General. All commercially available reagents were used without further purification. All solvents were used after distillation. Tetrahydrofuran (THF), diethyl ether and toluene were refluxed over and distilled from sodium-benzophenone ketyl. Dichloromethane was refluxed over and distilled from P_2O_5. Dimethylformamide (DMF) was distilled from CaH_2 under reduced pressure. Preparative separation was performed by column chromatography on silica gel. ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400MHz spectrometer and chemical shifts were represented as δ-values relative to the internal standard TMS. IR spectra were recorded on a FT-IR Spectrometer. High-resolution mass spectra (HRMS) were measured on a ESI-TOF MS.

(trans)-2-[(1*S*,2*R*,4*S*)-4-Hydroxy-1,2-epoxy-2,6,6-trimethylcyclohexyl]-1-iodoethylene (9). To a solution of iodine (1.28 g, 5.04 mmol), Na_2CO_3 (1.07 g, 10.1 mmol) in dichloromethane (25.2 mL) was added dropwise a solution of stannane **8** (1.19 g, 2.52 mmol) in dichloromethane (3 mL) at 0 ºC. After being stirred for 15 min at 0 ºC, the mixture was poured into a saturated aqueous $Na_2S_2O_3$ solution, and then extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 10% to 50% ethyl acetate in hexane) afforded iodide **9** (764 mg, 98%) as a colorless oil: $[\alpha]^{23}_D$ –82.0 (c 0.99, $CHCl_3$); IR (KBr disk, cm^{-1}) 3449, 2963, 2870, 1695, 1466, 1303, 1184, 1122, 1047, 953, 914; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.75 (d, *J* =14.2 Hz, 1H), 6.25 (d, *J* =14.2, 1H), 3.85 (m, 1H), 2.34 (ddd, *J* =14.7, 5.0, 1.8 Hz, 1H), 1.60 (m, 2H), 1.21 (dd, *J* =11.9, 11.9 Hz, 1H), 1.21 (s, 3H), 1.14 (s, 3H), 0.97 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 142.1, 79.7, 72.7, 66.6, 64.3, 47.1, 40.9, 35.1, 29.6, 25.0, 20.2.

(2*E*,4*E*)-5-[(1'*S*,2'*R*,4'*S*)-4'-Hydroxy-1',2'-epoxy-2',6',6'-trimethylcyclohexa-1'-yl]-3-methylpenta-2,4-diene-1-ol (11). To a solution of vinyl iodide **9** (71 mg, 0.23 mmol) and stannane **10** (208 mg, 0.58 mmol) in DMF (1.15 mL) was added bis(acetonitrile)dichloropalladium(II) (3 mg, 0.012 mmol) and lithium chloride (19 mg, 0.46 mmol). After being stirred for 20 min at room temperature, the reaction mixture was poured into water, and then extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 30% to 60% ethyl acetate in hexane) afforded alcohol **11** (50 mg, 86%) as a white solid: $[\alpha]^{25}_D$ –62.9 (c 1.14, MeOH); IR (KBr disk, cm^{-1}) 3449, 2963, 2870, 1695,

1466, 1303, 1184, 1122, 1047, 953, 914; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.20 (d, *J* =15.6 Hz, 1H), 5.85 (d, *J* =15.6, 1H), 5.65 (t, *J* =6.9 Hz, 1H), 4.26 (d, *J* =6.4 Hz, 2H), 3.86 (m, 1H), 2.34 (ddd, *J* =14.2, 3.2, 1.9 Hz, 1H), 1.78 (s, 3H), 1.58 (m, 2H), 1.21 (dd, *J* =12.9, 10.6 Hz, 1H), 1.15 (s, 3H), 1.11 (s, 3H), 0.94 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 137.0, 135.6, 130.6, 124.8, 70.4, 67.1, 64.5, 59.6, 47.4, 41.2, 35.5, 29.9, 25.1, 20.2, 13.0; ESI-HRMS m/z calcd for $C_{15}H_{24}O_3Na$ $(M+Na)^+$ 275.1623, found 275.1610.

(3*E*,5*E*)-6-[(1'*S*,2'*R*,4'*S*)-4'-Hydroxy-1',2'-epoxy-2',6',6'-trimethylcyclohex-1'-yl]-4-methylhexa-1,3,5-triene (6). A mixture of diene alcohol **11** (74 mg, 0.29 mmol) and manganese dioxide (1.17 g) in diethyl ether (2.35 mL) was stirred at room temperature for 20 min. The precipitate was filtered through a pad of Celite, and the filtrate was concentrated *in vacuo* to afford crude aldehyde, which was used in the next reaction without further purification.

To a suspension of methyltriphenylphosphonium bromide (314 mg, 0.88 mmol) in THF (1.32 mL) was added dropwise sodium bis(trimethylsilyl)amide (1.0M in THF, 0.88 mL, 0.88 mmol) at 0 ºC. After the mixture was stirred for 5 min at 0 ºC, a solution of the crude aldehyde obtained above in THF (0.30 mL) was added. After being stirred for 5 min at room temperature, the resulting mixture was poured into water, and extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 10% to 50% ethyl acetate in hexane) afforded triene **6** (47 mg, 72%) as a white solid: $[\alpha]^{25}_D$ –52.6 (c 0.77, $CHCl_3$); IR (KBr disk, cm^{-1}) 3451, 2963, 2929, 2367, 1655, 1560, 1420, 1381, 1217, 985, 906, 758; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.69 (dddd, *J* =17.0, 10.1, 6.4, 0.9 Hz, 1H), 6.25 (d, *J* =15.6, 1H), 6.09 (d, *J* =11.5 Hz, 1H), 5.89 (d, *J* =15.1 Hz, 1H), 5.25 (d, *J* =16.9 Hz, 1H), 5.14 (d, *J* =10.0 Hz, 1H), 3.90 (m, 1H), 2.37 (ddd, *J* =13.7, 5.1, 2.0 Hz, 1H), 1.88 (s, 3H), 1.62 (m, 2H), 1.24 (dd, *J* =12.8, 11.0 Hz, 1H), 1.18 (s, 3H), 1.14 (s, 3H), 0.97 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 137.4, 135.0, 133.4, 132.0, 124.8, 118.2, 70.5, 67.2, 64.6, 47.5, 41.3, 35.6, 29.9, 25.2, 20.3, 13.1; ESI-HRMS m/z calcd for $C_{16}H_{24}O_2Na$ $(M+Na)^+$ 271.1674, found 271.1662.

C30-violaxanthin derivative (3). To a solution of triene **6** (16 mg, 0.064 mmol) in toluene (0.65 mL) was added Grubbs second-generation catalyst (3 mg, 0.003 mmol). After being stirred for 15 min at 45 ºC, the reaction mixture was poured into water, and then extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 30% to 60%

ethyl acetate in hexane) afforded C30-violaxanthin derivative **3** (8 mg, 53%) as a yellow oil: $[\alpha]^{24}_{D}$ –47.4 (c 0.65, $CHCl_3$); IR (neat, cm^{-1}) 3570, 3451, 3019, 2964, 1660, 1626, 1215, 976, 758; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.58 (dd, *J* =7.8, 2.8 Hz, 1H), 6.27 (d, *J* =15.6, 1H), 6.19 (d, *J* =9.7 Hz, 1H), 5.89 (d, *J* =15.6 Hz, 1H), 3.90 (m, 1H), 2.38 (ddd, *J* =14.2, 5.0, 1.8 Hz, 1H), 1.90 (s, 3H), 1.62 (m, 2H), 1.22 (dd, *J* =12.8, 11.0 Hz, 1H), 1.18 (s, 3H), 1.14 (s, 3H), 0.97 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 137.4, 135.0, 133.4, 132.0, 124.8, 118.2, 70.5, 67.2, 64.6, 47.5, 41.3, 35.6, 29.9, 25.2, 20.3, 13.1; ESI-HRMS m/z calcd for $C_{30}H_{44}O_4Na$ $(M+Na)^+$ 491.3137, found 491.3151.

(2*E*,4*E*,6*E*)-7-(Tributylstannyl)-3,7-dimethylhexa-2,4,6-triene-1-ol (13). To a solution of ester **12** (2.08 g, 4.44 mmol) in dichloromethane (44.4 mL) was added dropwise diisobutylaluminium hydride (1.0 M in toluene, 13.3 mL, 13.3 mmol) at –78 °C. After the reaction mixture was stirred for 10 min at the same temperature, aqueous potassium sodium (+)-tartrate tetrahydrate solution was added, and then resulting mixture was extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 10% to 30% ethyl acetate in hexane in 3% triethyl amine) afforded alcohol **13** (1.60 g, 84%) as a yellow oil: IR (neat, cm^{-1}) 3393, 2853, 1714, 1616, 1464, 1373, 1253, 1072, 960, 758; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.63 (dd, *J* =15.1, 10.5 Hz, 1H), 6.26 (dd, *J* =11.0, 1.4 Hz, 1H), 6.21 (d, *J* =15.6 Hz, 1H), 5.70 (t, *J* =6.9 Hz, 1H), 4.31 (t, *J* =5.9 Hz, 2H), 2.03 (d, *J* =1.4 Hz, 3H), 1.84 (s, 3H), 1.49 (m, 6H), 1.31 (m, 6H), 0.90 (m, 15H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 145.5, 139.5, 137.4, 136.0, 130.3, 123.5, 59.9, 29.5, 27.8, 20.4, 14.1, 13.0, 9.5.

(2*E*,4*E*,6*E*,8*E*)-9-[(1'*S*,2'*R*,4'*S*)-4'-Hydroxy-1',2'-epoxy-2',6',6'-trimethylcyclohexa-1'-yl]-3,7-dimethylnona-2,4,6,8-tetraene-1-ol (14). To a solution of vinyl iodide **9** (308 mg, 0.99 mmol) and stannane **13** (470 mg, 1.10 mmol) in DMF (5.0 mL) was added diisopropylethylamine (0.52 mL, 3.00 mmol), $Pd(PPh_3)_4$ (58 mg, 0.050 mmol) and lithium chloride (84 mg, 2.00 mmol). After being stirred for 30 min at 65 °C, the reaction mixture was poured into water, and then extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 30% to 50% ethyl acetate in hexane) afforded **14** (202 mg, 64%) as a white solid: $[\alpha]^{25}_{D}$ –26.4 (c 0.99, MeOH); IR (KBr disk, cm^{-1}) 3449, 2963, 2870, 1695, 1466, 1303, 1184, 1122, 1047, 953, 914; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.54 (dd, *J* =15.1, 11.0

Hz, 1H), 6.28 (d, *J* =15.1, 1H), 6.25 (d, *J* =14.9 Hz, 1H), 6.12 (d, *J* =11.5 Hz, 1H), 5.85 (d, *J* =15.6 Hz, 1H), 5.68 (t, *J* =6.9 Hz, 1H), 4.28 (d, *J* =6.8 Hz, 2H), 3.87 (m, 1H), 2.35 (ddd, *J* =14.2, 5.1, 1.9 Hz, 1H), 1.89 (s, 3H), 1.83 (s, 3H), 1.59 (m, 2H), 1.21 (dd, *J* =12.9, 10.6 Hz, 1H), 1.16 (s, 3H), 1.12 (s, 3H), 0.95 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 137.7, 137.5, 137.0, 134.8, 131.9, 131.0, 125.1, 124.3, 70.6, 67.3, 64.6, 59.8, 47.5, 41.3, 35.6, 29.9, 25.2, 20.3, 13.3, 13.0; ESI-HRMS m/z calcd for $C_{20}H_{30}O_3Na$ $(M+Na)^+$ 341.2093, found 341.2079.

(3*E*,5*E*,7*E*,9*E*)-10-[(1'*S*,2'*R*,4'*S*)-4'-Hydroxy-1',2'-epoxy-2',6',6'-trimethylcyclohex-1'-yl]-4,8-dimethyldeca-1,3,5,7,9-pentaene (4). A mixture of alcohol **14** (129 mg, 0.41 mmol) and manganese dioxide (1.62 g) in THF (3.24 mL) was stirred at room temperature for 50 min. The precipitate was filtered through a pad of Celite, and the filtrate was concentrated *in vacuo* to afford crude aldehyde, which was used in the next reaction without further purification.

To a suspension of methyltriphenylphosphonium bromide (434 mg, 1.22 mmol) in THF (2.03 mL) was added dropwise sodium bis(trimethylsilyl)amide (1.0M in THF, 1.22 mL, 1.22 mmol) at 0 ºC. The mixture was stirred for 5 min at -20 ºC, and then a solution of crude aldehyde in THF (0.30 mL) was added. After being stirred for 5 min at the same temperature, the resulting mixture was poured into water, and extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 20% to 50% ethyl acetate in hexane) afforded pentaene **4** (89 mg, 70%) as a yellow solid: $[\alpha]^{24}_D$ –14.9 (c 0.20, $CHCl_3$); IR (KBr disk, cm^{-1}) 3449, 3017, 2929, 1655, 1381, 1215, 1045, 908, 758; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.71 (dddd, *J* =16.5, 11.5, 10.1, 1.4 Hz, 1H), 6.59 (d, *J* =15.1, 11.0 Hz, 1H), 6.33 (d, *J* =15.1 Hz, 1H), 6.28 (d, *J* =15.5 Hz, 1H), 6.17 (d, *J* =11.4 Hz, 1H), 6.13 (d, *J* =11.0 Hz, 1H), 5.87 (d, *J* =15.5 Hz, 1H), 5.26 (d, *J* =16.5 Hz, 1H), 5.14 (d, *J* =10.0 Hz, 1H), 3.90 (m, 1H), 2.37 (ddd, *J* =14.2, 5.0, 1.8 Hz, 1H), 1.92 (s, 3H), 1.91 (s, 3H), 1.62 (m, 2H), 1.21 (dd, *J* =12.9, 10.6 Hz, 1H), 1.18 (s, 3H), 1.14 (s, 3H), 0.97 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.3, 137.6, 136.5, 134.6, 133.6, 132.6, 132.3, 125.2, 124.2, 118.1, 70.6, 67.3, 64.6, 60.7, 53.8, 47.5, 41.3, 35.7, 29.9, 25.2, 21.3, 20.3, 14.5, 13.3, 13.0; ESI-HRMS m/z calcd for $C_{21}H_{30}O_2Na$ $(M+Na)^+$ 337.2143, found 337.2150.

