Supplementary Information

Enantioselective 1,4-addition of cyclopropylboronic acid catalyzed by rhodium/chiral diene complexes

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Contents of Supplementary Information:

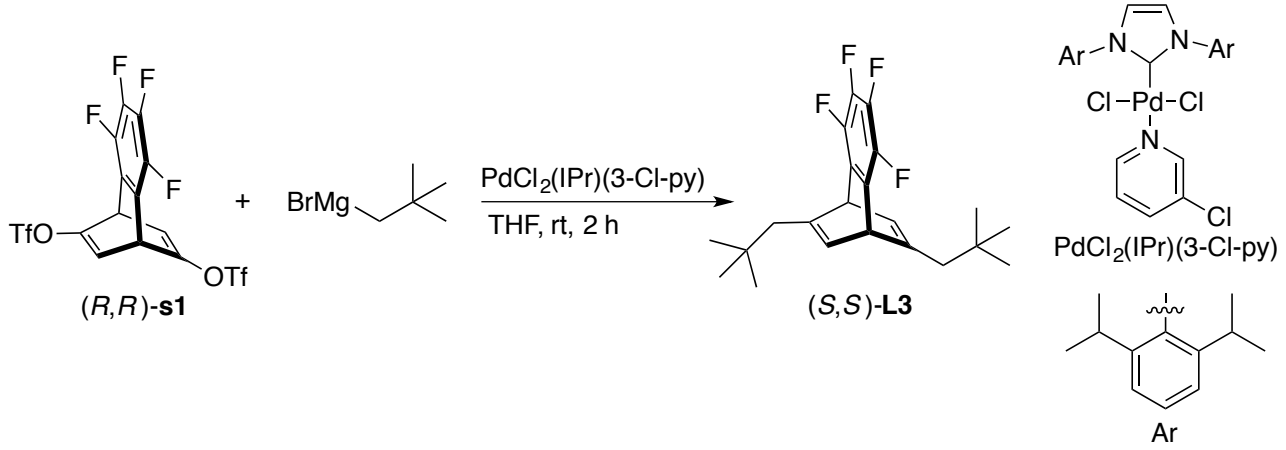
1. General

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) and CD_2Cl_2-d_2 ($CDHCl_2$, δ 5.30) for ^{1}H NMR, and $CDCl_3$ (δ 77.00) for ^{13}C NMR. The following abbreviations are used; s, singlet: d, doublet: t, triplet: q, quartet: sept, septet: m, multiplet: br, broad. High-resolution mass spectra (TOF-MS) were obtained with a Bruker micrOTOF spectrometer. Flash column chromatography was performed with Silica Gel 60 N (spherical, neutral) (Cica-Reagent). 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

Toluene and 1,4-dioxane were purified by passing through a neutral alumina column under N_2. Rhodium complexes $[RhCl((S,S)\text{-Fc-tfb*})]_2$,[1] $[RhCl((R,R)\text{-Ph-tfb*})]_2$,[1] $[RhCl((S,S)\text{-Bn-tfb*})]_2$,[1] $[Rh(OH)((S,S)\text{-Bn-tfb*})]_2$,[2] $[RhCl((R)\text{-}\mathbf{L1})]_2$,[3] $[RhCl((R)\text{-}\mathbf{L2})]_2$,[4] and $[RhCl((R)\text{-binap})]_2$[5] were prepared according to the reported procedures. Ligand (*S*,*S*)-**L3** $[RhCl((S,S)\text{-}\mathbf{L3})]_2$, and $[Rh(OH)((S,S)\text{-}\mathbf{L3})]_2$ were prepared as shown below.

3. Preparation of (*S*,*S*)-L3, $[RhCl((S,S)\text{-L3})]_2$, and $[Rh(OH)((S,S)\text{-L3})]_2$



Ligand L3: To a solution of (*R*,*R*)-**s1**[1] (527 mg, 1.0 mmol) and $PdCl_2$(IPr)(3-chloropyridine)[6] (34.0 mg, 0.050 mmol) in THF (4 mL) was added

1 T. Nishimura, H. Kumamoto, M. Nagaosa and T. Hayashi, *Chem. Commun.*, 2009, 5713.
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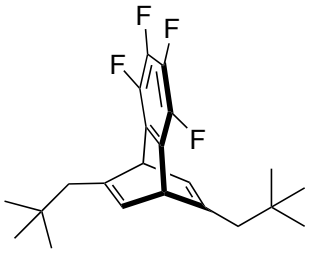
4 T. Nishimura, A. Noishiki, G. C. Tsui and T. Hayashi, *J. Am. Chem. Soc.*, 2012, **134**, 5056.
5 T. Hayashi, M. Takahashi, Y. Takaya and M. Ogasawara, *J. Am. Chem. Soc.*, 2002, **124**, 5052.
6 C. J. O'Brien, E. A. B. Kantchev, C. Valente, N. Hadei, G. A. Chass, A. Lough, A. C. Hopkinson and M. G. Organ, *Chem. Eur. J.*, 2006, **12**, 4743.

neopentylmagnesium bromide (0.91 M in THF, 5.5 mL, 5.0 mmol), prepared from neopentyl bromide with Mg, at room temperature and the mixture was stirred for 2 h. Saturated NH_4Cl (aq.) was added to the mixture and it was extracted with diethyl ether. The organic layer was passed through a short column of alumina with Et_2O, and the solvent was removed on a rotary evaporator. The residue was subjected to flash column chromatography on silica gel with hexane to give (*S*,*S*)-**L3** (311 mg, 0.81 mmol, 81% yield). ^{1}H NMR ($CDCl_3$) δ 0.87 (s, 18H), 2.09 (d, *J* = 13.6 Hz, 2H), 2.14 (d, *J* = 13.6 Hz, 2H), 4.91 (d, *J* = 5.5 Hz, 2H), 6.39 (d, *J* = 5.5 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 29.8 (6C), 32.3 (2C), 47.5, (2C), 47.7 (2C), 130.6–130.8 (m, 2C), 135.0 (2C), 136.1–142.2 (m, 4C), 152.8 (2C). HRMS (APCI) calcd for $C_{22}H_{26}F_4$ $(M)^+$ 366.1965, found 366.1968. $[\alpha]^{20}_D$ +32 (*c* 0.99, $CHCl_3$) for (*S*,*S*)-**L3**.



(*S*,*S*)-**L3**

+ $[RhCl(C_2H_4)_2]_2$ $\xrightarrow[CH_2Cl_2]{}$ $[RhCl((S,S)\text{-}\mathbf{L3})]_2$

[RhCl((*S*,*S*)-L3)]$_2$: To a suspension of $[RhCl(C_2H_4)_2]_2$[7] (236 mg, 0.61 mmol) in dichloromethane (4 mL) was added (*S*,*S*)-**L3** (311 mg, 0.81 mmol) in dichloromethane (1 mL) at room temperature and the mixture was stirred for 3 h. The mixture was concentrated under vacuum. The residue was subjected to flash column chromatography on silica gel with hexane, and then, dichloromethane under air to give $[RhCl((S,S)\text{-}\mathbf{L3})]_2$ (309 mg, 0.31 mmol, 76% yield). ^{1}H NMR ($CDCl_3$) δ 0.66 (s, 36H), 1.58 (d, *J* = 14.0 Hz, 4H), 2.14 (d, *J* = 14.0 Hz, 4H), 3.39 (d, *J* = 5.8 Hz, 4H), 5.39 (d, *J* = 5.8 Hz, 4H). HRMS (ESI) calcd for $C_{22}H_{26}Cl_2F_4Rh$ $(M/2+Cl)^-$ 539.0408, found 539.0405. $[\alpha]^{20}_D$ +11 (*c* 0.26, $CHCl_3$) for $[RhCl((S,S)\text{-}\mathbf{L3})]_2$.

$[RhCl((S,S)\text{-}\mathbf{L3})]_2$ $\xrightarrow[THF,\ rt]{1\ M\ KOHaq}$ $[Rh(OH)((S,S)\text{-}\mathbf{L3})]_2$

[Rh(OH)((*S*,*S*)-L3)]$_2$: To a solution of $[RhCl((S,S)\text{-}\mathbf{L3})]_2$ (236 mg, 0.31 mmol) in THF (2 mL) was added KOHaq (1 M, 6.1 mL, 6.1 mmol) at room temperature and the mixture was stirred for 0.5 h. Most of THF was removed under vacuum, and dichloromethane (1 mL) was added. The mixture was washed with 1 M KOHaq (1 mL) and H_2O (1 mL x 3) under nitrogen atmosphere. The organic layer was passed through a short column of Na_2SO_4 with dichloromethane and concentrated on a rotary evaporator. The residue was dried under vacuum to give $[Rh(OH)((S,S)\text{-}\mathbf{L3})]_2$ (268 mg, 0.28 mmol, 90% yield). ^{1}H NMR (CD_2Cl_2) δ 0.61 (s, 36H), 1.02 (d,

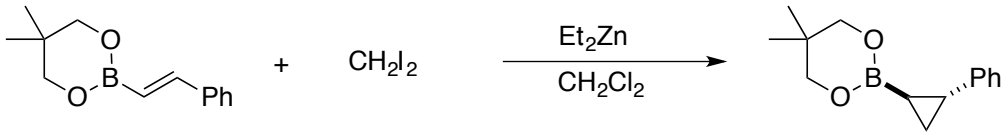
7 R. Uson, L. A. Oro and J. A. Cabeza, *Inorg. Synth.,* 1985, **23**, 126.

J = 13.6 Hz, 4H), 2.66 (d, J = 13.6 Hz, 4H), 2.95 (d, J = 5.5 Hz, 4H), 5.31 (d, J = 5.5 Hz, 4H). HRMS (ESI) calcd for $C_{22}H_{26}F_4Rh$ $(M/2–OH)^+$ 469.1020, found 469.10108. $[\alpha]^{20}_D$ –12 (*c* 0.25, CH_2Cl_2) for $[RhCl((S,S)\text{-}\mathbf{L3})]_2$.

4. Preparation of electron-deficient alkenes 1 and 4

Compounds **1a** (CAS: 16212-08-1),[8] **1b** (CAS: 876293-46-8),[9] **1c** (CAS: 35836-45-4),[9] **1d** (CAS: 107772-61-2),[9] **1e** (CAS: 1380035-31-3),[9] **1f** (CAS: 71964-05-1),[8] **1g** (CAS: 121033-92-9),[10] **1h** (CAS: 1380035-23-3),[8] **1i** (CAS: 14554-08-6),[11] and **1j** (CAS: 17299-32-0)[12] were prepared according to the reported procedures. Compounds **4e** (CAS: 710969-63-4),[13] **4f** (CAS: 710969-63-4),[14] **4g** (CAS: 28638-59-7),[15] **4h** (CAS: 5153-70-8),[15] and **4i** (CAS: 5576-97-6)[15] were prepared according to the reported procedures. Cyclopropylboronic acid (**2**), compounds **4a**–**d**, and **4j** were purchased from commercial suppliers and used as received. Cyclopropylboronate **10** was prepared as shown below.[16]

5. Preparation of compounds 10 (CAS: 1612136-76-1) and 10-d_2



s2 **10**

To a solution of diiodomethane (1.21 mL, 15 mmol) in dichloromethane (25 mL) at 0 °C was added diethylzinc (1 M in toluene, 7.5 mL, 7.5 mmol), and the mixture was stirred at the same temperature for 2 h. Compound **s2** (648 mg, 3.00 mmol) in dichloromethane (5 mL) was added to the mixture at 0 °C, and the mixture was stirred at room temperature for 36 h. Saturated NH_4Cl (aq.) was added to the mixture and it was extracted with dichloromethane. The organic layer was dried over Na_2SO_4, filtered, and concentrated on a rotary evaporator. The residue was subjected to flash column chromatography on silica gel with hexane/ethyl acetate (2:1) to give **10** (581 mg, 2.52 mmol, 84% yield). ^{1}H NMR ($CDCl_3$) δ 0.16–0.25 (m, 1H), 0.92–0.98 (m, 1H), 0.97 (s, 6H), 1.08–

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9 T. Nishimura, Y. Takiguchi and T. Hayashi, *J. Am. Chem. Soc.,* 2012, **134**, 9086.
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16 P. R. Blakemore, S. P. Marsden and H. D. Vater, *Org. Lett.,* 2006, **8**, 773.

1.14 (m, 1H), 2.00–2.06 (m, 1H), 3.59 (s, 4H), 7.08 (d, J = 7.5 Hz, 2H), 7.12 (t, J = 7.5 Hz, 1H), 7.24 (t, J = 7.5 Hz, 2H).

Compound **10-d_2** was prepared in 81% yield according to the same procedures for **10** using diiodomethane-d_2. ^{1}H NMR ($CDCl_3$) δ 0.17 (d, J = 5.5 Hz, 1H), 0.96 (s, 6H), 2.02 (d, J = 5.5 Hz, 1H), 3.58 (s, 4H), 7.07 (d, J = 7.5 Hz, 2H), 7.11 (t, J = 7.5 Hz, 1H), 7.23 (t, J = 7.5 Hz, 2H). HRMS (ESI) calcd for $C_{14}H_{17}BD_2NaO_2$ $(M+Na)^+$ 255.1498, found 255.1495.

6. General procedure for Table 1

A rhodium catalyst (0.0030 mmol of Rh), **1a** (25.8 mg, 0.10 mmol), K_3PO_4 (21.2 mg, 0.10 mmol) and cyclopropylboronic acid (**2**) (21.5 mg, 0.25 mmol) were placed in a Schlenk tube under nitrogen. Toluene (0.4 mL) was added and the mixture was stirred at 60 °C for 12 h. The mixture was passed through a short column of silica gel with ethyl acetate as eluent. The solvent was removed on a rotary evaporator and the yield of the product was determined by ^{1}H NMR using 1,4-dimethoxybenzene as an internal standard. For isolation of the product, the crude mixture was subjected to preparative TLC on silica gel with toluene to give **3a**. The ee of **3a** was determined by chiral HPLC (Daicel chiralpak AD-H).

7. General procedure for Scheme 2

$[Rh(OH)((S,S)\text{-Fc-tfb*})]_2$ (4.4 mg, 0.0060 mmol of Rh), **1** (0.20 mmol), K_3PO_4 (42.4 mg, 0.20 mmol), and cyclopropylboronic acid (**2**) (43.0 mg, 0.50 mmol) were placed in a Schlenk tube under nitrogen. 1,4-Dioxane or toluene (0.8 mL) was added and the mixture was stirred at 60 °C for 24 h. The mixture was passed through a short column of silica gel with ethyl acetate as eluent. The solvent was removed on a rotary evaporator and the residue was subjected to preparative TLC on silica gel with hexane/ethyl acetate to give **3**.

8. General procedure for Scheme 3

$[Rh(OH)((S,S)\text{-Bn-tfb*})]_2$ (3.2 mg, 0.0060 mmol of Rh), **4** (0.20 mmol), K_3PO_4 (42.4 mg, 0.20 mmol), and cyclopropylboronic acid (**2**) (60.1 mg, 0.70 mmol) were placed in a Schlenk tube under nitrogen. 1,4-Dioxane (0.8 mL) was added and the mixture was stirred at 60 °C for 12 h. The mixture was passed through a short column of silica gel with ethyl acetate as eluent. The solvent was removed on a rotary evaporator and the residue was subjected to preparative TLC on silica gel with hexane/ethyl acetate to give **5**. For nitroalkenes **4g–i**, the reaction was conducted in the presence of $[Rh(OH)((S,S)\text{-}\mathbf{L3})]_2$ (2.8 mg, 0.0060 mmol of Rh) and KHF_2 (15.6 mg, 0.20 mmol) in toluene (0.8 mL) instead of $[Rh(OH)((S,S)\text{-Bn-tfb*})]_2$ and K_3PO_4, respectively.

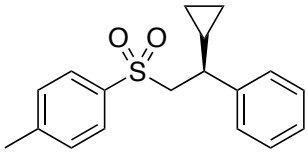
9. General procedure for eq 3

$[Rh(OH)((S,S)\text{-Bn-tfb*})]_2$ (1.6 mg, 0.0030 mmol of Rh), **4j** (7.0 mg, 0.10 mmol), K_3PO_4

(21.2 mg, 0.10 mmol), and cyclopropylboronate **10** (69.0 mg, 0.30 mmol) were placed in a Schlenk tube under nitrogen. 1,4-Dioxane (0.8 mL) and methanol (12 μL, 0.30 mmol) were added and the mixture was stirred at 80 °C for 24 h. The mixture was passed through a short column of silica gel with ethyl acetate as eluent. The solvent was removed on a rotary evaporator and the residue was subjected to preparative TLC on silica gel with hexane/ethyl acetate to give **11**.

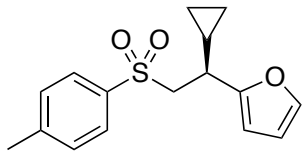
10. Characterization of the products

The absolute configuration of the product **3a** was determined by X-ray crystallographic analysis. For others, they were assigned by consideration of the stereochemical pathway.



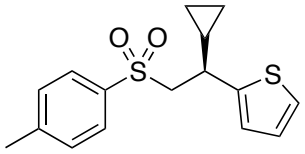
3a

Compound 3a (Table 1, entry 2, 96% yield, 97% ee). The ee was measured by HPLC (Chiralcel OD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 22.6 min (*R*), t_2 = 25.2 min (*S*)); $[\alpha]^{20}_D$ +31 (*c* 1.08, $CHCl_3$) for 97% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.14–0.20 (m, 1H), 0.29–0.35 (m, 1H), 0.39–0.45 (m, 1H), 0.57–0.64 (m, 1H), 1.01–1.08 (m, 1H), 2.37 (s, 3H), 2.51 (ddd, *J* = 9.5, 8.0, 5.5 Hz, 1H), 3.60 (dd, *J* = 14.3, 5.5 Hz, 1H), 3.63 (dd, *J* = 14.3, 8.0 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 2H), 7.12–7.19 (m, 5H), 7.55 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.8, 5.8, 18.1, 21.5, 45.7, 62.3, 126.6, 127.5, 127.8, 128.4, 129.5, 137.1, 141.7, 144.0. HRMS (ESI) calcd for $C_{18}H_{20}NaO_2S$ $(M+Na)^+$ 323.1076, found 323.1067.



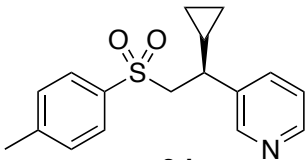
3b

Compound 3b (Scheme 2, 97% yield, 93% ee). The ee was measured by HPLC (Chiralpak AD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 22.7 min (*R*), t_2 = 24.9 min (*S*)); $[\alpha]^{20}_D$ +18 (*c* 1.00, $CHCl_3$) for 93% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.20–0.28 (m, 2H), 0.45–0.49 (m, 2H), 1.03–1.10 (m, 1H), 2.40 (s, 3H), 2.71 (td, *J* = 8.8, 4.8 Hz, 1H), 3.50 (dd, *J* = 14.3, 4.8 Hz, 1H), 3.72 (dd, *J* = 14.3, 8.8 Hz, 1H), 5.96 (d, *J* = 2.7 Hz, 1H), 6.15 (dd, *J* = 2.7, 1.4 Hz, 1H), 7.11 (d, *J* = 1.4 Hz, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.64 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.6, 4.9, 16.0, 21.5, 38.9, 59.9, 106.3, 110.0, 127.8, 129.6, 136.9, 141.4, 144.1, 153.7. HRMS (ESI) calcd for $C_{16}H_{18}NaO_3S$ $(M+Na)^+$ 313.0869, found 313.0873.



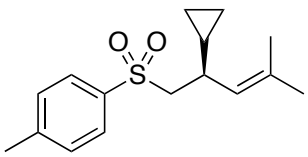
3c

Compound 3c (Scheme 2, 97% yield, 93% ee). The ee was measured by HPLC (Chiralpak AD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 25.7 min (*S*), t_2 = 27.5 min (*R*)); $[\alpha]^{20}_D$ +21 (*c* 0.99, $CHCl_3$) for 93% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.27–0.38 (m, 2H), 0.51–0.57 (m, 1H), 0.58–0.63 (m, 1H), 1.04–1.11 (m, 1H), 2.40 (s, 3H), 2.88 (dt, *J* = 9.5, 6.1 Hz, 1H), 3.61 (d, *J* = 6.1 Hz, 2H), 6.72 (d, *J* = 3.4 Hz, 1H), 6.81 (dd, *J* = 5.5, 3.4 Hz, 1H), 7.07 (d, *J* = 5.5 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.64 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 5.3, 5.8, 19.1, 21.5, 40.9, 63.2, 123.8, 123.5, 126.5, 127.9, 129.6, 137.1, 144.3, 145.3. HRMS (ESI) calcd for $C_{16}H_{18}NaO_2S_2$ $(M+Na)^+$ 329.0640, found 329.0642.



3d

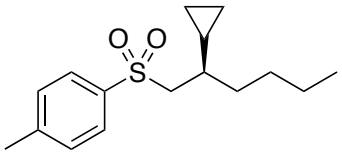
Compound 3d (Scheme 2, 51% yield, 96% ee). The ee was measured by HPLC (Chiralpak AD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 25.7 min (*R*), t_2 = 32.6 min (*S*)); $[\alpha]^{20}_D$ +30 (*c* 1.01, $CHCl_3$) for 96% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.14–0.20 (m, 1H), 0.31–0.37 (m, 1H), 0.43–0.49 (m, 1H), 0.61–0.67 (m, 1H), 0.99–1.06 (m, 1H), 2.38 (s, 3H), 2.48 (dt, *J* = 9.5, 6.8 Hz, 1H), 3.62 (d, *J* = 6.8 Hz, 2H), 7.09 (dd, *J* = 8.1, 4.1 Hz, 1H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.35–7.39 (m, 1H), 7.55 (d, *J* = 8.1 Hz, 2H), 8.32 (s, 1H), 8.40 (d, *J* = 4.1 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 4.9, 5.9, 18.1, 21.5, 43.5, 61.6, 123.3, 127.8, 129.7, 134.6, 136.7, 137.1, 144.5, 148.1, 149.2. HRMS (ESI) calcd for $C_{17}H_{19}NNaO_2S$ $(M+Na)^+$ 324.1029, found 324.1020.



3e

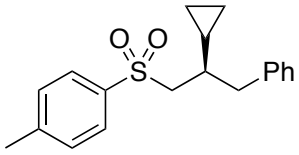
Compound 3e (Scheme 2, 78% yield, 83% ee). The ee was measured by HPLC (Chiralpak AS-H column, hexane/2-propanol = 80:20, flow 0.5 mL/min, 254 nm, t_1 = 33.9 min (*S*), t_2 = 48.9 min (*R*)); $[\alpha]^{20}_D$ +37 (*c* 1.03, $CHCl_3$) for 83% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.09–0.18 (m, 2H), 0.33–0.44 (m, 2H), 0.71–0.78 (m, 1H), 1.52 (s, 3H), 1.53 (s, 3H), 2.36–2.46 (m, 1H), 2.43 (s, 3H), 3.18 (dd, *J* = 14.3, 8.2 Hz, 1H), 3.31 (dd, *J* = 14.3, 4.1 Hz, 1H), 4.63 (d, *J* = 10.2 Hz, 1H), 7.31

(d, J = 8.1 Hz, 2H), 7.71 (d, J = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 3.0, 3.7, 16.6, 18.2, 21.5, 25.7, 37.3, 61.8, 124.2, 128.0, 129.5, 133.7, 137.6, 144.1. HRMS (ESI) calcd for $C_{16}H_{22}NaO_2S$ $(M+Na)^+$ 301.1233, found 301.1231.



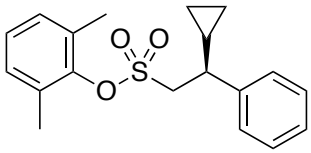
3f

Compound 3f (Scheme 2, 94% yield, 96% ee). The ee was measured by HPLC (Chiralpak IC column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 44.1 min (*R*), t_2 = 46.3 min (*S*)); $[\alpha]^{20}_D$ –27 (*c* 1.00, $CHCl_3$) for 96% ee (*R*). ^{1}H NMR ($CDCl_3$) δ –0.02–0.03 (m, 1H), 0.17–0.22 (m, 1H), 0.33–0.39 (m, 1H), 0.50–0.56 (m, 1H), 0.58–0.65 (m, 1H), 0.82–0.90 (m, 3H), 1.20–1.30 (m, 4H), 1.32–1.41 (m, 1H), 1.43–1.51 (m, 1H), 1.59–1.67 (m, 1H), 2.45 (s, 3H), 3.14 (dd, J = 14.3, 7.5 Hz, 1H), 3.21 (dd, J = 14.3, 4.1 Hz, 1H), 7.34 (d, J = 8.1 Hz, 2H), 7.78 (d, J = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 3.7, 6.0, 14.0, 16.5, 21.6, 22.9, 28.5, 34.4, 39.2, 61.5, 127.8, 129.8, 137.6, 144.3. HRMS (ESI) calcd for $C_{16}H_{24}NaO_2S$ $(M+Na)^+$ 303.1389, found 303.1387.



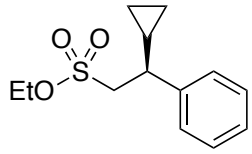
3g

Compound 3g (Scheme 2, 92% yield, 97% ee). The ee was measured by HPLC (Chiralpak IC column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 55.3 min (*R*), t_2 = 66.8 min (*S*)); $[\alpha]^{20}_D$ –15 (*c* 1.01, $CHCl_3$) for 97% ee (*R*). ^{1}H NMR ($CDCl_3$) δ –0.02–0.09 (m, 2H), 0.35–0.40 (m, 1H), 0.42–0.49 (m, 1H), 0.60–0.69 (m, 1H), 1.47–1.53 (m, 1H), 2.44 (s, 3H), 2.89 (dd, J = 13.6, 6.8 Hz, 1H), 2.91 (dd, J = 13.6, 5.5 Hz, 1H), 3.12 (dd, J = 14.3, 4.1 Hz, 1H), 3.20 (dd, J = 14.3, 8.2 Hz, 1H), 7.17–7.22 (m, 3H), 7.24–7.27 (m, 2H), 7.33 (d, J = 8.1 Hz, 2H), 7.76 (d, J = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.5, 5.7, 16.0, 21.6, 39.7, 40.9, 59.7, 126.1, 127.7, 128.1, 129.8, 132.3, 138.6, 144.4. HRMS (ESI) calcd for $C_{19}H_{22}NaO_2S$ $(M+Na)^+$ 337.1233, found 337.1232.



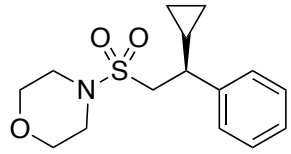
3h

Compound 3h (Scheme 2, 80% yield, 98% ee). The ee was measured by HPLC (Chiralpak AS-H column, hexane/2-propanol = 90:10, flow 1.0 mL/min, 254 nm, t_1 = 5.6 min (*S*), t_2 = 6.7 min (*R*); $[\alpha]^{20}_D$ +8 (*c* 1.36, $CHCl_3$) for 98% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.21–0.26 (m, 1H), 0.49–0.56 (m, 2H), 0.72–0.78 (m, 1H), 1.20–1.27 (m, 1H), 2.32 (s, 6H), 2.73 (dt, *J* = 9.6, 6.8 Hz, 1H), 3.84–3.92 (m, 2H), 7.02–7.07 (m, 3H), 7.25–7.31 (m, 3H), 7.33–7.78 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 4.6, 6.2, 17.2, 17.6, 46.4, 58.7, 126.7, 127.2, 127.5, 128.7, 129.2, 132.1, 141.8, 146.8. HRMS (ESI) calcd for $C_{19}H_{22}NaO_3S$ $(M+Na)^+$ 353.1182, found 353.1174.



3i

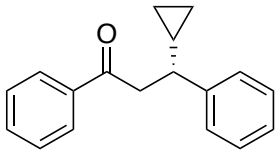
Compound 3i (Scheme 2, 86% yield, 92% ee). The ee was measured by HPLC (Chiralpak AS-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 30.4 min (*S*), t_2 = 36.8 min (*R*)); $[\alpha]^{20}_D$ +27 (*c* 1.00, $CHCl_3$) for 92% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.19–0.25 (m, 1H), 0.40–0.45 (m, 1H), 0.47–0.53 (m, 1H), 0.67–0.73 (m, 1H), 1.12–1.18 (m, 1H), 1.14 (t, *J* = 7.0 Hz, 3H), 2.50 (dt, *J* = 9.5, 7.8 Hz, 1H), 3.58 (d, *J* = 7.8 Hz, 2H), 3.95 (dq, *J* = 9.5, 7.0 Hz, 1H), 4.03 (dq, *J* = 9.5, 7.0 Hz, 1H), 7.25 (d, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.7, 5.9, 14.7, 17.5, 46.5, 56.5, 65.8, 127.1, 127.5, 128.6, 142.0. HRMS (ESI) calcd for $C_{13}H_{18}NaO_3S$ $(M+Na)^+$ 277.0869, found 277.0866.



3j

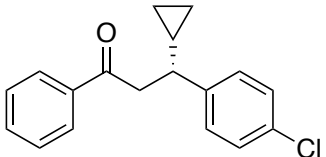
Compound 3j (Scheme 2, 96% yield, 98% ee). The ee was measured by HPLC (Chiralpak AD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 24.2 min (*R*), t_2 = 27.6 min (*S*)); $[\alpha]^{20}_D$ +35 (*c* 0.95, $CHCl_3$) for 98% ee (*S*). ^{1}H NMR ($CDCl_3$) δ 0.18–0.23 (m, 1H), 0.37–0.49 (m, 2H), 0.63–0.70 (m, 1H), 1.05–1.12 (m, 1H), 2.47 (dt, *J* = 8.9, 5.5 Hz, 1H), 2.92–3.04 (m, 4H), 3.39 (dd, *J* = 14.3, 5.5 Hz, 1H), 3.44 (dd, *J* = 14.3, 8.9 Hz, 1H), 3.49–3.56 (m, 4H), 7.22 (d, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ

4.7, 5.9, 18.0, 45.3, 46.2, 55.4, 66.4, 127.1, 127.4, 128.7, 142.5. HRMS (ESI) calcd for $C_{15}H_{21}NNaO_3S$ $(M+Na)^+$ 318.1134, found 318.1136.



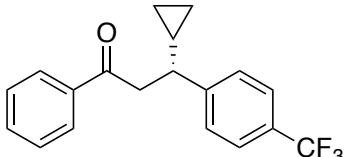
5a

Compound 5a (Scheme 3, 80% yield, 84% ee). The ee was measured by HPLC (Chiralpak IC column, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 11.5 min (*R*), t_2 = 12.6 min (*S*)); $[\alpha]^{20}_D$ +37 (*c* 0.90, $CHCl_3$) for 84% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.16–0.20 (m, 1H), 0.22–0.27 (m, 1H), 0.41–0.46 (m, 1H), 0.52–0.58 (m, 1H), 1.08–1.15 (m, 1H), 2.66 (ddd, *J* = 9.6, 7.5, 6.8 Hz, 1H), 3.42 (dd, *J* = 16.3, 6.8 Hz, 1H), 3.46 (dd, *J* = 16.3, 7.5 Hz, 1H), 7.18–7.22 (m, 1H), 7.28–7.32 (m, 4H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.94 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.3, 5.5, 17.6, 45.7, 46.4, 126.3, 127.4, 128.1, 128.3, 128.5, 132.8, 137.4, 144.8, 199.2. HRMS (ESI) calcd for $C_{18}H_{18}NaO$ $(M+Na)^+$ 273.1250, found 273.1248.



5b

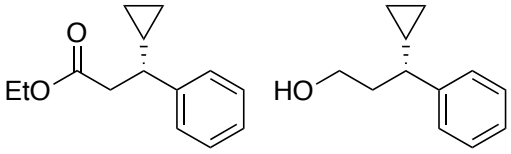
Compound 5b (Scheme 3, 89% yield, 84% ee). The ee was measured by HPLC (Chiralpak IC column, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 10.9 min (*R*), t_2 = 11.6 min (*S*)); $[\alpha]^{20}_D$ +46 (*c* 0.96, $CHCl_3$) for 84% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.13–0.18 (m, 1H), 0.22–0.28 (m, 1H), 0.41–0.47 (m, 1H), 0.52–0.58 (m, 1H), 1.03–1.10 (m, 1H), 2.62 (ddd, *J* = 9.5, 7.5, 6.1 Hz, 1H), 3.40 (dd, *J* = 16.3, 6.1 Hz, 1H), 3.43 (dd, *J* = 16.3, 7.5 Hz, 1H), 7.21 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 8.8 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 8.79 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.4, 5.6, 17.5, 45.4, 45.7, 128.0, 128.5, 128.6, 128.8, 131.9, 133.0, 137.2, 143.3, 198.8. HRMS (ESI) calcd for $C_{18}H_{17}ClNaO$ $(M+Na)^+$ 307.0860, found 307.0851.



5c

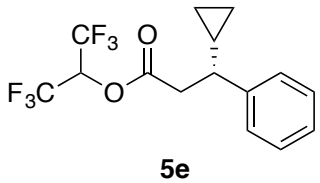
Compound 5c (Scheme 3, 95% yield, 86% ee). The ee was measured by HPLC (Chiralpak IA column x 2, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 28.3 min (*S*), t_2 = 30.2 min (*R*)); $[\alpha]^{20}_D$ +40 (*c* 0.89, $CHCl_3$) for 86% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.16–0.22 (m,

1H), 0.27–0.33 (m, 1H), 0.44–0.49 (m, 1H), 0.55–0.63 (m, 1H), 1.07–1.14 (m, 1H), 2.67–2.73 (m, 1H), 3.45 (dd, J = 16.3, 6.1 Hz, 1H), 3.49 (dd, J = 16.3, 8.2 Hz, 1H), 7.40 (d, J = 8.1 Hz, 2H), 7.45 (t, J = 8.1 Hz, 2H), 7.53–7.57 (m, 3H), 7.92 (d, J = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.5, 5.6, 17.4, 45.2, 46.0, 124.3 (q, $J_{F\text{-}C}$ = 273 Hz), 125.3 (q, $J_{F\text{-}C}$ = 3 Hz), 127.7, 128.0, 128.5 (q, $J_{F\text{-}C}$ = 30 Hz), 128.6, 130.1, 137.1, 149.0, 198.5. HRMS (ESI) calcd for $C_{19}H_{17}F_3NaO$ $(M+Na)^+$ 341.1124, found 341.1124.



5d **5d'**

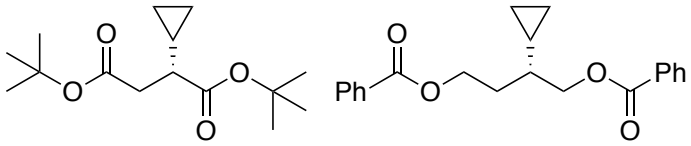
Compound 5d (Scheme 3, 63% yield, 81% ee). The ee of **5d** was determined by HPLC analysis of 3-cyclopropyl-3-phenylpropan-1-ol (**5d'**), which was obtained by treatment of **5d** with DIBAL-H (2 equiv) in toluene (69% yield). **Compound 5d**: $[\alpha]^{20}_D$ +28 (*c* 0.72, $CHCl_3$) for 81% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.13–0.18 (m, 1H), 0.25–0.31 (m, 1H), 0.39–0.45 (m, 1H), 0.55–0.61 (m, 1H), 1.00–1.07 (m, 1H), 1.13–1.19 (m, 3H), 2.34–2.41 (m, 1H), 2.71 (dd, J = 15.0, 8.1 Hz, 1H), 2.77 (dd, J = 15.0, 7.5 Hz, 1H), 4.00–4.10 (m, 2H), 7.19–7.26 (m, 3H), 7.30 (t, J = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.0, 5.3, 14.1, 17.2, 41.8, 47.2, 60.2, 126.4, 127.3, 128.3, 144.1, 172.3. HRMS (ESI) calcd for $C_{14}H_{18}NaO_2$ $(M+Na)^+$ 241.1199, found 241.1199. **Compound 5d'**: The ee was measured by HPLC (Chiralcel OJ-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 16.9 min (*S*), t_2 = 19.7 min (*R*)); $[\alpha]^{20}_D$ +27 (*c* 0.71, $CHCl_3$) for 81% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.06–0.12 (m, 1H), 0.23–0.29 (m, 1H), 0.36–0.42 (m, 1H), 0.58–0.64 (m, 1H), 0.96–1.04 (m, 1H), 1.19 (br s, 1H), 1.92–2.01 (m, 2H), 2.05–2.12 (m, 1H), 3.56 (dt, J = 10.2, 6.8 Hz, 1H), 3.65 (dt, J = 10.2, 6.1 Hz, 1H), 7.19–7.23 (m, 3H), 7.31 (t, J = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 3.8, 5.5, 17.4, 39.5, 47.6, 61.1, 126.2, 127.5, 128.4, 145.3. HRMS (ESI) calcd for $C_{12}H_{16}NaO$ $(M+Na)^+$ 199.1093, found 199.1096.



