Supplementary Information

Asymmetric hydroarylation of vinyl ethers catalyzed by a hydroxoiridium complex: azoles as effective directing groups

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1. General

All anaerobic and moisture-sensitive manipulations were carried out with standard Schlenk techniques under predried nitrogen. NMR spectra were recorded on a JEOL JNM ECA-600 spectrometer (600 MHz for ^{1}H, 150 MHz for ^{13}C). Chemical shifts are reported in δ (ppm) referenced to the residual peaks of $CDCl_3$ (δ 7.26), CD_3OD (δ 3.30), and $(CD_3)_2SO$ (δ 2.50) for ^{1}H NMR, and $CDCl_3$ (δ 77.00), CD_3OD (δ 49.00), and $(CD_3)_2SO$ (δ 39.50) for ^{13}C NMR. The following abbreviations are used; s, singlet: d, doublet: t, triplet: q, quartet: m, multiplet: br, broad. Infrared (IR) spectra were recorded on a Thermo Fisher Scientific Nicolet iS5 spectrometer. Melting points were determined on MPA100 (OptiMelt) Automated Melting Point System. High-resolution mass spectra (TOF-MS) were obtained with a Bruker micrOTOF spectrometer. Flash column chromatography was performed with Silica Gel 60 N (Wako). Preparative thin-layer chromatography was performed with Silica Gel 60 PF_{254} (Merck). Alumina (activated 200) for column chromatography was purchased from Nacalai Tesque.

2. Materials

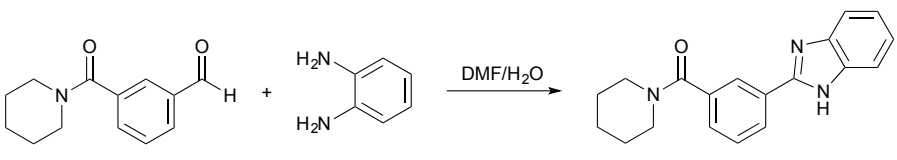
Dehydrated 1,4-dioxane and THF were purchased and used after deoxygenated by bubbling N_2. Other solvents and chemicals were purchased from commercial suppliers and used as received. $[Ir(OH)(cod)]_2$ was prepared according to the reported procedure.[1]

3. Preparation of azoles 1 and vinyl ethers 2

Compounds **1a** (CAS: 6528-83-2),[2] **1b** (CAS: 22868-35-5),[2] **1c** (CAS: 77738-96-6),[2] **1d** (CAS: 400073-80-5),[2] **1f** (CAS: 36677-36-8),[2] **1g** (CAS: 2963-64-6),[2] **1h** (CAS: 2562-81-4),[2] **1i** (CAS: 3878-18-0),[2] **1j** (CAS: 953071-79-9),[2] **1k** (CAS: 18818-49-0),[2] **1l** (CAS: 1224442-29-8),[2] **1n** (CAS: 21202-37-9),[3] **1o** (CAS: 23746-77-2),[4] **1r** (CAS: 36779-16-5),[5] **1s** (CAS: 1268691-73-1),[5] **1t** (CAS: 773139-10-9),[5] and **1v** (CAS: 638141-28-3)[6] were prepared according to the reported procedures.

Vinyl ethers **2a**–**2c**, **2g**, and **2i** were purchased from commercial suppliers and used as received. Vinyl ethers **2d** (CAS: 935-04-6), **2e** (CAS: 108388-36-9), **2f** (CAS: 26437-93-4), and **2h** (CAS: 17957-93-6) were prepared according to the reported procedure.[7]

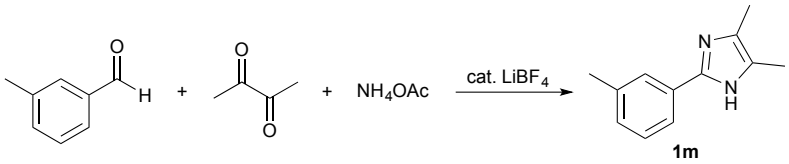
Compounds **1e**, **1m**, **1p**, **1q**, **1u**, and **1w** were prepared as shown below.



1e

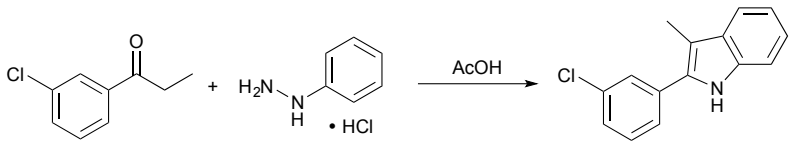
Compound 1e. To a solution of 1,2-phenylenediamine (703 mg, 6.5 mmol) in

DMF/H_2O (58 mL/7 mL) was added 3-(piperidine-1-carbonyl)benzaldehyde (1.41 g, 6.5 mmol), and the mixture was stirred at 80 ºC overnight in an open flask. EtOAc was added to the mixture and it was washed with H_2O. The organic layer was dried over Na_2SO_4, filtered, and concentrated on a rotary evaporator. The residue was subjected to column chromatography on silica gel with hexane/EtOAc/triethylamine (6:12:1) to give a yellow solid. The solid was dissolved in EtOAc and the solution was passed through a short column of alumina with EtOAc as an eluent. After the solvent was removed on a rotary evaporator, the residue was washed with hexane and dried under vacuum to give **1e** as a colorless solid (942 mg, 3.1 mmol, 47% yield). ^{1}H NMR ($CDCl_3$) δ 1.36–1.51 (br, 1H), 1.57–1.73 (br, 4H), 1.97–2.31 (br, 1H), 3.18–3.33 (br, 2H), 3.68–3.82 (br, 2H), 7.17–7.25 (m, 4H), 7.31–7.53 (br, 1H), 7.58–7.83 (br, 1H), 8.00 (s, 1H), 8.04 (d, J = 7.2 Hz, 1H), 12.42 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 24.4, 25.6, 26.4, 43.4, 48.8, 111.2 (br), 119.2 (br), 122.3 (br), 123.0 (br), 124.7, 127.2, 128.1, 129.0, 130.7, 135.0 (br), 136.2, 143.9 (br), 151.1, 170.3. HRMS (APCI) calcd for $C_{19}H_{20}N_3O$ $(M+H)^+$ 306.1601, found 306.1613. m.p. = 100–103 °C. IR (neat) 2934, 2854, 1600, 1435, 1276, 734, 711 cm^{-1}.



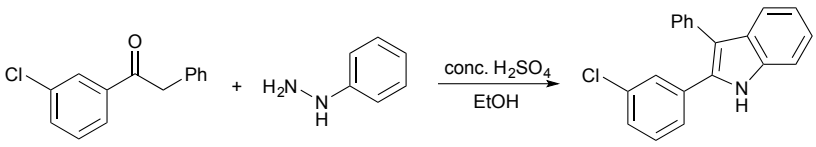
1m

Compound 1m.[8] A mixture of 3-methylbenzaldehyde (601 mg, 5.0 mmol), diacetyl (430 mg, 5.0 mmol), ammonium acetate (771 mg, 10 mmol), and $LiBF_4$ (47 mg, 10 mol%) was stirred at 120 ºC for 2 days. EtOAc was added to the mixture and the resulting mixture was washed with saturated $NaHCO_3$ solution and brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated on a rotary evaporator. The residue was subjected to column chromatography on silica gel with hexane/EtOAc/triethylamine (10:10:1) to give a yellow solid. The solid was dissolved in EtOAc and the solution was passed through a short column of alumina with EtOAc as an eluent. After the solvent was removed on a rotary evaporator, the residue was recrystallized from hot $CHCl_3$/hexane to give **1m** as a brown solid (150 mg, 0.81 mmol, 16% yield). ^{1}H NMR ($CDCl_3$) δ 2.17 (s, 6H), 2.25 (s, 3H), 7.05 (d, J = 7.8 Hz, 1H), 7.19 (t, J = 7.8 Hz, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.66 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 10.7, 21.2, 121.7, 125.5, 128.0, 128.6, 130.4, 138.3, 144.2. HRMS (APCI) calcd for $C_{12}H_{15}N_2$ $(M+H)^+$ 187.1230, found 187.1227. m.p. = 182–185 °C. IR (neat) 2917, 2623, 1604, 1425, 849, 784, 718, 693 cm^{-1}.



1p

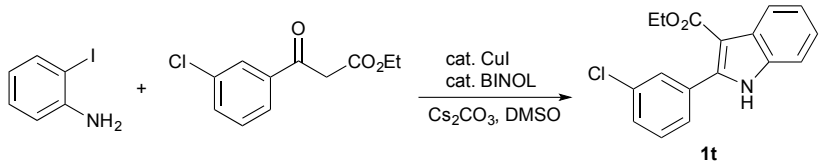
Compound 1p.[9] Phenylhydrazine hydrochloride (723 mg, 5.0 mmol) was added to a solution of 3'-chloropropiophenone (2.63 g, 15.6 mmol) in AcOH (25 mL), and the solution was stirred at 120 ºC for 2 h under nitrogen. EtOAc was added to the mixture and the resulting mixture was washed with brine and saturated $NaHCO_3$ solution. The organic layer was dried over Na_2SO_4, filtered, and concentrated on a rotary evaporator. The residue was subjected to column chromatography on silica gel with hexane/EtOAc (9:1) to give a yellow solid. The solid was dissolved in EtOAc and the solution was passed through a short column of alumina with EtOAc as an eluent. After the solvent was removed on a rotary evaporator, the residue was washed with hexane and dried under vacuum to give **1p** as a colorless solid (576 mg, 2.4 mmol, 48% yield). ^{1}H NMR ($CDCl_3$) δ 2.47 (s, 3H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.56 (s, 1H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.97 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 9.6, 109.7, 110.8, 119.1, 119.7, 122.8, 125.8, 127.2, 127.5, 129.9, 130.0, 132.5, 134.7, 135.1, 135.9. HRMS (APCI) calcd for $C_{15}H_{11}{}^{35}ClN$ $(M–H)^-$ 240.0586, found 240.0580. m.p. = 103–106 °C. IR (neat) 3386, 2919, 1600, 1455, 876, 792, 748, 736, 721, 696, 675 cm^{-1}.



1q

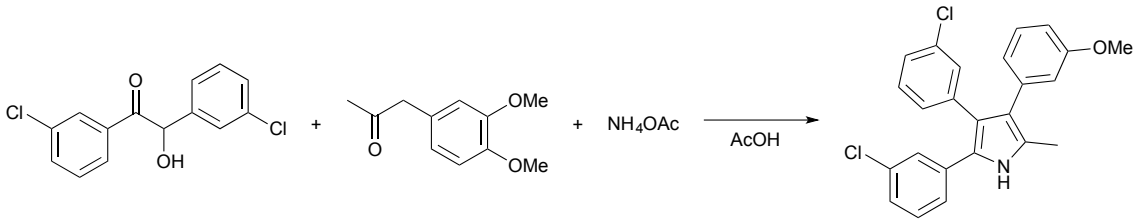
Compound 1q.[10] Concentrated sulfuric acid (2.0 g, 20 mmol) was added to a solution of phenylhydrazine (1.1 g, 10 mmol), 3'-chloro-2-phenylacetophenone (2.3 g, 10 mmol) in EtOH (40 mL), and the solution was refluxed overnight under nitrogen. The solution was cooled to room temperature, diluted with H_2O, and extracted with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated on a rotary evaporator. The residue was subjected to column chromatography on silica gel with hexane/EtOAc (20:1) to give a yellow solid. The solid was dissolved in EtOAc and the solution was passed through a short column of alumina with EtOAc as an eluent. After the solvent was removed on a rotary evaporator, the residue was washed with hexane and dried under vacuum to give **1q** as a colorless solid (642 mg, 2.1 mmol, 21% yield). ^{1}H NMR ($CDCl_3$) δ 7.18 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.25–7.31 (m, 3H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.39–7.48 (m, 6H), 7.69 (d, *J* = 7.5 Hz, 1H), 8.20 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 111.0, 116.0, 119.9, 120.6, 123.1, 126.47, 126.54, 127.6, 127.7, 128.6, 129.9, 130.1,

132.4, 134.48, 134.51, 134.53, 136.0. HRMS (APCI) calcd for $C_{20}H_{13}{}^{35}ClN$ $(M–H)^-$ 302.0742, found 302.0751. m.p. = 134–137 °C. IR (neat) 3395, 3060, 1599, 1437, 880, 845, 790, 775, 747, 740, 702, 682 cm^{-1}.



1t

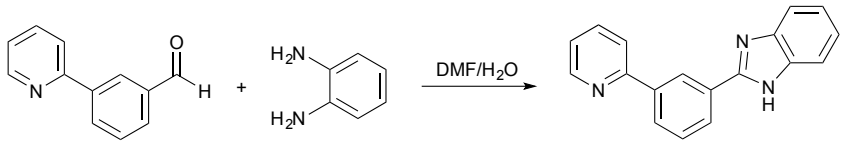
Compound 1t (CAS: 773139-10-9).[5] 2-Iodoaniline (2.0 g, 9.1 mmol), ethyl (3-chlorobenzoyl)acetate (2.3 g, 10 mmol), CuI (173 mg, 0.91 mmol), (*rac*)-binol (521 mg, 1.8 mmol), and Cs_2CO_3 (3.0 g, 9.1 mmol) were placed in a two-neck flask under nitrogen. DMSO (20 mL) was added to the mixture, and the solution was stirred at 50 ºC for 2 days. Saturated NH_4Cl solution was added to the mixture and the resulting mixture was extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated on a rotary evaporator. The residue was subjected to column chromatography on silica gel with hexane/EtOAc (8:1) to give a yellow solid. The solid was dissolved in EtOAc and the solution was passed through a short column of alumina with EtOAc as an eluent. After the solvent was removed on a rotary evaporator, the residue was washed with hexane and dried under vacuum to give **1t** as a colorless solid (978 mg, 3.3 mmol, 36% yield). ^1H NMR ($CDCl_3$) δ 1.33 (t, J = 7.1 Hz, 3H), 4.31 (q, J = 7.1 Hz, 2H), 7.27–7.31 (m, 2H), 7.34–7.42 (m, 3H), 7.54 (d, J = 7.5 Hz, 1H), 7.65 (s, 1H), 8.22–8.26 (m, 1H), 8.60 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 14.2, 59.8, 105.4, 111.0, 122.3, 123.6, 127.5, 127.9, 129.2, 129.3, 129.7, 133.8, 134.0, 135.2, 142.4, 165.1. HRMS (APCI) calcd for $C_{17}H_{13}{}^{35}ClNO_2$ $(M–H)^-$ 298.0640, found 298.0635.



1u

Compound 1u.[11] 2-Hydroxy-1,2-bis(3-chlorophenyl)ethanone (2.9 g, 10 mmol) and 3,4-dimethoxyphenylacetone (2.0 g, 10 mmol) were added to a solution of ammonium acetate (15 g, 0.20 mol) in AcOH (50 mL) under nitrogen, and the solution was refluxed overnight. EtOAc was added to the mixture and the resulting mixture was washed with saturated $NaHCO_3$ solution and brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated on a rotary evaporator. The residue was subjected to column chromatography on silica gel with hexane/EtOAc (5:1 to 3:2) to give a yellow solid. The solid was dissolved in EtOAc and the solution was passed through a

short column of alumina with EtOAc as an eluent. After the solvent was removed on a rotary evaporator, the residue was washed with hexane and dried under vacuum to give **1u** as a colorless solid (3.31 g, 7.6 mmol, 72% yield). ^{1}H NMR ($CDCl_3$) δ 2.39 (s, 3H), 3.62 (s, 3H), 3.88 (s, 3H), 6.51 (s, 1H), 6.71 (d, *J* = 7.8 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 7.01–7.05 (m, 1H), 7.09–7.18 (m, 5H), 7.27 (d, *J* = 7.8 Hz, 1H), 8.17 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 12.0, 55.5, 55.7, 111.9, 113.8, 120.9, 122.2, 122.6, 125.1, 125.7, 125.9, 126.1, 126.31, 126.35, 127.6, 129.0, 129.3, 129.8, 130.6, 133.8, 134.38, 134.45, 137.6, 147.1, 148.2. HRMS (APCI) calcd for $C_{25}H_{22}{}^{35}Cl_2NO_2$ $(M+H)^+$ 438.1022, found 438.1021. m.p. = 136–139 °C. IR (neat) 3409, 2959, 1594, 1509, 1242, 1218, 1138, 1022, 884, 798, 783, 764, 711, 690, 668 cm^{-1}.



1w

Compound 1w. Compound **1w** was prepared from 3-(pyridin-2-yl)benzaldehyde (916 mg, 5.0 mmol) and 1,2-phenylenediamine (541 mg, 5.0 mmol) according to the procedure for **1e**. The crude product was subjected to column chromatography on silica gel with hexane/EtOAc (1:2) to give a yellow solid. The solid was dissolved in EtOAc and the solution was passed through a short column of alumina with EtOAc as an eluent. After the solvent was removed on a rotary evaporator, the residue was washed with hexane and dried under vacuum to give **1w** as a colorless solid (1.03 g, 3.8 mmol, 76% yield). ^{1}H NMR ($(CD_3)_2SO$) δ 7.17–7.29 (m, 2H), 7.43 (t, *J* = 5.9 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 1H), 7.65–7.74 (m, 2H), 7.97 (t, *J* = 7.3 Hz, 1H), 8.09 (d, *J* = 8.2 Hz, 1H), 8.20 (d, *J* = 7.3 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 8.74 (d, *J* = 3.6 Hz, 1H), 8.92 (s, 1H), 13.05 (br s, 1H); ^{13}C NMR ($(CD_3)_2SO$) δ 111.4, 118.9, 120.4, 121.7, 122.6, 123.0, 124.5, 127.0, 127.8, 129.5, 130.7, 135.0, 137.4, 139.3, 143.8, 149.6, 151.0, 155.4. HRMS (APCI) calcd for $C_{18}H_{14}N_3$ $(M+H)^+$ 272.1182, found 272.1182. m.p. = 195–197 °C. IR (neat) 3046, 2636, 1581, 1567, 1532, 1443, 1424, 779, 765, 747, 741, 723, 688 cm^{-1}.

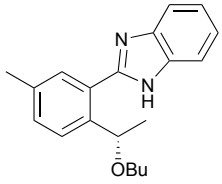
4. General procedure for Table 1

$[Ir(OH)(cod)]_2$ (1.6 mg, 0.0050 mmol of Ir, 5 mol% of Ir) and ligands (0.0060 mmol, 6 mol%) were placed in a Schlenk tube under nitrogen. Solvent (0.4 mL) was added to the tube and the mixture was stirred at room temperature for 15 min. 2-(*m*-Tolyl)benzimidazole (**1a**, 20.8 mg, 0.10 mmol) and butyl vinyl ether (**2a**, 20.0 mg, 0.20 mmol) were added to the mixture. The Schlenk tube was capped with a glass stopper and heated for 20 h with stirring. The solvent was removed on a rotary evaporator, and the residue was subjected to preparative TLC on silica gel with hexane/EtOAc/$CHCl_3$ (3:1:1) to give **3aa**.

5. General procedure for Table 2, Schemes 2 and 3

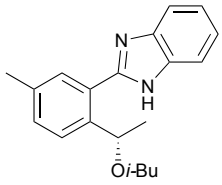
$[Ir(OH)(cod)]_2$ (3.2 mg, 0.010 mmol of Ir, 5 mol% of Ir) and (*R*,*R*)-QuinoxP* (4.0 mg, 0.012 mmol, 6 mol%) were placed in a Schlenk tube under nitrogen. THF (0.8 mL in the reaction at 50 ºC) or 1,4-dioxane (0.8 mL in the reaction at 80 ºC) was added to the tube and the mixture was stirred at room temperature for 15 min. Azoles (**1**, 0.20 mmol) and vinyl ethers (**2**, 0.30 mmol) were added to the mixture. The Schlenk tube was capped with a glass stopper and heated at 50 ºC or 80 ºC for 20 h with stirring. The solvent was removed on a rotary evaporator, and the residue was subjected to preparative TLC on silica gel to give **3**.

6. Characterization of the products



3aa

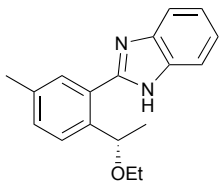
Compound 3aa (Table 2, Entry 1, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 29.0 min (major), t_2 = 38.0 min (minor)); $[\alpha]^{20}_D$ –66 (*c* 0.99, $CHCl_3$) for 93% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.93 (t, *J* = 7.5 Hz, 3H), 1.38–1.51 (m, 2H), 1.43 (d, *J* = 6.8 Hz, 3H), 1.63–1.72 (m, 2H), 2.42 (s, 3H), 3.48–3.57 (m, 2H), 4.75 (q, *J* = 6.8 Hz, 1H), 7.20–7.31 (m, 4H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 1H), 8.24 (s, 1H), 12.25 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.9, 19.5, 20.1, 20.9, 31.9, 68.1, 79.6, 111.0, 119.6, 122.2, 122.7, 129.4, 130.2, 132.7, 134.3, 135.8, 135.9, 138.7, 143.9, 152.1. HRMS (APCI) calcd for $C_{20}H_{25}N_2O$ $(M+H)^+$ 309.1961, found 309.1956. m.p. = 180–183 °C. IR (neat) 2978, 2931, 2873, 1449, 1423, 1261, 1097, 1074, 1057, 823, 752, 739 cm^{-1}.



3ab

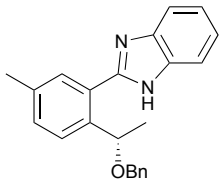
Compound 3ab (Table 2, Entry 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 20.7 min (major), t_2 = 24.0 min (minor)); $[\alpha]^{20}_D$ –58 (*c* 0.97, $CHCl_3$) for 87% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.99 (d, *J* = 6.8 Hz, 6H), 1.43 (d, *J* = 7.0 Hz, 3H), 1.95–2.13 (m, 1H), 2.43 (s, 3H), 3.26–3.30 (m, 1H), 3.31–3.35 (m, 1H), 4.74 (q, *J* = 7.0 Hz, 1H), 7.20–7.31 (m, 4H), 7.47 (d, *J* = 7.2 Hz, 1H), 7.85 (d, *J* = 7.2 Hz, 1H), 8.25 (s, 1H), 12.29 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 19.47, 19.51, 20.0, 20.9, 28.7, 75.2, 80.0, 111.0,

119.6, 122.1, 122.7, 129.4, 130.2, 130.3, 132.7, 134.3, 135.7, 138.8, 143.9, 152.0. HRMS (APCI) calcd for $C_{20}H_{25}N_2O$ $(M+H)^+$ 309.1961, found 309.1959. m.p. = 181–184 °C. IR (neat) 2955, 2872, 2677, 2361, 1449, 1423, 1364, 1264, 1100, 1074, 1060, 832, 752, 740 cm^{-1}.



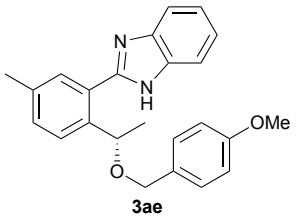
3ac

Compound 3ac (Table 2, Entry 3, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 24.5 min (major), t_2 = 28.3 min (minor)); $[\alpha]^{20}_D$ –48 (*c* 1.04, $CHCl_3$) for 84% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 1.31 (t, *J* = 7.2 Hz, 3H), 1.43 (d, *J* = 6.8 Hz, 3H), 2.41 (s, 3H), 3.53–3.64 (m, 2H), 4.77 (q, *J* = 6.8 Hz, 1H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.24–7.31 (m, 3H), 7.50 (d, *J* = 6.8 Hz, 1H), 7.85 (d, *J* = 6.8 Hz, 1H), 8.21 (s, 1H), 12.24 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 15.3, 20.3, 20.9, 63.6, 79.1, 111.0, 119.5, 122.1, 122.7, 129.4, 130.1, 130.2, 132.7, 134.3, 136.0, 138.7, 143.8, 152.1. HRMS (APCI) calcd for $C_{18}H_{21}N_2O$ $(M+H)^+$ 281.1648, found 281.1649. m.p. = 156–159 °C. IR (neat) 2968, 1423, 1363, 1109, 1086, 826, 768, 748, 739 cm^{-1}.



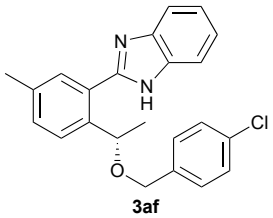
3ad

Compound 3ad (Table 2, Entry 4, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 34.9 min (major), t_2 = 39.4 min (minor)); $[\alpha]^{20}_D$ –73 (*c* 1.06, $CHCl_3$) for 93% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 1.46 (d, *J* = 6.8 Hz, 3H), 2.43 (s, 3H), 4.51 (d, *J* = 11.5 Hz, 1H), 4.64 (d, *J* = 11.5 Hz, 1H), 4.89 (q, *J* = 6.8 Hz, 1H), 7.19–7.41 (m, 10H), 7.83 (d, *J* = 7.5 Hz, 1H), 8.19 (d, *J* = 5.4 Hz, 1H), 11.90 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 20.5, 20.9, 70.1, 78.5, 78.6, 111.0, 119.5, 122.1, 122.7, 128.0, 128.1, 128.7, 129.6, 130.16, 130.20, 130.4, 132.8, 134.2, 135.8, 137.3, 138.8, 143.8, 151.9. HRMS (APCI) calcd for $C_{23}H_{23}N_2O$ $(M+H)^+$ 343.1805, found 343.1801. m.p. = 169–172 °C. IR (neat) 2891, 1454, 1418, 1270, 1089, 1072, 1051, 828, 749, 699 cm^{-1}.



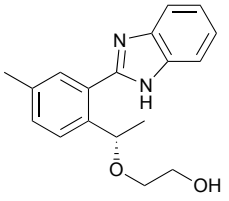
3ae

Compound 3ae (Table 2, Entry 5, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 41.8 min (major), t_2 = 47.1 min (minor)); $[\alpha]^{20}_D$ –82 (*c* 1.02, $CHCl_3$) for 92% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 1.45 (d, *J* = 6.8 Hz, 3H), 2.44 (s, 3H), 3.82 (s, 3H), 4.44 (d, *J* = 11.6 Hz, 1H), 4.58 (d, *J* = 11.6 Hz, 1H), 4.87 (q, *J* = 6.8 Hz, 1H), 6.91 (d, *J* = 8.1 Hz, 2H), 7.21–7.30 (m, 6H), 7.33 (d, *J* = 7.5 Hz, 1H), 7.84 (d, *J* = 7.5 Hz, 1H), 8.22 (s, 1H), 11.98 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 20.5, 20.9, 55.3, 69.8, 78.4, 111.1, 114.1, 119.5, 122.1, 122.7, 129.3, 129.6, 129.7, 130.27, 130.33, 132.9, 134.2, 135.8, 138.8, 143.8, 151.9, 159.5. HRMS (APCI) calcd for $C_{24}H_{25}N_2O_2$ $(M+H)^+$ 373.1911, found 373.1901. m.p. = 167–170 °C. IR (neat) 2892, 1612, 1511, 1423, 1301, 1108, 1088, 1034, 827, 808, 770, 754 cm^{-1}.



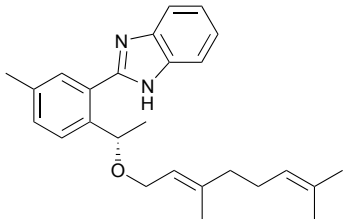
3af

Compound 3af (Table 2, Entry 6, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 35.6 min (major), t_2 = 40.5 min (minor)); $[\alpha]^{20}_D$ –60 (*c* 1.04, $CHCl_3$) for 96% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 1.47 (d, *J* = 7.0 Hz, 3H), 2.45 (s, 3H), 4.47 (d, *J* = 11.6 Hz, 1H), 4.59 (d, *J* = 11.6 Hz, 1H), 4.89 (q, *J* = 7.0 Hz, 1H), 7.23–7.30 (m, 6H), 7.32–7.40 (br, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.84 (br s, 1H), 8.19 (s, 1H), 11.66 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 20.7, 20.9, 69.3, 78.2, 111.0, 119.5, 122.2, 122.8, 128.8, 129.3, 129.5, 129.8, 130.4, 132.6, 133.9, 134.1, 135.9, 136.0, 138.8, 143.7, 151.8. HRMS (APCI) calcd for $C_{23}H_{22}{}^{35}ClN_2O$ $(M+H)^+$ 377.1415, found 377.1424. m.p. = 169–172 °C. IR (neat) 2974, 2360, 1490, 1422, 1106, 1087, 1075, 1014, 829, 808, 769, 753 cm^{-1}.



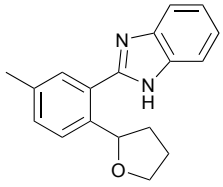
3ag

Compound 3ag (Table 2, Entry 7, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (1:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OJ–H, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 21.8 min (major), t_2 = 40.5 min (minor)); $[\alpha]^{20}_D$ –22 (*c* 0.97, MeOH) for 92% ee (*S*). ^{1}H NMR (CD_3OD) δ 1.37 (d, *J* = 6.1 Hz, 3H), 2.40 (s, 3H), 3.38–3.44 (m, 2H), 3.58–3.68 (m, 2H), 4.81–4.89 (m, 1H), 7.24–7.29 (m, 2H), 7.36 (d, *J* = 7.8 Hz, 1H), 7.49 (s, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.55–7.75 (br, 2H); ^{13}C NMR (CD_3OD) δ 21.0, 22.4, 49.9, 62.2, 70.8, 76.6, 115.7 (br), 123.7, 128.5, 130.9, 132.00, 132.04, 138.8, 140.6, 153.3. HRMS (APCI) calcd for $C_{18}H_{21}N_2O_2$ $(M+H)^+$ 297.1598, found 297.1607. m.p. = 78–81 °C. IR (neat) 3051, 2974, 2906, 1425, 1102, 1074, 1063, 942, 831, 769, 748, 739, 705 cm^{-1}.



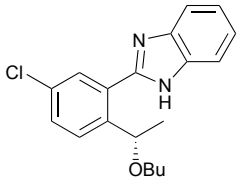
3ah

Compound 3ah (Table 2, Entry 8, viscous yellow oil). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 19.8 min (major), t_2 = 22.8 min (minor)); $[\alpha]^{20}_D$ –91 (*c* 1.06, $CHCl_3$) for 92% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 1.42 (d, *J* = 6.8 Hz, 3H), 1.56 (s, 3H), 1.60 (s, 3H), 1.67 (s, 3H), 2.02–2.13 (m, 4H), 2.41 (s, 3H), 4.00–4.06 (m, 1H), 4.06–4.13 (m, 1H), 4.77–4.83 (m, 1H), 5.09 (t, *J* = 6.1 Hz, 1H), 5.43 (t, *J* = 7.1 Hz, 1H), 7.19–7.30 (m, 4H), 7.46 (d, *J* = 6.8 Hz, 1H), 7.84 (d, *J* = 6.8 Hz, 1H), 8.22 (s, 1H), 12.26 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 16.4, 17.8, 20.4, 20.9, 25.6, 26.3, 39.6, 64.5, 78.5, 111.1, 119.5, 119.7, 122.1, 122.6, 123.7, 129.5, 130.20, 130.24, 131.8, 132.8, 134.3, 136.1, 138.7, 142.0, 143.8, 152.1. HRMS (APCI) calcd for $C_{26}H_{33}N_2O$ $(M+H)^+$ 389.2587, found 389.2594. IR (neat) 2971, 2923, 1448, 1418, 1365, 1270, 1096, 1073, 1040, 827, 768, 742 cm^{-1}.



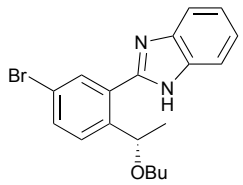
3ai

Compound 3ai (Table 2, Entry 9, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralpak IA, hexane/$CHCl_3$/ethanol = 18:6:1, flow 0.5 mL/min, 254 nm, t_1 = 13.2 min (major), t_2 = 15.6 min (minor)); $[\alpha]^{20}_D$ +2 (*c* 0.87, $CHCl_3$) for 3% ee. ^{1}H NMR ($CDCl_3$) δ 2.07–2.22 (m, 3H), 2.23–2.31 (m, 1H), 2.41 (s, 3H), 4.03–4.08 (m, 1H), 4.12–4.18 (m, 1H), 5.01 (dd, *J* = 8.1, 6.1 Hz, 1H), 7.25–7.31 (m, 3H), 7.43 (d, *J* = 8.2 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.85 (d, *J* = 7.2 Hz, 1H), 8.00 (s, 1H), 11.52 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 20.9, 26.2, 29.4, 68.0, 78.6, 111.0, 119.6, 122.1, 122.7, 126.7, 130.4, 131.2, 132.0, 133.6, 134.3, 138.7, 143.9, 152.0. HRMS (APCI) calcd for $C_{18}H_{19}N_2O$ $(M+H)^+$ 279.1492, found 279.1495. m.p. = 211–214 °C. IR (neat) 2871, 2671, 1454, 1428, 1275, 1061, 828, 746 cm^{-1}.



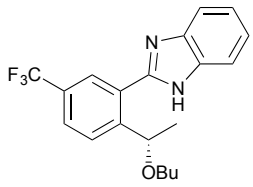
3ba

Compound 3ba (Scheme 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (5:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 52.1 min (major), t_2 = 65.3 min (minor)); $[\alpha]^{20}_D$ –64 (*c* 1.07, $CHCl_3$) for 98% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.93 (t, *J* = 7.5 Hz, 3H), 1.38–1.50 (m, 2H), 1.43 (d, *J* = 6.8 Hz, 3H), 1.63–1.71 (m, 2H), 3.48–3.57 (m, 2H), 4.78 (q, *J* = 6.8 Hz, 1H), 7.27–7.34 (m, 3H), 7.38 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 1H), 8.40 (d, *J* = 2.0 Hz, 1H), 12.15 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.5, 20.1, 31.9, 68.4, 79.1, 111.2, 119.8, 122.5, 123.2, 129.4, 131.3, 131.4, 131.9, 134.3, 134.7, 137.4, 143.8, 150.4. HRMS (APCI) calcd for $C_{19}H_{22}{}^{35}ClN_2O$ $(M+H)^+$ 329.1415, found 329.1425. m.p. = 126–129 °C. IR (neat) 2962, 2928, 2871, 1452, 1424, 1371, 1096, 1072, 970, 884, 828, 767, 756, 745 cm^{-1}.



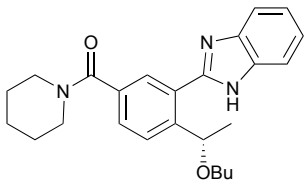
3ca

Compound 3ca (Scheme 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (8:1:2) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 29.3 min (major), t_2 = 40.0 min (minor)); $[\alpha]^{20}_D$ –46 (*c* 0.96, $CHCl_3$) for 95% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.94 (t, *J* = 7.5 Hz, 3H), 1.38–1.49 (m, 2H), 1.43 (d, *J* = 6.8 Hz, 3H), 1.64–1.70 (m, 2H), 3.48–3.57 (m, 2H), 4.76 (q, *J* = 6.8 Hz, 1H), 7.24 (d, *J* = 8.2 Hz, 1H), 7.28–7.33 (m, 2H), 7.46–7.52 (m, 1H), 7.53 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.84–7.88 (m, 1H), 8.56 (s, 1H), 12.11 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.4, 20.2, 31.8, 68.4, 78.8, 111.2, 119.7, 122.5, 122.6, 123.2, 131.3, 131.5, 132.4, 134.3, 134.6, 138.2, 143.7, 150.2. HRMS (APCI) calcd for $C_{19}H_{22}{}^{79}BrN_2O$ $(M+H)^+$ 373.0910, found 373.0918. m.p. = 93–96 °C. IR (neat) 2930, 2870, 2360, 1451, 1429, 1369, 1152, 1098, 1069, 967, 825, 766, 757, 743 cm^{-1}.



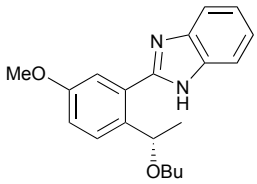
3da

Compound 3da (Scheme 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (8:1:2) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H column, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 18.9 min (major), t_2 = 21.4 min (minor)); $[\alpha]^{20}_D$ –61 (*c* 1.01, $CHCl_3$) for 94% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.94 (t, *J* = 7.5 Hz, 3H), 1.39–1.50 (m, 2H), 1.46 (d, *J* = 6.8 Hz, 3H), 1.64–1.71 (m, 2H), 3.54 (t, *J* = 6.8 Hz, 2H), 4.87 (q, *J* = 6.8 Hz, 1H), 7.29–7.34 (m, 2H), 7.48–7.54 (m, 2H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.85–7.90 (m, 1H), 8.66 (s, 1H), 12.05 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.4, 20.3, 31.8, 68.7, 78.7, 111.2, 119.8, 122.6, 123.3, 123.6 (q, *J* = 272 Hz), 126.0, 128.8, 130.1, 130.5, 130.9 (q, *J* = 33 Hz), 134.3, 143.3, 143.7, 150.2. HRMS (APCI) calcd for $C_{20}H_{22}F_3N_2O$ $(M+H)^+$ 363.1679, found 363.1673. m.p. = 115–118 °C. IR (neat) 2934, 2868, 2359, 1399, 1329, 1309, 1170, 1133, 1121, 1082, 979, 845, 767, 750, 730 cm^{-1}.



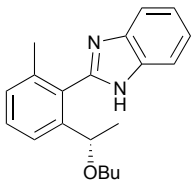
3ea

Compound 3ea (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc/$CHCl_3$ (1:3:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 34.6 min (major), t_2 = 43.9 min (minor)); $[\alpha]^{20}_D$ –55 (*c* 1.22, $CHCl_3$) for 93% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.94 (t, *J* = 7.2 Hz, 3H), 1.38–1.48 (m, 2H), 1.45 (d, *J* = 6.8 Hz, 3H), 1.51–1.61 (m, 2H), 1.63–1.73 (m, 6H), 3.36–3.46 (m, 2H), 3.47–3.56 (m, 2H), 3.64–3.73 (m, 1H), 3.74–3.83 (m, 1H), 4.83 (q, *J* = 6.8 Hz, 1H), 7.27–7.32 (m, 2H), 7.42–7.52 (m, 3H), 7.83–7.87 (m, 1H), 8.34 (s, 1H), 11.94 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.4, 20.8, 24.5, 25.5, 26.5, 31.9, 43.1, 48.8, 68.5, 78.2, 111.1, 119.7, 122.2, 122.9, 127.9, 129.6, 129.78, 129.84, 134.3, 136.6, 141.3, 143.8, 150.9, 169.2. HRMS (APCI) calcd for $C_{25}H_{32}N_3O_2$ $(M+H)^+$ 406.2489, found 406.2479. IR (neat) 3052, 2932, 2860, 1602, 1443, 1367, 1286, 1273, 1098, 1004, 852, 767, 739, 703 cm^{-1}.



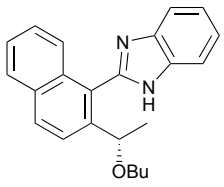
3fa

Compound 3fa (Scheme 2, colorless solid). A solution of hexane/EtOAc (2:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 25.0 min (major), t_2 = 27.9 min (minor)); $[\alpha]^{20}_D$ –55 (*c* 1.21, $CHCl_3$) for 78% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.94 (t, *J* = 7.3 Hz, 3H), 1.38–1.50 (m, 2H), 1.42 (d, *J* = 6.8 Hz, 3H), 1.63–1.72 (m, 2H), 3.47–3.52 (m, 1H), 3.52–3.58 (m, 1H), 3.91 (s, 3H), 4.74 (q, *J* = 6.8 Hz, 1H), 6.95 (dd, *J* = 8.1, 2.7 Hz, 1H), 7.24–7.32 (m, 3H), 7.49 (br s, 1H), 7.86 (br s, 1H), 7.94 (s, 1H), 12.28 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.9, 19.5, 20.1, 31.9, 55.6, 67.9, 79.1, 111.1, 116.0, 116.2, 119.6, 122.2, 122.8, 131.0, 131.1, 131.5, 134.3, 143.8, 151.9, 159.6. HRMS (APCI) calcd for $C_{20}H_{25}N_2O_2$ $(M+H)^+$ 325.1911, found 325.1905. m.p. = 127–130 °C. IR (neat) 2929, 2872, 1443, 1425, 1239, 1098, 1065, 1035, 984, 860, 830, 754, 738, 613 cm^{-1}.



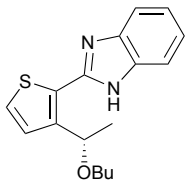
3ga

Compound 3ga (Scheme 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 52.3 min (major), t_2 = 62.2 min (minor)); $[\alpha]^{20}_D$ –4 (*c* 0.17, $CHCl_3$) for 83% ee (*S*). ^{1}H NMR (CD_3OD) δ 0.82 (t, *J* = 7.5 Hz, 3H), 1.21–1.30 (m, 2H), 1.32 (d, *J* = 6.6 Hz, 3H), 1.35–1.47 (m, 2H), 2.10 (s, 3H), 3.17 (dt, *J* = 9.5, 6.3 Hz, 1H), 3.25 (dt, *J* = 9.5, 6.9 Hz, 1H), 4.10 (q, *J* = 6.6 Hz, 1H), 7.24–7.31 (m, 3H), 7.42–7.48 (m, 2H), 7.54–7.66 (br, 2H); ^{13}C NMR (CD_3OD) δ 14.2, 19.8, 20.3, 24.3, 33.0, 69.5, 75.9, 112.5 (br), 119.0 (br), 123.8 (br), 124.1, 129.8, 131.2, 131.3, 139.0, 145.9, 152.3. HRMS (APCI) calcd for $C_{20}H_{25}N_2O$ $(M+H)^+$ 309.1961, found 309.1953. m.p. = 257–260 °C. IR (neat) 2972, 2930, 2862, 1446, 1421, 1365, 1263, 1100, 1056, 967, 790, 761, 749, 733 cm^{-1}.



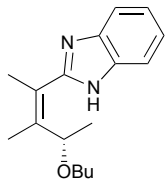
3ha

Compound 3ha (Scheme 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 4:1, flow 0.5 mL/min, 254 nm, t_1 = 8.0 min (major), t_2 = 11.4 min (minor)); $[\alpha]^{20}_D$ +14 (*c* 0.21, $CHCl_3$) for 78% ee (*S*). ^{1}H NMR (CD_3OD) δ 0.82 (t, *J* = 7.5 Hz, 3H), 1.23–1.35 (m, 2H), 1.37–1.49 (m, 2H), 1.44 (d, *J* = 6.2 Hz, 3H), 3.16–3.29 (m, 2H), 4.29 (q, *J* = 6.2 Hz, 1H), 7.25 (d, *J* = 8.2 Hz, 1H), 7.31–7.37 (m, 2H), 7.42 (t, *J* = 7.1 Hz, 1H), 7.50 (t, *J* = 7.1 Hz, 1H), 7.59–7.72 (br, 2H), 7.74 (d, *J* = 8.9 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 8.09 (d, *J* = 8.9 Hz, 1H); ^{13}C NMR (CD_3OD) δ 14.2, 20.3, 23.9, 33.0, 69.6, 76.0, 112.5 (br), 119.5 (br), 123.9 (br), 124.1, 126.3, 127.3, 127.9, 128.2, 129.1, 131.8, 134.0, 134.1, 135.4 (br), 143.6, 151.4. HRMS (APCI) calcd for $C_{23}H_{25}N_2O$ $(M+H)^+$ 345.1961, found 345.1951. m.p. = 238–241 °C. IR (neat) 2968, 2930, 2865, 2360, 1449, 1095, 823, 746, 732 cm^{-1}.



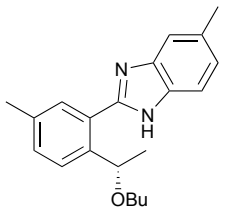
3ia

Compound 3ia (Scheme 2, colorless solid). A solution of hexane/EtOAc/AcOH (90:10:5) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 32.3 min (major), t_2 = 56.1 min (minor)); $[\alpha]^{20}_D$ –87 (*c* 1.19, $CHCl_3$) for 56% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.91 (t, *J* = 7.3 Hz, 3H), 1.36–1.47 (m, 2H), 1.56 (d, *J* = 6.8 Hz, 3H), 1.59–1.68 (m, 2H), 3.49 (dt, *J* = 9.5, 6.6 Hz, 1H), 3.55 (dt, *J* = 9.5, 6.6 Hz, 1H), 4.89 (q, *J* = 6.8 Hz, 1H), 6.96 (d, *J* = 5.1 Hz, 1H), 7.23–7.28 (m, 2H), 7.37 (d, *J* = 5.1 Hz, 1H), 7.43–7.47 (m, 1H), 7.78–7.83 (m, 1H), 11.95 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.4, 21.3, 31.8, 68.9, 75.0, 110.8, 119.4, 122.4, 122.9, 127.3, 129.8, 130.2, 134.3, 141.3, 143.9, 147.1. HRMS (APCI) calcd for $C_{17}H_{21}N_2OS$ $(M+H)^+$ 301.1369, found 301.1371. m.p. = 108–111 °C. IR (neat) 2954, 2928, 2865, 1453, 1406, 1278, 1114, 1097, 766, 745, 665 cm^{-1}.



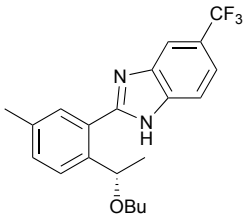
3ja

Compound 3ja (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc/$CHCl_3$ (3:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 24.0 min (major), t_2 = 25.1 min (minor)); $[\alpha]^{20}_D$ +2 (*c* 1.49, $CHCl_3$) for 15% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.88 (t, *J* = 7.5 Hz, 3H), 1.27 (d, *J* = 6.7 Hz, 3H), 1.28–1.40 (m, 2H), 1.45–1.56 (m, 2H), 1.88 (s, 3H), 2.19 (s, 3H), 3.23–3.29 (m, 1H), 3.31–3.36 (m, 1H), 4.34 (q, *J* = 6.7 Hz, 1H), 7.20–7.25 (m, 2H), 7.32–7.49 (br, 1H), 7.66–7.82 (br, 1H), 10.99 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.9, 14.9, 18.9, 19.5, 32.1, 67.7, 75.9, 110.6, 119.3, 122.0, 122.7, 124.0, 133.47, 133.54, 140.8, 143.3, 153.4. The double bond geometry of **3ja** was assigned by NOE experiments. HRMS (APCI) calcd for $C_{17}H_{25}N_2O$ $(M+H)^+$ 273.1961, found 273.1954. IR (neat) 3051, 2958, 2930, 2871, 1450, 1409, 1363, 1270, 1094, 768, 749 cm^{-1}.



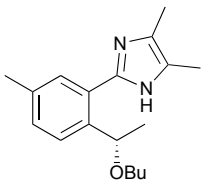
3ka

Compound 3ka (Scheme 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (5:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 26.9 min (major), t_2 = 36.7 min (minor)); $[\alpha]^{20}_D$ –75 (*c* 1.00, $CHCl_3$) for 94% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.95 (t, *J* = 7.1 Hz, 3H), 1.37–1.51 (m, 2H), 1.43 (d, *J* = 7.2 Hz, 3H), 1.63–1.72 (m, 2H), 2.42 (s, 3H), 2.52 (s, 3H), 3.46–3.59 (m, 2H), 4.77 (q, *J* = 7.2 Hz, 1H), 7.12 (d, *J* = 7.5 Hz, 1H), 7.20–7.85 (br, 2H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 5.4 Hz, 1H), 8.21 (s, 1H), 12.22 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.5, 20.2, 20.9, 21.7, 31.9, 68.1, 79.4, 111.1 (br), 119.1 (br), 124.0, 129.4, 130.0, 130.1, 132.3 (br), 132.6, 136.0, 138.6, 151.7. HRMS (APCI) calcd for $C_{21}H_{27}N_2O$ $(M+H)^+$ 323.2118, found 323.2119. m.p. = 176–179 °C. IR (neat) 2970, 2929, 2865, 1449, 1400, 1278, 1098, 1073, 1056, 828, 805, 602 cm^{-1}.



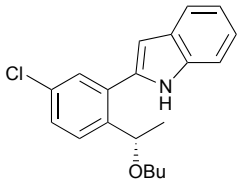
3la

Compound 3la (Scheme 2, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (5:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 18.6 min (major), t_2 = 24.7 min (minor)); $[\alpha]^{20}_D$ –50 (*c* 1.06, $CHCl_3$) for 83% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.94 (t, *J* = 7.2 Hz, 3H), 1.38–1.50 (m, 2H), 1.42 (d, *J* = 6.6 Hz, 3H), 1.65–1.72 (m, 2H), 2.44 (s, 3H), 3.52 (dt, *J* = 9.6, 6.8 Hz, 1H), 3.57 (dt, *J* = 9.6, 6.8 Hz, 1H), 4.75 (q, *J* = 6.6 Hz, 1H), 7.24–7.28 (m, 2H), 7.50–7.79 (m, 2H), 7.88–8.15 (m, 1H), 8.23–8.30 (m, 1H), 12.57 and 12.66 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.4, 20.3, 20.9, 31.8, 68.3, 79.6, 108.7 (br), 111.4 (br), 117.1 (br), 119.4 (br), 124.7 (q, *J* = 32 Hz), 124.9 (q, *J* = 272 Hz), 128.5, 130.3, 130.9, 132.8, 136.3, 138.9, 154.3 (br). HRMS (APCI) calcd for $C_{21}H_{24}F_3N_2O$ $(M+H)^+$ 377.1835, found 377.1847. m.p. = 160–163 °C. IR (neat) 2974, 2931, 2861, 1328, 1160, 1113, 1075, 1052, 935, 892, 836, 816, 666 cm^{-1}.



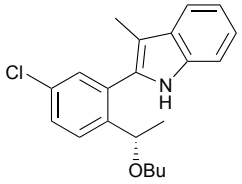
3ma

Compound 3ma (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc (1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 14.6 min (major), t_2 = 17.7 min (minor)); $[\alpha]^{20}_D$ –49 (*c* 1.24, $CHCl_3$) for 72% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.88 (t, *J* = 7.5 Hz, 3H), 1.32–1.39 (m, 2H), 1.41 (d, *J* = 6.8 Hz, 3H), 1.54–1.61 (m, 2H), 2.22 (s, 6H), 2.35 (s, 3H), 3.35–3.47 (m, 2H), 4.65 (q, *J* = 6.8 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 1H), 7.98 (s, 1H), 11.52 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 9.6, 12.3, 13.8, 19.4, 19.7, 20.8, 31.9, 67.5, 79.5, 121.8 (br), 128.1, 129.9, 130.0, 130.8, 133.8, 133.9 (br), 138.2, 143.6. HRMS (APCI) calcd for $C_{18}H_{27}N_2O$ $(M+H)^+$ 287.2118, found 287.2116. IR (neat) 2954, 2926, 2866, 1607, 1447, 1405, 1367, 1097, 825 cm^{-1}.



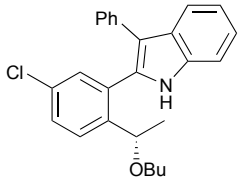
3oa

Compound 3oa (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc (9:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 26.8 min (major), t_2 = 30.0 min (minor)); $[\alpha]^{20}_D$ –52 (*c* 1.05, $CHCl_3$) for 76% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.94 (t, *J* = 7.5 Hz, 3H), 1.39 (d, *J* = 6.8 Hz, 3H), 1.40–1.48 (m, 2H), 1.60–1.68 (m, 2H), 3.38–3.46 (m, 2H), 4.70 (q, *J* = 6.8 Hz, 1H), 6.70 (s, 1H), 7.15 (t, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 8.1 Hz, 1H), 7.31 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.675 (d, *J* = 8.3 Hz, 1H), 7.681 (d, *J* = 2.2 Hz, 1H), 10.11 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.9, 19.5, 20.5, 32.0, 68.0, 77.2, 102.8, 111.1, 120.0, 120.6, 122.3, 127.6, 128.5, 130.4, 130.5, 133.8, 134.2, 136.2, 136.6, 137.8. HRMS (APCI) calcd for $C_{20}H_{23}{}^{35}ClNO$ $(M+H)^+$ 328.1463, found 328.1460. IR (neat) 3399, 3275, 3058, 2958, 2930, 2871, 1473, 1454, 1343, 1300, 1085, 1030, 1009, 946, 823, 794, 745, 681 cm^{-1}.



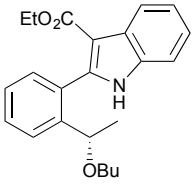
3pa

Compound 3pa (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc/$CHCl_3$ (18:2:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralpak AD–H × 2, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 28.1 min (major), t_2 = 30.0 min (minor)); $[\alpha]^{20}_D$ –18 (*c* 1.02, $CHCl_3$) for 65% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.91 (t, *J* = 7.5 Hz, 3H), 1.29 (d, *J* = 6.7 Hz, 3H), 1.34–1.44 (m, 2H), 1.53–1.60 (m, 2H), 2.29 (s, 3H), 3.31 (t, *J* = 6.5 Hz, 2H), 4.44 (q, *J* = 6.7 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 8.2 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.38–7.43 (m, 2H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 1H), 8.63 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 9.3, 13.9, 19.5, 21.7, 32.1, 68.1, 75.0, 109.9, 110.7, 119.0, 119.5, 122.3, 128.6, 128.7, 129.0, 131.1, 131.9, 132.9, 133.7, 135.7, 141.2. HRMS (APCI) calcd for $C_{21}H_{23}{}^{35}ClNO$ $(M–H)^-$ 340.1474, found 340.1470. IR (neat) 3401, 3312, 3057, 2958, 2929, 2869, 1457, 1336, 1094, 1016, 828, 741 cm^{-1}.



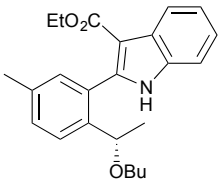
3qa

Compound 3qa (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc/$CHCl_3$ (8:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 20.8 min (minor), t_2 = 23.3 min (major)); $[\alpha]^{20}_D$ –4 (*c* 1.25, $CHCl_3$) for 68% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.86 (t, *J* = 7.1 Hz, 3H), 1.03 (d, *J* = 6.6 Hz, 3H), 1.20–1.32 (m, 2H), 1.34–1.46 (m, 2H), 2.71–2.78 (m, 1H), 2.89–2.96 (m, 1H), 4.37 (q, *J* = 6.6 Hz, 1H), 7.21–7.26 (m, 2H), 7.28–7.48 (m, 9H), 7.87 (d, *J* = 7.5 Hz, 1H), 8.69 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 19.3, 22.2, 31.9, 67.9, 74.6, 111.0, 116.2, 119.7, 120.5, 122.7, 126.2, 127.2, 128.4, 128.6, 129.0, 129.5, 131.2, 131.6, 132.8, 133.3, 134.7, 135.8, 141.6. HRMS (APCI) calcd for $C_{26}H_{25}{}^{35}ClNO$ $(M–H)^-$ 402.1630, found 402.1643. IR (neat) 3396, 3275, 3058, 2957, 2930, 2870, 1456, 1094, 1066, 829, 773, 741, 714, 700 cm^{-1}.