Violaxanthin (1). To a solution of pentaene **4** (27 mg, 0.086 mmol) in toluene (0.86 mL) was added Grubbs second-generation catalyst (7 mg, 0.0086 mmol). After being stirred for 10 min at 60 ºC, the reaction mixture was poured into water, and then extracted with ethyl acetate. The

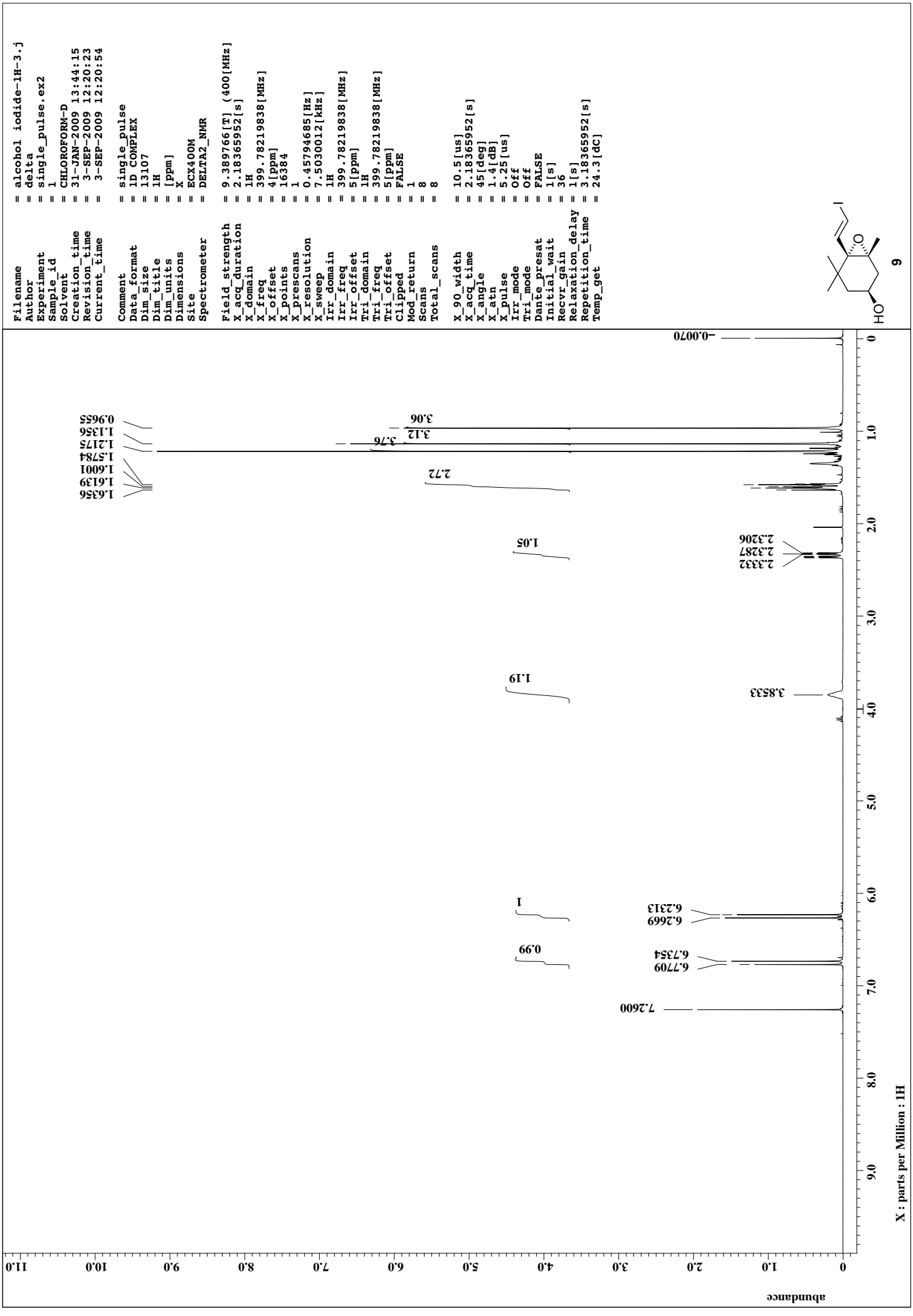
organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 30% to 60% ethyl acetate in hexane) afforded violaxanthin (**1**) (16 mg, 67%) as a crude product in a red film. The separation by preparative HPLC [column: Develosil CN-UG (0.6 x 25 cm); mobile phase: acetone / *n*-hexane = 1 / 11; flow rate: 2.0 mL / min.; UV detect: 470 nm; retention time: (all-*trans*-isomer) 40 min., in the dark, was afforded the desired optically active violaxanthin (**1**) as a red film: IR (neat, cm^{-1}) 3467, 3019, 2928, 1901, 1630, 1469, 1368, 1215, 972, 756; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.63 (m, 1H), 6.60 (dd, *J* =15.1, 11.4, 1H), 6.37 (d, *J* =15.1 Hz, 1H), 6.29 (d, *J* =15.1 Hz, 1H), 6.28 (m, 1H), 6.19 (d, *J* =11.0 Hz, 1H), 5.88 (d, *J* =15.6 Hz, 1H), 3.91 (m, 1H), 2.39 (ddd, *J* =14.2, 5.1, 1.4 Hz, 1H), 1.96 (s, 3H), 1.93 (s, 3H), 1.61 (m, 2H), 1.23 (m, 1H), 1.19 (s, 3H), 1.15 (s, 3H), 0.98 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.5, 137.7, 136.8, 134.7, 133.2, 132.6, 130.5, 125.1, 124.2, 70.7, 67.3, 64.7, 60.8, 47.6, 41.4, 35.7, 29.9, 25.3, 20.4, 14.6, 13.3, 13.1; ESI-HRMS m/z calcd for $C_{40}H_{56}O_4Na$ $(M+Na)^+$ 623.4076, found 623.4073.

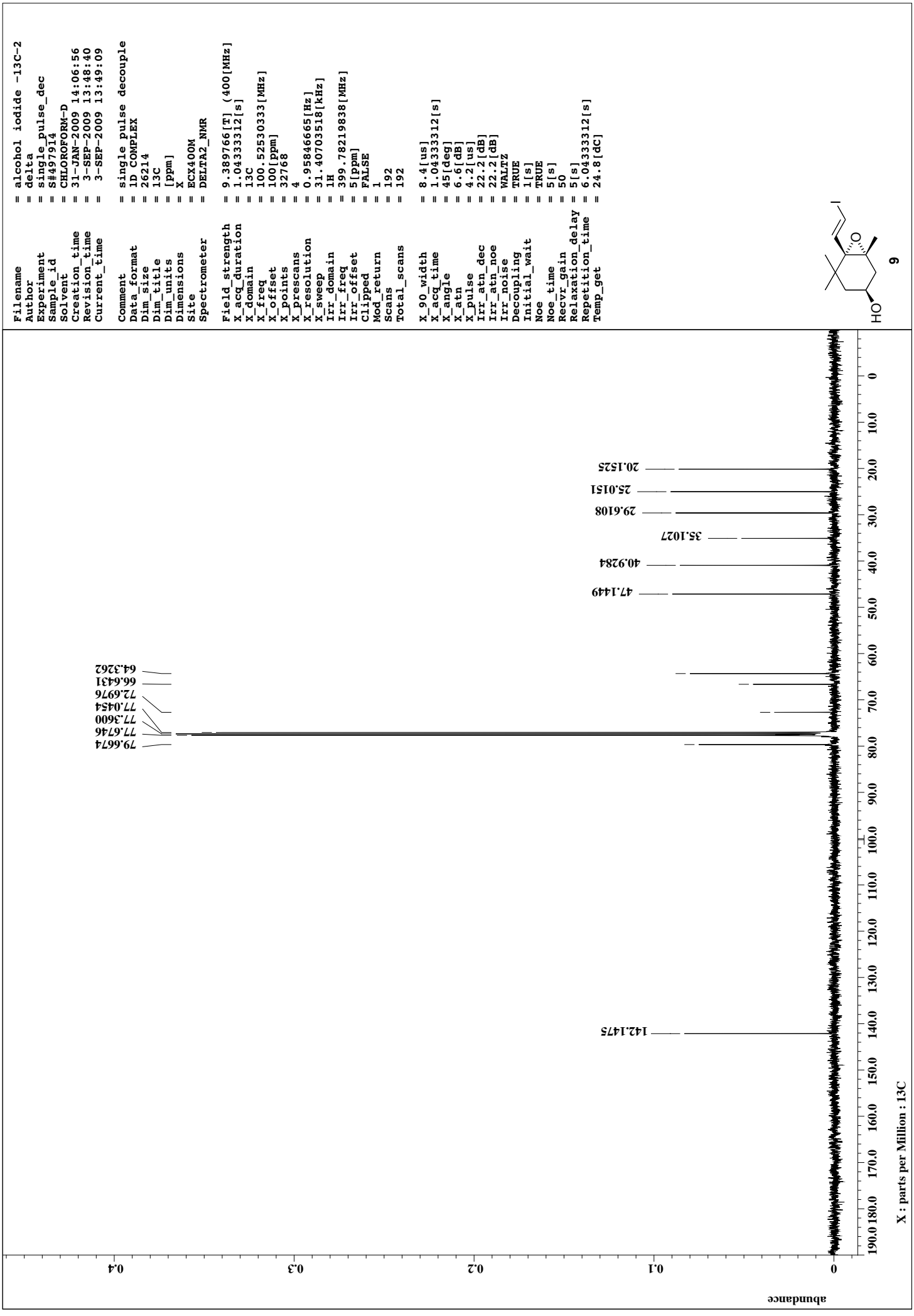
(3E, 5E, 7E)-10-[(1'R,2'R,4'S)-2',4'-Dihydroxy-2',6',6'-trimethylcyclohexylidene]-4,8-dimethyldeca-1,3,5,7,9-pentaene (5). A mixture of allenic alcohol **15** (165 mg, 0.52 mmol) and manganese dioxide (2.07 g) in ethyl acetate (5.18 mL) was stirred at room temperature for 20 min. The precipitate was filtered through a pad of Celite, and the filtrate was concentrated *in vacuo* to afford crude aldehyde, which was used in the next reaction without further purification.

