Supplementary Information

Stereoselective hydroacylation of bicyclic alkenes with 2-hydroxybenzaldehydes catalyzed by hydroxoiridium/diene complexes

Midori Nagamoto and Takahiro Nishimura*

Department of Chemistry, Graduate School of Science, Kyoto University, Sakyo, Kyoto 606-8502, Japan. Fax: +81 75 753 3988; Tel: +81 75 753 3987; E-mail: tnishi@kuchem.kyoto-u.ac.jp

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 peak of $CDCl_3$ (δ 7.26) 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: m, multiplet: br, broad. High-resolution mass spectra (ESI-TOF) 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).

2. Materials

Toluene was purified by passing through a neutral alumina column under N_2. Iridium complexes $[Ir(OH)(cod)]_2$[1] and $[IrCl((S,S)\text{-Me-tfb*})]_2$[2] were prepared according to the reported procedures.

3. Preparation of salicylaldehydes 1 and bicyclic alkenes 2

Salicylaldehydes **1k** and **1n** were prepared according to the reported procedures.[3] Bicyclic alkenes **1a** (CAS: 573-57-9),[4] **1b** (CAS: 26002-73-3),[4] **1c** (CAS: 19061-36-0),[4] **1d** (CAS: 111211-88-2),[5] **1e** (CAS: 96691-93-9),[6] **1f** (CAS: 573-57-9),[7] **1g** (CAS: 4453-90-1),[8] **1h** (CAS: 7350-72-3),[9] **1j** (CAS: 129-64-6),[10] **1k** (CAS: 75715-21-8),[11] **1l** (CAS: 15971-63-8),[12] **1n** (CAS: 4705-93-5),[13] and **1o** (CAS: 19396-42-0)[14] were prepared according to the reported procedures. Other materials were purchased from commercial suppliers and used as received.

4. General procedure for iridium-catalyzed addition of salicylaldehyde (1a) to oxabenzonorbornadiene 2a (Table 1)

$[Ir(OH)(cod)]_2$ (1.6 mg, 0.0050 mmol of Ir, 5 mol% of Ir) and **2a** (17.3 mg, 0.12 mmol)

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were placed in a Schlenk tube under N_2. 1,4-Dioxane (0.4 mL) and salicylaldehyde (**1a**: 12.2 mg, 0.10 mmol) were added successively. The Schlenk tube was capped with a glass stopper and heated at 60 °C for 6 h with stirring. The mixture was concentrated on a rotary evaporator. The yields of the products were determined by ^{1}H NMR using 1,4-dimethoxybenezene as an internal standard. For entries 3–7 of Table 1, $[IrCl(cod)]_2$ (1.7 mg, 0.0050 mmol of Ir, 5 mol% of Ir) and base (0.10 mmol, 10 mol%) were used instead of $[Ir(OH)(cod)]_2$.

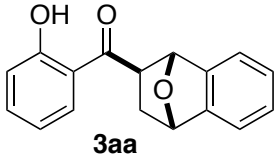
5. General procedure for iridium-catalyzed addition of salicylaldehyde (1a) to bicyclic alkenes 2 (Scheme 1)

$[Ir(OH)(cod)]_2$ (3.2 mg, 0.010 mmol of Ir, 5 mol% of Ir) and bicyclic alkene **2** (for solid materials, 0.24 mmol) were placed in a Schlenk tube under N_2. 1,4-Dioxane (0.8 mL) and salicylaldehyde (**1a**: 24.4 mg, 0.20 mmol) were added successively (liquid bicyclic alkene **2** was added at this time). The Schlenk tube was capped with a glass stopper and heated at 60 °C for 6 h with stirring. The mixture was concentrated on a rotary evaporator, and the residue was subjected to preparative TLC on silica gel with EtOAc/hexane to give **3**. For bicyclic alkenes **2j** and **2k**, the reaction of **1a** (0.24 mmol) with **2j** or **2k** (0.20 mmol) was conducted for an ease of isolation of the product.

6. General procedure for iridium-catalyzed addition of salicylaldehydes 1 to 2-norbornene (2i) (Scheme 2)

$[Ir(OH)(cod)]_2$ (3.2 mg, 0.010 mmol of Ir, 5 mol% of Ir) and 2-norbornene **(2i)** (0.40 mmol) were placed in a Schlenk tube under N_2. 1,4-Dioxane (0.8 mL) and salicylaldehyde (**1a**: 24.4 mg, 0.20 mmol) were added successively. The Schlenk tube was capped with a glass stopper and heated at 60 °C for 6 h with stirring. The mixture was concentrated on a rotary evaporator, and the residue was subjected to preparative TLC on silica gel with hexane/EtOAc to give **3**.

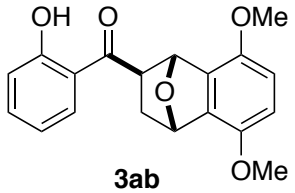
7. Characterization of the products



3aa

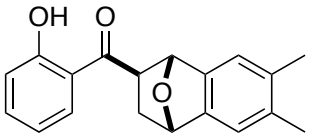
Compound 3aa (Scheme 1, 52.0 mg, 97% yield, CAS: 1028939-89-0). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.94 (dd, J = 11.6, 8.9 Hz, 1H), 2.50 (dt, J = 11.6, 4.8 Hz, 1H), 3.48 (dd, J = 8.9, 4.8 Hz, 1H), 5.53 (d, J = 4.8 Hz, 1H), 5.71 (s, 1H), 6.89 (t, J = 8.1 Hz, 1H), 7.03 (d, J = 8.1 Hz, 1H), 7.21–7.26 (m, 2H), 7.30–7.39

(m, 2H), 7.49 (td, J = 8.1, 1.4 Hz, 1H), 7.64 (dd, J = 8.1, 1.4 Hz, 1H), 12.29 (s, 1H).



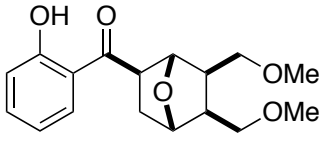
3ab

Compound 3ab (Scheme 1, 63.5 mg, 97% yield). A solution of $CHCl_3$/EtOAc (10:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.88 (dd, J = 11.6, 8.9 Hz, 1H), 2.55 (dt, J = 11.6, 4.8 Hz, 1H), 3.49 (dd, J = 8.9, 4.8 Hz, 1H), 3.82 (s, 3H), 3.85 (s, 3H), 5.69 (d, J = 4.8 Hz, 1H), 5.84 (s, 1H), 6.71 (s, 2H), 6.90 (td, J = 8.2, 1.4 Hz, 1H), 7.03 (dd, J = 8.2, 1.4 Hz, 1H), 7.48 (td, J = 8.2, 1.4 Hz, 1H), 7.77 (d, J = 8.2, 1.4 Hz, 1H), 12.30 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 31.6, 47.7, 56.0, 56.1, 77.2, 79.3, 111.1, 111.6, 118.7, 118.8, 118.9, 130.0, 133.6, 135.1, 136.3, 146.4, 146.8, 162.9, 204.8. HRMS (ESI) calcd for $C_{19}H_{18}NaO_5$ $(M+Na)^+$ 349.1046, found 349.1043.



3ac

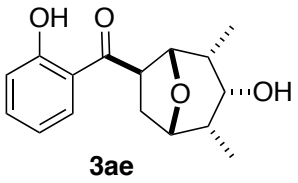
Compound 3ac (Scheme 1, 52.5 mg, 93% yield). CH_2Cl_2 was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.88 (dd, J = 11.6, 8.9 Hz, 1H), 2.28 (s, 3H), 2.29 (s, 3H), 2.48 (dt, J = 11.6, 4.8 Hz, 1H), 3.45 (dd, J = 8.9, 4.8 Hz, 1H), 5.53 (d, J = 4.8 Hz, 1H), 5.63 (s, 1H), 6.89 (t, J = 7.5 Hz, 1H), 7.03 (d, J = 7.5 Hz, 1H), 7.10 (s, 1H), 7.14 (s, 1H), 7.48 (t, J = 7.5 Hz, 1H), 7.64 (d, J = 7.5 Hz, 1H), 12.31 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 20.0, 33.1, 48.3, 79.0, 80.8, 118.7, 118.9, 120.2, 120.7, 129.7, 135.1, 135.3, 136.3, 142.3, 143.9, 163.0, 205.3. HRMS (ESI) calcd for $C_{19}H_{18}NaO_3$ $(M+Na)^+$ 317.1148, found 317.1144.



3ad

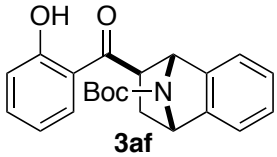
Compound 3ad (Scheme 1, 53.8 mg, 91% yield). A solution of hexane/EtOAc (1:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.86 (dd, J = 12.2, 9.6 Hz, 1H), 2.23–2.30 (m, 2H), 2.30–2.36 (m, 1H), 3.22–3.29 (m, 2H), 3.32 (s, 3H), 3.33 (s, 3H), 3.34–3.36 (m, 1H), 3.38 (dt, J = 8.9, 4.8 Hz, 1H), 3.52 (dd, J = 8.9, 4.8 Hz, 1H), 4.54 (d, J = 4.8 Hz, 1H), 4.75 (s, 1H), 6.90 (t, J = 7.7 Hz, 1H), 6.98 (d, J = 7.7 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 7.67 (d, J = 7.7 Hz, 1H), 12.25 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 33.7, 45.8, 46.0, 49.7, 58.78, 58.81, 70.5, 70.8, 79.0, 81.2, 118.3,

118.7, 118.9, 129.7, 136.1, 163.1, 204.3. HRMS (ESI) calcd for $C_{17}H_{22}NaO_5$ $(M+Na)^+$ 329.1356, found 329.1352.



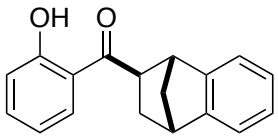
3ae

Compound 3ae (Scheme 1, 52.5 mg, 95% yield). A solution of $CHCl_3$/EtOAc (7:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.01 (d, *J* = 7.5 Hz, 3H), 1.06 (d, *J* = 7.5 Hz, 3H), 1.56 (br s, 1H), 1.96–2.03 (m, 1H), 2.08–2.22 (m, 2H), 2.69 (dd, *J* = 12.2, 9.5 Hz, 1H), 3.79 (s, 1H), 4.15–4.20 (m, 1H), 4.38 (dd, *J* = 9.5, 4.8 Hz, 1H), 4.46 (s, 1H), 6.90 (t, *J* = 8.2 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 7.46 (t, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 12.36 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 12.9, 13.3, 31.4, 38.7, 38.9, 45.5, 71.7, 78.7, 78.9, 118.3, 118.6, 188.7, 130.3, 136.1, 163.1, 207.0. HRMS (ESI) calcd for $C_{16}H_{20}NaO_4$ $(M+Na)^+$ 299.1254, found 299.1249.



3af

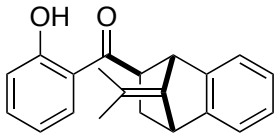
Compound 3af (Scheme 1, 68.2 mg, 95% yield). $CHCl_3$ was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.34 (s, 9H), 1.64–1.72 (m, 1H), 2.78–2.85 (m, 1H), 3.44 (s, 1H), 5.37 (br s, 2H), 6.94 (br t, *J* = 8.2 Hz, 1H), 7.03 (d, *J* = 8.2 Hz, 1H), 7.19–7.24 (m, 2H), 7.28–7.43 (m, 2H), 7.50 (br t, *J* = 8.2 Hz, 1H), 7.70 (br d, *J* = 8.2 Hz, 1H), 12.31 (br s, 1H); ^{13}C NMR ($CDCl_3$, 50 °C) δ 28.1, 30.9 (br), 49.3 (br), 60.9 (br), 64.4, 80.5, 118.8, 118.9, 119.0, 119.3 (br), 120.0, 126.7, 127.1, 129.4, 136.2, 144.5, 145.8, 153.8 (br), 163.1, 204.0. HRMS (ESI) calcd for $C_{22}H_{23}NNaO_4$ $(M+Na)^+$ 388.1519, found 388.1516.



3ag

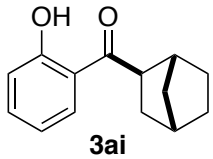
Compound 3ag (Scheme 1, 49.2 mg, 92% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.71 (ddd, *J* = 11.5, 9.5, 2.7 Hz, 1H), 1.83 (d, *J* = 9.5 Hz, 1H), 1.92 (d, *J* = 9.5 Hz, 1H), 2.32 (ddd, *J* = 11.5, 5.5, 4.1 Hz, 1H), 3.29 (dd, *J* = 9.5, 5.5 Hz, 1H), 3.48 (d, *J* = 2.7 Hz, 1H), 3.64 (s, 1H), 6.82 (t, *J* = 8.2 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 7.12–7.18 (m, 2H), 7.24–7.32 (m, 2H), 7.47 (td, *J* = 8.2, 1.3 Hz, 1H), 7.71 (dd, *J* = 8.2, 1.3

Hz, 1H), 12.46 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 33.2, 43.8, 47.3, 47.7, 47.8, 118.6, 118.85, 118.94, 120.7, 121.1, 125.9, 126.3, 130.0, 136.1, 147.1, 148.6, 162.8, 208.1. HRMS (ESI) calcd for $C_{18}H_{16}NaO_2$ $(M+Na)^+$ 287.1043, found 287.1036.



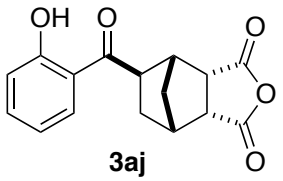
3ah

Compound 3ah (Scheme 1, 57.7 mg, 95% yield). A solution of hexane/EtOAc (7:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.660 (s, 3H), 1.665 (s, 3H), 1.80 (dd, *J* = 11.5, 9.5 Hz, 1H), 2.28 (ddd, *J* = 11.5, 5.1, 3.8 Hz, 1H), 3.33 (dd, *J* = 9.5, 5.1 Hz, 1H), 3.91 (d, *J* = 3.8 Hz, 1H), 4.12 (s, 1H), 6.89 (td, *J* = 8.2, 1.4 Hz, 1H), 7.01 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.12–7.17 (m, 2H), 7.23–7.31 (m, 2H), 7.46 (td, *J* = 8.2, 1.4 Hz, 1H), 7.69 (dd, *J* = 8.2, 1.4 Hz, 1H), 12.43 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 20.0, 20.1, 33.1, 44.2, 47.4, 48.4, 114.5, 118.6, 118.78, 118.82, 120.2, 120.4, 125.8, 126.2, 129.9, 135.9, 145.2, 146.5, 147.9, 162.7, 206.8. HRMS (ESI) calcd for $C_{21}H_{20}NaO_2$ $(M+Na)^+$ 327.1356, found 327.1352.



3ai

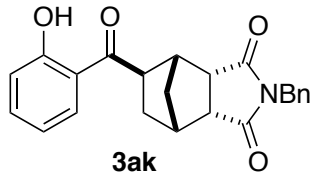
Compound 3ai (CAS: 220459-44-9, Scheme 2, 428.6 mg, 99% yield obtained in the reaction of 2.0 mmol of **1a**). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.19 (d, *J* = 10.2 Hz, 1H), 1.29–1.34 (m, 1H), 1.40–1.69 (m, 5H), 2.00–2.07 (m, 1H), 2.37 (s, 1H), 2.55 (s, 1H), 3.25 (dd, *J* = 9.2, 5.8 Hz, 1H), 6.89 (t, *J* = 8.2 Hz, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 7.44 (t, *J* = 8.2 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 12.49 (s, 1H).



3aj

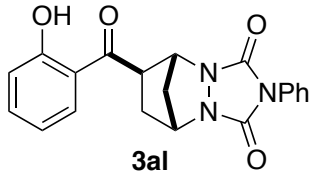
Compound 3aj (Scheme 1, 56.0 mg, 98% yield). A solution of CH_2Cl_2/AcOH (100:1) was used for column chromatography on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.62 (d, *J* = 10.9 Hz, 1H), 1.67–1.74 (m, 1H), 1.86 (dd, *J* = 10.9, 1.4 Hz, 1H), 2.36–2.43 (m, 1H), 2.50–3.00 (m, 1H), 3.10 (d, *J* = 5.5 Hz, 1H), 3.43–3.48 (m, 1H), 3.49 (ddd, *J* = 10.2, 5.5, 2.0 Hz, 1H), 3.58 (dd, *J* = 10.2, 5.5 Hz, 1H), 6.95 (t, *J* = 8.1 Hz, 1H), 6.99 (d, *J* = 8.1 Hz, 1H), 7.49 (t, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 8.1 Hz,

1H), 12.07 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.0, 40.1, 44.1, 44.5, 49.4, 49.5, 117.9, 118.7, 119.4, 129.9, 136.8, 163.1, 171.2, 171.8, 204.1. HRMS (ESI) calcd for $C_{16}H_{14}NaO_5$ $(M+Na)^+$ 309.0733, found 309.0730.



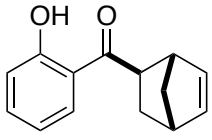
3ak

Compound 3ak (Scheme 1, 74.6 mg, 99% yield). A solution of hexane/EtOAc (4:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.20–1.28 (m, 1H), 1.55 (d, *J* = 10.6 Hz, 1H), 1.73 (d, *J* = 10.6 Hz, 1H), 1.85–1.91 (m, 1H), 2.82 (d, *J* = 4.8 Hz, 1H), 2.83 (d, *J* = 5.4 Hz, 1H), 3.01 (d, *J* = 5.5 Hz, 1H), 3.13 (dd, *J* = 9.5, 4.8 Hz, 1H), 3.21 (dd, *J* = 9.5, 5.5 Hz, 1H), 4.65 (d, *J* = 13.6 Hz, 1H), 4.70 (d, *J* = 13.6 Hz, 1H), 6.81 (t, *J* = 7.5 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 7.27–7.31 (m, 3H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.50–7.55 (m, 2H), 12.09 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.5, 39.3, 40.2, 42.3, 43.2, 43.5, 47.9, 48.1, 117.8, 118.4, 119.1, 128.2, 128.8, 129.4, 130.0, 136.3, 162.9, 177.3, 177.5, 205.3. HRMS (ESI) calcd for $C_{23}H_{21}NNaO_4$ $(M+Na)^+$ 398.1363, found 398.1365.



3al

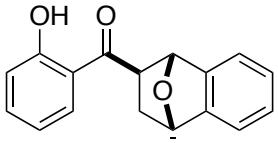
Compound 3al (Scheme 1, 73.1 mg, 99% yield). A solution of $CHCl_3$/EtOAc (7:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 2.03–2.06 (m, 1H), 2.08 (d, *J* = 10.9 Hz, 1H), 2.32 (ddd, *J* = 13.6, 8.9, 2.0 Hz, 1H), 2.39 (ddd, *J* = 13.6, 5.5, 2.7 Hz, 1H), 4.01 (dd, *J* = 8.9, 5.5 Hz, 1H), 4.77 (s, 1H), 4.90 (s, 1H), 6.99 (t, *J* = 8.1 Hz, 1H), 7.03 (t, *J* = 8.1 Hz, 1H), 7.40 (t, *J* = 8.1 Hz, 1H), 7.47–7.56 (m, 5H), 7.88 (d, *J* = 8.1 Hz, 1H), 11.96 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 32.1, 37.2, 47.3, 60.0, 62.5, 117.9, 119.0, 119.6, 125.3, 128.4, 129.2, 129.9, 131.6, 137.3, 156.8, 156.9, 163.2, 202.7. HRMS (ESI) calcd for $C_{20}H_{17}N_3NaO_4$ $(M+Na)^+$ 386.1111, found 386.1107.



3am

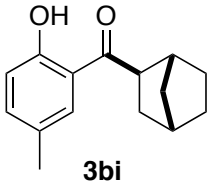
Compound 3am (Scheme 1, 37.2 mg, 85% yield) (CAS: 1028939-58-3). A solution of hexane/EtOAc (40:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.44 (d, *J* =

8.8 Hz, 1H), 1.49–1.58 (m, 2H), 2.02 (ddd, *J* = 11.6, 4.8, 3.4 Hz, 1H), 2.99 (s, 1H), 3.11 (s, 1H), 3.16 (dd, *J* = 8.8, 4.4 Hz, 1H), 6.24–6.30 (m, 2H), 7.89 (t, *J* = 8.1 Hz, 1H), 6.98 (d, *J* = 8.1 Hz, 1H), 7.45 (td, *J* = 8.1, 1.4 Hz, 1H), 6.98 (dd, *J* = 8.1, 1.4 Hz, 1H), 12.48 (s, 1H).



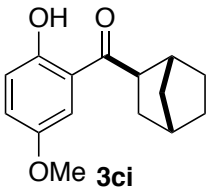
3ao

Compound 3ao (eq 1, 54.0 mg, 96% yield). CH_2Cl_2 was used for preparative TLC on silica gel. The structure of **3ao** was determined by NOE experiments. ^{1}H NMR ($CDCl_3$) δ 1.89 (s, 3H), 1.98 (dd, *J* = 11.6, 8.8 Hz, 1H), 2.21 (dd, *J* = 11.6, 4.8 Hz, 1H), 3.54 (dd, *J* = 8.8, 4.8 Hz, 1H), 5.64 (s, 1H), 6.87 (t, *J* = 8.2 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 7.20–7.27 (m, 3H), 7.34 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.47 (td, *J* = 8.2, 1.4 Hz, 1H), 7.60 (d, *J* = 8.2, 1.4 Hz, 1H), 12.31 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 17.2, 38.6, 50.7, 79.9, 86.0, 118.2, 118.6, 118.86, 118.89, 118.91, 126.8, 127.2, 129.7, 136.3, 145.2, 148.3, 163.0, 205.1. HRMS (ESI) calcd for $C_{18}H_{16}NaO_3$ $(M+Na)^+$ 303.0992, found 303.0987.



3bi

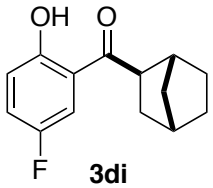
Compound 3bi (Scheme 2, 42.7 mg, 93% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.18 (d, *J* = 10.2 Hz, 1H), 1.29–1.34 (m, 1H), 1.41–1.46 (m, 2H), 1.49–1.67 (m, 3H), 1.97–2.02 (m, 1H), 2.31 (s, 3H), 2.35 (s, 1H), 2.53 (s, 1H), 3.22 (dd, *J* = 8.2, 5.4 Hz, 1H), 6.87 (d, *J* = 8.2 Hz, 1H), 7.25 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.78 (d, *J* = 2.0 Hz, 1H), 12.31 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 20.7, 28.9, 29.6, 34.1, 36.2, 36.4, 41.3, 49.1, 118.3, 127.7, 129.7, 136.8, 160.9, 207.8. HRMS (ESI) calcd for $C_{15}H_{17}O_2$ $(M–H)^–$ 229.1234, found 229.1238.



3ci

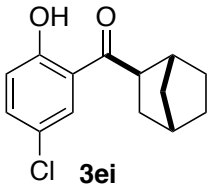
Compound 3ci (Scheme 2, 48.9 mg, 99% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.18 (d, *J* = 10.2 Hz, 1H), 1.29–1.34 (m, 1H), 1.41–1.46 (m, 1H), 1.49–1.67 (m, 4H), 1.97–2.02 (m, 1H), 2.31 (s, 3H), 2.36 (s, 1H), 2.53

(s, 1H), 3.22 (dd, J = 8.8, 5.4 Hz, 1H), 6.87 (d, J = 8.2 Hz, 1H), 7.25 (dd, J = 8.2, 2.0 Hz, 1H), 7.52 (d, J = 2.0 Hz, 1H), 12.31 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.9, 29.6, 33.9, 36.2, 36.3, 41.3, 49.3, 56.0, 113.4, 118.2, 119.3, 123.2, 151.5, 157.3, 207.3. HRMS (ESI) calcd for $C_{15}H_{18}NaO_3$ $(M+Na)^+$ 269.1148, found 269.1150.



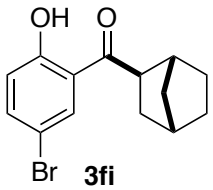
3di

Compound 3di (Scheme 2, 46.0 mg, 98% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.19 (d, J = 9.5 Hz, 1H), 1.29–1.34 (m, 1H), 1.39–1.47 (m, 2H), 1.49–1.68 (m, 3H), 1.98–2.04 (m, 1H), 2.37 (s, 1H), 2.53 (s, 1H), 3.14 (dd, J = 8.9, 5.5 Hz, 1H), 6.93 (dd, J = 8.9, 4.8 Hz, 1H), 7.15–7.21 (m, 1H), 7.41 (dd, J = 9.2, 3.1 Hz, 1H), 12.18 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.8, 29.6, 33.8, 36.2, 36.3, 41.4, 49.4, 114.9, (d, $J_{F\text{-}C}$ = 23 Hz), 118.2 (d, $J_{F\text{-}C}$ = 6 Hz), 119.8 (d, $J_{F\text{-}C}$ = 7 Hz), 123.4 (d, $J_{F\text{-}C}$ = 23 Hz), 154.7 (d, $J_{F\text{-}C}$ = 238 Hz), 159.1, 207.0. HRMS (ESI) calcd for $C_{14}H_{14}FO_2$ $(M–H)^–$ 233.0983, found 233.0979.



3ei

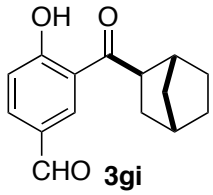
Compound 3ei (Scheme 2, 46.1 mg, 92% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.20 (d, J = 10.9 Hz, 1H), 1.29–1.34 (m, 1H), 1.40–1.46 (m, 2H), 1.50–1.69 (m, 3H), 1.96–2.01 (m, 1H), 2.37 (s, 1H), 2.53 (s, 1H), 3.16 (dd, J = 9.2, 5.8 Hz, 1H), 6.93 (d, J = 8.8 Hz, 1H), 7.38 (dd, J = 8.8, 2.7 Hz, 1H), 7.69 (d, J = 2.7 Hz, 1H), 12.37 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.9, 29.6, 34.1, 36.2, 36.4, 41.3, 49.3, 119.3, 120.2, 123.4, 129.2, 135.7, 161.5, 207.1. HRMS (ESI) calcd for $C_{14}H_{14}ClO_2$ $(M–H)^–$ 249.0688, found 249.0685.



3fi

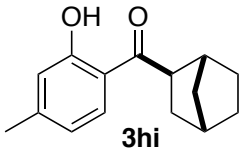
Compound 3fi (Scheme 2, 54.3 mg, 92% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.20 (d, J = 9.5 Hz, 1H), 1.29–1.34 (m, 1H), 1.40–1.46 (m, 2H), 1.50–1.69 (m, 3H), 1.95–2.00 (m, 1H), 2.37 (s, 1H), 2.53 (s, 1H), 3.16 (dd,

J = 8.8, 5.4 Hz, 1H), 6.88 (d, J = 8.9 Hz, 1H), 7.51 (dd, J = 8.9, 2.4 Hz, 1H), 7.83 (d, J = 2.4 Hz, 1H), 12.39 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.8, 29.6, 34.1, 36.2, 36.4, 41.2, 49.3, 110.3, 119.9, 120.6, 132.3, 138.5, 161.9, 207.0. HRMS (ESI) calcd for $C_{14}H_{14}BrO_2$ $(M–H)^-$ 293.0183, found 293.0177.



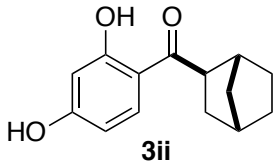
3gi

Compound 3gi (Scheme 2, 45.6 mg, 93% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.22 (d, J = 10.0 Hz, 1H), 1.31–1.36 (m, 1H), 1.42–1.45 (m, 2H), 1.57–1.69 (m, 3H), 1.95–2.01 (m, 1H), 2.38 (s, 1H), 2.55 (s, 1H), 3.31 (dd, J = 9.1, 6.4 Hz, 1H), 7.08 (d, J = 9.1 Hz, 1H), 7.96 (d, J = 9.1 Hz, 1H), 8.30 (s, 1H), 9.89 (s, 1H), 13.07 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.8, 29.6, 34.3, 36.3, 36.5, 41.2, 49.2, 118.4, 119.7, 128.0, 133.0, 136.3, 168.0, 189.8, 208.0. HRMS (ESI) calcd for $C_{15}H_{15}O_3$ $(M–H)^-$ 243.1027, found 243.1027.



3hi

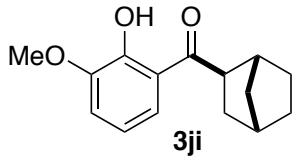
Compound 3hi (Scheme 2, 43.4 mg, 94% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.18 (d, J = 10.2 Hz, 1H), 1.28–1.33 (m, 1H), 1.40–1.46 (m, 2H), 1.50 (ddd, J = 10.2, 9.2, 2.8 Hz, 1H), 1.57–1.67 (m, 2H), 1.99–2.04 (m, 1H), 2.34 (s, 3H), 2.36 (s, 1H), 2.52 (s, 1H), 3.21 (dd, J = 8.8, 5.4 Hz, 1H), 6.69 (d, J = 8.2 Hz, 1H), 6.78 (s, 1H), 7.64 (d, J = 8.2 Hz, 1H), 12.50 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 21.8, 28.9, 29.7, 33.9, 36.2, 36.3, 41.5, 49.1, 116.5, 118.6, 119.9, 129.9, 147.3, 163.1, 207.3. HRMS (ESI) calcd for $C_{15}H_{17}O_2$ $(M–H)^-$ 229.1234, found 229.1238.



3ii

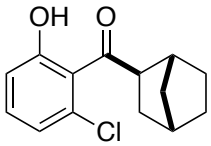
Compound 3ii (Scheme 2, 45.3 mg, 97% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.18 (d, J = 9.1 Hz, 1H), 1.25–1.33 (m, 1H), 1.39–1.53 (m, 3H), 1.56–1.70 (m, 2H), 1.99–2.05 (m, 1H), 2.36 (s, 1H), 2.51 (s, 1H), 3.15 (dd, J = 9.1, 5.5 Hz, 1H), 5.36 (br s, 1H), 6.37 (s, 1H), 6.38 (d, J = 9.1 Hz, 1H), 7.68 (d, J = 9.1 Hz, 1H), 12.90 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.9, 29.7, 33.9, 36.2, 36.4, 41.5, 48.9, 103.6, 107.5, 113.2,

132.3, 162.0, 165.5, 206.4. HRMS (ESI) calcd for $C_{14}H_{15}O_3$ $(M–H)^-$ 231.1027, found 231.1030.



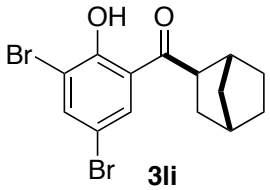
3ji

Compound 3ji (Scheme 2, 45.8 mg, 93% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.17 (d, *J* = 10.0 Hz, 1H), 1.27–1.32 (m, 1H), 1.39–1.44 (m, 2H), 1.47–1.53 (m, 1H), 1.55–1.66 (m, 2H), 1.99–2.02 (m, 1H), 2.35 (s, 1H), 2.53 (s, 1H), 3.22 (dd, *J* = 8.6, 5.9 Hz, 1H), 3.89 (s, 3H), 6.81 (t, *J* = 8.2 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 12.80 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.9, 29.7, 33.8, 36.2, 36.3, 41.5, 49.6, 56.2, 116.4, 117.9, 118.7, 121.3, 149.1, 153.4, 208.3. HRMS (ESI) calcd for $C_{15}H_{18}NaO_3$ $(M+Na)^+$ 269.1148, found 269.1147.



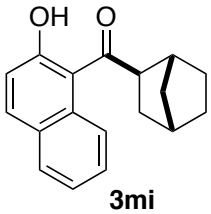
3ki

Compound 3ki (Scheme 2, 46.4 mg, 92% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.15 (d, *J* = 10.2 Hz, 1H), 1.23–1.30 (m, 1H), 1.36–1.42 (m, 1H), 1.48–1.62 (m, 4H), 1.99–2.02 (m, 1H), 2.34 (s, 1H), 2.53 (s, 1H), 3.67 (dd, *J* = 8.5, 5.8 Hz, 1H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.94 (d, *J* = 8.2 Hz, 1H), 7.24 (t, *J* = 8.2 Hz, 1H), 11.19 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.7, 29.9, 34.2, 36.2, 36.4, 42.3, 53.6, 117.2, 121.1, 122.3, 133.6, 133.7, 162.0, 209.6. HRMS (ESI) calcd for $C_{14}H_{14}ClO_2$ $(M–H)^-$ 249.0688, found 249.0681.



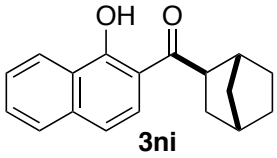
3li

Compound 3li (Scheme 2, 72.8 mg, 97% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.21 (d, *J* = 10.0 Hz, 1H), 1.29–1.34 (m, 1H), 1.39–1.45 (m, 2H), 1.52–1.69 (m, 3H), 1.94–1.99 (m, 1H), 2.38 (s, 1H), 2.53 (s, 1H), 3.16 (dd, *J* = 8.6, 5.9 Hz, 1H), 7.818 (s, 1H), 7.824 (s, 1H), 13.12 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.8, 29.5, 34.2, 36.3, 36.4, 41.3, 49.4, 110.2, 113.4, 120.2, 131.6, 140.9, 158.6, 206.8. HRMS (ESI) calcd for $C_{14}H_{13}Br_2O_2$ $(M–H)^-$ 370.9288, found 370.9283.



3mi

Compound 3mi (Scheme 2, 47.4 mg, 89% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.21–1.30 (m, 1H), 1.32–1.39 (m, 1H), 1.53–1.63 (m, 3H), 1.91 (d, *J* = 10.0 Hz, 1H), 2.00–2.05 (m, 1H), 2.40 (s, 1H), 2.58 (s, 1H), 3.46 (dd, *J* = 8.2, 5.4 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 1H), 7.37 (t, *J* = 9.1 Hz, 1H), 7.54 (t, *J* = 9.1 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.84 (d, *J* = 9.1 Hz, 1H), 8.03 (d, *J* = 9.1 Hz, 1H), 12.29 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 28.5, 29.9, 36.2, 36.3, 36.6, 42.9, 53.3, 115.8, 119.6, 123.7, 124.5, 127.7, 128.6, 129.3, 131.7, 136.2, 161.5, 211.2. HRMS (ESI) calcd for $C_{18}H_{17}O_2$ $(M–H)^-$ 265.1234, found 265.1230.