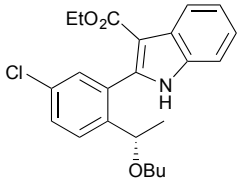
3ra

Compound 3ra (Scheme 2, colorless solid). A solution of hexane/EtOAc (10:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H × 2, hexane/2-propanol = 9:1, flow 0.5 mL/min, 254 nm, t_1 = 26.5 min (minor), t_2 = 28.3 min (major)); $[\alpha]^{20}_{D}$ –4 (*c* 1.23, $CHCl_3$) for 87% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.87 (t, *J* = 7.5 Hz, 3H), 1.15 (t, *J* = 7.1 Hz, 3H), 1.28–1.38 (m, 2H), 1.31 (d, *J* = 6.4 Hz, 3H), 1.46–1.56 (m, 2H), 3.24–3.32 (m, 2H), 4.11–4.22 (m, 2H), 4.35 (q, *J* = 6.4 Hz, 1H), 7.27–7.38 (m, 4H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 8.26 (d, *J* = 7.5 Hz, 1H), 9.08 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.9, 14.1, 19.4, 22.0, 32.1, 59.4, 68.2, 75.2, 106.2, 111.0, 121.9, 122.0, 123.1, 126.3, 126.8, 127.0, 129.5, 131.1, 131.4, 135.0, 142.5, 143.5, 165.0. HRMS (APCI) calcd for $C_{23}H_{26}NO_3$ $(M–H)^-$ 364.1918, found 364.1905. m.p. = 97–100 °C. IR (neat) 3255, 2958, 2931, 2870, 2360, 1676, 1663, 1456, 1431, 1281, 1193, 1135, 1102, 1079, 1051, 1034, 792, 767, 749 cm^{-1}.



3sa

Compound 3sa (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc (10:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralpak AD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 22.8 min (major), t_2 = 24.2 min (minor)); $[\alpha]^{20}_{D}$ –4 (*c* 1.08, $CHCl_3$) for 80% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.87 (t, *J* = 7.5 Hz, 3H), 1.17 (t, *J* = 7.2 Hz, 3H), 1.26–1.38 (m, 2H), 1.29 (d, *J* = 6.7 Hz, 3H), 1.46–1.54 (m, 2H), 2.36 (s, 3H), 3.22–3.31 (m, 2H), 4.11–4.23 (m, 2H), 4.32 (q, *J* = 6.7 Hz, 1H), 7.22 (s, 1H), 7.25–7.32 (m, 3H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 8.25 (d, *J* = 7.5 Hz, 1H), 9.13 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.9, 14.1, 19.4, 20.9, 22.0, 32.1, 59.3, 68.1, 75.0, 106.0, 111.0, 121.8, 121.9, 123.0, 126.3, 127.1, 130.2, 131.2, 131.5, 135.0, 136.4, 139.5, 143.7, 165.0. HRMS (APCI) calcd for $C_{24}H_{28}NO_3$ $(M–H)^-$ 378.2075, found 378.2069. IR (neat) 3272, 2958, 2930, 2871, 1700, 1665, 1456, 1438, 1220, 1188, 1114, 1089, 1048, 743 cm^{-1}.



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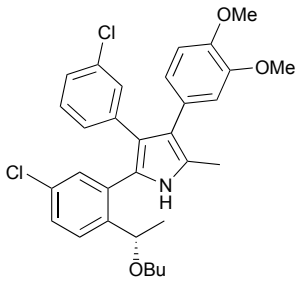
Compound 3ta (Scheme 2, colorless solid). A solution of hexane/EtOAc (9:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralpak AD–H × 2, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 19.5 min (major), t_2 = 21.2 min (minor)); $[\alpha]^{20}_D$ –6 (*c* 0.92, $CHCl_3$) for 89% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.87 (t, *J* = 7.5 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H), 1.28 (d, *J* = 6.4 Hz, 3H), 1.29–1.37 (m, 2H), 1.44–1.55 (m, 2H), 3.22–3.29 (m, 2H), 4.11–4.23 (m, 2H), 4.31 (q, *J* = 6.4 Hz, 1H), 7.28–7.33 (m, 2H), 7.35–7.40 (m, 2H), 7.45 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.52 (d, *J* = 8.7 Hz, 1H), 8.23–8.27 (m, 1H), 9.10 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 13.8, 14.1, 19.4, 22.0, 32.0, 59.6, 68.3, 74.6, 106.6, 111.1, 121.9, 122.2, 123.4, 126.9, 127.8, 129.5, 130.9, 132.4, 133.0, 135.1, 141.3, 141.4, 164.8. HRMS (APCI) calcd for $C_{23}H_{25}{}^{35}ClNO_3$ $(M–H)^-$ 398.1528, found 398.1521. m.p. = 93–96 °C. IR (neat) 3272, 2931, 2869, 2360, 1663, 1442, 1211, 1153, 1117, 1083, 1049, 1034, 791, 746 cm^{-1}.



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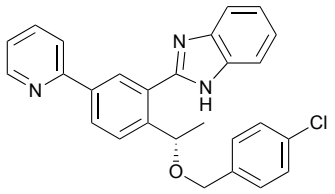
Compound 3ua (Scheme 2, viscous yellow oil). A solution of hexane/EtOAc/$CHCl_3$ (5:1:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 98:2, flow 0.5 mL/min, 254 nm, t_1 = 29.7 min (major), t_2 = 34.3 min (minor)); $[\alpha]^{20}_D$ –2 (*c* 0.77, $CHCl_3$) for 42% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.86 (t, *J* = 7.2 Hz, 3H), 1.18 (d, *J* = 6.6 Hz, 3H), 1.23–1.34 (m, 2H), 1.39–1.49 (m, 2H), 2.36 (s, 3H), 2.90–2.96 (m, 1H), 3.02–3.08 (m, 1H), 3.63 (s, 3H), 3.88 (s, 3H), 4.42 (q, *J* = 6.6 Hz, 1H), 6.55 (d, *J* = 2.5 Hz, 1H), 6.73 (dd, *J* = 2.5, 8.5 Hz, 1H), 6.82 (t, *J* = 8.5 Hz, 2H), 6.93 (s, 1H), 7.00–7.07 (m, 2H), 7.20 (d, *J* = 2.5 Hz, 1H), 7.25 (dd, *J* = 2.5, 8.5 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 1H), 8.97 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 12.0, 13.8, 19.3, 21.1, 32.0, 55.6, 55.8, 67.4, 75.3, 110.9, 113.9, 120.96, 121.02, 122.2, 124.7, 125.2, 125.6, 127.7, 128.0, 128.6, 128.9, 129.1, 130.1, 131.5, 132.9, 133.6, 133.7, 137.8, 140.0, 147.0, 148.3. HRMS (APCI) calcd for $C_{31}H_{34}{}^{35}Cl_2NO_3$ $(M+H)^+$ 538.1910, found 538.1916. IR (neat) 3339, 2957, 2931, 2870, 1592, 1508, 1464, 1245, 1219, 1156, 1137, 1093, 1027, 887, 787, 759, 737, 693 cm^{-1}.



3wf

Compound 3wf (Scheme 3, colorless solid). A solution of hexane/EtOAc/$CHCl_3$ (1:3:1) was used as an eluent for preparative TLC. The ee was measured by HPLC (Chiralcel OD–H, hexane/2-propanol = 10:1, flow 0.5 mL/min, 254 nm, t_1 = 25.2 min (major), t_2 = 44.5 min (minor)); $[\alpha]^{20}_D$ –22 (*c* 1.01, $CHCl_3$) for 97% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 1.46 (d, *J* = 6.2 Hz, 3H), 4.37 (d, *J* = 11.6 Hz, 1H), 4.47 (d, *J* = 11.6 Hz, 1H), 5.14 (q, *J* = 6.2 Hz, 1H), 7.19–7.24 (m, 3H), 7.24–7.30 (m, 4H), 7.31–7.51 (br, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.68 (d, *J* = 4.1 Hz, 2H), 7.71–7.93 (br, 1H), 8.10 (d, *J* = 7.8 Hz, 1H), 8.65 (d, *J* = 4.1 Hz, 2H), 11.84 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 21.4, 69.6, 76.9, 111.0 (br), 119.6 (br), 120.7, 122.5, 122.7 (br), 128.1, 128.7, 129.2, 129.6, 129.8, 129.9, 133.7, 134.2 (br), 136.0, 136.9, 139.4, 140.7, 143.7 (br), 149.6, 151.4, 156.0. HRMS (APCI) calcd for $C_{27}H_{23}{}^{35}ClN_3O$ $(M+H)^+$ 440.1530, found 440.1543. m.p. = 65–68 °C. IR (neat) 2973, 2360, 1465, 1451, 1432, 1087, 1062, 1015, 902, 806, 782, 768, 743, 669 cm^{-1}.

7. X-Ray data of 3wf

A white crystal of **3wf** suitable for X-ray crystallographic analysis was obtained by recrystallization from toluene/pentane. The ORTEP drawing of **3wf** is shown in Figure S1. The crystal structure has been deposited at the Cambridge Crystallographic Centre (deposition number: CCDC 1521370). The data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif. X-Ray data were collected on a Rigaku XtaLAB P200 using a graphite monochromater with Cu-*K*a radiation (λ = 1.54187 Å) at 93 K. The structure was solved by direct method (SHELXS-2014) and refined with full-matrix least-square technique (SHELXL-2014).[12] The absolute structure was deduced based on Flack parameter 0.033(13).[13] The data for **3wf** is summarized in Table S1.

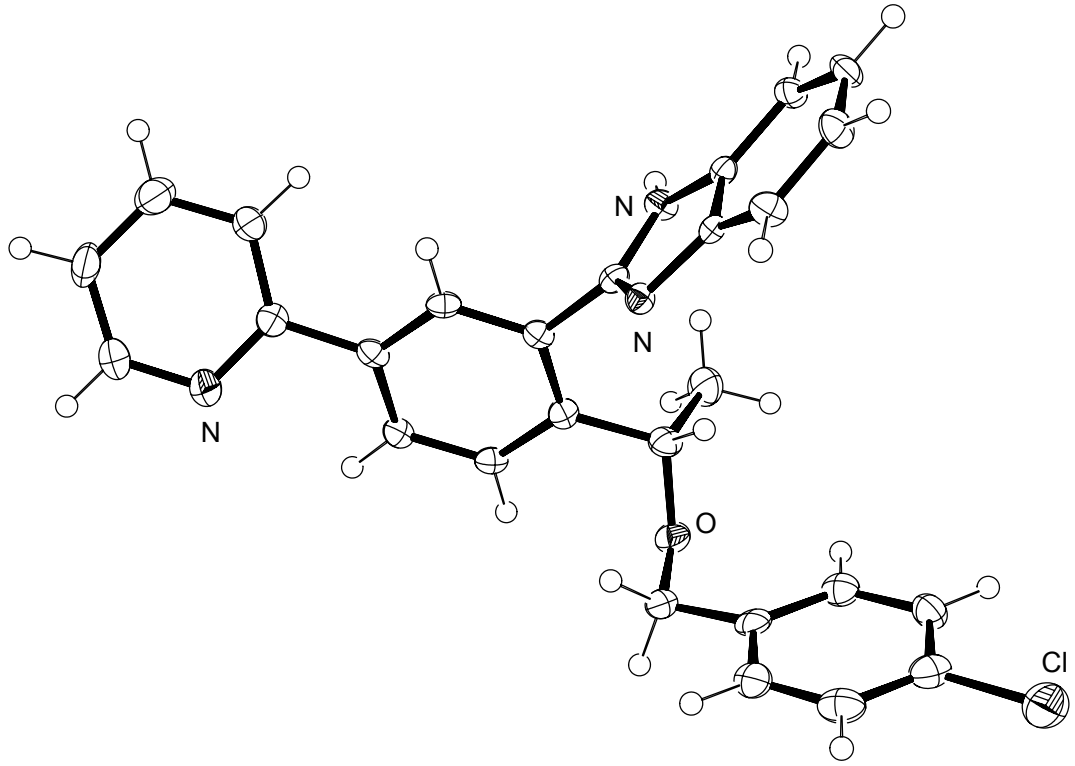


Figure S1. ORTEP illustration of **3wf** with thermal ellipsoids drawn at 50% probability level.

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

Empirical formula	$C_{27}H_{22}ClN_3O$
Formula weight	439.92
Temperature	93(2) K
Wavelength	1.54187 Å
Crystal system	Orthorhombic
Space group	$P\ 2_12_12_1$ (# 19)
Unit cell dimensions	a = 9.645(4) Å
	b = 11.952(5) Å
	c = 19.826(8) Å
Volume	2285.5(16) $Å^3$
Z	4
Density (calculated) [Mg/m^3]	1.279
Absorption coefficient [mm^{-1}]	1.663
F(000)	920
Reflections collected	14207
Independent reflections	4134 [*R*(int) = 0.0634]
Completeness to θ (%)	97.4
Goodness-of-fit on F^2	1.043
R_1 [$I>2\sigma(I)$]	0.0449
wR_2 (all data)	0.1031
Flack parameter	0.033(13)
Largest diff. peak and hole [$e/Å^3$]	0.384 and -0.416

8. References

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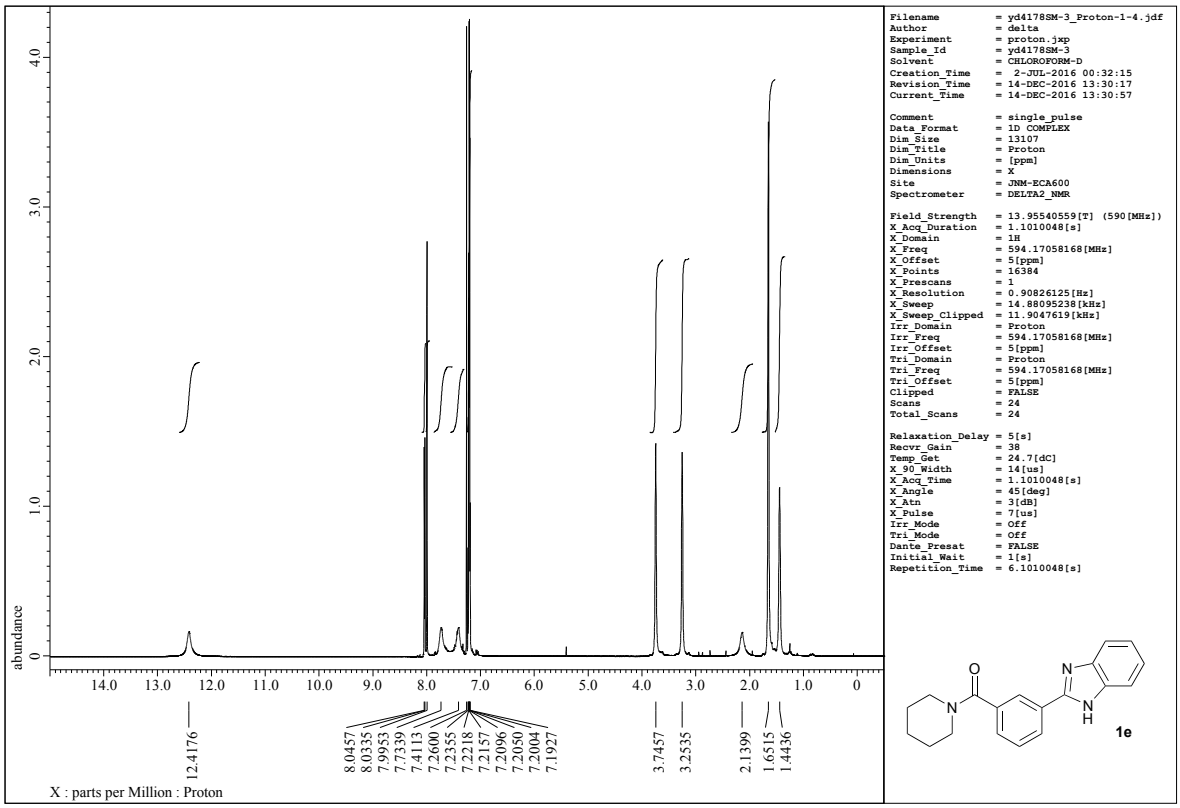
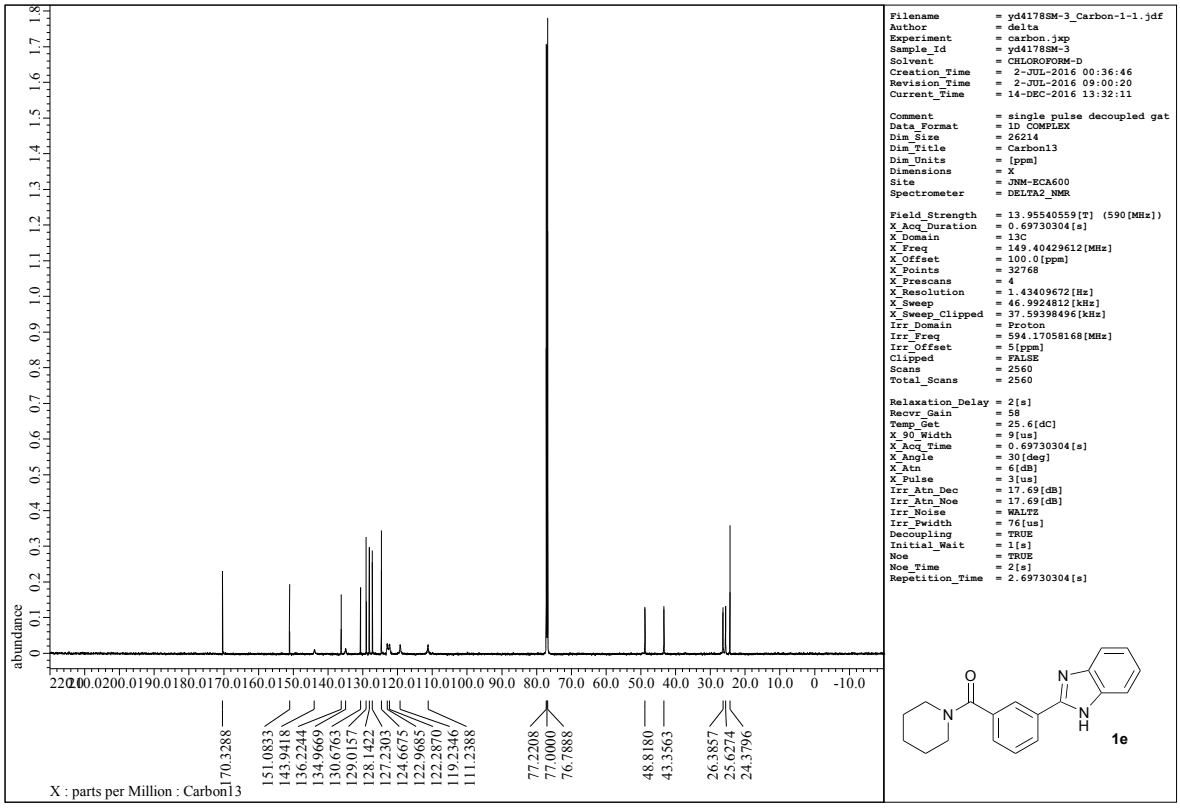
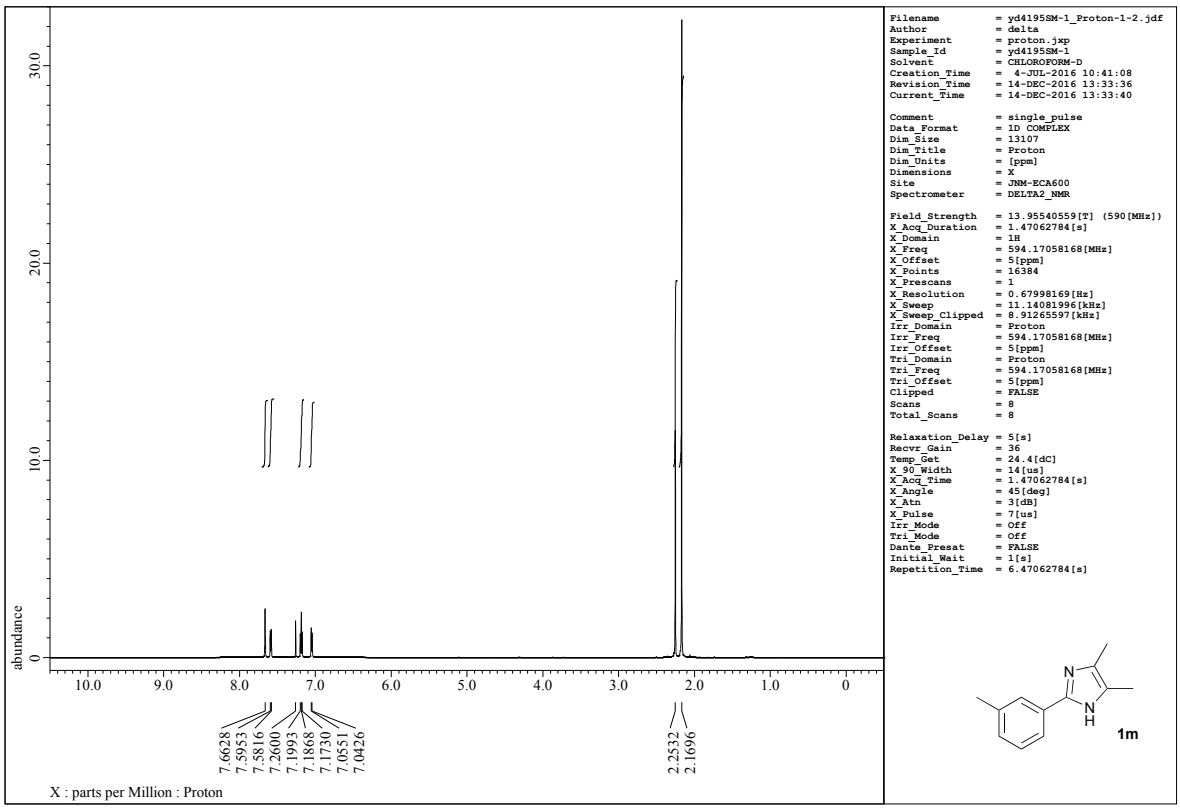
9. ^{1}H, ^{13}C NMR spectra and chiral HPLC charts



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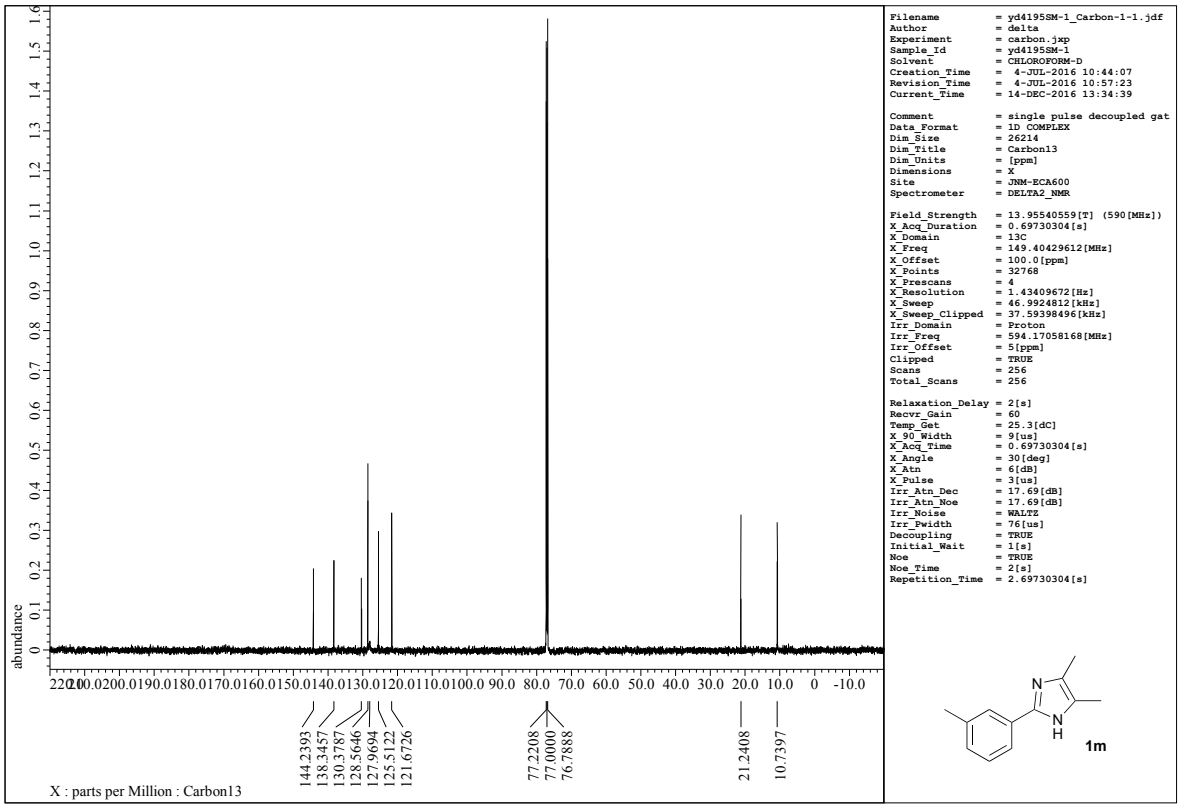
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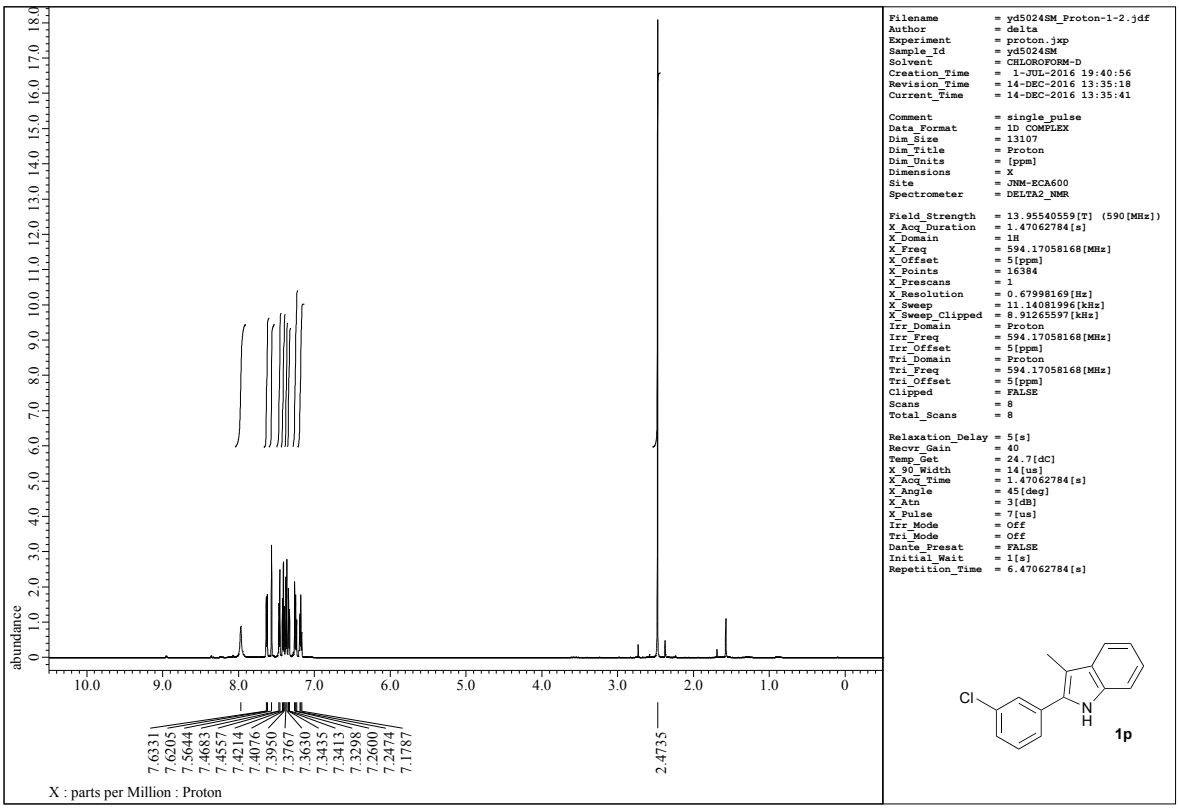
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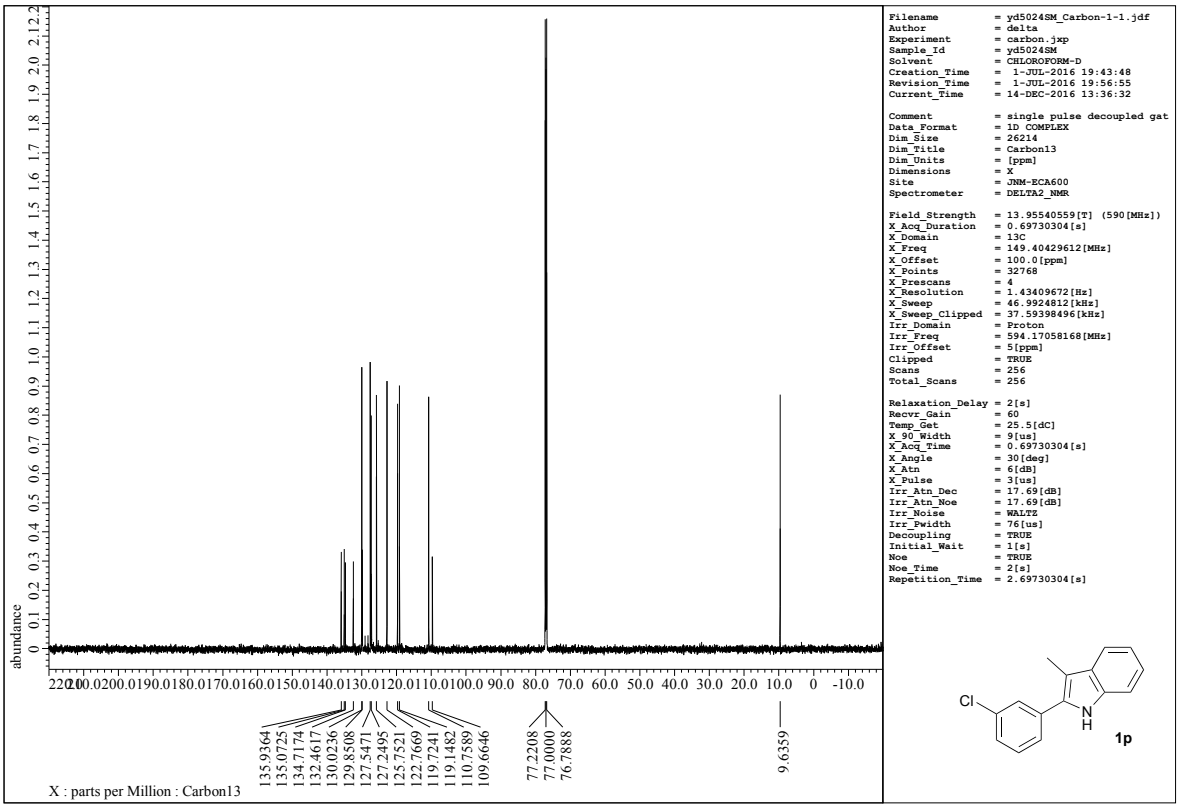
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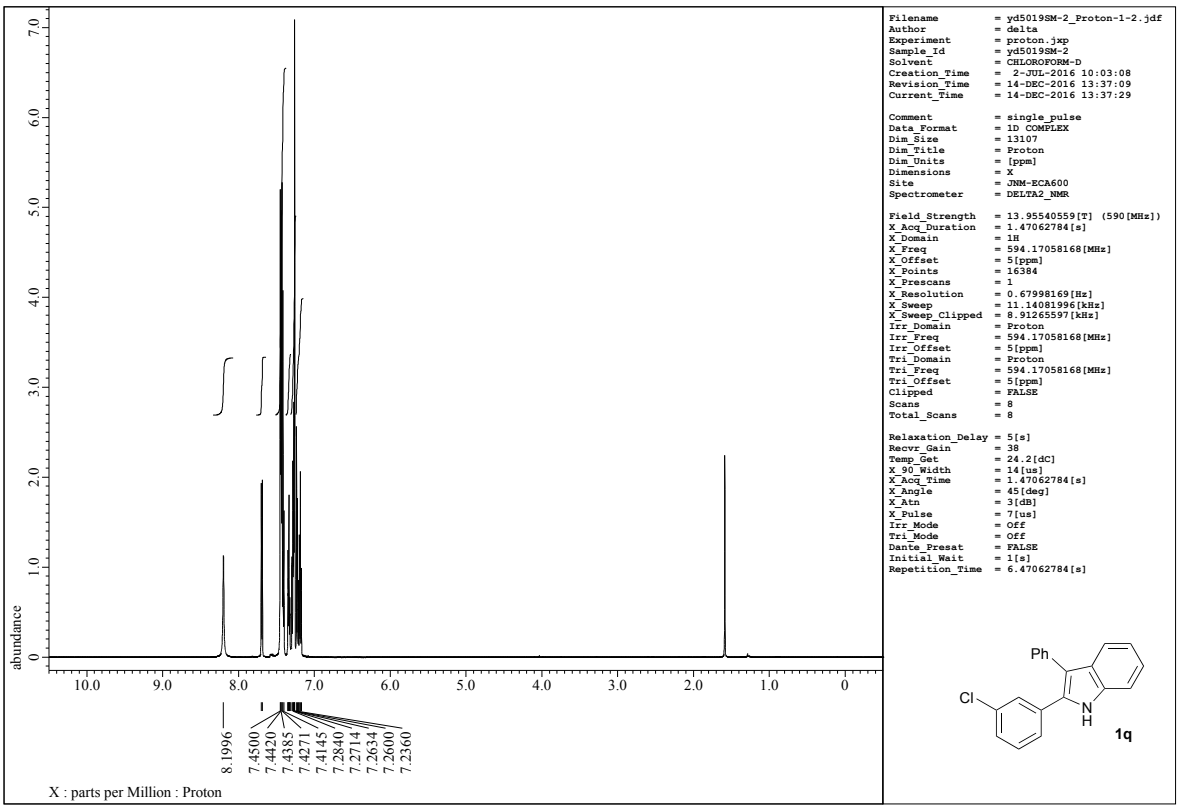
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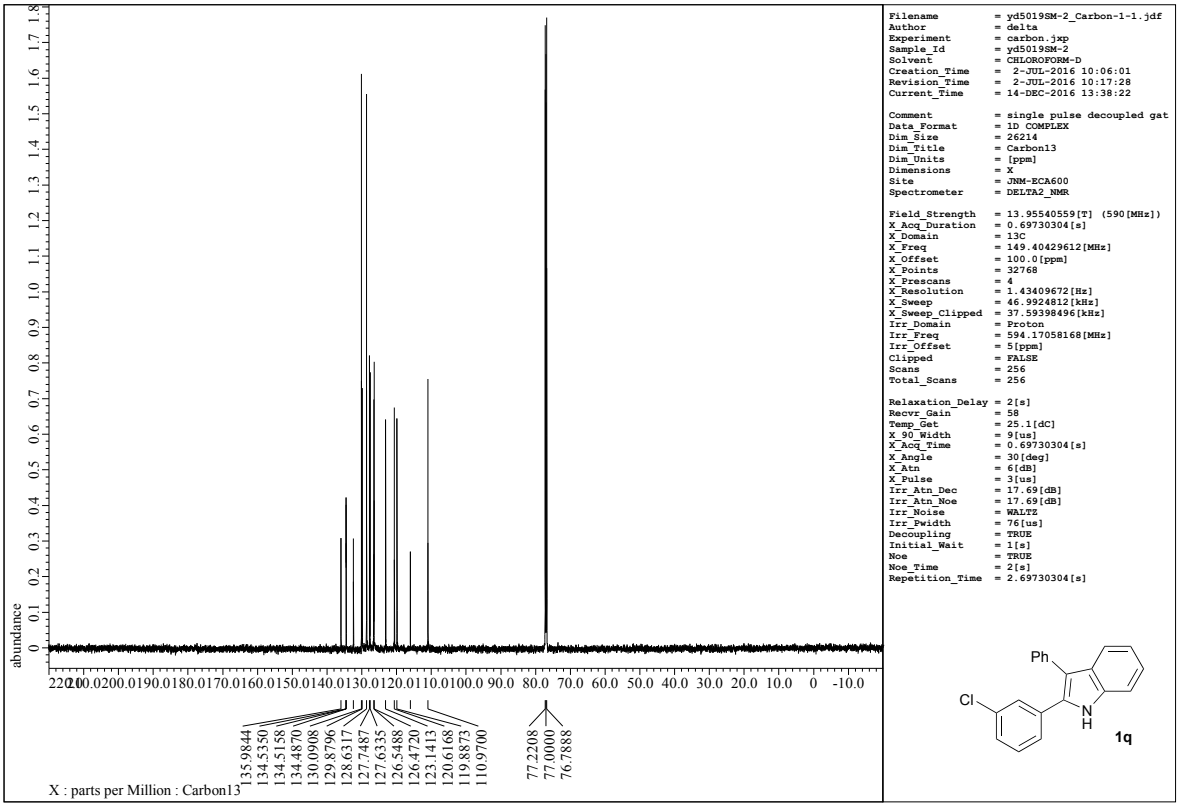
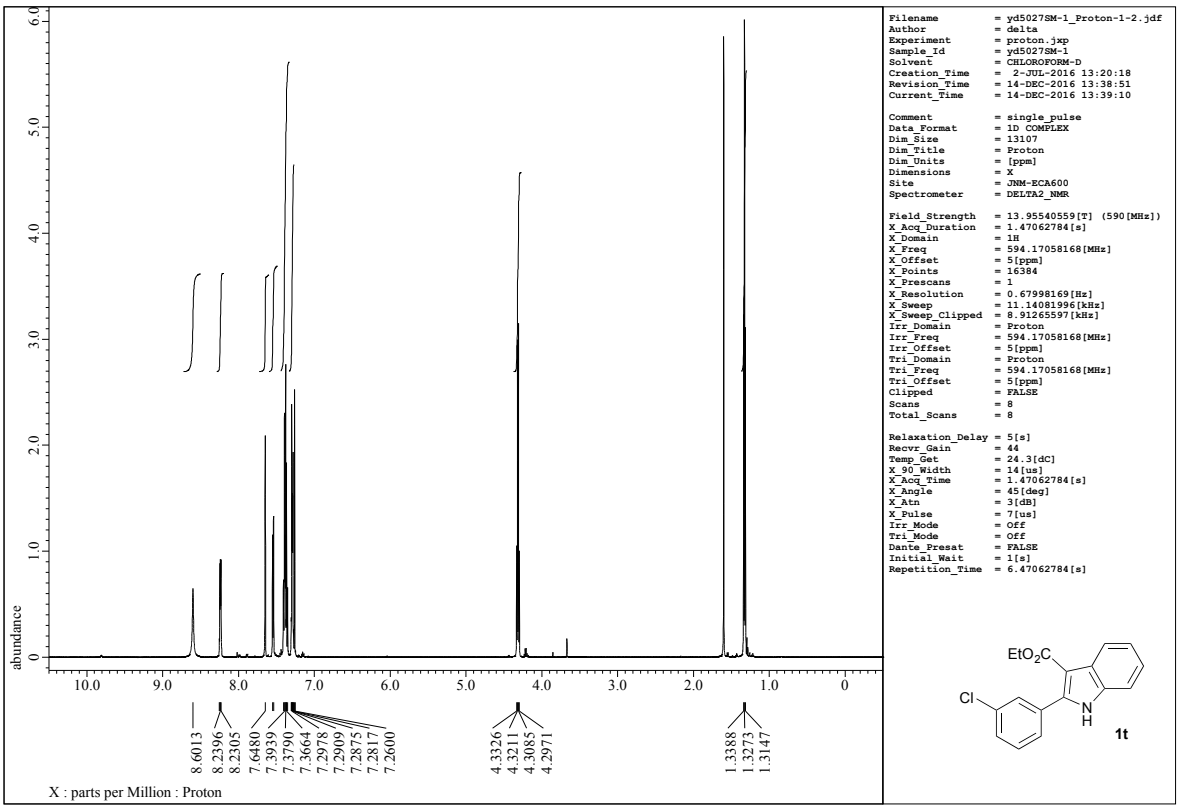
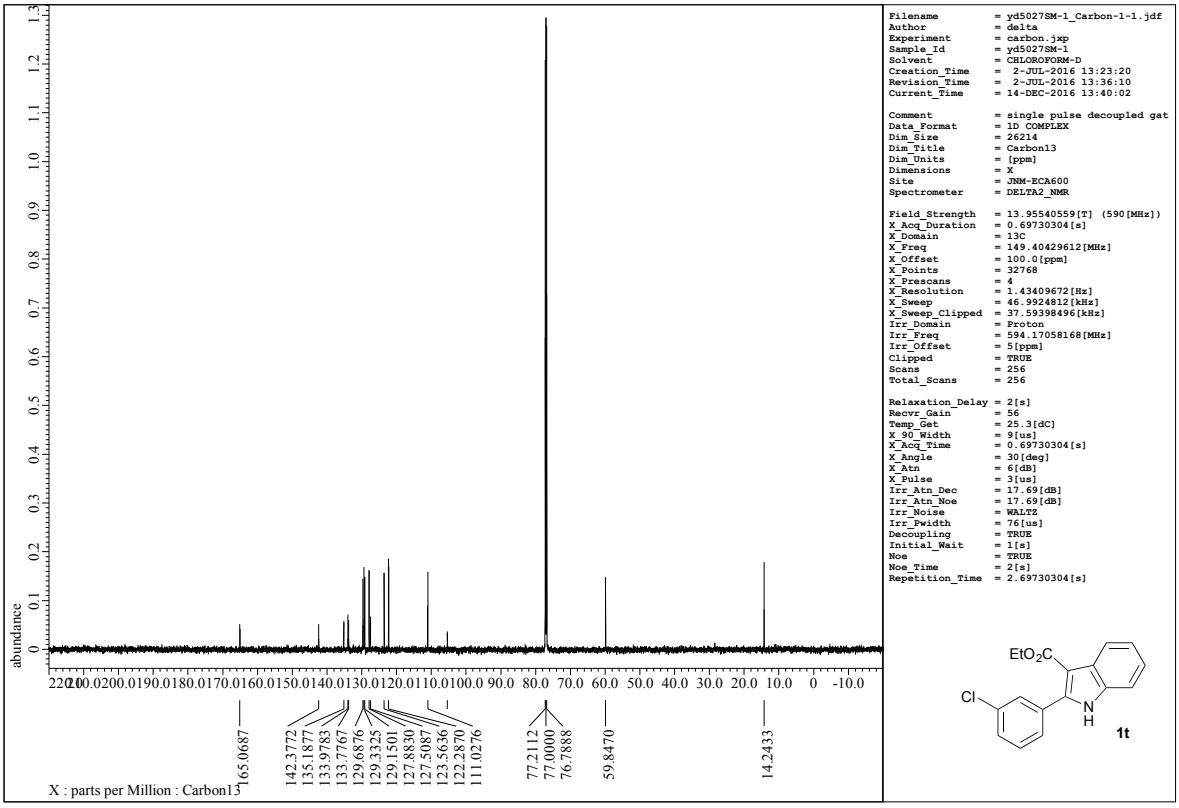
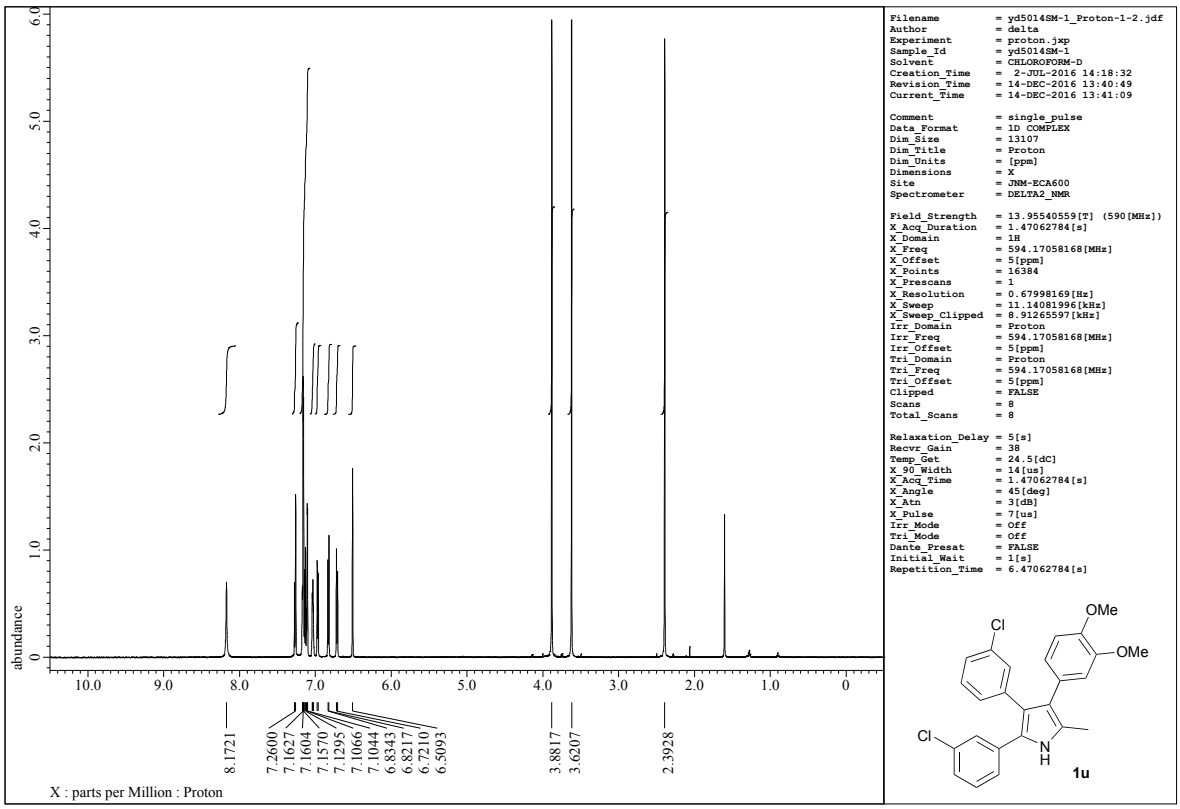
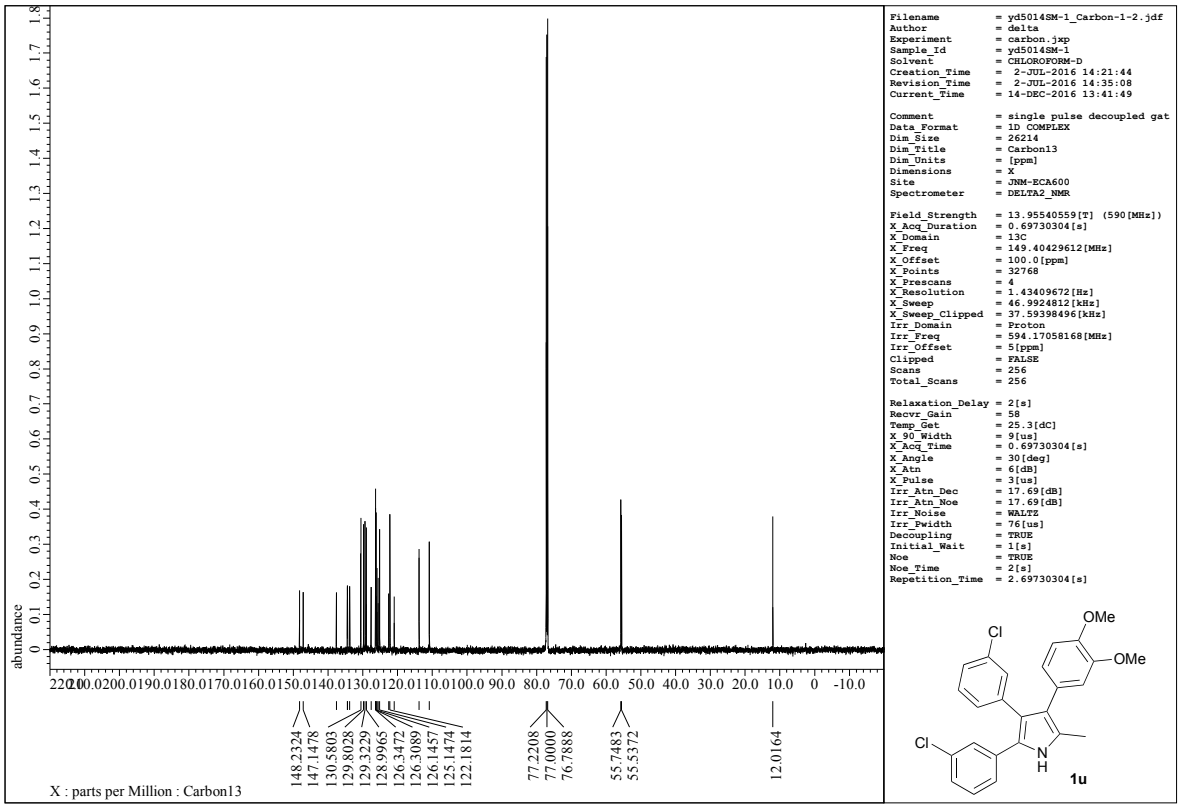
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 24.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Ph
Cl
N
H
1q

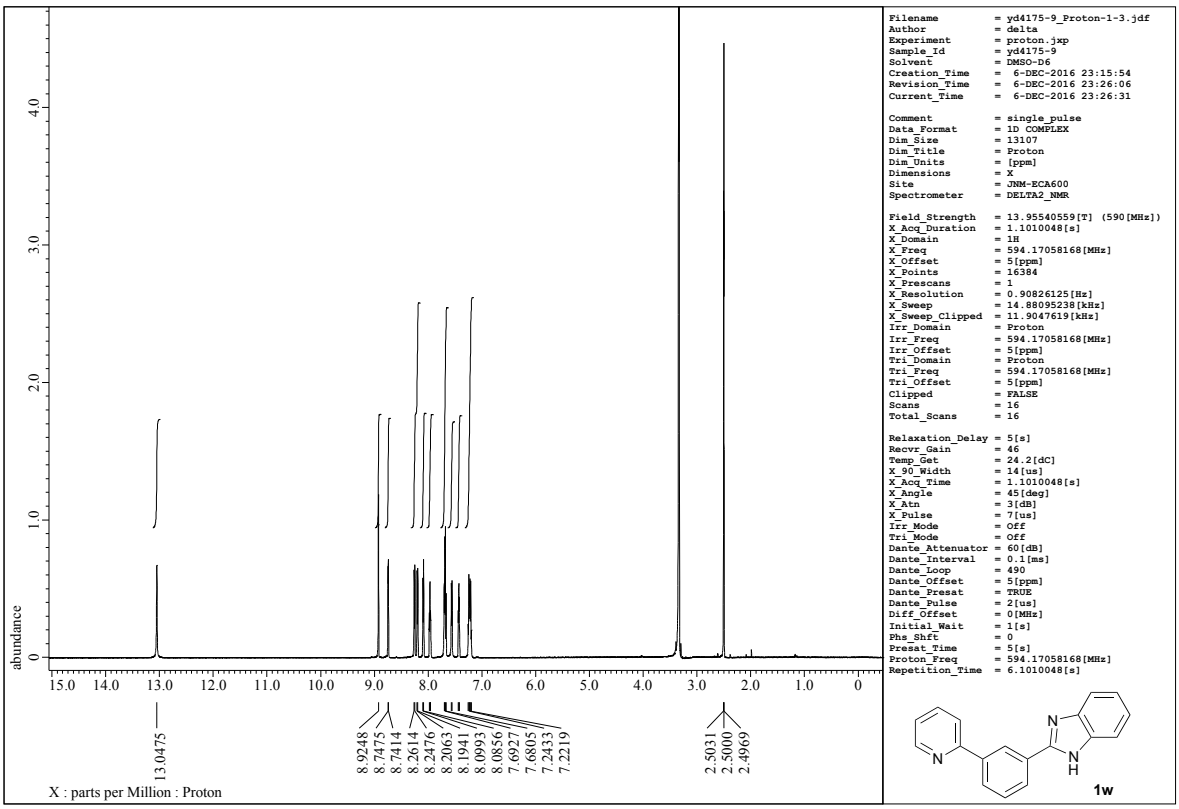

abundance
220 200 190 180 170 160 150 140 130 120 110 100 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
135.9844
134.5350
134.5158
134.4870
130.0908
129.8796
128.6317
127.7487
127.6335
126.5488
126.4720
123.1413
120.6168
119.8873
110.9700
77.2208
77.0000
76.7888
X : parts per Million : Carbon13
Filename = yd5019SM-2_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd5019SM-2
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2016 10:06:01
Revision_Time = 2-JUL-2016 10:17:28
Current_Time = 14-DEC-2016 13:38:22
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 25.1[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
Ph
Cl
N
H
1q

