

Revised (2)

Supporting Information

**Efficient Stereochemical Relay En Route to
Leucascandrolide A**

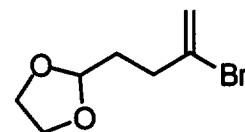
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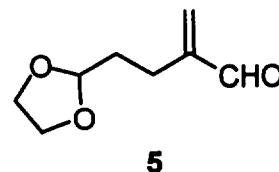
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ether (200 mL) and water (200 mL). The organic layer was separated, washed with water (300 mL), saturated aqueous solution of NaHCO_3 (200 mL), dried over anhydrous MgSO_4 . Concentration under reduced pressure gave 12.4 g of the crude aldehyde **11** (74% yield), which was used for the next step without further purification.

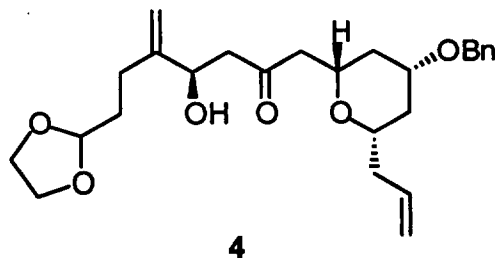
A 100-mL round-bottomed flask, equipped with the Dean-Stark trap was charged with aldehyde **11** (4.66 g, 28.6 mmol), ethylene glycol (1.86 g, 30 mmol), TsOH (50 mg) and benzene (50 mL). The resulting mixture was heated under a gentle reflux for 5 h, partitioned between ether (30 mL) and saturated aqueous solution of NaHCO_3 (50 mL). The aqueous layer was extracted with ether (30 mL), dried over anhydrous MgSO_4 , filtered and concentrated. The resulting dark-brown oil was subjected to the bulb-to-bulb distillation (100 °C oven temperature, 2 mm Hg) to give 5.62 g (96% yield) of the corresponding acetal, as a pale-yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 1.91 (m, 2H), 2.54 (m, 2H), 3.84 (m, 2H), 3.95 (m, 2H), 4.88 (t, 1H, $J = 4.5$ Hz), 5.38 (d, 1H, $J = 1.7$ Hz), 5.59 (q, 1H, $J = 1.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 32.3, 35.8, 65.0, 103.1, 116.8, 133.6; IR (neat) 2957, 2881, 1629, 1406, 1138, 1037, 886 cm^{-1} .



Aldehyde 5. A solution of vinyl bromide (3.70 g, 17.8 mmol), prepared in the previous step, in THF (50 mL) was treated dropwise with *n*-butyllithium (7.2 mL, 2.5 M in hexane) at -78 °C, followed by addition of dimethylformamide (6.9 mL) after a 20 min period. The reaction mixture was allowed to warm to ambient temperature, quenched by addition of water (200 mL), extracted with ether (2x300 mL), dried over anhydrous MgSO_4 , filtered and concentrated. Flash chromatography on silica gel (elution with ether:hexane; 1:3, 1:1) afforded 0.81 g of starting bromide and 1.15 g of aldehyde **5** (53% yield) as a colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.80 (m, 2H), 2.36 (t, 2H, $J = 8.0$ Hz), 3.83 (m, 2H), 3.94 (m, 2H), 4.86 (t, 1H, $J = 4.5$ Hz), 6.00 (s, 1H), 6.26 (s, 1H), 9.52 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 22.3, 31.7, 64.9, 103.7, 134.0, 149.5, 194.4; IR (neat) 2952, 2884, 1688, 1138, 1035, 945 cm^{-1} .

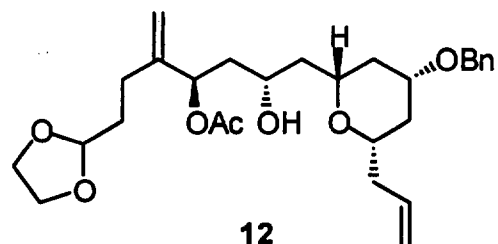


Ketone 4 Dicyclohexylboron chloride (2.5 mL of 1.0 M solution in hexane, 2.5 mmol) in ether (20 mL) was cooled to 0 °C, and treated with triethyl amine (0.39 mL, 2.8 mmol), followed by addition of ketone **6** (473 mg, 1.64 mmol) in ether (6 mL). The resulting white suspension was stirred for 15 min at 0 °C, cooled to -78 °C, and treated with aldehyde **5** (442 mg, 2.83



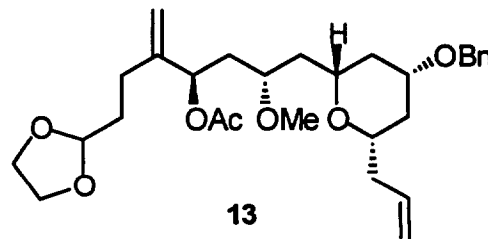
mmol) in ether (6 mL) over a 10 min period. The reaction mixture was stirred for 5 h at -78 C, quenched by addition of 21 mL of methanol:pH 7 buffer (6:1). Upon warming to ambient temperature, 9 mL of methanol-30% hydrogen peroxide (2:1) was added. The stirring was continued for 4 h. The resulting colorless solution was partitioned between ethyl acetate (100 mL) and saturated aqueous solution of NaHCO_3 (50 mL). The organic layer was washed with 10% solution of Na_2SO_3 , dried over anhydrous MgSO_4 , filtered and concentrated. Flash chromatography on silica gel (elution with ethyl acetate:hexane; 1:1) afforded 554 mg of ketone **4** (76% yield) as a colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 1.20 (m, 3H), 1.84 (m, 2H), 2.05 (m, 2H), 2.06-2.30 (m, 4H), 2.43 (dd, 1H, $J = 15.0, 4.5$ Hz), 2.66 (dd, 1H, $J = 17.0, 9.0$ Hz), 2.75 (m, 2H), 3.33 (m, 1H), 3.55 (dddd, 1H, $J = 11.0, 11.0, 5.0, 5.0$ Hz), 3.75 (m, 1H), 3.83 (, 2H), 3.94 (m, 2H), 4.52 (m, 1H), 4.53 (s, 2H), 4.88 (m, 2H), 5.01 (d, 1H, $J = 9$ Hz), 5.03 (d, 1H, $J = 16.5$ Hz), 5.08 (s, 1H), 5.75 (dddd, 1H, $J = 17.0, 10.0, 7.0, 7.0$ Hz); 7.26-7.34 (m, 5H); ^{13}C NMR (125 MHz, CDCl_3) δ 26.1, 32.1, 37.3, 37.8, 40.3, 49.4, 49.7, 64.9, 69.7, 70.3, 72.2, 74.2, 75.2, 104.0, 110.1, 117.1, 127.6, 128.4, 134.3, 138.4, 149.2, 209.8; IR (neat) 3451, 2916, 2849, 1710, 1352, 1069, 906, 733, 697 cm^{-1} .

Alcohol 12. A solution of ketone **4** (120 mg, 0.27 mmol) and acetaldehyde (48 mg, 1.1 mmol) in THF (3 mL) was cooled to -10 °C and treated with SmI_2 (0.80 mL, 0.1 M solution in THF). The reaction mixture was stirred for 15 min, quenched by addition of saturated aqueous solution of NaHCO_3 (15 mL), extracted with ethyl acetate (50 mL), dried over anhydrous MgSO_4 ,



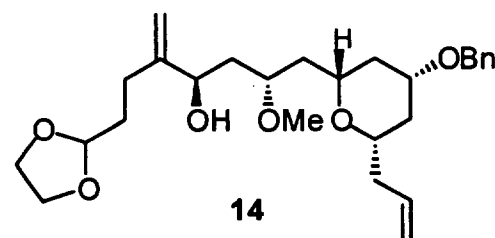
filtered and concentrated. Flash chromatography on silica gel (elution with ethyl acetate:hexane; 2:1) afforded 122 mg of alcohol **12** (93% yield) as a colorless oil. ^1H NMR (500 MHz, C_6D_6) δ 1.15 (m, 3H), 1.60 (dt, 1H, $J = 14.0, 9.5$ Hz), 1.72 (s, 3H), 1.65-1.85 (m, 4H), 1.95 (m, 1H), 2.00-2.10 (m, 3H), 2.40 (m, 2H), 2.95 (m, 1H), 3.18 (m, 2H), 3.33 (m, 1H), 3.35 (m, 2H), 3.52 (m, 2H), 3.77 (s, 1H), 3.95 (t, 1H, $J = 9.0$ Hz), 4.34 (d, 1H, $J = 12.5$ Hz), 4.36 (d, 1H, $J = 12.5$ Hz), 4.84 (t, 1H, $J = 4.5$ Hz), 4.89 (s, 1H), 4.98 (m, 2H), 5.15 (s, 1H), 5.66 (dddd, 1H, $J = 17.0, 10.0, 7.0, 7.0$ Hz); 5.87 (dd, 1H, $J = 9.5, 2.5$ Hz), 7.13 (t, $J = 7.0$ Hz), 7.22 (t, 2H, $J = 7.0$ Hz), 7.34 (d, 2H, $J = 7$ Hz); ^{13}C NMR (125 MHz, C_6D_6) δ 20.7, 26.9, 32.7, 37.8, 38.8, 40.7, 42.6, 43.3, 64.8, 67.7, 69.4, 73.8, 74.3, 75.2, 76.5, 104.2, 110.4, 117.5, 127.5, 127.6, 128.6, 134.7, 139.6, 148.9, 169.6; IR (neat) 3492, 2917, 2860, 1736, 1642, 1368, 1236, 1070, 904, 736, 698 cm^{-1} .

Methyl Ether 13. A solution of alcohol **12** (110 mg, 0.225 mmol), 2,6-di-*tert*-butylpyridine (0.76 mL, 3.37 mmol) and methyl triflate (0.323 mL, 2.25 mmol) was stirred for 14 h at ambient temperature, and quenched by addition of aqueous solution of ammonium hydroxide (10 mL). The product was extracted with ether (2x50 mL), dried over anhydrous MgSO₄, filtered and concentrated.



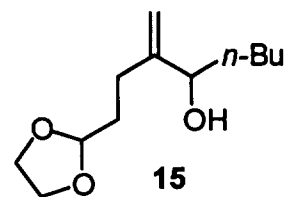
The excess 2,6-di-*tert*-butylpyridine was removed by bulb-to-bulb distillation (80 °C, 0.5 mm Hg). Flash chromatography on silica gel (elution with ethyl acetate:hexane; 1:2) afforded 81 mg of methyl ether **13** (72% yield) as a colorless oil. ¹H NMR (500 MHz, C₆D₆) δ 1.19 (q, 1H, *J* = 11.5 Hz), 1.26 (q, 1H, *J* = 11.5 Hz), 1.43 (ddd, 1H, *J* = 14.0, 7.5, 3.5 Hz), 1.77 (s, 3H), 1.80-1.90 (m, 5H), 2.00-2.10 (m, 3H), 2.27 (m, 1H), 2.40 (m, 2H), 2.98 (m, 1H), 3.17 (s, 3H), 3.20-3.28 (m, 2H), 3.33 (m, 1H), 3.35 (m, 2H), 3.50 (m, 2H), 4.37 (s, 2H), 4.83 (t, 1H, *J* = 4.5 Hz), 4.89 (s, 1H), 5.03 (m, 2H), 5.17 (s, 1H), 5.84 (dd, 1H, *J* = 9.5, 2.5 Hz), 5.90 (m, 1H); 7.12 (t, *J* = 7.0 Hz), 7.22 (t, 2H, *J* = 7.0 Hz), 7.35 (d, 2H, *J* = 7 Hz); ¹³C NMR (125 MHz, C₆D₆) δ 20.7, 26.8, 32.7, 38.1, 39.0, 39.4, 39.8, 40.9, 56.5, 64.8, 69.4, 72.1, 73.8, 74.7, 74.8, 75.2, 104.2, 110.5, 116.6, 127.5, 127.6, 128.5, 135.5, 139.7, 148.8, 169.3; IR (neat) 2939, 2880, 1736, 1368, 1235, 1070, 906, 736, 698 cm⁻¹.

Alcohol 14. Lithium aluminum hydride (38 mg, 1 mmol) was suspended in ether (2 mL), cooled to -78 °C, and treated with methyl ether **13** (66 mg, 0.13 mmol) in ether (2 mL). The reaction mixture was stirred for 30 min at -78 °C, quenched by dropwise addition of water (0.2 mL). The resulting suspension was allowed to reach ambient temperature, vigorously

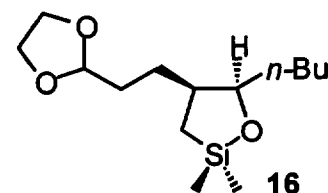


stirred for 1 h, diluted with ether, dried with anhydrous Na₂SO₄, filtered and concentrated. Flash chromatography on silica gel (elution with ethyl acetate:hexane; 1:2) afforded 51 mg of alcohol **14** (86% yield) as a colorless oil. ¹H NMR (500 MHz, C₆D₆) δ 1.20 (q, 1H, *J* = 11.5 Hz), 1.26 (q, 1H, *J* = 11.5 Hz), 1.46 (ddd, 1H, *J* = 14.0, 7.5, 3.5 Hz), 1.80-1.85 (m, 4H), 1.93 (ddd, 1H, *J* = 14.0, 9.0, 4.5 Hz), 2.00-2.04 (m, 2H), 2.10 (m, 1H), 2.28 (m, 2H), 2.40 (m, 1H), 3.00 (m, 1H), 3.08 (s, 3H), 3.20-3.28 (m, 2H), 3.35 (m, 2H), 3.69 (m, 1H), 4.37 (s, 2H), 4.43 (m, 1H), 4.85 (t, 1H, *J* = 4.5 Hz), 4.95 (s, 1H), 5.04 (m, 2H), 5.33 (s, 1H), 5.86 (dddd, 1H, *J* = 17.0, 10.0, 7.0, 7.0 Hz), 7.12 (t, *J* = 7.0 Hz), 7.22 (t, 2H, *J* = 7.0 Hz), 7.35 (d, 2H, *J* = 7 Hz); ¹³C NMR (125 MHz, C₆D₆) δ 26.7, 33.0, 37.9, 39.0, 38.9, 39.3, 39.5, 40.9, 56.0, 64.8, 69.4, 72.3, 74.8, 75.2, 76.4, 104.4, 108.9, 116.8, 127.5, 127.6, 128.5, 135.3, 139.7, 152.2; IR (neat) 3452, 2942, 2878, 1642, 1354, 1071, 904, 736, 698 cm⁻¹.

Alcohol 15. Aldehyde **5** (312 mg, 2.0 mmol) in THF (10 mL) was cooled to $-78\text{ }^{\circ}\text{C}$, and treated with *n*-butyllithium (0.88 mL, 2.5 M solution in hexane). After 15 min, the reaction was quenched by addition of saturated aqueous solution of NaHCO_3 (15 mL), extracted with ether (50 mL), dried over anhydrous MgSO_4 , filtered and concentrated. Flash chromatography on silica gel (elution with ether:hexane; 2:1) afforded 380 mg of alcohol **15** (87% yield) as a colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 0.87 (t, 3H, $J = 7.0$ Hz), 1.20-1.38 (m, 4H), 1.53 (m, 2H), 1.78 (br s, 1H), 1.85 (m, 2H), 2.10 (m, 1H), 2.21 (m, 1H), 3.81 (m, 2H), 3.95 (m, 2H), 4.06 (t, 1H, $J = 7.0$ Hz), 4.83 (s, 1H), 4.87 (t, 1H, $J = 4.5$ Hz), 5.01 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 14.0, 22.6, 25.3, 27.8, 32.2, 35.1, 64.9, 75.6, 104.2, 109.8, 151.1; IR (neat) 3439, 2953, 2870, 1692, 1409, 1135, 1031, 899, 731 cm^{-1} .

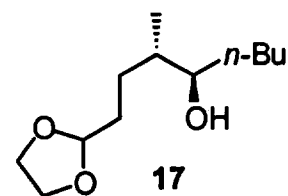


Silane 16. A solution of alcohol **15** (142 mg, 0.66 mmol) in CH_2Cl_2 (0.50 mL) was treated with tetramethyldisilazane (0.35 mL, 2.0 mmol). After 12 h, ^1H NMR analysis indicated complete consumption of the starting alcohol. The excess tetramethyldisilazane was removed under high vacuum. The



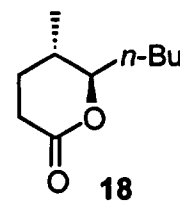
resulting silyl ether was dissolved in C_6H_6 (7 mL) and treated with H_2PtCl_6 [30 μL , 0.05 M in THF, (0.3 mol%)]. After 30 min at $50\text{ }^{\circ}\text{C}$, ^1H NMR analysis indicated quantitative formation of the silacycle **16**, as 85:15 mixture of diastereomers. Major isomer: ^1H NMR (400 MHz, C_6D_6) δ 0.10 (s, 3H), 0.15 (s, 3H), 0.90 (t, 3H, $J = 7.0$ Hz), 1.20-1.90 (m, 10H), 2.00 (m, 1H), 3.39 (m, 2H), 3.56 (m, 2H), 3.99 (ddd, 1H, $J = 10.4, 5.6, 3.2$ Hz), 4.82 (t, 1H, $J = 4.5$ Hz); ^{13}C NMR (100 MHz, C_6D_6) δ 0.2, 1.2, 14.4, 16.2, 23.0, 26.9, 28.7, 31.4, 33.2, 42.5, 64.8, 104.8; IR (neat) 2953, 2871, 1408, 1250, 1033, 840, 796 cm^{-1} .