5e

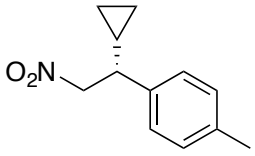
Compound 5e (Scheme 3, 70% yield, 84% ee). The ee was measured by HPLC (Chiralpak AD-H column x 2, hexane/2-propanol = 100:1, flow 0.5 mL/min, 224 nm, t_1 = 15.1 min (*S*), t_2 = 15.5 min (*R*)); $[\alpha]^{20}_D$ +17 (*c* 0.85, $CHCl_3$) for 86% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.18–0.23 (m, 1H), 0.26–0.31 (m, 1H), 0.43–0.50 (m, 1H), 0.58–0.65 (m, 1H), 1.03–1.10 (m, 1H), 2.43 (ddd, J = 8.9, 8.2, 7.5 Hz, 1H), 2.98 (dd, J = 15.0, 8.2 Hz, 1H), 3.01 (dd, J = 15.0, 7.5 Hz, 1H), 5.68 (sept, J

= 6.1 Hz, 1H), 7.20–7.26 (m, 3H), 7.32 (d, J = 7.5 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 4.1, 5.3, 17.2, 40.5, 47.0, 66.3 (sept, $J_{F\text{-}C}$ = 34 Hz), 120.4 (q, $J_{F\text{-}C}$ = 282 Hz), 126.9, 127.1, 128.5, 142.7, 169.0. HRMS (APCI) calcd for $C_{15}H_{14}F_6O_2$ $(M)^+$ 340.0893, found 340.0887.



5f **5f'**

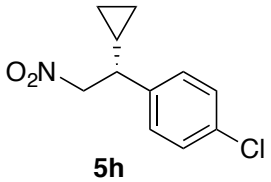
Compound 5f (Scheme 3, 99% yield, 81% ee). The ee of **5f** was determined by HPLC analysis of **5f'**, which was obtained by treatment of **5f** with DIBAL-H (4 equiv) in toluene, and then, benzoyl chloride (2.4 equiv) in the presence of triethyl amine (2.4 equiv) and 4-dimethylaminopyridine (10 mol %) in dichloromethane (65% yield). **Compound 5f**: $[\alpha]^{20}_D$ +46 (*c* 0.89, $CHCl_3$) for 81% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.13–0.18 (m, 1H), 0.37–0.43 (m, 1H), 0.45–0.52 (m, 2H), 0.80–0.87 (m, 1H), 1.42 (s, 9H), 1.44 (s, 9H), 1.91 (td, J = 9.5, 5.4 Hz, 1H), 2.41 (dd, J = 16.3, 5.4 Hz, 1H), 2.67 (dd, J = 16.3, 9.5 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 3.6, 4.0, 13.6, 28.0, 28.0, 37.9, 47.1, 80.2, 80.4, 171.2, 173.6. HRMS (ESI) calcd for $C_{15}H_{26}NaO_4$ $(M+Na)^+$ 293.1723, found 293.1719. **Compound 5f'**: The ee was measured by HPLC (Chiralpak IC column, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 29.9 min (*R*), t_2 = 36.4 min (*S*)); $[\alpha]^{20}_D$ –3 (*c* 0.88, $CHCl_3$) for 81% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.20–0.29 (m, 2H), 0.50–0.56 (m, 1H), 0.58–0.64 (m, 1H), 0.69–0.77 (m, 1H), 1.23–1.32 (m, 1H), 2.01 (dq, J = 14.0, 6.8 Hz, 1H), 2.13 (dq, J = 14.0, 6.9 Hz, 1H), 4.34 (dd, J = 10.9, 6.8 Hz, 1H), 4.49 (dt, J = 10.9, 5.4 Hz, 1H), 4.50–4.59 (m, 2H), 7.42 (t, J = 8.1 Hz, 2H), 7.44 (t, J = 8.1 Hz, 2H), 7.54 (t, J = 8.1 Hz, 1H), 7.55 (t, J = 8.1 Hz, 1H), 8.02 (d, J = 8.1 Hz, 2H), 8.05 (d, J = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 3.4, 4.4, 13.1, 31.6, 40.8, 63.1, 68.1, 128.3, 128.4, 129.48, 129.51, 130.3, 132.86, 132.88, 166.5, 166.6. HRMS (ESI) calcd for $C_{21}H_{22}NaO_4$ $(M+Na)^+$ 361.1410, found 361.1409.



5g

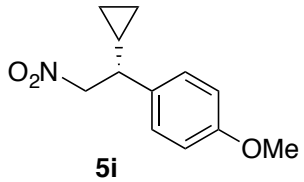
Compound 5g (Scheme 3, 92% yield, 89% ee). The ee was measured by HPLC (Chiralcel OD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 12.3 min (*S*), t_2 = 14.6 min (*R*)); $[\alpha]^{20}_D$ +34 (*c* 1.10, $CHCl_3$) for 89% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.16–0.21 (m, 1H), 0.30–0.37 (m, 1H), 0.48–0.53 (m, 1H), 0.64–0.70 (m, 1H), 1.04–1.12 (m, 1H), 2.34 (s, 3H), 2.69 (ddd, J = 9.6, 8.1, 7.5 Hz, 1H), 3.42 (dd, J = 11.6, 8.1 Hz, 1H), 3.46 (dd, J = 11.6, 7.5 Hz, 1H), 7.13 (d, J = 8.1 Hz, 2H), 7.16 (d, J = 8.1 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 3.4, 5.2, 14.4, 21.0, 48.8, 80.9,

127.2, 129.5, 136.6, 137.2. HRMS (ESI) calcd for $C_{12}H_{15}NNaO_2$ $(M+Na)^+$ 228.0995, found 228.0989.



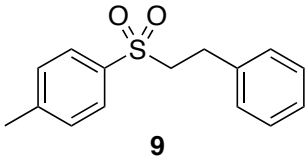
5h

Compound 5h (Scheme 3, 80% yield, 89% ee). The ee was measured by HPLC (Chiralcel OD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 16.5 min (*S*), t_2 = 19.2 min (*R*)); $[\alpha]^{20}_D$ +39 (*c* 0.99, $CHCl_3$) for 89% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.15–0.21 (m, 1H), 0.31–0.38 (m, 1H), 0.48–0.55 (m, 1H), 0.65–0.71 (m, 1H), 1.01–1.19 (m, 1H), 2.69 (ddd, *J* = 10.2, 8.5, 7.1 Hz, 1H), 4.65 (dd, *J* = 11.9, 8.5 Hz, 1H), 4.69 (dd, *J* = 11.9, 7.1 Hz, 1H), 7.18 (d, *J* = 8.9 Hz, 2H), 7.32 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 3.6, 5.3, 14.3, 48.6, 80.5, 128.7, 129.0, 133.4, 138.2. HRMS (ESI) calcd for $C_{11}H_{12}ClNNaO_2$ $(M+Na)^+$ 248.0449, found 248.0451.



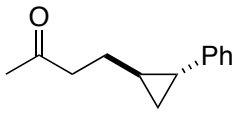
5i

Compound 5i (Scheme 3, 70% yield, 89% ee). The ee was measured by HPLC (Chiralcel OD-H column, hexane/2-propanol = 90:10, flow 0.5 mL/min, 254 nm, t_1 = 18.8 min (*S*), t_2 = 24.9 min (*R*)); $[\alpha]^{20}_D$ +26 (*c* 1.08, $CHCl_3$) for 89% ee (*R*). ^{1}H NMR ($CDCl_3$) δ 0.15–0.20 (m, 1H), 0.29–0.34 (m, 1H), 0.47–0.53 (m, 1H), 0.63–0.68 (m, 1H), 1.02–1.10 (m, 1H), 2.68 (dt, *J* = 10.2, 7.8 Hz, 1H), 3.79 (s, 3H), 4.64 (dd, *J* = 11.9, 7.8 Hz, 1H), 4.67 (dd, *J* = 11.9, 7.8 Hz, 1H), 6.88 (d, *J* = 8.9 Hz, 2H), 7.16 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 3.4, 5.2, 14.5, 48.4, 55.2, 81.0, 114.2, 128.3, 131.6, 158.9. HRMS (ESI) calcd for $C_{12}H_{15}NNaO_3$ $(M+Na)^+$ 244.0944, found 244.0944.



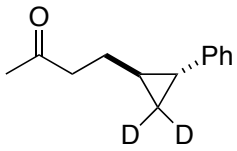
9

Compound 9 [CAS: 19719-87-0] (eq 2, 26% yield). ^{1}H NMR ($CDCl_3$) δ 2.46 (s, 3H), 3.01–3.06 (m, 2H), 3.31–3.36 (m, 2H), 7.11 (d, *J* = 7.5 Hz, 2H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.82 (d, *J* = 8.1 Hz, 2H).



11

Compound 11 (eq 3, 92% yield, 25% ee). The ee was measured by HPLC (Chiralpak IA column, hexane/2-propanol = 100:1, flow 0.5 mL/min, 254 nm, t_1 = 14.6 min (*major*), t_2 = 16.0 min (*minor*)). ^{1}H NMR ($CDCl_3$) δ 0.76–0.81 (m, 1H), 0.88–0.92 (m, 1H), 1.01–1.09 (m, 1H), 1.62–1.72 (m, 3H), 2.15 (s, 3H), 2.59 (t, *J* = 7.5 Hz, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 7.13 (t, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 16.1, 23.0, 23.3, 28.5, 30.1, 43.3, 125.3, 125.6, 128.2, 143.4, 208.7. HRMS (ESI) calcd for $C_{13}H_{16}NaO$ $(M+Na)^+$ 211.1093, found 211.1090.



11-*d*$_2$

Compound 11-*d*$_2$ (eq 4, 50% yield). ^{1}H NMR ($CDCl_3$) δ 1.03 (dd, *J* = 11.6, 6.8 Hz, 1H), 1.61–1.71 (m, 3H), 2.15 (s, 3H), 2.58 (t, *J* = 7.2 Hz, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 7.13 (t, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.8 Hz, 2H). HRMS (ESI) calcd for $C_{13}H_{14}D_2NaO$ $(M+Na)^+$ 213.1219, found 213.1222.

11. X-Ray data of 3a

A colorless crystal of **3a** suitable for X-ray crystallographic analysis was obtained by recrystallization from hexane/2-propanol. The ORTEP drawing of **3a** is shown in Figure S1. The crystal structure has been deposited at the Cambridge Crystallographic Centre (deposition number: CCDC 1047801). 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*α radiation (λ = 1.54187 Å) at 93 K. The structure was solved by direct method (SHELXS-97) and refined with full-matrix least-square technique (SHELXL-97).[17] The data for **3a** is summarized in Table S1.

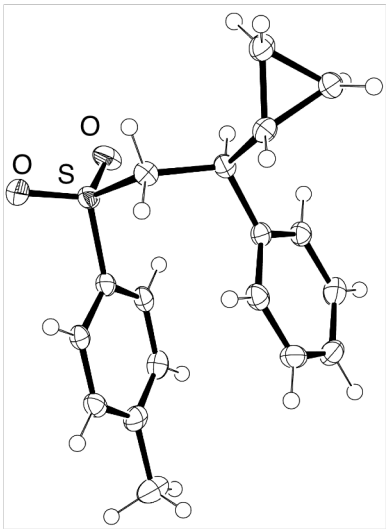


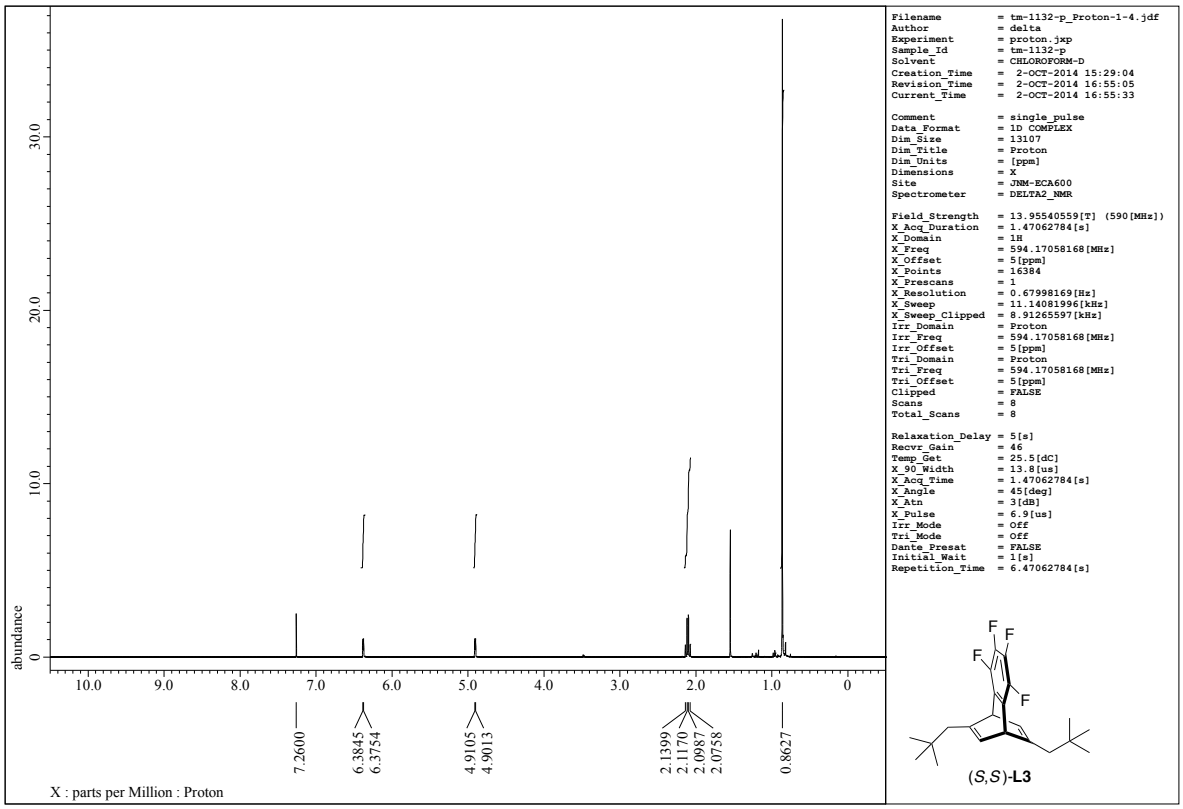
Figure S1. ORTEP illustration of **3a** drawn at 50% probability level.

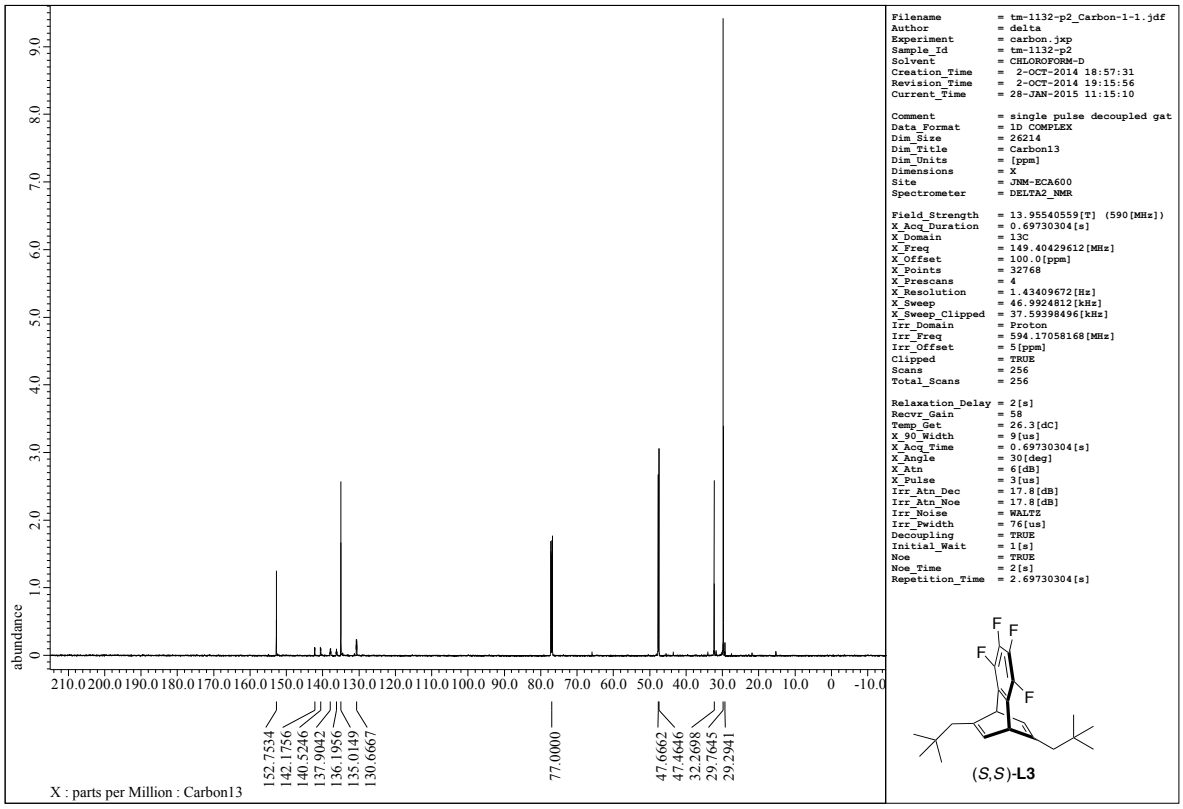
17 G. M. Sheldrick, Program for the solution and refinement of crystal structures, University of Göttingen, Göttingen, Germany, 1997.

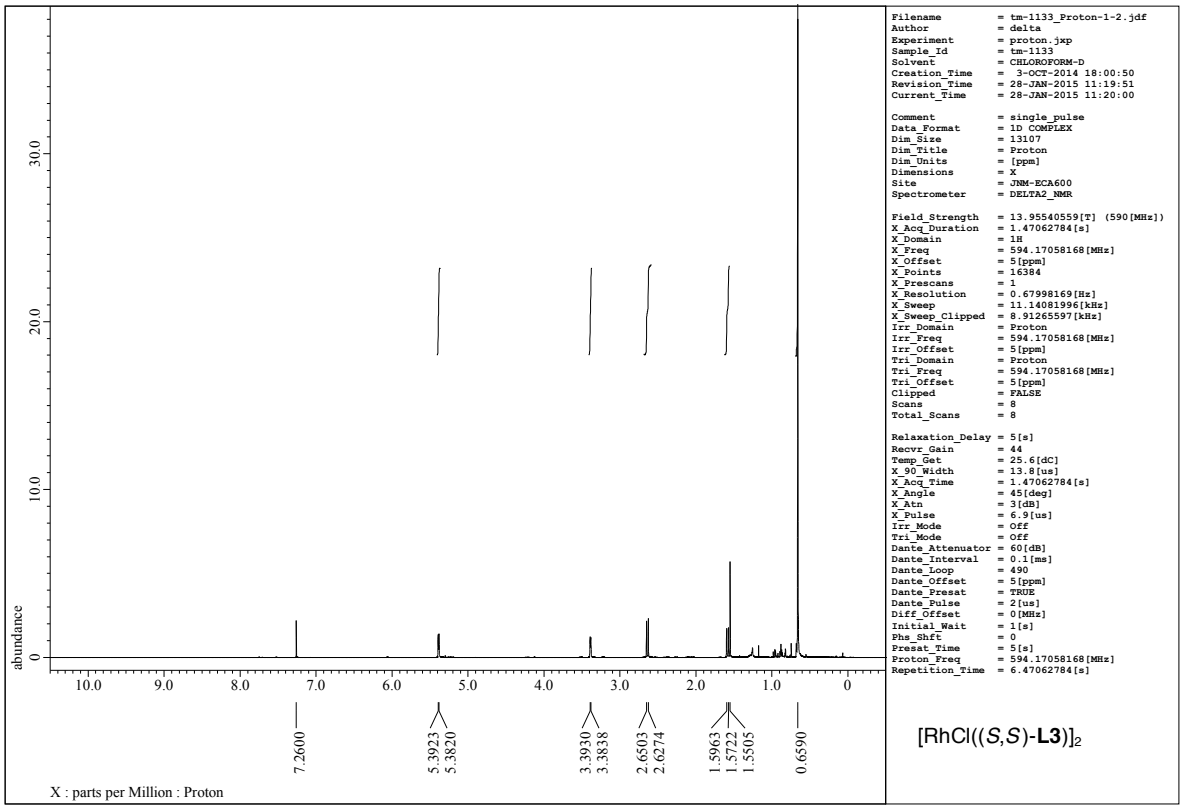
Table S1. Crystal data and structure refinement for **3a**

Empirical formula	$C_{18}H_{20}O_2S$
Formula weight	300.40
Temperature	93(2) K
Crystal system	Monoclinic
Space group	$P\,2_1$ (#4)
Unit cell dimensions	a = 7.323(5) Å
	b = 12.346(9) Å
	c = 9.152(6) Å
	β = 108.447(17)°
Volume	784.9(9) $Å^3$
Z	2
Density (calculated) [Mg/m^3]	1.271
μ (mm^{-1})	1.837
F(000)	320
Reflections collected	10183
Independent reflections	2650 [R(int) = 0. 0388]
Completeness to θ (%)	99.1%
Goodness-of-fit	1.026
R_1 [I>2σ (I)]	0.0323
wR_2 (all data)	0.0839
Flack parameter	–0.007(14)
Largest diff. peak and hole [$e^-/Å^{-3}$]	0.318 and –0.229

12. ^{1}H and ^{13}C NMR spectra and HPLC charts







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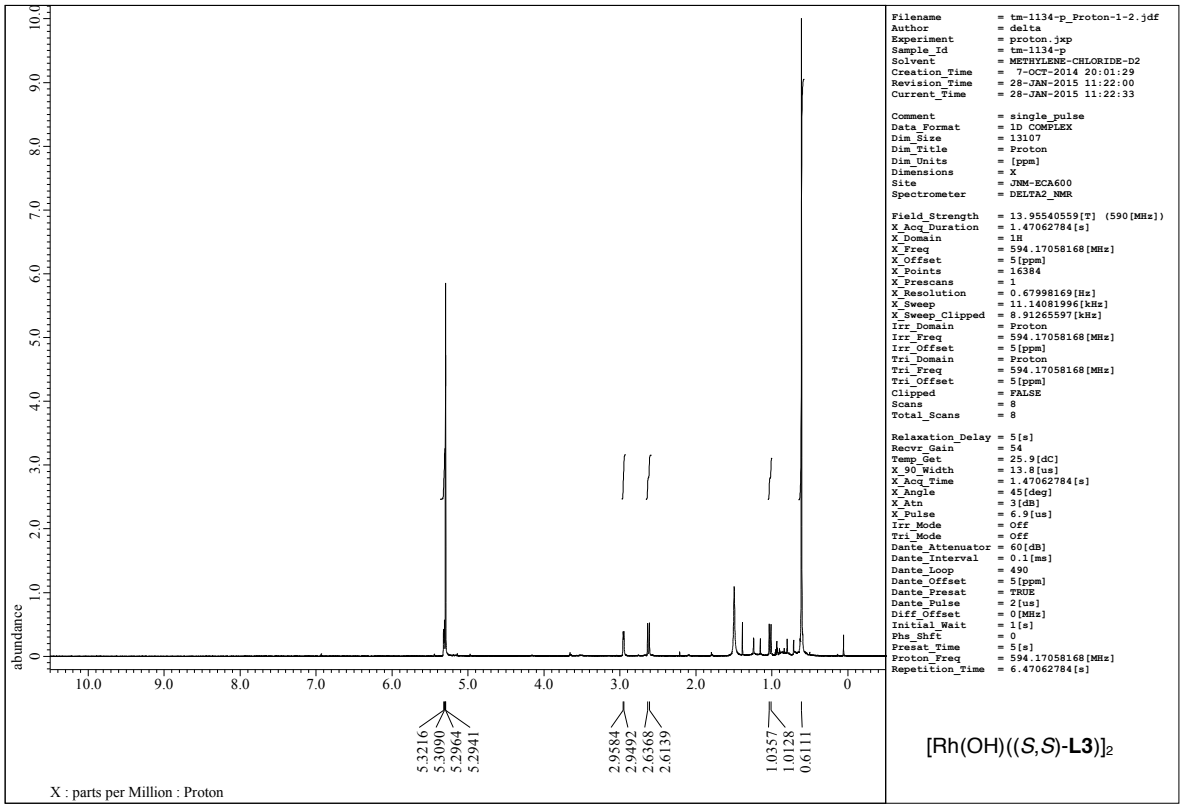
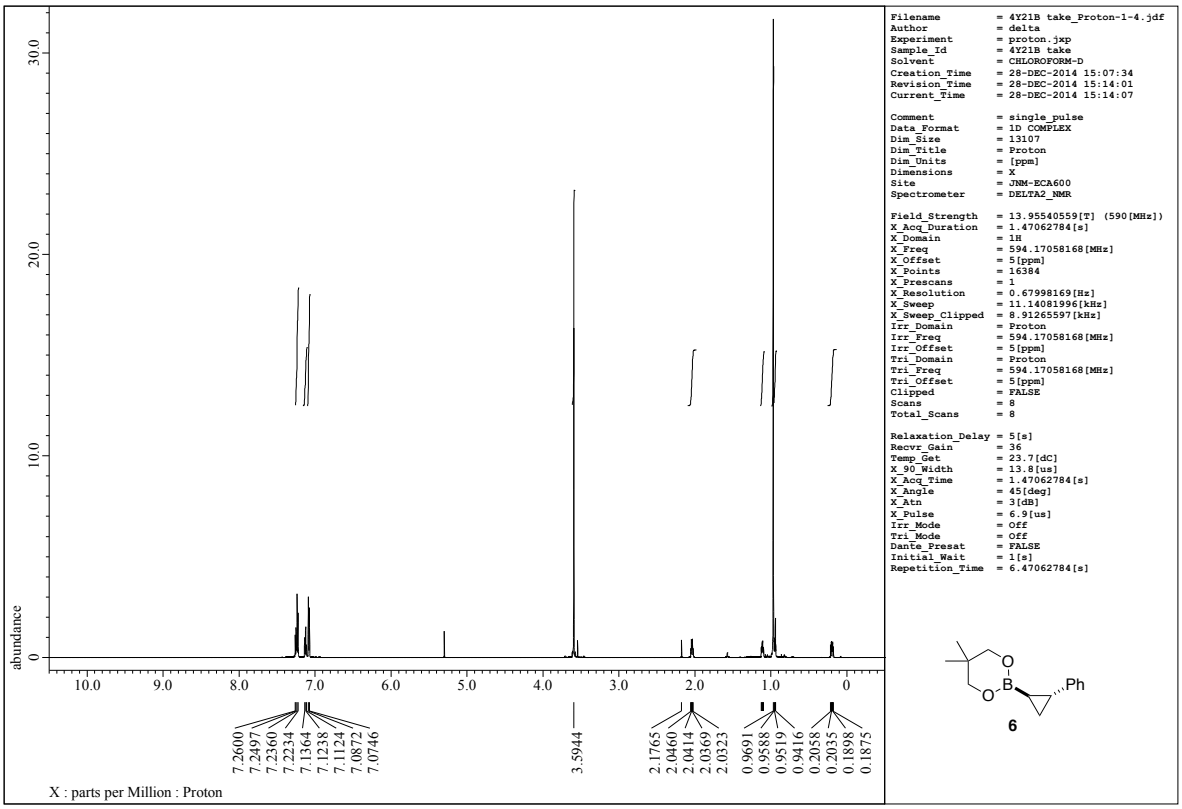


[Rh(OH)((*S*,*S*)-**L3**)]$_2$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3.5944
2.1765 2.0460 2.0414 2.0369 2.0323
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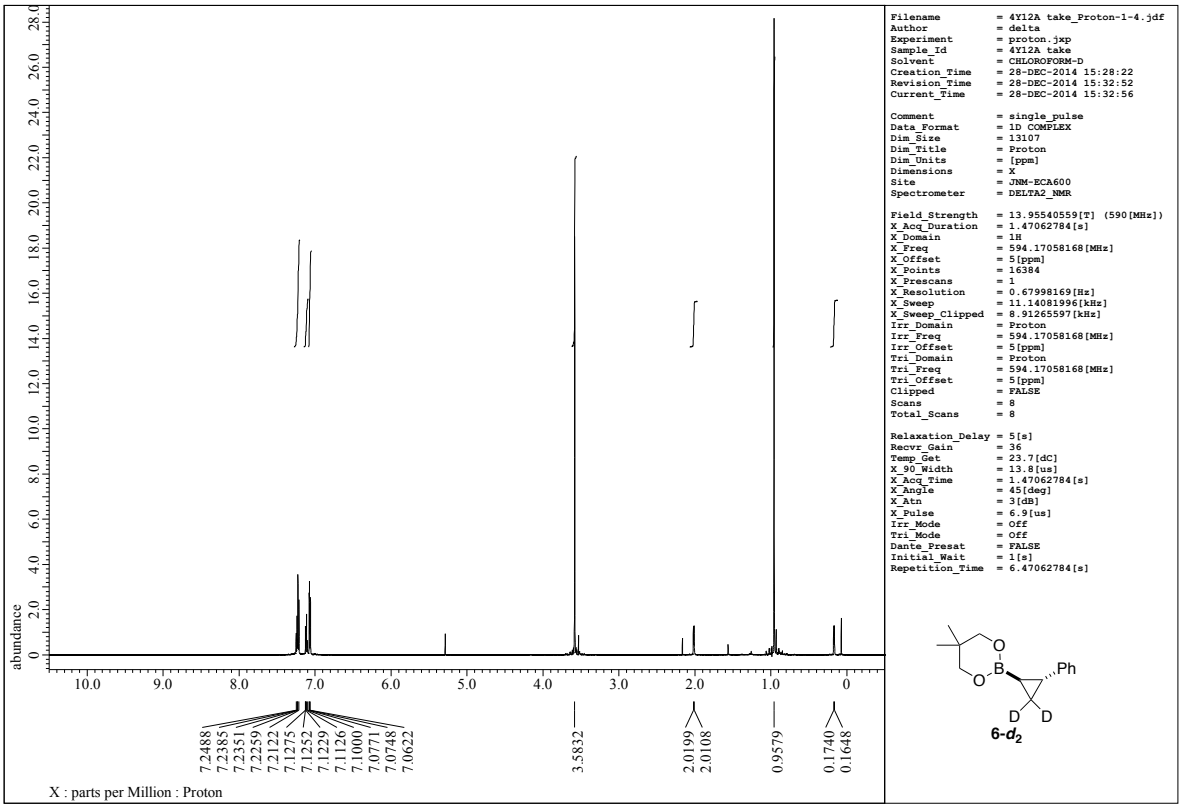
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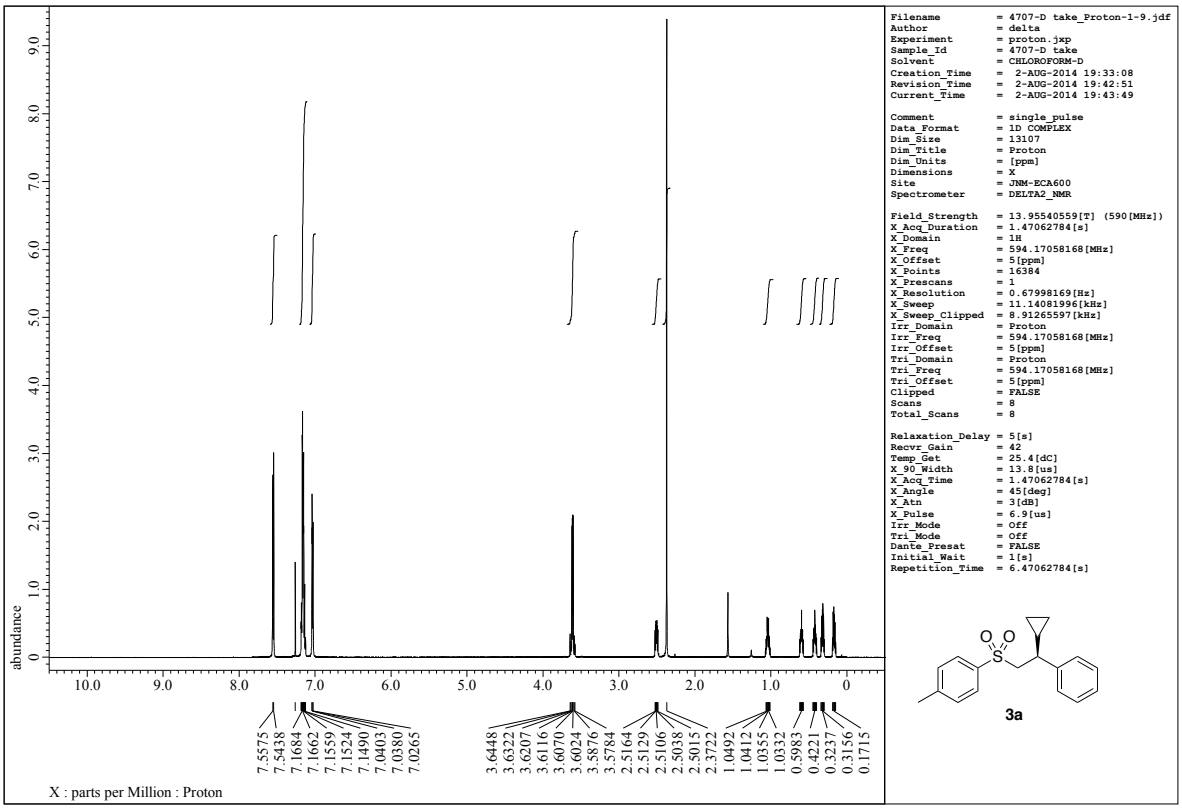
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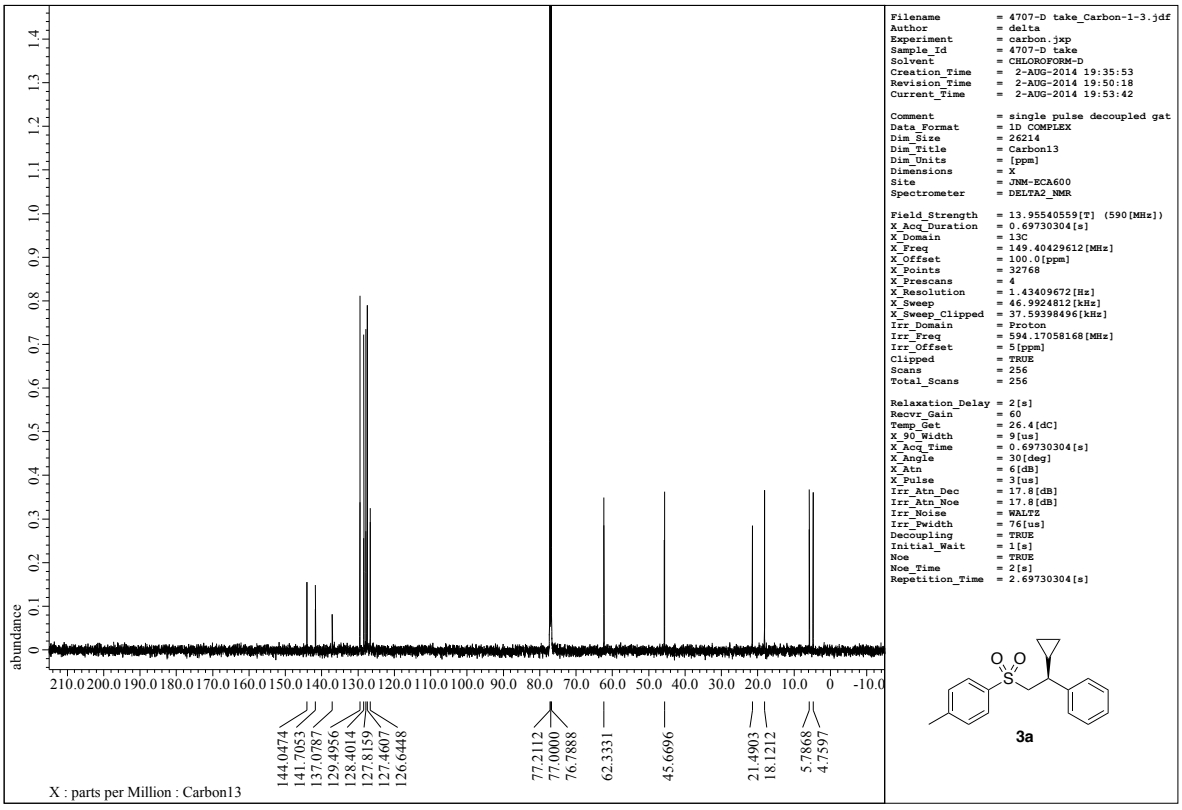
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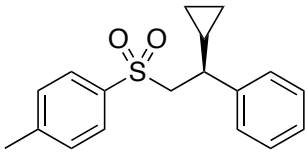

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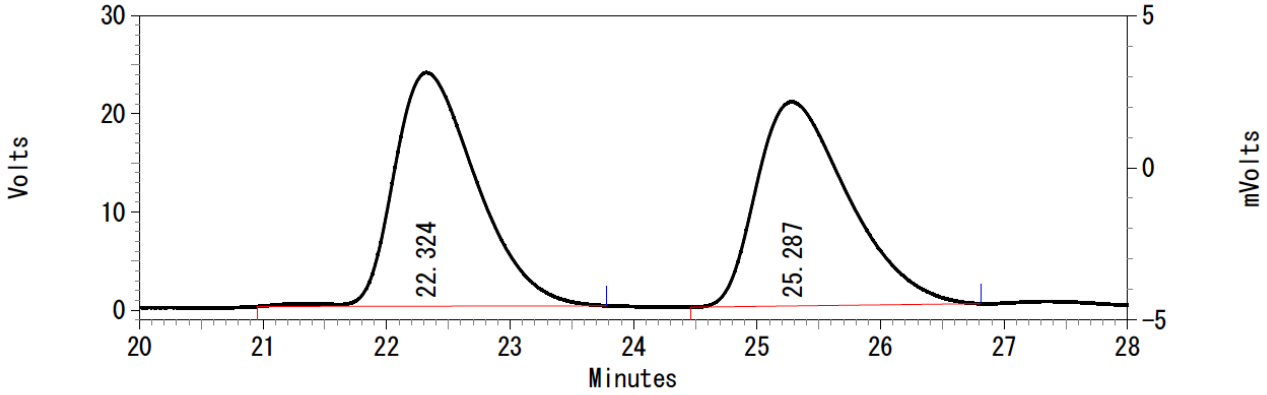

