

**Supporting Information for**  
**“Facile Preparation of Allenic Hydroxyketones via Rearrangement of**  
**Propargylic Alcohols” Michael E. Jung and Joseph Pontillo**

**General Procedures.** All reactions were conducted under an argon atmosphere. THF was distilled over sodium/benzophenone, benzene over calcium hydride and methanol over magnesium methoxide. Commercially available propargyl alcohol, 3-butyne-2-ol, 2-butyne-1-ol, 3-methyl-1-pentyne-3-ol, and 1-phenyl-2-propyne-1-ol (Aldrich Chemical Co.) were distilled prior to use. All other chemicals were used as received from Aldrich Chemical Co. Thin layer chromatography (TLC) was done on silica gel (0.25 mm thickness) aluminum plates. Plates were viewed under UV light (254 nm) and with *p*-anisaldehyde dip. Column chromatography was performed on 230-400 mesh silica gel. 400 MHz  $^1\text{H}$  and 100 MHz  $^{13}\text{C}$  NMR spectra were recorded on a Bruker ARX-400 spectrometer, while infrared spectra were recorded on a Nicolet Fourier transform spectrometer. High resolution mass spectra were performed by the UCLA Mass Spectrometry Laboratory.

**2-Methyl-1-phenoxy-3-butyne-2-ol (5):** To (trimethylsilyl)acetylene (0.051 g, 0.52 mmol) in 2 mL THF at  $-78\text{ }^\circ\text{C}$  was added *n*-BuLi (1.88 M in pentane, 0.26 mL, 0.48 mmol) dropwise, and stirring was continued for 20 min. 1-Phenoxyacetone (**8**, 0.060 g, 0.40 mmol) in 0.5 mL THF was then added dropwise *via* cannula. This was followed by 2 x 0.25 mL THF rinses, and stirring was continued at  $-78\text{ }^\circ\text{C}$  for 1 h. Ammonium chloride (0.100 g, 1.87 mmol) was then added in one portion, and the mixture was warmed to room temperature. After diluting with 15 mL of  $\text{Et}_2\text{O}$ , the mixture was successively washed with 5 mL saturated aqueous  $\text{NH}_4\text{Cl}$  and 2 x 5 mL brine. Drying over  $\text{MgSO}_4$  and concentrating at reduced pressure gave a yellow oil (0.098 g), which was then dissolved in 3 mL MeOH. To this solution was added  $\text{K}_2\text{CO}_3$  (0.061 g, 0.44 mmol) in one portion, and the resulting suspension was stirred for 2 h. The mixture was quenched with 2 mL sat. aqueous  $\text{NH}_4\text{Cl}$ , then extracted with 4 x 5 mL  $\text{Et}_2\text{O}$ . The combined extracts were washed with 2 x 10 mL brine, dried over  $\text{MgSO}_4$ , and concentrated to give a yellow oil. Subjection of the crude to flash column chromatography (20%  $\text{Et}_2\text{O}$ /pentane) gave propargyl alcohol **5** as a pale yellow oil (0.067 g, 95%):  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  7.33-7.21 (m, 2H), 7.01-6.88 (m, 3H), 4.06 (d,  $J=8.9$  Hz, 1H), 3.95 (d,  $J=8.9$  Hz, 1H), 3.12 (s, 1H), 2.51 (s, 1H), 1.63 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ) 158.4, 129.6, 121.5, 114.9, 85.4, 75.2, 72.2, 67.0, 25.9; IR (neat) 3411, 3291, 3000, 2929, 1599, 1496, 1246, 1051, 754, 693  $\text{cm}^{-1}$ .

**2-Methyl-1-phenoxy-3-buten-2-ol (15):** A mixture of 2-methyl-1-phenoxy-3-butyne-2-ol (**5**) (0.096 g, 0.54 mmol), quinoline (0.055 g, 0.42 mmol) and 5% Pd on  $\text{BaSO}_4$  (0.016 g, 0.0075 mmol) in 5 mL absolute  $\text{EtOH}$  was hydrogenated (balloon) for 10 min. Following filtration through a pipette column of Celite (3 cm) and elution with a further 3 x 2 mL  $\text{Et}_2\text{O}$ , concentration at reduced pressure gave a yellow oil, which was

subjected to flash column chromatography (20% Et<sub>2</sub>O/pentane). 2-Methyl-1-phenoxy-3-buten-2-ol (**15**) was isolated as a colorless oil (0.091 g, 94%): <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.31-7.28 (m, 2H), 7.00-6.93 (m, 3H), 6.03 (dd, *J*=10.8, 6.5 Hz, 1H), 5.41 (d, *J*=17 Hz, 1H), 5.20 (d, *J*=10.8 Hz, 1H), 3.89 (d, *J*=8.9 Hz, 1H), 3.84 (d, *J*=8.9 Hz, 1H), 2.95 (s, 1H), 1.41 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) 158.6, 141.8, 129.5, 121.2, 114.7, 114.0, 74.8, 72.5, 24.5; IR (neat) 3413, 2936, 2929, 1599, 1497, 1246, 1049, 754, 691 cm<sup>-1</sup>.

**General Procedure: Allenic Hydroxyketones via Rearrangement of Propargylic Alcohols.** To a mixture of 0.26 mmol of the propargylic alcohol and 0.013 mmol Rh<sub>2</sub>(OAc)<sub>4</sub> in 2 mL benzene at room temperature was added, dropwise over 5 min, a solution of 0.52 mmol 3-diazo-2-butanone (**6**) in 2 mL benzene. The yellow solution was then immediately filtered through a pipette column of Celite (3 cm), eluted with a further 3 x 2 mL Et<sub>2</sub>O, and carefully concentrated under reduced pressure (5 °C stillpot bath, 12 mm Hg) to give crude yellow oils, which were subjected to flash column chromatography (Et<sub>2</sub>O/pentane).

**3-Hydroxy-3,6-dimethyl-7-phenyloxyhepta-4,5-dien-2-ones, (9) and (10):** Employment of the general procedure with 2-methyl-1-phenoxy-3-butyne-2-ol (**5**) gave 0.037 g of a pale yellow liquid (58%, 76% based on 0.011 g recovered starting material) as an inseparable 9:1 mixture of diastereomers. Major diastereomer **9**: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.31-7.26 (m, 2H), 6.98-6.90 (m, 3H), 5.28-5.27 (m, 1H), 4.54 (m, 2H), 3.93 (s, 1H), 2.23 (s, 3H), 1.86 (d, *J*=2.9 Hz, 3H), 1.43 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 209.7, 201.3, 158.3, 129.5, 121.2, 115.0, 101.3, 97.1, 77.6, 69.0, 24.2, 23.4, 15.7. Minor diastereomer **10**: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.31-7.26 (m, 2H), 6.98-6.90 (m, 3H), 5.24 Hz (m, 1 H), 4.54 (m, 2H), 3.96 (s, 1H), 2.20 (s, 3H), 1.86 (d, *J*=2.9 Hz, 3H), 1.41 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 209.7, 201.3, 158.3, 129.1, 121.2, 114.8, 101.3, 97.1, 77.4, 69.0, 24.2, 23.4, 15.7. IR (mixture, neat) 3467, 3000, 2928, 1969, 1713, 1599, 1496, 1356, 1238, 756, 693 cm<sup>-1</sup>; HRMS (CI) *m/e* (M+NH<sub>4</sub><sup>+</sup>) calcd for C<sub>15</sub>H<sub>22</sub>NO<sub>3</sub> 264.1600, found 264.1593.

**3-Hydroxy-3-methyl-6-phenylhexa-4,5-dien-2-ones (14a):** Employment of the general procedure with 1-phenyl-2-propyne-1-ol (**13a**) gave 0.039 g of a pale yellow liquid (75%) as an inseparable 3:1 mixture of diastereomers. Major diastereomer **14a**: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.35-7.22 (m, 5H), 6.45 (d, *J*=6.4 Hz, 1H), 5.66 (d, *J*=6.4 Hz, 1H), 4.13 (s, 1H), 2.31 (s, 3H), 1.54 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 209.4, 204.7, 133.0, 128.8, 127.7, 126.9, 99.9, 98.7, 78.0, 24.2, 23.7. Minor diastereomer **14a**: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.35-7.22 (m, 5H), 6.43 (d, *J*=6.4 Hz, 1H), 5.65 (d, *J*=6.4 Hz, 1H), 4.19 (s, 1H), 2.29 (s, 3H), 1.54 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 209.4, 204.5, 133.0, 128.8, 127.7, 126.9, 100.3, 98.7, 77.6, 24.2, 23.6. IR (mixture, neat) 3459, 3033, 2988, 1950, 1713, 1458, 1356, 1129, 783, 693 cm<sup>-1</sup>.

**3-Hydroxy-3-methylhexa-4,5-dien-2-ones (14b):** Employment of the general procedure with propargyl alcohol (**13b**) gave 0.022 g of **14b** as a colorless liquid (68%): <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 5.19 (t, *J*=6.7 Hz, 1H), 4.96 (dd, *J*=4.0, 1.6 Hz, 2H), 4.03

(s, 1H), 2.22 (s, 3H), 1.45 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  209.6, 207.5, 95.3, 79.0, 51.6, 24.0, 23.5; IR (neat) 3467, 2988, 2853, 1956, 1714, 1358, 1128, 858, 615  $\text{cm}^{-1}$ .

**3-Hydroxy-3-methylhepta-4,5-dien-2-ones (14c):** Employment of the general procedure with 3-butyn-2-ol (**13c**) gave 0.023 g of a pale yellow liquid (62%) as an inseparable 3:2 mixture of diastereomers. Major diastereomer **14c**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  5.41-5.35 (m, 1H), 5.14-5.12 (m, 1H), 4.00 (s, 1H), 2.22 (s, 3H), 1.72 (d,  $J=3.2$  Hz, 3H), 1.44 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  209.4, 204.0, 129.1, 95.6, 90.2, 24.0, 23.5, 13.9. Minor diastereomer **14c**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  5.41-5.35 (m, 1H), 5.14-5.12 (m, 1H), 3.98 (s, 1H), 2.24 (s, 3H), 1.70 (d,  $J=3.2$  Hz, 3H), 1.44 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  209.4, 204.0, 129.1, 95.6, 90.2, 24.0, 23.4, 13.8. IR (mixture, neat) 3465, 2990, 2930, 1950, 1714, 1356, 1130, 1086, 872, 629  $\text{cm}^{-1}$ .

**3-Hydroxy-3,6-dimethylocta-4,5-dien-2-ones (14d):** Employment of the general procedure with 3-methyl-1-pentyn-3-ol (**13d**) gave 0.020 g of a pale yellow liquid (45%) as an inseparable 3:2 mixture of diastereomers. Major diastereomer **14d**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  5.14-5.10 (m, 1H), 3.97 (s, 1H), 2.23 (s, 3H), 2.03-2.01 (m, 2H), 1.75 (s, 3H), 1.43 (s, 3H), 1.03 (t,  $J=6.8$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  210.4, 200.4, 106.6, 96.3, 77.7, 27.0, 23.9, 23.4, 18.6, 12.2. Minor diastereomer **14d**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  5.14-5.10 (m, 1H), 3.90 (s, 1H), 2.23 (s, 3H), 2.03-2.01 (m, 2H), 1.74 (s, 3H), 1.43 (s, 3H), 1.03 (t,  $J=6.8$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  210.3, 200.4, 106.7, 95.9, 77.8, 26.9, 24.1, 23.6, 18.8, 12.3. IR (mixture, neat) 3465, 2990, 2930, 1950, 1714, 1356, 1130, 1086, 872, 629  $\text{cm}^{-1}$ .

**3-Hydroxy-3,4-dimethylhexa-4,5-dien-2-ones (14e):** Employment of the general procedure with 2-butyn-1-ol (**13e**) gave 0.016 g of **14e** as a pale yellow liquid (44%):  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  4.90-4.83 (m, 2H), 4.09 (s, 1H), 2.20 (s, 3H), 1.56 (t,  $J=3.1$  Hz, 3H), 1.46 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  210.5, 206.5, 101.4, 77.4, 57.7, 23.6, 23.1, 13.8; IR (neat) 3463, 2986, 2924, 2857, 1958, 1713, 1358, 1129, 855, 617  $\text{cm}^{-1}$ .

**(E) and (Z) 3-Hydroxy-3,6-dimethyl-7-phenoxyhept-5-en-2-ones (16) and (17):** Employment of the general procedure with 2-methyl-1-phenoxy-3-buten-2-ol (**15**) gave 0.043 g of a colorless liquid (67%, 92% based on 0.013 g recovered starting material) as an inseparable 7:1 mixture of diastereomers. Major diastereomer **16**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  7.29-7.25 (m, 2H), 6.93-6.87 (m, 3H), 5.49 (t,  $J=4.6$  Hz, 1H), 4.43 (s, 2H), 3.76 (s, 1H), 2.50 (d,  $J=6.6$  Hz, 2H), 2.17 (s, 3H), 1.75 (s, 3H), 1.37 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  221.8, 158.6, 135.0, 129.4, 121.7, 120.8, 114.9, 78.7, 73.5, 37.6, 25.1, 23.8, 14.2. Minor diastereomer **17**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  7.29-7.25 (m, 2H), 6.93-6.87 (m, 3H), 5.35 (t,  $J=4.6$  Hz, 1H), 4.40 (s, 2H), 3.84 (s, 1H), 2.50 (d,  $J=6.6$  Hz, 2H), 2.19 (s, 3H), 1.85 (s, 3H), 1.38 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  221.8, 158.6, 135.0, 129.4, 121.7, 120.8, 114.6, 78.7, 73.5, 37.6, 25.1, 23.8, 14.2. IR (mixture, neat) 3476, 2983, 2926, 1709, 1599, 1495, 1356, 1242, 1172, 1008, 756, 693  $\text{cm}^{-1}$ .