Alcohol 17. Cyclic silane **16**, obtained upon concentration of the crude hydrosilylation reaction mixture was treated with TBAF (2.6 mmol) in DMF (2.5 mL). The resulting solution was heated to $75\text{ }^{\circ}\text{C}$ for 24 h. The excess DMF was removed by bulb-to-bulb distillation ($50\text{ }^{\circ}\text{C}$, 0.5 mm Hg). Flash chromatography on silica gel (elution with ethyl

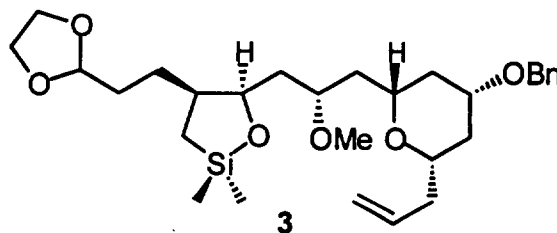


acetate:hexane; 1:2) afforded 121 mg of alcohol **17** (82% yield from **15**) as a colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 0.87 (d, 3H, $J = 7.0$ Hz), 0.88 (t, 3H, $J = 7.0$ Hz), 1.20-1.90 (m, 10H), 2.74 (m, 1H), 3.41 (m, 1H), 3.82 (m, 2H), 3.95 (m, 2H), 4.83 (t, 1H, $J = 4.5$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 14.0, 15.2, 22.7, 26.0, 28.2, 31.6, 33.1, 38.6, 64.8, 75.7, 104.7.

Lactone 18. A solution of alcohol 17 (110 mg, .50 mmol) in 6 mL of THF-water (5:1) containing a drop of concentrated H₂SO₄ was heated to 80 °C for 10 h, then partitioned between saturated aqueous solution of NaHCO₃ (1 mL), and ether (20 mL). The organic layer was separated, dried over anhydrous MgSO₄, filtered and concentrated. Flash chromatography on silica gel (elution with ether:pentane; 1:1) afforded 62 mg of the corresponding lactol as a colorless oil. The oxidation was conducted by addition of bromine (15 μL) to the solution of the lactol in acetic acid (0.4 mL) and water (0.64 mL). After 1 h, the reaction mixture was partitioned between saturated aqueous solution of NaHCO₃, and ether (20 mL). The organic layer was separated, dried over anhydrous MgSO₄, filtered and concentrated. Flash chromatography on silica gel (elution with ether:pentane; 1:1) afforded 61 mg of lactone 18 (86% from 17) as a colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 0.89 (t, 3H, *J* = 7.0 Hz), 0.97 (t, 3H, *J* = 7.0 Hz), 1.20-1.70 (m, 8H), 1.87 (m, 1H), 2.45 (ddd, 1H, *J* = 17.0, 10.0, 6.8 Hz), 2.60 (ddd, 1H, *J* = 17.0, 6.4, 4.4 Hz), 3.91 (ddd, 1H, *J* = 10.0, 8.0, 3.0 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 13.9, 17.4, 22.6, 26.5, 27.8, 29.5, 32.2, 33.1, 85.9, 174.0.

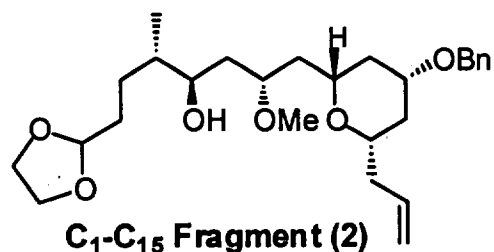


Silane 3. A solution of alcohol 13 (46 mg, 0.10 mmol) in CDCl₃ (0.50 mL) was treated with tetramethyldisilazane (0.10 mL, 0.56 mmol). After 15 min, ¹H NMR analysis indicated complete consumption of the starting alcohol. The excess tetramethyldisilazane was removed



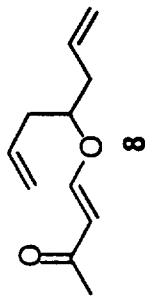
under high vacuum. The resulting silyl ether was dissolved in C₆D₆ (1 mL) and treated with H₂PtCl₆ (0.5 mol%). After 10 min at 57 °C, ¹H NMR analysis indicated quantitative formation of the silacycle 3, as 87:13 mixture of diastereomers. Major isomer: ¹H NMR (500 MHz, C₆D₆) δ 0.11 (s, 3H), 0.17 (s, 3H), 0.48 (dd, 1H, *J* = 14.5, 11.0 Hz), 0.80 (dd, 1H, *J* = 14.5, 7.0 Hz), 1.25 (q, 1H, *J* = 11.5 Hz), 1.36 (q, 1H, *J* = 11.5 Hz), 1.46-2.38 (m, 2H), 3.10 (m, 1H), 3.33 (s, 3H), 3.20-3.28 (m, 2H), 3.28 (m, 2H), 3.35 (m, 2H), 3.90 (m, 1H), 4.38 (s, 2H), 4.50 (m, 1H), 4.85 (t, 1H, *J* = 4.5 Hz), 5.04 (m, 2H), 5.92 (m, 1H), 7.11 (t, *J* = 7.0 Hz), 7.21 (t, 2H, *J* = 7.0 Hz), 7.34 (d, 2H, *J* = 7 Hz).

Alcohol 2. Cyclic silane **3**, obtained upon concentration of the crude hydrosilylation reaction mixture was treated with TBAF (0.4 mmol) in *d*-DMF (0.5 mL). The resulting solution was heated to 70 °C for 15 min. At this point, ¹H NMR analysis indicated complete consumption of the starting silane **3**. The excess DMF was removed by bulb-to-bulb distillation



(50 °C, 0.5 mm Hg). Flash chromatography on silica gel (elution with ethyl acetate:hexane; 1:1) afforded 24 mg of alcohol **2** (54% yield from **14**) as a colorless oil. ¹H NMR (500 MHz, C₆D₆) δ 0.93 (d, 3H, *J* = 6.5 Hz), 1.22 (q, 1H, *J* = 11.5 Hz), 1.28 (q, 1H, *J* = 11.5 Hz), 1.48-2.03 (m, H), 2.10 (m, 1H), 2.30 (m, 1H), 2.80 (br s, 1H), 3.00 (m, 1H), 3.07 (s, 3H), 3.26 (m, 2H), 3.36 (m, 2H), 3.56 (m, 2H), 3.67 (m, 1H), 3.78 (m, 1H), 4.37 (s, 2H), 4.85 (t, 1H, *J* = 4.5 Hz), 5.04 (m, 2H), 5.87 (dddd, 1H, *J* = 17.0, 10.0, 7.0, 7.0 Hz), 7.12 (t, *J* = 7.0 Hz), 7.22 (t, 2H, *J* = 7.0 Hz), 7.35 (d, 2H, *J* = 7 Hz); ¹³C NMR (125 MHz, C₆D₆) δ 15.4, 27.0, 32.2, 36.3, 37.9, 38.9, 39.3, 39.4, 40.9, 56.2, 64.8, 69.4, 72.4, 74.9, 75.2, 76.8, 105.2, 116.8, 127.5, 127.6, 128.5, 135.2, 139.7; IR (neat) 3470, 2919, 2870, 1354, 1071, 736, 697 cm⁻¹.

^1H NMR and ^{13}C NMR Spectra



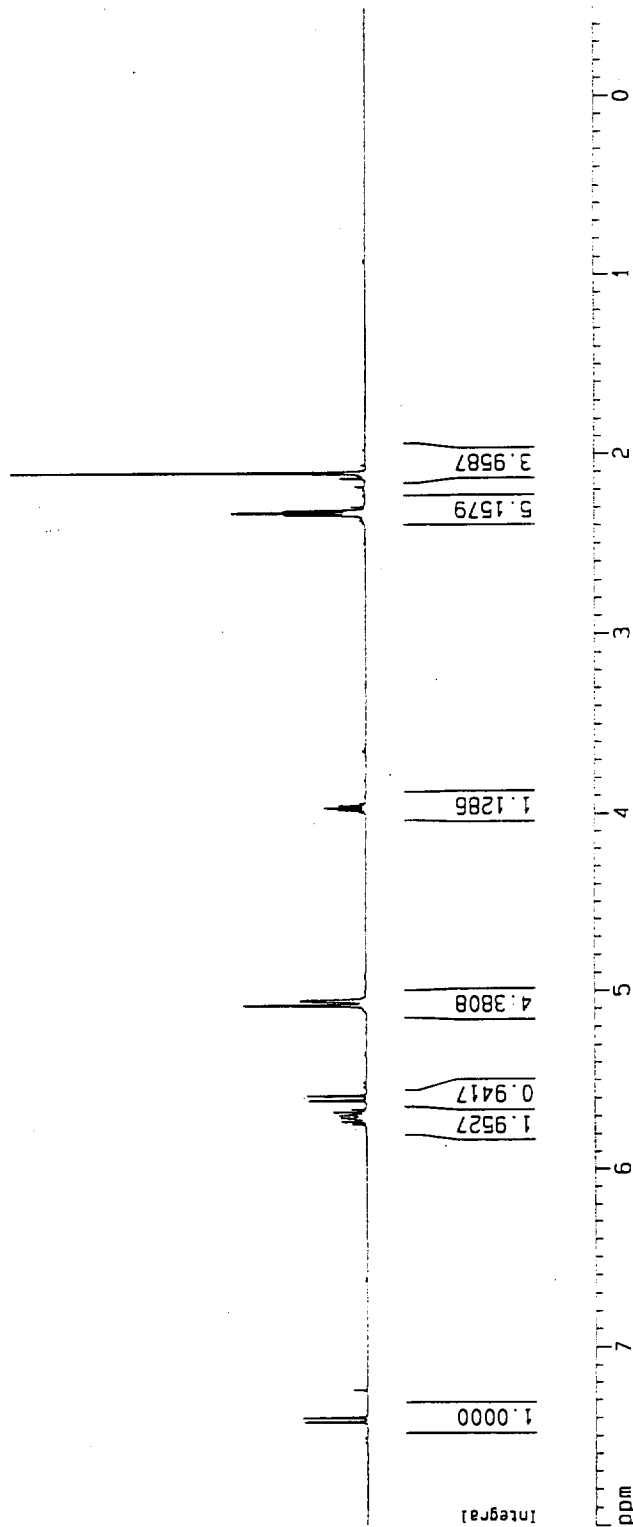
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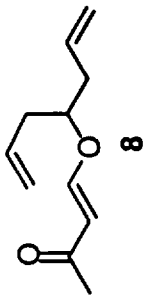
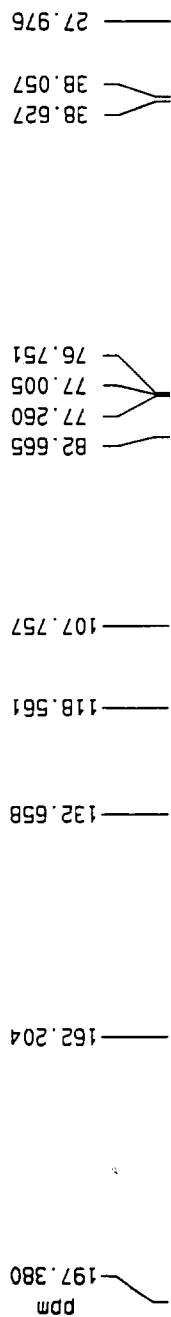
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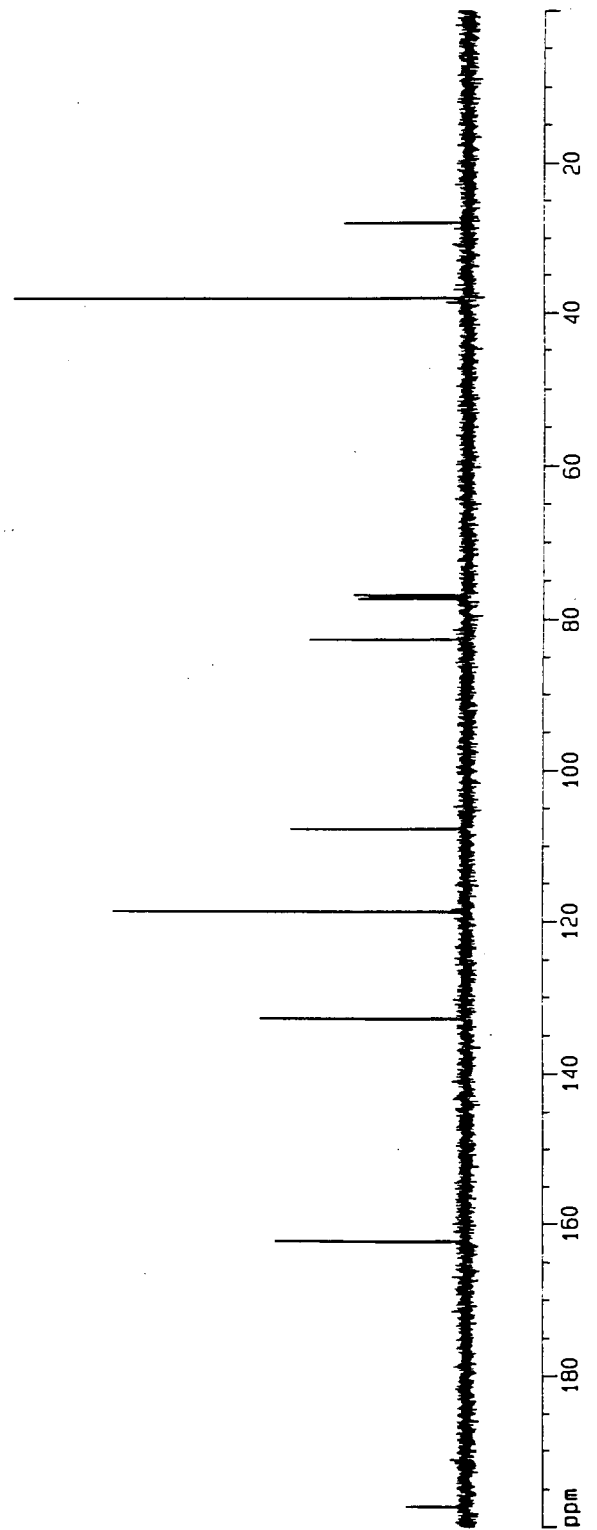
***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 28.00 dB
 SF02 500.1317628 MHz

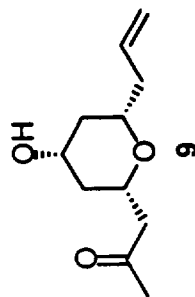
F2 - Processing parameters
 SI 32768
 SF 125.7578007 MHz
 HOW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CK 20.00 cm
 F1P 200.000 ppm
 F1 25151.56 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1257.57800 Hz/cm



