144[MHz]
Tri_Offset         = 5[ppm]
Clipped            = FALSE
Scans              = 4
Total_Scans        = 4

Relaxation_Delay   = 5[s]
Recvr_Gain         = 40
Temp_Get           = 21.3[dC]
X_90_Width         = 11[us]
X_Acq_Time         = 4.41450496[s]
X_Angle            = 45[deg]
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

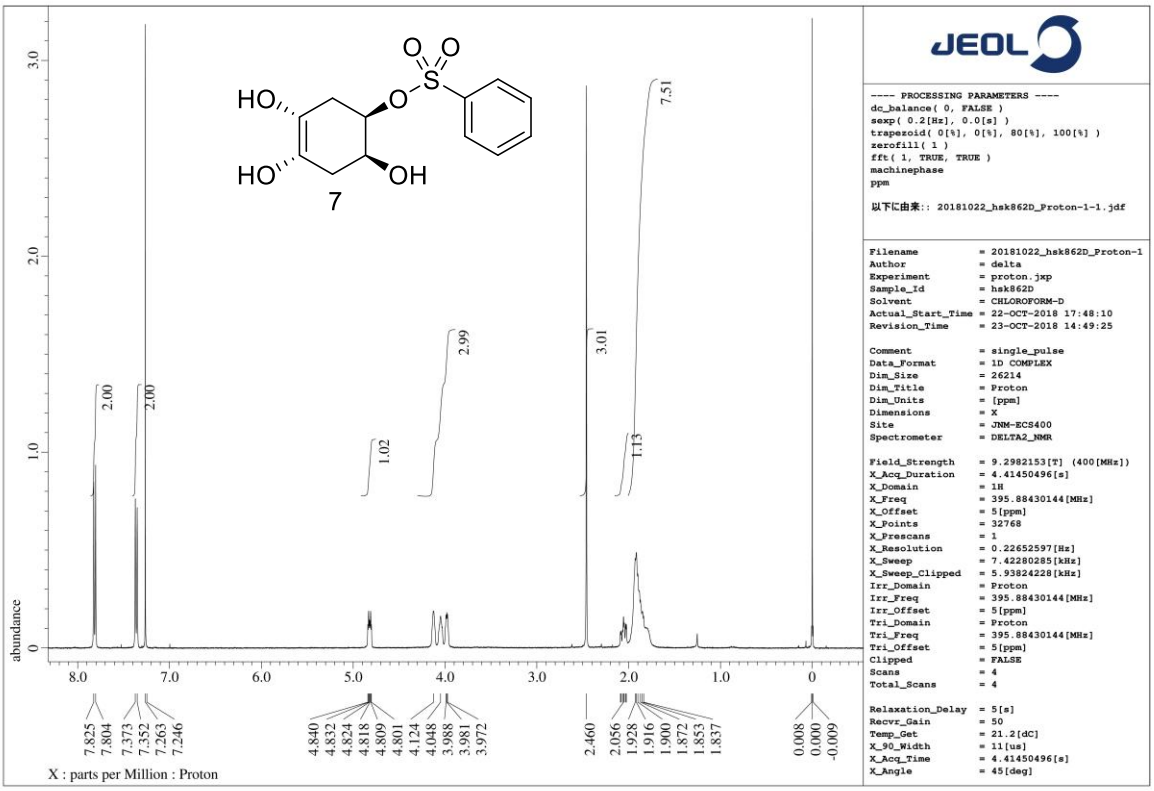
以下に由来:: 20181023_hsk871Bcarb_Carbon-1-1.jdf

Filename           = 20181023_hsk871Bcarb_Carb
Author             = delta
Experiment         = carbon.jxp
Sample_Id          = hsk871Bcarb
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 23-OCT-2018 19:26:11
Revision_Time      =  8-DEC-2018 15:48:01

Comment            = single pulse decoupled ga
Data_Format        = 1D COMPLEX
Dim_Size           = 26214
Dim_Title          = Carbon13
Dim_Units          = [ppm]
Dimensions         = X
Site               = JNM-ECS400SL
Spectrometer       = DELTA2_NMR

Field_Strength     = 9.20197068[T] (390[MHz])
X_Acq_Duration     = 1.06430464[s]
X_Domain           = 13C
X_Freq             = 98.51479726[MHz]
X_Offset           = 100[ppm]
X_Points           = 32768
X_Prescans         = 4
X_Resolution       = 0.93958061[Hz]
X_Sweep            = 30.78817734[kHz]
X_Sweep_Clipped    = 24.63054187[kHz]
Irr_Domain         = Proton
Irr_Freq           = 391.78655441[MHz]
Irr_Offset         = 5[ppm]
Clipped            = FALSE
Scans              = 907
Total_Scans        = 907

Relaxation_Delay   = 2[s]
Recvr_Gain         = 50
Temp_Get           = 21.4[dC]
X_90_Width         = 10.51[us]
X_Acq_Time         = 1.06430464[s]
X_Angle            = 30[deg]
X_Atn              = 4[dB]
X_Pulse            = 3.50333333[us]
Irr_Atn_Dec        = 20.416[dB]
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

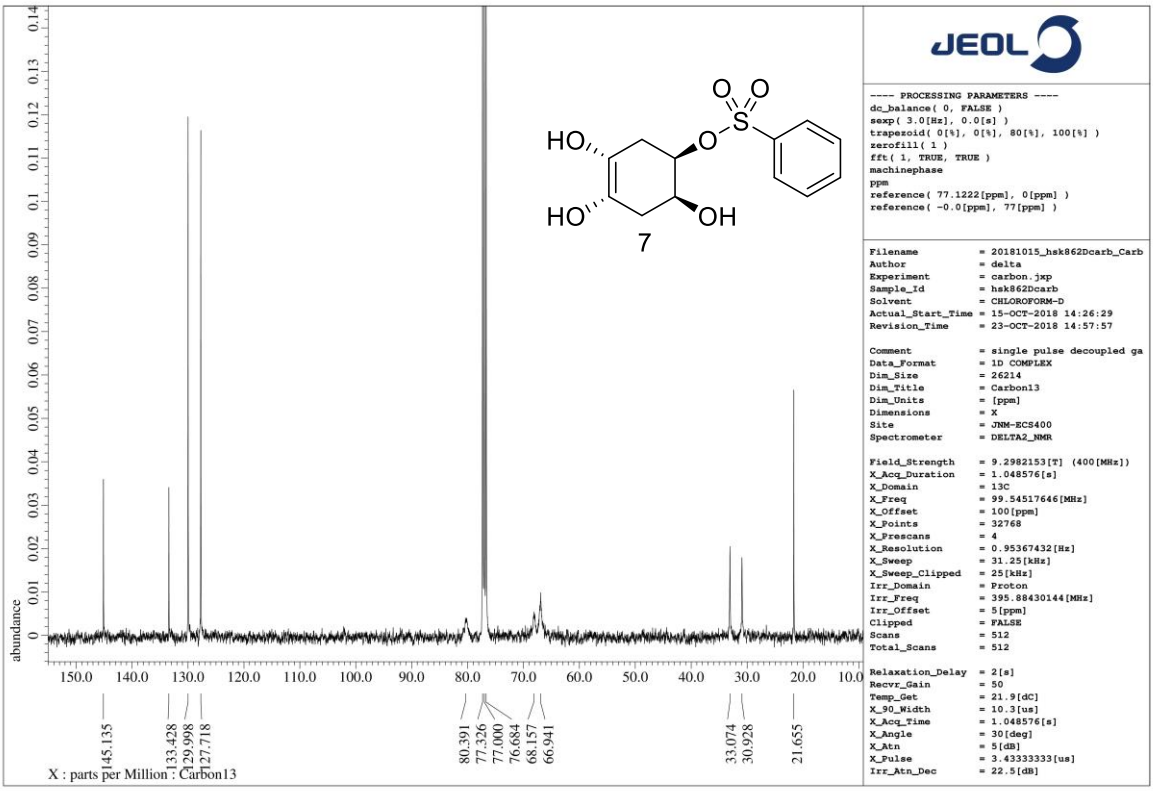
以下に由来:: 20181022_hsk862D_Proton-1-1.jdf

Filename            = 20181022_hsk862D_Proton-1
Author              = delta
Experiment          = proton.jxp
Sample_Id           = hsk862D
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 22-OCT-2018 17:48:10
Revision_Time       = 23-OCT-2018 14:49:25

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 4.41450496[s]
X_Domain            = 1H
X_Freq              = 395.88430144[MHz]
X_Offset            = 5[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22652597[Hz]
X_Sweep             = 7.42280285[kHz]
X_Sweep_Clipped     = 5.93824228[kHz]
Irr_Domain          = Proton
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = Proton
Tri_Freq            = 395.88430144[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 4
Total_Scans         = 4

Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 21.2[dC]
X_90_Width          = 11[us]
X_Acq_Time          = 4.41450496[s]
X_Angle             = 45[deg]
```



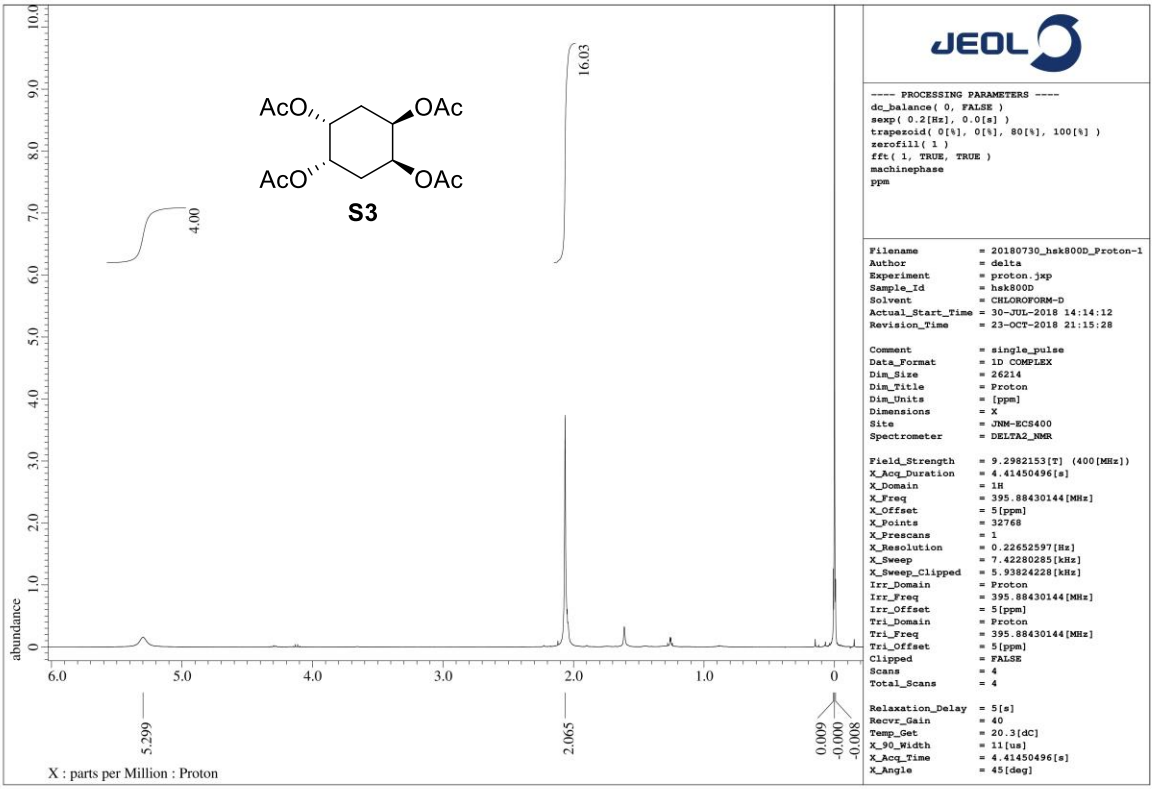

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.1222[ppm], 0[ppm] )
reference( -0.0[ppm], 77[ppm] )

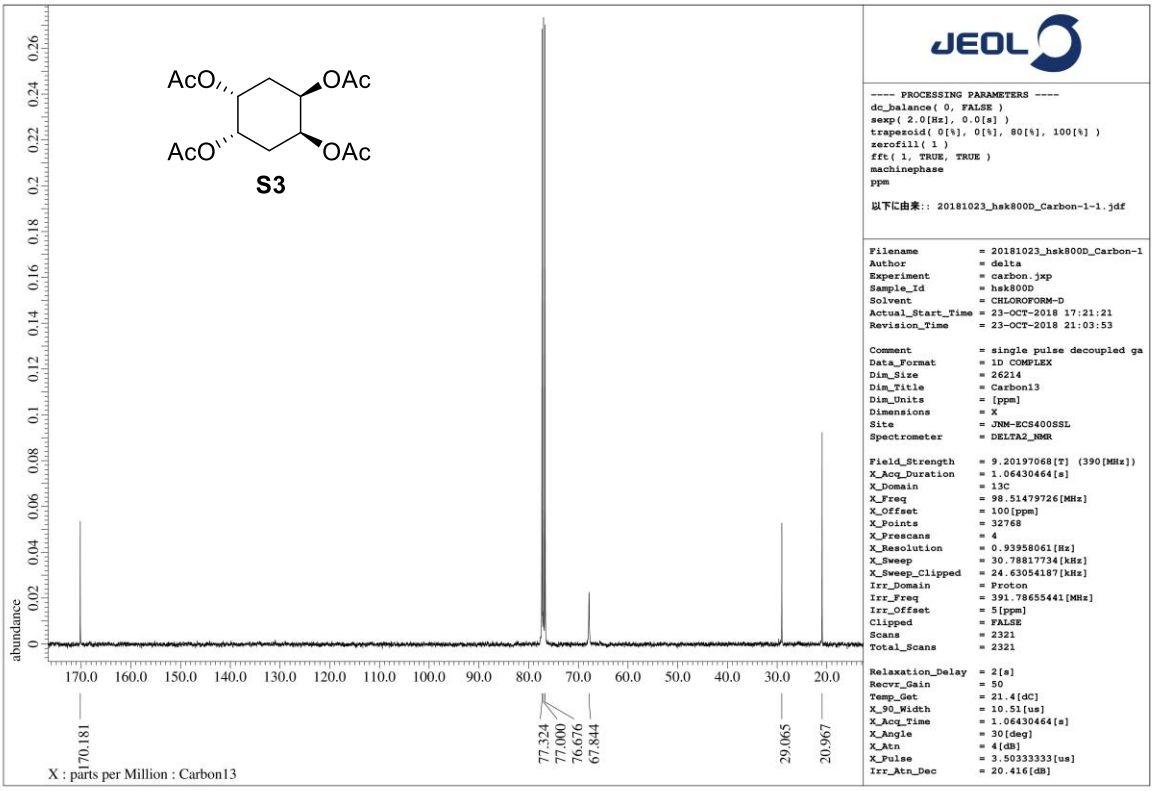
Filename            = 20181015_hsk862Dcarb_Carb
Author              = delta
Experiment          = carbon.jxp
Sample_Id           = hsk862Dcarb
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 15-OCT-2018 14:26:29
Revision_Time       = 23-OCT-2018 14:57:57

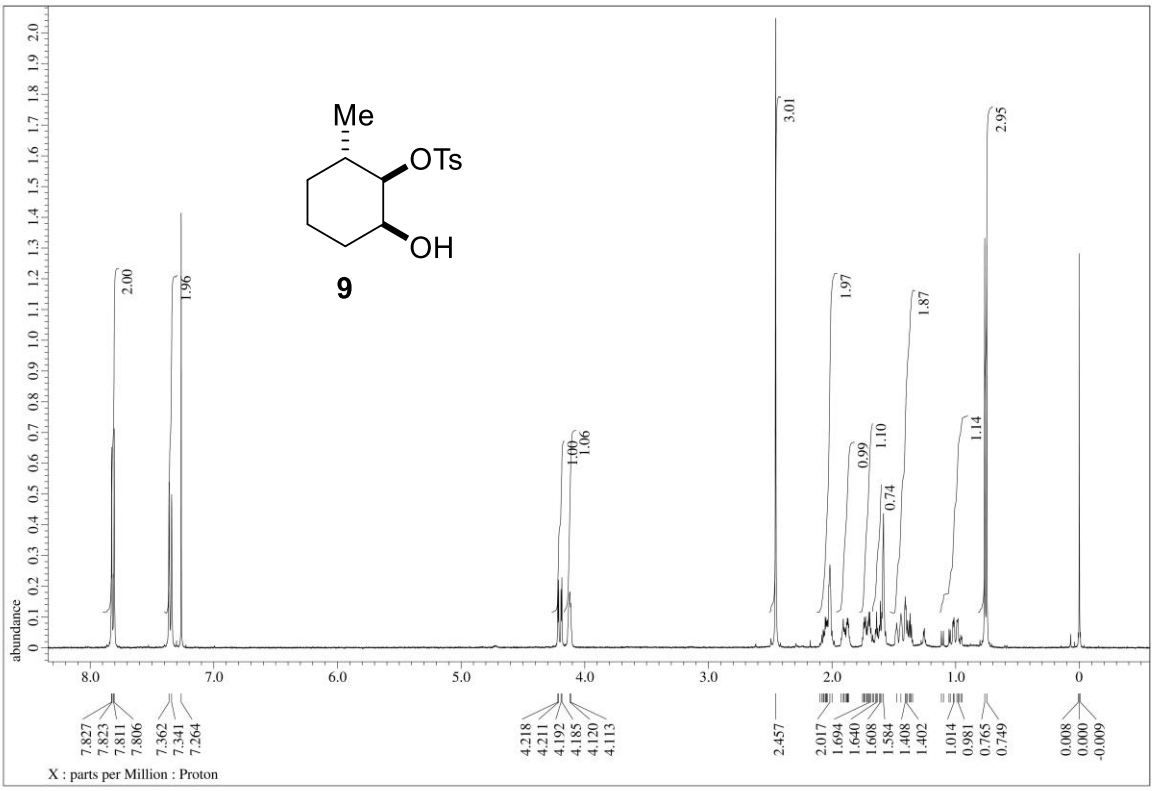
Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

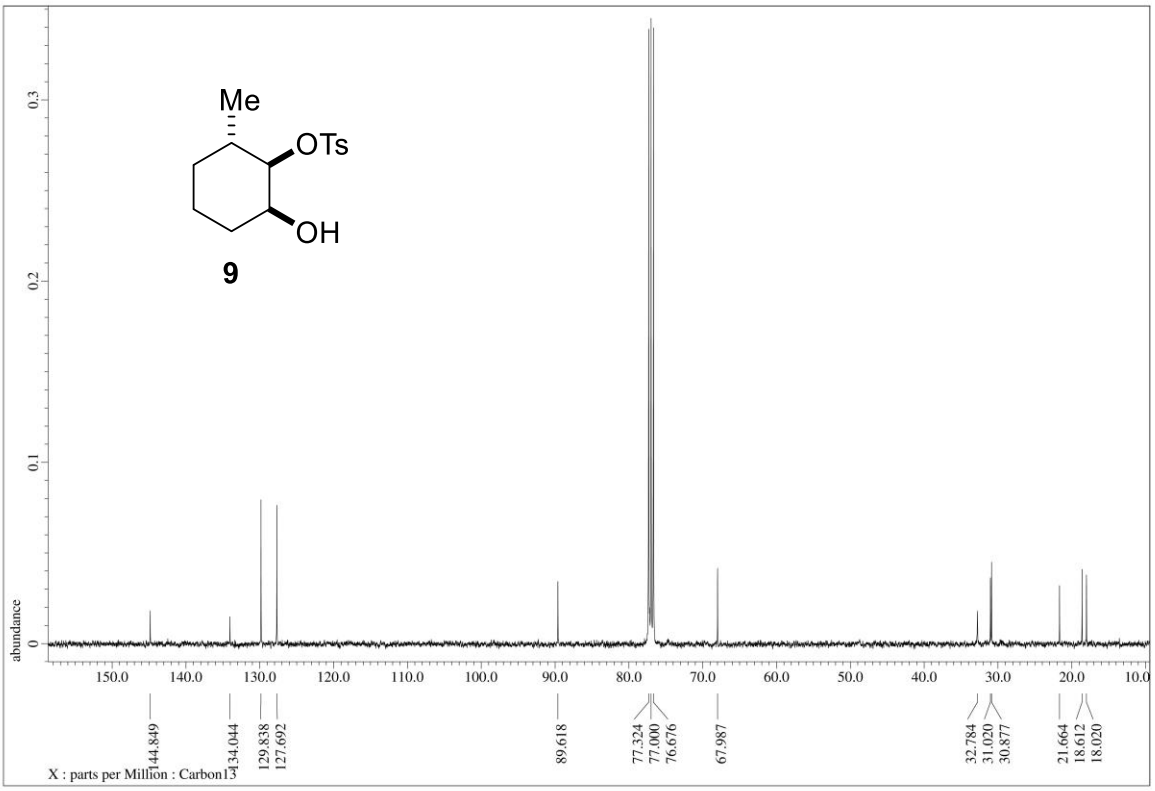
Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 1.048576[s]
X_Domain            = 13C
X_Freq              = 99.54517646[MHz]
X_Offset            = 100[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95367432[Hz]
X_Sweep             = 31.25[kHz]
X_Sweep_Clipped     = 25[kHz]
Irr_Domain          = Proton
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 512
Total_Scans         = 512

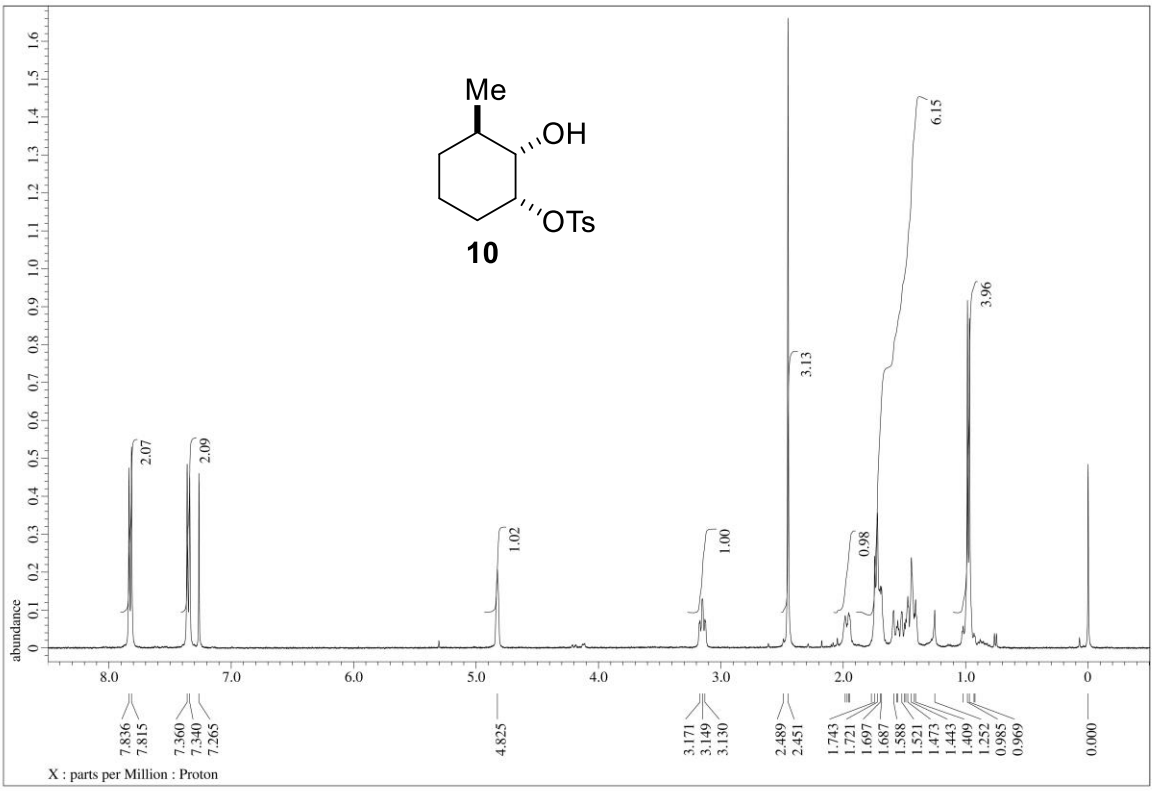
Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 21.9[dC]
X_90_Width          = 10.3[us]
X_Acq_Time          = 1.048576[s]
X_Angle             = 30[deg]
X_Atn               = 5[dB]
X_Pulse             = 3.43333333[us]
Irr_Atn_Dec         = 22.5[dB]
```