**2-Hydroxy-2,5-dimethyl-1-phenyl-6-phenoxyhepta-3,4-dien-1-ones (19):** Employment of the general procedure with 2-methyl-1-phenoxy-3-buten-2-ol (**5**) and

$\alpha$ -diazopropiophenone (**18**) gave 0.044 g of a pale yellow liquid (55%, 81% based on 0.015 g recovered starting material) as an inseparable (>15:1) mixture of diastereomers. Major diastereomer **19**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  8.09 (d,  $J=7.8$  Hz, 2H), 7.24-7.45 (m, 5 H), 6.95-6.86 (m, 3H), 5.58-5.56 (m, 1H), 4.47 (s, 1H), 4.46 (s, 3H), 1.86 (s, 3H), 1.65 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  201.9, 201.7, 158.3, 133.3, 133.2, 130.2, 129.4, 128.4, 128.3, 121.1, 115.0, 101.6, 98.3, 68.8, 26.4, 15.2. IR (neat) 3444, 2984, 2932, 1970, 1676, 1599, 1495, 1448, 1238, 754, 693  $\text{cm}^{-1}$ .

**3-Hydroxy-6-methyl-3-phenyl-7-phenoxyhepta-4,5-dien-2-ones 20**: Employment of a modification of the general procedure (addition of  $\text{Rh}_2(\text{OAc})_4$  in one portion to a mixture of 2-methyl-1-phenoxy-3-butyn-2-ol (**5**) and  $\alpha$ -diazopropiophenone (**18**) in 4 mL benzene at room temperature, and stirring 15 min) gave 0.042 g of a pale yellow liquid (52%, 75% based on 0.014 g recovered starting material) as an inseparable (>15:1) mixture of isomers. Major diastereomer **20**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  7.52-7.26 (m, 7 H), 6.96-6.87 (m, 3H), 5.84-5.81 (m, 1H), 4.55 (s, 3H), 4.41 (s, 1H), 2.09 (s, 3H), 1.87 (d,  $J=3.2$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  207.1, 201.2, 158.2, 140.3, 129.6, 129.5, 128.6, 126.7, 121.1, 114.9, 101.5, 95.5, 82.0, 68.7, 24.7, 15.7. IR (neat) 3449, 3100, 2950, 2932, 1970, 1713, 1599, 1495, 1449, 1238, 1172, 756, 693  $\text{cm}^{-1}$ .

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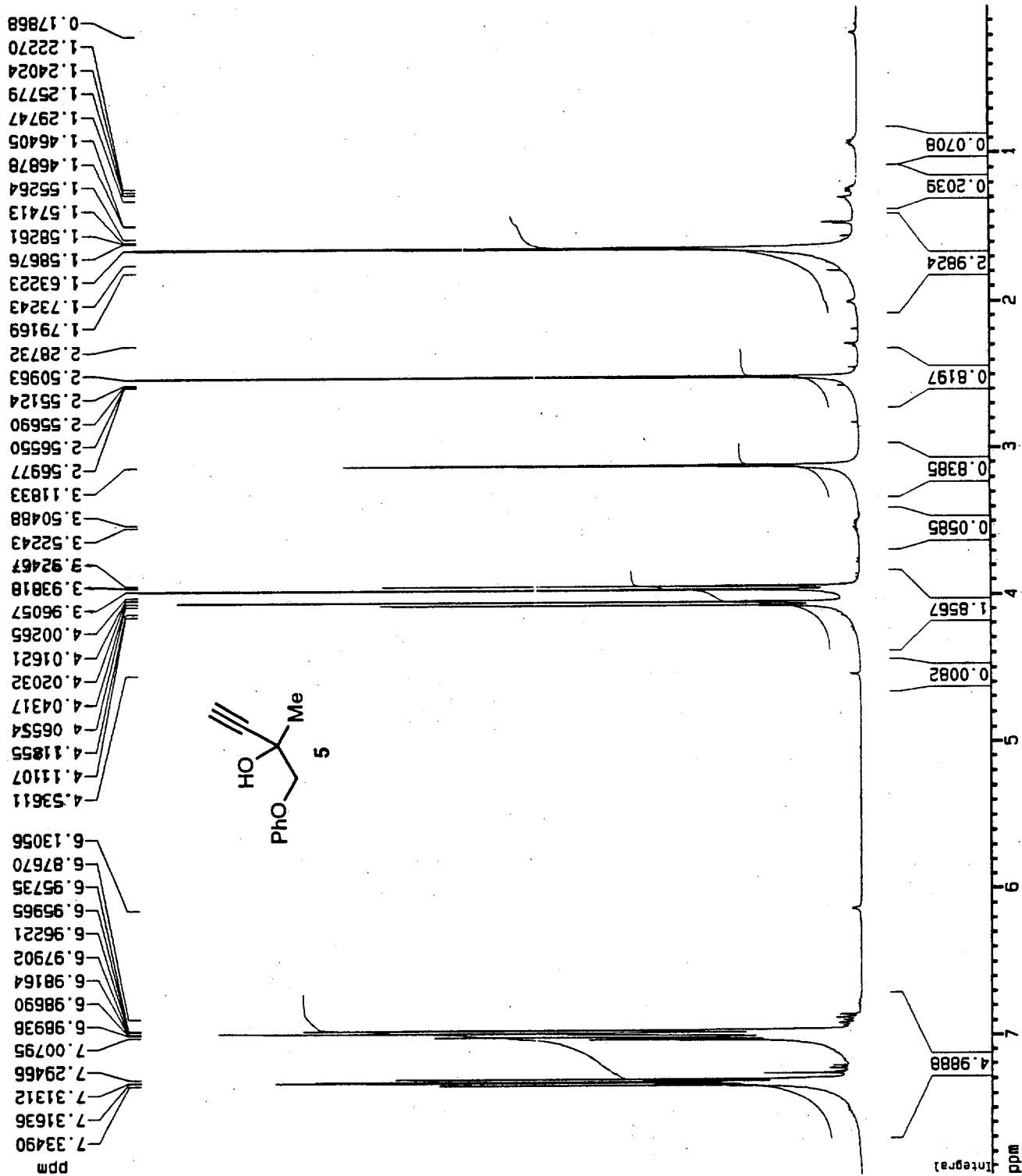
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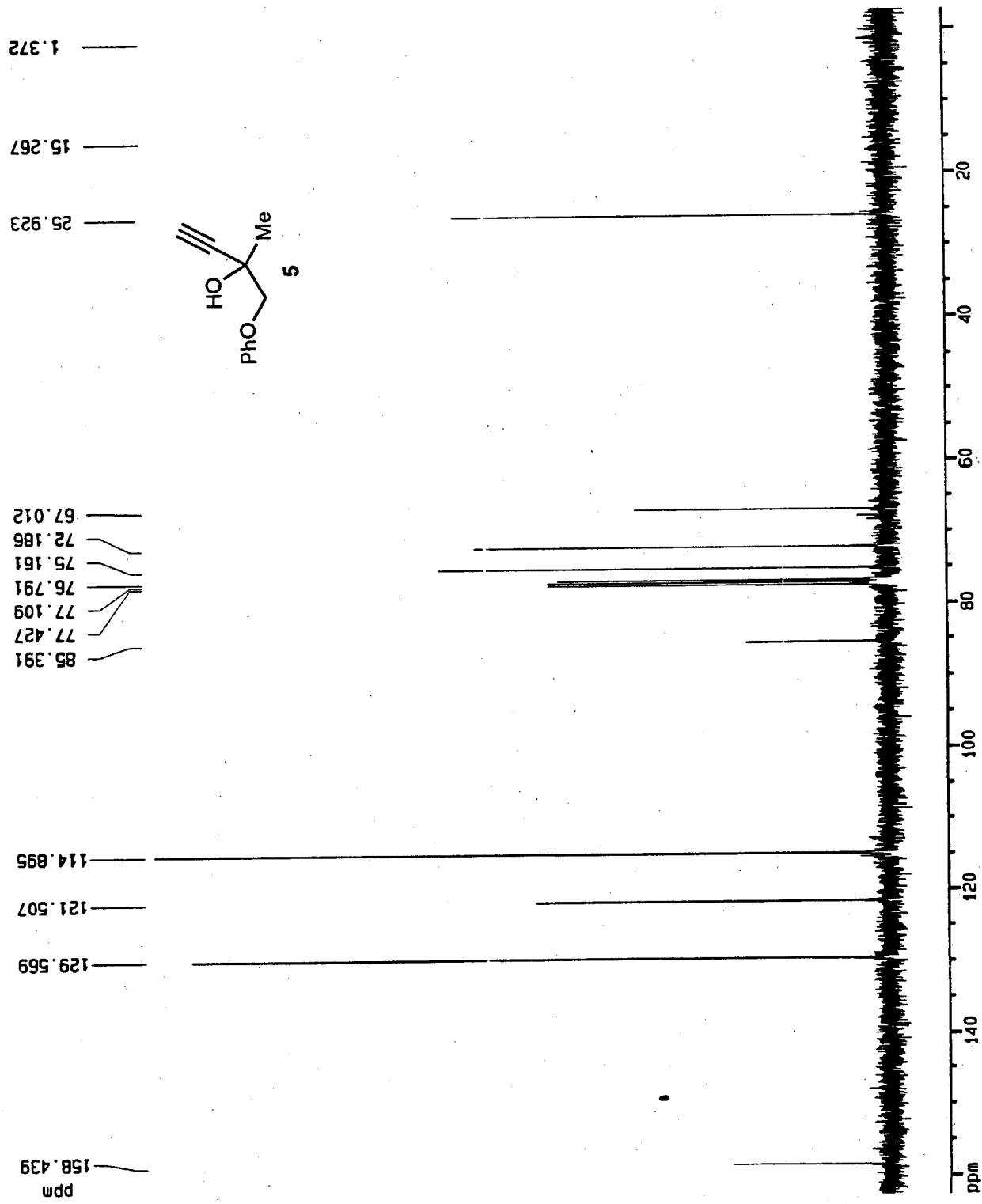
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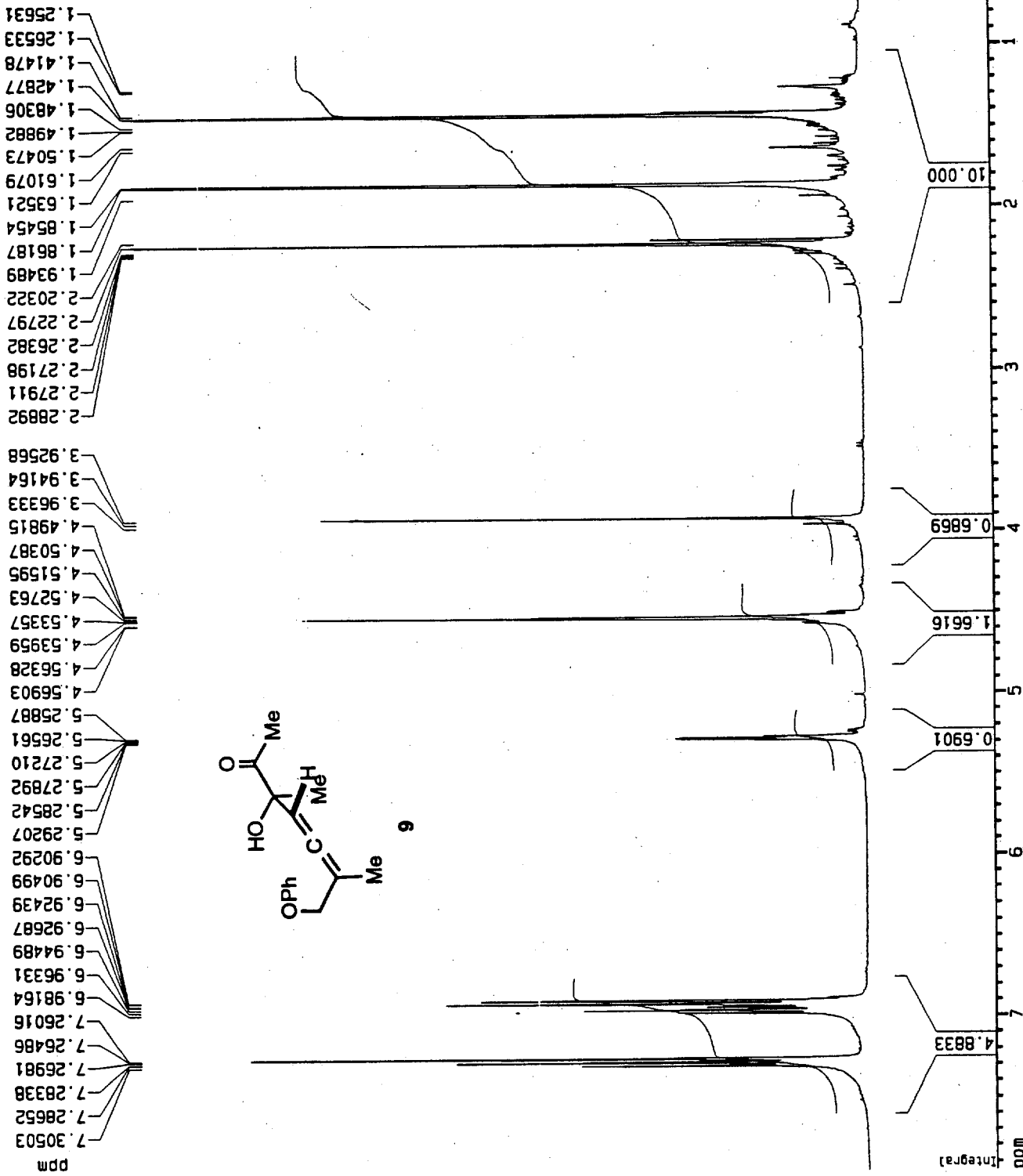
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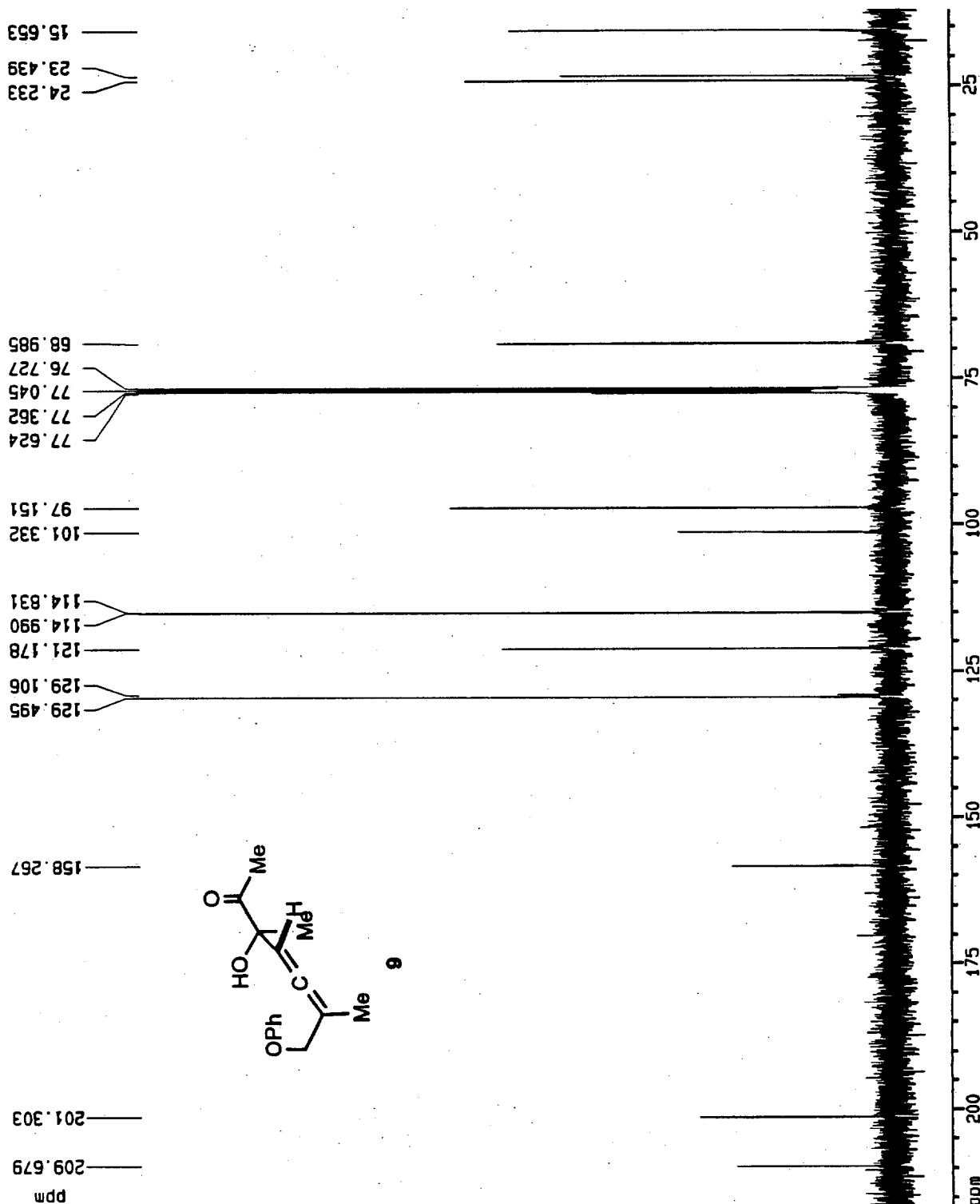
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Default parameters for C-13 with proton decoupling