UV Results

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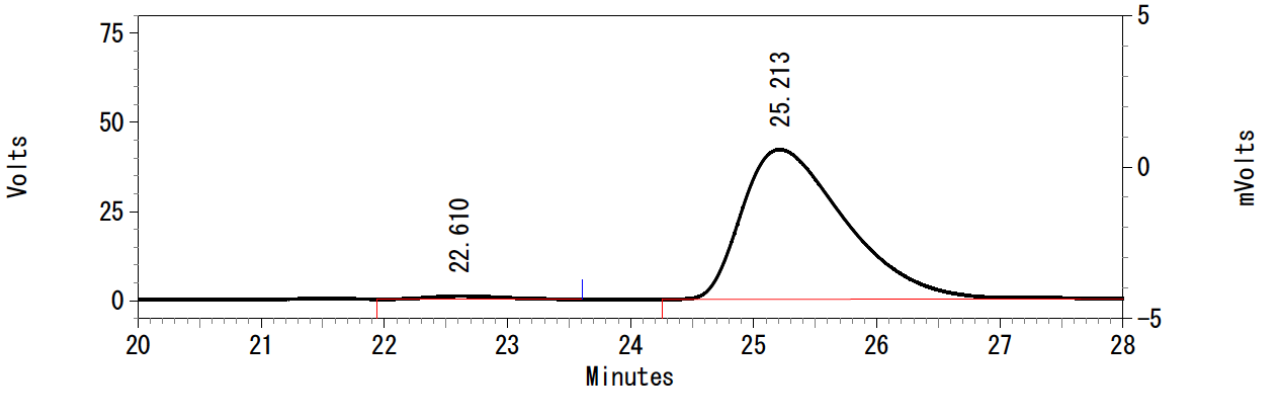

UV Results

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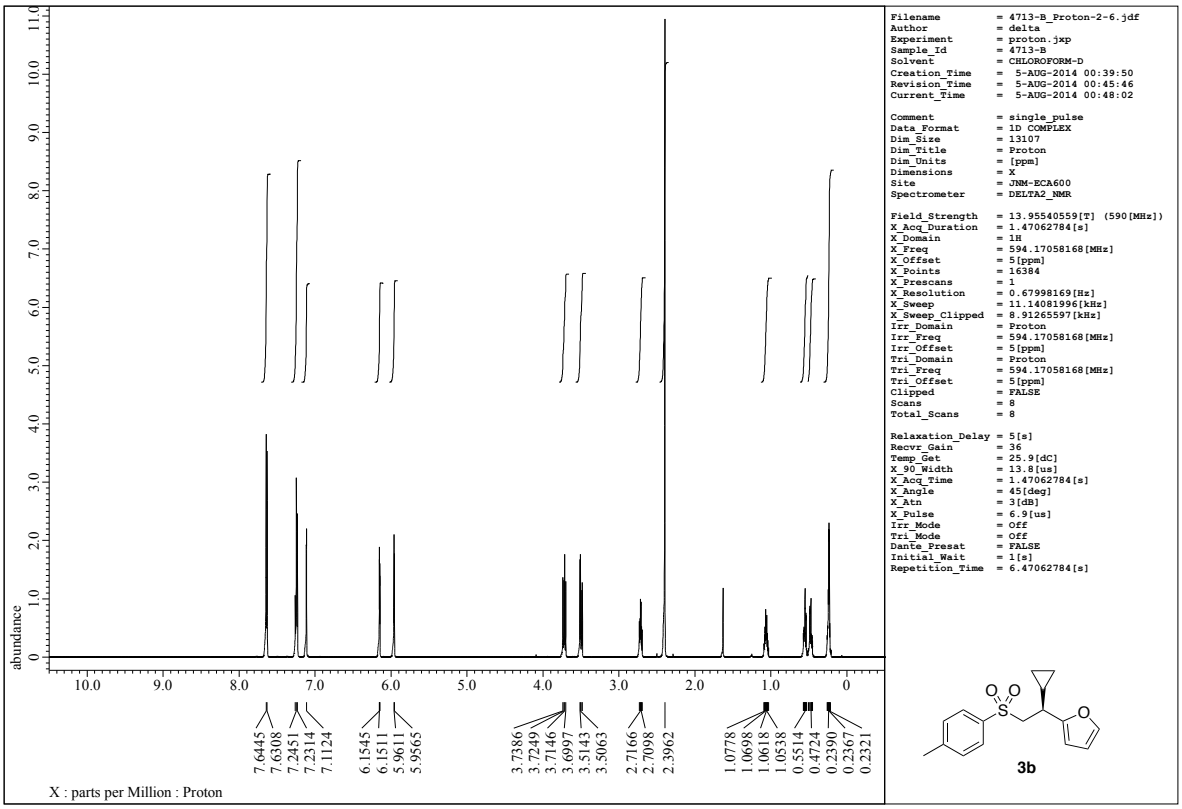
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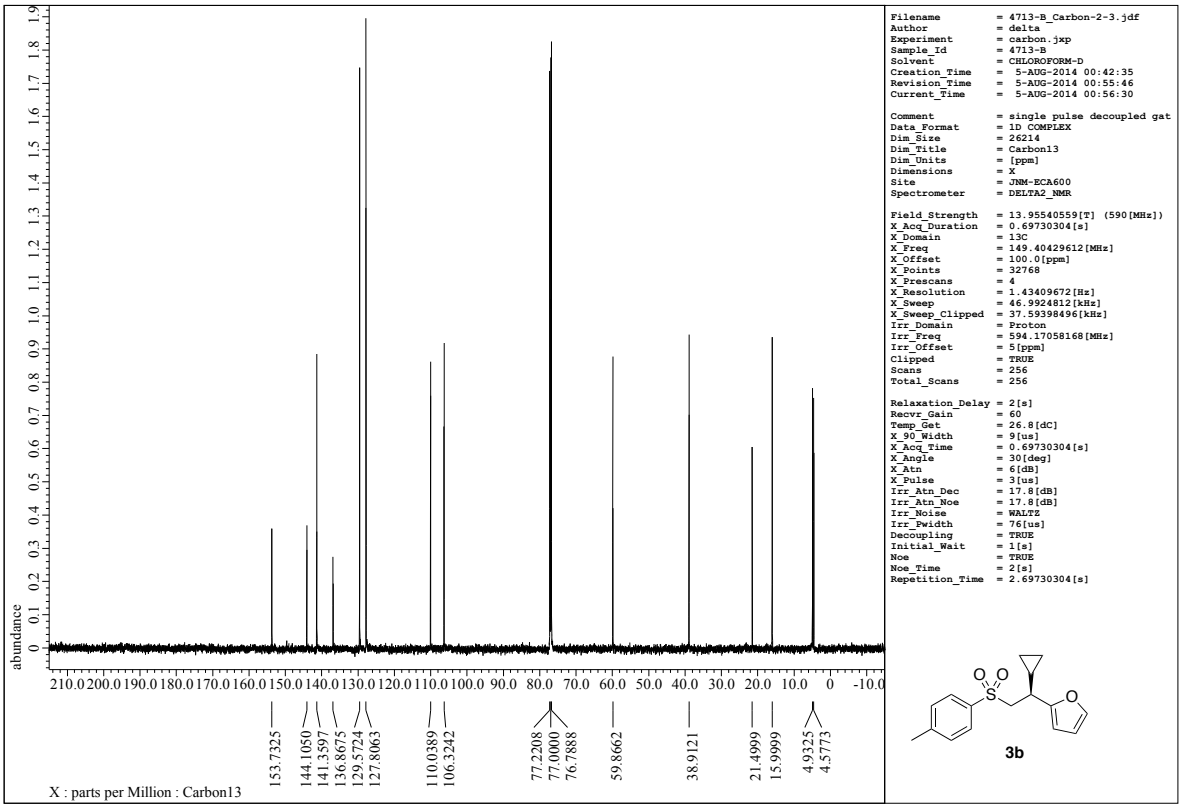
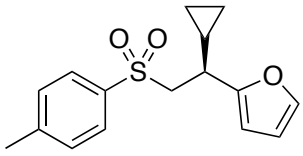
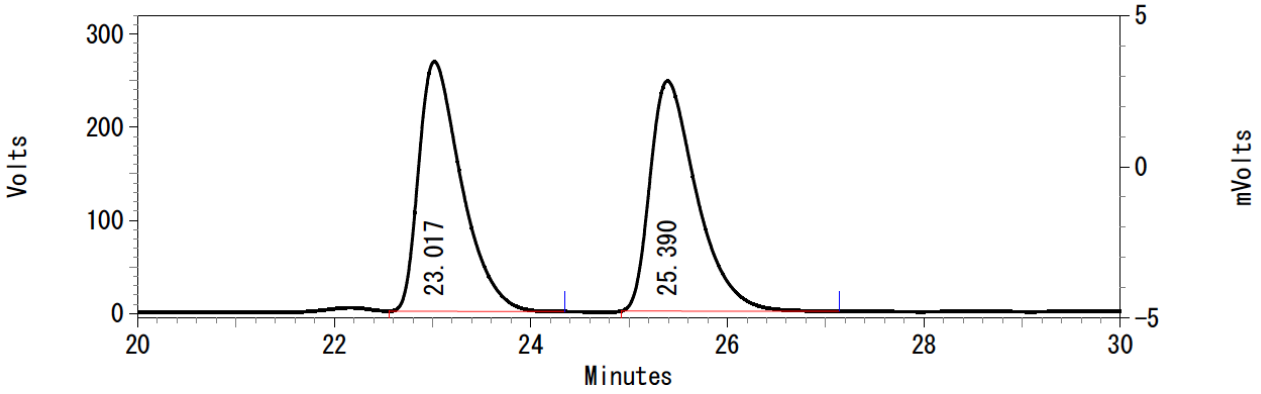
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
3b


abundance
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
153.7325 144.1050 141.3597 136.8675 129.5724 127.8063 110.0389 106.3242 77.2208 77.0000 76.7888 59.8662 38.9121 21.4999 15.9999 4.9325 4.5773
X : parts per Million : Carbon13
Filename = 4713-B_Carbon-2-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4713-B
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 00:42:35
Revision_Time = 5-AUG-2014 00:55:46
Current_Time = 5-AUG-2014 00:56:30
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 = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 26.8[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
3b

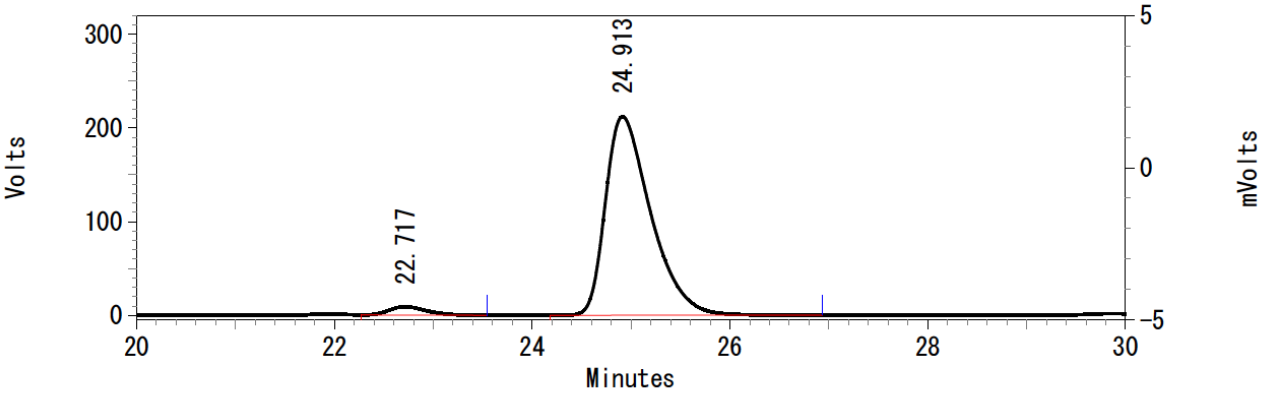


3b



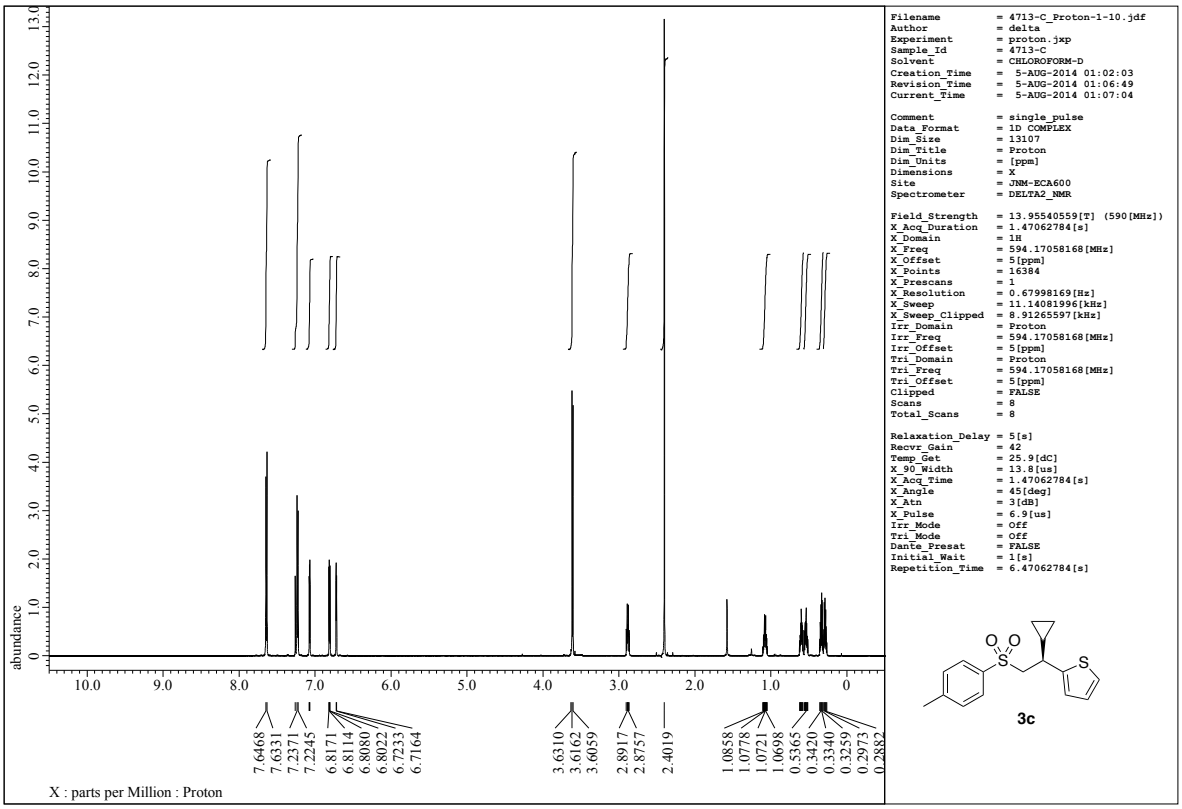
UV Results

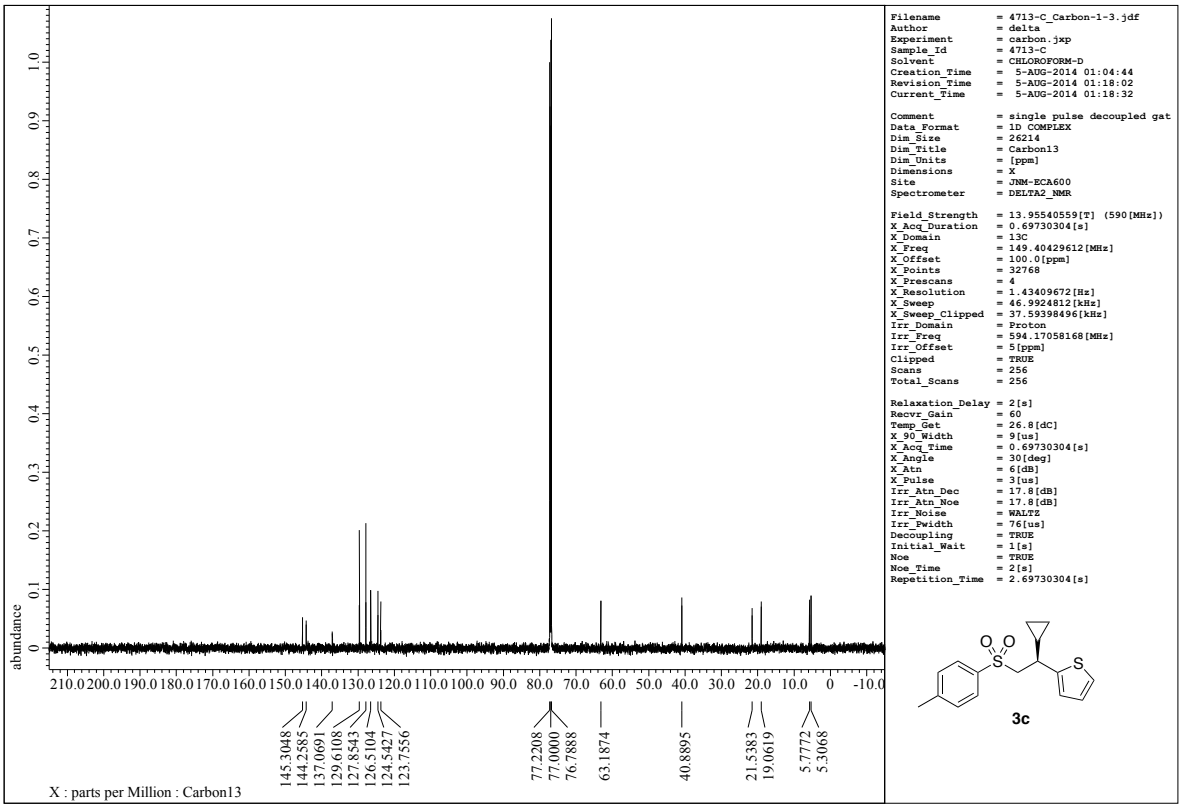
Pk #	Retention Time	Area	Area Percent	Height
1	23.017	8103366	49.900	268107
2	25.390	8135925	50.100	246945
Totals		16239291	100.000	515052

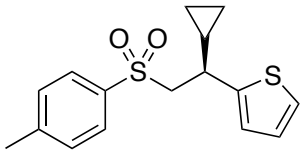


UV Results

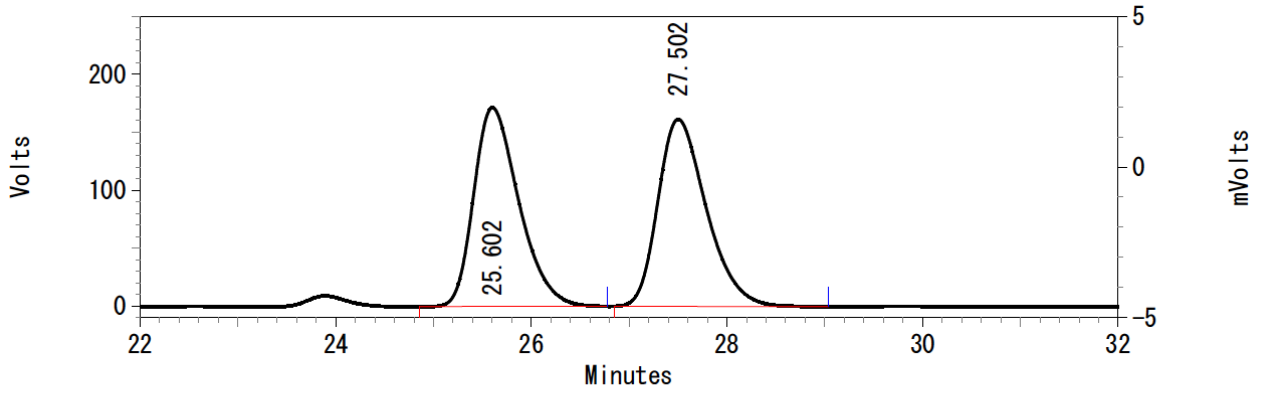
Pk #	Retention Time	Area	Area Percent	Height
1	22.717	232349	3.333	8949
2	24.913	6739243	96.667	212014
Totals		6971592	100.000	220963


abundance
X : parts per Million : Proton
7.6468
7.6331
7.2371
7.2245
6.8171
6.8114
6.8080
6.8022
6.7233
6.7164
3.6310
3.6162
3.6059
2.8917
2.8757
2.4019
1.0858
1.0778
1.0721
1.0698
0.5365
0.3420
0.3340
0.3259
0.2973
0.2882
Filename = 4713-C_Proton-1-10.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4713-C
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 01:02:03
Revision_Time = 5-AUG-2014 01:06:49
Current_Time = 5-AUG-2014 01:07:04
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 = 25.9[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
3c


abundance
X : parts per Million : Carbon13
145.3048
144.2585
137.0691
129.6108
127.8543
126.5104
124.5427
123.7556
77.2208
77.0000
76.7888
63.1874
40.8895
21.5383
19.0619
5.7772
5.3068
Filename = 4713-C_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4713-C
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 01:04:44
Revision_Time = 5-AUG-2014 01:18:02
Current_Time = 5-AUG-2014 01:18:32
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 = 26.8[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
3c

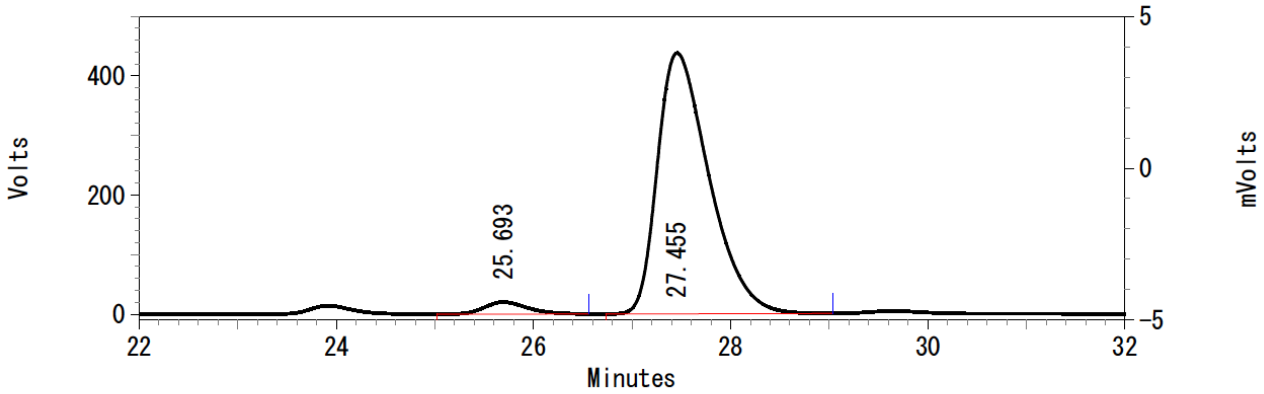


3c



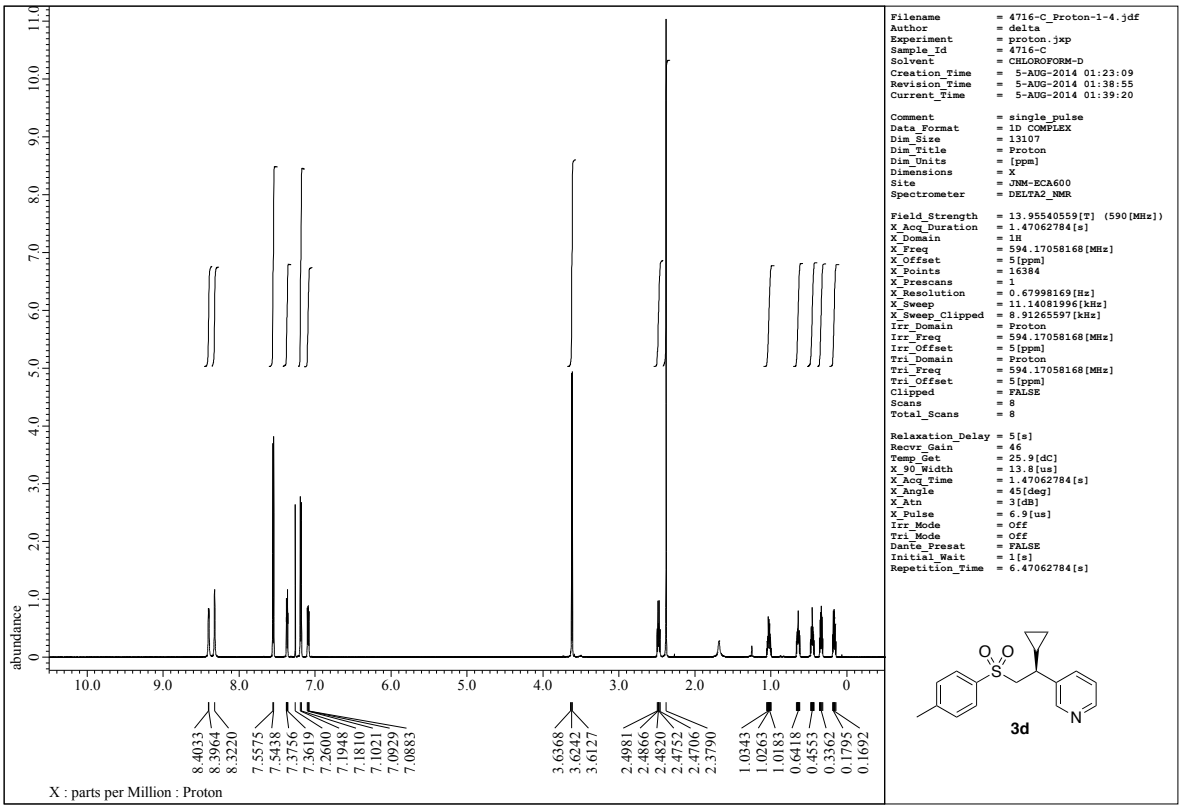
UV Results

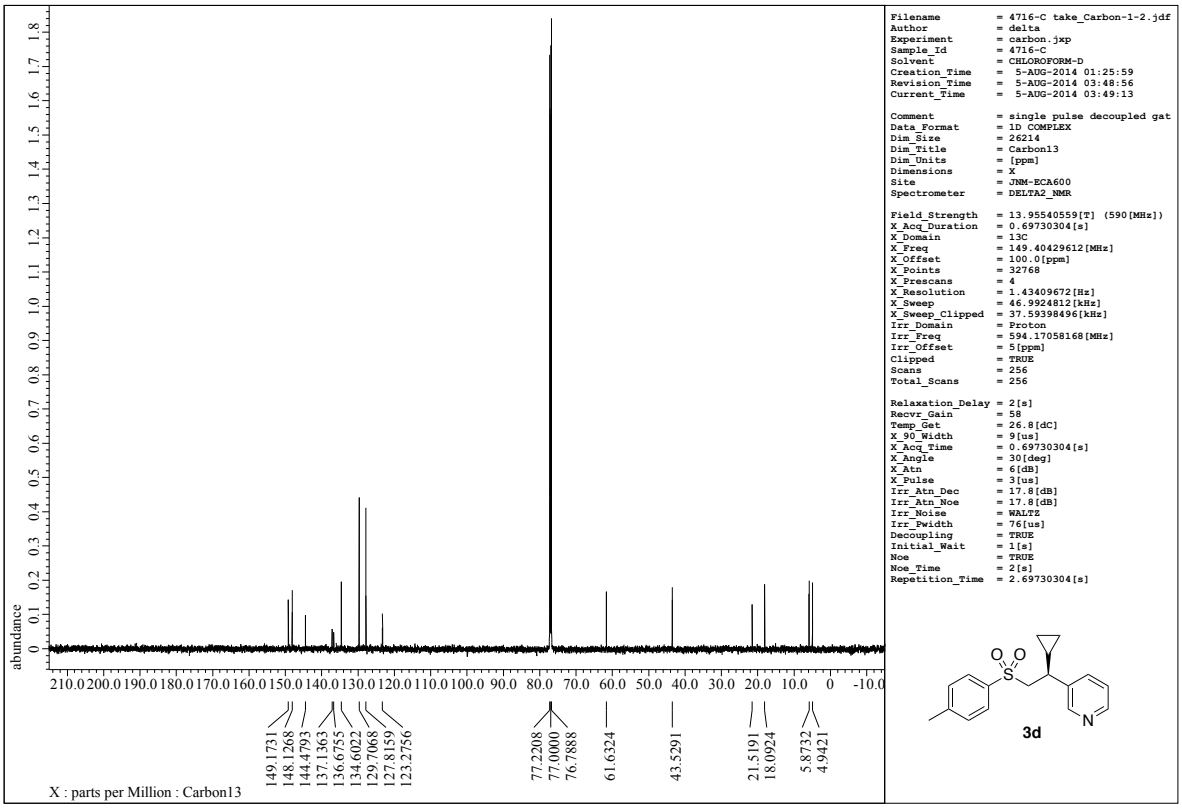
Pk #	Retention Time	Area	Area Percent	Height
1	25.602	5495009	49.772	171405
2	27.502	5545415	50.228	161382
Totals		11040424	100.000	332787

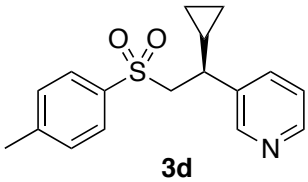


UV Results

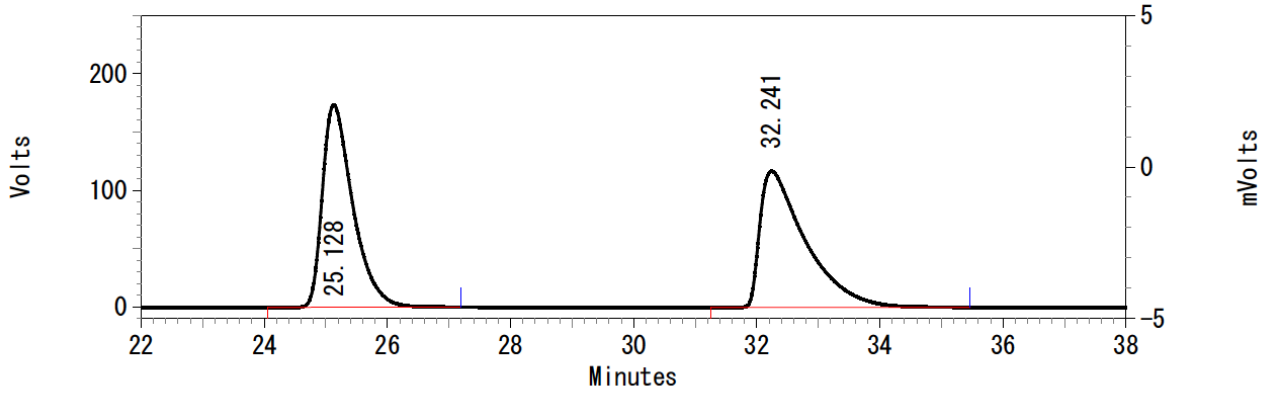
Pk #	Retention Time	Area	Area Percent	Height
1	25.693	605241	3.658	20100
2	27.455	15940342	96.342	437905
Totals		16545583	100.000	458005


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.4033 8.3964 8.3220 7.5575 7.5438 7.3756 7.3619 7.2600 7.1948 7.1810 7.1021 7.0929 7.0883
3.6368 3.6242 3.6127 2.4981 2.4866 2.4820 2.4752 2.4706 2.3790 1.0343 1.0263 1.0183 0.6418 0.4553 0.3362 0.1795 0.1692
X : parts per Million : Proton
Filename = 4716-C_Proton-1-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4716-C
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 01:23:09
Revision_Time = 5-AUG-2014 01:38:55
Current_Time = 5-AUG-2014 01:39:20
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 = 46
Temp_Get = 25.9[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O O S N
3d


abundance
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
149.1731 148.1268 144.4793 137.1363 136.6755 134.6022 129.7068 127.8159 123.2756
77.2208 77.0000 76.7888 61.6324 43.5291 21.5191 18.0924 5.8732 4.9421
X : parts per Million : Carbon13
Filename = 4716-C take_Carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4716-C
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 01:25:59
Revision_Time = 5-AUG-2014 03:48:56
Current_Time = 5-AUG-2014 03:49:13
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 = 26.8[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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 O S N
3d

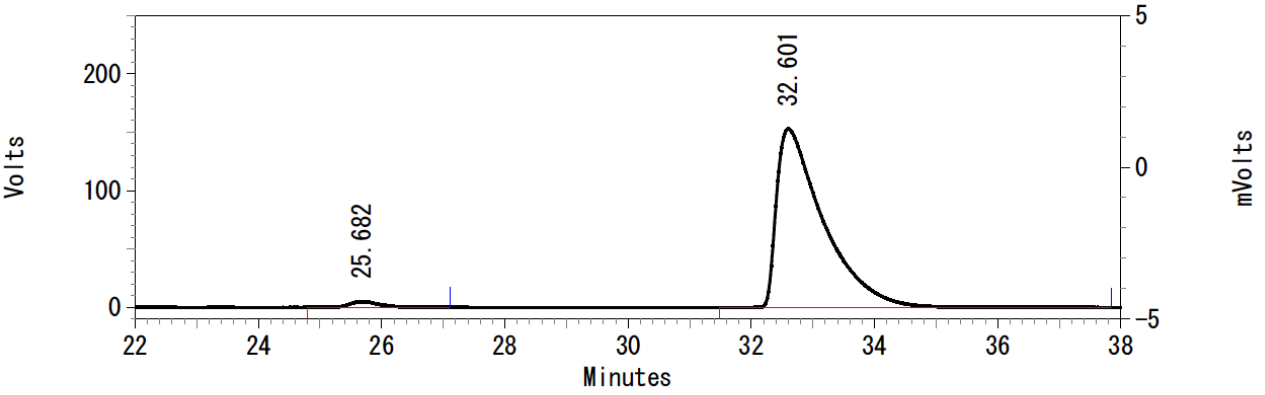


3d



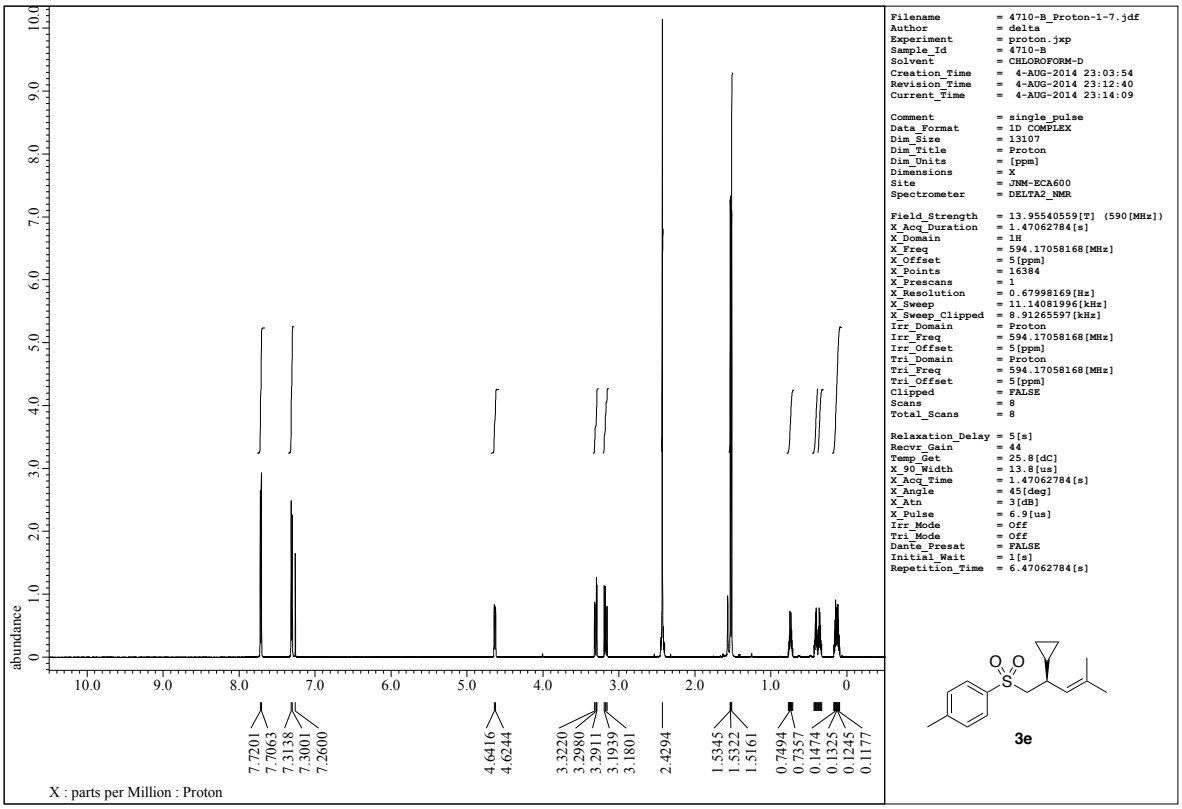
UV Results

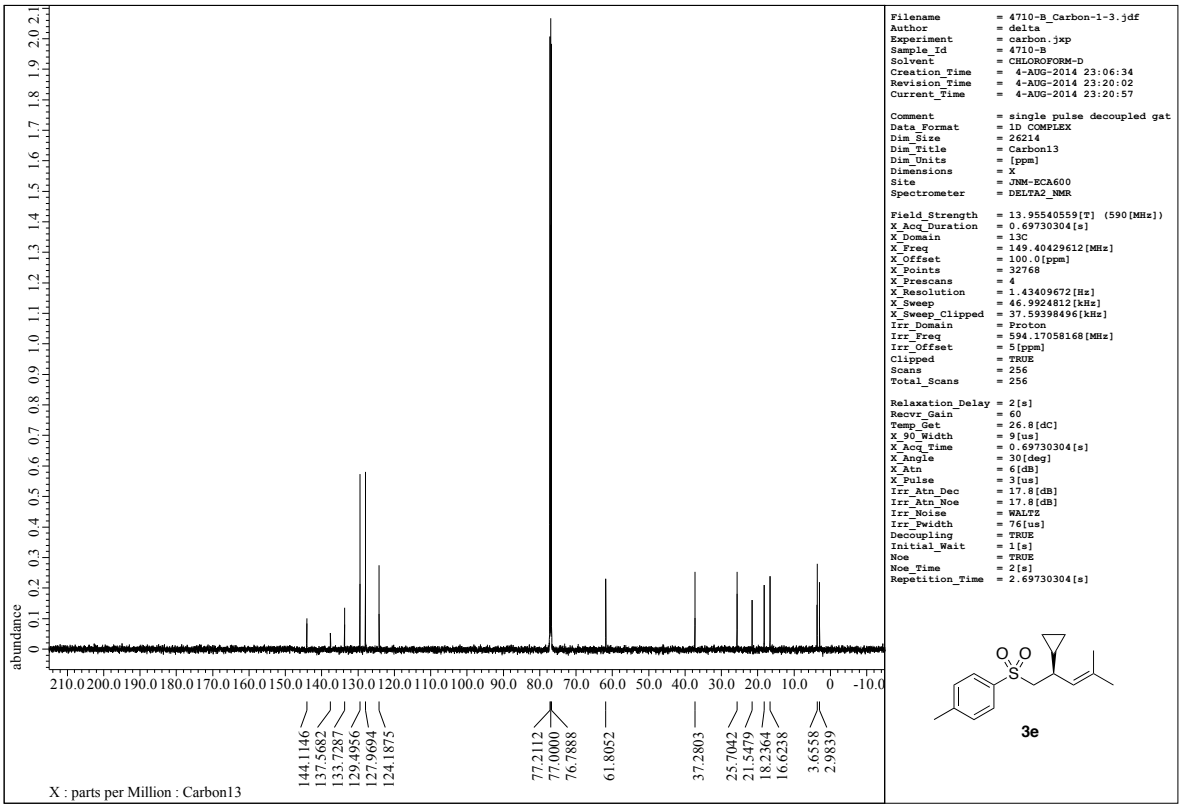
Pk #	Retention Time	Area	Area Percent	Height
1	25.128	5957255	49.834	173666
2	32.241	5996836	50.166	116703
Totals		11954091	100.000	290369