3ni

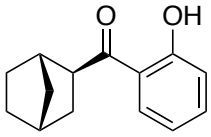
Compound 3ni (Scheme 2, 47.1 mg, 88% yield). A solution of hexane/EtOAc (5:1) was used for preparative TLC on silica gel. ^{1}H NMR ($CDCl_3$) δ 1.20 (d, *J* = 10.0 Hz, 1H), 1.31–1.36 (m, 1H), 1.45–1.70 (m, 5H), 2.07–2.12 (m, 1H), 2.39 (s, 1H), 2.60 (s, 1H), 3.30 (dd, *J* = 8.6, 5.9 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 1H), 7.51 (t, *J* = 8.1 Hz, 1H), 7.61 (t, *J* = 8.1 Hz, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 8.45 (d, *J* = 8.1 Hz, 1H), 14.20 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 29.0, 29.7, 33.7, 36.32, 36.35, 41.5, 49.5, 112.2, 118.0, 124.4, 124.5, 125.5, 125.8, 127.3, 129.8, 137.0, 162.9, 207.7. HRMS (ESI) calcd for $C_{18}H_{17}O_2$ $(M–H)^-$ 265.1234, found 265.1233.

8. General procedure for iridium-catalyzed asymmetric hydroacylation of 2-norbornene (2i) with 2-hydroxybenzaldehydes 1 (Scheme 3)

[IrCl((*S*,*S*)-Me-tfb*)]$_2$ (4.8 mg, 0.010 mmol of Ir, 5 mol% of Ir), Na_2CO_3 (2.2 mg, 0.020 mmol), and 2-norbornene (**2i**) (0.40 mmol) were placed in a Schlenk tube under N_2. Toluene (0.8 mL) was added and the mixture was stirred at 0°C for a few minutes. 2-Hydroxybenzaldehydes **1** (0.20 mmol) was added, and the Schlenk tube was capped with a glass stopper and the mixture was stirred at 10 °C for 48 h. The mixture was passed through a short column of silica gel with EtOAc and the solvent was removed on a rotary evaporator. The residue was subjected to preparative TLC on silica gel with hexane/EtOAc to give **3**.

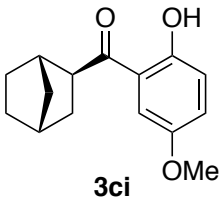
9. Data for Scheme 3

The absolute configuration of **3li** was determined to be 1*S*,2*S*,4*R* by X-ray crystallographic analysis of compound **4**, which was derived from **3li** and TsCl in pyridine (vide infra). For others, they were assigned by analogy with **3li**.



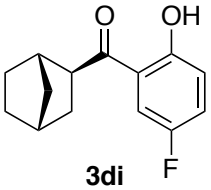
3ai

Compound 3ai (Scheme 3, 42.0 mg, 97% yield, 86% ee). The ee was measured by HPLC (Chiralcel OD-H column × 2, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 19.0 min (major), t_2 = 19.9 min (minor); $[\alpha]^{20}_D$ +30 (*c* 0.99, $CHCl_3$) for 86% ee (1*S*,2*S*,4*R*).



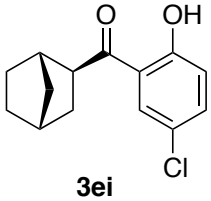
3ci

Compound 3ci (Scheme 3, 35.0 mg, 71% yield, 82% ee). The ee was measured by HPLC (Chiralpak AD–H column, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 12.1 min (minor), t_2 = 12.9 min (major); $[\alpha]^{20}_D$ +19 (*c* 1.01, $CHCl_3$) for 82% ee (1*S*,2*S*,4*R*).



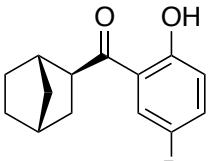
3di

Compound 3di (Scheme 3, 44.4 mg, 95% yield, 87% ee). The ee was measured by HPLC (Chiralpak AD–H column, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 9.0 min (minor), t_2 = 10.0 min (major); $[\alpha]^{20}_D$ +33 (*c* 1.00, $CHCl_3$) for 87% ee (1*S*,2*S*,4*R*).



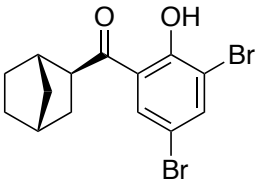
3ei

Compound 3ei (Scheme 3, 47.3 mg, 94% yield, 88% ee). The ee was measured by HPLC (Chiralpak AD–H column, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 8.6 min (minor), t_2 = 9.3 min (major); $[\alpha]^{20}_D$ +22 (*c* 1.01, $CHCl_3$) for 88% ee (1*S*,2*S*,4*R*).



3fi

Compound 3fi (Scheme 3, 55.6 mg, 94% yield, 87% ee). The ee was measured by HPLC (Chiralpak AD–H column, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 8.8 min (minor), t_2 = 9.3 min (major); $[\alpha]^{20}_D$ +18 (*c* 0.98, $CHCl_3$) for 87% ee (1*S*,2*S*,4*R*).



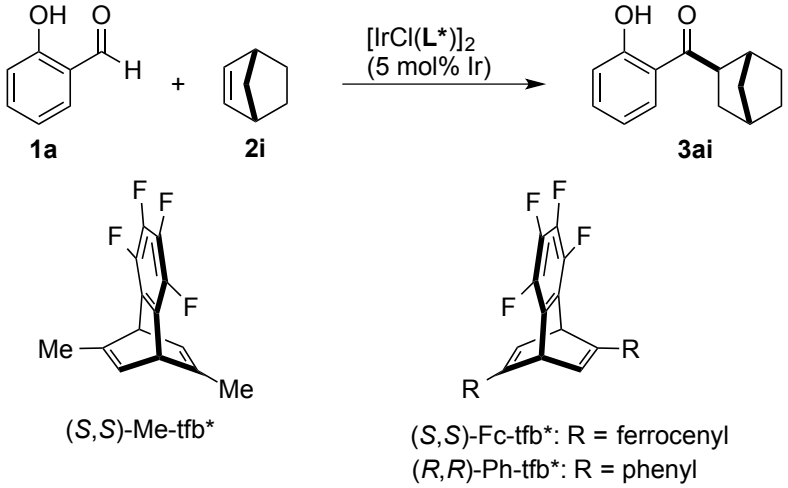
3li

Compound 3li (Scheme 3, 63.6 mg, 85% yield, 88% ee). The ee was measured by HPLC (Chiralcel OJ-H column × 2, hexane/2-propanol = 95:5, flow 0.5 mL/min, 254 nm, t_1 = 21.3 min (minor), t_2 = 22.1 min (major); $[\alpha]^{20}_D$ +20 (*c* 1.00, $CHCl_3$) for 88% ee (1*S*,2*S*,4*R*).

10. Condition screening of the asymmetric hydroacylation of 2-norbornene (2i) with salicylaldehyde (1a)

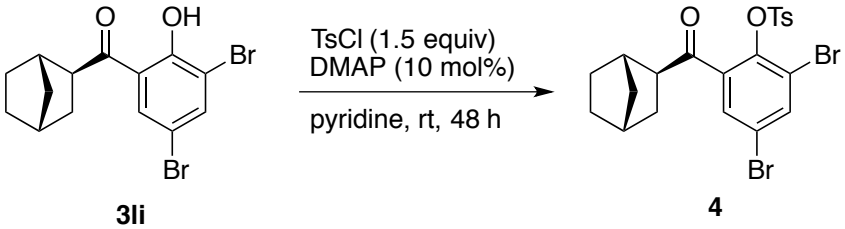
$[IrCl(R\text{-}tfb^*)]_2$ (0.0050 mmol of Ir, 5 mol% of Ir), base (0.010 mmol), and 2-norbornene (**2i**) (18.8 mg, 0.20 mmol) were placed in a Schlenk tube under N_2. Solvent (0.4 mL) and salicylaldehyde (**1a**) (12.2 mg, 0.10 mmol) was added successively, and the Schlenk tube was capped with a glass stopper. The mixture was stirred under the conditions shown in Table S1, and the mixture was passed through a short column of silica gel with EtOAc. The solvent was removed on a rotary evaporator. After an isolation of **3ai** by preparative TLC on silica gel with hexane/EtOAc, the ee was measure by chiral HPLC analysis (Daicel Chiralcel OD-H).

Table S1. Condition screening



Entry	Ligand	Base (mol%)	Solvent	Conditions	Yield [%]	Ee [%]
1	(*S*,*S*)-Me-tfb*	KOHaq (1 M, 10)	1,4-Dioxane	80 °C, 16 h	30	65
2	(*S*,*S*)-Fc-tfb*	KOHaq (1 M, 10)	1,4-Dioxane	80 °C, 16 h	65	52
3	(*R*,*R*)-Ph-tfb*	KOHaq (1 M, 10)	1,4-Dioxane	80 °C, 16 h	77	47
4	(*S*,*S*)-Me-tfb*	Na_2CO_3 (10)	1,4-Dioxane	60 °C, 12 h	98	69
5	(*S*,*S*)-Me-tfb*	Na_2CO_3 (10)	1,4-Dioxane	40 °C, 12 h	99	72
6	(*S*,*S*)-Me-tfb*	Na_2CO_3 (10)	1,4-Dioxane	25 °C, 12 h	91	75
7	(*S*,*S*)-Me-tfb*	Na_2CO_3 (10)	Toluene	25 °C, 24 h	93	82
8	(*S*,*S*)-Me-tfb*	Na_2CO_3 (10)	CH_2Cl_2	25 °C, 24 h	92	80
9	(*S*,*S*)-Me-tfb*	Na_2CO_3 (10)	Toluene	10 °C, 48 h	97	86

11. Transformation of 3li into 4



Compound **3li** (37.0 mg, 0.10 mmol, 88% ee), tosyl chloride (28.6 mg, 0.15 mmol), and 4-dimethylaminopyridine (DMAP, 1.2 mg, 0.010 mmol) in pyridine (0.40 mL) were stirred at room temperature for 48 h. Aqueous HCl (3 M, 0.50 mL) was added to the mixture and it was extracted with CH_2Cl_2. The organic layer was passed through a pad of silica gel with CH_2Cl_2 as an eluent, and concentrated on a rotary evaporator. The residue was subjected to preparative TLC on silica gel with hexane/CH_2Cl_2 (3:1) to give **4** as a white solid (33.3 mg, 0.063 mmol, 63% yield, 89% ee). The ee was measured by HPLC (Chiralpak ID column × 2, hexane/chloroform/ethanol = 180:60:1, flow 0.5 mL/min, 254 nm, t_1 = 49.9 min (minor), t_2 = 51.6 min (major); $[\alpha]^{20}_D$ –15 (*c* 0.50, $CHCl_3$)

for 89% ee (1*S*,2*S*,4*R*)). ^{1}H NMR ($CDCl_3$) δ 1.07 (d, *J* = 9.5 Hz, 1H), 1.18–1.27 (m, 2H), 1.33–1.40 (m, 2H), 1.46–1.54 (m, 2H), 1.80–1.86 (m, 1H), 2.27 (s, 2H), 2.45 (s, 3H), 3.10 (dd, *J* = 8.9, 5.5 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.56 (d, *J* = 2.0 Hz, 1H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.75 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 21.7, 28.7, 29.7, 33.4, 36.0, 36.2, 40.8, 52.9, 119.6, 121.0, 128.8, 130.0, 132.0, 132.1, 138.1, 138.2, 142.8, 146.4, 201.1. HRMS (ESI) calcd for $C_{21}H_{20}Br_2NaO_4S$ $(M+Na)^+$ 548,9348, found 548.9341.

12. X-Ray data of 4

A colorless crystal of **4** suitable for X-ray crystallographic analysis was obtained by recrystallization from CH_2Cl_2/methanol. The ORTEP drawing of **4** is shown in Figure S1. The crystal structure has been deposited at the Cambridge Crystallographic Centre (deposition number: CCDC 1402140). The data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

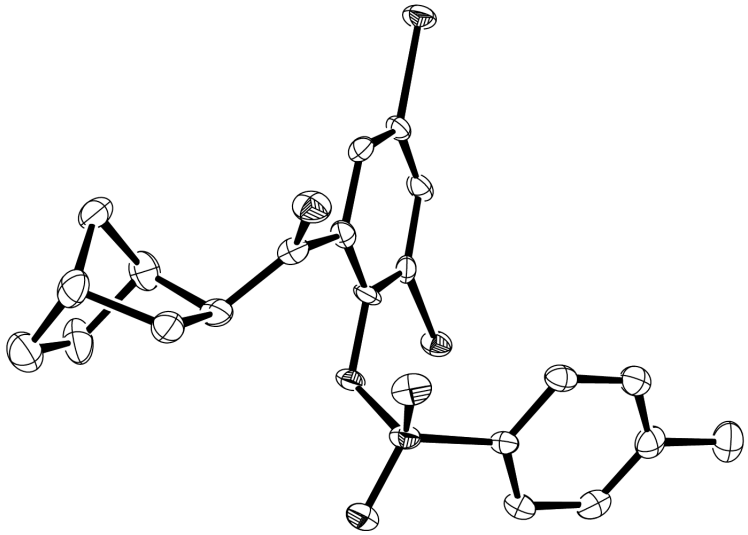


Figure S1. ORTEP illustration of (1*S*,2*S*,4*R*)-**4** with thermal ellipsoids drawn at 50% probability level (hydrogen atoms are omitted for clarity). One of four independent molecules is shown.

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).[15] The absolute structure was deduced based on Flack parameter 0.002(13).[16] The data for **4** are summarized in Table S2.

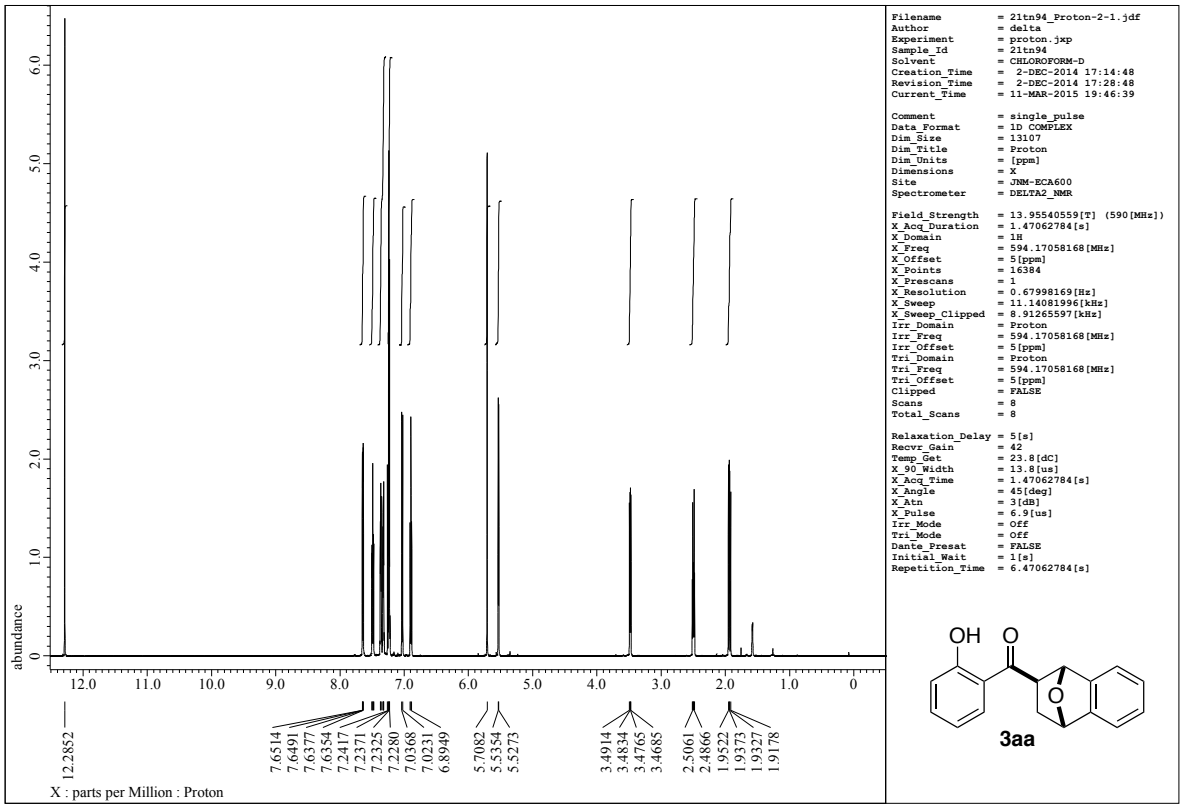
15 G. M. Sheldrick, Program for the solution and refinement of crystal structures, University of Göttingen, Göttingen, Germany, 1997.

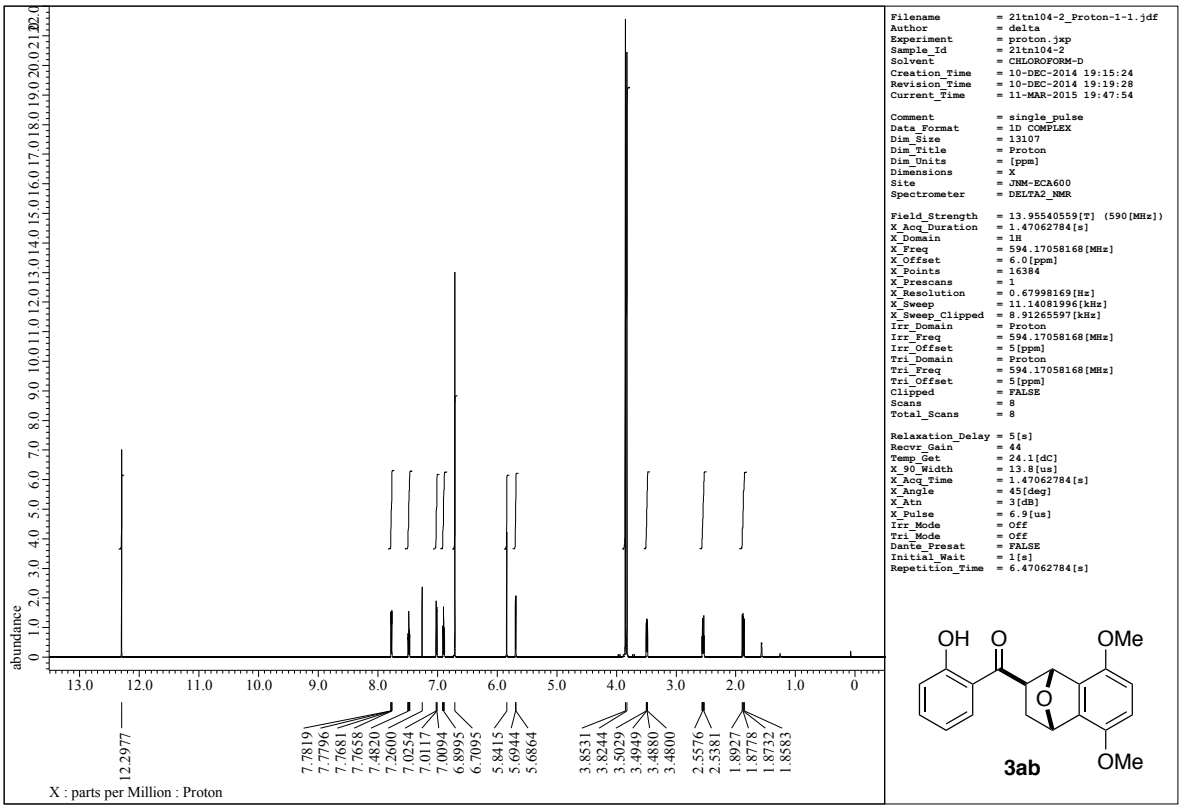
16 H. D. Flack, *Acta Cryst.*, 1983, **A39**, 876.

Table S2. Crystal data and structure refinement for **4**.

Empirical formula	$C_{21}H_{20}Br_2O_4S$
Formula weight	528.25
Temperature	93(2) K
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 10.927(3) Å
	b = 19.507(4) Å
	c = 19.810(6) Å
	β = 105.742(8)°
Volume	4064.2(19) $Å^3$
Z	4
Density (calculated) [Mg/m^3]	1.727
μ (mm^{-1})	6.237
F(000)	2112
No. of reflections	26845
Independent reflections	12241 [*R*(int) = 0.0371]
No. of parameters	1013
Completeness to θ (%)	97.7
Goodness-of-fit	1.048
R_1 [$I>2\sigma(I)$]	0.0346
wR_2 (all data)	0.0888
Flack parameter	0.002(13)
Largest diff. peak and hole [$e^-/Å^{-3}$]	0.906 and –0.773

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

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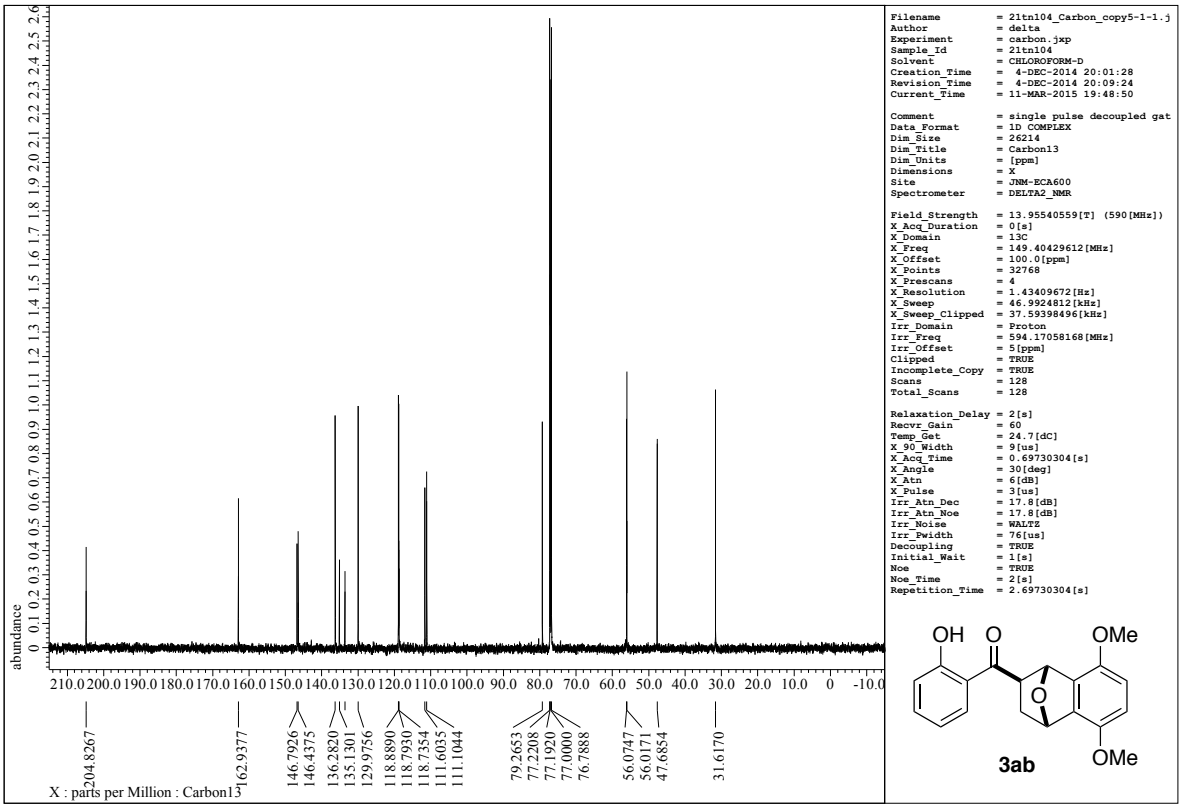
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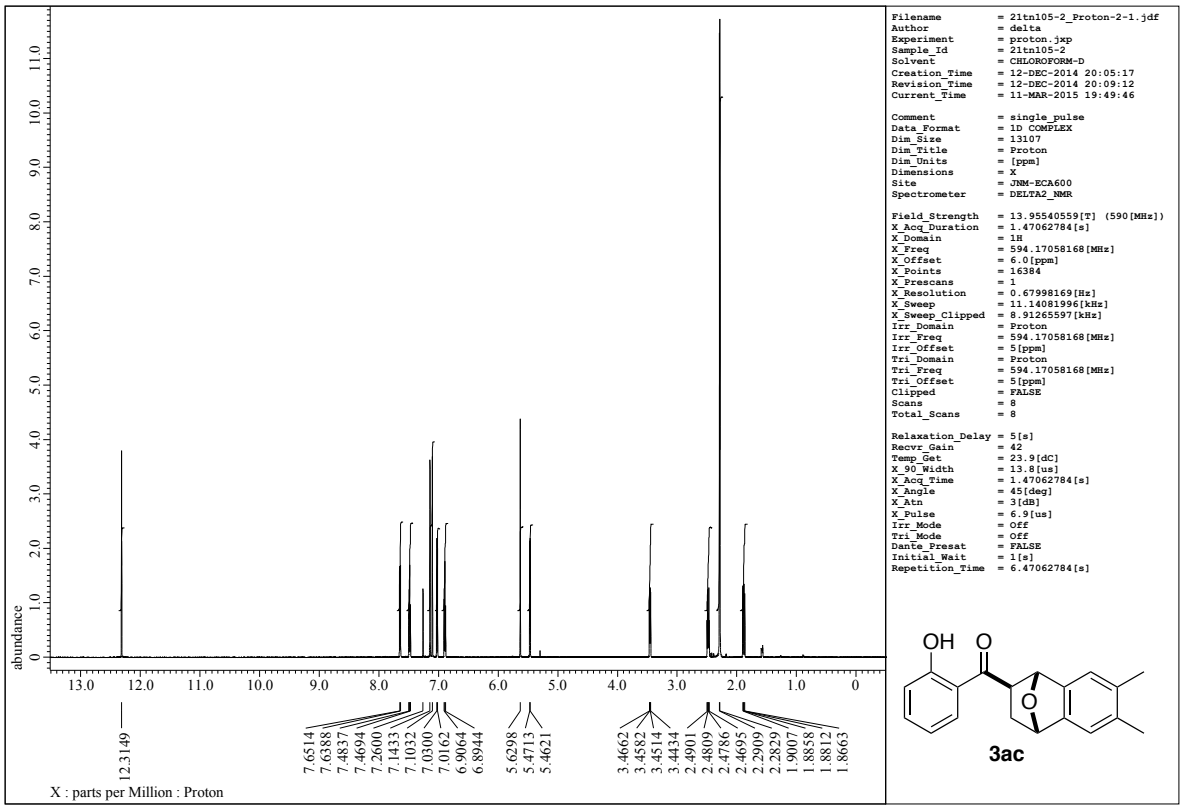
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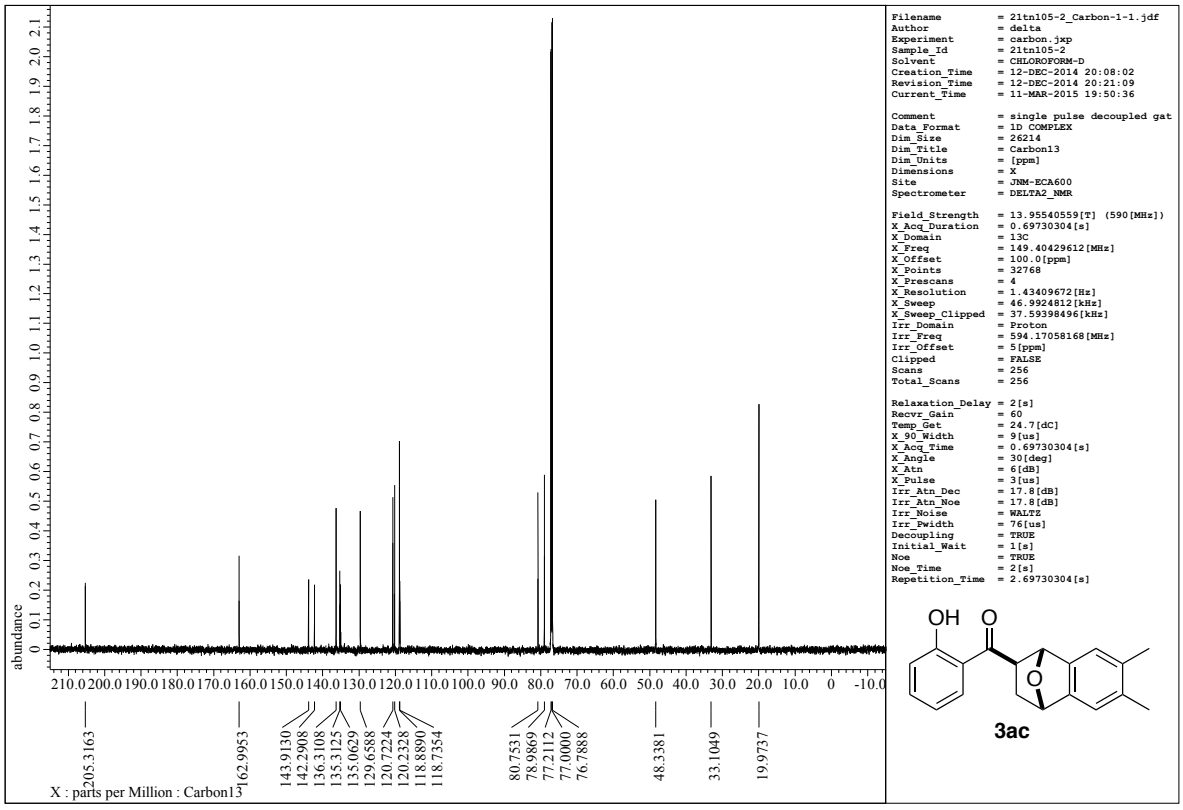
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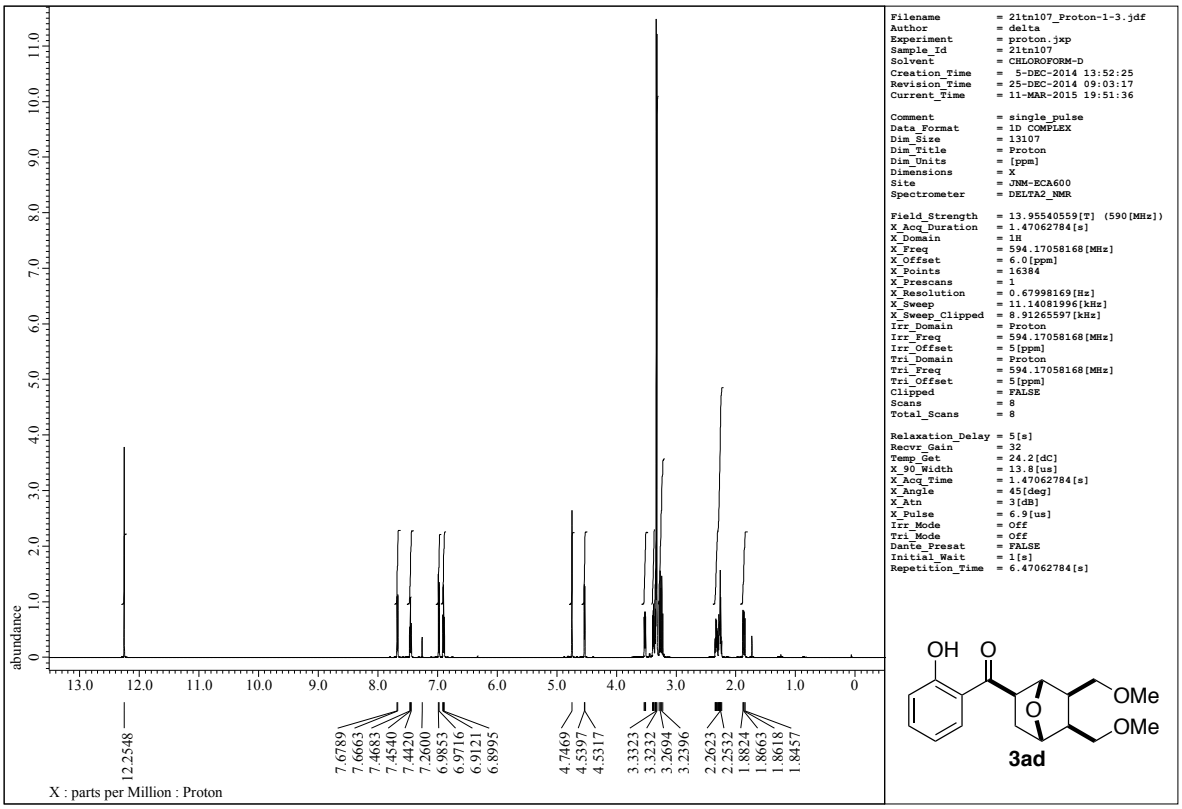
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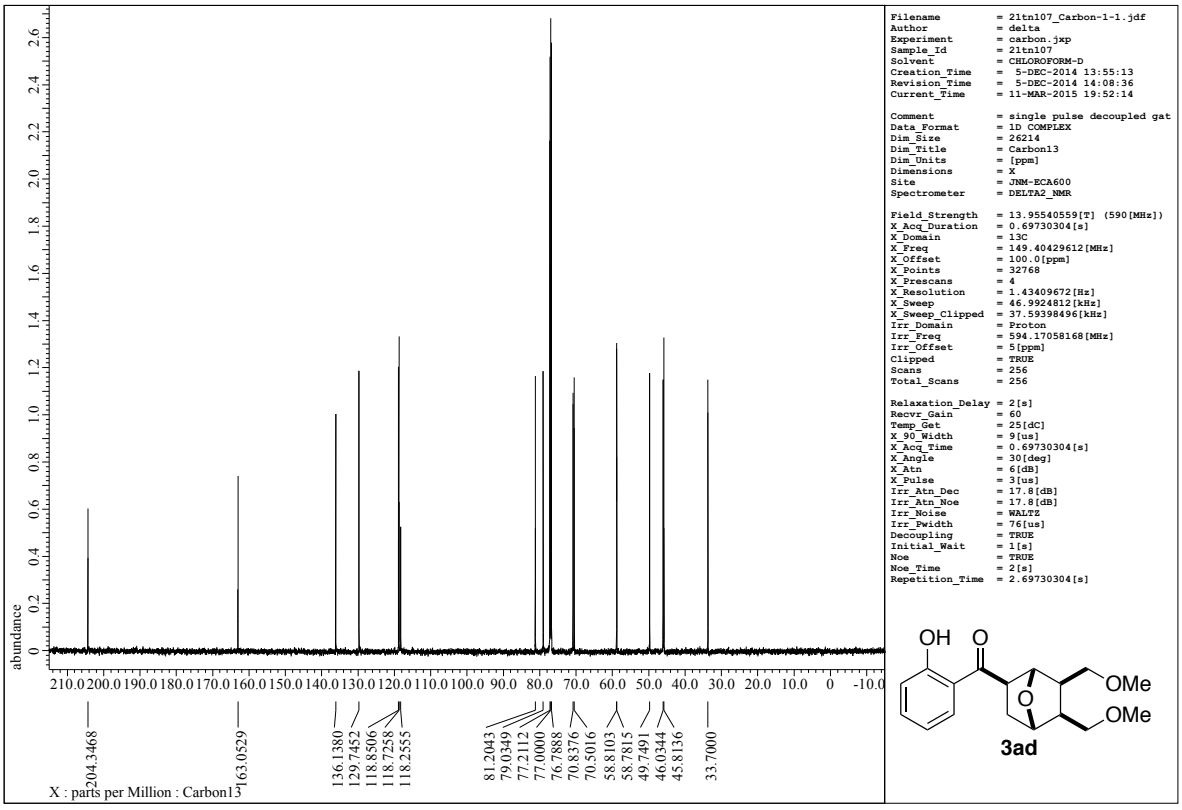
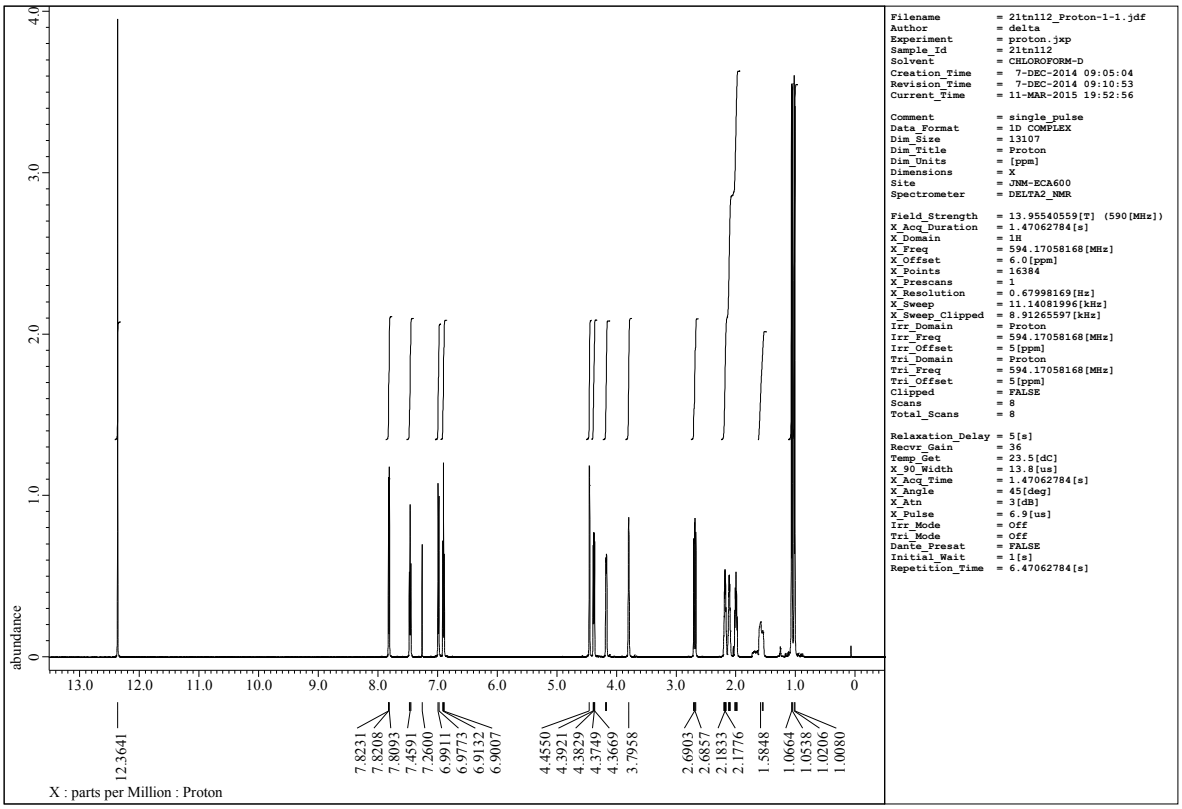
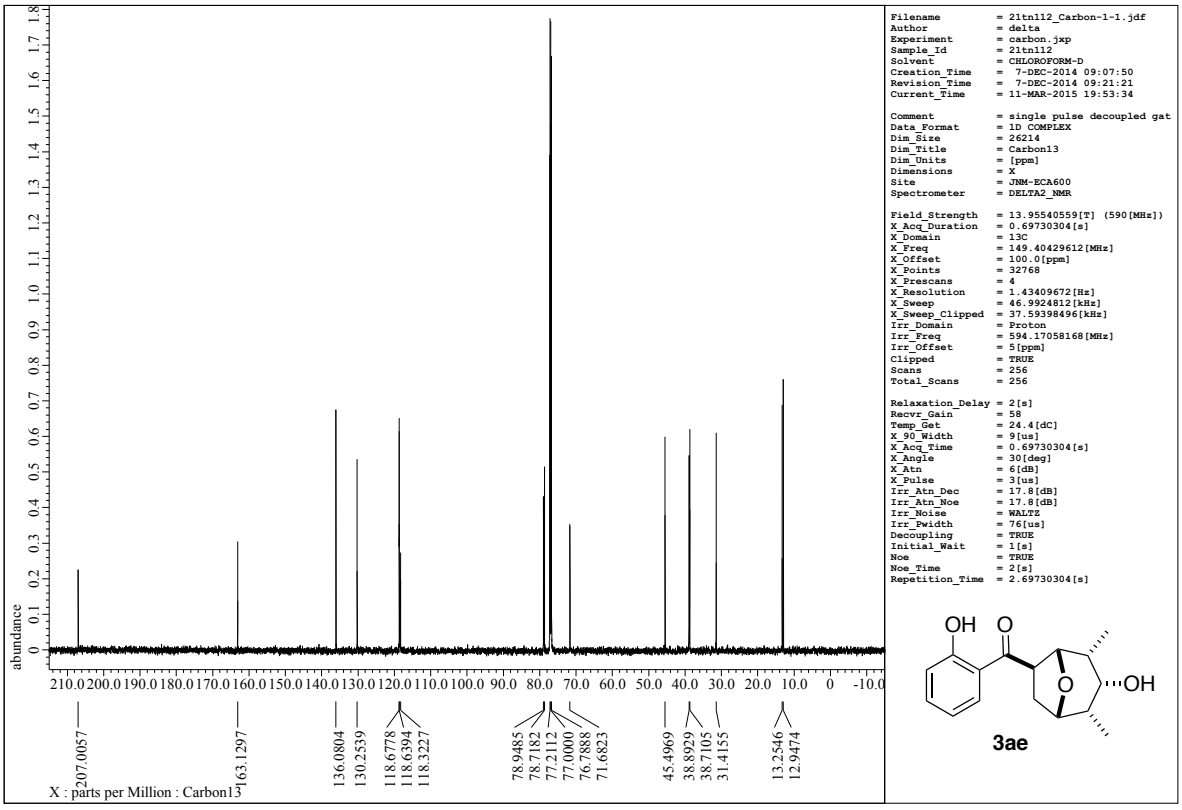
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 32
Temp_Get = 24.2[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]
OH
O
OMe
OMe
O
3ad