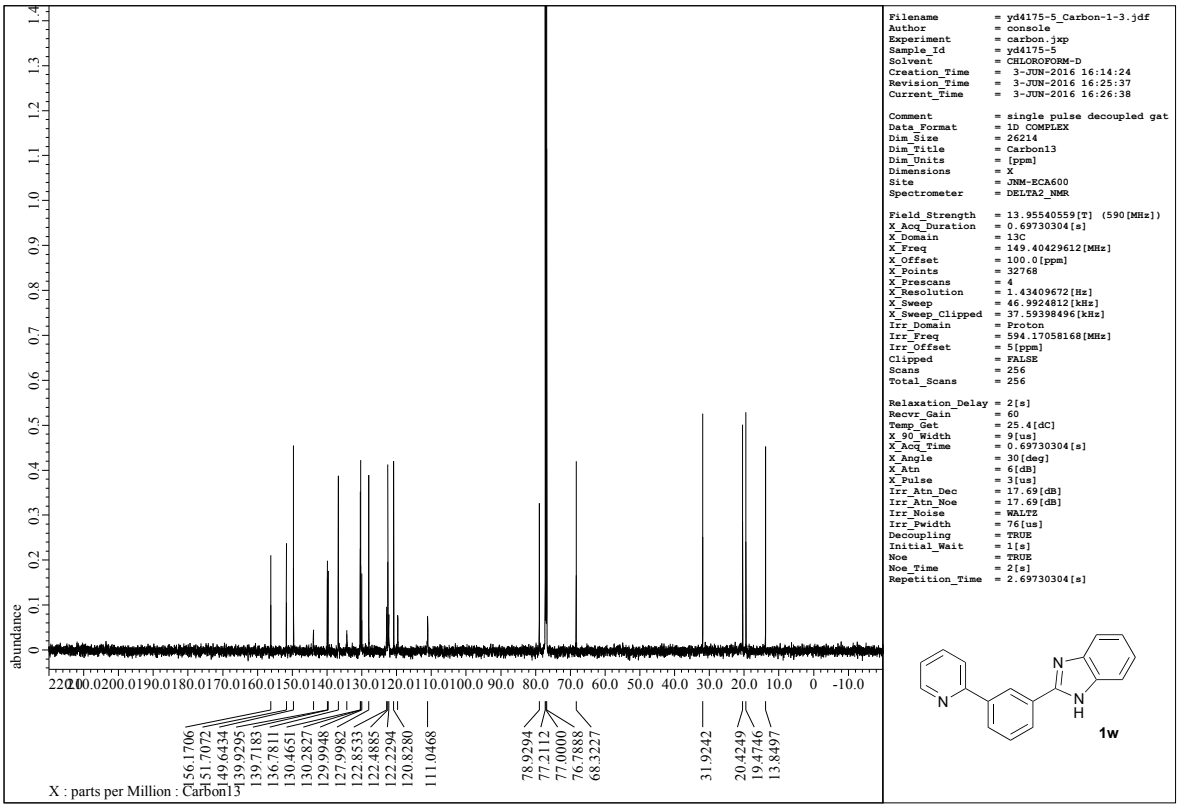

abundance
8.6013
8.2396
8.2305
7.6480
7.3939
7.3790
7.3664
7.2978
7.2909
7.2875
7.2817
7.2600
4.3326
4.3211
4.3085
4.2971
1.3388
1.3273
1.3147
X : parts per Million : Proton
Filename = yd5027SM-1_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd5027SM-1
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2016 13:20:18
Revision_Time = 14-DEC-2016 13:38:51
Current_Time = 14-DEC-2016 13:39:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 24.3[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
EtO2C
Cl
N
H
1t

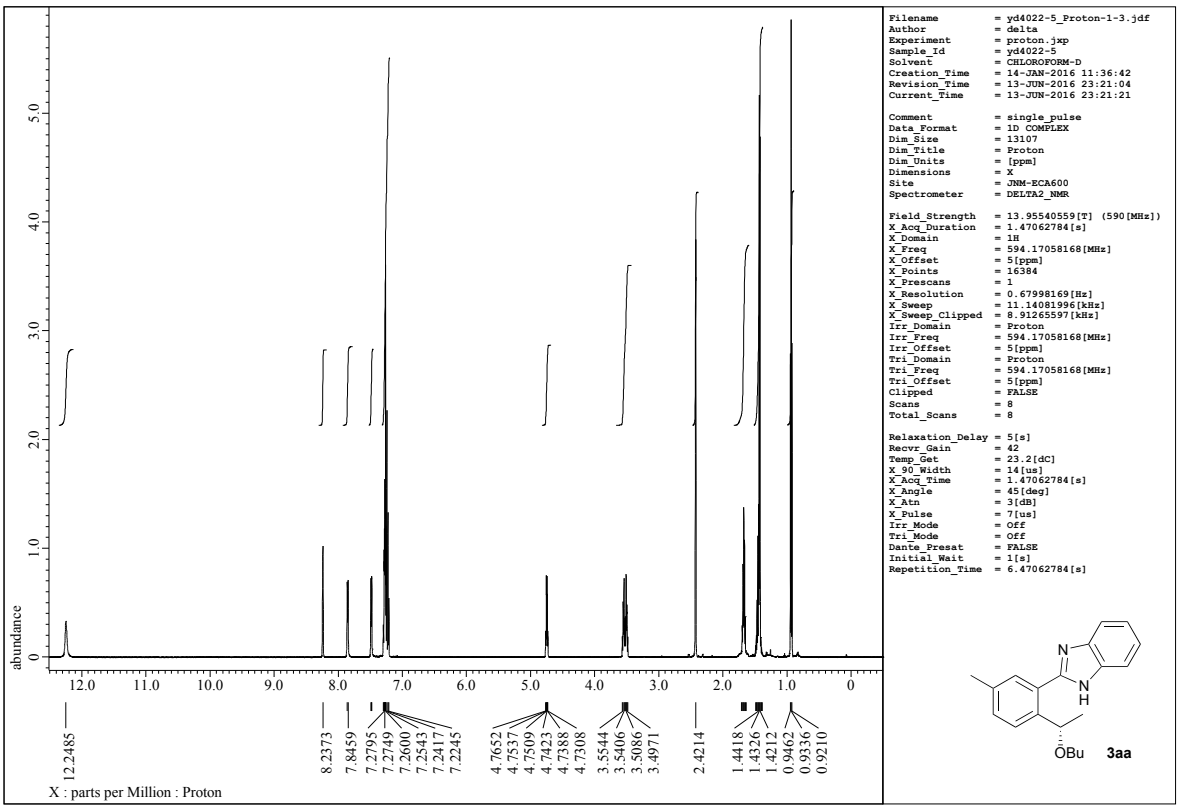

abundance
165.0687
142.3772
135.1877
133.9783
133.7767
129.6876
129.3325
129.1501
127.8830
127.5087
123.5636
122.2870
111.0276
77.2112
77.0000
76.7888
59.8470
14.2433
X : parts per Million : Carbon13
Filename = yd5027SM-1_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd5027SM-1
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2016 13:23:20
Revision_Time = 2-JUL-2016 13:36:10
Current_Time = 14-DEC-2016 13:40:02
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 25.3[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
EtO2C
Cl
N
H
1t

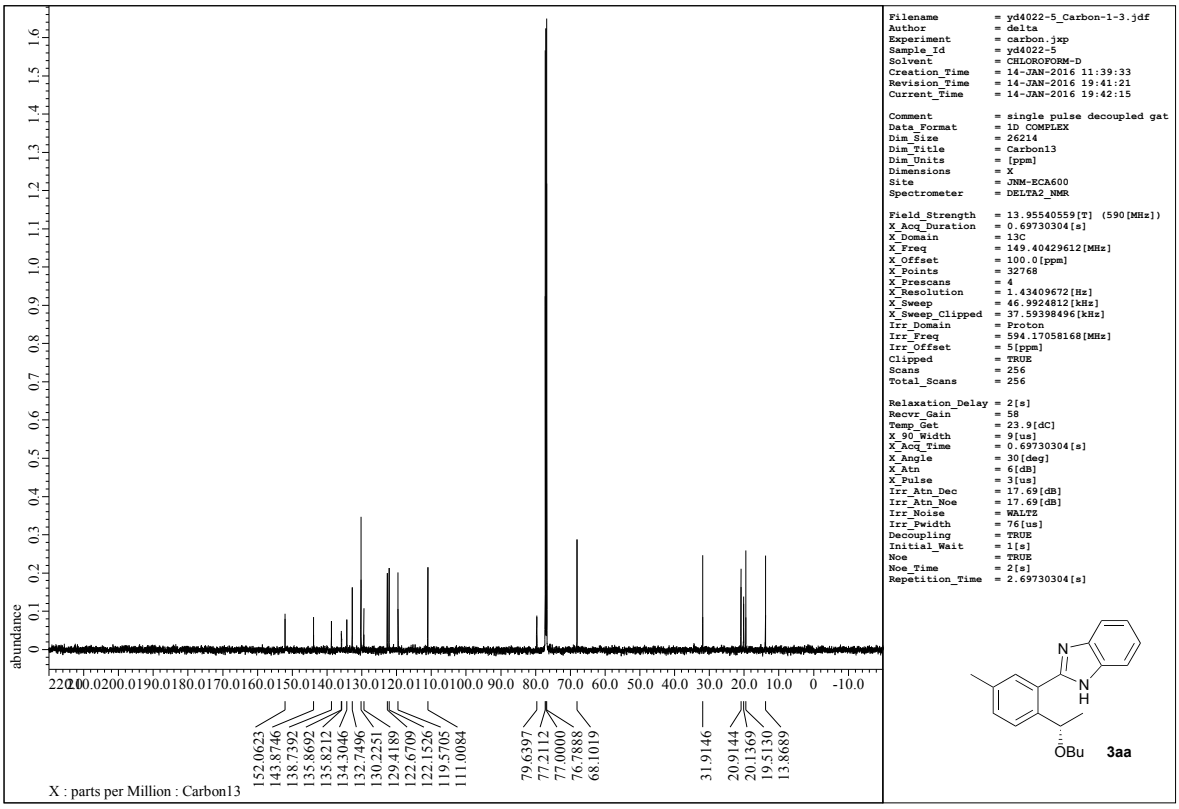

abundance
8.1721
7.2600
7.1627
7.1604
7.1570
7.1295
7.1066
7.1044
6.8343
6.8217
6.7210
6.5093
3.8817
3.6207
2.3928
X : parts per Million : Proton
Filename = yd5014SM-1_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd5014SM-1
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2016 14:18:32
Revision_Time = 14-DEC-2016 13:40:49
Current_Time = 14-DEC-2016 13:41:09
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 24.5[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
OMe
OMe
Cl
Cl
N
H
1u

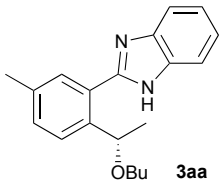

abundance
148.2324
147.1478
130.5803
129.8028
129.3229
128.9965
126.3472
126.3089
126.1457
125.1474
122.1814
77.2208
77.0000
76.7888
55.7483
55.5372
12.0164
X : parts per Million : Carbon13
Filename = yd5014SM-1_Carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd5014SM-1
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2016 14:21:44
Revision_Time = 2-JUL-2016 14:35:08
Current_Time = 14-DEC-2016 13:41:49
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 25.3[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
OMe
OMe
Cl
Cl
N
H
1u


abundance
13.0475
8.9248
8.7475
8.7414
8.2614
8.2476
8.2063
8.1941
8.0993
8.0856
7.6927
7.6805
7.2433
7.2219
2.5031
2.5000
2.4969
X : parts per Million : Proton
Filename = yd4175-9_Proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4175-9
Solvent = DMSO-D6
Creation_Time = 6-DEC-2016 23:15:54
Revision_Time = 6-DEC-2016 23:26:06
Current_Time = 6-DEC-2016 23:26:31
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 24.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.1010048[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Attenuator = 60[dB]
Dante_Interval = 0.1[ms]
Dante_Loop = 490
Dante_Offset = 5[ppm]
Dante_Presat = TRUE
Dante_Pulse = 2[us]
Diff_Offset = 0[MHz]
Initial_Wait = 1[s]
Phs_Shft = 0
Presat_Time = 5[s]
Proton_Freq = 594.17058168[MHz]
Repetition_Time = 6.1010048[s]
1w

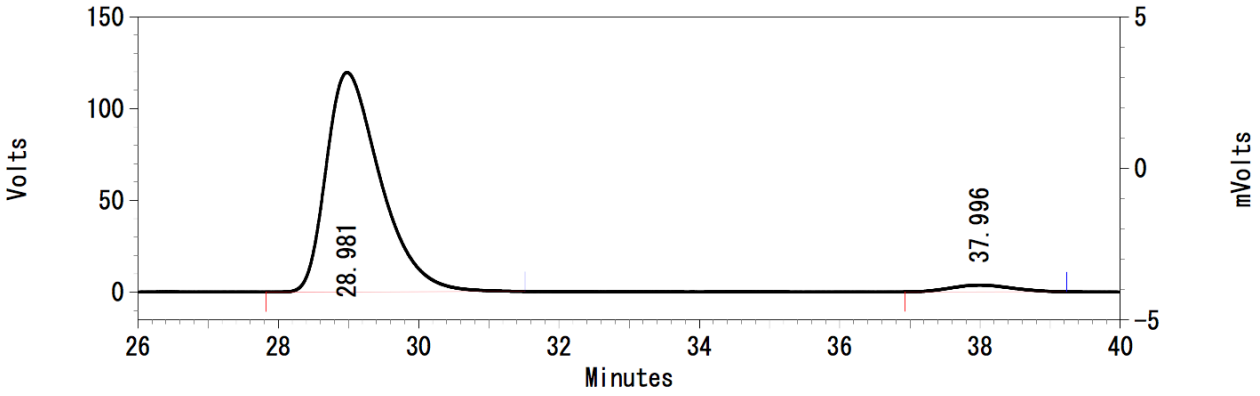

abundance
156.1706
151.7072
149.6434
139.9295
139.7183
136.7811
130.4651
130.2827
129.9948
127.9982
122.8533
122.4885
122.2294
120.8280
111.0468
78.9294
77.2112
77.0000
76.7888
68.3227
31.9242
20.4249
19.4746
13.8497
X : parts per Million : Carbon13
Filename = yd4175-5_Carbon-1-3.jdf
Author = console
Experiment = carbon.jxp
Sample_Id = yd4175-5
Solvent = CHLOROFORM-D
Creation_Time = 3-JUN-2016 16:14:24
Revision_Time = 3-JUN-2016 16:25:37
Current_Time = 3-JUN-2016 16:26:38
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.4[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
1w


abundance
X : parts per Million : Proton
12.2485
8.2373
7.8459
7.2795
7.2749
7.2600
7.2543
7.2417
7.2245
4.7652
4.7537
4.7509
4.7423
4.7388
4.7308
3.5544
3.5406
3.5086
3.4971
2.4214
1.4418
1.4326
1.4212
0.9462
0.9336
0.9210
Filename = yd4022-5_Proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4022-5
Solvent = CHLOROFORM-D
Creation_Time = 14-JAN-2016 11:36:42
Revision_Time = 13-JUN-2016 23:21:04
Current_Time = 13-JUN-2016 23:21:21
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 23.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OBu
3aa


abundance
X : parts per Million : Carbon13
152.0623
143.8746
138.7392
135.8692
135.8212
134.3046
132.7496
130.2251
129.4189
122.6709
122.1526
119.5705
111.0084
79.6397
77.2112
77.0000
76.7888
68.1019
31.9146
20.9144
20.1369
19.5130
13.8689
Filename = yd4022-5_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4022-5
Solvent = CHLOROFORM-D
Creation_Time = 14-JAN-2016 11:39:33
Revision_Time = 14-JAN-2016 19:41:21
Current_Time = 14-JAN-2016 19:42:15
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 23.9[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OBu
3aa

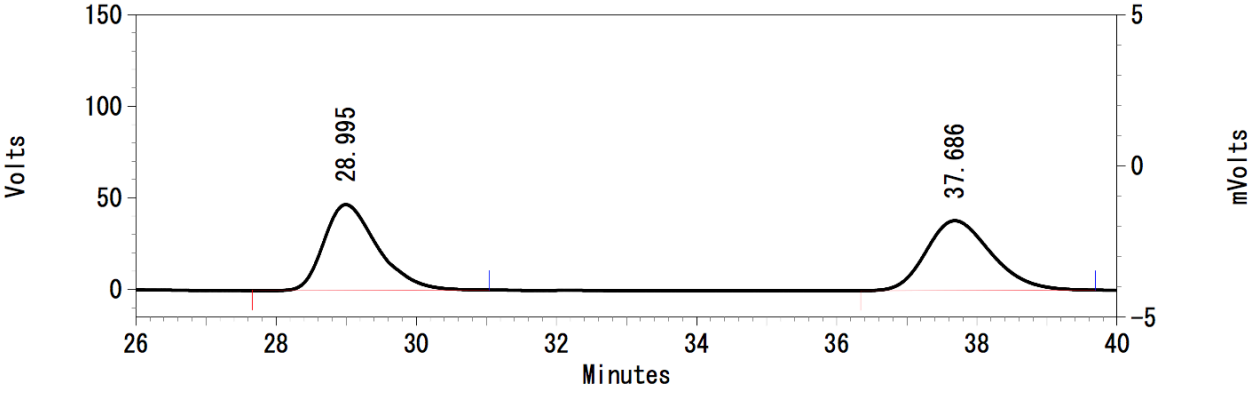


3aa



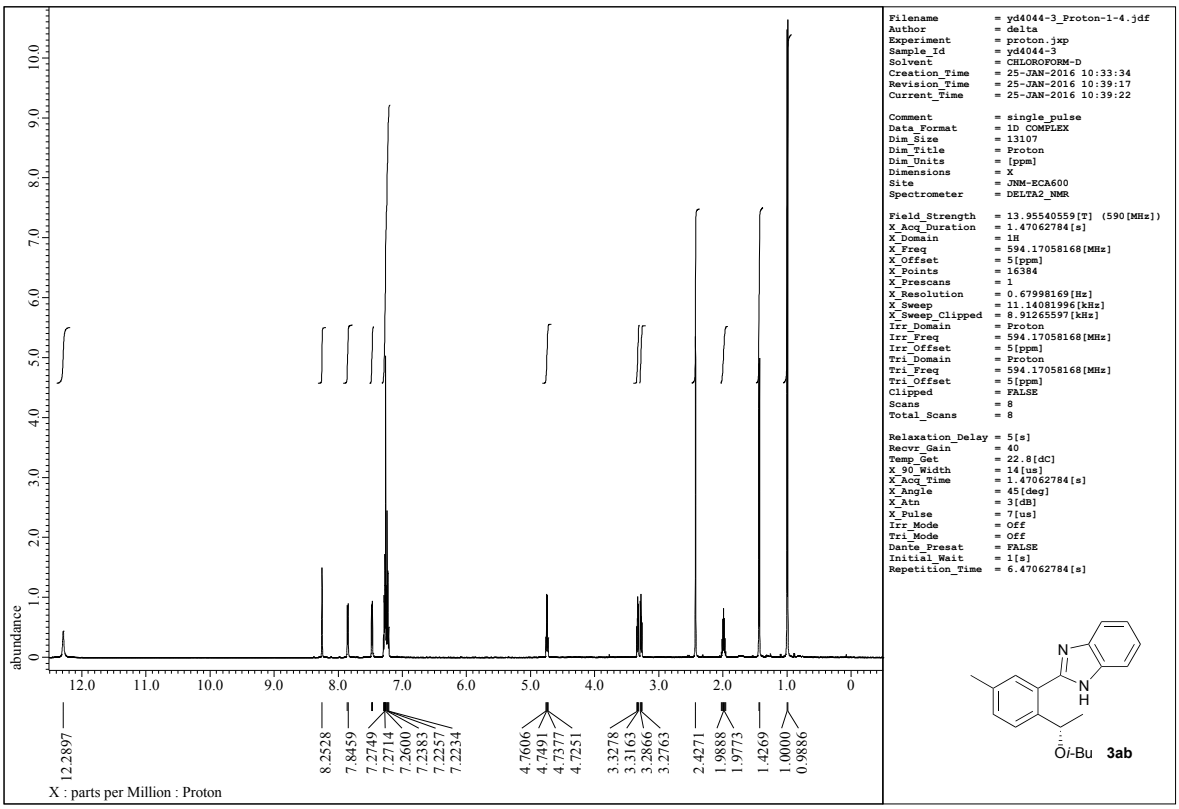
UV Results

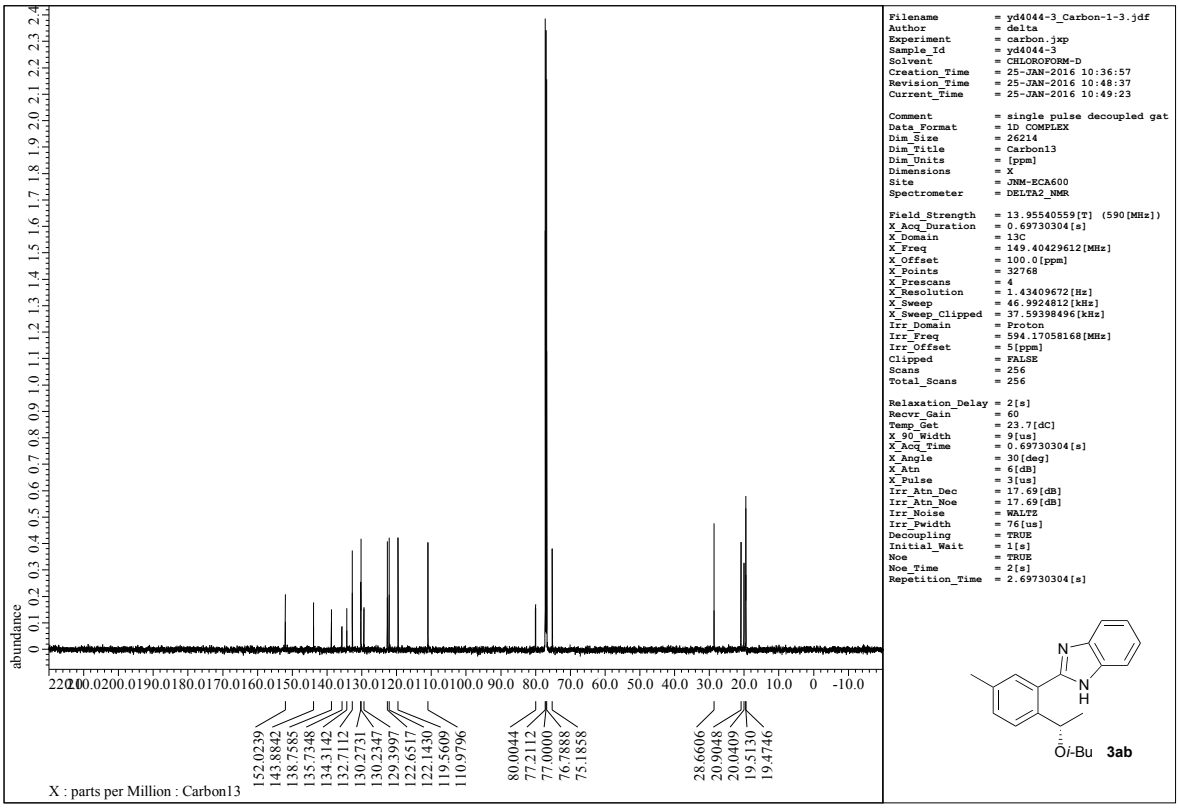
Pk #	Retention Time	Area	Area Percent	Height
1	28.981	6397579	96.643	119399
2	37.996	222247	3.357	3649

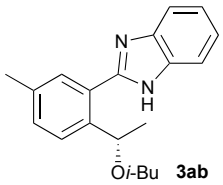


UV Results

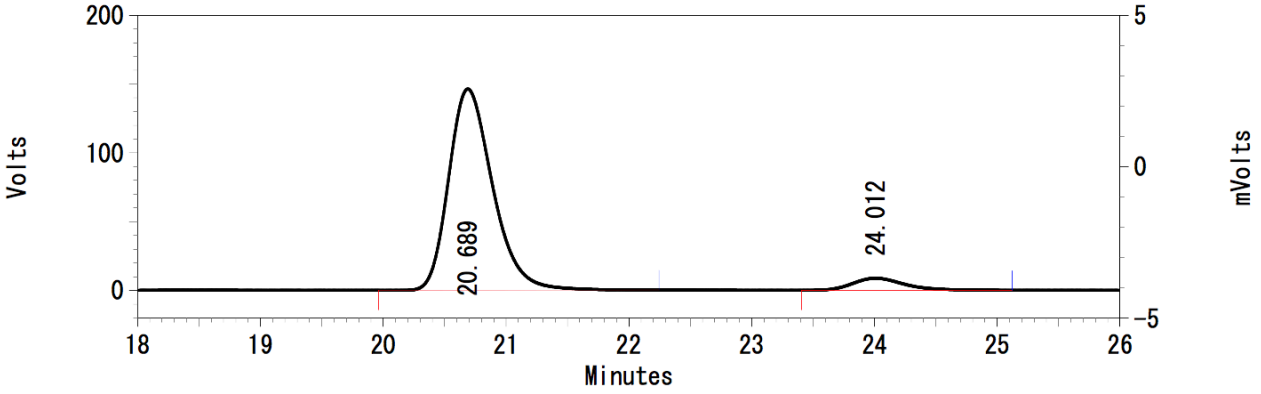
Pk #	Retention Time	Area	Area Percent	Height
1	28.995	2481290	50.236	46750
2	37.686	2457971	49.764	38075


abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.2897
8.2528 7.8459 7.2749 7.2714 7.2600 7.2383 7.2257 7.2234
4.7606 4.7491 4.7377 4.7251
3.3278 3.3163 3.2866 3.2763
2.4271 1.9888 1.9773 1.4269 1.0000 0.9886
X : parts per Million : Proton
Filename = yd4044-3_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4044-3
Solvent = CHLOROFORM-D
Creation_Time = 25-JAN-2016 10:33:34
Revision_Time = 25-JAN-2016 10:39:17
Current_Time = 25-JAN-2016 10:39:22
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 22.8[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
Oi-Bu 3ab


abundance
220.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
152.0239 143.8842 138.7585 135.7348 134.3142 132.7112 130.2731 130.2347 129.3997 122.6517 122.1430 119.5609 110.9796
80.0044 77.2112 77.0000 76.7888 75.1858
28.6606 20.9048 20.0409 19.5130 19.4746
X : parts per Million : Carbon13
Filename = yd4044-3_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4044-3
Solvent = CHLOROFORM-D
Creation_Time = 25-JAN-2016 10:36:57
Revision_Time = 25-JAN-2016 10:48:37
Current_Time = 25-JAN-2016 10:49:23
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 23.7[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
Oi-Bu 3ab

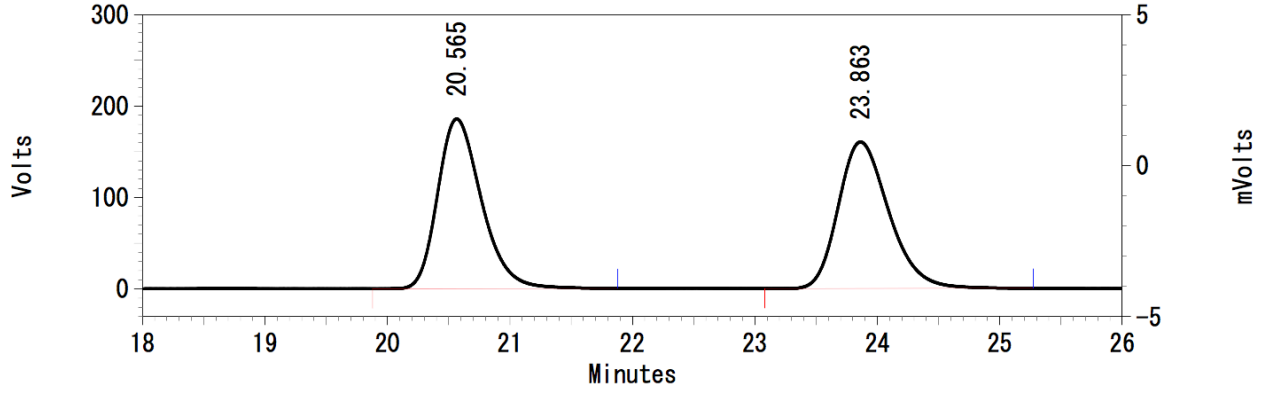


3ab



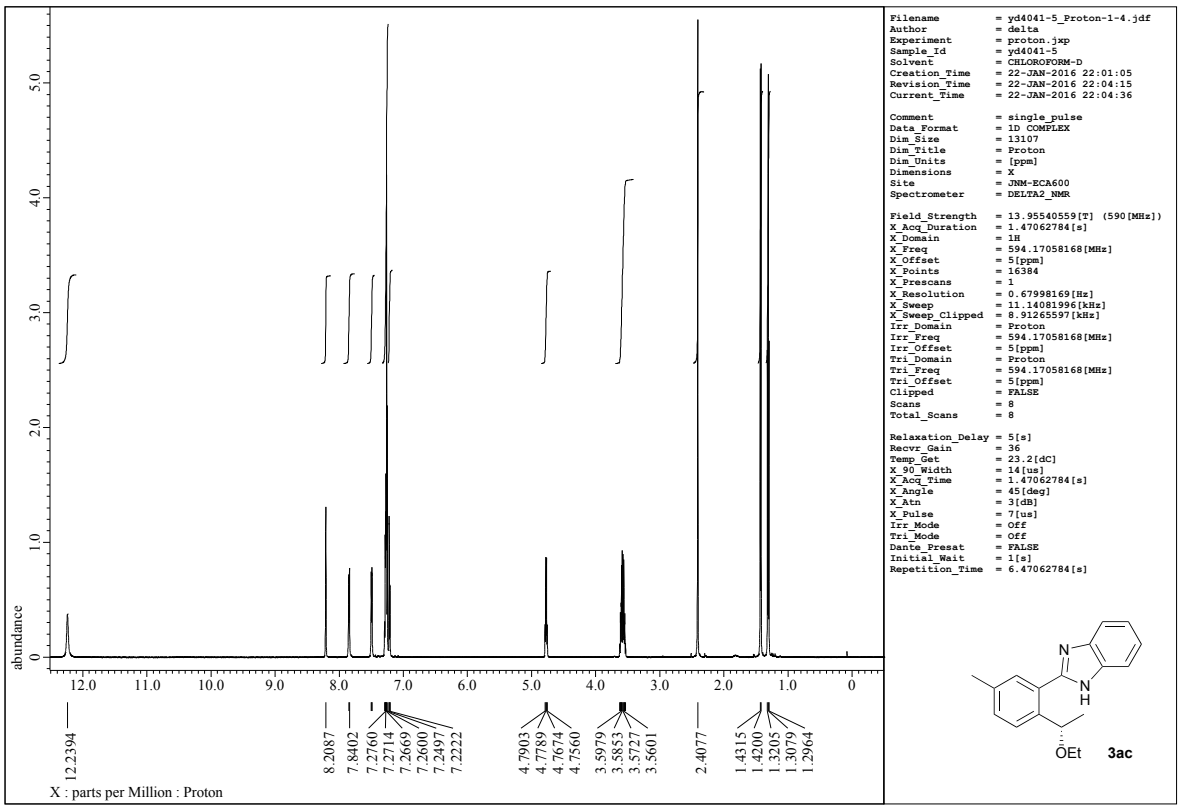
UV Results

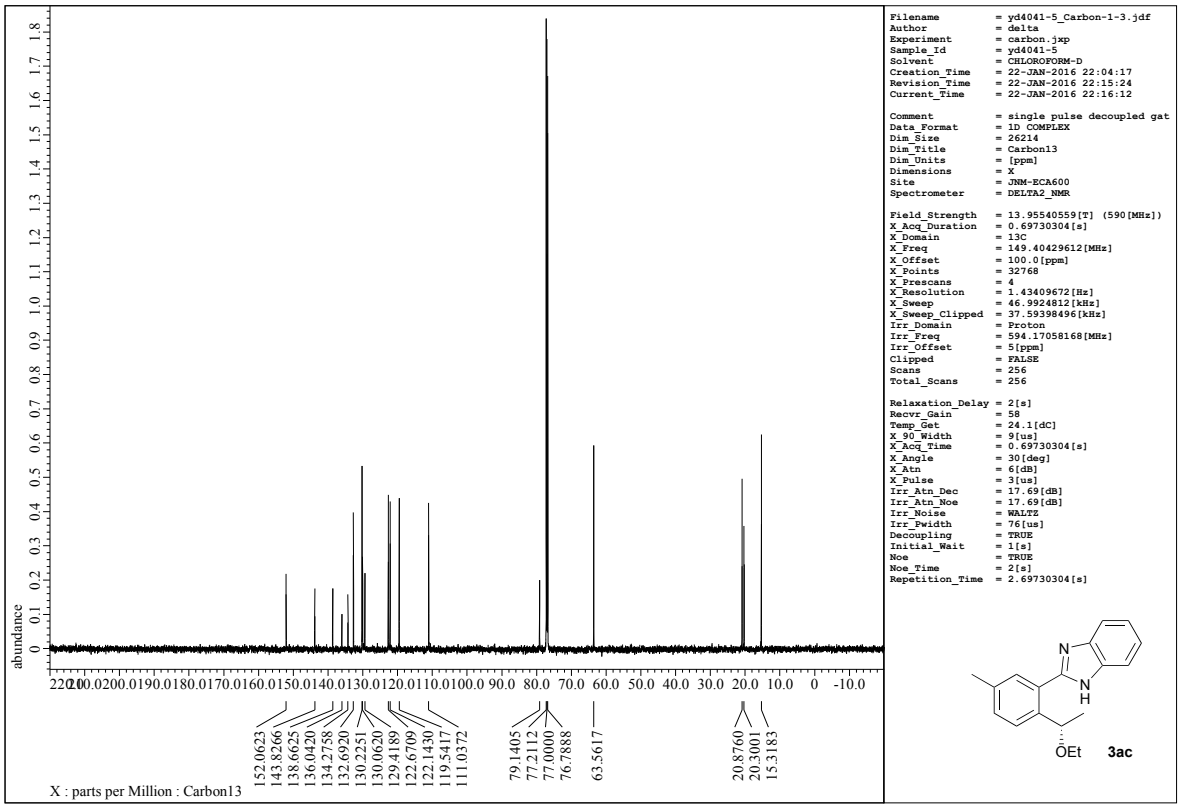
Pk #	Retention Time	Area	Area Percent	Height
1	20.689	3636201	93.397	146137
2	24.012	257075	6.603	8762

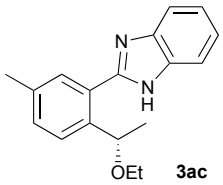


UV Results

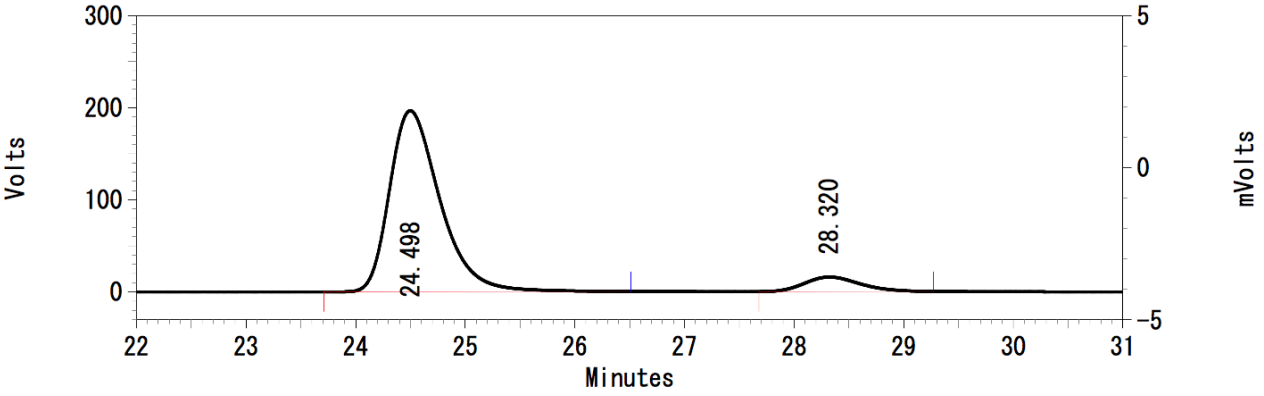
Pk #	Retention Time	Area	Area Percent	Height
1	20.565	4614875	50.061	185368
2	23.863	4603654	49.939	160235


abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.2394
8.2087 7.8402 7.2760 7.2714 7.2669 7.2600 7.2497 7.2222
4.7903 4.7789 4.7674 4.7560
3.5979 3.5853 3.5727 3.5601
2.4077
1.4315 1.4200 1.3205 1.3079 1.2964
X : parts per Million : Proton
Filename = yd4041-5_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4041-5
Solvent = CHLOROFORM-D
Creation_Time = 22-JAN-2016 22:01:05
Revision_Time = 22-JAN-2016 22:04:15
Current_Time = 22-JAN-2016 22:04:36
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 23.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OEt
3ac


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
152.0623
143.8266
138.6625
136.0420
134.2758
132.6920
130.2251
130.0620
129.4189
122.6709
122.1430
119.5417
111.0372
79.1405
77.2112
77.0000
76.7888
63.5617
20.8760
20.3001
15.3183
X : parts per Million : Carbon13
Filename = yd4041-5_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4041-5
Solvent = CHLOROFORM-D
Creation_Time = 22-JAN-2016 22:04:17
Revision_Time = 22-JAN-2016 22:15:24
Current_Time = 22-JAN-2016 22:16:12
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 24.1[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OEt
3ac

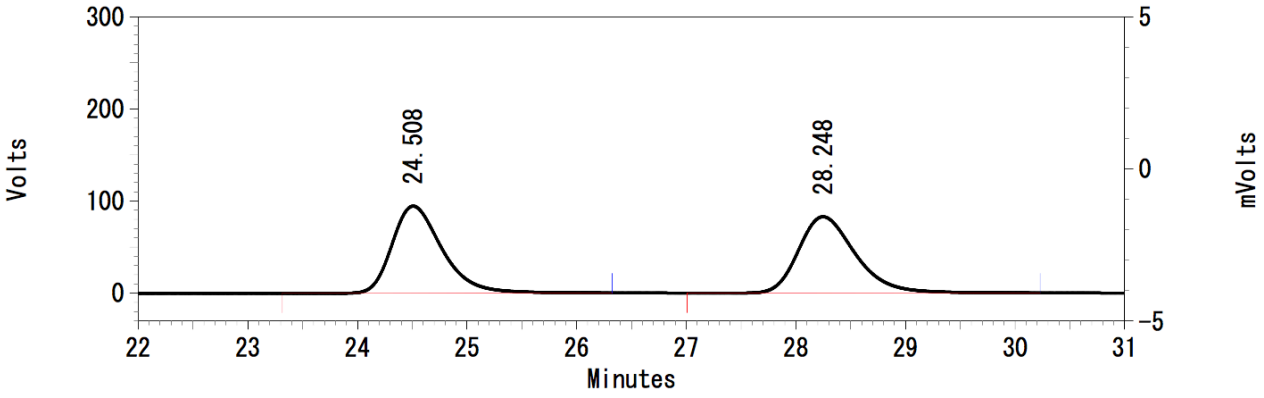


3ac



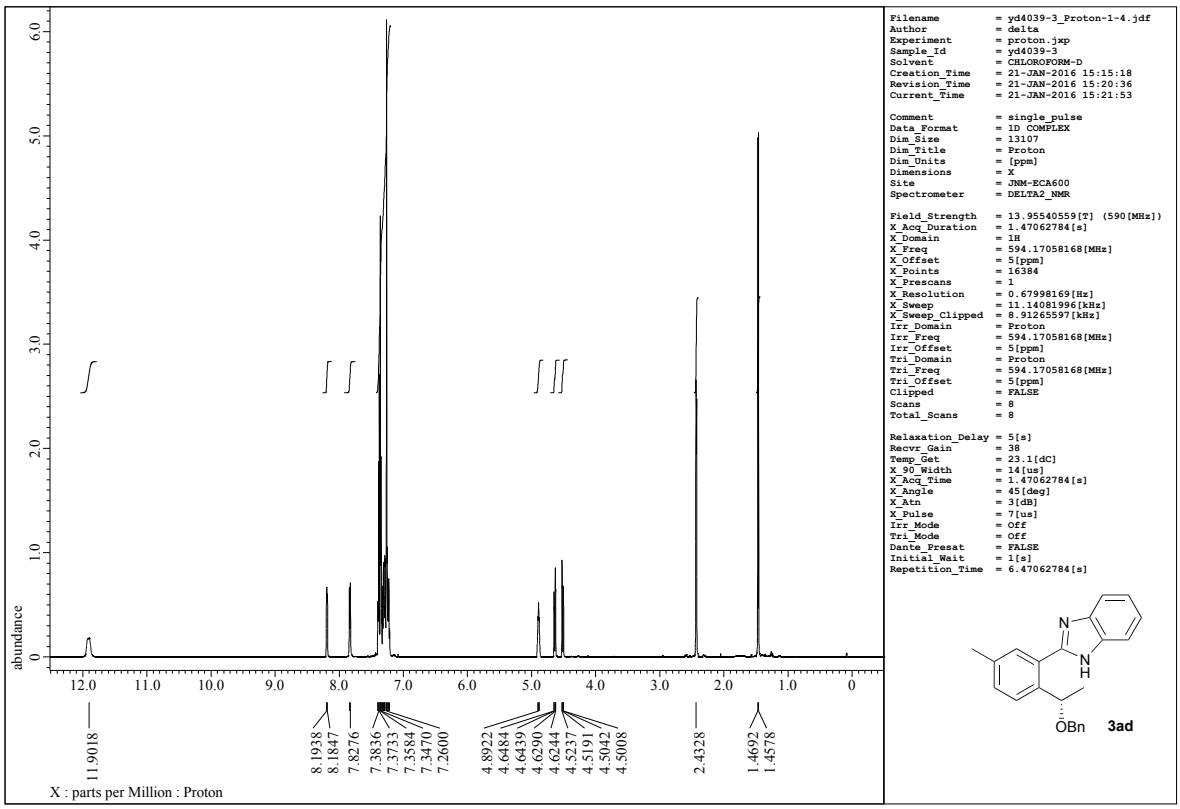
UV Results

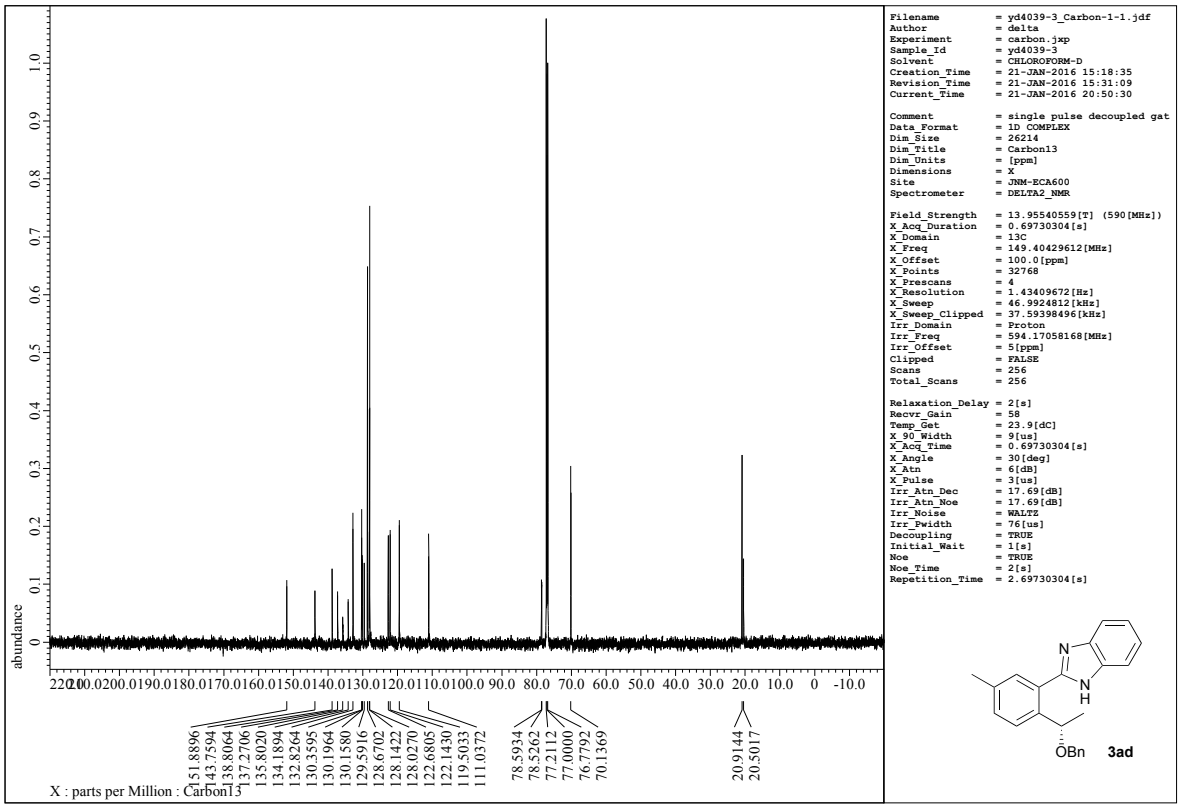
Pk #	Retention Time	Area	Area Percent	Height
1	24.498	6275931	91.850	196449
2	28.320	556863	8.150	15766

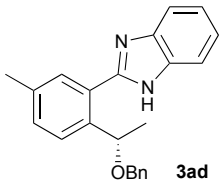


UV Results

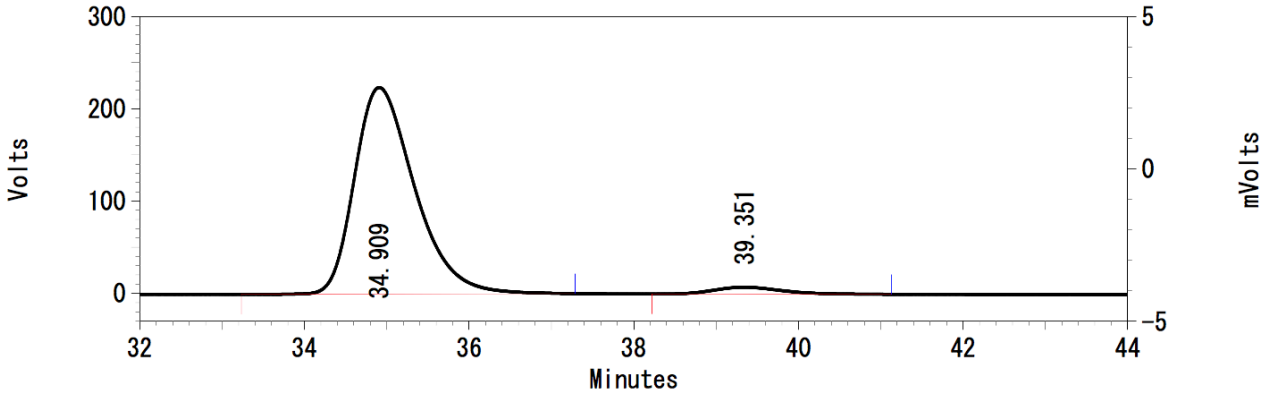
Pk #	Retention Time	Area	Area Percent	Height
1	24.508	2990656	50.064	94340
2	28.248	2983003	49.936	82708


abundance
X : parts per Million : Proton
11.9018
8.1938
8.1847
7.8276
7.3836
7.3733
7.3584
7.3470
7.2600
4.8922
4.6484
4.6439
4.6290
4.6244
4.5237
4.5191
4.5042
4.5008
2.4328
1.4692
1.4578
Filename = yd4039-3_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4039-3
Solvent = CHLOROFORM-D
Creation_Time = 21-JAN-2016 15:15:18
Revision_Time = 21-JAN-2016 15:20:36
Current_Time = 21-JAN-2016 15:21:53
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 23.1[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OBn
3ad


abundance
X : parts per Million : Carbon13
151.8896
143.7594
138.8064
137.2706
135.8020
134.1894
132.8264
130.3595
130.1964
130.1580
129.5916
128.6702
128.1422
128.0270
122.6805
122.1430
119.5033
111.0372
78.5934
78.5262
77.2112
77.0000
76.7792
70.1369
20.9144
20.5017
Filename = yd4039-3_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4039-3
Solvent = CHLOROFORM-D
Creation_Time = 21-JAN-2016 15:18:35
Revision_Time = 21-JAN-2016 15:31:09
Current_Time = 21-JAN-2016 20:50:30
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 23.9[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OBn
3ad

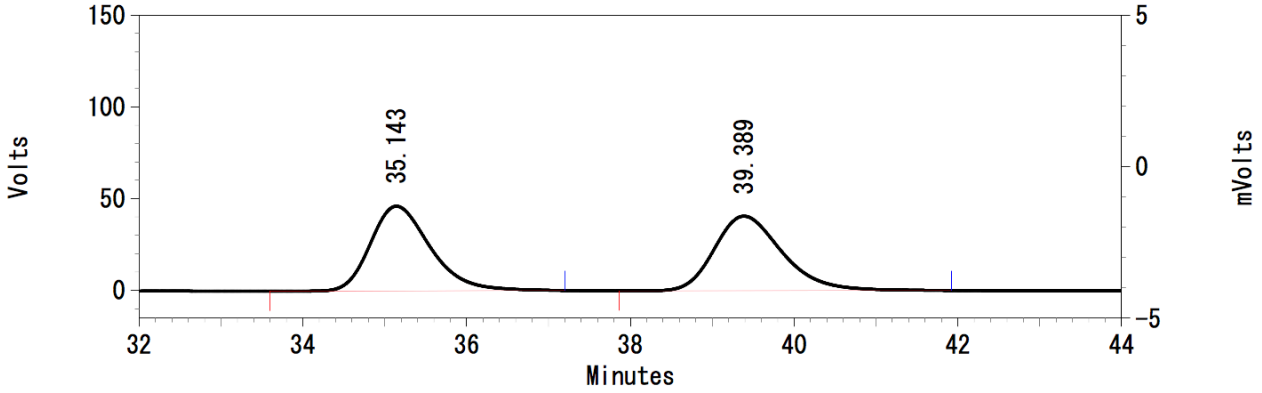


3ad



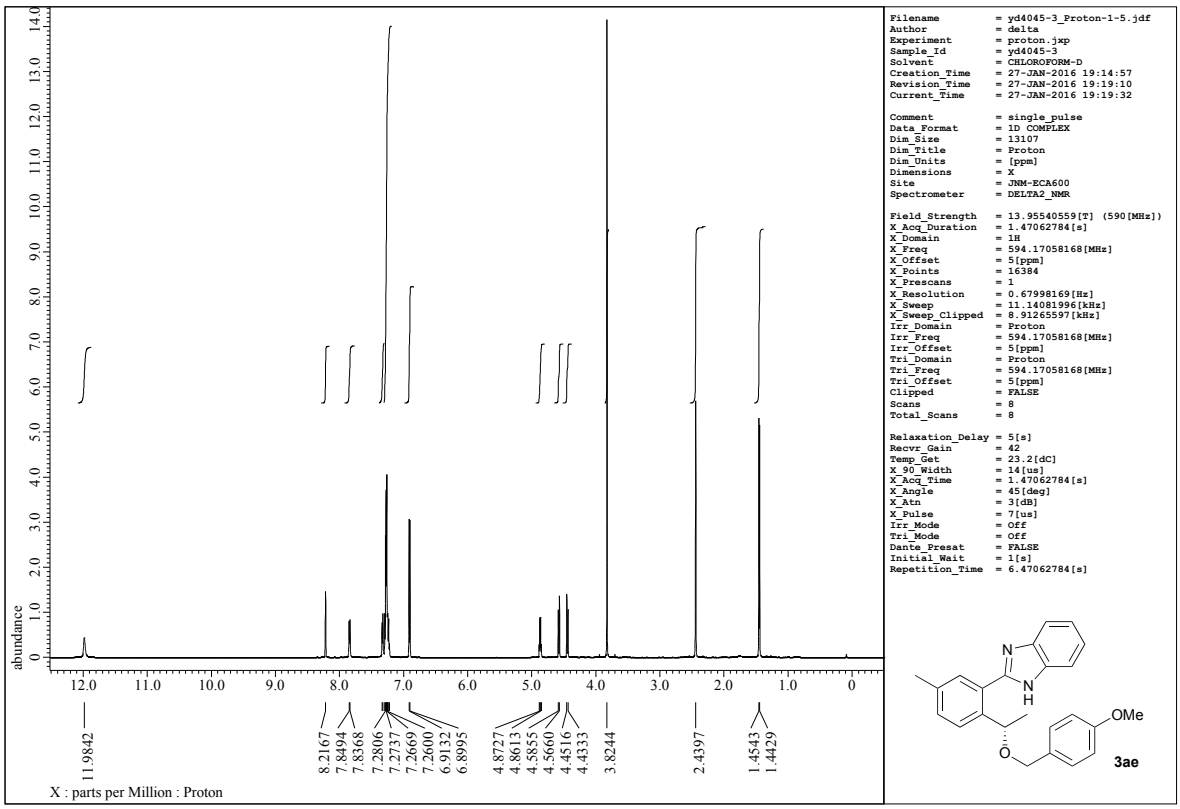
UV Results

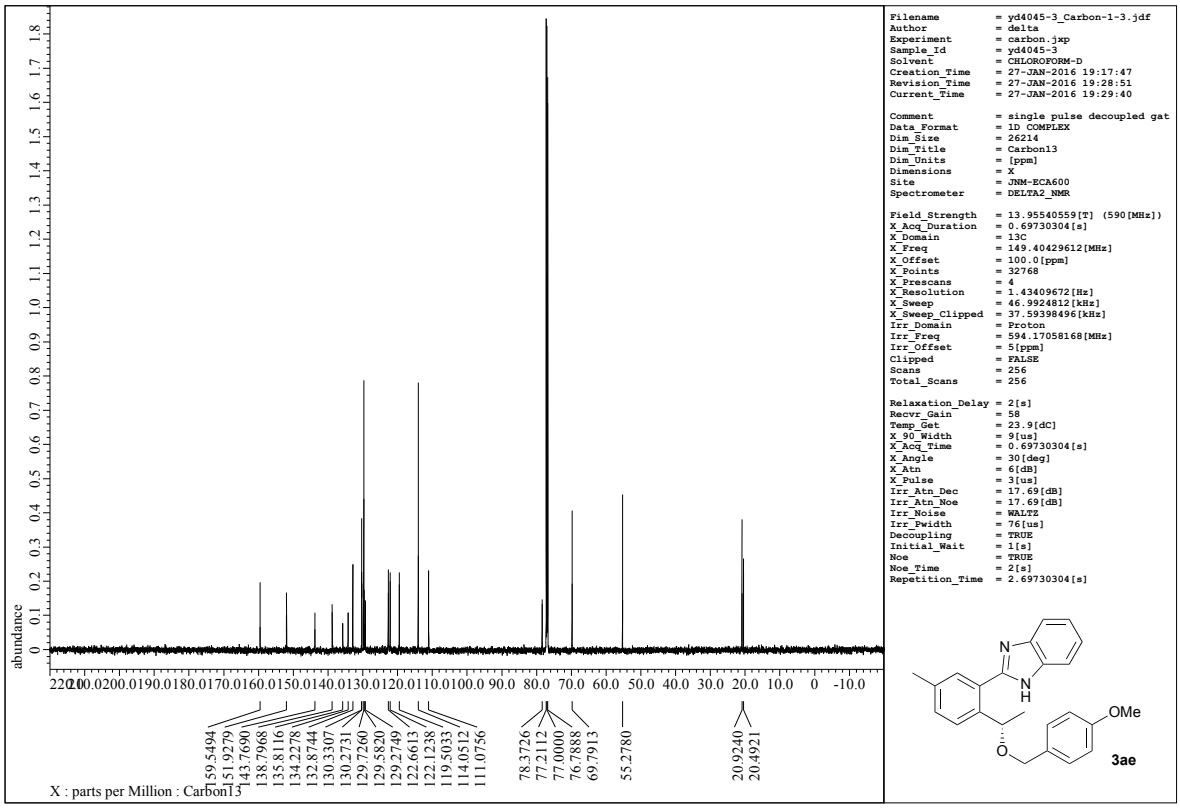
Pk #	Retention Time	Area	Area Percent	Height
1	34.909	11349853	96.367	223693
2	39.351	427877	3.633	7540