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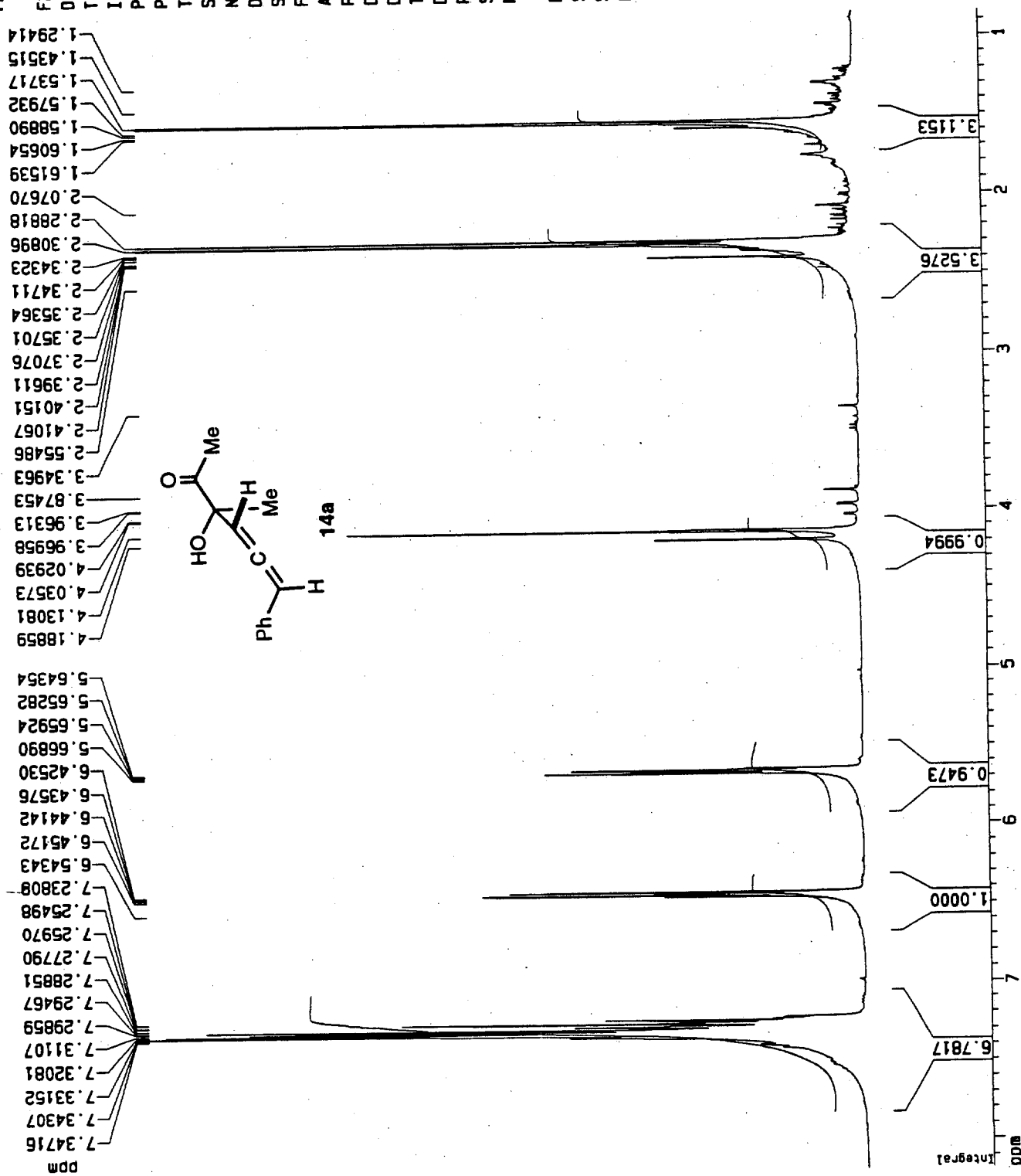
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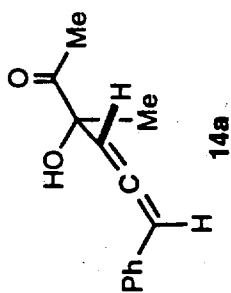
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Default parameters for C-13 with proton decoupling

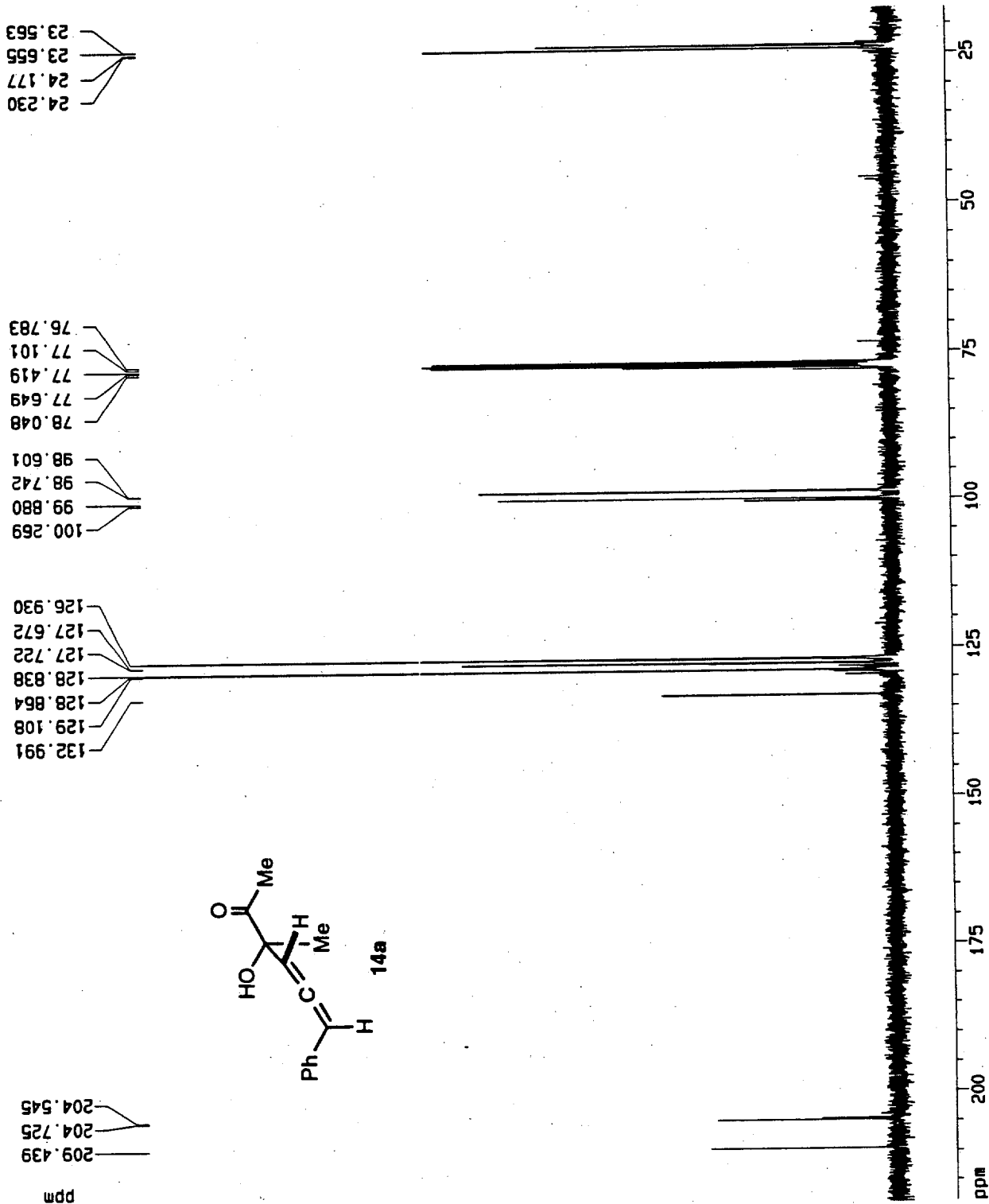


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 FIDRES 0.423855 Hz  
 AQ 1.1796980 sec  
 RG 32768  
 DM 18.000 usec  
 DE 25.71 usec  
 TE 300.0 K  
 D12 0.0000200 sec  
 DL5 23.50 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 D1 2.0000000 sec  
 P1 6.25 usec  
 SF01 100.6248445 MHz  
 NUCLEUS 13C  
 D11 0.0300000 sec

F2 - Processing parameters  
 SI 65536  
 SF 100.6127710 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 218.420 ppm  
 F1 21975.80 Hz  
 F2P 17.425 ppm  
 F2 1753.32 Hz  
 PPMCH 10.04956 ppm/cm  
 HZCM 1011.12396 Hz/cm