abundance
X : parts per Million : Carbon13
204.3468
163.0529
136.1380
129.7452
118.8506
118.7258
118.2555
81.2043
79.0349
77.2112
77.0000
76.7888
70.8376
70.5016
58.8103
58.7815
49.7491
46.0344
45.8136
33.7000
Filename = 21tn107_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn107
Solvent = CHLOROFORM-D
Creation_Time = 5-DEC-2014 13:55:13
Revision_Time = 5-DEC-2014 14:08:36
Current_Time = 11-MAR-2015 19:52:14
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 25[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]
OH
O
OMe
OMe
O
3ad

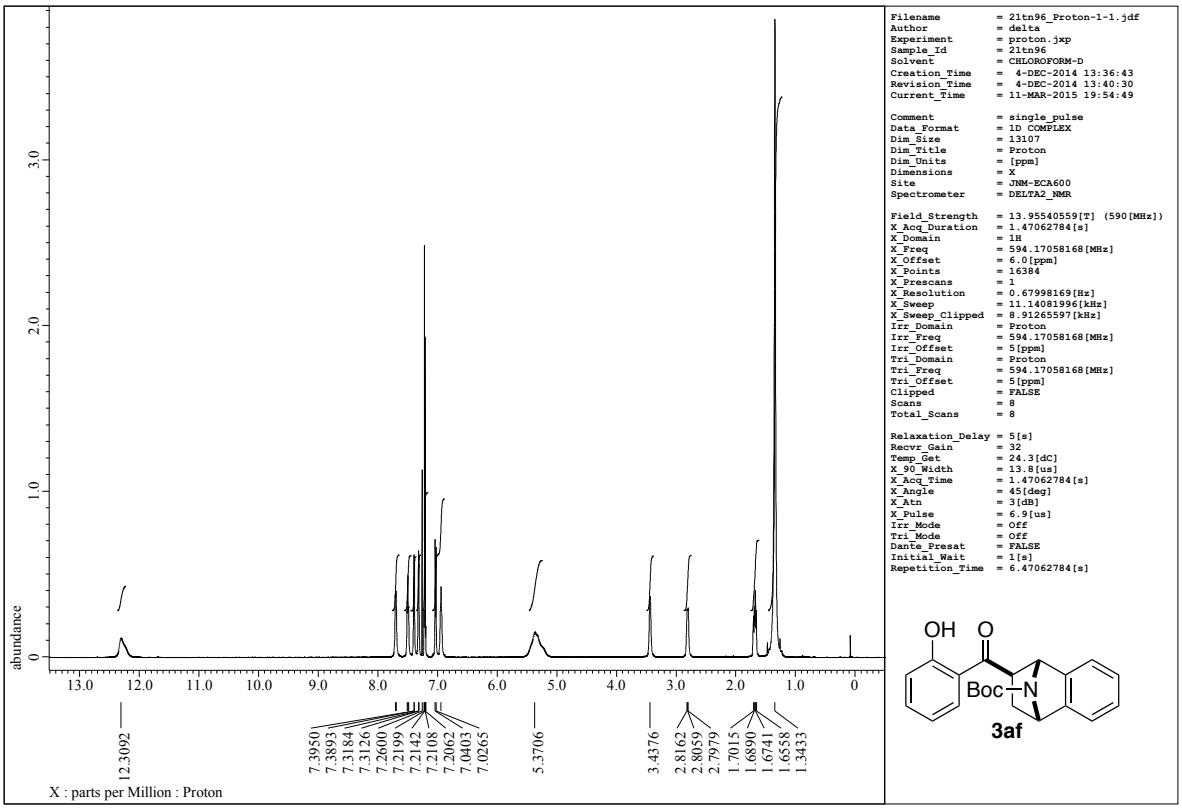


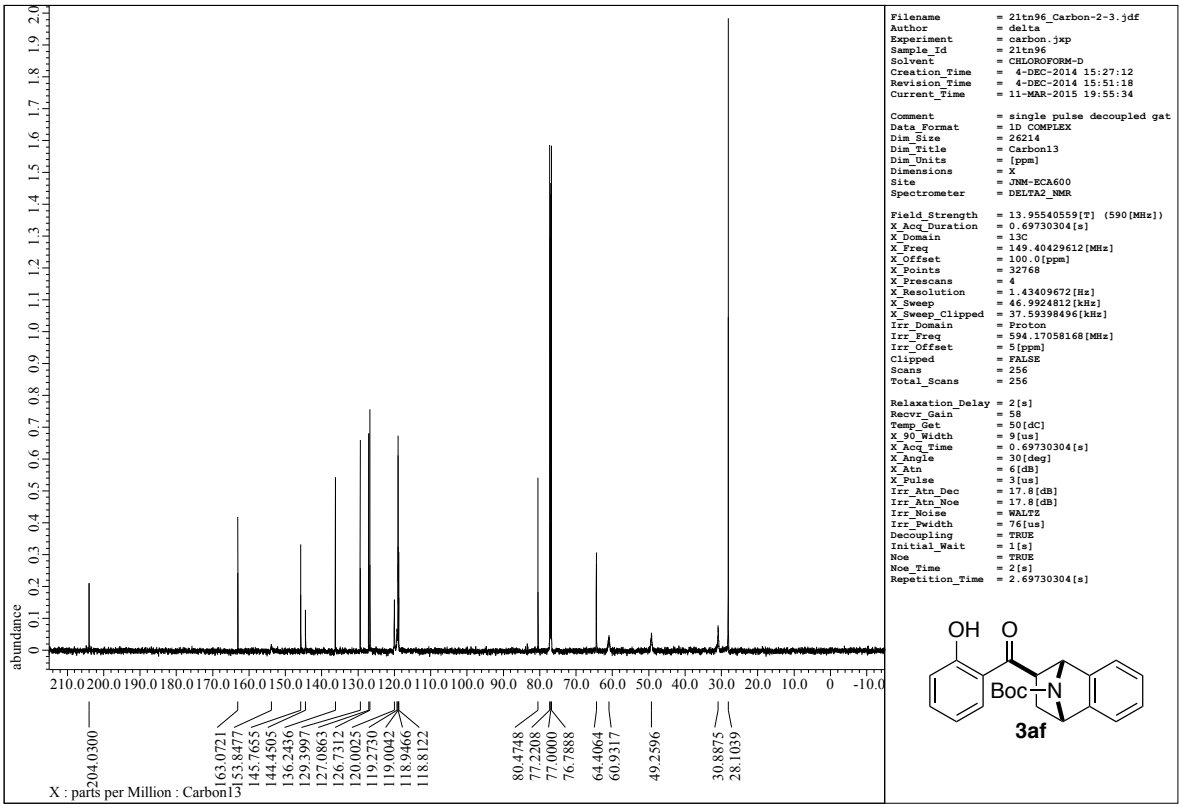

```
Filename          = 21tn112_Proton-1-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 21tn112
Solvent           = CHLOROFORM-D
Creation_Time     =  7-DEC-2014 09:05:04
Revision_Time     =  7-DEC-2014 09:10:53
Current_Time      = 11-MAR-2015 19:52:56

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA600
Spectrometer      = DELTA2_NMR

Field_Strength    = 13.95540559[T] (590[MHz])
X_Acq_Duration    = 1.47062784[s]
X_Domain          = 1H
X_Freq            = 594.17058168[MHz]
X_Offset          = 6.0[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          = 23.5[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]
```

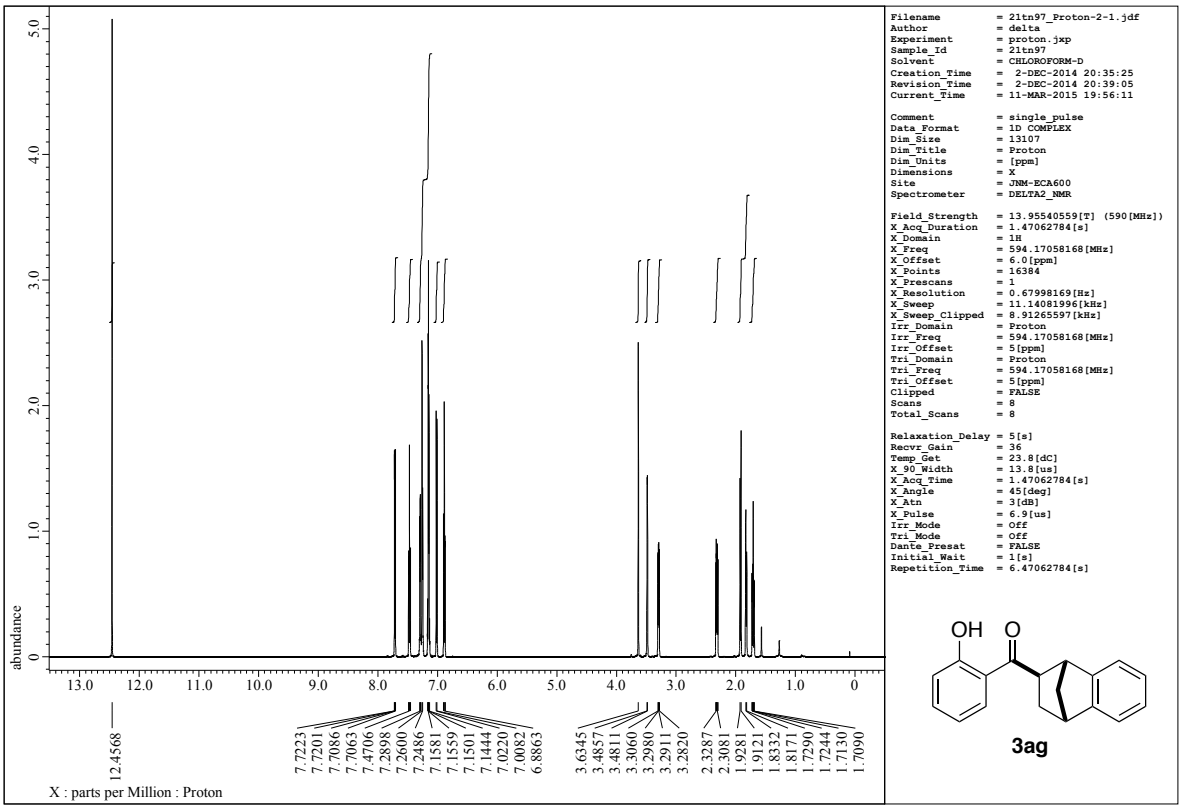


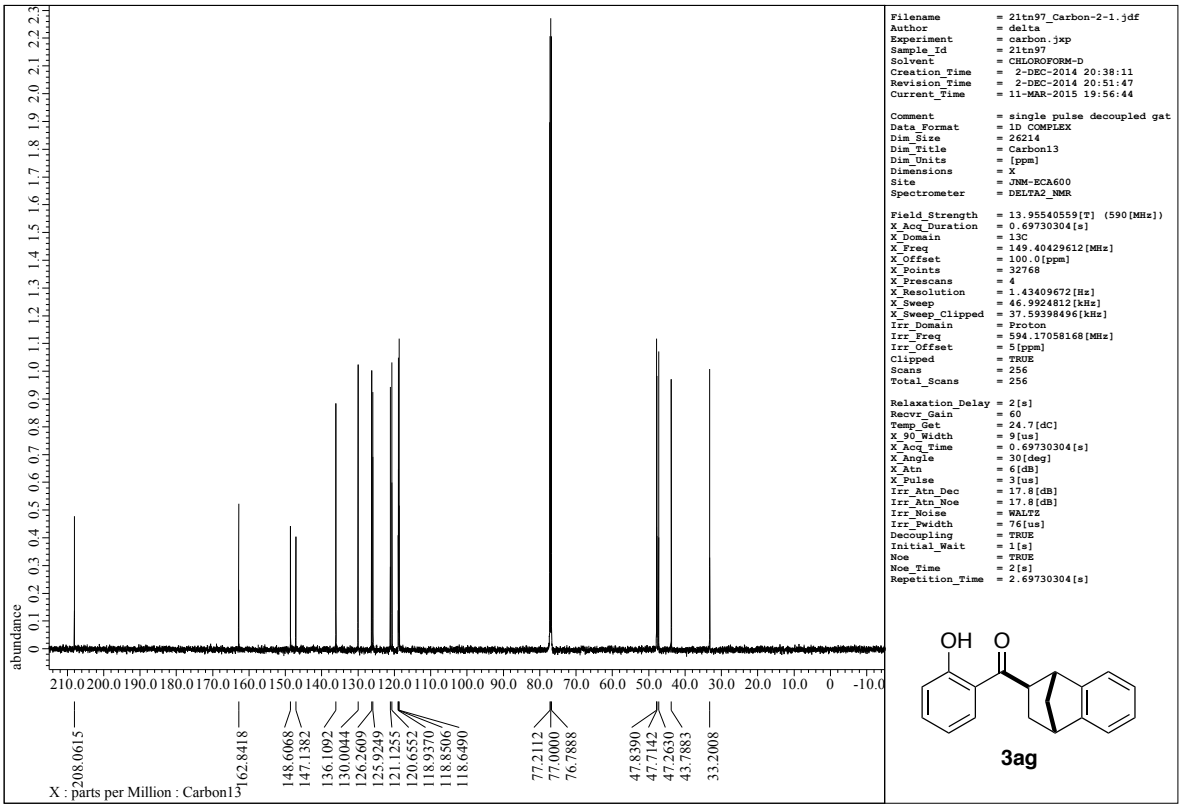

```
Filename          = 21tn112_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 21tn112
Solvent           = CHLOROFORM-D
Creation_Time     =  7-DEC-2014 09:07:50
Revision_Time     =  7-DEC-2014 09:21:21
Current_Time      = 11-MAR-2015 19:53:34

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA600
Spectrometer      = DELTA2_NMR

Field_Strength    = 13.95540559[T] (590[MHz])
X_Acq_Duration    = 0.69730304[s]
X_Domain          = 13C
X_Freq            = 149.40429612[MHz]
X_Offset          = 100.0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.43409672[Hz]
X_Sweep           = 46.9924812[kHz]
X_Sweep_Clipped   = 37.59398496[kHz]
Irr_Domain        = Proton
Irr_Freq          = 594.17058168[MHz]
Irr_Offset        = 5[ppm]
Clipped           = 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]
```

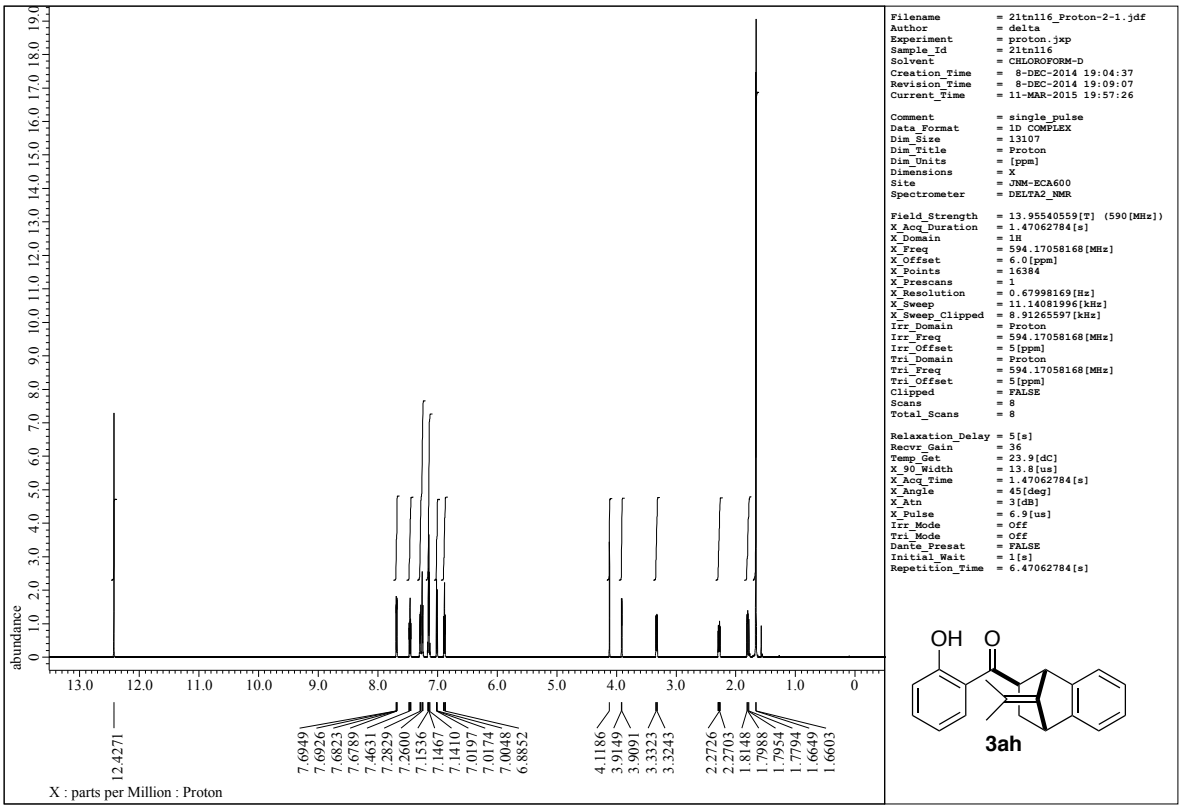

3ae

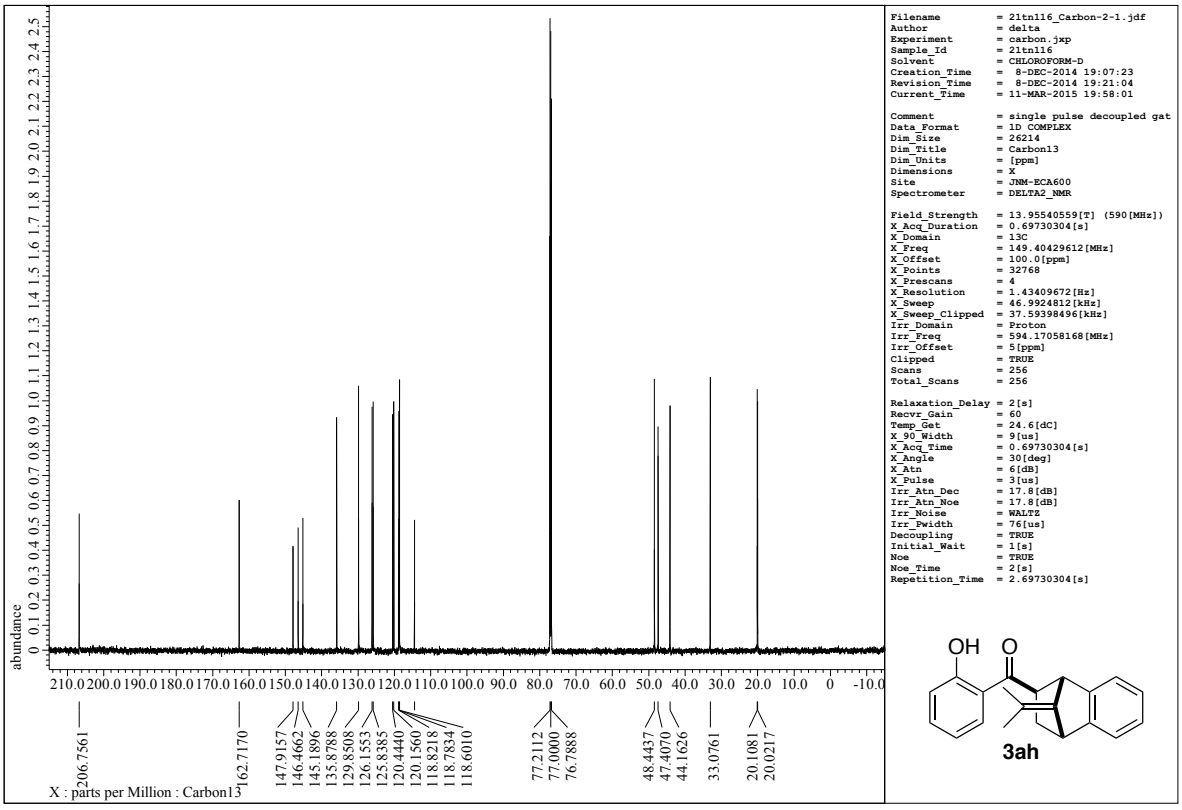

abundance
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.3092
7.3950
7.3893
7.3184
7.3126
7.2600
7.2199
7.2142
7.2108
7.2062
7.0403
7.0265
5.3706
3.4376
2.8162
2.8059
2.7979
1.7015
1.6890
1.6741
1.6558
1.3433
X : parts per Million : Proton
Filename = 21tn96_Proton-1-1.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn96
Solvent = CHLOROFORM-D
Creation_Time = 4-DEC-2014 13:36:43
Revision_Time = 4-DEC-2014 13:40:30
Current_Time = 11-MAR-2015 19:54:49
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 = 6.0[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 = 24.3[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]
OH O
Boc N
3af

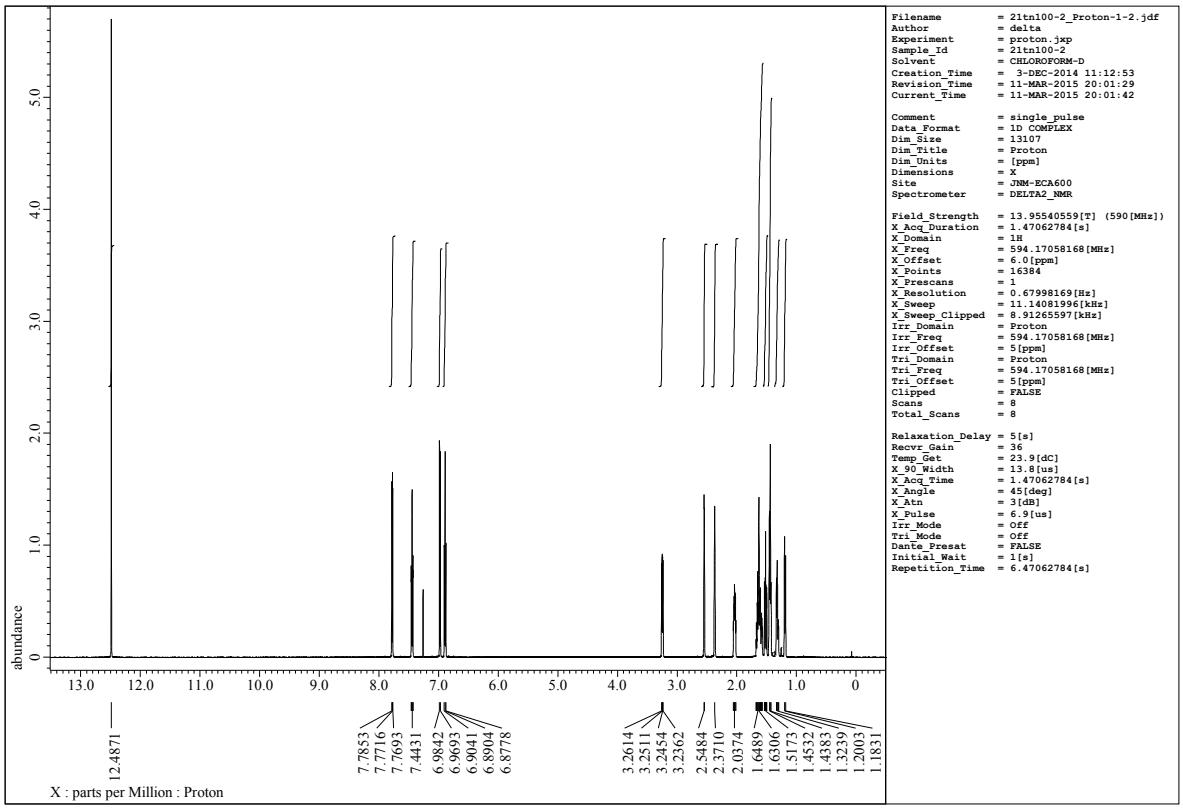

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
204.0300
163.0721
153.8477
145.7655
144.4505
136.2436
129.3997
127.0863
126.7312
120.0025
119.2730
119.0042
118.9466
118.8122
80.4748
77.2208
77.0000
76.7888
64.4064
60.9317
49.2596
30.8875
28.1039
X : parts per Million : Carbon13
Filename = 21tn96_Carbon-2-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn96
Solvent = CHLOROFORM-D
Creation_Time = 4-DEC-2014 15:27:12
Revision_Time = 4-DEC-2014 15:51:18
Current_Time = 11-MAR-2015 19:55:34
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 50[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]
OH O
Boc N
3af