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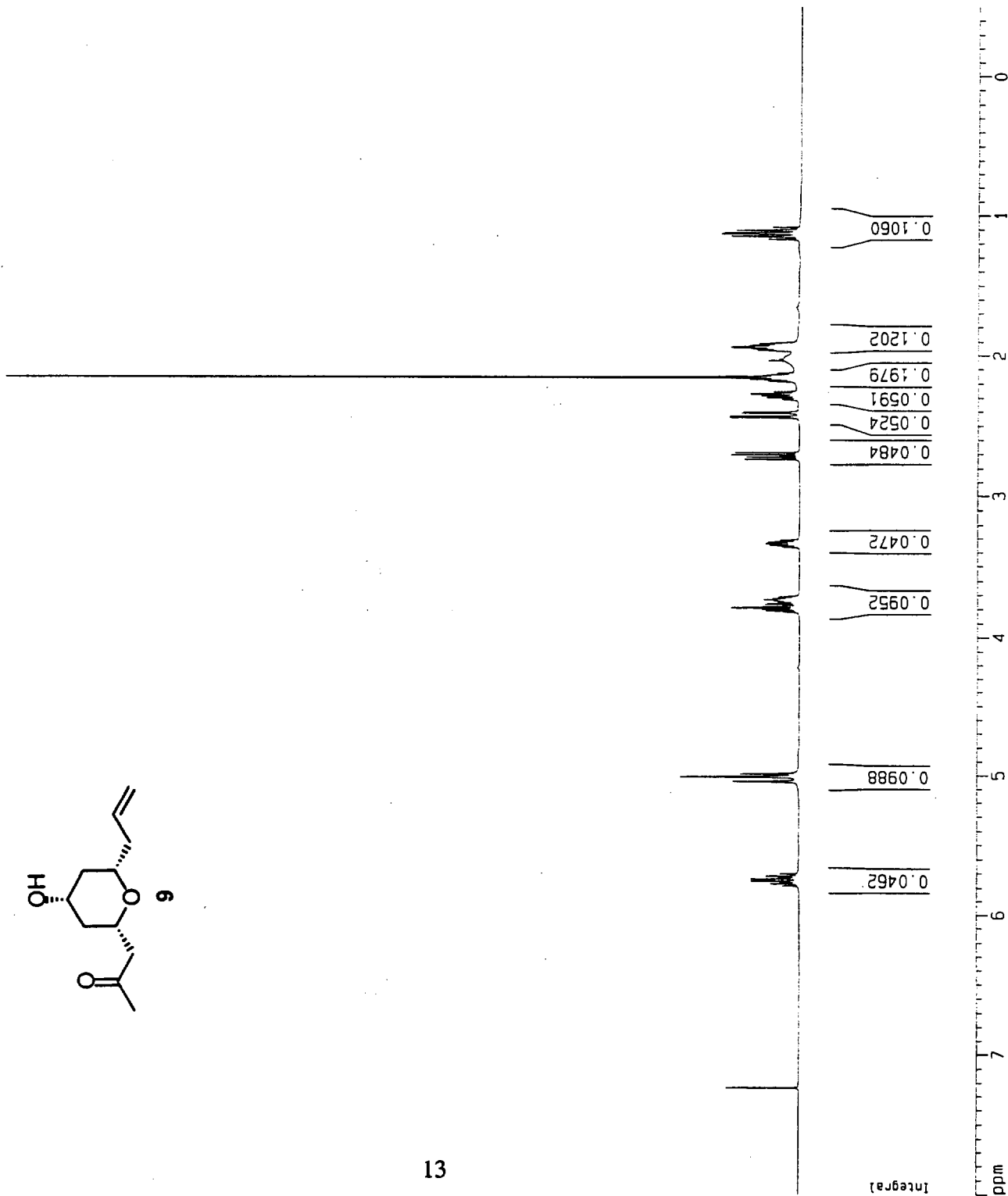
Current Data Parameters
 NAME proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001121
 Time 10.07
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 64
 DM 96.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 0.00 dB
 SF01 500.1320118 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300239 MHz
 NDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 212.55527 Hz/cm



```

Current Data Parameters
NAME          carbon
EXPNO         1
PROCNO        1

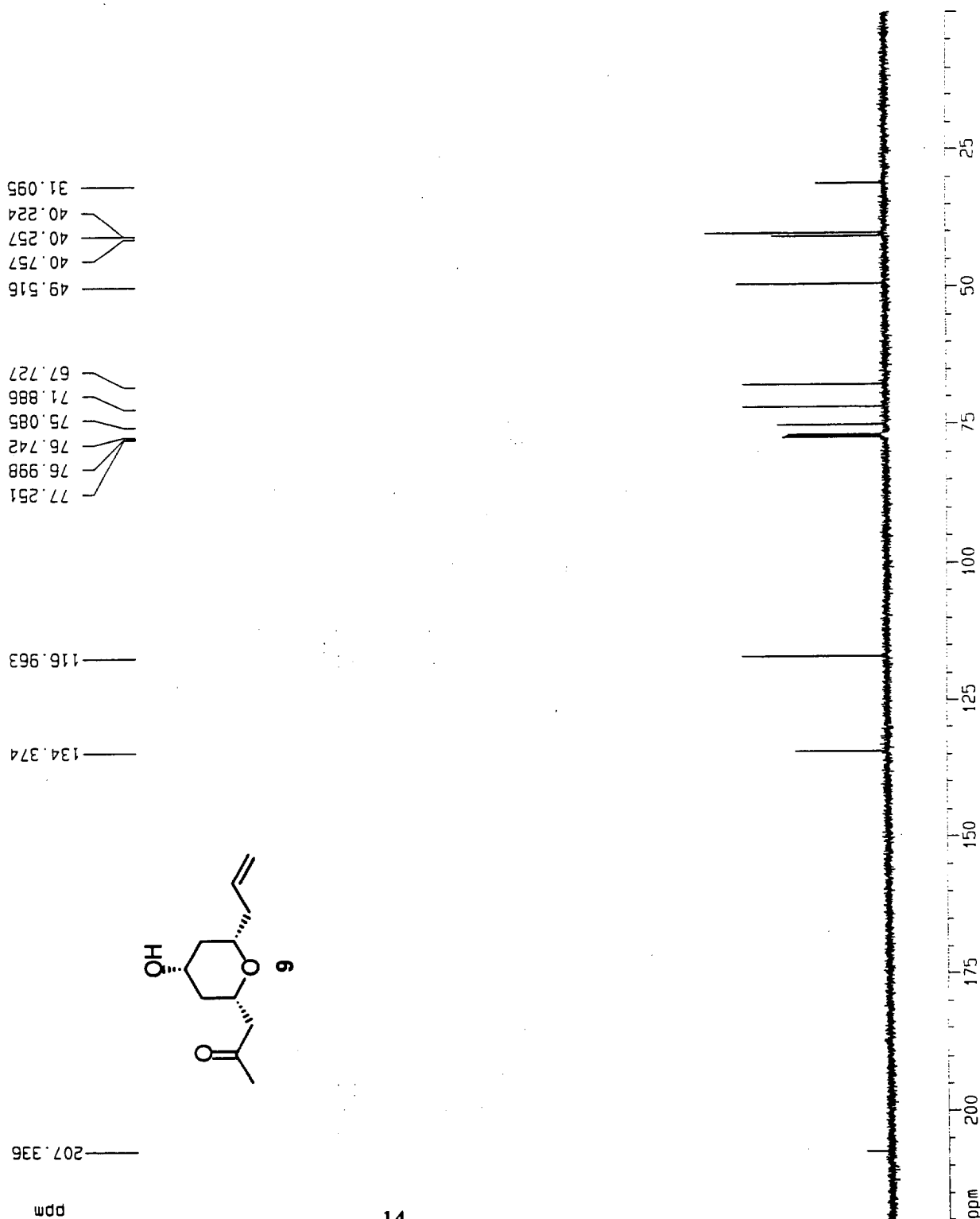
F2 - Acquisition Parameters
Date_         20001121
Time          10.09
INSTRUM       spect
PROBHD        5 mm QNP 1H
PULPROG       zgpg
TD             65536
SOLVENT       CDCl3
NS             33
DS             0
SWH            39662.539 Hz
FIDRES        0.605507 Hz
AQ             0.8256036 sec
RG             1024
DW             12.600 usec
DE             7.50 usec
TE             300.0 K
D1             2.0000000 sec
d11            0.0300000 sec

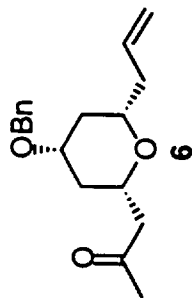
===== CHANNEL f1 =====
NUC1           13C
P1             5.00 usec
PL1            0.00 dB
SF01           125.7736214 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         100.00 usec
PL2            120.00 dB
PL12          20.00 dB
SF02           500.1320005 MHz

F2 - Processing parameters
SI             32768
SF             125.7577958 MHz
RG             EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40

10 NMR1 plot parameters
CX             20.000 cm
F1P           220.000 ppm
F1            27666.71 Hz
F2            0.000 ppm
F2P           0.00 Hz
PPMCH         11.00000 ppm/cm
HZCM          1383.33582 Hz/cm
    
```





Current Data Parameters
 NAME sk-proton
 EXPNO 3
 PROCNO 1

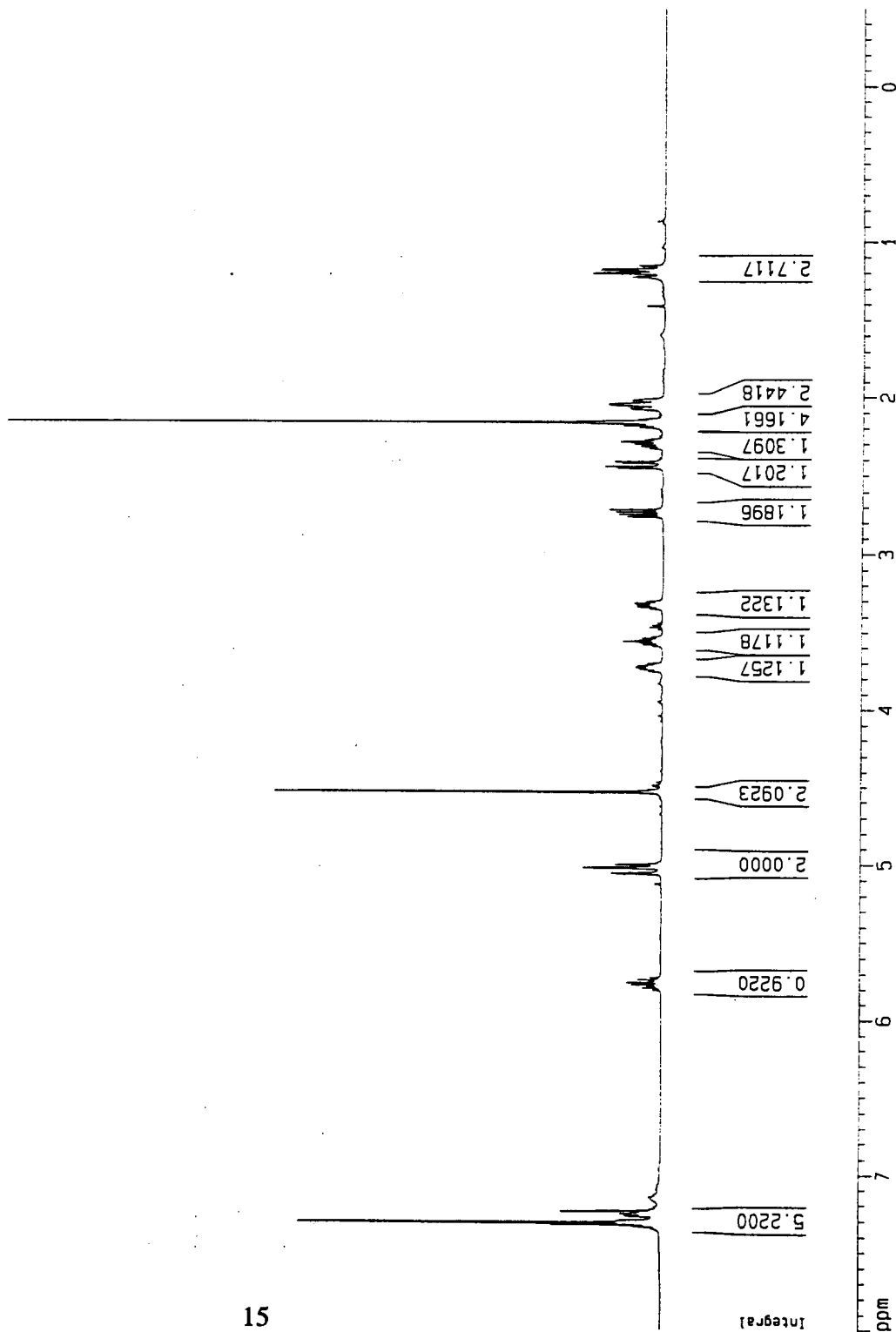
F2 - Acquisition Parameters
 Date_ 2001206
 Time 17.38
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 4
 DS 0
 SWH 15015.015 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912244 sec
 RG 50.8
 DM 33.300 usec
 DE 7.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 4.00 dB
 SF01 500.1317628 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300234 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 212.55527 Hz/cm

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Current Data Parameters
 NAME sk-carbon
 EXPNO 1
 PROCNO 1

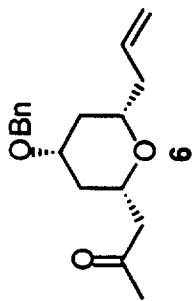
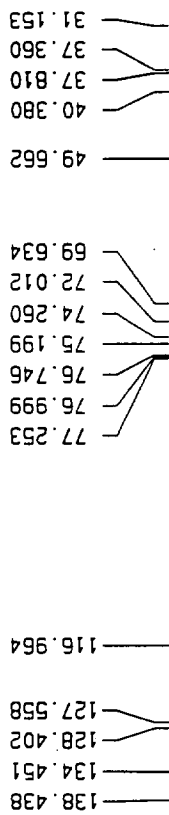
F2 - Acquisition Parameters
 Date_ 20001206
 Time 17.43
 INSTRUM Spect
 PROBHD 5 mm Multinu
 PULPROG zgdc
 TD 65536
 SOLVENT CDCl3
 NS 110
 DS 1
 SMH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 9195.2
 DW 12.600 usec
 DE 4.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 8.00 usec
 PL1 -3.00 dB
 SF01 125.7736214 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPO2 100.00 usec
 PL2 120.00 dB
 PL12 28.00 dB
 SF02 500.1317628 MHz

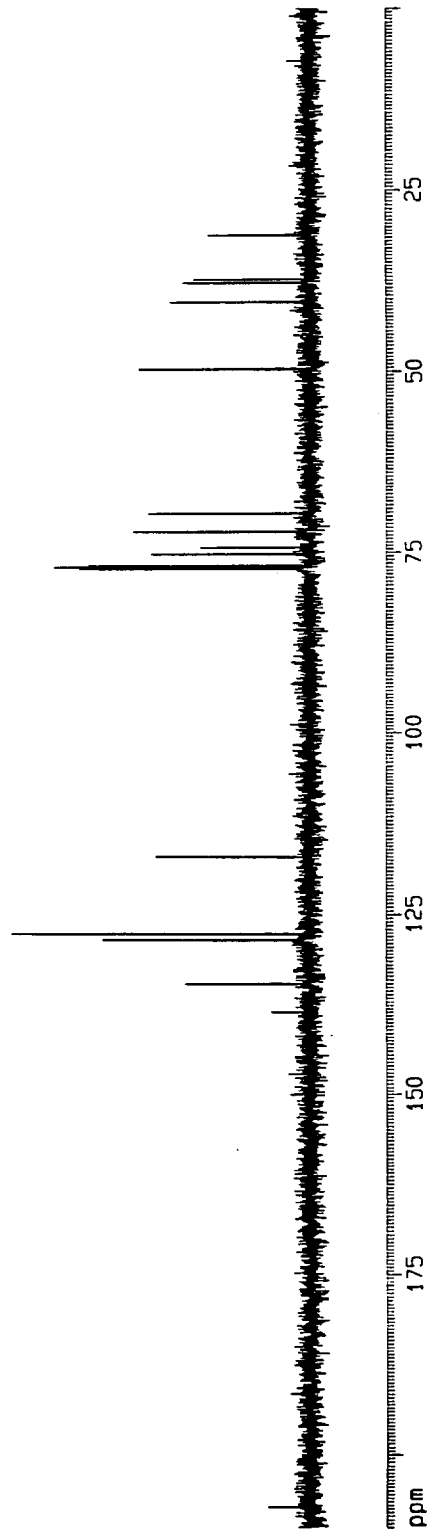
F2 - Processing parameters
 SI 32768
 SF 125.7577958 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 20.00 cm
 F1P 210.000 ppm
 F1 26409.14 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.50000 ppm/cm
 HZCM 1320.45691 Hz/cm



207.273 ppm

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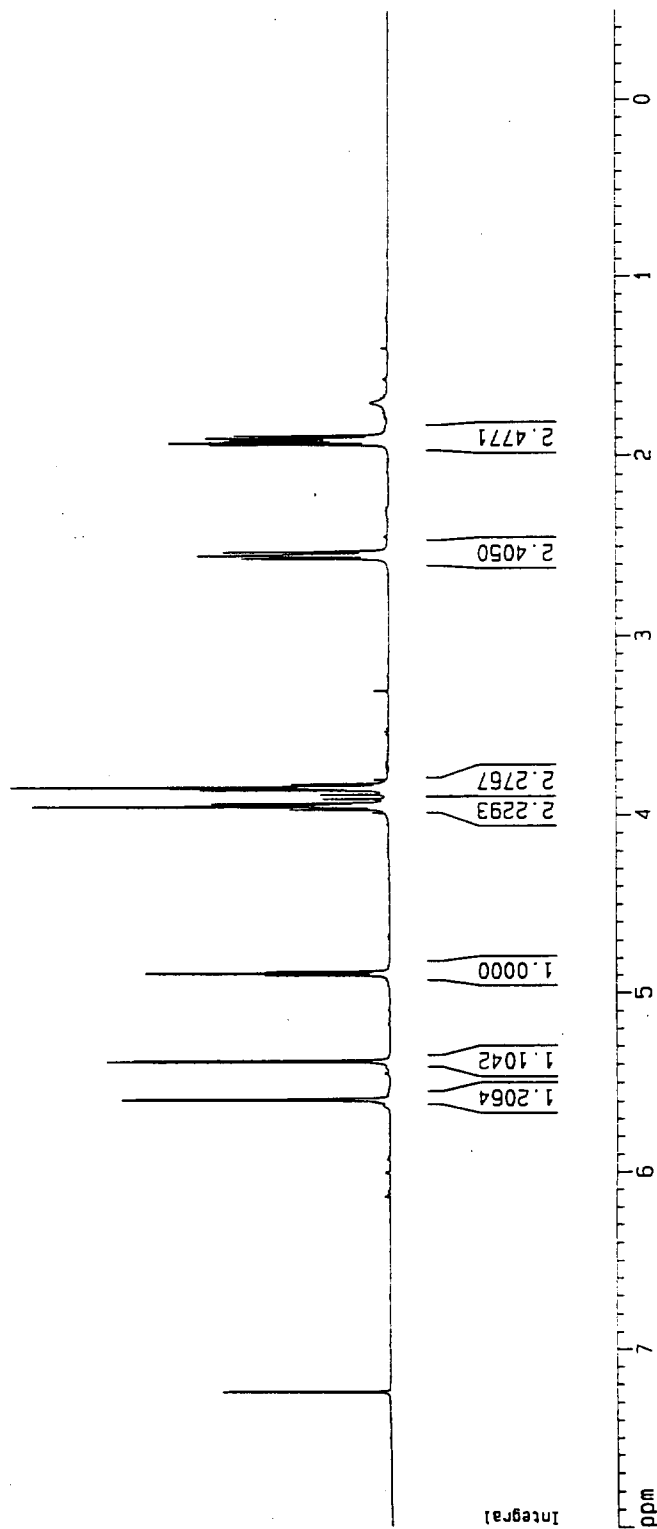
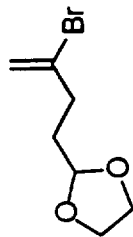