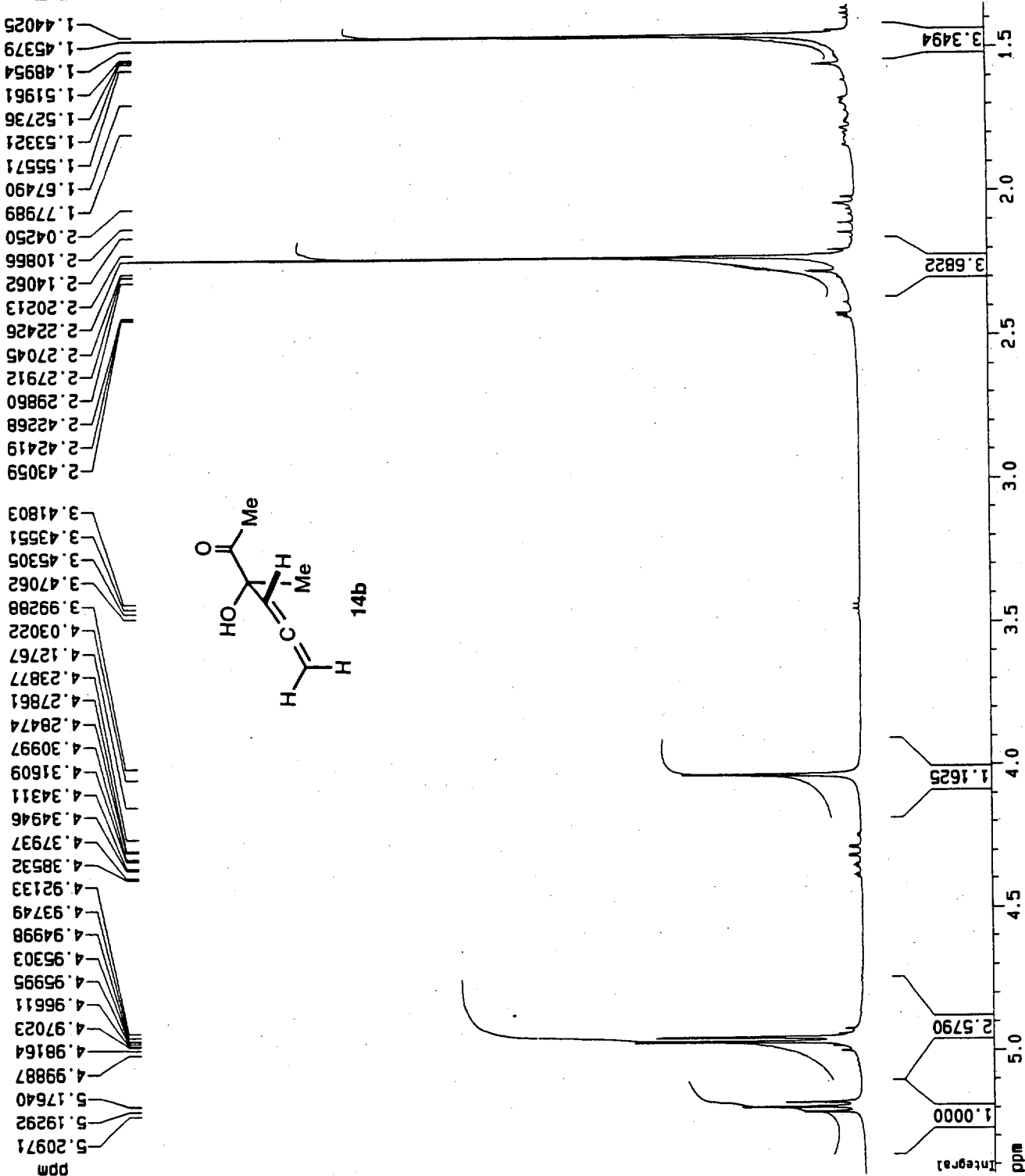
proton default parameters

Current Data Parameters  
 NAME allene  
 EXPNO 1  
 PROCNO 1

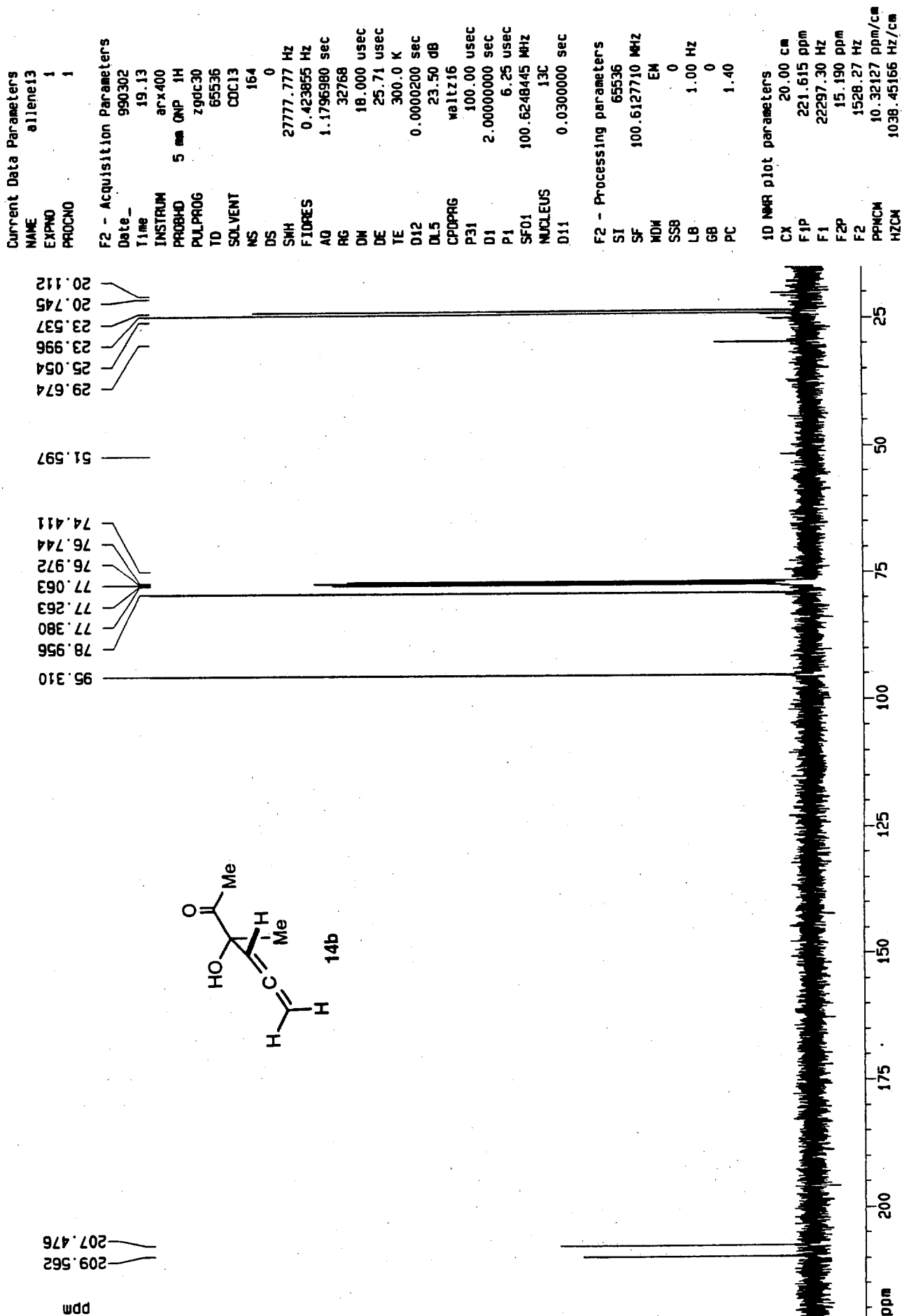
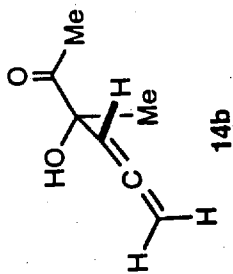
F2 - Acquisition Parameters  
 Date\_ 990302  
 Time 19.02  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 256  
 DM 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 P1 8.25 usec  
 SF01 400.132408 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 5.431 ppm  
 F1 2173.14 Hz  
 F2P 1.350 ppm  
 F2 540.22 Hz  
 PPMCM 0.20405 ppm/cm  
 HZCM 81.64597 Hz/cm



Default parameters for C-13 with proton decoupling



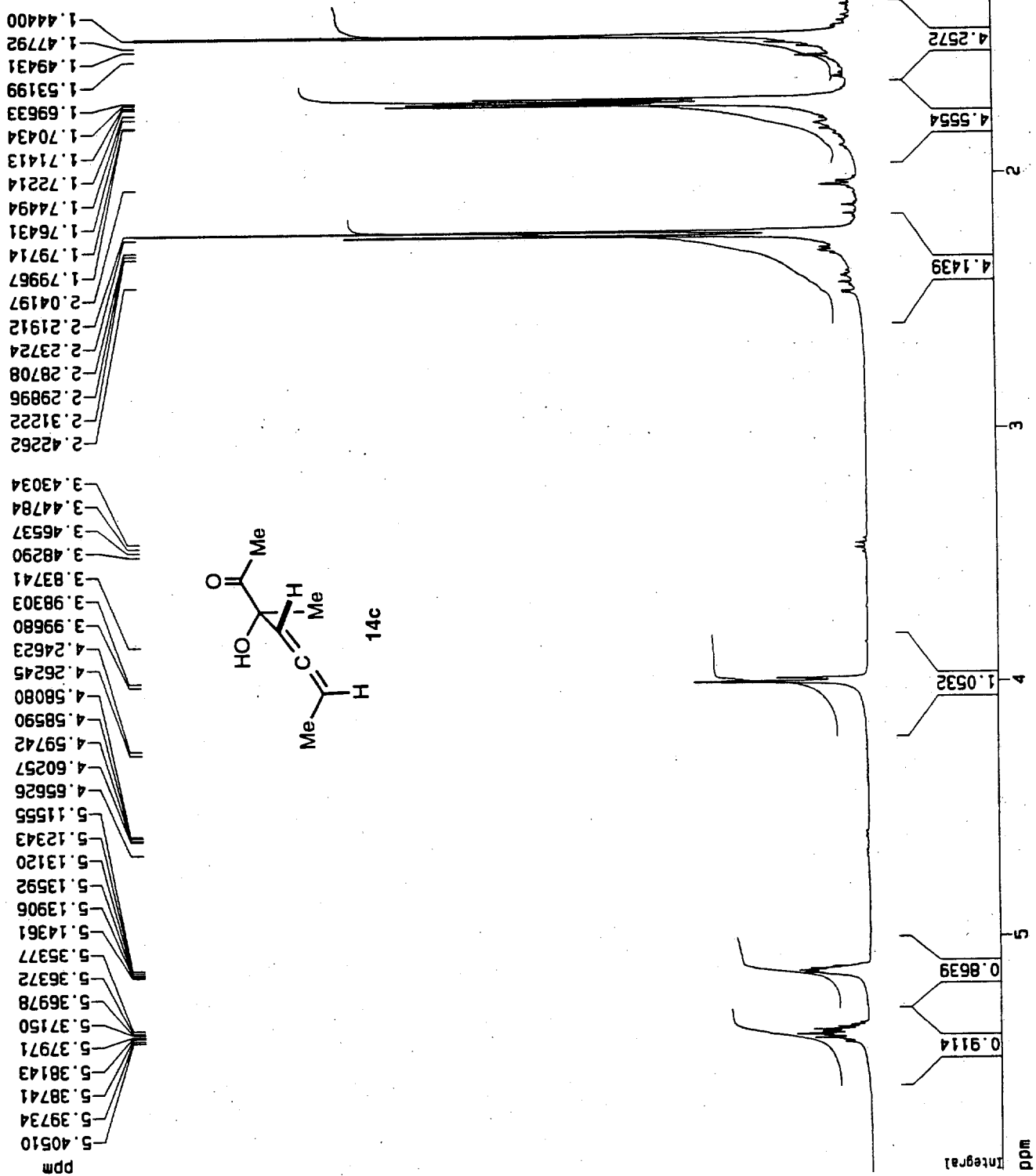
proton default parameters

Current Data Parameters  
 NAME alleneme  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990303  
 Time 12.01  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zg30  
 TO 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 360  
 DW 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 P1 8.25 usec  
 SF01 400.1324008 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 MVM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 5.929 ppm  
 F1 2372.45 Hz  
 F2P 1.307 ppm  
 F2 523.16 Hz  
 PPMCM 0.23109 ppm/cm  
 HZCM 92.46426 Hz/cm



- 5.40510
- 5.39734
- 5.38741
- 5.38143
- 5.37971
- 5.37150
- 5.36978
- 5.36372
- 5.35377
- 5.14361
- 5.13906
- 5.13592
- 5.13120
- 5.12343
- 5.11555
- 4.65626
- 4.60257
- 4.59742
- 4.58590
- 4.58080
- 4.26245
- 4.24623
- 3.99680
- 3.98303
- 3.83741
- 3.48290
- 3.46537
- 3.44784
- 3.43034
- 2.42262
- 2.31222
- 2.29896
- 2.28708
- 2.23724
- 2.21912
- 2.04197
- 1.79967
- 1.79714
- 1.76431
- 1.74494
- 1.72214
- 1.71413
- 1.70434
- 1.69633
- 1.53199
- 1.49431
- 1.47792
- 1.44400