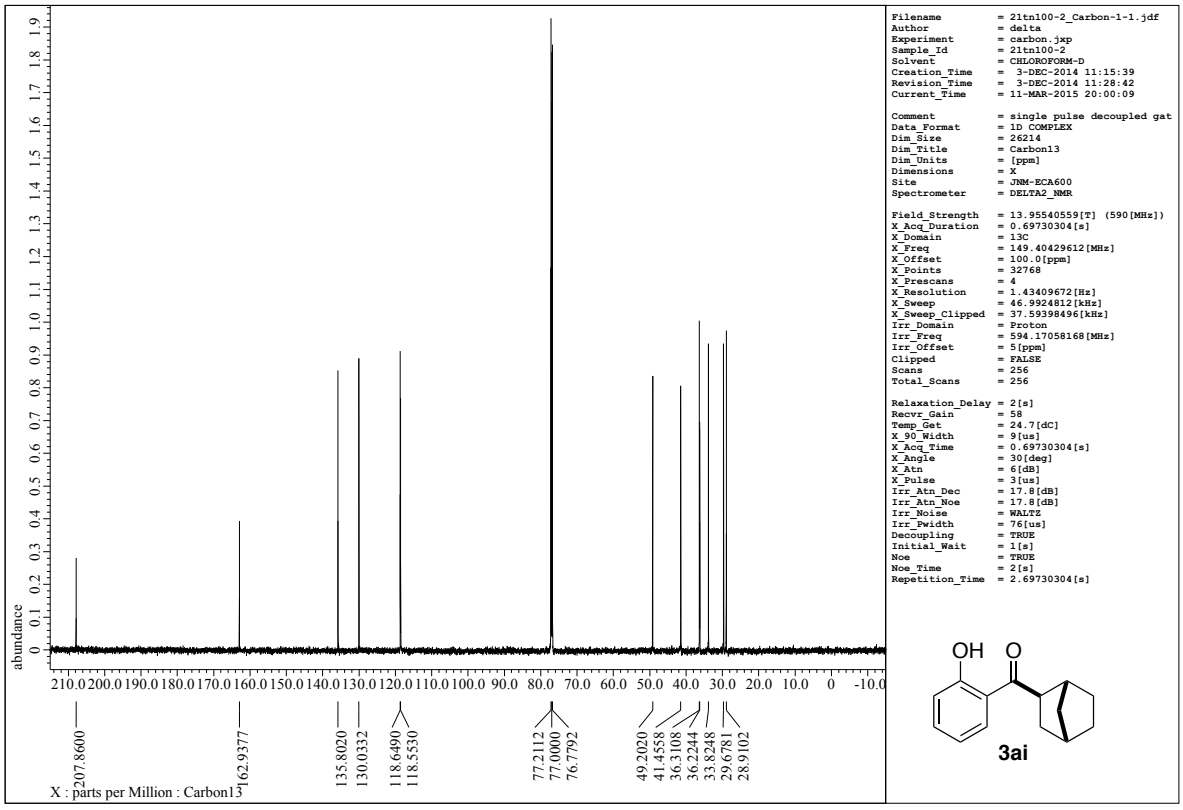

abundance
X : parts per Million : Proton
12.4568
7.7223
7.7201
7.7086
7.7063
7.4706
7.2898
7.2600
7.2486
7.1581
7.1559
7.1501
7.1444
7.0220
7.0082
6.8863
3.6345
3.4857
3.4811
3.3060
3.2980
3.2911
3.2820
2.3287
2.3081
1.9281
1.9121
1.8332
1.8171
1.7290
1.7244
1.7130
1.7090
Filename = 21tn97_Proton-2-1.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn97
Solvent = CHLOROFORM-D
Creation_Time = 2-DEC-2014 20:35:25
Revision_Time = 2-DEC-2014 20:39:05
Current_Time = 11-MAR-2015 19:56:11
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 = 6.0[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 = 23.8[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]
OH
O
3ag

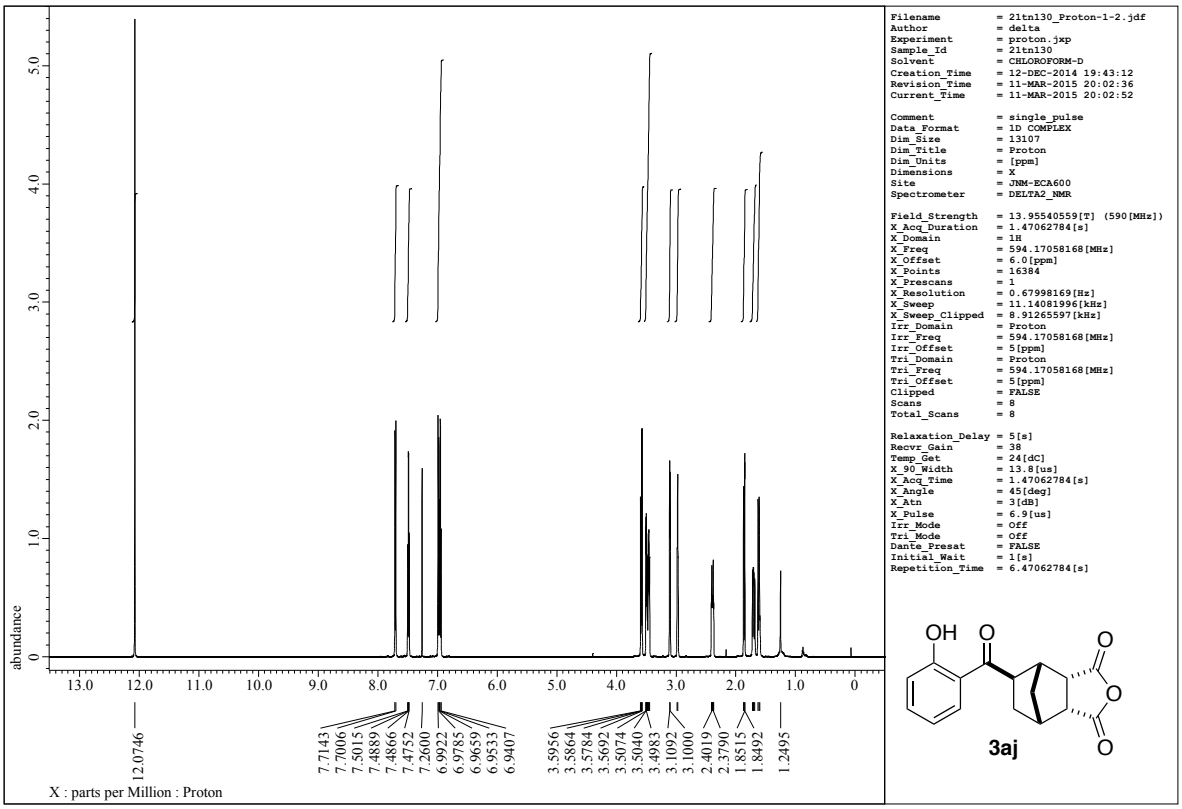

abundance
X : parts per Million : Carbon13
208.0615
162.8418
148.6068
147.1382
136.1092
130.0044
126.2609
125.9249
121.1255
120.6552
118.9370
118.8506
118.6490
77.2112
77.0000
76.7888
47.8390
47.7142
47.2630
43.7883
33.2008
Filename = 21tn97_Carbon-2-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn97
Solvent = CHLOROFORM-D
Creation_Time = 2-DEC-2014 20:38:11
Revision_Time = 2-DEC-2014 20:51:47
Current_Time = 11-MAR-2015 19:56:44
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 = 24.7[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]
OH
O
3ag

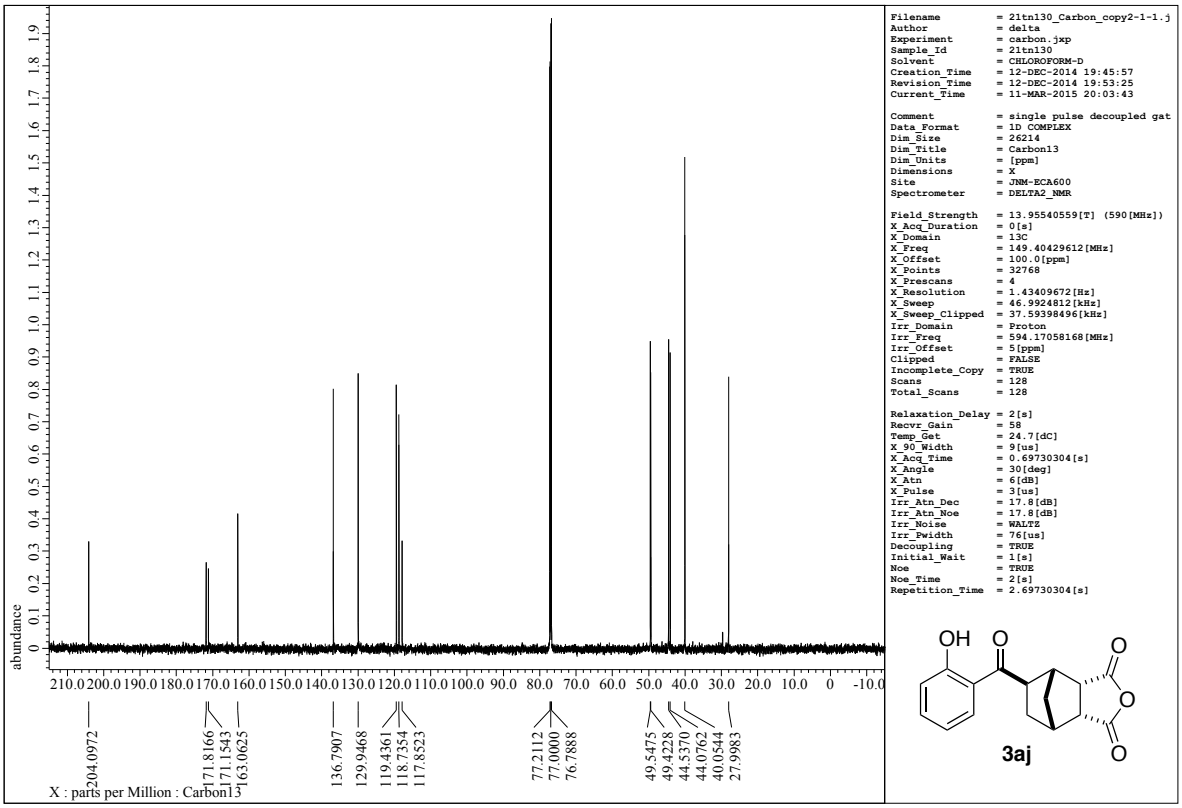

abundance
X : parts per Million : Proton
12.4271
7.6949
7.6926
7.6823
7.6789
7.4631
7.2829
7.2600
7.1536
7.1467
7.1410
7.0197
7.0174
7.0048
6.8852
4.1186
3.9149
3.9091
3.3323
3.3243
2.2726
2.2703
1.8148
1.7988
1.7954
1.7794
1.6649
1.6603
Filename = 21tn116_Proton-2-1.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn116
Solvent = CHLOROFORM-D
Creation_Time = 8-DEC-2014 19:04:37
Revision_Time = 8-DEC-2014 19:09:07
Current_Time = 11-MAR-2015 19:57:26
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 = 6.0[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 = 23.9[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]
OH
O
3ah

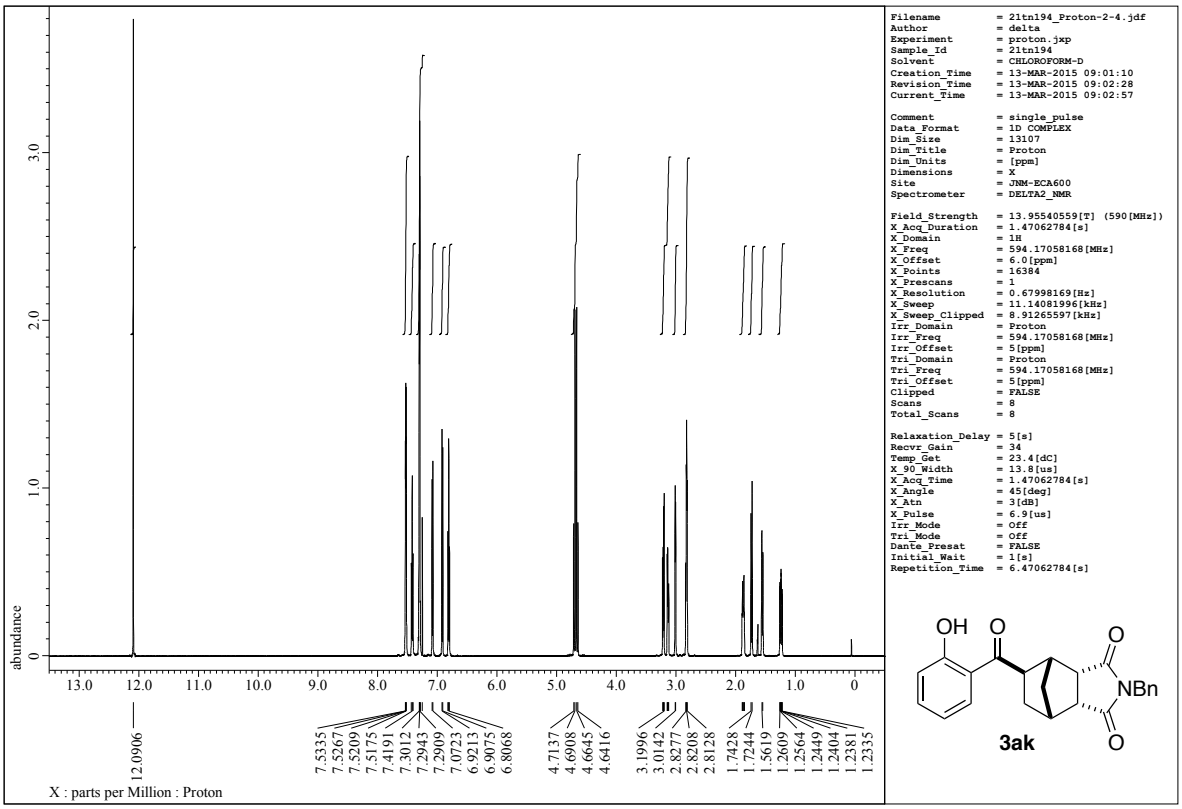

abundance
X : parts per Million : Carbon13
206.7561
162.7170
147.9157
146.4662
145.1896
135.8788
129.8508
126.1553
125.8385
120.4440
120.1560
118.8218
118.7834
118.6010
77.2112
77.0000
76.7888
48.4437
47.4070
44.1626
33.0761
20.1081
20.0217
Filename = 21tn116_Carbon-2-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn116
Solvent = CHLOROFORM-D
Creation_Time = 8-DEC-2014 19:07:23
Revision_Time = 8-DEC-2014 19:21:04
Current_Time = 11-MAR-2015 19:58:01
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
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]
OH
O
3ah

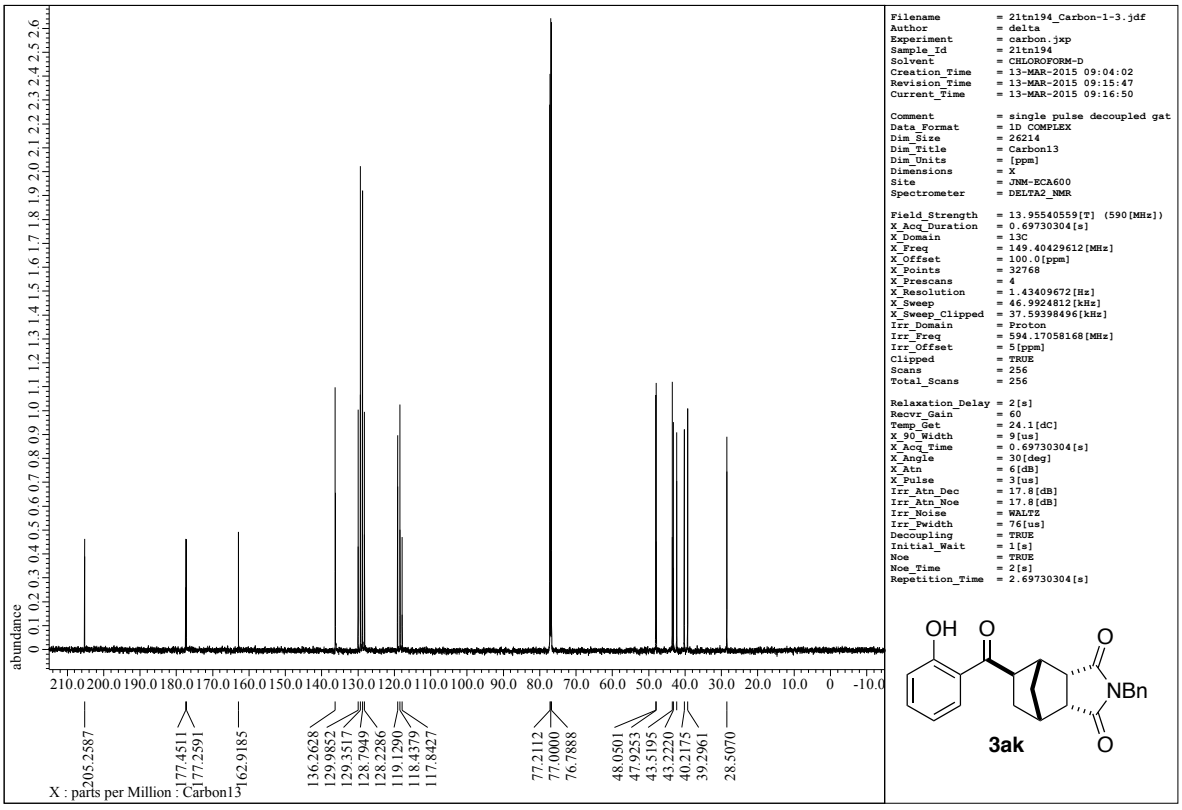

abundance
12.4871
7.7853
7.7716
7.7693
7.4431
6.9842
6.9693
6.9041
6.8904
6.8778
3.2614
3.2511
3.2454
3.2362
2.5484
2.3710
2.0374
1.6489
1.6306
1.5173
1.4532
1.4383
1.3239
1.2003
1.1831
X : parts per Million : Proton
Filename = 21tn100-2_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn100-2
Solvent = CHLOROFORM-D
Creation_Time = 3-DEC-2014 11:12:53
Revision_Time = 11-MAR-2015 20:01:29
Current_Time = 11-MAR-2015 20:01:42
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 = 6.0[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 = 23.9[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]

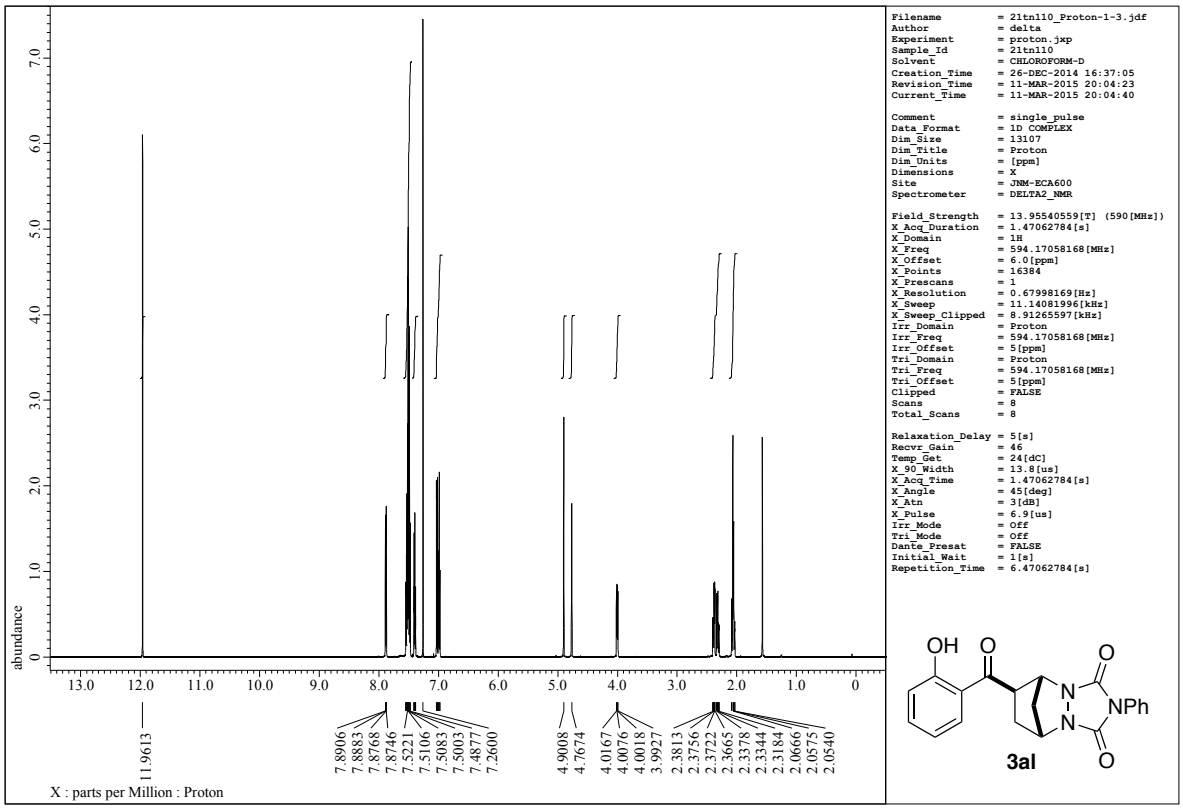

abundance
207.8600
162.9377
135.8020
130.0332
118.6490
118.5530
77.2112
77.0000
76.7792
49.2020
41.4558
36.3108
36.2244
33.8248
29.6781
28.9102
X : parts per Million : Carbon13
Filename = 21tn100-2_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn100-2
Solvent = CHLOROFORM-D
Creation_Time = 3-DEC-2014 11:15:39
Revision_Time = 3-DEC-2014 11:28:42
Current_Time = 11-MAR-2015 20:00:09
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]
OH
O
3ai

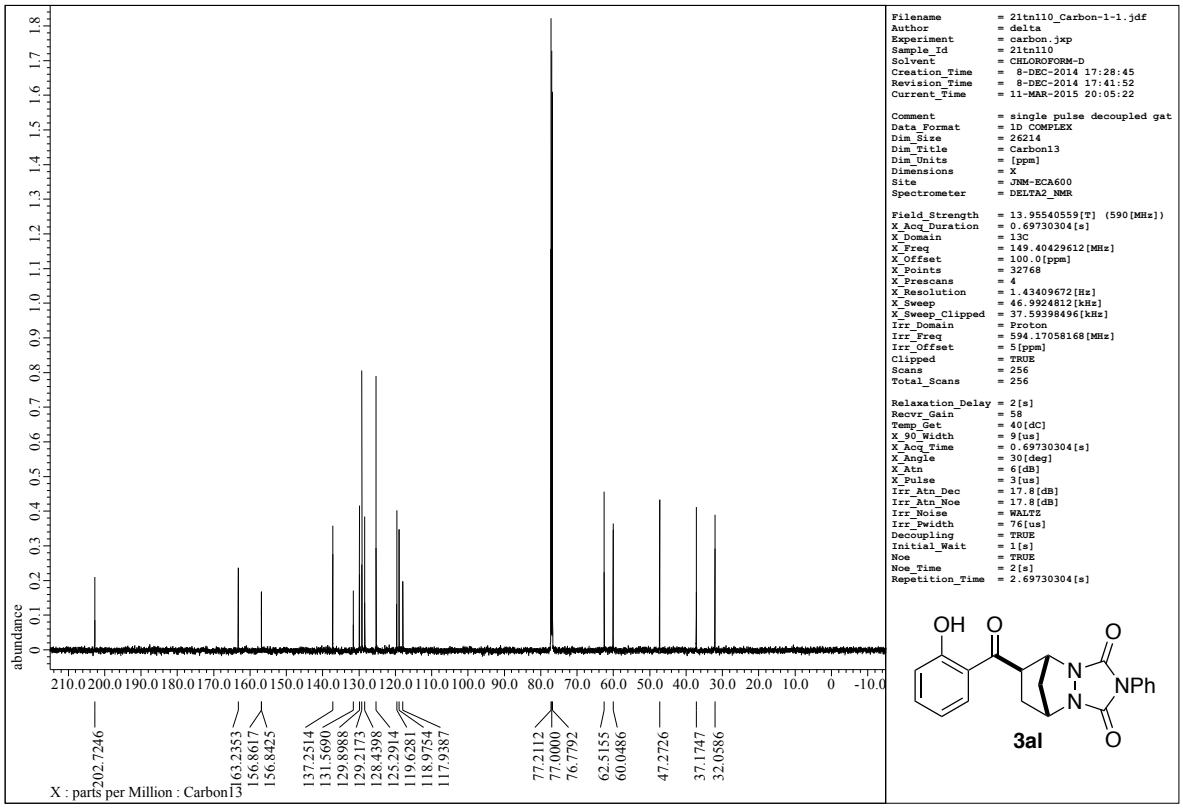

Filename = 21tn130_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn130
Solvent = CHLOROFORM-D
Creation_Time = 12-DEC-2014 19:43:12
Revision_Time = 11-MAR-2015 20:02:36
Current_Time = 11-MAR-2015 20:02:52
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 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 = 6.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 24[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]
abundance
X : parts per Million : Proton
12.0746
7.7143
7.7006
7.5015
7.4889
7.4866
7.4752
7.2600
6.9922
6.9785
6.9659
6.9533
6.9407
3.5956
3.5864
3.5784
3.5692
3.5074
3.5040
3.4983
3.1092
3.1000
2.4019
2.3790
1.8515
1.8492
1.2495
OH
O
O
O
O
3aj

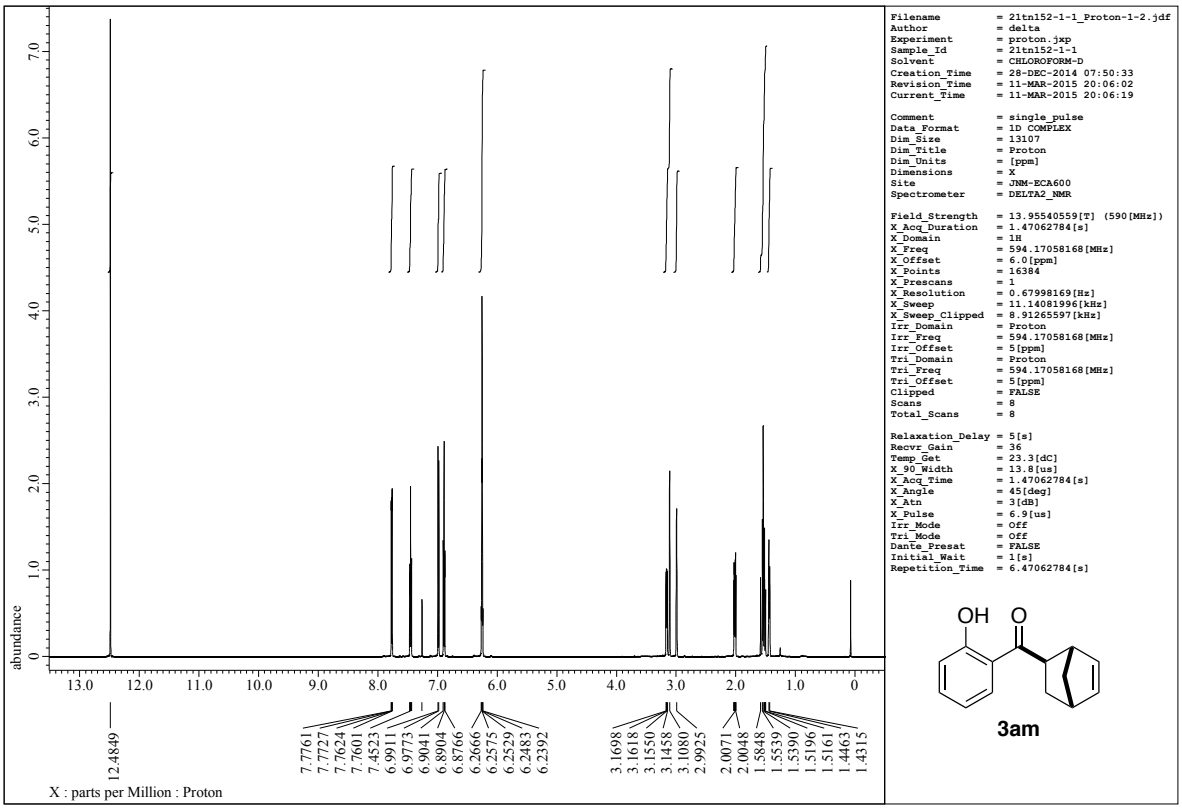

Filename = 21tn130_Carbon_copy2-1-1.j
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn130
Solvent = CHLOROFORM-D
Creation_Time = 12-DEC-2014 19:45:57
Revision_Time = 12-DEC-2014 19:53:25
Current_Time = 11-MAR-2015 20:03:43
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 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[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
Incomplete_Copy = TRUE
Scans = 128
Total_Scans = 128
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]
abundance
X : parts per Million : Carbon13
204.0972
171.8166
171.1543
163.0625
136.7907
129.9468
119.4361
118.7354
117.8523
77.2112
77.0000
76.7888
49.5475
49.4228
44.5370
44.0762
40.0544
27.9983
OH
O
O
O
O
3aj

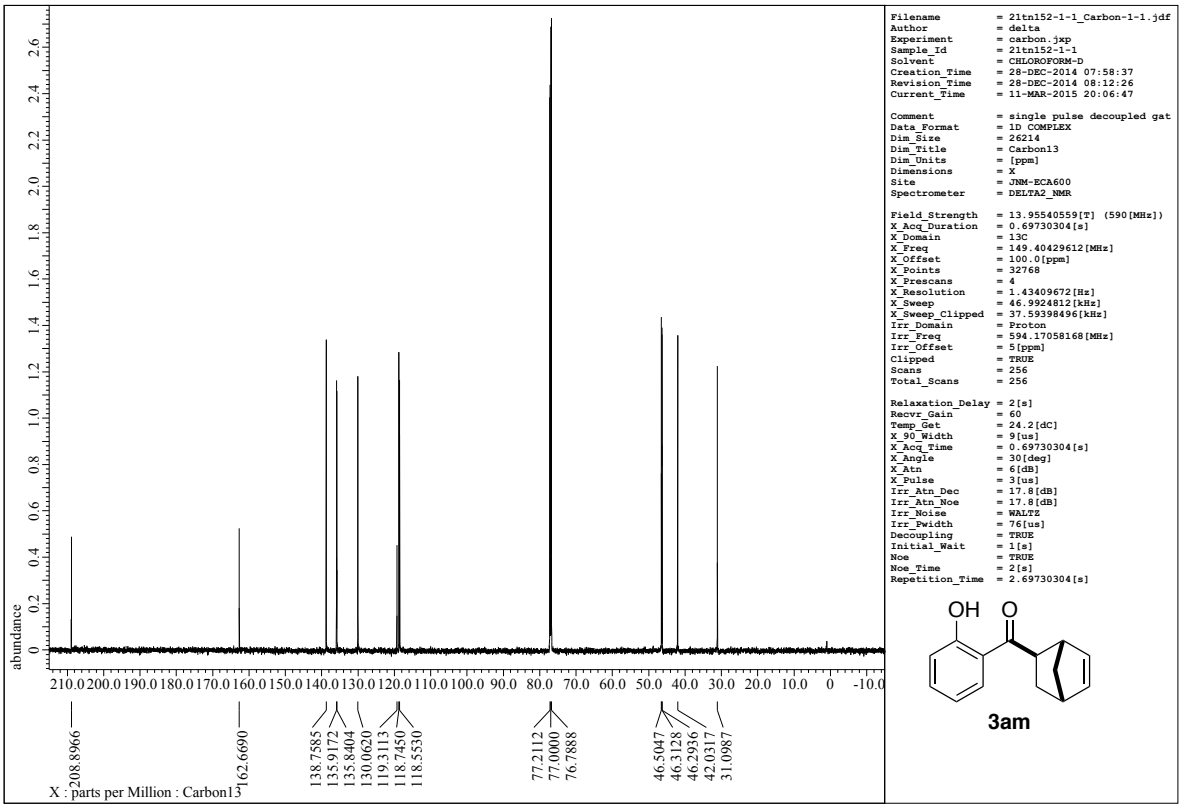

abundance
X : parts per Million : Proton
12.0906
7.5335
7.5267
7.5209
7.5175
7.4191
7.3012
7.2943
7.2909
7.0723
6.9213
6.9075
6.8068
4.7137
4.6908
4.6645
4.6416
3.1996
3.0142
2.8277
2.8208
2.8128
1.7428
1.7244
1.5619
1.2609
1.2564
1.2449
1.2404
1.2381
1.2335
Filename = 21tn194_Proton-2-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn194
Solvent = CHLOROFORM-D
Creation_Time = 13-MAR-2015 09:01:10
Revision_Time = 13-MAR-2015 09:02:28
Current_Time = 13-MAR-2015 09:02:57
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 6.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 34
Temp_Get = 23.4[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]
OH
O
O
NBn
O
3ak

