

SUPPLEMENTARY INFORMATION

**Substitution of a Bridgehead Bromide by Primary Organolithium
Reagent**

Michael Harmata* and Sumrit Wacharasindhu

**Department of Chemistry
University of Missouri-Columbia
Columbia, Missouri 65211**

General information:

All reactions were carried out under an atmosphere of nitrogen in oven-dried glassware with magnetic stir bar. THF was distilled from sodium/benzophenone and HMPA were distilled from CaH_2 . Chromatographic separations were carried out using Silicycle ultra pure silica gel (230-400 mesh). Analytical thin layer chromatography was performed on EM Reagent 0.25 mm silica gel 60-F plates. Visualization of the developed chromatogram was performed by phosphomolybdic acid stain solution followed by heating. Infrared spectra were recorded on a Perkin Elmer 1600 series FT-IR spectrometer. ^1H NMR is recorded on a Bruker ARX-250 (250 MHz), DRX-300 (300 MHz), DRX-500 (500 MHz) spectrometer and are reported in ppm from internal tetramethyl silane. Data are reported as (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, ddd = doublet of doublet of doublet, integration, coupling constant (Hz), proton assignments). ^{13}C NMR spectra were recorded on a Bruker ARX-250 (62.5 MHz), DRX-300 (75 MHz), DRX-500 (125 MHz) spectrometer and are reported in ppm from internal tetramethylsilane with solvent resonance employed as the internal standard (CDCl_3 at 77.0 ppm).

General procedure for monosubstitution reaction:

To a solution of iodohexane (47 μL , 0.33 mmol) in ether (0.33 mL) was added t-BuLi (0.70 mmol) dropwise at -78°C . The mixture was stirred at -78°C for 45 min, then 5 min at room temperature. The solution was transferred by syringe to a solution of **1**, (50 mg, 0.22 mmol) in THF/HMPA (20%, 2.2 mL) at -78°C . The reaction mixture was stirred at -78°C for 4 h, quenched with MeOH (1 mL), warmed to room temperature, and diluted with distilled water. The mixture was extracted with ether (3 X 10 mL), washed with brine (5 mL), dried over MgSO_4 , filtered and concentrated under reduced pressure. The residue was purified by flash chromatography using 5 % EtOAc/Hexanes to yield ketone **10** (25 mg, 49%) as colorless oil. ^1H NMR (250 MHz, CDCl_3): δ 6.17-6.03 (m, 2H), 2.81-2.70 (m, 1H), 2.65 (d, $J = 2.2$ Hz, 1H), 2.34 (t, $J = 5.9$ Hz, 1H), 2.04 (d, $J = 11.1$ Hz, 1H), 1.91-1.59 (m, 3H), 1.59-1.47 (m, 2H), 1.47-1.35 (m, 3H), 1.35-0.825 (m, 7H), 0.96-0.81 (t, $J = 5.9$ Hz, 3H); ^{13}C NMR (75.5 MHz, CDCl_3): δ 214.6, 136.5, 135.5, 54.3, 48.6, 48.3, 45.5, 38.1, 31.7, 31.5, 30.1, 29.2, 24.5, 23.2, 22.6, 14.1; IR (neat) 3056, 2992, 2953, 2930, 2856, 1748, 1480, 1465, 1335, 1097 cm^{-1} ; Anal. calcd for $\text{C}_{16}\text{H}_{24}\text{O}$: C, 82.70, H; 10.41 Found: C, 82.82; H 10.32.

General procedure for disubstitution reaction:

To a solution of iodohexane (94 μL , 0.66 mmol) in ether (0.66 mL) was added t-BuLi (1.41 mmol) dropwise at -78°C . The mixture was stirred at -78°C for 45 min, then 5 min at room temperature. The solution was transferred by syringe to a solution of **1** (50 mg, 0.22 mmol) in a mixture of THF/HMPA (20%, 2.2 mL) at -78°C . The reaction mixture was stirred at -78°C for 4 h, quenched with MeOH (1 mL), warmed to room temperature and diluted with distilled water. The mixture was extracted by ether (3 X 10

mL), washed with brine (5 mL), dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography using 5 % EtOAc/Hex to yield an alcohol **15** (43mg, 62%) as colorless oil. ¹H NMR (300 MHz, CDCl₃): δ 6.50 (s, 2H), 4.23-4.13 (t, *J* = 2.7 Hz, 1H), 2.75-2.45 (m, 2H), 2.26-2.09 (m, 2H), 1.81-1.09 (m, 25H), 0.97-0.74 (m, 6H); ¹³C NMR (75.5 MHz, CDCl₃): δ 141.4, 141.1, 86.1, 51.3, 48.3, 44.6, 44.5, 42.5, 37.5, 36.4, 32.7, 32.0, 31.8, 30.6, 30.1, 29.4, 27.6, 25.1, 23.0, 22.6, 14.1; IR (neat) 3603, 3015, 2941, 2847, 1503, 1466, 1376, 1339, 1286, 1066, 747 cm⁻¹ Anal. calcd for C₂₂H₃₈O: C, 82.95, H; 12.02 Found: C, 83.12; H 11.79.