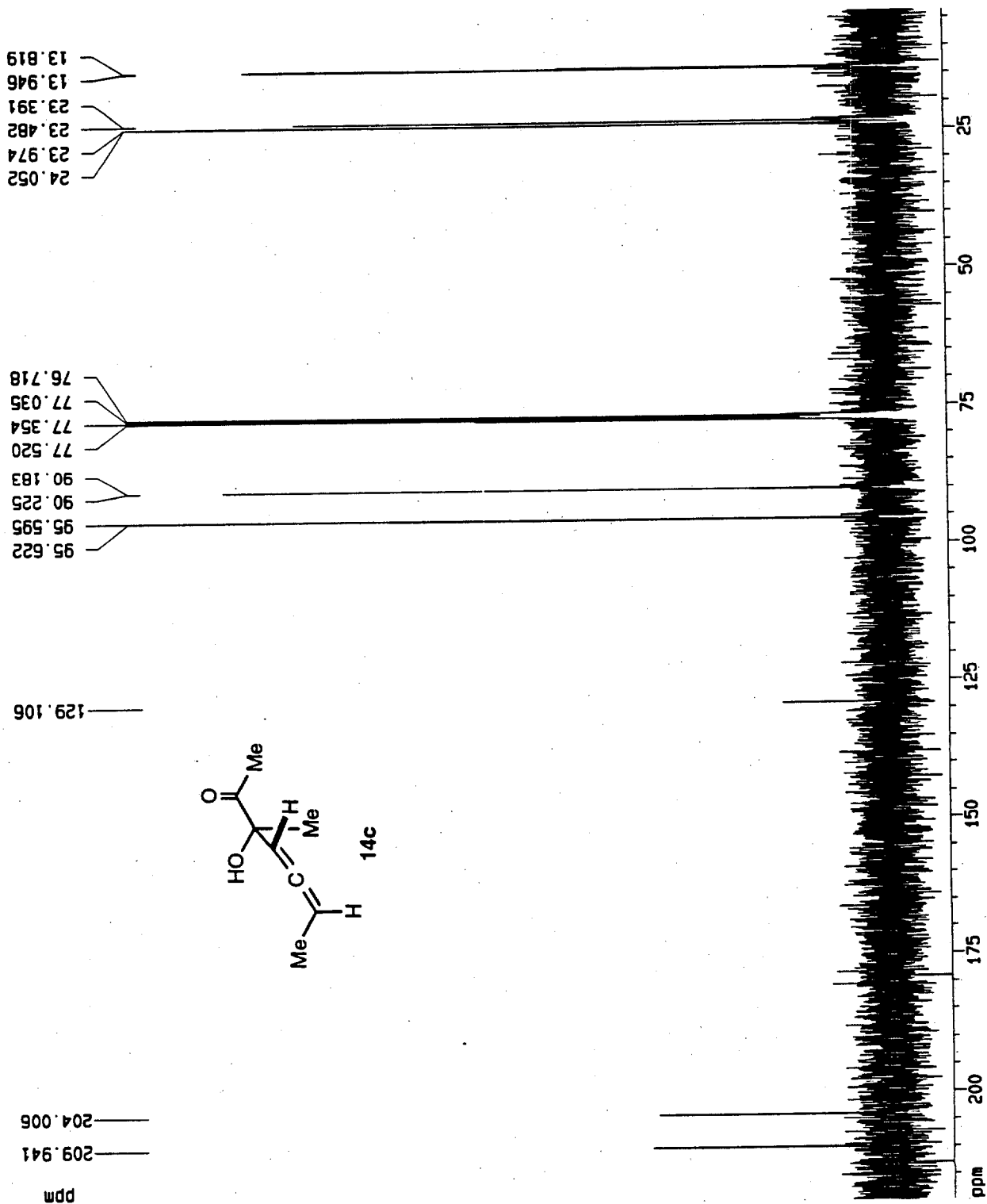
Default parameters for C-13 with proton decoupling

Current Data Parameters  
 NAME allenem13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990303  
 Time 12.13  
 INSTRUM arx400  
 PROBHD 5 mm CNP 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT COC13  
 NS 200  
 DS 0  
 SNH 27777.777 Hz  
 FIDRES 0.423855 Hz  
 AQ 1.1796980 sec  
 RG 32768  
 DM 18.000 usec  
 DE 25.71 usec  
 TE 300.0 K  
 D12 0.0000200 sec  
 DL5 23.50 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 D1 2.0000000 sec  
 P1 6.25 usec  
 SFO1 100.6248445 MHz  
 NUCLEUS 13C  
 D11 0.0300000 sec

F2 - Processing parameters  
 SI 65536  
 SF 100.6127710 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 219.698 ppm  
 F1 22104.40 Hz  
 F2P 3.686 ppm  
 F2 370.86 Hz  
 PPMCM 10.80059 ppm/cm  
 HZCM 1086.67700 Hz/cm



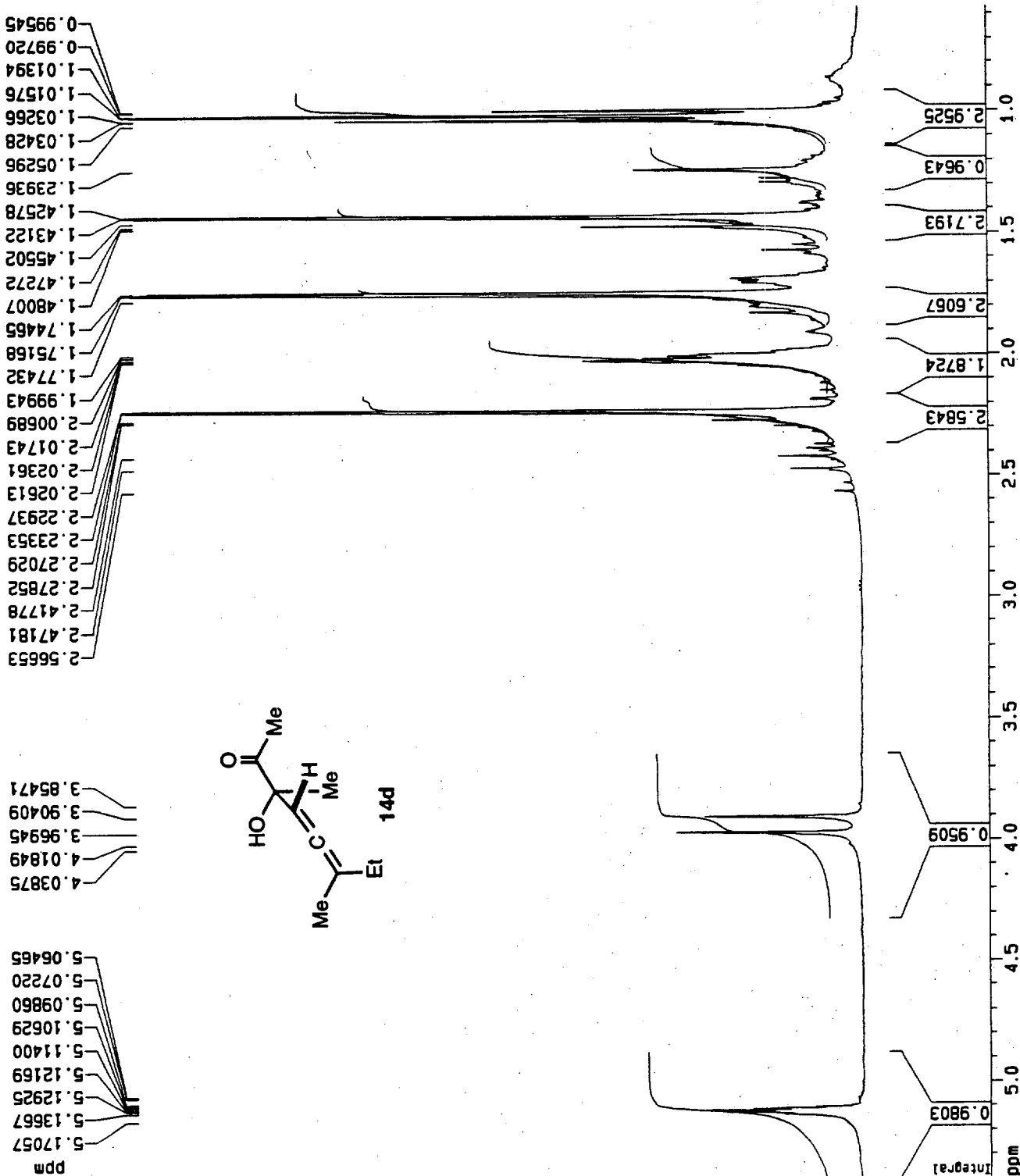
proton default parameters

Current Data Parameters  
 NAME allenetert  
 EXPNO 1  
 PROCNO 1

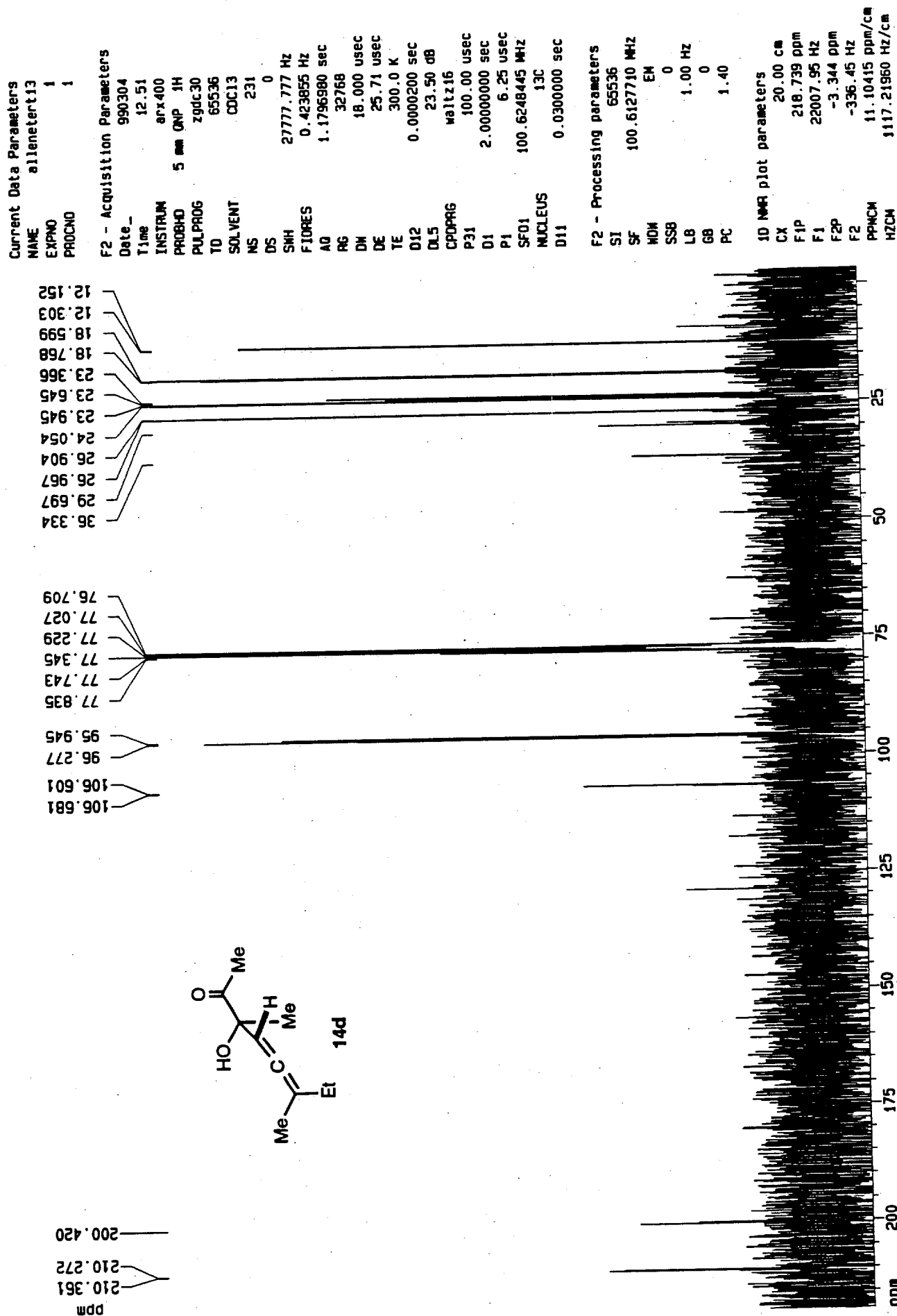
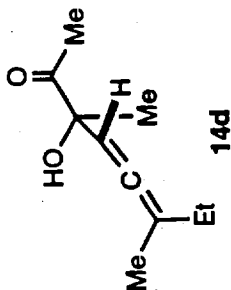
F2 - Acquisition Parameters  
 Date\_ 990304  
 Time 12.38  
 INSTRUM arx400  
 PROBHD 5 mm GNP 1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 24  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 360  
 DM 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 P1 8.25 usec  
 SFO1 400.132408 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 WOH EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 5.397 ppm  
 F1 2159.50 Hz  
 F2P 0.568 ppm  
 F2 227.37 Hz  
 PPMCM 0.24144 ppm/cm  
 HZCM 96.60618 Hz/cm