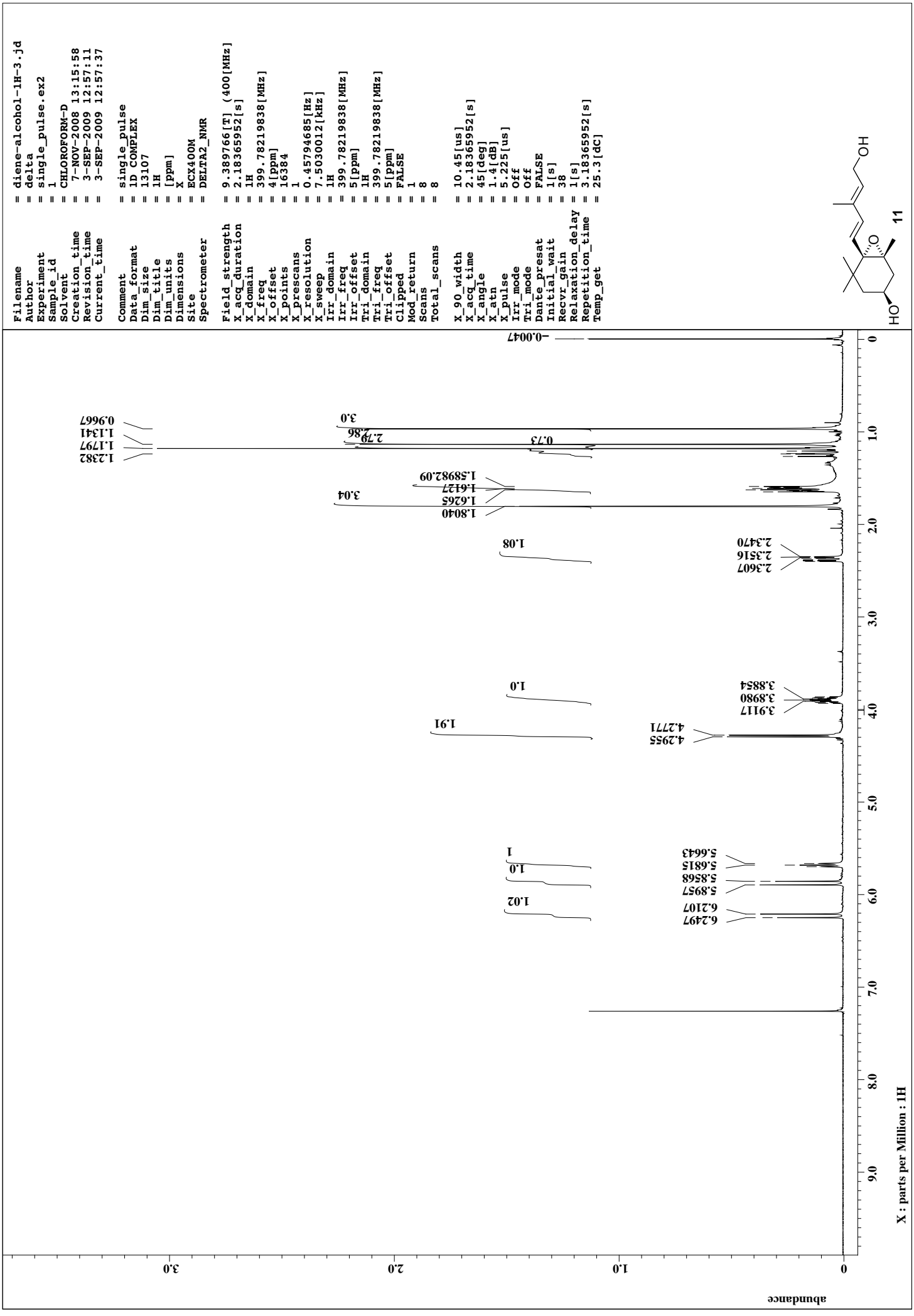
To a suspension of methyltriphenylphosphonium bromide (195 mg, 0.54 mmol) in THF (1.10 mL) was added dropwise sodium bis(trimethylsilyl)amide (1.0M in THF, 0.53 mL, 0.53 mmol) at 0 ºC. The mixture was stirred for 5 min at 0 ºC, and then a solution of crude aldehyde (69 mg, 0.22 mmol) in THF (0.30 mL) was added. After being stirred for 10 min at the same temperature, the resulting mixture was poured into water, and extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 20% to 50% ethyl acetate in hexane) afforded **5** (30 mg, 44%) as a yellow solid: $[\alpha]^{24}_D$ –28.1 (c 0.57 $CHCl_3$); IR (KBr disk, cm^{-1}) 3335, 2926, 1929, 1455, 1439, 1375, 1161, 956; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.72 (dddd, *J* =16.5, 10.9, 10.1, 1.4 Hz, 1H), 6.45 (dd, *J* =15.1, 11.4 Hz, 1H), 6.30 (d, *J* =15.1 Hz, 1H), 6.12 (d, *J* =10.5 Hz, 1H), 6.09 (d, *J* =10.5 Hz, 1H), 6.02 (s, 1H), 5.26 (d, *J* =16.5 Hz, 1H), 5.14 (d, *J* =10.6 Hz, 1H), 4.13 (m, 1H), 2.26 (ddd, *J* =12.8, 4.1, 2.2 Hz, 1H), 2.00 (m, 1H), 1.93 (m, 1H), 1.92 (s, 3H), 1.79 (s, 3H), 1.35 (s, 3H), 1.33 (s, 3H), 1.06 (s, 3H); ^{13}C NMR (CD_3OD, 100 MHz) δ 204.4, 138.9, 138.2, 135.4, 134.1, 133.8, 130.0, 127.2, 119.3, 118.6, 104.6, 74.0, 65.6, 37.5,

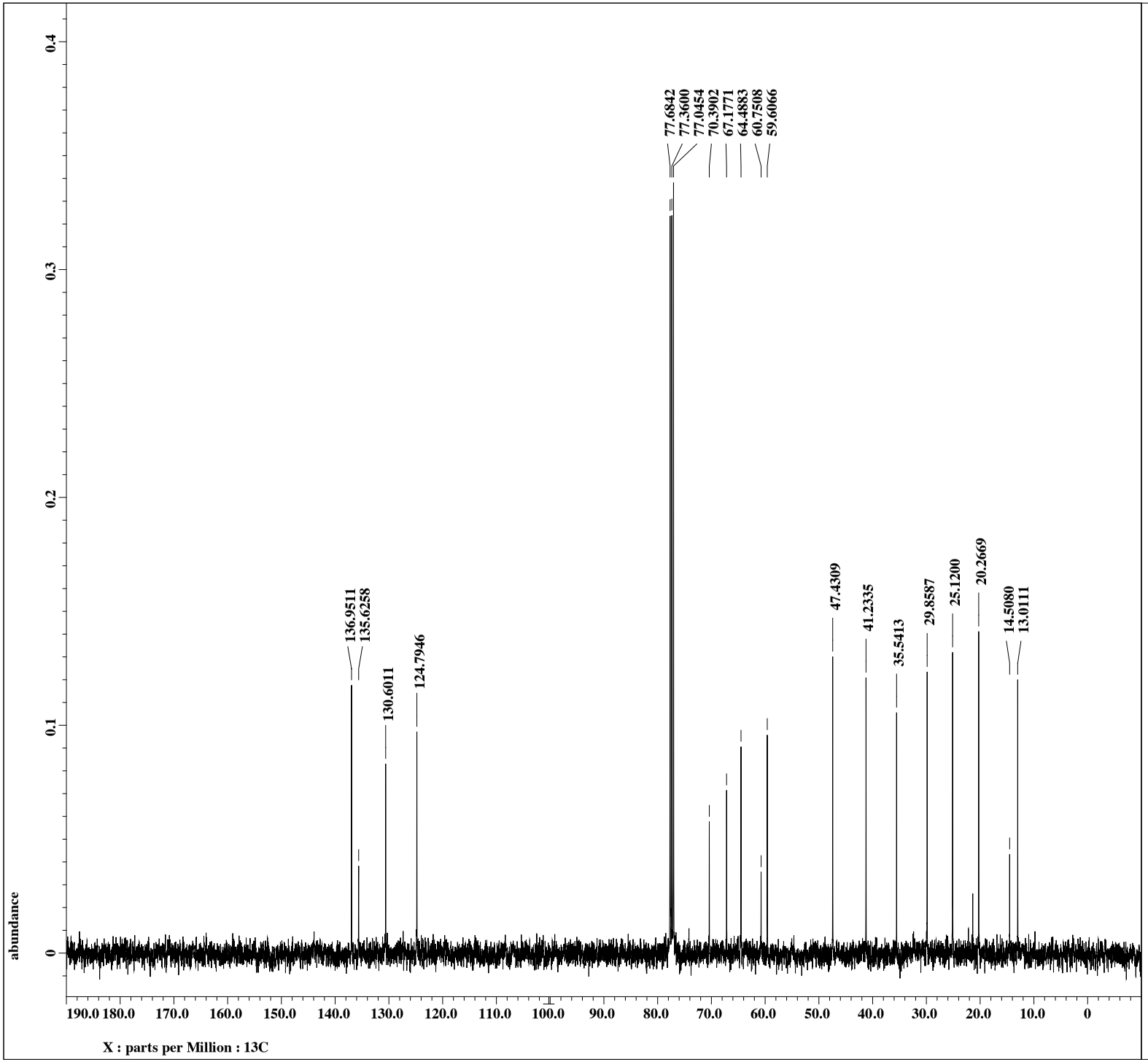
33.8, 32.2, 30.4, 15.0, 13.5; ESI-HRMS m/z calcd for $C_{21}H_{30}O_2Na$ $(M+Na)^+$ 337.2143, found 337.2139.

Mimulaxanthin (2). To a solution of allenic tetraene **5** (31 mg, 0.099 mmol) in toluene (1.91 mL) was added Grubbs second-generation catalyst (4 mg, 0.0048 mmol) at 4 times at 5 min intervals. After being stirred for 5 min at 60 °C, the reaction mixture was poured into water, and then extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification by silica gel column chromatography (from 50% ethyl acetate in hexane to 15% methanol in chloroform) afforded mimulaxanthin (**2**) (17 mg, 56%) as a crude product in a red film. The separation by preparative HPLC [column: Develosil CN-UG (0.6 x 25 cm); mobile phase: acetone / *n*-hexane = 1 / 6; flow rate: 2.0 mL / min.; UVdetect: 468 nm; retention time: (all-*trans*-isomer) 49 min., in the dark, was afforded the desired optically active mimulaxanthin (**2**) as a red film: IR (KBr disk, cm^{-1}) 3449, 2926, 2372, 1655, 1458, 1263, 1070, 958; ^1H NMR (CD_3OD, 400 MHz) δ 6.67 (dd, *J* =7.2, 2.7 Hz, 1H), 6.60 (dd, *J* =15.1, 11.4, 1H), 6.35 (d, *J* =15.1 Hz, 1H), 6.27 (d, *J* =10.1 Hz, 1H), 6.12 (d, *J* =8.2 Hz, 1H), 6.04 (s, 1H), 4.20 (m, 1H), 2.19 (m, 1H), 1.96 (s, 3H), 1.87 (m, 2H), 1.82 (s, 3H), 1.33 (s, 3H), 1.30 (s, 3H), 1.06 (s, 3H); ^{13}C NMR (CD_3OD, 100 MHz) δ 204.6, 139.2, 138.3, 134.5, 133.9, 132.1, 130.3, 126.9, 119.3, 104.7, 74.0, 65.6, 37.5, 33.8, 32.2, 30.4, 28.7, 28.5, 28.1, 15.0, 13.5; ESI-HRMS m/z calcd for $C_{40}H_{56}O_4Na$ $(M+Na)^+$ 623.4076, found 623.4063.

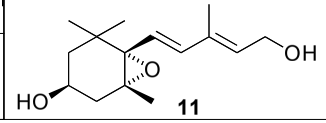

Filename = alcohol iodide-1H-3.j
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 31-JAN-2009 13:44:15
Revision_time = 3-SEP-2009 12:20:23
Current_time = 3-SEP-2009 12:20:54
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.3[dC]
I
O
HO
9
abundance
X : parts per Million : 1H
-0.0070
7.2600
6.7709
6.7354
6.2669
6.2313
3.8533
2.3332
2.3287
2.3206
1.6356
1.6139
1.6001
1.5784
1.2175
1.1356
0.9655
3.76
3.12
3.06
2.72
1.19
1.05
0.99
1


Filename = alcohol iodide -13C-2
Author = delta
Experiment = single_pulse_dec
Sample_id = S#497914
Solvent = CHLOROFORM-D
Creation_time = 31-JAN-2009 14:06:56
Revision_time = 3-SEP-2009 13:48:40
Current_time = 3-SEP-2009 13:49:09
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 192
Total_scans = 192
X_90_width = 8.4[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.2[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.8[dC]
I
O
HO
9
abundance
0
0.1
0.2
0.3
0.4
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C
142.1475
79.6674
77.6746
77.3600
77.0454
72.6976
66.6431
64.3262
47.1449
40.9284
35.1027
29.6108
25.0151
20.1525

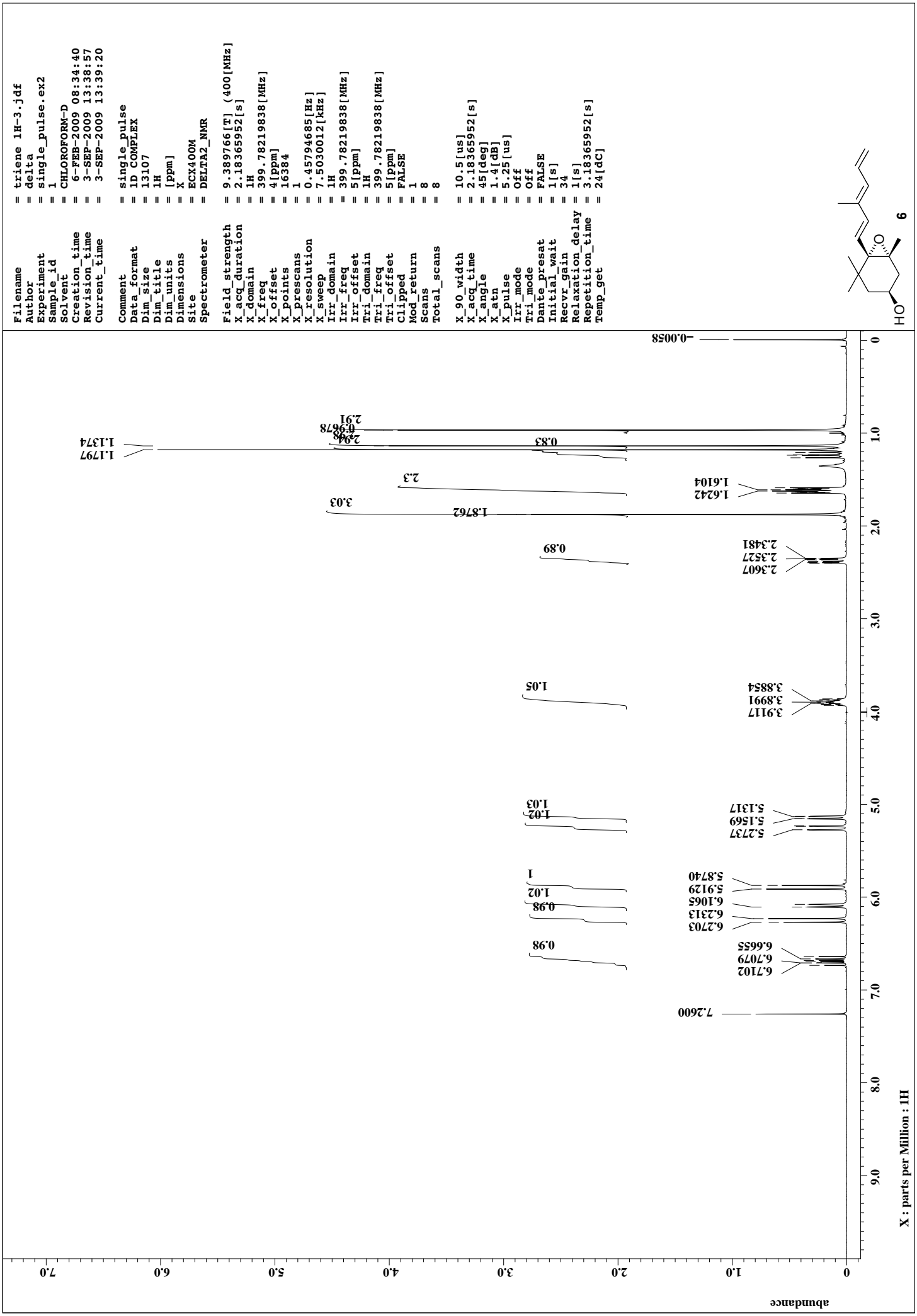

Filename = diene-alcohol-1H-3.jd
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 7-NOV-2008 13:15:58
Revision_time = 3-SEP-2009 12:57:11
Current_time = 3-SEP-2009 12:57:37
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.45[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.225[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 25.3[dC]
OH
HO
11
-0.0047
0.9667
1.1341
1.1797
1.2382
3.0
2.79
2.86
0.73
1.58982.09
1.6127
1.6265
1.8040
3.04
1.08
2.3470
2.3516
2.3607
1.0
3.8854
3.8980
3.9117
1.91
4.2771
4.2955
1.0
1.0
5.6643
5.6815
5.8568
5.8957
1.02
6.2107
6.2497
abundance
X : parts per Million : 1H