COMPOUND 5: colorless oil; ¹H NMR (300 MHz, CDCl₃): δ 6.16-6.04 (m, 2H), 2.78-2.75 (m, 1H), 2.66 (d, *J* = 2.4 Hz, 1H), 2.34 (t, *J* = 12.0 Hz, 1H), 2.04 (d, *J* = 11.1 Hz, 1H), 1.87-1.72 (m, 2H), 1.72-1.60 (m, 1H), 1.60-1.46 (m, 2H), 1.46-1.14 (m, 6H), 0.91 (t, *J* = 14.1 Hz, 3H); ¹³C NMR (75.48 MHz, CDCl₃): δ 214.5, 136.5, 135.5, 54.2, 48.6, 48.3, 45.5, 38.1, 31.2, 29.2, 26.8, 23.5, 23.2, 14.0; IR (neat) 3060, 2961, 2876, 1751, 1469, 1344, 1101cm⁻¹; Anal. calcd for C₁₄H₂₀O: C, 82.30, H; 9.87 Found: C, 82.50; H 9.74.

COMPOUND 6: colorless oil; ¹H NMR (250 MHz, CDCl₃): δ 6.50 (s, 2H), 4.18 (d, *J* = 3.1 Hz, 1H), 2.62-2.50 (m, 2H), 2.31-2.06 (m, 2H), 1.75-1.13 (m, 17H), 1.06-0.75 (m, 6H); ¹³C NMR (62.9 MHz, CDCl₃): δ 141.45, 141.06, 86.1, 51.2, 48.3, 44.6, 44.5, 42.5, 37.2, 36.4, 32.5, 27.5, 27.4, 25.3, 23.9, 23.4, 14.2, 14.1; IR (neat) 3604, 2946, 2927, 1463, 1349 cm⁻¹; Anal. calcd for C₁₈H₃₀O: C, 82.39, H; 11.52 Found: C, 82.54; H 11.36.

COMPOUND 7: colorless oil; ¹H NMR (300 MHz, CDCl₃): δ 6.17-6.06 (m, 2H), 2.81-2.72 (m, 1H), 2.66 (d, *J* = 2.4 Hz, 1H), 2.36 (t, *J* = 6.0 Hz, 1H), 2.06 (d, *J* = 11.0 Hz, 1H), 1.90-1.41 (m, 7H), 0.94 (t, *J* = 8.6 Hz, 1H); ¹³C NMR (75.48 MHz, CDCl₃): δ 214.5, 136.5, 135.6, 54.6, 48.73, 47.90, 45.5, 38.1, 28.8, 24.1, 23.2, 9.0; IR (neat) 3056, 2953, 2880, 1744, 1458, 1335 cm⁻¹; Anal. calcd for C₁₂H₁₆O: C 81.77; H, 9.15. Found: C 81.58; H, 8.99.

COMPOUND 8: colorless oil; ¹H NMR (300 MHz, CDCl₃): δ 6.16-6.04 (m, 2H), 2.78-2.71 (m, 2H), 2.64 (d, *J* = 2.4 Hz, 1H), 2.34 (t, *J* = 6 Hz, 1H), 2.04 (d, *J* = 11.1 Hz, 1H), 1.88-1.58 (m, 3H), 1.58-1.33 (m, 5H), 1.33-1.17 (m, 1H), 0.93 (t, *J* = 6.7 Hz, 3H); ¹³C NMR (75.48 MHz, CDCl₃): δ 214.5, 136.5, 135.5, 54.3, 48.6, 48.4, 45.5, 38.1, 34.0, 29.2, 23.2, 17.9, 14.9; IR (neat) 2949, 2872, 1748, 1454, 1339, 1098, 743 cm⁻¹; Anal. calcd for C₁₃H₁₈O: C, 82.06, H 9.53. Found: C, 82.11; H, 9.39.