Default parameters for C-13 with proton decoupling





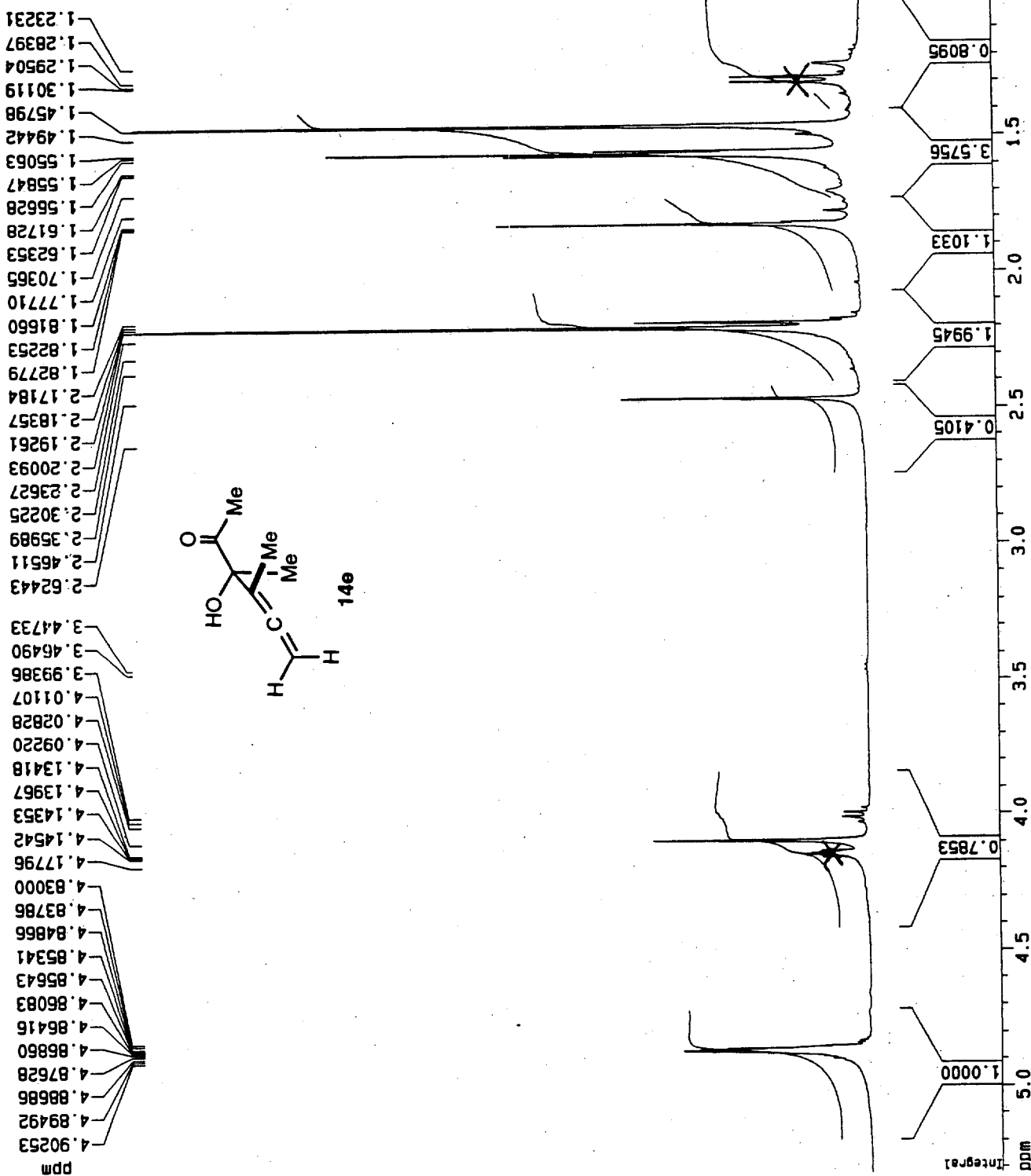
proton default parameters

Current Data Parameters  
 NAME alleneison  
 EXPNO 1  
 PROCNO 1

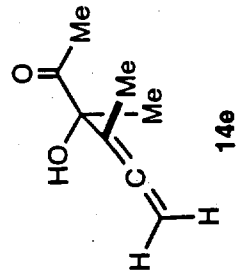
F2 - Acquisition Parameters  
 Date\_ 990303  
 Time 15.41  
 INSTRUM arx400  
 PROBHD 5 mm ONP 1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 24  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 360  
 DM 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 P1 8.25 usec  
 SF01 400.1324008 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 NDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 5.320 ppm  
 F1 2128.65 Hz  
 F2P 0.990 ppm  
 F2 396.01 Hz  
 PPMCM 0.21651 ppm/cm  
 HZCM 86.63226 Hz/cm



Default parameters for C-13 with proton decoupling

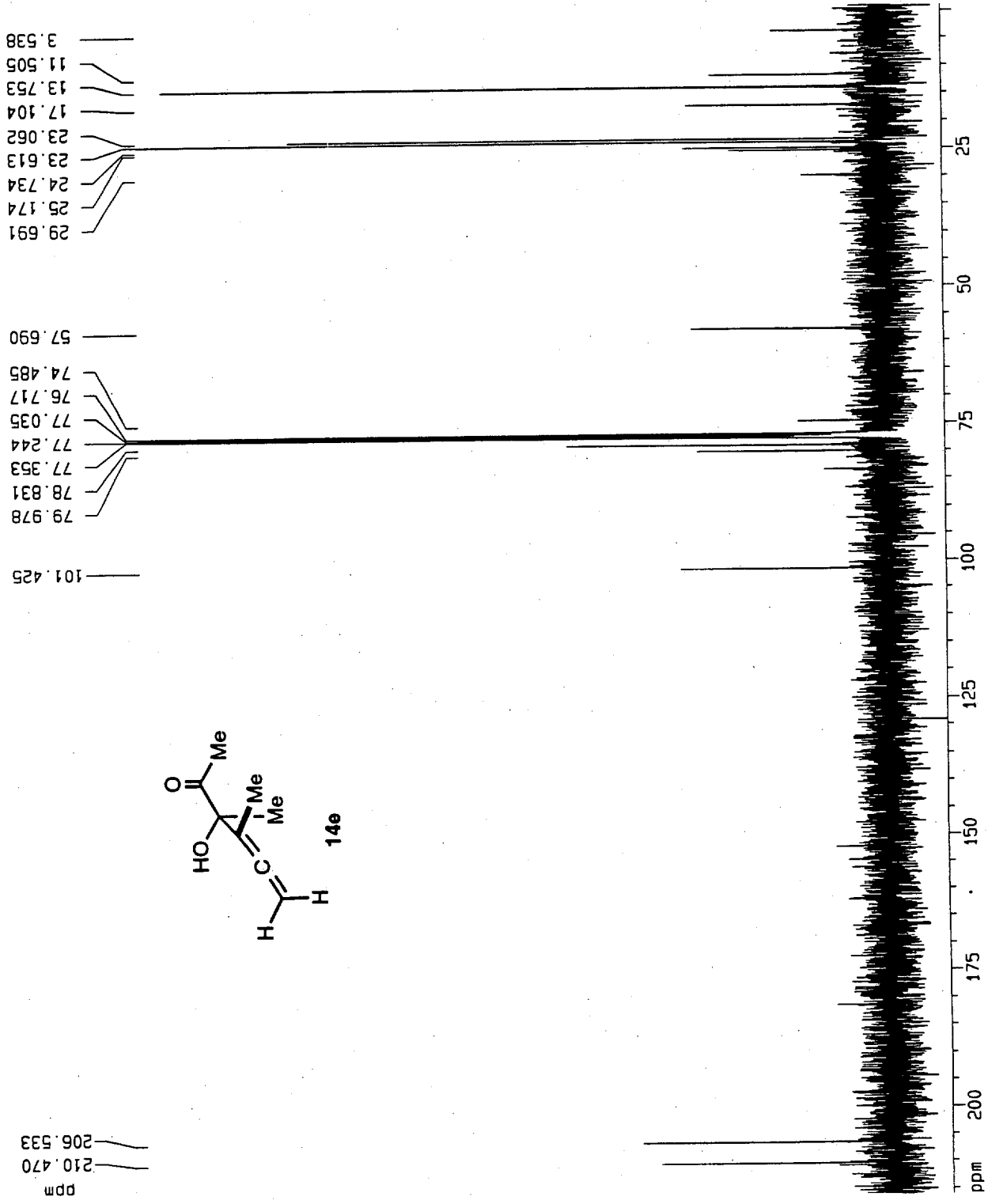


Current Data Parameters  
 NAME alleneisom13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990303  
 Time 15.54  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zgpg30  
 TO 65536  
 SOLVENT CDCl3  
 NS 242  
 DS 0  
 SWH 27777.777 Hz  
 FIDRES 0.423855 Hz  
 AQ 1.1796980 sec  
 RG 32768  
 DM 18.000 usec  
 DE 25.71 usec  
 TE 300.0 K  
 D12 0.0000200 sec  
 DL5 23.50 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 D1 2.00000000 sec  
 P1 6.25 usec  
 SF01 100.6248445 MHz  
 NUCLEUS 13C  
 D11 0.0300000 sec

F2 - Processing parameters  
 SI 65536  
 SF 100.6127710 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D-NMR plot parameters  
 CX 20.00 cm  
 F1P 216.183 ppm  
 F1 21750.75 Hz  
 F2P -1.107 ppm  
 F2 -111.39 Hz  
 PPKCM 10.86450 ppm/cm  
 HZCM 1093.10693 Hz/cm



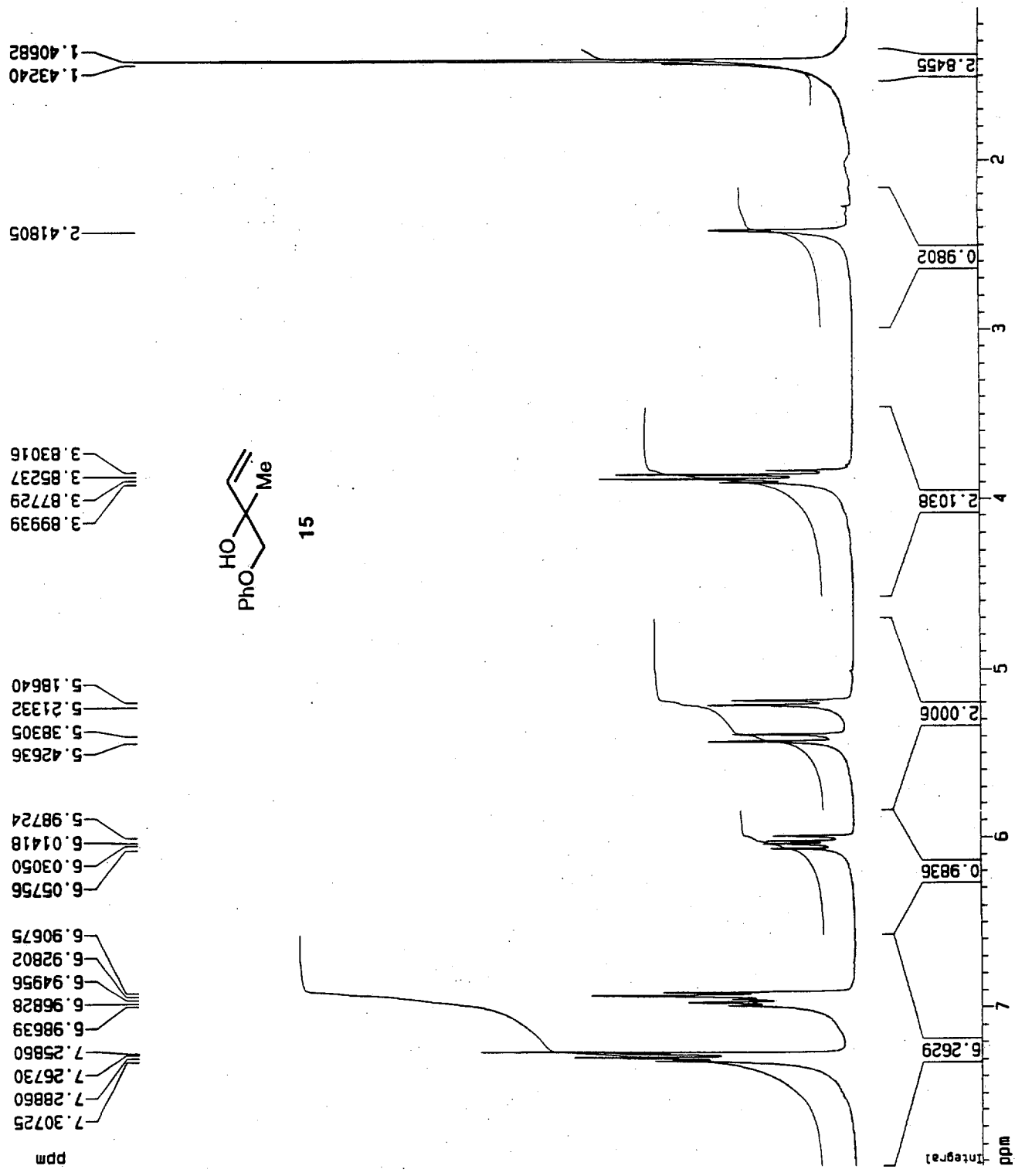
proton default parameters

Current Data Parameters  
 NAME ene  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990503  
 Time 6.55  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 1024  
 DM 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 P1 8.25 usec  
 SF01 400.1324008 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 HDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 7.931 ppm  
 F1 3173.59 Hz  
 F2P 1.104 ppm  
 F2 441.73 Hz  
 PPMCM 0.34137 ppm/000  
 HZCM 136.59293 Hz/c