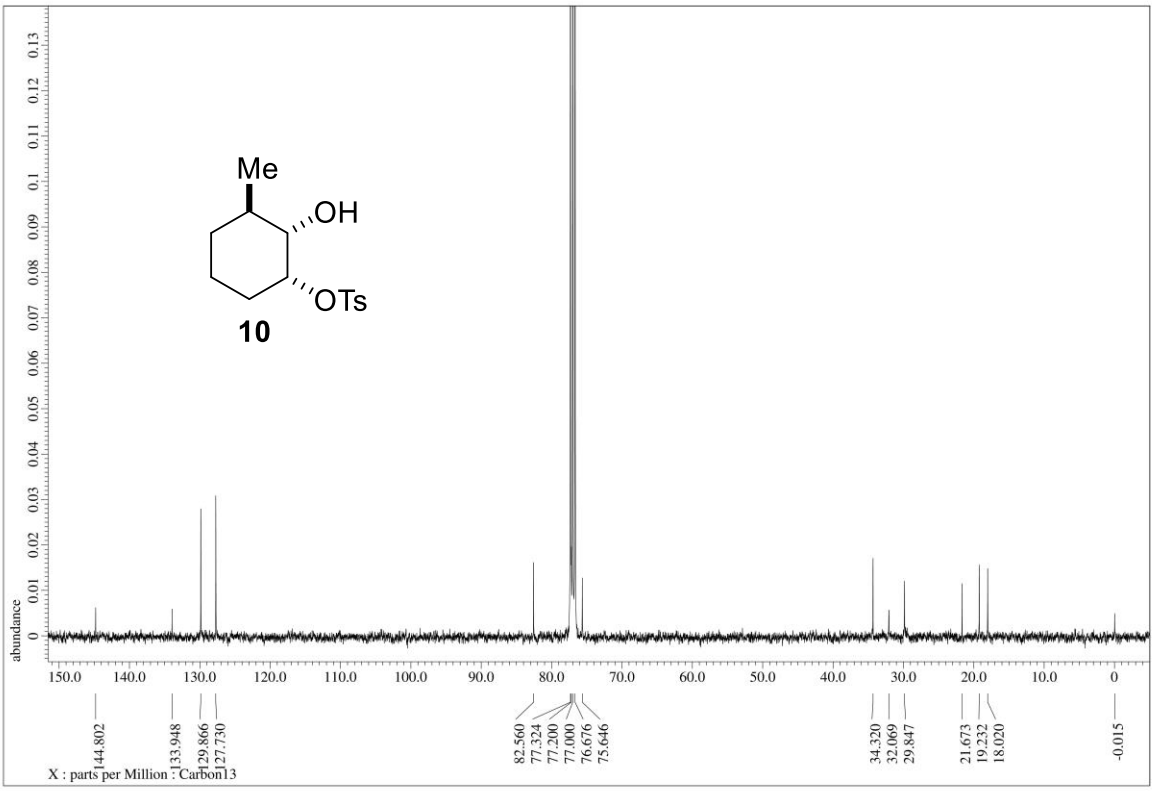

AcO
OAc
AcO
OAc
S3
16.03
4.00
abundance
6.0
5.0
4.0
3.0
2.0
1.0
0
5.299
2.065
0.009
-0.000
-0.008
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20180730_hsk800D_Proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = hsk800D
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-JUL-2018 14:14:12
Revision_Time = 23-OCT-2018 21:15:28
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 4.41450496[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22652597[Hz]
X_Sweep = 7.42280285[kHz]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 4
Total_Scans = 4
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 20.3[dC]
X_90_Width = 11[us]
X_Acq_Time = 4.41450496[s]
X_Angle = 45[deg]

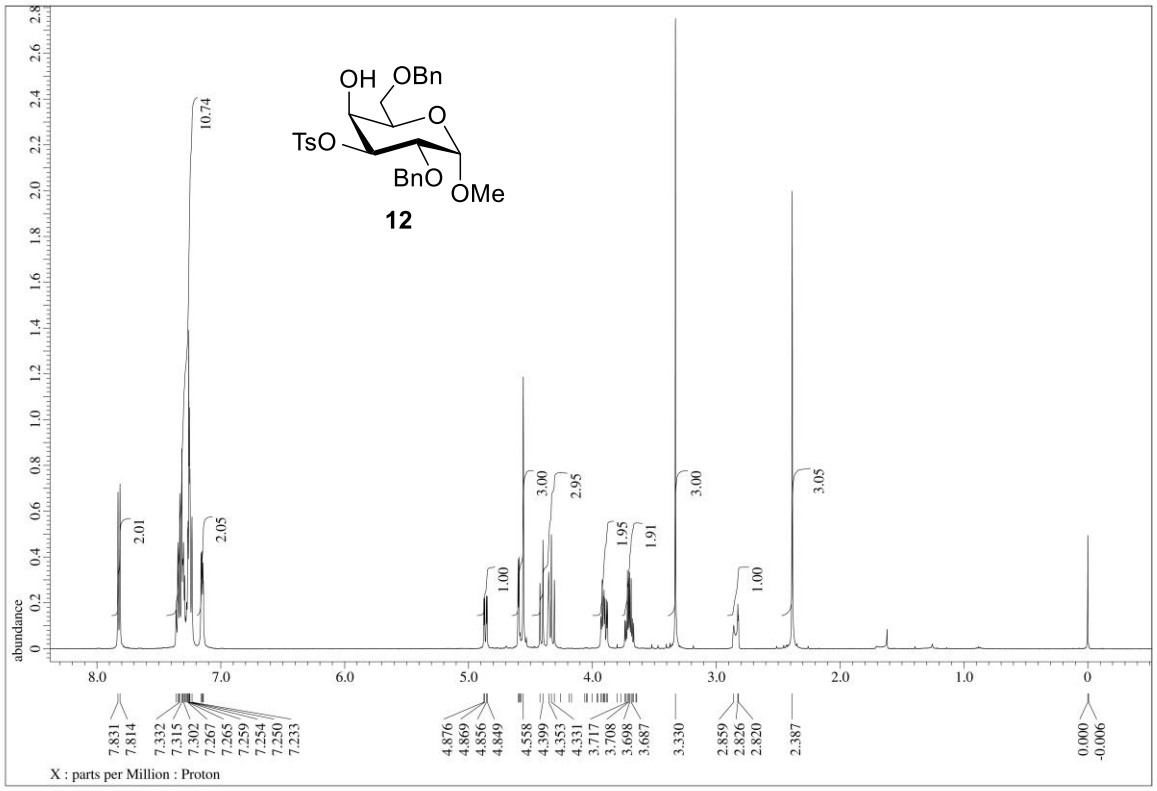

AcO
OAc
AcO
OAc
S3
abundance
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
170.181
77.324
77.000
76.676
67.844
29.065
20.967
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: 20181023_hsk800D_Carbon-1-1.jdf
Filename = 20181023_hsk800D_Carbon-1
Author = delta
Experiment = carbon.jxp
Sample_Id = hsk800D
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-OCT-2018 17:21:21
Revision_Time = 23-OCT-2018 21:03:53
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400SSL
Spectrometer = DELTA2_NMR
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
X_Sweep_Clipped = 24.63054187[kHz]
Irr_Domain = Proton
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 2321
Total_Scans = 2321
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 10.51[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4[dB]
X_Pulse = 3.50333333[us]
Irr_Atn_Dec = 20.416[dB]