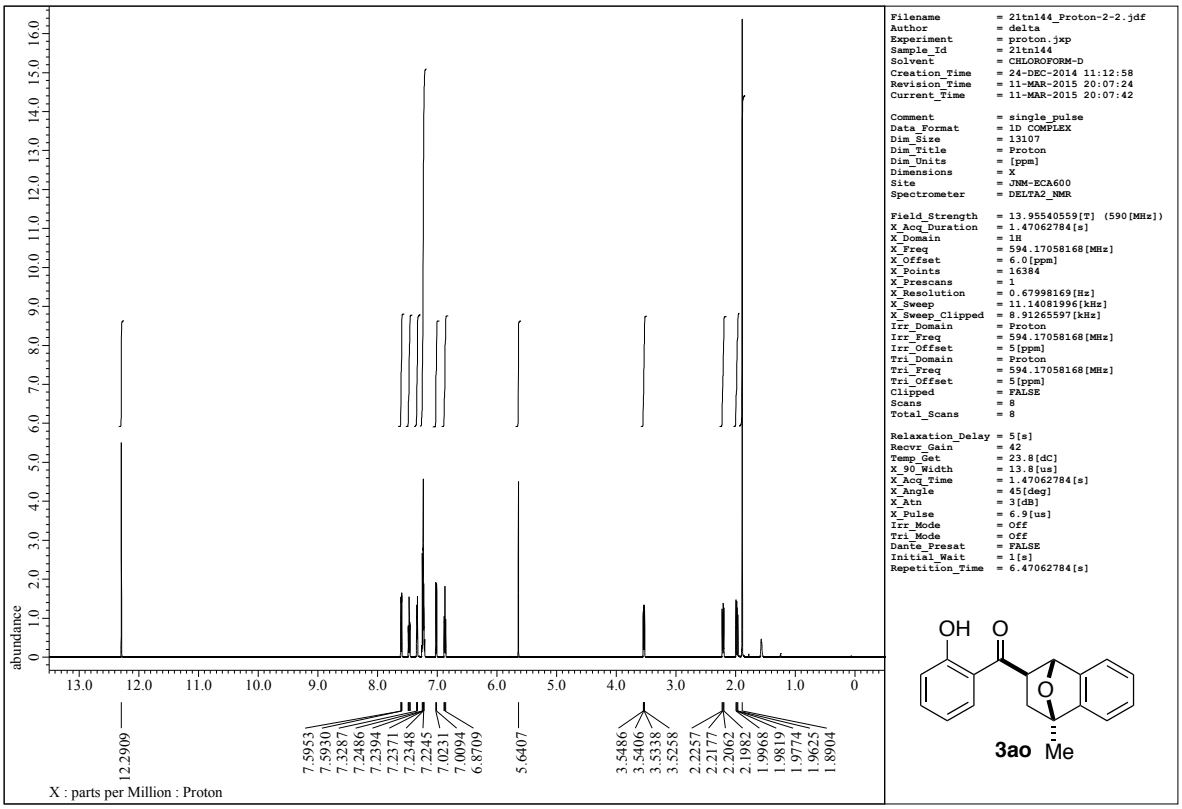

abundance
X : parts per Million : Carbon13
205.2587
177.4511
177.2591
162.9185
136.2628
129.9852
129.3517
128.7949
128.2286
119.1290
118.4379
117.8427
77.2112
77.0000
76.7888
48.0501
47.9253
43.5195
43.2220
40.2175
39.2961
28.5070
Filename = 21tn194_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn194
Solvent = CHLOROFORM-D
Creation_Time = 13-MAR-2015 09:04:02
Revision_Time = 13-MAR-2015 09:15:47
Current_Time = 13-MAR-2015 09:16:50
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 = 24.1[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.8[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]
OH
O
O
NBn
O
3ak


abundance
X : parts per Million : Proton
11.9613
7.8906
7.8883
7.8768
7.8746
7.5221
7.5106
7.5083
7.5003
7.4877
7.2600
4.9008
4.7674
4.0167
4.0076
4.0018
3.9927
2.3813
2.3756
2.3722
2.3665
2.3378
2.3344
2.3184
2.0666
2.0575
2.0540
Filename = 21tn110_Proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn110
Solvent = CHLOROFORM-D
Creation_Time = 26-DEC-2014 16:37:05
Revision_Time = 11-MAR-2015 20:04:23
Current_Time = 11-MAR-2015 20:04:40
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 = 6.0[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 = 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]
OH
O
N
N
NPh
O
3al


abundance
X : parts per Million : Carbon13
202.7246
163.2353
156.8617
156.8425
137.2514
131.5690
129.8988
129.2173
128.4398
125.2914
119.6281
118.9754
117.9387
77.2112
77.0000
76.7792
62.5155
60.0486
47.2726
37.1747
32.0586
Filename = 21tn110_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn110
Solvent = CHLOROFORM-D
Creation_Time = 8-DEC-2014 17:28:45
Revision_Time = 8-DEC-2014 17:41:52
Current_Time = 11-MAR-2015 20:05:22
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 40[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]
OH
O
N
N
NPh
O
3al


abundance
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.4849
7.7761 7.7727 7.7624 7.7601 7.4523 6.9911 6.9773 6.9041 6.8904 6.8766 6.2666 6.2575 6.2529 6.2483 6.2392
3.1698 3.1618 3.1550 3.1458 3.1080 2.9925 2.0071 2.0048 1.5848 1.5539 1.5390 1.5196 1.5161 1.4463 1.4315
X : parts per Million : Proton
Filename = 21tn152-1-1_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn152-1-1
Solvent = CHLOROFORM-D
Creation_Time = 28-DEC-2014 07:50:33
Revision_Time = 11-MAR-2015 20:06:02
Current_Time = 11-MAR-2015 20:06:19
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 6.0[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 = 23.3[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]
OH O
3am


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
208.8966
162.6690
138.7585 135.9172 135.8404 130.0620 119.3113 118.7450 118.5530
77.2112 77.0000 76.7888
46.5047 46.3128 46.2936 42.0317 31.0987
X : parts per Million : Carbon13
Filename = 21tn152-1-1_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn152-1-1
Solvent = CHLOROFORM-D
Creation_Time = 28-DEC-2014 07:58:37
Revision_Time = 28-DEC-2014 08:12:26
Current_Time = 11-MAR-2015 20:06:47
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.2[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.8[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]
OH O
3am


abundance
X : parts per Million : Proton
12.2909
7.5953
7.5930
7.3287
7.2486
7.2394
7.2371
7.2348
7.2245
7.0231
7.0094
6.8709
5.6407
3.5486
3.5406
3.5338
3.5258
2.2257
2.2177
2.2062
2.1982
1.9968
1.9819
1.9774
1.9625
1.8904
Filename = 21tn144_Proton-2-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn144
Solvent = CHLOROFORM-D
Creation_Time = 24-DEC-2014 11:12:58
Revision_Time = 11-MAR-2015 20:07:24
Current_Time = 11-MAR-2015 20:07:42
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 = 6.0[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 = 23.8[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]
OH
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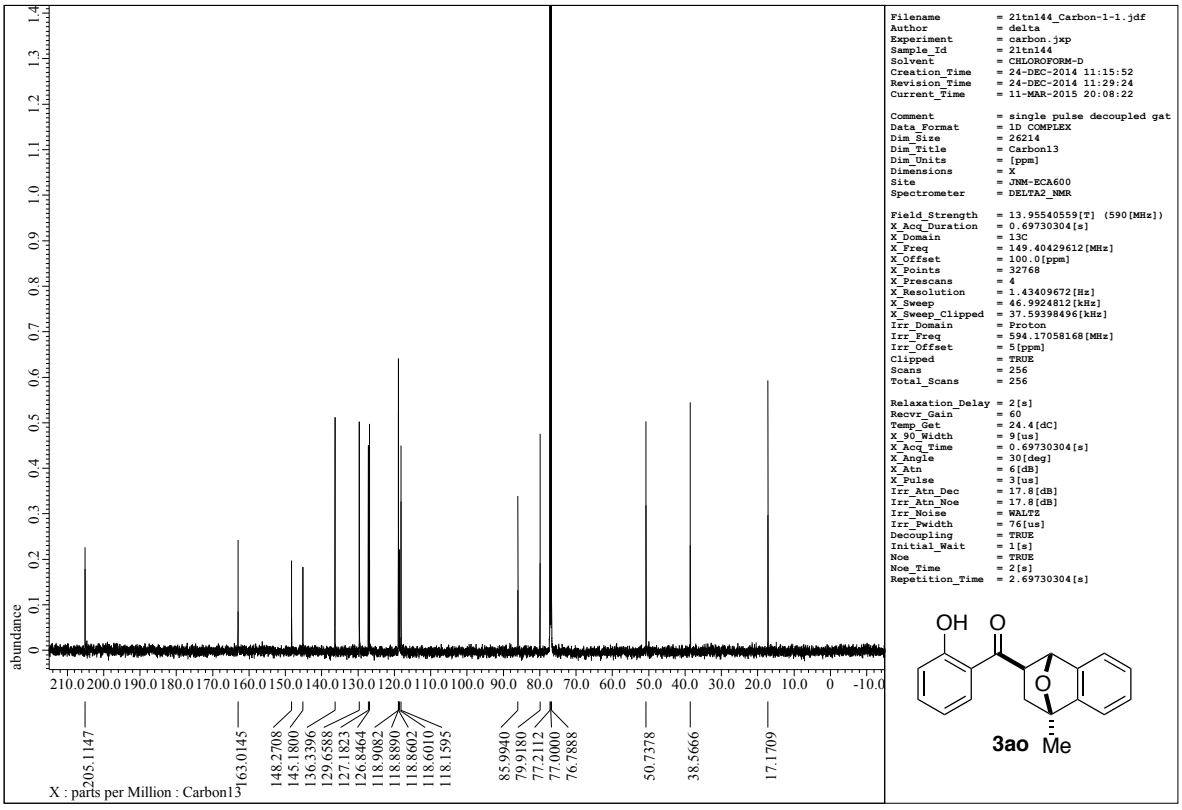
3ao
Me


abundance
X : parts per Million : Carbon13
205.1147
163.0145
148.2708
145.1800
136.3396
129.6588
127.1823
126.8464
118.9082
118.8890
118.8602
118.6010
118.1595
85.9940
79.9180
77.2112
77.0000
76.7888
50.7378
38.5666
17.1709
Filename = 21tn144_Carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn144
Solvent = CHLOROFORM-D
Creation_Time = 24-DEC-2014 11:15:52
Revision_Time = 24-DEC-2014 11:29:24
Current_Time = 11-MAR-2015 20:08:22
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 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]
OH
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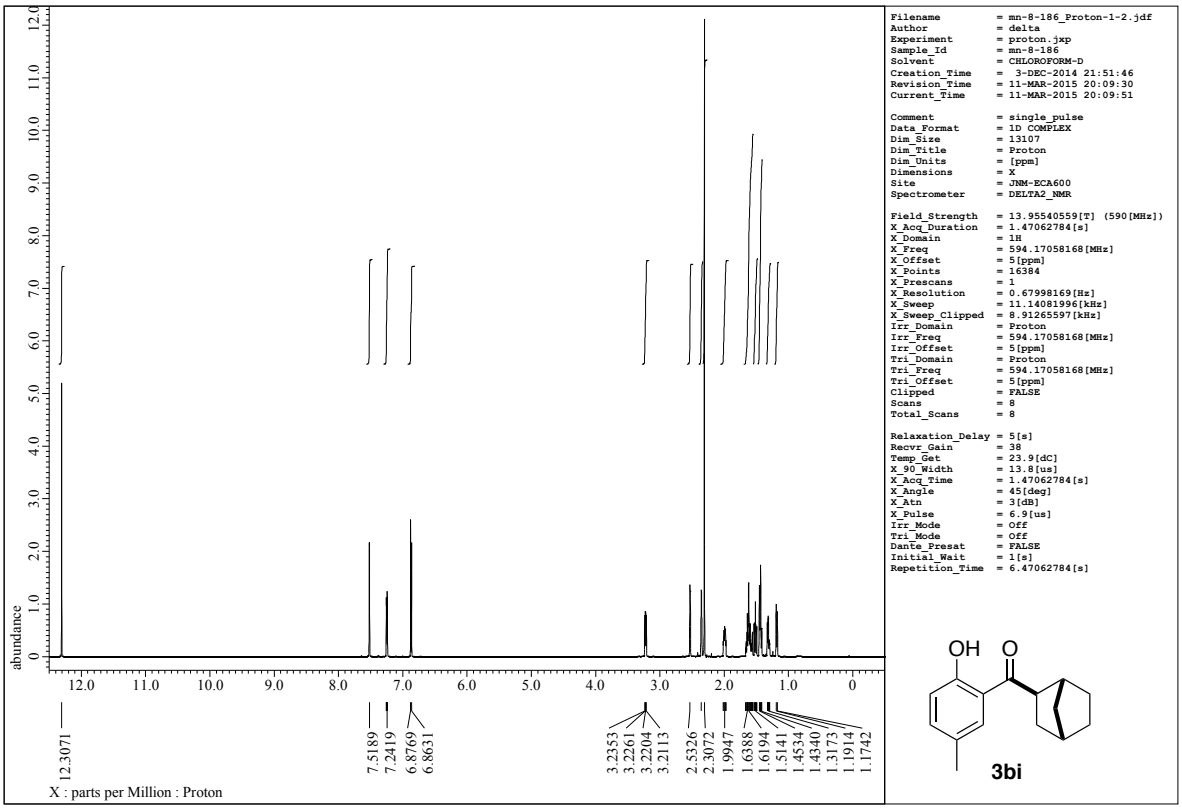
3ao
Me


abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.3071
7.5189
7.2419
6.8769
6.8631
3.2353
3.2261
3.2204
3.2113
2.5326
2.3072
1.9947
1.6388
1.6194
1.5141
1.4534
1.4340
1.3173
1.1914
1.1742
X : parts per Million : Proton
Filename = mn-8-186_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-186
Solvent = CHLOROFORM-D
Creation_Time = 3-DEC-2014 21:51:46
Revision_Time = 11-MAR-2015 20:09:30
Current_Time = 11-MAR-2015 20:09:51
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]
OH
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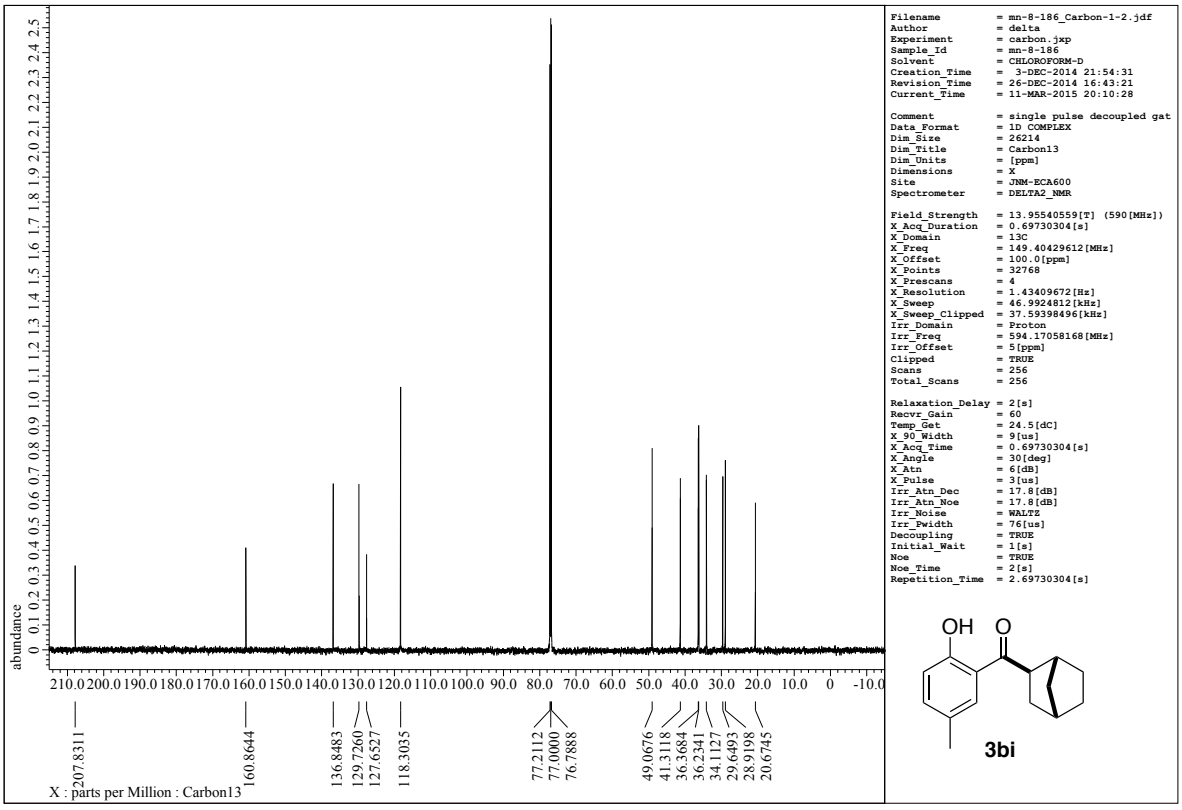
3bi


abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5
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
207.8311
160.8644
136.8483
129.7260
127.6527
118.3035
77.2112
77.0000
76.7888
49.0676
41.3118
36.3684
36.2341
34.1127
29.6493
28.9198
20.6745
X : parts per Million : Carbon13
Filename = mn-8-186_Carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-186
Solvent = CHLOROFORM-D
Creation_Time = 3-DEC-2014 21:54:31
Revision_Time = 26-DEC-2014 16:43:21
Current_Time = 11-MAR-2015 20:10:28
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 = 24.5[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]
OH
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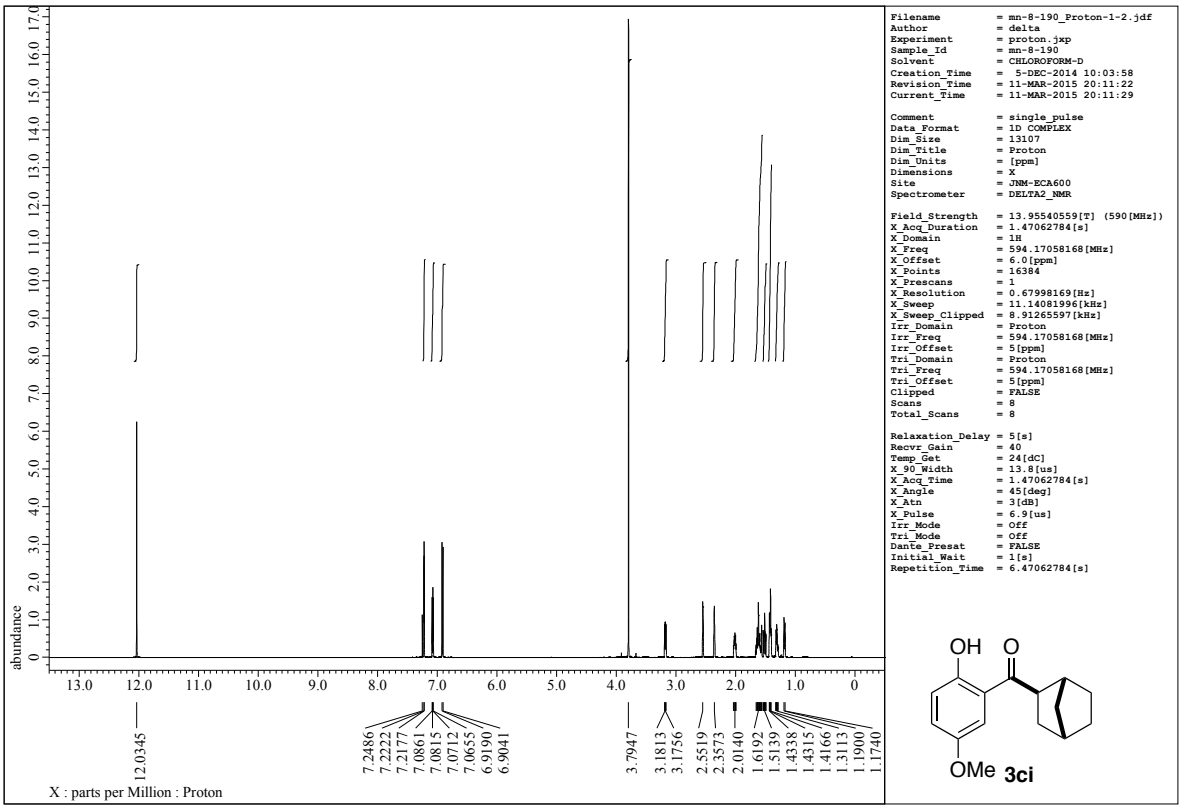
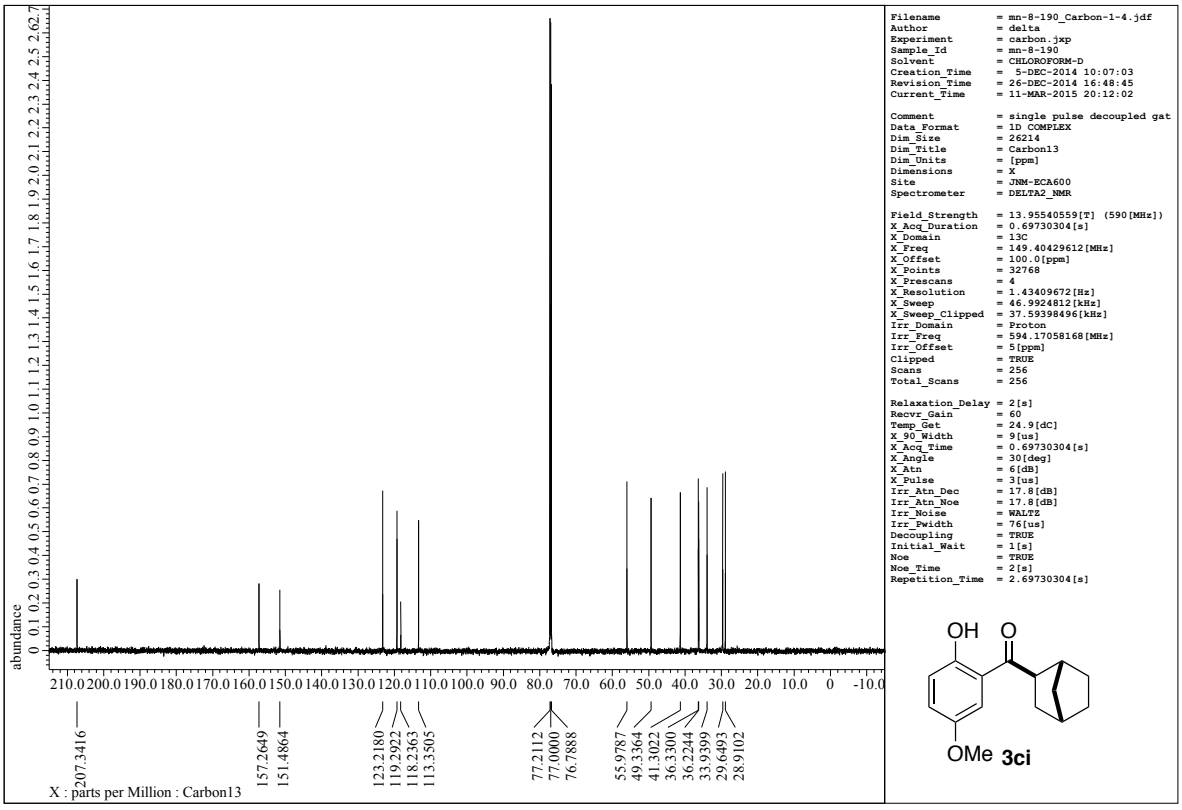
3bi


abundance
X : parts per Million : Proton
12.0345
7.2486
7.2222
7.2177
7.0861
7.0815
7.0712
7.0655
6.9190
6.9041
3.7947
3.1813
3.1756
2.5519
2.3573
2.0140
1.6192
1.5139
1.4338
1.4315
1.4166
1.3113
1.1900
1.1740
Filename = mn-8-190_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-190
Solvent = CHLOROFORM-D
Creation_Time = 5-DEC-2014 10:03:58
Revision_Time = 11-MAR-2015 20:11:22
Current_Time = 11-MAR-2015 20:11:29
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 = 6.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 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]
OH
O
OMe
3ci


abundance
X : parts per Million : Carbon13
207.3416
157.2649
151.4864
123.2180
119.2922
118.2363
113.3505
77.2112
77.0000
76.7888
55.9787
49.3364
41.3022
36.3300
36.2244
33.9399
29.6493
28.9102
Filename = mn-8-190_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-190
Solvent = CHLOROFORM-D
Creation_Time = 5-DEC-2014 10:07:03
Revision_Time = 26-DEC-2014 16:48:45
Current_Time = 11-MAR-2015 20:12:02
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 = 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]
OH
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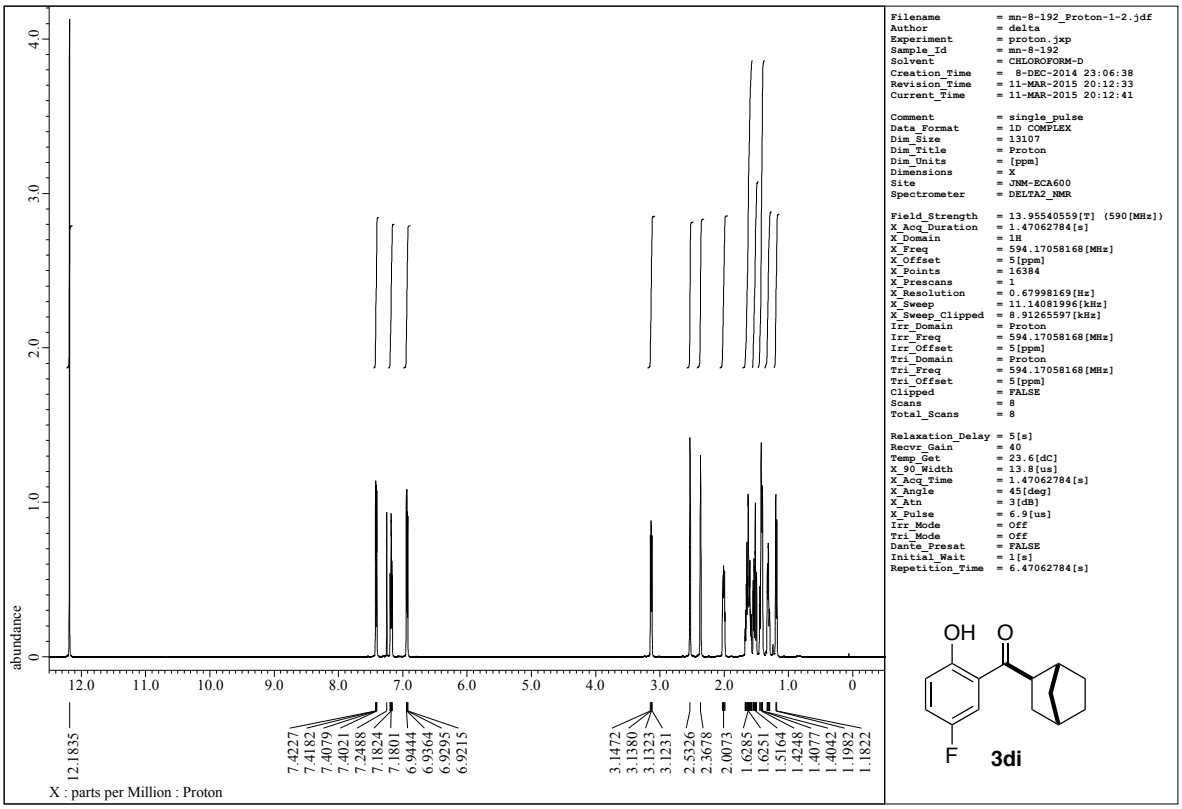
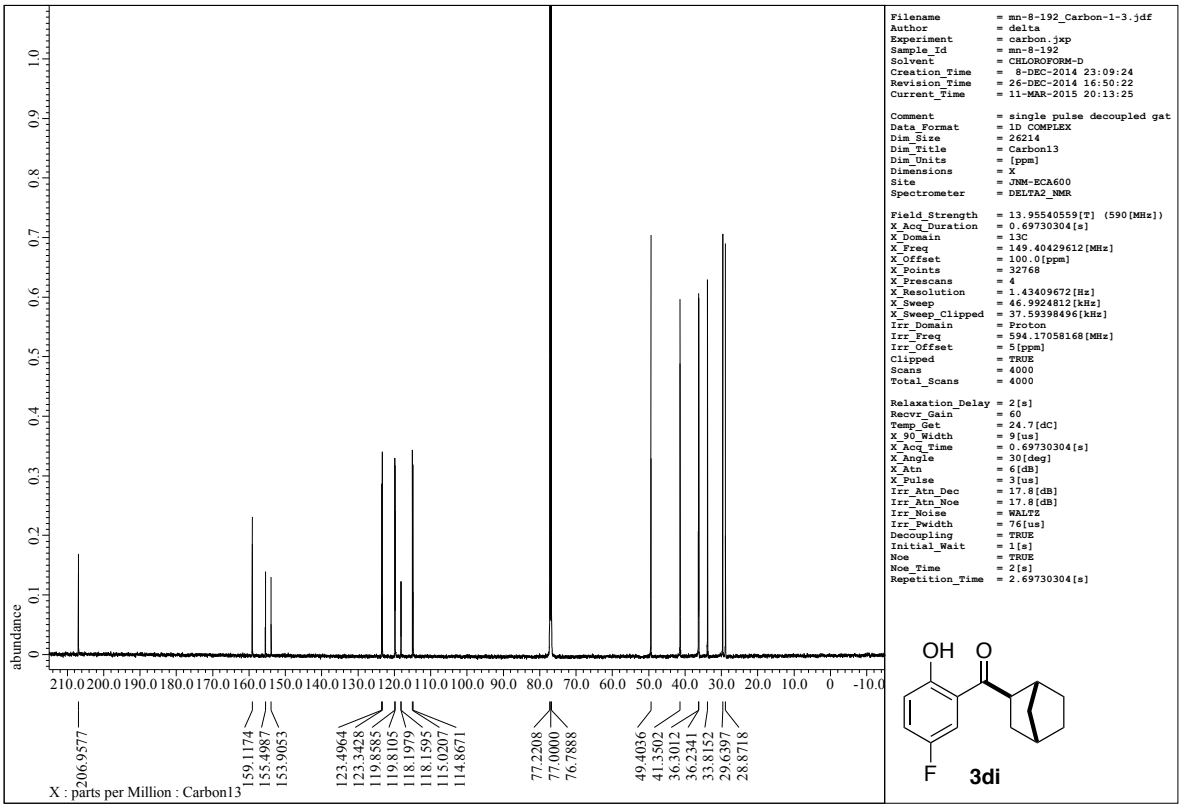
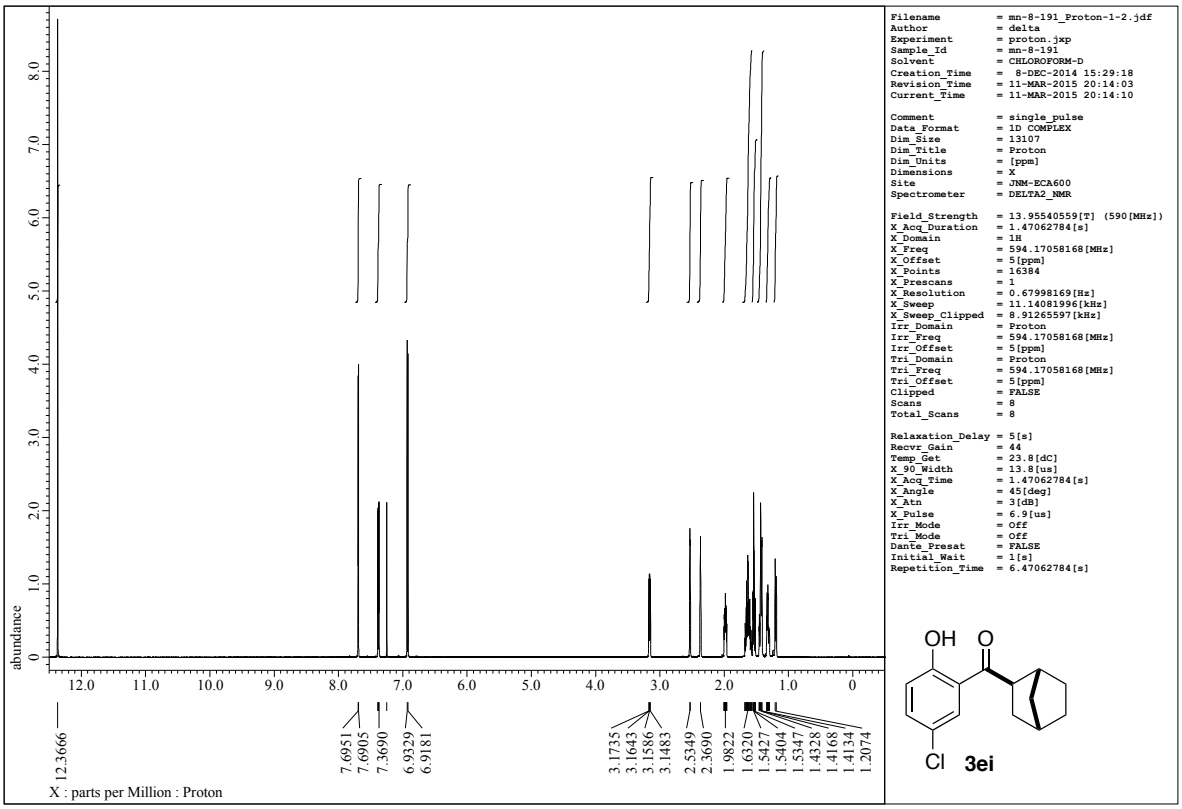
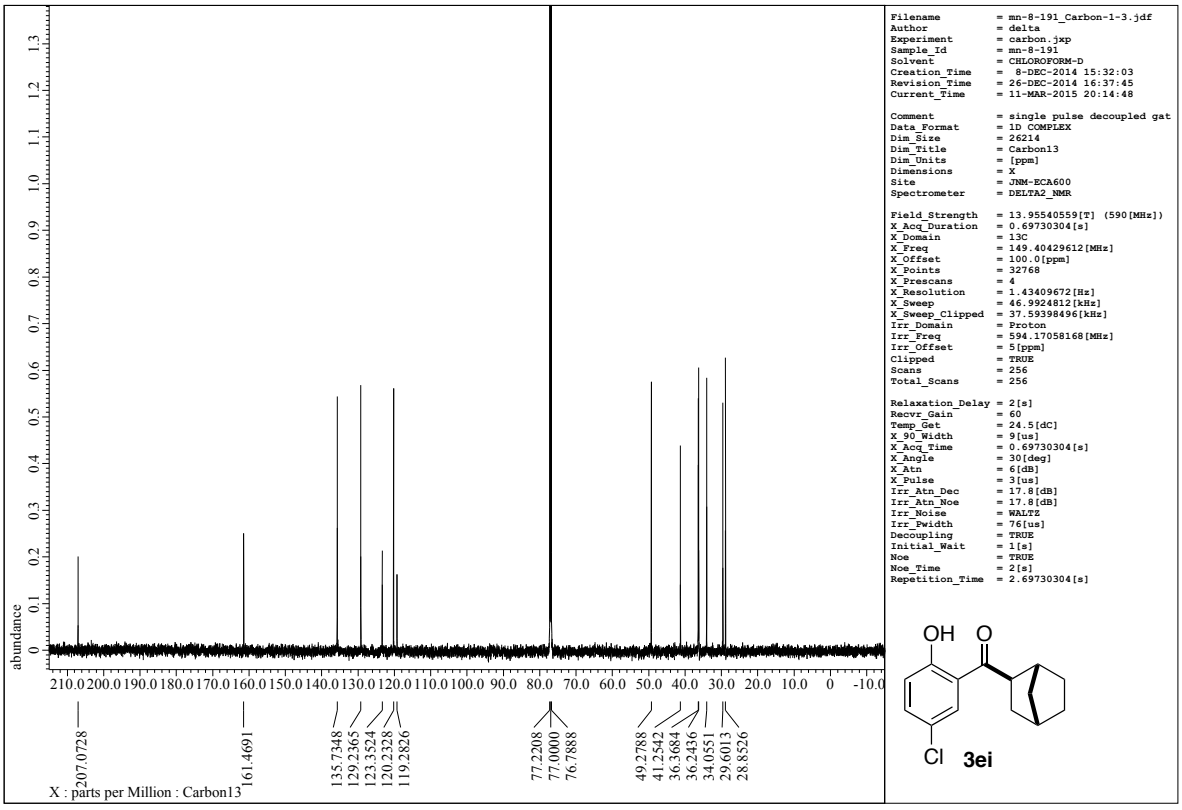
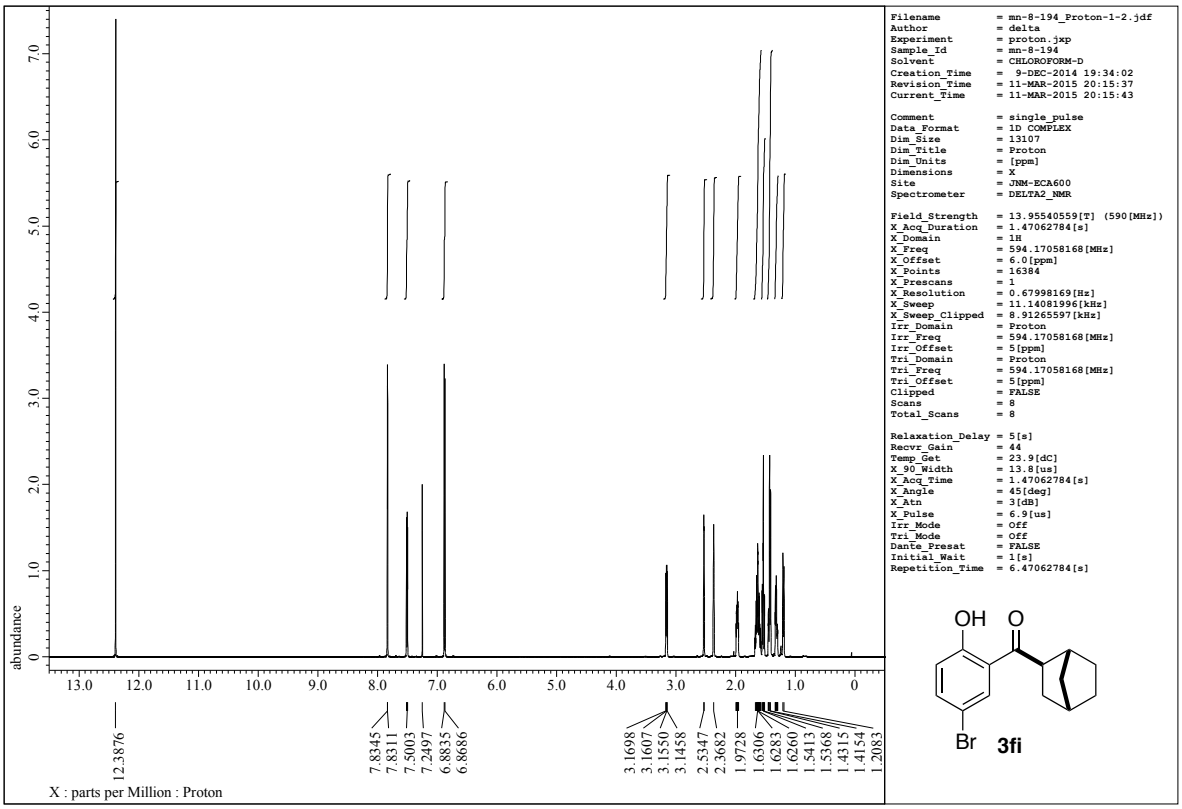
OMe
3ci

