Supporting Information for

## A Convergent Assembly of the Spiroacetal Subunit of Didemnaketal B

Haruhiko Fuwa\*, Sayaka Noji, and Makoto Sasaki

Graduate School of Life Sciences, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

\*Corresponding author. Email: hfuwa@bios.tohoku.ac.jp

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General methods. All reactions sensitive to moisture and/or air were carried out under an atmosphere of argon in dry, freshly distilled solvents under anhydrous conditions using oven-dried glassware unless otherwise noted. Anhydrous dichloromethane (CH<sub>2</sub>Cl<sub>2</sub>) was purchased from Kanto Chemical Co. Inc. and used directly without further drying. Anhydrous tetrahydrofuran, diethyl ether, and toluene were purchased from Wako Pure Chemical Industries, Ltd. and further purified by a Glass Contour solvent purification system under an atmosphere of argon immediately prior to use. Diisopropylethylamine, triethylamine, 2,6-lutidine, acetonitrile (CH<sub>3</sub>CN), benzene, and methanol were distilled from calcium hydride under an atmosphere of argon. Hexamethyphosphoramide (HMPA) and N.N.-dimethylpropyleneurea (DMPU) were distilled from calcium hydride under reduced pressure. N,N-dimethylformamide (DMF) and dimethyl sulfoxide (DMSO) were distilled from magnesium sulfate under reduced pressure. All other chemicals were purchased at highest commercial grade and used directly. Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F<sub>254</sub> plates (0.25-mm thickness). Flash column chromatography was carried out using Kanto chemical silica gel 60N (40-100 mesh, spherical, neutral) or Fuji Silysia silica gel BW-300 (200-400 mesh). Optical rotations were recorded on a JASCO P-1020 digital polarimeter. IR spectra were recorded on a JASCO FT/IR-4100 spectrometer. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on a JEOL JNM-ECA-600 spectrometer, and chemical shift values are reported in ppm ( $\delta$ ) downfield from tetramethylsilane with reference to internal solvent [<sup>1</sup>H NMR, CHCl<sub>3</sub> (7.24), C<sub>6</sub>HD<sub>5</sub> (7.15); <sup>13</sup>C NMR, CDCl<sub>3</sub> (77.0), C<sub>6</sub>D<sub>6</sub> (128.0)] unless otherwise noted. Coupling constants (J) are reported in Hertz (Hz). The following abbreviations were used to designate the multiplicities: s = singlet; d = doublet; t = triplet; m = multiplet; br = broad. FAB mass spectra were recorded on a JEOL JMS-700 spectrometer and ESI-TOF mass spectra were measured on a Bruker microTOF focus spectrometer.



Sulfone 12. To a solution of alcohol 11 (0.8965 g, 4.977 mmol) in THF (40 mL) cooled to 0 °C were added 1-phenyl-1H-tetrazole-5-thiol (1.33 g, 7.46 mmol), Ph<sub>3</sub>P (1.96 g, 7.47 mmol), and DEAD (2.2 M solution in toluene, 3.40 mL, 7.48 mmol), and the resultant solution was stirred at room temperature for 25 min. The reaction was quenched with saturated aqueous NaHCO<sub>3</sub> solution at 0 °C, and the resultant mixture was diluted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (8 to 15% EtOAc/hexanes) gave sulfide S1 (1.6017 g, 95%) as a colorless oil:  $[\alpha]_D^{26}$  -8.0 (c 1.00, CHCl<sub>3</sub>); IR (film) 2930, 1595, 1498, 1454, 1385, 1014, 962, 759, 695, 443 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.57-7.49 (m, 5H), 7.33–7.23 (m, 5H), 4.49 (d, J = 12.0 Hz, 1H), 4.47 (d, J = 12.0 Hz, 1H), 3.54 (dd, J = 12.7, 6.2 Hz, 1H), 3.47 (dd, J = 9.6, 4.9 Hz, 1H), 3.40 (dd, J = 9.6, 5.8 Hz, 1H), 3.38 (dd, J = 12.7, 6.8 Hz, 1H), 2.29 (m, 1H), 1.08 (d, J = 6.8 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) & 154.7, 138.2, 133.7, 130.0, 129.7 (2C), 128.3 (2C), 127.6 (3C), 123.8 (2C), 73.5, 73.1, 37.1, 33.6, 16.5; HRMS (ESI) calcd for  $C_{18}H_{20}N_4OSNa$  [(M + Na)<sup>+</sup>] 363.1250, found 363.1259.

To a solution of sulfide S1 (0.6626 g, 1.948 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) cooled

to 0 °C was added *m*-CPBA (77% purity, 1.07 g, 4.77 mmol), and the resultant solution was stirred at room temperature for 22 h. The reaction was quenched with 3.0 M aqueous NaOH solution at 0 °C, and the resultant mixture was stirred at room temperature for 10 min. The resultant mixture was diluted with EtOAc, and the organic layer was washed successively with 3.0 M aqueous NaOH solution, saturated aqueous NH<sub>4</sub>Cl solution, and brine. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (10 to 15% EtOAc/hexanes) gave sulfone 12 (0.7321 g, 100%) as a colorless viscous oil:  $[\alpha]_D^{28}$  -14.0 (c 1.00, C<sub>6</sub>H<sub>6</sub>); IR (film) 2861, 1496, 1455, 1336, 1152, 1096, 764, 689, 634, 520 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.63—7.53 (m, 5H), 7.36—7.25 (m, 5H), 4.48 (d, J = 11.6 Hz, 1H), 4.43 (d, J = 11.6 Hz, 1H), 4.03 (dd, J = 14.8, 5.2 Hz, 1H), 3.56 (dd, J = 14.8, 7.5 Hz, 1H), 3.52 (dd, J = 9.3, 4.8 Hz, 1H), 3.36 (dd, J = 9.3, 6.5 Hz, 1H), 2.60 (m, 1H), 1.18 (d, J = 6.9 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) & 154.0, 137.8, 133.0, 131.4, 129.6 (2C), 128.4 (2C), 127.8, 127.6 (2C), 125.2 (2C), 73.1, 73.0, 59.0, 29.3, 17.1; HRMS (ESI) calcd for  $C_{18}H_{20}N_4O_3SNa [(M + Na)^+] 395.1148$ , found 395.1151.



**Olefin 14.** To a solution of sulfone **12** (2.565 g, 6.893 mmol) in THF/DMPU (4:1, v/v, 40 mL) cooled to -78 °C was added dropwise KHMDS (0.5 M solution in toluene, 12 mL, 6.0 mmol), and the resultant mixture was stirred at -78 °C for 40 min. To this

solution was added dropwise a solution of aldehyde 13 (0.7355 g, 3.311 mmol) in THF (17 mL + 10 mL rinse), and the resultant mixture was allowed to warm to room temperature over a period of 11 h 20 min. The reaction was quenched with saturated aqueous NH<sub>4</sub>Cl solution at 0 °C, and the mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (3 to 15% EtOAc/hexanes) gave olefin 14 (0.9981 g, 82%, E/Z = 16:1 by 600 MHz <sup>1</sup>H NMR analysis) as a yellow oil:  $[\alpha]_D^{24} + 2.1$  (c 1.80, C<sub>6</sub>H<sub>6</sub>); IR (film) 2852, 1612, 1513, 1454, 1361, 1248, 1093, 1037, 971, 698 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.35—7.30 (m, 4H), 7.29—7.22 (m, 3H), 6.89—6.85 (m, 2H), 5.42 (ddd, J = 15.4, 6.5, 6.5 Hz, 1H), 5.36 (dd, J = 15.4, 6.9 Hz, 1H), 4.51 (d, J = 12.0 Hz, 1H), 4.49 (d, J = 12.0Hz, 1H), 4.41 (s, 2H), 3.79 (s, 3H), 3.34 (dd, J = 8.9, 6.5 Hz, 1H), 3.29 (dd, J = 8.9, 6.2 Hz, 1H), 3.26 (dd, J = 9.3, 6.9 Hz, 1H), 3.21 (dd, J = 9.3, 6.5 Hz, 1H), 2.46 (m, 1H), 2.14 (ddd, J = 12.7, 6.5, 6.5 Hz, 1H), 1.89—1.74 (m, 2H), 1.01 (d, J = 6.5 Hz, 3H), 0.89 (d, J = 6.5 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  159.0, 138.7, 134.4, 130.8, 129.1 (2C), 128.3 (2C), 127.9, 127.5 (2C), 127.4, 113.7 (2C), 75.5, 75.0, 72.8, 72.6, 55.2, 36.9, 36.7, 33.6, 17.3, 16.8; HRMS (ESI) calcd for  $C_{24}H_{32}O_3Na \left[(M + Na)^+\right]$  391.2244, found 391.2255.



**1,2-Diol 15.** To a solution of olefin **14** (1.437 g, 3.902 mmol, E/Z = 16:1) in *t*-BuOH/H<sub>2</sub>O (1:1, v/v, 34 mL) were added (DHQ)<sub>2</sub>PHAL (60.8 mg, 78.1 µmol),

K<sub>3</sub>Fe(CN)<sub>6</sub> (3.85 g, 11.7 mmol), and K<sub>2</sub>CO<sub>3</sub> (1.62 g, 11.7 mmol). The resultant mixture was cooled to 0 °C, treated with OsO<sub>4</sub> (0.039 M solution in *t*-BuOH, 1.0 mL, 39 µmol) and MeSO<sub>2</sub>NH<sub>2</sub> (371.0 mg, 3.900 mmol), and stirred vigorously at 0 °C for 15 h 20 min. The reaction was quenched with solid Na<sub>2</sub>SO<sub>3</sub>, and the mixture was stirred at room temperature for 10 min. The resultant mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (10 to 50% EtOAc/hexanes) to give 1,2-diol 15 (1.442 g) along with unreacted olefin 14 (0.0837 g, 6%, E/Z = 5:2). The former material was further purified by recrystallization from CH<sub>2</sub>Cl<sub>2</sub>/hexanes to give 1.2-diol **15** (1.265 g, 81%, dr >20:1 by 600 MHz  $^{1}$ H NMR analysis) as a colorless solid: mp 89.0—89.5 °C;  $[\alpha]_D^{23}$  +4.5 (c 1.00, CHCl<sub>3</sub>); IR (film) 3341, 2936, 1514, 1248, 1100, 1032, 816, 698 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.36–7.26 (m, 5H), 7.25–7.20 (m, 2H), 6.89–6.81 (m, 2H), 4.50 (s, 2H), 4.43 (d, J =11.7 Hz, 1H), 4.41 (d, J = 11.7 Hz, 1H), 3.78 (s, 3H), 3.67 (ddd, J = 10.0, 3.0, 3.0 Hz, 1H), 3.54—3.50 (m, 2H), 3.31—3.24 (m, 3H), 2.04 (m, 1H), 1.98 (m, 1H), 1.69 (ddd, J = 14.1, 10.0, 5.9 Hz, 1H), 1.29 (ddd, J = 14.1, 7.6, 3.0 Hz, 1H), 0.92 (d, J = 7.3 Hz, 3H), 0.91 (d, J = 6.8 Hz, 3H) (two protons missing presumably due to H/D exchange); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 159.1, 137.6, 130.4, 129.2 (2C), 128.5 (2C), 127.8, 127.7 (2C), 113.7 (2C), 78.7, 76.2, 74.1, 73.4, 72.7, 69.9, 55.2, 39.5, 35.8, 30.9, 17.5, 14.6; HRMS (ESI) calcd for  $C_{24}H_{34}O_5Na[(M + Na)^+]$  425.2298, found 425.2305.



Alcohol 16. To a solution of 1,2-diol 15 (92.6 mg, 0.230 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (2.3 mL) cooled to 0 °C were added 2,6-lutidine (0.11 mL, 0.94 mmol) and TIPSOTf (0.18 mL, 0.67 mmol). The resultant solution was stirred at 0 °C for 2 h and then at room temperature for 1 h. The reaction was quenched with saturated aqueous NH<sub>4</sub>Cl solution at 0 °C, and the resultant mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (3 to 5% EtOAc/hexanes) gave silvl ether S2 (166.6 mg, 100%) as a colorless oil:  $\left[\alpha\right]_{D}^{25}$  -28.3 (c 1.00, CHCl<sub>3</sub>); IR (film) 2944, 2866, 1513, 1463, 1248, 1097, 997, 882, 678 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) & 7.32-7.26 (m, 4H), 7.26-7.19 (m, 3H), 6.89-6.80 (m, 2H), 4.47 (d, J = 12.0 Hz, 1H), 4.43 (d, J = 12.0 Hz, 1H), 4.40 (s, 2H), 3.95 (ddd, J =9.3, 3.8, 2.7 Hz, 1H), 3.86 (dd, J = 4.1, 3.8 Hz, 1H), 3.78 (s, 3H), 3.64 (dd, J = 9.3, 3.1 Hz, 1H), 3.31 (dd, J = 9.3, 7.6 Hz, 1H), 3.30 (dd, J = 8.9, 3.4 Hz, 1H), 3.14 (dd, J = 8.9, 3.4 Hz, 1H7.6 Hz, 1H), 2.20 (m, 1H), 1.97 (m, 1H), 1.46 (ddd, J = 12.4, 9.3, 3.8 Hz, 1H), 1.41 (ddd, J = 12.4, 9.6, 2.7 Hz, 1H), 1.14 (d, J = 6.8 Hz, 3H), 1.06-0.98 (m, 42H), 0.92 (d, J = 0.000 Hz, 0.0000 Hz, 0.000 Hz,J = 6.5 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  159.0, 138.9, 131.0, 128.9 (2C), 128.2 (2C), 127.6 (2C), 127.3, 113.7 (2C), 78.0, 76.4, 74.3, 73.5, 72.9, 72.4, 55.2, 35.8, 35.0,

29.8, 18.4 (7C), 18.33 (3C), 18.31 (3C), 17.4, 13.1 (6C); HRMS (ESI) calcd for  $C_{42}H_{74}O_5Si_2Na [(M + Na)^+] 737.4967$ , found 737.4963.