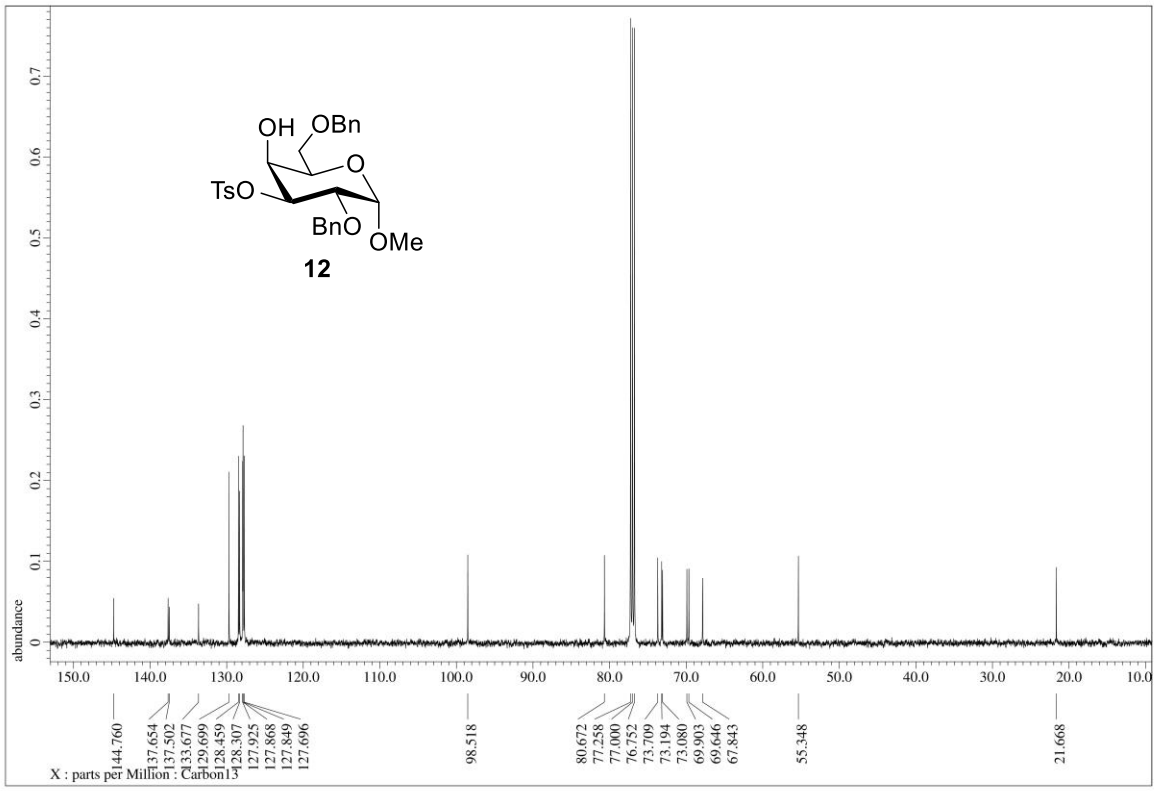

Me
OTs
OH
9
abundance
X : parts per Million : Proton


Me
OTs
OH
9
abundance
X : parts per Million : Carbon13

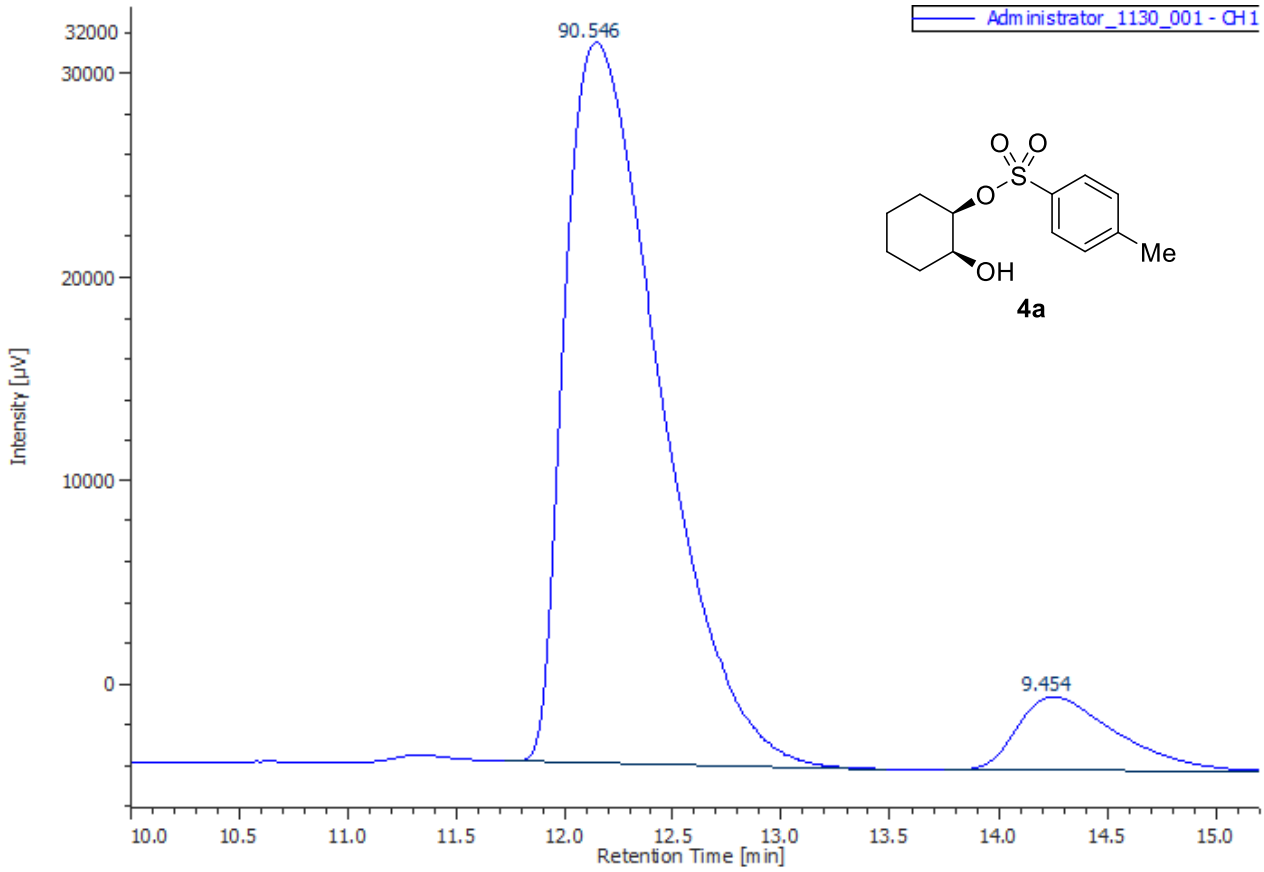

Me
OH
OTs
10
abundance
X : parts per Million : Proton

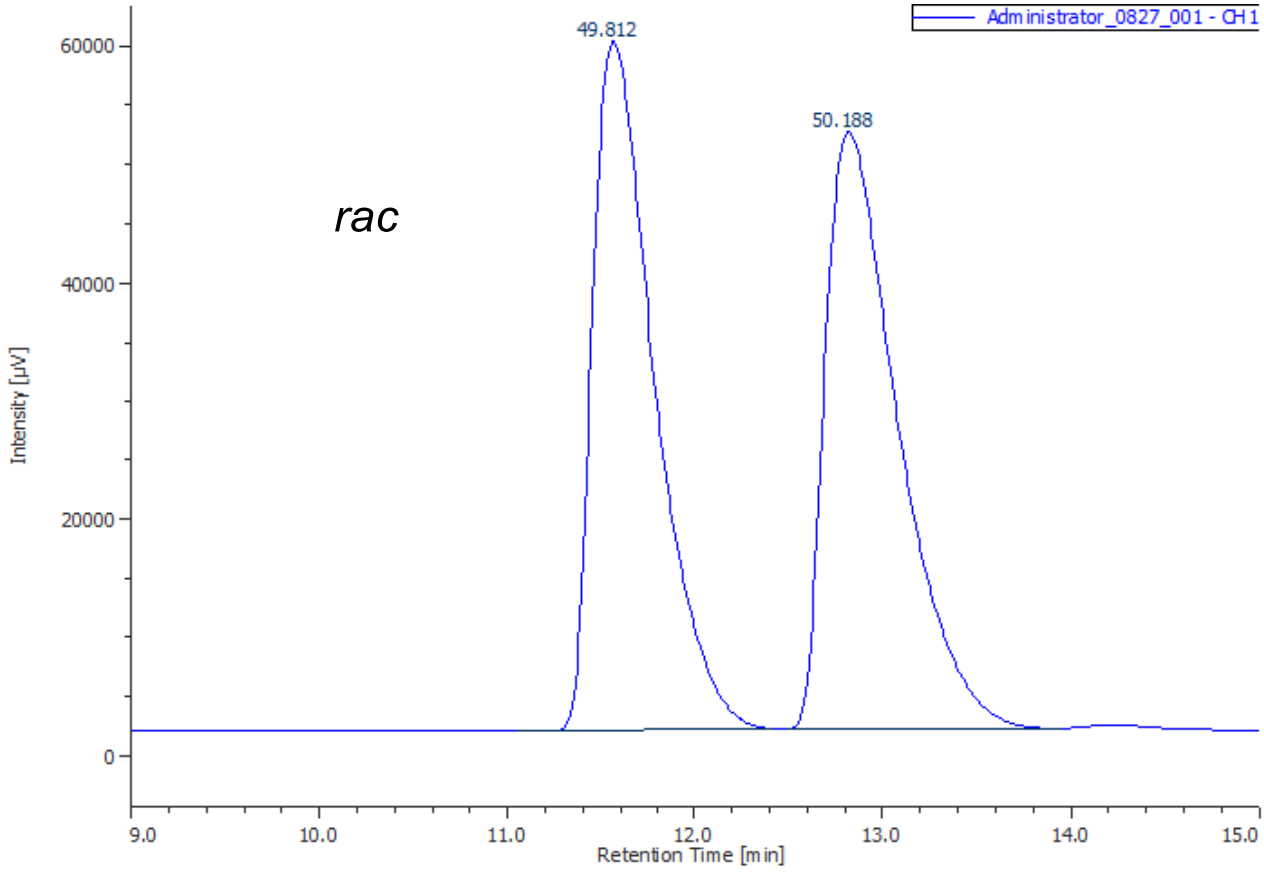

Me
OH
OTs
10
abundance
X : parts per Million : Carbon13

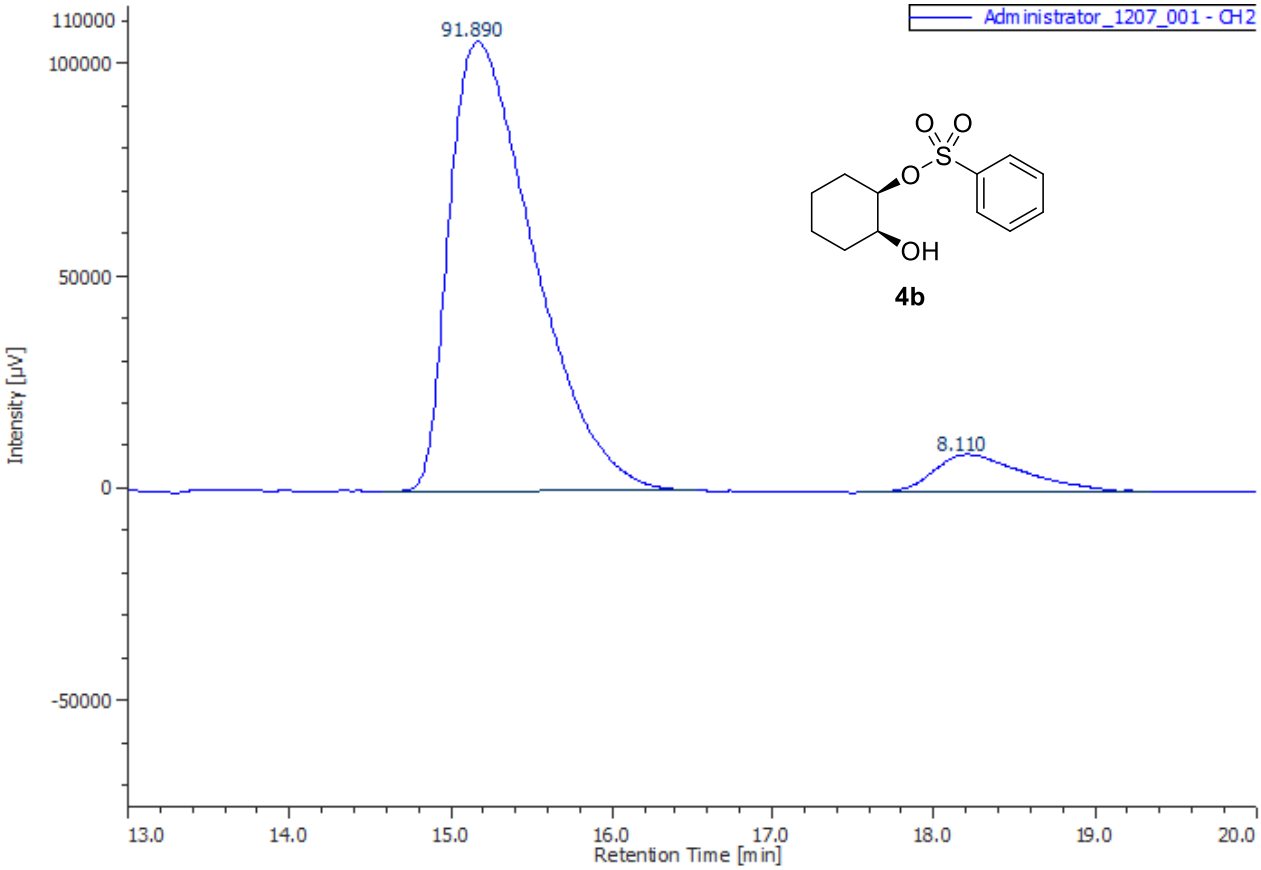

OH
OBn
O
TsO
BnO
OMe
12
abundance
X : parts per Million : Proton


OH
OBn
O
TsO
BnO
OMe
12
abundance
X : parts per Million : Carbon13

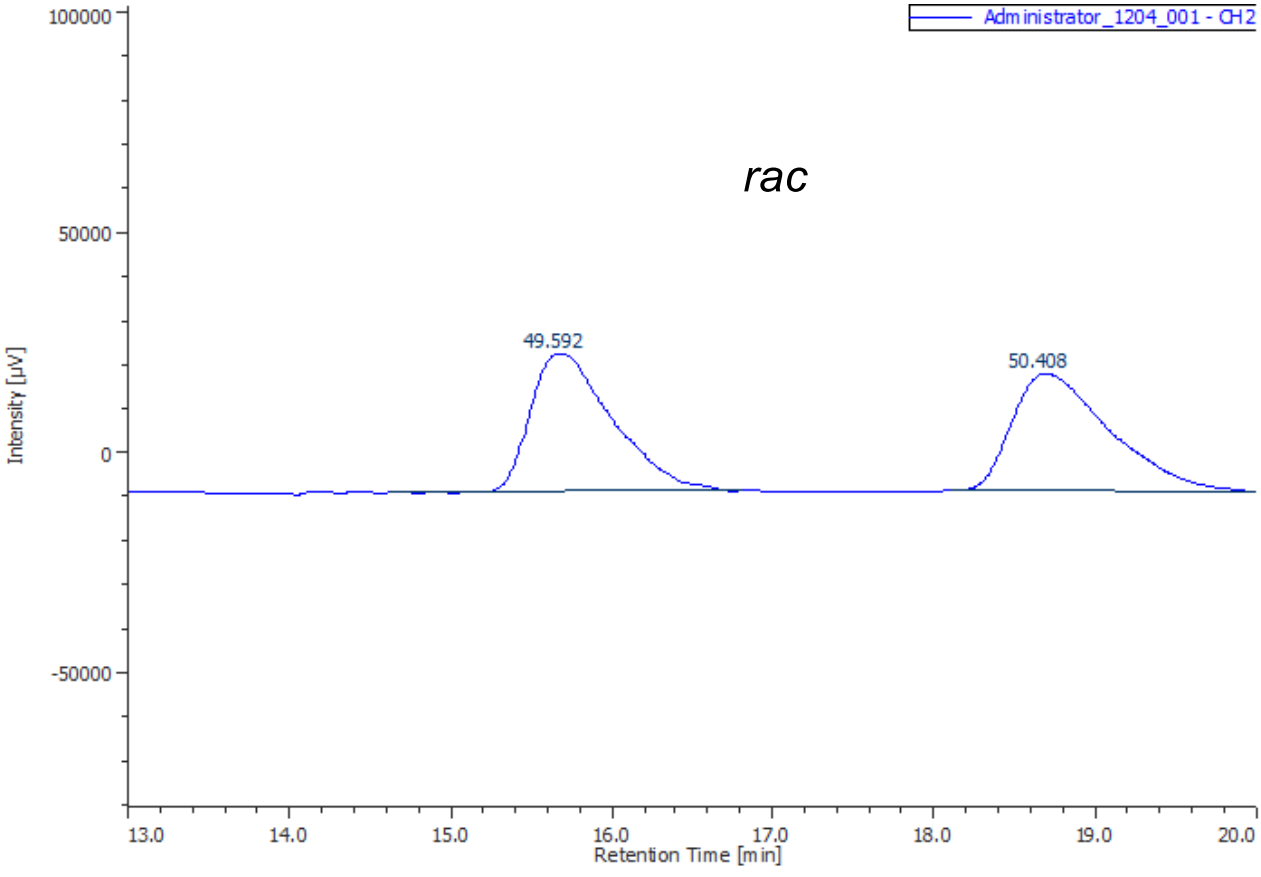
17. HPLC spectra

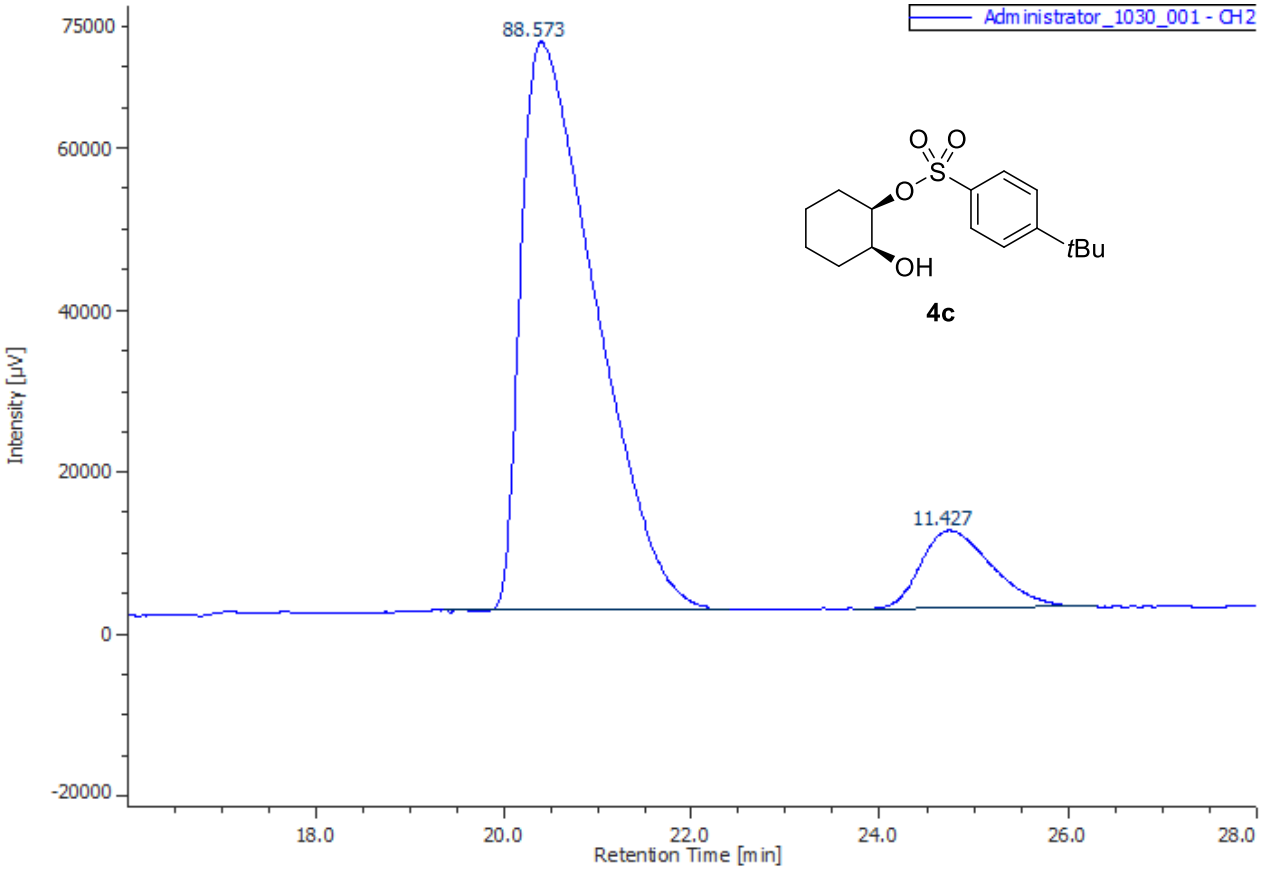




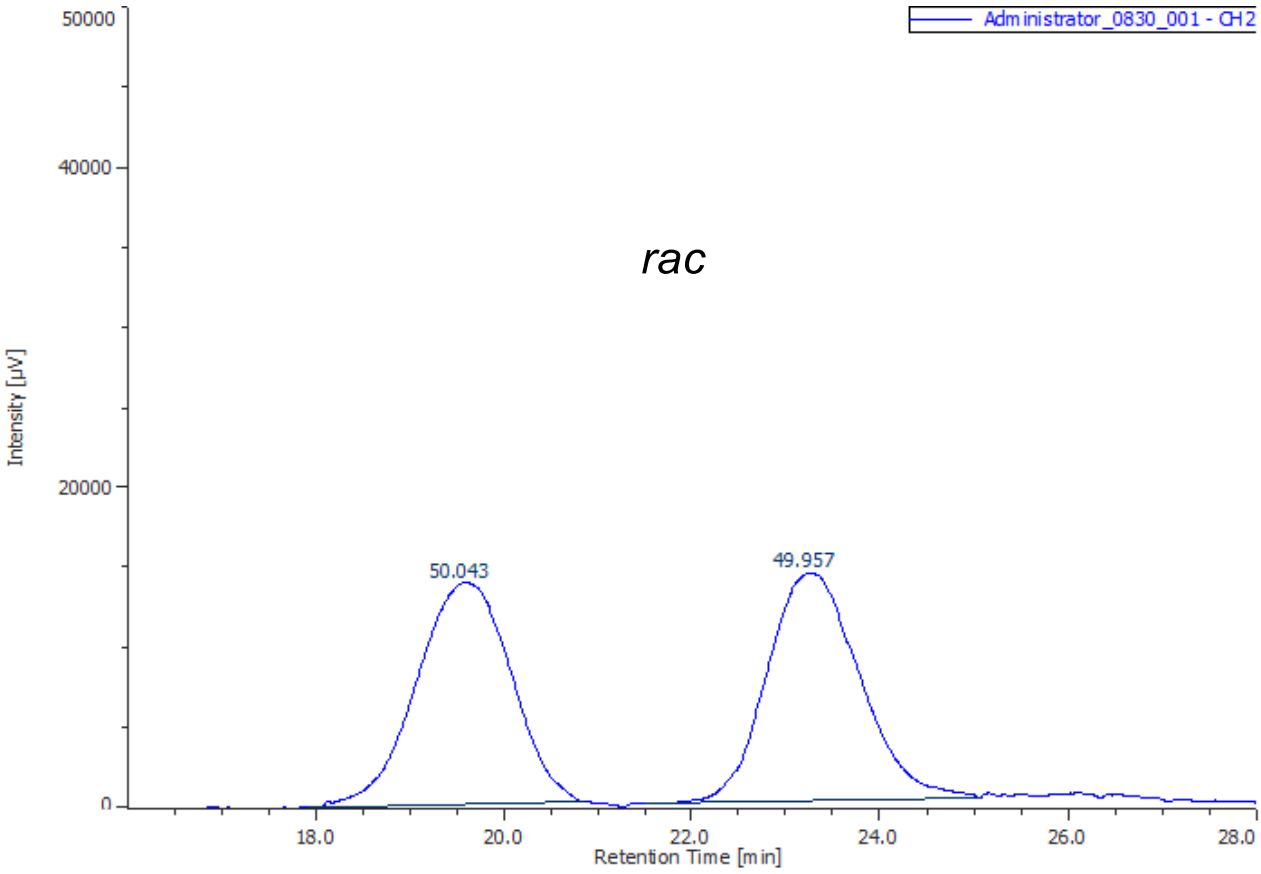

Administrator_1207_001 - CH2
91.890
8.110
110000
100000
50000
0
-50000
Intensity [µV]
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
Retention Time [min]
O
O
S
O
OH

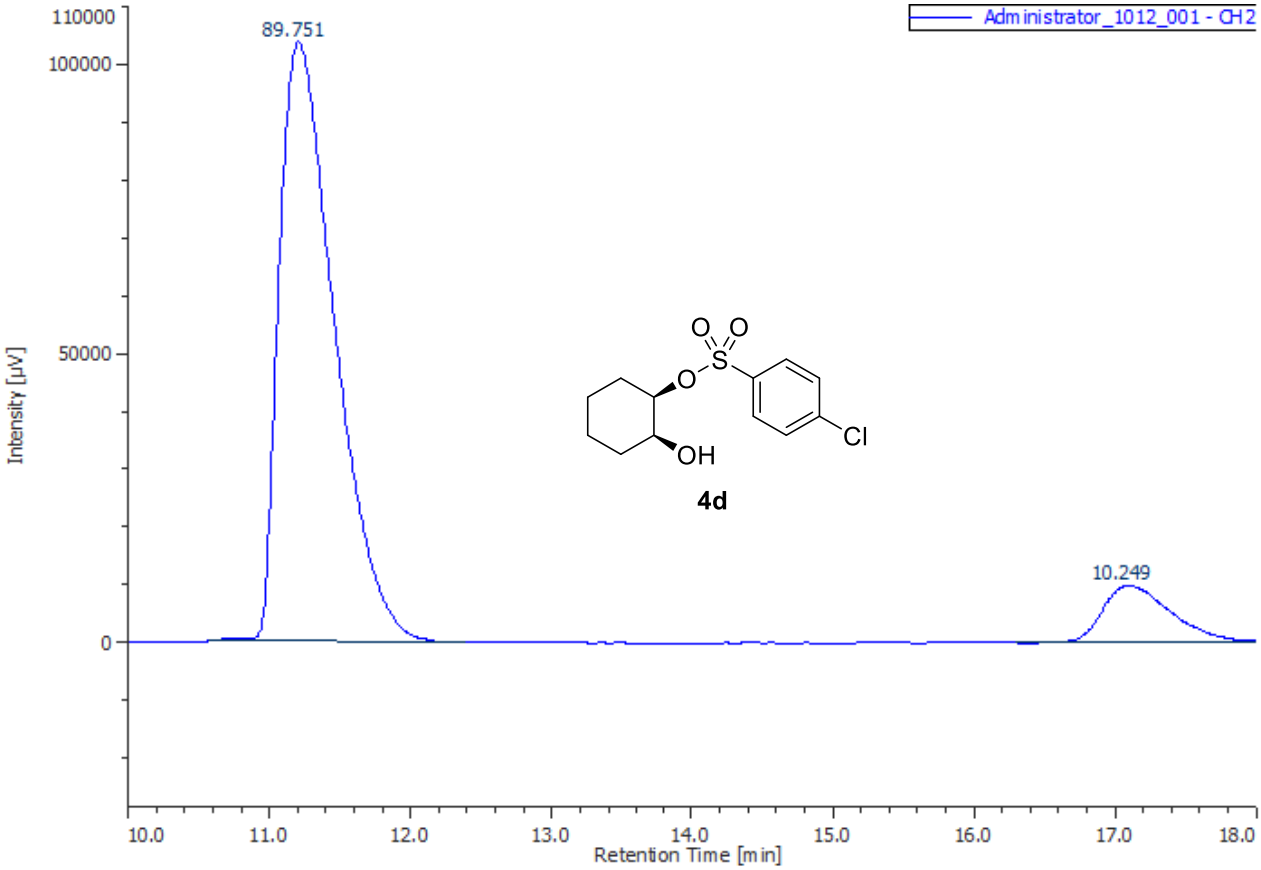
4b


Administrator_1204_001 - CH2
rac
49.592
50.408
100000
50000
0
-50000
Intensity [µV]
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
Retention Time [min]

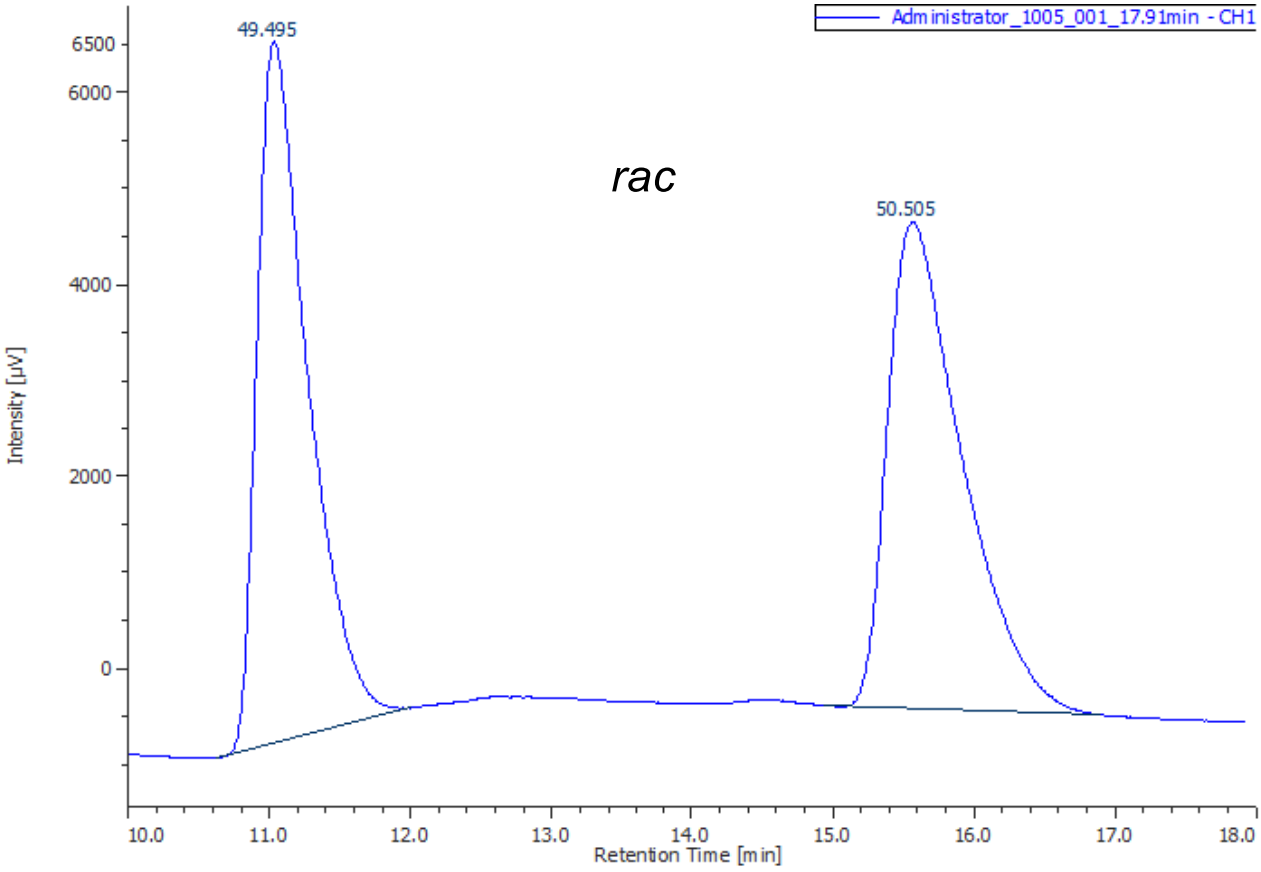

Administrator_1030_001 - CH2
88.573
11.427
Intensity [µV]
Retention Time [min]
OH
tBu

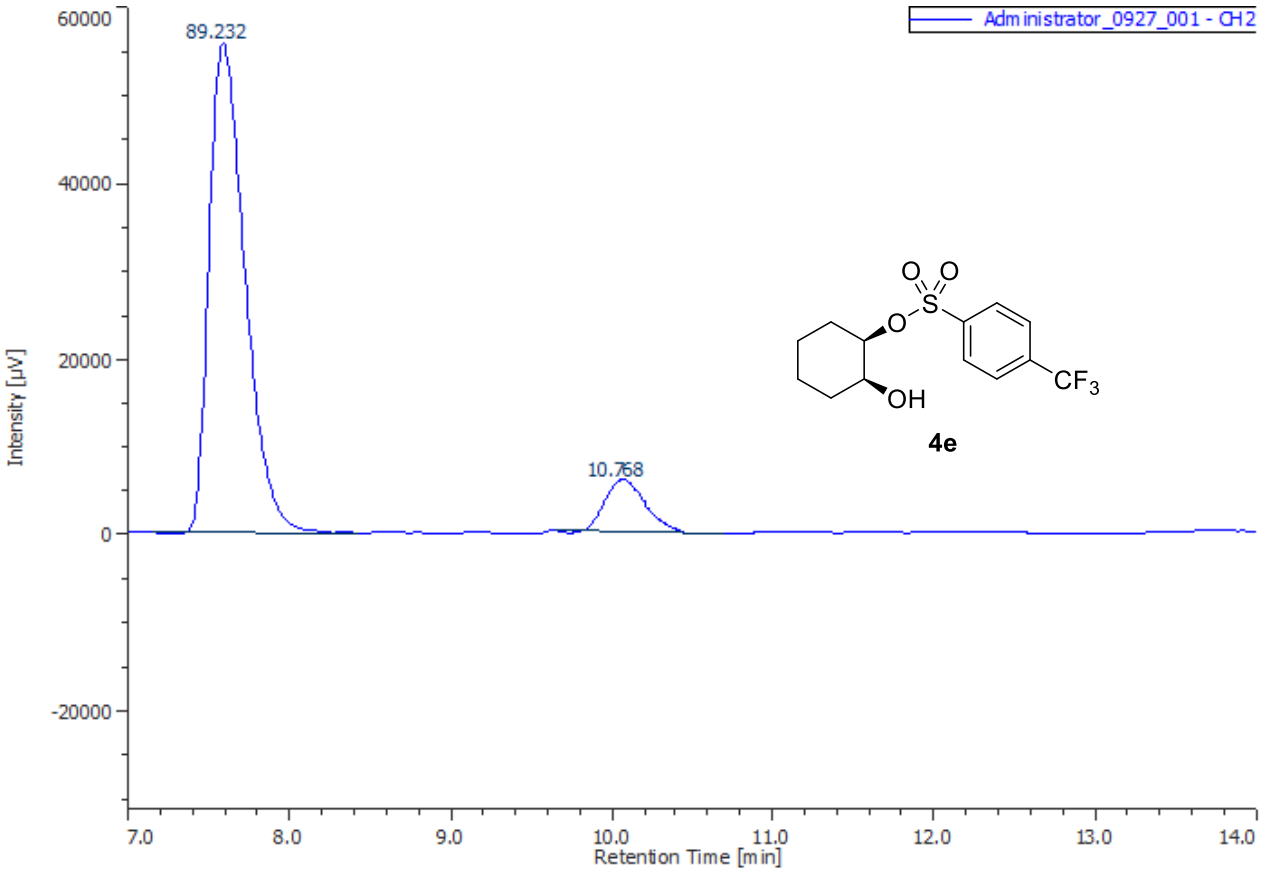
4c

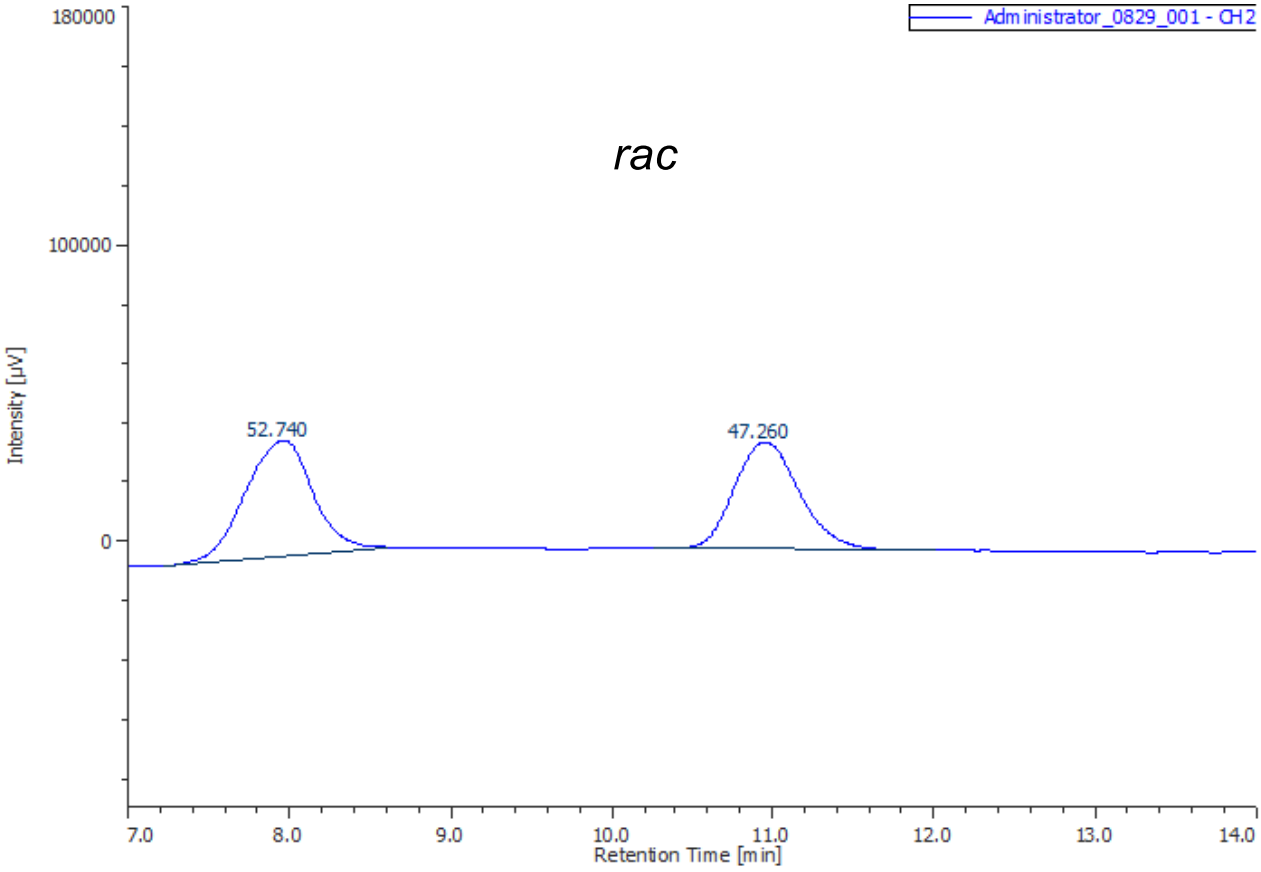

Administrator_0830_001 - CH2
rac
50.043
49.957
Intensity [µV]
Retention Time [min]