COMPOUND 9: colorless oil; H NMR (250 MHz, CDCl₃): δ 6.16-6.04 (m, 2H), 2.78-2.68 (m, 1H), 2.65 (d, *J* = 2.4 Hz, 1H), 2.34 (t, *J* = 12.0, 1H), 2.04 (d, *J* = 11.1 Hz, 1H), 1.89-1.13 (m, 13H), 0.88 (t, *J* = 13.3 Hz, 3H); ¹³C NMR (62.9 MHz, CDCl₃): δ 214.5, 136.6, 135.5, 54.3, 48.6, 48.3, 45.5, 38.1, 32.7, 31.5, 29.2, 24.3, 23.2, 22.6, 14.02; IR (neat) 3056, 2953, 2872, 1748, 1450, 1335, 1090, 963, 898, 743, 710 cm⁻¹; Anal. calcd for C₁₅H₂₂O: C, 82.52, H; 10.16 Found: C, 82.69; H 10.12.

COMPOUND 11: colorless oil; ^1H NMR (300 MHz, CDCl_3): δ 6.16-6.05 (m, 2H), 2.80-2.71 (m, 1H), 2.65 (d, $J = 2.1$ Hz, 1H), 2.34 (t, $J = 5.7$ Hz, 1H), 2.04 (d, $J = 11.1$ Hz, 1H), 1.90-1.58 (m, 3H), 1.58-1.46 (m, 2H), 1.46-1.11 (m, 12H), 0.88 (t, $J = 6.5$ Hz, 3H); ^{13}C NMR (75.5 MHz, CDCl_3): δ 214.5, 136.5, 135.5, 54.2, 48.6, 48.3, 45.4, 38.1, 31.8, 31.5, 30.4, 29.2, 29.2, 24.5, 23.2, 22.6, 14.1; IR (neat) 3056, 2925, 2855, 1752, 1482, 1458, 1380, 1339, 1098 cm^{-1} ; Anal. calcd for $\text{C}_{17}\text{H}_{26}\text{O}$: C, 82.87, H; 10.64 Found: C, 82.66; H 10.67

COMPOUND 12: colorless oil; ^1H NMR (250 MHz, CDCl_3): δ 6.50 (s, 2H), 4.14 (d, $J = 3.2$ Hz, 1H), 2.67-2.47 (m, 2H), 2.19 (d, $J = 8.7$ Hz, 2H), 1.73-1.30 (m, 9H), 0.97 (t, $J = 7.4$ Hz, 3H), 0.84 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (62.9 MHz, CDCl_3): δ 141.5, 140.9, 86.0, 51.5, 47.6, 44.6, 44.5, 41.8, 36.1, 29.7, 27.3, 24.9, 9.5, 7.38; IR (neat), 3598, 2922, 2852, 1496, 1468 cm^{-1} ; Anal. calcd for $\text{C}_{14}\text{H}_{22}\text{O}$: C, 81.50, H; 10.75 Found: C, 82.36; H 10.66