To a solution of silvl ether S2 (27.9 mg, 39.0 µmol) in CH<sub>2</sub>Cl<sub>2</sub>/pH 7 buffer (10:1, v/v, 0.77 mL) cooled to 0 °C was added DDQ (9.8 mg, 43 µmol). The resultant mixture was stirred at room temperature for 2 h 40 min, after which point an additional portion of DDQ (0.90 mg, 3.96 µmol) was added to the reaction mixture. After being stirred at room temperature for further 45 min, the reaction was quenched with saturated aqueous NaHCO<sub>3</sub> solution at 0 °C. The resultant mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was passed through a pad of silica gel (5 to 8% EtOAc/hexanes) and then purified by preparative HPLC to give alcohol 16 (20.6 mg, 89%) as a colorless oil:  $[\alpha]_D^{25}$  -35.7 (*c* 1.00, CHCl<sub>3</sub>); IR (film) 3375, 2944, 2867, 1463, 1110, 882, 733, 677, 416 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.33—7.29 (m, 4H), 7.25 (m, 1H), 4.48 (d, J = 12.0 Hz, 1H), 4.46 (d, J = 12.0 Hz, 1H), 3.95 (ddd, J = 9.2, 3.8, 2.8Hz, 1H), 3.88 (dd, J = 4.1, 3.8 Hz, 1H), 3.65 (dd, J = 9.2, 3.1 Hz, 1H), 3.45 (m, 1H), 3.37 (m, 1H), 3.31 (dd, J = 8.9, 8.9 Hz, 1H), 2.20 (m, 1H), 1.82 (m, 1H), 1.46 (ddd, J =13.7, 9.2, 3.8 Hz, 1H), 1.41 (ddd, J = 13.7, 9.3, 2.8 Hz, 1H), 1.29 (br s, 1H), 1.15 (d, J =6.9 Hz, 3H), 1.09–0.97 (m, 42H), 0.90 (d, J = 6.8 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) & 138.9, 128.2 (2C), 127.6 (2C), 127.4, 77.9, 74.4, 73.3, 72.9, 69.2, 35.4, 35.0, 32.2, 18.33 (6C), 18.30 (6C), 17.4, 16.7, 13.1 (6C); HRMS (ESI) calcd for  $C_{34}H_{66}O_4Si_2Na [(M + Na)^+] 617.4392$ , found 617.4393.



**Iodide 9.** To a solution of alcohol **16** (113.7 mg, 0.1913 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (2.0 mL) cooled to 0 °C were added Et<sub>3</sub>N (53  $\mu$ L, 0.38 mmol), DMAP (3.0 mg, 20  $\mu$ mol) and TsCl (55.0 mg, 0.289 mmol), and the resultant solution was stirred at room temperature for 12 h. The reaction was quenched with H<sub>2</sub>O at 0 °C, and the resultant mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residual crude tosylate was used in the next reaction without further purification.

To a solution of the above tosylate in acetone (2.5 mL) was added NaI (143 mg, 0.954 mmol), and the resultant mixture was stirred at 50 °C for 15 h. After being cooled to room temperature, the reaction mixture was diluted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (1 to 1.5% EtOAc/hexanes) gave iodide **9** (131.8 mg, 98% for the two steps) as a colorless oil:  $[\alpha]_D^{25}$  –33.7 (*c* 1.00, CHCl<sub>3</sub>); IR (film) 2944, 2866, 1462, 1110, 882, 732, 679 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.35—7.29 (m, 4H), 7.25 (m, 1H), 4.49 (s, 2H), 3.91 (ddd, *J* = 8.9, 3.8, 2.8 Hz, 1H), 3.87 (dd, *J* = 4.1, 3.8 Hz, 1H), 3.66 (dd, *J* = 9.3, 3.1 Hz, 1H), 3.33 (dd, *J* = 8.9, 8.9 Hz, 1H), 3.21 (dd, *J* = 9.3, 4.4 Hz, 1H), 3.12 (dd, *J* = 9.6, 6.5 Hz, 1H), 2.21 (m, 1H), 1.72 (m, 1H), 1.56 (ddd, *J* = 13.4, 8.6, 2.8 Hz, 1H), 1.51 (ddd, *J* = 13.4, 8.9, 3.8 Hz, 1H), 1.16 (d, *J* = 6.9 Hz, 3H), 1.08—0.99 (m, 42H), 0.96 (d, *J* = 6.5 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  138.8, 128.2 (2C), 127.6 (2C), 127.3, 77.9,

74.5, 73.4, 73.0, 39.3, 35.0, 31.2, 20.4, 19.2, 18.35 (6C), 18.33 (3C), 18.29 (3C), 17.5, 13.1 (6C); HRMS (ESI) calcd for  $C_{34}H_{65}IO_3Si_2Na$  [(M + Na)<sup>+</sup>] 727.3409, found 727.3438.



**Diene 18.** To a mixture of epoxide **17** (3.28 g, 16.9 mmol) and CuI (322 mg, 1.69 mmol) in THF (140 mL) cooled to -35 °C was added vinylmagnesium bromide (1.0 M solution in THF, 20.3 mL, 20.3 mmol), and the resultant mixture was allowed to warm to -20 °C over a period of 30 min. The reaction was quenched with saturated aqueous NH<sub>4</sub>Cl solution. The resultant mixture was allowed to warm to room temperature and then extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (10 to 20% EtOAc/hexanes) gave a homoallylic alcohol, which was contaminated with some impurities but was used in the next reaction without further purification.

To a solution of the above homoallylic alcohol in  $CH_2Cl_2$  (140 mL) cooled to 0 °C were added *i*-Pr<sub>2</sub>NEt (9.00 mL, 49.2 mmol) and acryloyl chloride (1.73 ml, 21.3 mmol), and the resultant solution was stirred at 0 °C for 3 h. The reaction was quenched with saturated aqueous NaHCO<sub>3</sub> solution, and the resultant mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (6 to 7.5% EtOAc/hexanes) gave diene **18** (4.41 g, 95% for the two steps) as a colorless oil:  $[\alpha]_D^{24}$  –8.6 (*c* 1.00, C<sub>6</sub>H<sub>6</sub>); IR (film) 2933, 1723, 1613, 1514, 1406, 1249, 1195, 1037, 809 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) 8 7.25—7.20 (m, 2H), 6.87—6.83 (m, 2H), 6.39 (dd, *J* = 17.5, 1.4 Hz, 1H), 6.11 (dd, *J* = 17.5, 10.6 Hz, 1H), 5.81 (dd, *J* = 10.6, 1.4 Hz, 1H), 5.72 (dddd, *J* = 17.2, 10.0, 7.2, 7.2 Hz, 1H), 5.14 (m, 1H) 5.07 (dddd, *J* = 17.2, 1.4, 1.4, 1.0 Hz, 1H), 5.04 (dddd, *J* = 10.0, 2.1, 1.4, 1.0 Hz, 1H), 4.49 (d, *J* = 11.7 Hz, 1H), 4.42 (d, *J* = 11.7 Hz, 1H), 3.78 (s, 3H), 3.53 (dd, *J* = 10.6, 5.5 Hz, 1H), 3.51 (dd, *J* = 10.6, 4.8 Hz, 1H), 2.42 (ddddd, *J* = 14.1, 7.2, 7.2, 2.1, 1.4 Hz, 1H), 2.39 (ddddd, *J* = 14.1, 7.2, 7.2, 1.0, 1.0 Hz, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) 8 165.7, 159.2, 133.1, 130.8, 130.1, 129.2 (2C), 128.6, 118.0, 113.8 (2C), 72.8, 72.1, 70.1, 55.3, 35.4; HRMS (ESI) calcd for C<sub>16</sub>H<sub>20</sub>O<sub>4</sub>Na [(M + Na)<sup>+</sup>] 299.1254, found 299.1258.



 $\alpha$ , $\beta$ -Unsaturated lactone 19. To a solution of diene 18 (0.510 g, 1.85 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (150 mL) was added Ti(O*i*-Pr)<sub>4</sub> (0.17 mL, 0.57 mmol), and the resultant solution was stirred at 45 °C for 1 h. To this mixture was added a solution of the Grubbs second-generation catalyst (80 mg, 94 µmol) in CH<sub>2</sub>Cl<sub>2</sub> (30 mL), and the resultant solution was stirred at 45 °C for 12 h. After being cooled to room temperature, the reaction mixture was treated with Et<sub>3</sub>N and stirred at room temperature for 1.5 h under air. The resultant mixture was passed through a pad of silica gel (EtOAc) and concentrated under reduced pressure. Purification of the residue by flash

chromatography on silica gel (15 to 40% EtOAc/hexanes) gave α,β-unsaturated lactone **19** (0.437 g, 95%) as a pale brown oil:  $[\alpha]_D^{24}$  –94.4 (*c* 1.00, CHCl<sub>3</sub>); IR (film) 2910, 1719, 1611, 1513, 1246, 1085, 1050, 814 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.29—7.20 (m, 2H), 6.91—6.84 (m, 3H), 6.00 (ddd, *J* = 9.6, 2.8, 1.0 Hz, 1H), 4.58 (dddd, *J* = 11.7, 4.8, 4.8, 4.1 Hz, 1H), 4.53 (d, *J* = 11.6 Hz, 1H) 4.50 (d, *J* = 11.6 Hz, 1H), 3.79 (s, 3H), 3.66 (dd, *J* = 10.3, 4.8 Hz, 1H), 3.64 (dd, *J* = 10.3, 4.8 Hz, 1H), 2.53 (dddd, *J* = 18.5, 11.7, 2.8, 2.8 Hz, 1H), 2.37 (dddd, *J* = 18.5, 5.5, 4.1, 1.0 Hz, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 163.7, 159.3, 144.9, 129.7, 129.4 (2C), 121.2, 113.8 (2C), 76.6, 73.3, 70.4, 55.3, 26.2; HRMS (ESI) calcd for C<sub>14</sub>H<sub>16</sub>O<sub>4</sub>Na [(M + Na)<sup>+</sup>] 271.0935, found 271.0939.



**Lactone 20.** To a suspension of CuI (286 mg, 1.50 mmol) in diethyl ether (10 mL) cooled to -10 °C was added MeLi (1.09 M solution in diethyl ether, 2.70 mL, 2.97 mmol), and the resultant mixture was stirred at -10 °C for 1 h. To this mixture was added a solution of  $\alpha$ , $\beta$ -unsaturated lactone **19** (0.241 g, 0.971 mmol) in diethyl ether (5 mL +2 mL rinse). The resultant solution was stirred at -10 °C for 40 min. The reaction was quenched with saturated aqueous NH<sub>4</sub>Cl solution, and the resultant mixture was filtered through a pad of Celite, and the filtrate was extracted with diethyl ether. The organic layer was washed with brine. The aqueous layer was cooled to 0 °C and carefully acidified with 1 M aqueous HCl solution (pH = ca. 4). The resultant mixture was dried over

Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (30 to 80% EtOAc/hexanes) gave lactone **20** (0.183 g, 72%):  $[\alpha]_D^{25}$  +26.6 (*c* 1.00, CHCl<sub>3</sub>); IR (film) 2955, 1735, 1612, 1513, 1247, 1173, 1080, 1032, 819, 419 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.26—7.20 (m, 2H), 6.89—6.83 (m, 2H), 4.54 (dddd, *J* = 8.6, 5.2, 4.8, 4.8 Hz, 1H), 4.48 (d, *J* = 11.7 Hz, 1H) 4.46 (d, *J* = 11.7 Hz, 1H), 3.78 (s, 3H), 3.57 (dd, *J* = 10.3, 4.8 Hz, 1H), 3.53 (dd, *J* = 10.3, 5.2 Hz, 1H), 2.55 (ddd, *J* = 16.5, 5.5, 0.7 Hz, 1H), 2.18 (m, 1H), 2.11 (dd, *J* = 16.5, 8.9 Hz, 1H), 1.91 (dddd, *J* = 14.0, 8.6, 6.2, 0.7 Hz, 1H), 1.55 (ddd, *J* = 14.0, 6.5, 4.8 Hz, 1H), 1.04 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  171.6, 159.3, 129.8, 129.3 (2C), 113.8 (2C), 76.1, 73.2, 71.3, 55.2, 37.6, 31.7, 23.7, 21.1; HRMS (ESI) calcd for C<sub>15</sub>H<sub>20</sub>O<sub>4</sub>Na [(M + Na)<sup>+</sup>] 287.1254, found 287.1257.



Alcohol 24. To a suspension of CuCN (430 mg, 4.80 mmol) in THF (10 mL) cooled to

0 °C was added Me<sub>2</sub>PhSiLi (ca. 0.96 M in THF, 10 mL, 9.6 mmol). After being stirred at 0 °C for 20 min, the reaction mixture was cooled to -78 °C. To this mixture was added a solution of alkyne 21 (0.940 g, 2.49 mmol) in THF (6 mL + 3 mL rinse twice). The resultant mixture was stirred at -78 °C for 2 h and then at 0 °C for 2 h. The reaction was quenched with a 9:1 mixture of saturated aqueous NH<sub>4</sub>Cl solution and 28% NH<sub>4</sub>OH solution at 0 °C, filtered through a pad of Celite, and the filtrate was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (hexanes) gave vinyl silane 22 (1.361 g), which was contaminated with silane byproducts and used in the next reaction without further purification. <sup>1</sup>H NMR spectrum of the crude product indicated that the regioselectivity of the reaction was ca. 7:1. Data for 22: <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.72—7.60 (m, 5H), 7.52–7.26 (m, 10H), 5.77 (ddq, J = 6.9, 6.9, 1.7 Hz, 1H), 3.74–3.62 (m, 2H), 2.15—2.00 (m, 2H), 1.64 (d, J = 1.7 Hz, 3H), 1.65—1.57 (m, 2H), 1.40—1.31 (m, 2H), 1.16 (m, 1H), 1.03 (s, 9H), 0.83 (d, J = 6.5 Hz, 3H), 0.30 (s, 6H); HRMS (FAB) calcd for  $C_{33}H_{47}OSi_2 [(M + Na)^+] 515.3165$ , found 515.3163.

To a solution of the above vinyl silane **22** in CH<sub>3</sub>CN/THF (3:1, v/v, 24 mL) was added NIS (1.13 g, 5.04 mmol), and the resultant mixture was stirred at room temperature for 18 h. The reaction was quenched with a 1:1 mixture of saturated aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution and saturated aqueous NaHCO<sub>3</sub> solution at 0 °C, and the resultant mixture was stirred vigorously at room temperature until the layers became colorless. The resultant mixture was diluted with EtOAc, washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (0 to 0.5% diethyl ether/hexanes) gave an

inseparable mixture of vinyl iodide **23** and its isomers (1.207 g), which was used in the next reaction without further purification. <sup>1</sup>H NMR spectrum of the crude product indicated that E/Z = ca. 6:1 for the major regioisomer. Data for **23**: <sup>1</sup>H NMR (600 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$  7.84—7.72 (m, 5H), 7.30—7.18 (m, 5H), 6.06 (m, 1H), 3.76—3.58 (m, 2H), 2.08 (s, 3H), 1.75—1.61 (m, 2H), 1.54—1.43 (m, 2H), 1.26 (m, 1H), 1.19 (s, 9H), 1.09 (m, 1H), 0.88 (dddd, J = 13.7, 9.2, 7.6, 6.2 Hz, 1H), 0.68 (d, J = 6.5 Hz, 3H); HRMS (FAB) calcd for C<sub>25</sub>H<sub>36</sub>IOSi [(M + Na)<sup>+</sup>] 507.1580, found 507.1582.