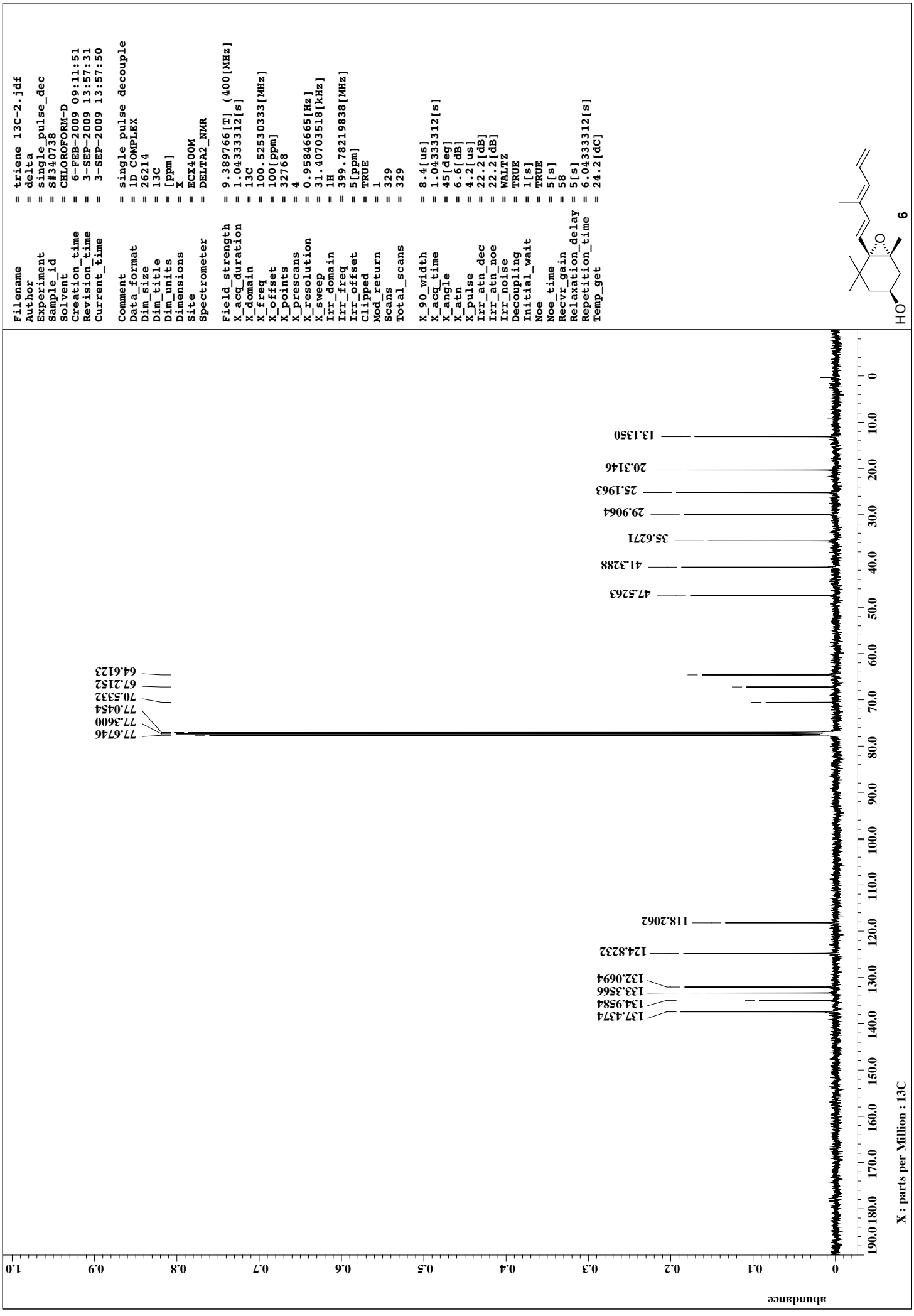


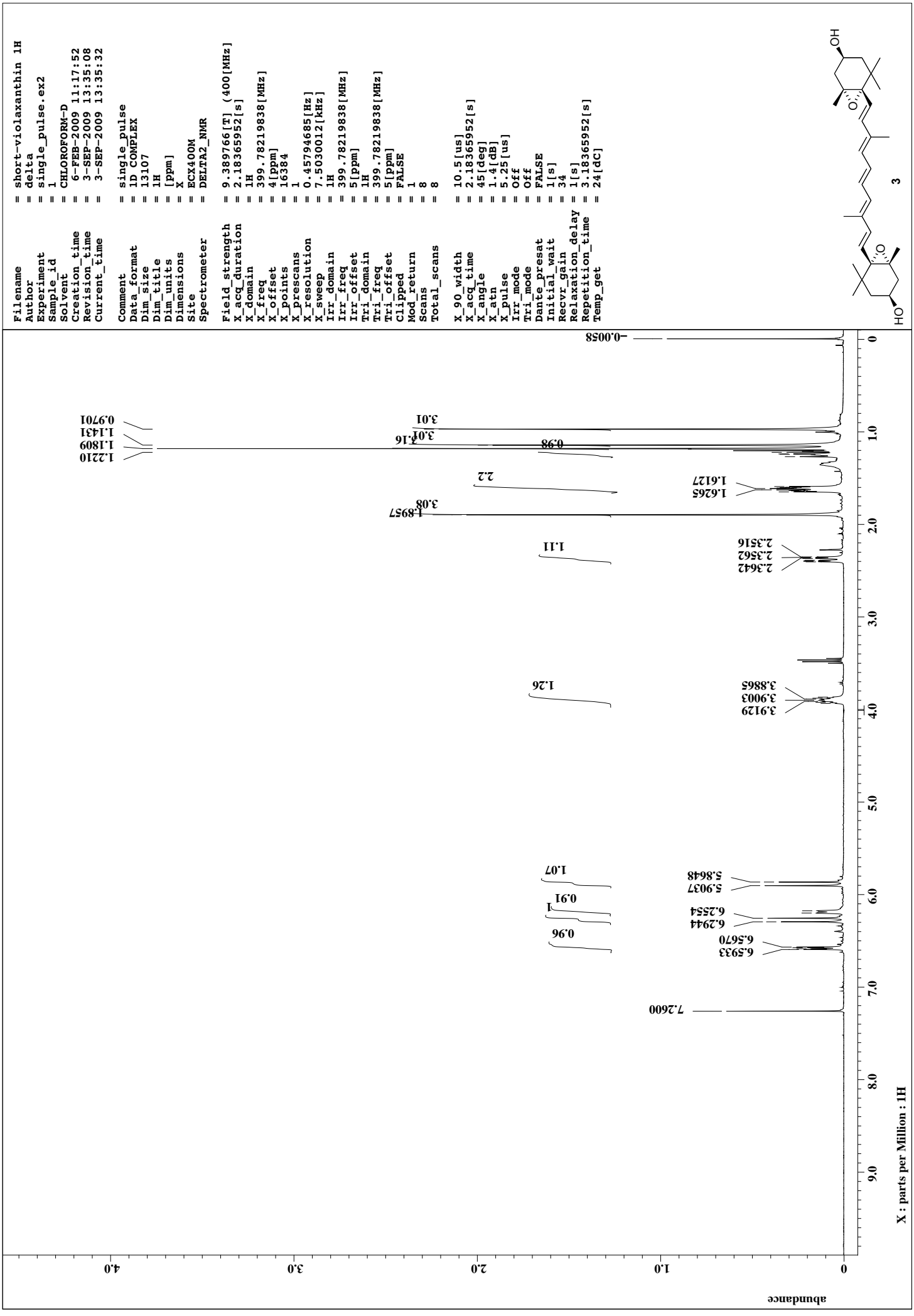

```
Filename          = diene-alcohol-13C-3.j
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#377181
Solvent           = CHLOROFORM-D
Creation_time     =  5-FEB-2009 09:43:06
Revision_time     =  3-SEP-2009 13:53:39
Current_time      =  3-SEP-2009 13:54:00

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX400M
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 42
Total_scans       = 42

X_90_width        = 8.4[us]
X_acq_time        = 1.04333312[s]
X_angle           = 45[deg]
X_atn             = 6.6[dB]
X_pulse           = 4.2[us]
Irr_atn_dec       = 22.2[dB]
Irr_atn_noe       = 22.2[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 5[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.04333312[s]
Temp_get          = 24.4[dC]
```