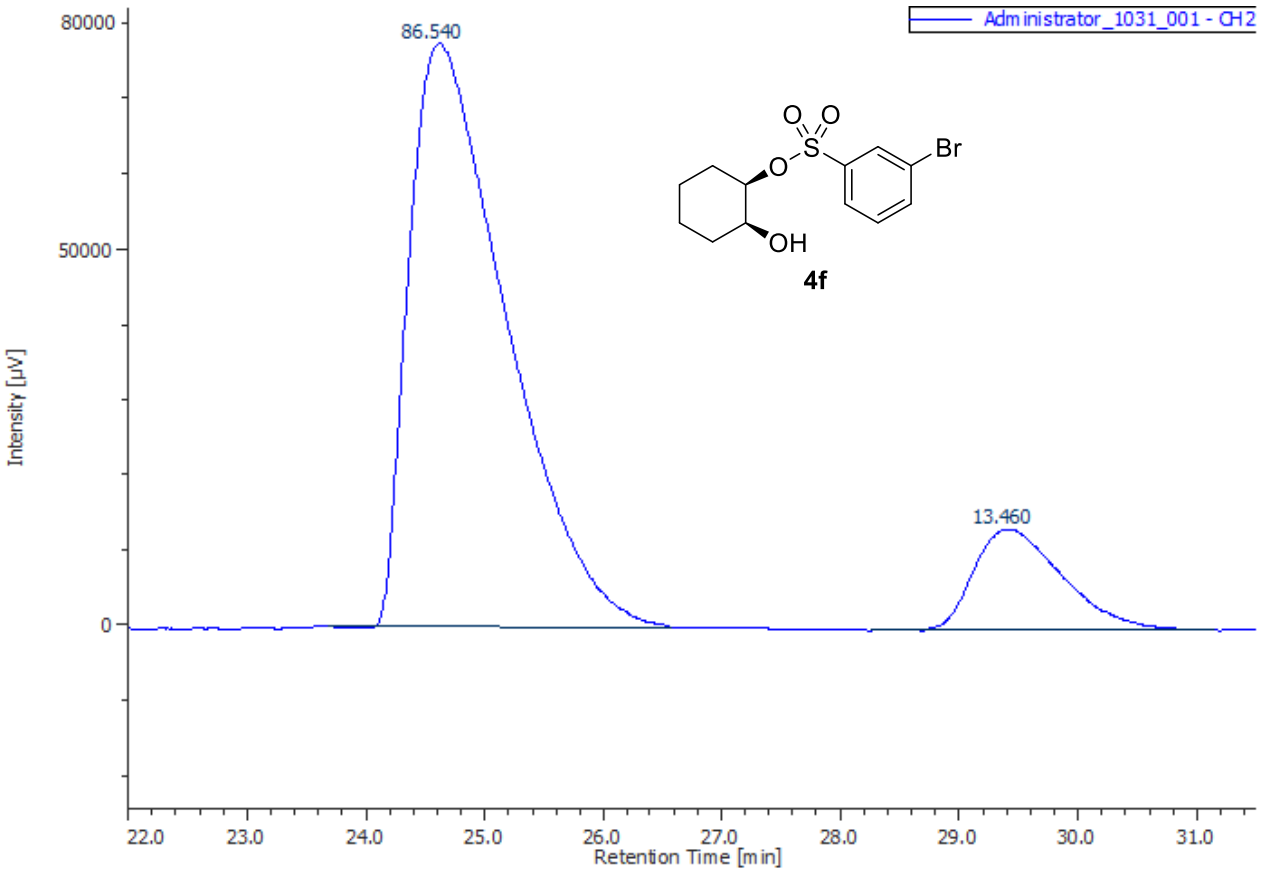

Administrator_1012_001 - CH2
89.751
10.249
110000
100000
50000
0
Intensity [µV]
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
Retention Time [min]
O
O
S
O
OH
Cl

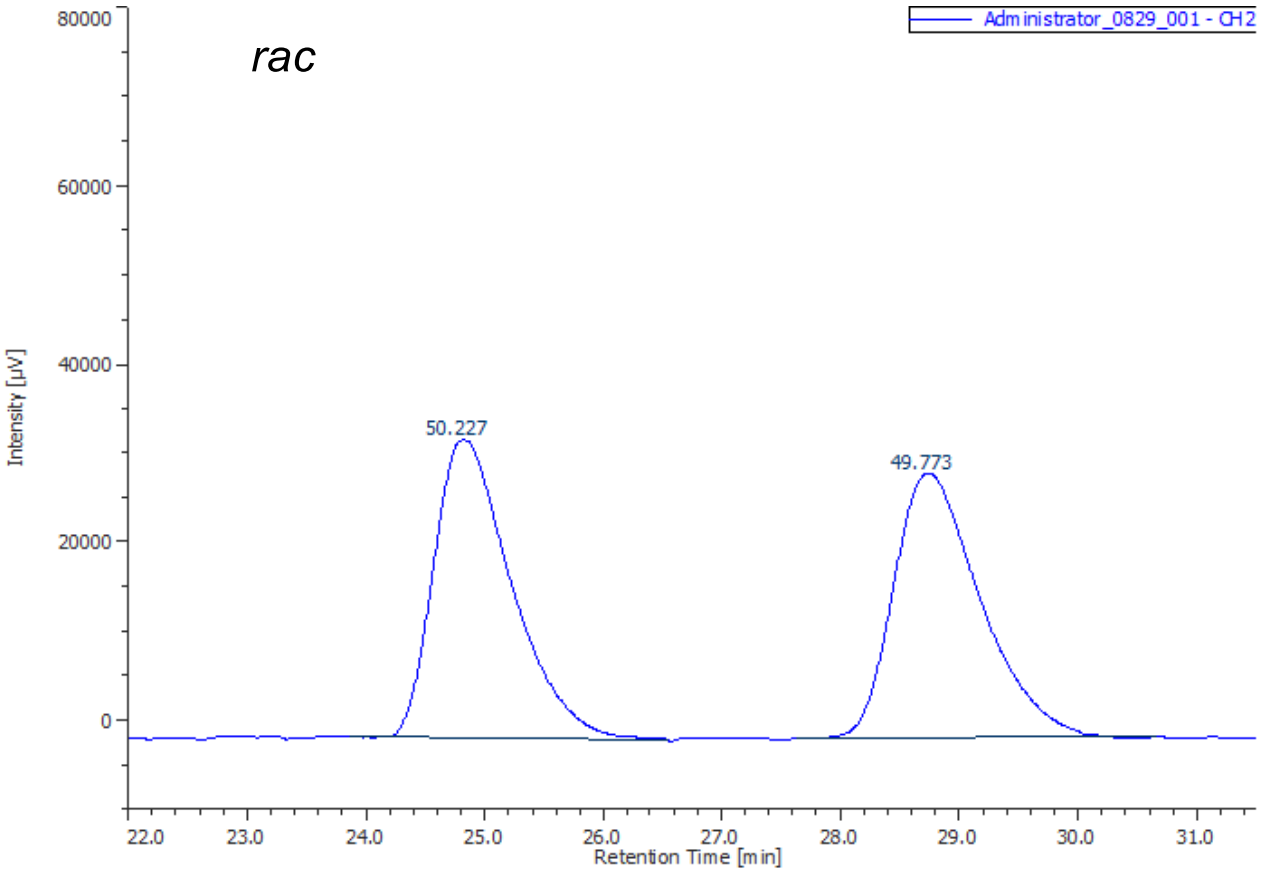
4d

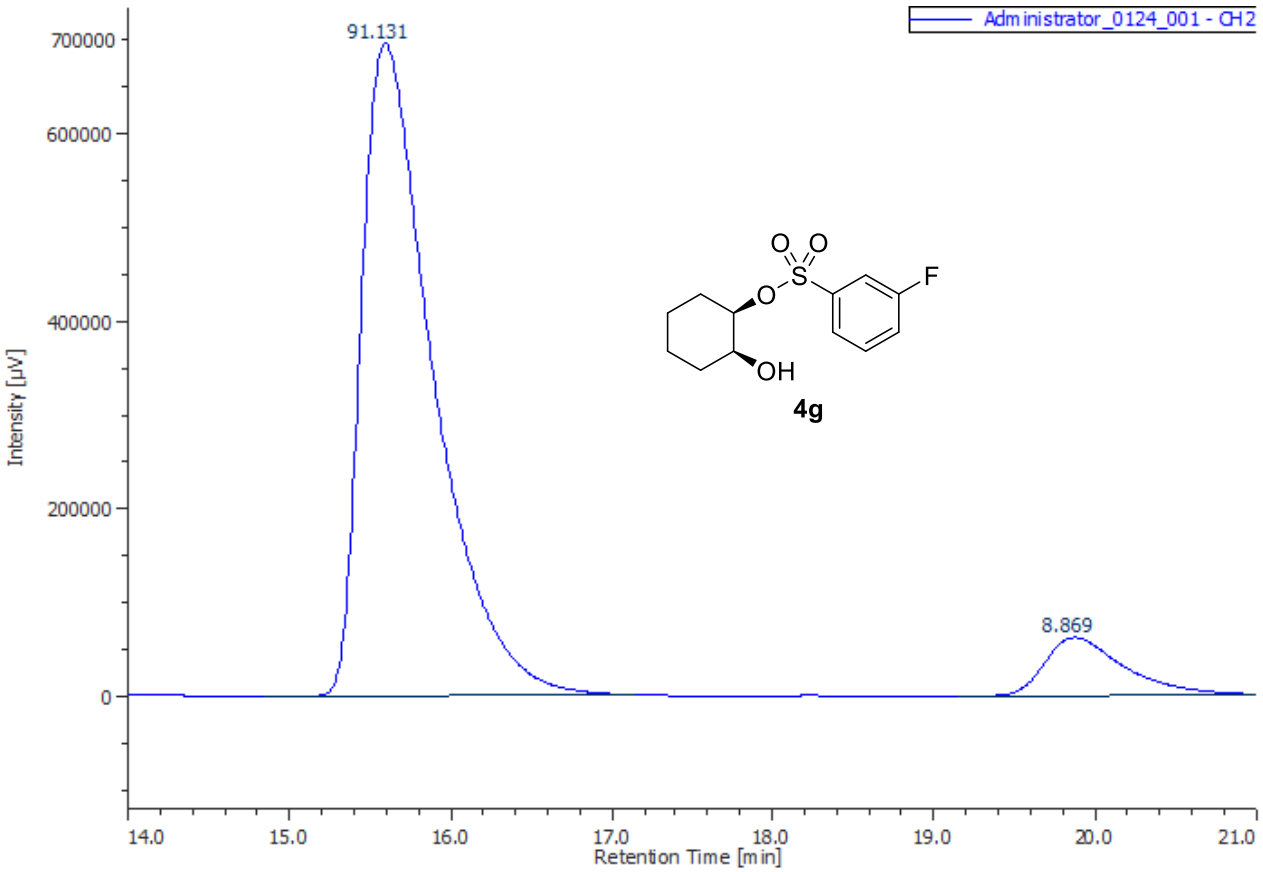

Administrator_1005_001_17.91min - CH1
49.495
50.505
rac
6500
6000
4000
2000
0
Intensity [µV]
10.0
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
Retention Time [min]


Administrator_0927_001 - CH2
89.232
10.768
60000
40000
20000
0
-20000
Intensity [µV]
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
Retention Time [min]
O
O
S
O
OH
CF3
4e

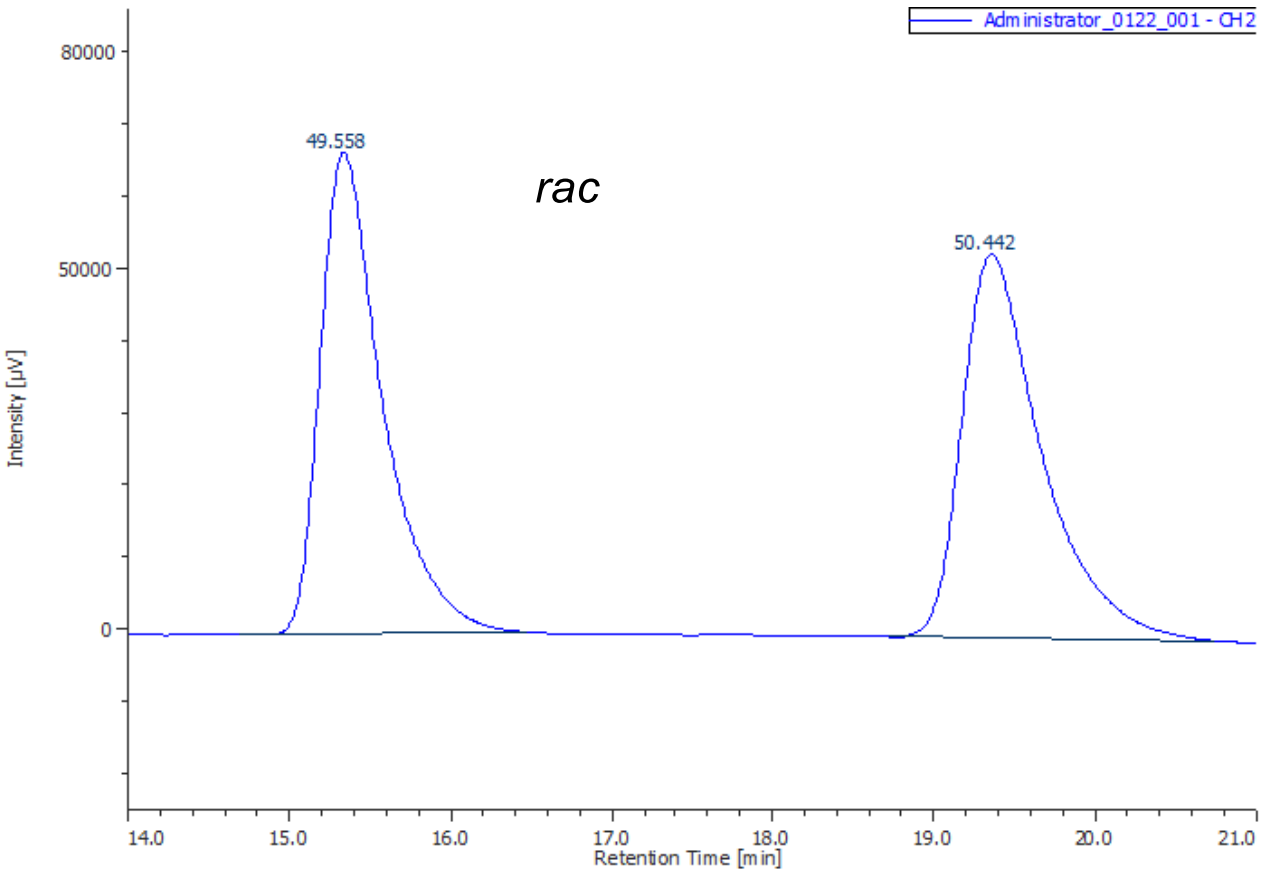

Administrator_0829_001 - CH2
rac
180000
100000
0
Intensity [µV]
52.740
47.260
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
Retention Time [min]

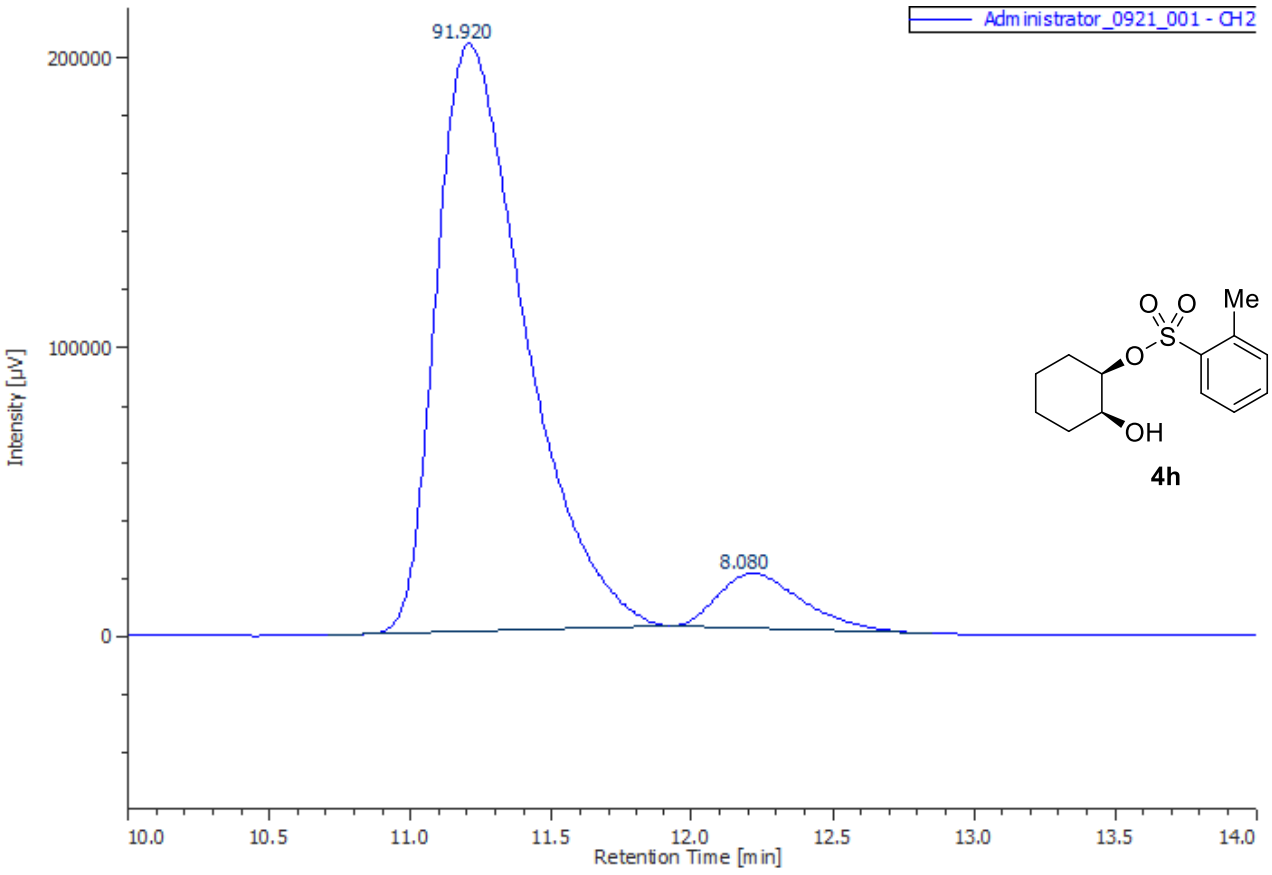

Administrator_1031_001 - CH2
86.540
13.460
80000
50000
0
Intensity [µV]
22.0
23.0
24.0
25.0
26.0
27.0
28.0
29.0
30.0
31.0
Retention Time [min]
O
O
S
O
Br
OH
4f


Administrator_0829_001 - CH2
rac
80000
60000
40000
20000
0
Intensity [µV]
50.227
49.773
22.0
23.0
24.0
25.0
26.0
27.0
28.0
29.0
30.0
31.0
Retention Time [min]