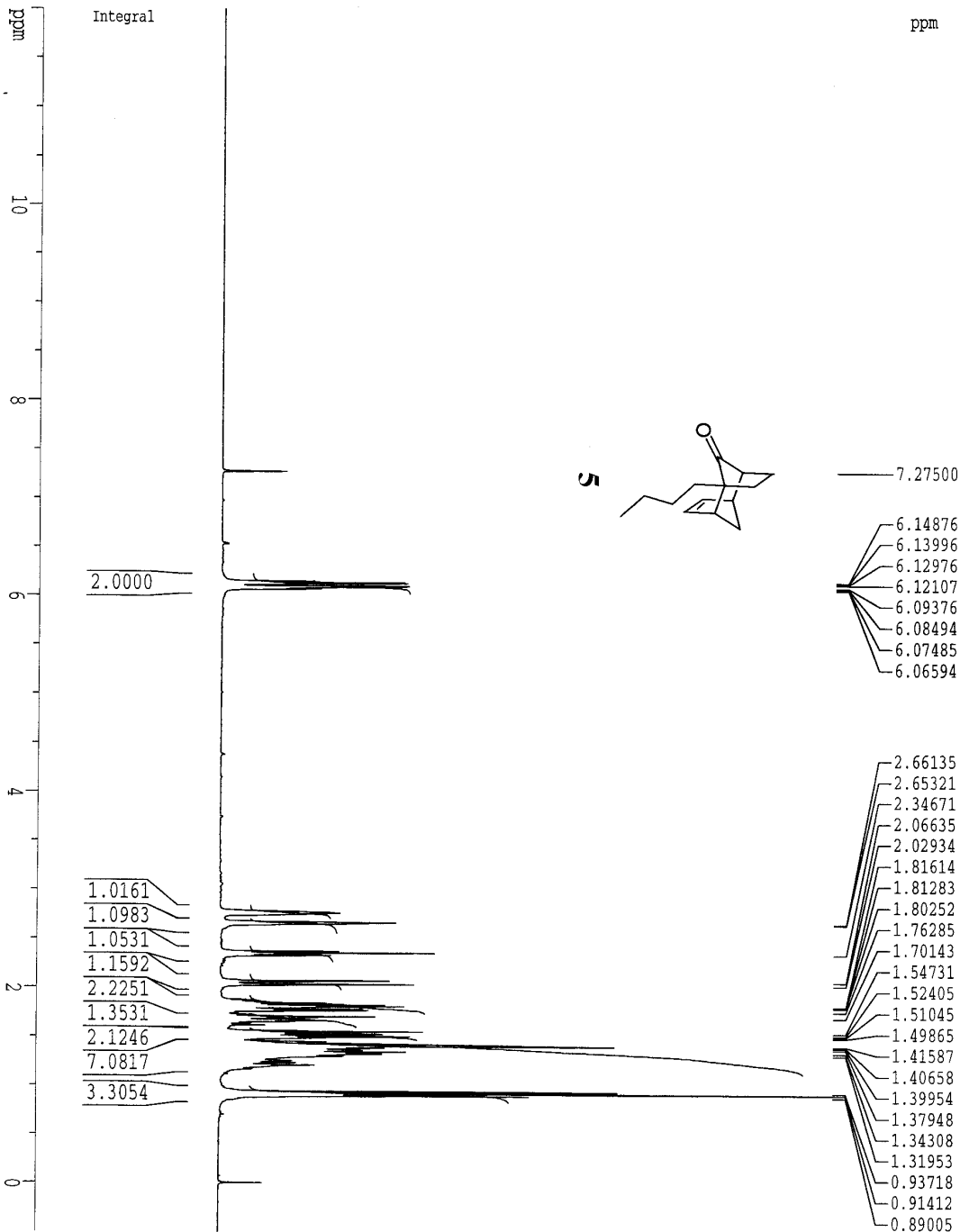
COMPOUND 13: colorless oil; ^1H NMR (250 MHz, CDCl_3): δ 6.49 (s, 2H), 4.16 (d, $J = 3.0$ Hz, 1H), 2.66-2.47 (m, 2H), 2.26-2.10 (m, 2H), 1.75-1.10 (m, 13H), 1.00-0.87 (m, 6H); ^{13}C NMR (62.9 MHz, CDCl_3): δ 141.4, 141.0, 86.1, 51.3, 48.3, 44.6, 44.5, 42.5, 39.9, 36.4, 35.3, 27.5, 18.4, 16.2, 15.3, 14.8; IR (neat) 3608, 2958, 2932, 1463, 1338 cm^{-1} ; Anal. calcd for $\text{C}_{16}\text{H}_{26}\text{O}$: C, 81.99, H; 11.18 Found: C, 82.10; H 11.13.

COMPOUND 14: colorless oil; ^1H NMR (250 MHz, CDCl_3): δ 6.50 (s, 2H), 4.16 (d, $J = 2.9$ Hz, 1H), 2.66-2.46 (m, 2H), 2.26-2.11 (m, 2H), 1.74-1.09 (m, 21H), 1.00-0.75 (m, 6H); ^{13}C NMR (62.9 MHz, CDCl_3): δ 141.4, 141.1, 86.1, 51.3, 48.3, 44.6, 44.5, 42.5, 37.4, 36.4, 33.1, 32.7, 32.6, 27.6, 24.8, 22.8, 22.7, 22.6, 14.1; IR (neat) 3583, 3047, 3015, 2953, 2929, 2855, 1736, 1544, 1495, 1470, 1376, 1266, 1172, 1057, 906 cm^{-1} Anal. calcd for $\text{C}_{20}\text{H}_{34}\text{O}$: C, 82.69, H; 11.80 Found: C, 82.80; H 12.00.

COMPOUND 16: colorless oil; ^1H NMR (250 MHz, CDCl_3): δ 6.49 (s, 2H), 4.16 (d, $J = 2.6$ Hz, 1H), 2.66-2.47 (m, 2H), 2.28-2.11 (m, 2H), 1.77-1.07 (m, 29H), 0.94-0.81 (m, 6H); ^{13}C NMR (62.9 MHz, CDCl_3): δ 141.4, 141.1, 86.1, 51.3, 48.2, 44.6, 45.5, 42.5, 37.5, 36.4, 32.7, 31.9, 31.9, 30.8, 29.4, 29.3, 27.6, 25.2, 23.1, 22.6, 14.1; IR (neat) 3603, 3342, 3068, 3019, 2949, 2925, 2851, 1597, 1454, 1376, 963, 747 cm^{-1} ; Anal. calcd for $\text{C}_{24}\text{H}_{42}\text{O}$: C, 83.17, H; 12.21, Found: C, 82.01; H 12.01.