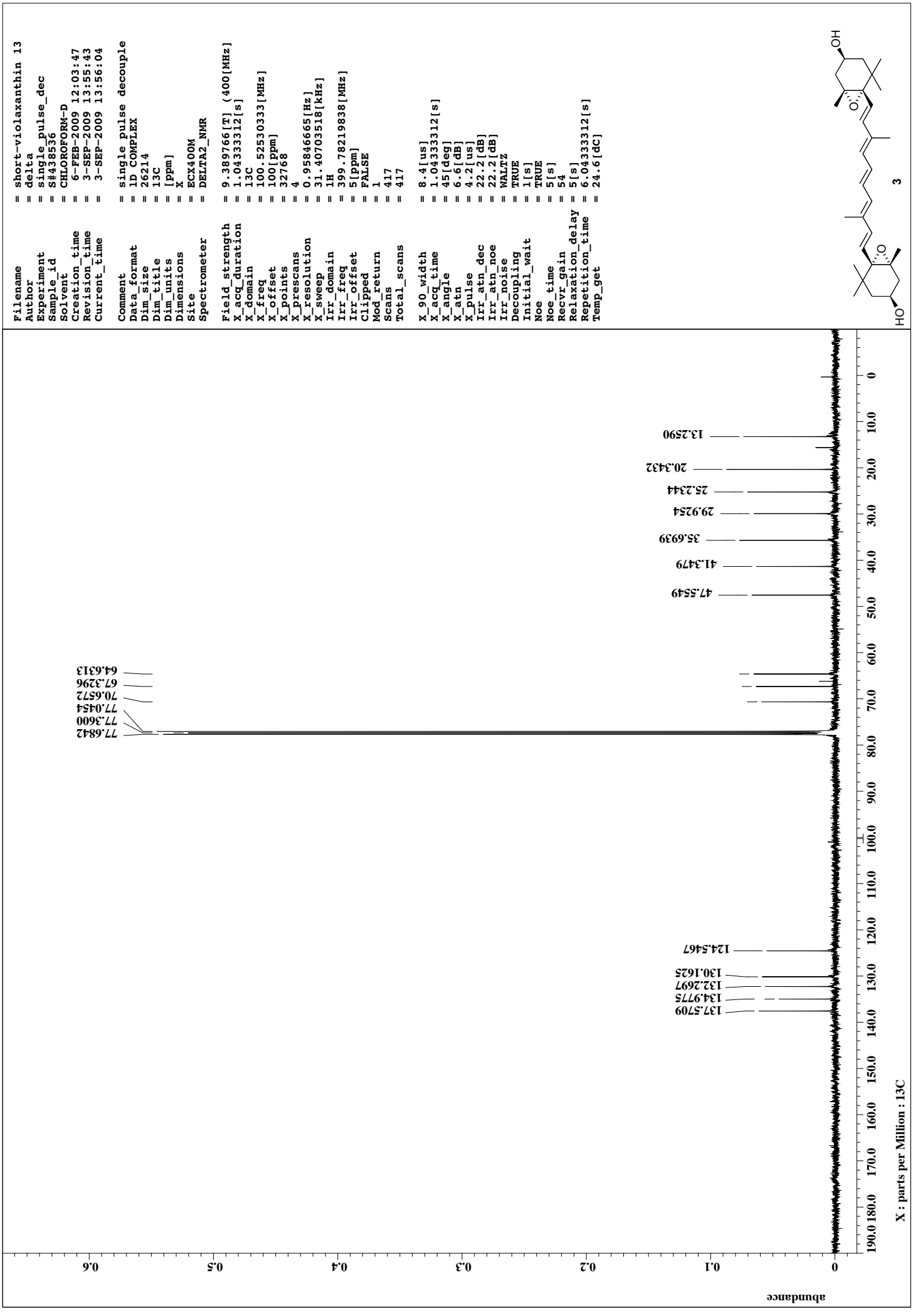


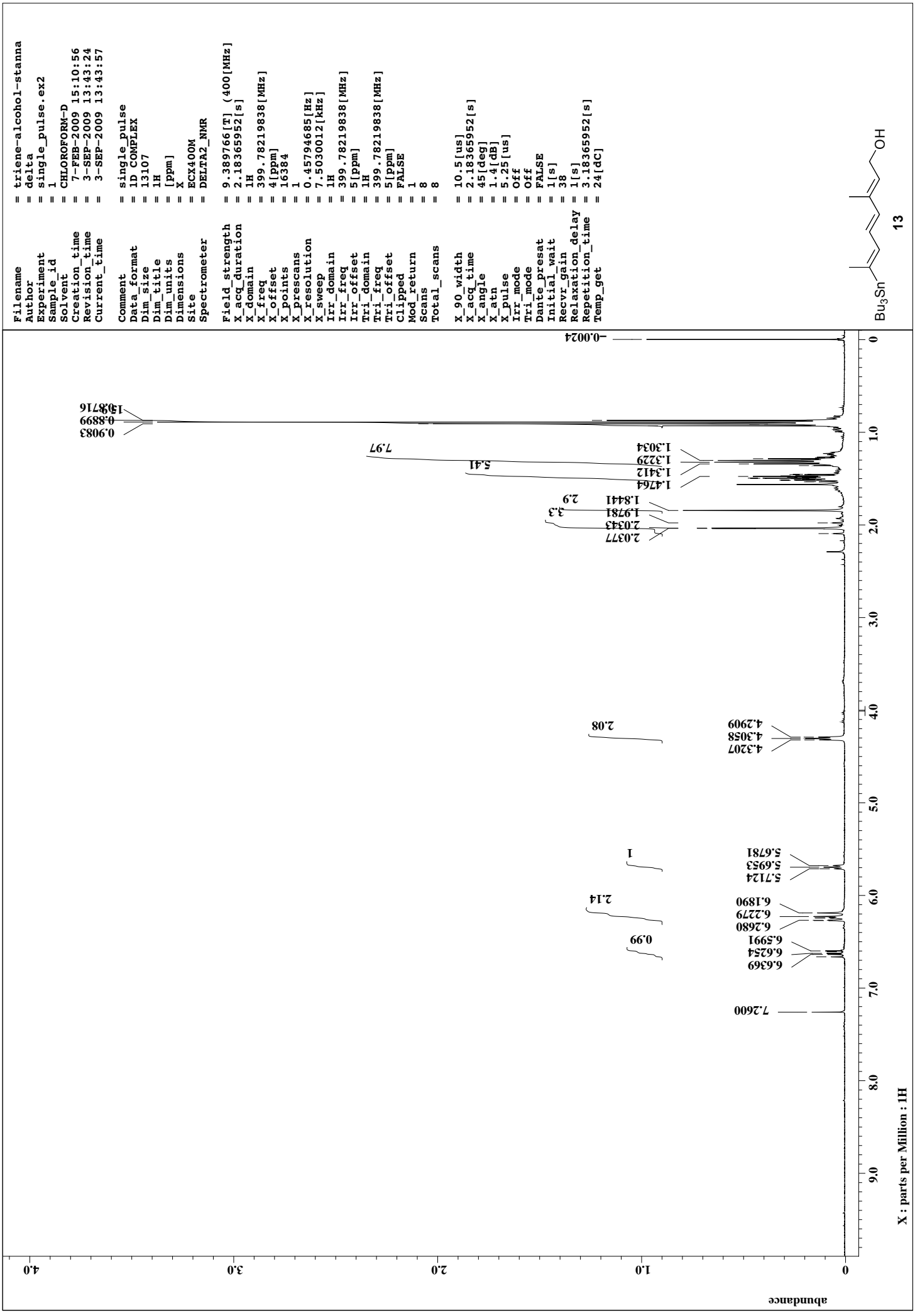
11

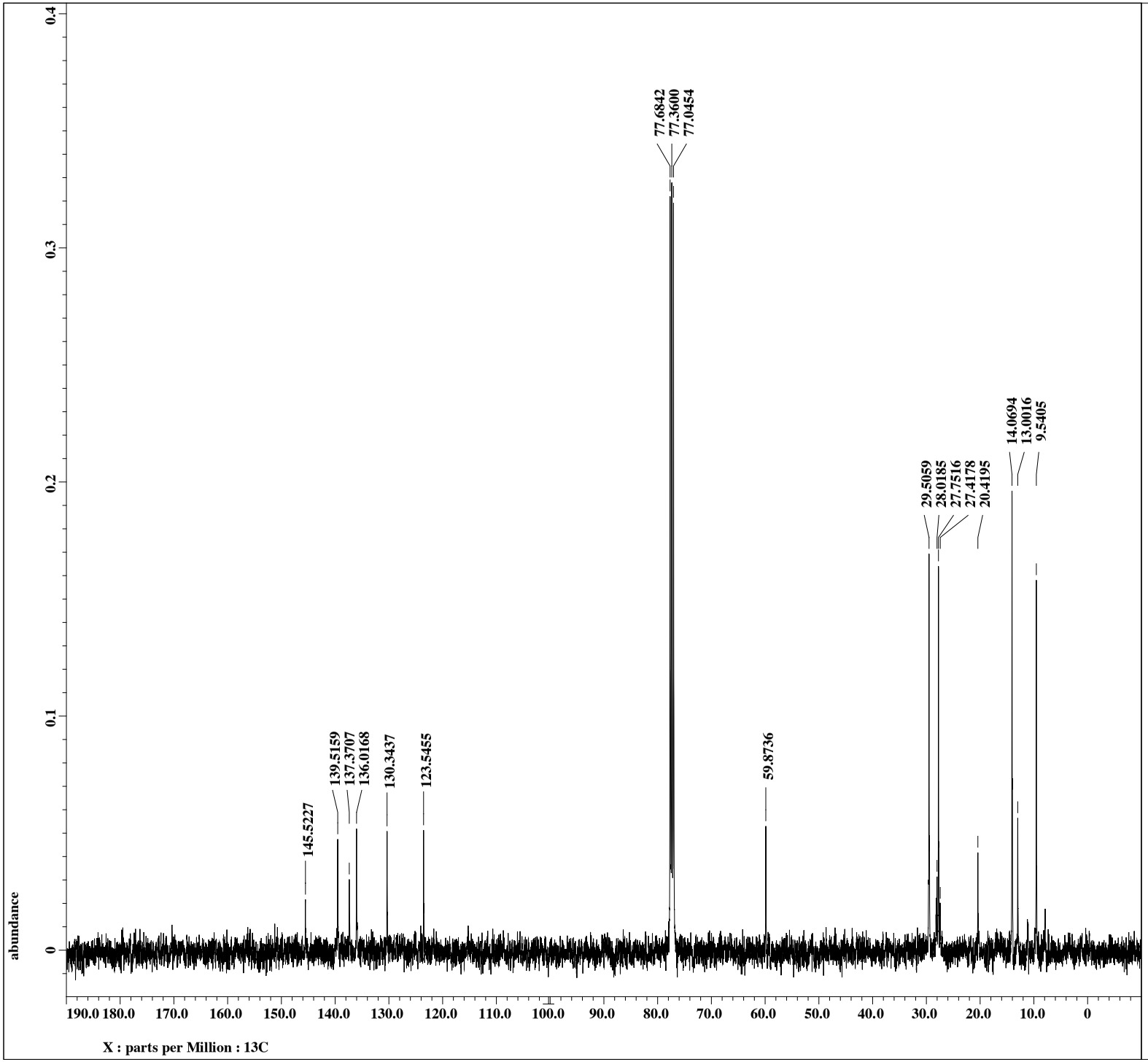

Filename = triene 1H-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 6-FEB-2009 08:34:40
Revision_time = 3-SEP-2009 13:38:57
Current_time = 3-SEP-2009 13:39:20
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24[dC]
HO
6
abundance
X : parts per Million : 1H
-0.0058
7.2600
6.7102
6.7079
6.6655
6.2703
6.2313
6.1065
5.9129
5.8740
5.2737
5.1569
5.1317
3.9117
3.8991
3.8854
2.3607
2.3527
2.3481
1.6242
1.6104
1.8762
3.03
2.3
0.89
1.05
1.02
1.03
0.98
0.98
1
0.83
2.94
2.91
1.1797
1.1374


Filename = triene 13C-2.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = S#340738
Solvent = CHLOROFORM-D
Creation_time = 6-FEB-2009 09:11:51
Revision_time = 3-SEP-2009 13:57:31
Current_time = 3-SEP-2009 13:57:50
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = TRUE
Mod_return = 1
Scans = 329
Total_scans = 329
X_90_width = 8.4[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.2[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 58
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.2[dC]
HO
6
abundance
X : parts per Million : 13C
13.1350
20.3146
25.1963
29.9064
35.6271
41.3288
47.5263
64.6123
67.2152
70.5332
77.0454
77.3600
77.6746
118.2062
124.8232
132.0694
133.3566
134.9584
137.4374

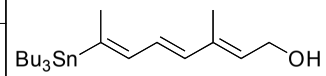

Filename = short-violaxanthin 1H
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 6-FEB-2009 11:17:52
Revision_time = 3-SEP-2009 13:35:08
Current_time = 3-SEP-2009 13:35:32
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 34
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24[dC]
OH
O
O
HO
3
-0.0058
7.2600
6.5933
6.5670
6.2944
6.2554
5.9037
5.8648
3.9129
3.9003
3.8865
2.3642
2.3562
2.3516
1.6265
1.6127
1.8957
3.08
2.2
0.98
3.16
3.01
3.01
1.2210
1.1809
1.1431
0.9701
1.07
0.91
1
0.96
1.26
1.11
abundance
X : parts per Million : 1H


Filename = short-violaxanthin 13
Author = delta
Experiment = single_pulse_dec
Sample_id = S#438536
Solvent = CHLOROFORM-D
Creation_time = 6-FEB-2009 12:03:47
Revision_time = 3-SEP-2009 13:55:43
Current_time = 3-SEP-2009 13:56:04
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 417
Total_scans = 417
X_90_width = 8.4[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.2[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 54
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.6[dC]
OH
O
O
HO
3
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
137.5709
134.9775
132.2697
130.1625
124.5467
77.6842
77.3600
77.0454
70.6572
67.3296
64.6313
47.5549
41.3479
35.6939
29.9254
25.2344
20.3432
13.2590

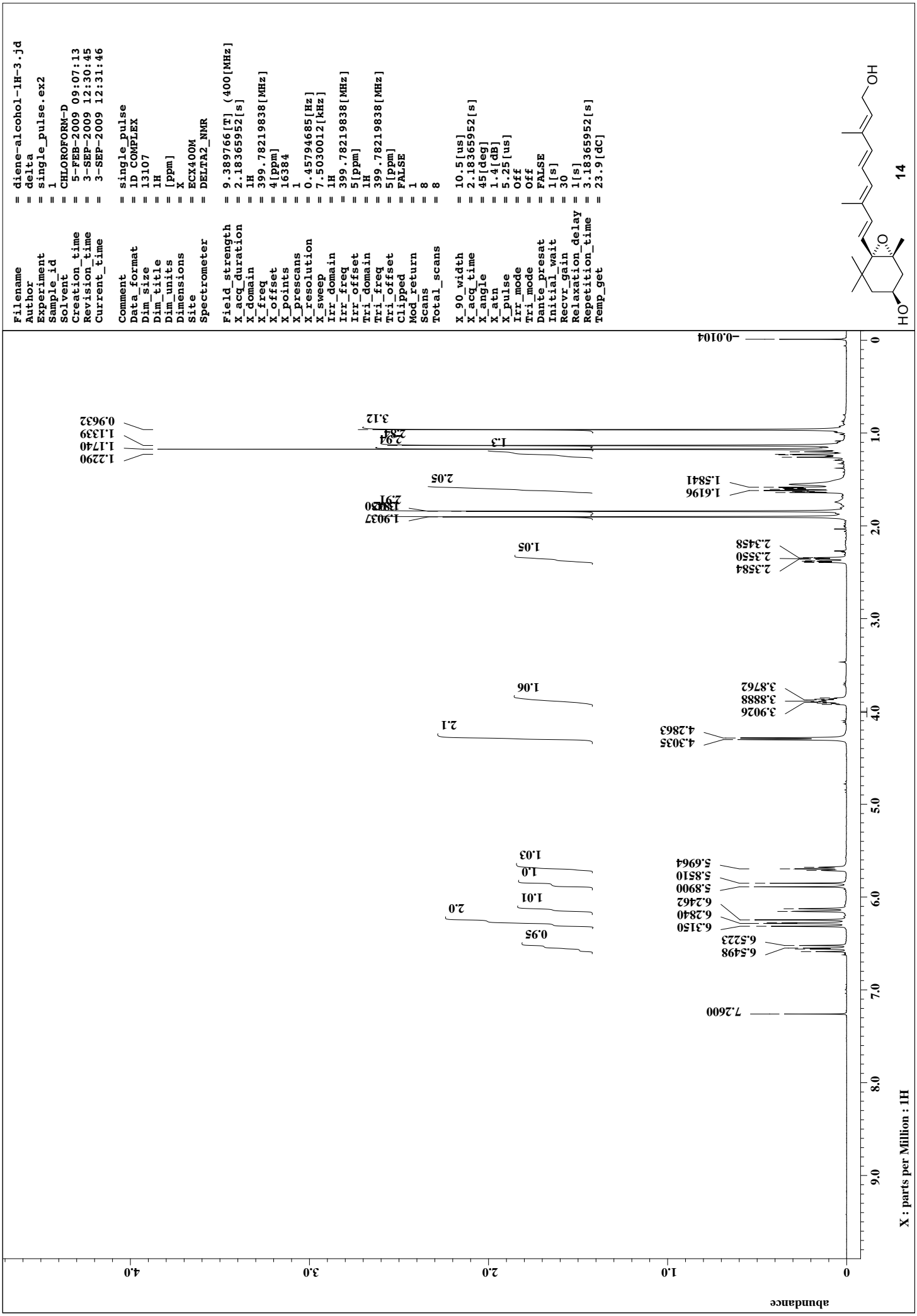

Filename = triene-alcohol-stanna
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 7-FEB-2009 15:10:56
Revision_time = 3-SEP-2009 13:43:24
Current_time = 3-SEP-2009 13:43:57
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24[dC]
OH
Bu3Sn
13
abundance
X : parts per Million : 1H
-0.0024
0.9083
0.8899
15.8716
7.97
5.41
1.3034
1.3229
1.3412
1.4764
1.8441
2.9
1.9781
3.3
2.0343
2.0377
4.3207
4.3058
4.2909
2.08
5.6781
5.6953
5.7124
1
6.1890
6.2279
6.2680
2.14
6.5991
6.6254
6.6369
0.99
7.2600