To a solution of the above vinyl iodide **23** in THF (15 mL) was added TBAF (1.0 M solution in THF, 11.6 mL, 11.6 mmol). The resultant solution was stirred at room temperature for 1 h 50 min and then concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (1 to 3% EtOAc/benzene) followed by preparative HPLC gave alcohol **24** (0.372 g, 57% for the three steps) as a colorless oil:  $[\alpha]_D^{26}$  –6.9 (*c* 1.00, C<sub>6</sub>H<sub>6</sub>); IR (film) 3345, 2923, 1458, 1377, 1373, 1057, 419 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  6.12 (ddq, *J* = 7.6, 7.6, 1.4 Hz, 1H), 3.71—3.61 (m, 2H), 2.35 (d, *J* = 1.4 Hz, 3H), 2.09—1.95 (m, 2H), 1.63—1.51 (m, 2H), 1.49—1.30 (m, 2H), 1.21 (dddd, *J* = 13.4, 9.3, 7.6, 5.8 Hz, 1H), 0.89 (d, *J* = 6.5 Hz, 3H) (one proton missing presumably due to H/D exchange); <sup>13</sup>C NMR (150 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$  141.6, 93.6, 60.6, 39.8, 36.2, 29.2, 28.3, 27.3, 19.4; HRMS (ESI) calcd for C<sub>9</sub>H<sub>18</sub>IO [(M + H)<sup>+</sup>] 269.0397, found 269.0398.



**Vinyl iodide 6.** To a solution of alcohol **24** (0.238 g, 0.888 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (9 mL) were added PhI(OAc)<sub>2</sub> (315 mg, 0.978 mmol) and TEMPO (14.0 mg, 89.6  $\mu$ mol), and the resultant solution was stirred at room temperature for 3.5 h. To the reaction mixture were added additional portions of PhI(OAc)<sub>2</sub> (86.0 mg, 0.263 mmol) and TEMPO (14 mg, 89.6  $\mu$ mol), and the resultant mixture was stirred at room temperature for 2 h. The reaction was quenched with a 1:1 mixture of saturated aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution and saturated aqueous NaHCO<sub>3</sub> solution at 0 °C, and the resultant solution was stirred at room temperature for Lac, and the organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residual crude aldehyde was used in the next reaction without further purification.

To a solution of the above aldehyde,  $NaH_2PO_4$  (120 mg, 1.00 mmol), and 2-methyl-2-butene (1.90 mL, 17.8 mmol) in *t*-BuOH/H<sub>2</sub>O (5:1, v/v, 9 mL) cooled to 0 °C was added NaClO<sub>2</sub> (280 mg, 3.12 mmol), and the resultant mixture was stirred at room temperature for 50 min. The reaction mixture was cooled to 0 °C and carefully acidified with 1 M aqueous HCl solution (pH = ca. 4). The resultant mixture was extracted repeatedly with CHCl<sub>3</sub>, and the organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was passed through a pad of silica gel (5 to 10 % EtOAc/hexanes) to give a carboxylic acid (0.244 g, ca. 97%), which was used in the next reaction without further purification.

To a solution of the above carboxylic acid in methanol/benzene (1:1, v/v, 8 mL) cooled to 0  $^{\circ}$ C was added TMSCHN<sub>2</sub> (2.0 M solution in hexanes, 1.29 mL, 2.58 mmol). The reaction mixture was stirred at room temperature for 35 min and then concentrated under reduced pressure. Purification of the residue by flash

chromatography on silica gel (1% EtOAc/hexanes) to give vinyl iodide **6** (0.256 g, 97% for the three steps) as a colorless oil:  $[\alpha]_D^{25}$  –5.4 (*c* 1.13, C<sub>6</sub>H<sub>6</sub>); IR (film) 2952, 1737, 1435, 1202, 1160, 1058 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$  6.01 (dd, *J* = 7.6, 7.6 Hz, 1H), 3.33 (s, 3H), 2.06 (s, 3H), 2.00 (dd, *J* = 15.1, 5.8 Hz, 1H), 1.87 (dd, *J* = 15.1, 7.9 Hz, 1H), 1.78 (m, 1H), 1.70—1.55 (m, 2H), 1.05 (dddd, *J* = 13.4, 9.7, 6.2, 6.2 Hz, 1H), 0.86 (dddd, *J* = 13.4, 9.7, 7.9, 6.2 Hz, 1H), 0.73 (d, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (150 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$  172.5, 141.1, 93.8, 50.9, 41.2, 35.6, 29.9, 28.2, 27.3, 19.5; HRMS (ESI) calcd for C<sub>10</sub>H<sub>17</sub>IO<sub>2</sub>Na [(M + Na)<sup>+</sup>] 319.0165, found 319.0159.



**Enol phosphate 10.** To a solution of lactone **20** (0.947 g, 3.59 mmol) in THF (35 mL) were added HMPA (1.87 mL, 10.8 mmol) and (PhO)<sub>2</sub>P(O)Cl (0.89 mL, 4.3 mmol), and the resultant solution was cooled to -78 °C. To this solution was added KHMDS (0.5 M solution in toluene, 9.30 mL, 4.65 mmol), and the resultant solution was stirred at -78 °C for 40 min. The reaction was quenched with 3% NH<sub>4</sub>OH solution. The resultant mixture was diluted with diethyl ether and allowed to warm to room temperature over a period of 40 min. The resultant mixture was extracted with EtOAc, and the organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was passed through a pad of silica gel (eluted with 15% EtOAc/hexanes) to give enol phosphate **10**, which was immediately used in the next reaction.



Endocyclic enol ether 25. To a solution of iodide 9 (1.086 g, 1.542 mmol) in diethyl ether (15 mL) was added B-MeO-9-BBN (1.0 M solution in hexanes, 4.0 mL, 4.0 mmol). To this solution cooled to -78 °C was added t-BuLi (1.59 M in pentane, 2.90 mL, 4.61 mmol) at once. The resultant mixture was stirred at -78 °C for 5 min and then THF (15 mL) was added. The resultant solution was allowed to warm to room temperature over a period of 3 h 25 min. To this solution was added 3 M aqueous Cs<sub>2</sub>CO<sub>3</sub> solution (1.54 mL, 4.62 mmol), and the resultant mixture was stirred at room temperature for 20 min. To this mixture were added a solution of the above crude enol phosphate 10 in DMF (10 mL + 5 mL rinse) and PdCl<sub>2</sub>(dppf)•CH<sub>2</sub>Cl<sub>2</sub> (126 mg, 0.154 mmol). The resultant mixture was stirred at 50 °C for 16 h. The reaction mixture was diluted with H<sub>2</sub>O and extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (0.5 to 1% EtOAc/hexanes) gave endocyclic enol ether 25 (1.021 g, 81%) as a colorless oil:  $\left[\alpha\right]_{D}^{24}$  -5.5 (c 1.00, C<sub>6</sub>H<sub>6</sub>); IR (film) 2945, 2866, 1513, 1462, 1248, 1095, 882, 678 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, C<sub>6</sub>D<sub>6</sub>) δ 7.37-7.32 (m, 2H), 7.26-7.22 (m, 2H), 7.21-7.16 (m, 2H), 7.09 (m, 1H), 6.83-6.78 (m, 2H), 4.50 (d, J = 4.1 Hz, 1H), 4.49 (d, J = 12.0 Hz, 1H) 4.46 (d, J = 12.0 Hz, 1H),

4.42 (s, 2H), 4.21 (m, 1H), 4.17 (m, 1H), 4.15 (dd, J = 5.2, 3.8 Hz, 1H), 3.79 (dd, J = 8.9, 3.4 Hz, 1H), 3.66 (dd, J = 9.6, 5.2 Hz, 1H), 3.61 (dd, J = 7.9, 7.9 Hz, 1H), 3.51 (dd, J = 9.6, 6.2 Hz, 1H), 3.31 (s, 3H), 2.46 (m, 1H), 2.25 (m, 1H), 2.20—2.11 (m, 2H), 2.05 (m, 1H), 1.88 (ddd, J = 13.0, 10.0, 2.7 Hz, 1H), 1.79 (ddd, J = 13.4, 8.9, 5.8 Hz, 1H), 1.66 (br dd, J = 11.3, 11.3 Hz, 1H), 1.51 (ddd, J = 13.4, 2.8, 2.8 Hz, 1H), 1.47 (d, J = 6.8 Hz, 3H), 1.24—1.13 (m, 42H), 1.11 (d, J = 6.9 Hz, 3H), 0.97 (d, J = 6.9 Hz, 3H); 1<sup>3</sup>C NMR (150 MHz, C<sub>6</sub>D<sub>6</sub>) & 159.7, 152.1, 139.5, 131.0, 129.5 (2C), 128.4 (2C), 128.3 (2C), 127.5, 114.1 (2C), 103.4, 77.9, 75.1, 73.7, 73.31, 73.29, 72.2, 71.2, 54.7, 43.9, 39.2, 36.6, 32.1, 27.6, 24.5, 23.1, 20.0, 18.74 (3C), 18.71 (3C), 18.68 (3C), 18.6 (3C), 17.3, 13.6 (6C); HRMS (ESI) calcd for C<sub>49</sub>H<sub>84</sub>O<sub>6</sub>Si<sub>2</sub>Na [(M + Na)<sup>+</sup>] 847.5699, found 847.5676.



**Spiroacetal 26.** To a solution of endocyclic enol ether **25** (1.275 g, 1.546 mmol) in THF (8 mL) was added TBAF (1.0 M solution in THF, 15.2 mL, 15.2 mmol). The resultant solution was stirred at room temperature for 3 h 10 min and then concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (20 to 30% EtOAc/benzene) gave dihydroxy enol ether **7** (0.8194 g), which was used in the next reaction without further purification:  $[\alpha]_D^{25}$  +43.5 (*c* 1.00, C<sub>6</sub>H<sub>6</sub>); IR (film) 3461,

2953, 2867, 1513, 1455, 1248, 1092, 420 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$ 7.28—7.22 (m, 2H), 7.21—7.11 (m, 4H), 7.06 (m, 1H), 6.84—6.79 (m, 2H), 4.50 (d, *J* = 4.1 Hz, 1H), 4.41 (d, *J* = 11.7 Hz, 1H) 4.38 (d, *J* = 11.7 Hz, 1H), 4.19 (s, 2H), 4.11 (m, 1H), 3.80 (br ddd, *J* = 9.6, 2.4, 2.4 Hz, 1H), 3.55 (dd, *J* = 10.0, 6.2 Hz, 1H), 3.41—3.35 (m, 3H), 3.34—3.27 (m, 2H), 3.30 (s, 3H), 2.80 (br s, 1H), 2.32 (m, 1H), 2.18—2.06 (m, 3H), 2.01 (m, 1H), 1.90 (ddd, *J* = 14.4, 10.0, 4.8 Hz, 1H), 1.66 (ddd, *J* = 13.4, 9.6, 6.2 Hz, 1H), 1.32 (m, 1H), 1.24 (ddd, *J* = 13.7, 8.9, 3.4 Hz, 1H), 1.03 (d, *J* = 6.5 Hz, 3H), 0.91 (d, *J* = 6.9 Hz, 3H), 0.90 (d, *J* = 6.8 Hz, 3H); <sup>13</sup>C NMR (150 MHz, C<sub>6</sub>D<sub>6</sub>)  $\delta$  159.7, 152.2, 138.4, 130.9, 129.6 (2C), 128.6 (2C), 128.5, 128.3 (2C), 114.1 (2C), 103.5, 78.6, 73.9, 73.4, 73.1, 72.4, 71.4, 70.1, 54.7, 42.5, 41.4, 36.5, 31.8, 28.0, 24.7, 23.2, 19.8, 15.0; HRMS (ESI) calcd for C<sub>31</sub>H<sub>44</sub>O<sub>6</sub>Na [(M + Na)<sup>+</sup>] 535.3041, found 535.3042.

To a solution of the above dihydroxy enol ether **7** in CH<sub>2</sub>Cl<sub>2</sub> (20 mL) cooled to 0 °C was added PPTS (79.0 mg, 0.314 mmol), and the resultant mixture was stirred at room temperature for 2 days. The reaction was quenched with saturated aqueous NaHCO<sub>3</sub> solution at 0 °C. The resultant mixture was diluted with EtOAc and washed with brine. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (10 to 13% EtOAc/hexanes) gave spiroacetal **26** (0.6651 g, 84% for the two steps) as a colorless oil:  $[\alpha]_D^{24}$  +25.1 (*c* 1.31, CHCl<sub>3</sub>); IR (film) 3494, 2930, 1613, 1513, 1455, 1247, 1090, 982, 698 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.33—7.28 (m, 4H), 7.27—7.20 (m, 3H), 6.86—6.82 (m, 2H), 4.48 (d, *J* = 11.6 Hz, 1H), 4.46 (s, 2H) 4.45 (d, *J* = 11.6 Hz, 1H), 3.96 (m, 1H), 3.87 (ddd, *J* = 11.7, 3.4, 3.0 Hz, 1H), 3.77 (s, 3H), 3.60 (dd, *J* = 9.3, 5.8 Hz, 1H), 3.47 (dd, *J* = 9.3, 5.8 Hz, 1H), 3.41 (dd, *J* = 10.3, 6.2 Hz, 1H), 3.36 (dd, *J* = 10.3, 4.1 Hz, 1H), 3.26 (ddd, *J* = 7.5, 6.2, 3.4 Hz, 1H), 2.75 (d, *J* = 6.2 Hz,

1H), 2.11—2.00 (m, 2H), 1.97 (m, 1H), 1.65 (ddd, J = 13.0, 3.8, 1.4 Hz, 1H), 1.61 (dd, J = 14.1, 5.8 Hz, 1H), 1.53 (ddd, J = 13.0, 11.7, 5.8 Hz, 1H), 1.51—1.45 (m, 2H), 1.29 (br ddd, J = 13.0, 2.7, 2.4 Hz, 1H), 1.16 (m, 1H), 1.14 (d, J = 7.2 Hz, 3H), 0.99 (m, 1H), 0.98 (d, J = 6.8 Hz, 3H), 0.86 (d, J = 6.5 Hz, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  159.0, 138.5, 130.7, 129.0 (2C), 128.3 (2C), 127.5 (2C), 127.4, 113.6 (2C), 98.2, 77.2, 73.5, 73.3, 73.1, 72.9, 69.6, 64.7, 55.2, 44.4, 40.5, 35.74, 35.68, 33.0, 24.8, 24.6, 22.1, 21.1, 14.8; HRMS (ESI) calcd for C<sub>31</sub>H<sub>44</sub>O<sub>6</sub>Na [(M + Na)<sup>+</sup>] 535.3041, found 535.3045.