COMPOUND 25: colorless oil; ^1H NMR (250 MHz, CDCl_3): δ 6.16-6.06 (m, 2H), 2.75 (s, 2H), 2.38-2.33 (t, $J = 6.0$ Hz, 1H), 2.08-2.04 (d, $J = 11$ Hz, 1H), 1.88-0.94 (m, 16H); ^{13}C NMR (62.9 MHz, CDCl_3): δ 214.4, 136.7, 135.3, 54.4, 48.2, 47.3, 45.3, 37.9, 36.9, 36.8, 34.8, 34.1, 29.6, 25.0, 24.7, 23.3; IR (neat) 2950, 2878, 1756, 1448 cm^{-1} ; HRMS calcd for $\text{C}_{16}\text{H}_{22}\text{ONa}$ $[\text{M} + \text{Na}]^+$ 253.15628, found 253.15686.

COMPOUND 26: colorless oil; ^1H NMR (250 MHz, CDCl_3): δ 6.16-6.06 (m, 2H), 5.89-5.73 (m, 1H) 5.05-4.91 (m, 2H), 2.78-2.65 (m, 2H), 2.35 (t, $J = 5.9$ Hz, 3H), 2.12-2.03 (m, 3H), 1.87-1.65 (m, 3H), 1.57-1.23 (m, 8H); ^{13}C NMR (62.9 MHz, CDCl_3): δ 214.4, 138.9, 136.6, 135.5, 114.3, 54.27, 48.6, 48.3, 45.5, 38.1, 33.6, 31.3, 29.6, 29.2, 24.0, 23.2; IR (neat) 3060, 2929, 1744, 1642 cm^{-1} ; HRMS calcd for $\text{C}_{16}\text{H}_{22}\text{ONa}$ $[\text{M} + \text{Na}]^+$ 253.15628, found 253.1581