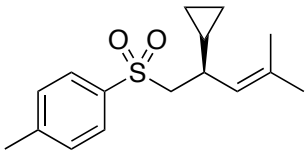


UV Results

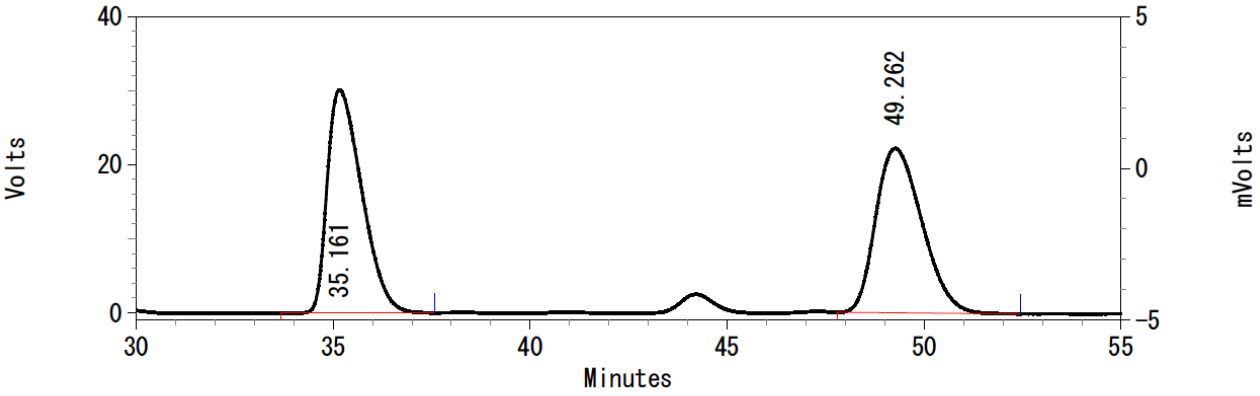
Pk #	Retention Time	Area	Area Percent	Height
1	25.682	172016	2.086	5011
2	32.601	8074724	97.914	152785
Totals		8246740	100.000	157796


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.7201 7.7063 7.3138 7.3001 7.2600
4.6416 4.6244
3.3220 3.2980 3.2911 3.1939 3.1801
2.4294
1.5345 1.5322 1.5161
0.7494 0.7357 0.1474 0.1325 0.1245 0.1177
X : parts per Million : Proton
Filename = 4710-B_Proton-1-7.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4710-B
Solvent = CHLOROFORM-D
Creation_Time = 4-AUG-2014 23:03:54
Revision_Time = 4-AUG-2014 23:12:40
Current_Time = 4-AUG-2014 23:14:09
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 = 44
Temp_Get = 25.8[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O O S
3e


abundance
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
144.1146 137.5682 133.7287 129.4956 127.9694 124.1875
77.2112 77.0000 76.7888
61.8052
37.2803
25.7042 21.5479 18.2364 16.6238
3.6558 2.9839
X : parts per Million : Carbon13
Filename = 4710-B_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4710-B
Solvent = CHLOROFORM-D
Creation_Time = 4-AUG-2014 23:06:34
Revision_Time = 4-AUG-2014 23:20:02
Current_Time = 4-AUG-2014 23:20:57
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 = 26.8[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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 O S
3e

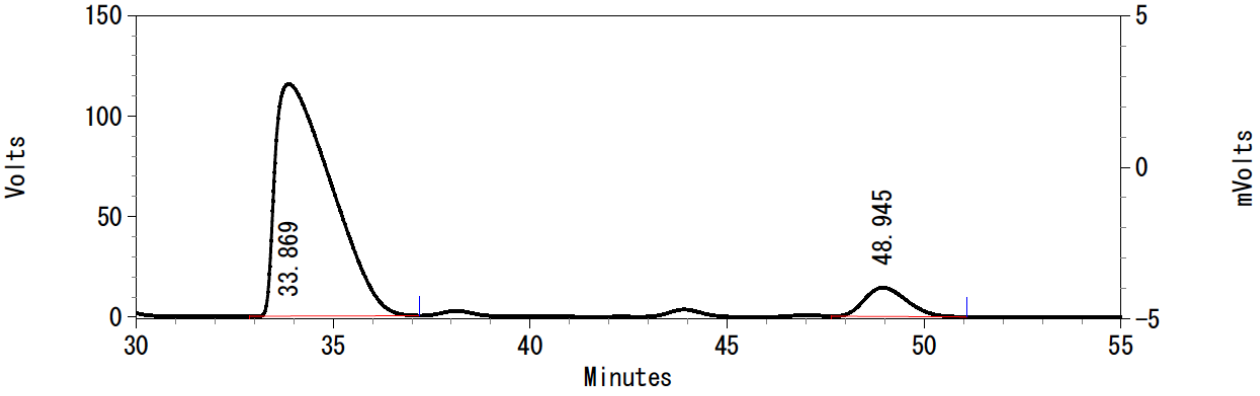


3e



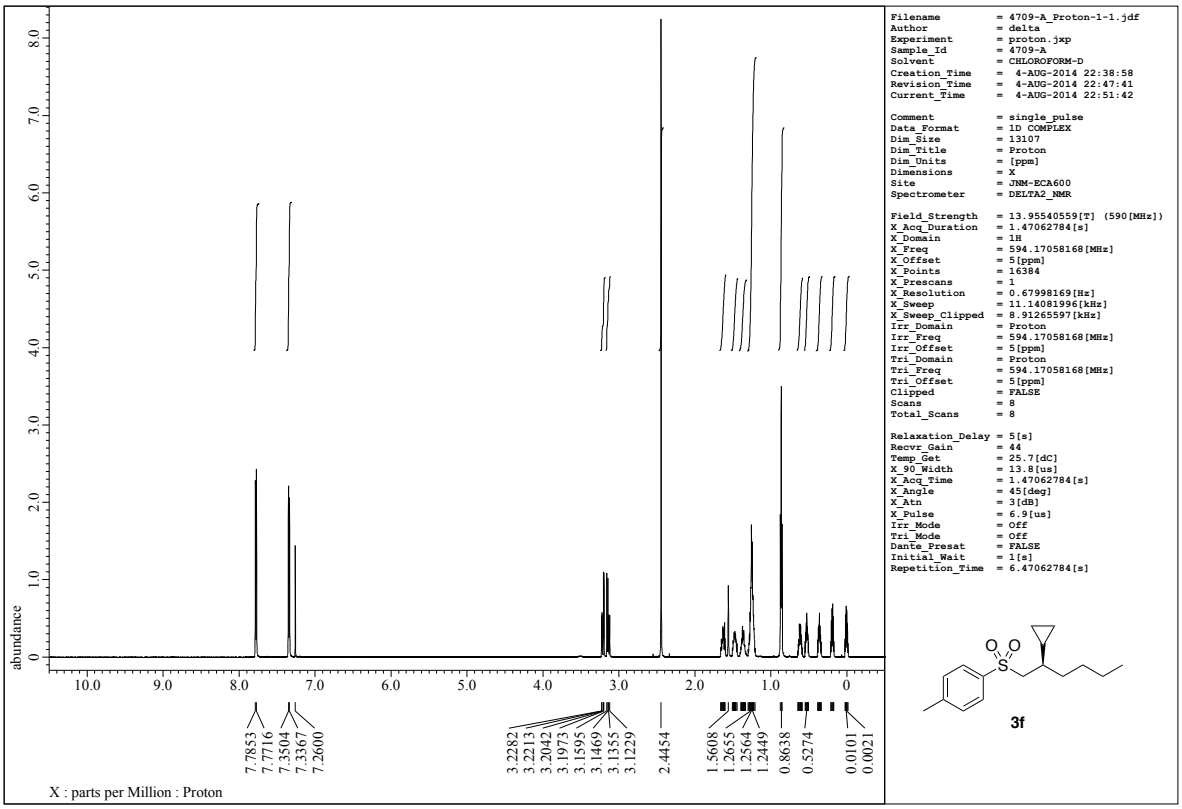
UV Results

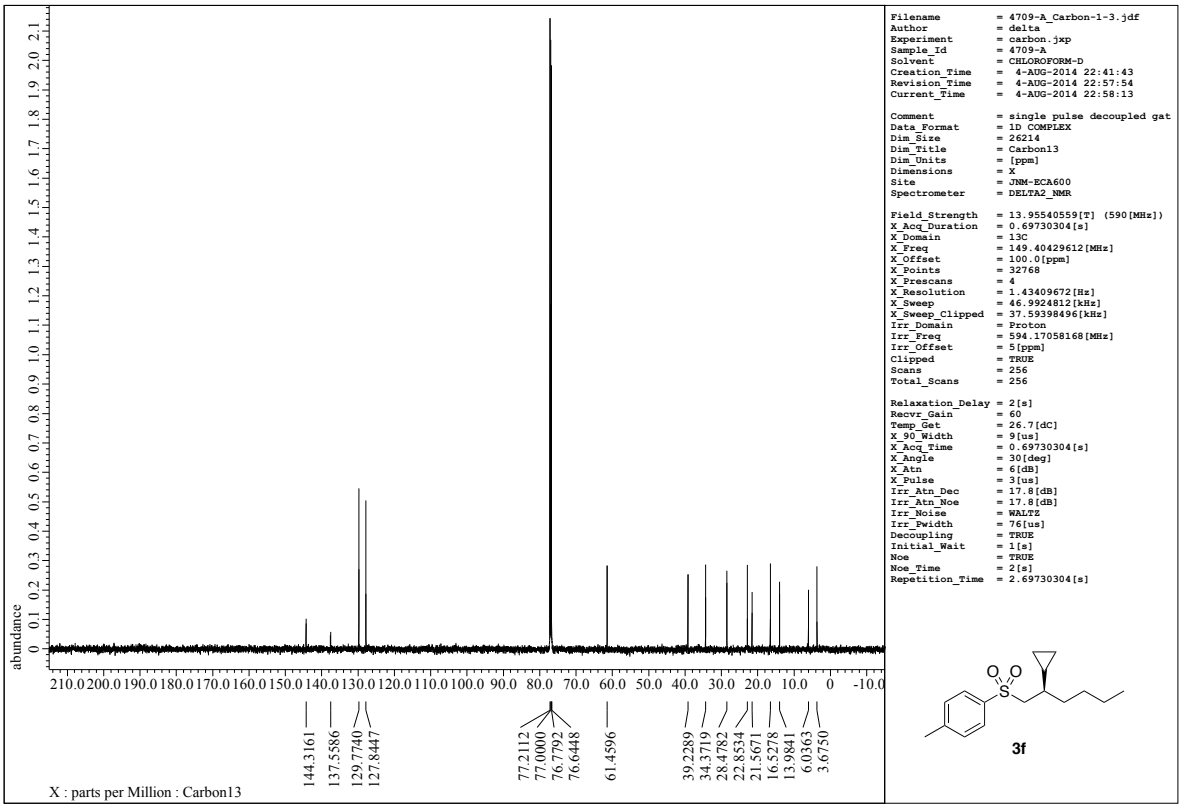
Pk #	Retention Time	Area	Area Percent	Height
1	35.161	1832656	50.345	30123
2	49.262	1807517	49.655	22182
Totals		3640173	100.000	52305

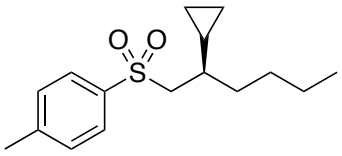


UV Results

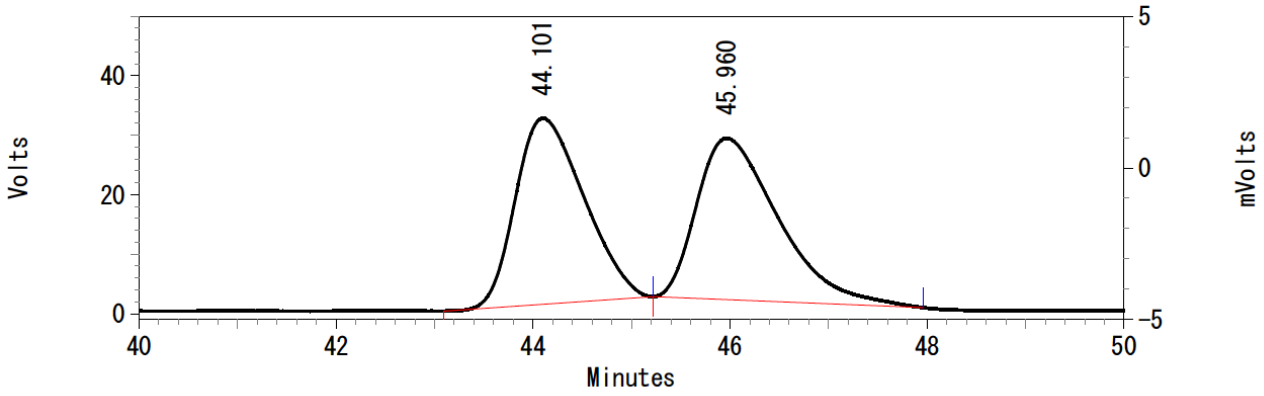
Pk #	Retention Time	Area	Area Percent	Height
1	33.869	11337396	91.331	115456
2	48.945	1076075	8.669	14311
Totals		12413471	100.000	129767


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.7853 7.7716 7.3504 7.3367 7.2600
3.2282 3.2213 3.2042 3.1973 3.1595 3.1469 3.1355 3.1229
2.4454
1.5608 1.2655 1.2564 1.2449
0.8638
0.5274
0.0101 0.0021
X : parts per Million : Proton
Filename = 4709-A_Proton-1-1.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4709-A
Solvent = CHLOROFORM-D
Creation_Time = 4-AUG-2014 22:38:58
Revision_Time = 4-AUG-2014 22:47:41
Current_Time = 4-AUG-2014 22:51:42
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 = 25.7[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
3f


abundance
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
144.3161
137.5586
129.7740
127.8447
77.2112
77.0000
76.7792
76.6448
61.4596
39.2289
34.3719
28.4782
22.8534
21.5671
16.5278
13.9841
6.0363
3.6750
X : parts per Million : Carbon13
Filename = 4709-A_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4709-A
Solvent = CHLOROFORM-D
Creation_Time = 4-AUG-2014 22:41:43
Revision_Time = 4-AUG-2014 22:57:54
Current_Time = 4-AUG-2014 22:58:13
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 = 26.7[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
3f

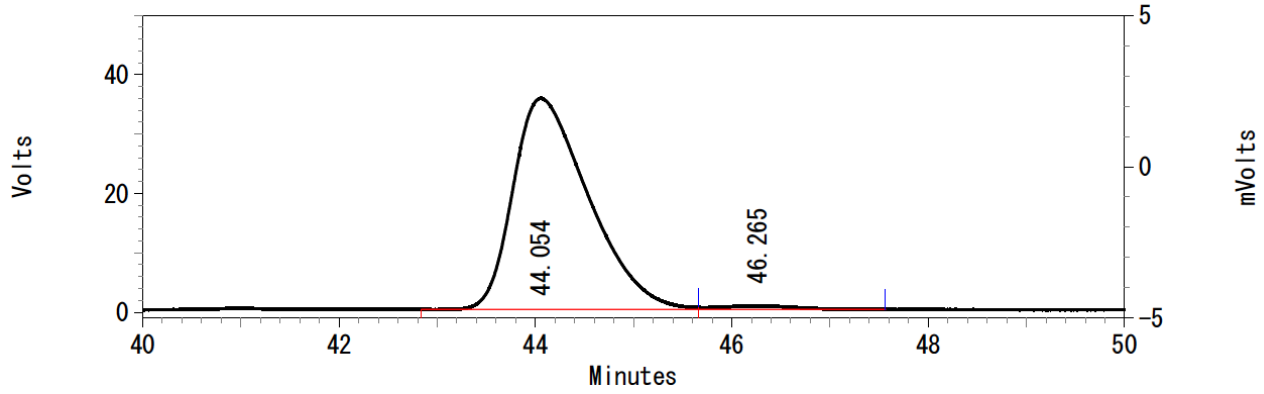


3f



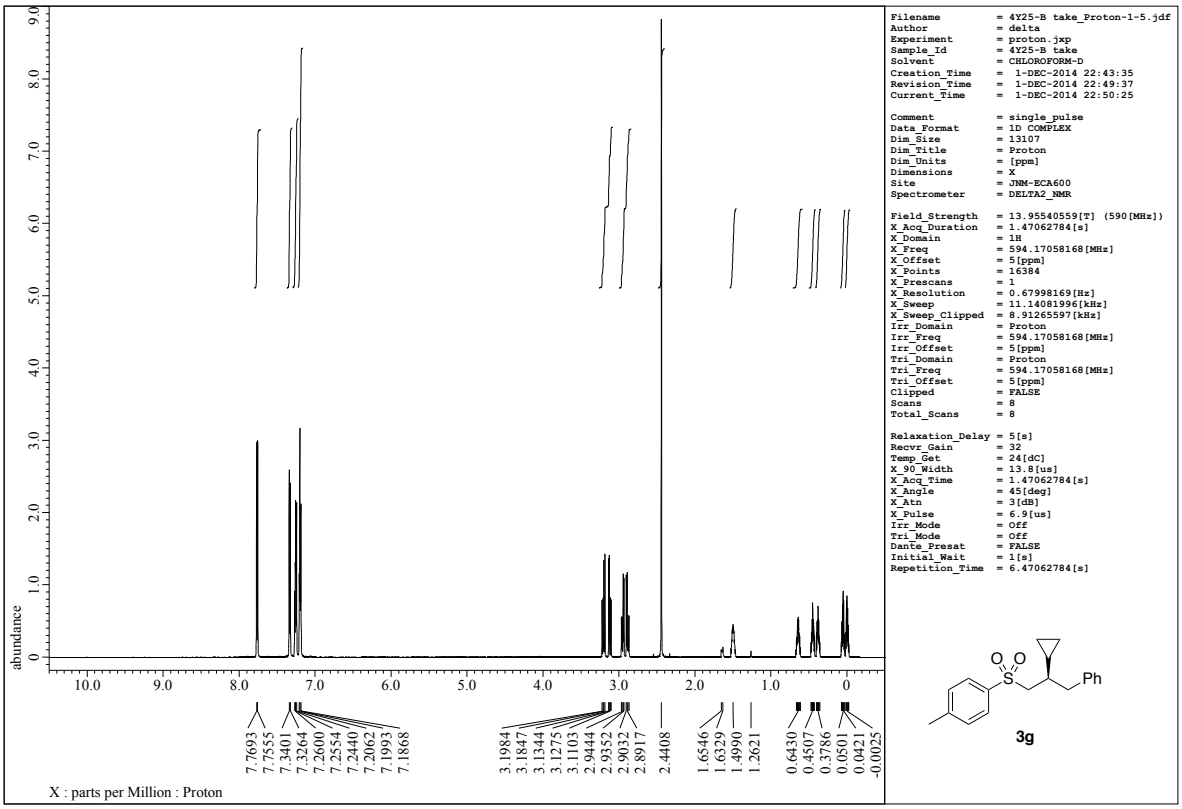
UV Results

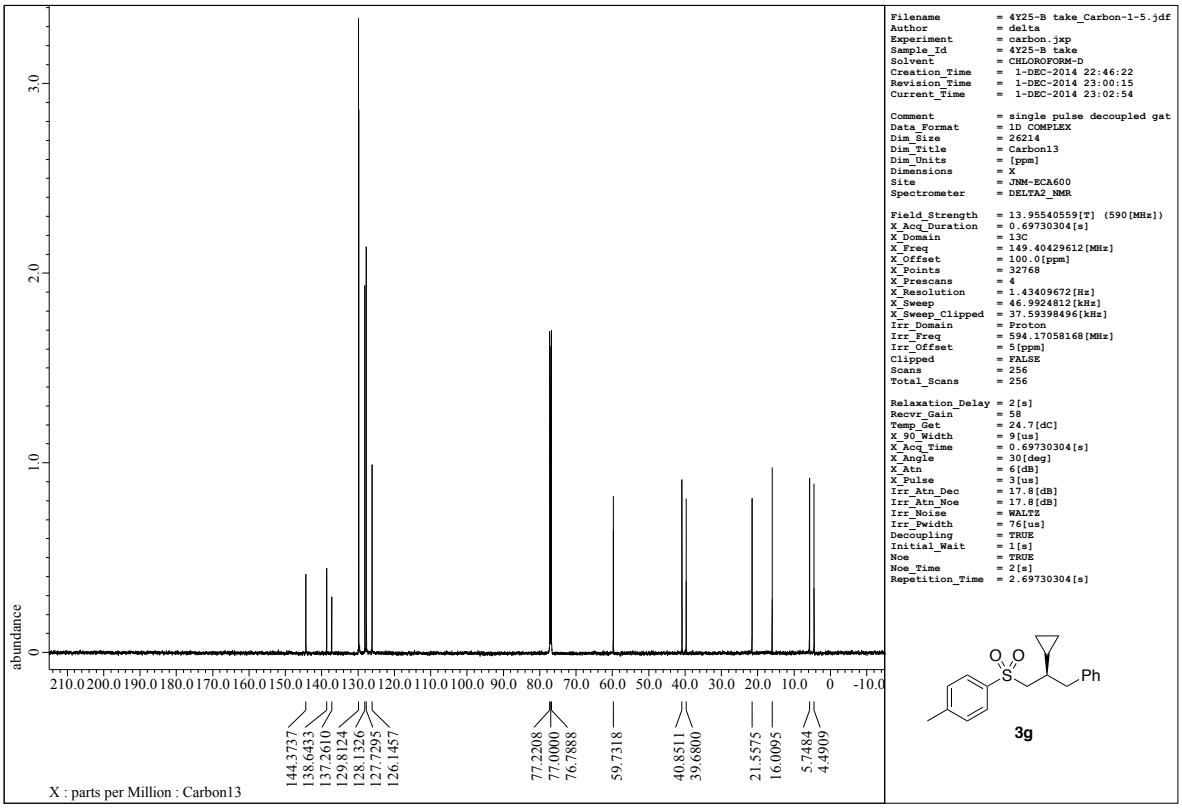
Pk #	Retention Time	Area	Area Percent	Height
1	44.101	1508893	49.149	31275
2	45.960	1561116	50.851	27145
Totals		3070009	100.000	58420

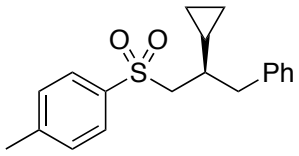


UV Results

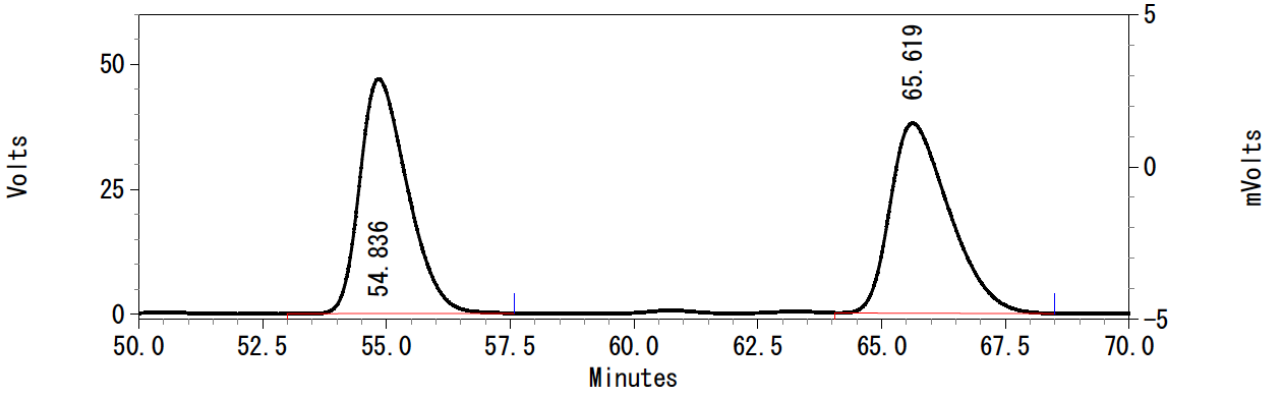
Pk #	Retention Time	Area	Area Percent	Height
1	44.054	1902192	98.335	35565
2	46.265	32209	1.665	604
Totals		1934401	100.000	36169


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.7693 7.7555 7.3401 7.3264 7.2600 7.2554 7.2440 7.2062 7.1993 7.1868
3.1984 3.1847 3.1344 3.1275 3.1103 2.9444 2.9352 2.9032 2.8917 2.4408
1.6546 1.6329 1.4990 1.2621
0.6430 0.4507 0.3786 0.0501 0.0421 -0.0025
X : parts per Million : Proton
Filename = 4Y25-B take_Proton-1-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Y25-B take
Solvent = CHLOROFORM-D
Creation_Time = 1-DEC-2014 22:43:35
Revision_Time = 1-DEC-2014 22:49:37
Current_Time = 1-DEC-2014 22:50:25
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 = 24[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O O S Ph
3g


abundance
3.0 2.0 1.0 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
144.3737 138.6433 137.2610 129.8124 128.1326 127.7295 126.1457
77.2208 77.0000 76.7888 59.7318 40.8511 39.6800 21.5575 16.0095 5.7484 4.4909
X : parts per Million : Carbon13
Filename = 4Y25-B take_Carbon-1-5.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Y25-B take
Solvent = CHLOROFORM-D
Creation_Time = 1-DEC-2014 22:46:22
Revision_Time = 1-DEC-2014 23:00:15
Current_Time = 1-DEC-2014 23:02:54
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 = 24.7[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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 O S Ph
3g

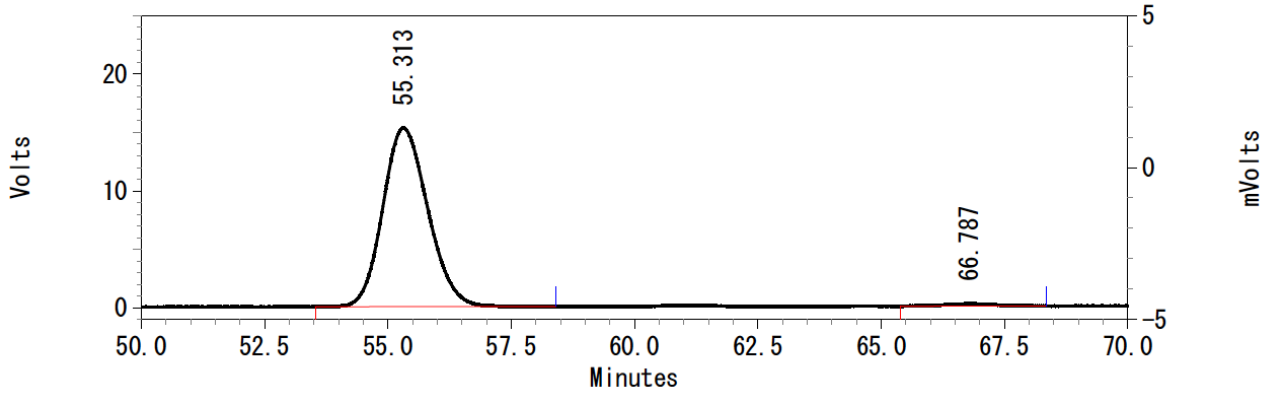


3g



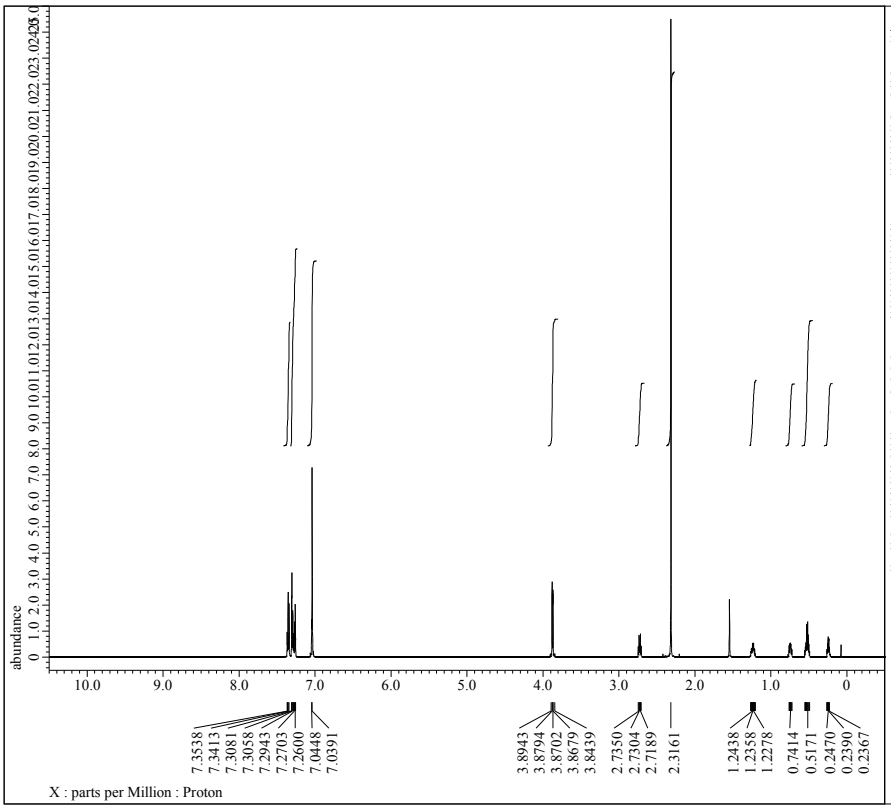
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	54.836	3136472	49.821	46923
2	65.619	3158968	50.179	37980
Totals		6295440	100.000	84903

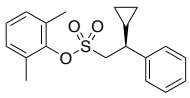


UV Results

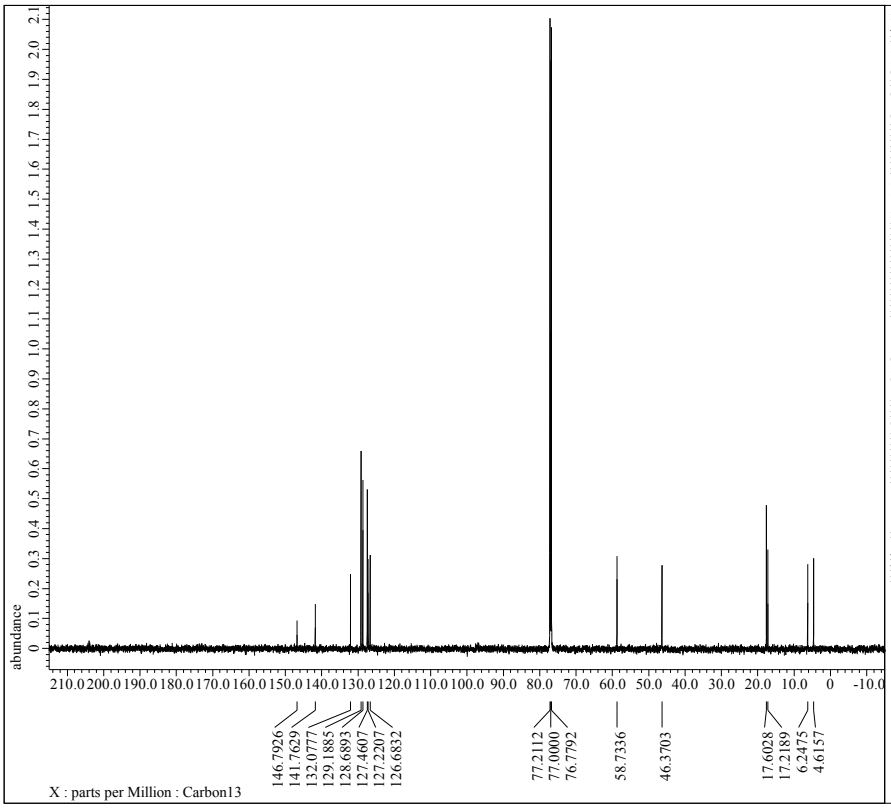
Pk #	Retention Time	Area	Area Percent	Height
1	55.313	969692	98.554	15267
2	66.787	14227	1.446	200
Totals		983919	100.000	15467



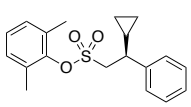

```
Filename          = 4716-B_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 4716-B
Solvent           = CHLOROFORM-D
Creation_Time     =  5-AUG-2014 01:46:24
Revision_Time     =  5-AUG-2014 01:52:43
Current_Time      =  5-AUG-2014 01:53:00

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          = 25.8[dC]
X_90_Width        = 13.8[us]
X_Acq_Time        = 1.47062784[s]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 6.9[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.47062784[s]
```



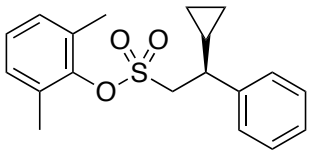
3h



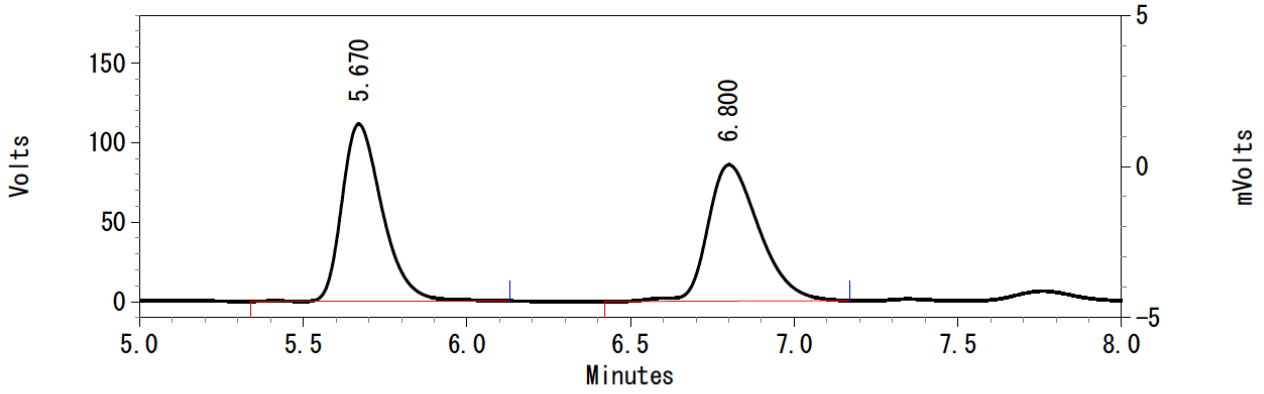

```
Filename          = 4716-B_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 4716-B
Solvent           = CHLOROFORM-D
Creation_Time     =  5-AUG-2014 01:49:10
Revision_Time     =  5-AUG-2014 02:02:27
Current_Time      =  5-AUG-2014 02:03:20

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          = 26.8[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       = 17.8[dB]
Irr_Atn_Noe       = 17.8[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]
```