Current Data Parameters
 NAME dsrh1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20000919
 Time 11.46
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4882.812 Hz
 FIDRES 0.149012 Hz
 AQ 3.3554933 sec
 RG 80.5
 DW 102.400 usec
 DE 7.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 P1 7.70 usec
 SF01 400.1317512 MHz
 NUC1 1H
 PL1 -6.00 dB

F2 - Processing parameters
 SI 32768
 SF 400.1300172 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCH 0.42500 ppm/cm
 HZCM 170.05525 Hz/cm



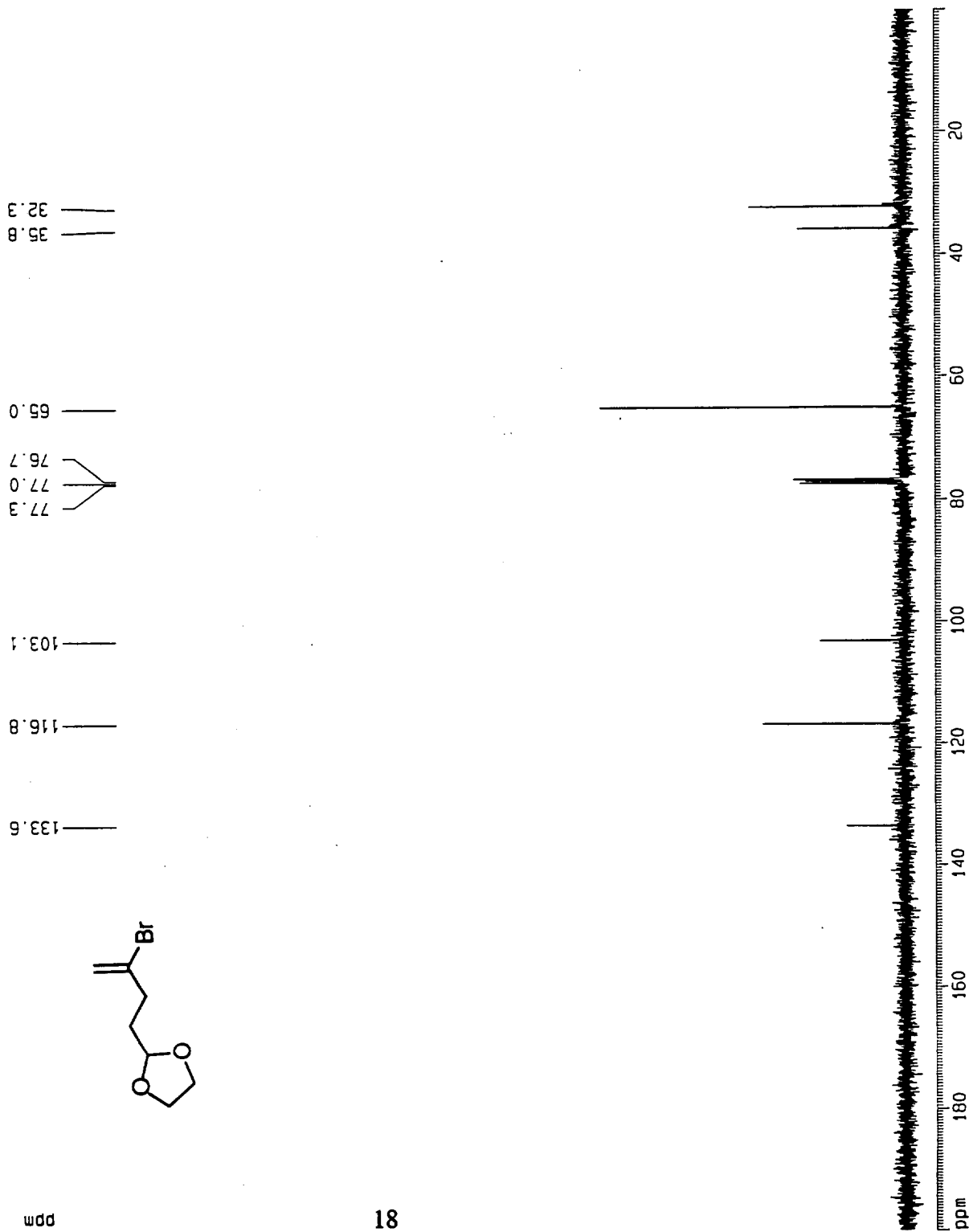
Current Data Parameters
 NAME carbon
 EXPNO 1
 PROCNO 1

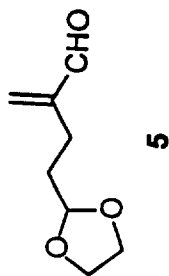
F2 - Acquisition Parameters
 Date_ 20000919
 Time 11:50
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zgpgc
 TD 65536
 SOLVENT CDCl3
 NS 49
 DS 0
 SMH 29239.766 Hz
 FIDRES 0.446163 Hz
 AQ 1.1207156 sec
 RG 2048
 DW 17.100 usec
 DE 7.50 usec
 TE 300.0 K

d11 0.0300000 sec
 PL12 24.00 dB
 CPDPRG2 waltz16
 PCPO2 105.00 usec
 SF02 400.1315715 MHz
 NUC2 1H
 PL2 0.00 dB
 D1 2.5000000 sec
 P1 8.00 usec
 SF01 100.6263545 MHz
 NUC1 13C
 PL1 -6.00 dB

F2 - Processing parameters
 SI 32768
 SF 100.6127724 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 200.000 ppm
 F1 20122.55 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1006.12769 Hz/cm





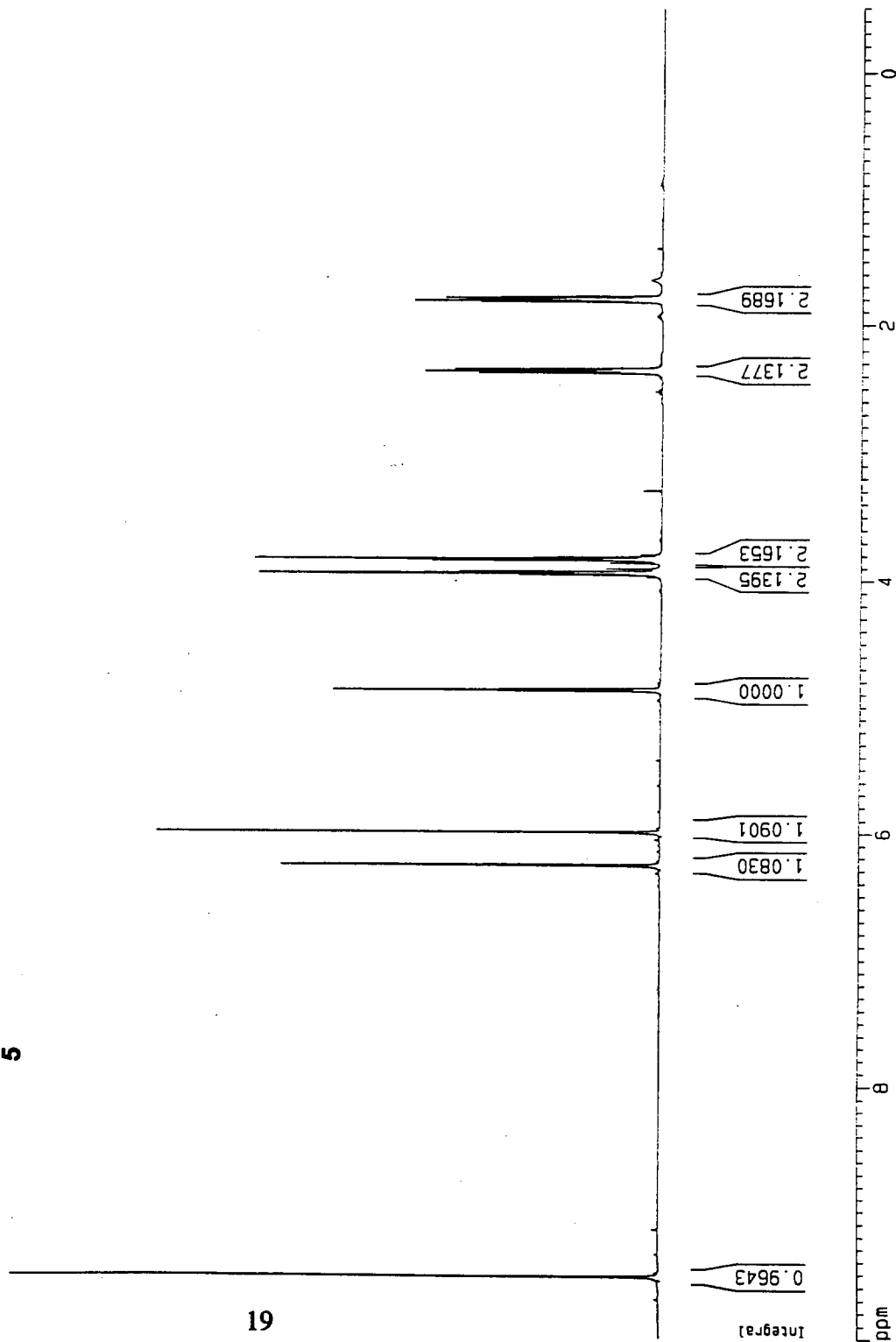
Current Data Parameters
 NAME proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001219
 Time 13.12
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6384500 sec
 RG 128
 DW 50.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 0.00 dB
 SF01 500.1318178 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300237 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 5001.30 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPRCM 0.52500 ppm/cm
 HZCM 262.56827 Hz/cm



Current Data Parameters
 NAME carbon
 EXPNO 1
 PROCNO 1

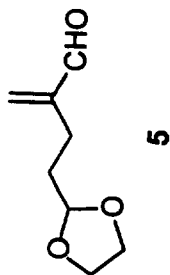
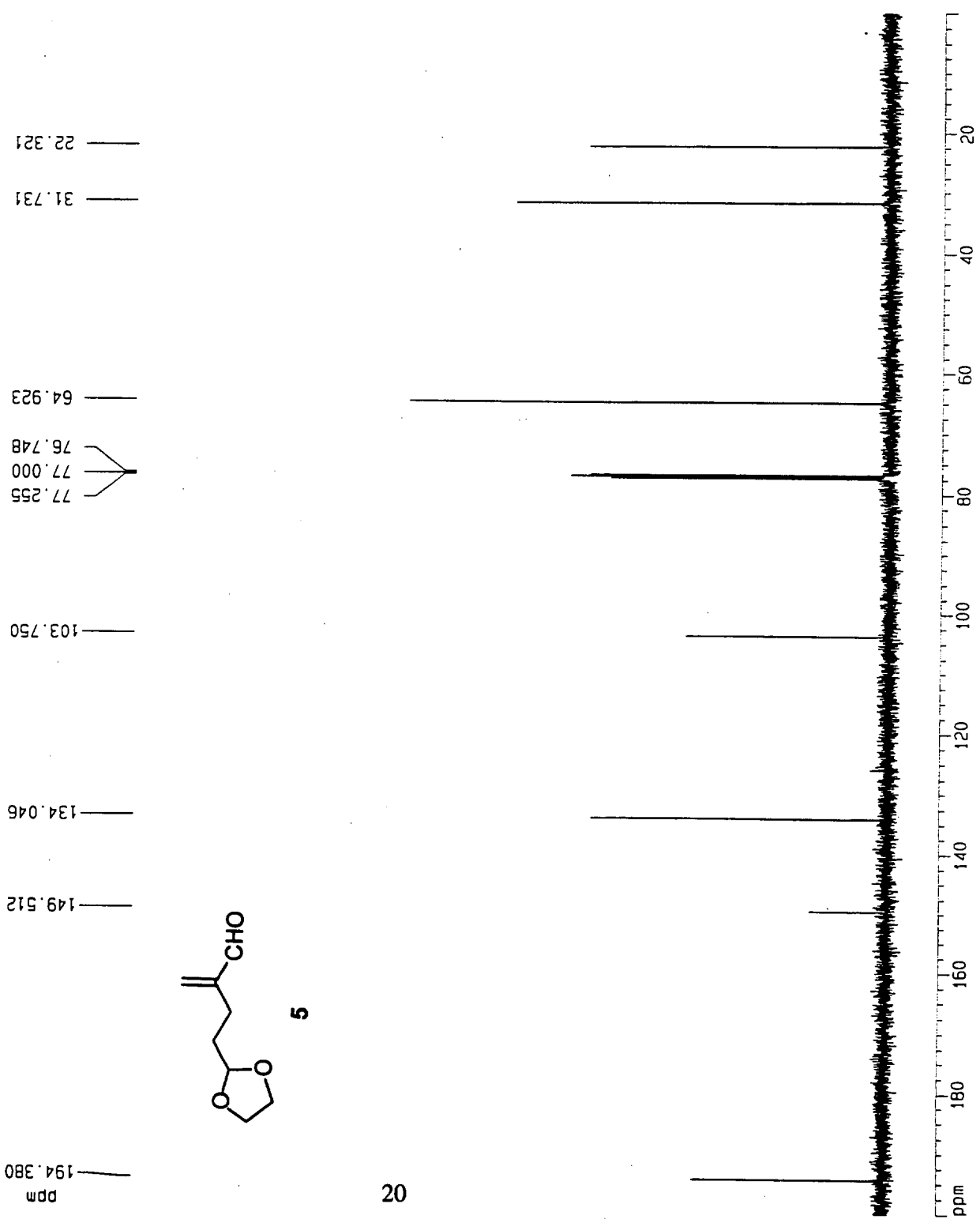
F2 - Acquisition Parameters
 Date_ 20001219
 Time 13.15
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TD 65536
 SOLVENT Tol
 NS 55
 DS 0
 SMH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 1024
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

***** CHANNEL f2 *****
 CPROG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.757946 MHz
 MOW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 20.00 cm
 FIP 200.000 ppm
 F1 25151.56 Hz
 F2 0.000 ppm
 F2P 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1257.57800 Hz/cm



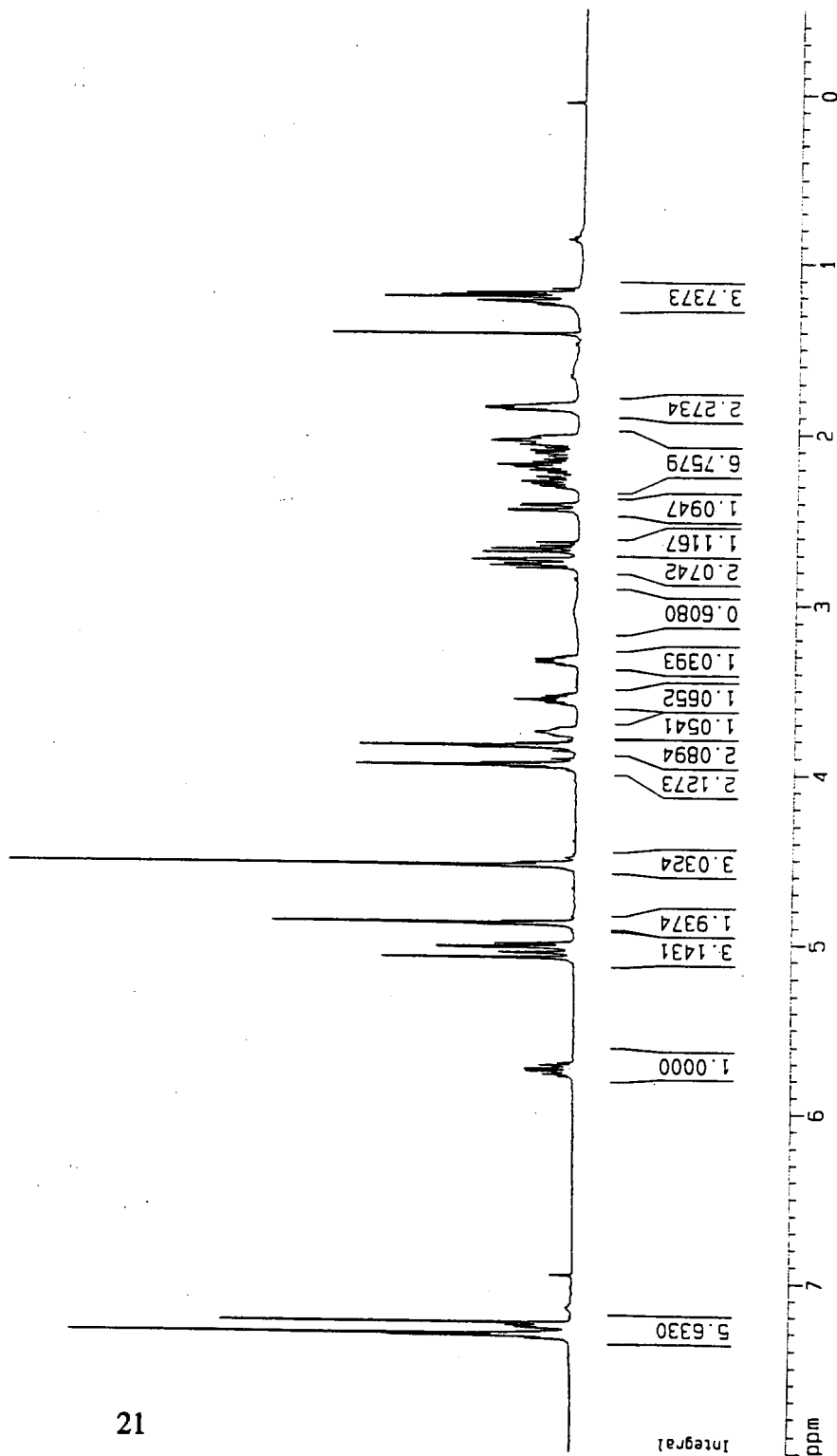
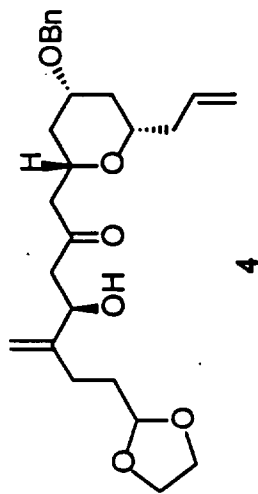
Current Data Parameters
 NAME proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001220
 Time 20.17
 INSTRUM spect
 PROBHD 5 mm ONP 1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6384500 sec
 RG 256
 DM 50.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 0.00 dB
 SF01 500.1318178 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300231 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 212.55527 Hz/cm