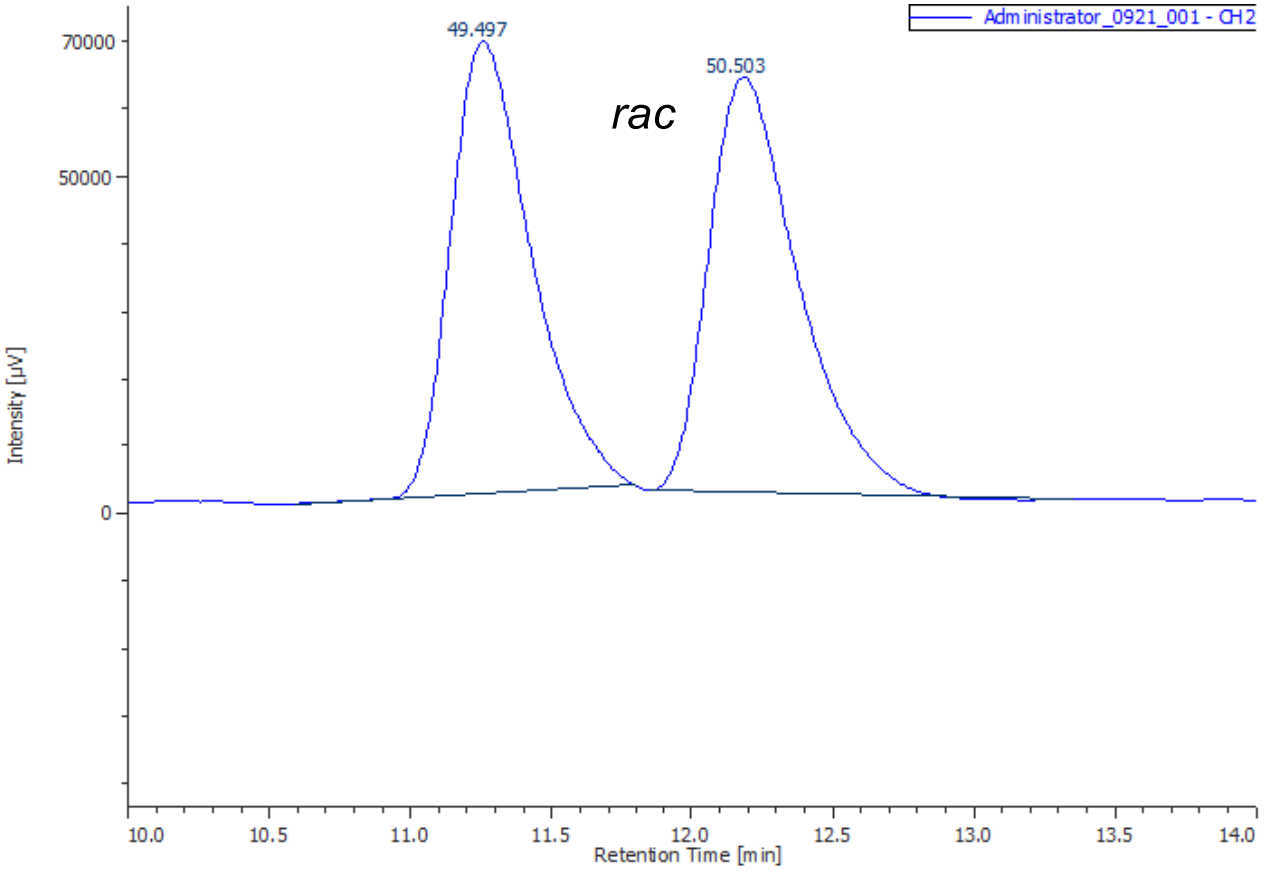

Administrator_0124_001 - CH2
91.131
8.869
Intensity [µV]
Retention Time [min]
4g

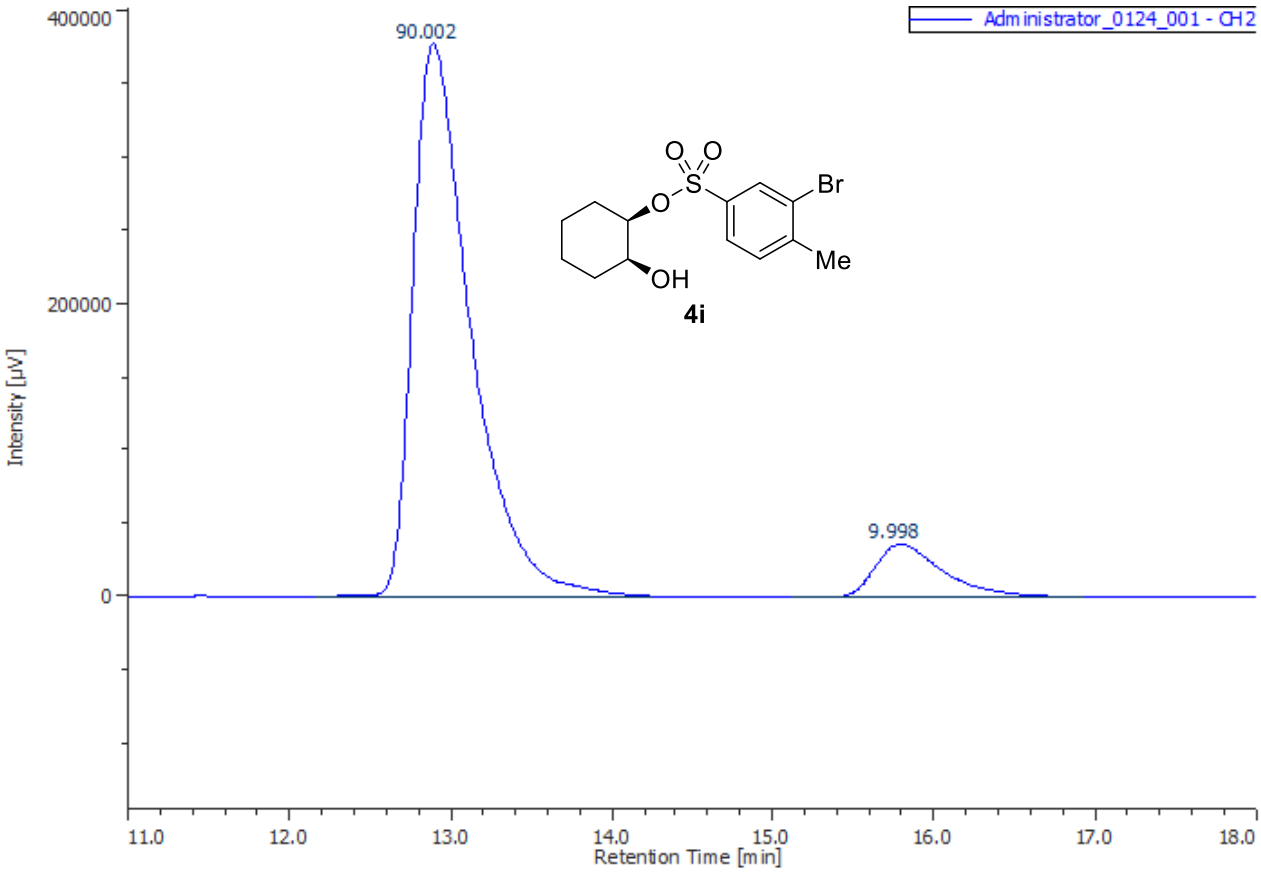
i

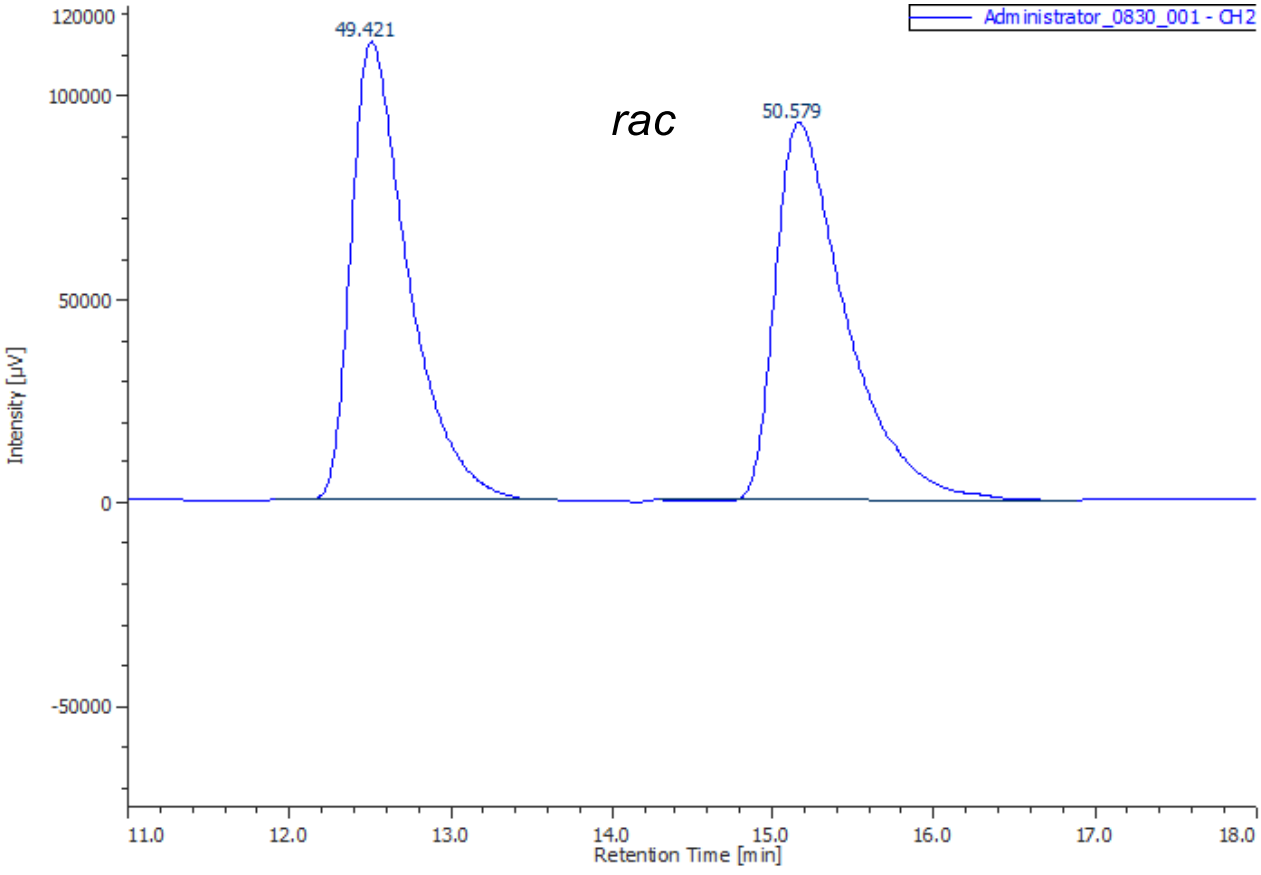

Administrator_0122_001 - CH2
49.558
50.442
rac
Intensity [µV]
Retention Time [min]

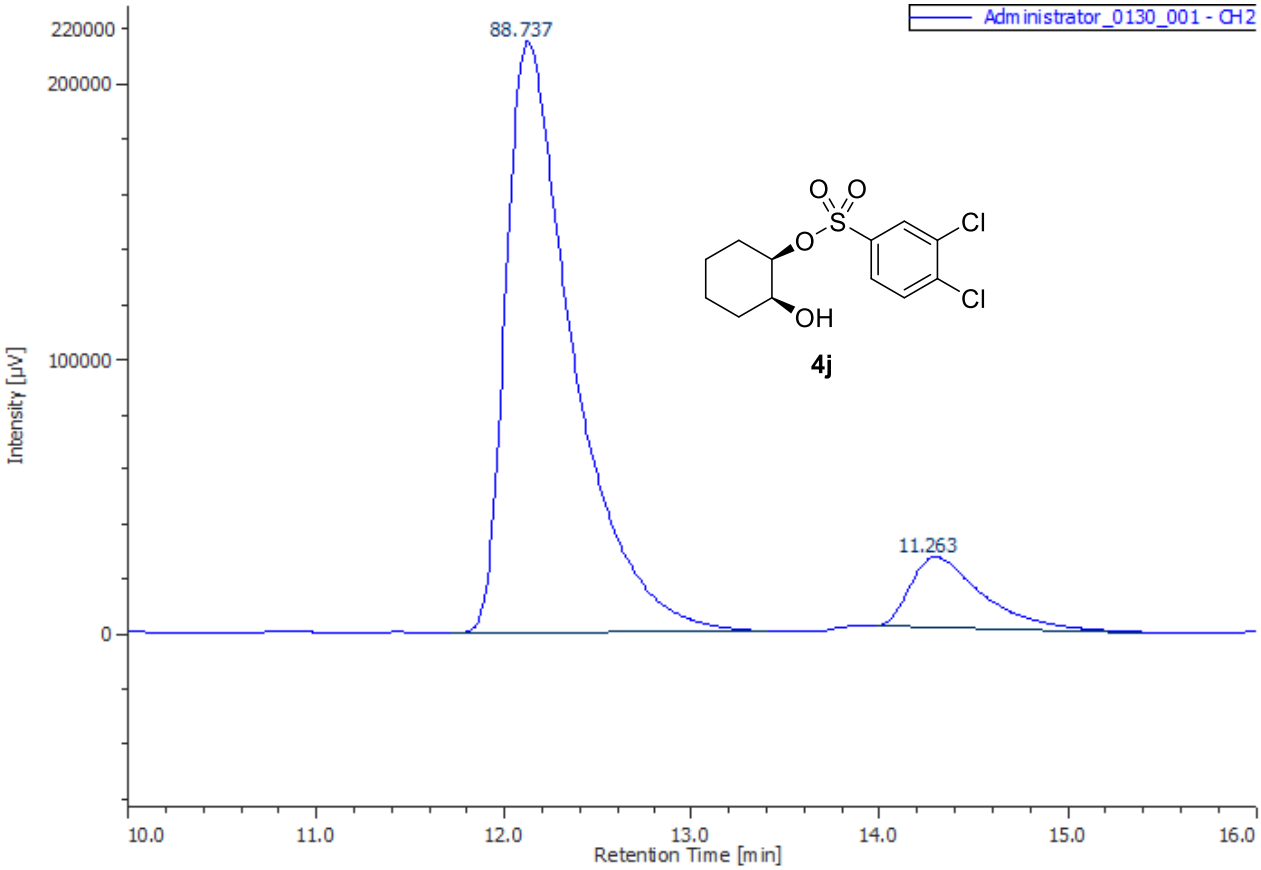

Administrator_0921_001 - CH2
91.920
8.080
200000
100000
0
Intensity [µV]
10.0
10.5
11.0
11.5
12.0
12.5
13.0
13.5
14.0
Retention Time [min]
O
O
S
O
Me
OH

4h

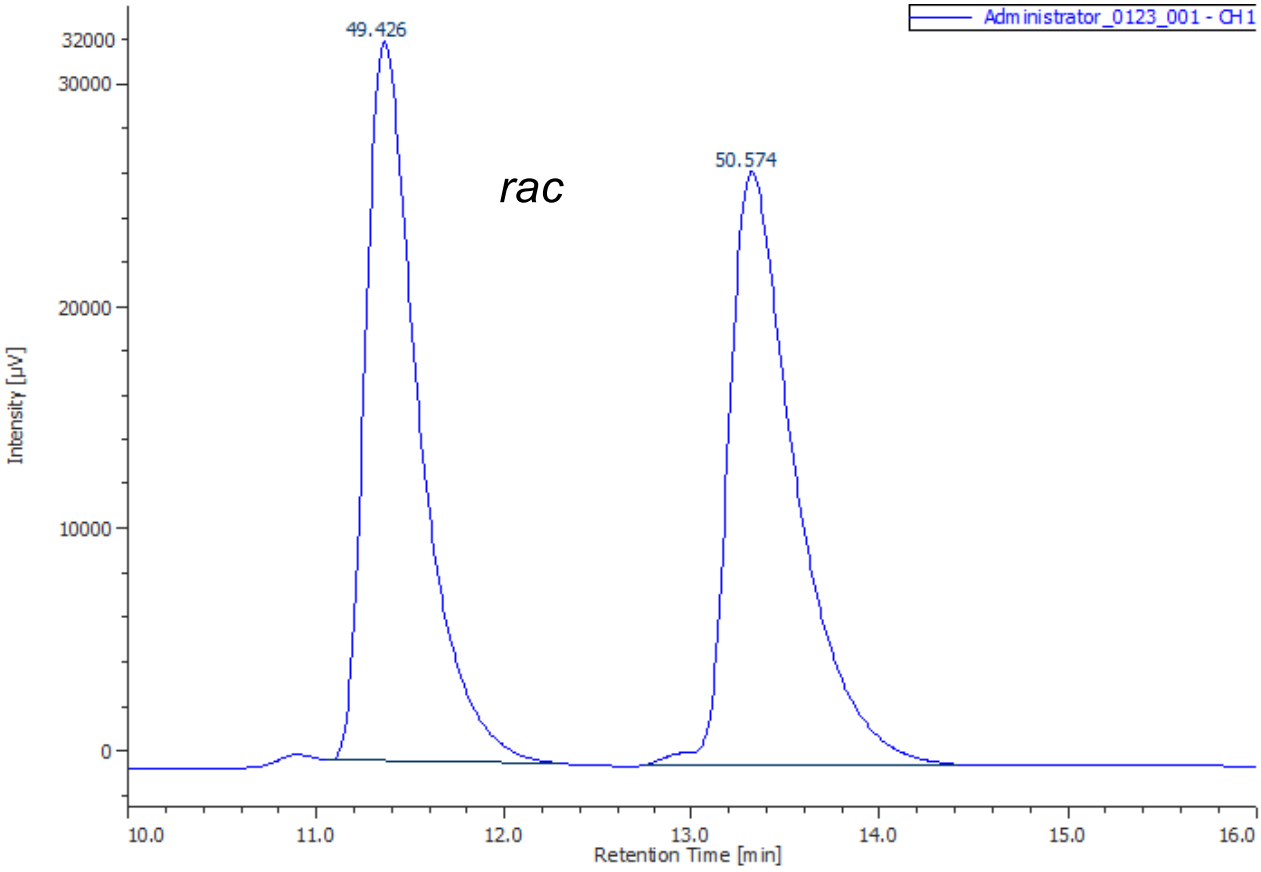

Administrator_0921_001 - CH2
49.497
50.503
rac
70000
50000
0
Intensity [µV]
10.0
10.5
11.0
11.5
12.0
12.5
13.0
13.5
14.0
Retention Time [min]

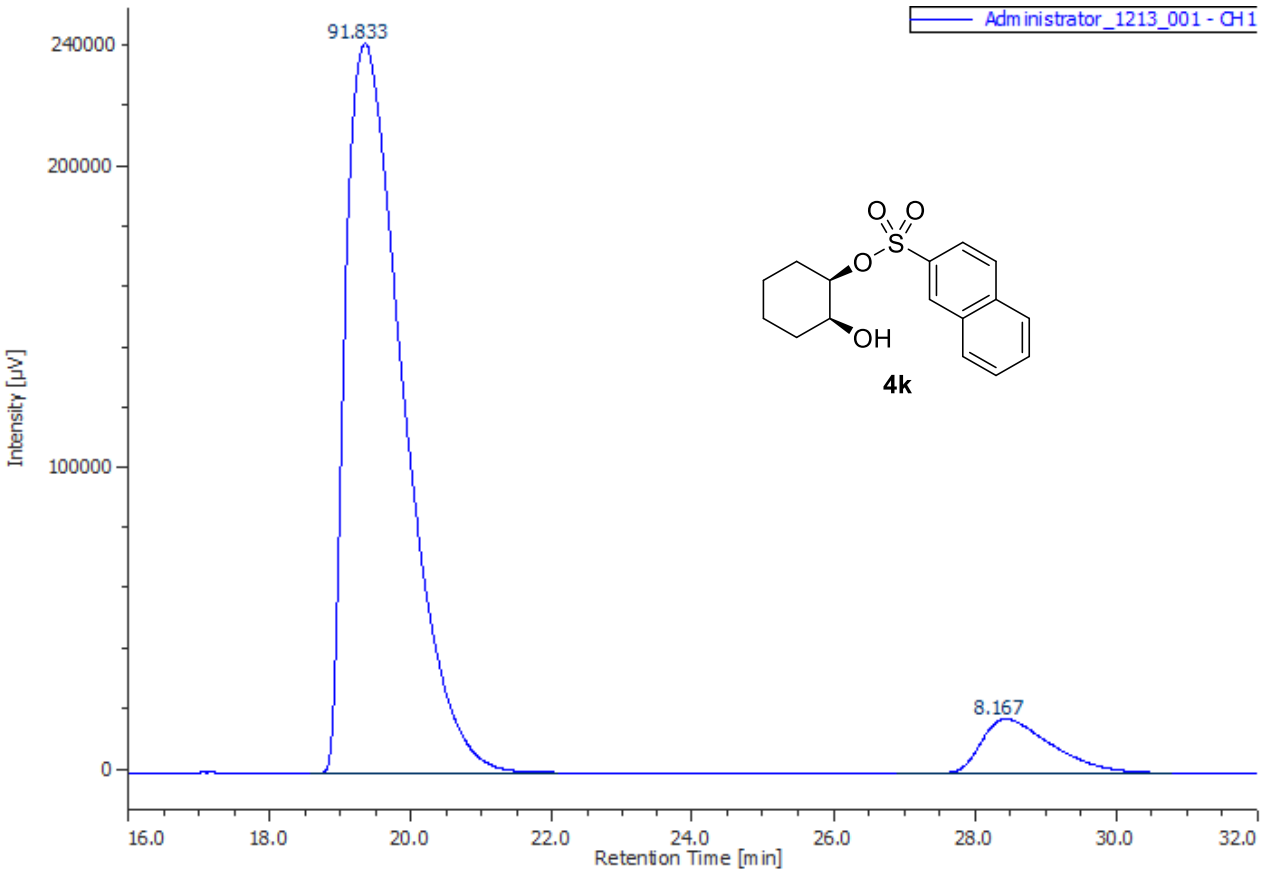

Administrator_0124_001 - CH2
90.002
9.998
400000
200000
0
Intensity [µV]
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
Retention Time [min]
O
O
S
O
Br
Me
OH
4i

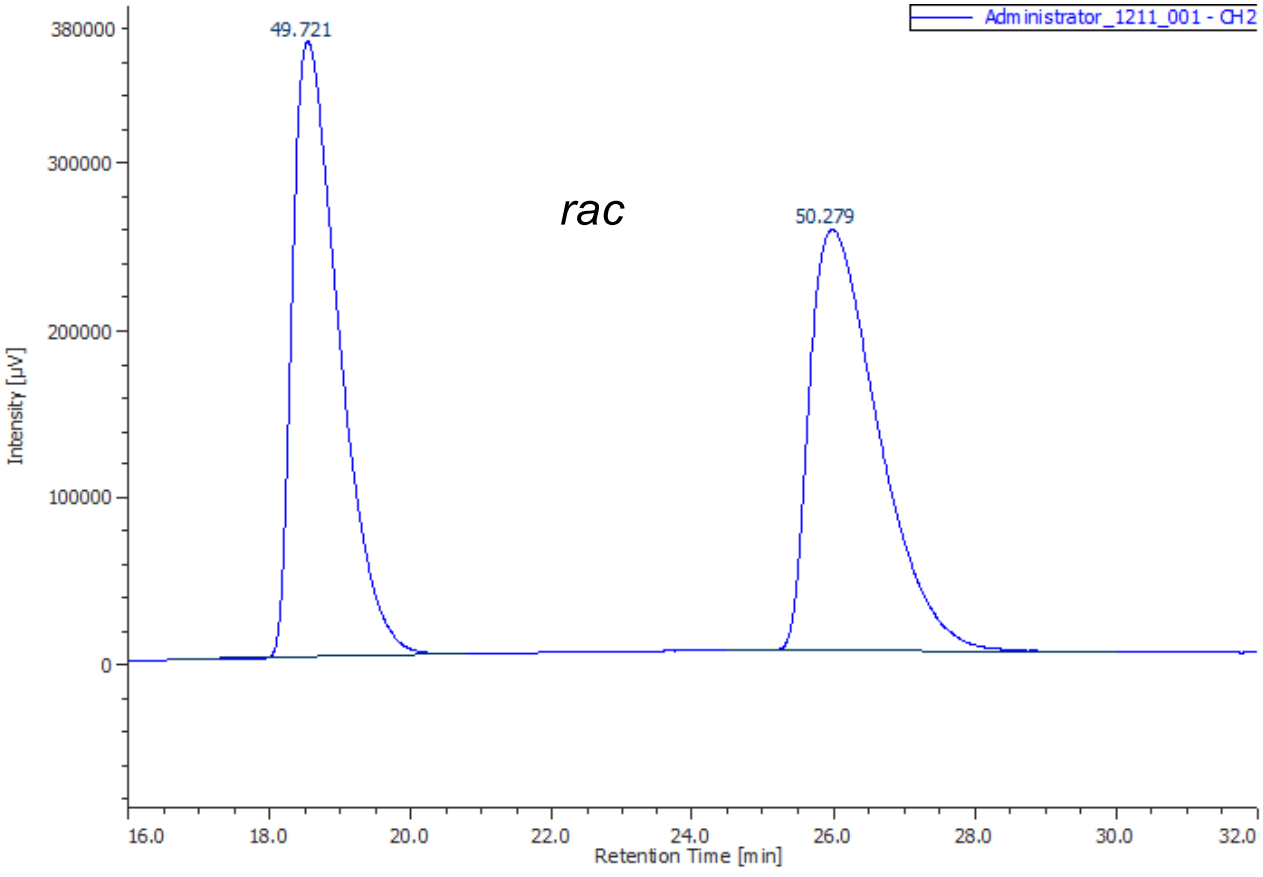

Administrator_0830_001 - CH2
49.421
50.579
rac
120000
100000
50000
0
-50000
Intensity [µV]
11.0
12.0
13.0
14.0
15.0
16.0
17.0
18.0
Retention Time [min]