3h

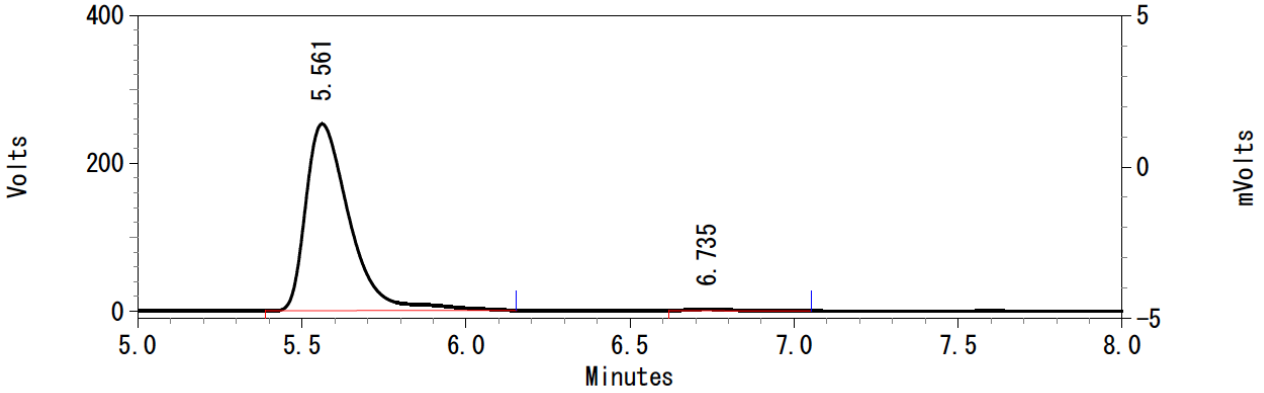


3h



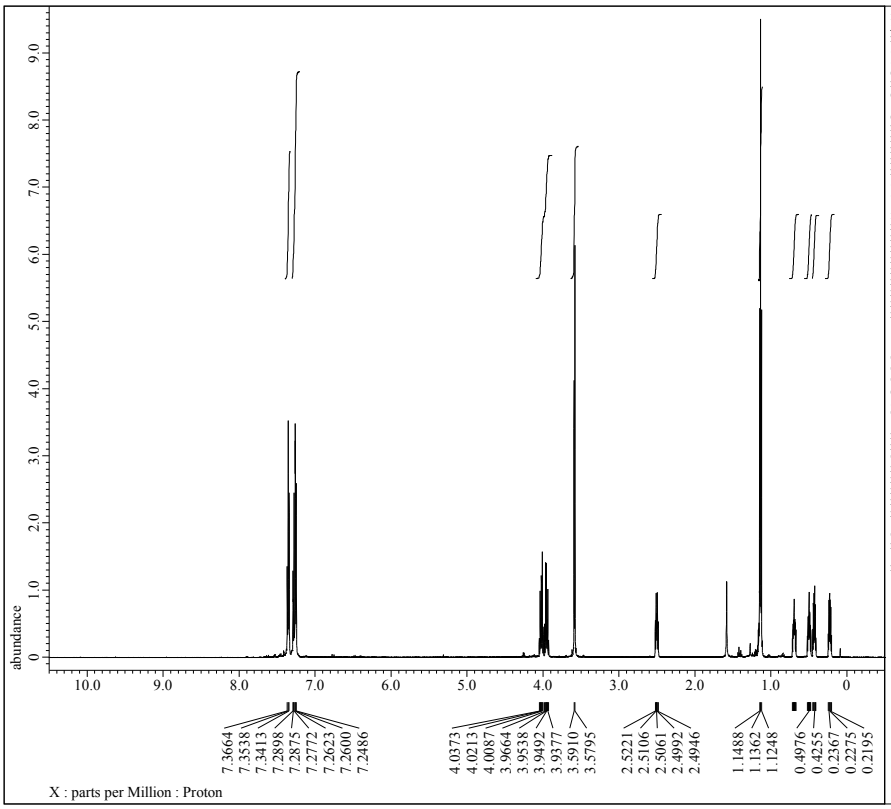
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	5.670	951693	50.486	111293
2	6.800	933379	49.514	85634
Totals		1885072	100.000	196927

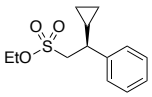


UV Results

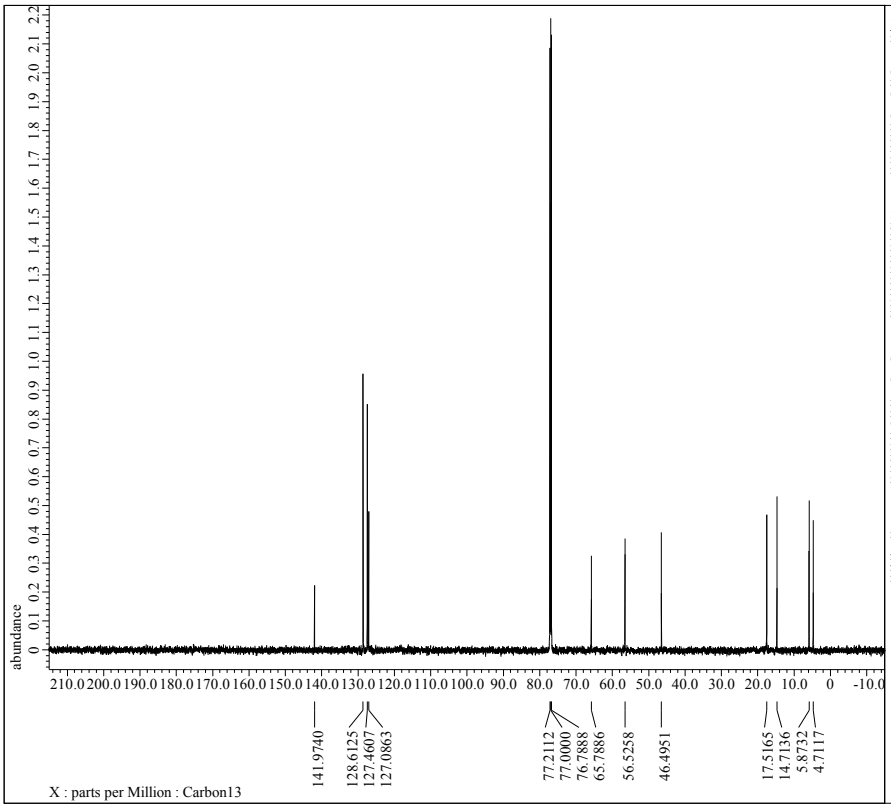
Pk #	Retention Time	Area	Area Percent	Height
1	5.561	2341857	99.115	252591
2	6.735	20909	0.885	2127
Totals		2362766	100.000	254718



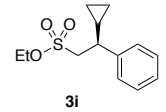

```
Filename          = 4713-A_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 4713-A
Solvent           = CHLOROFORM-D
Creation_Time     =  5-AUG-2014 02:08:14
Revision_Time     =  5-AUG-2014 02:16:01
Current_Time      =  5-AUG-2014 02:16:31

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    = 1.47062784[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          = 25.9[dC]
X_90_Width        = 13.8[us]
X_Acq_Time        = 1.47062784[s]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 6.9[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.47062784[s]
```



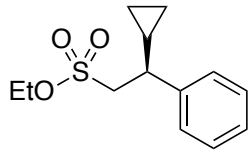
3i



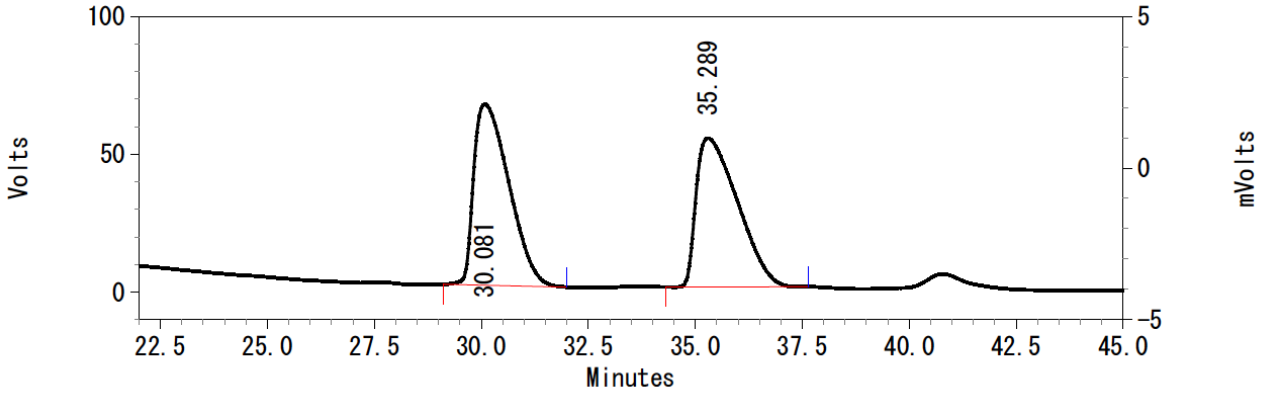

```
Filename          = 4713-A take_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 4713-A
Solvent           = CHLOROFORM-D
Creation_Time     =  5-AUG-2014 02:11:00
Revision_Time     =  5-AUG-2014 03:50:25
Current_Time      =  5-AUG-2014 03:50:39

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           = TRUE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 26.8[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       = 17.8[dB]
Irr_Atn_Noe       = 17.8[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]
```



3i

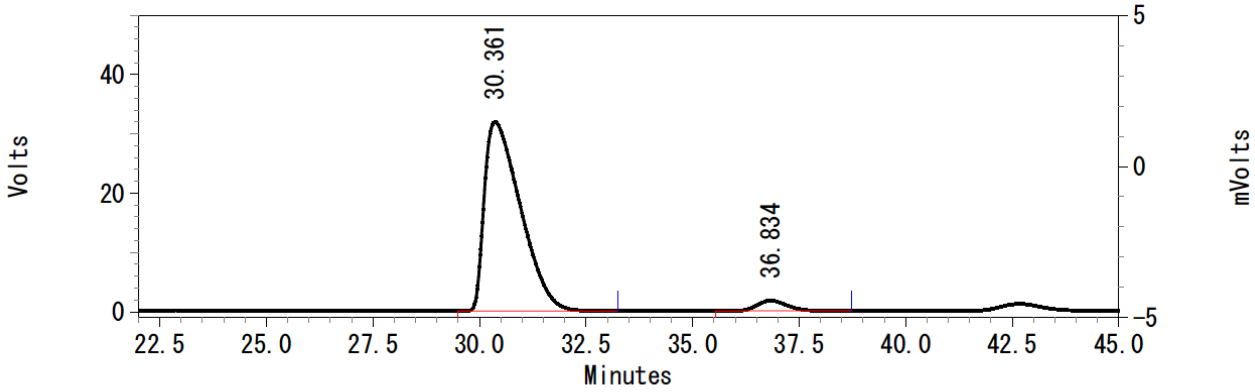


3i



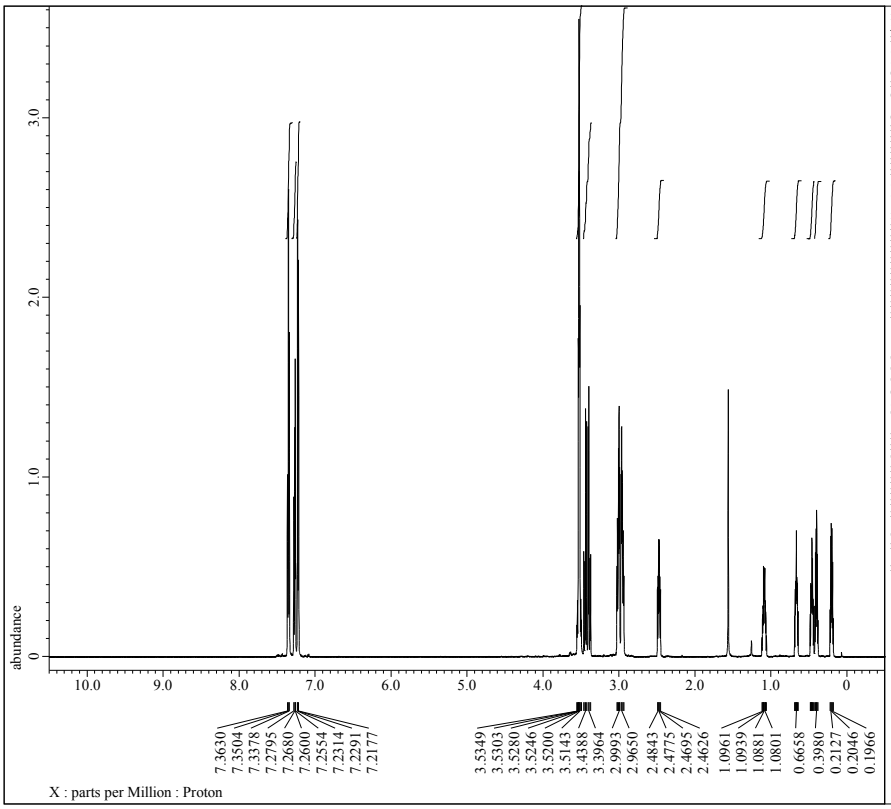
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	30.081	3763709	50.972	65737
2	35.289	3620162	49.028	53944
Totals		7383871	100.000	119681

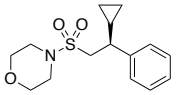


UV Results

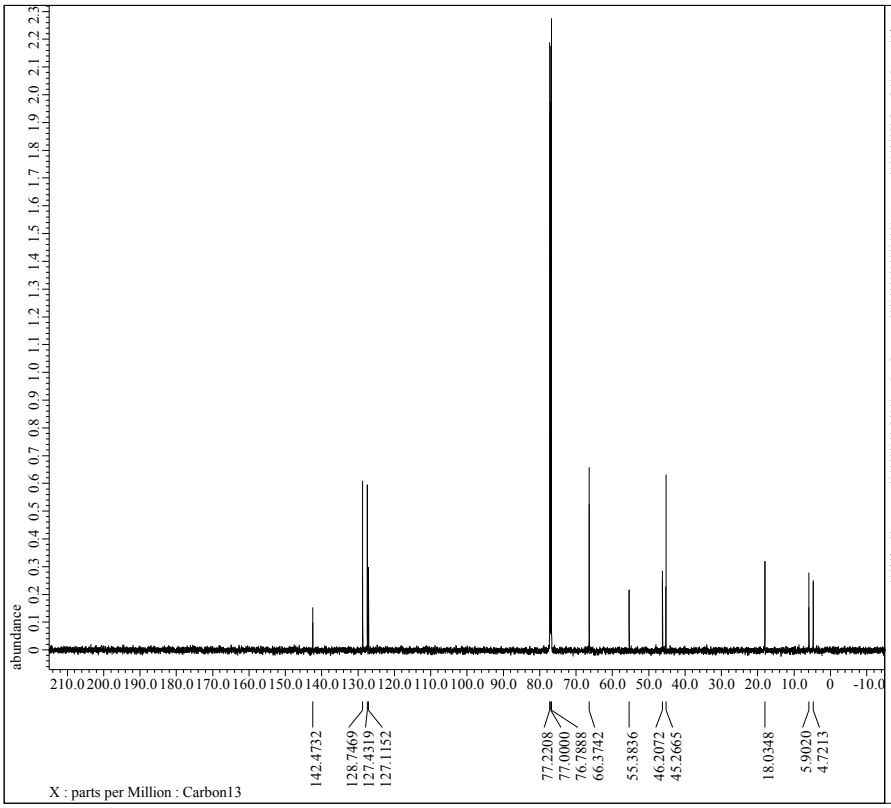
Pk #	Retention Time	Area	Area Percent	Height
1	30.361	1878149	95.755	31869
2	36.834	83256	4.245	1747
Totals		1961405	100.000	33616



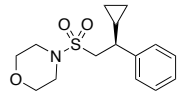

```
Filename          = 4710-C_Proton-1-8.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 4710-C
Solvent           = CHLOROFORM-D
Creation_Time     =  4-AUG-2014 23:26:23
Revision_Time     =  4-AUG-2014 23:34:52
Current_Time      =  4-AUG-2014 23:36:21

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        = 44
Temp_Get          = 25.9[dC]
X_90_Width        = 13.8[us]
X_Acq_Time        = 1.47062784[s]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 6.9[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.47062784[s]
```



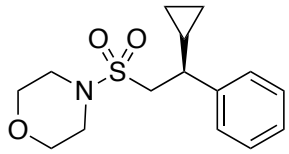
3j



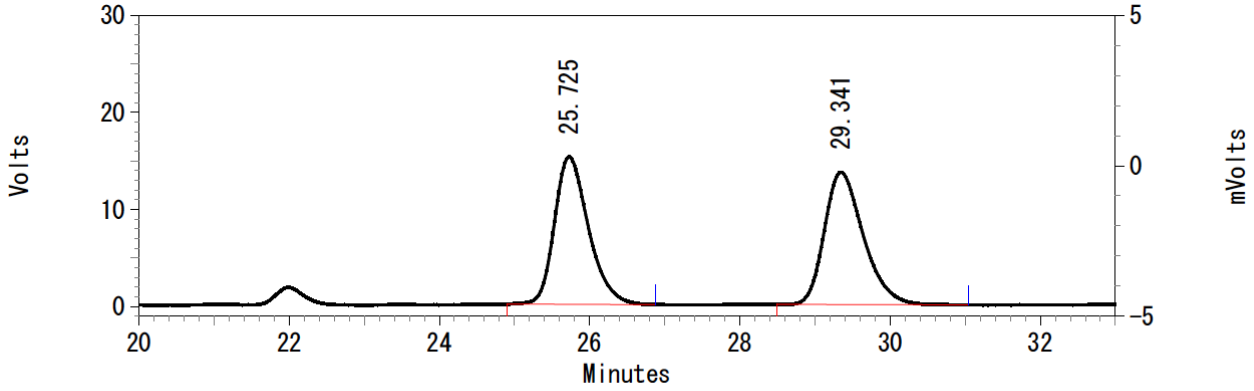

```
Filename          = 4710-C_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 4710-C
Solvent           = CHLOROFORM-D
Creation_Time     =  4-AUG-2014 23:29:08
Revision_Time     =  4-AUG-2014 23:42:28
Current_Time      =  4-AUG-2014 23:43:17

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             = 256
Total_Scans       = 256

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 26.8[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       = 17.8[dB]
Irr_Atn_Noe       = 17.8[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]
```



3j

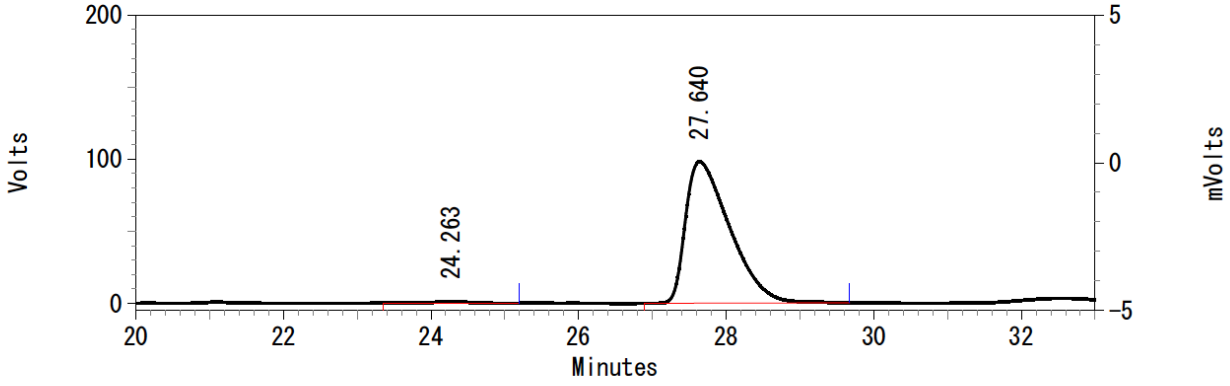


3j



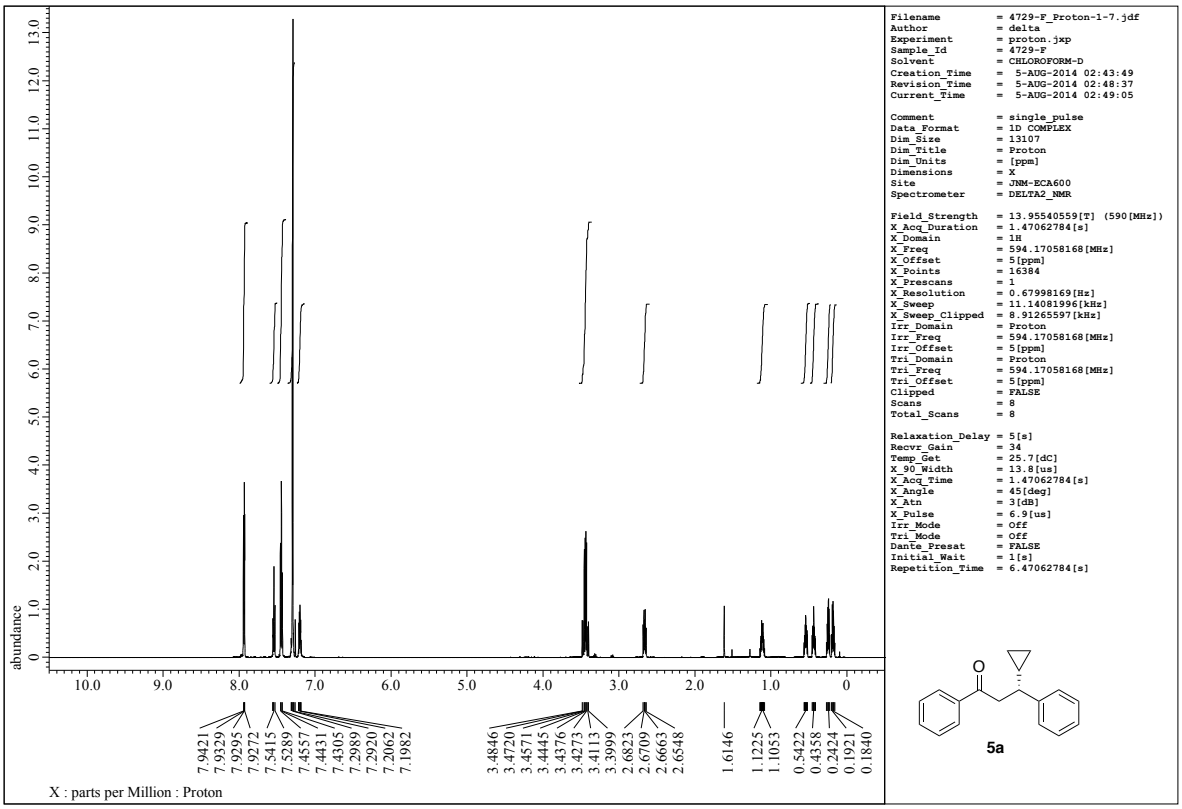
UV Results

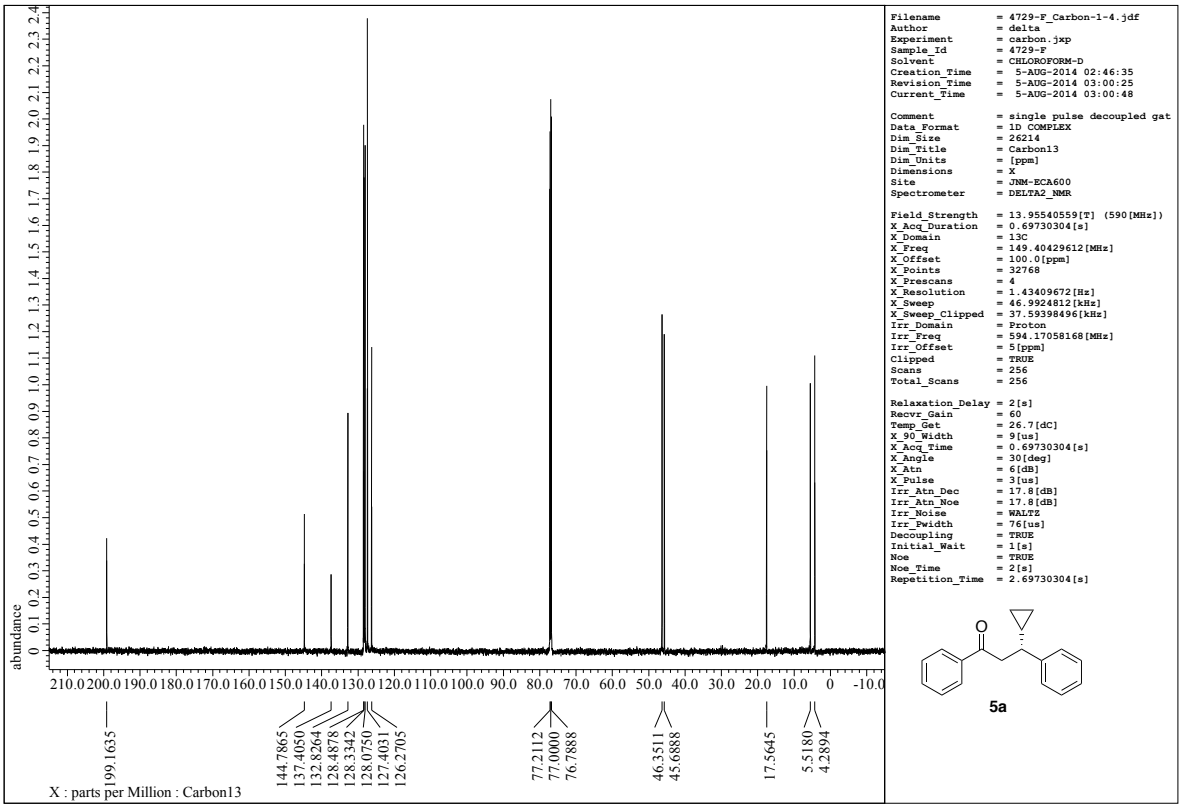
Pk #	Retention Time	Area	Area Percent	Height
1	25.725	478815	49.377	15194
2	29.341	490890	50.623	13622
Totals		969705	100.000	28816

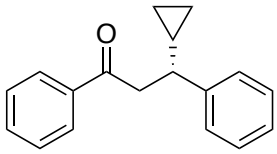


UV Results

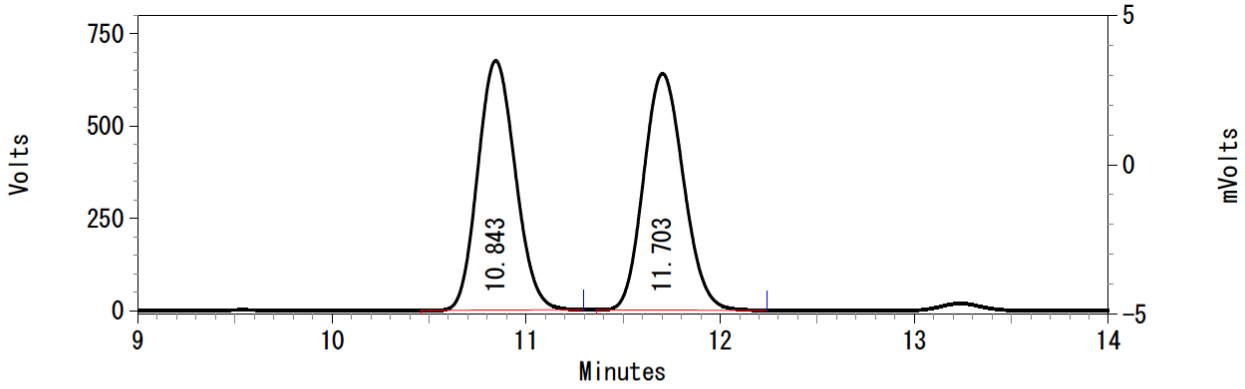
Pk #	Retention Time	Area	Area Percent	Height
1	24.263	39416	0.953	1275
2	27.640	4095299	99.047	98172
Totals		4134715	100.000	99447


abundance
X : parts per Million : Proton
7.9421
7.9329
7.9295
7.9272
7.5415
7.5289
7.4557
7.4431
7.4305
7.2989
7.2920
7.2062
7.1982
3.4846
3.4720
3.4571
3.4445
3.4376
3.4273
3.4113
3.3999
2.6823
2.6709
2.6663
2.6548
1.6146
1.1225
1.1053
0.5422
0.4358
0.2424
0.1921
0.1840
Filename = 4729-F_Proton-1-7.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4729-F
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 02:43:49
Revision_Time = 5-AUG-2014 02:48:37
Current_Time = 5-AUG-2014 02:49:05
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 = 34
Temp_Get = 25.7[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O
5a


abundance
X : parts per Million : Carbon13
199.1635
144.7865
137.4050
132.8264
128.4878
128.3342
128.0750
127.4031
126.2705
77.2112
77.0000
76.7888
46.3511
45.6888
17.5645
5.5180
4.2894
Filename = 4729-F_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4729-F
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 02:46:35
Revision_Time = 5-AUG-2014 03:00:25
Current_Time = 5-AUG-2014 03:00:48
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 = 26.7[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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
5a

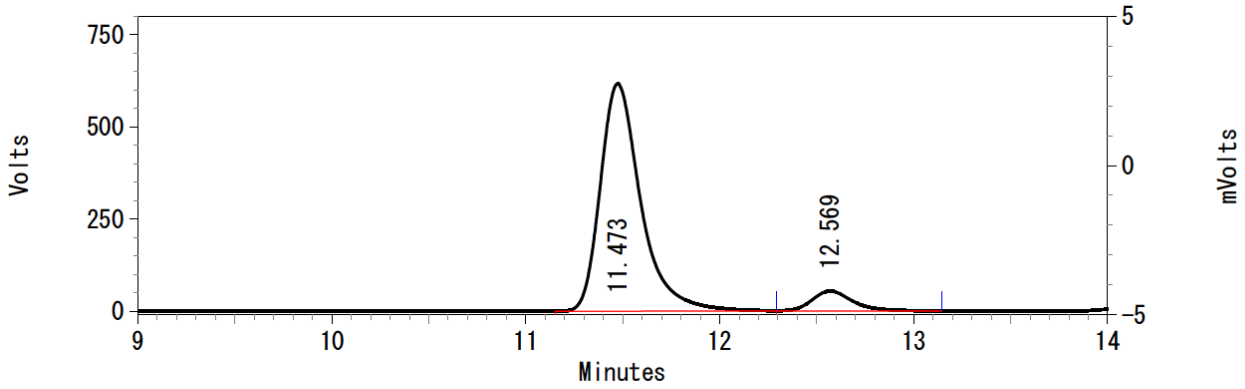


5a



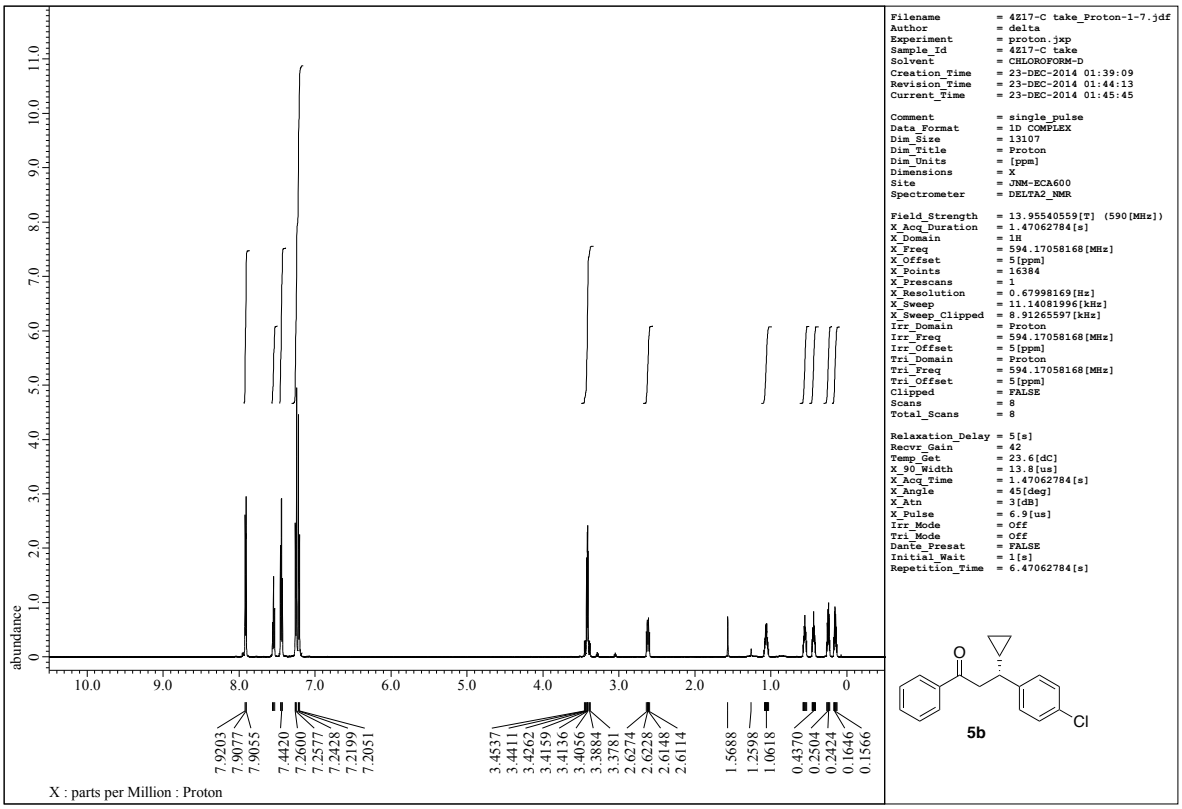
UV Results

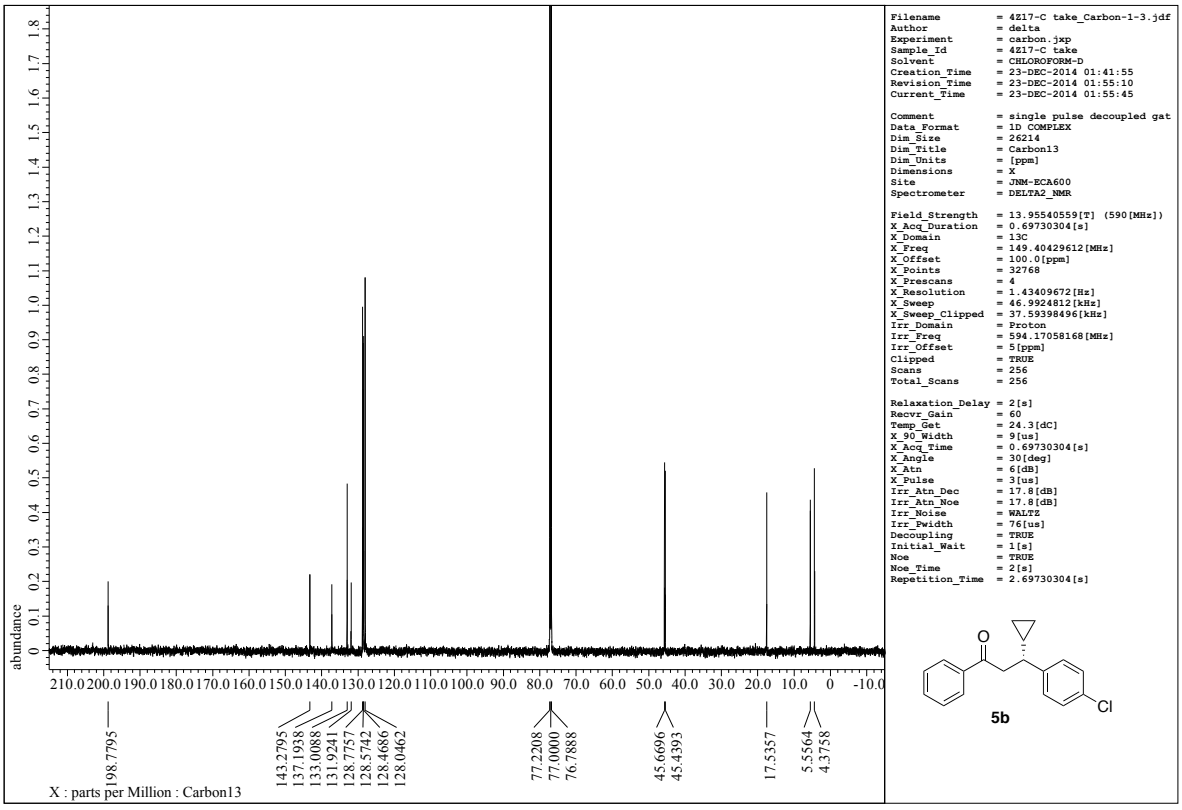
Pk #	Retention Time	Area	Area Percent	Height
1	10.843	9056769	49.768	674647
2	11.703	9141098	50.232	640237
Totals		18197867	100.000	1314884