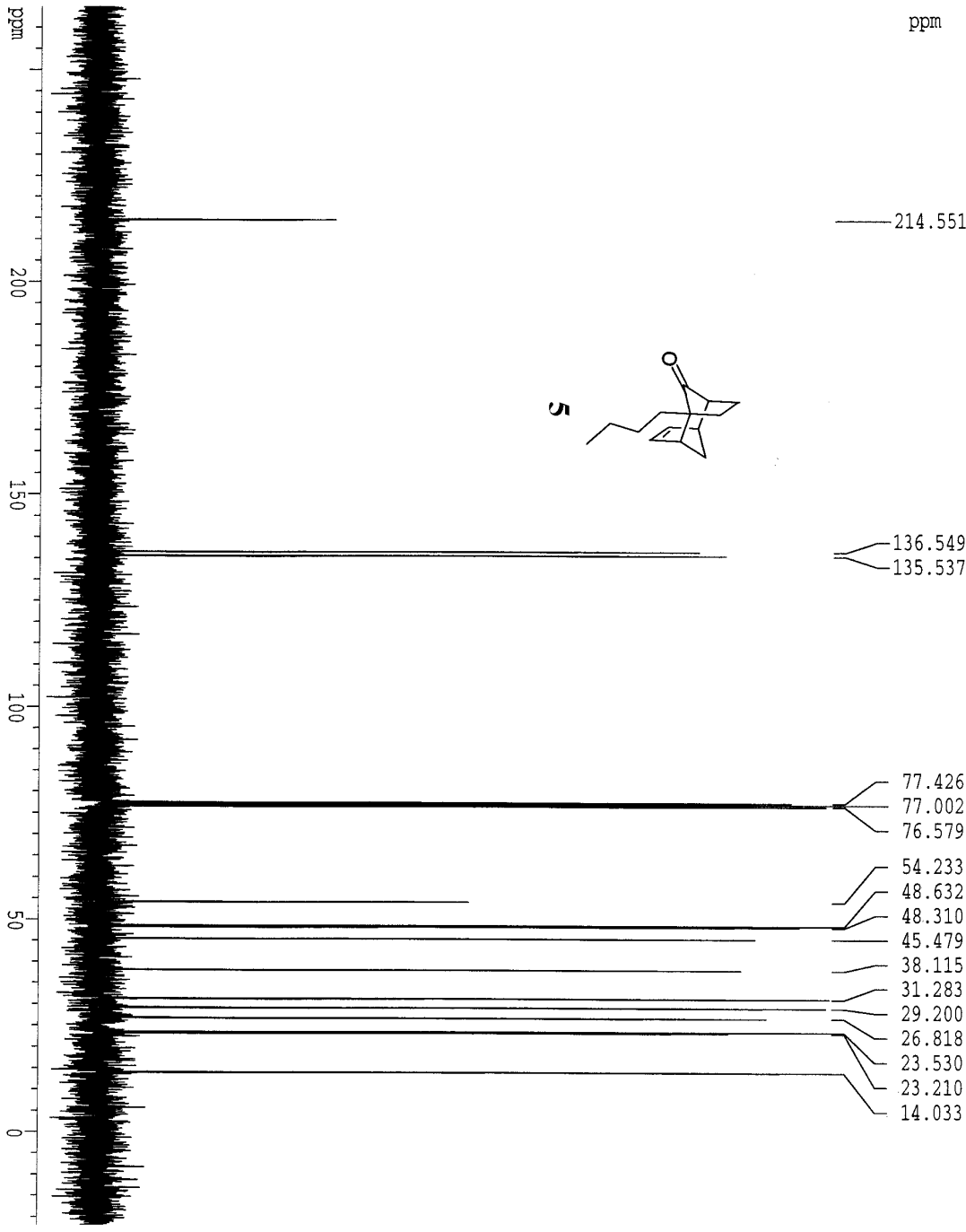
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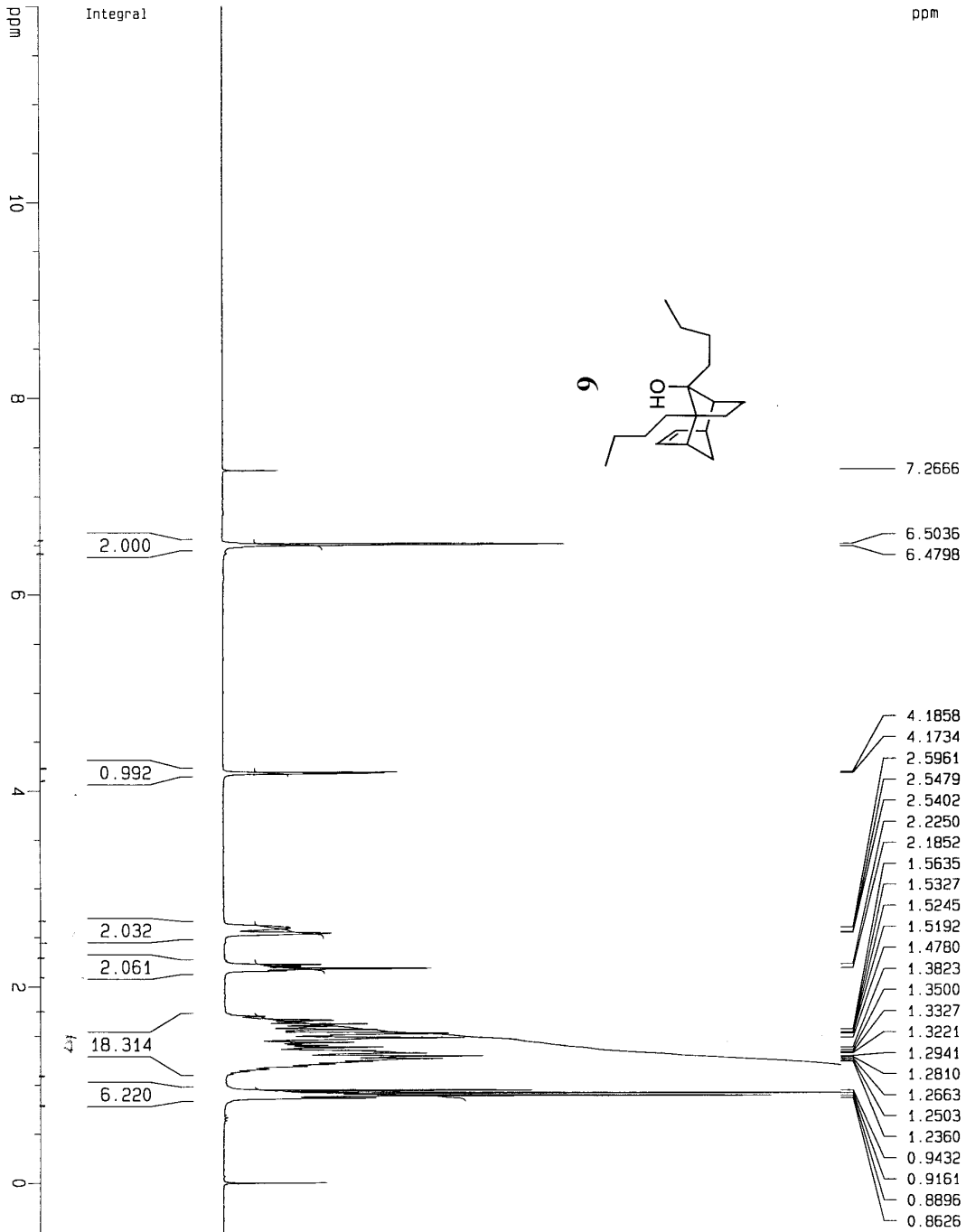