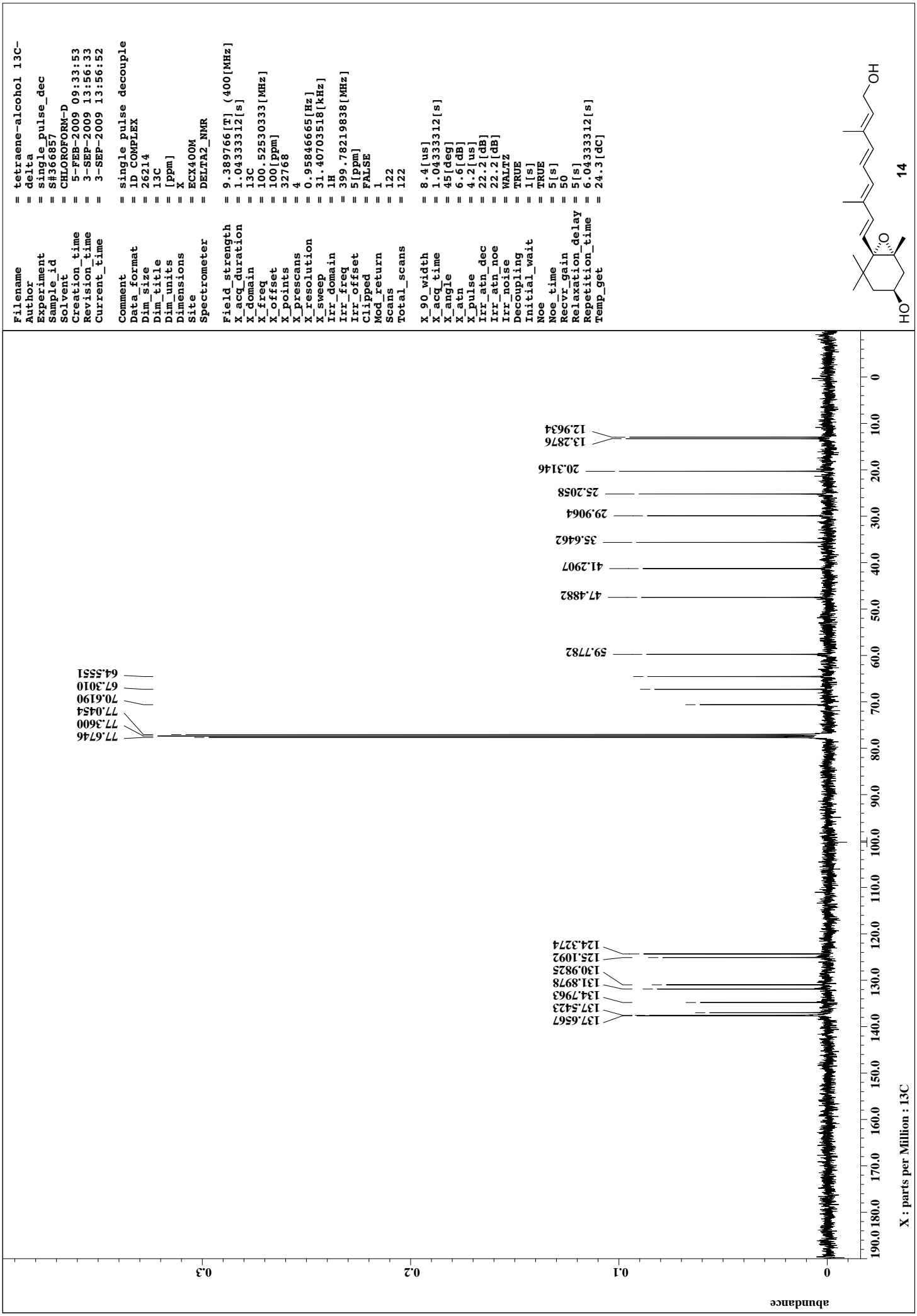



```
Filename          = triene-alcohol-stanna
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#521216
Solvent           = CHLOROFORM-D
Creation_time     =  7-FEB-2009 14:12:12
Revision_time     =  3-SEP-2009 13:58:52
Current_time      =  3-SEP-2009 13:59:13

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX400M
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 330
Total_scans       = 330

X_90_width        = 8.4[us]
X_acq_time        = 1.04333312[s]
X_angle           = 45[deg]
X_atn             = 6.6[dB]
X_pulse           = 4.2[us]
Irr_atn_dec       = 22.2[dB]
Irr_atn_noe       = 22.2[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 5[s]
Recvr_gain        = 60
Relaxation_delay  = 5[s]
Repetition_time   = 6.04333312[s]
Temp_get          = 24.2[dC]
```

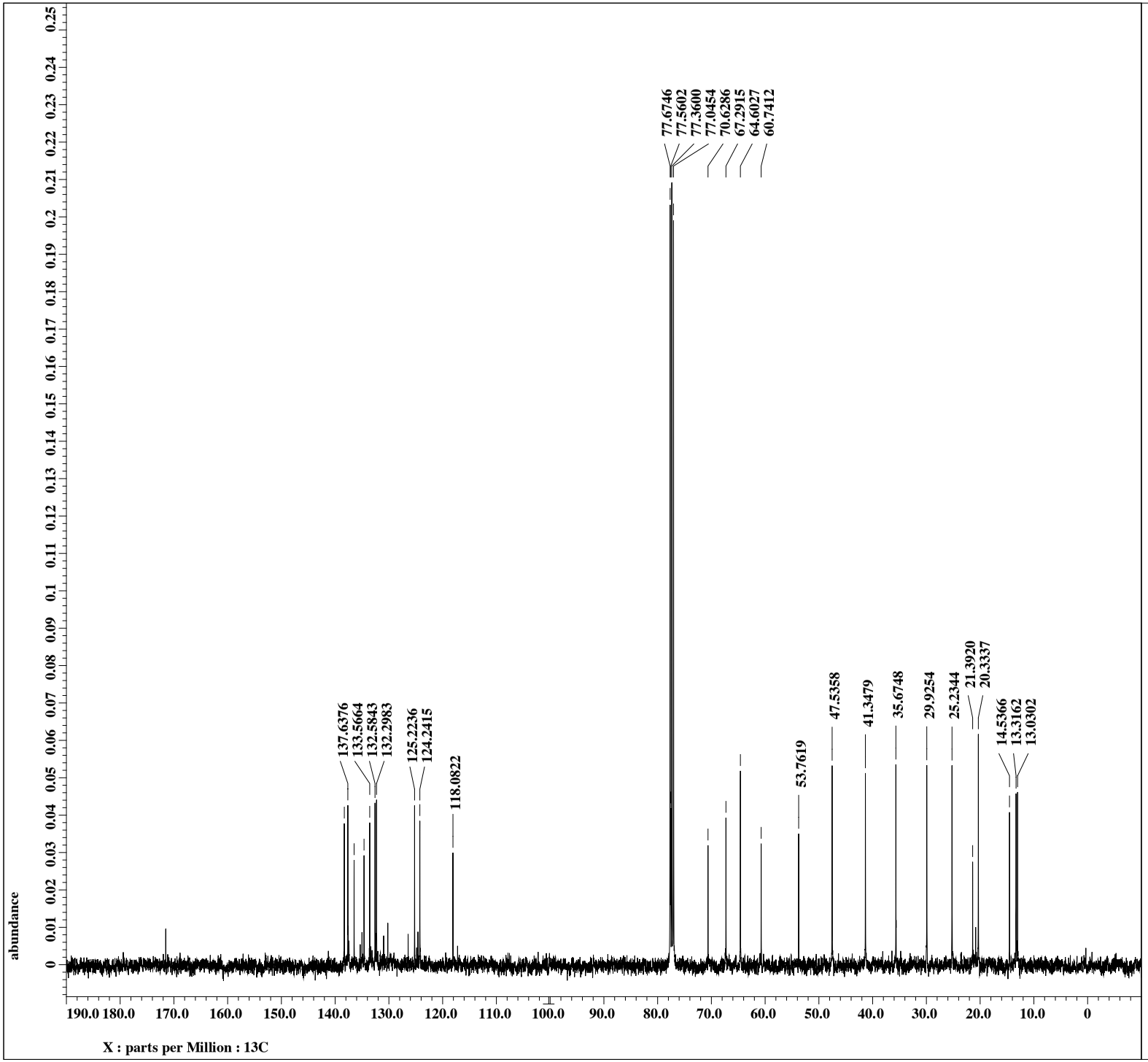


13

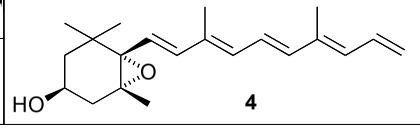

Filename = diene-alcohol-1H-3.jd
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 5-FEB-2009 09:07:13
Revision_time = 3-SEP-2009 12:30:45
Current_time = 3-SEP-2009 12:31:46
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 23.9[dC]
OH
HO
14
abundance
X : parts per Million : 1H
-0.0104
7.2600
6.5498
6.5223
6.3150
6.2840
6.2462
5.8900
5.8510
5.6964
4.3035
4.2863
3.9026
3.8888
3.8762
2.3584
2.3550
2.3458
1.9037
1.6196
1.5841
1.3
3.12
2.94
2.84
1.2290
1.1740
1.1339
0.9632
2.1
2.0
1.06
1.05
2.05
1.03
1.0
1.01
0.95


Filename = tetraene-alcohol 13C-
Author = delta
Experiment = single_pulse_dec
Sample_id = S#366857
Solvent = CHLOROFORM-D
Creation_time = 5-FEB-2009 09:33:53
Revision_time = 3-SEP-2009 13:56:33
Current_time = 3-SEP-2009 13:56:52
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 122
Total_scans = 122
X_90_width = 8.4[us]
X_acq_time = 1.04333312[s]
X_angle = 45[deg]
X_atn = 6.6[dB]
X_pulse = 4.2[us]
Irr_atn_dec = 22.2[dB]
Irr_atn_noe = 22.2[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 5[s]
Recvr_gain = 50
Relaxation_delay = 5[s]
Repetition_time = 6.04333312[s]
Temp_get = 24.3[dC]
OH
HO
14
12.9634
13.2876
20.3146
25.2058
29.9064
35.6462
41.2907
47.4882
59.7782
64.5551
67.3010
70.6190
77.0454
77.3600
77.6746
124.3274
125.1092
130.9825
131.8978
134.7963
137.5423
137.6567
abundance
X : parts per Million : 13C

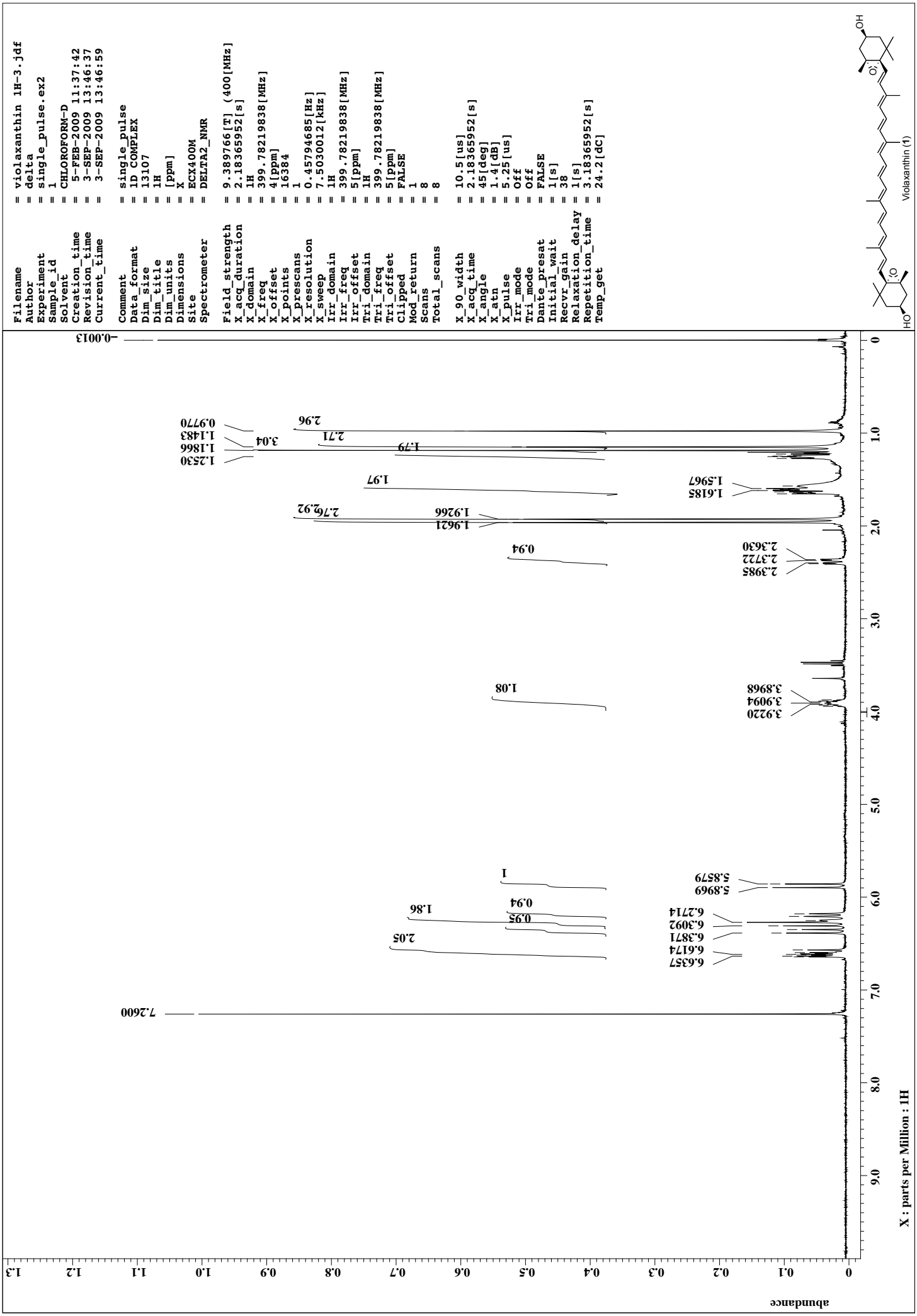

Filename = pentaene-1H-2.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 11-MAR-2009 19:27:22
Revision_time = 3-SEP-2009 13:31:12
Current_time = 3-SEP-2009 13:31:51
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.1[dC]
OH
4
7.2600
6.6059
6.5968
6.5681
6.3539
6.3035
6.2646
5.8969
5.8579
5.2886
5.1638
5.1386
3.9220
3.9094
3.8968
2.3745
2.3699
2.3619
1.9323
1.9209
1.6173
1.5669
0.9770
1.1866
1.1477
0.0013
X : parts per Million : 1H
abundance