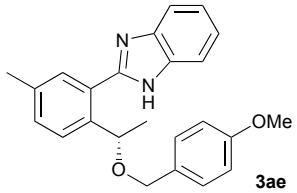


UV Results

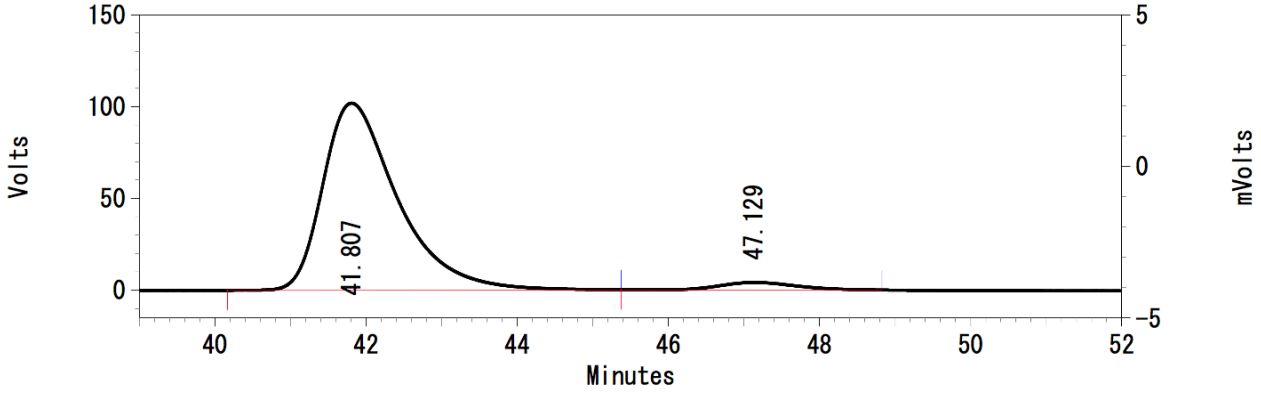
Pk #	Retention Time	Area	Area Percent	Height
1	35.143	2338314	50.047	46110
2	39.389	2333917	49.953	40566


Filename = yd4045-3_Proton-1-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4045-3
Solvent = CHLOROFORM-D
Creation_Time = 27-JAN-2016 19:14:57
Revision_Time = 27-JAN-2016 19:19:10
Current_Time = 27-JAN-2016 19:19:32
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 23.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
abundance
11.9842
8.2167
7.8494
7.8368
7.2806
7.2737
7.2669
7.2600
6.9132
6.8995
4.8727
4.8613
4.5855
4.5660
4.4516
4.4333
3.8244
2.4397
1.4543
1.4429
X : parts per Million : Proton
N
N
H
OMe
O
3ae


Filename = yd4045-3_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4045-3
Solvent = CHLOROFORM-D
Creation_Time = 27-JAN-2016 19:17:47
Revision_Time = 27-JAN-2016 19:28:51
Current_Time = 27-JAN-2016 19:29:40
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 23.9[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
abundance
159.5494
151.9279
143.7690
138.7968
135.8116
134.2278
132.8744
130.3307
130.2731
129.7260
129.5820
129.2749
122.6613
122.1238
119.5033
114.0512
111.0756
78.3726
77.2112
77.0000
76.7888
69.7913
55.2780
20.9240
20.4921
X : parts per Million : Carbon13
N
N
H
OMe
O
3ae

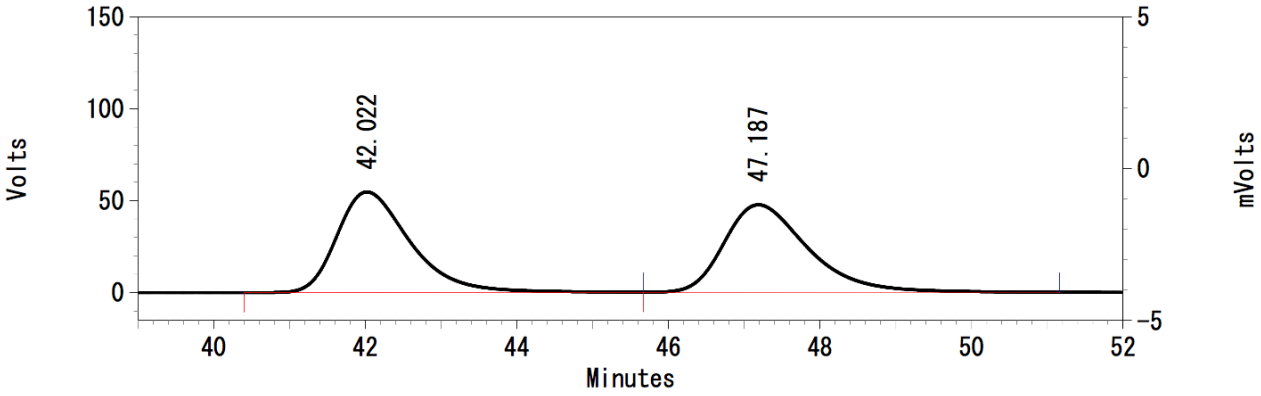


3ae



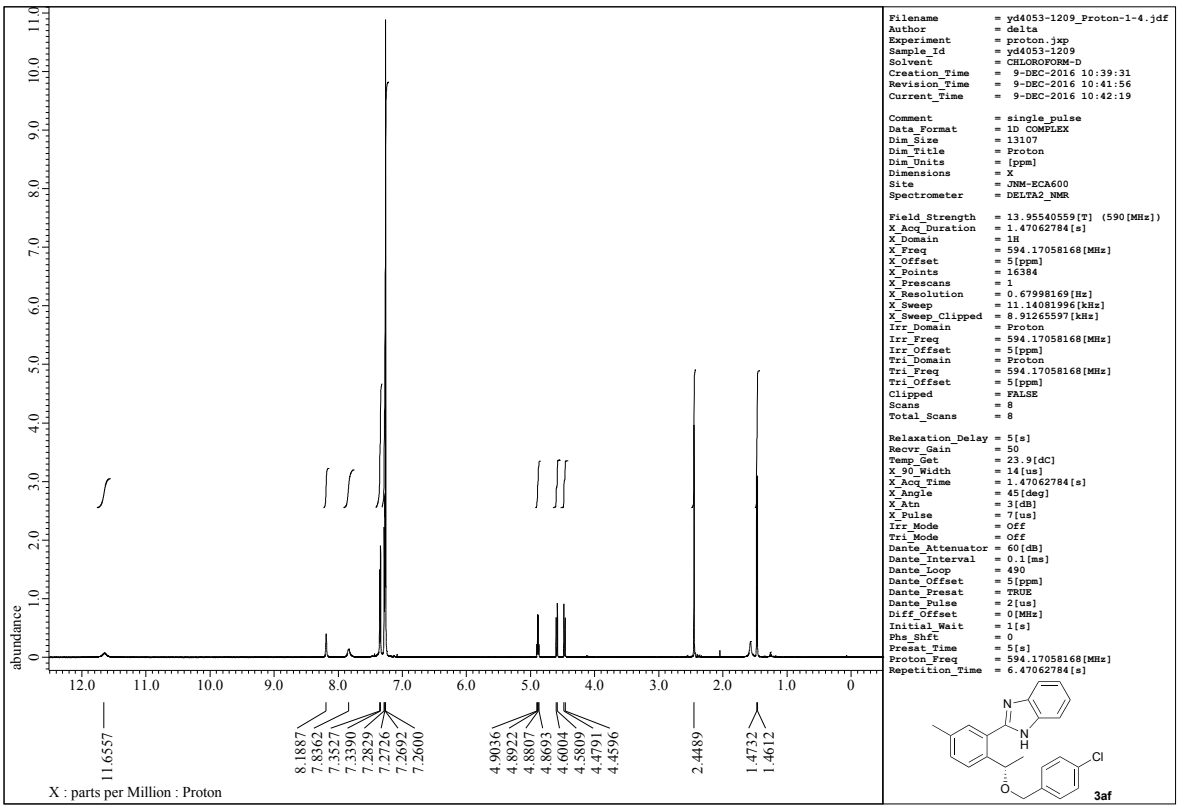
UV Results

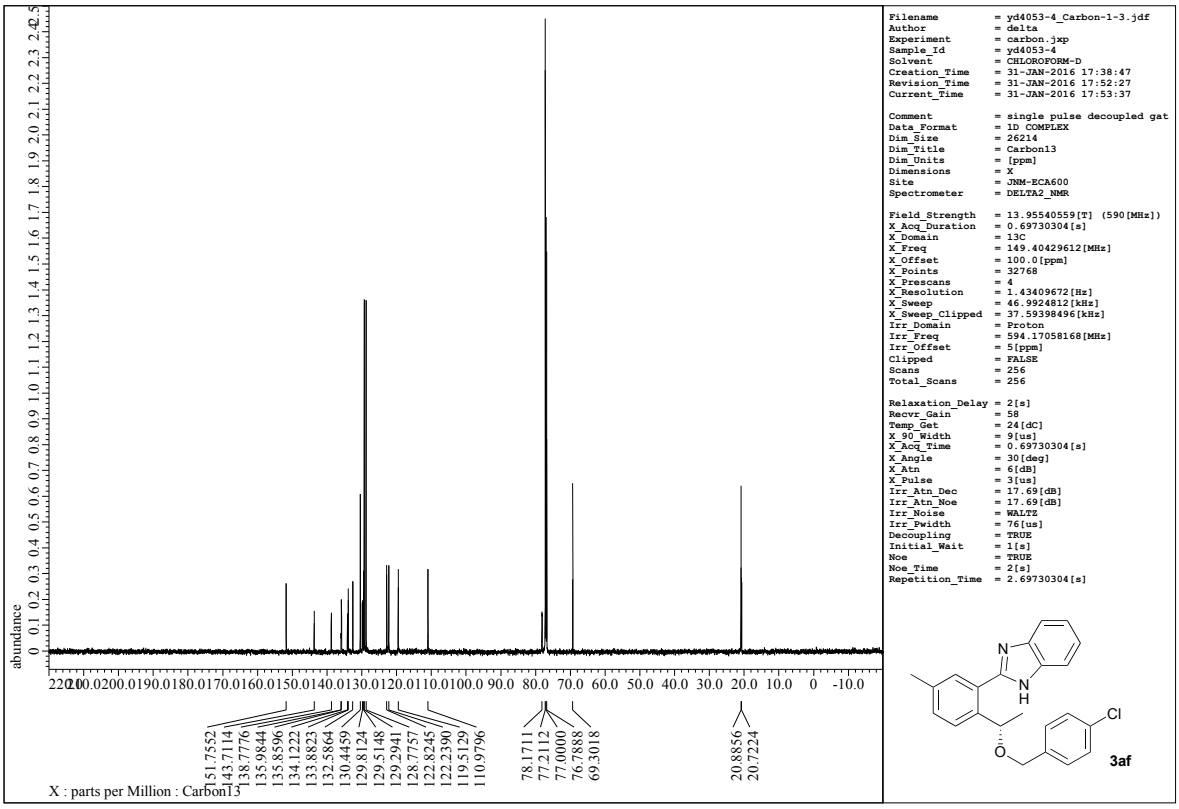
Pk #	Retention Time	Area	Area Percent	Height
1	41.807	7002882	95.873	101851
2	47.129	301474	4.127	4143

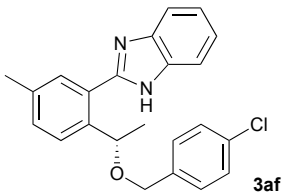


UV Results

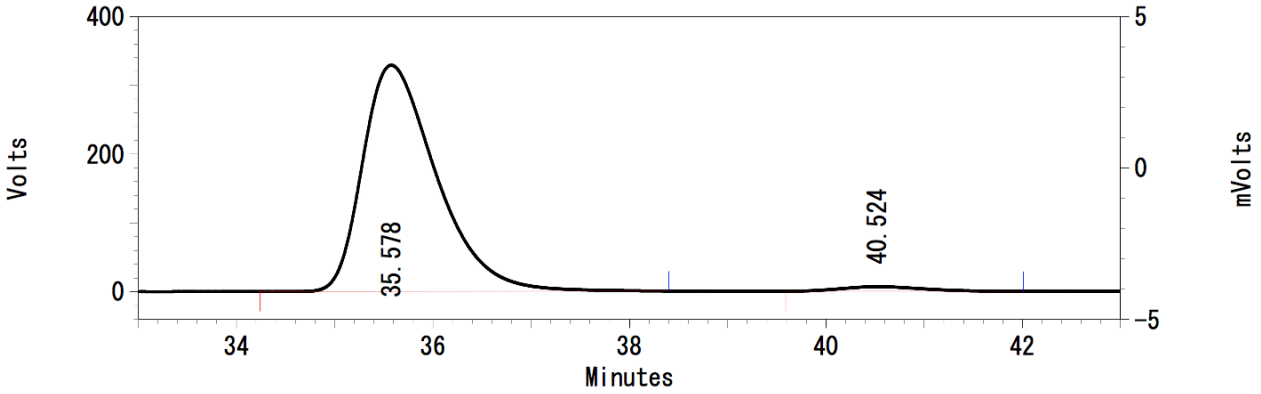
Pk #	Retention Time	Area	Area Percent	Height
1	42.022	3695214	50.095	54673
2	47.187	3681198	49.905	47596


abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
11.6557
8.1887 7.8362 7.3527 7.3390 7.2829 7.2726 7.2692 7.2600
4.9036 4.8922 4.8807 4.8693 4.6004 4.5809 4.4791 4.4596
2.4489
1.4732 1.4612
X : parts per Million : Proton
Filename = yd4053-1209_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4053-1209
Solvent = CHLOROFORM-D
Creation_Time = 9-DEC-2016 10:39:31
Revision_Time = 9-DEC-2016 10:41:56
Current_Time = 9-DEC-2016 10:42:19
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 23.9[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Attenuator = 60[dB]
Dante_Interval = 0.1[ms]
Dante_Loop = 490
Dante_Offset = 5[ppm]
Dante_Presat = TRUE
Dante_Pulse = 2[us]
Diff_Offset = 0[MHz]
Initial_Wait = 1[s]
Phs_Shft = 0
Presat_Time = 5[s]
Proton_Freq = 594.17058168[MHz]
Repetition_Time = 6.47062784[s]
N
H
O
Cl
3af


abundance
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
151.7552 143.7114 138.7776 135.9844 135.8596 134.1222 133.8823 132.5864 130.4459 129.8124 129.5148 129.2941 128.7757 122.8245 122.2390 119.5129 110.9796
78.1711 77.2112 77.0000 76.7888 69.3018
20.8856 20.7224
X : parts per Million : Carbon13
Filename = yd4053-4_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4053-4
Solvent = CHLOROFORM-D
Creation_Time = 31-JAN-2016 17:38:47
Revision_Time = 31-JAN-2016 17:52:27
Current_Time = 31-JAN-2016 17:53:37
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 24[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
H
O
Cl
3af

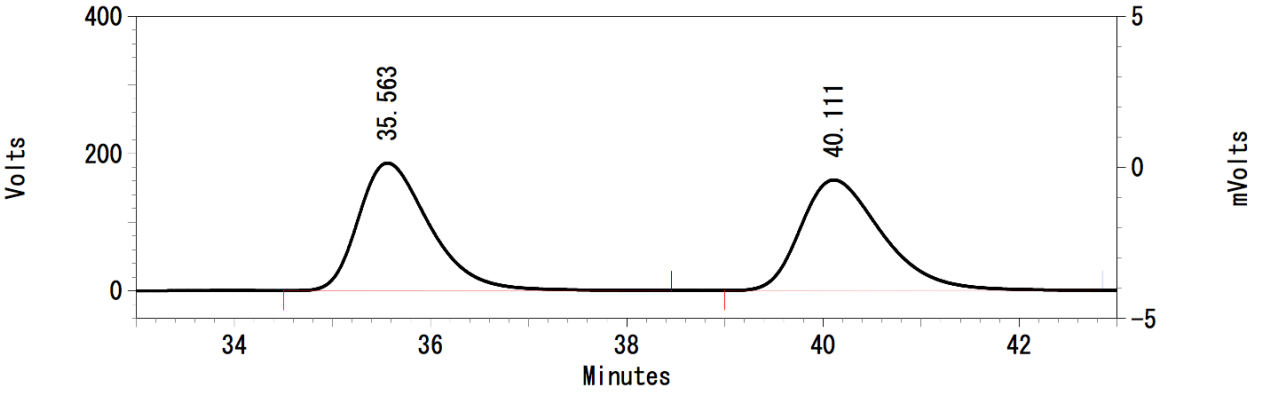


3af



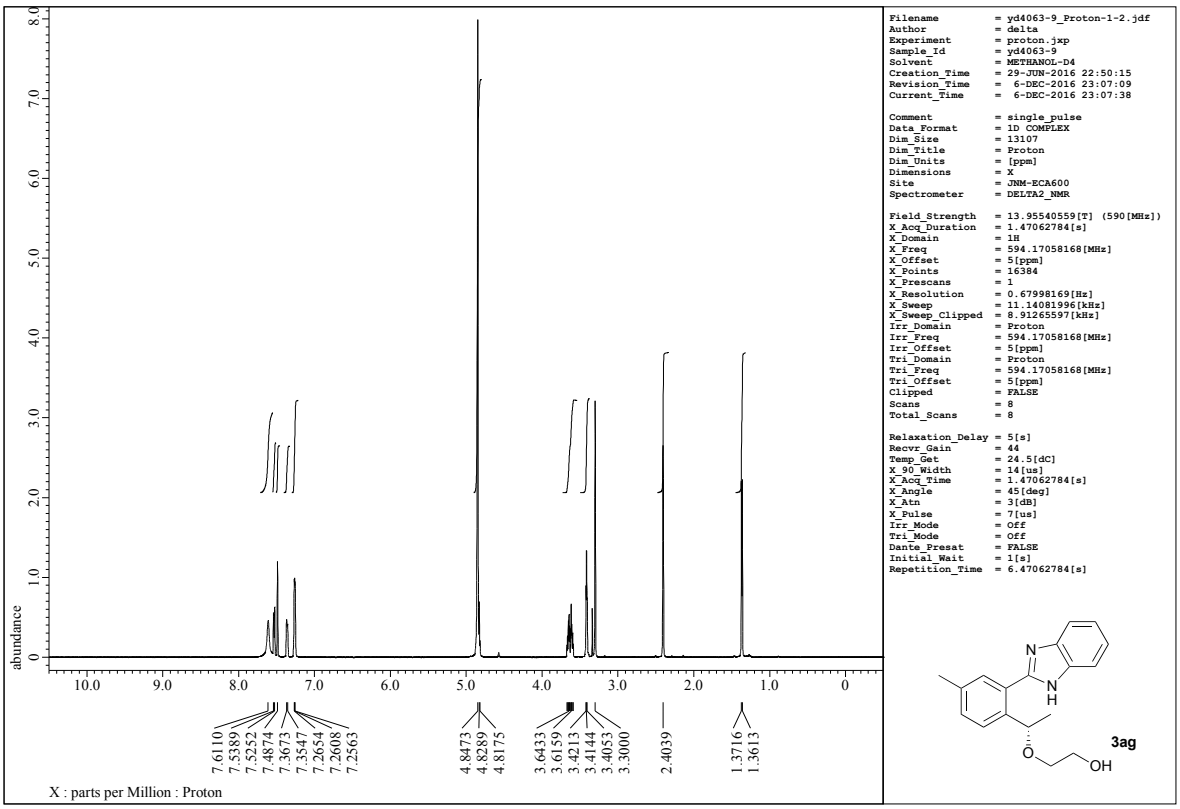
UV Results

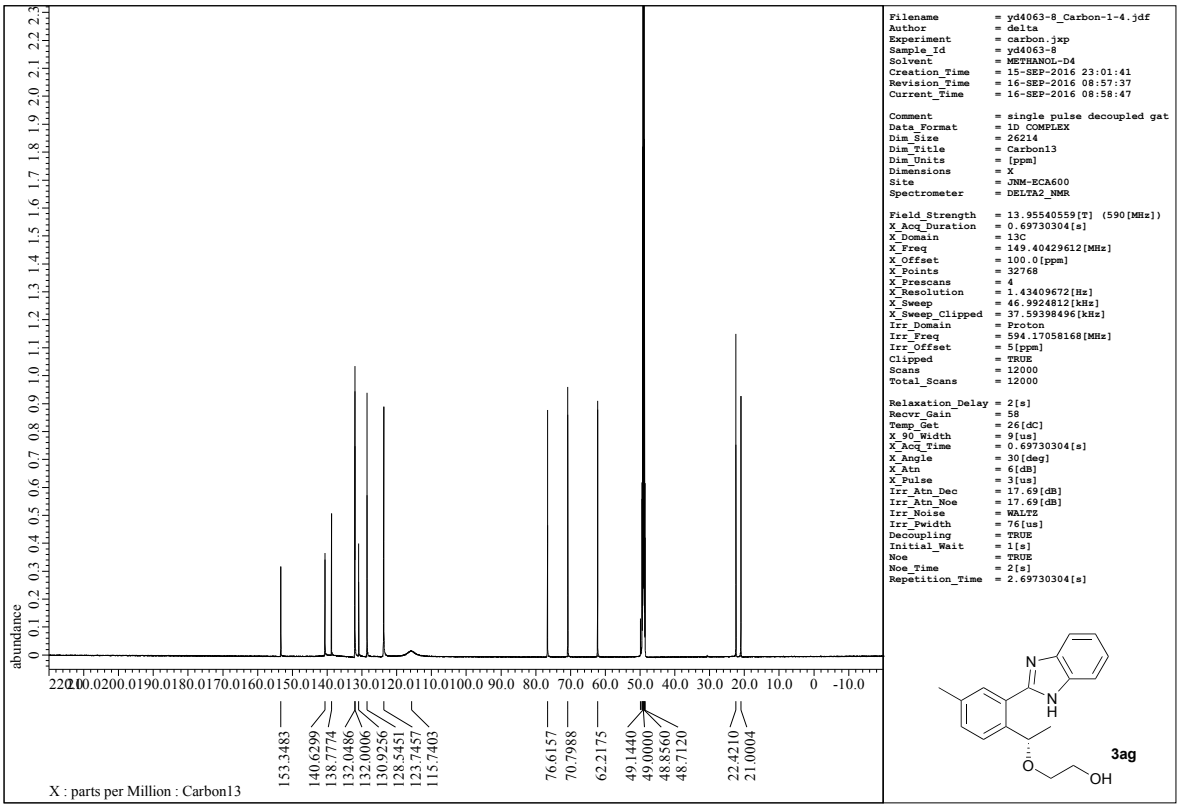
Pk #	Retention Time	Area	Area Percent	Height
1	35.578	17112594	97.833	328495
2	40.524	379114	2.167	6593

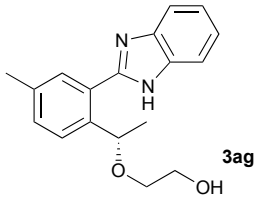


UV Results

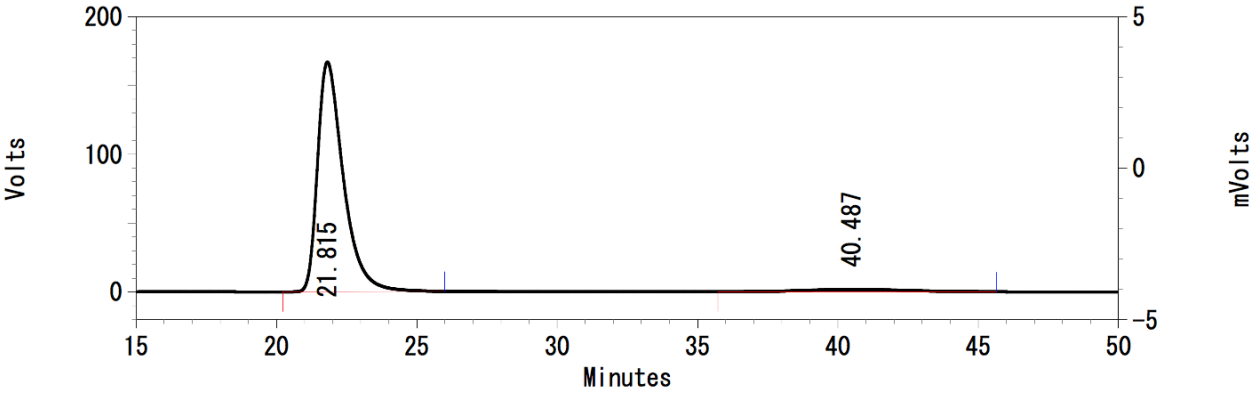
Pk #	Retention Time	Area	Area Percent	Height
1	35.563	9343966	50.143	185792
2	40.111	9290564	49.857	160920


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.6110 7.5389 7.5252 7.4874 7.3673 7.3547 7.2654 7.2608 7.2563
4.8473 4.8289 4.8175
3.6433 3.6159 3.4213 3.4144 3.4053 3.3000
2.4039
1.3716 1.3613
X : parts per Million : Proton
Filename = yd4063-9_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4063-9
Solvent = METHANOL-D4
Creation_Time = 29-JUN-2016 22:50:15
Revision_Time = 6-DEC-2016 23:07:09
Current_Time = 6-DEC-2016 23:07:38
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 24.5[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
O
OH
3ag


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
153.3483
140.6299 138.7774 132.0486 132.0006 130.9256 128.5451 123.7457 115.7403
76.6157 70.7988 62.2175 49.1440 49.0000 48.8560 48.7120
22.4210 21.0004
X : parts per Million : Carbon13
Filename = yd4063-8_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4063-8
Solvent = METHANOL-D4
Creation_Time = 15-SEP-2016 23:01:41
Revision_Time = 16-SEP-2016 08:57:37
Current_Time = 16-SEP-2016 08:58:47
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 12000
Total_Scans = 12000
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 26[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
O
OH
3ag

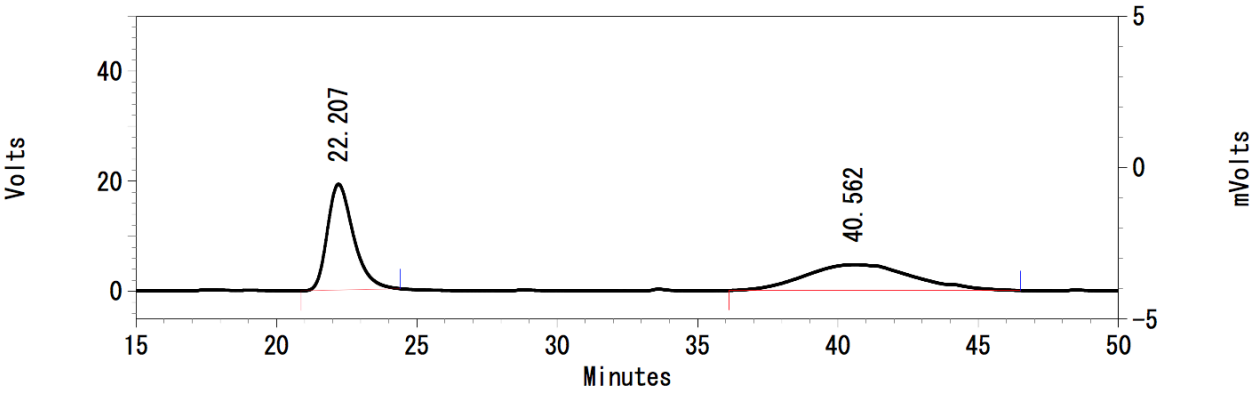


3ag



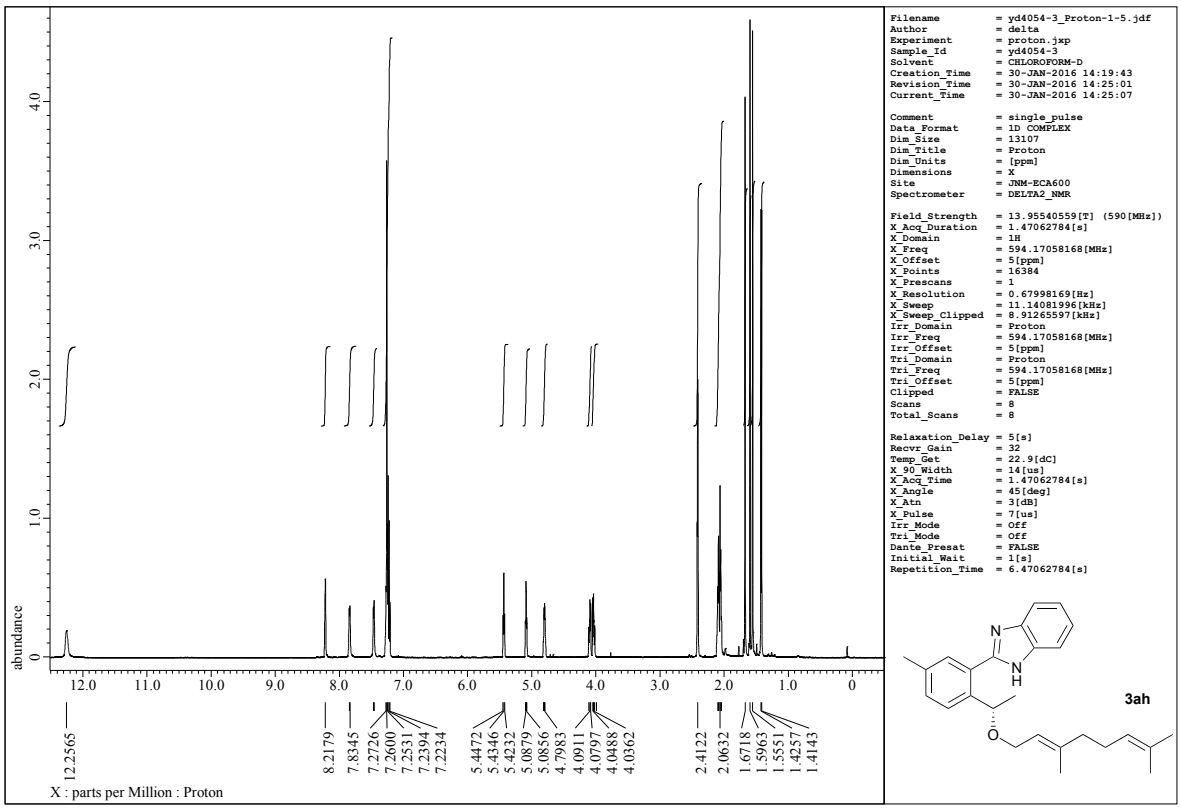
UV Results

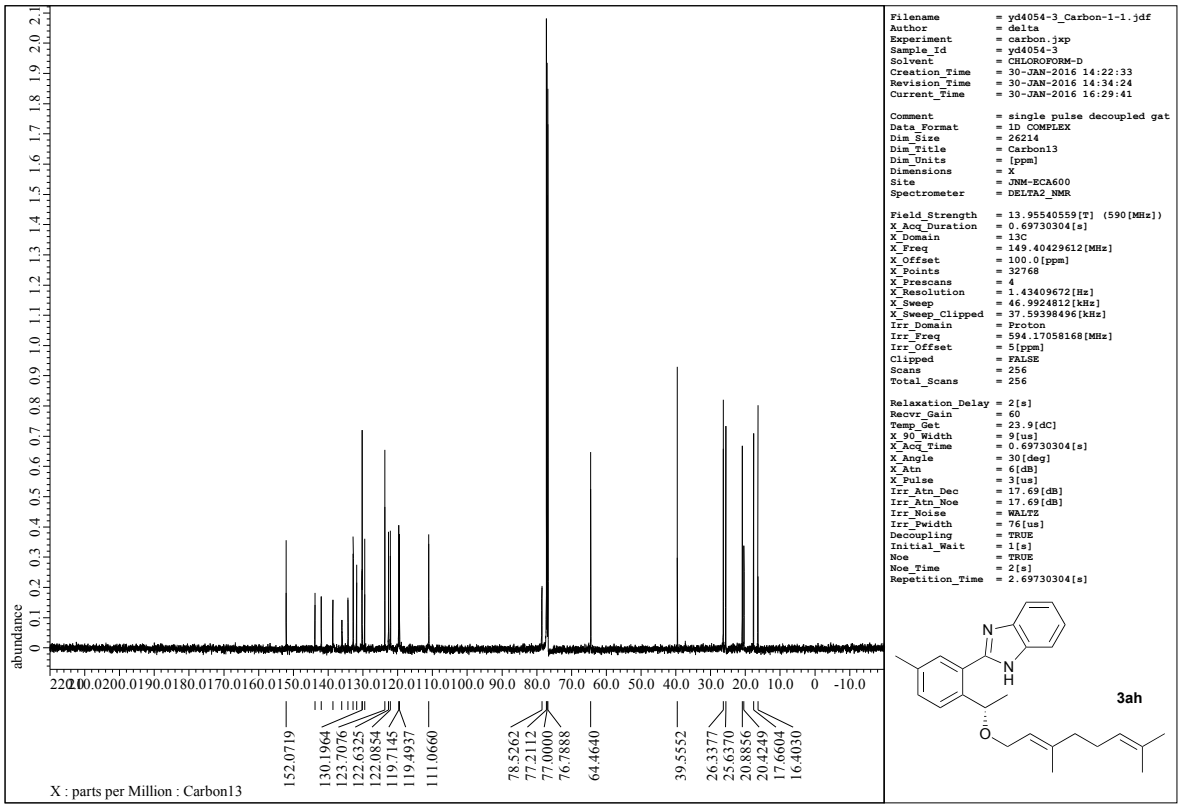
Pk #	Retention Time	Area	Area Percent	Height
1	21.815	10667183	96.020	166724
2	40.487	442153	3.980	1677

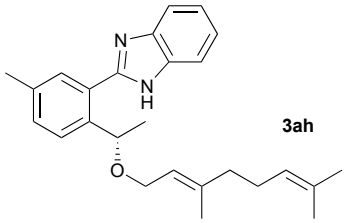


UV Results

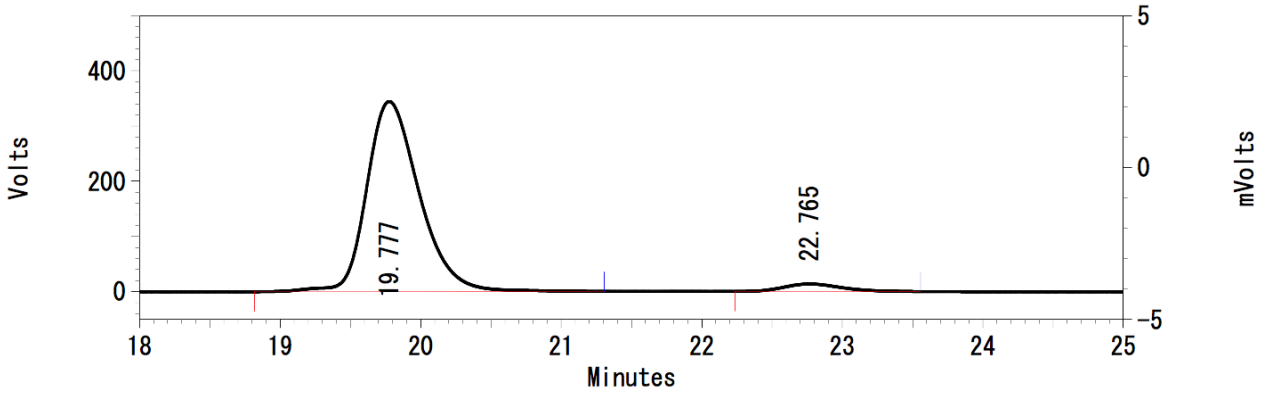
Pk #	Retention Time	Area	Area Percent	Height
1	22.207	1244553	49.859	19221
2	40.562	1251576	50.141	4691


Filename = yd4054-3_Proton-1-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4054-3
Solvent = CHLOROFORM-D
Creation_Time = 30-JAN-2016 14:19:43
Revision_Time = 30-JAN-2016 14:25:01
Current_Time = 30-JAN-2016 14:25:07
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 32
Temp_Get = 22.9[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.2565
8.2179 7.8345 7.2726 7.2600 7.2531 7.2394 7.2234
5.4472 5.4346 5.4232 5.0879 5.0856 4.7983 4.0911 4.0797 4.0488 4.0362
2.4122 2.0632 1.6718 1.5963 1.5551 1.4257 1.4143
X : parts per Million : Proton
N
N
H
O
3ah


Filename = yd4054-3_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4054-3
Solvent = CHLOROFORM-D
Creation_Time = 30-JAN-2016 14:22:33
Revision_Time = 30-JAN-2016 14:34:24
Current_Time = 30-JAN-2016 16:29:41
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 23.9[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
152.0719
130.1964 123.7076 122.6325 122.0854 119.7145 119.4937 111.0660
78.5262 77.2112 77.0000 76.7888 64.4640
39.5552 26.3377 25.6370 20.8856 20.4249 17.6604 16.4030
X : parts per Million : Carbon13
N
N
H
O
3ah

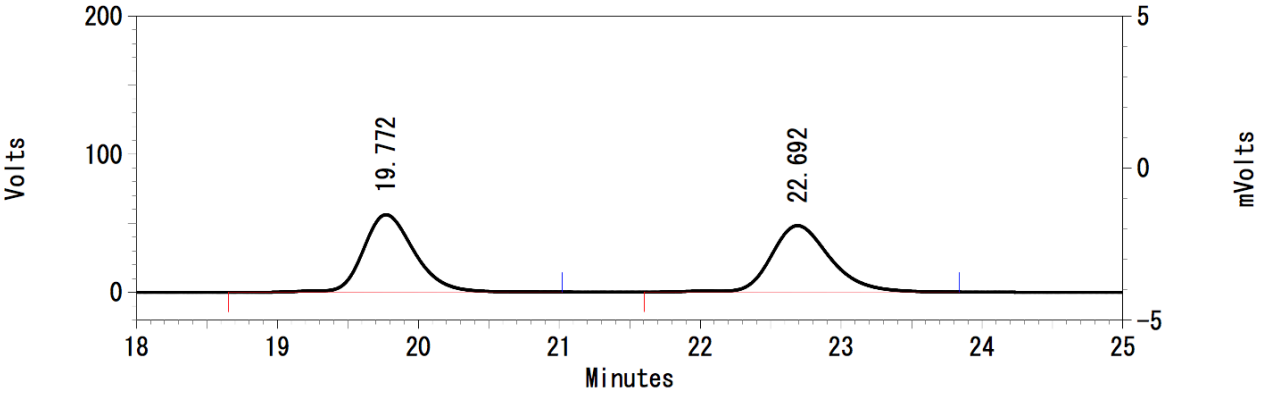


3ah



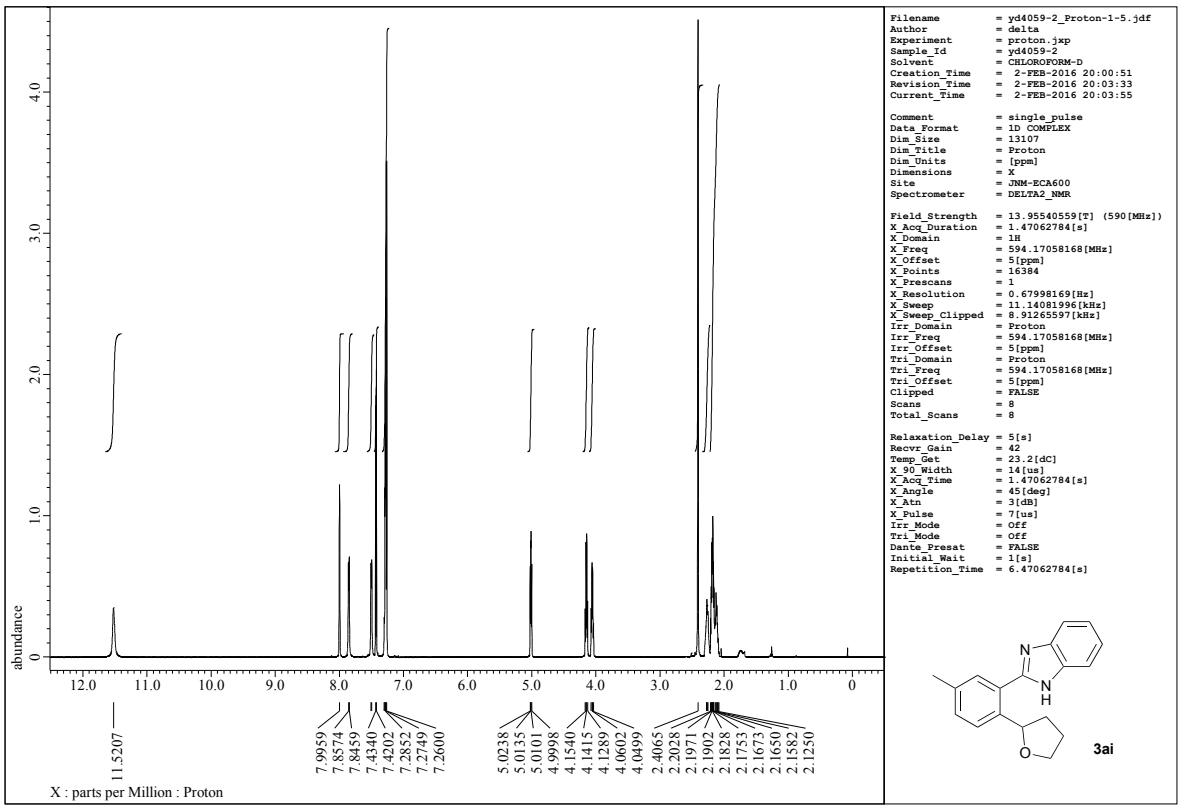
UV Results

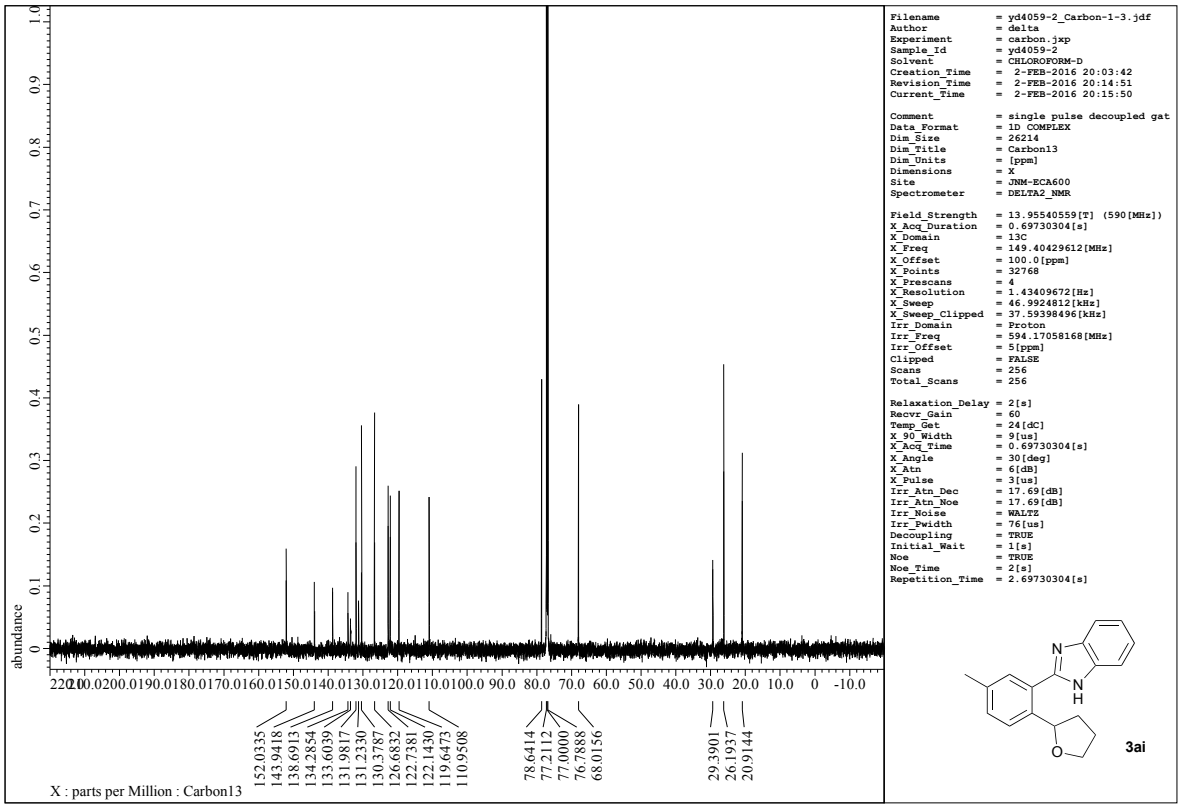
Pk #	Retention Time	Area	Area Percent	Height
1	19.777	8939902	95.870	344215
2	22.765	385077	4.130	13545

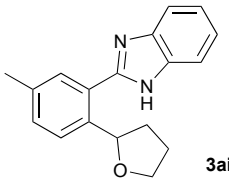


UV Results

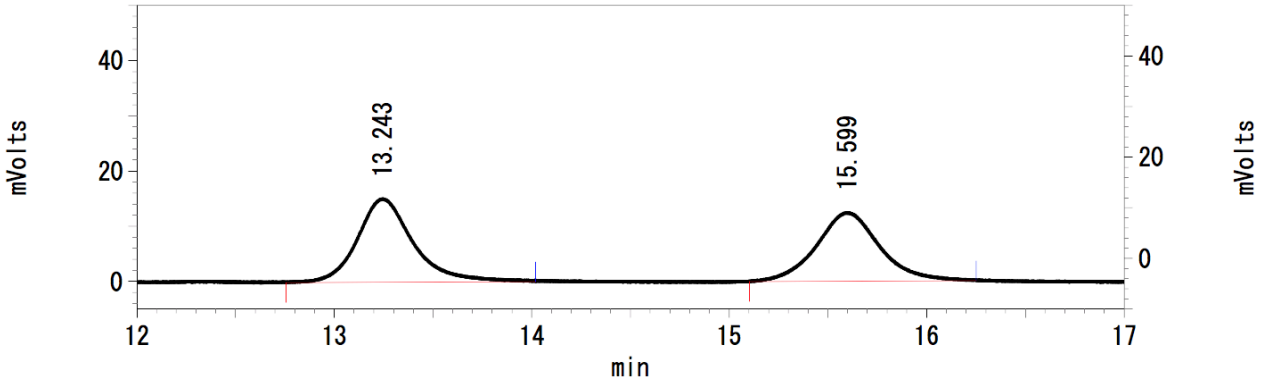
Pk #	Retention Time	Area	Area Percent	Height
1	19.772	1415934	50.153	56048
2	22.692	1407304	49.847	48097


abundance
X : parts per Million : Proton
11.5207
7.9959
7.8574
7.8459
7.4340
7.4202
7.2852
7.2749
7.2600
5.0238
5.0135
5.0101
4.9998
4.1540
4.1415
4.1289
4.0602
4.0499
2.4065
2.2028
2.1971
2.1902
2.1828
2.1753
2.1673
2.1650
2.1582
2.1250
Filename = yd4059-2_Proton-1-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4059-2
Solvent = CHLOROFORM-D
Creation_Time = 2-FEB-2016 20:00:51
Revision_Time = 2-FEB-2016 20:03:33
Current_Time = 2-FEB-2016 20:03:55
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 23.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
3ai

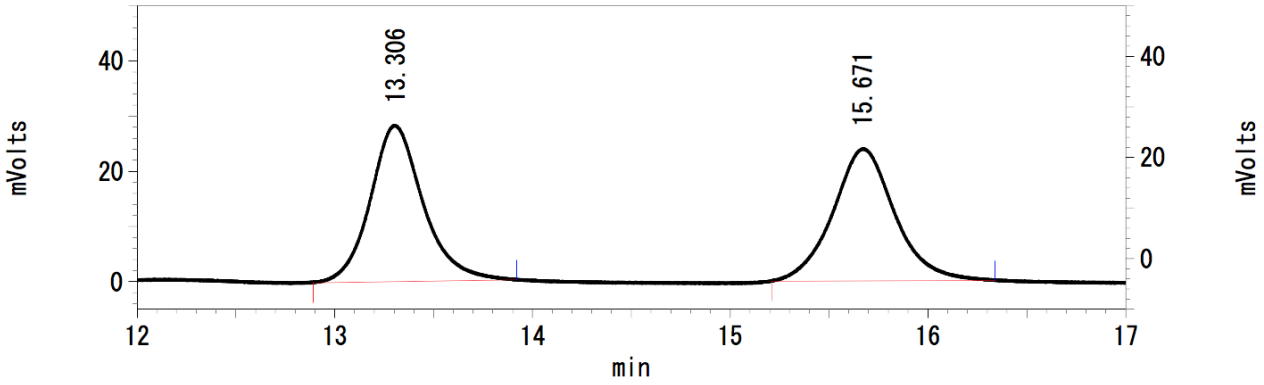

abundance
X : parts per Million : Carbon13
152.0335
143.9418
138.6913
134.2854
133.6039
131.9817
131.2330
130.3787
126.6832
122.7381
122.1430
119.6473
110.9508
78.6414
77.2112
77.0000
76.7888
68.0156
29.3901
26.1937
20.9144
Filename = yd4059-2_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4059-2
Solvent = CHLOROFORM-D
Creation_Time = 2-FEB-2016 20:03:42
Revision_Time = 2-FEB-2016 20:14:51
Current_Time = 2-FEB-2016 20:15:50
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
3ai



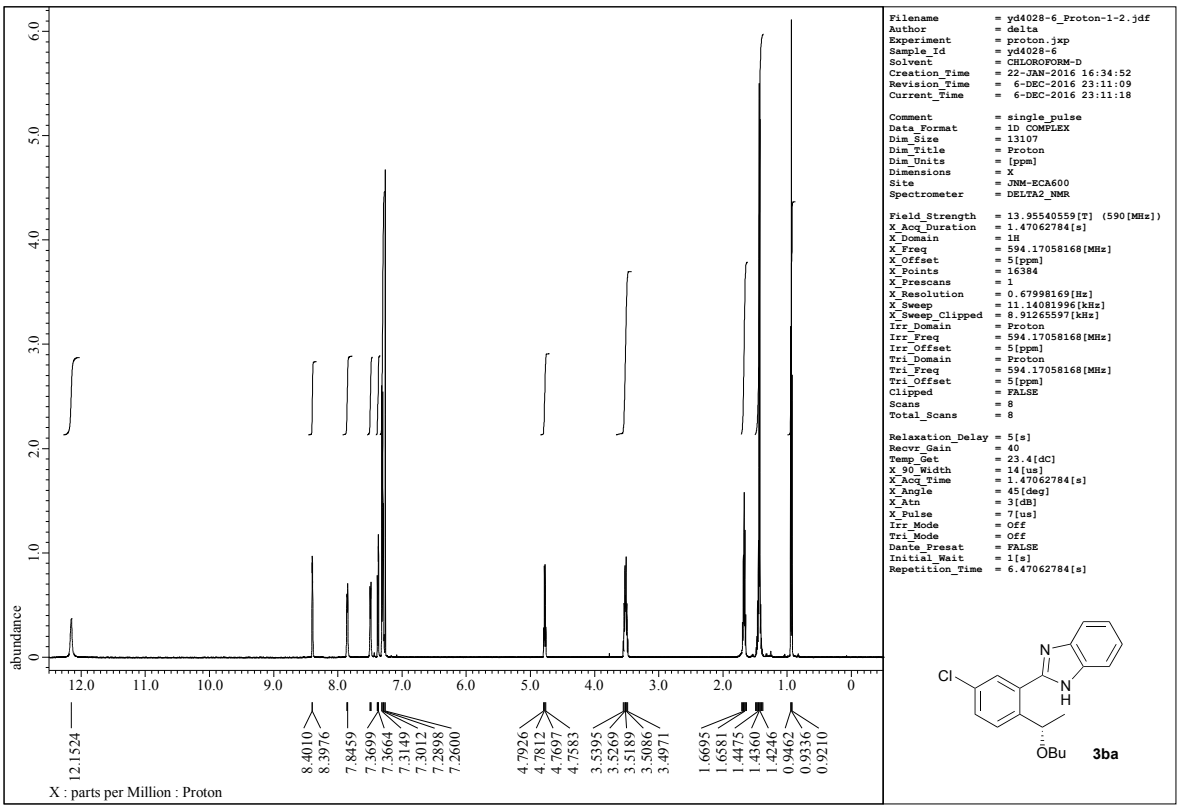
3ai

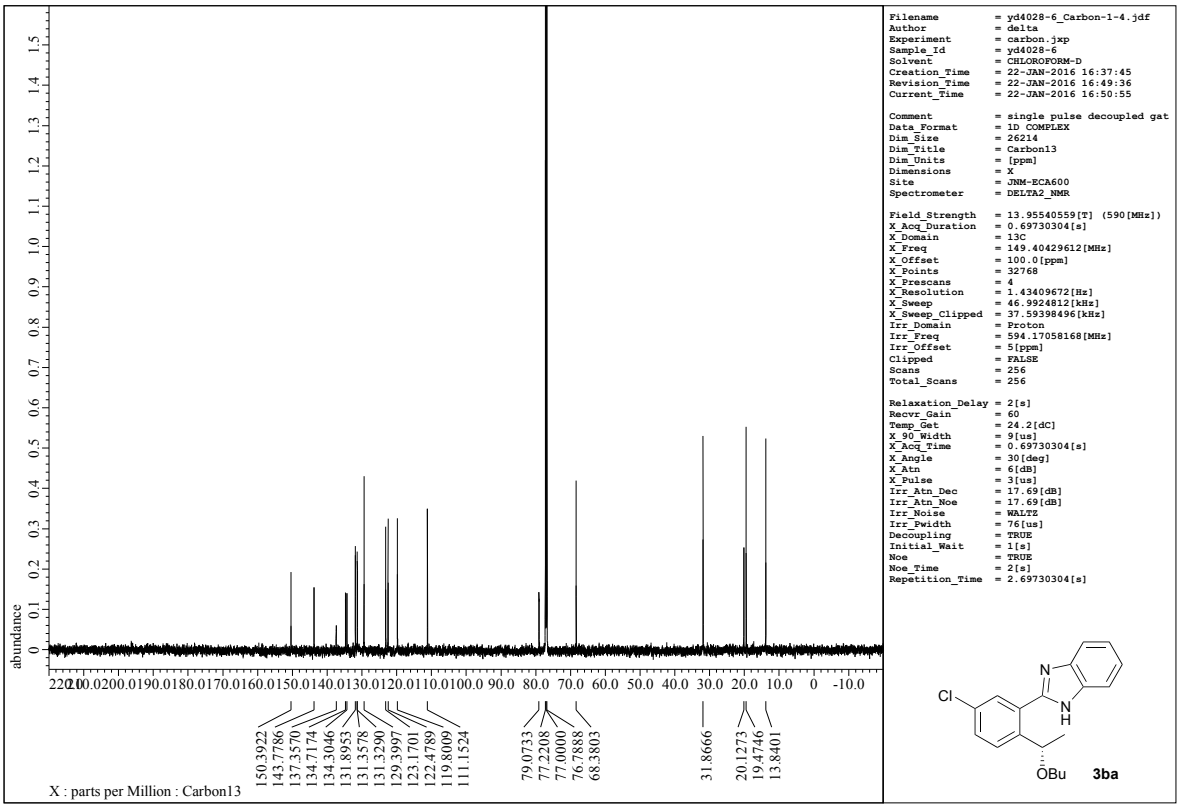


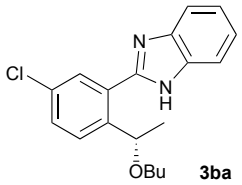
Pk #	Retention Time	Area	Area Percent
1	13.243	296211	51.651
2	15.599	277269	48.349