Aldehyde 5. To a solution of spiroacetal 26 (645.3 mg, 1.260 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (12 mL) cooled to 0 °C were added 2,6-lutidine (0.30 mL, 2.5 mmol) and TBSOTF (0.50 mL, 1.9 mmol), and the resultant solution was stirred at room temperature for 3 h 50 min. The reaction was quenched with saturated aqueous NH<sub>4</sub>Cl solution at 0 °C, and the resultant mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (3% EtOAc/hexanes) gave silyl ether **S3** (0.7592 g, 96%) as a colorless oil:  $[\alpha]_D^{25}$  +0.6 (*c* 1.96, CHCl<sub>3</sub>); IR (film) 2951, 2855, 1513,

1455, 1249, 1086, 1038, 984, 836, 775 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.33—7.28 (m, 4H), 7.26—7.20 (m, 3H), 6.86—6.82 (m, 2H), 4.50—4.42 (m, 4H), 3.94 (m, 1H), 3.78 (s, 3H), 3.73 (ddd, *J* = 12.0, 3.8, 2.1 Hz, 1H), 3.59 (dd, *J* = 8.9, 3.4 Hz, 1H), 3.49 (dd, *J* = 6.5, 3.8 Hz, 1H), 3.40 (dd, *J* = 10.0, 5.8 Hz, 1H), 3.35 (dd, *J* = 10.0, 5.2 Hz, 1H), 3.26 (dd, *J* = 8.9, 8.2 Hz, 1H), 2.04 (dddd, *J* = 14.8, 13.7, 6.9, 3.4 Hz, 1H), 1.98—1.88 (m, 2H), 1.64 (ddd, *J* = 13.1, 3.8, 1.4 Hz, 1H), 1.61—1.50 (m, 3H), 1.41 (dd, *J* = 13.7, 3.4 Hz, 1H), 1.32 (br ddd, *J* = 13.1, 2.8, 2.8 Hz, 1H), 1.13 (d, *J* = 7.2 Hz, 3H), 1.03 (d, *J* = 6.9 Hz, 3H), 0.99—0.89 (m, 2H), 0.85 (d, *J* = 6.5 Hz, 3H), 0.83 (s, 9H), 0.00 (s, 3H), -0.01 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  159.0, 139.0, 130.7, 129.2 (2C), 128.2 (2C), 127.5 (2C), 127.3, 113.6 (2C), 97.8, 76.1, 73.4, 73.3, 72.92, 72.88, 72.5, 64.4, 55.2, 44.7, 40.8, 35.9, 33.4, 33.2, 25.9 (3C), 25.2, 24.7, 22.3, 21.0, 18.1, 15.9, -4.3, -4.7; HRMS (ESI) calcd for C<sub>37</sub>H<sub>58</sub>O<sub>6</sub>SiNa [(M + Na)<sup>+</sup>] 649.3895, found 649.3894.

To a solution of silyl ether **S3** (23.6 mg, 37.8 µmol) in CH<sub>2</sub>Cl<sub>2</sub>/pH 7 buffer (10:1, v/v, 0.77 mL) cooled to 0 °C was added DDQ (9.5 mg, 42 µmol), and the resultant solution was stirred at room temperature for 2.5 h. The reaction was quenched with saturated aqueous NaHCO<sub>3</sub> solution at 0 °C, and the resultant mixture was stirred at room temperature for 10 min. The resultant mixture was extracted with EtOAc. The organic layer was washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (5:1:25, CHCl<sub>3</sub>/EtOAc/hexanes) gave alcohol **S4** (16.6 mg, 87%) as a colorless oil:  $[\alpha]_D^{24}$  +7.5 (*c* 1.00, CHCl<sub>3</sub>); IR (film) 3480, 2927, 1455, 1254, 1076, 981, 882, 836, 775 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.35—7.29 (m, 4H), 7.25 (m, 1H), 4.49 (d, *J* = 12.0 Hz, 1H), 4.45 (d, *J* = 12.0 Hz, 1H), 3.86 (dddd, *J* = 11.3, 6.9, 4.1, 3.4 Hz, 1H), 3.69

(ddd, J = 11.7, 3.8, 2.0 Hz, 1H), 3.59 (dd, J = 8.9, 3.5 Hz, 1H), 3.57 (m, 1H), 3.49 (dd, J = 6.5, 3.8 Hz, 1H), 3.47 (dd, J = 11.3, 6.9 Hz, 1H), 3.26 (dd, J = 8.9, 8.0 Hz, 1H), 2.04 (m, 1H), 1.98—1.83 (m, 2H), 1.63 (ddd, J = 13.1, 3.8, 1.7 Hz, 1H), 1.60—1.50 (m, 3H), 1.43 (ddd, J = 13.7, 4.1, 1.0 Hz, 1H), 1.21 (br ddd, J = 13.1, 3.4, 3.4 Hz, 1H), 1.14 (d, J = 7.2 Hz, 3H), 1.03 (d, J = 6.8 Hz, 3H), 1.01—0.89 (m, 2H), 0.86 (d, J = 6.5 Hz, 3H), 0.84 (s, 9H), 0.03 (s, 3H), 0.00 (s, 3H) (one proton missing presumably due to H/D exchange); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  138.9, 128.2 (2C), 127.5 (2C), 127.3, 97.7, 76.1, 73.2, 72.9, 72.7, 66.4, 65.4, 44.6, 40.9, 35.9, 33.1, 32.2, 25.9 (3C), 25.3, 24.6, 22.3, 21.0, 18.1, 15.9, -4.3, -4.6; HRMS (ESI) calcd for C<sub>29</sub>H<sub>50</sub>O<sub>5</sub>SiNa [(M + Na)<sup>+</sup>] 529.3320, found 529.3336.

To a solution of alcohol S4 (21.4 mg, 42.3 µmol) in CH<sub>2</sub>Cl<sub>2</sub>/t-BuOH (10:1, v/v, 0.88 mL) cooled to 0 °C was added Dess—Martin periodinane (90 mg, 0.21 mmol), and the resultant solution was stirred at room temperature for 1 h. The reaction was quenched with a 1:1 mixture of saturated aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution and saturated aqueous NaHCO<sub>3</sub> solution at 0 °C, and the resultant solution was stirred at room temperature for 15 min. The resultant mixture was extracted with diethyl ether, and the organic layer was washed with brine, dried over MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (7% EtOAc/hexanes) gave aldehyde **5** (21.2 mg, 99%) as a colorless oil:  $[\alpha]_D^{26}$  –10.8 (*c* 0.50, CHCl<sub>3</sub>); IR (film) 2952, 2927, 2855, 1739, 1456, 1076, 978, 836, 774 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  9.65 (s, 1H), 7.33—7.29 (m, 4H), 7.25 (m, 1H), 4.49 (d, *J* = 12.0 Hz, 1H), 4.43 (d, *J* = 12.0 Hz, 1H), 4.16 (dd, *J* = 11.7, 3.8 Hz, 1H), 3.69 (ddd, *J* = 11.7, 3.4, 2.0 Hz, 1H), 3.56 (dd, *J* = 8.9, 3.4 Hz, 1H), 3.48 (dd, *J* = 6.8, 3.4 Hz, 1H), 3.26 (dd, *J* = 8.9, 7.9 Hz, 1H), 2.06—1.93 (m, 3H), 1.72 (ddd, *J* = 13.4, 3.8,

1.7 Hz, 1H), 1.65 (ddd, J = 13.4, 11.7, 5.5 Hz, 1H), 1.64—1.59 (m, 2H), 1.55 (m, 1H), 1.44 (dd, J = 14.1, 4.1 Hz, 1H), 1.16 (d, J = 7.3 Hz, 3H), 1.05—0.92 (m, 2H), 1.01 (d, J = 6.9 Hz, 3H), 0.88 (d, J = 6.5 Hz, 3H), 0.83 (s, 9H), -0.02 (s, 3H), -0.03 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  202.8, 138.9, 128.2 (2C), 127.5 (2C), 127.3, 98.3, 75.9, 73.3, 73.1, 72.9, 70.9, 44.2, 40.6, 36.0, 32.9, 30.9, 25.9 (3C), 25.2, 24.4, 22.2, 20.5, 18.1, 15.7, -4.3, -4.6; HRMS (ESI) calcd for C<sub>29</sub>H<sub>48</sub>O<sub>5</sub>SiNa [(M + Na)<sup>+</sup>] 527.3163, found 527.3173.



**C9—C28 Subunit 4 and 21***-epi-***4.** To a mixture of NiCl<sub>2</sub>/CrCl<sub>2</sub> (1%, w/w, 38.1 mg, weighted in a glove box) was added a mixture of aldehyde **5** (15.6 mg, 30.9  $\mu$ mol) and vinyl iodide **6** (20.5 mg, 69.3  $\mu$ mol) in degassed DMF (0.5 mL + 0.4 mL rinse twice). The resultant mixture was stirred at room temperature for 13 h. The reaction was quenched with D/L-serine (1.0 M solution in saturated aqueous NaHCO<sub>3</sub> solution) at 0 °C. The resultant solution was stirred at room temperature for 15 min. The resultant mixture was extracted with diethyl ether, and the organic layer was washed with brine, dried over MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (3 to 10% EtOAc/hexanes) gave a 1.4:1 mixture of C9—C28 subunit **4** and **21***-epi***-4** (16.9 mg, 81%) as a colorless oil. Separation of the two diasteromeric alcohols by preparative TLC (13% EtOAc/hexanes,

developed thrice) gave C9—C28 subunit **4** (8.5 mg, 41%) and **21**-*epi*-**4** (5.0 mg, 24%). Data for **4**:  $[\alpha]_D^{27}$  +25.1 (*c* 0.37, CHCl<sub>3</sub>); IR (film) 3574, 2952, 2931, 1739, 1455, 1254, 1078, 1025, 837, 776 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.33—7.29 (m, 4H), 7.25 (m, 1H), 5.40 (ddq, *J* = 7.2, 7.2, 1.4 Hz, 1H), 4.48 (d, *J* = 12.0 Hz, 1H), 4.45 (d, *J* = 12.0 Hz, 1H), 3.75 (m, 1H), 3.73 (dd, *J* = 10.7, 3.1 Hz, 1H), 3.69 (m, 1H), 3.64 (s, 3H), 3.59 (dd, *J* = 8.9, 3.8 Hz, 1H), 3.51 (dd, *J* = 6.5, 3.8 Hz, 1H), 3.27 (dd, *J* = 8.9, 8.2 Hz, 1H), 2.70 (br s, 1H), 2.29 (dd, *J* = 14.8, 5.8 Hz, 1H), 2.11 (dd, *J* = 14.8, 7.9 Hz, 1H), 2.09—1.80 (m, 6H), 1.64 (m, 1H), 1.59 (d, *J* = 1.4 Hz, 3H), 1.61—1.50 (m, 3H), 1.42 (dd, *J* = 14.1, 3.8 Hz, 1H), 1.39—1.20 (m, 3H), 1.11 (m, 1H), 1.10 (d, *J* = 7.2 Hz, 3H), 1.04 (d, *J* = 6.9 Hz, 3H), 0.98 (m, 1H), 0.92 (d, *J* = 6.8 Hz, 3H), 0.87 (d, *J* = 6.8 Hz, 3H), 0.84 (s, 9H), 0.07 (s, 3H), 0.01 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  173.6, 138.9, 133.2, 130.1, 128.2 (2C), 127.5 (2C), 127.3, 97.8, 81.9, 76.1, 73.2, 72.9, 72.8, 66.9, 51.4, 44.7, 41.6, 40.9, 36.2, 35.8, 33.2, 32.7, 30.1, 25.9 (3C), 25.3, 25.0, 24.5, 22.3, 20.9, 19.5, 18.2, 16.0, 11.5, -4.1, -4.5; HRMS (ESI) calcd for C<sub>39</sub>H<sub>66</sub>O<sub>7</sub>SiNa [(M + Na)<sup>+</sup>] 697.4470, found 697.4482.

Data for **21**-*epi*-**4**:  $[\alpha]_D^{28}$  +15.3 (*c* 1.54, CHCl<sub>3</sub>); IR (film) 3481, 2952, 2928, 2856, 1740, 1455, 1254, 1076, 982, 837, 775 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.33—7.30 (m, 4H), 7.25 (m, 1H), 5.46 (dd, *J* = 7.2, 7.2 Hz, 1H), 4.48 (d, *J* = 12.0 Hz, 1H), 4.44 (d, *J* = 12.0 Hz, 1H), 4.08 (br s, 1H), 3.86 (ddd, *J* = 11.0, 3.8, 3.8 Hz, 1H), 3.70 (ddd, *J* = 12.1, 4.1, 2.1 Hz, 1H), 3.64 (s, 3H), 3.58 (dd, *J* = 8.9, 3.8 Hz, 1H), 3.49 (dd, *J* = 6.2, 4.1 Hz, 1H), 3.27 (dd, *J* = 8.9, 7.8 Hz, 1H), 2.37 (br s, 1H), 2.30 (dd, *J* = 14.8, 5.9 Hz, 1H), 2.11 (dd, *J* = 14.8, 8.2 Hz, 1H), 2.08—1.80 (m, 6H), 1.68—1.49 (m, 4H), 1.55 (s, 3H), 1.43—1.33 (m, 2H), 1.30—1.20 (m, 2H), 1.07 (d, *J* = 7.2 Hz, 3H), 1.02 (d, *J* = 6.8 Hz, 3H), 0.99 (m, 1H), 0.95 (m, 1H), 0.92 (d, *J* = 6.5 Hz, 3H), 0.85 (d, *J* = 6.9 Hz, 3H), 0.84

(s, 9H), 0.04 (s, 3H), 0.00 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  173.6, 138.9, 132.5, 128.2 (2C), 127.5 (2C), 127.3, 125.7, 98.3, 77.2, 76.3, 73.1, 72.9, 72.7, 66.4, 51.3, 44.7, 41.6, 41.1, 36.4, 35.9, 33.4, 30.1, 29.3, 26.0 (3C), 25.1, 24.9, 24.6, 22.3, 20.9, 19.6, 18.2, 15.9, 13.6, -3.9, -4.5; HRMS (ESI) calcd for C<sub>39</sub>H<sub>66</sub>O<sub>7</sub>SiNa [(M + Na)<sup>+</sup>] 697.4470, found 697.4476.