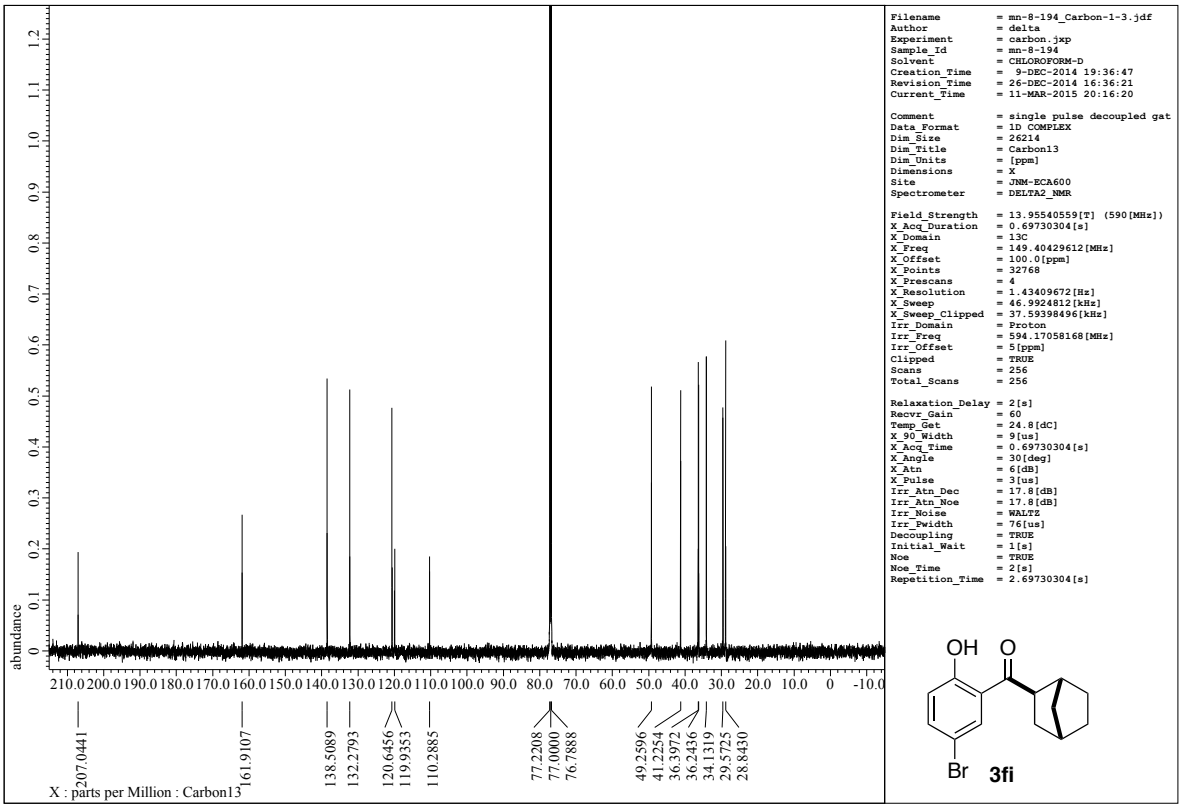

abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.1835
7.4227 7.4182 7.4079 7.4021 7.2488 7.1824 7.1801 6.9444 6.9364 6.9295 6.9215
3.1472 3.1380 3.1323 3.1231 2.5326 2.3678 2.0073 1.6285 1.6251 1.5164 1.4248 1.4077 1.4042 1.1982 1.1822
X : parts per Million : Proton
Filename = mn-8-192_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-192
Solvent = CHLOROFORM-D
Creation_Time = 8-DEC-2014 23:06:38
Revision_Time = 11-MAR-2015 20:12:33
Current_Time = 11-MAR-2015 20:12:41
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 23.6[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]
OH O F
3di

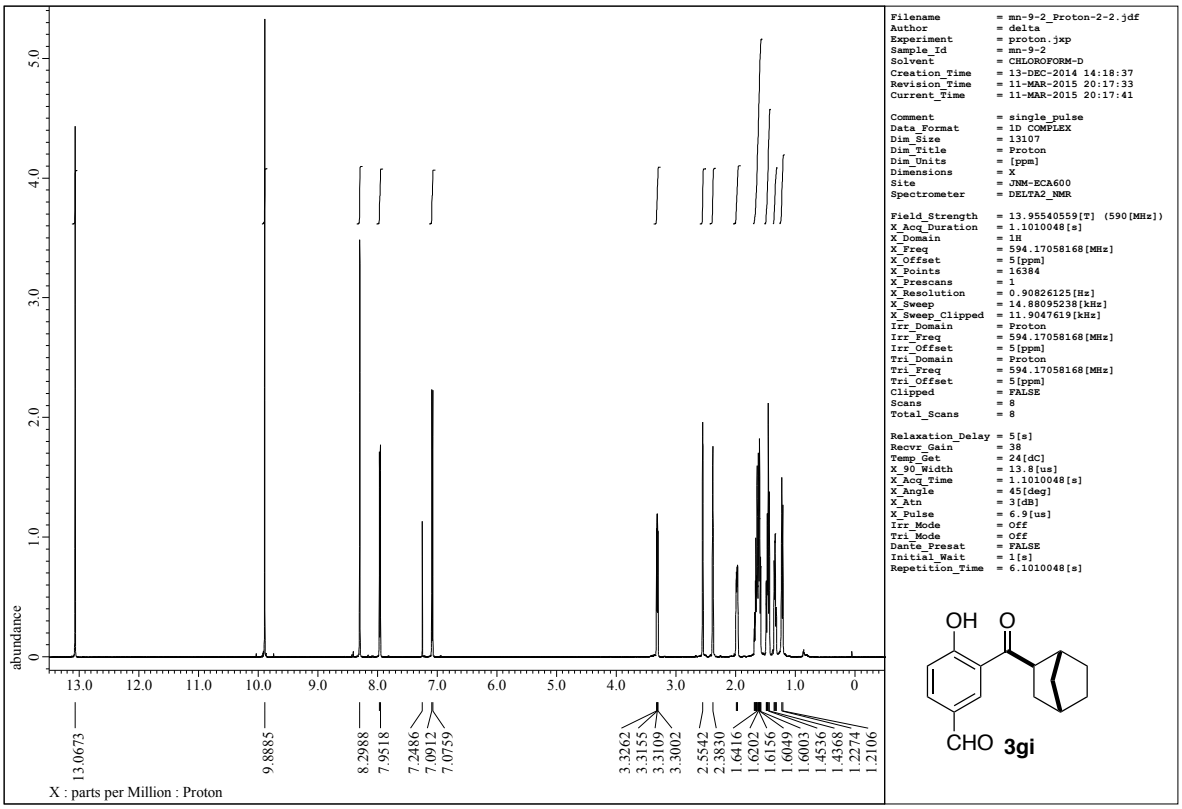

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
206.9577
159.1174 155.4987 153.9053
123.4964 123.3428 119.8585 119.8105 118.1979 118.1595 115.0207 114.8671
77.2208 77.0000 76.7888
49.4036 41.3502 36.3012 36.2341 33.8152 29.6397 28.8718
X : parts per Million : Carbon13
Filename = mn-8-192_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-192
Solvent = CHLOROFORM-D
Creation_Time = 8-DEC-2014 23:09:24
Revision_Time = 26-DEC-2014 16:50:22
Current_Time = 11-MAR-2015 20:13:25
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 = 4000
Total_Scans = 4000
Relaxation_Delay = 2[s]
Recvr_Gain = 60
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]
OH O F
3di

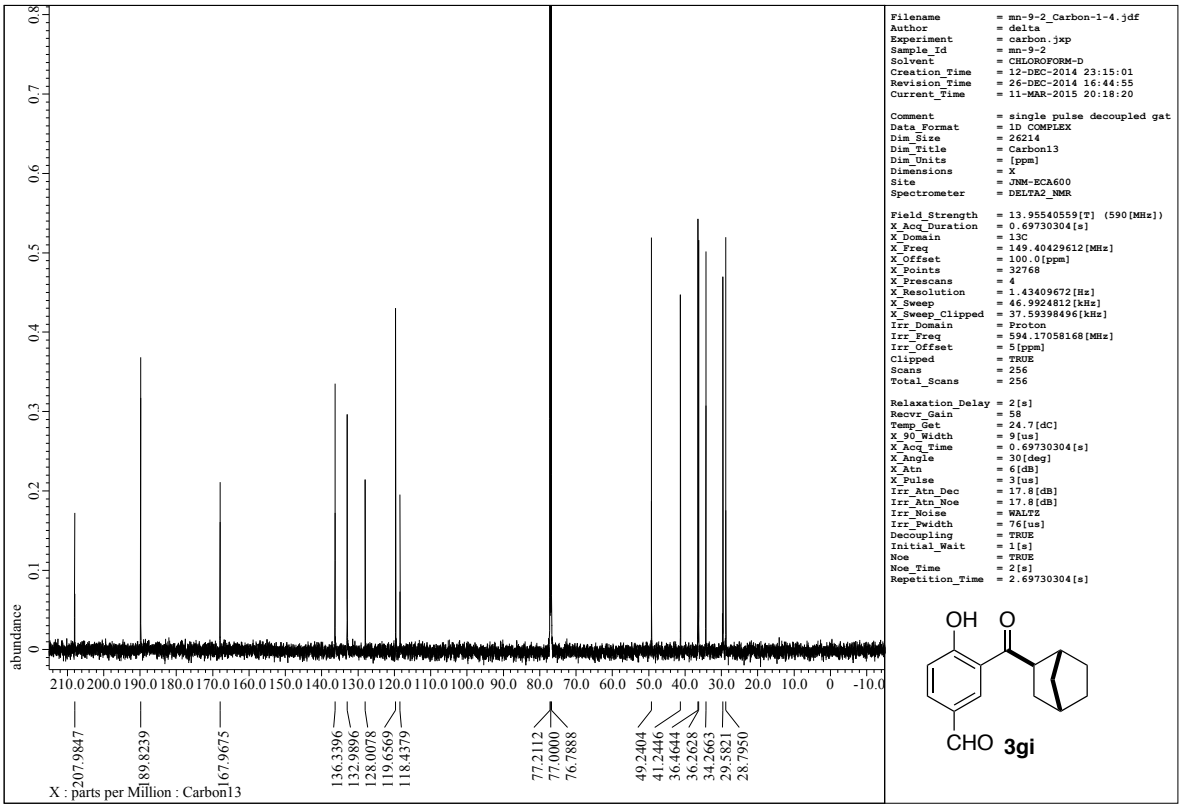

abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.3666
7.6951 7.6905 7.3690 6.9329 6.9181
3.1735 3.1643 3.1586 3.1483 2.5349 2.3690 1.9822 1.6320 1.5427 1.5404 1.5347 1.4328 1.4168 1.4134 1.2074
X : parts per Million : Proton
Filename = mn-8-191_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-191
Solvent = CHLOROFORM-D
Creation_Time = 8-DEC-2014 15:29:18
Revision_Time = 11-MAR-2015 20:14:03
Current_Time = 11-MAR-2015 20:14:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 23.8[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]
OH O
Cl
3ei

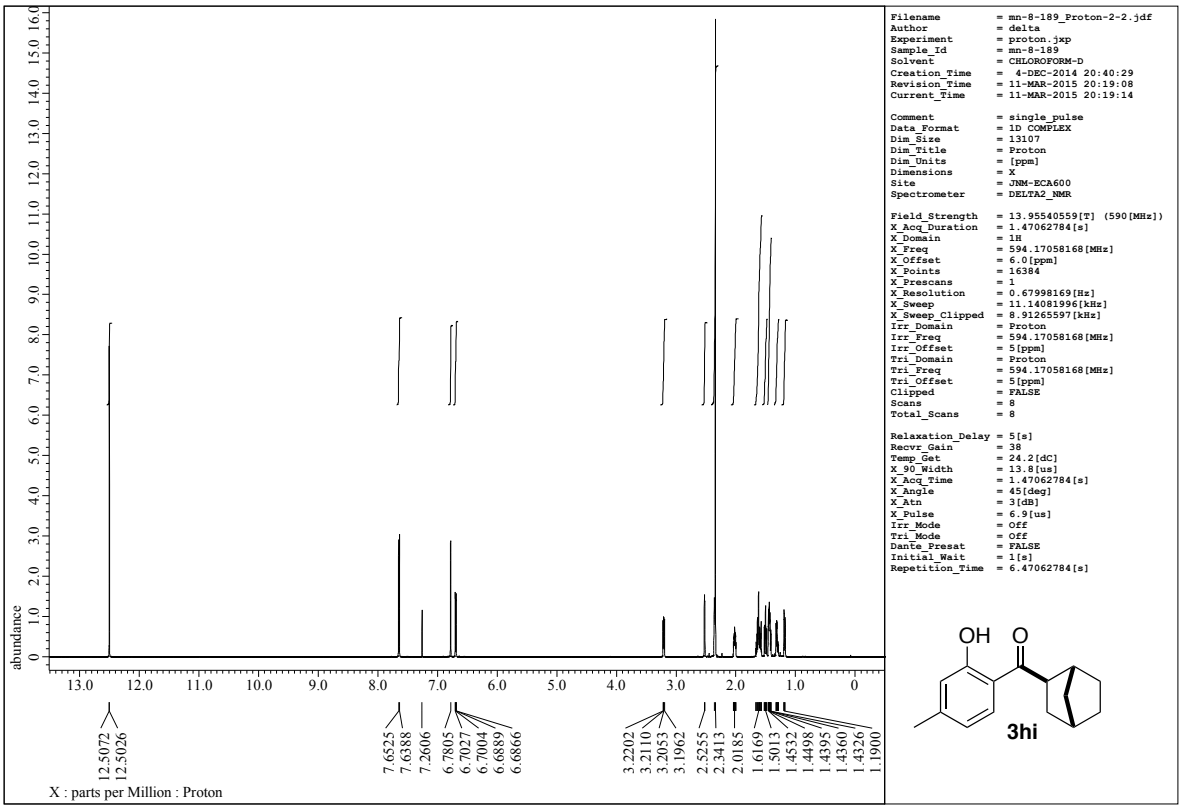

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
207.0728
161.4691
135.7348 129.2365 123.3524 120.2328 119.2826
77.2208 77.0000 76.7888
49.2788 41.2542 36.3684 36.2436 34.0551 29.6013 28.8526
X : parts per Million : Carbon13
Filename = mn-8-191_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-191
Solvent = CHLOROFORM-D
Creation_Time = 8-DEC-2014 15:32:03
Revision_Time = 26-DEC-2014 16:37:45
Current_Time = 11-MAR-2015 20:14:48
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 = 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]
OH O
Cl
3ei

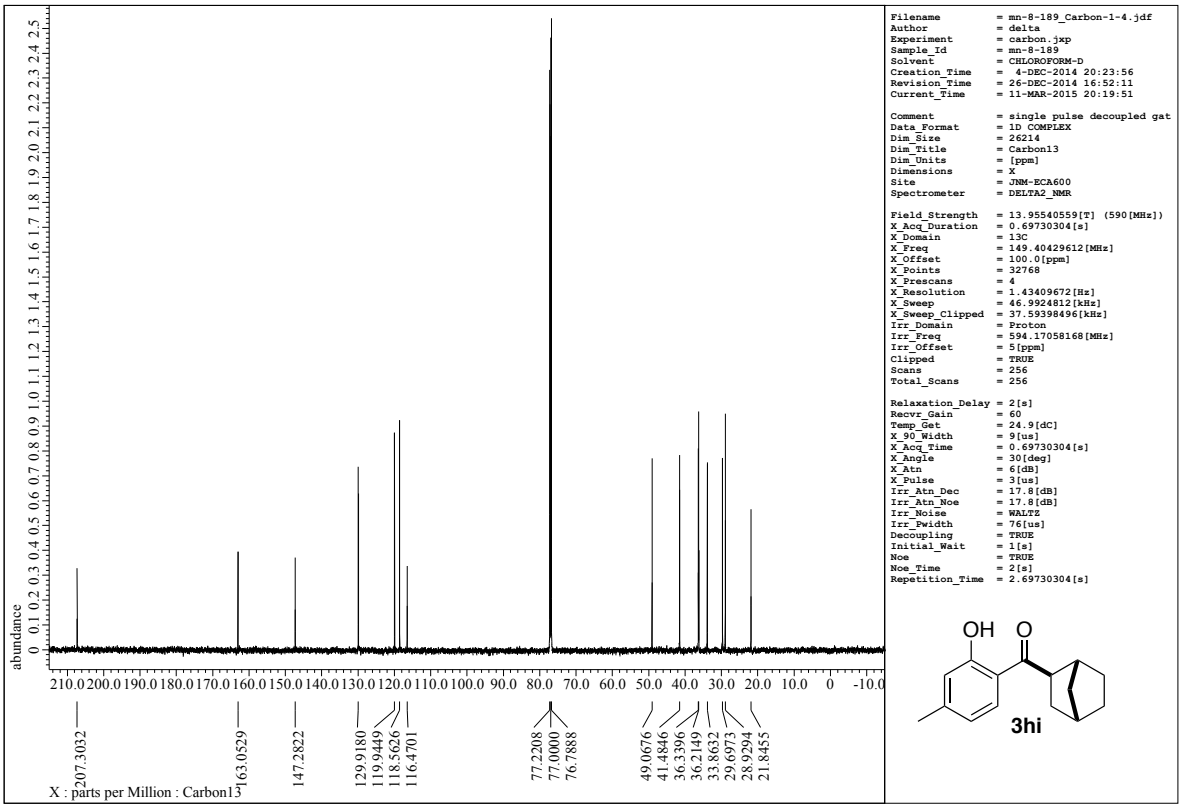

abundance
X : parts per Million : Proton
12.3876
7.8345
7.8311
7.5003
7.2497
6.8835
6.8686
3.1698
3.1607
3.1550
3.1458
2.5347
2.3682
1.9728
1.6306
1.6283
1.6260
1.5413
1.5368
1.4315
1.4154
1.2083
Filename = mn-8-194_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-194
Solvent = CHLOROFORM-D
Creation_Time = 9-DEC-2014 19:34:02
Revision_Time = 11-MAR-2015 20:15:37
Current_Time = 11-MAR-2015 20:15:43
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 = 6.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 23.9[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]
OH
O
Br
3fi

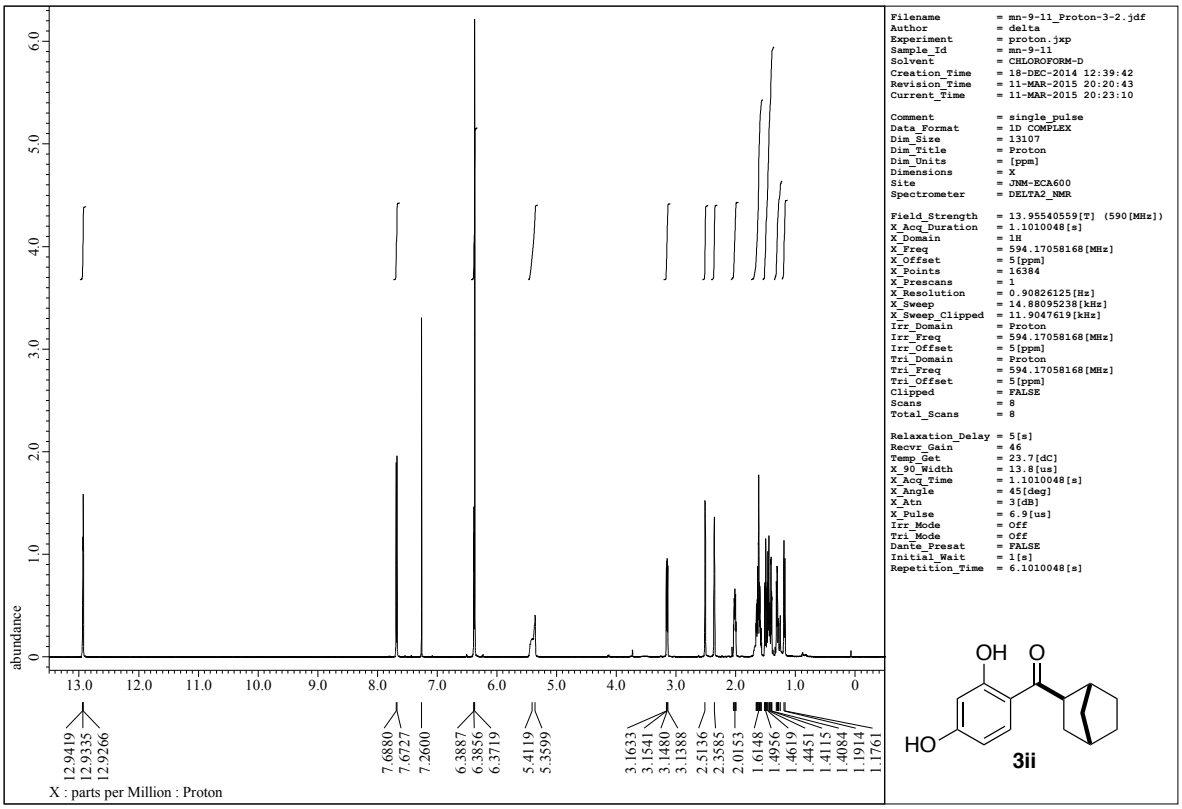

abundance
X : parts per Million : Carbon13
207.0441
161.9107
138.5089
132.2793
120.6456
119.9353
110.2885
77.2208
77.0000
76.7888
49.2596
41.2254
36.3972
36.2436
34.1319
29.5725
28.8430
Filename = mn-8-194_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-194
Solvent = CHLOROFORM-D
Creation_Time = 9-DEC-2014 19:36:47
Revision_Time = 26-DEC-2014 16:36:21
Current_Time = 11-MAR-2015 20:16:20
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 = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.8[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.8[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]
OH
O
Br
3fi

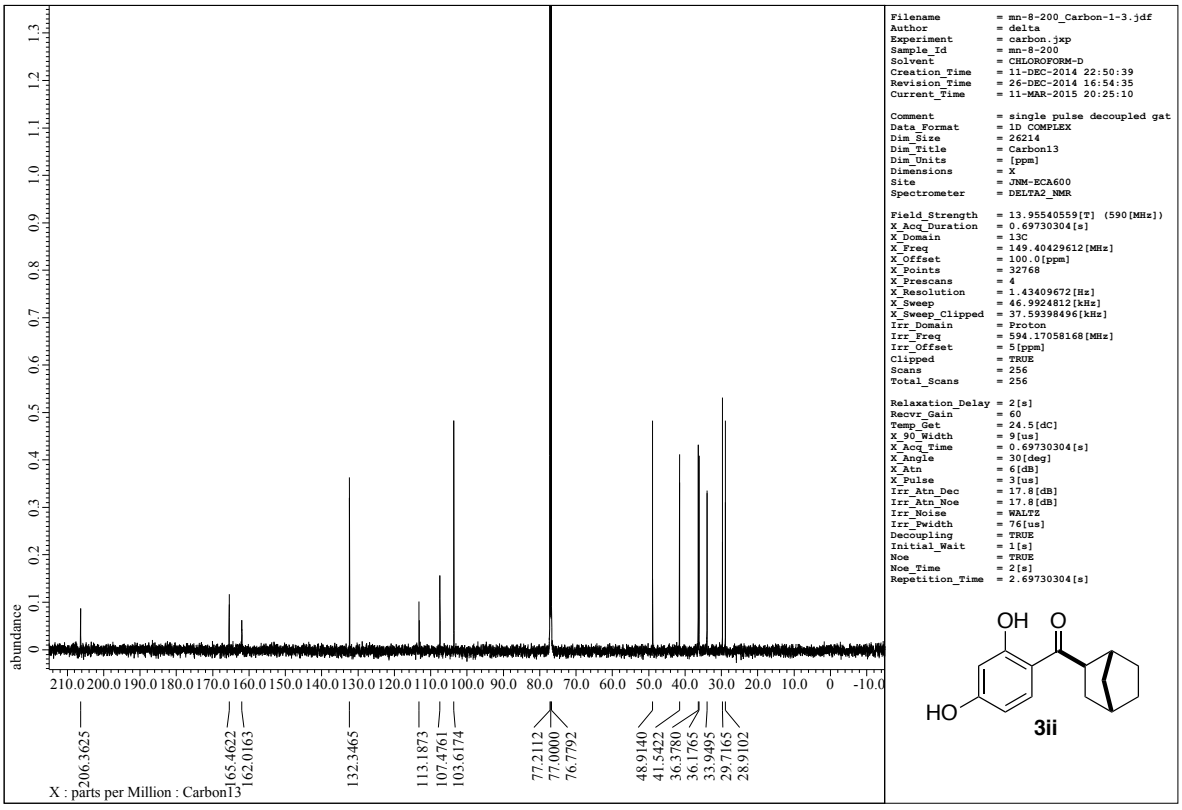

abundance
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
13.0673
9.8885
8.2988
7.9518
7.2486
7.0912
7.0759
3.3262
3.3155
3.3109
3.3002
2.5542
2.3830
1.6416
1.6202
1.6156
1.6049
1.6003
1.4536
1.4368
1.2274
1.2106
X : parts per Million : Proton
Filename = mn-9-2_Proton-2-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-9-2
Solvent = CHLOROFORM-D
Creation_Time = 13-DEC-2014 14:18:37
Revision_Time = 11-MAR-2015 20:17:33
Current_Time = 11-MAR-2015 20:17:41
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 24[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.1010048[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 = 6.1010048[s]
OH
O
CHO
3gi

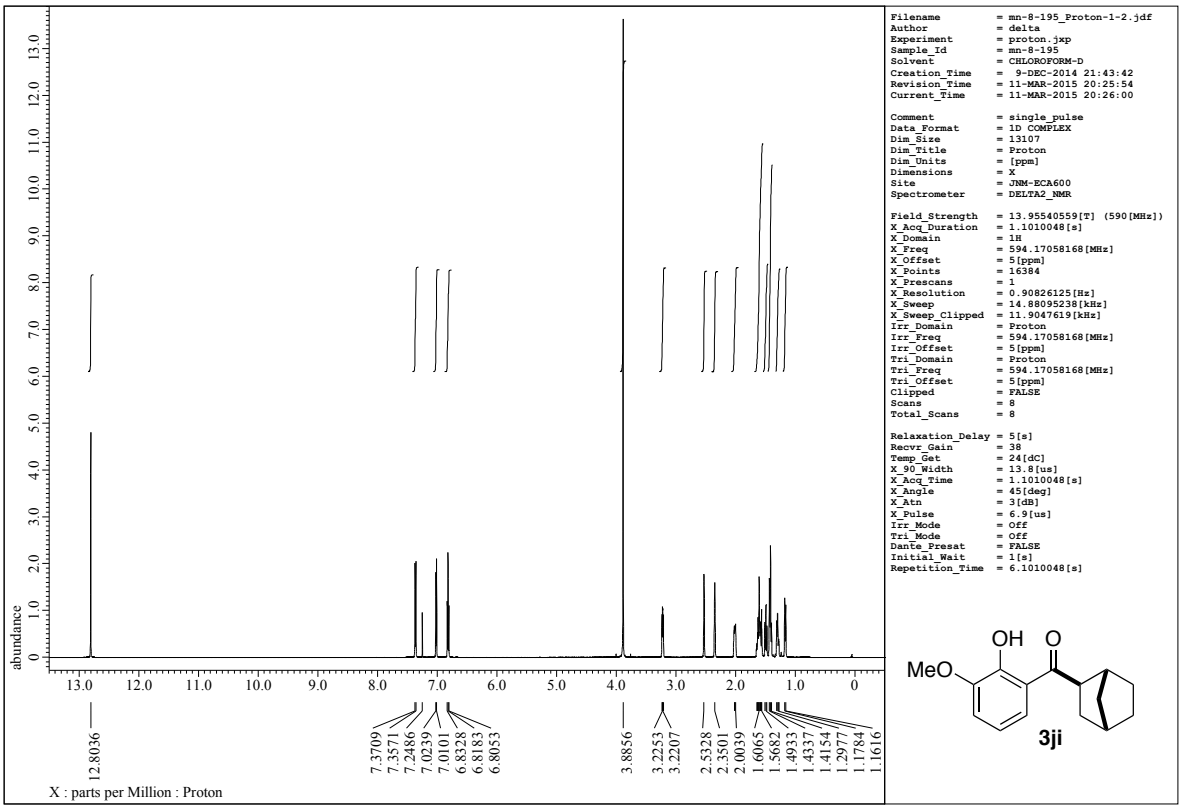

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
207.9847
189.8239
167.9675
136.3396
132.9896
128.0078
119.6569
118.4379
77.2112
77.0000
76.7888
49.2404
41.2446
36.4644
36.2628
34.2663
29.5821
28.7950
X : parts per Million : Carbon13
Filename = mn-9-2_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-9-2
Solvent = CHLOROFORM-D
Creation_Time = 12-DEC-2014 23:15:01
Revision_Time = 26-DEC-2014 16:44:55
Current_Time = 11-MAR-2015 20:18:20
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 = TRUE
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]
OH
O
CHO
3gi