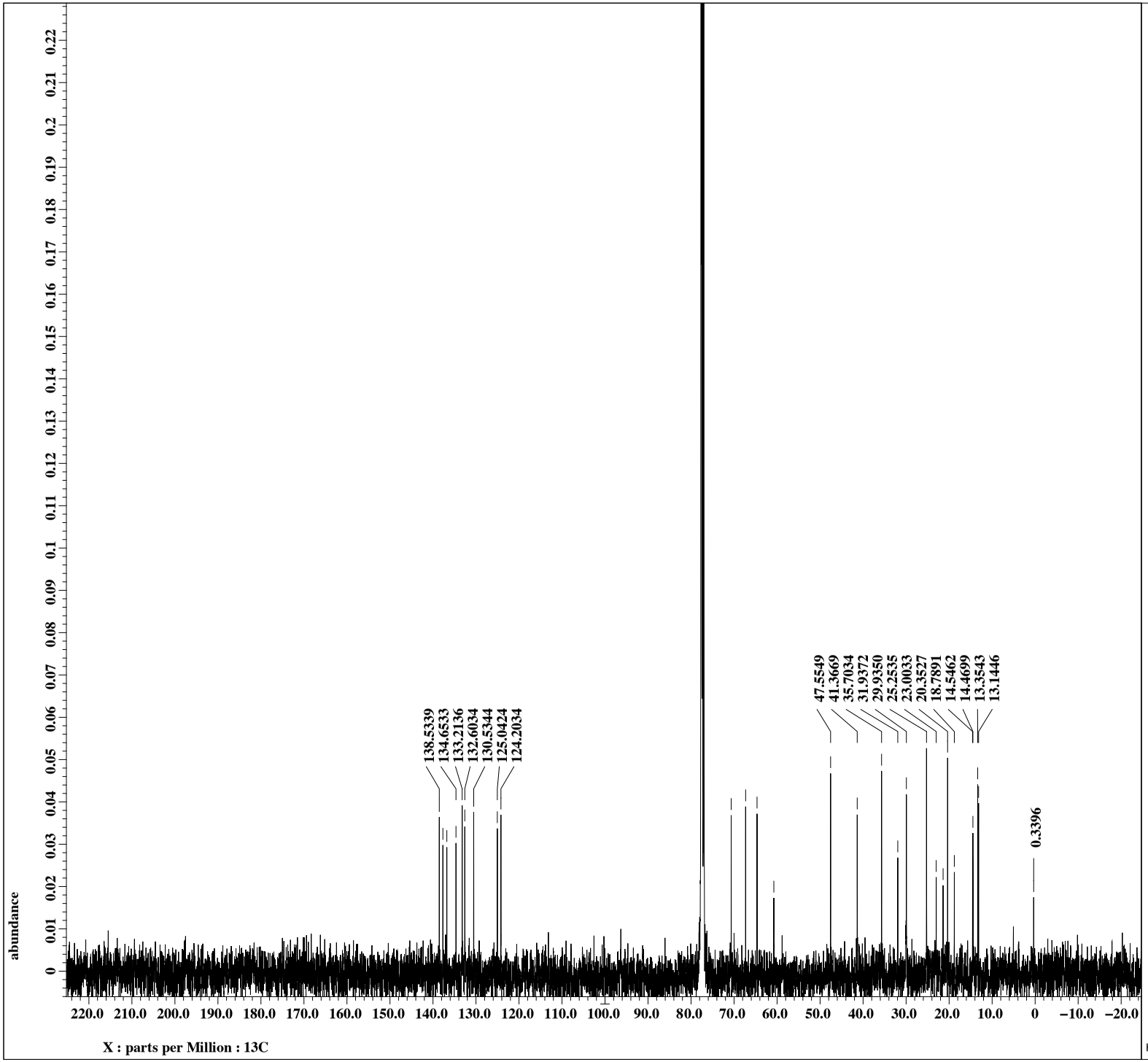



```
Filename          = pentaene-13C-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#675968
Solvent           = CHLOROFORM-D
Creation_time     =  6-FEB-2009 18:28:28
Revision_time     =  3-SEP-2009 13:54:31
Current_time      =  3-SEP-2009 13:54:53

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX400M
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 316
Total_scans       = 316

X_90_width        = 8.4[us]
X_acq_time        = 1.04333312[s]
X_angle           = 45[deg]
X_atn             = 6.6[dB]
X_pulse           = 4.2[us]
Irr_atn_dec       = 22.2[dB]
Irr_atn_noe       = 22.2[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 5[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.04333312[s]
Temp_get          = 24.8[dC]
```

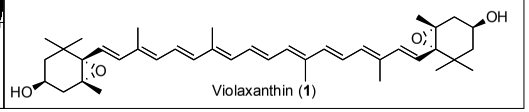


4

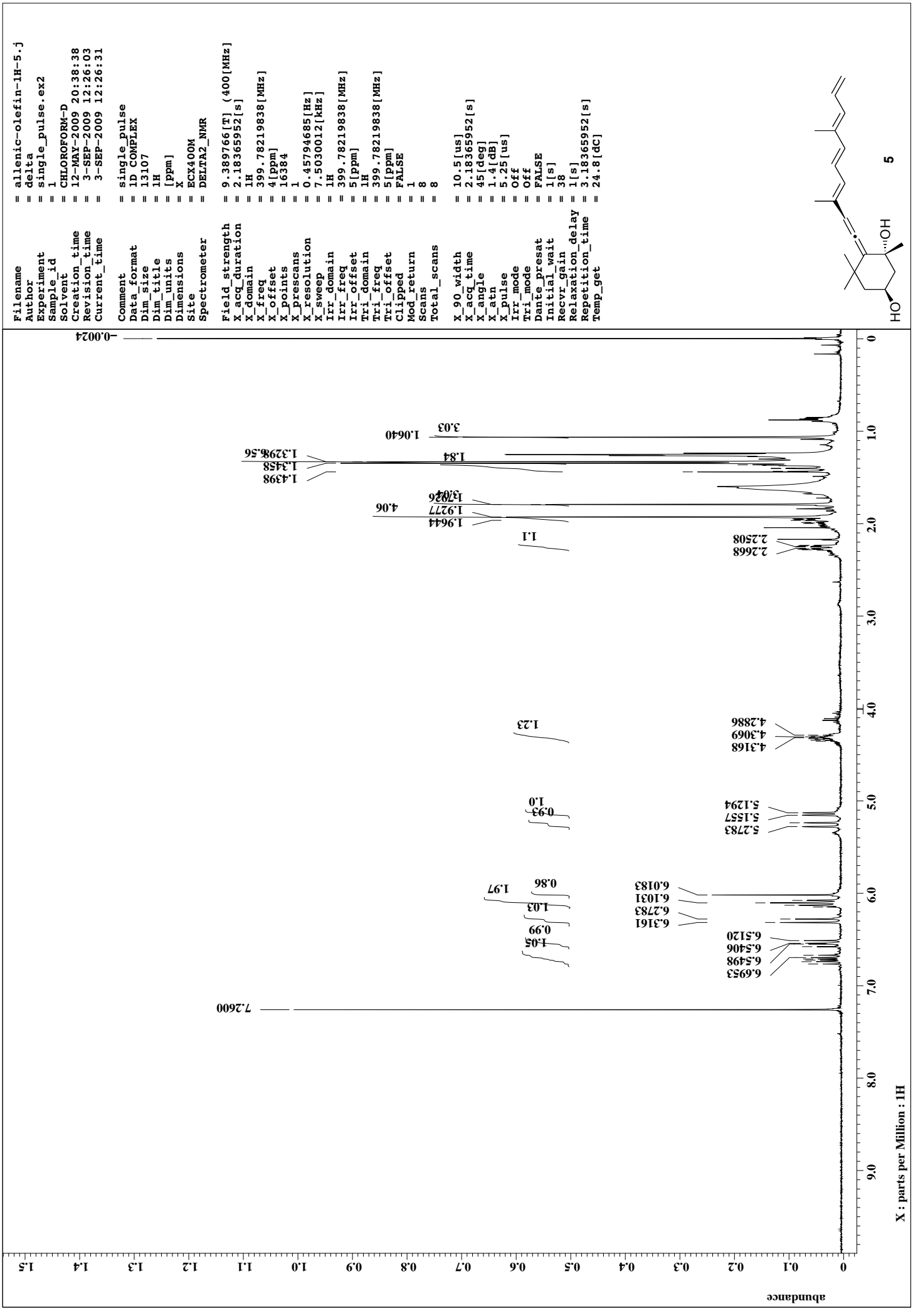

Filename = violaxanthin 1H-3.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 5-FEB-2009 11:37:42
Revision_time = 3-SEP-2009 13:46:37
Current_time = 3-SEP-2009 13:46:59
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.2[dC]
Violaxanthin (1)
7.2600
6.6357
6.6174
6.3871
6.3092
6.2714
5.8969
5.8579
2.05
1.86
0.95
0.94
1
1.08
3.9220
3.9094
3.8968
2.3985
2.3722
2.3630
0.94
1.9621
1.9266
2.76
2.92
1.97
1.6185
1.5967
1.79
2.71
2.96
3.04
1.2530
1.1866
1.1483
0.9770
-0.0013
abundance
X : parts per Million : 1H

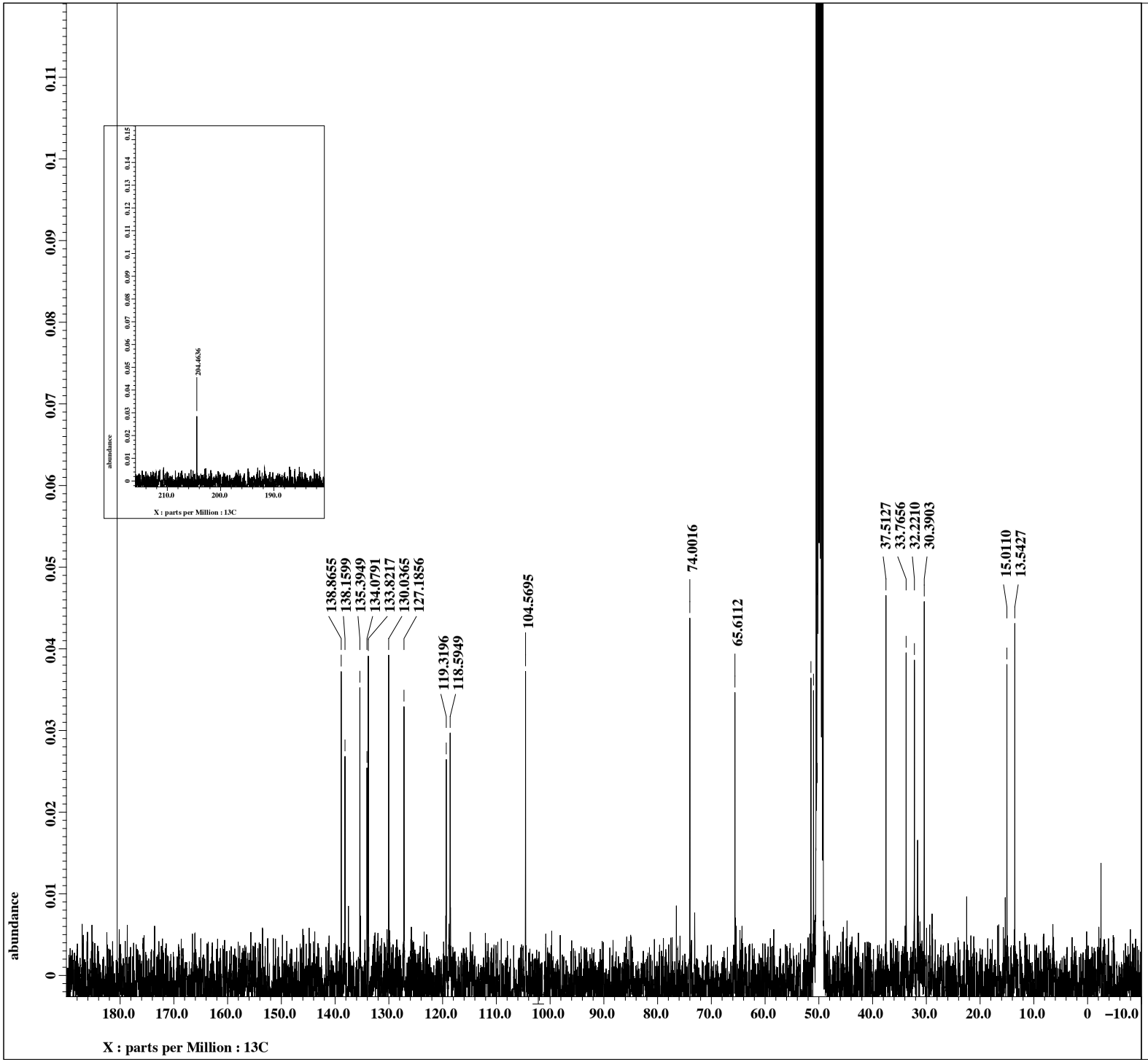



```
Filename          = violaxanthin 13C-2.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#482613
Solvent           = CHLOROFORM-D
Creation_time     =  5-FEB-2009 13:14:52
Revision_time     =  3-SEP-2009 13:59:37
Current_time      =  3-SEP-2009 14:00:02

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX400M
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Incomplete_copy   = TRUE
Mod_return        = 1
Scans             = 396
Total_scans       = 396

X_90_width        = 8.4[us]
X_acq_time        = 1.04333312[s]
X_angle           = 45[deg]
X_atn             = 6.6[dB]
X_pulse           = 4.2[us]
Irr_atn_dec       = 22.2[dB]
Irr_atn_noe       = 22.2[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 5[s]
Recvr_gain        = 60
Relaxation_delay  = 5[s]
Repetition_time   = 6.04333312[s]
Temp_get          = 25.2[dC]
```