**Conversion of 21**-*epi*-4 to 4. To a solution of a 1.4:1 mixture of C9—C28 subunit 4 and 21-*epi*-4 (24.5 mg, 36.3 µmol) in CH<sub>2</sub>Cl<sub>2</sub>/*t*-BuOH (10:1, v/v, 0.99 mL) cooled to 0 °C was added Dess—Martin periodinane (76 mg, 0.18 mmol), and the resultant solution was stirred at room temperature for 1 h. The reaction was quenched with a 1:1 mixture of saturated aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution and saturated aqueous NaHCO<sub>3</sub> solution at 0 °C, and the resultant solution was stirred at room temperature for a room temperature for 15 min. The resultant mixture was extracted with diethyl ether, and the organic layer was washed with brine, dried over MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (7% EtOAc/hexanes) gave enone **S5** (24.7 mg, 100%) as a colorless oil:  $[\alpha]_D^{26}$  +15.7 (*c* 1.15, CHCl<sub>3</sub>); IR

(film) 2952, 2926, 2857, 1739, 1683, 1455, 1255, 1074, 1025, 836 cm<sup>-1</sup>; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  7.35—7.27 (m, 4H), 7.25 (m, 1H), 6.57 (ddq, J = 7.2, 7.2, 1.0 Hz, 1H), 4.97 (dd, J = 11.0, 3.8 Hz, 1H), 4.47 (d, J = 12.0 Hz, 1H), 4.43 (d, J = 12.0 Hz, 1H), 3.64 (s, 3H), 3.61 (ddd, J = 11.7, 3.8, 2.4 Hz, 1H), 3.56 (dd, J = 8.9, 3.4 Hz, 1H), 3.47 (dd, J = 6.5, 3.8 Hz, 1H), 3.27 (dd, J = 8.9, 7.9 Hz, 1H), 2.29 (dd, J = 14.8, 5.9 Hz, 1H), 2.21 (m, 1H), 2.14 (dd, J = 14.8, 8.3 Hz, 1H), 2.03 (ddd, J = 14.5, 6.9, 3.4 Hz, 1H), 2.00—1.91 (m, 4H), 1.81 (ddd, J = 13.1, 3.8, 1.4 Hz, 1H), 1.77 (s, 3H), 1.71 (ddd, J = 13.1, 11.0, 5.5 Hz, 1H), 1.64 (dd, J = 13.7, 5.9 Hz, 1H), 1.57—1.49 (m, 2H), 1.48—1.39 (m, 2H), 1.31 (dddd, J = 13.4, 10.0, 7.6, 5.9 Hz, 1H), 1.18 (d, J = 6.9 Hz, 3H), 1.00—0.88 (m, 2H), 0.96 (d, J = 6.8 Hz, 3H), 0.84 (d, J = 6.5 Hz, 3H), 0.82 (s, 9H), -0.03 (s, 3H), -0.06 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  199.9, 173.2, 142.2, 138.9, 135.4, 128.2 (2C), 127.5 (2C), 127.3, 98.4, 76.2, 73.1, 73.0, 72.9, 67.4, 51.4, 44.3, 41.3, 40.7, 36.0, 35.42, 33.36, 33.3, 30.2, 26.5, 25.9 (3C), 25.00, 24.95, 22.2, 20.7, 19.6, 18.1, 15.8, 11.7, -4.1, -4.6; HRMS (ESI) calcd for C<sub>39</sub>H<sub>64</sub>O<sub>7</sub>SiNa [(M + Na)<sup>+</sup>] 695.4314, found 695.4331.

To a solution of enone **S5** (7.0 mg, 10  $\mu$ mol) in THF (0.5 mL) cooled to -78 °C was added dropwise L-selectride (1.0 M solution in THF, 0.04 mL, 0.04 mmol), and the resultant solution was stirred at -78 °C for 1 h. The reaction was quenched with saturated aqueous NaHCO<sub>3</sub> solution, and the resultant mixture was allowed to warm to 0 °C and treated with 30% aqueous H<sub>2</sub>O<sub>2</sub> solution (0.2 mL). After being stirred at room temperature for 1 h, the resultant mixture was extracted with EtOAc. The organic layer was washed successively with H<sub>2</sub>O, saturated aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> solution, and brine. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. Purification of the residue by flash chromatography on silica gel (5 to 10%)

EtOAc/hexanes) gave C9—C28 subunit 4 (5.8 mg, 82%, dr > 20:1 by 600 MHz  $^{1}$ H NMR analysis) as a colorless oil.



Figure S1. Stereochemical confirmation of compound 15 by conformational analysis on compound A.



**Figure S2.** Assignment of the absolute configuration of the C21 stereogenic center of compound **4** by modified Mosher method.



| <pre>Filename = C:\Users\delta\Documents\J Author = delta = delta Experiment = carbon.jxp Sample_Id = SN-II-112 Solvent = cNLOROFORM-D Solvent = 11-SEP-2010 15:34:55 Revision_Time = 11-SEP-2010 15:37:31 Current_Time = 11-SEP-2010 15:33:08</pre> | Comment = single pulse decoupled gat<br>Data_Format = 1D CONFLEX<br>Dim_Size = 26214<br>Dim_Title = 26214<br>Dim_Units = [apm]<br>Dim_Units = [apm]<br>Sinensions = Z<br>Site = ECA600<br>Spectrometer = DELTAA_NMR | <pre>Field_Strength = 14.09636928[T] (600[WHz]) X_Acq_Duration = 0.69206016[s] X_Freq = 150.91343039[MHz] X_Fresten = 150.91343039[MHz] X_Points = 100[ppm] X_Points = 32768 X_Prestens = 4.44464109[Hz] X_Sweep_clipped = 37.878789[KHz] Irr_Offset = 47.3484485[KHz] Irr_Offset = 77.33046[MHz] Irr_Offset = 70.1723046[MHz] Irr_Offset = 51ppm] Mod_Return = 1 Mod_Return = 1 Mod_Return = 20[us] Scans = 256 Total_Scans = 256</pre> | <pre>X_90_Width = 8.4[us]<br/>X_acq_rime = 0.69206016[s]<br/>X_angle = 0.69206016[s]<br/>X_angle = 30(deg]<br/>X_Pulse = 30(deg]<br/>X_Pulse = 18[dB]<br/>Irr_Ath_Dec = 18[dB]<br/>Irr_Ath_Noe = 18[dB]<br/>Irr_Ath_Noe = 18[dB]<br/>Irr_Pwidth = 76[us]<br/>Decoupling = TsUE<br/>Noe_rime = 2[s]</pre> | Recvr_Gain = 56<br>Relaxation_Delay = 2[8]<br>Repetition_Time = 2.69206016[8]<br>Temp_Get = 23.3[dC]<br>Mo Dh |                                               | S1 (150 MHz, CDCI <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
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|                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                          |                                                                                                               | 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0          | 6742.91<br>6742.91<br>2703.55<br>8641.75                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                          |                                                                                                               | 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 | 77.2106<br>77.2106<br>77.2106<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8453<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.8493<br>123.84 |
|                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                          | 331                                                                                                                                                                                                                                                                                                      |                                                                                                               | 190.0 180.0 170.0 160.0                       | X : parts per Million : Carbon13 : p                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |

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| <pre>= C:\Users\delta\Documents\J<br/>= delta<br/>= carbbn.jxp<br/>= SN-IT-115<br/>= SN-IT-115<br/>= CHLOROFORM-D<br/>= CHLOROFORM-D<br/>= 16-SEP-2010 14:11:51<br/>= 16-SEP-2010 14:11:51<br/>= 16-SEP-2010 14:12:52</pre> | <pre>= single pulse decoupled gat = 1D COMPLEX = 26214 = 26214 = Carbon13 = [ppm] = [ppm] = X = ZA600 = DELTA2_NMR</pre> | <pre>th = 14.09636928[r] (600[MHz]) on = 0.69206016[s] = 13C = 150.91343039[MHz] = 100[ppm] = 32768 = 4.4466109[Hz] = 4.7.34846485[KHz] ped = 37.878788[KHz] ped = 37.878788[KHz] = 4.7.34846485[KHz] = 4.7.34846485[KHz] = 4.7.34846485[KHz] = 1. ry = 20[us] = 219</pre> | <pre>= 8.4 [us] = 0.69206016[s] = 0.69206016[s] = 6.4 [dB] = 18 [dB] = 2.69206016[s] ime = 2.3.1[dC]</pre>                                                                                                               | Me Q, O Ph<br>S N N<br>N-N<br>S0 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
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| Filename<br>Author<br>Experiment<br>Sauwple_Id<br>Solvent<br>Creation_Tim<br>Revision_Time<br>Current_Time                                                                                                                  | Comment<br>Data_Format<br>Dim_size<br>Dim_Title<br>Dim_Units<br>Dim_Units<br>Site<br>Site                                | Field Streng<br>X_Acq_Duration<br>X_Pomain<br>X_Freq<br>X_Fred<br>X_Fred<br>X_Fred<br>X_Resolution<br>X_Sweep_Clip<br>X_Sweep_Clip<br>Irr_Domain<br>Irr_Offset<br>Clipped<br>Irr_Offset<br>Clipped<br>Prob_Recovel<br>Scans<br>Total_Scans                                 | x_90_width<br>X_Arg1e<br>X_Arg1e<br>X_Arg1e<br>X_Pulse<br>Irr_Atr_Noe<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Puidth<br>Noe Time<br>Recoupling<br>Relaxation_T<br>Repetition_T | Bn0<br>12 (15                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|                                                                                                                                                                                                                             |                                                                                                                          |                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                  | 190.0       180.0       17.1194       17.1194         190.0       180.0       17.1194       10.0       10.0         190.0       130.0       130.0       100.0       10.0       10.0       10.0         190.0       180.0       17.1194       10.0       10.0       10.0       10.0       10.0       10.0         190.0       130.0       130.0       130.0       100.0       80.0       70.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0       10.0 |



| <pre>filename = C:\Users\delta\Documents\J Author = delta Experiment = delta Experiment = carbon.jxp Sample_Id = SN-II-167-1 Sample_Id = SN-II-167-1 Sample_Id = CHLORFORM-D Creation_Time = 15-SEP-2010 13:24:56 Current_Time = 15-SEP-2010 13:35:11 Comment = 15-SEP-2010 13 Comment = 15-SEP-2010 13 Comment = 15-S</pre> | <pre>field_Strength = 14.09636928[T] (600[MHz]) X_Acq_Duration = 0.69206016[s] X_Domain = 13C X_Doffset = 15C X_Doffset = 150.91343039[MHz] X_Doffset = 150.91343039[MHz] X_Doffset = 100[ppm] X_Points = 32768 X_Prescans = 4.446109[Hz] X_Sweep_clipped = 1.4446109[Hz] X_SWEEp_clipped = 1.</pre> | <pre>x_90_width = 8.4[us] x_Acc_Time = 0.69206016[s] x_Acc_Time = 0.69206016[s] x_Artn = 0.4[db] x_hus = 0.4[db] x_pulse = 0.4[db] recurling = 0.4</pre> | Bno Me Me OMPM<br>14 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
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                                                                                                                                                               | 190.0 180.0 170.0<br>X : parts per Million : Carl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       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| <pre>rilename = C:\Users\delta\Documents\J Author = delta Author = delta Experiment = carbon.jxp Sample Id = SN-II-168-2-1 Solvent = HLCN0PORN-D Creation_Time = 15-SEP-2010 15:41:04 Revision_Time = 15-SEP-2010 15:45:50 Current_Time = 15-SEP-2010 15:46:08</pre> | Comment = single pulse decoupled gat<br>Data_Format = 1D CONFLEX<br>Dim_Size = 26214<br>Dim_Title = 2arbon13<br>Dim_Units = [ppm]<br>Dim_Units = X<br>Site = ZCA600<br>Spectrometer = DELTA2_NWR | <pre>Field_Strength = 14.09636928[T] (600[MHz]) X_Acq_Duration = 0.69206016[s] X_Domain = 13C X_Freq = 1.3C X_Freq = 150.91343039[MHz] X_Pfield = 150.91343039[MHz] X_Pointe = 100[ppm] X_Pointe = 32768 X_Prescans = 4.14496109[Hz] X_Sweep_Clipped = 1.44496109[Hz] X_Sweep_Clipped = 37.878788[KHz] Irr_Domain = 27.639 X_Sweep_Clipped = 37.878788[KHz] Irr_Domain = 20.1723046[MHz] Irr_Orfleet = 5[ppm] Clipped = FALSE Mod_Return = 1 Mod_Return = 1 Probe_Recovery = 80 Total_Scans = 80</pre> | <pre>x_90_width = 8.4[us]<br/>X_Acq_Time = 0.69206016[s]<br/>X_Angle = 0.69206016[s]<br/>X_Ant<br/>x_Ath = 6.4[db]<br/>Trr_Ath_Dec = 18[db]<br/>Trr_Ath_Noe = 18[db]<br/>Trr_Noise = 18[db]<br/>Trr_Noise = 18[db]<br/>Trr_Noise = 18[db]<br/>Trr_Noise = 18[db]<br/>Moe = 76[us]<br/>Moe = 77(Us]<br/>Moe = 1[s]<br/>Noe = 1[s]<br/>Noe = 2[s]<br/>Recuping = 2[s]<br/>Recur_dain = 2[s]<br/>Reptation_Time = 2.69206016[s]<br/>Temp_Get = 23.1[dc]</pre> | Bno in Me OH Me<br>OH<br>15 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
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| Filename = C:\Users\delta\Documents\.<br>Author = delta<br>Experiment = carbon.jxp<br>Exporiment = SN-III-45<br>Sample_Id = SN-III-45<br>Solvent = GHLOROFORM-D<br>Creation_Time = 14-SEP-2010 15:37:59<br>Revision_Time = 14-SEP-2010 15:49:40<br>Current_Time = 14-SEP-2010 15:50:15 | Comment = single pulse decoupled gat<br>Data_Format = 1D COMPLEX<br>Dim_Size = 26214<br>Dim_Title = Carbon13<br>Dim_Units = [ppm]<br>Dim_Units = K<br>Site = ZC600<br>Site = DELTA2_NMR | <pre>Field_Strength = 14.09636928[T] (600[MHz]) X_Acq_Duration = 0.69206016[s] X_Pomain = 13C X_Offset = 13C X_Offset = 100[ppm] X_Prescans = 100[ppm] X_Prescans = 100[ppm] X_Prescans = 4 4495109[Hz] X_Sweep_Clipped = 1.4445109[Hz] X_Sweep_Clipped = 7.87878788[KHz] Irr_Domain = 47.3484485[KHz] X_Sweep_Clipped = 37.87878788[KHz] Irr_Offset = 5[ppm] Irr_Offset = 5[ppm] Irr_Offset = 5[ppm] Irr_Offset = 5[ppm] Irr_Offset = 20[us] Scans = 238 Total_Scans = 238</pre> | <pre>X_90_Width = 8.4[us]<br/>X_Acq_Time = 0.69206016[s]<br/>X_Angle = 0.69206016[s]<br/>X_Angle = 30(deg]<br/>X_Ann = 6.4[dB]<br/>Irr_Atn_Dec = 18[dB]<br/>Irr_Atn_Dec = 18[dB]<br/>Irr_Atn_Noe = 18[dB]<br/>Irr_Moise = MALTZ<br/>Irr_Pwidth = 76[us]<br/>Deccupling = 76[us]<br/>Noe = TRUE<br/>Initial_Wait = 1[s]<br/>Noe = TRUE<br/>Noe-Time = 2[s]<br/>Relaxation_Delay = 2[s]<br/>Repetition_Time = 2.69016[s]<br/>Temp_Get = 23[dC]</pre> | SdIT, | Bno Othe O Me<br>OTiPS<br>S2 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
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| C:\Users\delta\Documents\J<br>delta<br>proton.jxp<br>pw-rr1-46<br>CHLOROFORM-D<br>26-MMY-2010 17:55:49<br>26-MMY-2010 17:55:49<br>27-MMY-2010 17:55:49<br>26-MMY-2010 17:55:49<br>27-MMY-2010 17:55<br>26-MMY-2010 17:55<br>27-MMY-2010 17:55<br>27-MMY-2010 17:55<br>27-MMY-2010 | <pre>14.09636928[T] (600[MHz]) 1H 2.9007984[a] 1H 2.9001723046[MHz] 5[Epm] 32768 1 32768 1 33766642[Hz] 11.26126136[KHz] 0.34366642[Hz] 11.26126136[KHz] 60.1723046[MHz] 7 5[Epm] 7 5[Epm] 7 5[Epm] 7 5[Um] 8 8</pre>                                                  | <pre>12.4[us] 2.9097984[s] 45[deg] 45[deg] 3[dB] 3[dB] 6.2[us] 0ff 0ff 1[s] 1[s] 1[s] 1[s] 1[s] 1[s] 1[s] 1[s]</pre>                                                                                       | 16 (600 MHz, CDCl <sub>3</sub> )                                                                 |
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| Filename<br>Author<br>Experiment<br>Sample<br>Sample<br>Sevent<br>Time<br>Creentor<br>Comment<br>Data<br>Data<br>Dia<br>Dia<br>Dia<br>Dia<br>Dia<br>Dia<br>Dia<br>Dia<br>Dia<br>Di                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Field_Strength<br>X_Acq_Duration<br>X_Preq<br>X_Offset<br>X_Offset<br>X_Prescans<br>X_Prescans<br>X_Sweep_<br>X_Sweep_<br>X_Sweep_<br>Irr_Domain<br>Tri_Freq<br>Tri_Domain<br>Tri_Freq<br>Tri_Offset<br>Clipped<br>Wod_Return<br>Prodal_Scover<br>Scans<br>Total_Scans | X_90_Width<br>X_Acq_Time<br>X_Angle<br>X_Angle<br>X_Ath<br>X_Ath<br>X_Puise<br>IrriMode<br>TriMode<br>TriMode<br>TriMode<br>Tritial_Mait<br>Recvr_Gain<br>Relaxation_Fa<br>Relaxation_Fa<br>Repetition_Tim |                                                                                                  |
| 08.84                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                                        | 00'E<br>1955<br>51'5<br>EI'I<br>II'I<br>60'T<br>FUI<br>97'7                                                                                                                                                | 5.0<br>5.0<br>5.0<br>5.0<br>5.0<br>5.0<br>5.0<br>5.0                                             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                        | <u>17.65.1</u>                                                                                                                                                                                             | 9.0 8.0 7.2460<br>9.0 8.0 7.0 6.0 6.0 7.2463<br>7.2463 7.2958<br>7.2958<br>X : parts per Million |