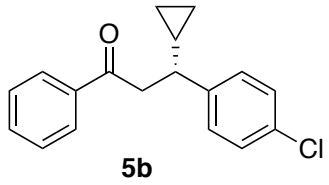


UV Results

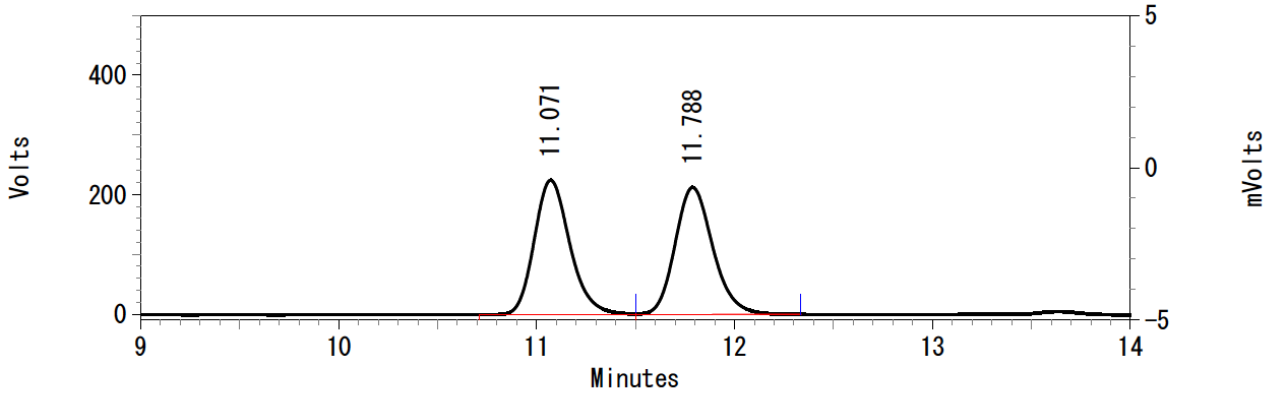
Pk #	Retention Time	Area	Area Percent	Height
1	11.473	8946687	91.871	616346
2	12.569	791587	8.129	53970
Totals		9738274	100.000	670316


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.9203 7.9077 7.9055 7.4420 7.2600 7.2577 7.2428 7.2199 7.2051
3.4537 3.4411 3.4262 3.4159 3.4136 3.4056 3.3884 3.3781
2.6274 2.6228 2.6148 2.6114
1.5688 1.2598 1.0618
0.4370 0.2504 0.2424 0.1646 0.1566
X : parts per Million : Proton
Filename = 4Z17-C take_Proton-1-7.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Z17-C take
Solvent = CHLOROFORM-D
Creation_Time = 23-DEC-2014 01:39:09
Revision_Time = 23-DEC-2014 01:44:13
Current_Time = 23-DEC-2014 01:45:45
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 = 23.6[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O
Cl
5b


abundance
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
198.7795
143.2795 137.1938 133.0088 131.9241 128.7757 128.5742 128.4686 128.0462
77.2208 77.0000 76.7888
45.6696 45.4393
17.5357
5.5564 4.3758
X : parts per Million : Carbon13
Filename = 4Z17-C take_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Z17-C take
Solvent = CHLOROFORM-D
Creation_Time = 23-DEC-2014 01:41:55
Revision_Time = 23-DEC-2014 01:55:10
Current_Time = 23-DEC-2014 01:55:45
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 = 24.3[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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
Cl
5b

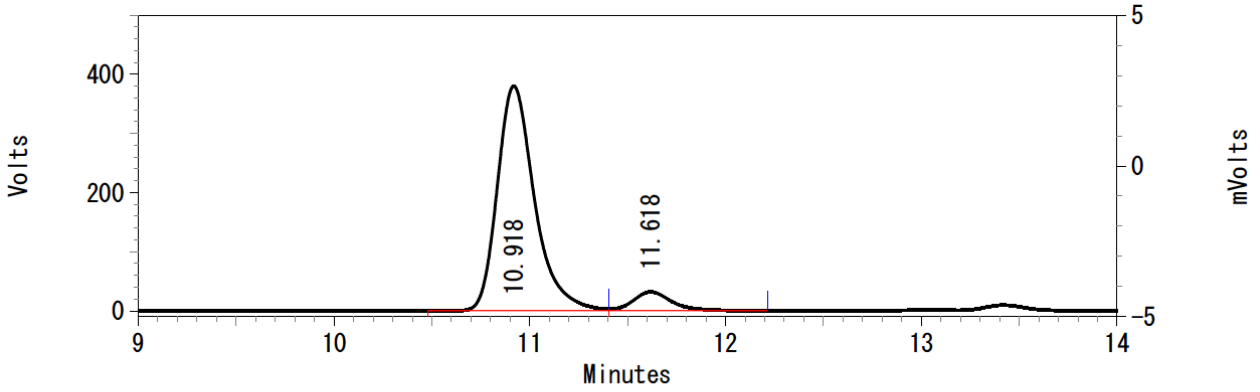


5b



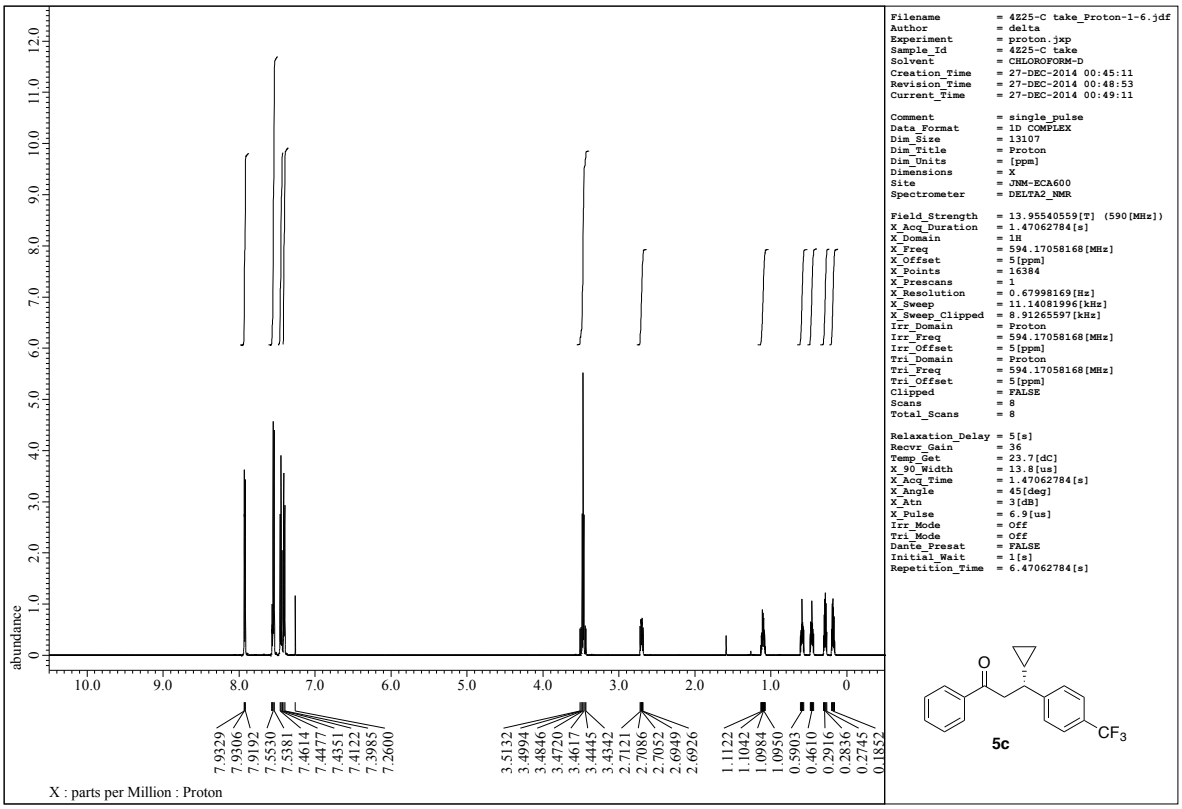
UV Results

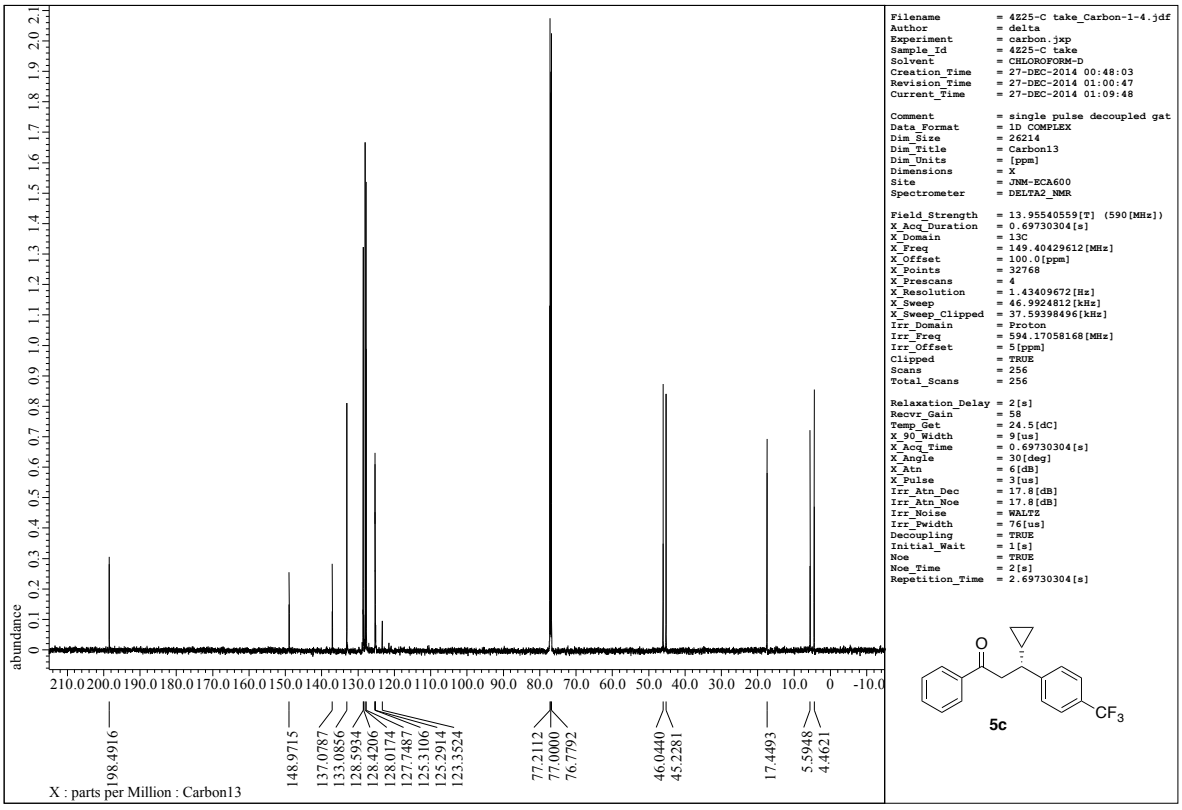
Pk #	Retention Time	Area	Area Percent	Height
1	11.071	2820373	49.895	224898
2	11.788	2832201	50.105	212748
Totals		5652574	100.000	437646

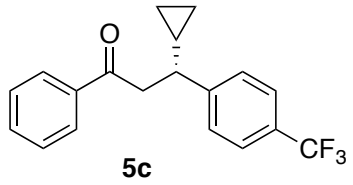


UV Results

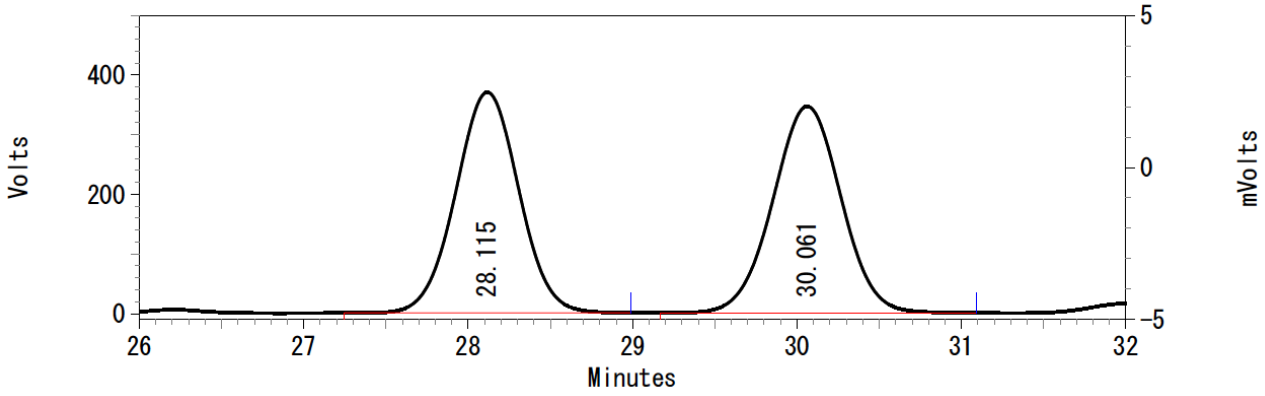
Pk #	Retention Time	Area	Area Percent	Height
1	10.918	5016013	92.195	380070
2	11.618	424646	7.805	31645
Totals		5440659	100.000	411715


abundance
X : parts per Million : Proton
7.9329
7.9306
7.9192
7.5530
7.5381
7.4614
7.4477
7.4351
7.4122
7.3985
7.2600
3.5132
3.4994
3.4846
3.4720
3.4617
3.4445
3.4342
2.7121
2.7086
2.7052
2.6949
2.6926
1.1122
1.1042
1.0984
1.0950
0.5903
0.4610
0.2916
0.2836
0.2745
0.1852
Filename = 4Z25-C take_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Z25-C take
Solvent = CHLOROFORM-D
Creation_Time = 27-DEC-2014 00:45:11
Revision_Time = 27-DEC-2014 00:48:53
Current_Time = 27-DEC-2014 00:49:11
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 = 23.7[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O
CF3
5c


abundance
X : parts per Million : Carbon13
198.4916
148.9715
137.0787
133.0856
128.5934
128.4206
128.0174
127.7487
125.3106
125.2914
123.3524
77.2112
77.0000
76.7792
46.0440
45.2281
17.4493
5.5948
4.4621
Filename = 4Z25-C take_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Z25-C take
Solvent = CHLOROFORM-D
Creation_Time = 27-DEC-2014 00:48:03
Revision_Time = 27-DEC-2014 01:00:47
Current_Time = 27-DEC-2014 01:09:48
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 = 24.5[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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
CF3
5c

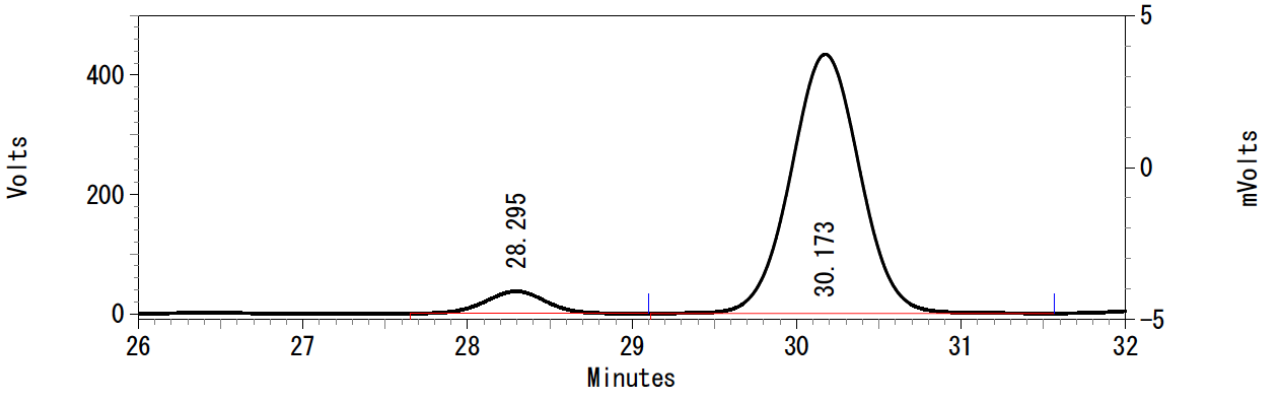


5c



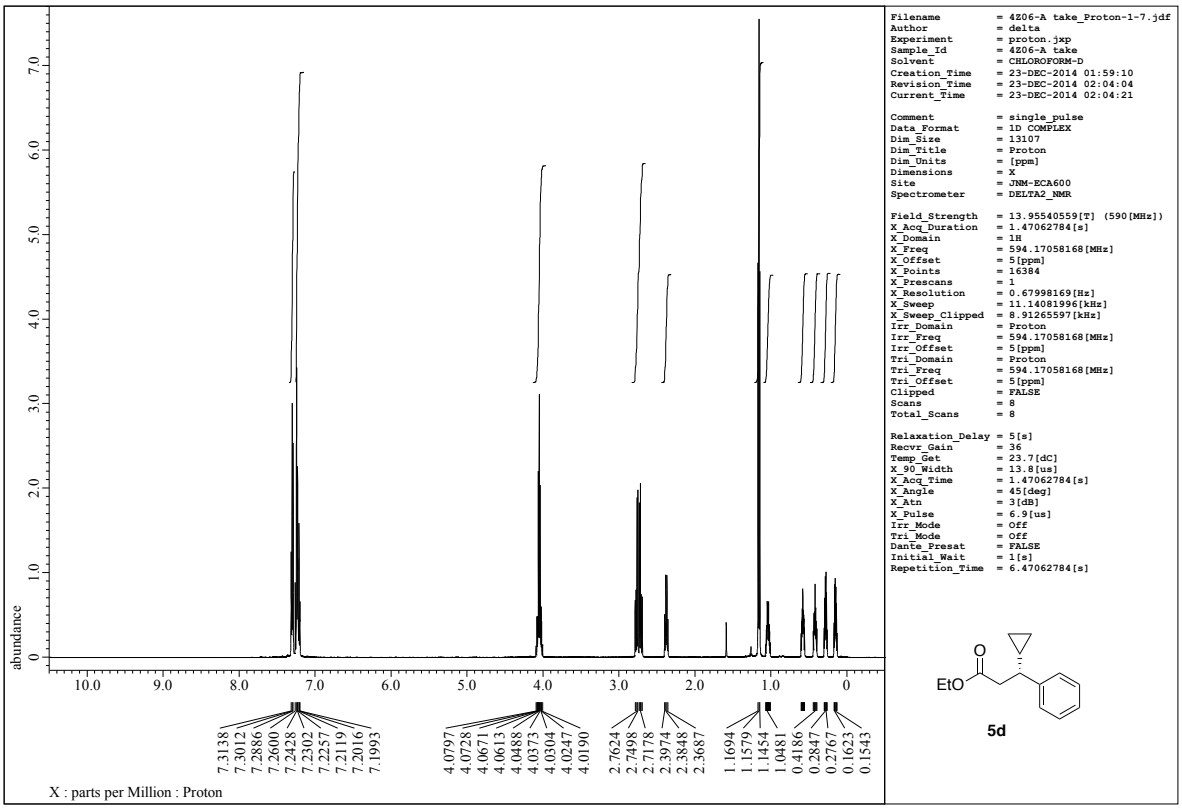
UV-970 Results

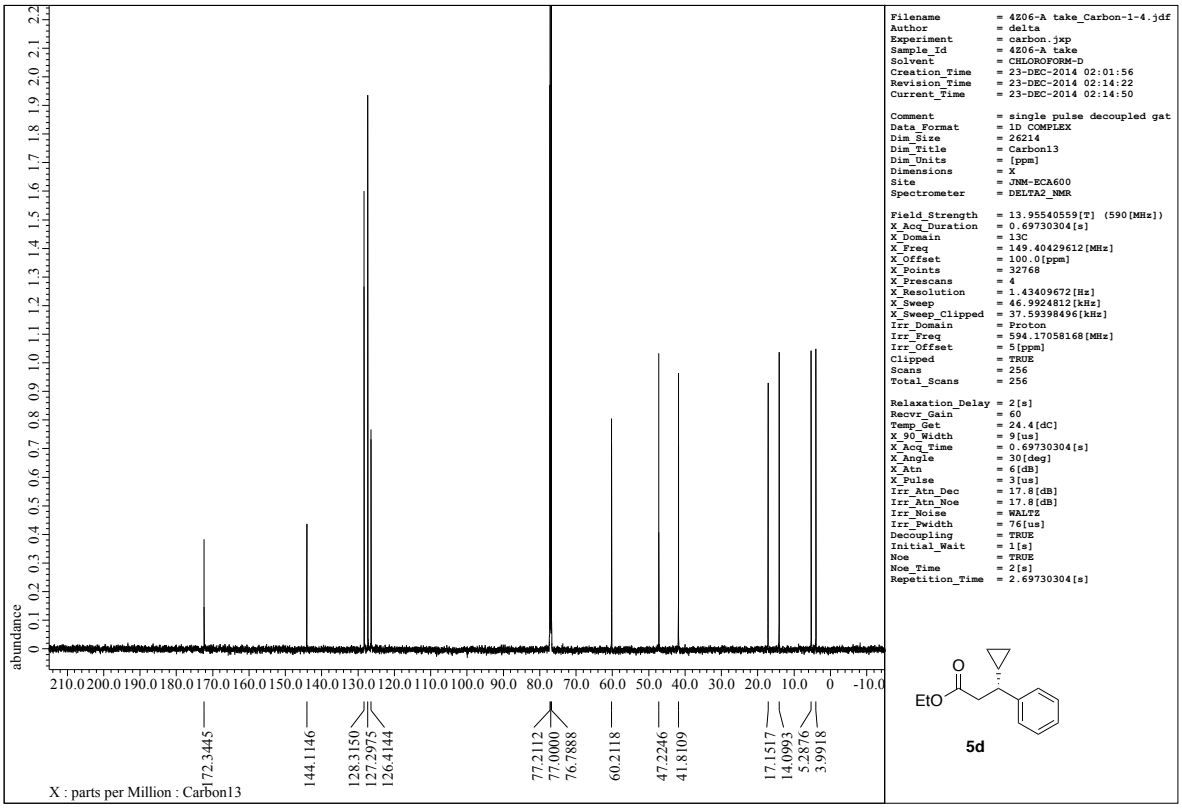
Pk #	Retention Time	Area	Area Percent	Height
1	28.115	9913308	49.701	369947
2	30.061	10032413	50.299	346556
Totals		19945721	100.000	716503

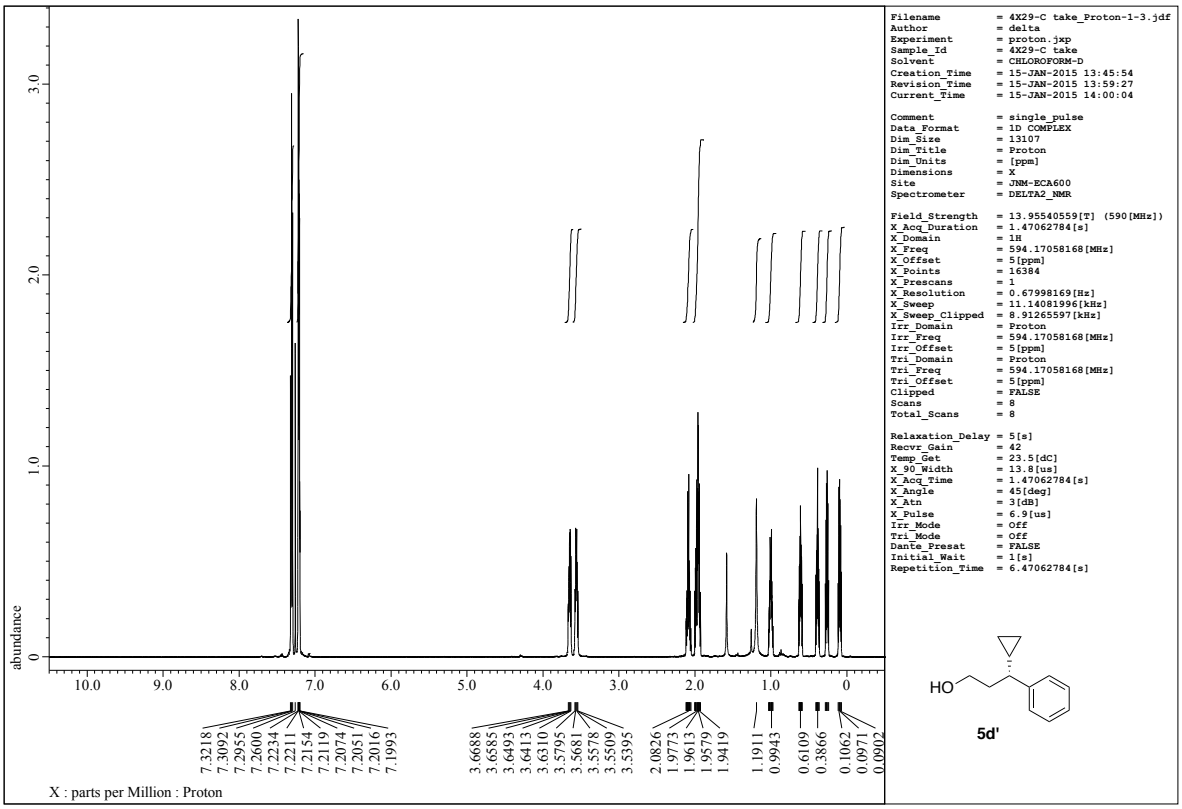


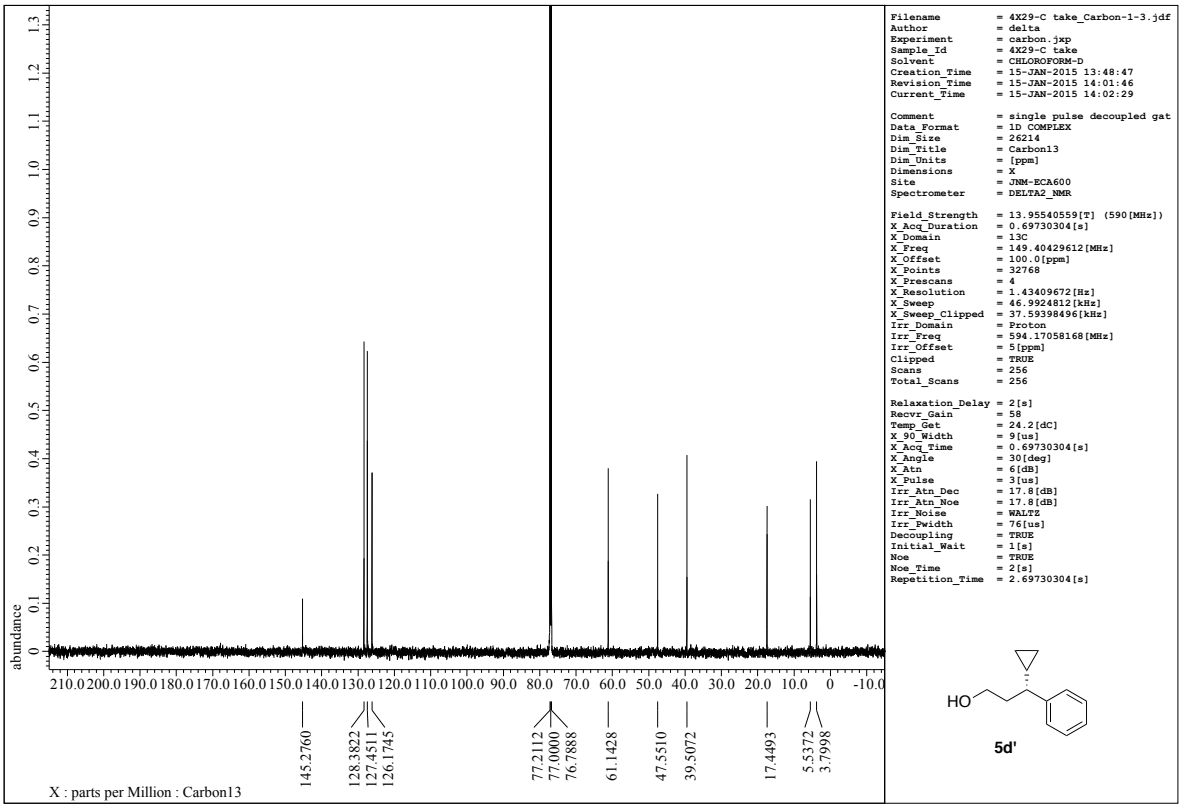
UV-970 Results

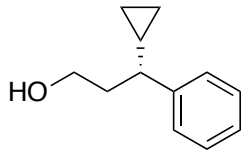
Pk #	Retention Time	Area	Area Percent	Height
1	28.295	948816	6.968	37132
2	30.173	12667533	93.032	434530
Totals		13616349	100.000	471662


abundance
X : parts per Million : Proton
7.3138
7.3012
7.2886
7.2600
7.2428
7.2302
7.2257
7.2119
7.2016
7.1993
4.0797
4.0728
4.0671
4.0613
4.0488
4.0373
4.0304
4.0247
4.0190
2.7624
2.7498
2.7178
2.3974
2.3848
2.3687
1.1694
1.1579
1.1454
1.1481
0.4186
0.2847
0.2767
0.1623
0.1543
Filename = 4Z06-A take_Proton-1-7.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Z06-A take
Solvent = CHLOROFORM-D
Creation_Time = 23-DEC-2014 01:59:10
Revision_Time = 23-DEC-2014 02:04:04
Current_Time = 23-DEC-2014 02:04:21
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 = 36
Temp_Get = 23.7[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
EtO
O
5d

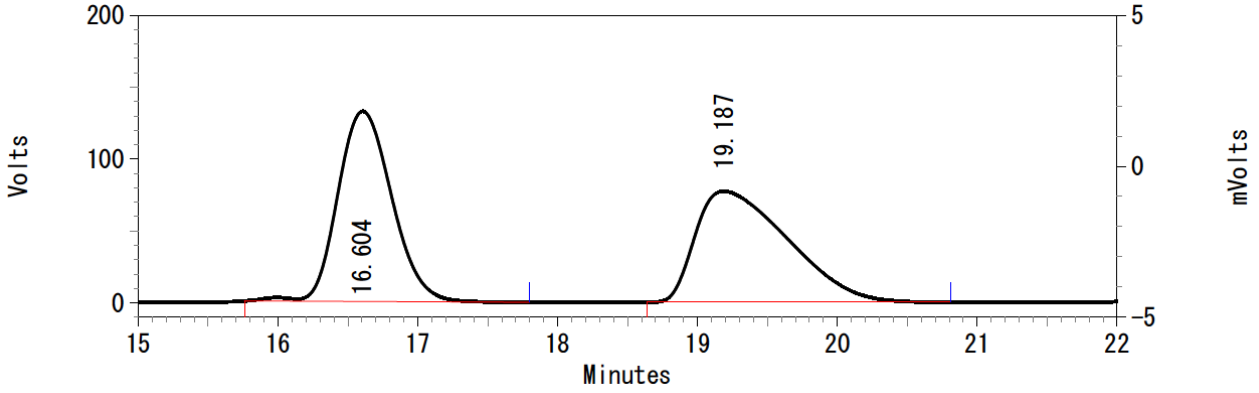

abundance
X : parts per Million : Carbon13
172.3445
144.1146
128.3150
127.2975
126.4144
77.2112
77.0000
76.7888
60.2118
47.2246
41.8109
17.1517
14.0993
5.2876
3.9918
Filename = 4Z06-A take_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Z06-A take
Solvent = CHLOROFORM-D
Creation_Time = 23-DEC-2014 02:01:56
Revision_Time = 23-DEC-2014 02:14:22
Current_Time = 23-DEC-2014 02:14:50
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 = TRUE
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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
EtO
O
5d


abundance
X : parts per Million : Proton
7.3218
7.3092
7.2955
7.2600
7.2234
7.2211
7.2154
7.2119
7.2074
7.2051
7.2016
7.1993
3.6688
3.6585
3.6493
3.6413
3.6310
3.5795
3.5681
3.5578
3.5509
3.5395
2.0826
1.9773
1.9613
1.9579
1.9419
1.1911
0.9943
0.6109
0.3866
0.1062
0.0971
0.0902
Filename = 4X29-C take_Proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4X29-C take
Solvent = CHLOROFORM-D
Creation_Time = 15-JAN-2015 13:45:54
Revision_Time = 15-JAN-2015 13:59:27
Current_Time = 15-JAN-2015 14:00:04
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 = 23.5[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
HO
5d'


abundance
X : parts per Million : Carbon13
145.2760
128.3822
127.4511
126.1745
77.2112
77.0000
76.7888
61.1428
47.5510
39.5072
17.4493
5.5372
3.7998
Filename = 4X29-C take_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4X29-C take
Solvent = CHLOROFORM-D
Creation_Time = 15-JAN-2015 13:48:47
Revision_Time = 15-JAN-2015 14:01:46
Current_Time = 15-JAN-2015 14:02:29
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 = 24.2[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
HO
5d'

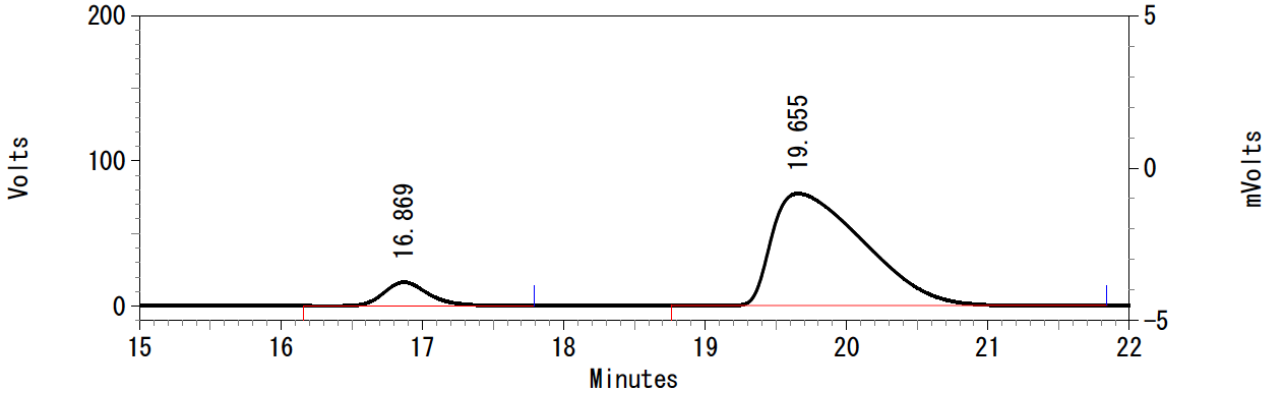


5d'



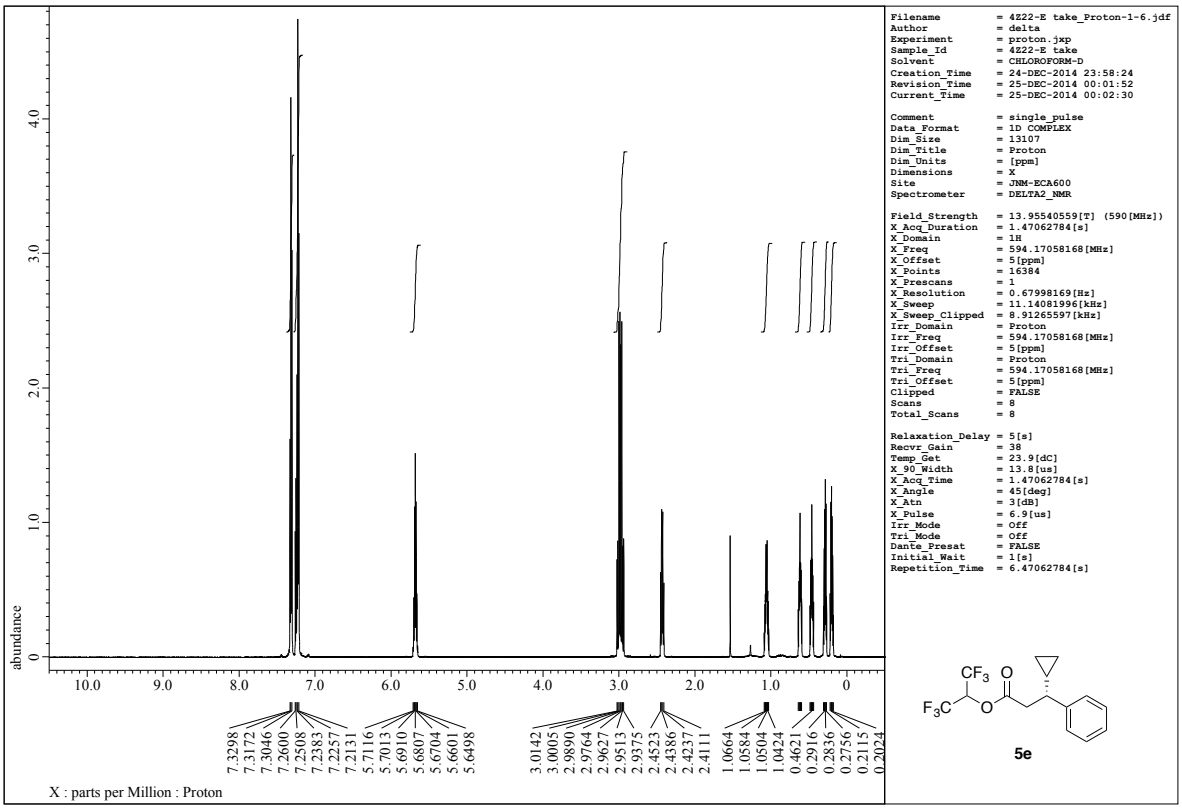
UV Results

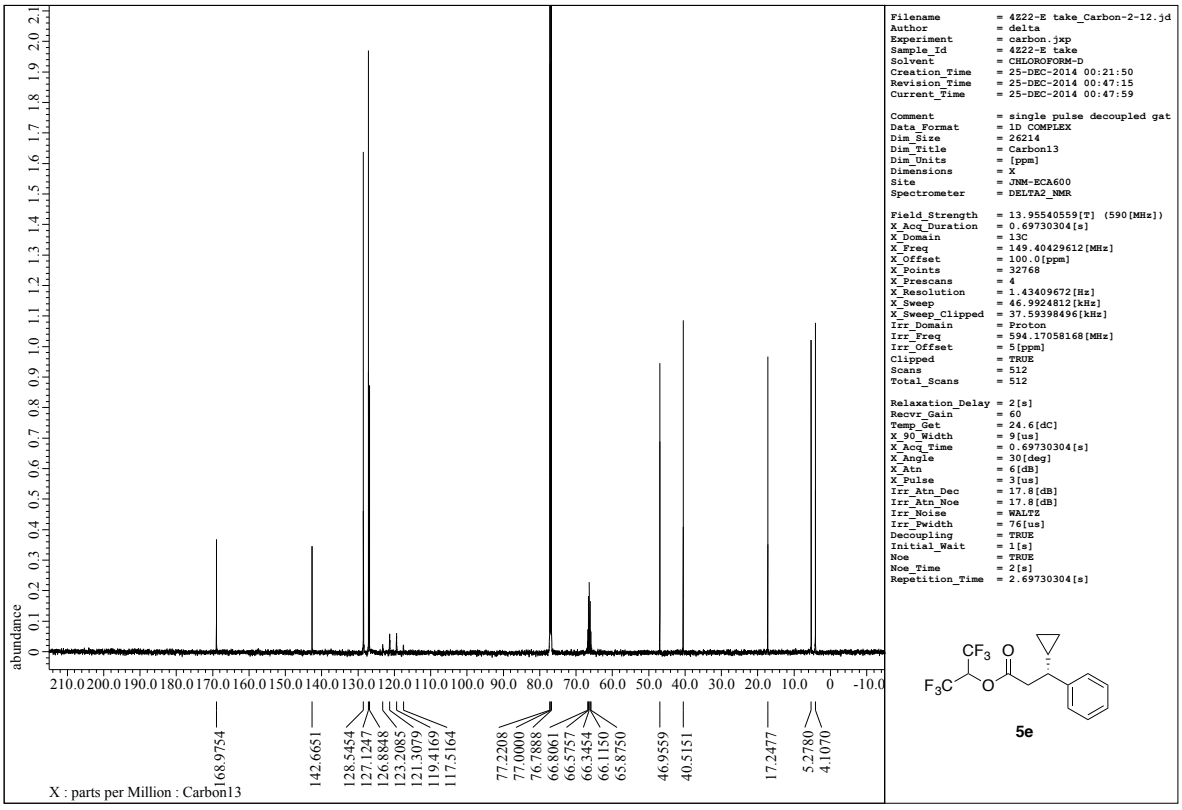
Pk #	Retention Time	Area	Area Percent	Height
1	16.604	3561444	50.076	132323
2	19.187	3550663	49.924	77258
Totals		7112107	100.000	209581