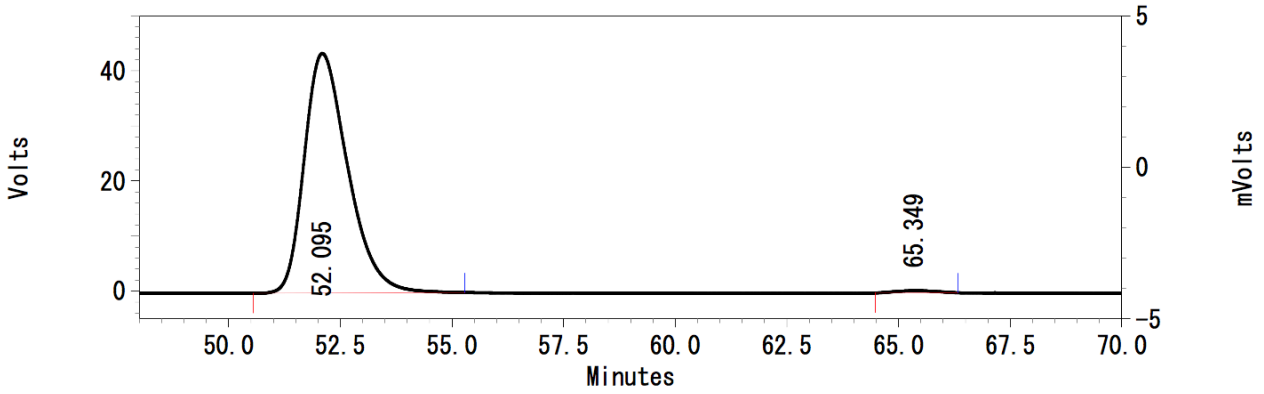
Pk #	Retention Time	Area	Area Percent
1	13.306	526083	50.248
2	15.671	520885	49.752


abundance
X : parts per Million : Proton
12.1524
8.4010
8.3976
7.8459
7.3699
7.3664
7.3149
7.3012
7.2898
7.2600
4.7926
4.7812
4.7697
4.7583
3.5395
3.5269
3.5189
3.5086
3.4971
1.6695
1.6581
1.4475
1.4360
1.4246
0.9462
0.9336
0.9210
Filename = yd4028-6_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4028-6
Solvent = CHLOROFORM-D
Creation_Time = 22-JAN-2016 16:34:52
Revision_Time = 6-DEC-2016 23:11:09
Current_Time = 6-DEC-2016 23:11:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 23.4[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Cl
N
N
H
OBu
3ba


abundance
X : parts per Million : Carbon13
150.3922
143.7786
137.3570
134.7174
134.3046
131.8953
131.3578
131.3290
129.3997
123.1701
122.4789
119.8009
111.1524
79.0733
77.2208
77.0000
76.7888
68.3803
31.8666
20.1273
19.4746
13.8401
Filename = yd4028-6_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4028-6
Solvent = CHLOROFORM-D
Creation_Time = 22-JAN-2016 16:37:45
Revision_Time = 22-JAN-2016 16:49:36
Current_Time = 22-JAN-2016 16:50:55
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.2[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
Cl
N
N
H
OBu
3ba

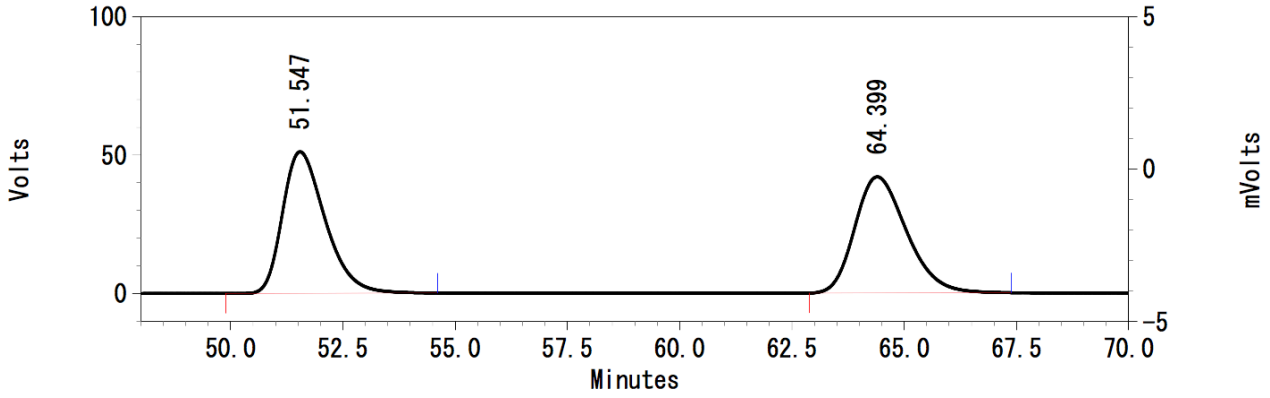


3ba



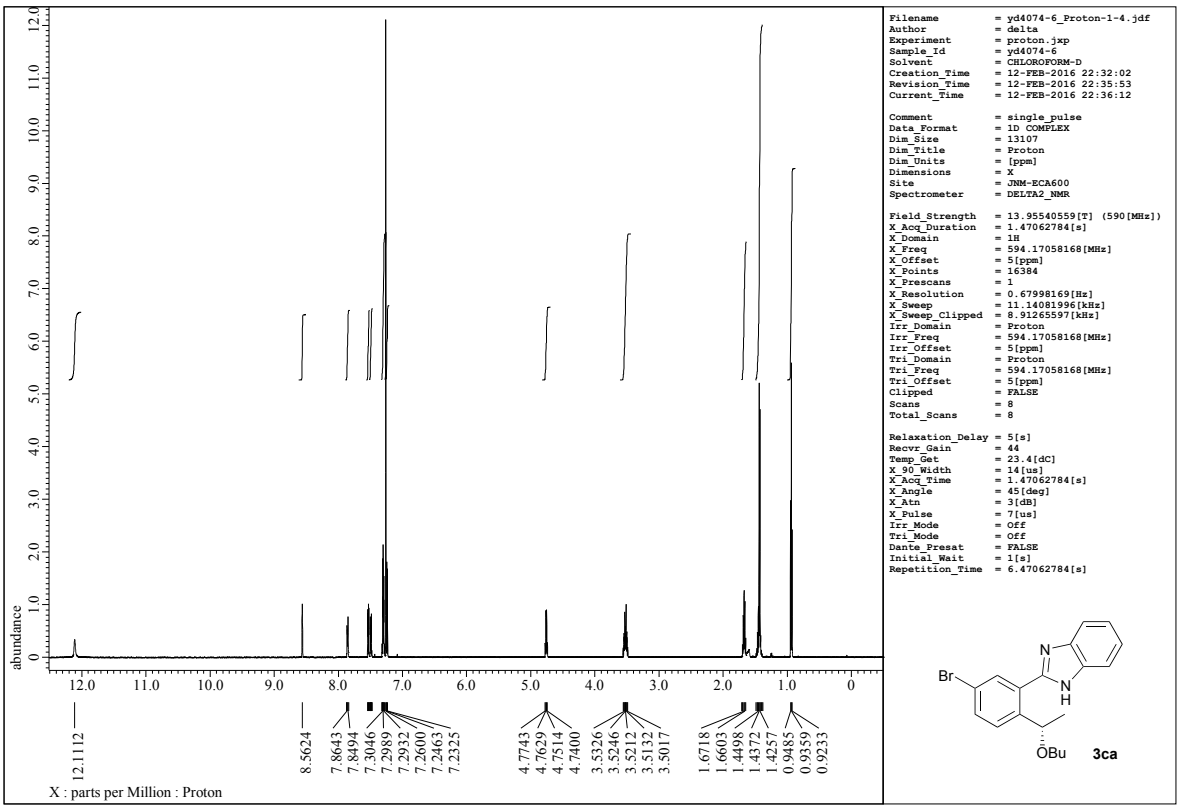
UV Results

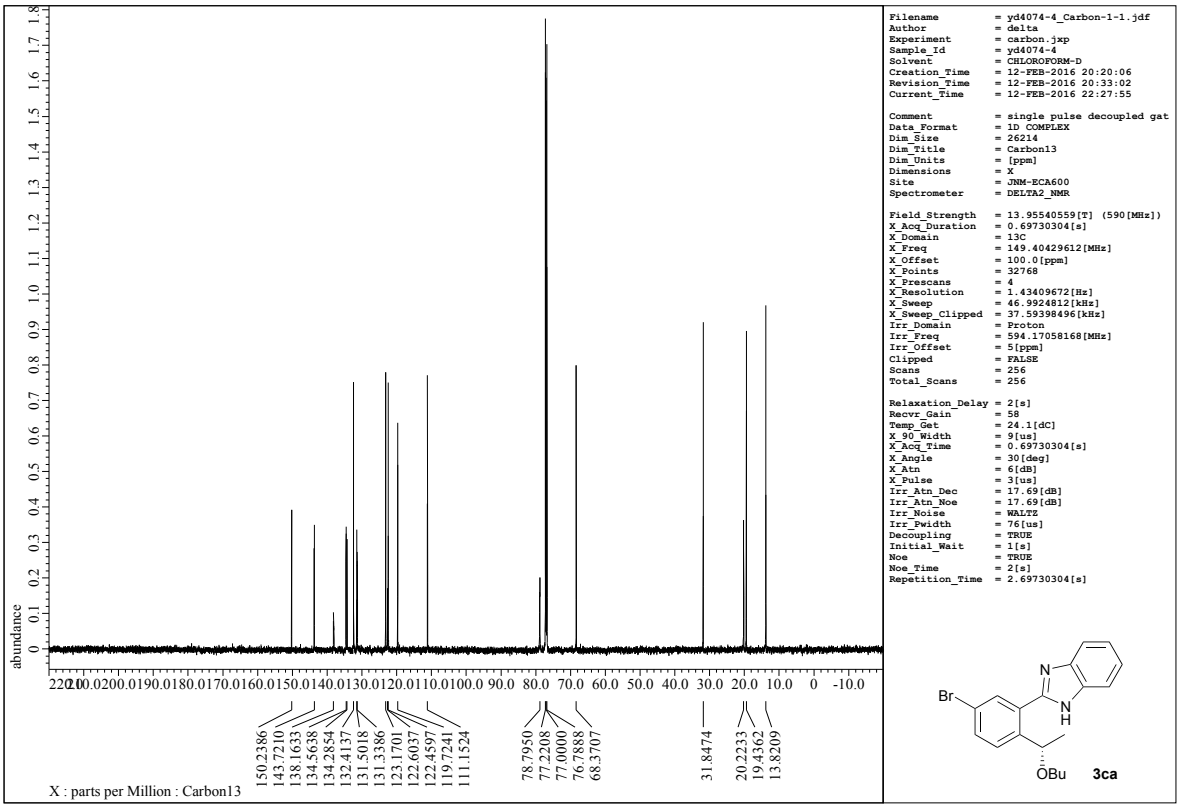
Pk #	Retention Time	Area	Area Percent	Height
1	52.095	2951760	99.178	43499
2	65.349	24472	0.822	398

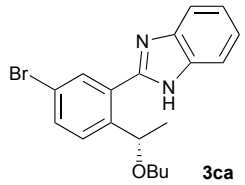


UV Results

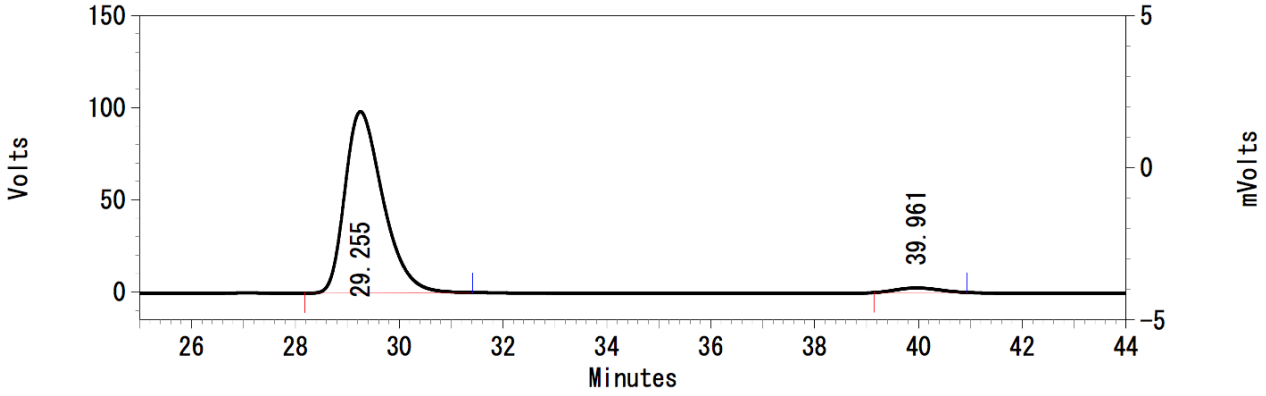
Pk #	Retention Time	Area	Area Percent	Height
1	51.547	3367419	50.086	51027
2	64.399	3355829	49.914	41876


abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.1112
8.5624
7.8643
7.8494
7.3046
7.2989
7.2932
7.2600
7.2463
7.2325
4.7743
4.7629
4.7514
4.7400
3.5326
3.5246
3.5212
3.5132
3.5017
1.6718
1.6603
1.4498
1.4372
1.4257
0.9485
0.9359
0.9233
X : parts per Million : Proton
Filename = yd4074-6_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4074-6
Solvent = CHLOROFORM-D
Creation_Time = 12-FEB-2016 22:32:02
Revision_Time = 12-FEB-2016 22:35:53
Current_Time = 12-FEB-2016 22:36:12
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 23.4[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Br
N
N
H
OBu
3ca


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
150.2386
143.7210
138.1633
134.5638
134.2854
132.4137
131.5018
131.3386
123.1701
122.6037
122.4597
119.7241
111.1524
78.7950
77.2208
77.0000
76.7888
68.3707
31.8474
20.2233
19.4362
13.8209
X : parts per Million : Carbon13
Filename = yd4074-4_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4074-4
Solvent = CHLOROFORM-D
Creation_Time = 12-FEB-2016 20:20:06
Revision_Time = 12-FEB-2016 20:33:02
Current_Time = 12-FEB-2016 22:27:55
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 24.1[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
Br
N
N
H
OBu
3ca

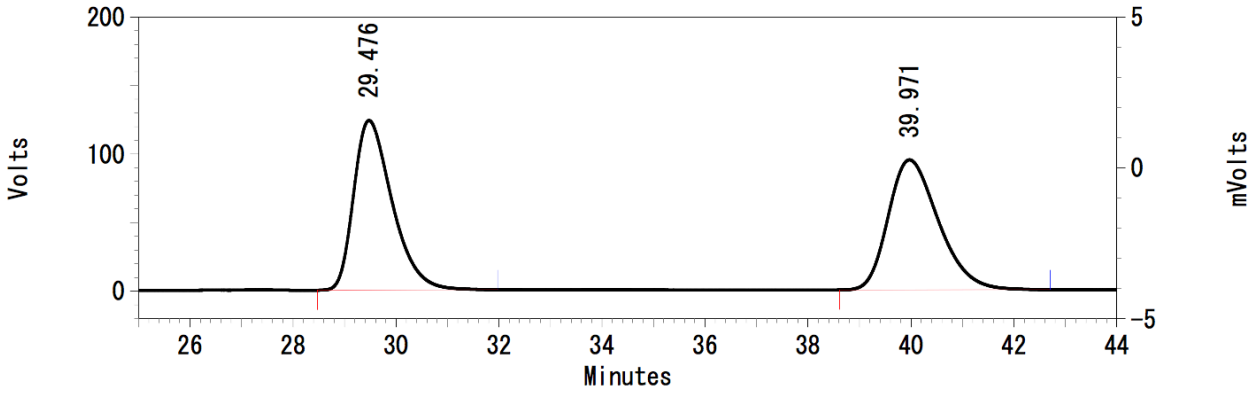


3ca



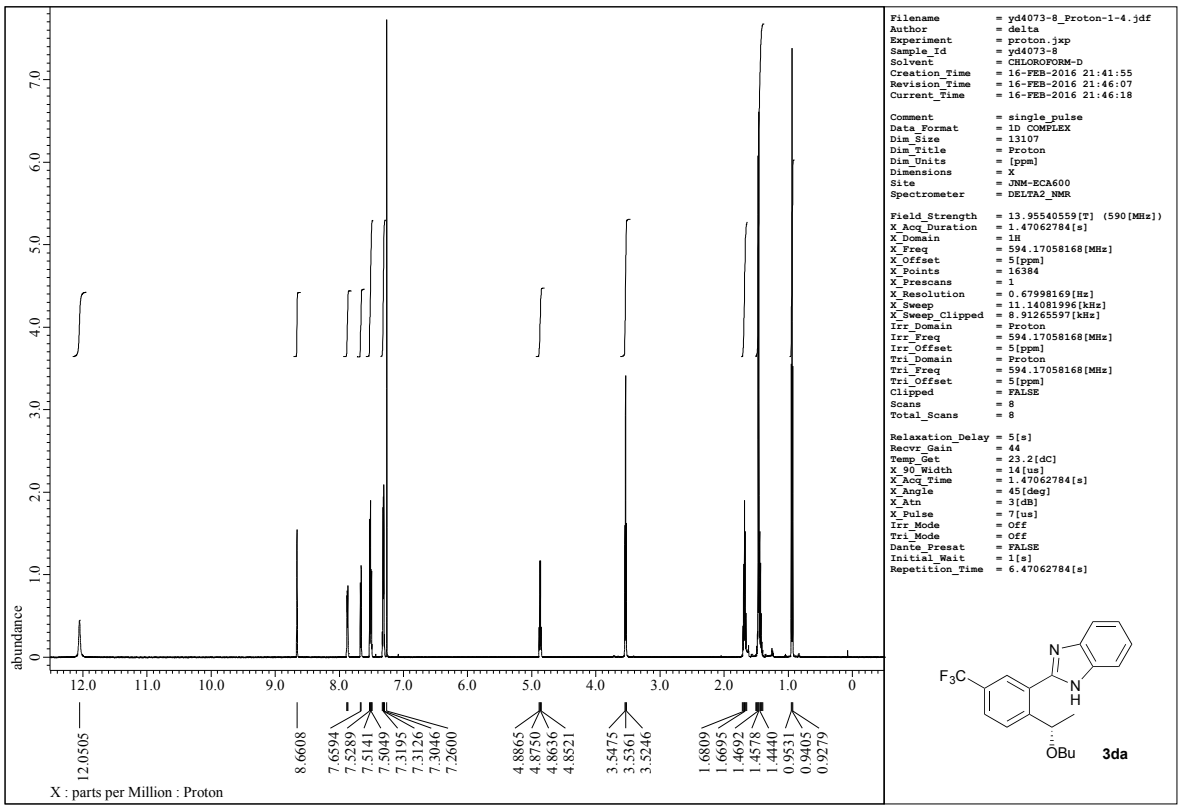
UV Results

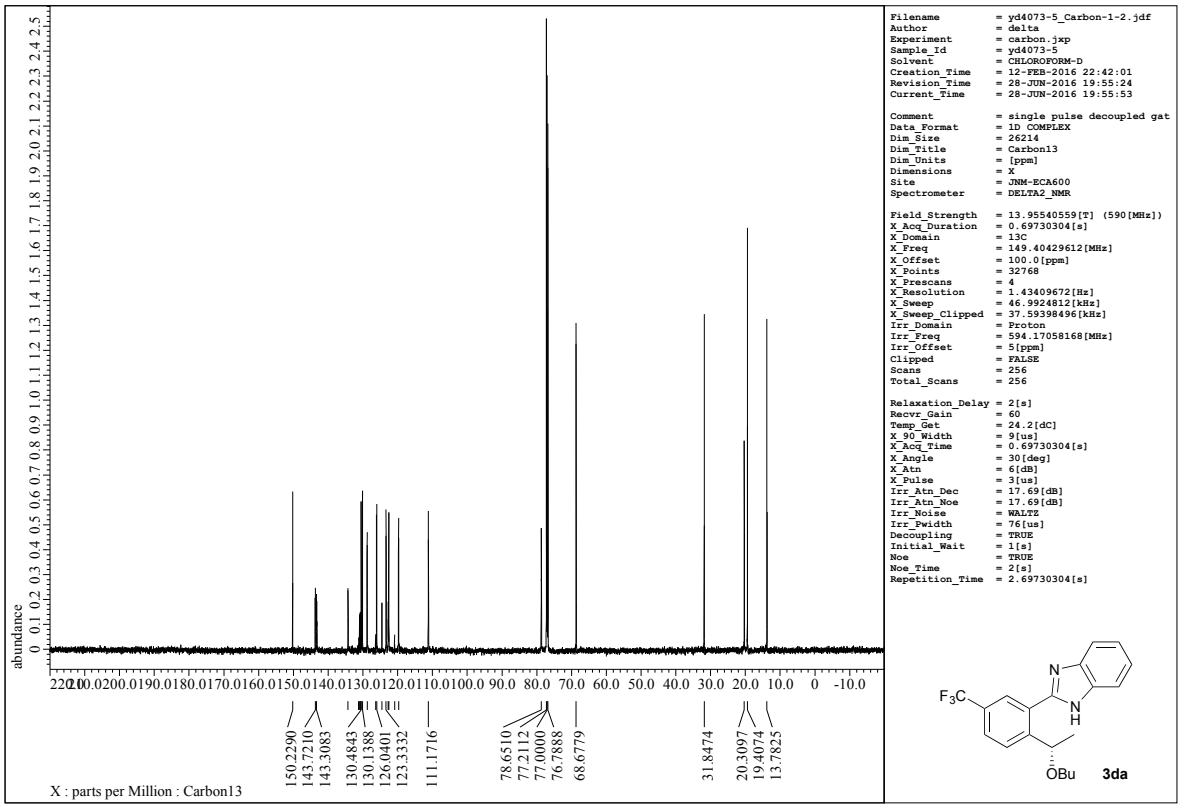
Pk #	Retention Time	Area	Area Percent	Height
1	29.255	4996725	97.271	98310
2	39.961	140172	2.729	2477

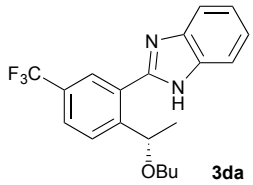


UV Results

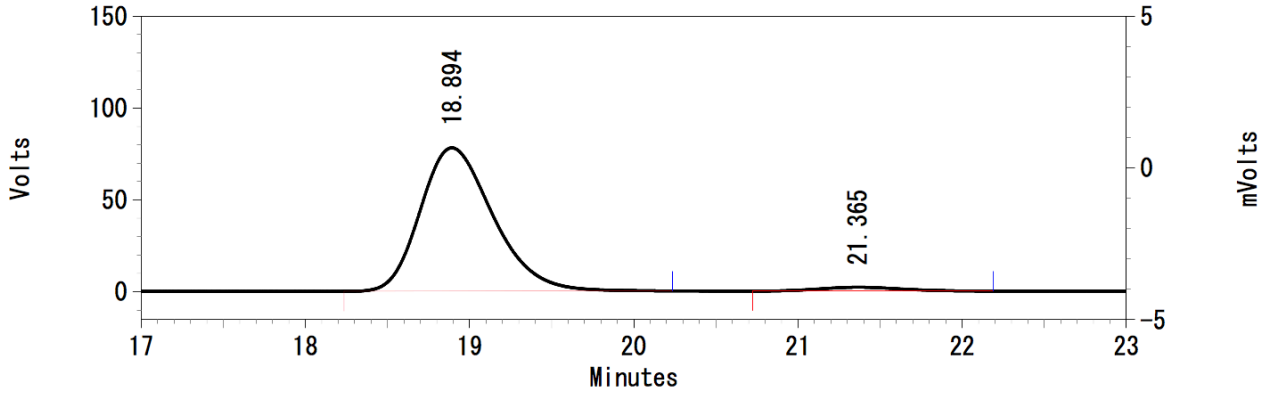
Pk #	Retention Time	Area	Area Percent	Height
1	29.476	6421788	49.988	123605
2	39.971	6424884	50.012	94804


Filename = yd4073-8_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4073-8
Solvent = CHLOROFORM-D
Creation_Time = 16-FEB-2016 21:41:55
Revision_Time = 16-FEB-2016 21:46:07
Current_Time = 16-FEB-2016 21:46:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 23.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
abundance
12.0505
8.6608
7.6594
7.5289
7.5141
7.5049
7.3195
7.3126
7.3046
7.2600
4.8865
4.8750
4.8636
4.8521
3.5475
3.5361
3.5246
1.6809
1.6695
1.4692
1.4578
1.4440
0.9531
0.9405
0.9279
X : parts per Million : Proton
F3C
N
H
OBu
3da


Filename = yd4073-5_Carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4073-5
Solvent = CHLOROFORM-D
Creation_Time = 12-FEB-2016 22:42:01
Revision_Time = 28-JUN-2016 19:55:24
Current_Time = 28-JUN-2016 19:55:53
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.2[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
abundance
150.2290
143.7210
143.3083
130.4843
130.1388
126.0401
123.3332
111.1716
78.6510
77.2112
77.0000
76.7888
68.6779
31.8474
20.3097
19.4074
13.7825
X : parts per Million : Carbon13
F3C
N
H
OBu
3da

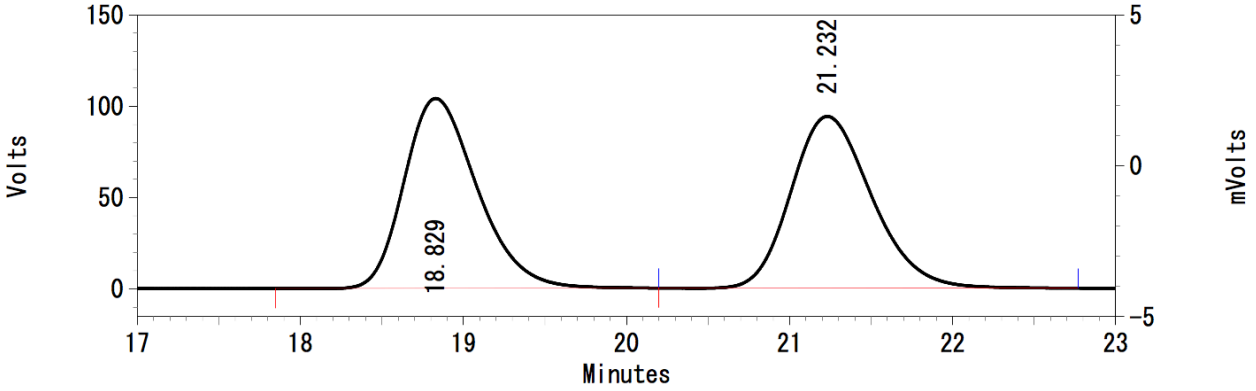


3da



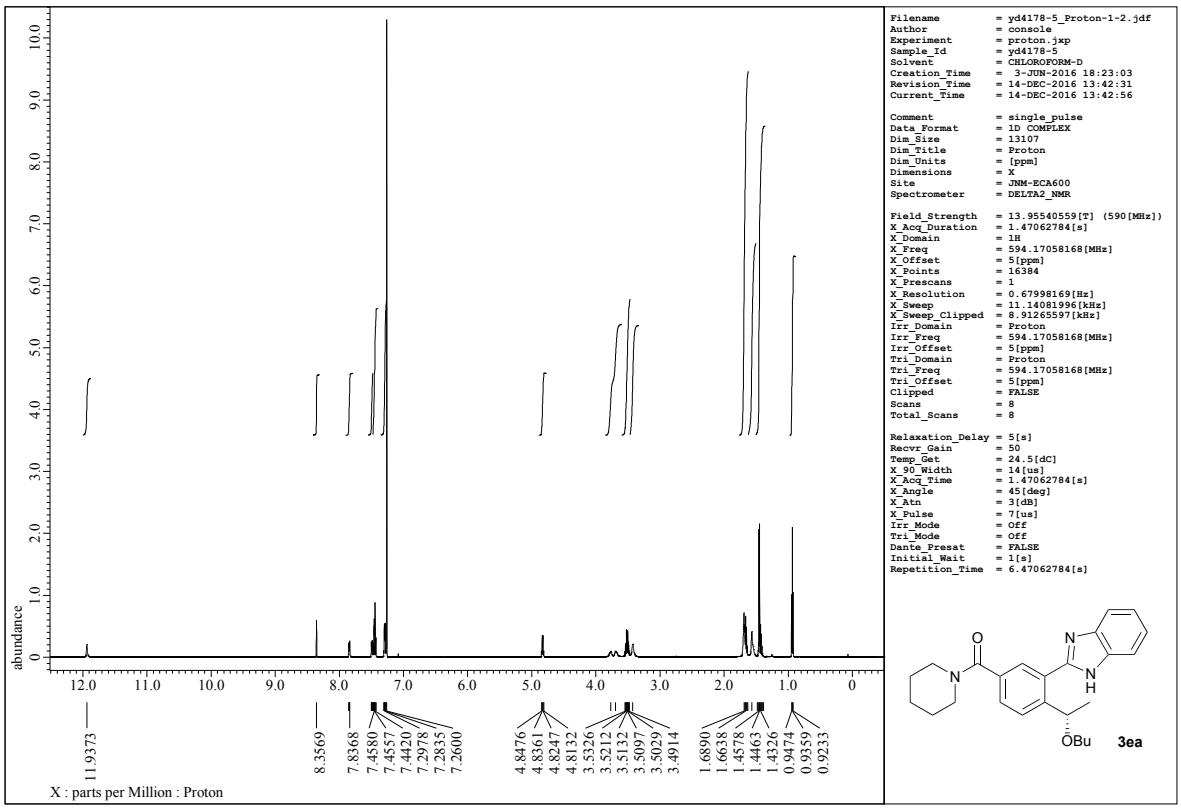
UV Results

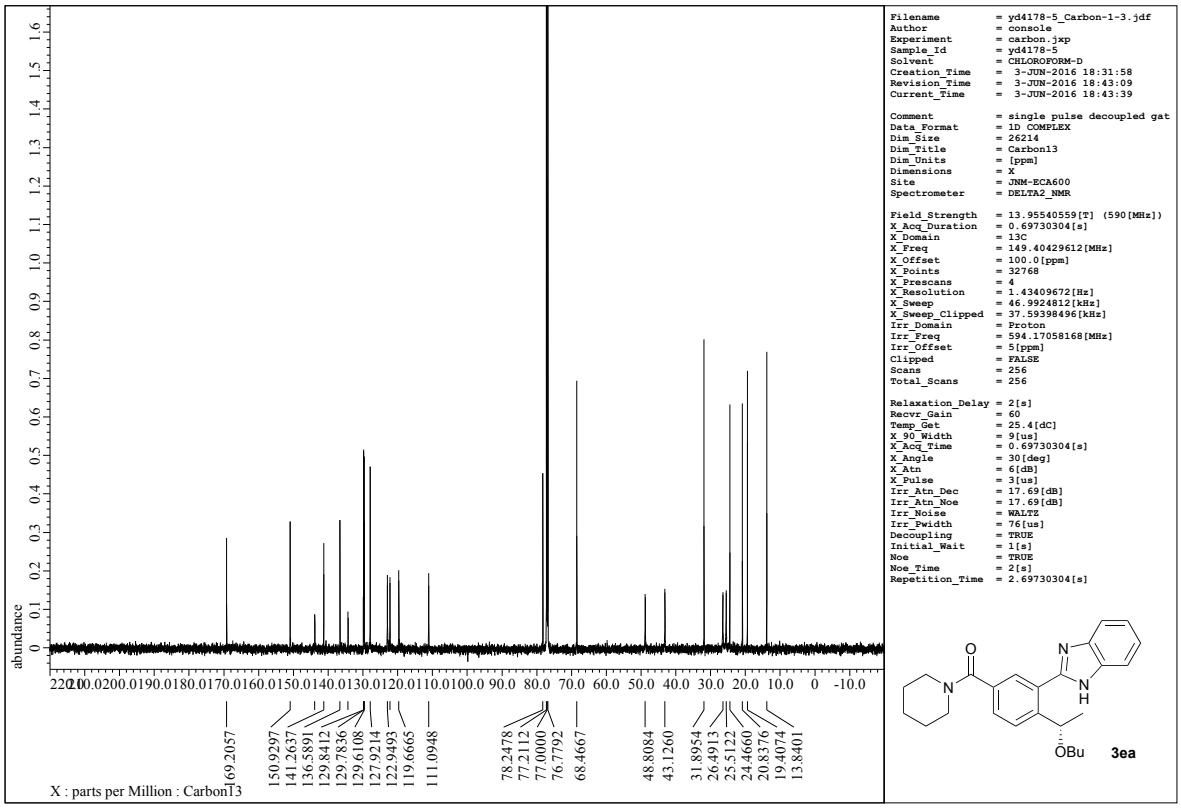
Pk #	Retention Time	Area	Area Percent	Height
1	18.894	2400719	97.184	77949
2	21.365	69559	2.816	2068

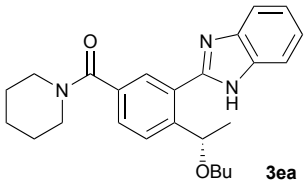


UV Results

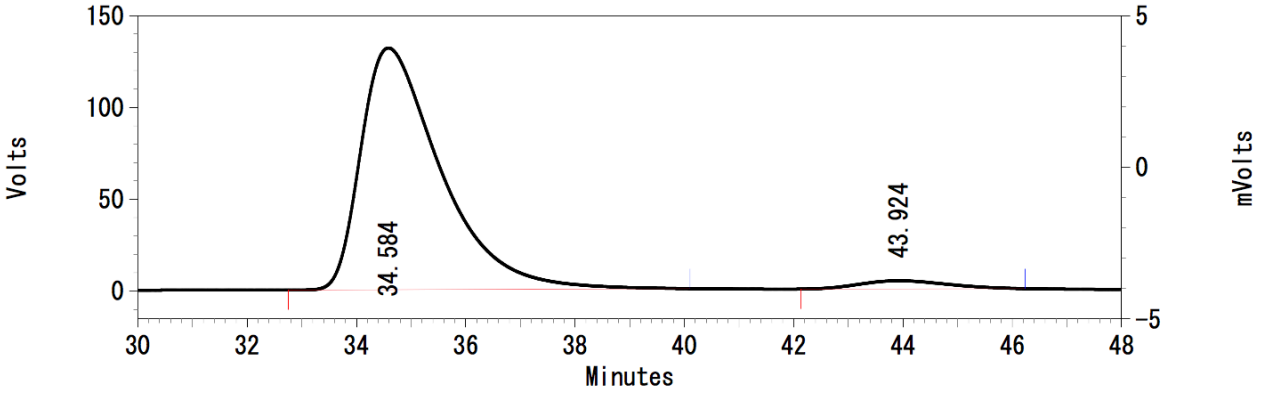
Pk #	Retention Time	Area	Area Percent	Height
1	18.829	3248187	50.018	103912
2	21.232	3245787	49.982	94017


abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
11.9373
8.3569
7.8368
7.4580
7.4557
7.4420
7.2978
7.2835
7.2600
4.8476
4.8361
4.8247
4.8132
3.5326
3.5212
3.5132
3.5097
3.5029
3.4914
1.6890
1.6638
1.4578
1.4463
1.4326
0.9474
0.9359
0.9233
X : parts per Million : Proton
Filename = yd4178-5_Proton-1-2.jdf
Author = console
Experiment = proton.jxp
Sample_Id = yd4178-5
Solvent = CHLOROFORM-D
Creation_Time = 3-JUN-2016 18:23:03
Revision_Time = 14-DEC-2016 13:42:31
Current_Time = 14-DEC-2016 13:42:56
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 24.5[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O
N
N
H
OBu
3ea


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
169.2057
150.9297
141.2637
136.5891
129.8412
129.7836
129.6108
127.9214
122.9493
119.6665
111.0948
78.2478
77.2112
77.0000
76.7792
68.4667
48.8084
43.1260
31.8954
26.4913
25.5122
24.4660
20.8376
19.4074
13.8401
X : parts per Million : Carbon13
Filename = yd4178-5_Carbon-1-3.jdf
Author = console
Experiment = carbon.jxp
Sample_Id = yd4178-5
Solvent = CHLOROFORM-D
Creation_Time = 3-JUN-2016 18:31:58
Revision_Time = 3-JUN-2016 18:43:09
Current_Time = 3-JUN-2016 18:43:39
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.4[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
O
N
N
H
OBu
3ea

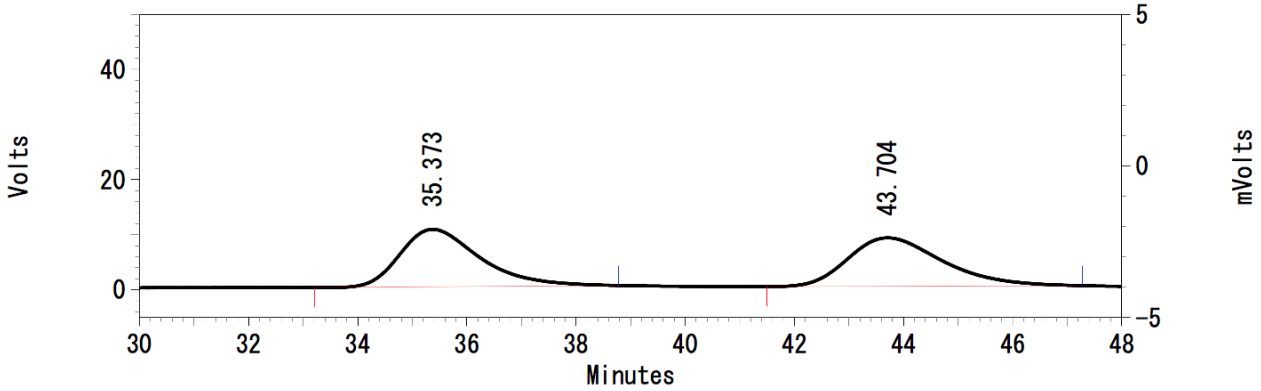


3ea



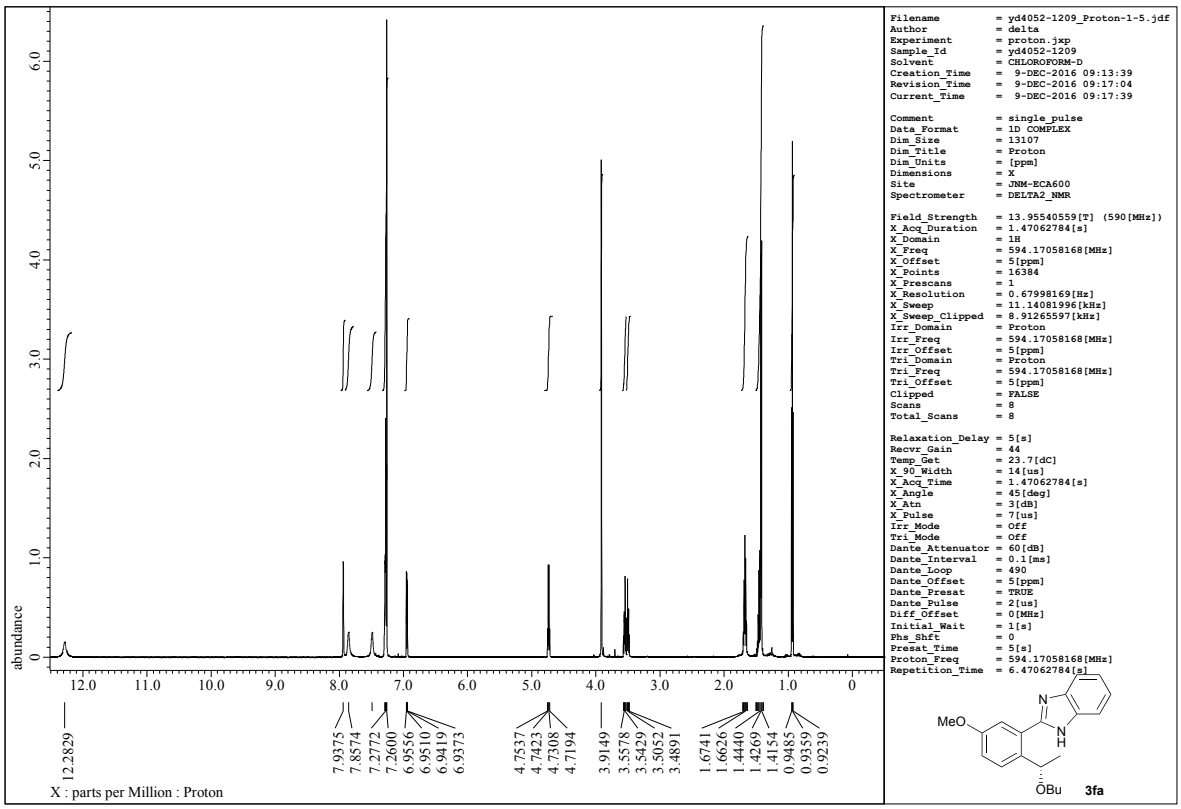
UV Results

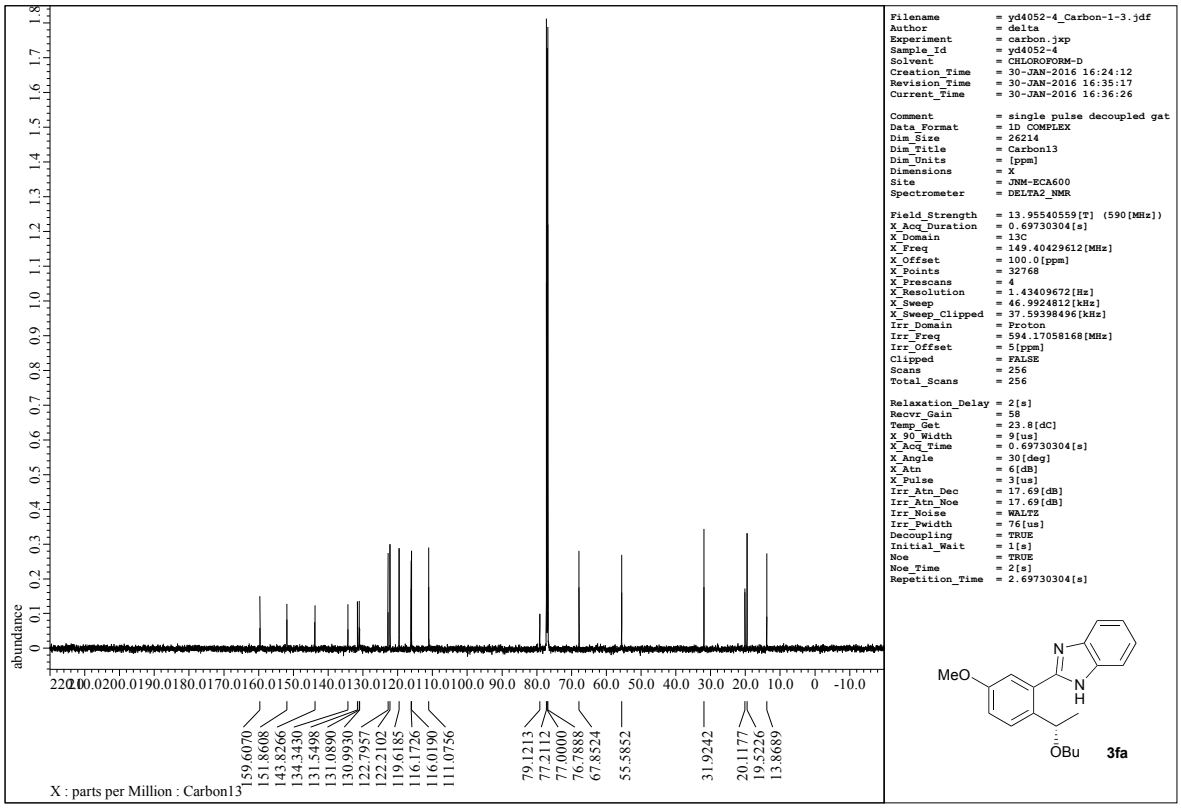
Pk #	Retention Time	Area	Area Percent	Height
1	34.584	13378169	96.425	131583
2	43.924	496026	3.575	4443

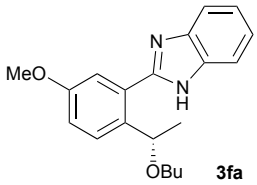


UV Results

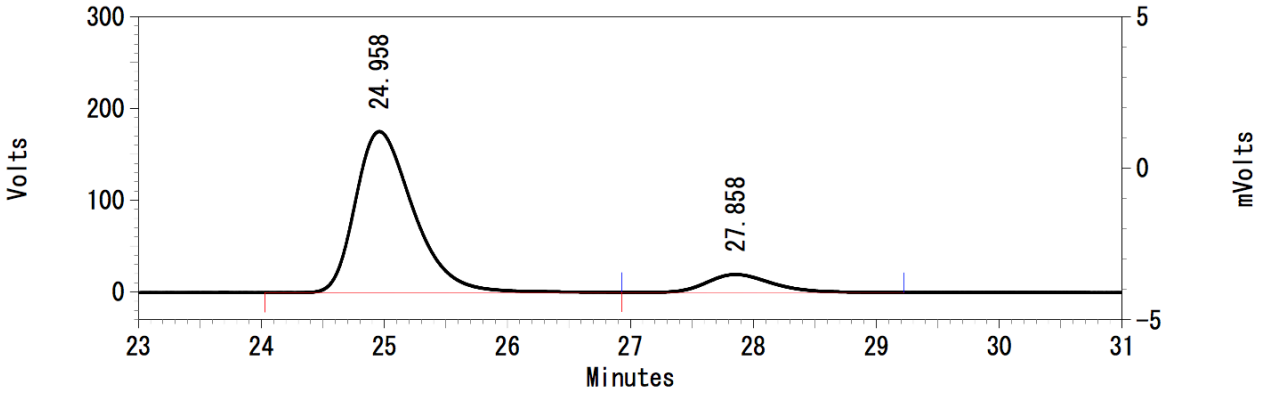
Pk #	Retention Time	Area	Area Percent	Height
1	35.373	1059130	49.969	10418
2	43.704	1060436	50.031	8790


abundance
12.2829
7.9375
7.8574
7.2772
7.2600
6.9556
6.9510
6.9419
6.9373
4.7537
4.7423
4.7308
4.7194
3.9149
3.5578
3.5429
3.5052
3.4891
1.6741
1.6626
1.4440
1.4269
1.4154
0.9485
0.9359
0.9239
X : parts per Million : Proton
Filename = yd4052-1209_Proton-1-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4052-1209
Solvent = CHLOROFORM-D
Creation_Time = 9-DEC-2016 09:13:39
Revision_Time = 9-DEC-2016 09:17:04
Current_Time = 9-DEC-2016 09:17:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 23.7[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Attenuator = 60[dB]
Dante_Interval = 0.1[ms]
Dante_Loop = 490
Dante_Offset = 5[ppm]
Dante_Presat = TRUE
Dante_Pulse = 2[us]
Diff_Offset = 0[MHz]
Initial_Wait = 1[s]
Phs_Shft = 0
Presat_Time = 5[s]
Proton_Freq = 594.17058168[MHz]
Repetition_Time = 6.47062784[s]
MeO
N
H
OBu
3fa


abundance
159.6070
151.8608
143.8266
134.3430
131.5498
131.0890
130.9930
122.7957
122.2102
119.6185
116.1726
116.0190
111.0756
79.1213
77.2112
77.0000
76.7888
67.8524
55.5852
31.9242
20.1177
19.5226
13.8689
X : parts per Million : Carbon13
Filename = yd4052-4_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4052-4
Solvent = CHLOROFORM-D
Creation_Time = 30-JAN-2016 16:24:12
Revision_Time = 30-JAN-2016 16:35:17
Current_Time = 30-JAN-2016 16:36:26
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 23.8[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
MeO
N
H
OBu
3fa

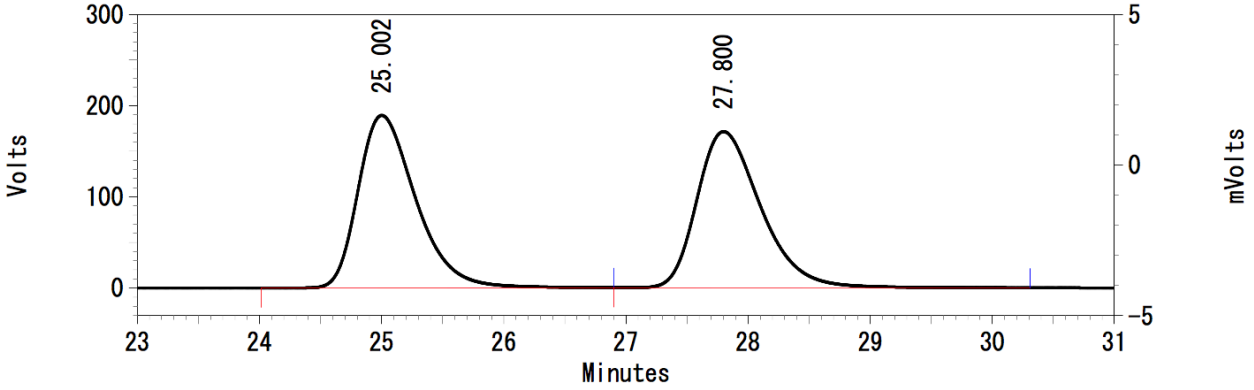


3fa



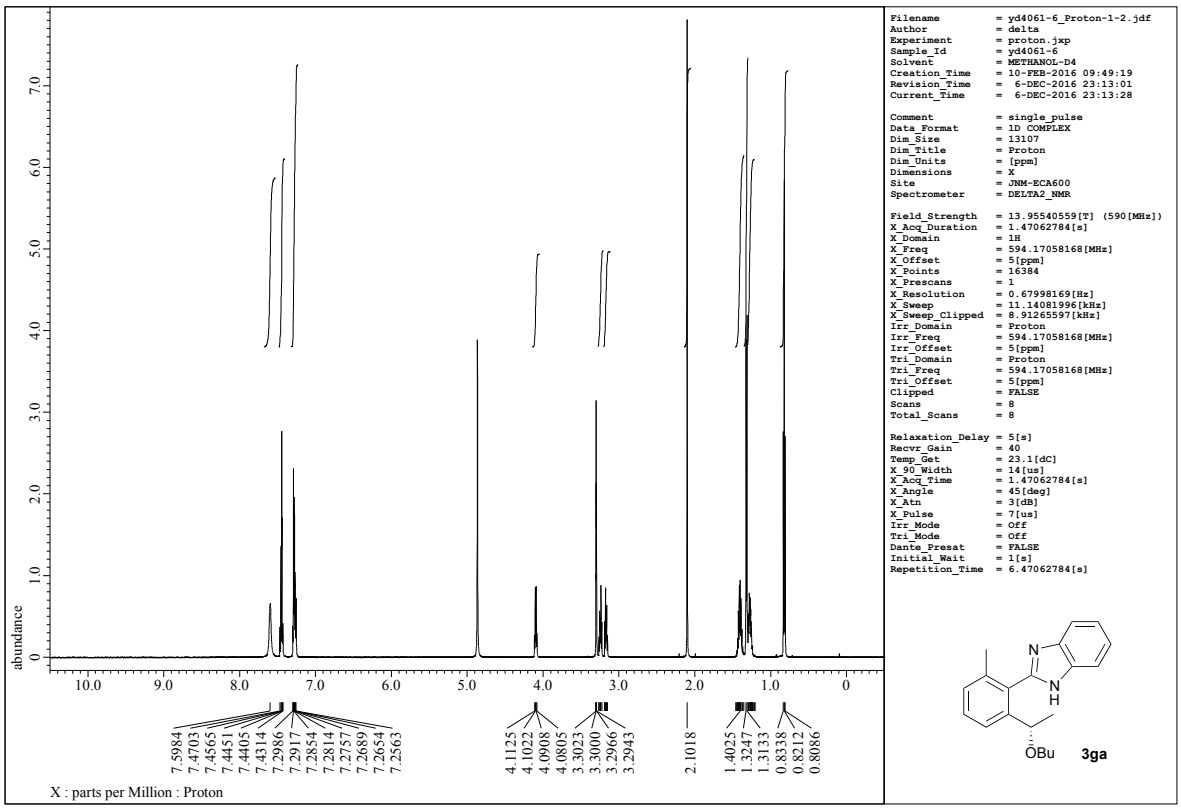
UV Results

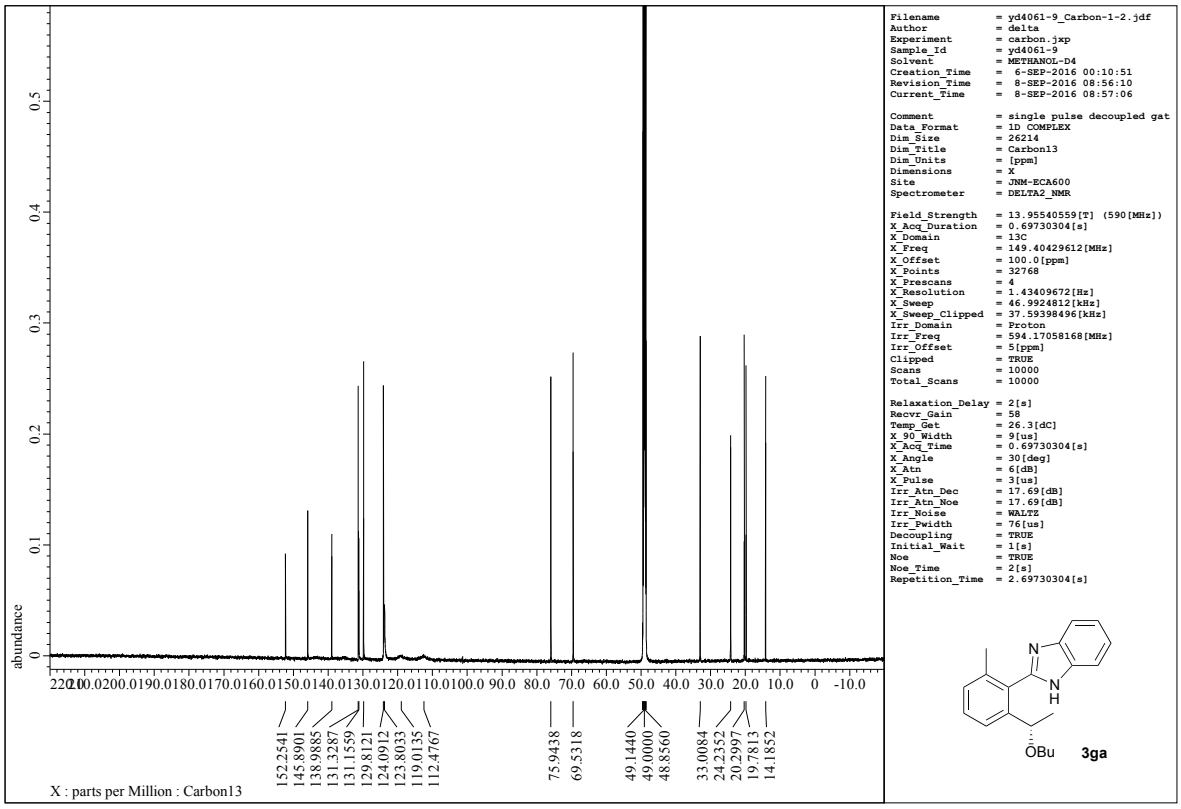
Pk #	Retention Time	Area	Area Percent	Height
1	24.958	5745367	88.904	175215
2	27.858	717075	11.096	19525