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Current Data Parameters
NAME          Carbon
EXPNO         1
PROCNO        1

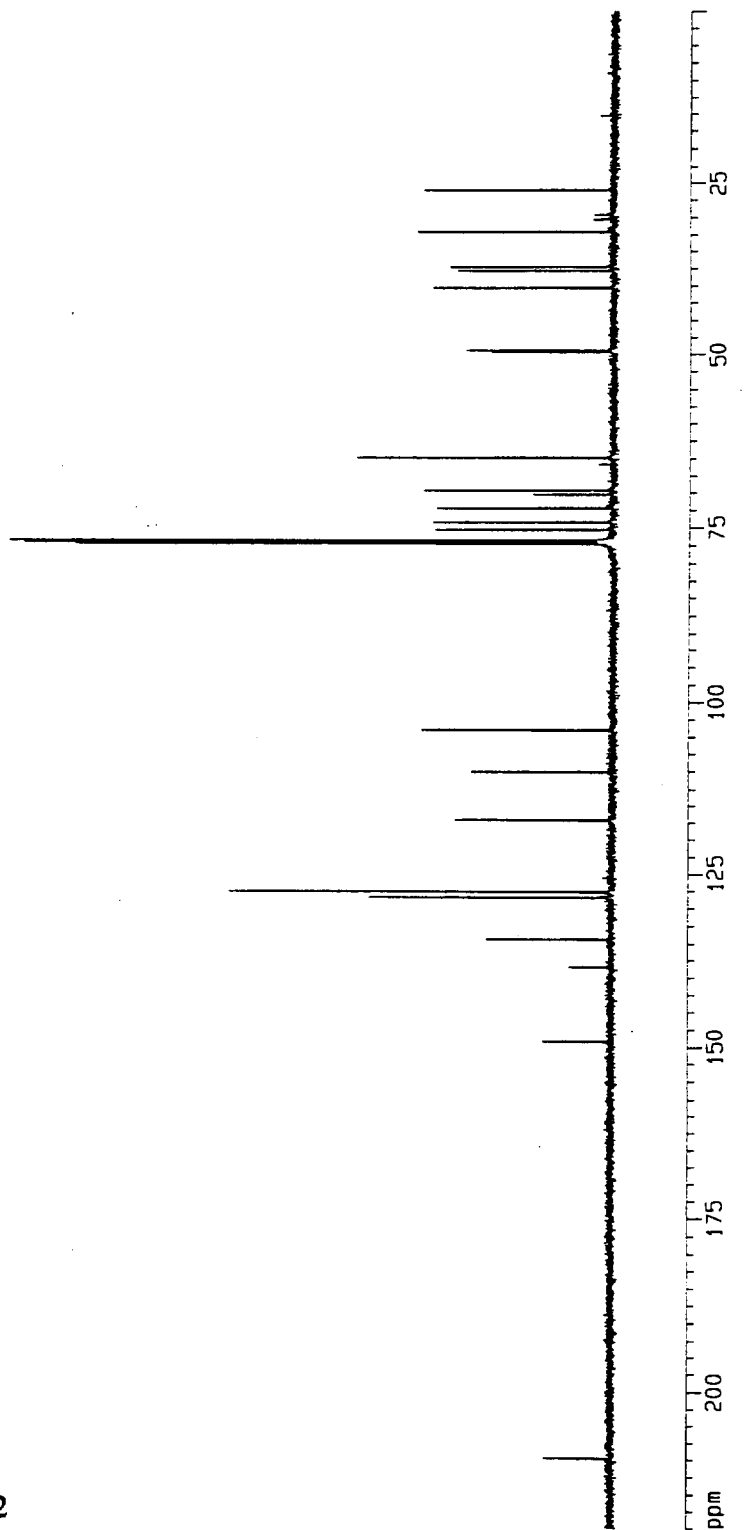
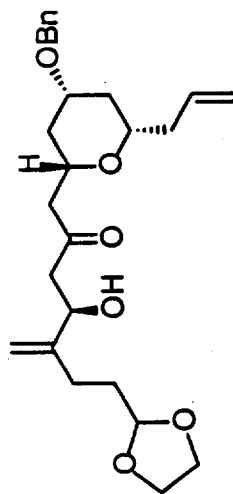
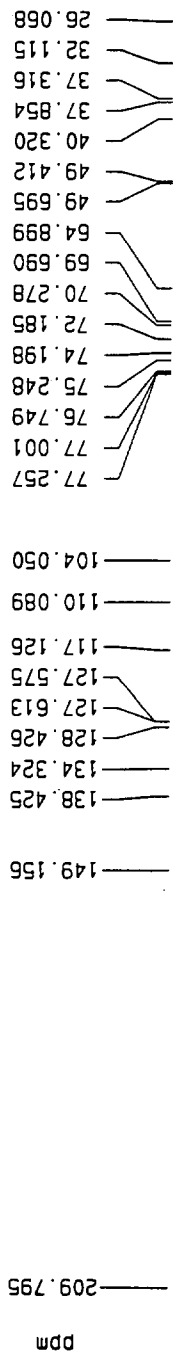
F2 - Acquisition Parameters
Date_         20001221
Time          0.37
INSTRUM      spect
PROBHD       5 mm QNP 1H
PULPROG      zgpg
TD            65536
SOLVENT      CDCl2
NS            1702
DS            0
SWH           39682.539 Hz
FIDRES       0.605507 Hz
AQ            0.8258036 sec
RG            1024
DM            12.600 usec
DE            7.50 usec
TE            300.0 K
D1            2.00000000 sec
d11           0.03000000 sec

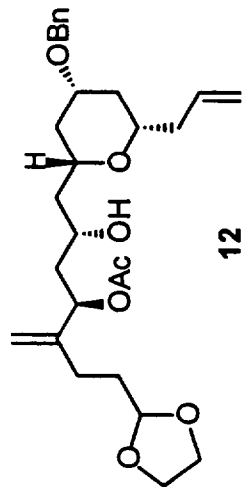
===== CHANNEL f1 =====
NUC1          13C
P1            5.00 usec
PL1           0.00 dB
SFO1          125.7736214 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2         100.00 usec
PL2           120.00 dB
PL12          20.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI            32768
SF            125.7577922 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

10 NMR plot parameters
CX            20.00 cm
F1P           220.000 ppm
F1            27666.71 Hz
F2P           0.000 ppm
F2            0.00 Hz
PPMCM         11.00000 ppm/cm
HZCM          1383.33569 Hz/cm
    
```





```

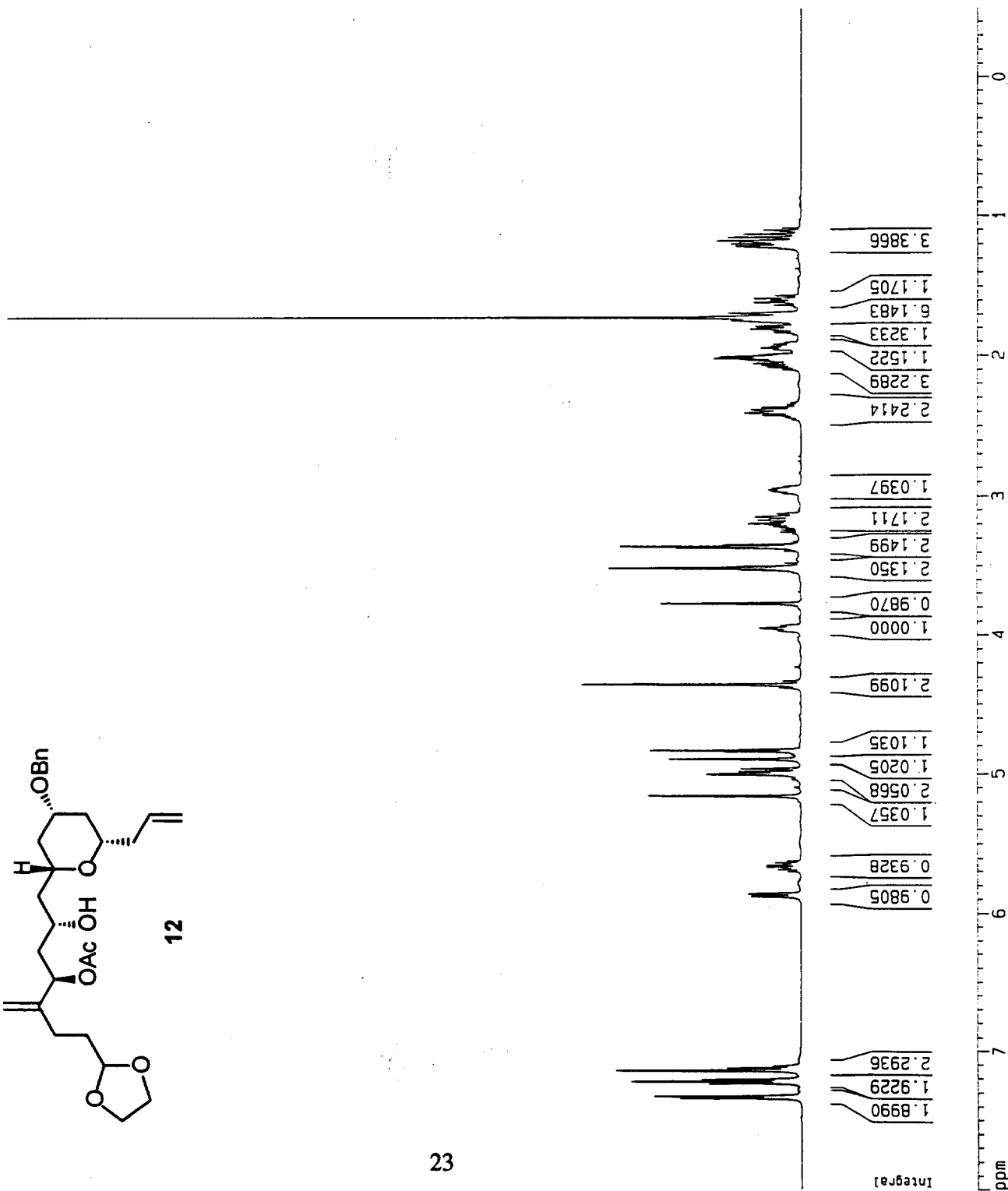
Current Data Parameters
NAME      proton
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20001221
Time     18:01
INSTRUM  spect
PROBHD   5 mm QNP 1H
PULPROG  zg
TD        32768
SOLVENT  C6D6
NS        4
DS        0
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        1.6384500 sec
RG         32
DM         50.000 usec
DE         4.50 usec
TE        300.0 K
TE        1.00000000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        5.00 usec
PL1       0.00 dB
SFO1     500.1318178 MHz

F2 - Processing parameters
SI        16384
SF        500.1300620 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
F1P       8.000 ppm
F1         4001.04 Hz
F2        -0.500 ppm
F2        -250.07 Hz
PPMCH    0.42500 ppm/cm
HZCM     212.55528 Hz/cm
    
```



```

Current Data Parameters
NAME          carbon
EXPNO         1
PROCNO        1

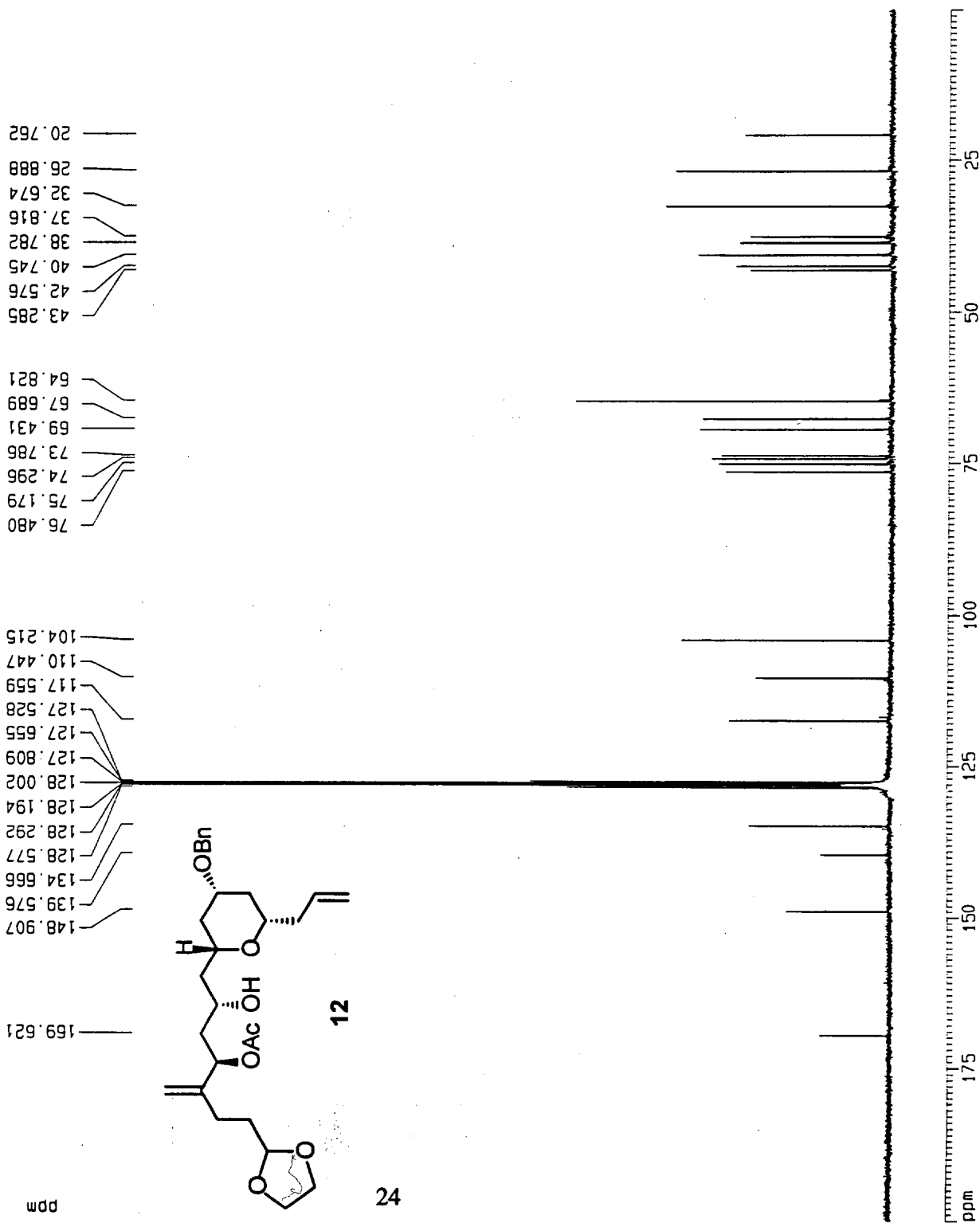
F2 - Acquisition Parameters
Date_         20001221
Time          18.07
INSTRUM       spect
PROBHD        5 mm QNP 1H
PULPROG       zgpg
TO            65536
SOLVENT       CDCl2
NS            101
DS            0
SWH           39682.539 Hz
FIDRES        0.605507 Hz
AQ            0.8258036 sec
RG            1024
DM            12.600 usec
DE            7.50 usec
TE            300.0 K
D1            2.0000000 sec
d11           0.0300000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            5.00 usec
PL1           0.00 dB
SF01          125.7736214 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         100.00 usec
PL2           120.00 dB
PL12          20.00 dB
SF02          500.1320005 MHz

F2 - Processing parameters
SI            32768
SF            125.7577666 MHz
HDM           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

10 NMR plot parameters
CX            20.00 cm
F1P           200.000 ppm
F1            25151.55 Hz
F2P           0.000 ppm
F2            0.00 Hz
PPMCM         10.00000 ppm/cm
HZCM          1257.57776 Hz/cm
    