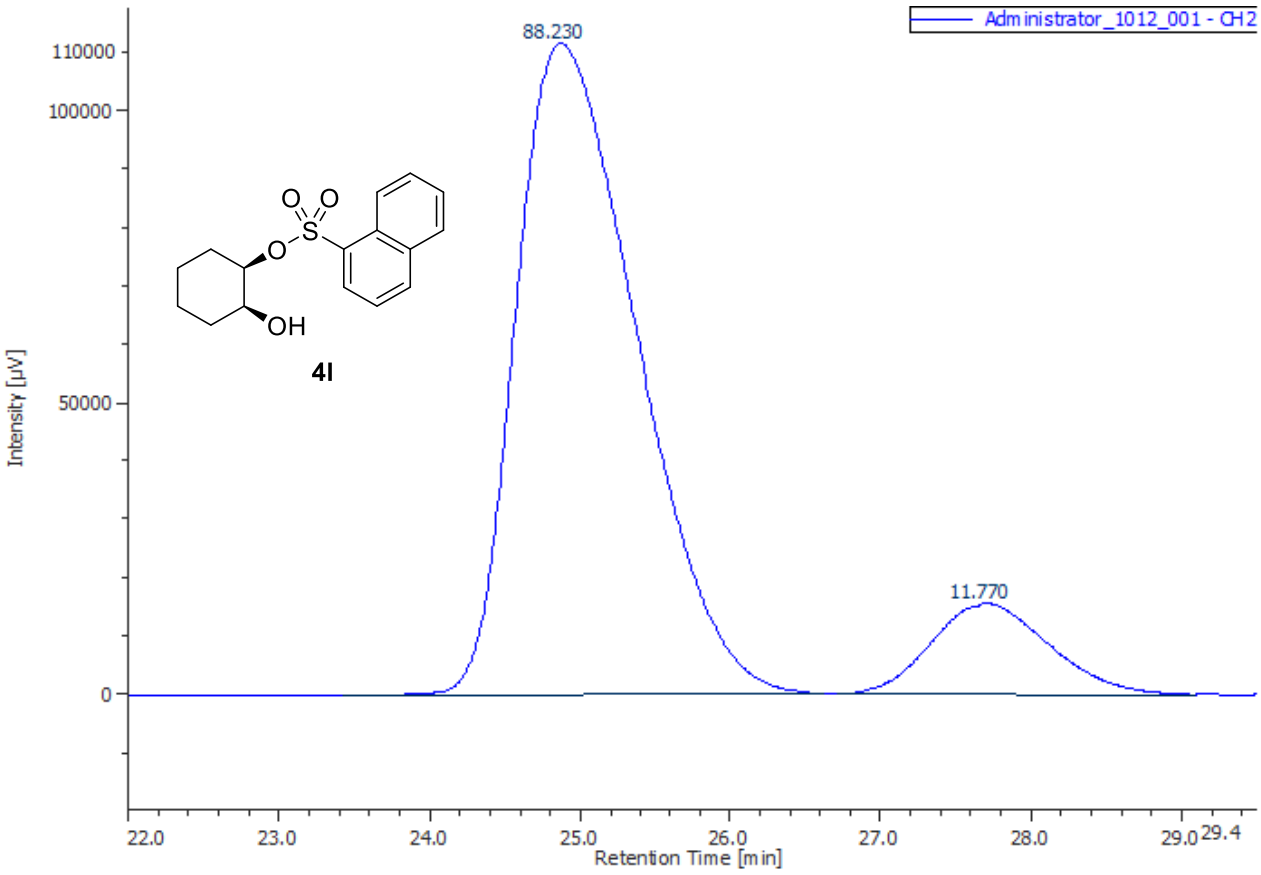

Administrator_0130_001 - CH2
88.737
11.263
220000
200000
100000
0
Intensity [µV]
10.0
11.0
12.0
13.0
14.0
15.0
16.0
Retention Time [min]
O
O
S
O
Cl
Cl
OH

4j

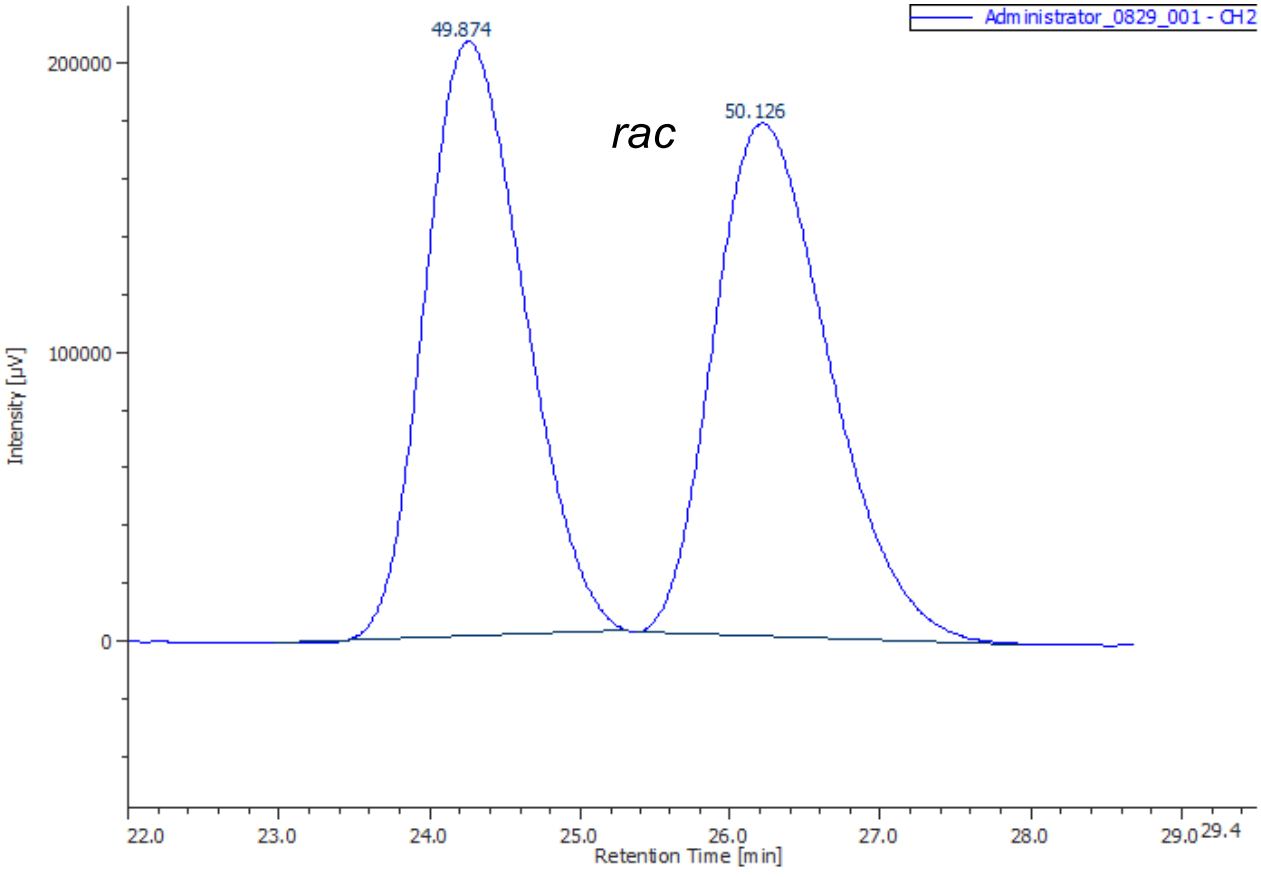

Administrator_0123_001 - CH1
49.426
50.574
rac
32000
30000
20000
10000
0
Intensity [µV]
10.0
11.0
12.0
13.0
14.0
15.0
16.0
Retention Time [min]

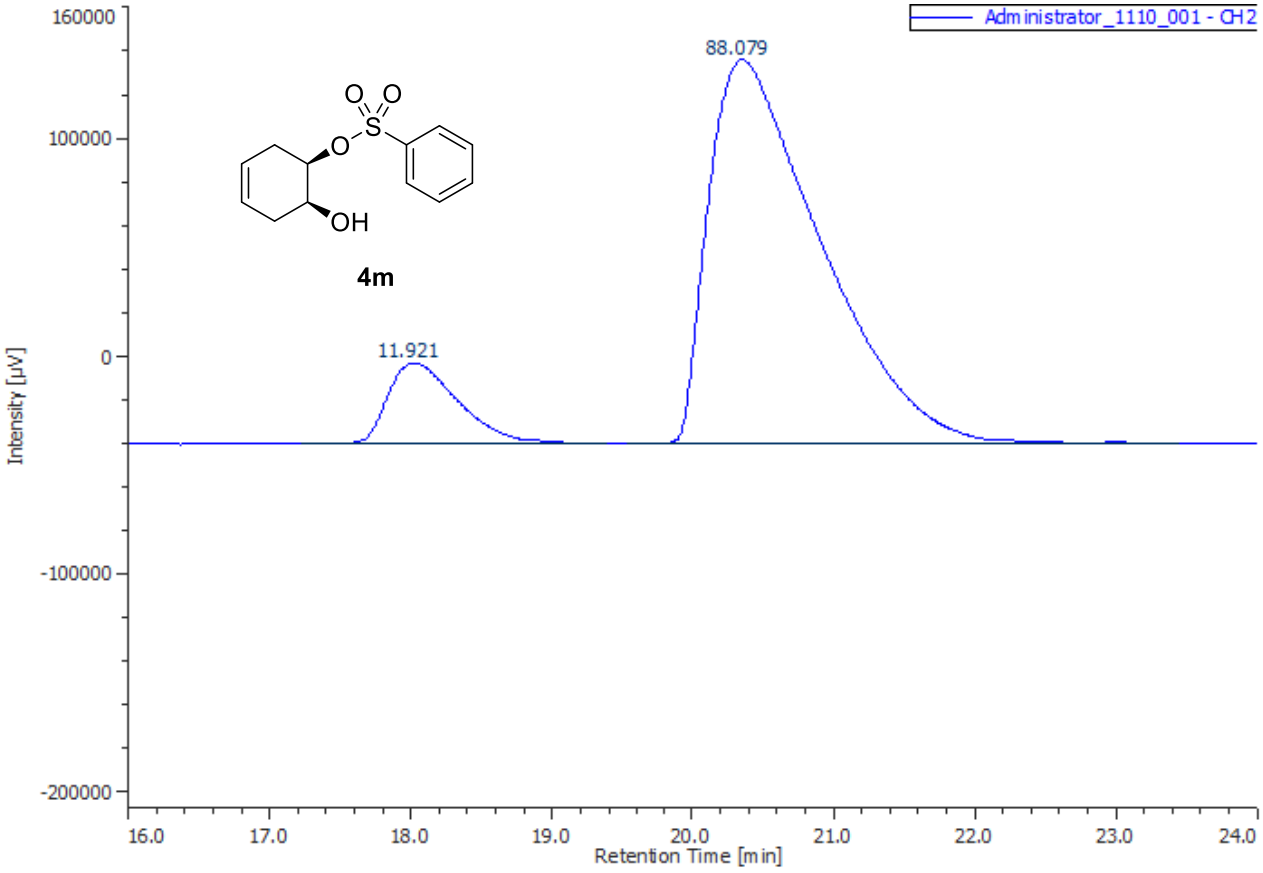

Administrator_1213_001 - CH1
91.833
8.167
Intensity [µV]
240000
200000
100000
0
16.0
18.0
20.0
22.0
24.0
26.0
28.0
30.0
32.0
Retention Time [min]
OH
4k

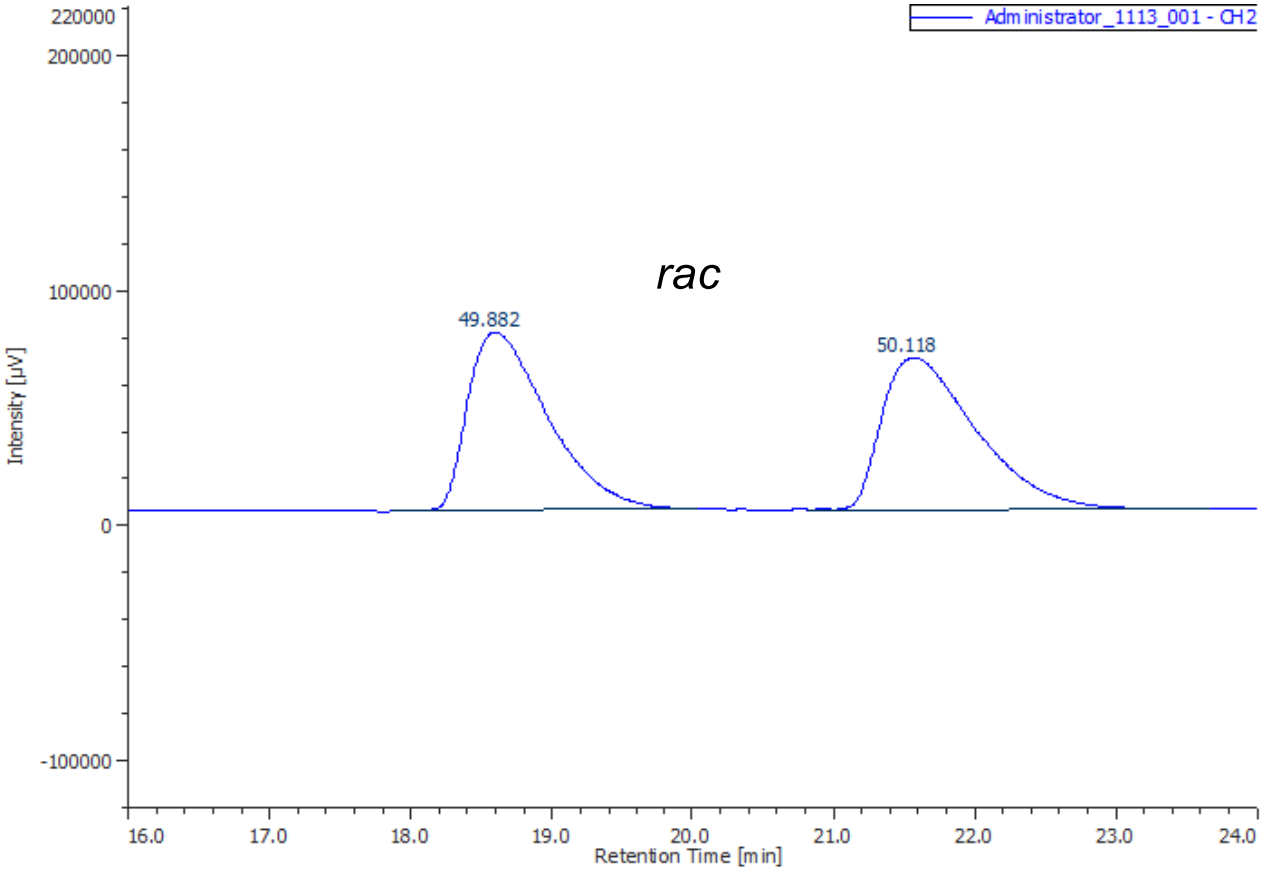

Administrator_1211_001 - CH2
49.721
50.279
rac
Intensity [µV]
380000
300000
200000
100000
0
16.0
18.0
20.0
22.0
24.0
26.0
28.0
30.0
32.0
Retention Time [min]

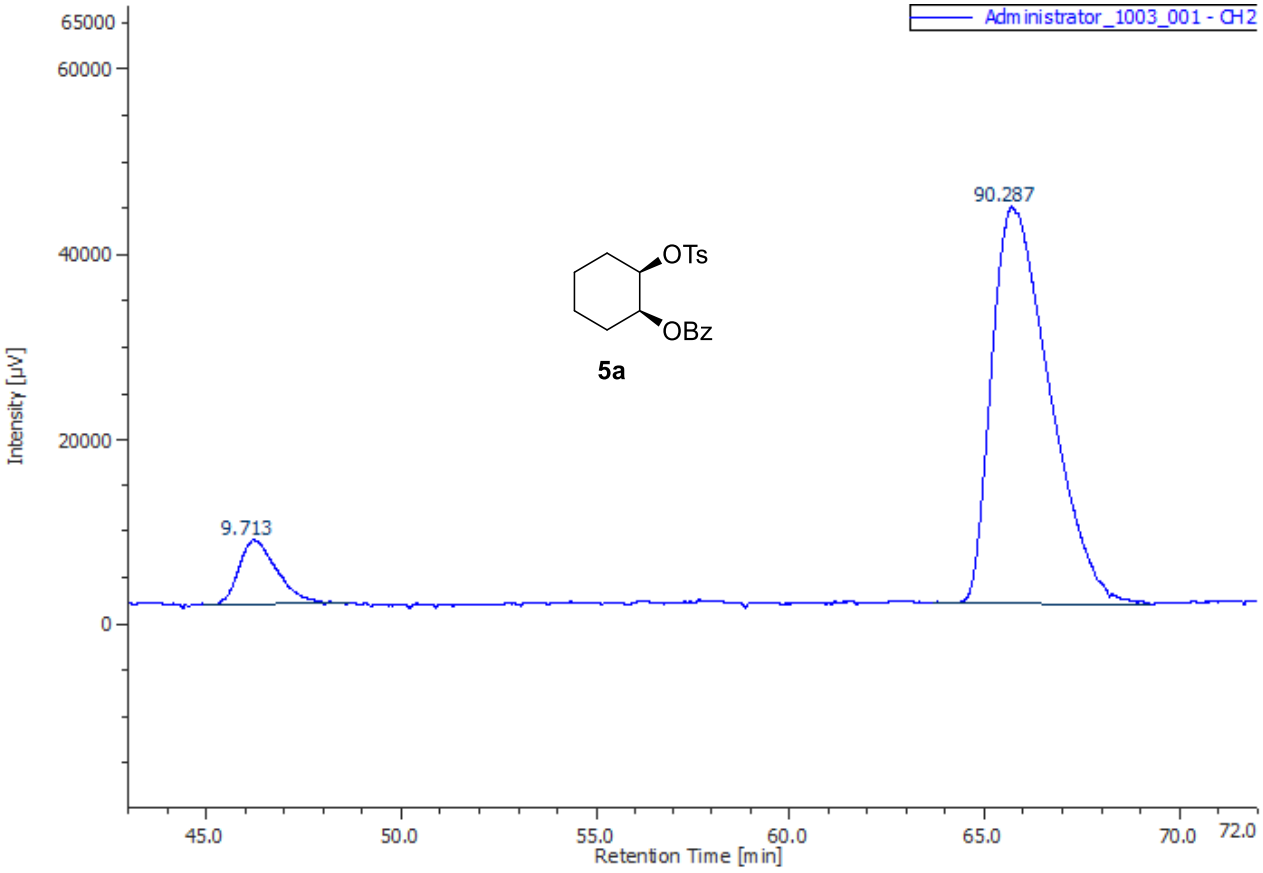

Administrator_1012_001 - CH2
88.230
11.770
110000
100000
50000
0
Intensity [µV]
22.0
23.0
24.0
25.0
26.0
27.0
28.0
29.0
29.4
Retention Time [min]
O
O
S
O
OH