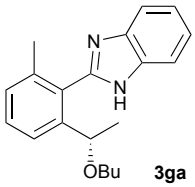


UV Results

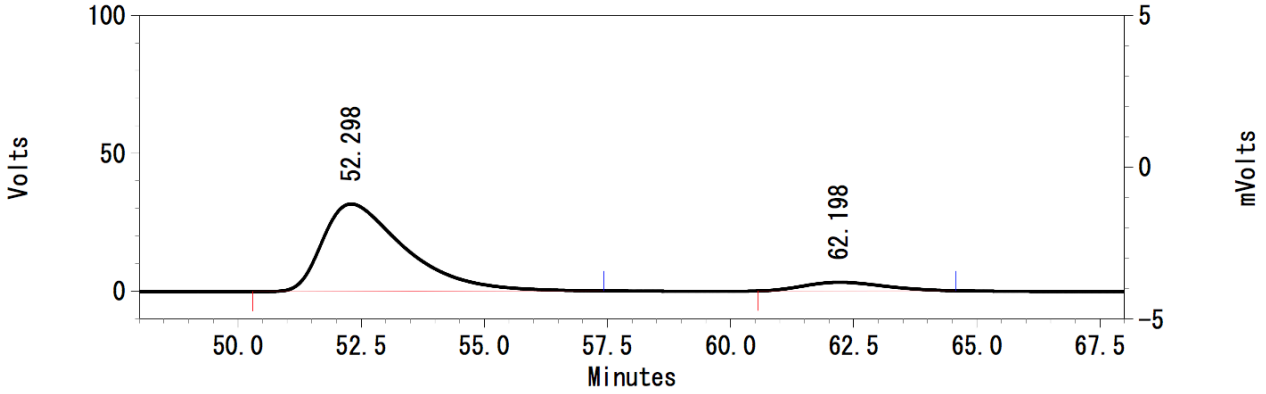
Pk #	Retention Time	Area	Area Percent	Height
1	25.002	6223368	49.913	189064
2	27.800	6245186	50.087	171248


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.5984 7.4703 7.4565 7.4451 7.4405 7.4314 7.2986 7.2917 7.2854 7.2814 7.2757 7.2689 7.2654 7.2563
4.1125 4.1022 4.0908 4.0805 3.3023 3.3000 3.2966 3.2943
2.1018
1.4025 1.3247 1.3133 0.8338 0.8212 0.8086
X : parts per Million : Proton
Filename = yd4061-6_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4061-6
Solvent = METHANOL-D4
Creation_Time = 10-FEB-2016 09:49:19
Revision_Time = 6-DEC-2016 23:13:01
Current_Time = 6-DEC-2016 23:13:28
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 23.1[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OBu
3ga


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
152.2541 145.8901 138.9885 131.3287 131.1559 129.8121 124.0912 123.8033 119.0135 112.4767
75.9438 69.5318
49.1440 49.0000 48.8560
33.0084 24.2352 20.2997 19.7813 14.1852
X : parts per Million : Carbon13
Filename = yd4061-9_Carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4061-9
Solvent = METHANOL-D4
Creation_Time = 6-SEP-2016 00:10:51
Revision_Time = 8-SEP-2016 08:56:10
Current_Time = 8-SEP-2016 08:57:06
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 10000
Total_Scans = 10000
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 26.3[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OBu
3ga

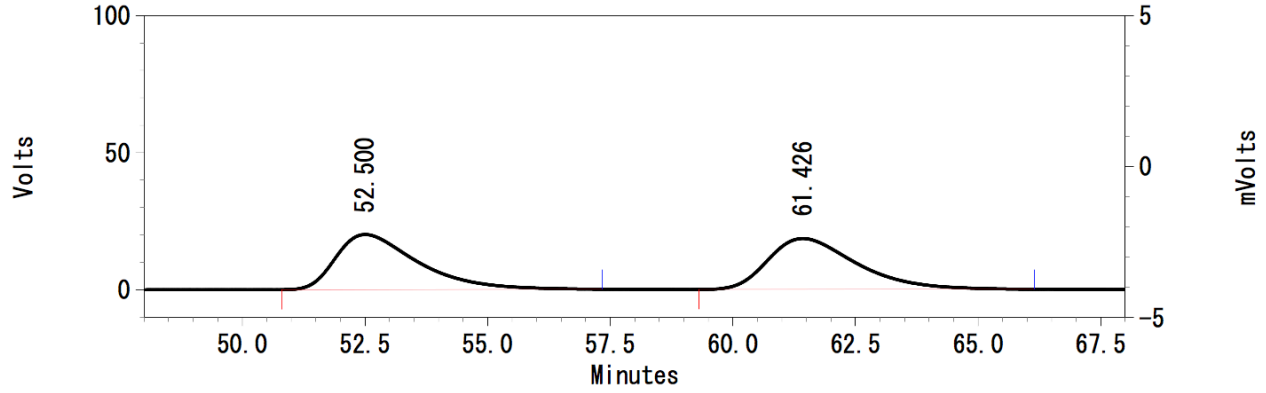


3ga



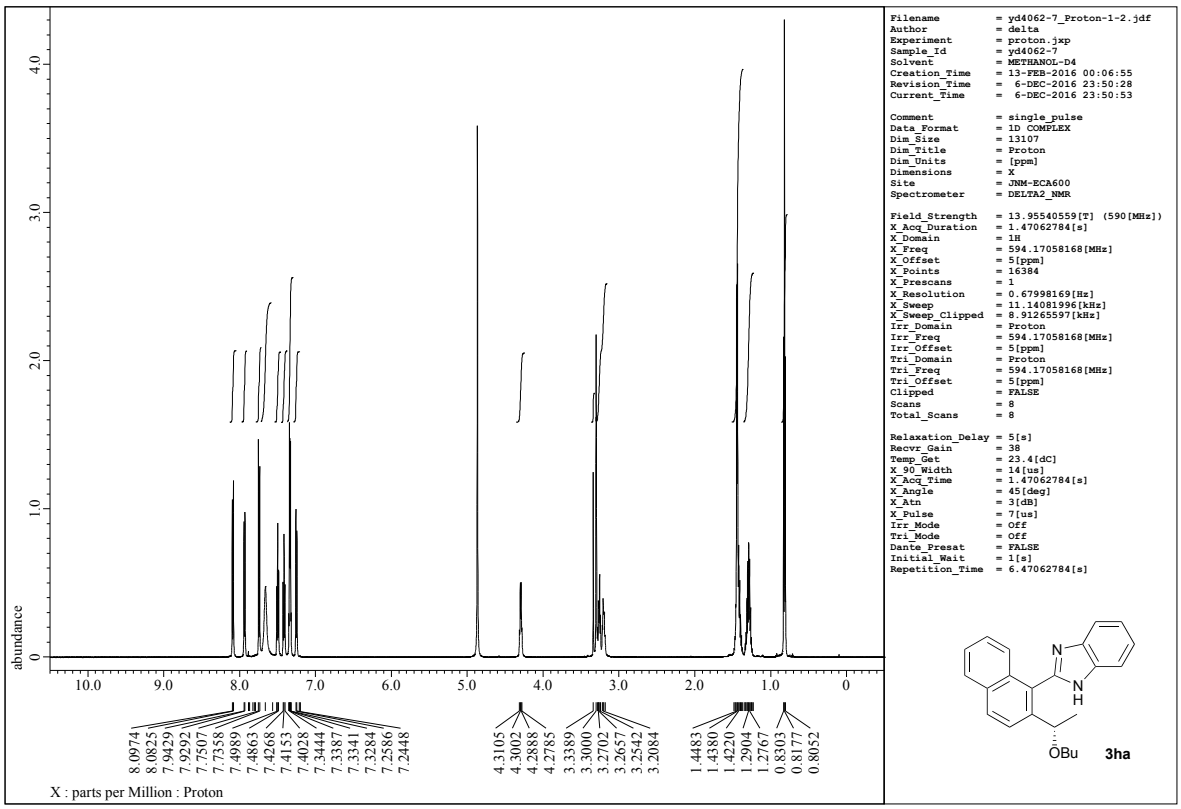
UV Results

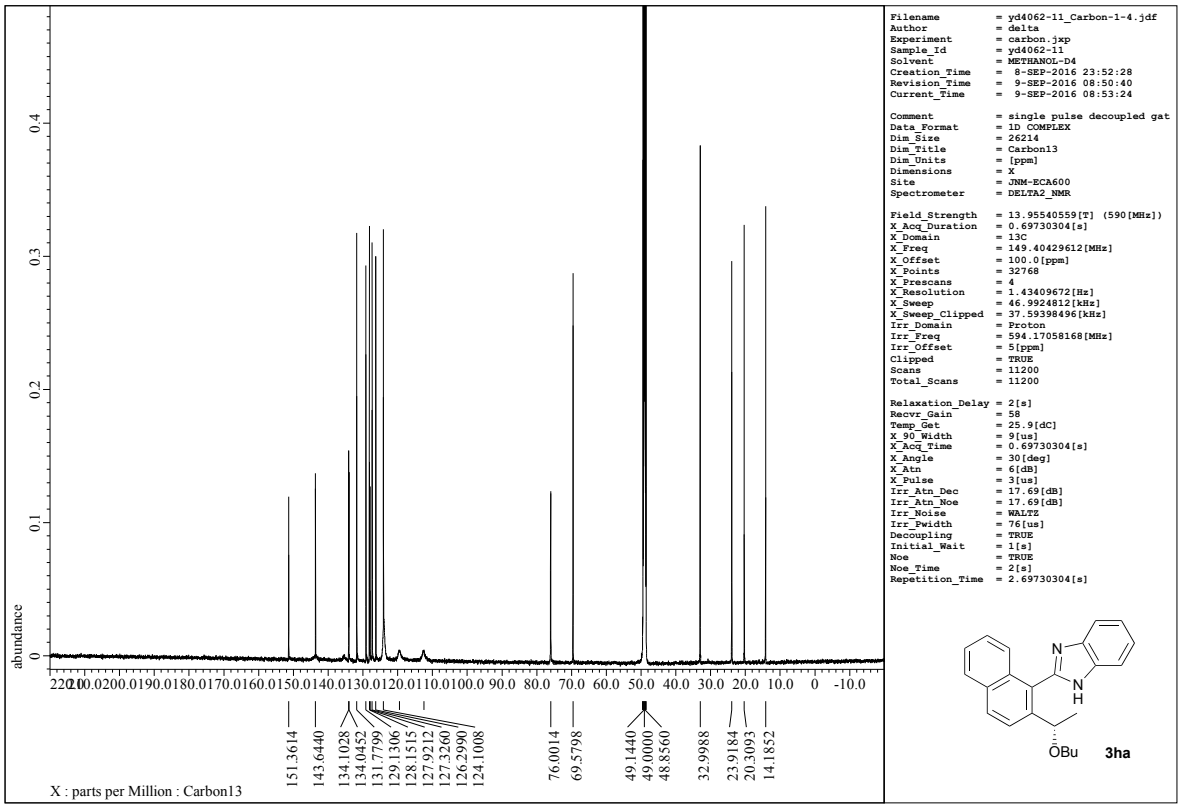
Pk #	Retention Time	Area	Area Percent	Height
1	52.298	3668256	91.328	31627
2	62.198	348319	8.672	3117

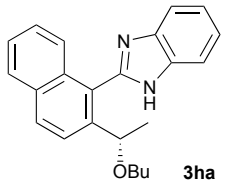


UV Results

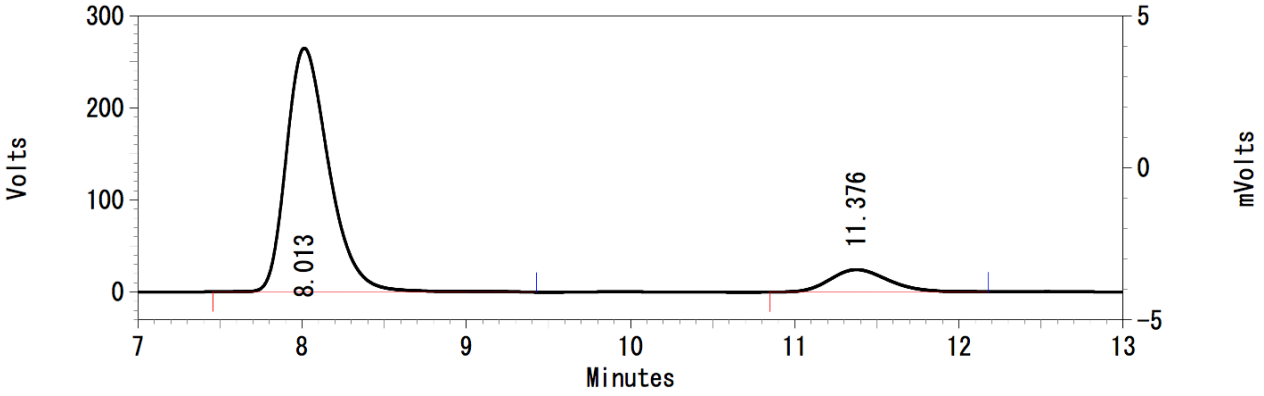
Pk #	Retention Time	Area	Area Percent	Height
1	52.500	2332582	50.029	20052
2	61.426	2329870	49.971	18540


abundance
X : parts per Million : Proton
8.0974
8.0825
7.9429
7.9292
7.7507
7.7358
7.4989
7.4863
7.4268
7.4153
7.4028
7.3444
7.3387
7.3341
7.3284
7.2586
7.2448
4.3105
4.3002
4.2888
4.2785
3.3389
3.3000
3.2702
3.2657
3.2542
3.2084
1.4483
1.4380
1.4220
1.2904
1.2767
0.8303
0.8177
0.8052
Filename = yd4062-7_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4062-7
Solvent = METHANOL-D4
Creation_Time = 13-FEB-2016 00:06:55
Revision_Time = 6-DEC-2016 23:50:28
Current_Time = 6-DEC-2016 23:50:53
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 23.4[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OBu
3ha


abundance
X : parts per Million : Carbon13
151.3614
143.6440
134.1028
134.0452
131.7799
129.1306
128.1515
127.9212
127.3260
126.2990
124.1008
76.0014
69.5798
49.1440
49.0000
48.8560
32.9988
23.9184
20.3093
14.1852
Filename = yd4062-11_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4062-11
Solvent = METHANOL-D4
Creation_Time = 8-SEP-2016 23:52:28
Revision_Time = 9-SEP-2016 08:50:40
Current_Time = 9-SEP-2016 08:53:24
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 11200
Total_Scans = 11200
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 25.9[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OBu
3ha

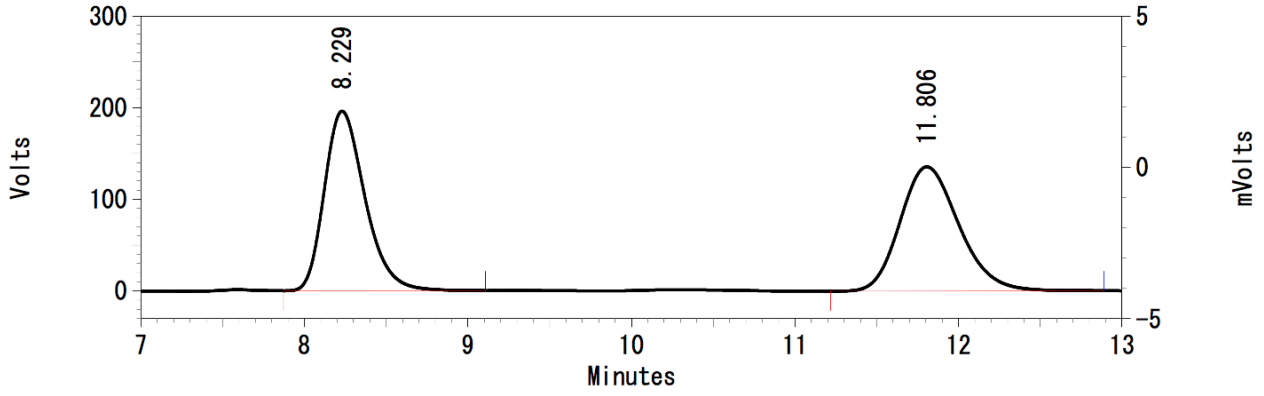


3ha



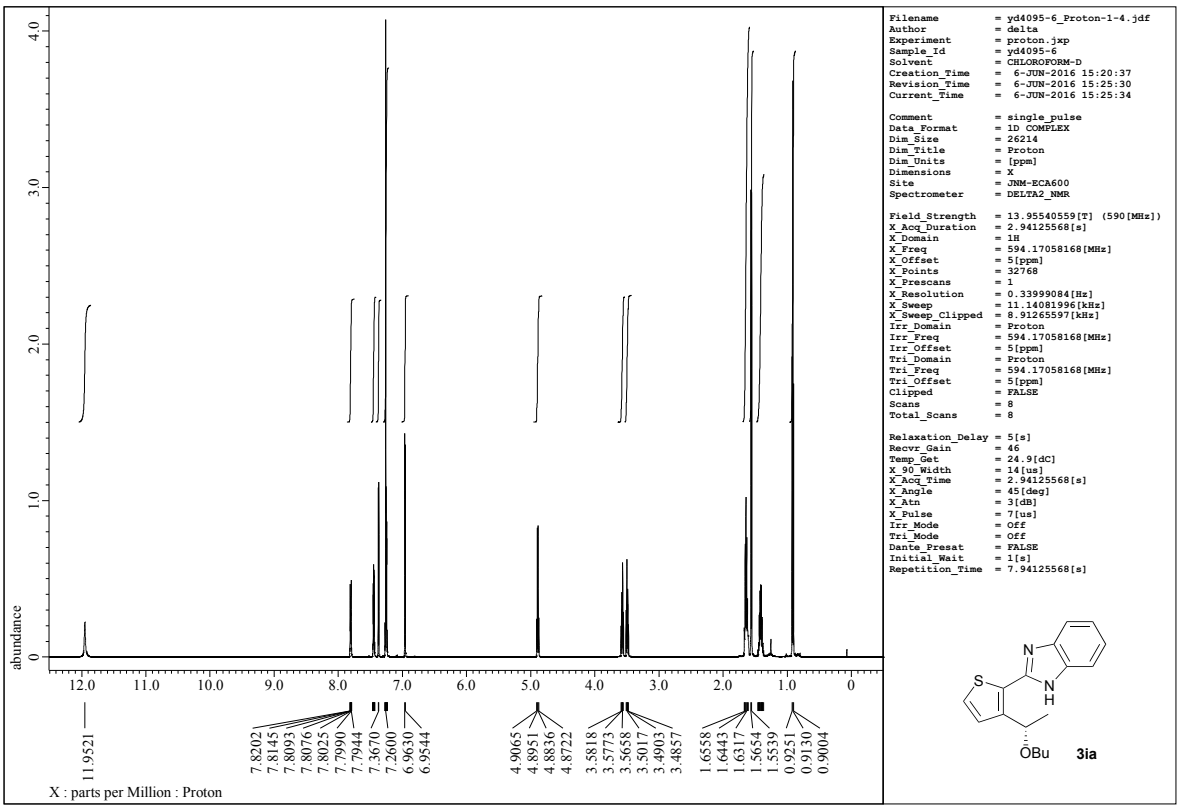
UV Results

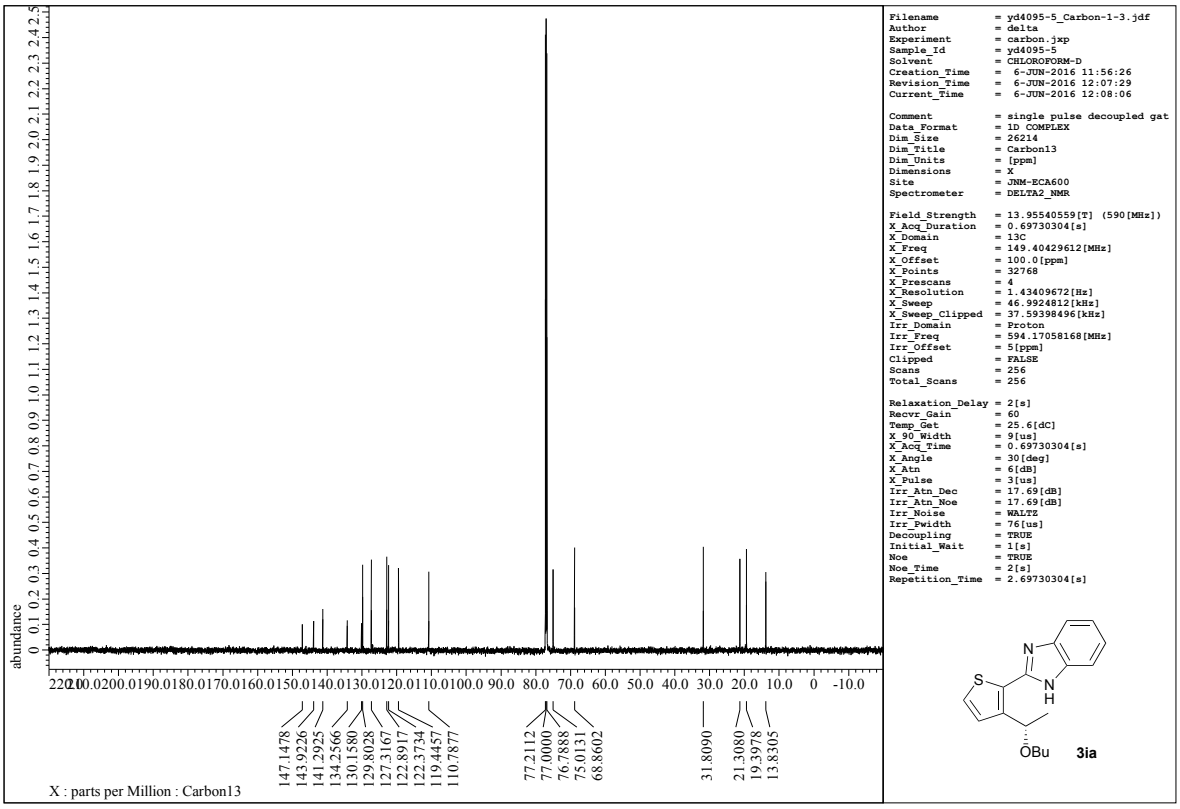
Pk #	Retention Time	Area	Area Percent	Height
1	8.013	4766114	88.901	264551
2	11.376	595058	11.099	24216

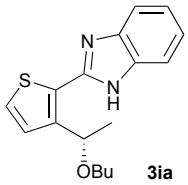


UV Results

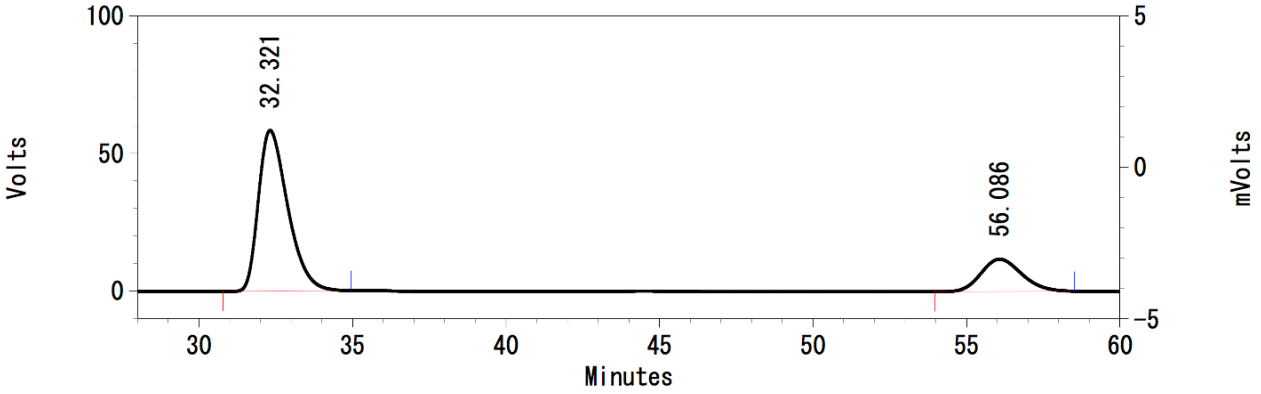
Pk #	Retention Time	Area	Area Percent	Height
1	8.229	3380402	49.965	195888
2	11.806	3385181	50.035	135449


abundance
X : parts per Million : Proton
11.9521
7.8202
7.8145
7.8093
7.8076
7.8025
7.7990
7.7944
7.3670
7.2600
6.9630
6.9544
4.9065
4.8951
4.8836
4.8722
3.5818
3.5773
3.5658
3.5017
3.4903
3.4857
1.6558
1.6443
1.6317
1.5654
1.5539
0.9251
0.9130
0.9004
Filename = yd4095-6_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4095-6
Solvent = CHLOROFORM-D
Creation_Time = 6-JUN-2016 15:20:37
Revision_Time = 6-JUN-2016 15:25:30
Current_Time = 6-JUN-2016 15:25:34
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 2.94125568[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.33999084[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 24.9[dC]
X_90_Width = 14[us]
X_Acq_Time = 2.94125568[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.94125568[s]
N
S
N
H
OBu
3ia


abundance
X : parts per Million : Carbon13
147.1478
143.9226
141.2925
134.2566
130.1580
129.8028
127.3167
122.8917
122.3734
119.4457
110.7877
77.2112
77.0000
76.7888
75.0131
68.8602
31.8090
21.3080
19.3978
13.8305
Filename = yd4095-5_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4095-5
Solvent = CHLOROFORM-D
Creation_Time = 6-JUN-2016 11:56:26
Revision_Time = 6-JUN-2016 12:07:29
Current_Time = 6-JUN-2016 12:08:06
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.6[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
S
N
H
OBu
3ia

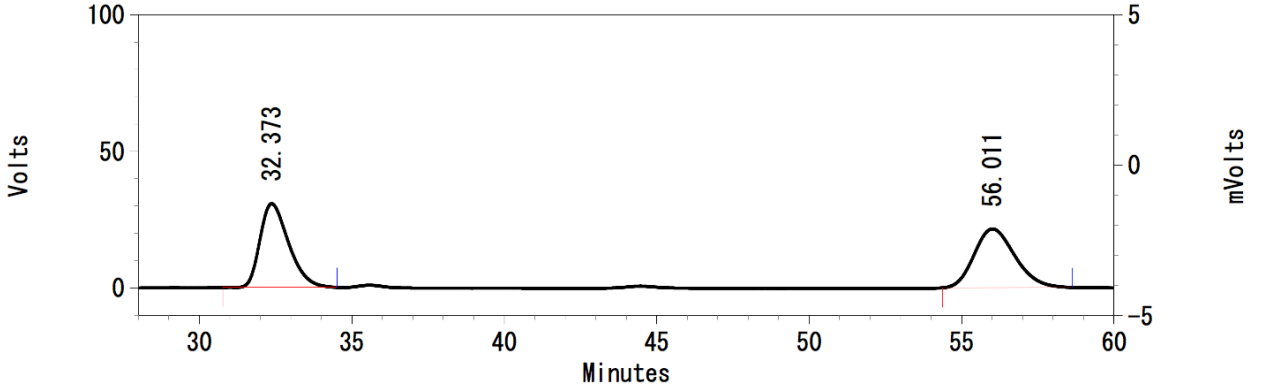


3ia



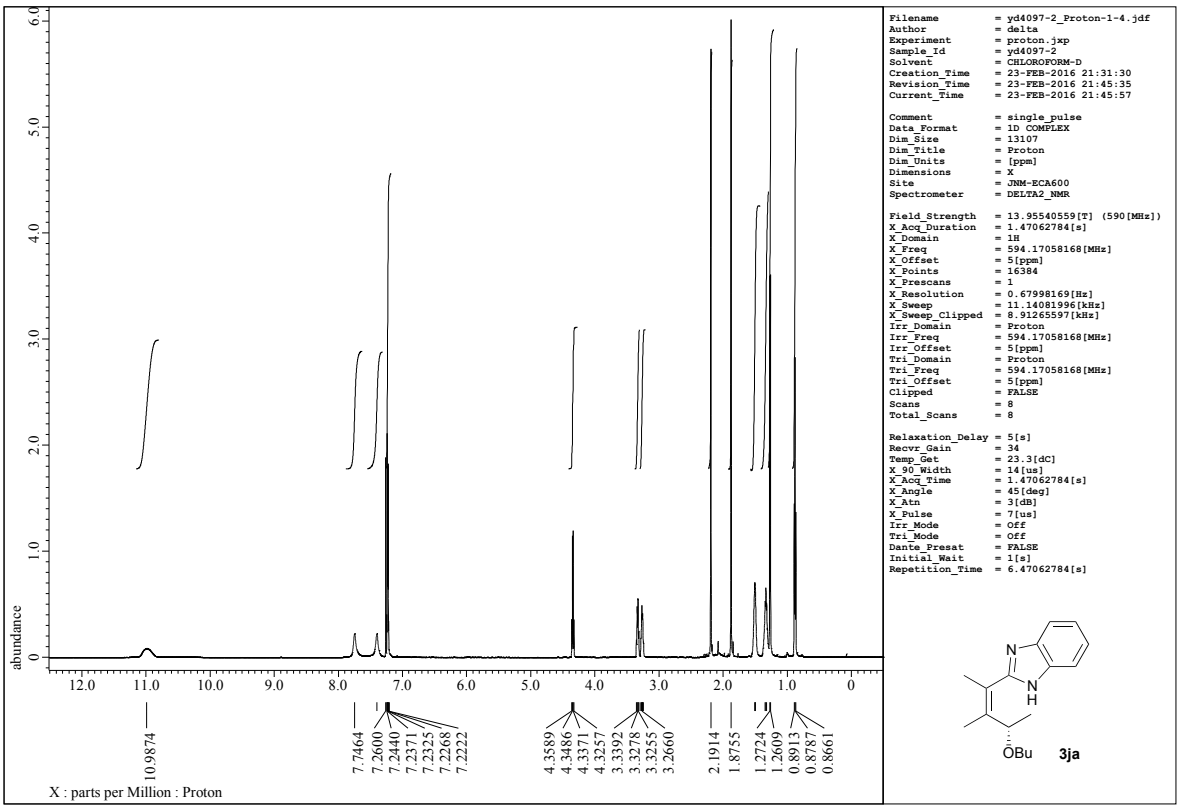
UV Results

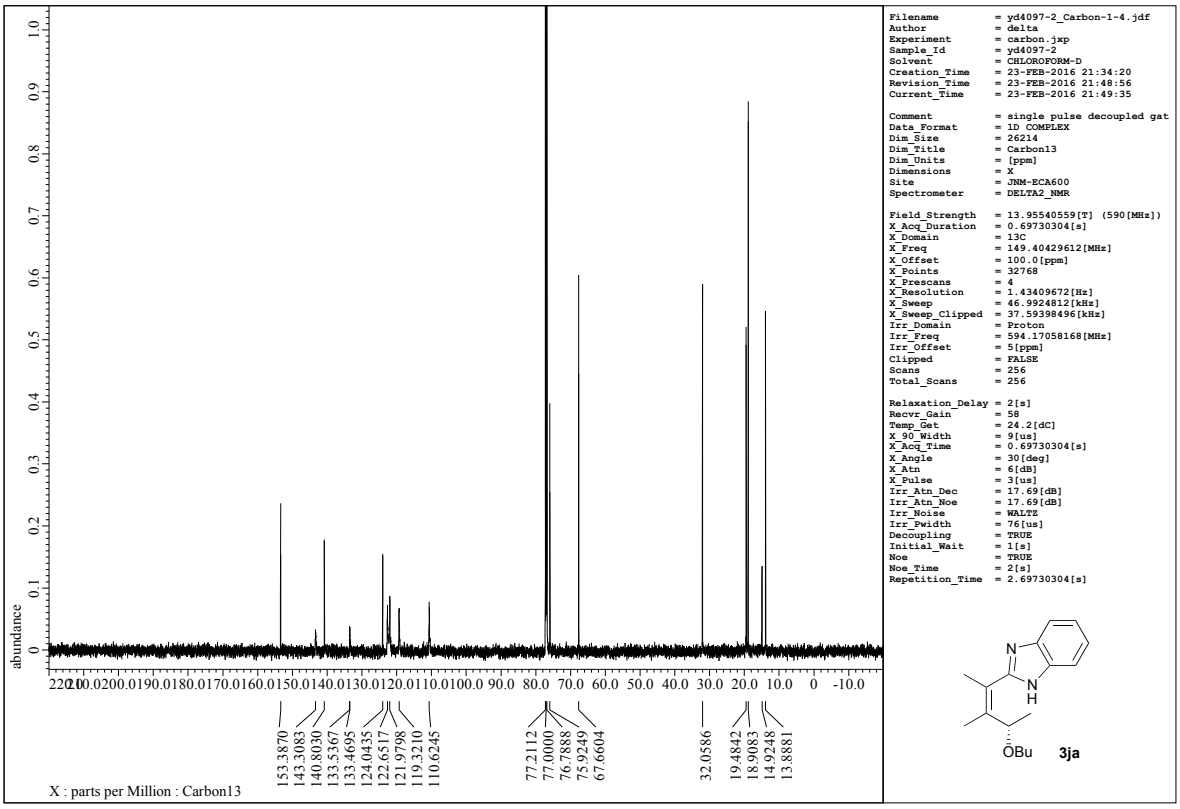
Pk #	Retention Time	Area	Area Percent	Height
1	32.321	3869078	78.135	58276
2	56.086	1082730	21.865	11725

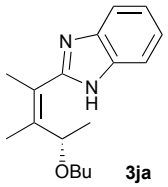


UV Results

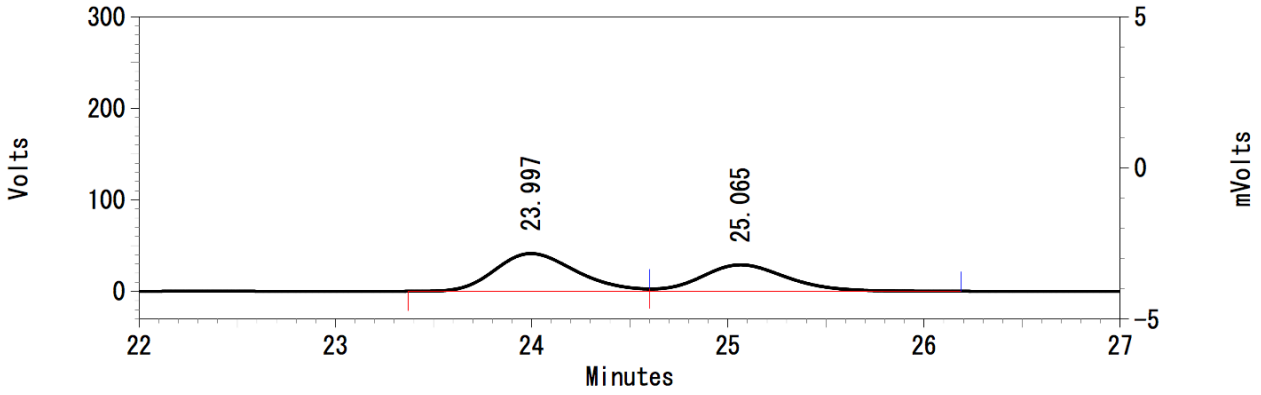
Pk #	Retention Time	Area	Area Percent	Height
1	32.373	1996410	50.062	30579
2	56.011	1991496	49.938	21478


abundance
X : parts per Million : Proton
10.9874
7.7464
7.2600
7.2440
7.2371
7.2325
7.2268
7.2222
4.3589
4.3486
4.3371
4.3257
3.3392
3.3278
3.3255
3.2660
2.1914
1.8755
1.2724
1.2609
0.8913
0.8787
0.8661
Filename = yd4097-2_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4097-2
Solvent = CHLOROFORM-D
Creation_Time = 23-FEB-2016 21:31:30
Revision_Time = 23-FEB-2016 21:45:35
Current_Time = 23-FEB-2016 21:45:57
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 23.3[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OBu
3ja


abundance
X : parts per Million : Carbon13
153.3870
143.3083
140.8030
133.5367
133.4695
124.0435
122.6517
121.9798
119.3210
110.6245
77.2112
77.0000
76.7888
75.9249
67.6604
32.0586
19.4842
18.9083
14.9248
13.8881
Filename = yd4097-2_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4097-2
Solvent = CHLOROFORM-D
Creation_Time = 23-FEB-2016 21:34:20
Revision_Time = 23-FEB-2016 21:48:56
Current_Time = 23-FEB-2016 21:49:35
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 24.2[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OBu
3ja

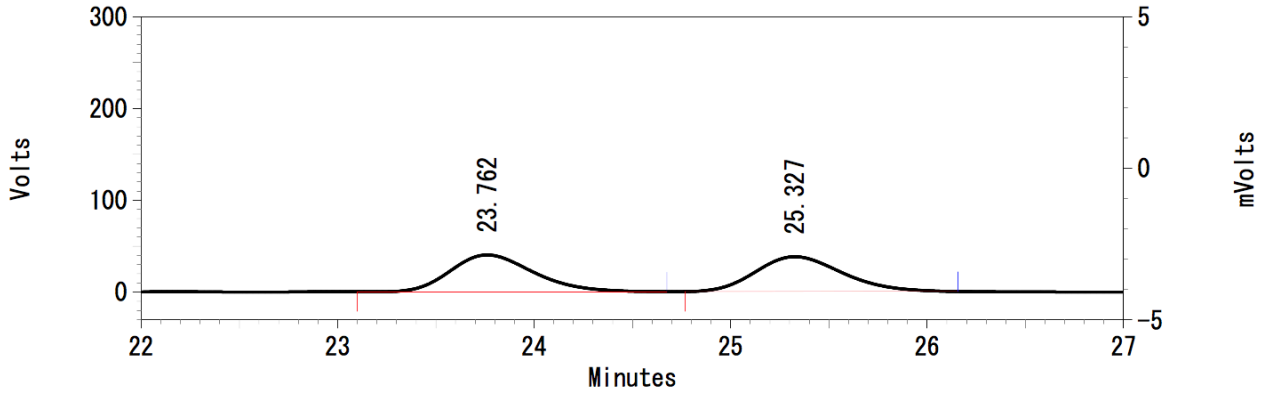


3ja



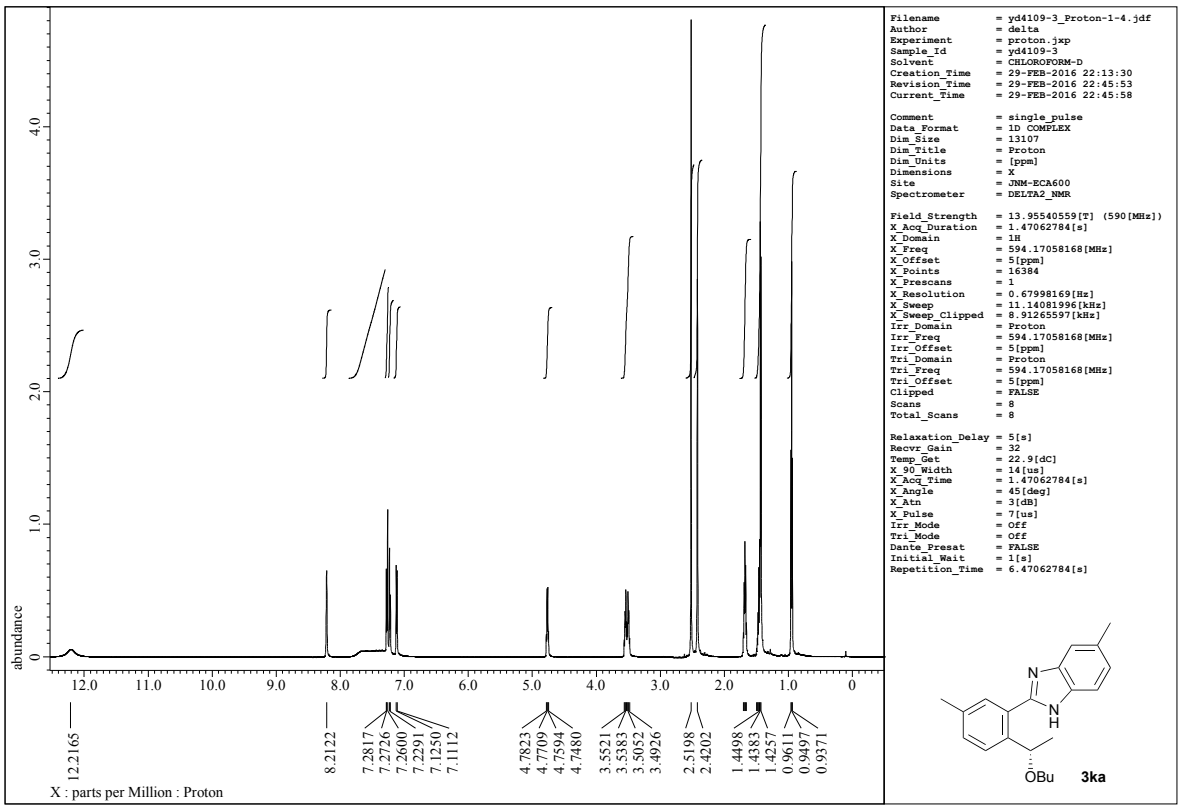
UV Results

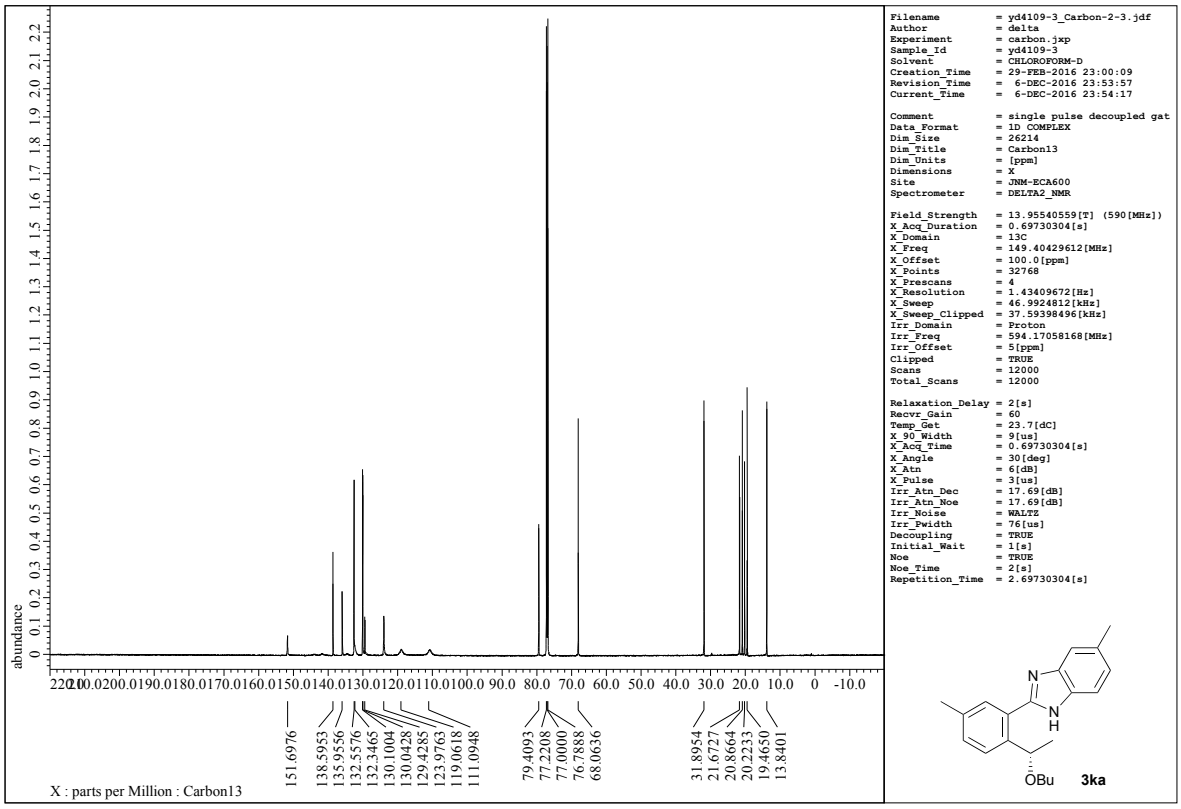
Pk #	Retention Time	Area	Area Percent	Height
1	23.997	1184081	57.527	41173
2	25.065	874219	42.473	28856

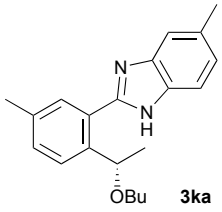


UV Results

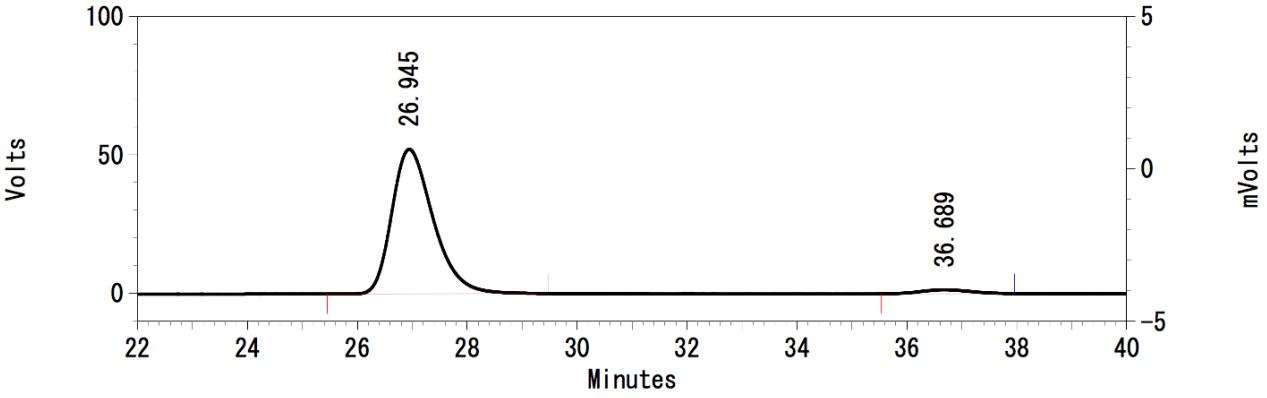
Pk #	Retention Time	Area	Area Percent	Height
1	23.762	1176327	50.214	40045
2	25.327	1166283	49.786	37927


abundance
X : parts per Million : Proton
12.2165
8.2122
7.2817
7.2726
7.2600
7.2291
7.1250
7.1112
4.7823
4.7709
4.7594
4.7480
3.5521
3.5383
3.5052
3.4926
2.5198
2.4202
1.4498
1.4383
1.4257
0.9611
0.9497
0.9371
Filename = yd4109-3_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4109-3
Solvent = CHLOROFORM-D
Creation_Time = 29-FEB-2016 22:13:30
Revision_Time = 29-FEB-2016 22:45:53
Current_Time = 29-FEB-2016 22:45:58
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 32
Temp_Get = 22.9[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OBu
3ka


abundance
X : parts per Million : Carbon13
151.6976
138.5953
135.9556
132.5576
132.3465
130.1004
130.0428
129.4285
123.9763
119.0618
111.0948
79.4093
77.2208
77.0000
76.7888
68.0636
31.8954
21.6727
20.8664
20.2233
19.4650
13.8401
Filename = yd4109-3_Carbon-2-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4109-3
Solvent = CHLOROFORM-D
Creation_Time = 29-FEB-2016 23:00:09
Revision_Time = 6-DEC-2016 23:53:57
Current_Time = 6-DEC-2016 23:54:17
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 12000
Total_Scans = 12000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 23.7[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OBu
3ka

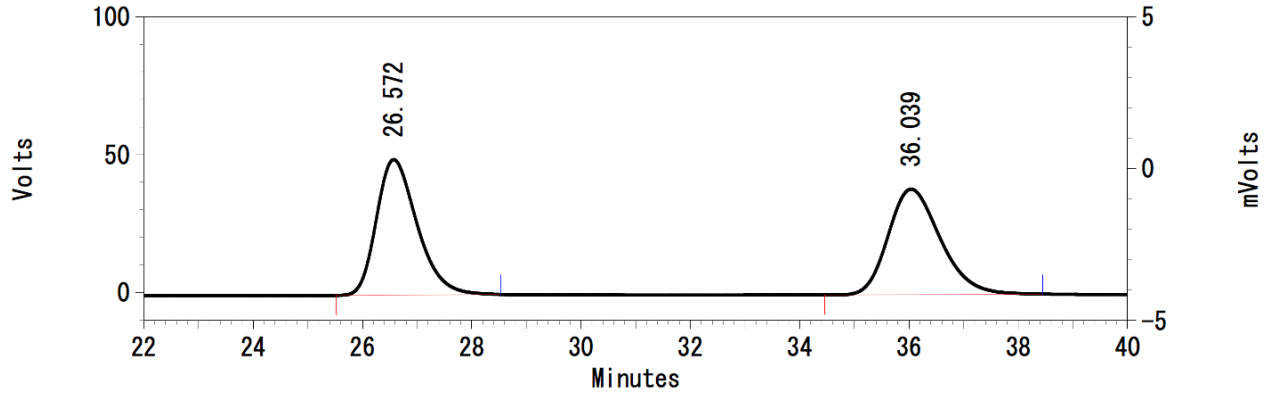


3ka



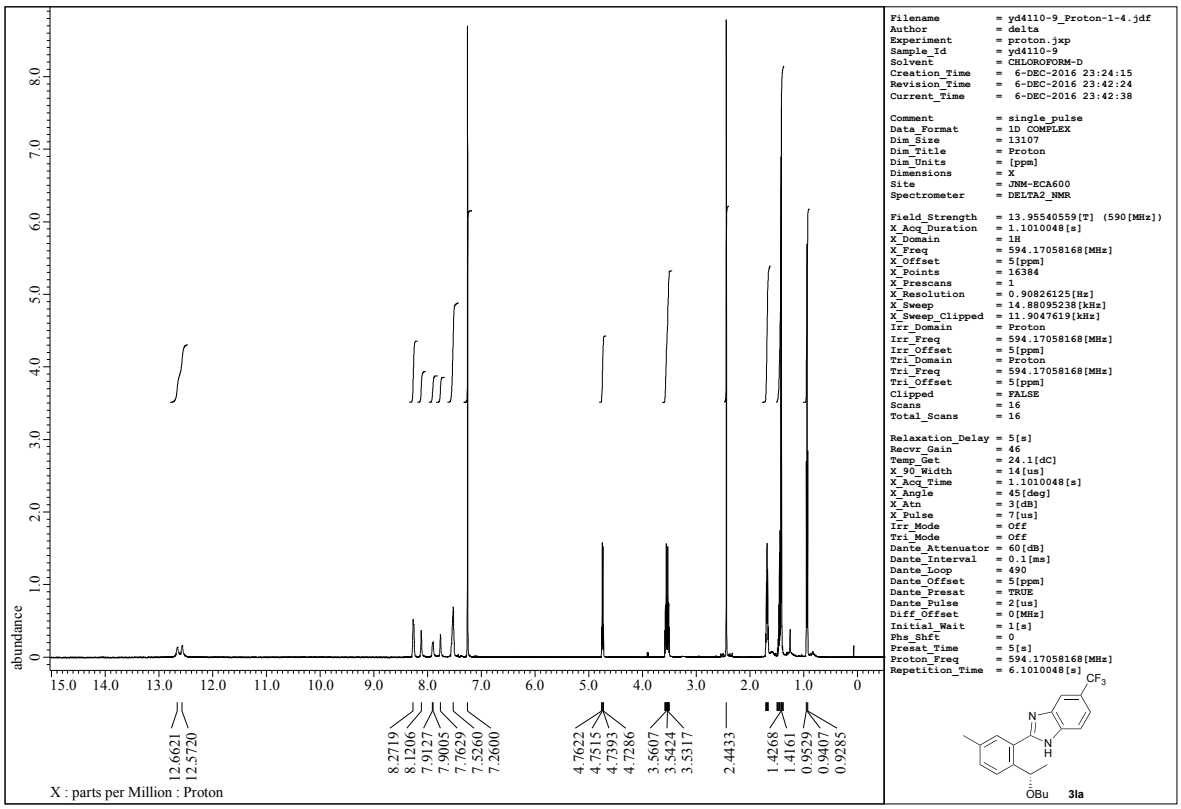
UV Results

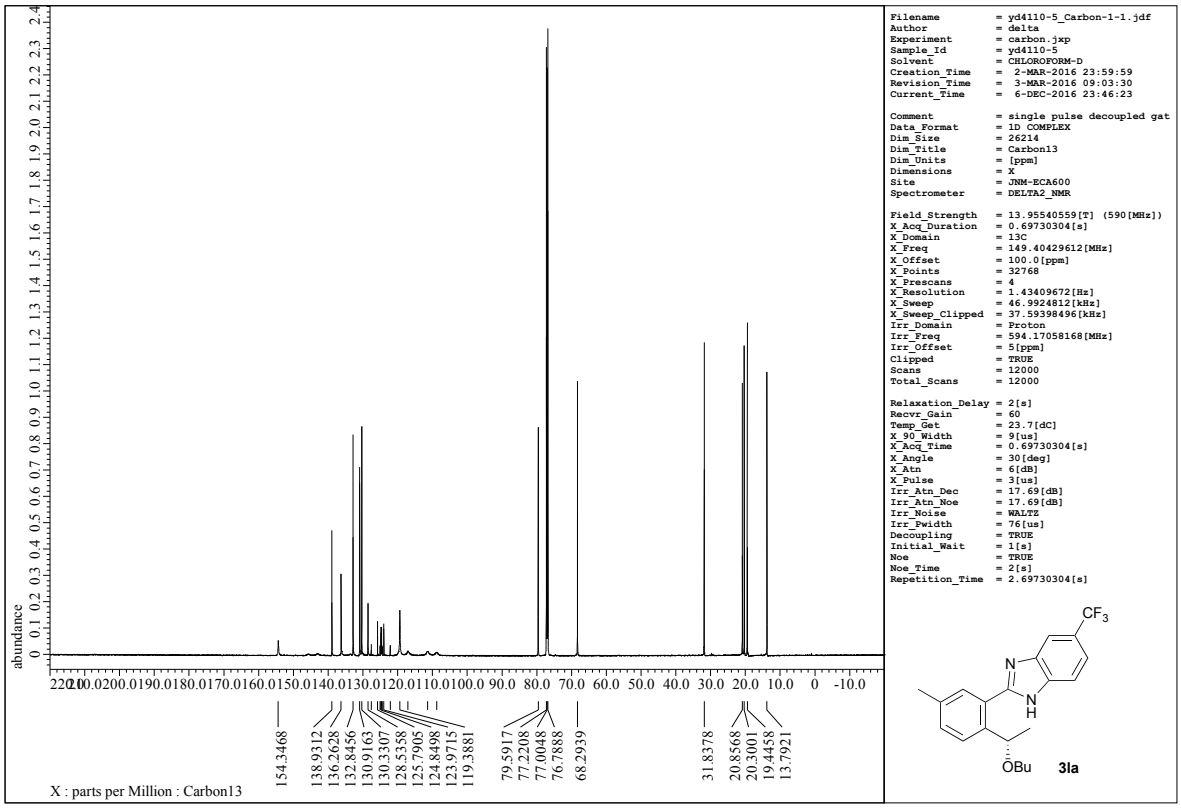
Pk #	Retention Time	Area	Area Percent	Height
1	26.945	2731600	96.850	52102
2	36.689	88857	3.150	1410