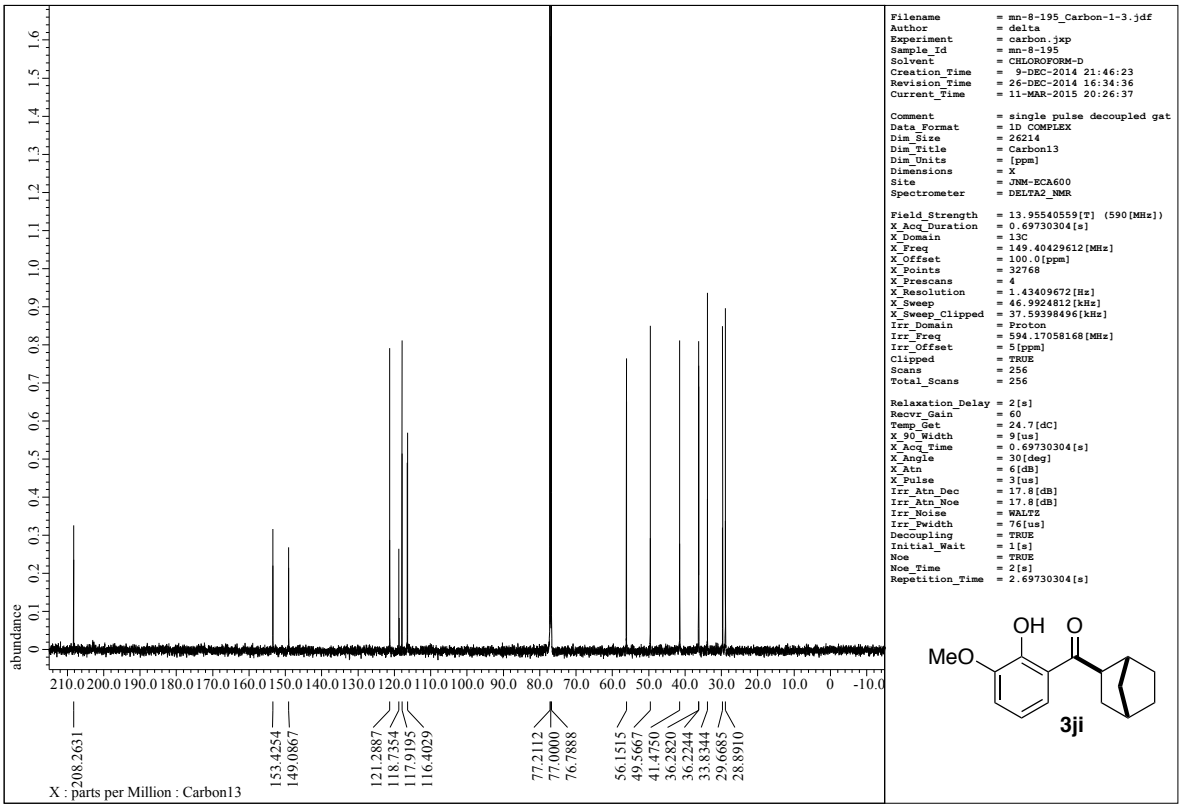

abundance
12.5072
12.5026
7.6525
7.6388
7.2606
6.7805
6.7027
6.7004
6.6889
6.6866
3.2202
3.2110
3.2053
3.1962
2.5255
2.3413
2.0185
1.6169
1.5013
1.4532
1.4498
1.4395
1.4360
1.4326
1.1900
X : parts per Million : Proton
Filename = mn-8-189_Proton-2-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-189
Solvent = CHLOROFORM-D
Creation_Time = 4-DEC-2014 20:40:29
Revision_Time = 11-MAR-2015 20:19:08
Current_Time = 11-MAR-2015 20:19:14
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 = 6.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 24.2[dC]
X_90_Width = 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]
OH
O
3hi

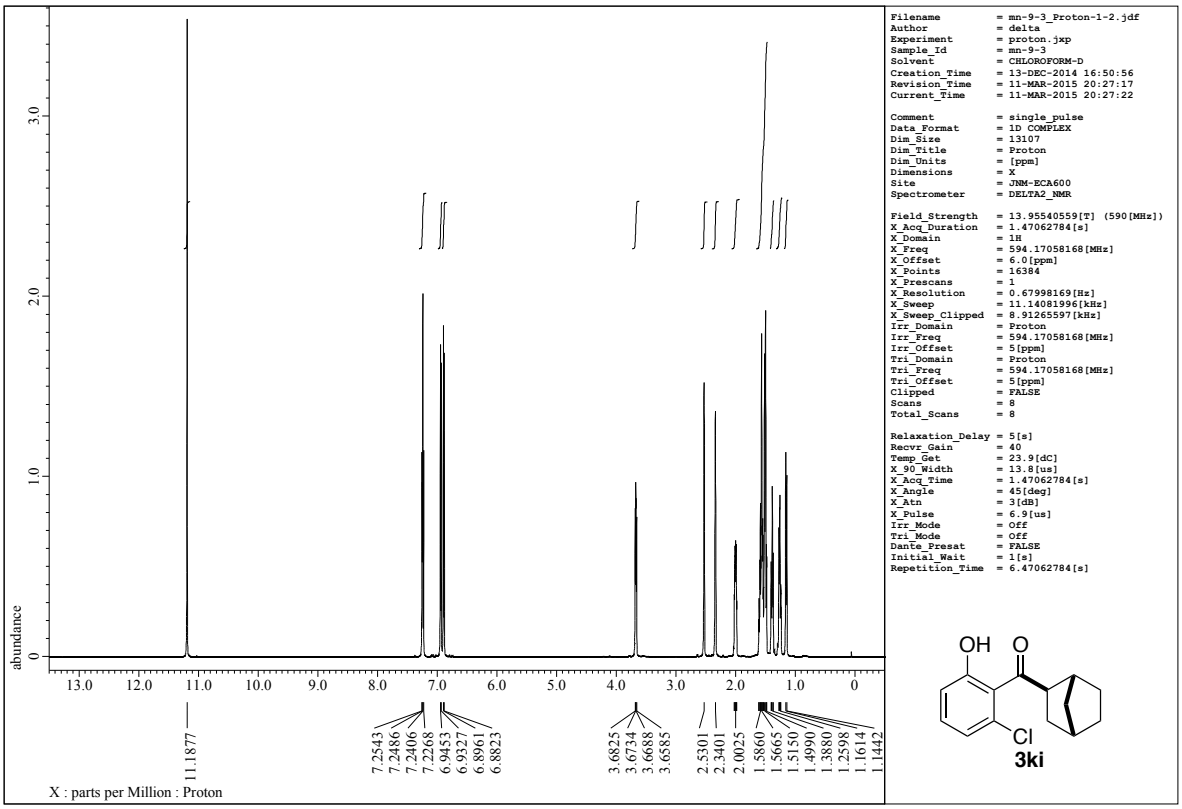

abundance
207.3032
163.0529
147.2822
129.9180
119.9449
118.5626
116.4701
77.2208
77.0000
76.7888
49.0676
41.4846
36.3396
36.2149
33.8632
29.6973
28.9294
21.8455
X : parts per Million : Carbon13
Filename = mn-8-189_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-189
Solvent = CHLOROFORM-D
Creation_Time = 4-DEC-2014 20:23:56
Revision_Time = 26-DEC-2014 16:52:11
Current_Time = 11-MAR-2015 20:19:51
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]
OH
O
3hi

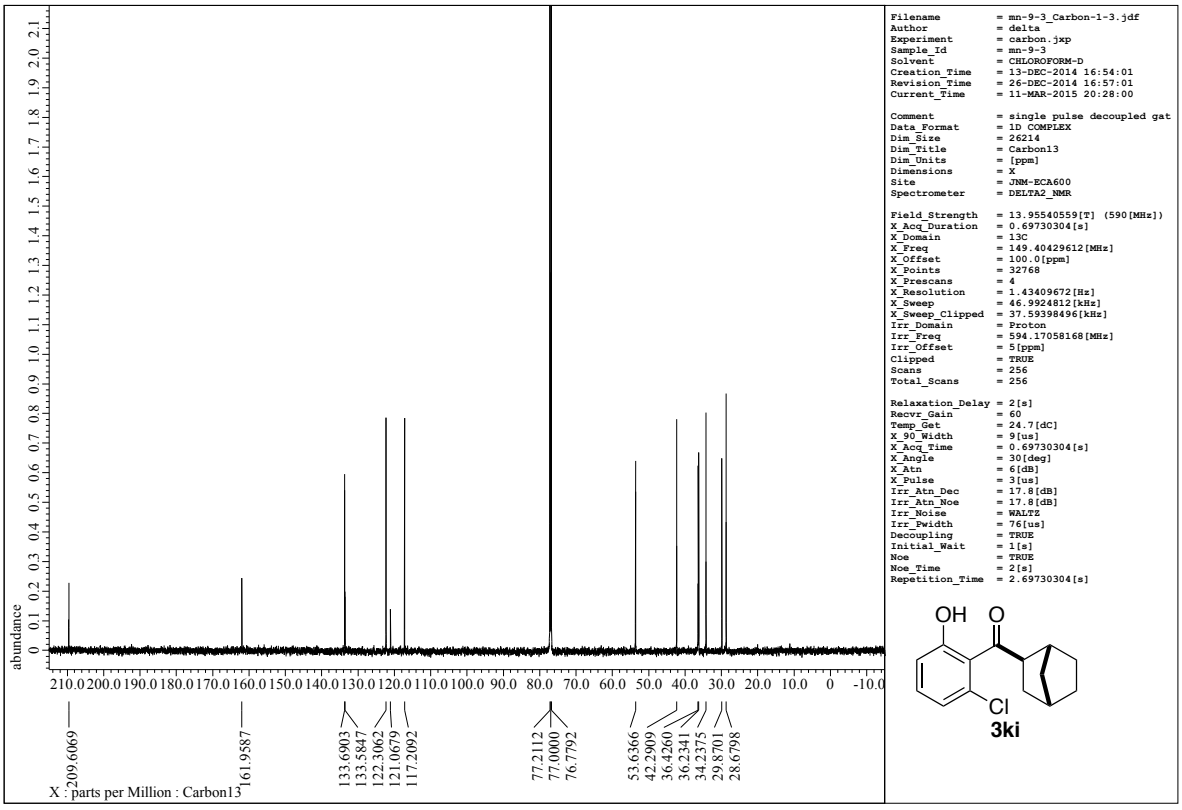

abundance
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.9419
12.9335
12.9266
7.6880
7.6727
7.2600
6.3887
6.3856
6.3719
5.4119
5.3599
3.1633
3.1541
3.1480
3.1388
2.5136
2.3585
2.0153
1.6148
1.4956
1.4619
1.4451
1.4115
1.4084
1.1914
1.1761
X : parts per Million : Proton
Filename = mn-9-11_Proton-3-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-9-11
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2014 12:39:42
Revision_Time = 11-MAR-2015 20:20:43
Current_Time = 11-MAR-2015 20:23:10
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.7[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.1010048[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 = 6.1010048[s]
OH
O
HO
3ii

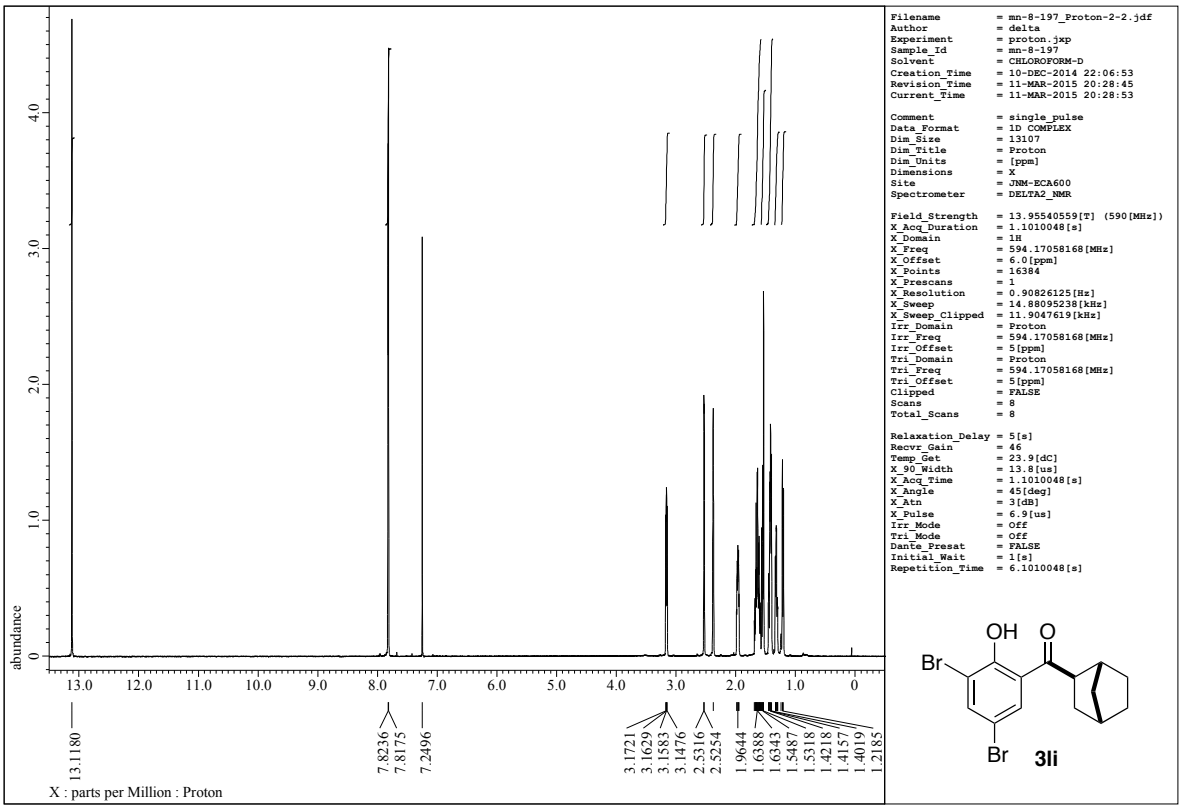

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
206.3625
165.4622
162.0163
132.3465
113.1873
107.4761
103.6174
77.2112
77.0000
76.7792
48.9140
41.5422
36.3780
36.1765
33.9495
29.7165
28.9102
X : parts per Million : Carbon13
Filename = mn-8-200_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-200
Solvent = CHLOROFORM-D
Creation_Time = 11-DEC-2014 22:50:39
Revision_Time = 26-DEC-2014 16:54:35
Current_Time = 11-MAR-2015 20:25:10
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 = 24.5[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]
OH
O
HO
3ii

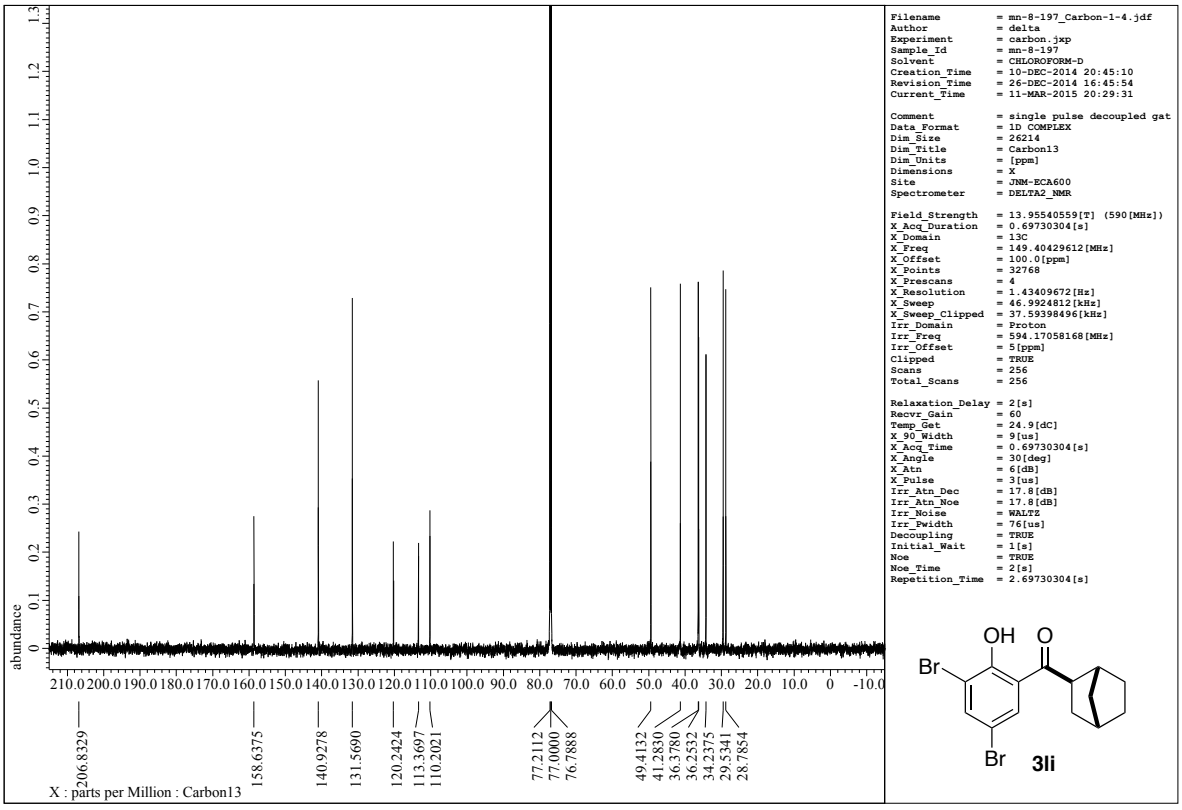

abundance
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
12.8036
7.3709
7.3571
7.2486
7.0239
7.0101
6.8328
6.8183
6.8053
3.8856
3.2253
3.2207
2.5328
2.3501
2.0039
1.6065
1.5682
1.4933
1.4337
1.4154
1.2977
1.1784
1.1616
X : parts per Million : Proton
Filename = mn-8-195_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-195
Solvent = CHLOROFORM-D
Creation_Time = 9-DEC-2014 21:43:42
Revision_Time = 11-MAR-2015 20:25:54
Current_Time = 11-MAR-2015 20:26:00
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 = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 24[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.1010048[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 = 6.1010048[s]
OH
O
MeO
3ji

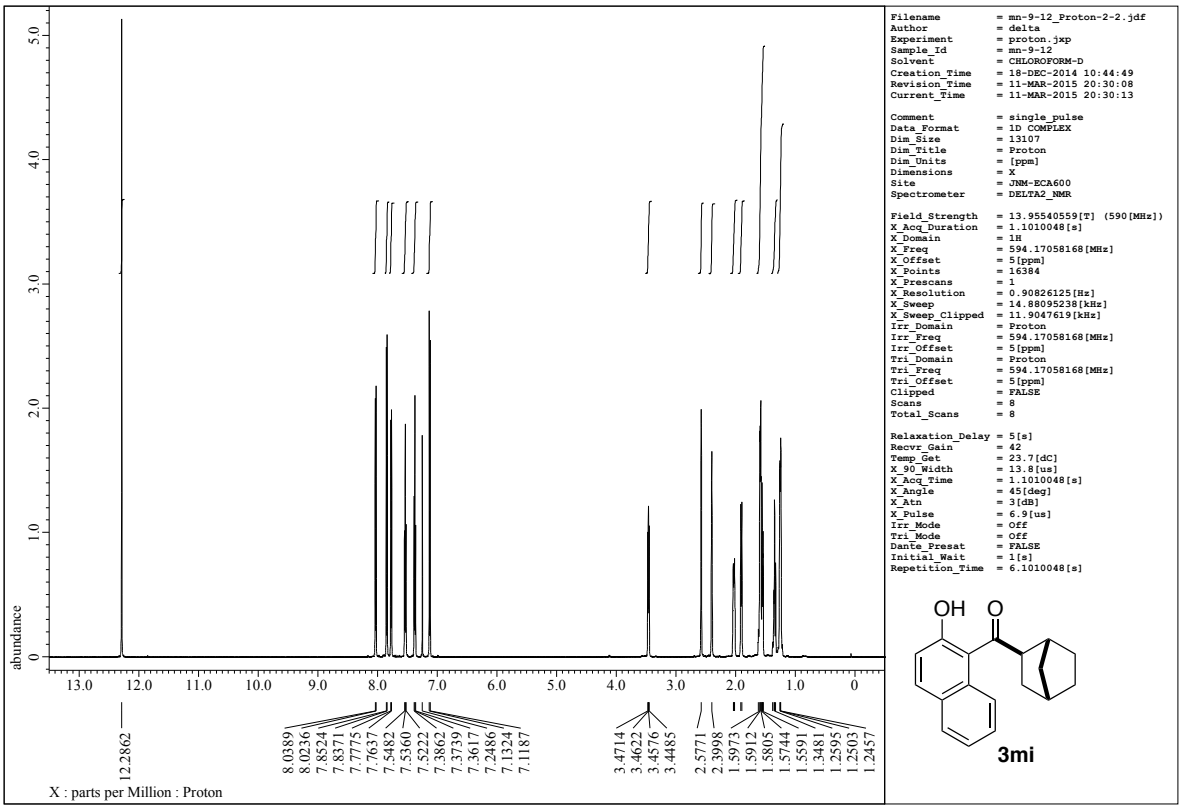

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
208.2631
153.4254
149.0867
121.2887
118.7354
117.9195
116.4029
77.2112
77.0000
76.7888
56.1515
49.5667
41.4750
36.2820
36.2244
33.8344
29.6685
28.8910
X : parts per Million : Carbon13
Filename = mn-8-195_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-195
Solvent = CHLOROFORM-D
Creation_Time = 9-DEC-2014 21:46:23
Revision_Time = 26-DEC-2014 16:34:36
Current_Time = 11-MAR-2015 20:26:37
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 60
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]
OH
O
MeO
3ji

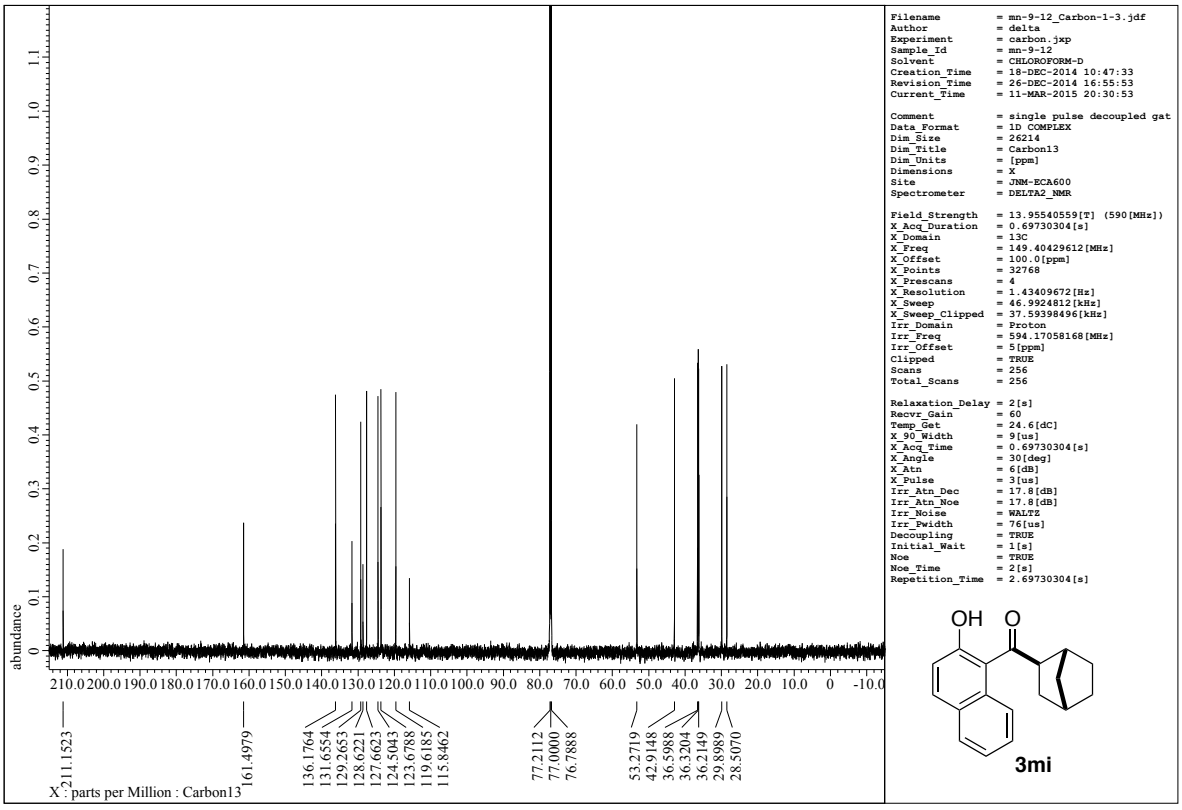

abundance
X : parts per Million : Proton
11.1877
7.2543
7.2486
7.2406
7.2268
6.9453
6.9327
6.8961
6.8823
3.6825
3.6734
3.6688
3.6585
2.5301
2.3401
2.0025
1.5860
1.5665
1.5150
1.4990
1.3880
1.2598
1.1614
1.1442
Filename = mn-9-3_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-9-3
Solvent = CHLOROFORM-D
Creation_Time = 13-DEC-2014 16:50:56
Revision_Time = 11-MAR-2015 20:27:17
Current_Time = 11-MAR-2015 20:27:22
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.47062784[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 6.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.67998169[Hz]
X_Sweep = 11.14081996[kHz]
X_Sweep_Clipped = 8.91265597[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 40
Temp_Get = 23.9[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]
OH
O
Cl
3ki

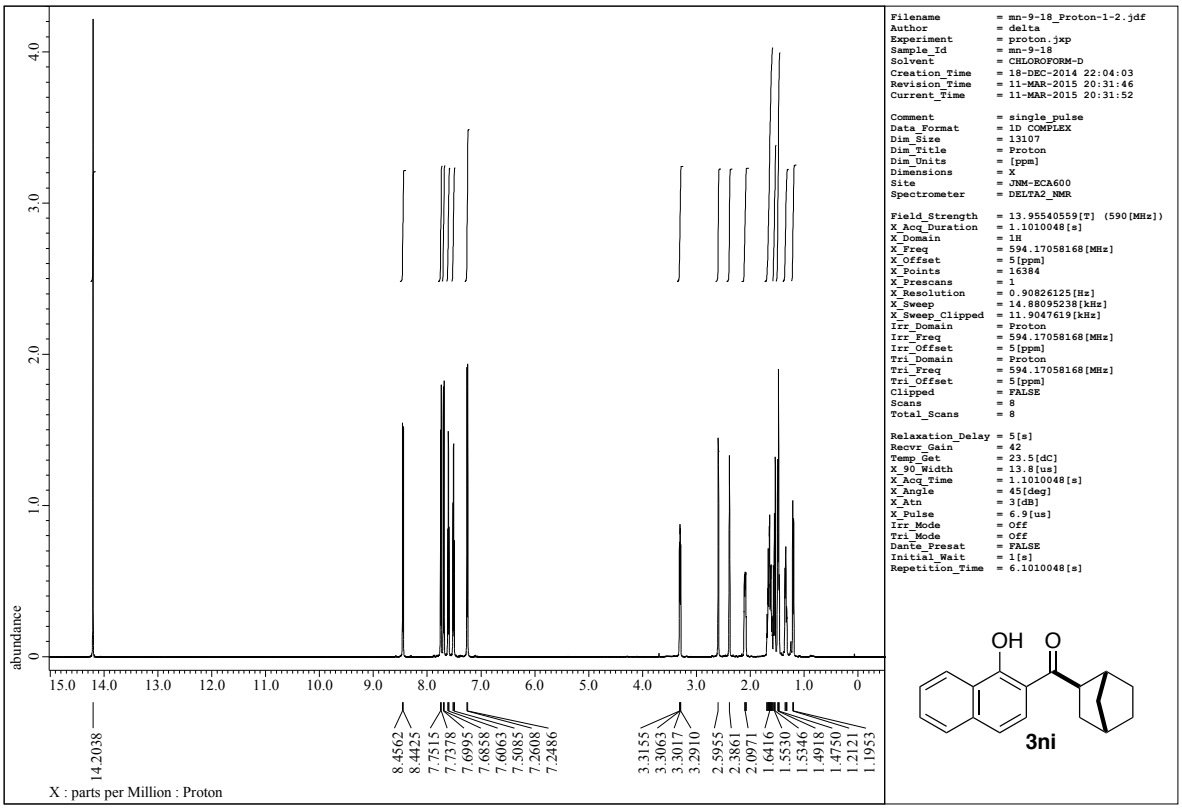

abundance
X : parts per Million : Carbon13
209.6069
161.9587
133.6903
133.5847
122.3062
121.0679
117.2092
77.2112
77.0000
76.7792
53.6366
42.2909
36.4260
36.2341
34.2375
29.8701
28.6798
Filename = mn-9-3_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-9-3
Solvent = CHLOROFORM-D
Creation_Time = 13-DEC-2014 16:54:01
Revision_Time = 26-DEC-2014 16:57:01
Current_Time = 11-MAR-2015 20:28:00
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 = 24.7[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]
OH
O
Cl
3ki

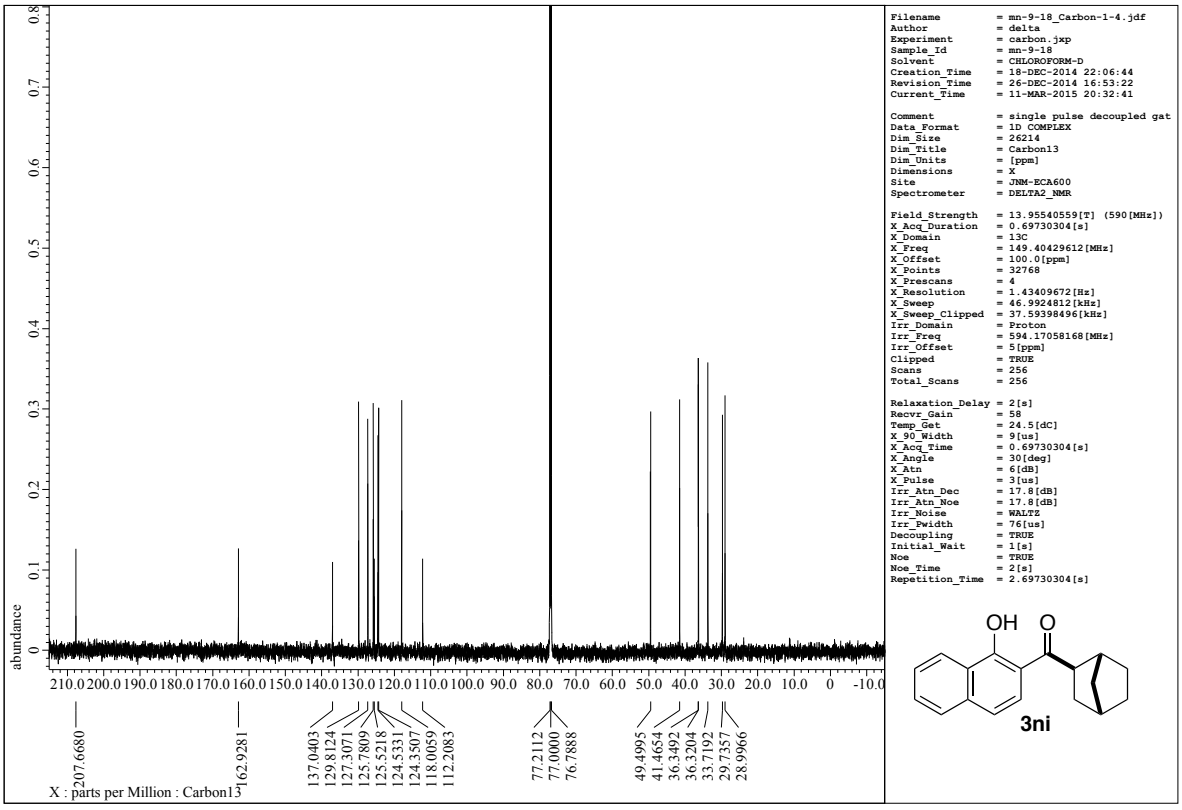

abundance
13.1180
7.8236
7.8175
7.2496
3.1721
3.1629
3.1583
3.1476
2.5316
2.5254
1.9644
1.6388
1.6343
1.5487
1.5318
1.4218
1.4157
1.4019
1.2185
X : parts per Million : Proton
Filename = mn-8-197_Proton-2-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-8-197
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2014 22:06:53
Revision_Time = 11-MAR-2015 20:28:45
Current_Time = 11-MAR-2015 20:28:53
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 6.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.9[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.1010048[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 = 6.1010048[s]
OH
O
Br
Br
3li

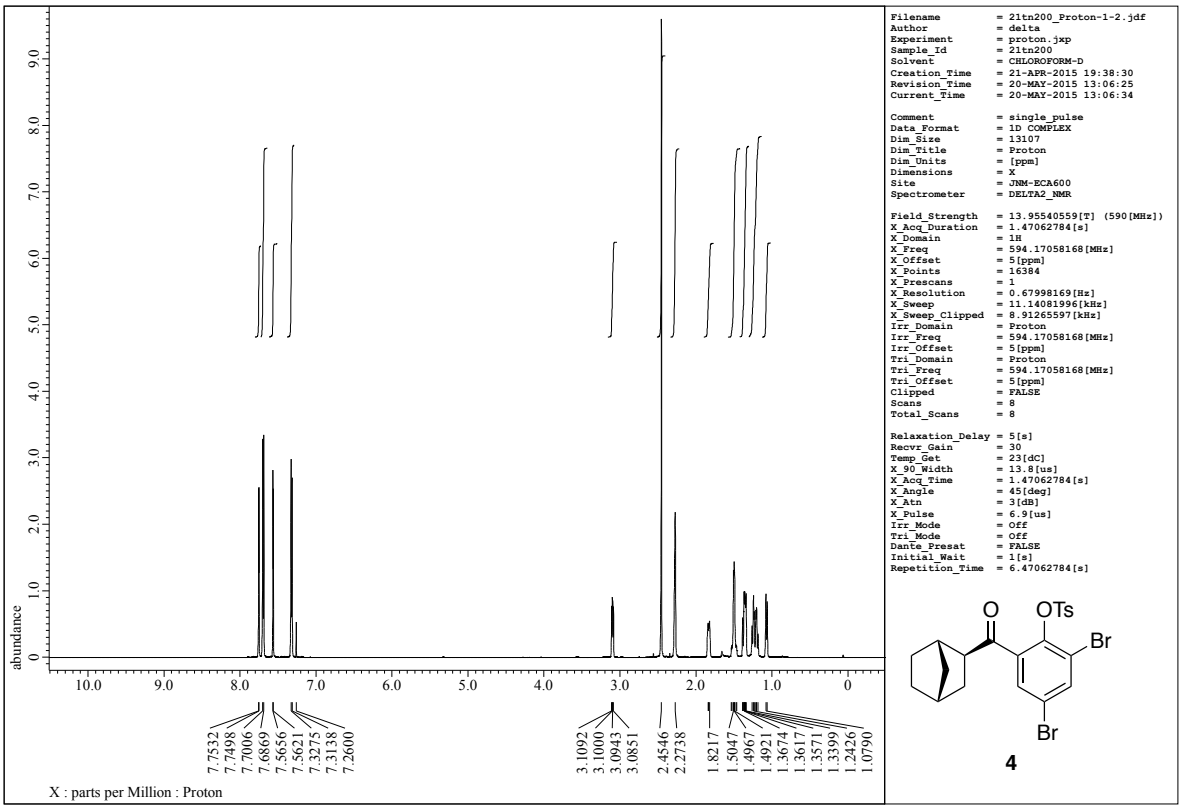

abundance
206.8329
158.6375
140.9278
131.5690
120.2424
113.3697
110.2021
77.2112
77.0000
76.7888
49.4132
41.2830
36.3780
36.2532
34.2375
29.5341
28.7854
X : parts per Million : Carbon13
Filename = mn-8-197_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-8-197
Solvent = CHLOROFORM-D
Creation_Time = 10-DEC-2014 20:45:10
Revision_Time = 26-DEC-2014 16:45:54
Current_Time = 11-MAR-2015 20:29:31
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]
OH
O
Br
Br
3li