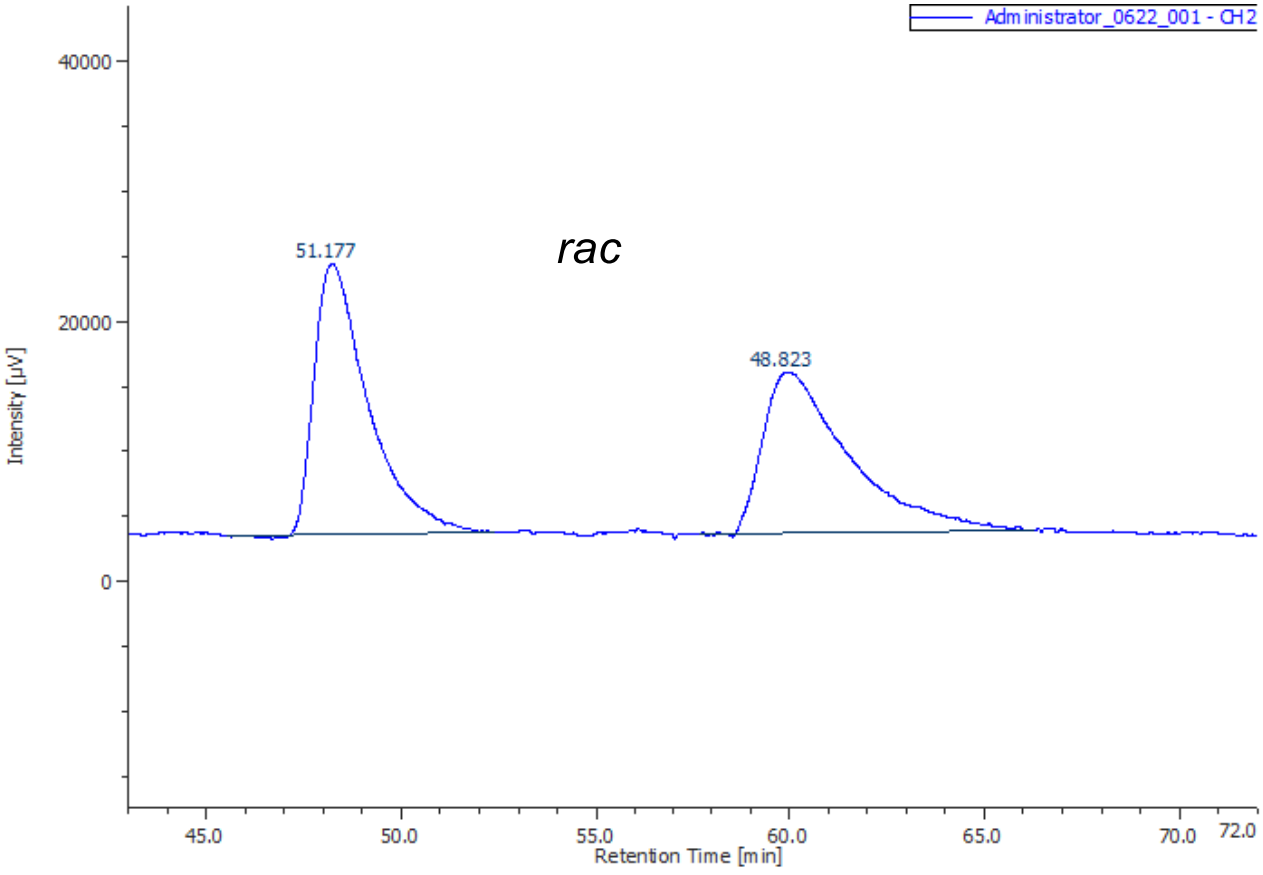
4l

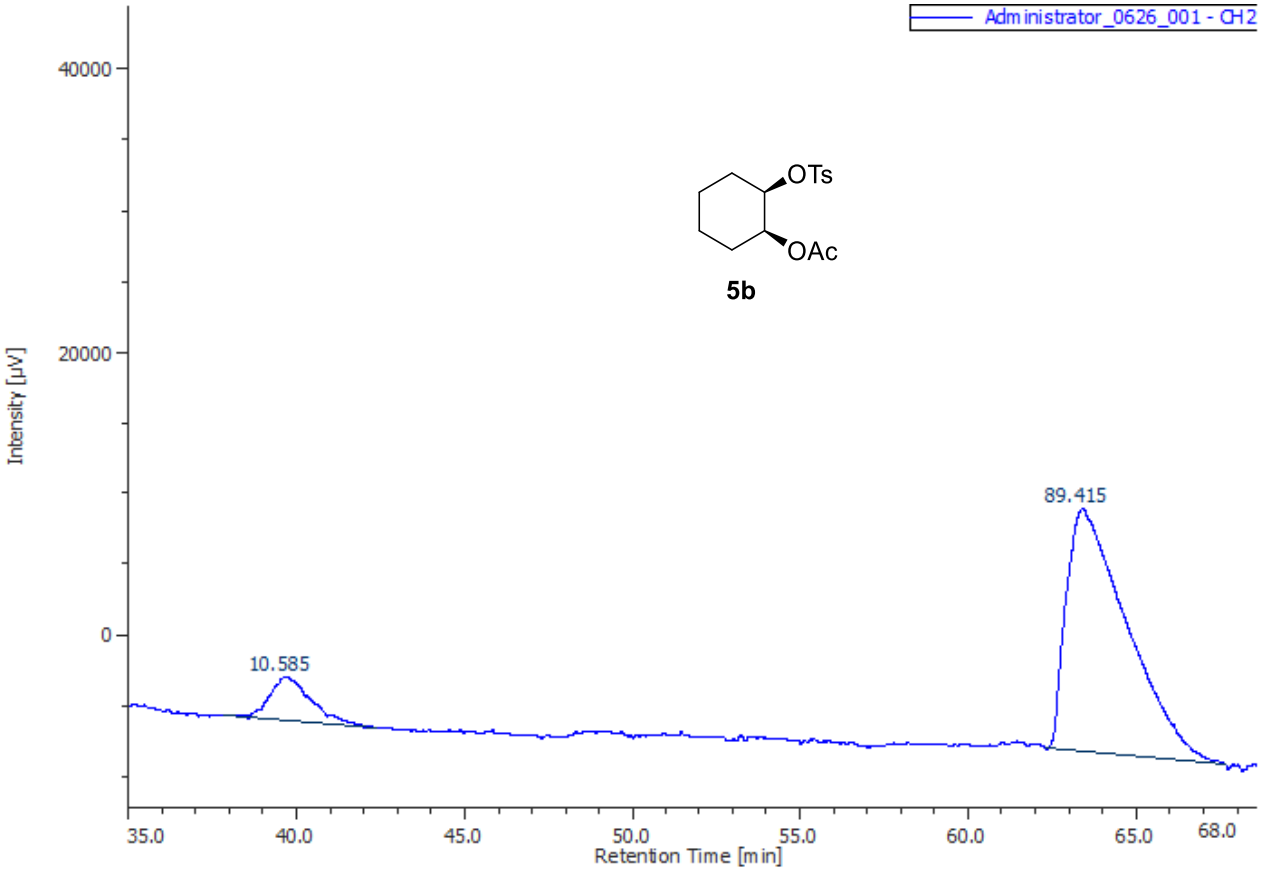

Administrator_0829_001 - CH2
49.874
50.126
rac
200000
100000
0
Intensity [µV]
22.0
23.0
24.0
25.0
26.0
27.0
28.0
29.0
29.4
Retention Time [min]

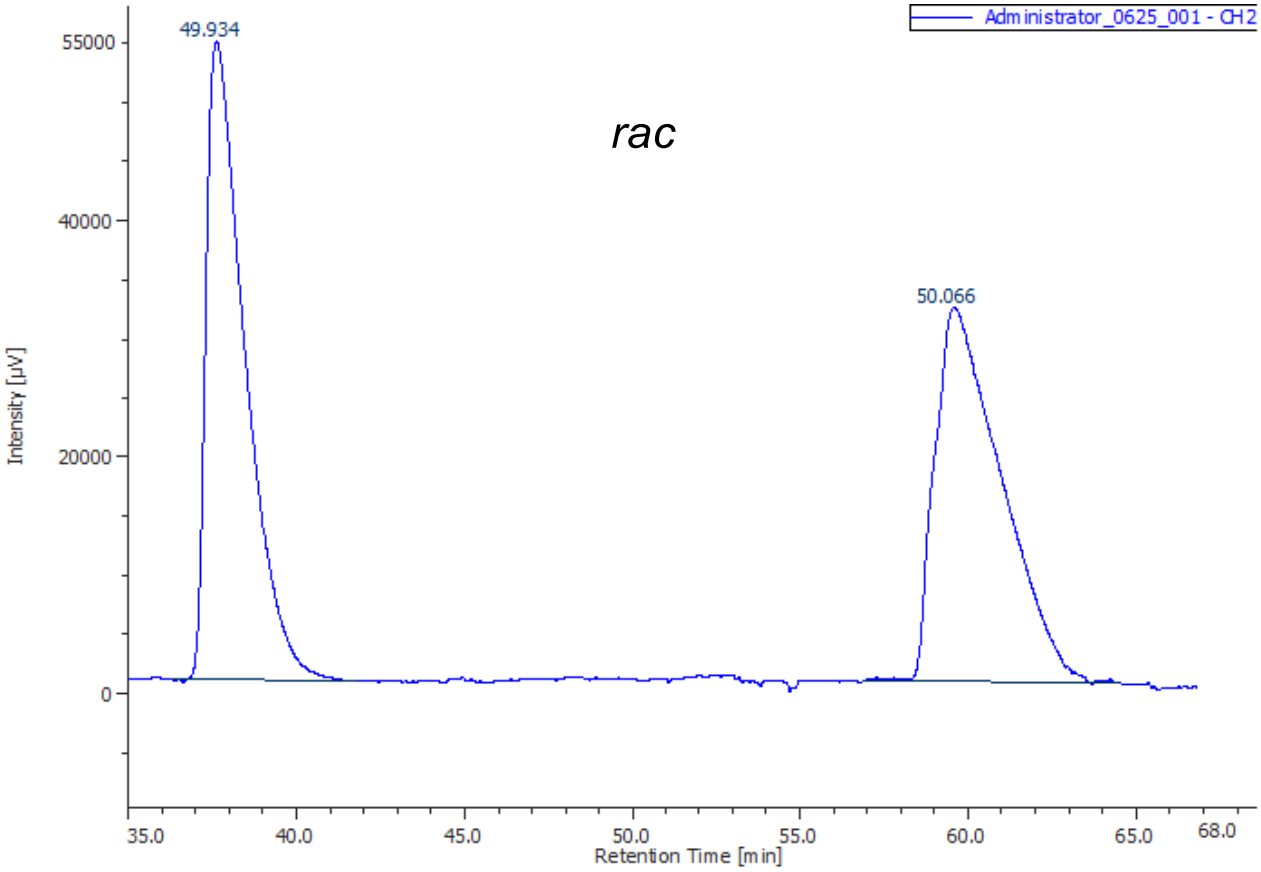

Administrator_1110_001 - CH2
88.079
11.921
4m
160000
100000
0
-100000
-200000
Intensity [µV]
16.0
17.0
18.0
19.0
20.0
21.0
22.0
23.0
24.0
Retention Time [min]

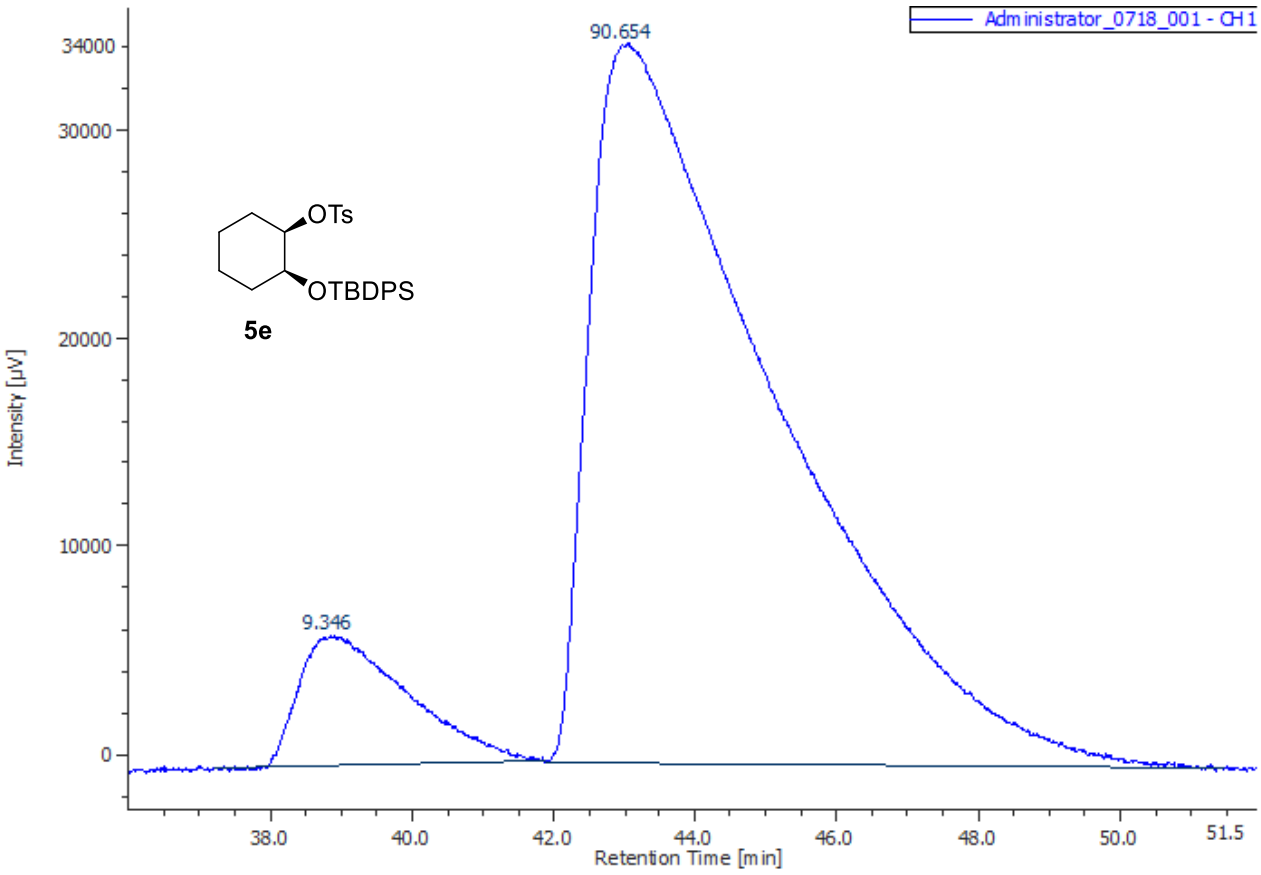

Administrator_1113_001 - CH2
rac
49.882
50.118
220000
200000
100000
0
-100000
Intensity [µV]
16.0
17.0
18.0
19.0
20.0
21.0
22.0
23.0
24.0
Retention Time [min]

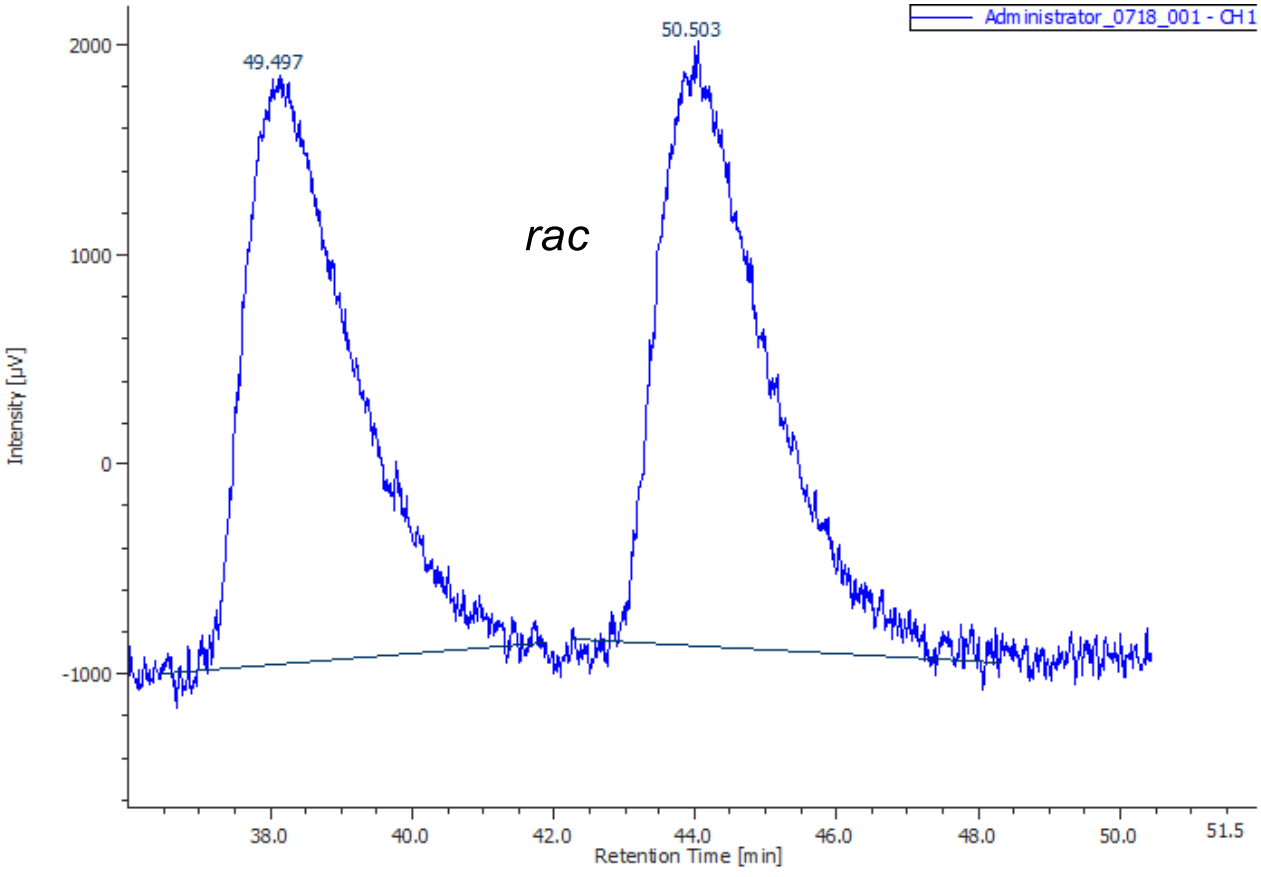

Administrator_1003_001 - CH2
65000
60000
40000
20000
0
Intensity [µV]
9.713
90.287
OTs
OBz
5a
45.0
50.0
55.0
60.0
65.0
70.0
72.0
Retention Time [min]

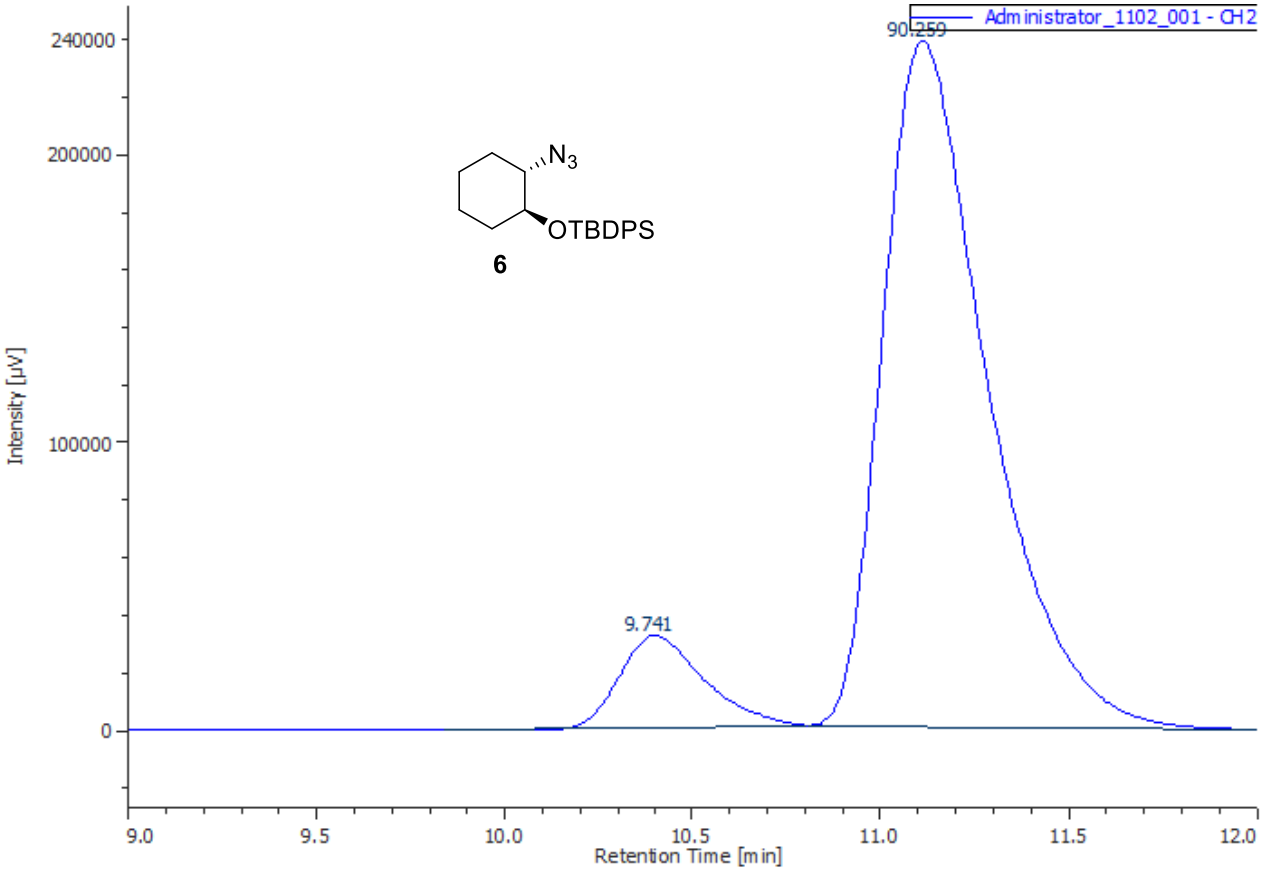

Administrator_0622_001 - CH2
40000
20000
0
Intensity [µV]
51.177
48.823
rac
45.0
50.0
55.0
60.0
65.0
70.0
72.0
Retention Time [min]

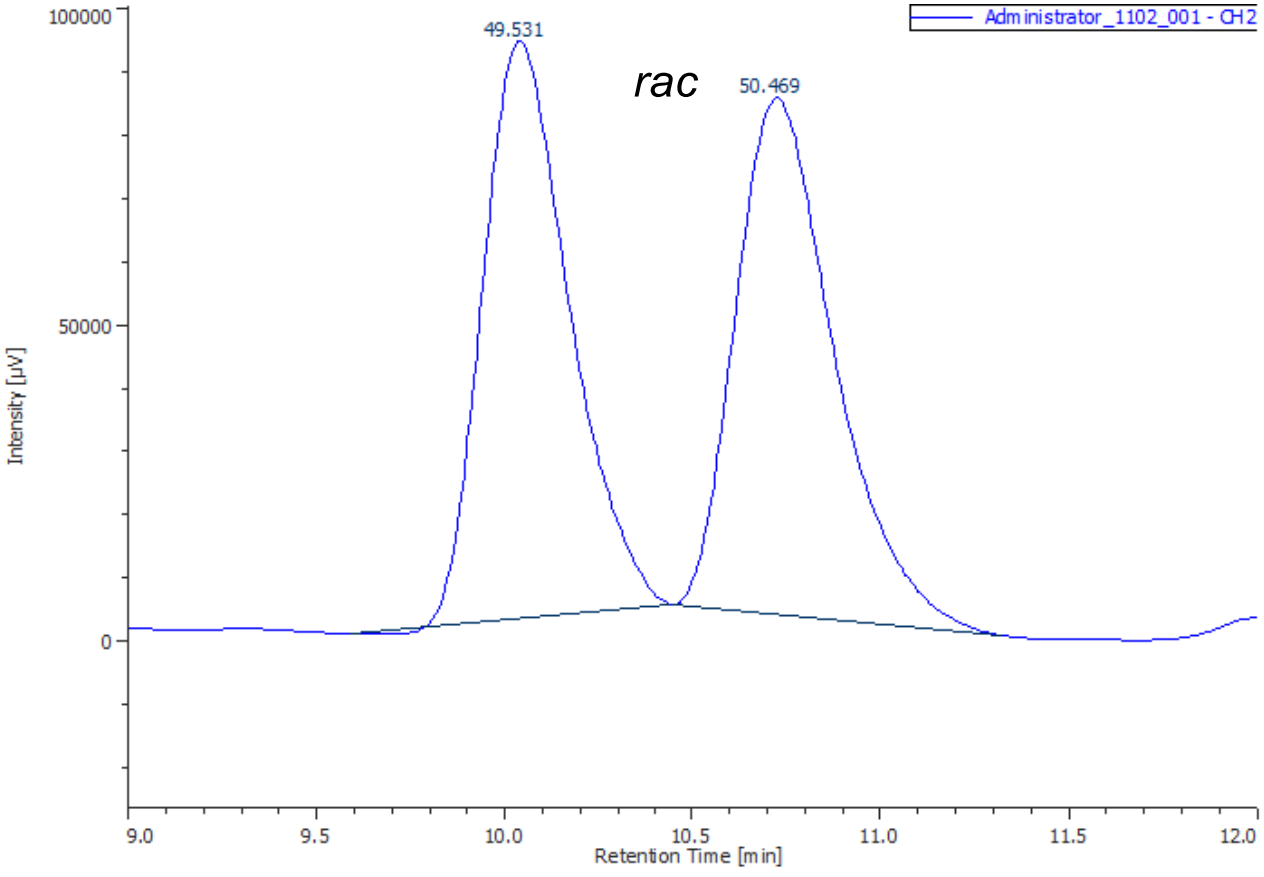

Administrator_0626_001 - CH2
OTs
OAc
5b
40000
20000
0
Intensity [µV]
89.415
10.585
35.0
40.0
45.0
50.0
55.0
60.0
65.0
68.0
Retention Time [min]