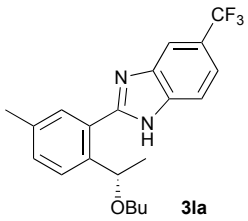


UV Results

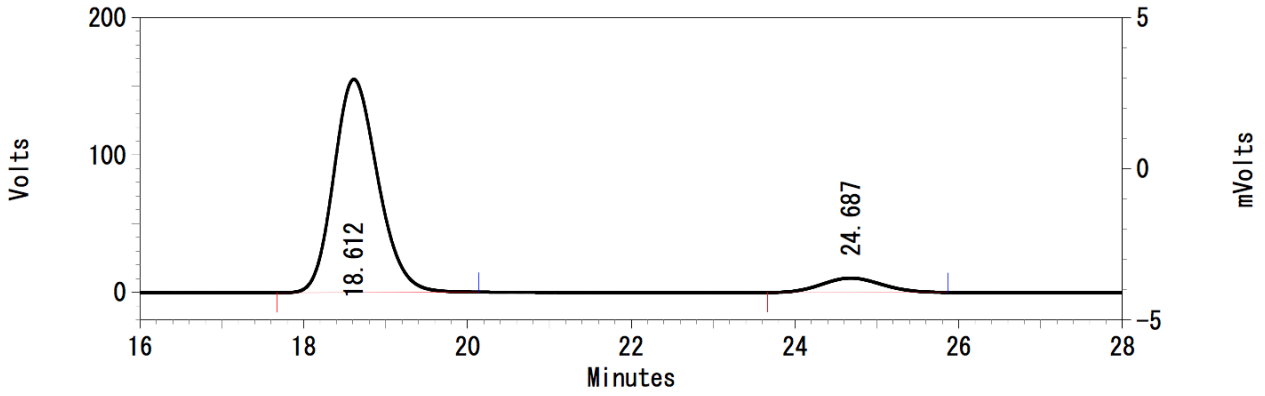
Pk #	Retention Time	Area	Area Percent	Height
1	26.572	2532773	49.988	49071
2	36.039	2534019	50.012	38200


abundance
15.0 14.0 13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.6621
12.5720
8.2719
8.1206
7.9127
7.9005
7.7629
7.5260
7.2600
4.7622
4.7515
4.7393
4.7286
3.5607
3.5424
3.5317
2.4433
1.4268
1.4161
0.9529
0.9407
0.9285
X : parts per Million : Proton
Filename = yd4110-9_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4110-9
Solvent = CHLOROFORM-D
Creation_Time = 6-DEC-2016 23:24:15
Revision_Time = 6-DEC-2016 23:42:24
Current_Time = 6-DEC-2016 23:42:38
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 24.1[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.1010048[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Attenuator = 60[dB]
Dante_Interval = 0.1[ms]
Dante_Loop = 490
Dante_Offset = 5[ppm]
Dante_Presat = TRUE
Dante_Pulse = 2[us]
Diff_Offset = 0[MHz]
Initial_Wait = 1[s]
Phs_Shft = 0
Presat_Time = 5[s]
Proton_Freq = 594.17058168[MHz]
Repetition_Time = 6.1010048[s]
CF3
N
N
H
OBu
3la


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
154.3468
138.9312
136.2628
132.8456
130.9163
130.3307
128.5358
125.7905
124.8498
123.9715
119.3881
79.5917
77.2208
77.0048
76.7888
68.2939
31.8378
20.8568
20.3001
19.4458
13.7921
X : parts per Million : Carbon13
Filename = yd4110-5_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4110-5
Solvent = CHLOROFORM-D
Creation_Time = 2-MAR-2016 23:59:59
Revision_Time = 3-MAR-2016 09:03:30
Current_Time = 6-DEC-2016 23:46:23
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 12000
Total_Scans = 12000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 23.7[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
CF3
N
N
H
OBu
3la

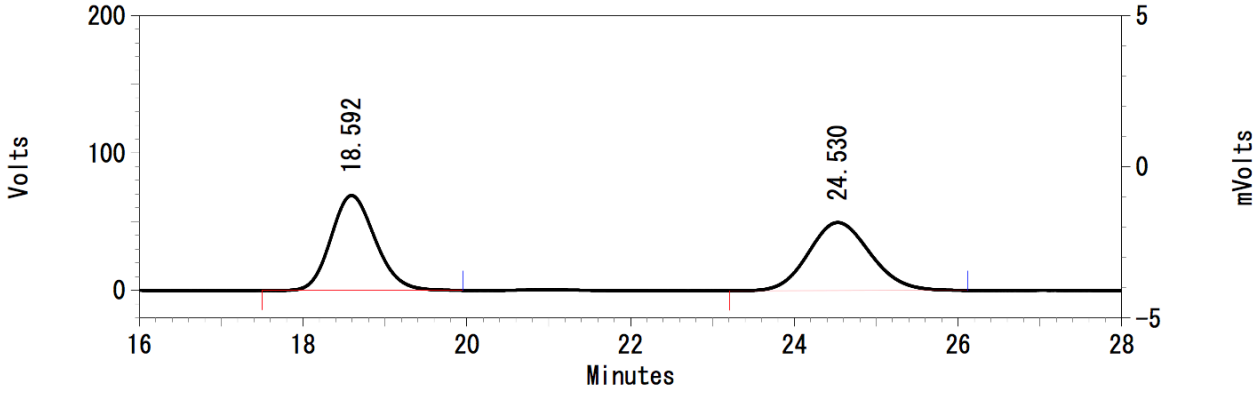


3la



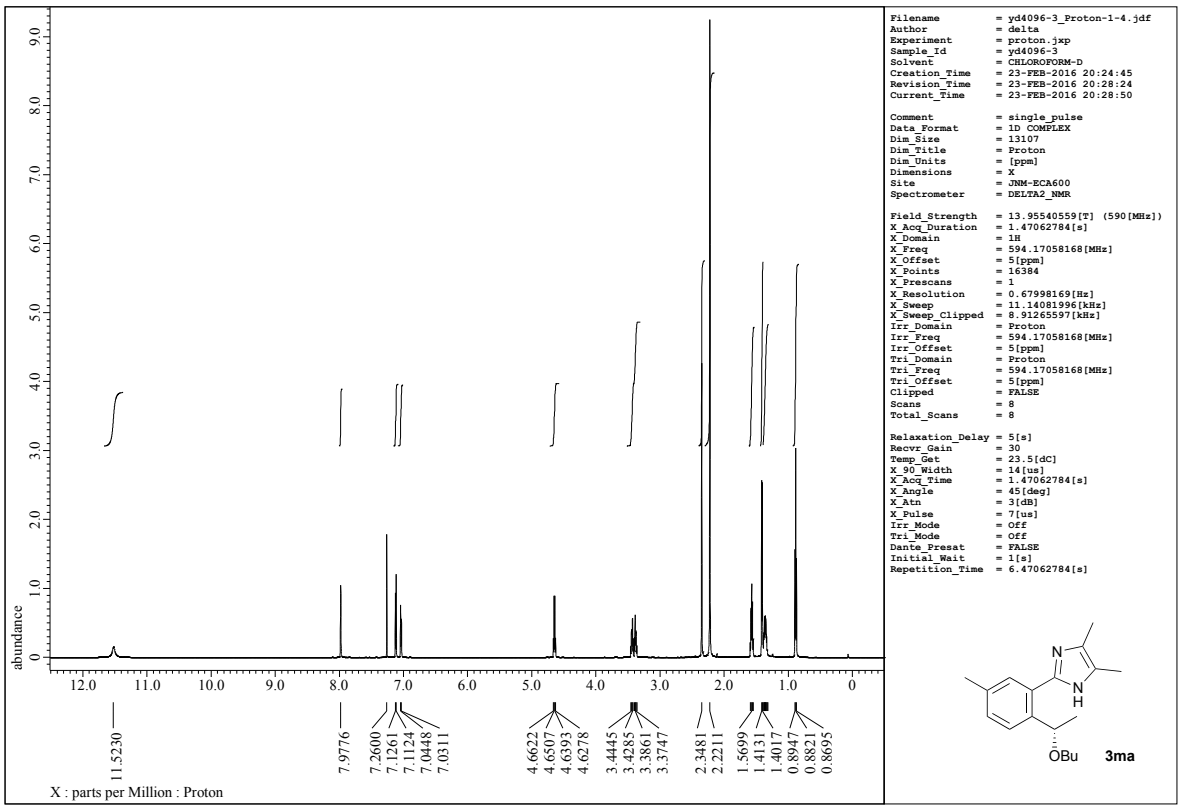
UV Results

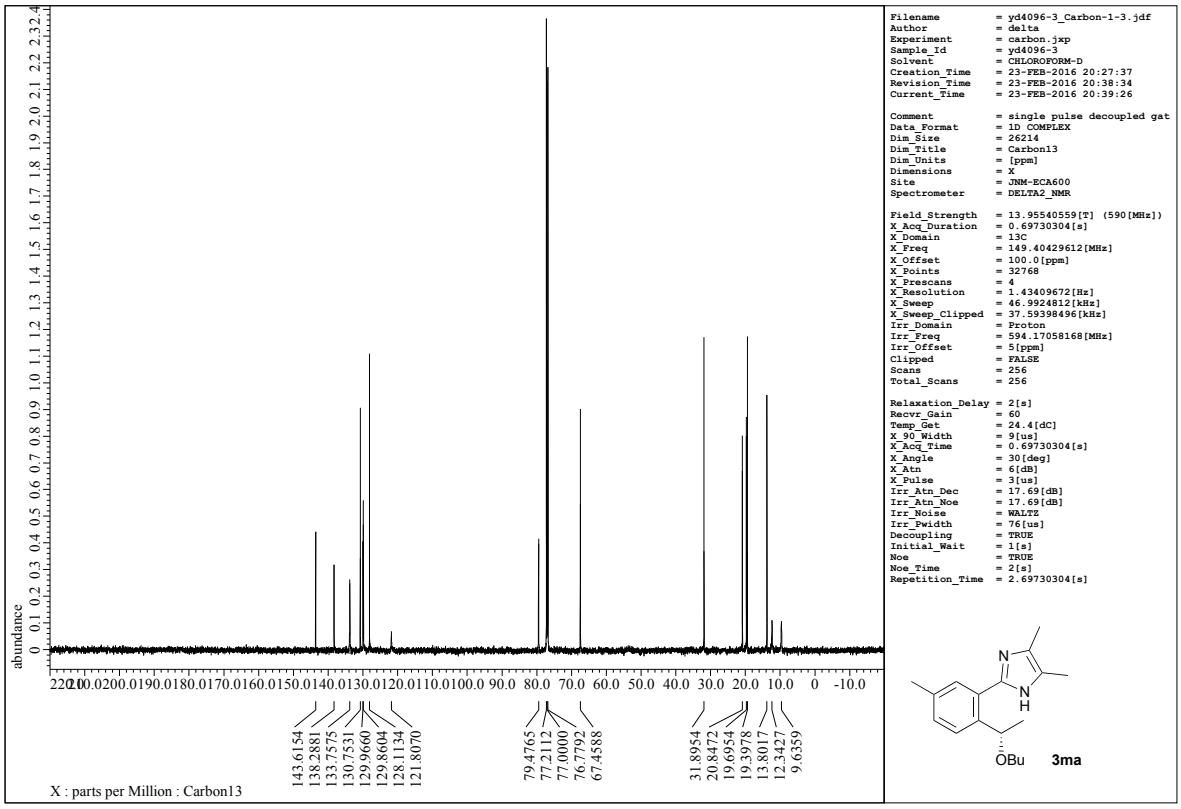
Pk #	Retention Time	Area	Area Percent	Height
1	18.612	5790021	91.506	155002
2	24.687	537444	8.494	10479

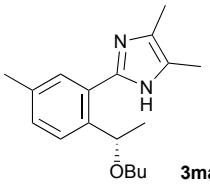


UV Results

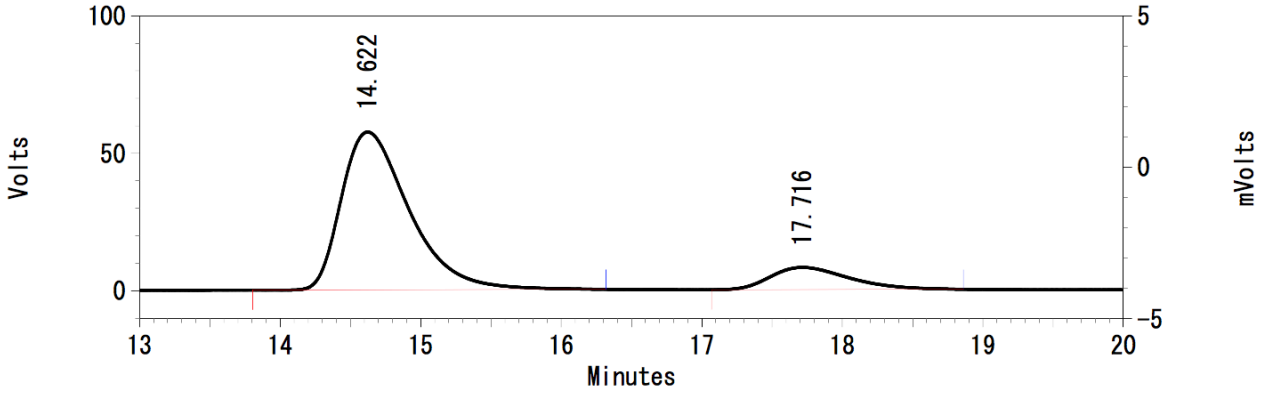
Pk #	Retention Time	Area	Area Percent	Height
1	18.592	2590112	49.948	69010
2	24.530	2595481	50.052	49467


abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
11.5230
7.9776
7.2600
7.1261
7.1124
7.0448
7.0311
4.6622
4.6507
4.6393
4.6278
3.4445
3.4285
3.3861
3.3747
2.3481
2.2211
1.5699
1.4131
1.4017
0.8947
0.8821
0.8695
X : parts per Million : Proton
Filename = yd4096-3_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4096-3
Solvent = CHLOROFORM-D
Creation_Time = 23-FEB-2016 20:24:45
Revision_Time = 23-FEB-2016 20:28:24
Current_Time = 23-FEB-2016 20:28:50
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 23.5[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
N
N
H
OBu
3ma


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
143.6154
138.2881
133.7575
130.7531
129.9660
129.8604
128.1134
121.8070
79.4765
77.2112
77.0000
76.7792
67.4588
31.8954
20.8472
19.6954
19.3978
13.8017
12.3427
9.6359
X : parts per Million : Carbon13
Filename = yd4096-3_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4096-3
Solvent = CHLOROFORM-D
Creation_Time = 23-FEB-2016 20:27:37
Revision_Time = 23-FEB-2016 20:38:34
Current_Time = 23-FEB-2016 20:39:26
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.4[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
N
N
H
OBu
3ma

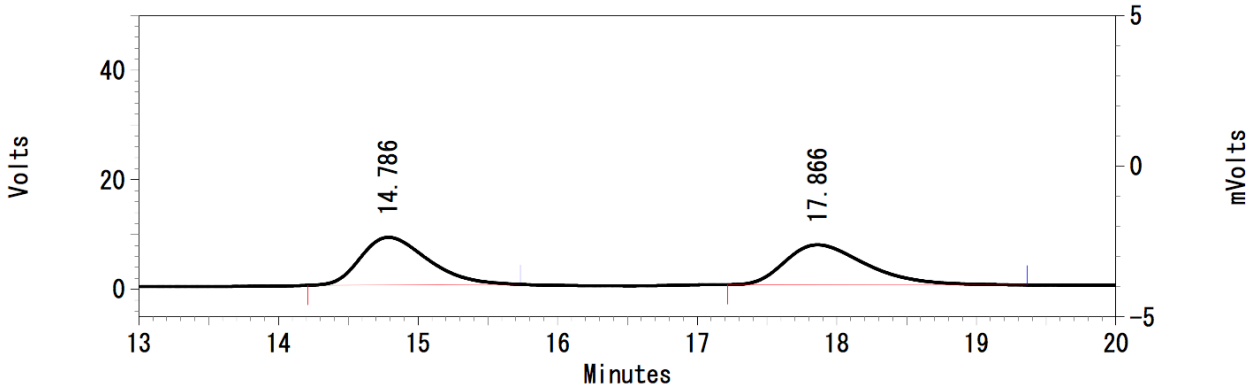


3ma



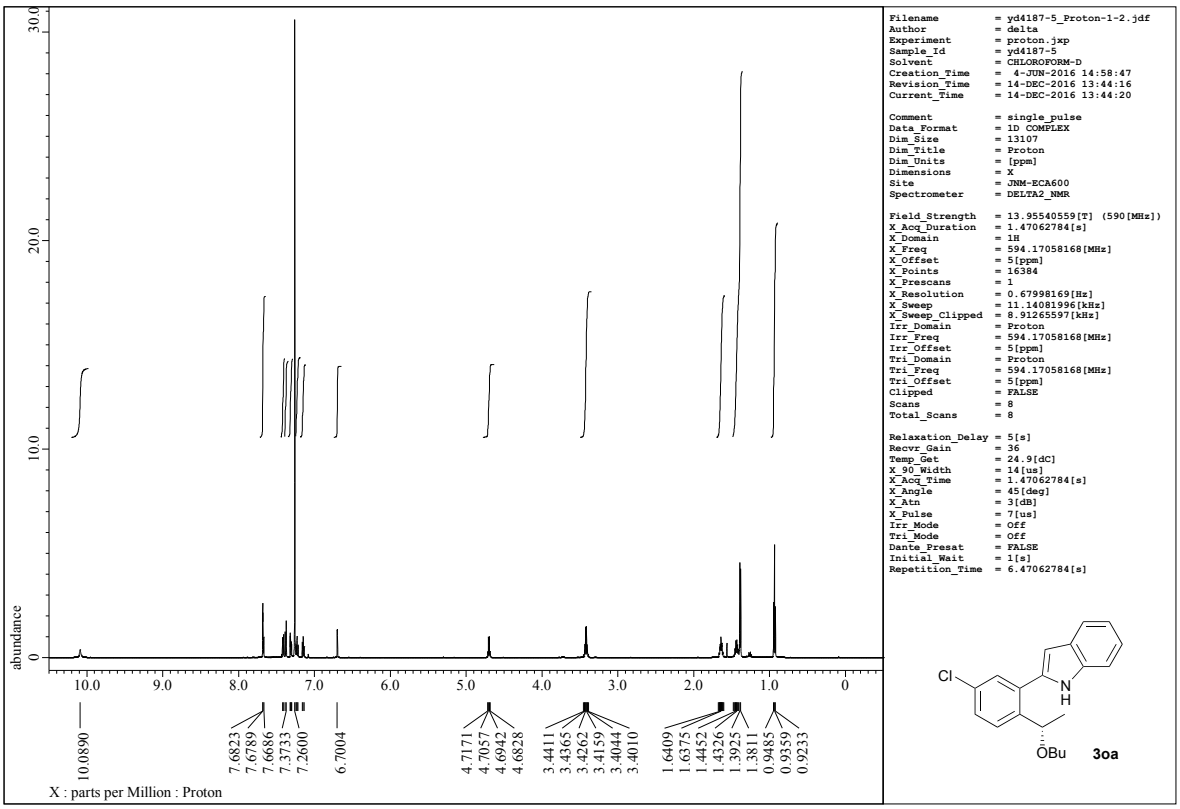
UV Results

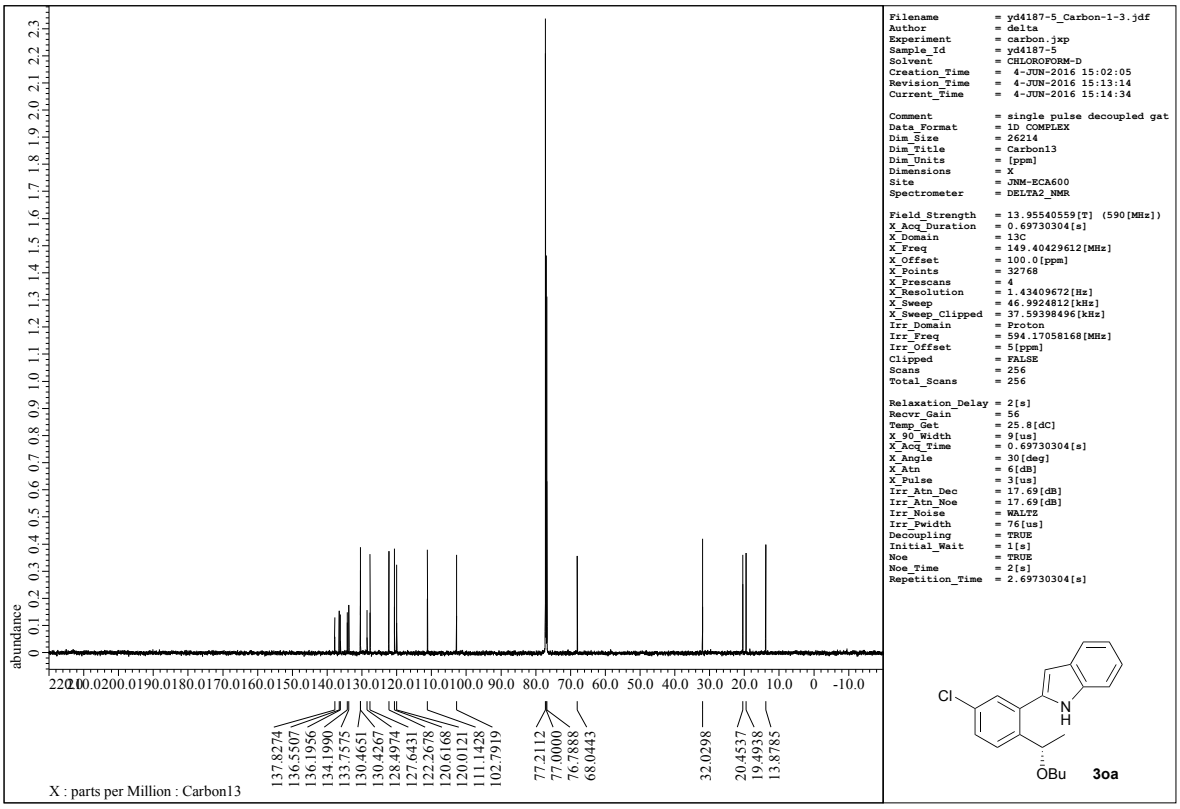
Pk #	Retention Time	Area	Area Percent	Height
1	14.622	1920644	86.004	57321
2	17.716	312548	13.996	8047

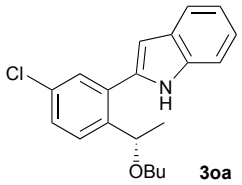


UV Results

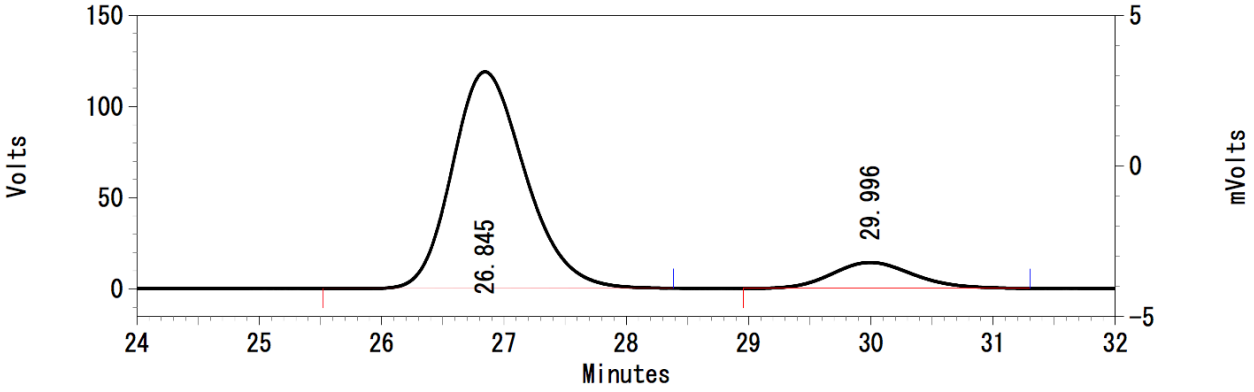
Pk #	Retention Time	Area	Area Percent	Height
1	14.786	291482	49.799	8689
2	17.866	293839	50.201	7292


abundance
10.0890
7.6823
7.6789
7.6686
7.3733
7.2600
6.7004
4.7171
4.7057
4.6942
4.6828
3.4411
3.4365
3.4262
3.4159
3.4044
3.4010
1.6409
1.6375
1.4452
1.4326
1.3925
1.3811
0.9485
0.9359
0.9233
X : parts per Million : Proton
Filename = yd4187-5_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4187-5
Solvent = CHLOROFORM-D
Creation_Time = 4-JUN-2016 14:58:47
Revision_Time = 14-DEC-2016 13:44:16
Current_Time = 14-DEC-2016 13:44:20
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 24.9[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Cl
N
H
OBu
3oa


abundance
137.8274
136.5507
136.1956
134.1990
133.7575
130.4651
130.4267
128.4974
127.6431
122.2678
120.6168
120.0121
111.1428
102.7919
77.2112
77.0000
76.7888
68.0443
32.0298
20.4537
19.4938
13.8785
X : parts per Million : Carbon13
Filename = yd4187-5_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4187-5
Solvent = CHLOROFORM-D
Creation_Time = 4-JUN-2016 15:02:05
Revision_Time = 4-JUN-2016 15:13:14
Current_Time = 4-JUN-2016 15:14:34
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 25.8[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
Cl
N
H
OBu
3oa

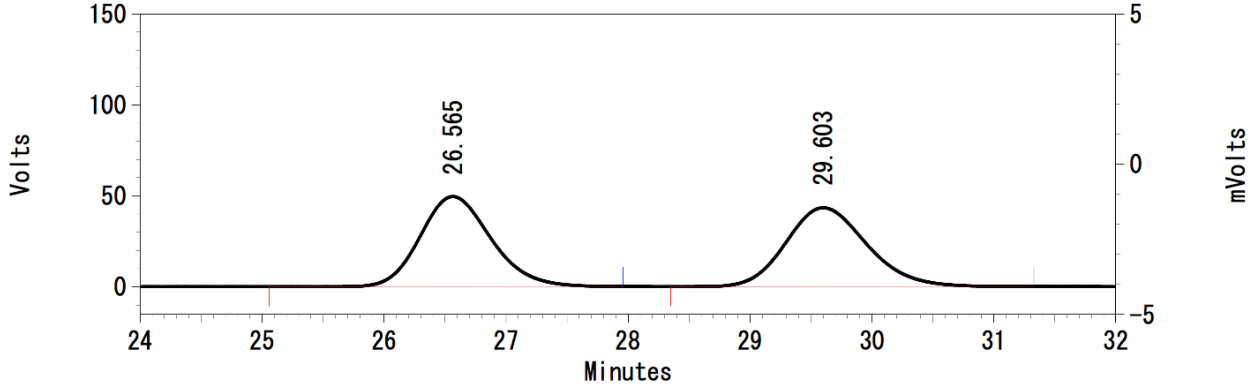


3oa



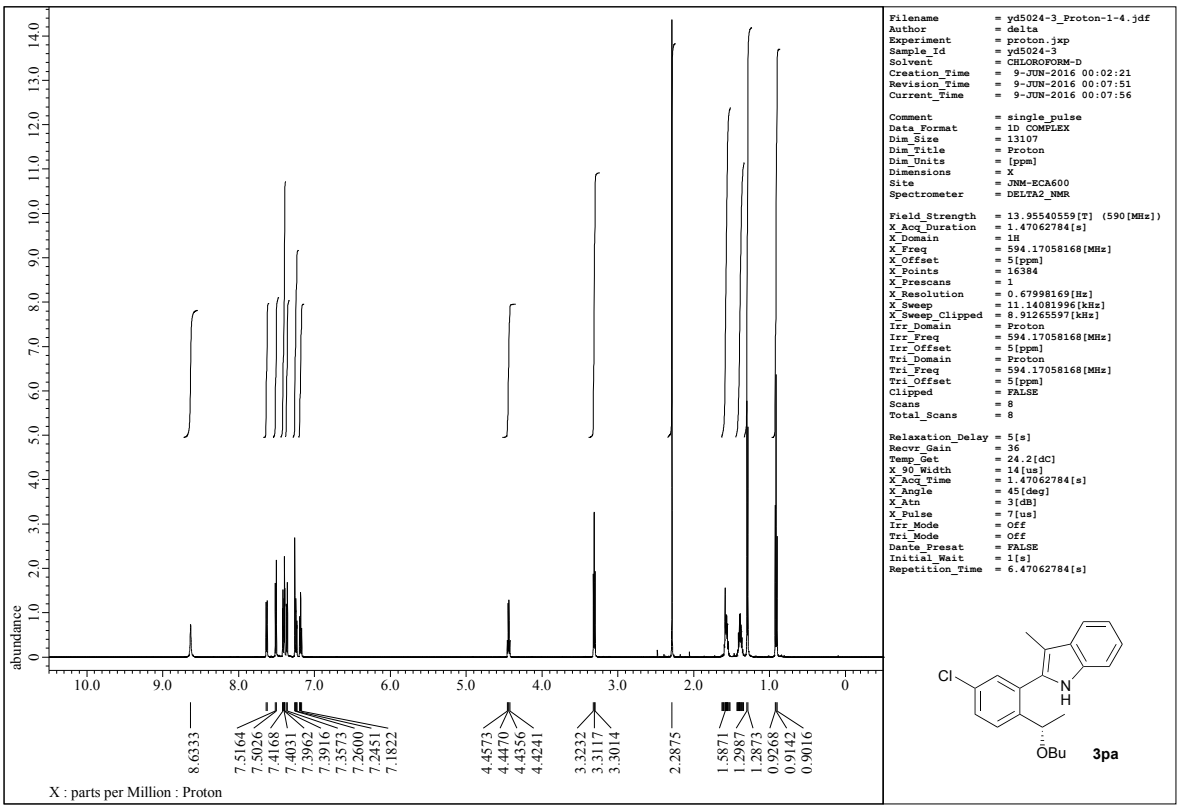
UV Results

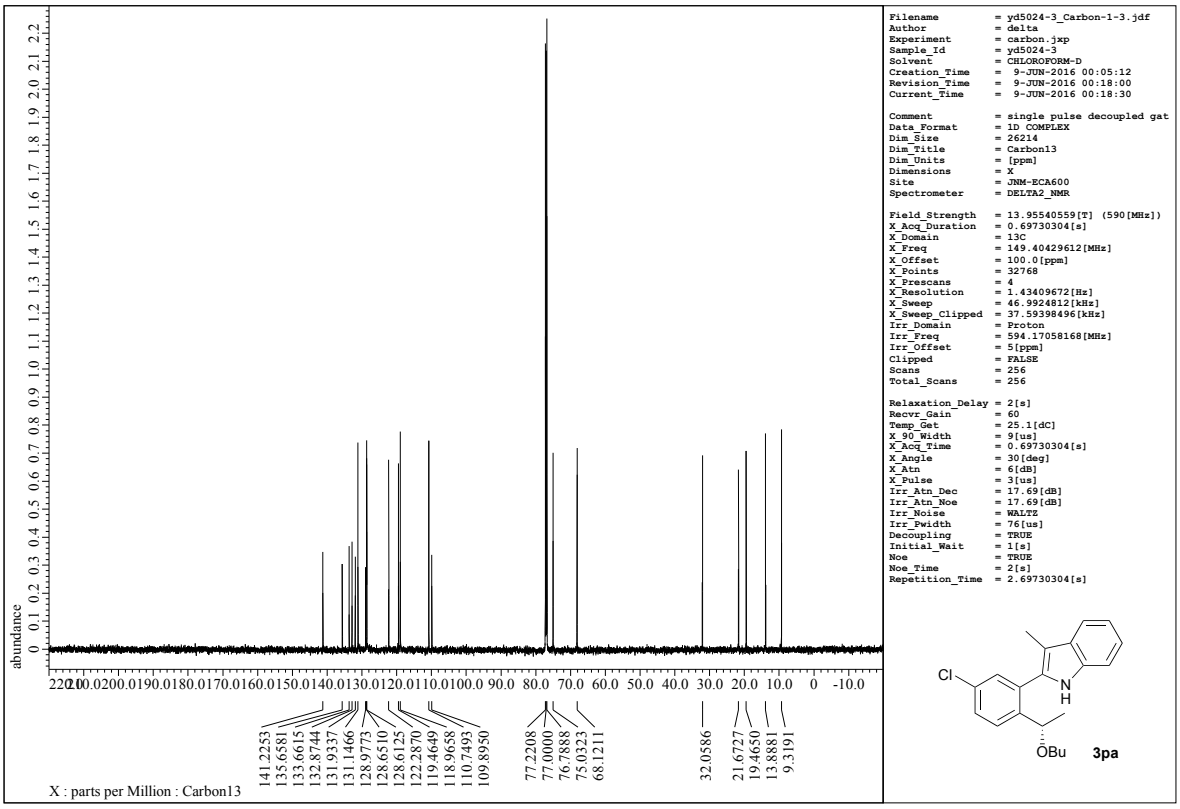
Pk #	Retention Time	Area	Area Percent	Height
1	26.845	4915852	88.224	118617
2	29.996	656164	11.776	14166

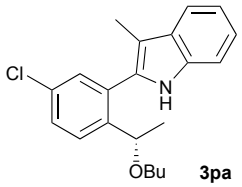


UV Results

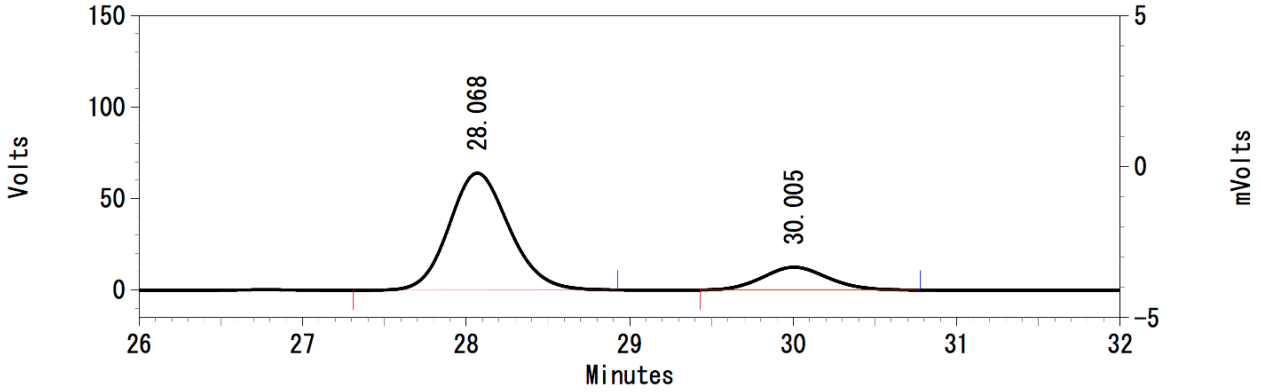
Pk #	Retention Time	Area	Area Percent	Height
1	26.565	2000068	50.013	49437
2	29.603	1999000	49.987	43265


abundance
X : parts per Million : Proton
8.6333
7.5164
7.5026
7.4168
7.4031
7.3962
7.3916
7.3573
7.2600
7.2451
7.1822
4.4573
4.4470
4.4356
4.4241
3.3232
3.3117
3.3014
2.2875
1.5871
1.2987
1.2873
0.9268
0.9142
0.9016
Filename = yd5024-3_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd5024-3
Solvent = CHLOROFORM-D
Creation_Time = 9-JUN-2016 00:02:21
Revision_Time = 9-JUN-2016 00:07:51
Current_Time = 9-JUN-2016 00:07:56
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 24.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Cl
N
H
OBu
3pa


abundance
X : parts per Million : Carbon13
141.2253
135.6581
133.6615
132.8744
131.9337
131.1466
128.9773
128.6510
128.6125
122.2870
119.4649
118.9658
110.7493
109.8950
77.2208
77.0000
76.7888
75.0323
68.1211
32.0586
21.6727
19.4650
13.8881
9.3191
Filename = yd5024-3_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd5024-3
Solvent = CHLOROFORM-D
Creation_Time = 9-JUN-2016 00:05:12
Revision_Time = 9-JUN-2016 00:18:00
Current_Time = 9-JUN-2016 00:18:30
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.1[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
Cl
N
H
OBu
3pa

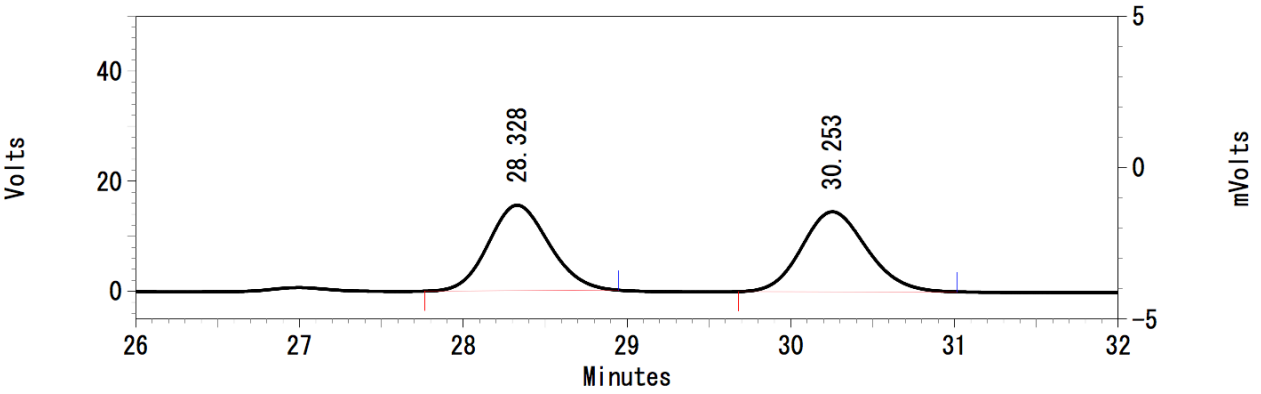


3pa



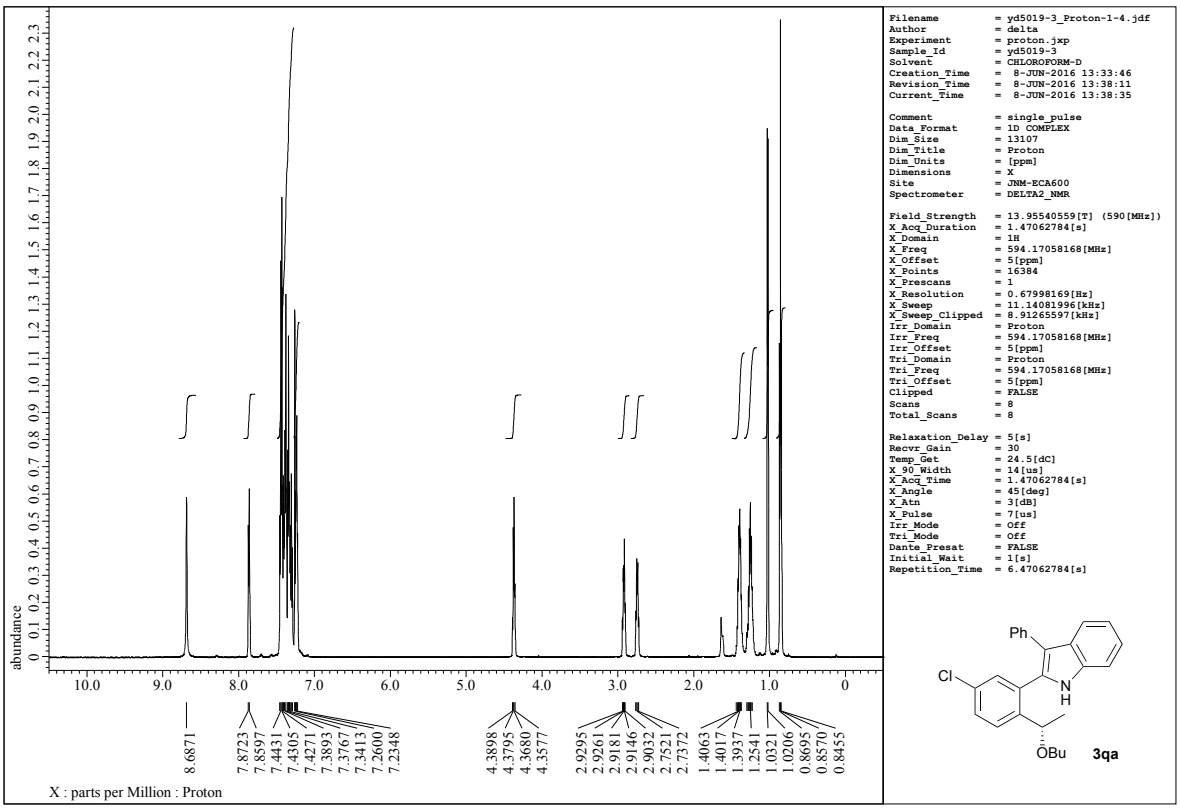
UV Results

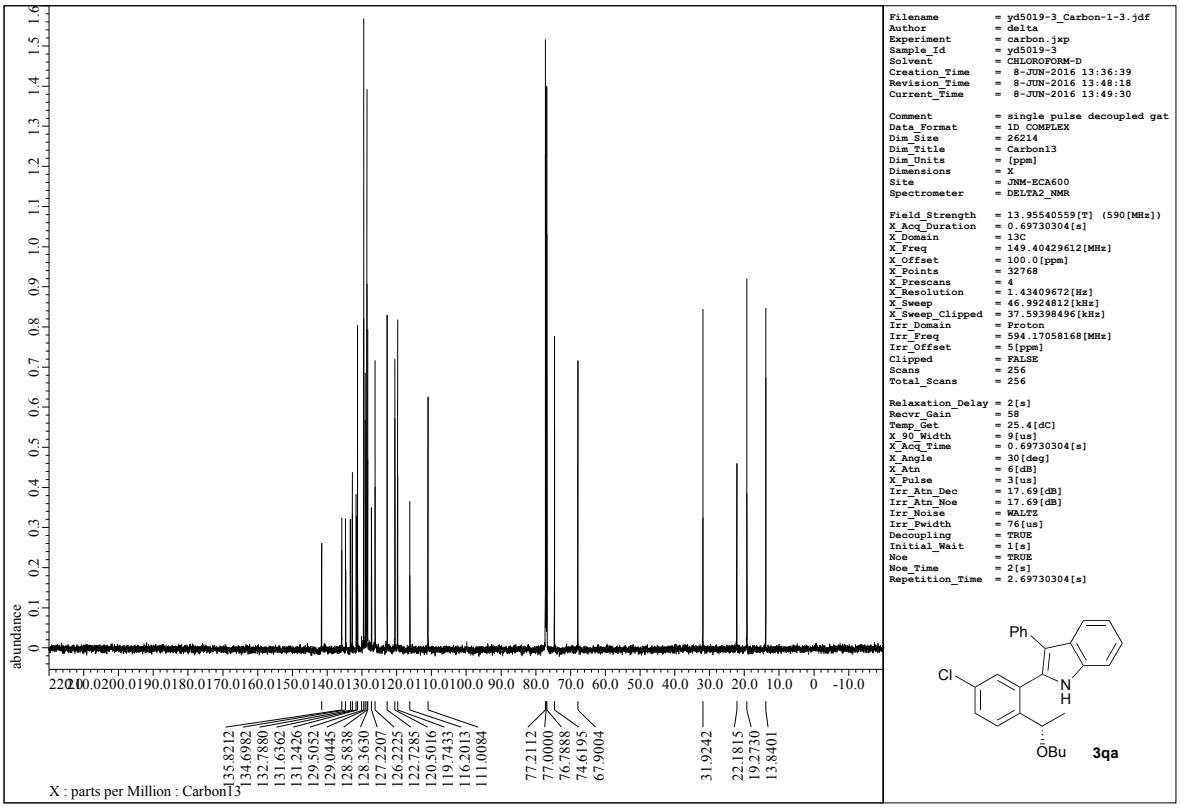
Pk #	Retention Time	Area	Area Percent	Height
1	28.068	1637300	82.472	63881
2	30.005	347980	17.528	12466

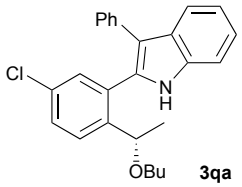


UV Results

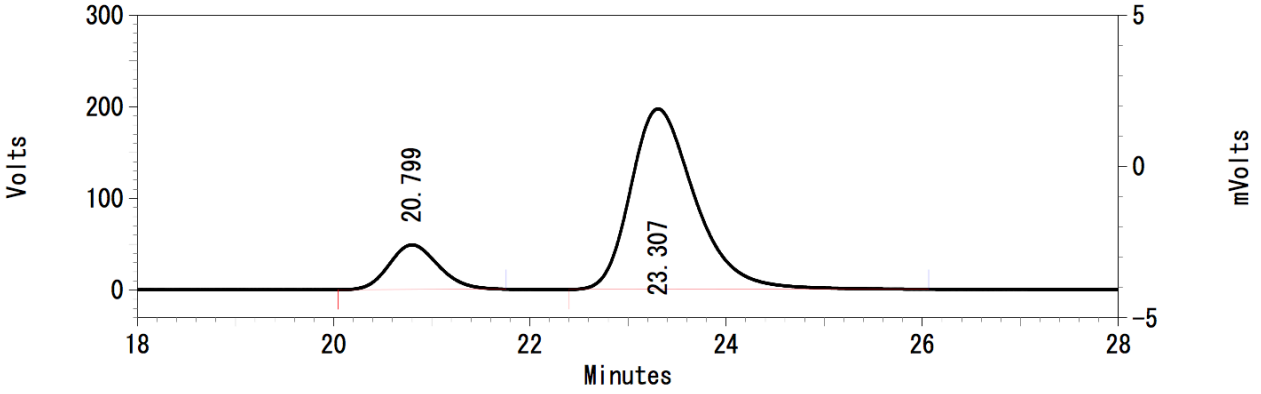
Pk #	Retention Time	Area	Area Percent	Height
1	28.328	400049	49.850	15522
2	30.253	402451	50.150	14518


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.6871
7.8723 7.8597 7.4431 7.4305 7.4271 7.3893 7.3767 7.3413 7.2600 7.2348
4.3898 4.3795 4.3680 4.3577
2.9295 2.9261 2.9181 2.9146 2.9032 2.7521 2.7372
1.4063 1.4017 1.3937 1.2541 1.0321 1.0206 0.8695 0.8570 0.8455
X : parts per Million : Proton
Filename = yd5019-3_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd5019-3
Solvent = CHLOROFORM-D
Creation_Time = 8-JUN-2016 13:33:46
Revision_Time = 8-JUN-2016 13:38:11
Current_Time = 8-JUN-2016 13:38:35
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 24.5[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Ph
Cl
N
H
OBu
3qa


abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
135.8212
134.6982
132.7880
131.6362
131.2426
129.5052
129.0445
128.5838
128.3630
127.2207
126.2225
122.7285
120.5016
119.7433
116.2013
111.0084
77.2112
77.0000
76.7888
74.6195
67.9004
31.9242
22.1815
19.2730
13.8401
X : parts per Million : Carbon13
Filename = yd5019-3_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd5019-3
Solvent = CHLOROFORM-D
Creation_Time = 8-JUN-2016 13:36:39
Revision_Time = 8-JUN-2016 13:48:18
Current_Time = 8-JUN-2016 13:49:30
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 25.4[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
Ph
Cl
N
H
OBu
3qa