| <pre>ilename = C:\Users\delta\Documents\J uthor = delta xperiment = carbon.jxp auple_Id = SN-III-46 olvent = CHLOROFORM-D olvent = 14-SFP-2010 16:36:31 evision_Time = 14-SFP-2010 16:45:04 urrent_Time = 14-SFP-2010 16:45:04</pre> | omment = single pulse decoupled gat<br>atFormat = 1D COMPLEX<br>im_Size = 26214<br>im_Title = 26214<br>im_Units = [ppm]<br>im_Units = [ppm]<br>im_Onits = x<br>ite = ECA600<br>ite = DELTA2_NTR | <pre>ield_Strength = 14.09636928[T] (600[MHz]) _Acq_Duration = 0.69206016[s] _Domain = 150.91343039[MHz] _freq = 150.91343039[MHz] _freq = 100[ppm] _points = 3768 _range= 1.4486405[Hz] _range= 1.4486405[Hz] _range= 1.4486405[Hz] _range= 1.4486405[Hz] _range= 1.4486405[Hz] _range= 1.4486405[Hz] rr_Offset = 5[ppm] rr_Offset = 5[ppm] rr_Offset = 5[ppm] lipped = FALSE od_Recovery = 20[us] coms = 85 otal_Scans = 85 otal_Scans = 85</pre> | <pre>90_Width = 8.4[us] Acq_Time = 0.69206016[s] Augle = 30[deg] Augle = 30[deg] Augle = 30[deg] Augle = 10[db] Fr_Atn_Dec = 18[db] Fr_Atn_Dec = 18[db] Fr_Nte = 18[db] Fr_Nte = 18[db] Fr_Nte = 16] eccupiing = 1[s] offus = 1[s] offus = 2[s] ecr_ane = 2[s] ecr_an</pre> | Bno TIPS<br>Bno TIPS<br>OTIPS<br>16 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
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| <pre>Filename = C:\Users\delta\Documents\J Author = delta Experiment = proton.jxp Sample_Id = SN-III-63 Solvent = CSILOROFORM-D Creation_Time = 12-JUN-2010 22:08:15 Revision_Time = 12-JUN-2010 22:15:15 Current_Time = 12-JUN-2010 22:15:15</pre> | Comment = single_pulse<br>Data_Format = 1D COMFLEX<br>Dim_Size = 26214<br>Dim_Title = Proton<br>Dim_Units = [ppm]<br>Dimensions = X<br>Site = ECA600<br>Spectrometer = DELTA2_NMR | <pre>Field_Strength = 14.09636928[T] (600[MHz]) X_Acq_Duration = 14 X_Domain = 14 X_Domain = 14 X_Orfset = 2.9097984[s] X_Orfset = 2.9097984[s] X_Pred = 5[ppm] X_Prise = 32768 X_Prise = 35768 X_Prise = 35768 X_Prise = 35768 X_Prise = 35768 X_Prise = 37768 X_Prise = 3776</pre> | <pre>X_90_Width = 12.4[us] X_Acg_Time = 2.9097984[s] X_Angle = 45[deg] X_Angle = 45[deg] X_Pulse = 3[dB] X_Pulse = 5.2[us] Irr_Mode = 6.2[us] Irr_Mode = 6.2[us] Irr_Mode = 0ff Trilial_Wait = 1[s] Recvr_Gain = 28 Relation_Delay = 1[s] Repetition_Time = 3.9097984[s] Temp_Get = 22.4[dC]</pre>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      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| <pre>rilename = C:\Users\delta\Documents\J ruthor = delta Superiment = delta Superiment = carbon.jxp sample_Id = SN-III-63 2 Solvent = SN-III-63 2 Solvent = 12-JUN-2010 22:14:07 reation_Time = 12-JUN-2010 22:13:6     'urrent_Time = 12-JUN-2010 22:21:24     'urrent_Time = single pulse decoupled gat ata_Format = ID CONFLEX</pre> | <pre>jim_Size = 26214<br/>jim_Tite = 26214<br/>jim_Title = Carbon13<br/>jim_Units = [ppm]<br/>jimensions = X<br/>ite = X<br/>Strength = 14.09636928[T] (600[MHz])<br/>field_Strength = 14.09636928[T] (600[MHz])<br/>[Acc_Duration = 0.69206016[s]<br/>[Domain = 130<br/>[Freq = 150.91343039[MHz]]<br/>[offiet = 100[ppm]</pre> | <pre></pre> | <pre>C_90_Width = 8.4[us] (_Acc_Time = 0.6926016[s] (_Angle = 0.6926016[s] (_Angle = 0.6926016[s] (_Angle = 0.6926016[s] (_Tr_An_Dec = 18[db] [rr_An_Dec = 18[db] [rr_An_Noe = 18[db] [rr_Noise = 18[db] [rr_Pidth = 76[us] noise = 78UE nitial_Wait = 1[s] nitial_Wait = 1[s] nitial_Wait = 1[s] nitial_Wait = 2[s] eccvr_Gain = 2[s] elecvr_Gain = 2.6 elecvr_Time = 2.6926016[s]</pre> | Bno is (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
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| <pre>Filename = C:\Users\delta\Documents\J Author = delta Experiment = delta Experiment = carbon.jxp Supule_1d = SH-ITI-198 Solvent = SH-ORV-D8 Creation_Time = 15-SEP-2010 18:46:29 Revision_Time = 15-SEP-2010 18:53:40 Current_Time = 15-SEP-2010 18:54:07</pre> | Comment = single pulse decoupled gat<br>Data_Format = 1D COMFLEX<br>Dim_Title = 26214<br>Dim_Title = Carbon13<br>Dim_Units = [ppm]<br>Dimensions = X<br>Site = DELTA2_NMR | <pre>Field_Strength = 14.09636928[T] (600[MHz]) X_Acq_Duration = 0.69206016[s] X_Domain = 13C X_Freq = 1.3C X_Freq = 150.91343039[WHz] X_Points = 32768 X_Points = 32768 X_Points = 32768 X_Points = 32768 X_Sweep_Clipped = 1.44496109[Hz] X_Sweep_Clipped = 37.878788[KHz] Irr_Domain = 47.3484845[KHz] Irr_Domain = 47.3484845[KHz] Irr_Domain = 5[ppm] Irr_Doffeet = 5[ppm] Clipped = FALSE Mod_Return = 1 Kod_Return =</pre> | <pre>x 90_Width = 8.4[us] X_Acq_Time = 0.69206016[s] X_Angle = 0.69206016[s] X_Angle = 30[deg] X_Ant = 5.4[dB] X_Ant = 2.8[us] Irr_Atn_Dec = 18[dB] Irr_Atn_Noe = 18[dB] Irr_Atn_Noe = 18[dB] Irr_Atn_Noe = 18[dB] Irr_Evidth = 76[us] Noe = 1[s] Noe = 1[s] Noe = 2[s] Revr_Gain = 2[s] Revr_Gain = 2[s] Revr_Gain = 2[s] Revr_Gain = 2[s] Repetition_Time = 2.8[dC] Temp_Get = 23[dC]</pre> | 18 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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S48



| ename = C:\USers\delta\Documents\J<br>hor = delta = Gelta<br>pje_Id = NrII-97-3<br>vent = NrII-97-3<br>vent = CHLORFORM-D<br>ation_Time = 7-0CT-2010 10:41:30<br>ation_Time = 7-0CT-2010 10:49:09<br>ision_Time = 7-0CT-2010 10:49:09<br>rent_Time = 7-0CT-2010 10:49:09<br>ment = single_Dulse<br>= 26214<br>_Title = Proton<br>_Title = Proton<br>_Title = roton | <pre>e = ECA600 ctrometer = DELTA2_NWR ctrometer = DELTA2_NWR id_Strength = 14.09636928[T] (600[WHz]) cq_Duration = 2.9097984[s] cq_Duration = 2.9097984[s] cq_Duration = 2.9097984[s] ffset = 5[Dpm] ffset = 5[Dpm] ffset = 11.26126[KHz] weep ints = 1.26126[KHz] weep ints = 2.0090901[KHz] weep ints = 2.0090901[KHz] momin = 2.0090901[KHz] momin = 2.0000001[KHz] coffset = 5[Dpm] coffse</pre>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | <pre>be_Recovery = 5[us] ns = 8 ns = 8 al_Scans = 8 0 width = 12.4[us] cq_rime = 12.909984[s] ngle = 2.909984[s] ngle = 45[deg] tn = 3[dB] tn = 3[dB] cd = 0ff mode = 0ff land = 0ff te_Presat = 1[s] vr_gain = 48 axation_belay = 1[s] vr_gain = 3.9097984[s] p_det = 22.2[dC] </pre> | HO | I —∕√<br>Me<br>24 (600 MHz, CDCI₃)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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| 2.1                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Filename<br>Author<br>Experiment<br>Sample_Id                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | = C:\Users\delta\Documents\J<br>= delta<br>= carbon.jxp<br>= SN-III-97<br>- PENTENE_F                              |
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| I.I                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Creation<br>Revision_1<br>Current_ri                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | ше = 23-JUL-2010 12:11:46<br>ime = 23-JUL-2010 12:11:45<br>ime = 23-JUL-2010 12:14:23<br>ae = 23-JUL-2010 12:14:35 |
| 0°I 6°0                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Comment<br>Data_Forme<br>Data_Forme<br>Dim_Title<br>Dim_Title<br>Dimensione<br>Spectromet                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | <pre>= single pulse decoupled gat = 1D COMPLEX = 26214 = 26214 = 262013 = [ppm] = x = DELTA2 NMR </pre>            |
| 8.0                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Field_Stre<br>X_Acq_Durs<br>X_Domain<br>X_Freq<br>X_Offset                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | <pre>sgth = 14.09636928[T] (600[MHz]) .ion = 0.69206016[s] = 13C = 15C = 150.91343039[MHz] = 100[Toum]</pre>       |
| <i>L</i> <sup>.</sup> 0 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | x_Points<br>X_Prescans<br>X_Resoluti<br>X_Sweep<br>X_Sweep_C1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | = 32768<br>= 4<br>20 = 4<br>= 47.34496109[Hz]<br>= 47.34848615[HHz]<br>[pped = 37.878788[KHz]                      |
| 9.0                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Irr_Domair<br>Irr_Freq<br>Irr_Offset<br>Clipped<br>Mod_Return                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | = Protom<br>= 600.1723046[WHz]<br>= 5[ppm]<br>= FALSE<br>= 1                                                       |
| <i>s</i> .0             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Probe_Recc<br>Scans<br>Total_Scar                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | /ery = 20[us]<br>= 46<br>= 46                                                                                      |
| •••••                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | X_90_Widt<br>X_Acq_Time<br>X_Angle<br>X_Ath<br>X_Ath                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | = 8.4 [us]<br>= 0.69266016[s]<br>= 30[deg]<br>= 5.4 [dB]<br>= 2.8 [ns]                                             |
| £.0                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | ITT ATD De<br>ITT ATD NO<br>ITT NOI86                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | = 18(dB)<br>= 18(dB)<br>= WALTZ<br>= 76[us]                                                                        |
| <b></b> 0.2             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Initial_Wa<br>Noe_Time<br>Recvr_Gain<br>Ralaxation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | .t = 1.105<br>= TRUE<br>= 2.[s]<br>Delav = 2.15<br>Delav = 2.15                                                    |
| I.0<br>Son              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Repetition<br>Temp_Get                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Time = 2.69206016[s]<br>= 22.9[dC]                                                                                 |
| 0<br>repunqe            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | a substantia de la constantia de la constan<br>La constantia de la constanti<br>La constantia de la consta | P                                                                                                                  |
|                         | 0.0210.0200.0190.0180.0170.0160.0150.0140.0130.0120.0110.0100.090.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 0 -10.0 -20.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Me                                                                                                                 |
|                         | <pre>8886<br/>1206<br/>9657<br/>9657<br/>9282<br/>0000<br/>8291<br/>0225<br/>0000<br/>8291<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0225<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0255<br/>0</pre> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | .(150 MHz, C <sub>6</sub> D <sub>6</sub> )                                                                         |
| ×                       | 422222719<br>93 33222719<br>93 33222719<br>94 50 50 50 50 50 50 50 50 50 50 50 50 50                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                    |