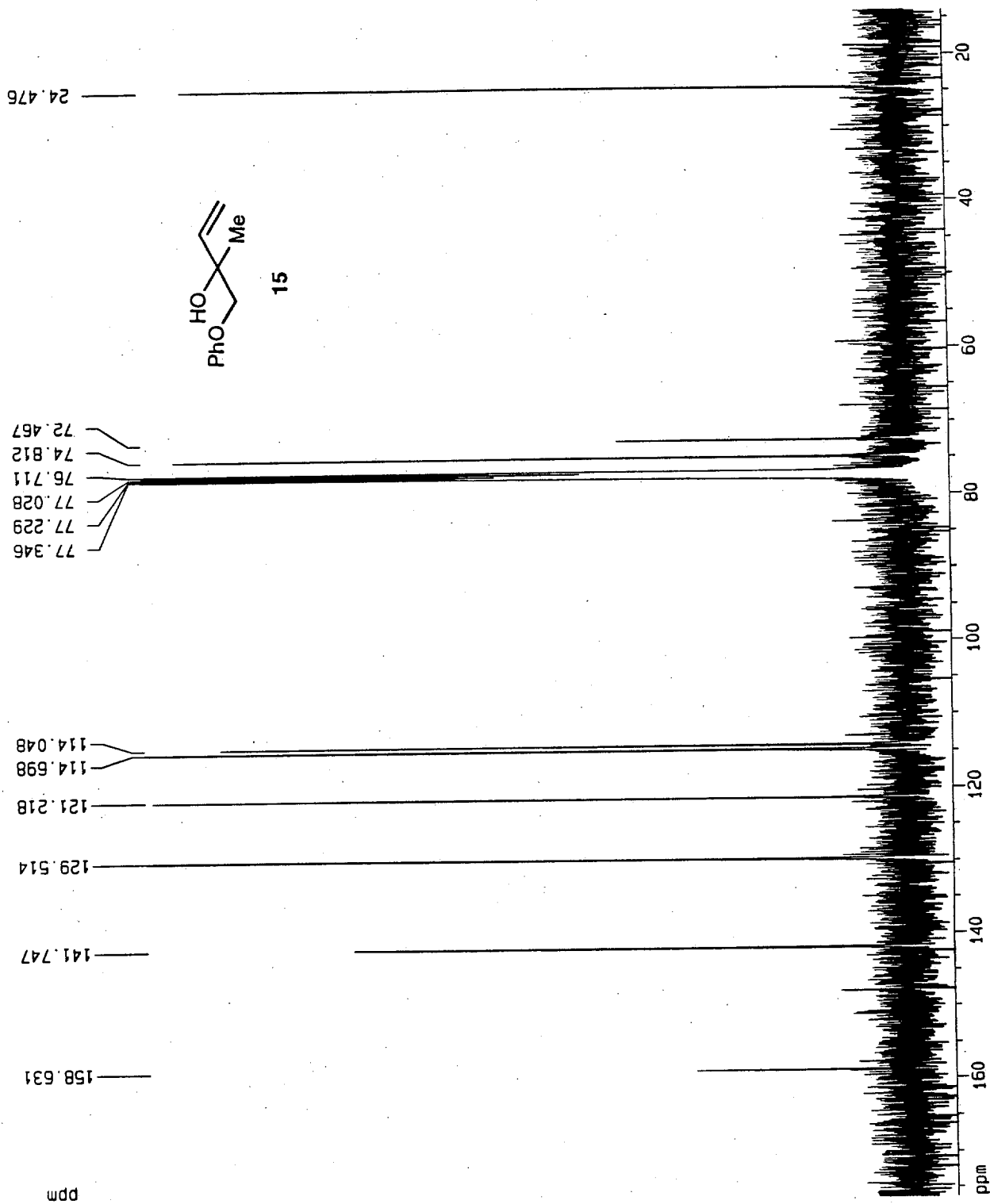
Default parameters for C-13 with proton decoupling

Current Data Parameters  
 NAME en13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990503  
 Time 8.37  
 INSTRUM arcx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2137  
 DS 0  
 SMH 27777.777 Hz  
 FIDRES 0.423855 Hz  
 AQ 1.1796980 sec  
 RG 32768  
 DM 18.000 usec  
 DE 25.71 usec  
 TE 300.0 K  
 D12 0.000200 sec  
 DL5 23.50 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 D1 2.0000000. sec  
 P1 6.25 usec  
 SFO1 100.6248445 MHz  
 NUCLEUS 13C  
 D11 0.0300000 sec

F2 - Processing parameters  
 SI 65536  
 SF 100.6127710 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 176.263 ppm  
 F1 17734.33 Hz  
 F2P 13.972 ppm  
 F2 1405.72 Hz  
 PPMCM 8.11458 ppm/cm  
 HZCM 816.43066 Hz/cm



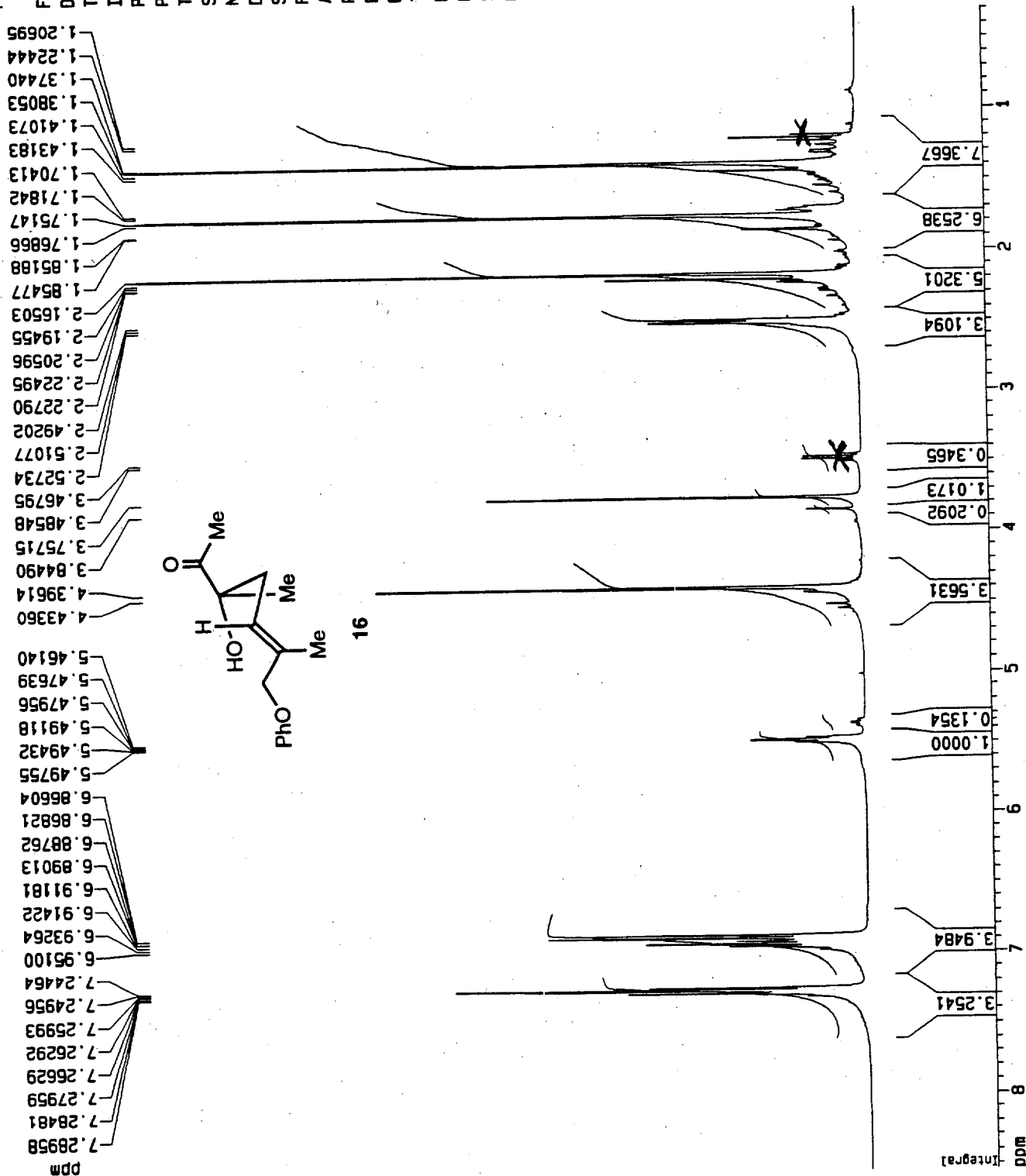
proton default parameters

Current Data Parameters  
 NAME allenealkene  
 EXPND 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990301  
 Time 18.31  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 360  
 DW 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 P1 8.25 usec  
 SF01 400.1324008 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 F1P 8.546 ppm  
 F1 3419.58 Hz  
 F2P 0.288 ppm  
 F2 115.37 Hz  
 PPMCH 0.41289 ppm/cm  
 HZCM 165.21057 Hz/cm



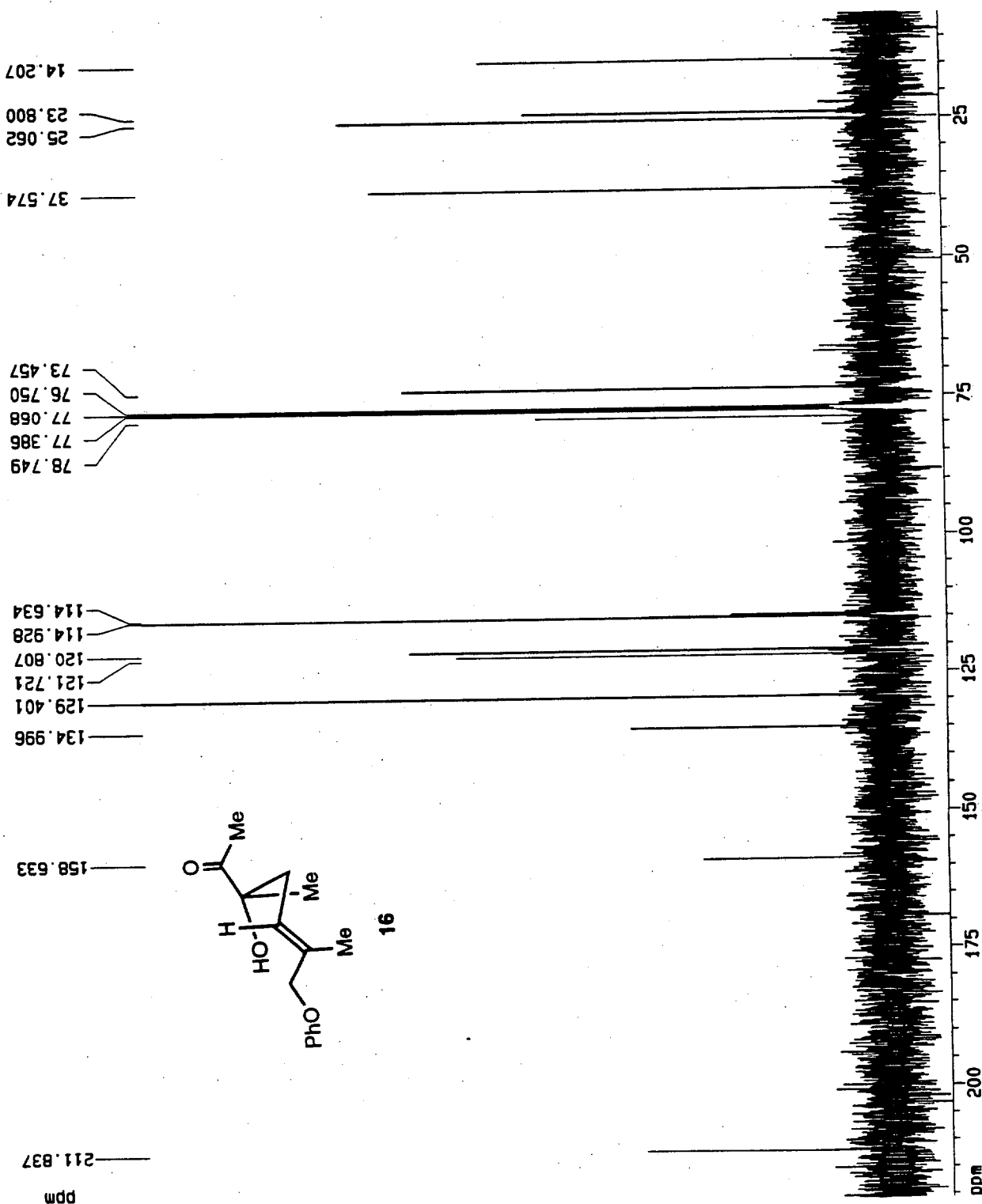
Default parameters for C-13 with proton decoupling

Current Data Parameters  
 NAME allenalken13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990301  
 Time 18.43  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zgpg30  
 TO 65536  
 SOLVENT CDC13  
 NS 200  
 DS 0  
 SMH 27777.777 Hz  
 FIDRES 0.423855 Hz  
 AQ 1.1796980 sec  
 RG 32768  
 DM 18.000 usec  
 DE 25.71 usec  
 TE 300.0 K  
 D12 0.0000200 sec  
 DL5 23.50 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 D1 2.00000000 sec  
 P1 6.25 usec  
 SF01 100.6248445 MHz  
 NUCLEUS 13C  
 D11 0.0300000 sec

F2 - Processing parameters  
 SI 65536  
 SF 100.6127710 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

10 NMR plot parameters  
 CX 20.00 cm  
 F1P 220.656 ppm  
 F1 22200.85 Hz  
 F2P 5.923 ppm  
 F2 595.91 Hz  
 PPMCM 10.73668 ppm/cm  
 HZCM 1080.24707 Hz/cm