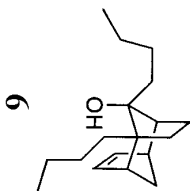
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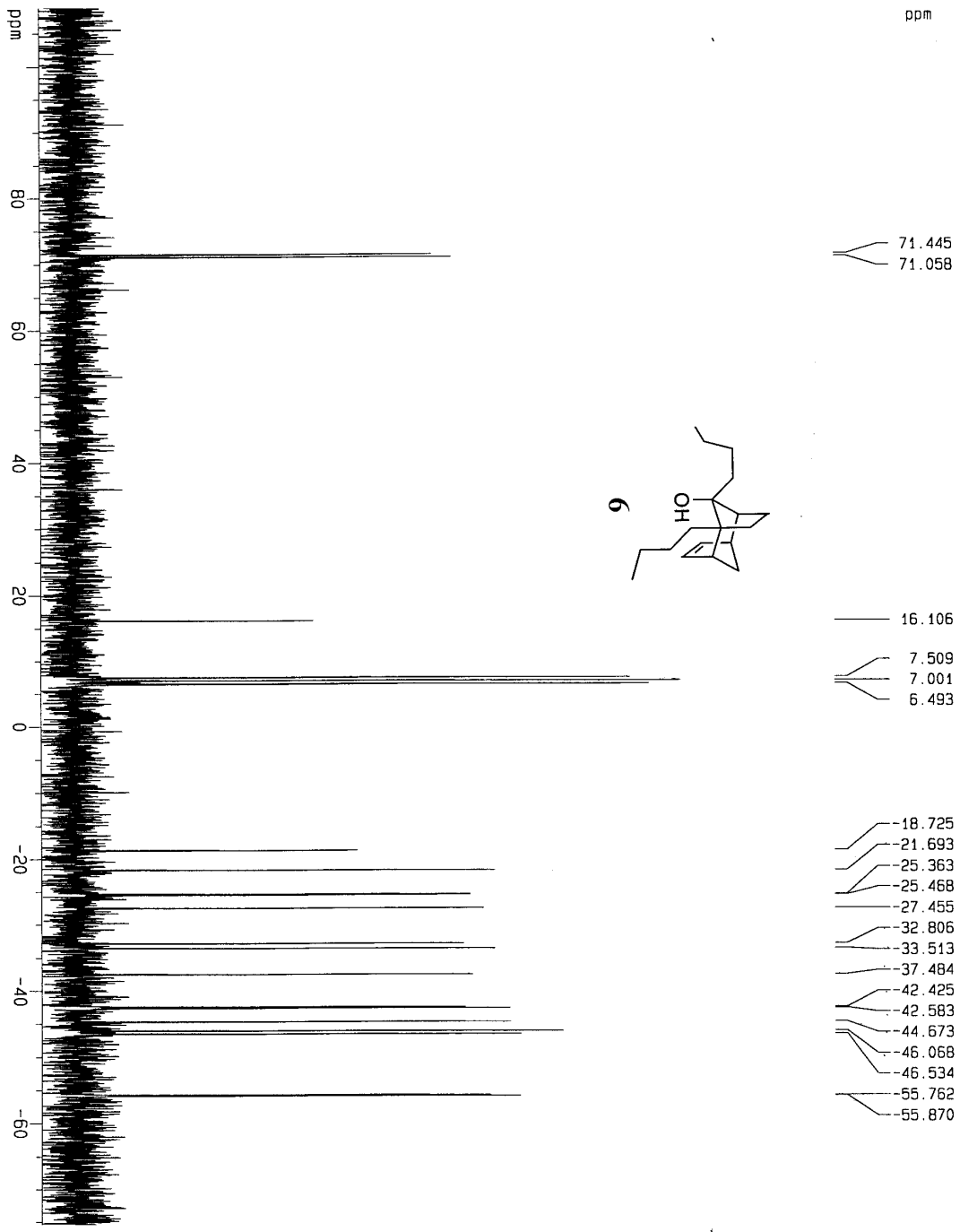