| <pre>= C:\Users\delta\Documents\J<br/>= delta<br/>= delta<br/>= carbon.jxp<br/>= SN-TII-93<br/>= BNZZNE-D6<br/>= 13-SEP-2010 13:37:46<br/>= 13-SEP-2010 13:37:59<br/>= 13-SEP-2010 13:37<br/>= 13-SEP-2010 13:37</pre> | <pre>ch = 14.09636928[r] (600[MHz]) cn = 0.69206016[s]     = 13C     = 13C     = 13C     = 13C     = 13C     = 13C     = 100[ppm]     = 37438039[MHz]     = 37488485[KHz] e 4     = 1.44496109[Hz] e 47.34048485[KHz] ped = 37.878788[kHz] ped = 37.878788[kHz] e 47.34048485[KHz] e 47.34048485[KHz] e 57.878788[kHz] e 600.1723046[MHz] e 77.820[mHz] e 77.820[mHz] e 178 e 178 e 178 e 178</pre> | = 8.4[us]<br>= 0.69206016[s]<br>= 30[deg]<br>= 4(dB]<br>= 2.4[dB]<br>= 18[dB]<br>= 18[dB]<br>= 18[dB]<br>= 18[dB]<br>= 16]<br>= 1[s]<br>= 76[us]<br>= 76[us]<br>= 1[s]<br>= 1[s]<br>= 2[s]<br>= 2[s]<br>= 2[s]<br>= 2[s]<br>= 2[dC]                                                                                                              | MeO <sub>2</sub> C<br>Me<br>Me<br>6 (150 MHz, C <sub>6</sub> D <sub>6</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
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| Filename<br>Author<br>Experiment<br>Sample_Id<br>Sample_Id<br>Solvent<br>Coornent<br>Current_Time<br>Comment<br>Data_Format<br>Dim_Units<br>Dim_Units<br>Dim_Units<br>Site<br>Spectrometer<br>Spectrometer                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Field_Strengt<br>X_Acq_Duration<br>X_Freq<br>X_Freq<br>X_Frescans<br>X_Points<br>X_Sweep_Clipt<br>ITY_Freq<br>TIX_Freq<br>TIX_Freq<br>Clipped<br>Clipped<br>Rode_Return<br>Probe_Recovel<br>Scans<br>Total_Scans                                                                                                                                                                                    | X_90_Width<br>X_Acd_Time<br>X_Angle<br>X_Angle<br>X_Aulse<br>X_Fulse<br>ITT_Atn_Dec<br>ITT_Atn_Noe<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_Noise<br>ITT_ITT_ITT_ITT_ITT_ITT_ITT_ITT_ITT_ITT | ,                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     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28,0000<br>128,1628<br>128,1628<br>128,1628<br>128,1628<br>128,0000<br>120,1228<br>128,0000<br>120,1228<br>128,0000<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0<br>120,0 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| <pre>Filename = C:\Users\delta\Documents\J Author = delta Author = delta Experiment = proton.jxp Sample_Id = SN-III-149 Sample_Id = BENZENE-D6 Color_Time = 21-SEP-2010 14:45:46 Current_Time = 21-SEP-2010 14:45:56 Current_Time = 21-SEP-2010 14:45:56</pre> | Comment = single_pulse<br>Data_Format = 1D COMFLEX<br>Dim_Size = 26214<br>Dim_Title = Proton<br>Dim_Title = Proton<br>Dim_Units = [ppm]<br>Dimensions = X<br>Site = ECA600<br>Spectrometer = DELTA2_NUR | <pre>Field_Strength = 14.09636928[T] (600[WHz]) X_Acq_Duration = 2.9097984[s] X_Domain = 1H X_Domain = 1H X_Freq = 600.1723046[WHz] X_offset = 5[ppm] X_offset = 32768 X_Presens = 1</pre> | X_Resolution = 0.3436642[Hz]<br>X_Sweep = 11.26126126[HHz]<br>X_sweep_clipped = 9.0090901[HHz]<br>Irr_Domain = Proton<br>Irr_Pred = 600.1723046[NHz]<br>Irr_Offset = 5[ppm] | Tri_Domain = Froton<br>Tri_Freq = 600.1723046[MHz]<br>Tri_Offset = 5[ppm]<br>Clipped = FALSE<br>Mod_Return = 1<br>Frobe_Recovery = 5[us]<br>Scams = 8<br>Total_Scams = 8 | X_90_Width = 12.4[us]<br>X_Acq_Time = 2.9097984[s]<br>X_Angle = 45[deg]<br>X_Ath = 3[dB]<br>X_Pulse = 6.2[us]<br>Irr_Mode = 0ff<br>Tri_Mode = 0ff | Dantereat = rALSE<br>Initial_Wait = 1[s]<br>Recvr_Gain = 40<br>Relaxation_Delay = 1[s]<br>Repetition_Time = 3.99994[s]<br>Remp_Get = 22.3[dC] | Me<br>TIPS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           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| <u>t</u>                                                                                                                                                                                                                                                       | 0.84                                                                                                                                                                                                    |                                                                                                                                                                                            |                                                                                                                                                                             |                                                                                                                                                                          |                                                                                                                                                   | 50<br>50<br>50<br>50<br>50<br>50<br>50<br>50<br>50<br>50                                                                                      | I A THE CHANNEL THE BEEN IN THE CASE OF TH | 5.0 4.0 3.0 2.0 1.0 0 | 6856.0<br>6151.1<br>8294.1<br>0274.1<br>2457.2<br>1124.2<br>1124.2<br>1124.2<br>1124.2<br>1124.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2<br>2025.2                                                                                                                                                                                                                                                                                                                                                                               |                                                                  |
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| <pre>&lt; : parts per Million : Proton : parts per Million</pre> |

| <pre>Filename = C:\Users\delta\Documents\J<br/>Author = delta<br/>Author = delta<br/>Experiment = carbon.jxp<br/>Sample_Id = SN_TIT-149<br/>Solvent = SN_TIT-149<br/>Solvent = 21-SEP-2010 14:59:08<br/>Creation_Time = 21-SEP-2010 14:59:08<br/>Current_Time = 21-SEP-2010 14:59:08<br/>Current_Time = 21-SEP-2010 14:59:08<br/>Current_Time = 21-SEP-2010 14:59:08<br/>Dim_Title = 1D REAL<br/>Dim_Title = 26214<br/>Dim_Title = Carbon13<br/>Dim_Units = Kpm]<br/>Dim_Units = Kpm]</pre> | <pre>Site = ECA600 Spectrometer = DELTA2_NMR Field_Strength = 14.0963928[T] (600[MHz]) X_Acq_Duration = 0.69206016[s] X_Domain = 130 X_Domain = 130 X_Diffset = 150.91343039[MHz] X_Diffset = 100[Dpm] X_Offset = 100[Dpm] X_Offset = 100[Dpm] X_Prescans = 4 X_Resolution = 47.3484485[KHz] X_Sweep = 51Dpm] Trr_Domain = Proton ITr_Pomain = 1 Trr_Domain = 1 Proba_Recovery = 20[us] Scans = 372 Scans = 372 Scans = 372</pre> | <pre>X_90_Width = 8.4[us] X_Acc_Time = 0.65206016[s] X_Angle = 0.65206016[s] X_Angle = 0.65206016[s] X_Ath = 0.6510[s] X_Pulse = 0.64(db] X_Pulse = 2.64(db] ITT_Ath_Dec = 18[dB] ITT_Ath_Nee = 2.65206016[s] Temp_Get = 2.65206016[s] </pre> | Bno in the mean of the office office of the office |
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|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | المانية المانية<br>المانية المانية المانية<br>والمانية المانية                                                                | Reprint provide the pro                               |



| <pre>rilename = C:\Users\delta\Documents\J Author = delta = delta Experiment = carbon.jxp Sample_Id = SN-III-73-1 Solvent = SN-III-73-1 Solvent = 19-UUN-2010 20:11:34 Evision_Time = 19-UUN-2010 20:21:45 Current_Time = 19-UUN-2010 20:21:45</pre> | Comment = single pulse decoupled gat<br>Data_permat = 1D COMPLEX<br>Dim_Size = 26214<br>Dim_Title = 26214<br>Dim_Title = Carbon13<br>Dim_Units = [ppm]<br>Simensions = X<br>Spectrometer = DELTA2_NWR | <pre>Field_Strength = 14.0963628[T] (600[MHz]) X_Acq_Duration = 0.69206016[s] X_Freq = 150.91343039[MHz] X_Freq = 150.91343039[MHz] X_Frescans = 100[ppm] X_Frescans = 44.4496109[Hz] X_Frescans = 44.4496109[Hz] X_Sweep_clipped = 37.87878788[KHz] Irr_Domain = 1.44496109[Hz] Y_Sweep_clipped = 37.87878788[KHz] Irr_Domain = 1.44496109[Hz] Y_Sweep_clipped = 20[us] Scans = 128 Total_Scans = 128</pre> | <pre>X_90_Width = 8.4[us]<br/>X_Acq_Time = 0.69206016[s]<br/>X_Attn = 0.69206016[s]<br/>X_Lulse = 30[deg]<br/>X_Lulse = 30[deg]<br/>X_Lulse = 2.8[us]<br/>ITT_Atn_Noe = 18[dB]<br/>ITT_Atn_Noe = 18[dB]<br/>ITT_Noise = 4.8.7<br/>ITT_Noise = 18[dB]<br/>ITT_Noise = 76[us]<br/>Decoupling = TRUE<br/>ITT_Pwidth = 1[s]<br/>Noe = 1[s]<br/>Noe = 1[s]<br/>Noe = 2[s]<br/>Recvr_Oain = 2[s]<br/>Repetition_Time = 2[s]<br/>Repetition_Time = 2[d]<br/>Temp_Get = 23[dC]</pre> | Bno in the off me off m |
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|                                                                                                                                                                                                                                                      |                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | parts per Million : Carbon13 : parts per Million                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |



S58

| <pre>Filename = C:\Users\delta\Documents\J Author = delta Author = delta Exporiment = carbon.jxp Sample_Id = SN-III-74 Solvent = 17-SEP-2010 1159:45 Creation_Time = 17-SEP-2010 12:03:22 Current_Time = 17-SEP-2010 12:03:46</pre> | Comment = single pulse decoupled gat<br>Data_Format = 1D COMPLEX<br>Dim_Size = 26214<br>Dim_Title = 26214<br>Dim_Units = [ppm]<br>Dim_Units = [ppm]<br>Dim_Bions = X<br>Site = ECA600<br>Spectrometer = DELTA2_NWR | <pre>Field_Strength = 14.0963628[T] (600[MHz]) X_Acq_Duration = 0.69206016[s] X_Domain = 13C X_Freq = 150.91343039[MHz] X_Freq = 150.91343039[MHz] X_Points = 32768 X_Prescans = 44496109[Hz] X_Prescans = 4 X_Sweep_clipped = 1.44496109[Hz] X_Sweep_clipped = 5[Dpm] Clipped = 5[Dpm] Clipped = 1. Mod_Return = 1 Mod_Return = 1 Scans = 58 Total_Scans = 58</pre> | <pre>X_90_Width = 8.4[us]<br/>X_Acq_Time = 0.69206016[s]<br/>X_Atn = 0.69206016[s]<br/>X_Atn = 6.4[db]<br/>X_Pulse = 3.0[ds]<br/>Trr_Atn_Nos = 18[db]<br/>Trr_Anden = 18[db]<br/>Trr_Noise = 18[db]<br/>Trr_Noise = 18[db]<br/>Trr_Noise = 76[us]<br/>Trr_Noise = WALTZ<br/>Trr_Noise = WALTZ<br/>Trr_Noise = 18[db]<br/>Trr_Andth = 76[us]<br/>Nos = 12[s]<br/>Nos = 12[s]<br/>Nos = 2.69206016[s]<br/>Retration_Time = 2.69206016[s]<br/>Temp_Get = 2.1[dC]</pre> | Me Me Me MPM<br>Ho Me<br>OBn<br>26 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
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|                                                                                                                                                                                                                                     |                                                                                                                                                                                                                    | \$59                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |



|   | <pre>= C:\Vsers\delta\Documents\J t = delta = delta = carbon.jxp t = carbon.jxp = cHLORORM-D Time = 13-SEP-2010 19:46:07 Time = 13-SEP-2010 20:00:56 ime = 13-SEP-2010 20:00:56</pre> | at = single pulse decoupled gat<br>= 1D COMPLEX<br>= 2 ComPLEX<br>= 2 Carbon13<br>= Carbon13<br>= 2 Carbon<br>= 2 Car600<br>ter = DELTA2_NWR | <pre>ength = 14.09636928[T] (600[WHz]) ation = 0.69206016[s] = 130.91343039[MHz] = 150.91343039[MHz] = 100[ppm] = 104496109[Hz] = 32768 ion = 47.34846485[HHz] n = 47.34846485[HHz] n = 47.34846485[HHz] n = 71.878788[KHz] n = 27.000 t = 510pm] n = 261 n n = 261</pre> | h = $0.69206016[s]$<br>= $0.69206016[s]$<br>= $0.69206016[s]$<br>= $0.69206016[s]$<br>= $0.69206016[s]$<br>= $0.69206016[s]$<br>= $0.69206016[s]$<br>= $1.[s]$<br>= $2.6[us]$<br>= $2.6[us]$<br>= $2.69206016[s]$<br>= $2.69206016[s]$ | TBSO<br>S3 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
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|   | Filename<br>Author<br>Experimer<br>Sample_Id<br>Solvent<br>Solvent<br>Revision<br>Current_1                                                                                           | Comment<br>Data_rorr<br>Dim_sire_<br>Dim_Title<br>Dim_Units<br>Dimension<br>Stectrome                                                        | Field_Str<br>X_Acq_Dur<br>X_Creet<br>X_Offset<br>X_Offset<br>X_Prescants<br>X_Sweep<br>X_Sweep<br>X_Sweep<br>X_Sweep<br>X_Sweep<br>Clipped<br>IITY_Offse<br>IITY_Offset<br>Frod_stetur<br>Prod_stetur<br>Prod_stetur<br>Prod_stetur                                       | X_90_widt<br>X_Acq_Tim<br>X_Atn<br>X_Atn<br>X_Atn<br>X_Pulse<br>X_Pulse<br>X_Pulse<br>ITT_Atn<br>ITT_Atn<br>ITT_Atn<br>ITT_Atn<br>ITT_Atn<br>ITT_Atn<br>Noe<br>Tan<br>Robertico<br>Repetitio                                           | 6169.4-                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| , |                                                                                                                                                                                       |                                                                                                                                              | -                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                        | 70.0<br>15.8934<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70.0<br>70. |
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|   |                                                                                                                                                                                       |                                                                                                                                              |                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                        | 210200.0 190.0 180.0 170.0 160.0 150.(<br>210200.0 190.0 180.0 170.0 160.0 150.(<br>59.0366<br>X : parts per Million : Carbon13 : parts p                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |



| 1900     1800     1700     200     200     100     0       1900     1800     1700     200     200     200     200     200       172     172     255     255     255     255     255       1900     1800     1700     200     200     200     255     255       1900     1800     1700     200     200     200     255     255       1900     1800     1900     1900     1900     100     000     000     000     000       15     15     15     15     15     15     15     15       15     15     15     15     15     15     15       16     15     15     15     15     15     15 | <pre>= C:\Users\delta\Documents\J = delta = carbon.jxp = sN-III-40 = SN-III-40 = CHLOROFORM-D = 17-SEP-2010 17:40:09 = 17-SEP-2010 11:36:00 = 17-SEP-2010 11:36:34</pre> | <pre>= single pulse decoupled gat<br/>= 1D CONFLEX<br/>= 262141<br/>= Carbon13<br/>= [ppm]<br/>= [ppm]<br/>= ECA600<br/>= DELTAA_NWR</pre> | <pre>th = 14.09636928[T] (600[WHz]) on = 0.69206016[s] = 130 = 130.91343039[MHz] = 100[ppm] = 100[ppm] = 32768 = 47.348488[NHz] e 47.34848485[NHz] ped = 77.000 = 77.000 = 600.1723046[MHz]</pre>            | = 7100<br>= TRUE<br>= 1<br>= 20[us]<br>= 720<br>= 720                        | = 8.4[us]<br>= 0.69206016[s]<br>= 30[deg]<br>= 2.8[us]<br>= 2.8[us]<br>= 18[dB]<br>= 18[dB]<br>= MALTZ<br>= 76[us]<br>= 1[s]    | $ = \frac{1000}{2[6]} = \frac{2[6]}{2[6]} = 56$ $ = 2.69206016[6]$ $ = 22.3[dC]$ | Me Me OH<br>TBSO <sup>,</sup> Me<br>OBn<br>S4 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
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| 4.1613                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Filename<br>Author<br>Experiment<br>Sample_Id<br>Solvent<br>Creation_Tim<br>Revision_Time                                                                                | Comment<br>Data_Format<br>Dim_Size<br>Dim_Tritle<br>Dim_Units<br>Dimensions<br>Site<br>Spectrometer                                        | Field Streng<br>X_Acq Duration<br>X_Dumain<br>X_Freq<br>X_Freq<br>X_Freq<br>X_Freq<br>X_Resolution<br>X_Sweep<br>X_Sweep<br>Clip<br>X_Sweep<br>Clip<br>X_Sweep<br>Clip<br>X_Sweep<br>Clip<br>X_Sweep<br>Clip | LILLOLISEC<br>Clipped<br>Mod_Return<br>Probe_Recove:<br>Scans<br>Total_Scans | X_90_width<br>X_Acq_Time<br>X_Angle<br>X_Atn<br>X_Pulse<br>Irr_Atn_Dec<br>Irr_Noise<br>Irr_Pwidth<br>Deccupling<br>Initial_wait | NOC Time<br>Recvr_Gain<br>Relaxation_D<br>Repetition_T<br>Temp_Get               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                          |                                                                                                                                            |                                                                                                                                                                                                              |                                                                              |                                                                                                                                 |                                                                                  | X: parts per Million : Carbon13 : parts per Million : Carbon13 |



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|   | <pre>= C:\Users\delta\Documents\J<br/>= delta<br/>= carbon.jxp<br/>= SN-III-113<br/>= SN-III-113<br/>= CHLCROFORM-D<br/>= 4-AUG-2010 17:42:28<br/>= 4-AUG-2010 17:42:28<br/>= 4-AUG-2010 17:42:49</pre> | <pre>= single pulse decoupled gat = 1D COMPLEX = 26214 = 26214 = Carbon13 = [ppm] = X = ECA600 = DELTA2_NUR</pre> | <pre>h = 14.0963628[T] (600[MHZ]) n = 0.69206016[s] = 13C = 150.91343039[MHZ] = 100[ppm] = 100[ppm] = 3768 = 4 = 47.3484846[yHz] = 47.3484846[yHz] = 47.3484846[xHZ] ad = 37.87878788[kHZ] = 600.1723046[MHZ] = 5[ppm] = 71 r = 20[us] r = 97</pre>   | <pre>= 8.4[us] = 0.69206016[s] = 0.69206016[s] = 3.0[dag] = 3.4[db] = 18[db] = 16[db] = 2163[dc] = 23.5[dc]</pre> | Mile<br>OBn<br>50 MHz, CDCI <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
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|   | Filename<br>Author<br>Experiment<br>Sample_Id<br>Solvent<br>Creation_Time<br>Revision_Time<br>Current_Time                                                                                              | Comment<br>Data_Format<br>Dim_Title<br>Dim_Title<br>Dim_Units<br>Dimensions<br>Site<br>Spectrometer               | Field_Strengt<br>X_Acq_Duration<br>X_Dommin<br>X_Offset<br>X_Points<br>X_Prescans<br>X_Prescans<br>X_Sweep_Clipp<br>X_Sweep_Clipp<br>X_Sweep_Clipp<br>Irr_Pred<br>Irr_Pred<br>Irr_Offset<br>Clipped<br>Scans<br>Probe_Recover<br>Scans<br>Total_Scans | X_90_Width<br>X_Acq_Time<br>X_Atq16<br>X_Atg16<br>X_Atg16<br>X_Pulse<br>Irr_Atg106<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Irr_Noise<br>Recoupling<br>Noe time<br>Relaxation_De<br>Repetition_De       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
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|   |                                                                                                                                                                                                         |                                                                                                                   |                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                                 | 72.9403<br>73.1764<br>73.1764<br>73.1764<br>73.1764<br>73.1764<br>73.1764<br>73.1764<br>75.784<br>75.784<br>75.784<br>75.784<br>75.784<br>75.784<br>76.786<br>70.0<br>80.0<br>90.0<br>70.0<br>90.0<br>90.0<br>90.0<br>90.0<br>90.0<br>9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
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                                  | <pre>C:\Users\delta\Documents\J = dalta = proton.jxp = srl.r1r=82-5 = St-JTL-2010 14:53:37 = 24-JUL-2010 14:57:49 = 24-JUL-2010 14:57:49</pre>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       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| <pre>= 14.09636928[T] (600[MHz]) = 2.9097984[s] = 14.09636928[T] (600[MHz]) = 1.1512046[MHz] = 5.5ppm] = 0.3436642[Hz] = 0.3436642[Hz] = 0.3436642[Hz] = 1.26126126[EHz] = 9.00900901[EHz] = 9.00900901[HHz] = 1.261213046[MHz] = 5.5pm] = 5.</pre> |
| <u>00'1</u>                                                   | 70.2                                                                | 17.2 12.1 27.0<br>89.0<br>89.0<br>84.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           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                                                                                                                                                                                                                                                                                                                                                                                                       | Me Co <sub>2</sub> Me D MHz, CDCI <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                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| X : parts per Million : Proton : parts per Million            |                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  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| <pre>C:\Users\delta\Documents\J = delta = carbon.jxp = carbon.jxp = SN-III-121-1-3 = CHLOR0FORM-D = 18-AUG-2010 21:18:25 = 18-AUG-2010 21:18:42 = sincle vulse decompled cat</pre> | = 1D COMPLEX<br>= 26214<br>= 26214<br>= Carboni3<br>= [ppm]<br>= X<br>= ZCA600<br>= DELTA2_NHR | h = 14.09636928[T] (600[WHz])<br>= 13C<br>= 13C<br>= 100[Dpm]<br>= 100[Dpm]<br>= 27688<br>= 4<br>= 4<br>= 4<br>= 4<br>= 4<br>= 1.44496109[Hz]<br>= 4<br>= 4<br>= 4<br>= 4<br>= 4<br>= 1.44496109[Hz]<br>= 327688[KHz]<br>= 4<br>= 7.3484865[KHz]<br>= 4<br>= 7.3484865[KHz]<br>= 6<br>= 1.44496109[Hz]<br>= 2.7120<br>= 6<br>= 1.220<br>= 1.2200<br>= 1.20 | <pre>= 8.4[us] = 0.6206016[s] = 0.6206016[s] = 30(deg] = 30(deg] = 30(deg] = 18[db] = 28] = 28] = 23.4[dC]</pre>                                         | Me CO <sub>2</sub> Me | Me<br>OBn<br>4 (150 MHz, CDCl <sub>3</sub> )                                                                                               |
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| Filename<br>Author<br>Experiment<br>Sample_Id<br>Solvent<br>Creation_Time<br>Revision_Time<br>Current_Time                                                                         | Dim_file<br>Dim_file<br>Dim_file<br>Dim_file<br>Dim_file<br>Dimensions<br>Site<br>Spectrometer | Field_Strengtl<br>X_Acq_Duration<br>X_Domain<br>X_Prend<br>X_Offset<br>X_Preseams<br>X_Preseams<br>X_Preseams<br>X_Preseams<br>X_Preseams<br>X_Preseams<br>Trr_Domain<br>Trr_Freq<br>Trr_Domain<br>Trr_Freq<br>Trr_Offset<br>Clipped<br>Mod_Return<br>Probe_Return<br>Probe_Return<br>Probe_Return<br>Probe_Return<br>Probe_Return<br>Probe_Return<br>Probe_Return<br>Probe_Return                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | X_90_width<br>X_Acq_Time<br>X_Augle<br>X_Augle<br>X_Aulse<br>X_Pulse<br>Trr_Aunoe<br>Trr_Aunoe<br>Trr_Aunoe<br>Trr_Noise<br>Trr_Noise<br>Trr_Pwidth<br>Decoupling<br>Initial wait<br>Noe<br>Time<br>Recvr_Gain<br>Relaxation_Tin<br>Tepetition_Tin<br>Tepedition_Tin | Me<br>Me              | TBSO                                                                                                                                       |
|                                                                                                                                                                                    |                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                      |                       | $ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c}$ |
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|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Comment<br>Data_Format<br>Dim_Size<br>Dim_Title<br>Dim_Units<br>Dimensions<br>Site<br>Spectrometer                                               | <pre>= single pulse decoupled gat = 1D COMPLEX = 26214 = Carbon13 = [ppm] = [ppm] = ECA600 = DELTA2_NMR</pre>                                                                                   |
| ·                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Field_Strength<br>X_Acq_Duration<br>X_Domain<br>X_Peeq<br>X_Offset<br>X_Pescens<br>X_Pescens<br>X_Sweep<br>X_Sweep_Clipped<br>Irr_Peq<br>Irr_Peq | = 14.09636928[T] (600[MHz])<br>= 0.69206016[s]<br>= 13C<br>= 150.91343039[MHz]<br>= 100[ppm]<br>= 32768<br>= 47.34848485[KHz]<br>= 47.34848485[KHz]<br>= 47.34848485[KHz]<br>= 500.1723046[MHz] |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Irr_Offset<br>Clipped<br>Mod_Return<br>Probe_Recovery<br>Scans<br>Total_Scans                                                                    | = 5 [ppm]<br>= FALSE<br>= 1<br>= 1<br>= 20[us]<br>= 452.0<br>= 452.0                                                                                                                            |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | X_90_Width<br>X_Acq_Time<br>X_Angle<br>X_Aun<br>X_Pulse<br>Irr_Atn_Dec<br>Irr_Atn_Nee<br>Irr_Poise<br>Irr_Width<br>Decoupling                    | = 8.4[us]<br>= 0.69206016[s]<br>= 30[dec]<br>= 6.4[db]<br>= 2.8[us]<br>= 18[db]<br>= 18[db]<br>= 18[db]<br>= 16[db]<br>= 76[us]<br>= 76[us]                                                     |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | Initial_Wait<br>Noe_Time<br>Noe_Time<br>Recvr_Gain<br>Reperition_Delay<br>Reperition_Time<br>Temp_Get                                            | = 1[s]<br>= TRUE<br>= 2[s]<br>= 56<br>= 2[s]<br>= 2.69206016[s]<br>= 2.69206016[s]                                                                                                              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                  | <del>Б</del> .                                                                                                                                                                                  |
| $190.0 \ 180.0 \ 170.0 \ 160.0 \ 150.0 \ 140.0 \ 130.0 \ 120.0 \ 100.0 \ 90.0 \ 80.0 \ 70.0 \ 60.0 \ 50.0 \ 40.0 \ 30.0 \ 20.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 \ 10.0 $ |                                                                                                                                                  | Me Me CO <sub>2</sub> Me                                                                                                                                                                        |
| : parts per Million : Carbon13 : parts per Million                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 51-<br>                                                                                                                                          | <i>∋pi-</i> 4 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                     |

| <pre>Filename = C:\Users\delta\Documents\J Author = dalta = SN-TII-135 Sumple_Id = NN-TII-135 Sumple_Id = NN-TII-135 Sumple_Id = NN-TII-135 Sumple_Id = Proton_135 Coleantion_Time = 25-MUG-2010 16:12:16 Current_Time = 25-MUG-2010 16:12 Current_Time = 25-MUG-2010 16:12 Current = 14.09535928[T] Current = 14 Current = 14.09535928[T] Current = 14.0953594[HHZ] Current = 14.</pre> | Tri_Offset = 5[ppm]<br>Clipped = FALSE<br>Mod_Return = 1<br>Probe_Recovery = 5[us]<br>Scans = 8<br>Scans = 8<br>Total_Scans = 8<br>X_acq_rime = 12.4[us]<br>X_ard_rime = 12.4[us]<br>X_ard_rime = 2.9097984[s]<br>X_ard_rime = 2.9097984[s]<br>X_ard_rime = 2.9097984[s]<br>X_ard_rime = 2.9097984[s]<br>Tri_Mode = 0ff<br>Tri_Mode = 0ff<br>Tri_Mode = 0ff<br>Tri_Mat = 1[s]<br>Recvr_dim = 3.6<br>Renetition_rime = 3.909784[s]                                                                                                                                                                                                           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| Z.I I.I 0.I 0.0 8.0 7.    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                        | <pre>Filename = C:\USers\delta\Documents\J<br/>Author = delta = C:\USers\delta\Documents\J<br/>Experiment = carbon.jxp<br/>Salvent = SN-III-136<br/>Salvent = SN-III-136<br/>Salvent = C=HLOROFORM-D<br/>Creation_Time = 2-SEP-2010 20:12:44<br/>Current_Time = 2-SEP-2010 20:20:440<br/>Current_Time = 2-SEP-2010 20:20:440<br/>Current_Time = 2-SEP-2010 20:20:440<br/>Current_Time = 2-SEP-2010 20:20:440<br/>Comment = 2-SEP-2010 20:20:440<br/>Field_Strength = 10.0505628[F] (600[MHz])<br/>X_Preq = 100(Ppm]<br/>X_Preq = 100(Ppm]<br/>X_Offset = 100(Ppm]<br/>X_Prescans = 4</pre> |
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| 0 9.0 2.0 4.0 £.0 2.0 I.0 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                        | $ \begin{array}{llllllllllllllllllllllllllllllllllll$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|                           | arts per Million : Carbon 13 : parts per Million : Carbon 13 : | 00000000000000000000000000000000000000 | Me Me Me Me Me Me Co <sub>2</sub> Me<br>TBSO <sup>111</sup> Me Me CO <sub>2</sub> Me S5 (150 MHz, CDCl <sub>3</sub> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |

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