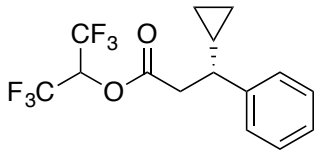


UV Results

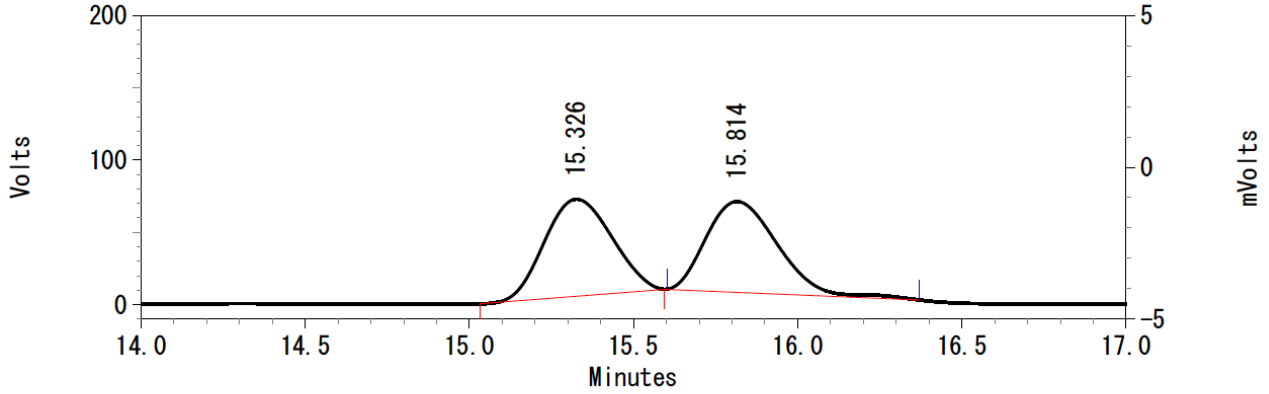
Pk #	Retention Time	Area	Area Percent	Height
1	16.869	356839	9.361	16247
2	19.655	3455289	90.639	77032
Totals		3812128	100.000	93279


abundance
X : parts per Million : Proton
7.3298
7.3172
7.3046
7.2600
7.2508
7.2383
7.2257
7.2131
5.7116
5.7013
5.6910
5.6807
5.6704
5.6601
5.6498
3.0142
3.0005
2.9890
2.9764
2.9627
2.9513
2.9375
2.4523
2.4386
2.4237
2.4111
1.0664
1.0584
1.0504
1.0424
0.4621
0.2916
0.2836
0.2756
0.2115
0.2024
Filename = 4Z22-E take_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Z22-E take
Solvent = CHLOROFORM-D
Creation_Time = 24-DEC-2014 23:58:24
Revision_Time = 25-DEC-2014 00:01:52
Current_Time = 25-DEC-2014 00:02:30
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 = 23.9[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
5e


abundance
X : parts per Million : Carbon13
168.9754
142.6651
128.5454
127.1247
126.8848
123.2085
121.3079
119.4169
117.5164
77.2208
77.0000
76.7888
66.8061
66.5757
66.3454
66.1150
65.8750
46.9559
40.5151
17.2477
5.2780
4.1070
Filename = 4Z22-E take_Carbon-2-12.jd
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Z22-E take
Solvent = CHLOROFORM-D
Creation_Time = 25-DEC-2014 00:21:50
Revision_Time = 25-DEC-2014 00:47:15
Current_Time = 25-DEC-2014 00:47:59
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 = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.6[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
5e

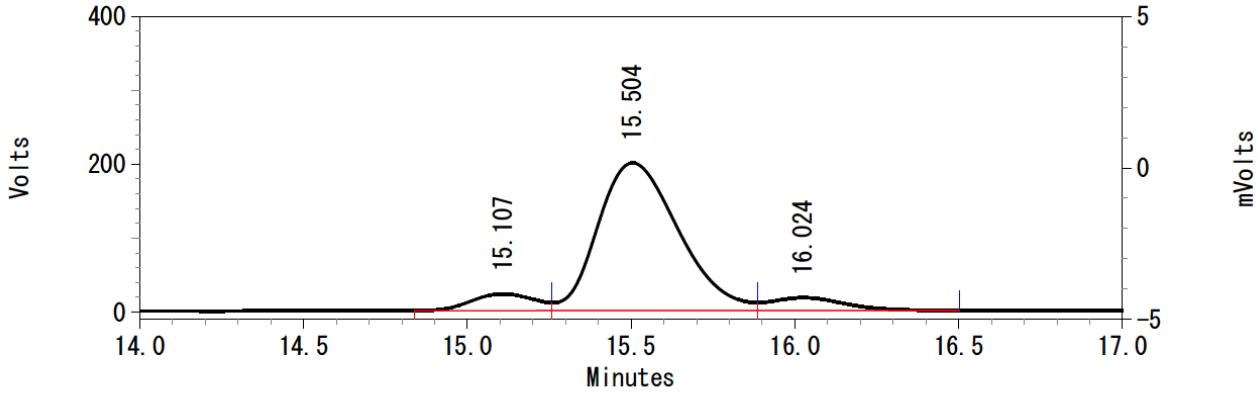


5e



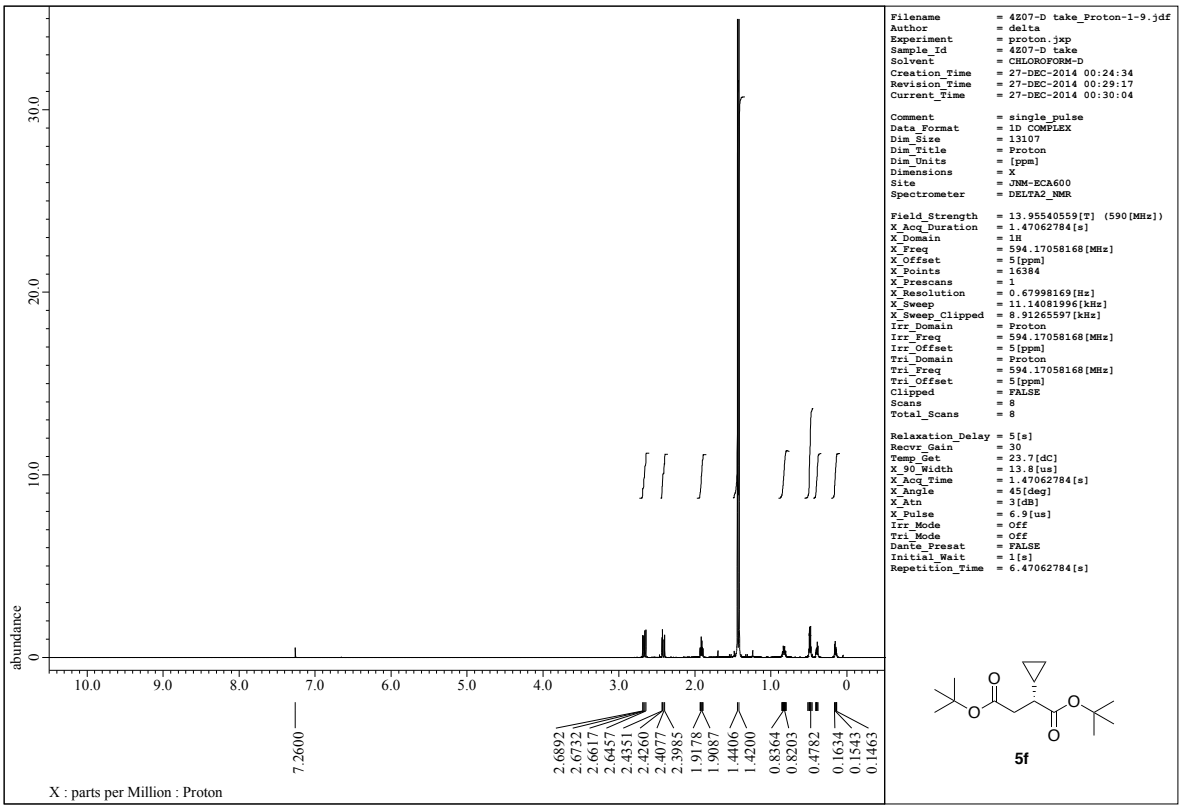
UV Results

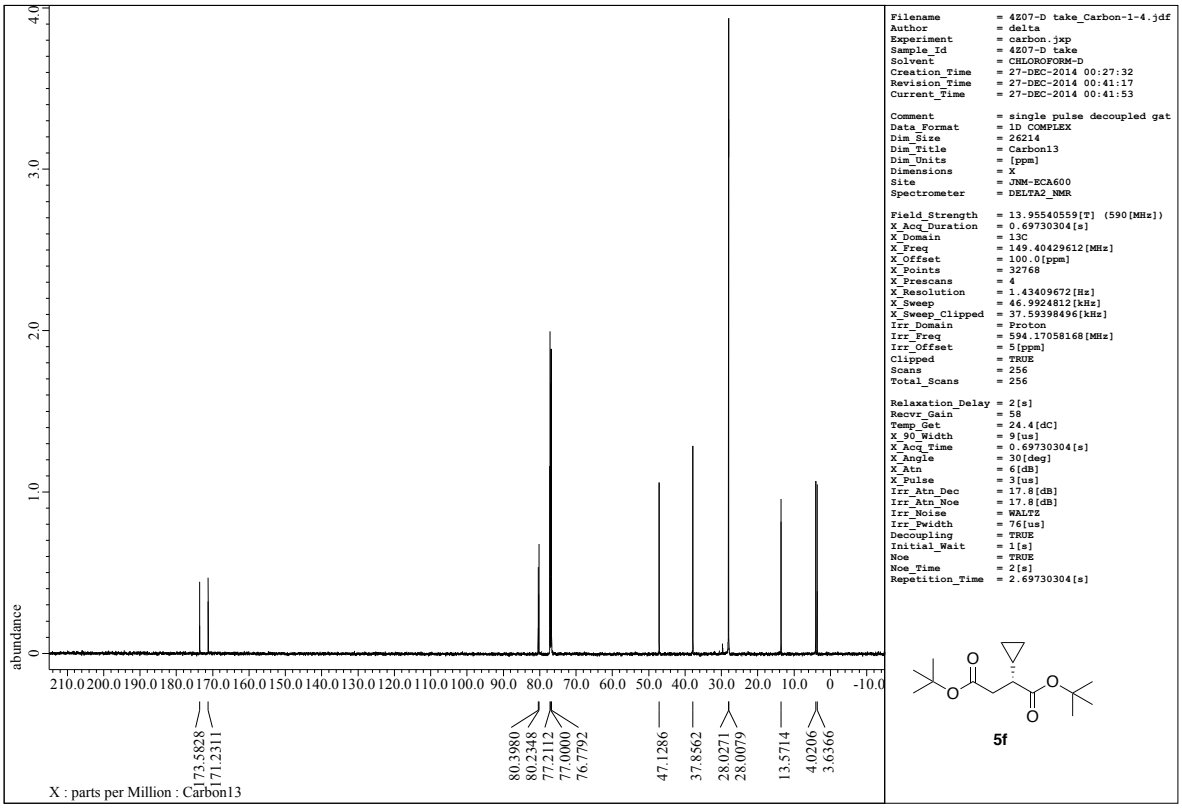
Pk #	Retention Time	Area	Area Percent	Height
1	15.326	957453	50.111	67105
2	15.814	953212	49.889	62816
Totals		1910665	100.000	129921

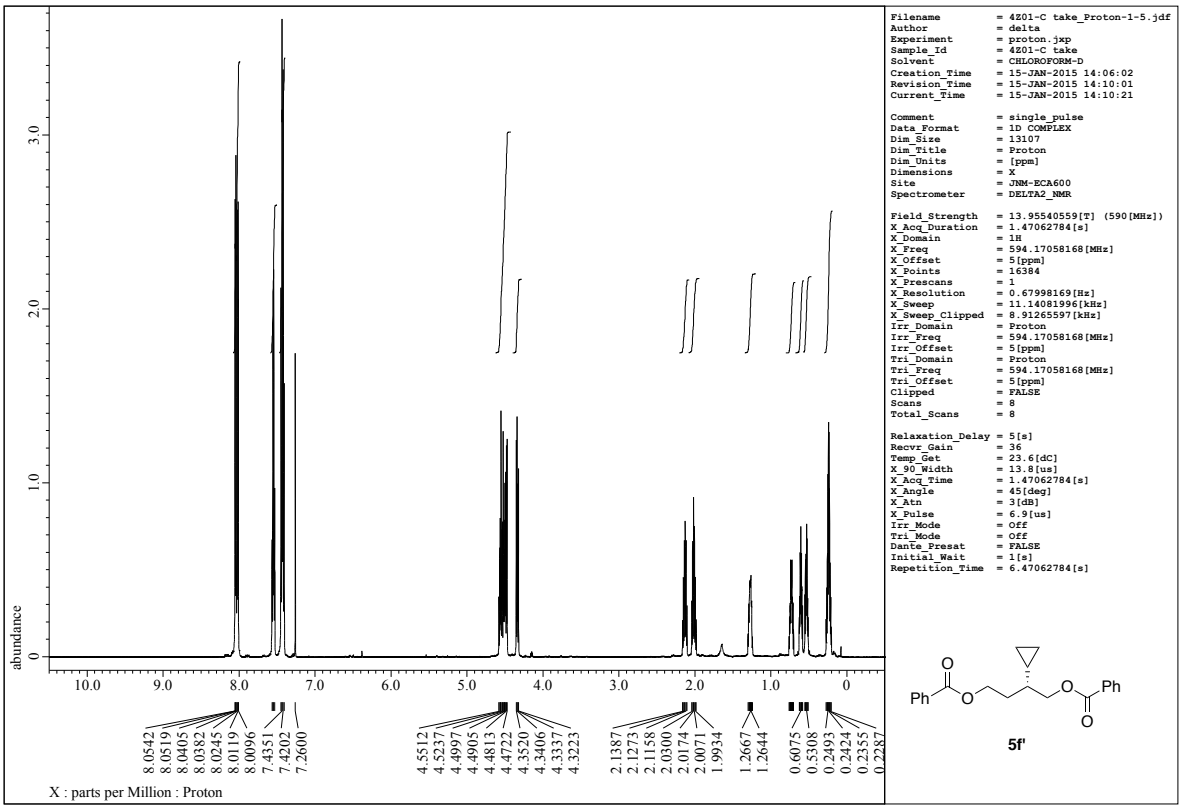


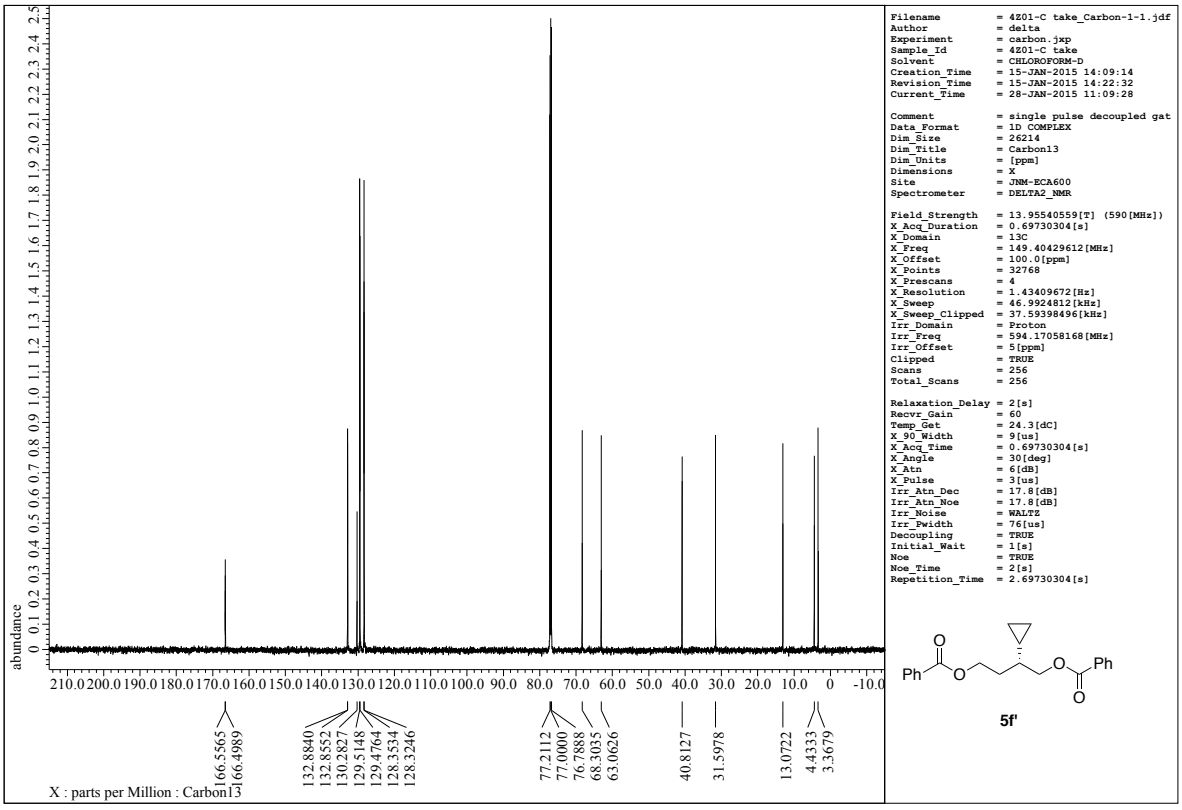
UV Results

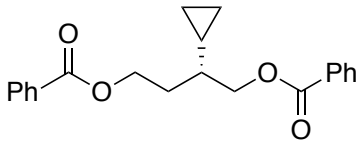
Pk #	Retention Time	Area	Area Percent	Height
1	15.107	302611	7.575	22637
2	15.504	3417984	85.559	199736
3	16.024	274275	6.866	17419
Totals		3994870	100.000	239792


abundance
30.0
20.0
10.0
0
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.2600
2.6892 2.6732 2.6617 2.6457 2.4351 2.4260 2.4077 2.3985 1.9178 1.9087 1.4406 1.4200 0.8364 0.8203 0.4782 0.1634 0.1543 0.1463
X : parts per Million : Proton
Filename = 4Z07-D take_Proton-1-9.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Z07-D take
Solvent = CHLOROFORM-D
Creation_Time = 27-DEC-2014 00:24:34
Revision_Time = 27-DEC-2014 00:29:17
Current_Time = 27-DEC-2014 00:30:04
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 = 23.7[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
5f

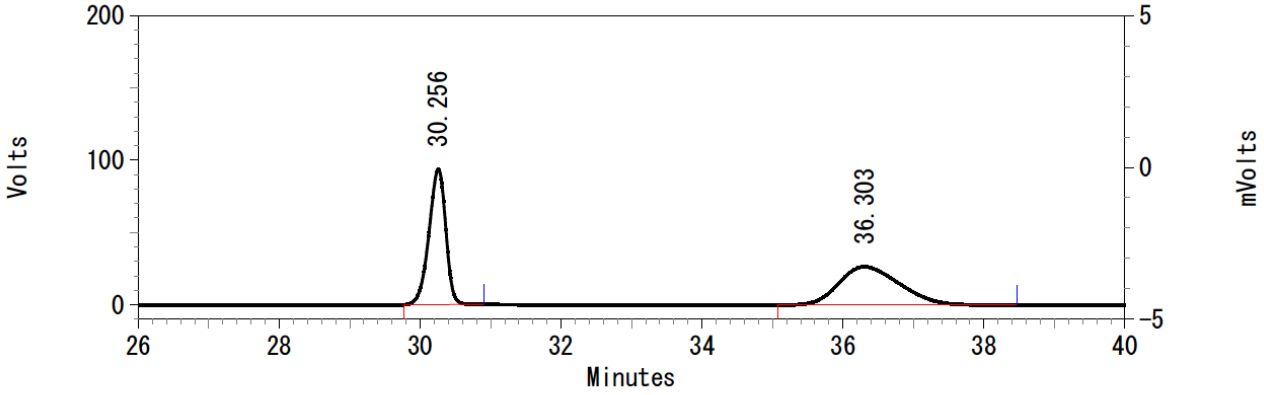

abundance
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
173.5828 171.2311
80.3980 80.2348 77.2112 77.0000 76.7792 47.1286 37.8562 28.0271 28.0079 13.5714 4.0206 3.6366
X : parts per Million : Carbon13
Filename = 4Z07-D take_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Z07-D take
Solvent = CHLOROFORM-D
Creation_Time = 27-DEC-2014 00:27:32
Revision_Time = 27-DEC-2014 00:41:17
Current_Time = 27-DEC-2014 00:41:53
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 = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
5f


abundance
8.0542
8.0519
8.0405
8.0382
8.0245
8.0119
8.0096
7.4351
7.4202
7.2600
4.5512
4.5237
4.4997
4.4905
4.4813
4.4722
4.3520
4.3406
4.3337
4.3223
2.1387
2.1273
2.1158
2.0300
2.0174
2.0071
1.9934
1.2667
1.2644
0.6075
0.5308
0.2493
0.2424
0.2355
0.2287
X : parts per Million : Proton
Filename = 4Z01-C take_Proton-1-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Z01-C take
Solvent = CHLOROFORM-D
Creation_Time = 15-JAN-2015 14:06:02
Revision_Time = 15-JAN-2015 14:10:01
Current_Time = 15-JAN-2015 14:10:21
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 = 36
Temp_Get = 23.6[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
Ph
O
O
O
O
Ph
5f'


abundance
166.5565
166.4989
132.8840
132.8552
130.2827
129.5148
129.4764
128.3534
128.3246
77.2112
77.0000
76.7888
68.3035
63.0626
40.8127
31.5978
13.0722
4.4333
3.3679
X : parts per Million : Carbon13
Filename = 4Z01-C take_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Z01-C take
Solvent = CHLOROFORM-D
Creation_Time = 15-JAN-2015 14:09:14
Revision_Time = 15-JAN-2015 14:22:32
Current_Time = 28-JAN-2015 11:09:28
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 = 24.3[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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
O
O
O
O
Ph
5f'

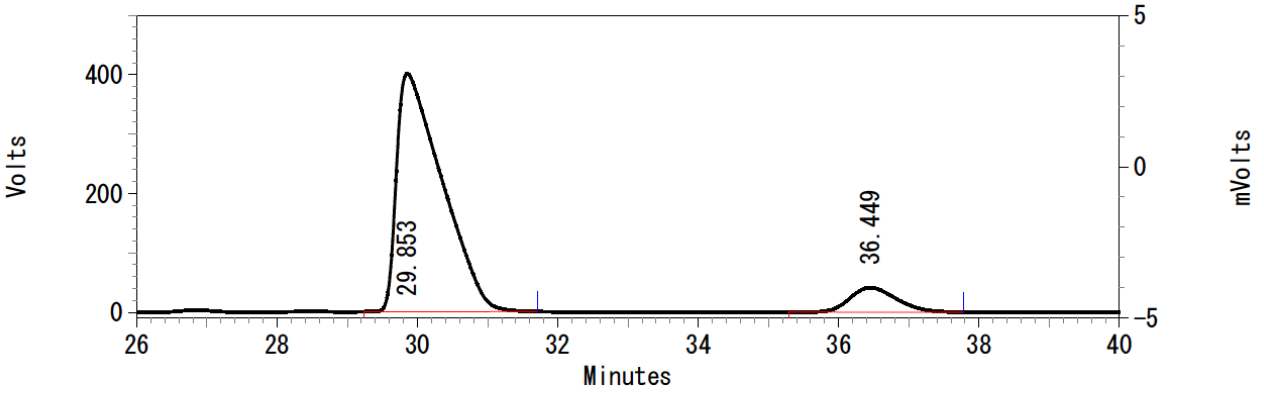


5f'



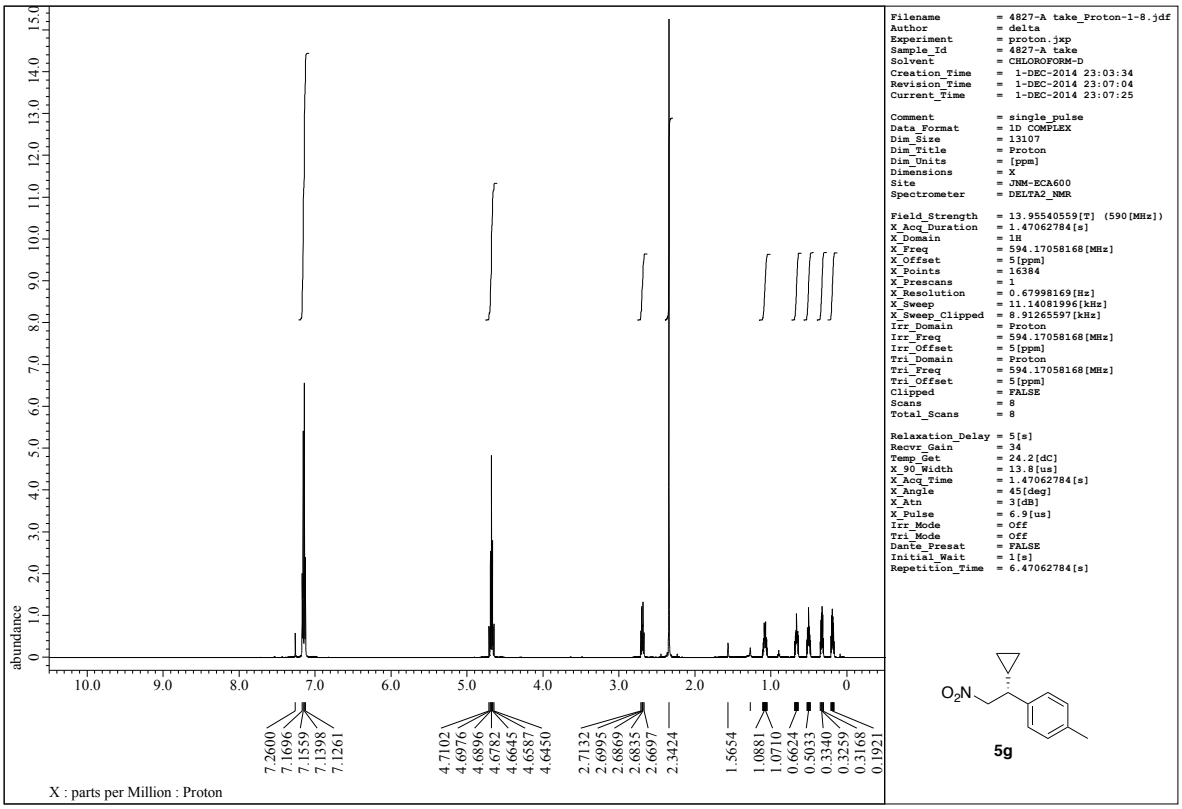
UV Results

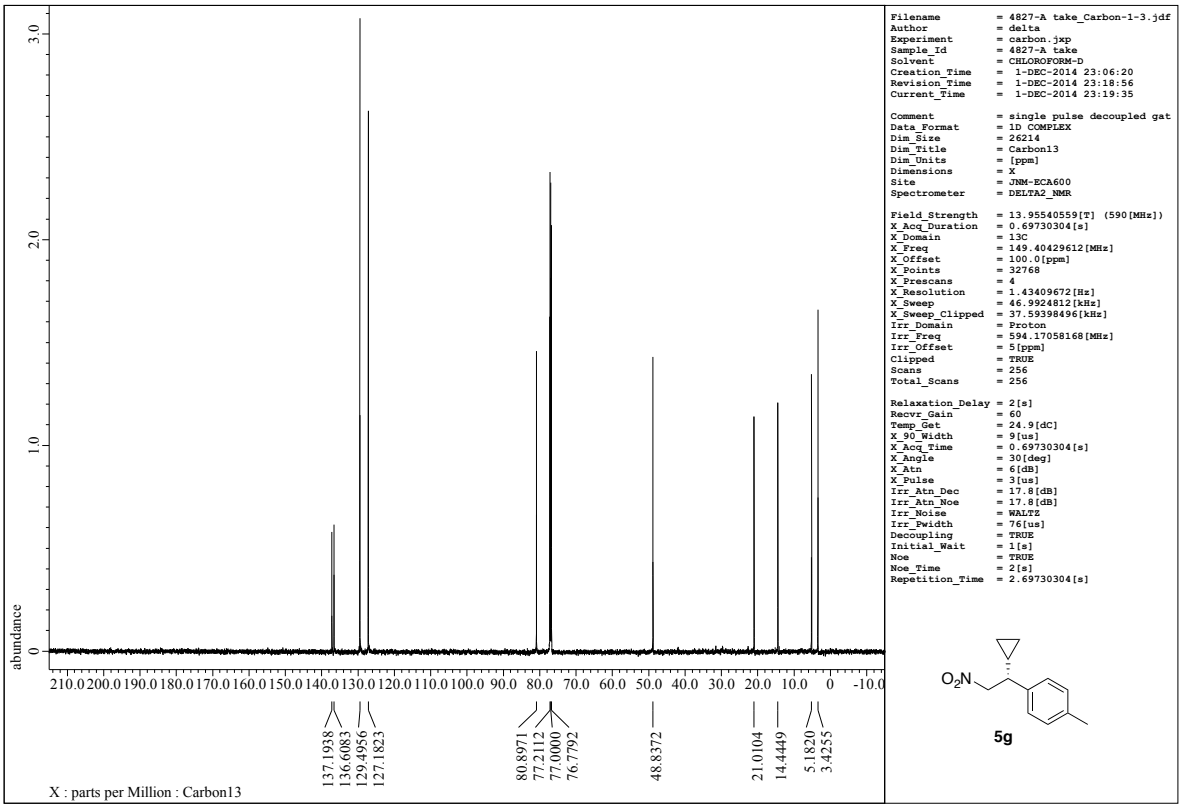
Pk #	Retention Time	Area	Area Percent	Height
1	30.256	1551683	49.515	93560
2	36.303	1582063	50.485	26422
Totals		3133746	100.000	119982

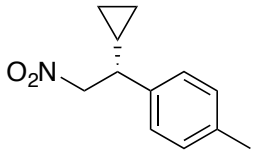


UV Results

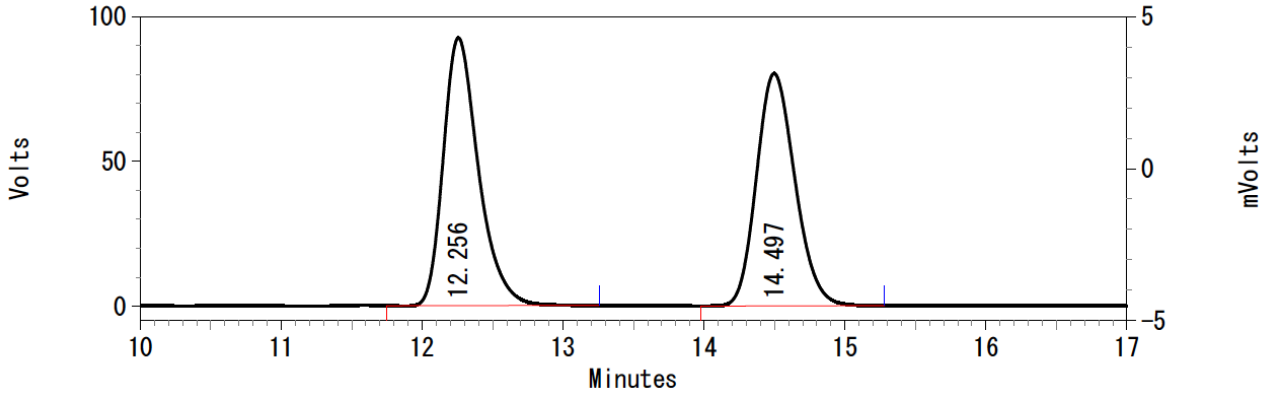
Pk #	Retention Time	Area	Area Percent	Height
1	29.853	18016172	90.447	401091
2	36.449	1902913	9.553	41211
Totals		19919085	100.000	442302


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.2600 7.1696 7.1559 7.1398 7.1261
4.7102 4.6976 4.6896 4.6782 4.6645 4.6587 4.6450
2.7132 2.6995 2.6869 2.6835 2.6697 2.3424
1.5654
1.0881 1.0710 0.6624 0.5033 0.3340 0.3259 0.3168 0.1921
X : parts per Million : Proton
Filename = 4827-A take_Proton-1-8.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4827-A take
Solvent = CHLOROFORM-D
Creation_Time = 1-DEC-2014 23:03:34
Revision_Time = 1-DEC-2014 23:07:04
Current_Time = 1-DEC-2014 23:07:25
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 = 24.2[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O2N
5g


abundance
3.0 2.0 1.0 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
137.1938 136.6083 129.4956 127.1823
80.8971 77.2112 77.0000 76.7792
48.8372
21.0104 14.4449 5.1820 3.4255
X : parts per Million : Carbon13
Filename = 4827-A take_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4827-A take
Solvent = CHLOROFORM-D
Creation_Time = 1-DEC-2014 23:06:20
Revision_Time = 1-DEC-2014 23:18:56
Current_Time = 1-DEC-2014 23:19:35
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 = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.9[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
O2N
5g