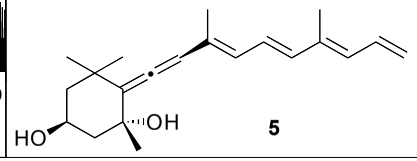


Violaxanthin (**1**)

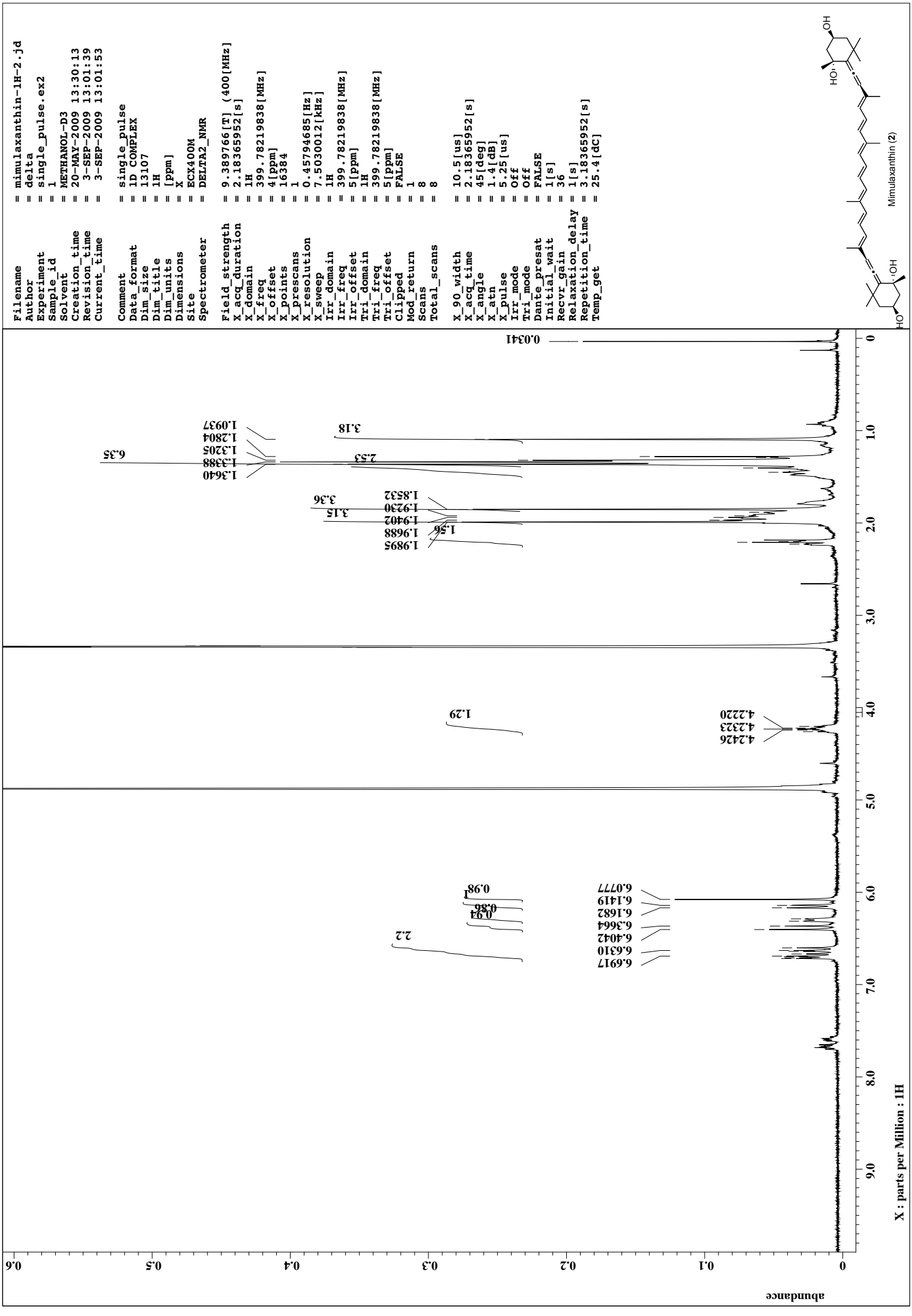

Filename = allenic-olefin-1H-5.j
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = CHLOROFORM-D
Creation_time = 12-MAY-2009 20:38:38
Revision_time = 3-SEP-2009 12:26:03
Current_time = 3-SEP-2009 12:26:31
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 24.8[dC]
HO
OH
5
7.2600
6.6953
6.5498
6.5406
6.5120
6.3161
6.2783
6.1031
6.0183
5.2783
5.1557
5.1294
4.3168
4.3069
4.2886
2.2668
2.2508
1.9644
1.9277
1.7026
1.3024
1.4398
1.3458
1.3298
1.0640
3.03
1.84
4.06
1.1
1.23
0.93
1.0
0.86
1.97
1.03
0.99
1.05
−0.0024
abundance
X : parts per Million : 1H

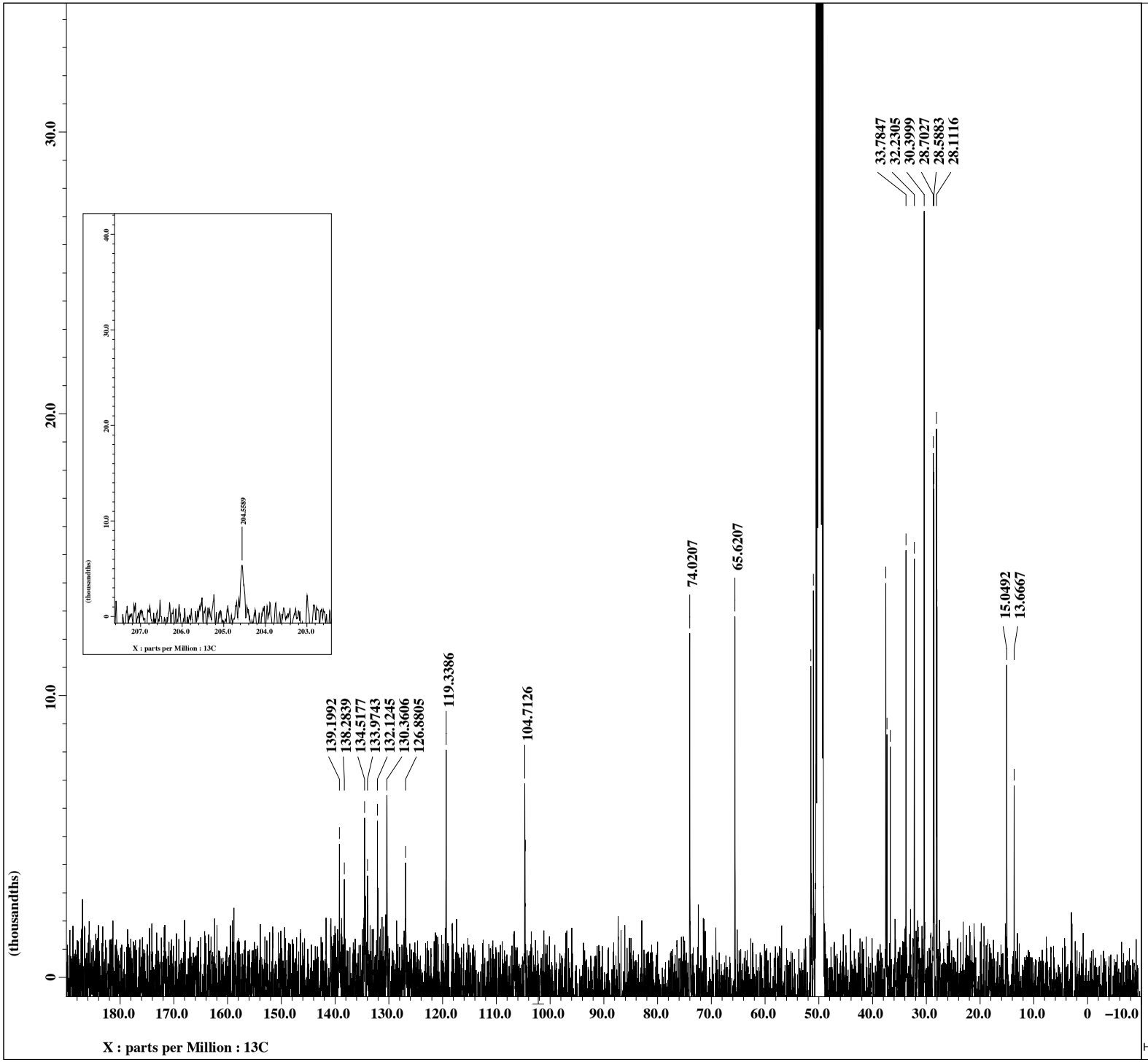



```
Filename          = allenic-olefin-13C-4.
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#356983
Solvent           = METHANOL-D3
Creation_time     = 13-MAY-2009 09:24:45
Revision_time     =  3-SEP-2009 13:51:12
Current_time      =  3-SEP-2009 13:52:37

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX400M
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 245
Total_scans       = 245

X_90_width        = 8.4[us]
X_acq_time        = 1.04333312[s]
X_angle           = 45[deg]
X_atn             = 6.6[dB]
X_pulse           = 4.2[us]
Irr_atn_dec       = 22.2[dB]
Irr_atn_noe       = 22.2[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 5[s]
Recvr_gain        = 56
Relaxation_delay  = 5[s]
Repetition_time   = 6.04333312[s]
Temp_get          = 24.9[dC]
```

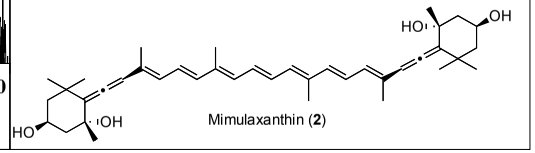


5


Filename = mimulaxanthin-1H-2.jd
Author = delta
Experiment = single_pulse.ex2
Sample_id = 1
Solvent = METHANOL-D3
Creation_time = 20-MAY-2009 13:30:13
Revision_time = 3-SEP-2009 13:01:39
Current_time = 3-SEP-2009 13:01:53
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECX400M
Spectrometer = DELTA2_NMR
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 4[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.5[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 1.4[dB]
X_pulse = 5.25[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 1[s]
Repetition_time = 3.18365952[s]
Temp_get = 25.4[dC]
Mimulaxanthin (2)
abundance
X : parts per Million : 1H
0.0341
1.0937
1.2804
1.3205
1.3388
1.3640
6.35
3.18
2.53
1.8532
1.9230
1.9402
1.56
1.9688
1.9895
3.15
3.36
1.29
4.2220
4.2323
4.2426
6.0777
6.1419
6.1682
6.3664
6.4042
6.6310
6.6917
2.2
0.98
1
0.86
0.94




```
Filename          = mimulaxanthin-13C-4.j
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#544193
Solvent           = METHANOL-D3
Creation_time     =  3-SEP-2009 14:55:42
Revision_time     =  3-SEP-2009 16:07:45
Current_time      =  3-SEP-2009 16:25:52

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX400M
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 470
Total_scans       = 470

X_90_width        = 9.2[us]
X_acq_time        = 1.04333312[s]
X_angle           = 45[deg]
X_atn             = 6.6[dB]
X_pulse           = 4.6[us]
Irr_atn_dec       = 22.2[dB]
Irr_atn_noe       = 22.2[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 5[s]
Recvr_gain        = 50
Relaxation_delay  = 5[s]
Repetition_time   = 6.04333312[s]
Temp_get          = 26.1[dC]
```



Mimulaxanthin (**2**)