```



```

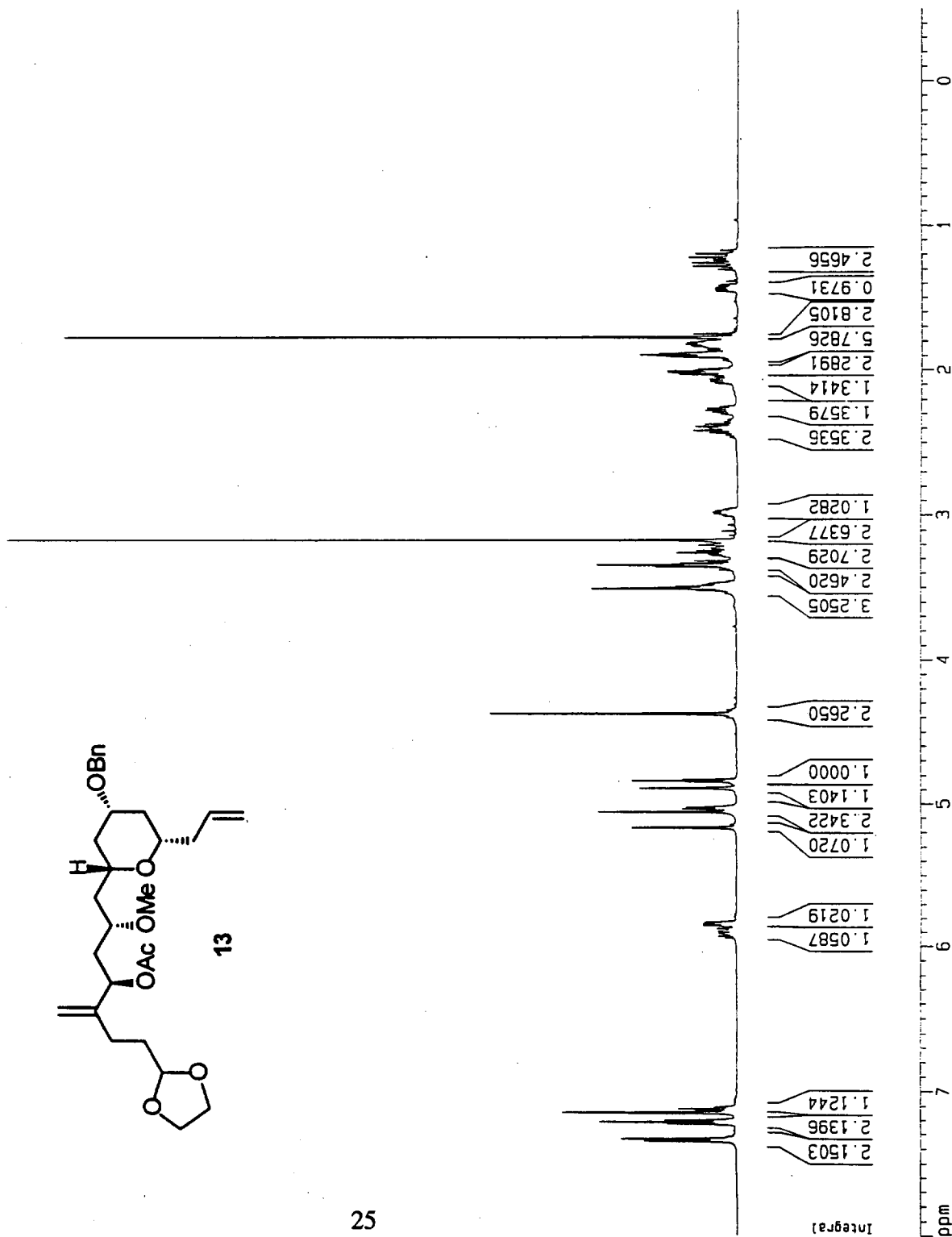
Current Data Parameters
NAME      proton
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20001222
Time     10.24
INSTRUM  spect
PROBHD   5 mm QNP 1H
PULPROG  zg
TD        32768
SOLVENT  C6D6
NS        4
DS        0
SMH       10000.000 Hz
FIDRES   0.305176 Hz
AQ        1.6384500 sec
RG        32
DM        50.000 usec
DE        4.50 usec
TE        300.0 K
D1        1.00000000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        5.00 usec
PL1       0.00 dB
SFO1      500.1318178 MHz

F2 - Processing parameters
SI        16384
SF        500.1300626 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
F1P       8.000 ppm
F1         4001.04 Hz
F2P       -0.500 ppm
F2        -250.07 Hz
PPMCHM    0.42500 ppm/cm
HZCM      212.55528 Hz/cm
    
```



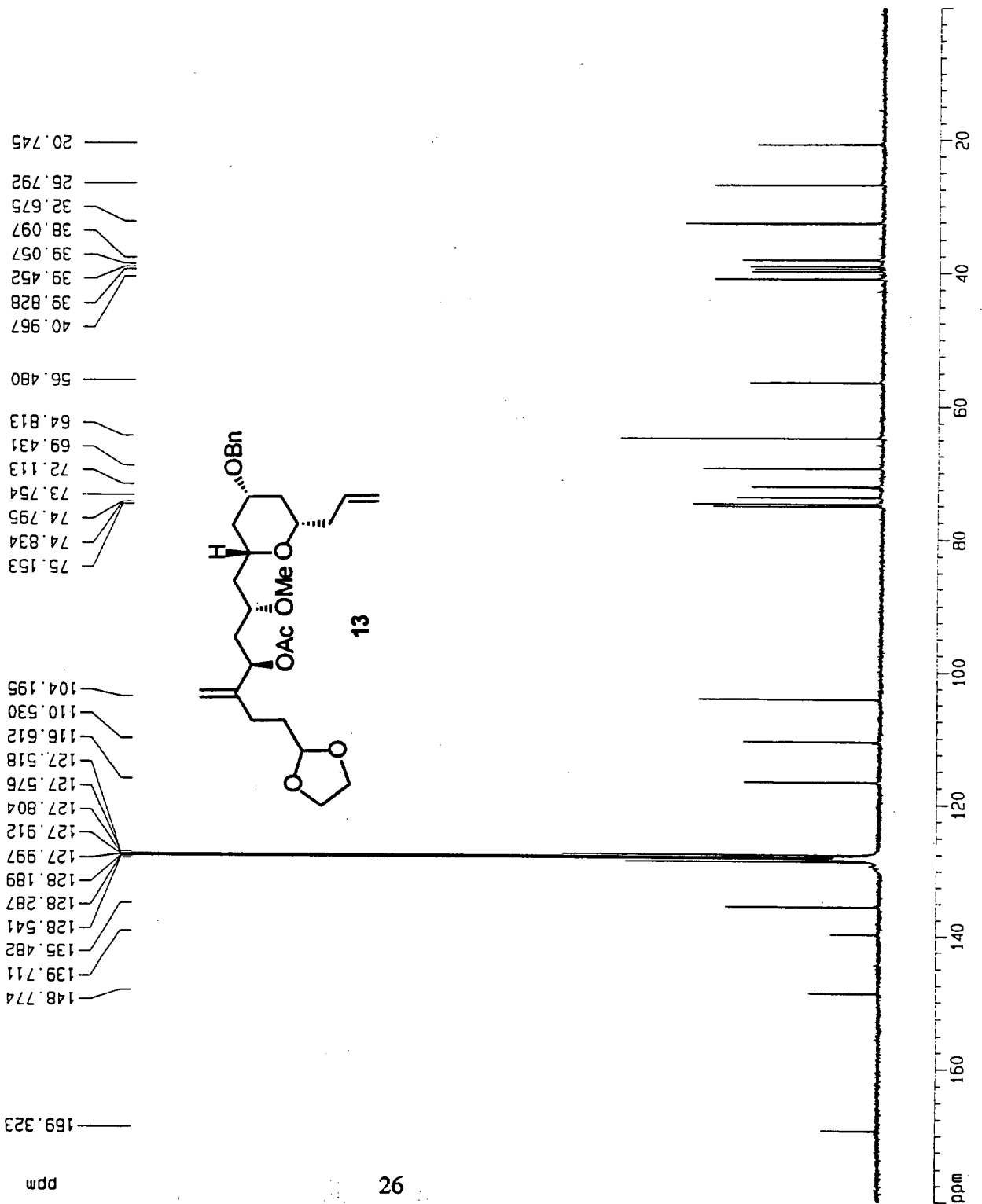
Current Data Parameters
 NAME carbon
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001222
 Time 10.33
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgdc
 TO 65536
 SOLVENT CDCl3
 NS 152
 DS 0
 SWH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 1024
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SFO1 125.7736214 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577666 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 1D NMR plot parameters
 CX 20.00 cm
 F1P 180.000 ppm
 F1 22636.40 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 9.00000 ppm/cm
 HZCM 1131.81995 Hz/cm



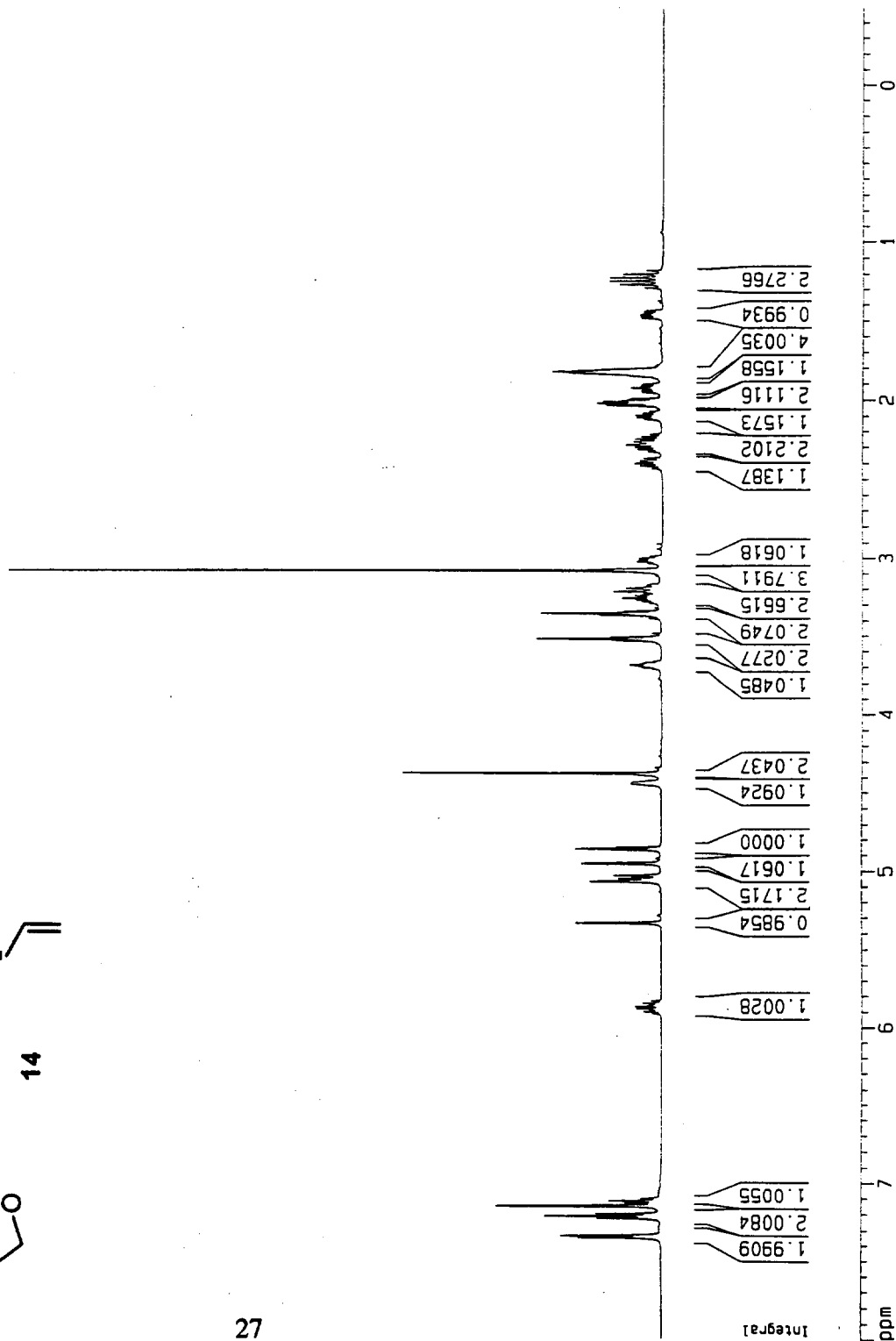
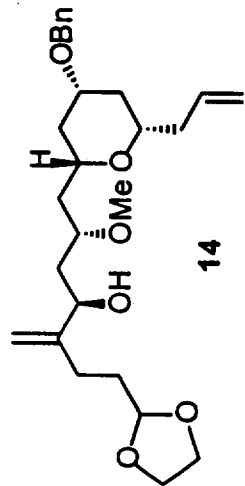
Current Data Parameters
 NAME proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001222
 Time 14.40
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT C606
 NS 4
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6384500 sec
 RG 32
 DM 50.000 usec
 DE 4.50 usec
 TE 300.0 K
 O1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 0.00 dB
 SF01 500.1318178 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300626 MHz
 HDW EH
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 212.55528 Hz/cm



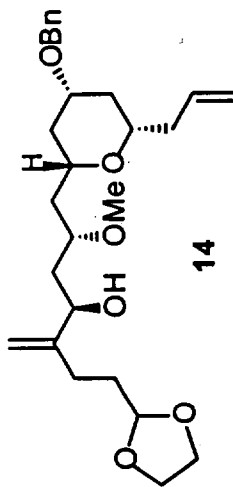
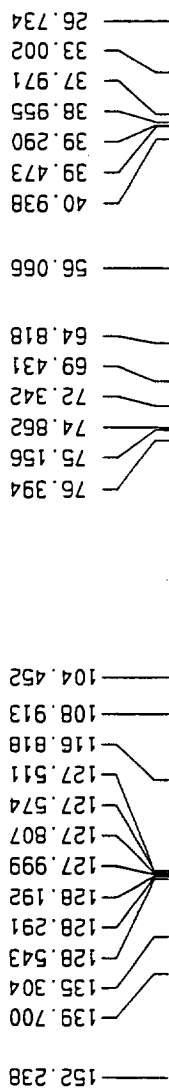
Current Data Parameters
 NAME carbon
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001222
 Time 14.47
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 123
 DS 0
 SWH 39882.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 1024
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

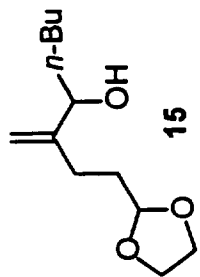
***** CHANNEL f1 *****
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577666 MHz
 NDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 ID NMR plot parameters
 CX 20.00 cm
 F1P 180.000 ppm
 F1 22636.40 Hz
 F2 0.000 ppm
 F2P 0.00 Hz
 PPMCH 9.00000 ppm/cm
 HZCM 1131.81995 Hz/cm



14



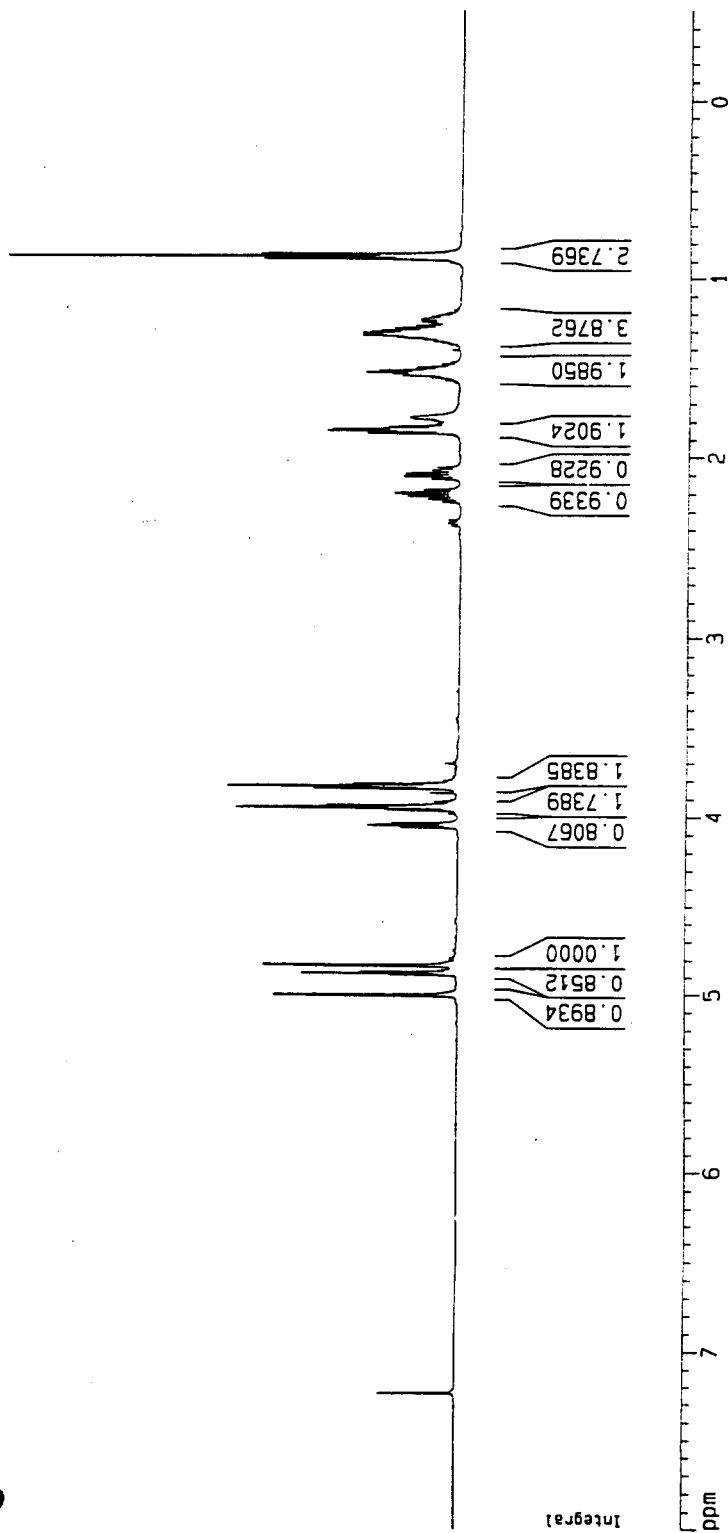
Current Data Parameters
 NAME sk-proton
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001206
 Time 17.52
 INSTRUM spect
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 4
 DS 0
 SMH 15015.015 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912244 sec
 RG 40.3
 DM 33.300 usec
 DE 7.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 4.00 dB
 SF01 500.1317628 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300234 MHz
 NDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 212.55527 Hz/cm