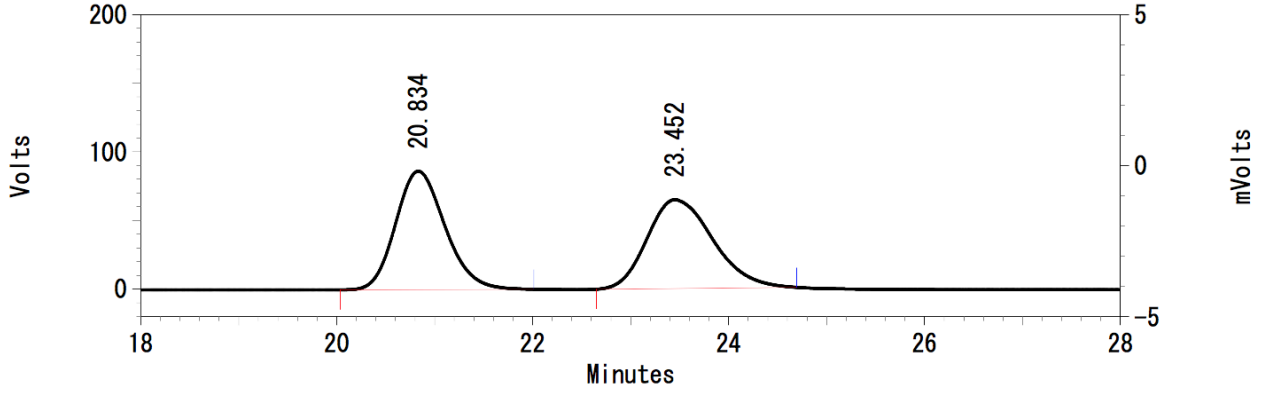


3qa



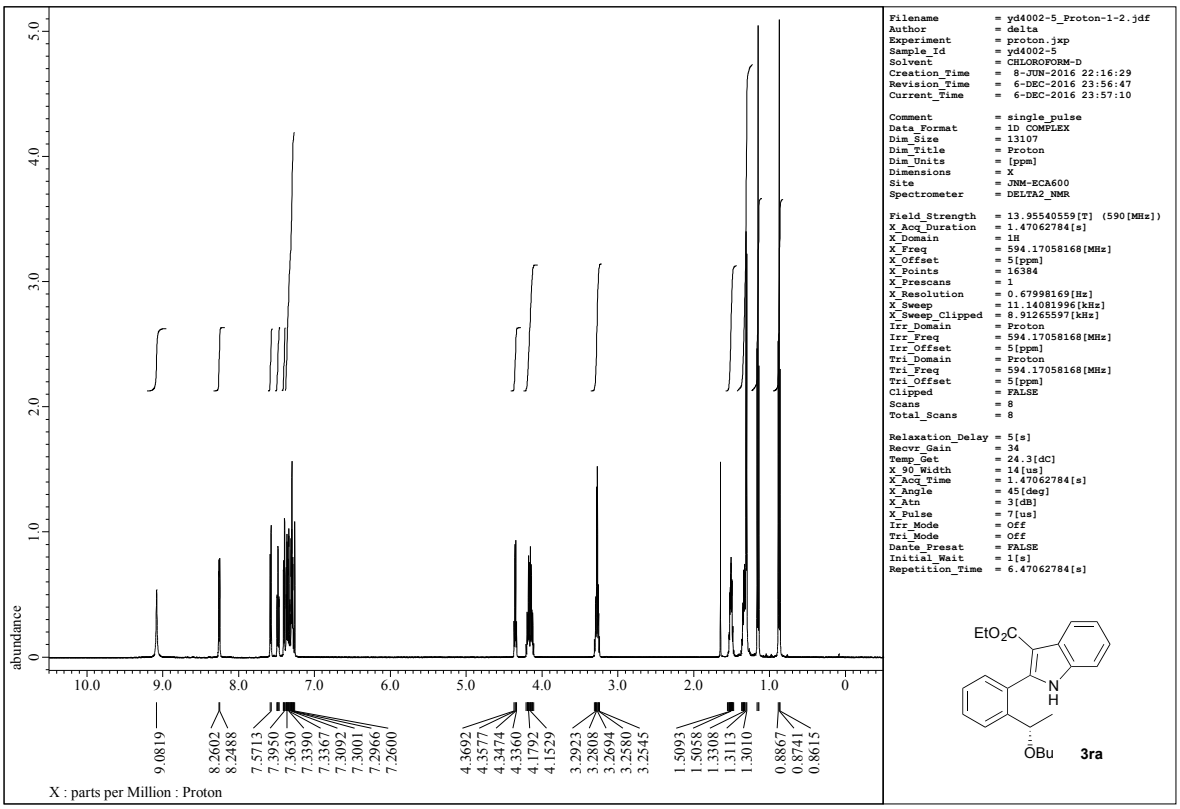
UV Results

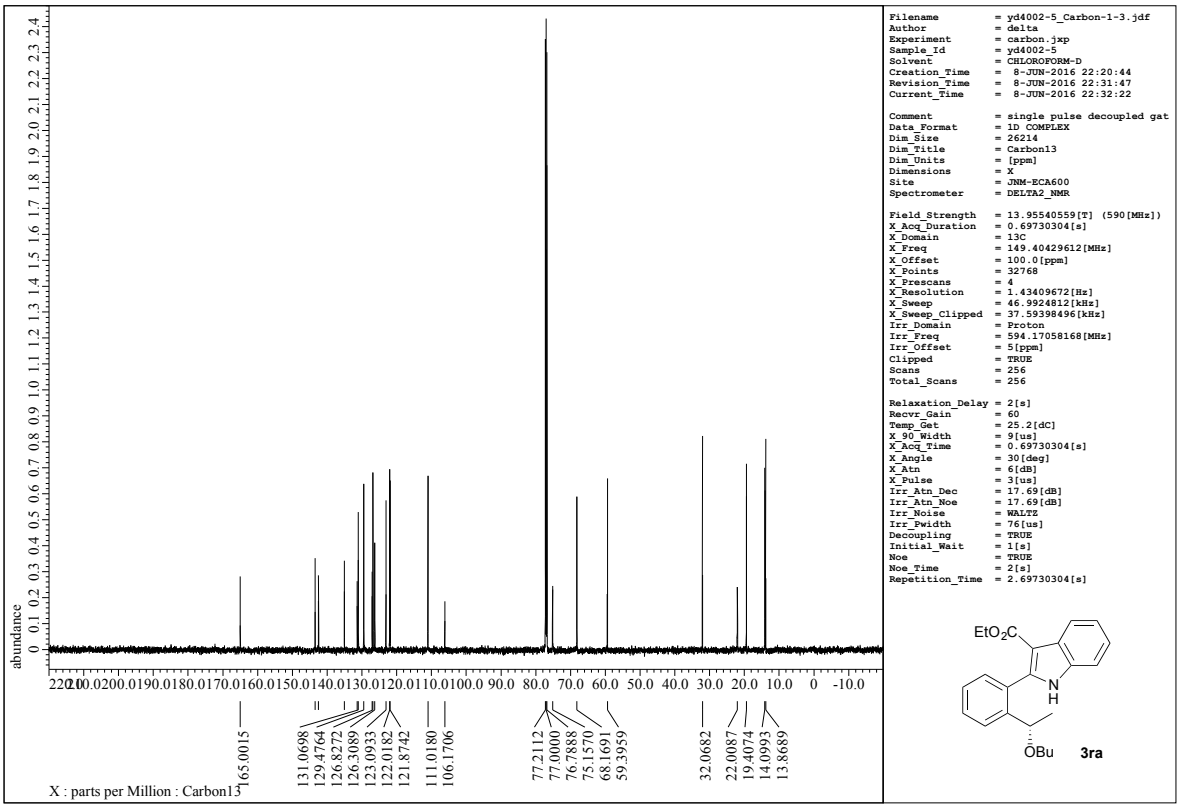
Pk #	Retention Time	Area	Area Percent	Height
1	20.799	1693486	15.851	48647
2	23.307	8990248	84.149	196863

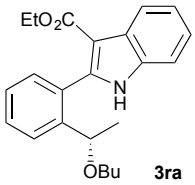


UV Results

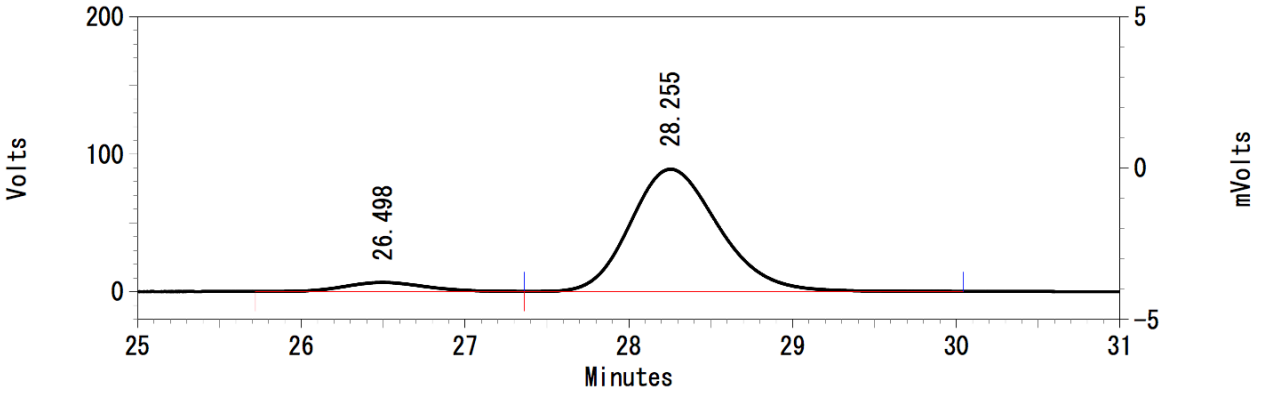
Pk #	Retention Time	Area	Area Percent	Height
1	20.834	3022567	50.041	86240
2	23.452	3017661	49.959	64659


abundance
X : parts per Million : Proton
9.0819
8.2602
8.2488
7.5713
7.3950
7.3630
7.3390
7.3367
7.3092
7.3001
7.2966
7.2600
4.3692
4.3577
4.3474
4.3360
4.1792
4.1529
3.2923
3.2808
3.2694
3.2580
3.2545
1.5093
1.5058
1.3308
1.3113
1.3010
0.8867
0.8741
0.8615
Filename = yd4002-5_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4002-5
Solvent = CHLOROFORM-D
Creation_Time = 8-JUN-2016 22:16:29
Revision_Time = 6-DEC-2016 23:56:47
Current_Time = 6-DEC-2016 23:57:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 24.3[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
EtO2C
N
H
OBu
3ra


abundance
X : parts per Million : Carbon13
165.0015
131.0698
129.4764
126.8272
126.3089
123.0933
122.0182
121.8742
111.0180
106.1706
77.2112
77.0000
76.7888
75.1570
68.1691
59.3959
32.0682
22.0087
19.4074
14.0993
13.8689
Filename = yd4002-5_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4002-5
Solvent = CHLOROFORM-D
Creation_Time = 8-JUN-2016 22:20:44
Revision_Time = 8-JUN-2016 22:31:47
Current_Time = 8-JUN-2016 22:32:22
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.2[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
EtO2C
N
H
OBu
3ra

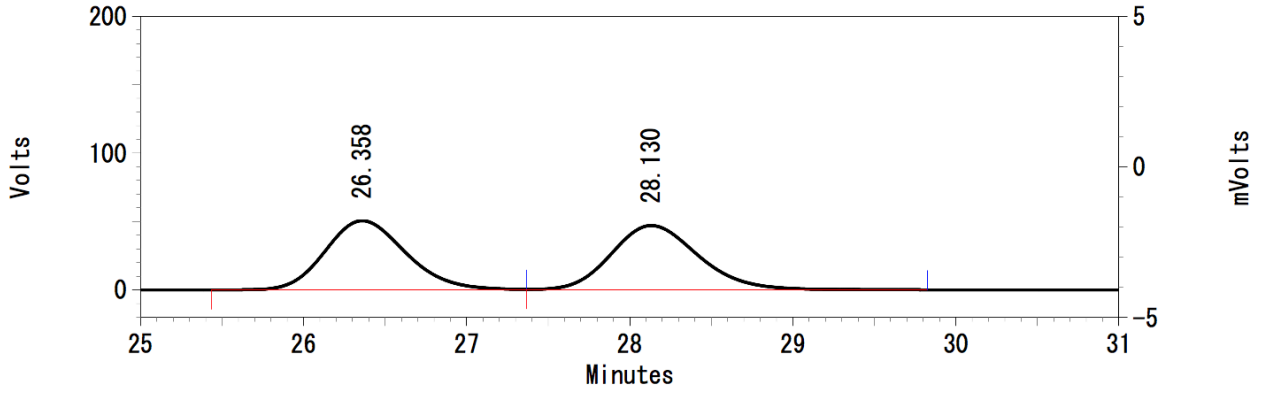


3ra



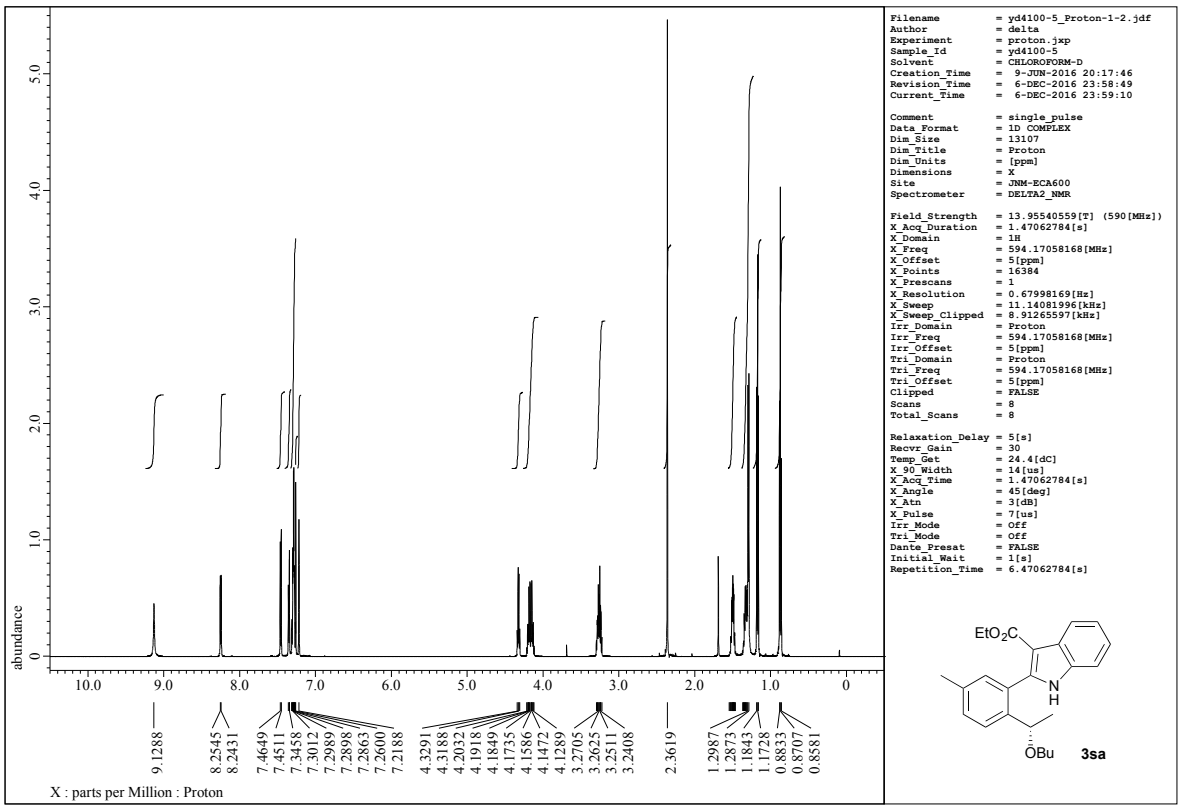
UV Results

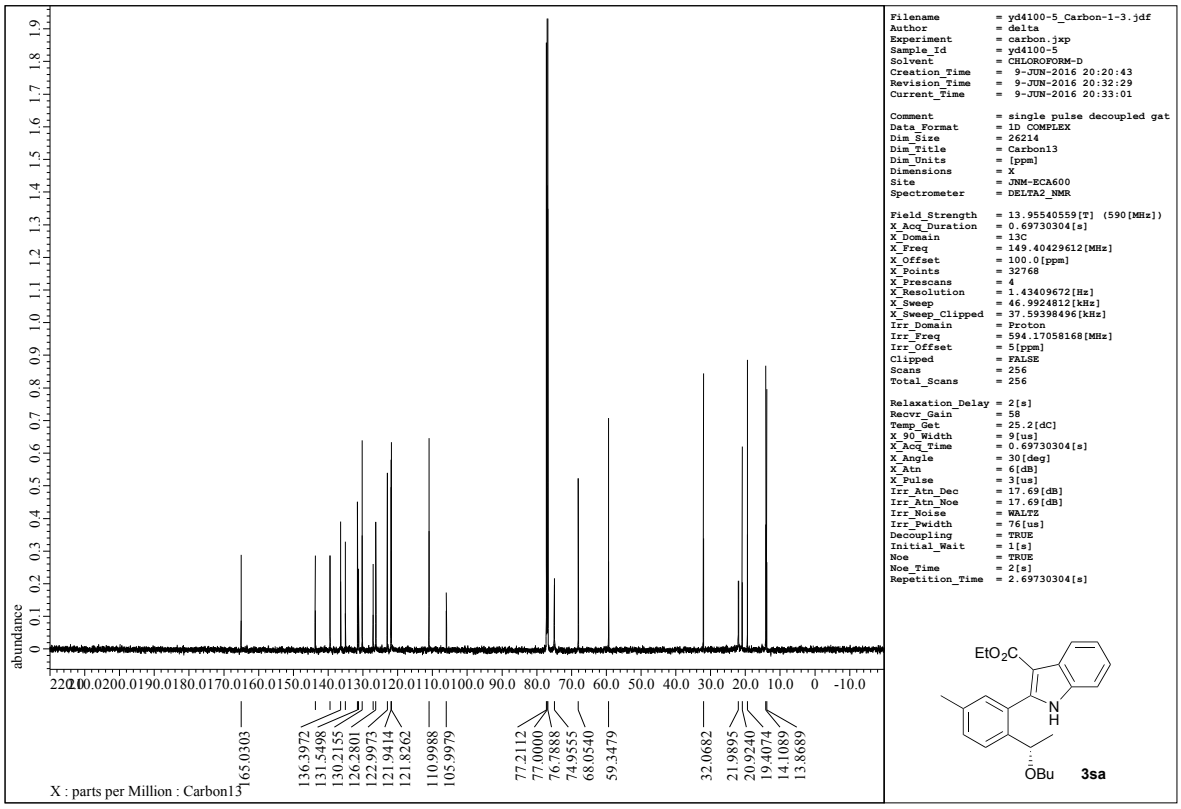
Pk #	Retention Time	Area	Area Percent	Height
1	26.498	225901	6.347	6563
2	28.255	3333538	93.653	88844

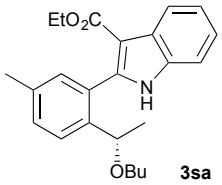


UV Results

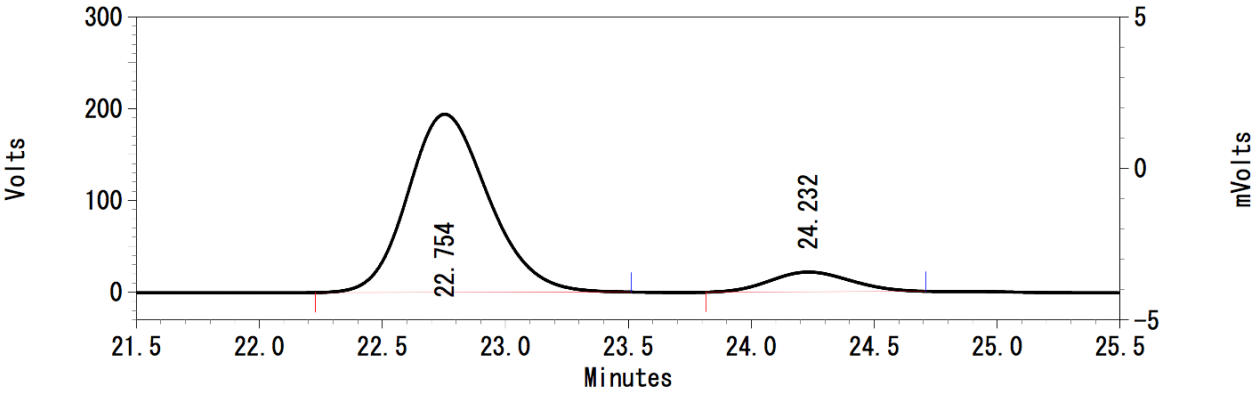
Pk #	Retention Time	Area	Area Percent	Height
1	26.358	1741733	49.870	50467
2	28.130	1750782	50.130	46937


abundance
X : parts per Million : Proton
9.1288
8.2545
8.2431
7.4649
7.4511
7.3458
7.3012
7.2989
7.2898
7.2863
7.2600
7.2188
4.3291
4.3188
4.2032
4.1918
4.1849
4.1735
4.1586
4.1472
4.1289
3.2705
3.2625
3.2511
3.2408
2.3619
1.2987
1.2873
1.1843
1.1728
0.8833
0.8707
0.8581
Filename = yd4100-5_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd4100-5
Solvent = CHLOROFORM-D
Creation_Time = 9-JUN-2016 20:17:46
Revision_Time = 6-DEC-2016 23:58:49
Current_Time = 6-DEC-2016 23:59:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 24.4[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
EtO2C
N
H
OBu
3sa


abundance
X : parts per Million : Carbon13
165.0303
136.3972
131.5498
130.2155
126.2801
122.9973
121.9414
121.8262
110.9988
105.9979
77.2112
77.0000
76.7888
74.9555
68.0540
59.3479
32.0682
21.9895
20.9240
19.4074
14.1089
13.8689
Filename = yd4100-5_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd4100-5
Solvent = CHLOROFORM-D
Creation_Time = 9-JUN-2016 20:20:43
Revision_Time = 9-JUN-2016 20:32:29
Current_Time = 9-JUN-2016 20:33:01
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 25.2[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
EtO2C
N
H
OBu
3sa

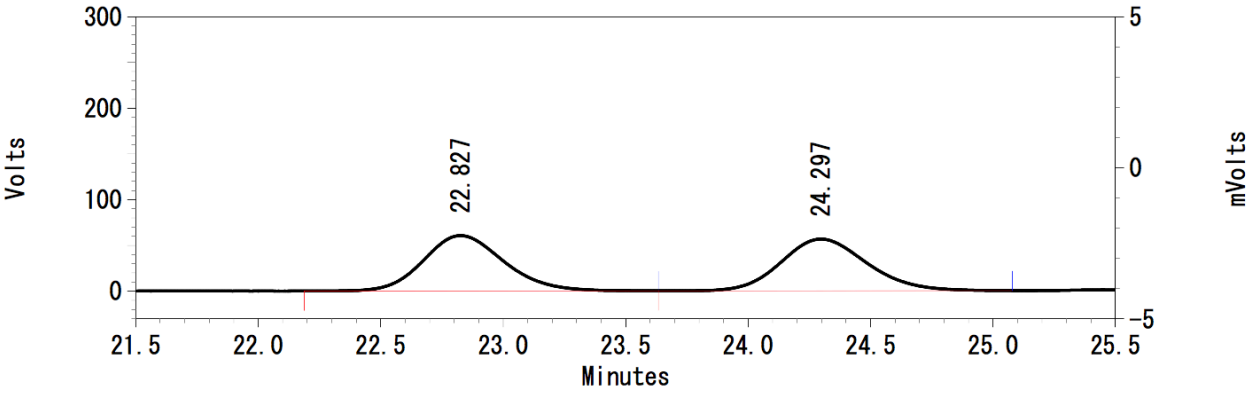


3sa



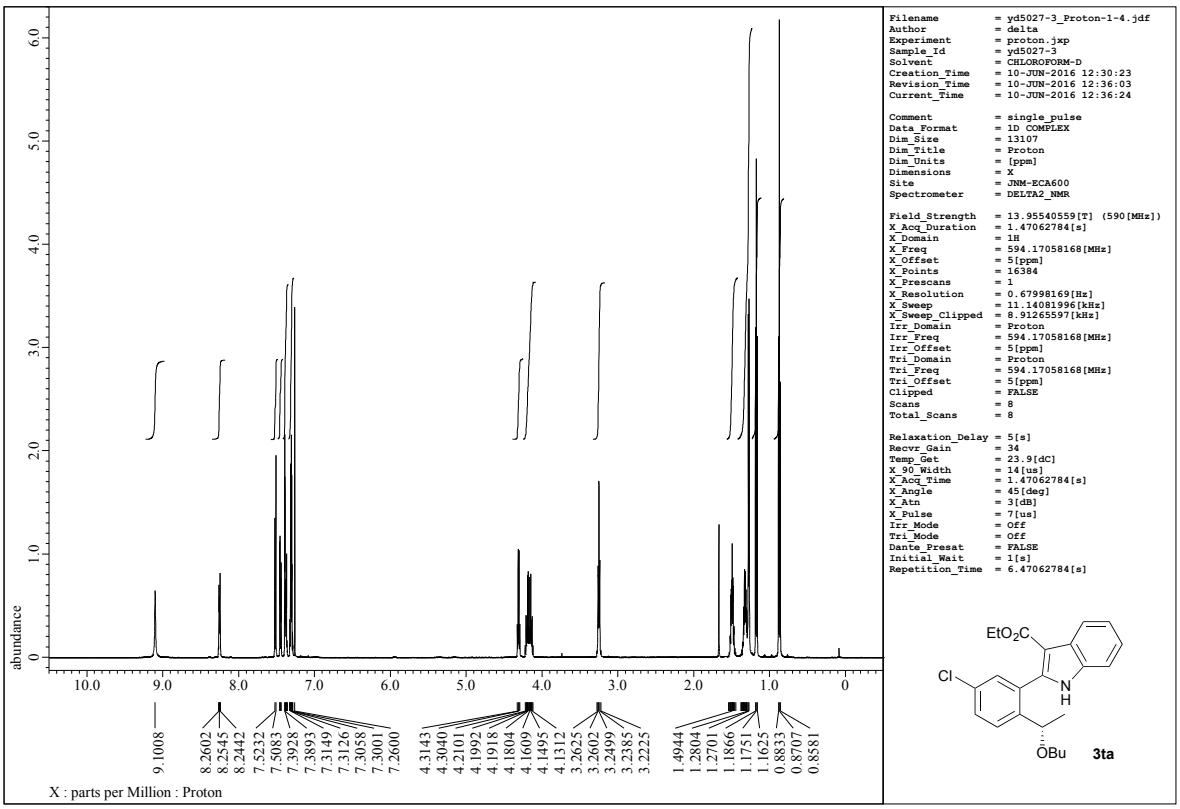
UV Results

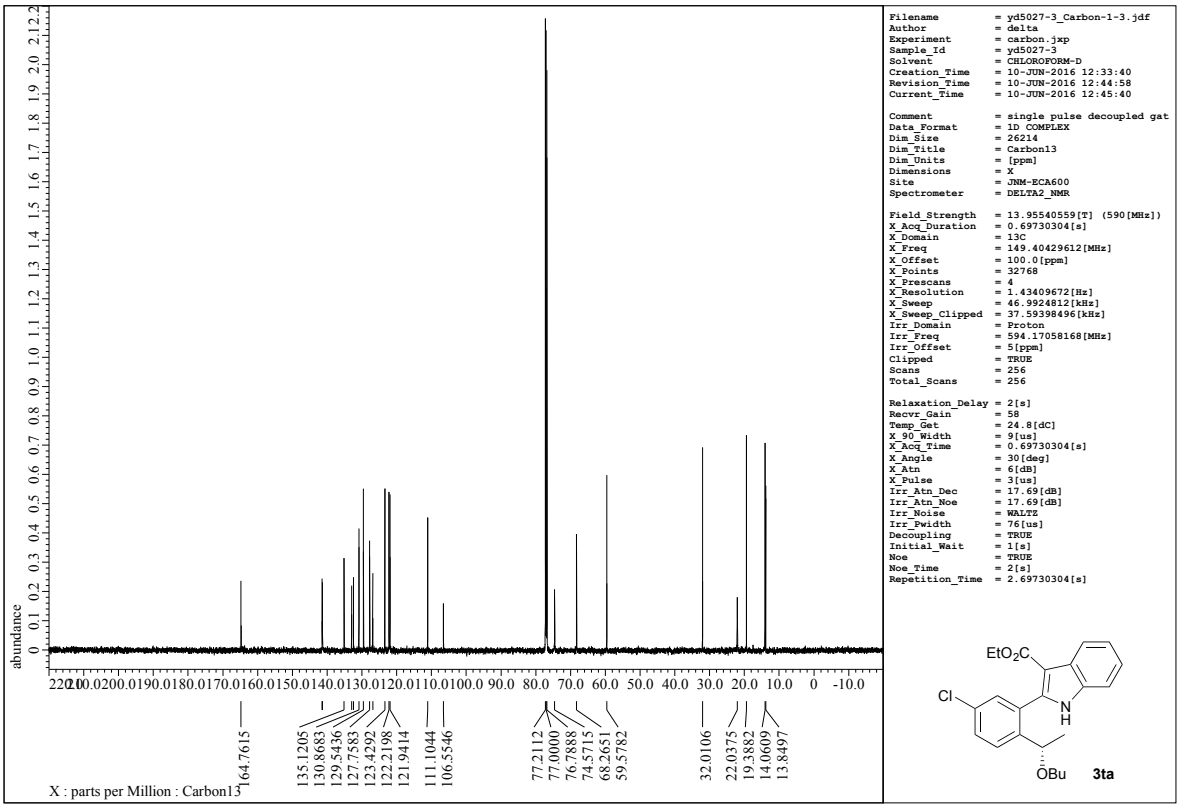
Pk #	Retention Time	Area	Area Percent	Height
1	22.754	4432312	90.083	193995
2	24.232	487954	9.917	21445

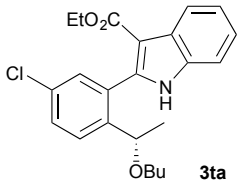


UV Results

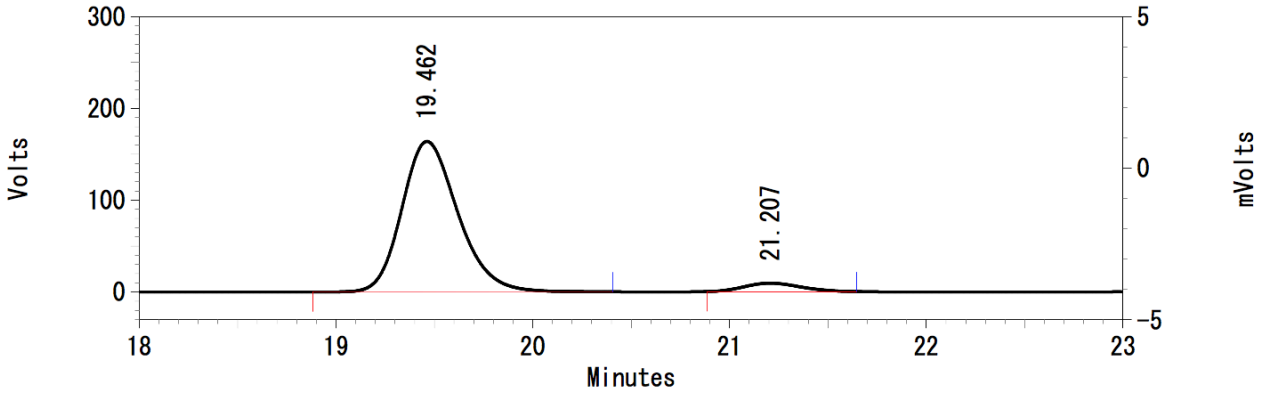
Pk #	Retention Time	Area	Area Percent	Height
1	22.827	1382839	50.192	60509
2	24.297	1372263	49.808	56387


abundance
9.1008
8.2602
8.2545
8.2442
7.5232
7.5083
7.3928
7.3893
7.3149
7.3126
7.3058
7.3001
7.2600
4.3143
4.3040
4.2101
4.1992
4.1918
4.1804
4.1609
4.1495
4.1312
3.2625
3.2602
3.2499
3.2385
3.2225
1.4944
1.2804
1.2701
1.1866
1.1751
1.1625
0.8833
0.8707
0.8581
X : parts per Million : Proton
Filename = yd5027-3_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd5027-3
Solvent = CHLOROFORM-D
Creation_Time = 10-JUN-2016 12:30:23
Revision_Time = 10-JUN-2016 12:36:03
Current_Time = 10-JUN-2016 12:36:24
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 23.9[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
EtO2C
Cl
N
H
OBu
3ta


abundance
164.7615
135.1205
130.8683
129.5436
127.7583
123.4292
122.2198
121.9414
111.1044
106.5546
77.2112
77.0000
76.7888
74.5715
68.2651
59.5782
32.0106
22.0375
19.3882
14.0609
13.8497
X : parts per Million : Carbon13
Filename = yd5027-3_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd5027-3
Solvent = CHLOROFORM-D
Creation_Time = 10-JUN-2016 12:33:40
Revision_Time = 10-JUN-2016 12:44:58
Current_Time = 10-JUN-2016 12:45:40
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 24.8[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
EtO2C
Cl
N
H
OBu
3ta

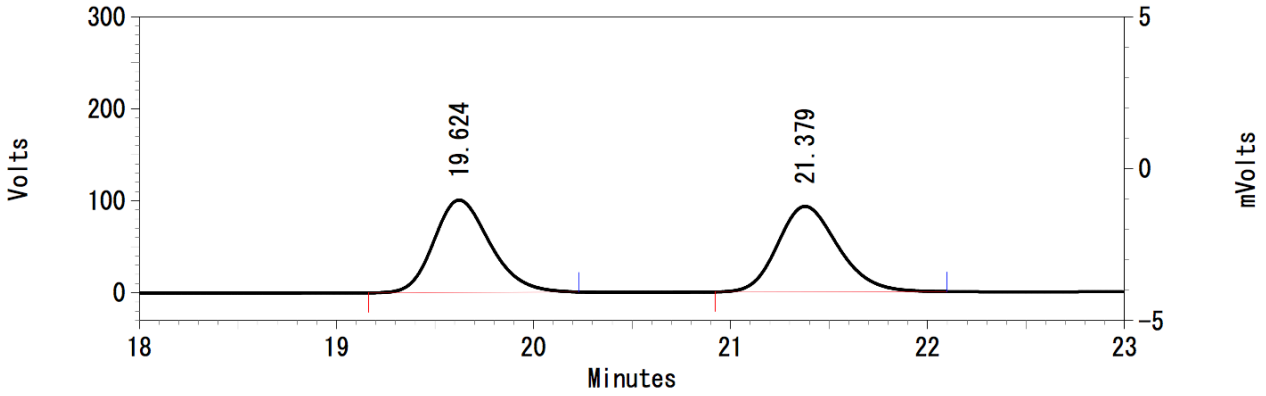


3ta



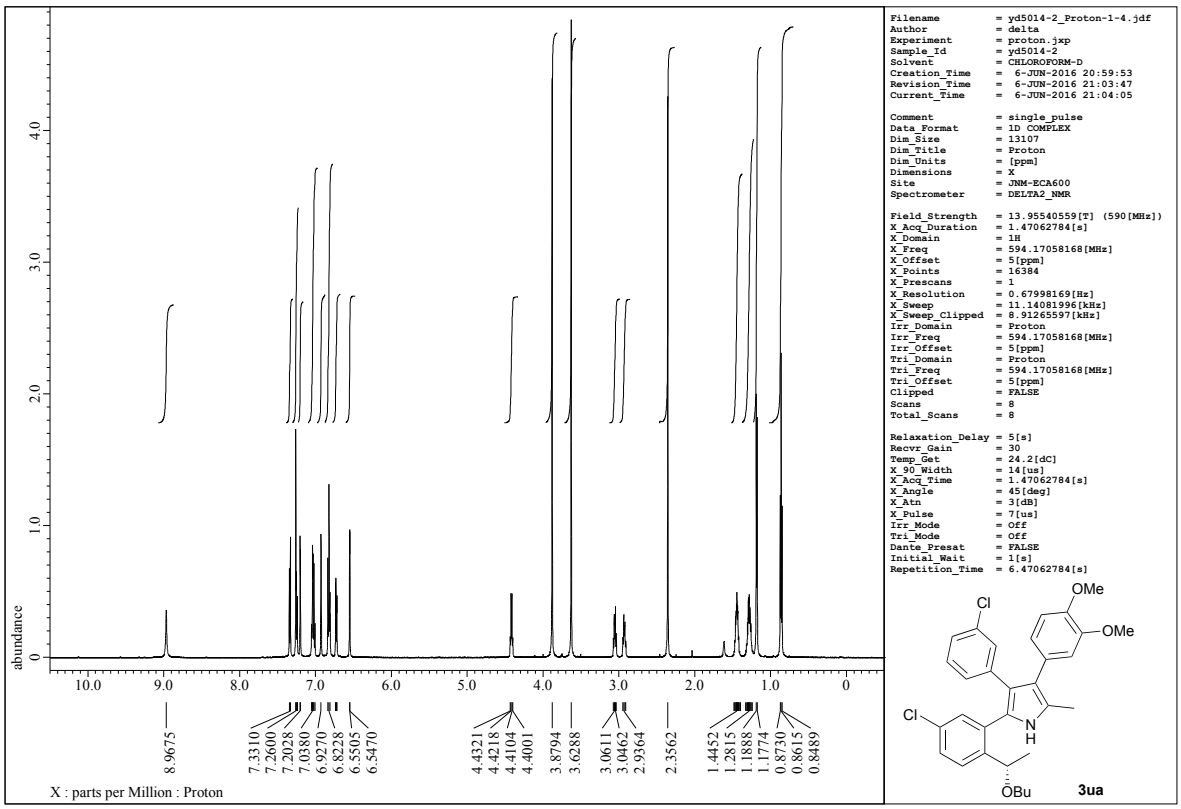
UV Results

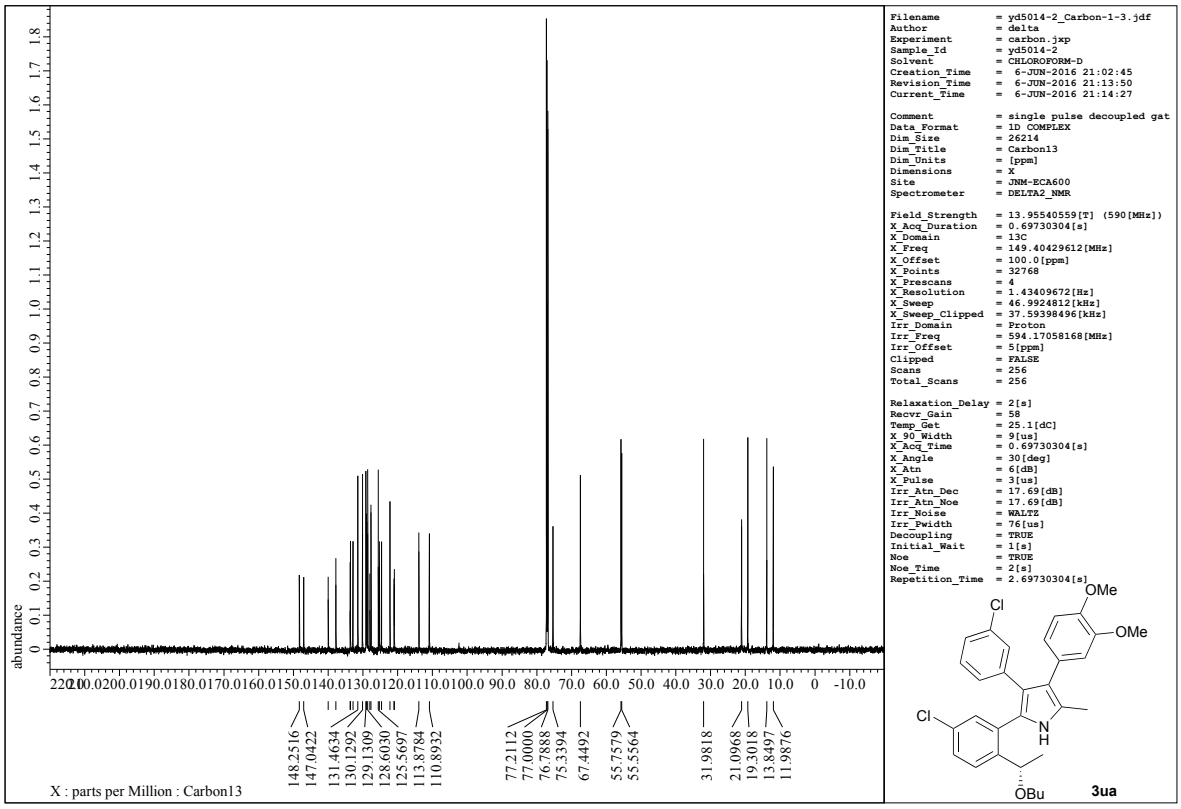
Pk #	Retention Time	Area	Area Percent	Height
1	19.462	3244182	94.631	163821
2	21.207	184052	5.369	9245

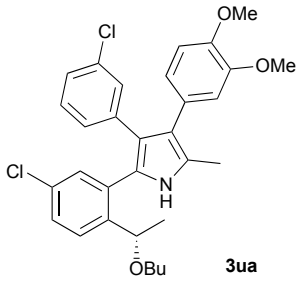


UV Results

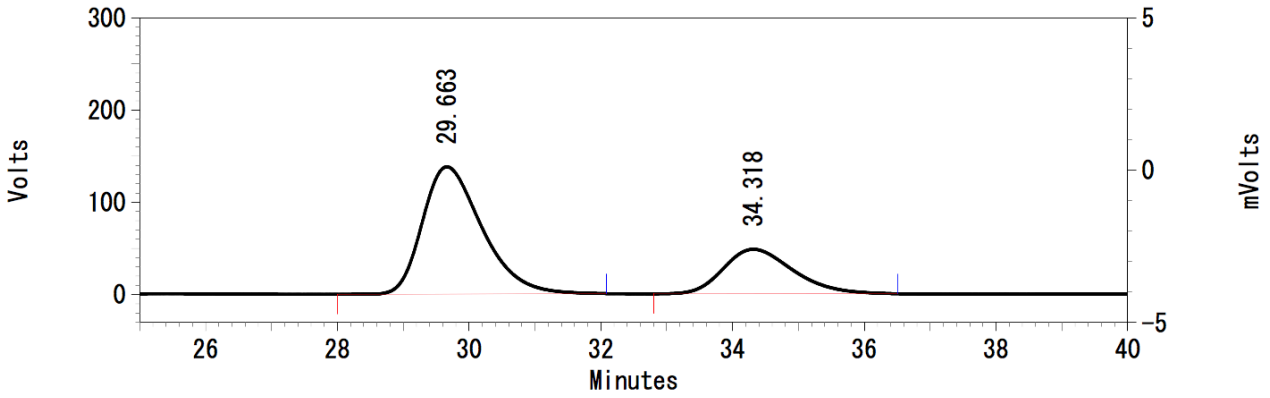
Pk #	Retention Time	Area	Area Percent	Height
1	19.624	1991338	50.140	100383
2	21.379	1980256	49.860	92806


abundance
X : parts per Million : Proton
8.9675
7.3310
7.2600
7.2028
7.0380
6.9270
6.8228
6.5505
6.5470
4.4321
4.4218
4.4104
4.4001
3.8794
3.6288
3.0611
3.0462
2.9364
2.3562
1.4452
1.2815
1.1888
1.1774
0.8730
0.8615
0.8489
Filename = yd5014-2_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd5014-2
Solvent = CHLOROFORM-D
Creation_Time = 6-JUN-2016 20:59:53
Revision_Time = 6-JUN-2016 21:03:47
Current_Time = 6-JUN-2016 21:04:05
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 30
Temp_Get = 24.2[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Cl
OMe
OMe
Cl
N
H
OBu
3ua


abundance
X : parts per Million : Carbon13
148.2516
147.0422
131.4634
130.1292
129.1309
128.6030
125.5697
113.8784
110.8932
77.2112
77.0000
76.7888
75.3394
67.4492
55.7579
55.5564
31.9818
21.0968
19.3018
13.8497
11.9876
Filename = yd5014-2_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd5014-2
Solvent = CHLOROFORM-D
Creation_Time = 6-JUN-2016 21:02:45
Revision_Time = 6-JUN-2016 21:13:50
Current_Time = 6-JUN-2016 21:14:27
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 25.1[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
Cl
OMe
OMe
Cl
N
H
OBu
3ua

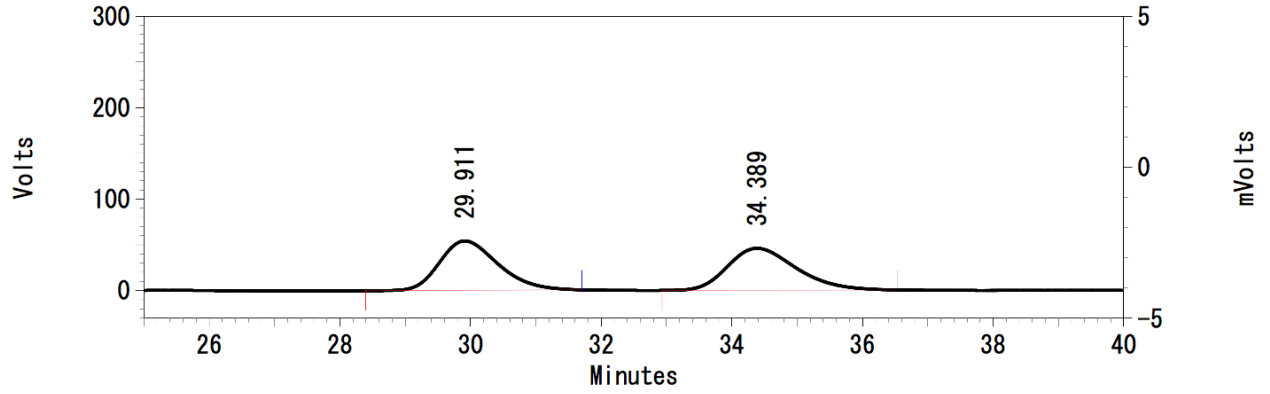


3ua



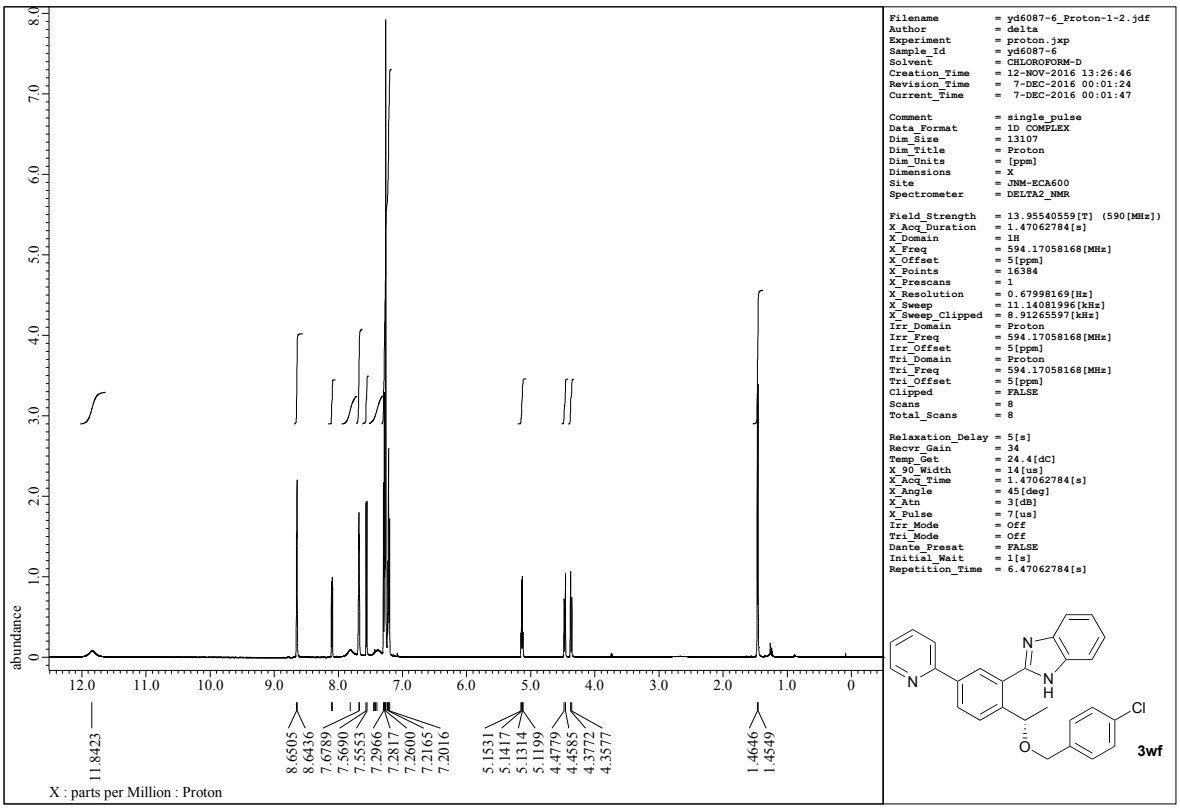
UV Results

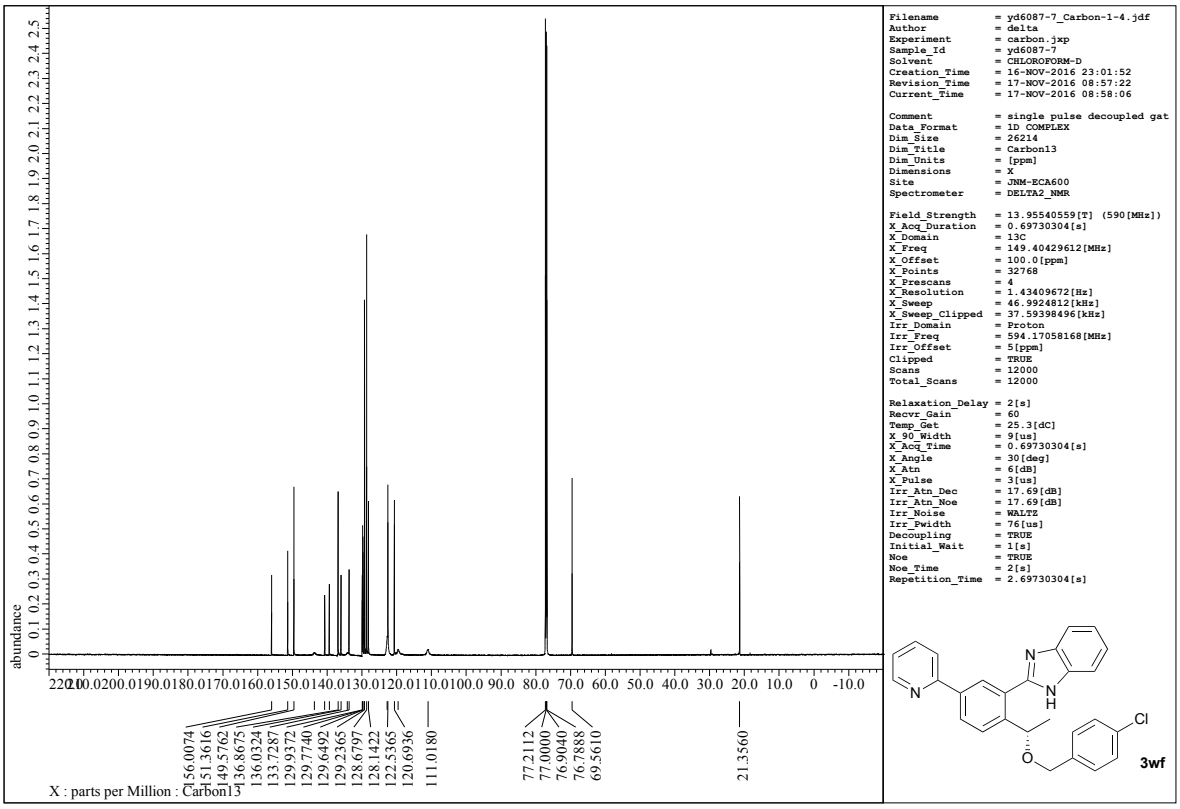
Pk #	Retention Time	Area	Area Percent	Height
1	29.663	8659003	71.008	137829
2	34.318	3535361	28.992	48125

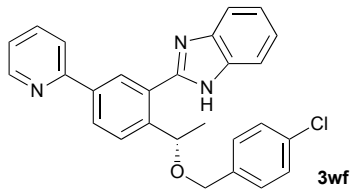


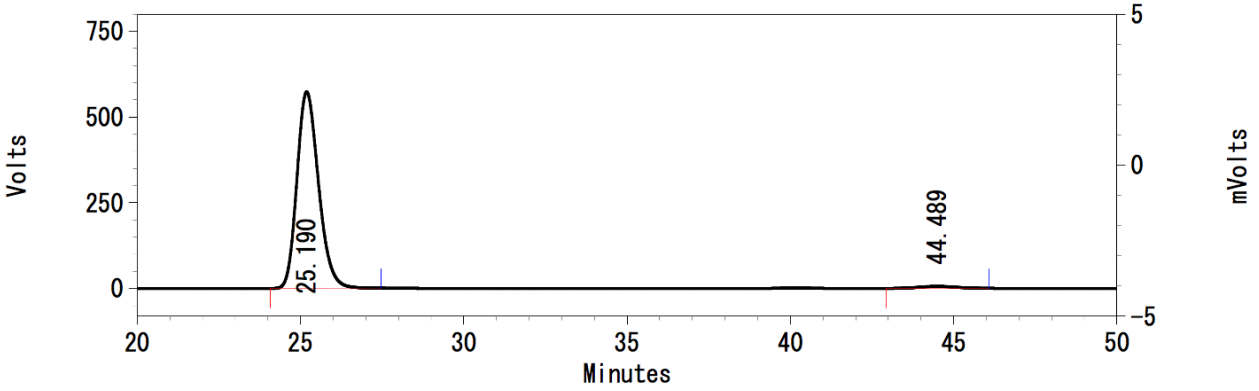
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	29.911	3358081	50.076	53928
2	34.389	3347929	49.924	45821


Filename = yd6087-6_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = yd6087-6
Solvent = CHLOROFORM-D
Creation_Time = 12-NOV-2016 13:26:46
Revision_Time = 7-DEC-2016 00:01:24
Current_Time = 7-DEC-2016 00:01:47
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 24.4[dC]
X_90_Width = 14[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 7[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
11.8423
8.6505 8.6436 7.6789 7.5690 7.5553 7.2966 7.2817 7.2600 7.2165 7.2016
5.1531 5.1417 5.1314 5.1199 4.4779 4.4585 4.3772 4.3577
1.4646 1.4549
X : parts per Million : Proton
N
N
H
Cl
O
3wf

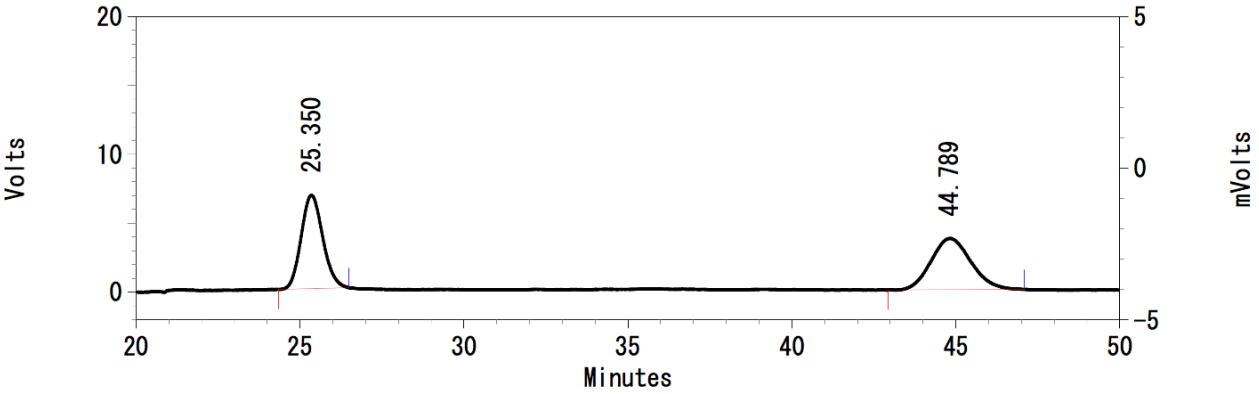

Filename = yd6087-7_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = yd6087-7
Solvent = CHLOROFORM-D
Creation_Time = 16-NOV-2016 23:01:52
Revision_Time = 17-NOV-2016 08:57:22
Current_Time = 17-NOV-2016 08:58:06
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 12000
Total_Scans = 12000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25.3[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.69[dB]
Irr_Atn_Noe = 17.69[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 76[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.69730304[s]
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
156.0074
151.3616
149.5762
136.8675
136.0324
133.7287
129.9372
129.7740
129.6492
129.2365
128.6797
128.1422
122.5365
120.6936
111.0180
77.2112
77.0000
76.9040
76.7888
69.5610
21.3560
X : parts per Million : Carbon13
N
N
H
Cl
O
3wf





UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	25.190	26396939	98.236	572989
2	44.489	474140	1.764	5784



UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	25.350	310665	49.758	6768
2	44.789	313681	50.242	3711