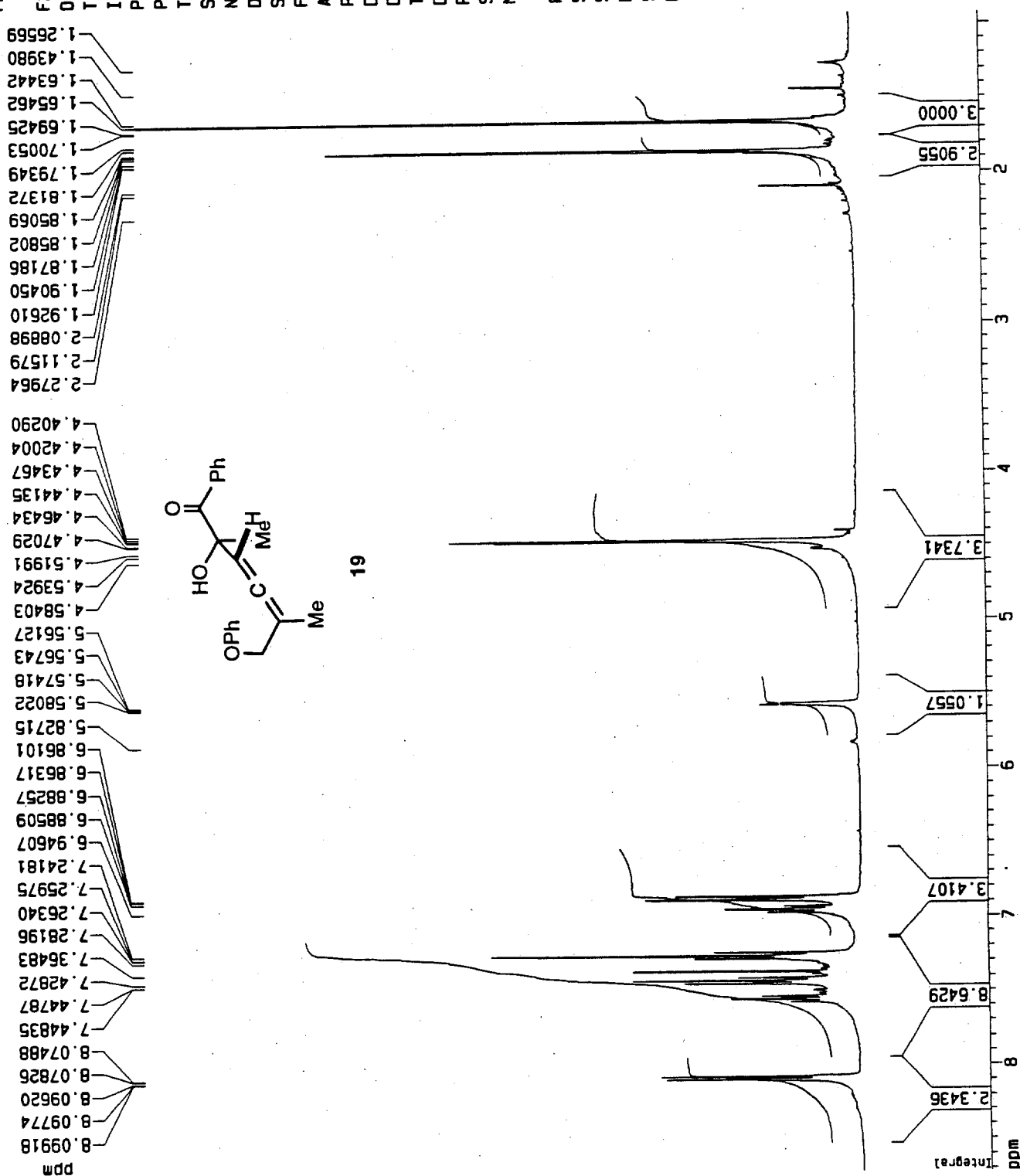
proton default parameters

Current Data Parameters  
 NAME allenePh  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990429  
 Time 13.33  
 INSTRUM arx400  
 PROBHD 5 mm ONP 1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SMH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 360  
 DM 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 P1 8.25 usec  
 SF01 400.1324008 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 8.722 ppm  
 F1 3489.95 Hz  
 F2P 0.924 ppm  
 F2 369.70 Hz  
 PPMCM 0.38991 ppm/cm  
 HZCM 156.01274 Hz/cm



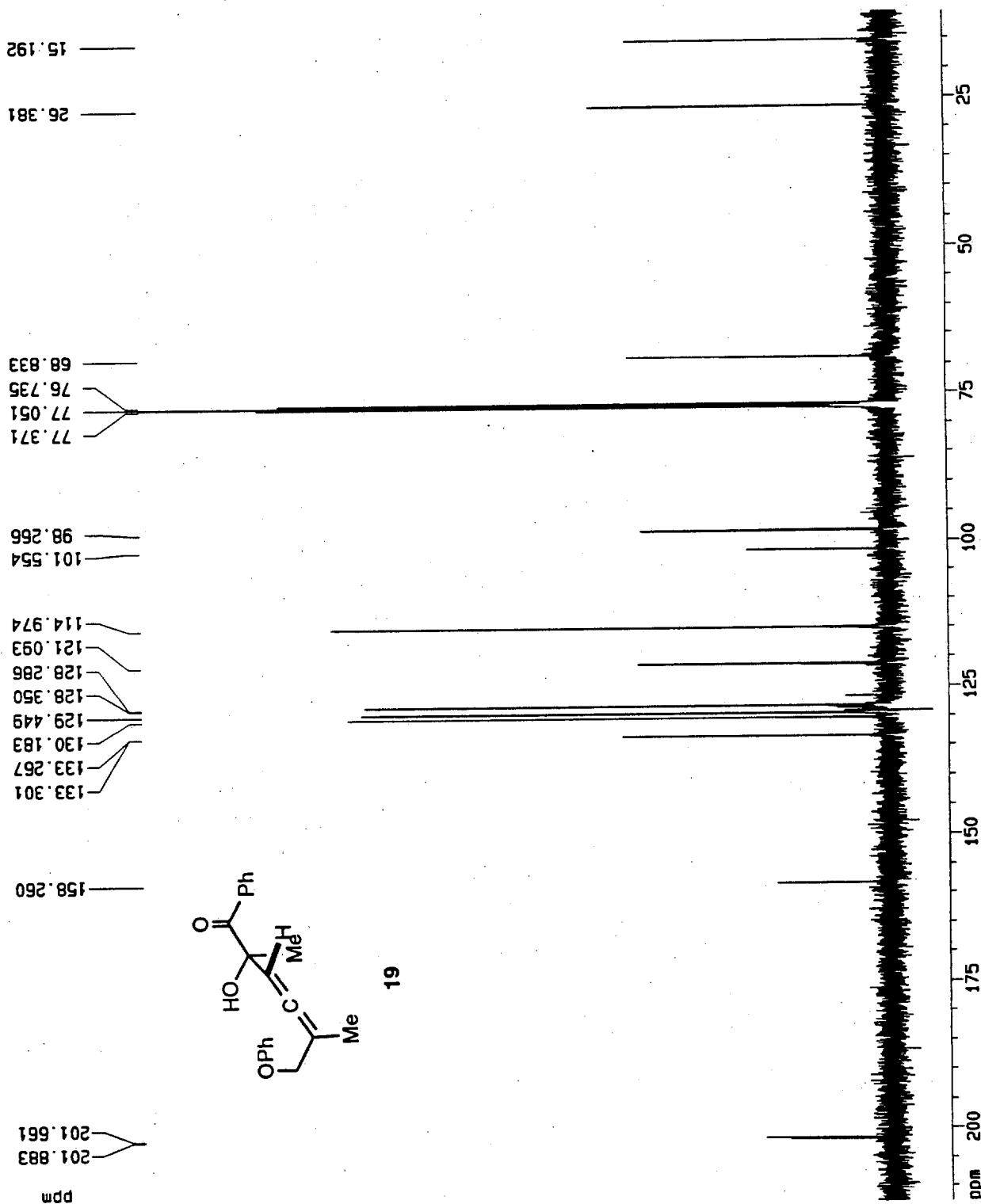
Default parameters for C-13 with proton decoupling

Current Data Parameters  
 NAME alleneP13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990429  
 Time 13.47  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 182  
 DS 0  
 SWH 27777.777 Hz  
 FIDRES 0.423855 Hz  
 AQ 1.1795980 sec  
 RG 32768  
 DM 18.000 usec  
 DE 25.71 usec  
 TE 300.0 K  
 D12 0.0000200 sec  
 DL5 23.50 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 D1 2.0000000 sec  
 P1 6.25 usec  
 SFO1 100.6248445 MHz  
 NUCLEUS 13C  
 D11 0.0300000 sec

F2 - Processing parameters  
 SI 65536  
 SF 100.6127710 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 FIP 212.715 ppm  
 F1 21401.89 Hz  
 F2P 10.485 ppm  
 F2 1054.91 Hz  
 PPMCM 10.11153 ppm/cm  
 HZCM 1017.34924 Hz/cm





proton default parameters

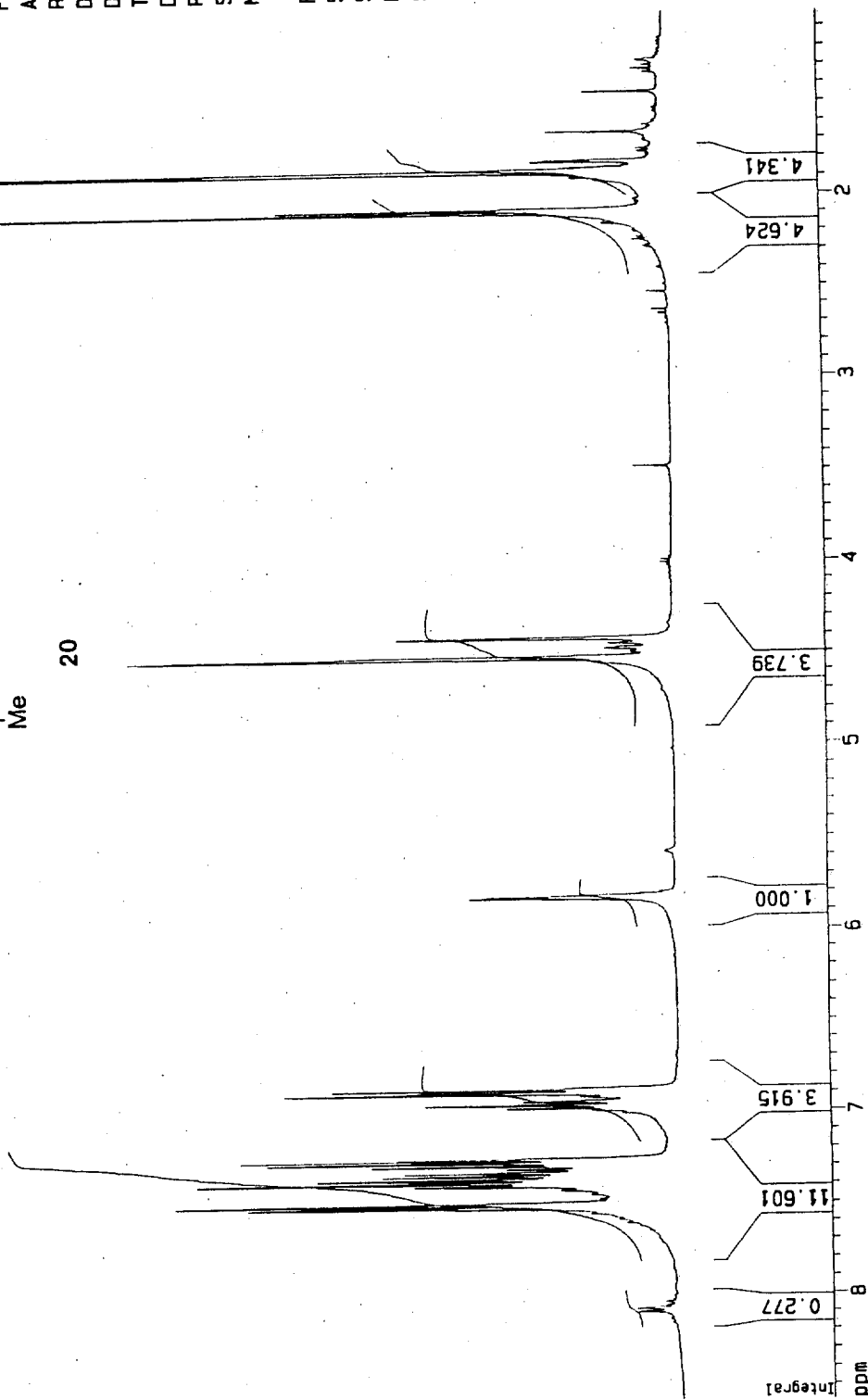
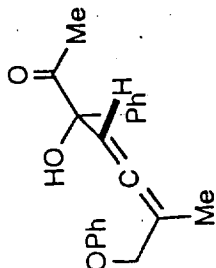
Current Data Parameters  
 NAME threethree  
 EXPNO 1  
 PROCND 1

F2 - Acquisition Parameters  
 Date\_ 990501  
 Time 20.28  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 8  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.123055 Hz  
 AQ 4.0632820 sec  
 RG 360  
 DW 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 P1 8.25 usec  
 SF01 400.1324008 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 65536  
 SF 400.1300173 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 8.583 ppm  
 F1 3434.40 Hz  
 F2P 1.016 ppm  
 F2 406.73 Hz  
 PPMCM 0.37834 ppm/0  
 HZCM 151.38329 Hz/c

7.52009  
7.51638  
7.50259  
7.49890  
7.38706  
7.37148  
7.36842  
7.35070  
7.33322  
7.29548  
7.27697  
7.27393  
7.25963  
7.25540  
6.89679  
6.89433  
6.87491  
5.83747  
5.83100  
5.82392  
5.81736  
5.81030  
5.80702  
4.55511  
4.54949  
4.52218  
4.49256  
4.48670  
4.47341  
4.46821  
4.44518  
4.41467  
3.47683  
2.25110  
2.15701  
2.14026  
2.09153  
2.07828  
2.07828  
1.92866  
1.91059  
1.90786  
1.87456  
1.86710  
1.85364  
1.82316  
1.81572  
1.65804  
1.44386



Default parameters for C-13 with proton decoupling

Current Data Parameters  
 NAME threethr13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 990501  
 Time 20.35  
 INSTRUM arx400  
 PROBHD 5 mm QNP 1H  
 PULPROG zgpg30  
 TO 65536  
 SOLVENT CDCl3  
 NS 128  
 DS 0  
 SMH 27777.777 Hz  
 FIDRES 0.423855 Hz  
 AQ 1.1796980 sec  
 RG 32768  
 DM 18.000 usec  
 DE 25.71 usec  
 TE 300.0 K  
 D12 0.000200 sec  
 DL5 23.50 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 O1 2.0000000 sec  
 P1 6.25 usec  
 SFO1 100.6248445 MHz  
 NUCLEUS 13C  
 D11 0.0300000 sec

F2 - Processing parameters  
 SI 65536  
 SF 100.6127710 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

10 NMR plot parameters  
 CX 20.00 cm  
 F1P 217.153 ppm  
 F1 21848.38 Hz  
 F2P 10.485 ppm  
 F2 1054.91 Hz  
 PPNOM 10.33341 ppm/cm  
 HZCN 1039.67346 Hz/cm