```

Current Data Parameters
NAME      Sk-carbon
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    2001206
Time     17.56
INSTRUM  spect
PROBHD   5 mm Multinu
PULPROG  zgdc
TD        65536
SOLVENT  CDCl3
NS        54
DS        1
SWH       39682.539 Hz
FIDRES   0.605507 Hz
AQ        0.8258036 sec
RG        9195.2
DM        12.600 usec
DE        4.50 usec
TE        300.0 K
D1        2.0000000 sec
d11       0.0300000 sec

===== CHANNEL f1 =====
NUC1      13C
P1        8.00 usec
PL1       -3.00 dB
SFO1     125.7736214 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    100.00 usec
PL2      120.00 dB
PL12     28.00 dB
SFO2     500.1317628 MHz

F2 - Processing parameters
SI        32768
SF        125.7577958 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

1D NMR plot parameters
CX        20.00 cm
F1P       160.000 ppm
F1        20121.25 Hz
F2P       0.000 ppm
F2        0.00 Hz
PP4CH    8.00000 ppm/cm
HZCH     1006.06238 Hz/cm
    
```

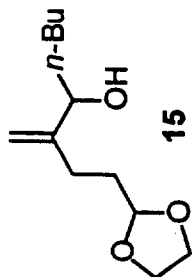
14.032
22.602
25.307
27.859
32.203
35.105

64.864
64.915
75.615
76.739
76.992
77.247

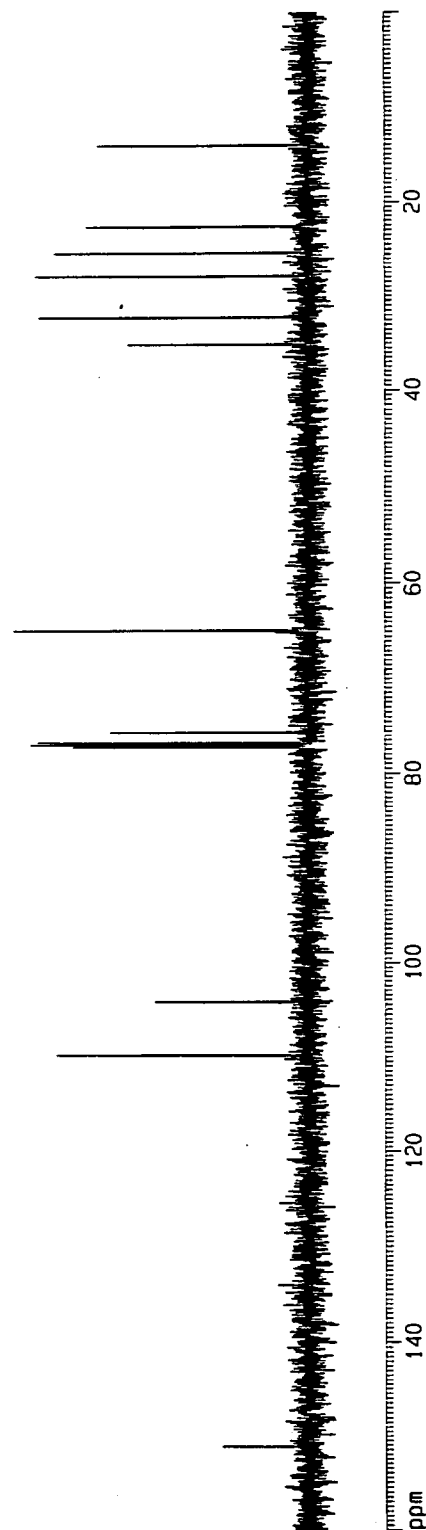
104.212
109.866

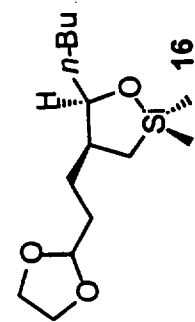
151.149

ppm



03





(18:15 mixture of diastereomers)

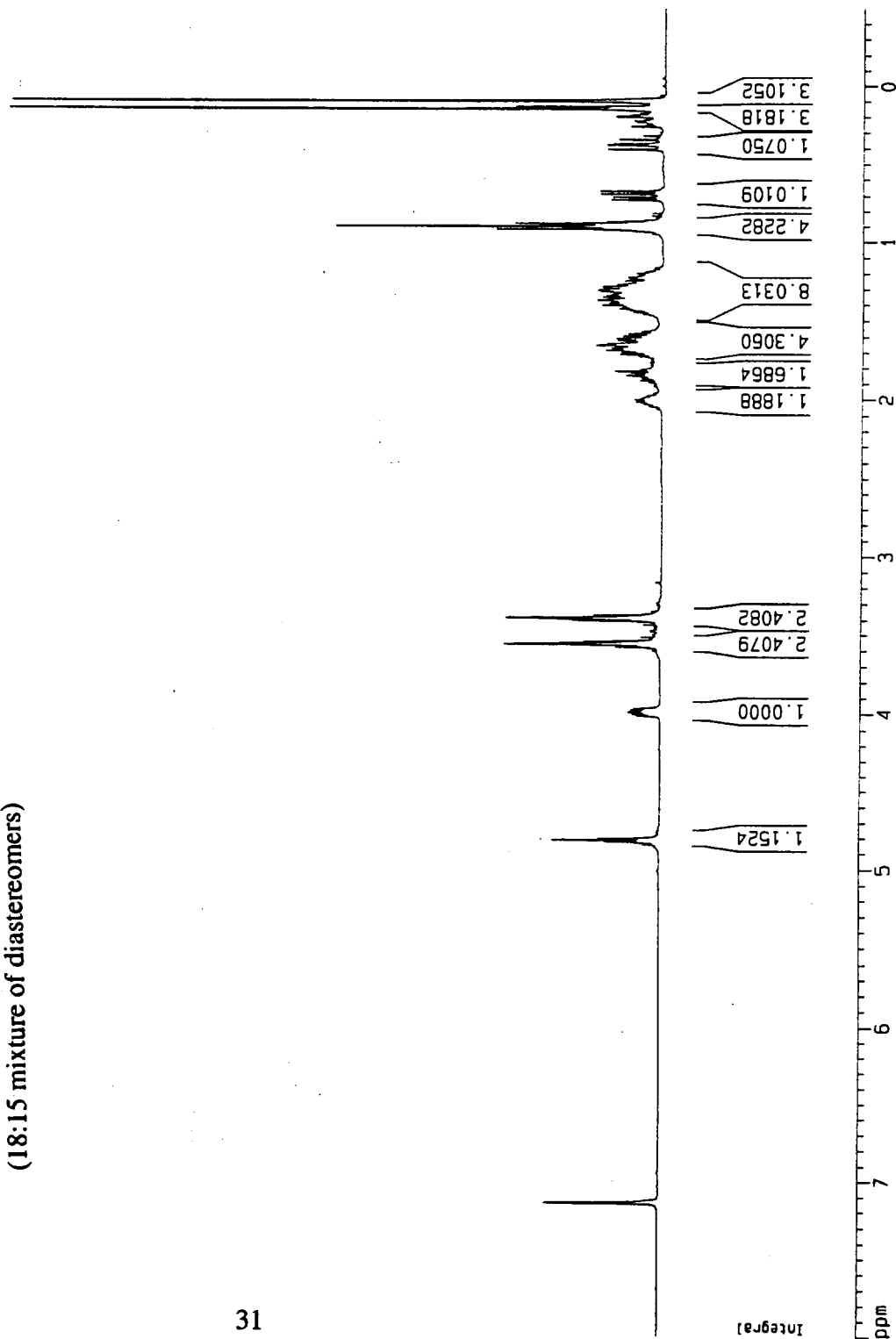
Current Data Parameters
 NAME sk-proton
 EXPNO 2
 PROCNO 1

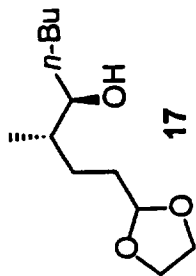
F2 - Acquisition Parameters
 Date_ 20001211
 Time 18.51
 INSTRUM spect
 PRBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT C6D6
 NS 4
 DS 0
 SWH 6510.417 Hz
 FIDRES 0.198682 Hz
 AQ 2.5166323 sec
 RG 22.6
 DM 76.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 8.50 usec
 PL1 0.00 dB
 SF01 400.1319246 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1299966 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 170.05525 Hz/cm





(18:15 mixture of diastereomers)

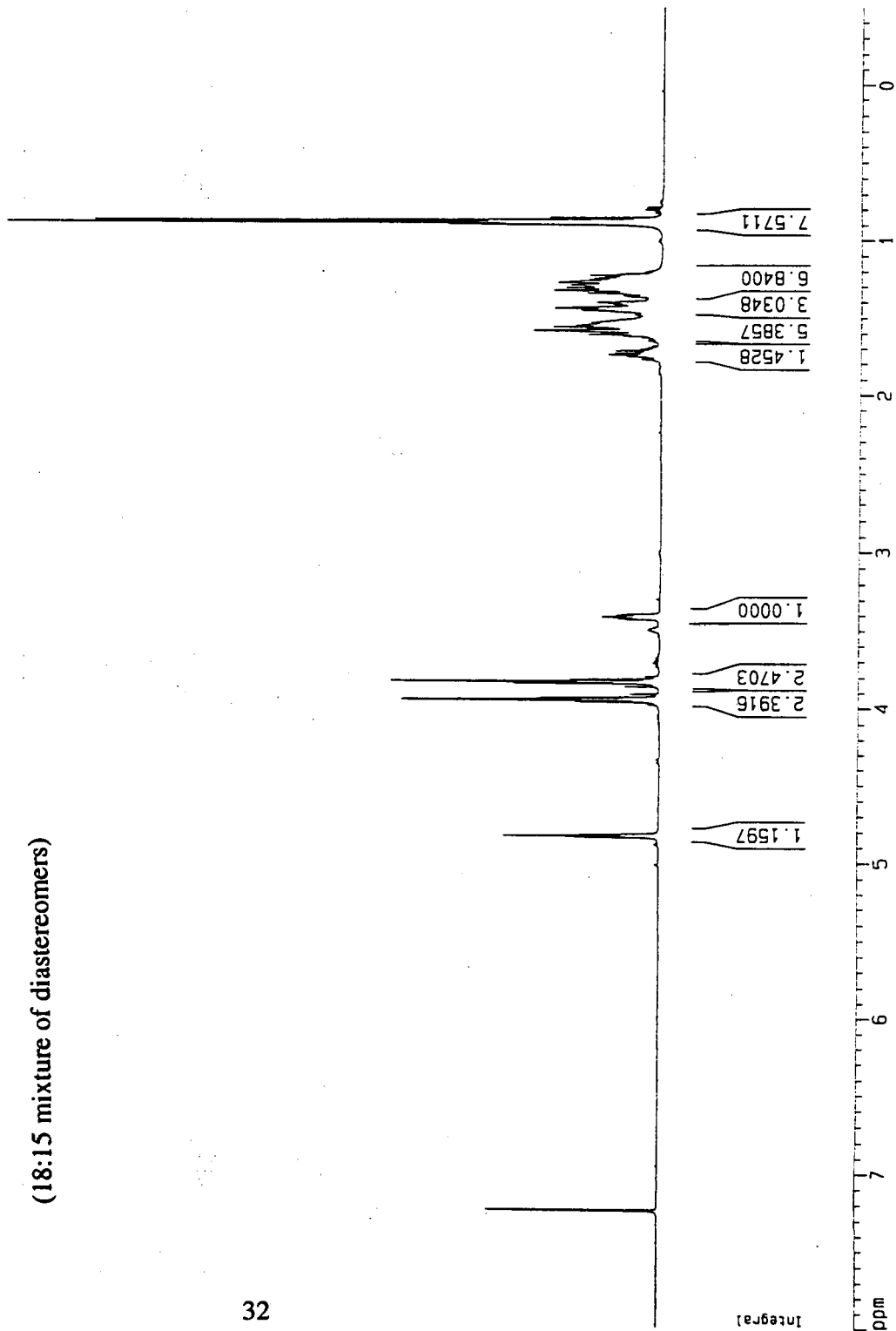
Current Data Parameters
 NAME proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001215
 Time 12.08
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 128
 DM 83.200 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 0.00 dB
 SFO1 500.1318178 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300232 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1 8.000 ppm
 F2 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCH 0.42500 ppm/cm
 HZCM 212.55527 Hz/cm



```

Current Data Parameters
NAME      carbon
EXPNO    1
PROCNO   1

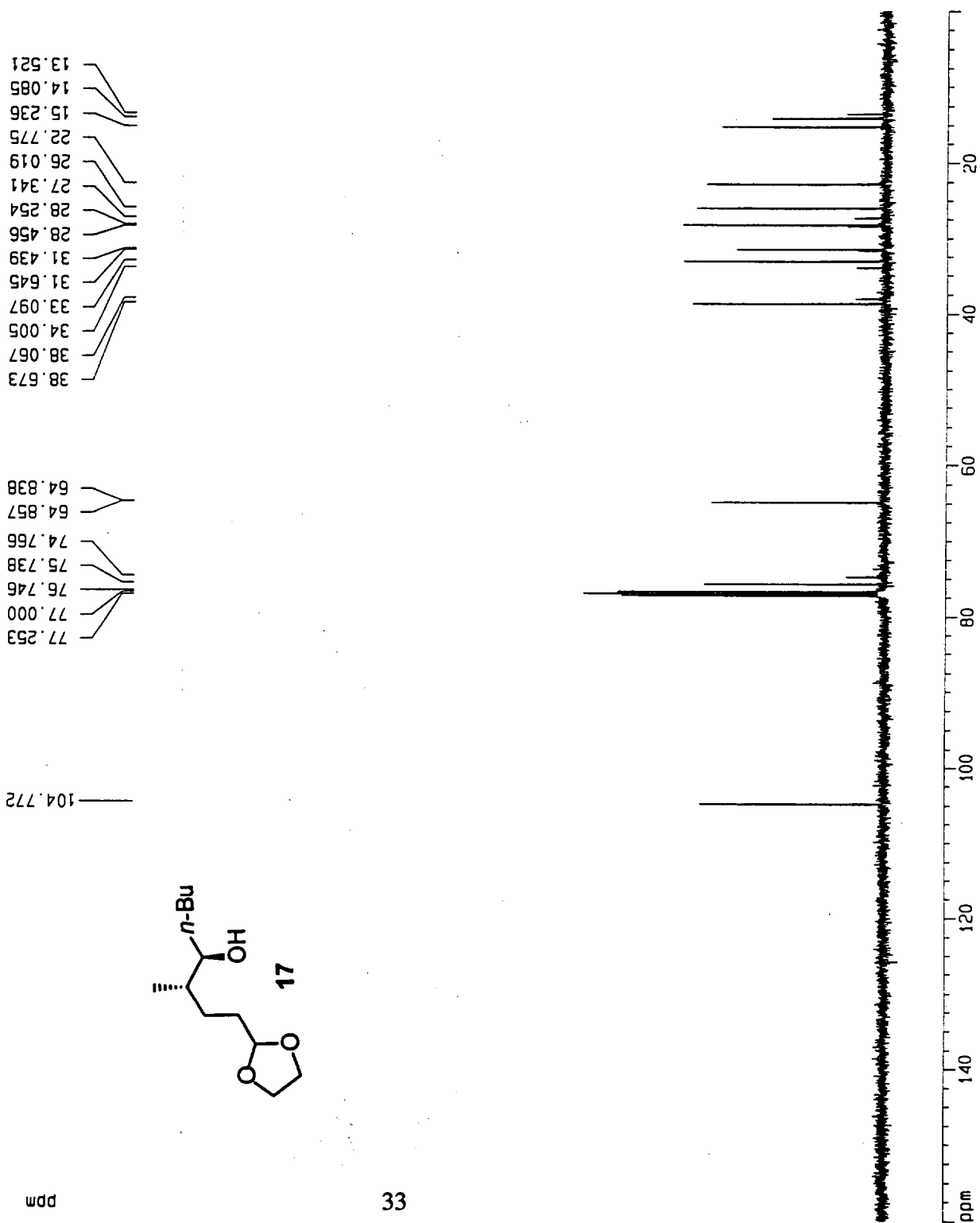
F2 - Acquisition Parameters
Date_    20001215
Time     12.14
INSTRUM  spect
PROBHD   5 mm QNP 1H
PULPROG  zgpg
TO       65536
SOLVENT  CDCl3
NS       103
DS       0
SWH      39682.539 Hz
FIDRES   0.605507 Hz
AQ       0.8258036 sec
RG       2048
DM       12.600 usec
DE       7.50 usec
TE       300.0 K
D1       2.00000000 sec
d11      0.03000000 sec