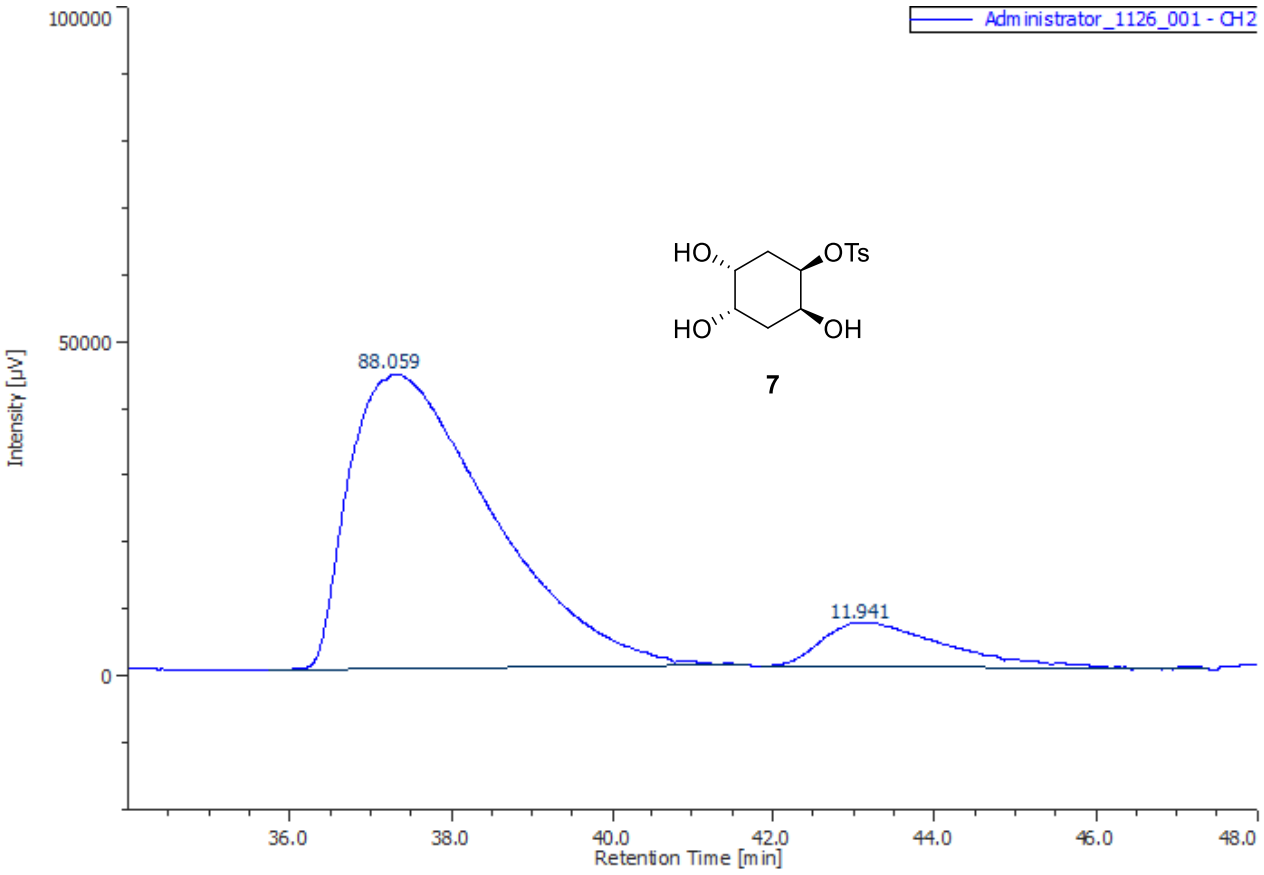

Administrator_0625_001 - CH2
rac
55000
40000
20000
0
Intensity [µV]
49.934
50.066
35.0
40.0
45.0
50.0
55.0
60.0
65.0
68.0
Retention Time [min]

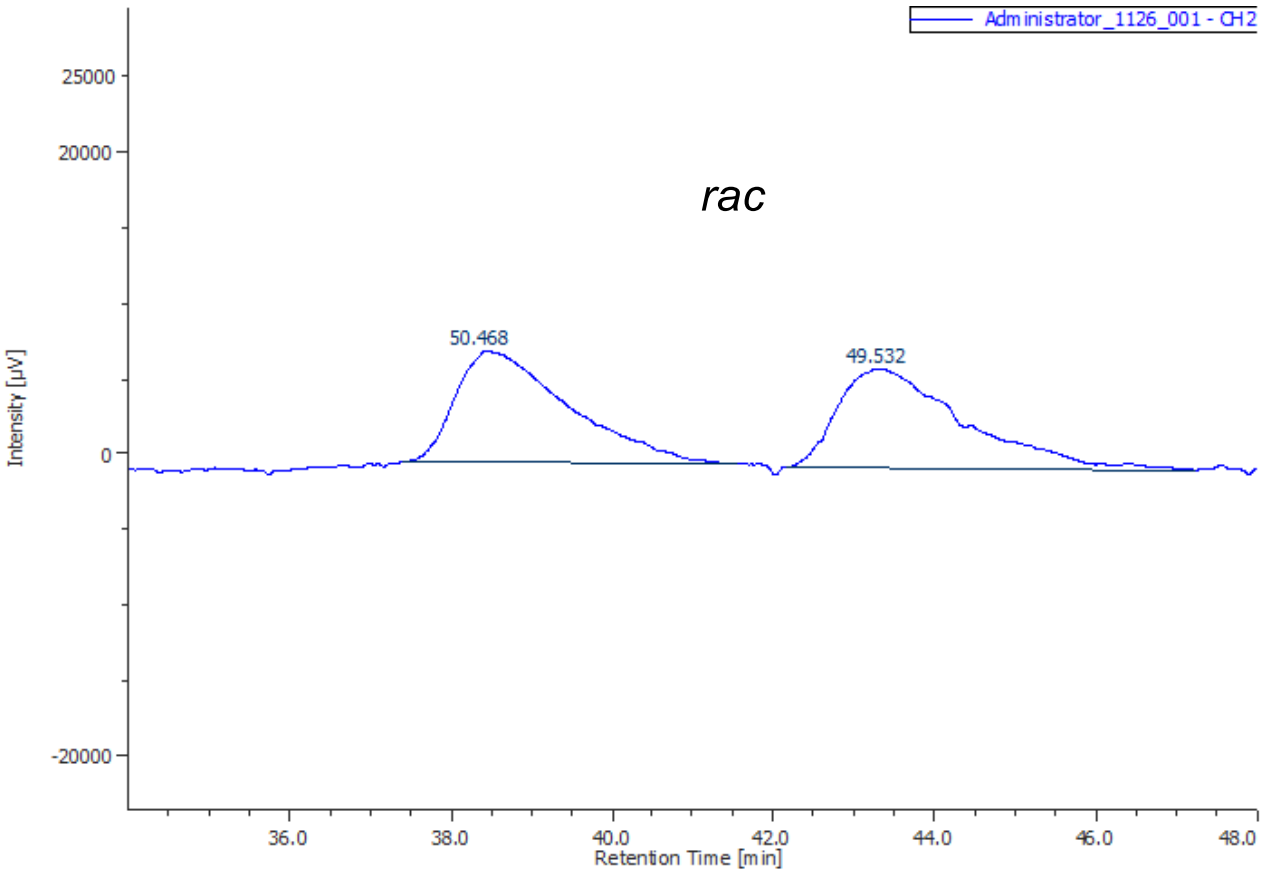

Administrator_0718_001 - CH1
90.654
9.346
OTs
OTBDPS
5e
Intensity [µV]
Retention Time [min]

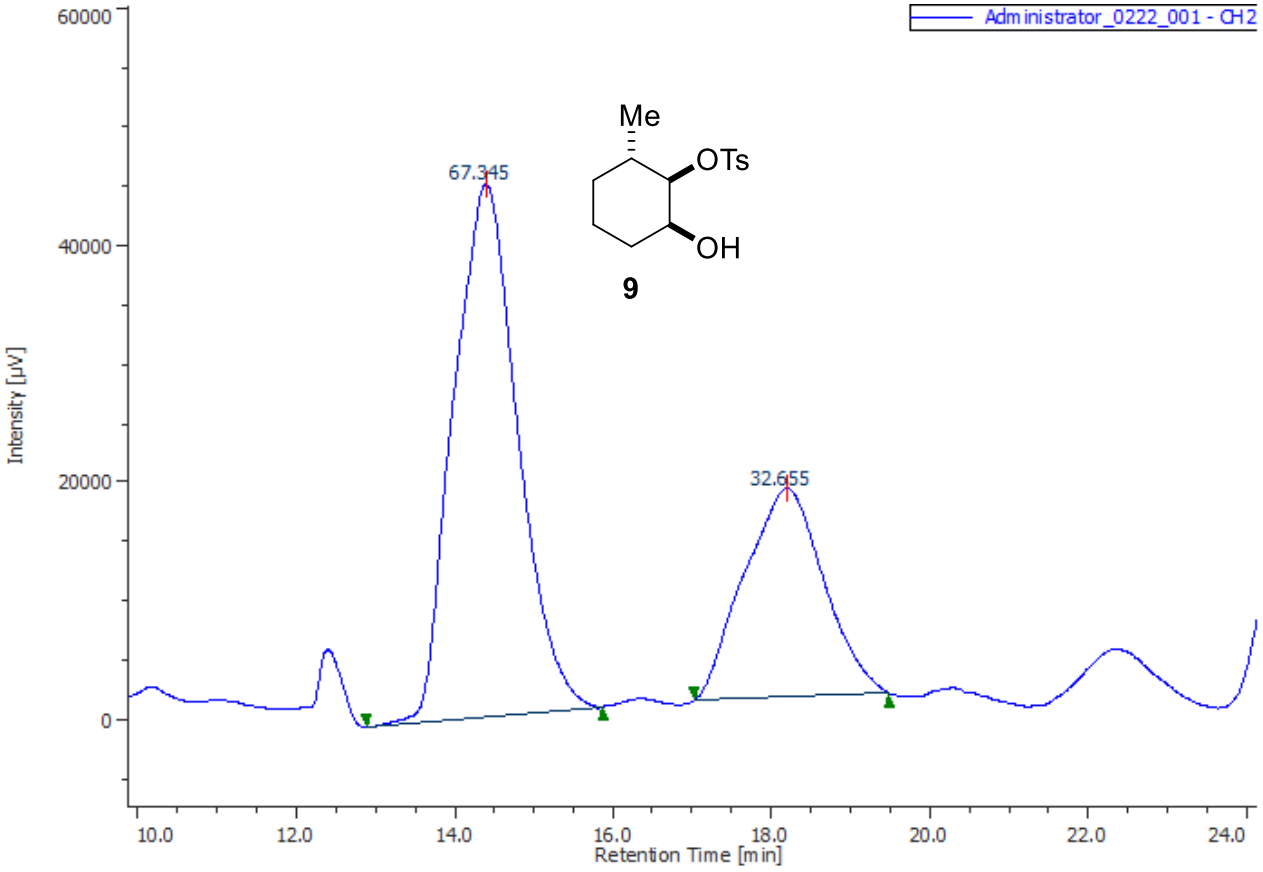

Administrator_0718_001 - CH1
49.497
50.503
rac
Intensity [µV]
Retention Time [min]

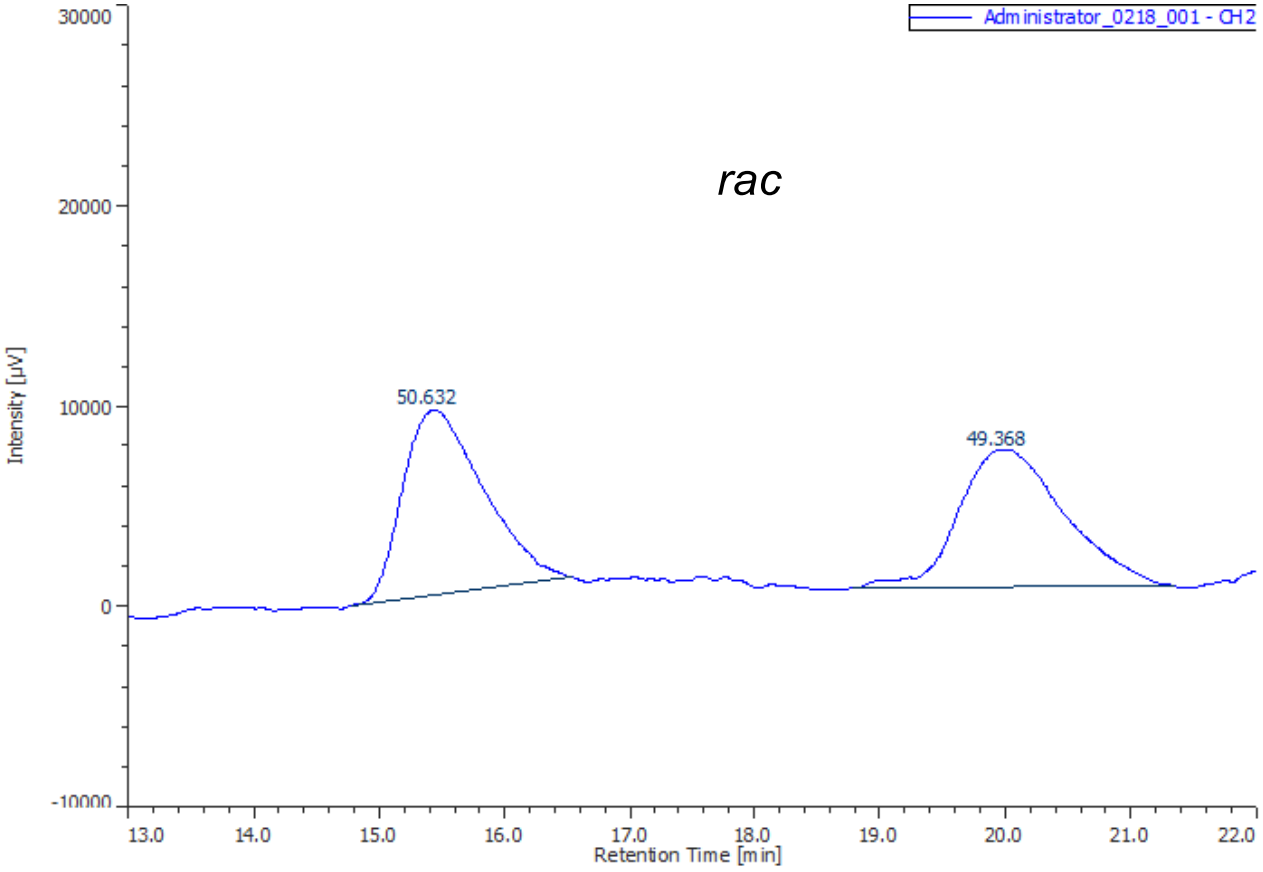

Administrator_1102_001 - CH2
90.259
9.741
240000
200000
100000
0
Intensity [µV]
9.0
9.5
10.0
10.5
11.0
11.5
12.0
Retention Time [min]
N3
OTBDPS
6

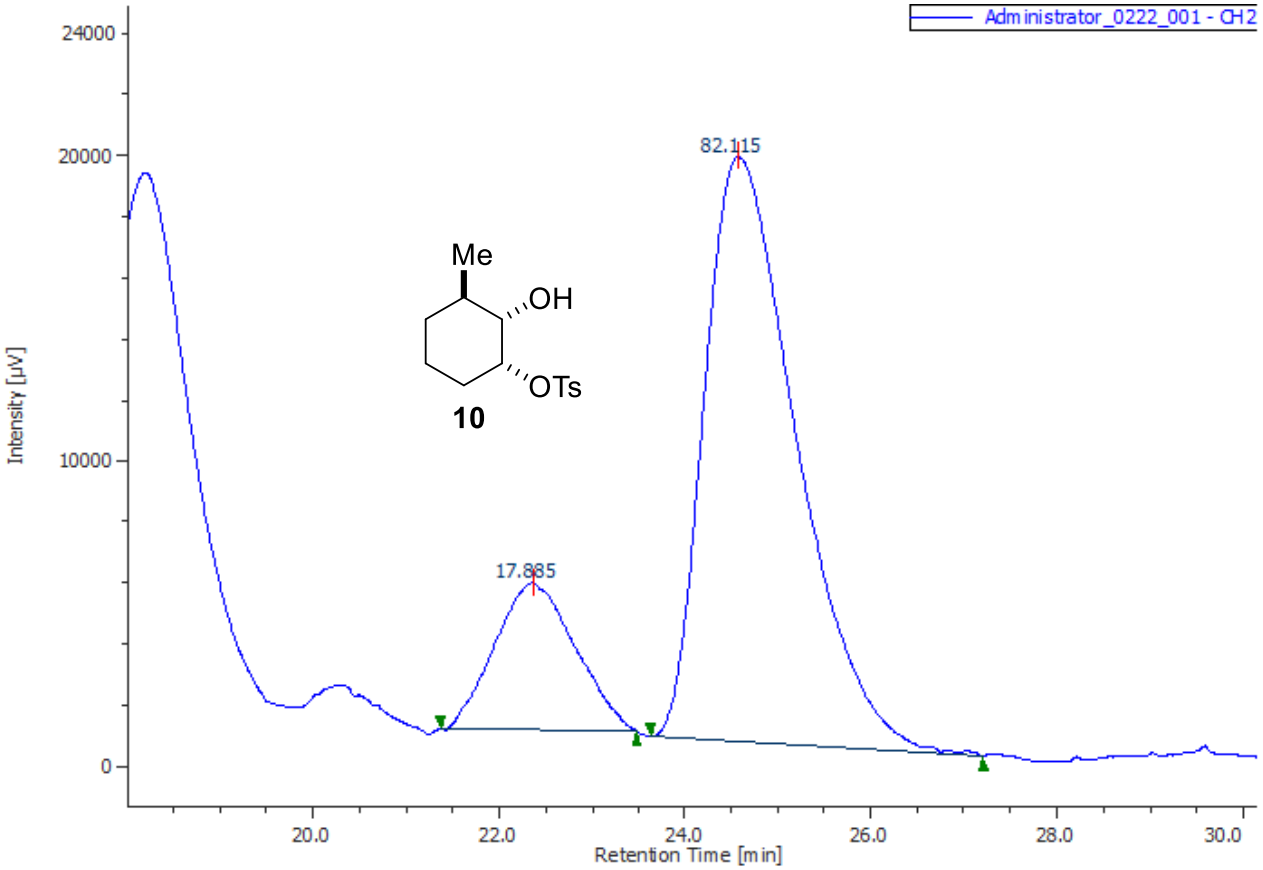

Administrator_1102_001 - CH2
49.531
rac
50.469
100000
50000
0
Intensity [µV]
9.0
9.5
10.0
10.5
11.0
11.5
12.0
Retention Time [min]

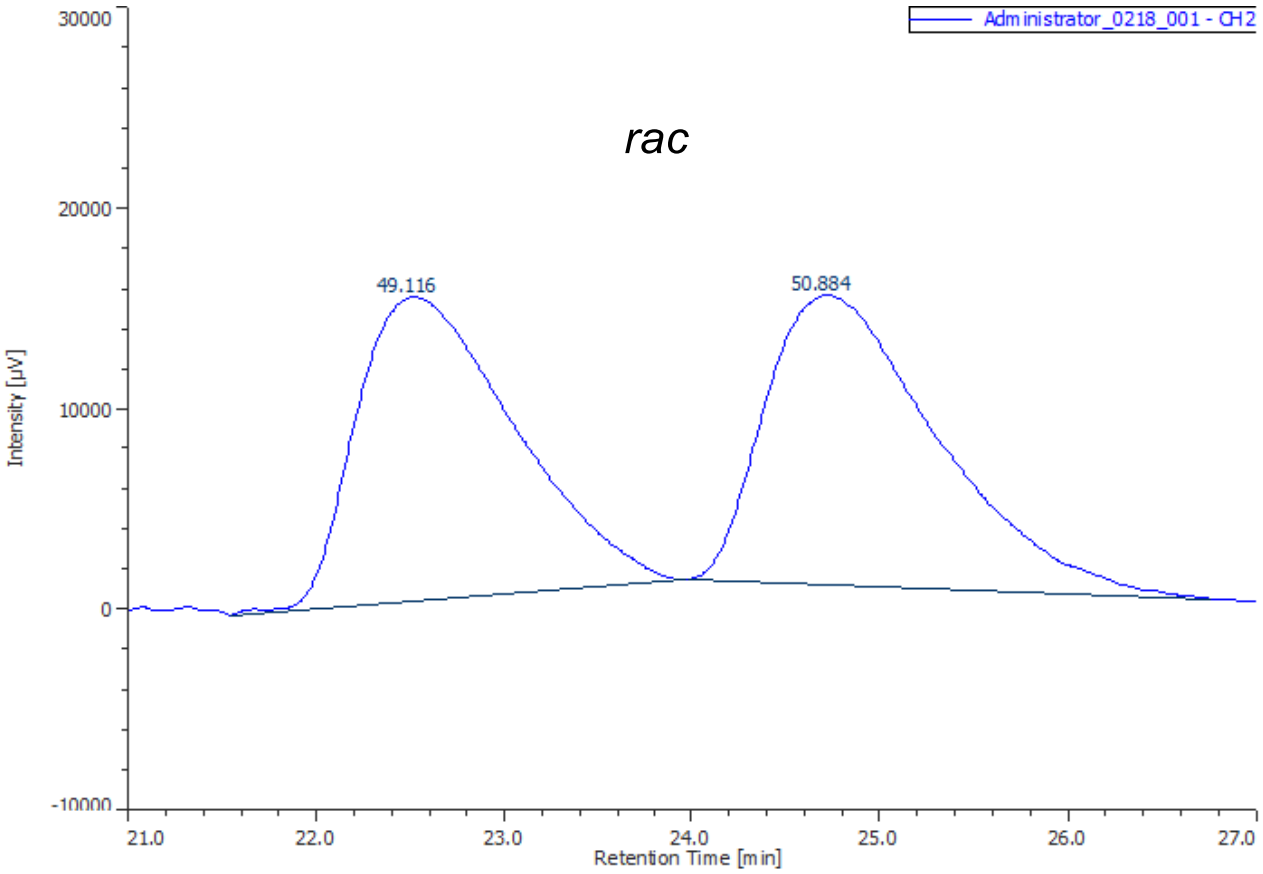

Administrator_1126_001 - CH2
100000
50000
0
Intensity [µV]
88.059
11.941
HO
OTs
HO
OH
7
36.0
38.0
40.0
42.0
44.0
46.0
48.0
Retention Time [min]


Administrator_1126_001 - CH2
25000
20000
0
-20000
Intensity [µV]
rac
50.468
49.532
36.0
38.0
40.0
42.0
44.0
46.0
48.0
Retention Time [min]


Administrator_0222_001 - CH2
Me
OTs
OH
9
67.345
32.655
60000
40000
20000
0
Intensity [µV]
10.0
12.0
14.0
16.0
18.0
20.0
22.0
24.0
Retention Time [min]


Administrator_0218_001 - CH2
rac
50.632
49.368
30000
20000
10000
0
-10000
Intensity [µV]
13.0
14.0
15.0
16.0
17.0
18.0
19.0
20.0
21.0
22.0
Retention Time [min]


Administrator_0222_001 - CH2
24000
20000
10000
0
Intensity [µV]
82.115
17.885
Me
OH
OTs
10
20.0
22.0
24.0
26.0
28.0
30.0
Retention Time [min]


Administrator_0218_001 - CH2
rac
30000
20000
10000
0
-10000
Intensity [µV]
49.116
50.884
21.0
22.0
23.0
24.0
25.0
26.0
27.0
Retention Time [min]