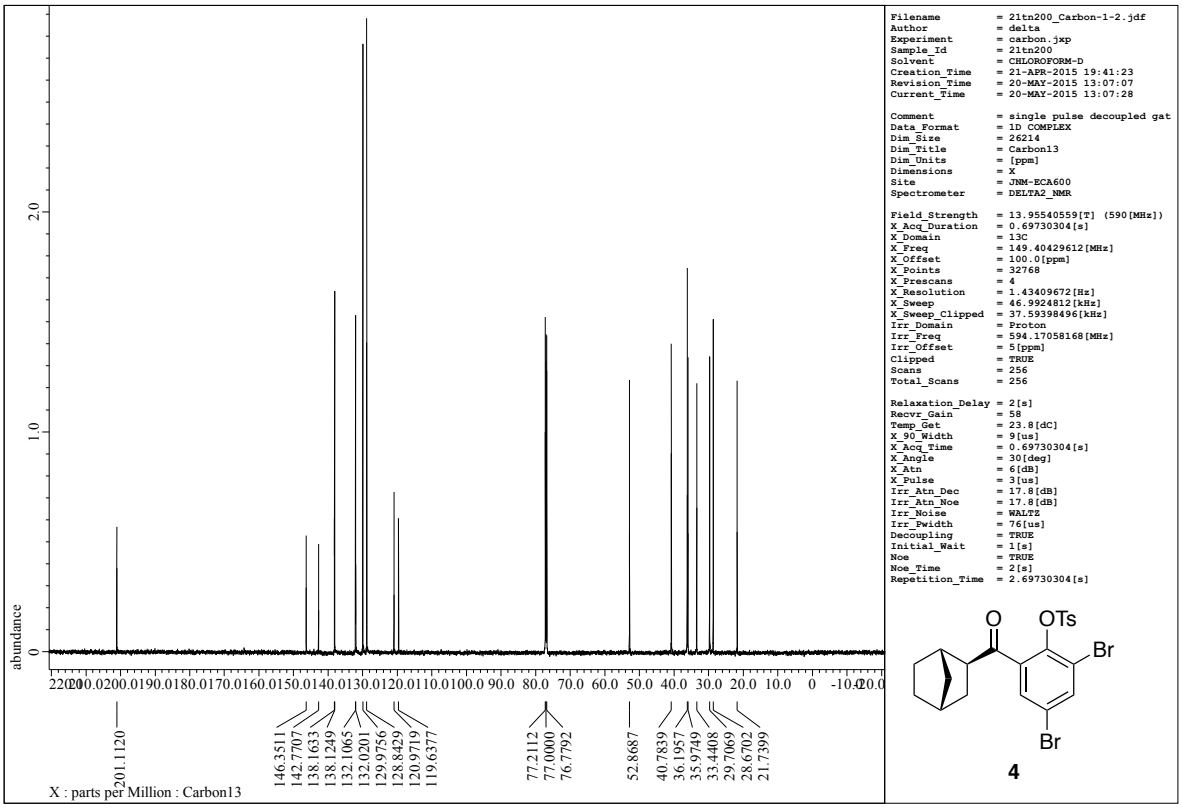

abundance
X : parts per Million : Proton
12.2862
8.0389
8.0236
7.8524
7.8371
7.7775
7.7637
7.5482
7.5360
7.5222
7.3862
7.3739
7.3617
7.2486
7.1324
7.1187
3.4714
3.4622
3.4576
3.4485
2.5771
2.3998
1.5973
1.5912
1.5805
1.5744
1.5591
1.3481
1.2595
1.2503
1.2457
Filename = mn-9-12_Proton-2-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-9-12
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2014 10:44:49
Revision_Time = 11-MAR-2015 20:30:08
Current_Time = 11-MAR-2015 20:30:13
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 23.7[dC]
X_90_Width = 13.8[us]
X_Acq_Time = 1.1010048[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 = 6.1010048[s]
OH
O
3mi


abundance
X : parts per Million : Carbon13
211.1523
161.4979
136.1764
131.6554
129.2653
128.6221
127.6623
124.5043
123.6788
119.6185
115.8462
77.2112
77.0000
76.7888
53.2719
42.9148
36.5988
36.3204
36.2149
29.8989
28.5070
Filename = mn-9-12_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-9-12
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2014 10:47:33
Revision_Time = 26-DEC-2014 16:55:53
Current_Time = 11-MAR-2015 20:30:53
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 = 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]
OH
O
3mi

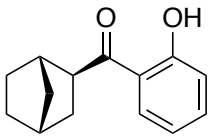

abundance
X : parts per Million : Proton
14.2038
8.4562
8.4425
7.7515
7.7378
7.6995
7.6858
7.6063
7.5085
7.2608
7.2486
3.3155
3.3063
3.3017
3.2910
2.5955
2.3861
2.0971
1.6416
1.5530
1.5346
1.4918
1.4750
1.2121
1.1953
Filename = mn-9-18_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = mn-9-18
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2014 22:04:03
Revision_Time = 11-MAR-2015 20:31:46
Current_Time = 11-MAR-2015 20:31:52
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 1.1010048[s]
X_Domain = 1H
X_Freq = 594.17058168[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.90826125[Hz]
X_Sweep = 14.88095238[kHz]
X_Sweep_Clipped = 11.9047619[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 594.17058168[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 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 = 1.1010048[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 = 6.1010048[s]
OH
O
3ni


abundance
X : parts per Million : Carbon13
207.6680
162.9281
137.0403
129.8124
127.3071
125.7809
125.5218
124.5331
124.3507
118.0059
112.2083
77.2112
77.0000
76.7888
49.4995
41.4654
36.3492
36.3204
33.7192
29.7357
28.9966
Filename = mn-9-18_Carbon-1-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = mn-9-18
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2014 22:06:44
Revision_Time = 26-DEC-2014 16:53:22
Current_Time = 11-MAR-2015 20:32:41
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA600
Spectrometer = DELTA2_NMR
Field_Strength = 13.95540559[T] (590[MHz])
X_Acq_Duration = 0.69730304[s]
X_Domain = 13C
X_Freq = 149.40429612[MHz]
X_Offset = 100.0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.43409672[Hz]
X_Sweep = 46.9924812[kHz]
X_Sweep_Clipped = 37.59398496[kHz]
Irr_Domain = Proton
Irr_Freq = 594.17058168[MHz]
Irr_Offset = 5[ppm]
Clipped = 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]
OH
O
3ni

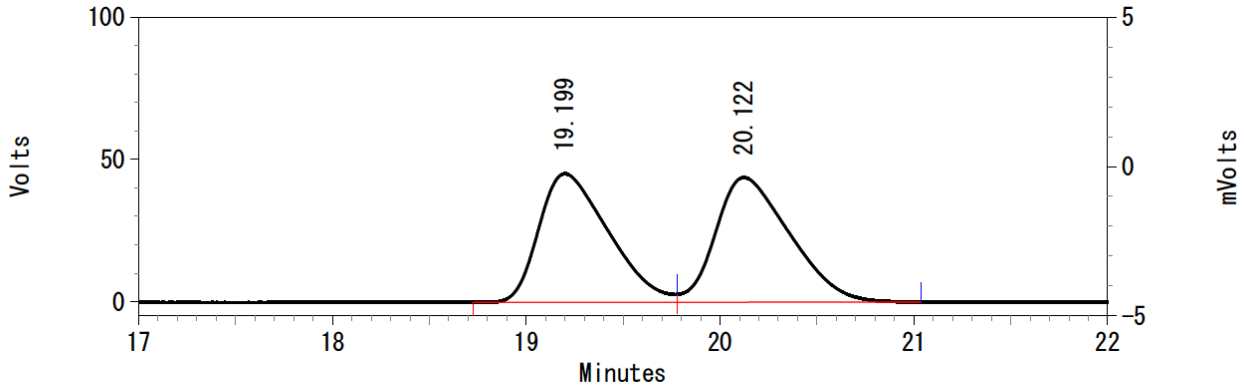

abundance
X : parts per Million : Proton
7.7532
7.7498
7.7006
7.6869
7.5656
7.5621
7.3275
7.3138
7.2600
3.1092
3.1000
3.0943
3.0851
2.4546
2.2738
1.8217
1.5047
1.4967
1.4921
1.3674
1.3617
1.3571
1.3399
1.2426
1.0790
Filename = 21tn200_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 21tn200
Solvent = CHLOROFORM-D
Creation_Time = 21-APR-2015 19:38:30
Revision_Time = 20-MAY-2015 13:06:25
Current_Time = 20-MAY-2015 13:06:34
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[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
OTs
Br
Br
4


abundance
X : parts per Million : Carbon13
201.1120
146.3511
142.7707
138.1633
138.1249
132.1065
132.0201
129.9756
128.8429
120.9719
119.6377
77.2112
77.0000
76.7792
52.8687
40.7839
36.1957
35.9749
33.4408
29.7069
28.6702
21.7399
Filename = 21tn200_Carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 21tn200
Solvent = CHLOROFORM-D
Creation_Time = 21-APR-2015 19:41:23
Revision_Time = 20-MAY-2015 13:07:07
Current_Time = 20-MAY-2015 13:07:28
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 = 58
Temp_Get = 23.8[dC]
X_90_Width = 9[us]
X_Acq_Time = 0.69730304[s]
X_Angle = 30[deg]
X_Atn = 6[dB]
X_Pulse = 3[us]
Irr_Atn_Dec = 17.8[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
OTs
Br
Br
4

14. Chiral HPLC charts

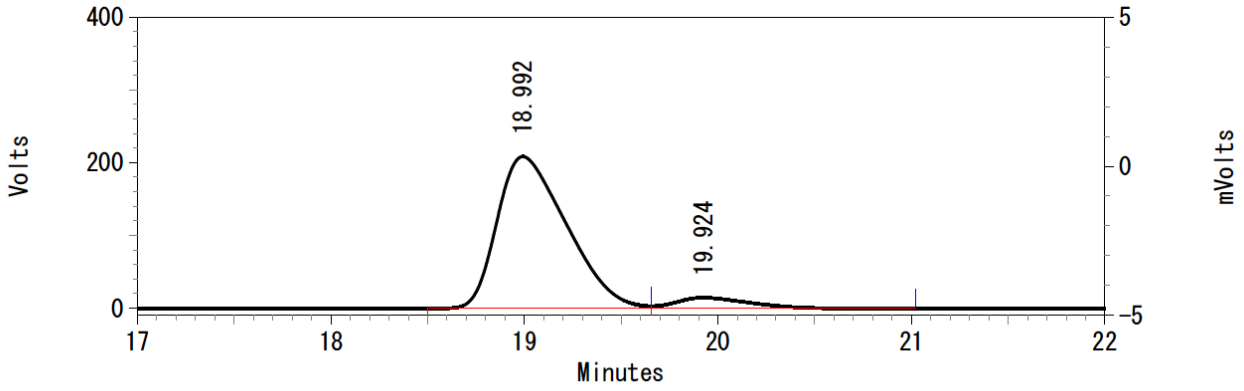


3ai



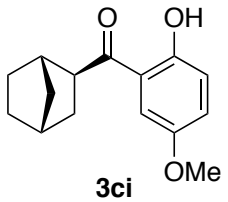
UV-970 Results

Pk #	Retention Time	Area	Area Percent	Height
1	19.199	1128167	49.265	45187
2	20.122	1161810	50.735	43855
Totals		2289977	100.000	89042

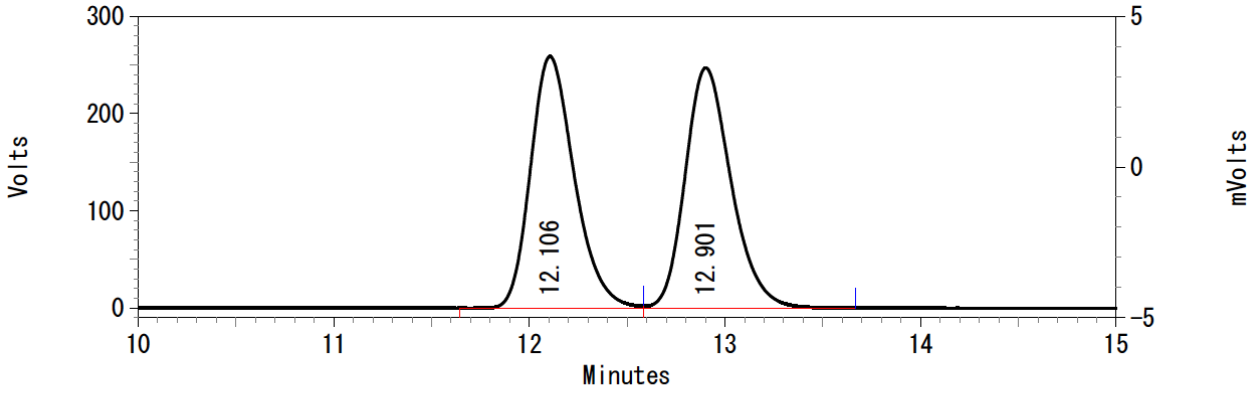


UV-970 Results

Pk #	Retention Time	Area	Area Percent	Height
1	18.992	5184274	93.059	208566
2	19.924	386680	6.941	14757
Totals		5570954	100.000	223323

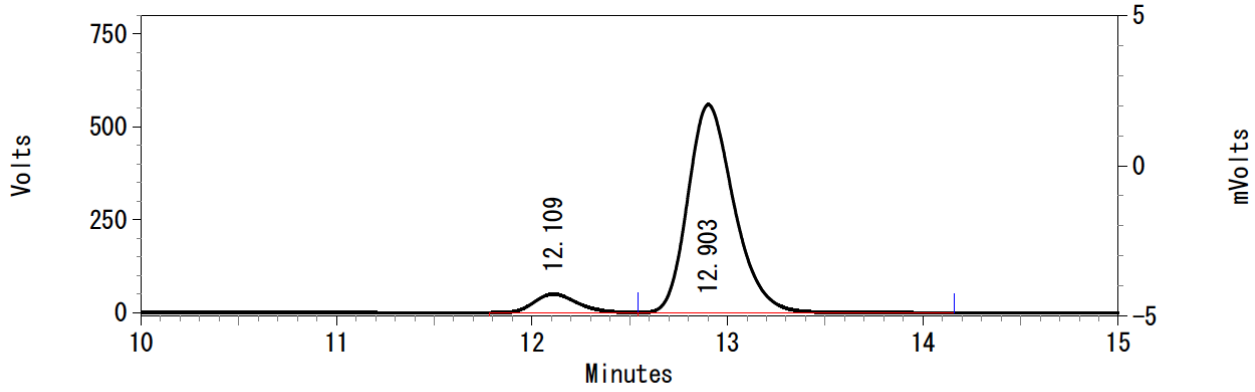


3ci



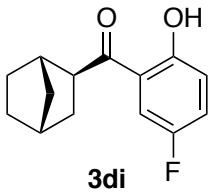
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	12.106	4035086	49.925	258846
2	12.901	4047194	50.075	247053
Totals		8082280	100.000	505899

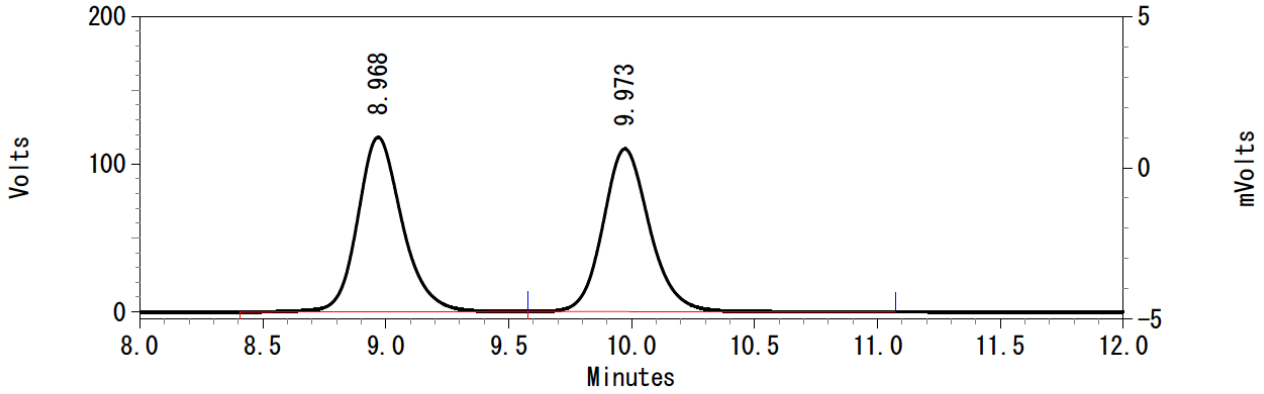


UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	12.109	786538	7.884	50502
2	12.903	9190447	92.116	559730
Totals		9976985	100.000	610232

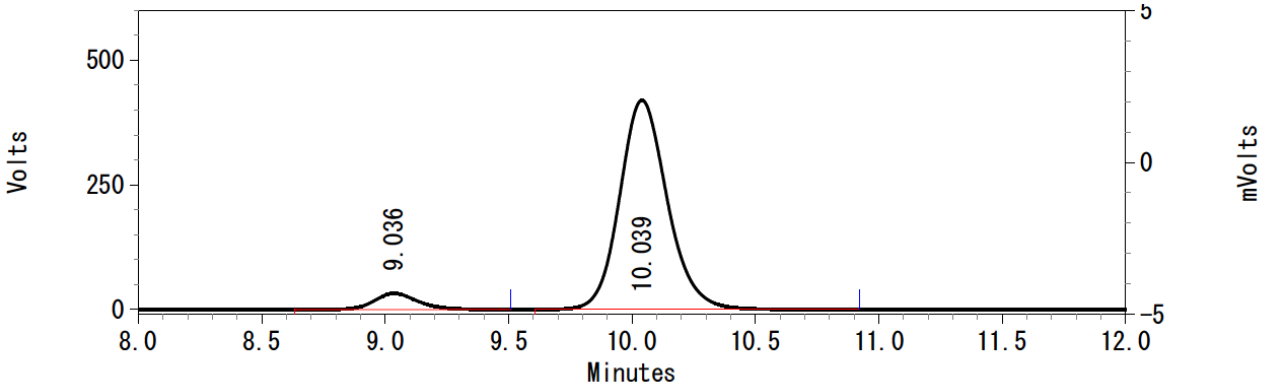


3di



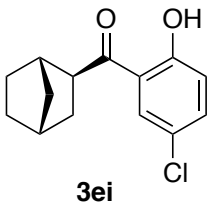
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	8.968	1488954	50.629	118114
2	9.973	1451946	49.371	110186
Totals		2940900	100.000	228300

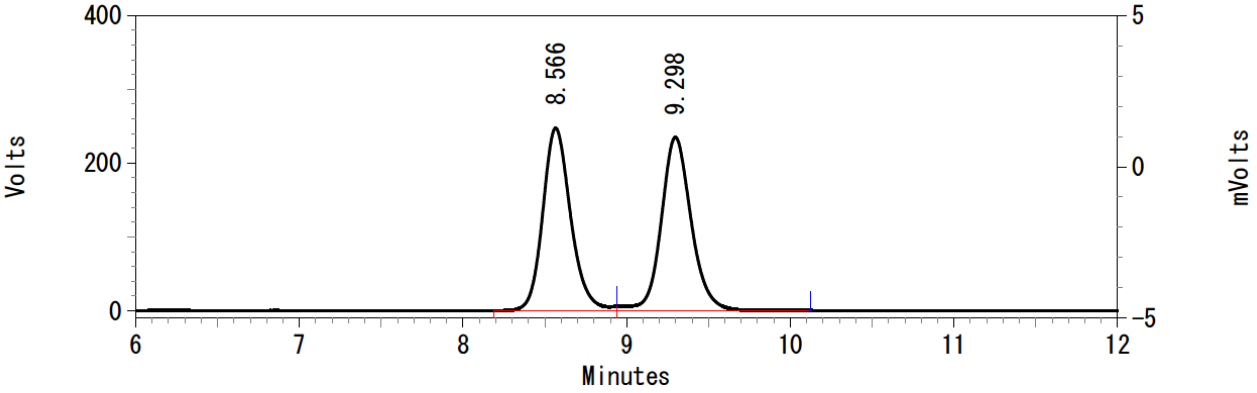


UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	9.036	399315	6.616	32333
2	10.039	5636387	93.384	419666
Totals		6035702	100.000	451999

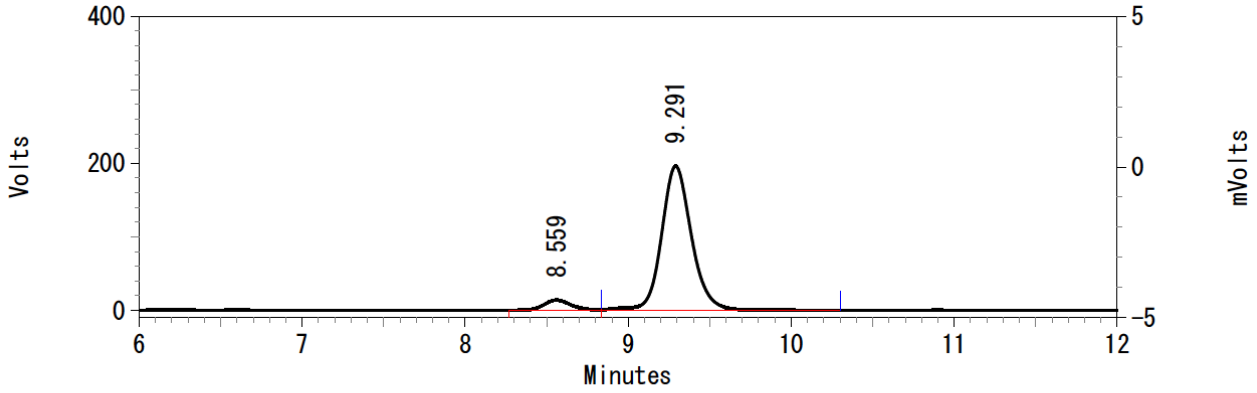


3ei



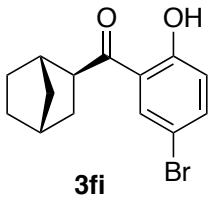
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	8.566	2943189	49.511	247323
2	9.298	3001288	50.489	234892
Totals		5944477	100.000	482215

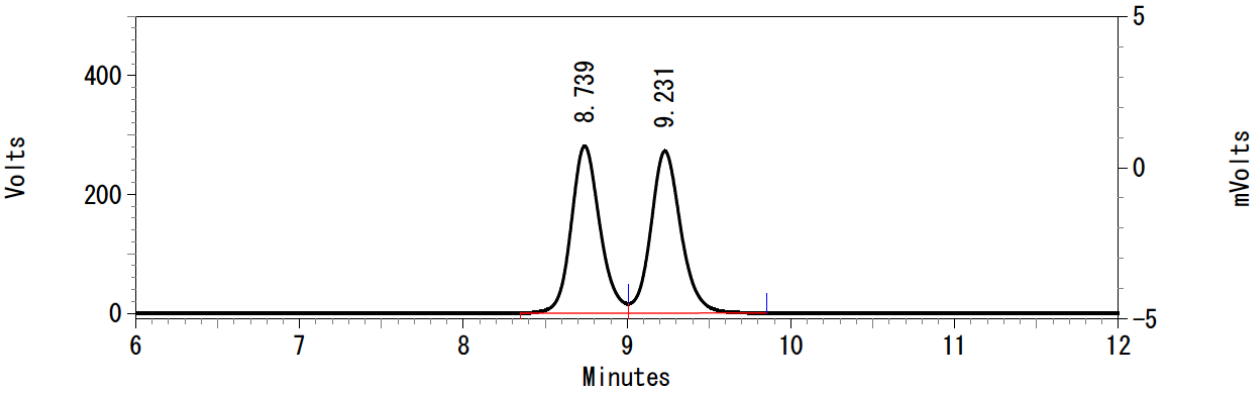


UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	8.559	165380	6.197	13963
2	9.291	2503190	93.803	196064
Totals		2668570	100.000	210027

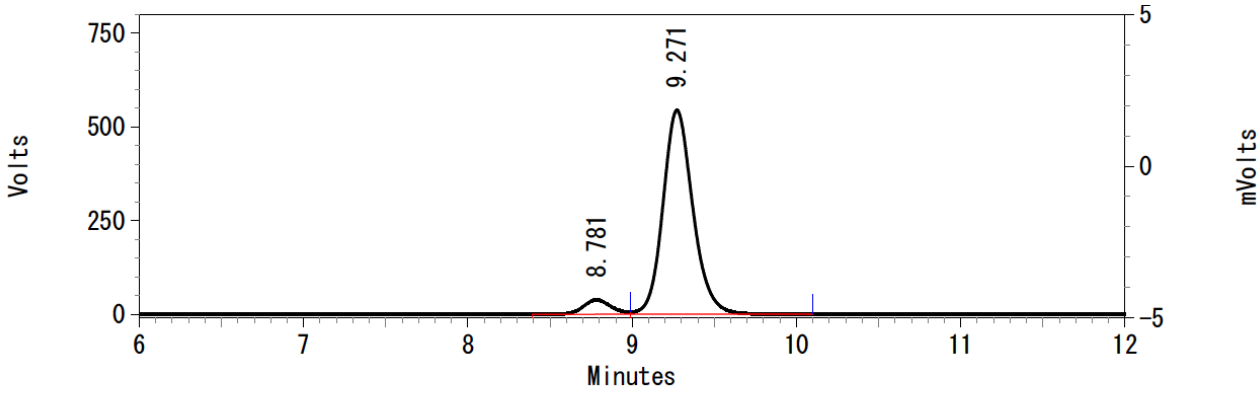


3fi



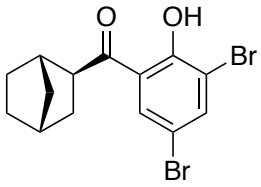
UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	8.739	3418389	49.584	281405
2	9.231	3475749	50.416	273031
Totals		6894138	100.000	554436

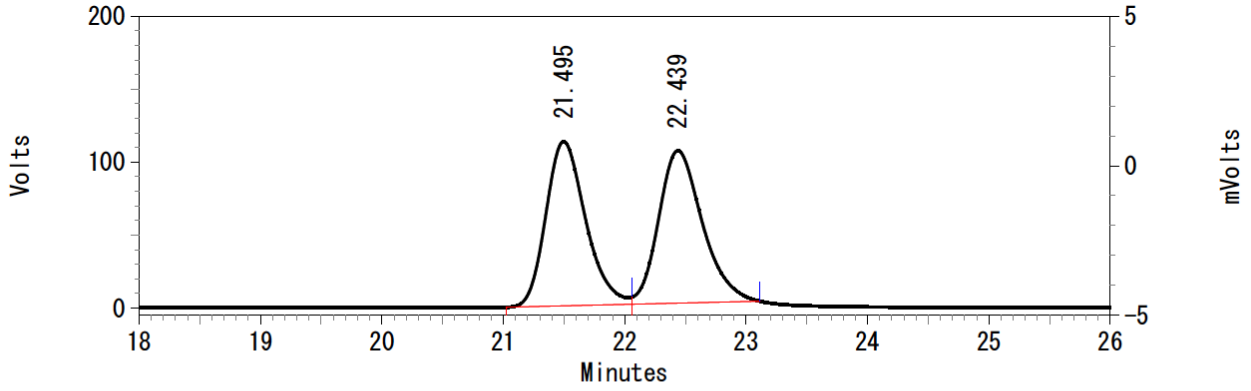


UV Results

Pk #	Retention Time	Area	Area Percent	Height
1	8.781	459774	6.259	38550
2	9.271	6886334	93.741	543782
Totals		7346108	100.000	582332

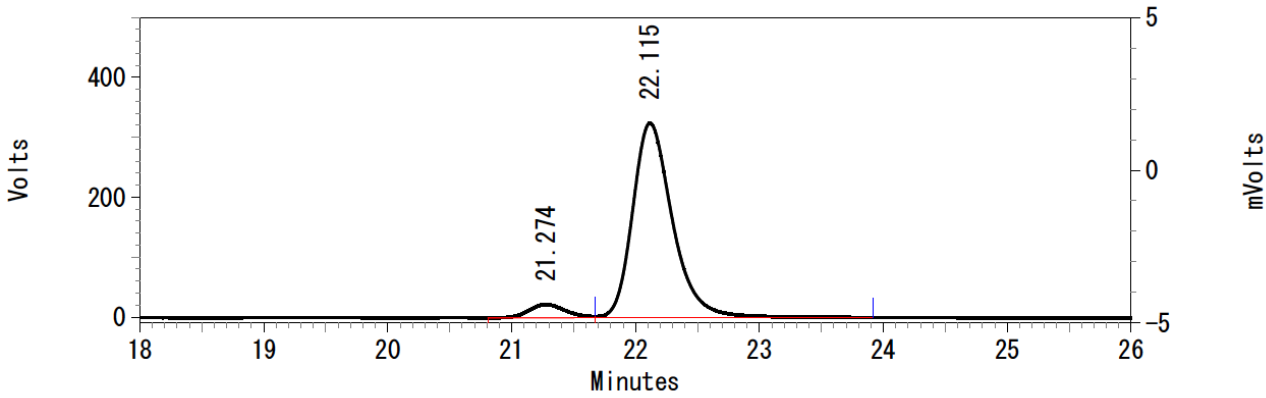


3li



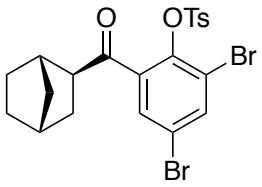
UV-970 Results

Pk #	Retention Time	Area	Area Percent	Height
1	21.495	2562183	49.456	112683
2	22.439	2618560	50.544	104535
Totals		5180743	100.000	217218

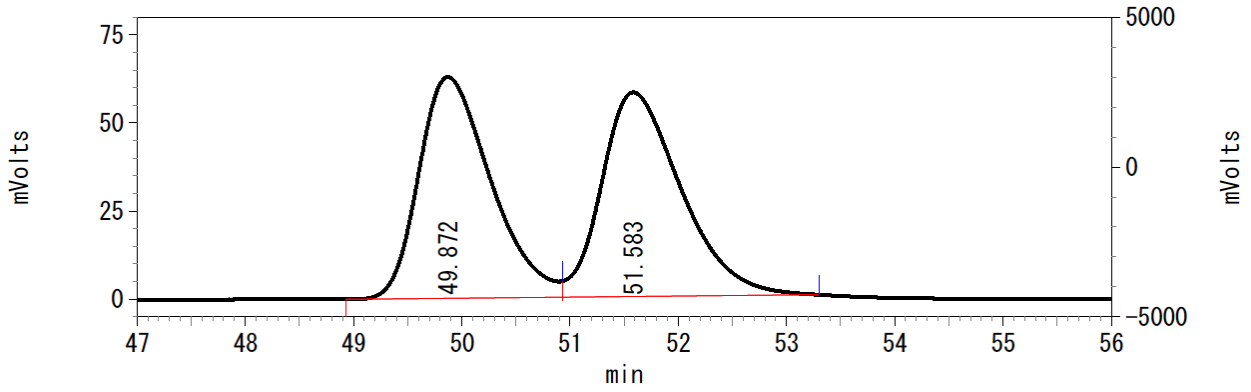


UV-970 Results

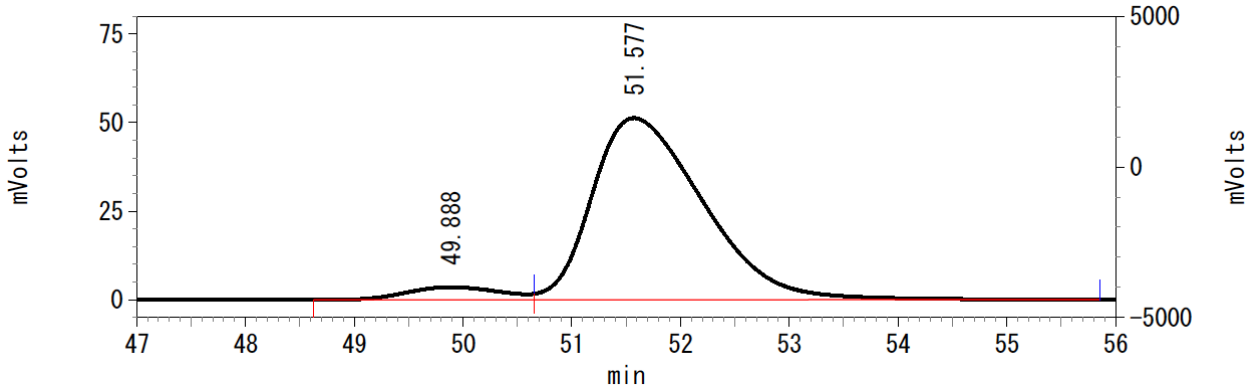
Pk #	Retention Time	Area	Area Percent	Height
1	21.274	449924	5.836	22231
2	22.115	7259271	94.164	324859
Totals		7709195	100.000	347090



4



Pk #	Retention Time	Area	Area Percent
1	49.872	2907422	49.623
2	51.583	2951609	50.377



Pk #	Retention Time	Area	Area Percent
1	49.888	218535	5.657
2	51.577	3644735	94.343