===== CHANNEL f1 =====
NUC1     13C
P1       5.00 usec
PL1      0.00 dB
SF01     125.7736214 MHz

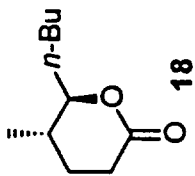
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    100.00 usec
PL2      120.00 dB
PL12     20.00 dB
SF02     500.1320005 MHz

F2 - Processing parameters
SI       32768
SF       125.7577934 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR pilot parameters
CX       20.00 cm
F1P      160.000 ppm
F1       20121.25 Hz
F2       0.000 ppm
PPMCM    8.00000 ppm/cm
HZCM     1006.06232 Hz/cm
    
```



ppm



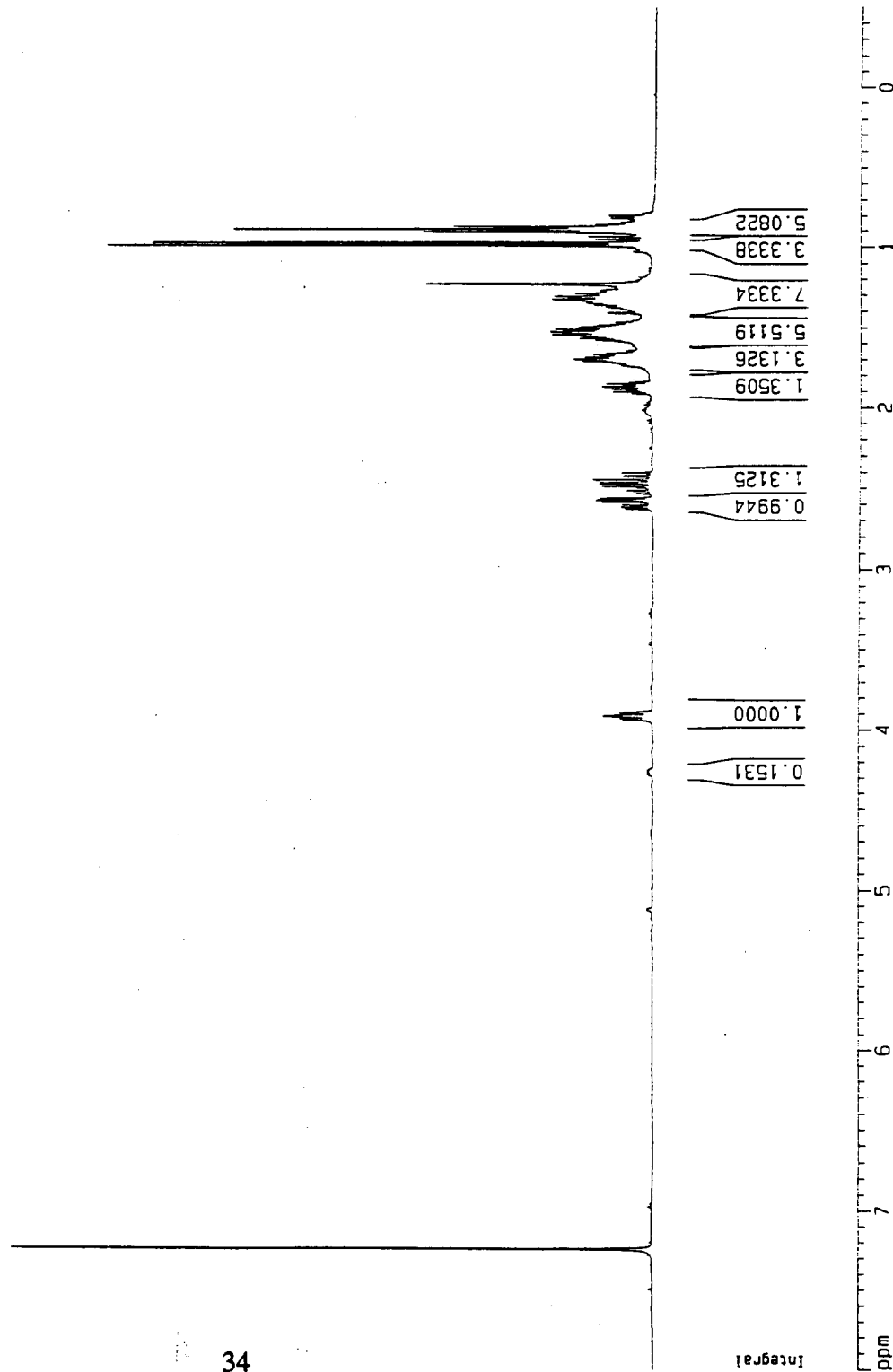
Current Data Parameters
 NAME sk-proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001218
 Time 18.17
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TO 32768
 SOLVENT COCl3
 NS 16
 DS 0
 SWH 6510.417 Hz
 FIDRES 0.198682 Hz
 AQ 2.5166323 sec
 RG 322.5
 DW 76.800 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.50 usec
 PL1 0.00 dB
 SF01 400.1319246 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300175 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 3201.04 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 170.05525 Hz/cm



Current Data Parameters
 NAME carbon
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20001218
 Time 16.32
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TO 65536
 SOLVENT tcl
 NS 418
 DS 0
 SWH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 1024
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

***** CHANNEL f1 *****
 NUC1 ¹³C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

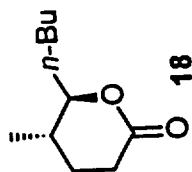
***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577922 MHz
 NQM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

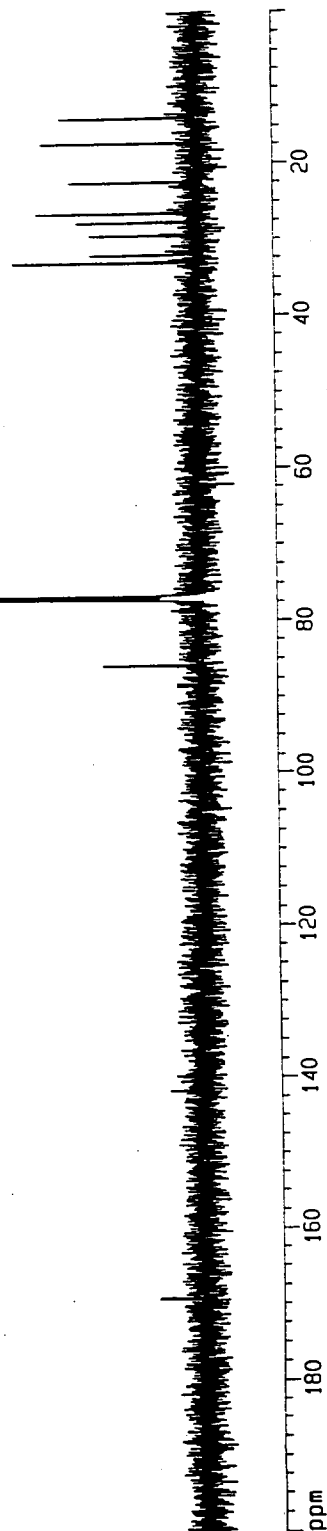
1D NMR plot parameters
 CX 20.00 cm
 FIP 200.000 ppm
 F1 25151.56 Hz
 F2 0.000 ppm
 F2 0.00 Hz
 PPMCM 10.00000 ppm/cm
 HZCM 1257.57788 Hz/cm

13.9530
 17.4397
 22.5813
 26.5591
 27.7903
 29.5261
 32.1848
 33.1169

76.7498
 77.0030
 77.2584
 85.8953



ppm



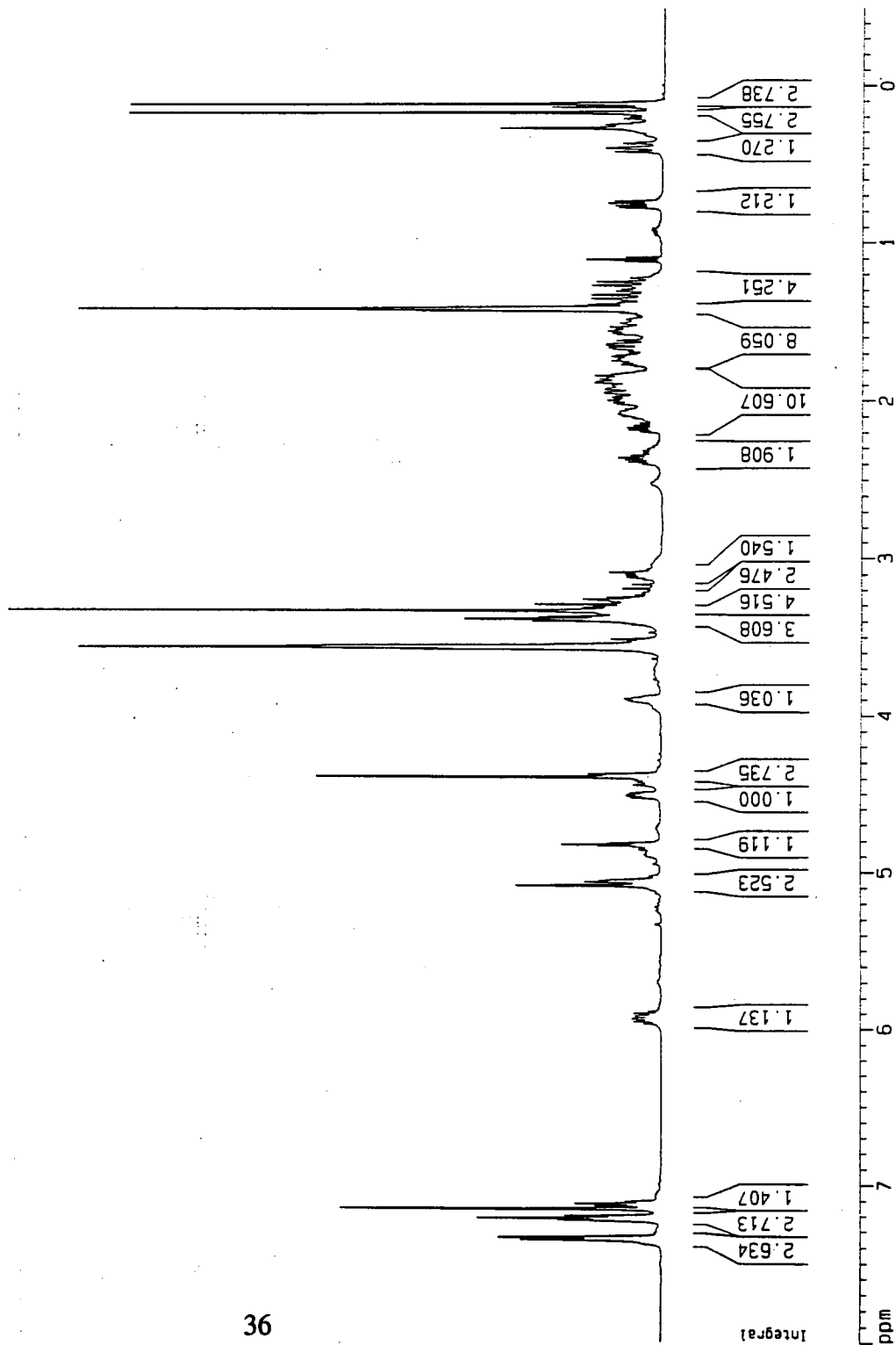
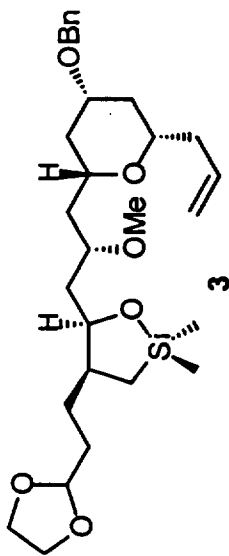
Current Data Parameters
 NAME proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001222
 Time 17.25
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT C6D6
 NS 4
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6384500 sec
 RG 32
 DM 50.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 0.00 dB
 SF01 500.1318178 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300620 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPHCM 0.42500 ppm/cm
 HZCM 212.55528 Hz/cm



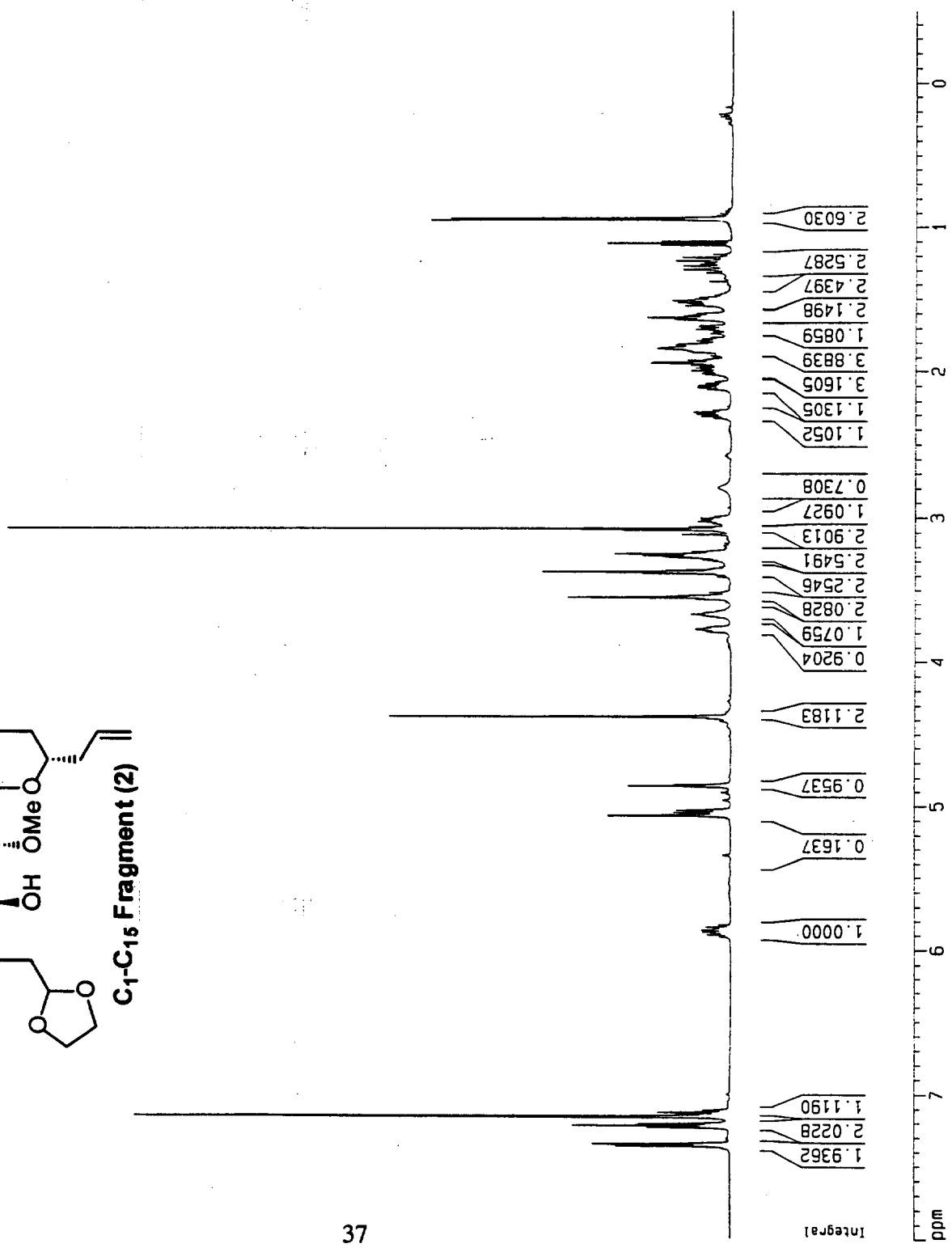
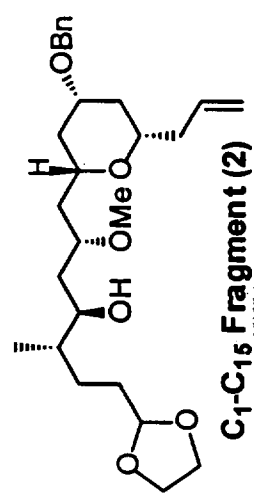
Current Data Parameters
 NAME proton
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001222
 Time 20.24
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zg
 TD 32768
 SOLVENT C6D6
 NS 4
 DS 0
 SMH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 1.6384500 sec
 RG 64
 DM 50.000 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.00 usec
 PL1 0.00 dB
 SF01 500.1318178 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300620 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 8.000 ppm
 F1 4001.04 Hz
 F2P -0.500 ppm
 F2 -250.07 Hz
 PPMCM 0.42500 ppm/cm
 HZCM 212.55528 Hz/cm



Current Data Parameters
 NAME carbon
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001222
 Time 20:31
 INSTRUM spect
 PROBHD 5 mm QNP 1H
 PULPROG zgpg
 TD 65536
 SOLVENT CDCl3
 NS 111
 DS 0
 SWH 39682.539 Hz
 FIDRES 0.605507 Hz
 AQ 0.8258036 sec
 RG 1024
 DM 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 0.00 dB
 SF01 125.7736214 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 20.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577666 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 180.000 ppm
 F1 22636.40 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 9.00000 ppm/cm
 HZCM 1131.81995 Hz/cm