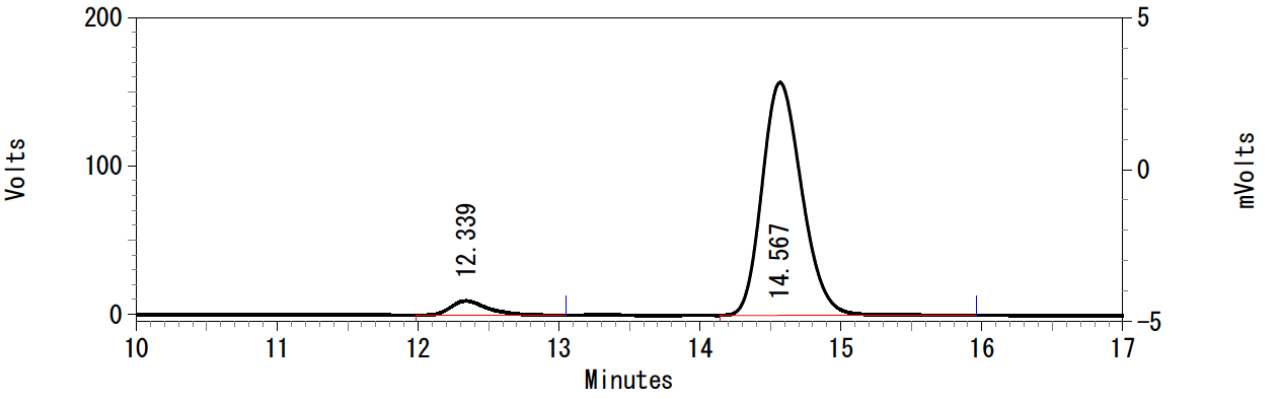


5g



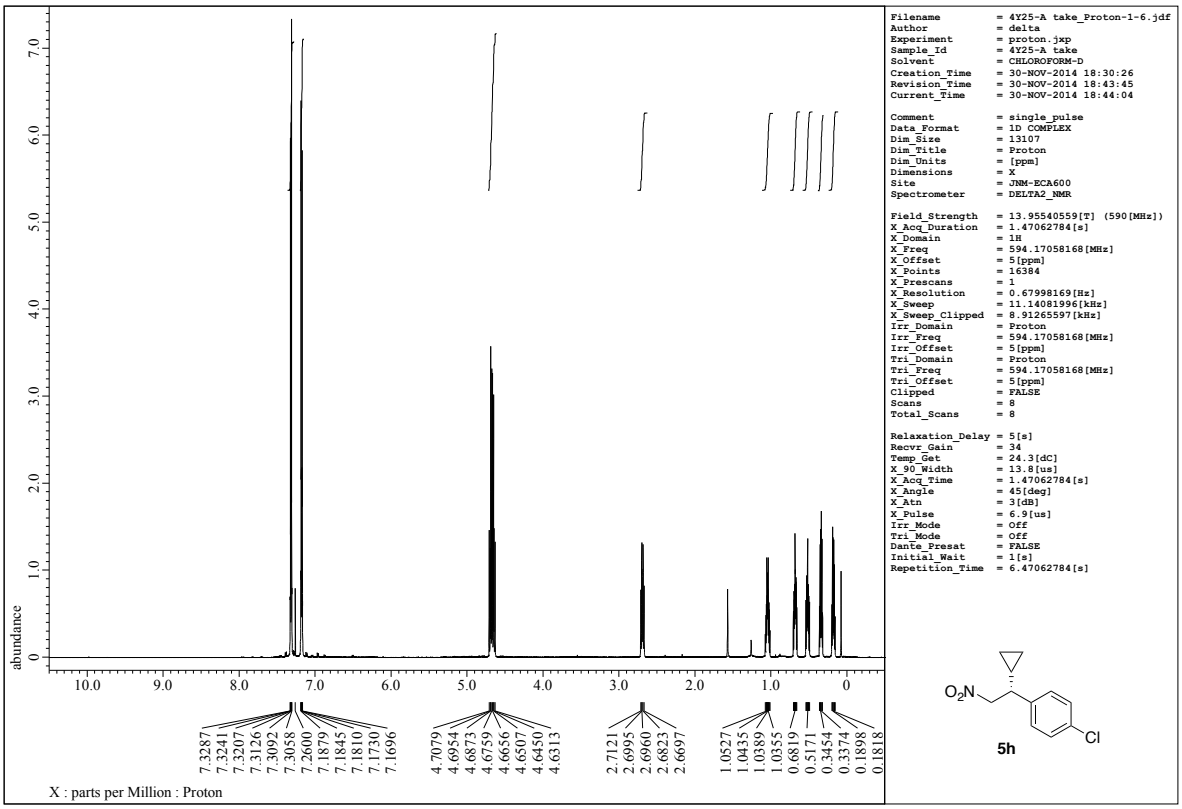
UV Results

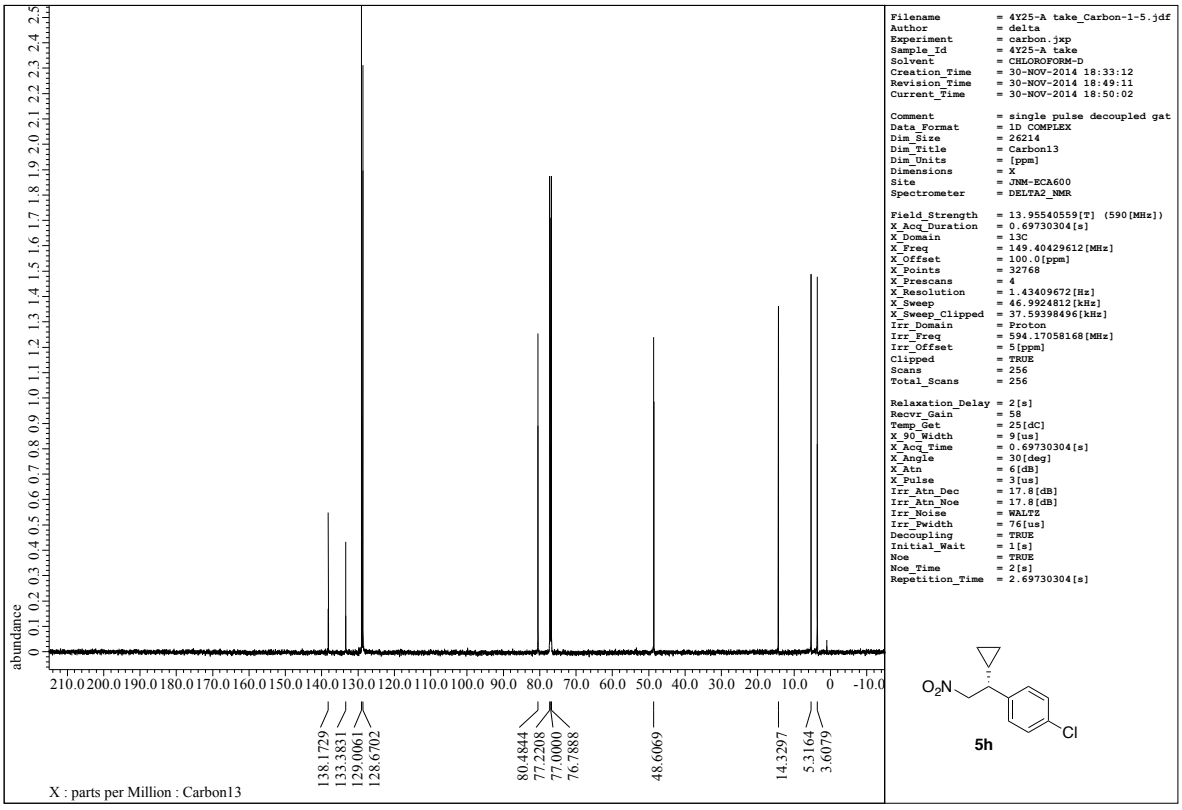
Pk #	Retention Time	Area	Area Percent	Height
1	12.256	1603227	51.247	92454
2	14.497	1525202	48.753	80250
Totals		3128429	100.000	172704

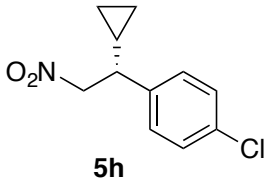


UV Results

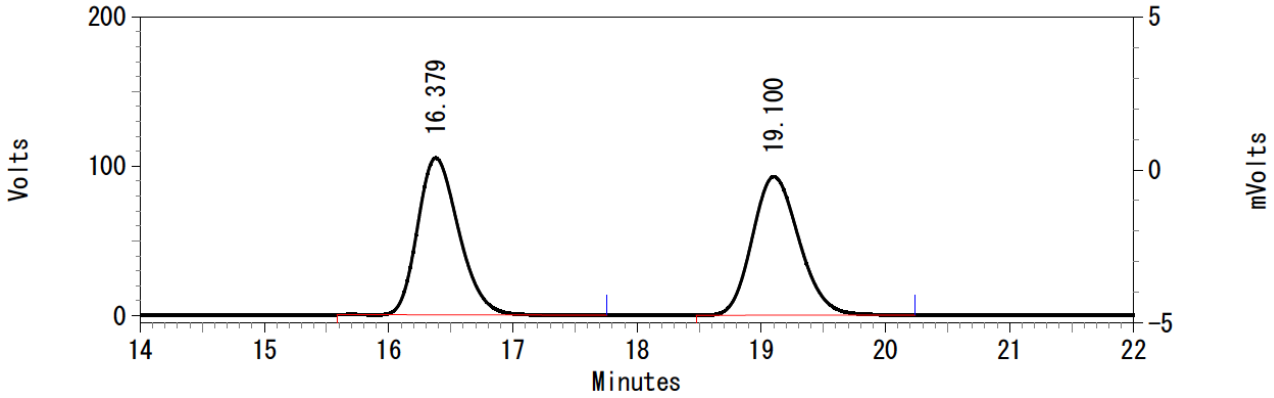
Pk #	Retention Time	Area	Area Percent	Height
1	12.339	177895	5.487	9683
2	14.567	3064111	94.513	156872
Totals		3242006	100.000	166555


abundance
7.3287
7.3241
7.3207
7.3126
7.3092
7.3058
7.2600
7.1879
7.1845
7.1810
7.1730
7.1696
4.7079
4.6954
4.6873
4.6759
4.6656
4.6507
4.6450
4.6313
2.7121
2.6995
2.6960
2.6823
2.6697
1.0527
1.0435
1.0389
1.0355
0.6819
0.5171
0.3454
0.3374
0.1898
0.1818
X : parts per Million : Proton
Filename = 4Y25-A take_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Y25-A take
Solvent = CHLOROFORM-D
Creation_Time = 30-NOV-2014 18:30:26
Revision_Time = 30-NOV-2014 18:43:45
Current_Time = 30-NOV-2014 18:44:04
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 = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O2N
Cl
5h


abundance
138.1729
133.3831
129.0061
128.6702
80.4844
77.2208
77.0000
76.7888
48.6069
14.3297
5.3164
3.6079
X : parts per Million : Carbon13
Filename = 4Y25-A take_Carbon-1-5.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Y25-A take
Solvent = CHLOROFORM-D
Creation_Time = 30-NOV-2014 18:33:12
Revision_Time = 30-NOV-2014 18:49:11
Current_Time = 30-NOV-2014 18:50:02
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 = 58
Temp_Get = 25[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
O2N
Cl
5h

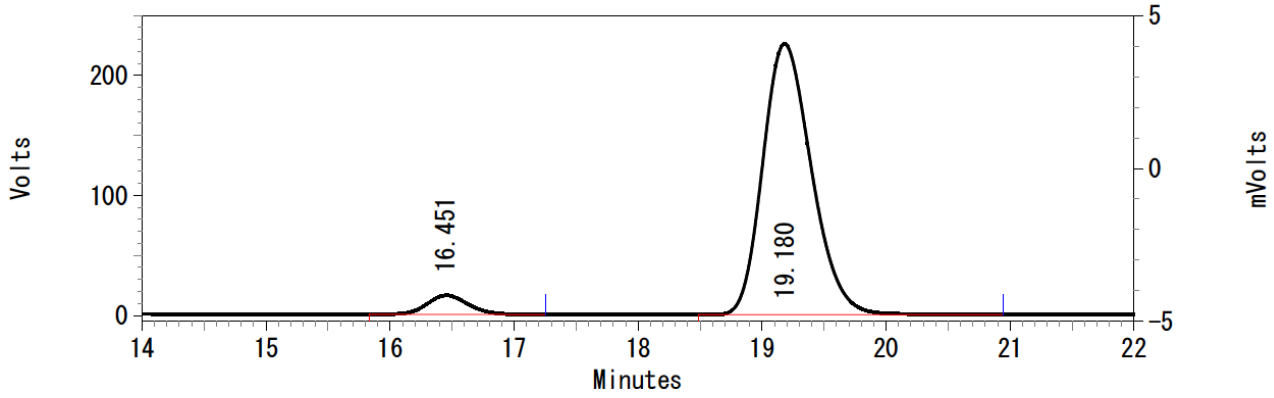


5h



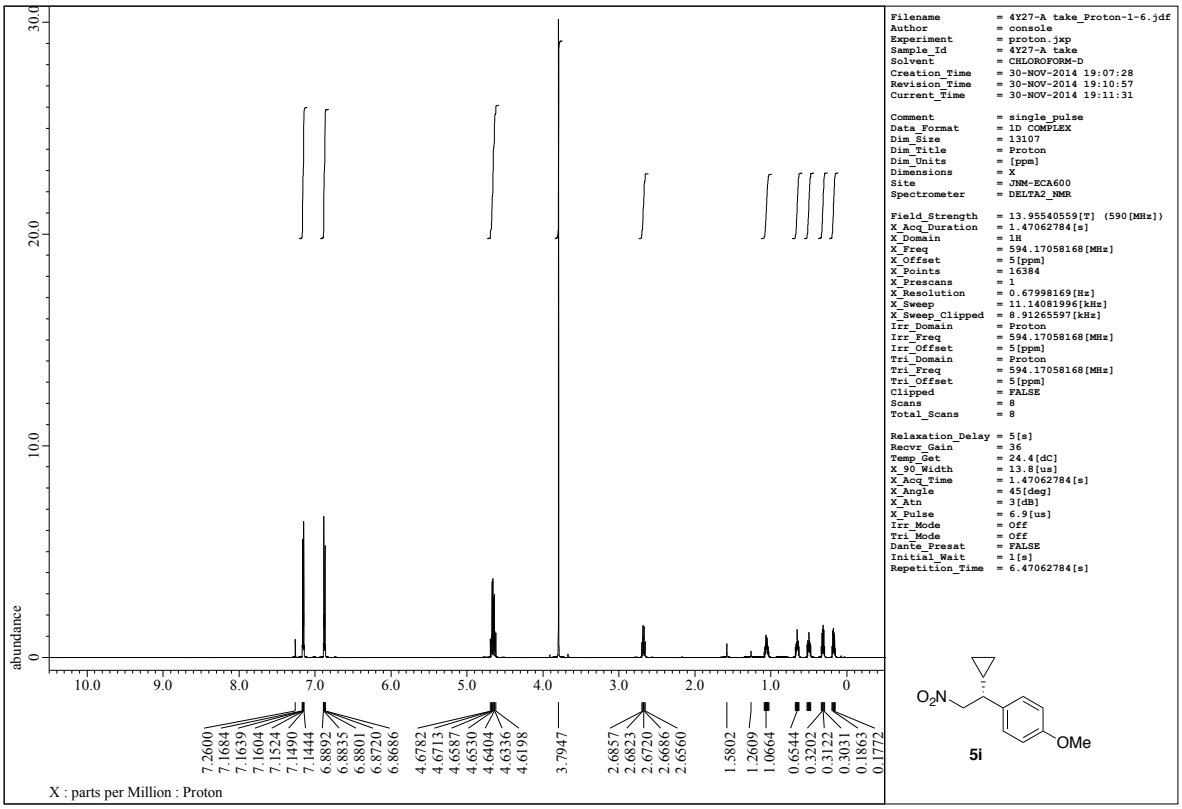
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	16.379	2416399	49.828	104918
2	19.100	2433098	50.172	92734
Totals		4849497	100.000	197652



UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	16.451	369533	5.657	15955
2	19.180	6163015	94.343	225778
Totals		6532548	100.000	241733


abundance
30.0
20.0
10.0
0
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.2600 7.1684 7.1639 7.1604 7.1524 7.1490 7.1444 6.8892 6.8835 6.8801 6.8720 6.8686
4.6782 4.6713 4.6587 4.6530 4.6404 4.6336 4.6198
3.7947
2.6857 2.6823 2.6720 2.6686 2.6560
1.5802 1.2609 1.0664 0.6544 0.3202 0.3122 0.3031 0.1863 0.1772
X : parts per Million : Proton
Filename = 4Y27-A take_Proton-1-6.jdf
Author = console
Experiment = proton.jxp
Sample_Id = 4Y27-A take
Solvent = CHLOROFORM-D
Creation_Time = 30-NOV-2014 19:07:28
Revision_Time = 30-NOV-2014 19:10:57
Current_Time = 30-NOV-2014 19:11:31
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 = 1.47062784[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 = 24.4[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
O2N
OMe
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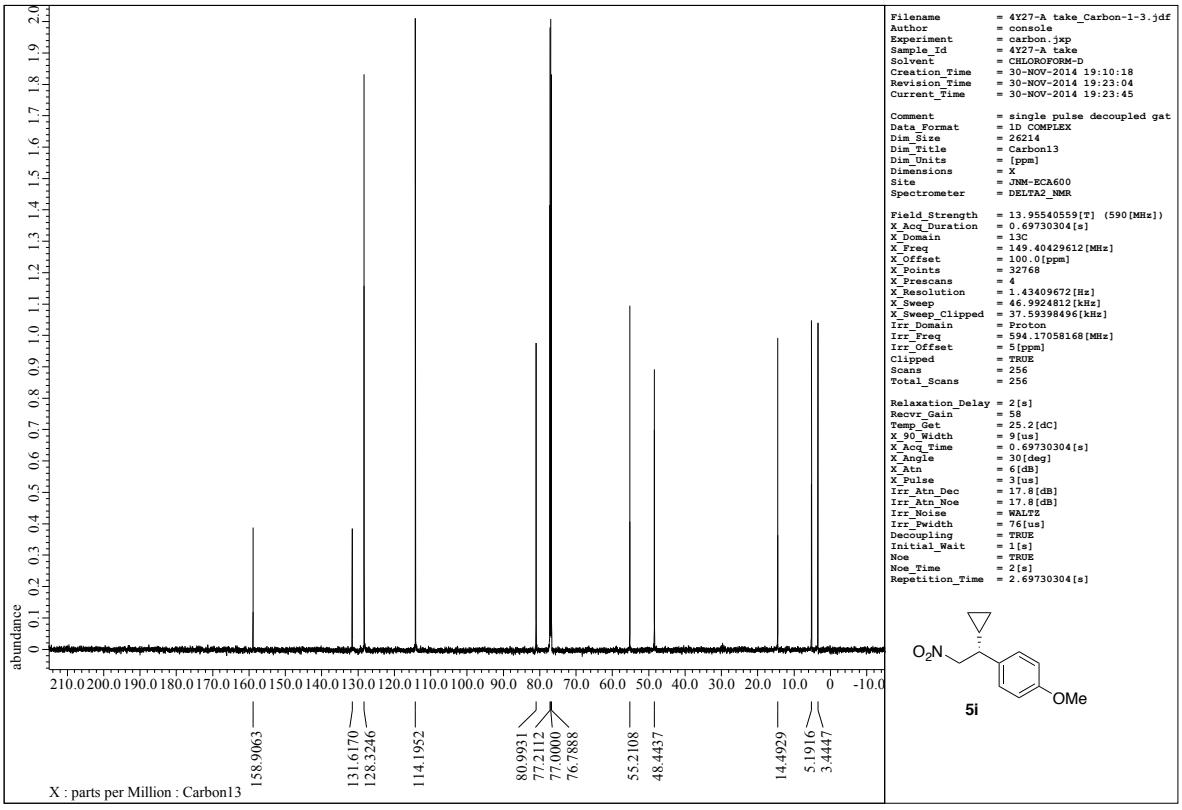
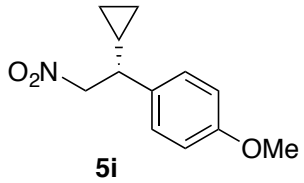
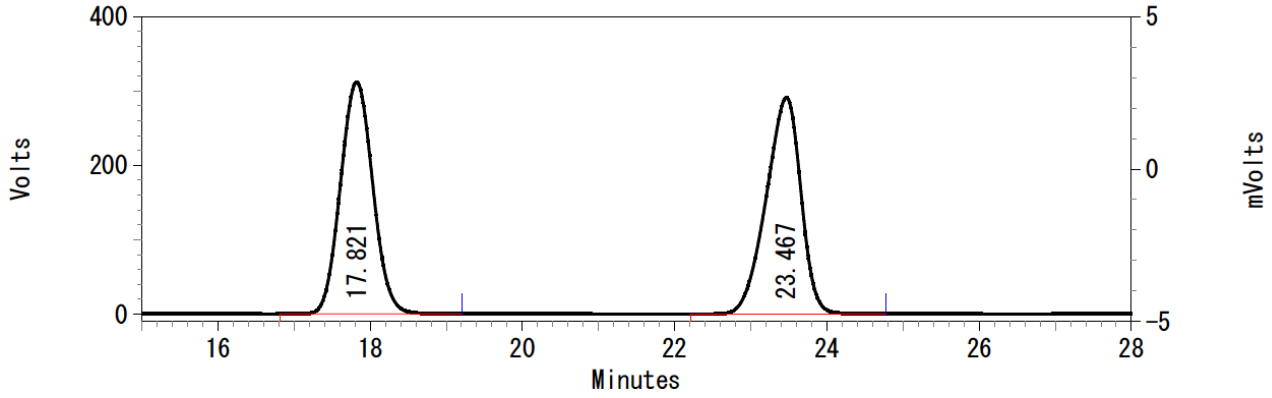

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
158.9063
131.6170 128.3246
114.1952
80.9931 77.2112 77.0000 76.7888
55.2108
48.4437
14.4929
5.1916
3.4447
X : parts per Million : Carbon13
Filename = 4Y27-A take_Carbon-1-3.jdf
Author = console
Experiment = carbon.jxp
Sample_Id = 4Y27-A take
Solvent = CHLOROFORM-D
Creation_Time = 30-NOV-2014 19:10:18
Revision_Time = 30-NOV-2014 19:23:04
Current_Time = 30-NOV-2014 19:23:45
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 = 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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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]
O2N
OMe
5i

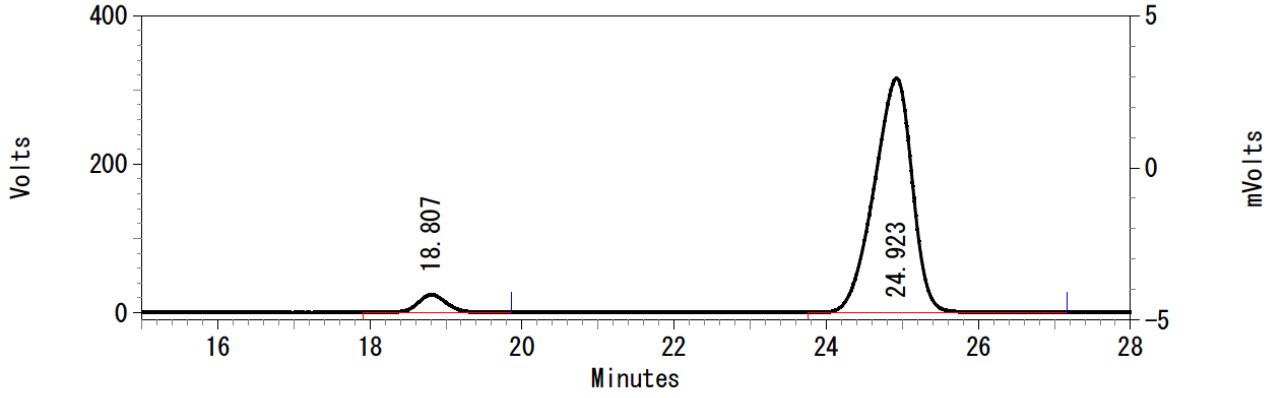


5i



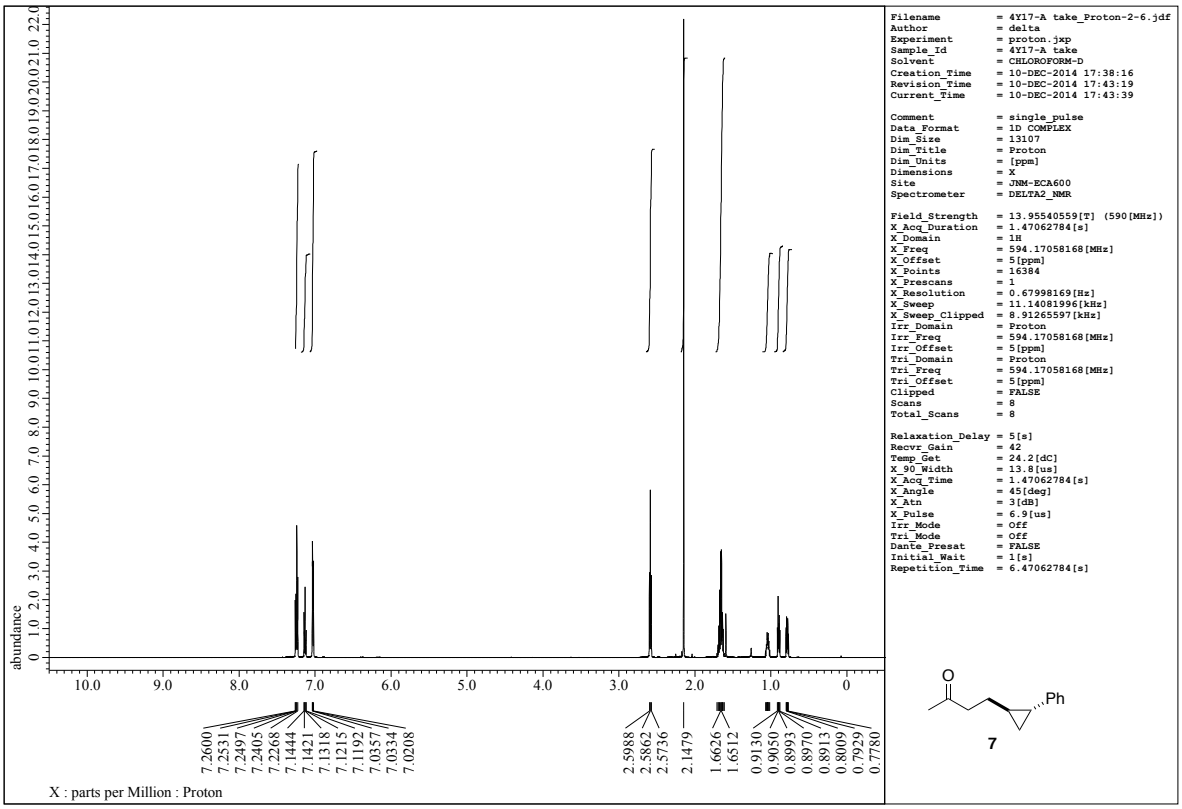
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	17.821	9223870	49.976	311518
2	23.467	9232810	50.024	291138
Totals		18456680	100.000	602656



UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	18.807	627933	5.411	23929
2	24.923	10977273	94.589	315078
Totals		11605206	100.000	339007


abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.2600 7.2531 7.2497 7.2405 7.2268 7.1444 7.1421 7.1318 7.1215 7.1192 7.0357 7.0334 7.0208
2.5988 2.5862 2.5736 2.1479 1.6626 1.6512 0.9130 0.9050 0.8993 0.8970 0.8913 0.8009 0.7929 0.7780
X : parts per Million : Proton
Filename = 4Y17-A take_Proton-2-6.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Y17-A take
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2014 17:38:16
Revision_Time = 10-DEC-2014 17:43:19
Current_Time = 10-DEC-2014 17:43:39
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 = 42
Temp_Get = 24.2[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
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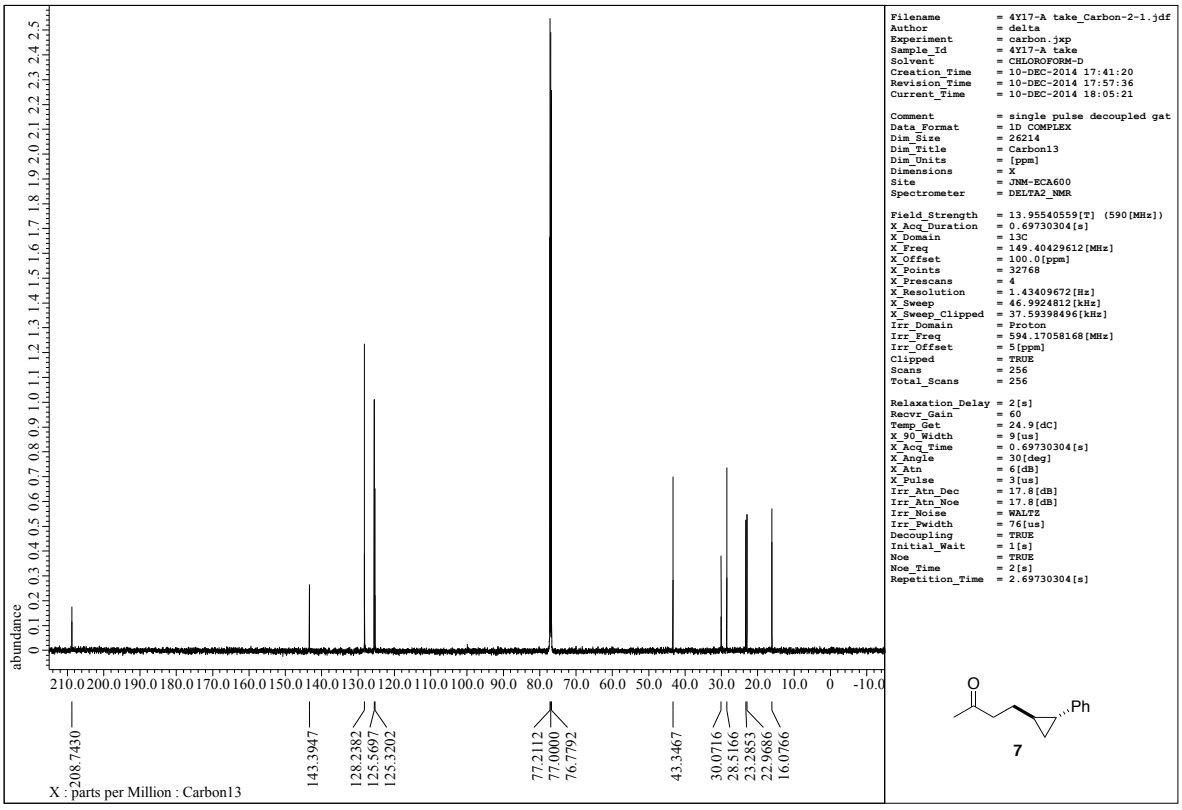
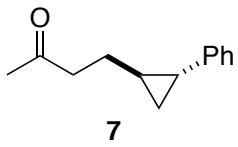
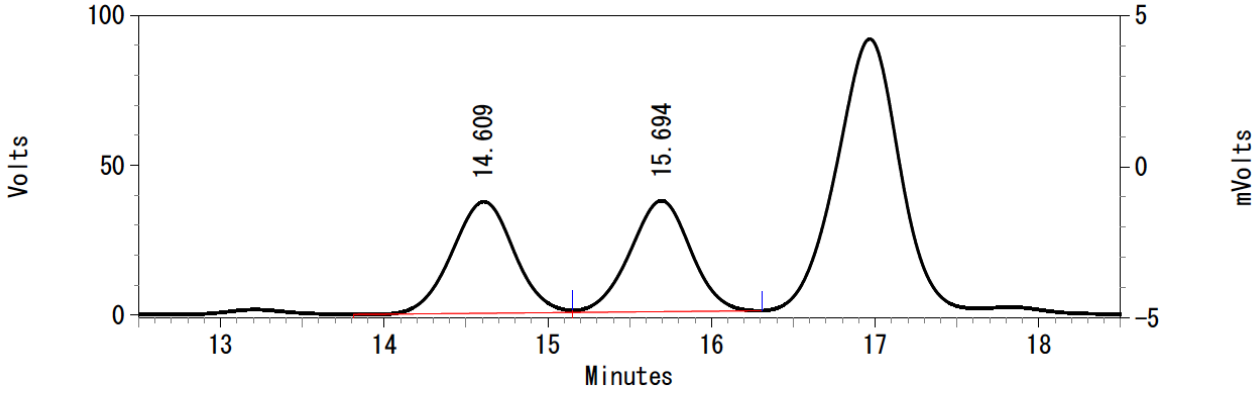

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
208.7430
143.3947
128.2382 125.5697 125.3202
77.2112 77.0000 76.7792
43.3467
30.0716 28.5166 23.2853 22.9686 16.0766
X : parts per Million : Carbon13
Filename = 4Y17-A take_Carbon-2-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 4Y17-A take
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2014 17:41:20
Revision_Time = 10-DEC-2014 17:57:36
Current_Time = 10-DEC-2014 18:05:21
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 = 24.9[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 = 17.8[dB]
Irr_Atn_Noe = 17.8[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
Ph
7

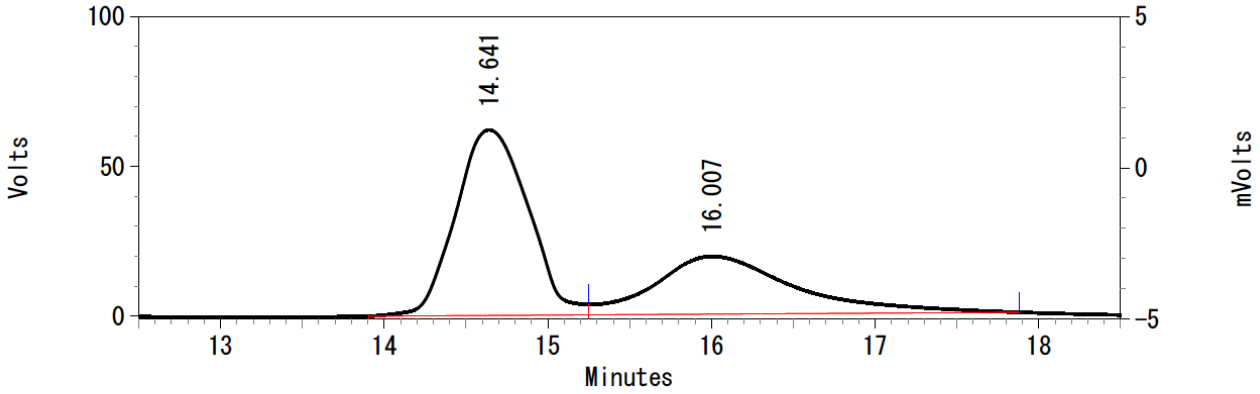


7



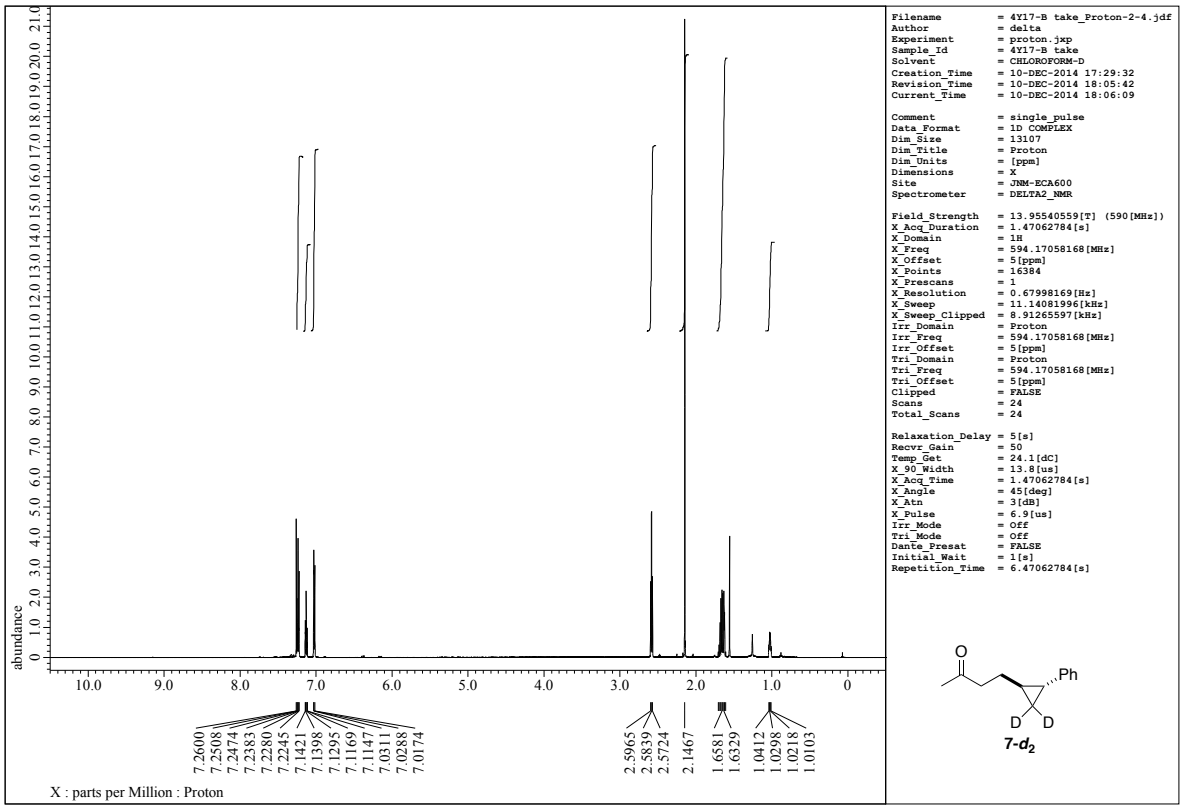
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	14.609	981738	50.765	37228
2	15.694	952157	49.235	37005
Totals		1933895	100.000	74233



UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	14.641	1894804	62.320	61893
2	16.007	1145624	37.680	19261
Totals		3040428	100.000	81154


abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2600
7.2508
7.2474
7.2383
7.2280
7.2245
7.1421
7.1398
7.1295
7.1169
7.1147
7.0311
7.0288
7.0174
2.5965
2.5839
2.5724
2.1467
1.6581
1.6329
1.0412
1.0298
1.0218
1.0103
X : parts per Million : Proton
Filename = 4Y17-B take_Proton-2-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 4Y17-B take
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2014 17:29:32
Revision_Time = 10-DEC-2014 18:05:42
Current_Time = 10-DEC-2014 18:06:09
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 = 24
Total_Scans = 24
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 24.1[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.47062784[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.9[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.47062784[s]
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***7-d*$_2$**