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 DS 2
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
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 DM 96.000 use
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1D NMR plot parameters
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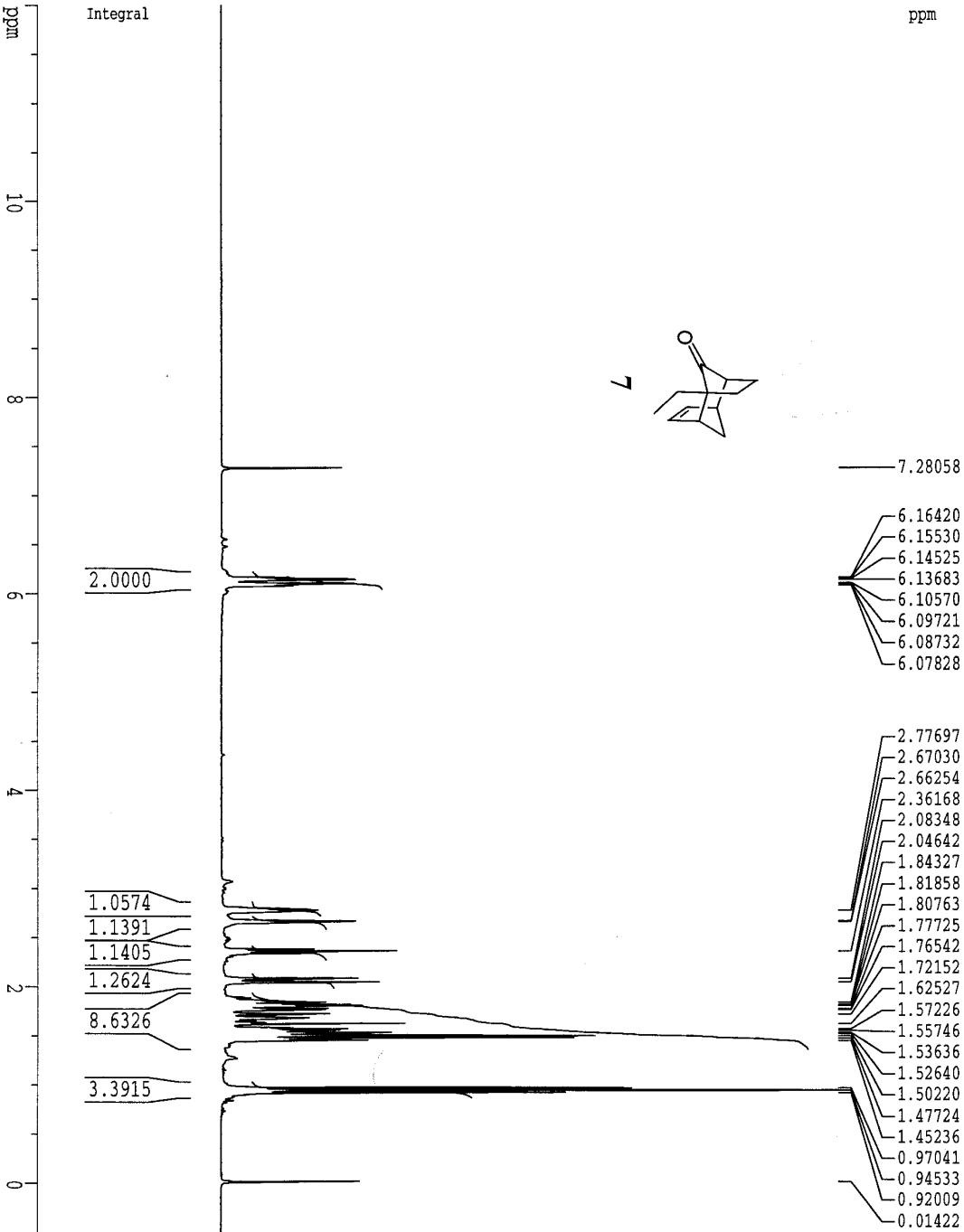


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 F2 -4740.78 Hz
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 HZCM 579.52081 Hz/



Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 SOLVENT CDC13

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 AQ 2.6542580 sec

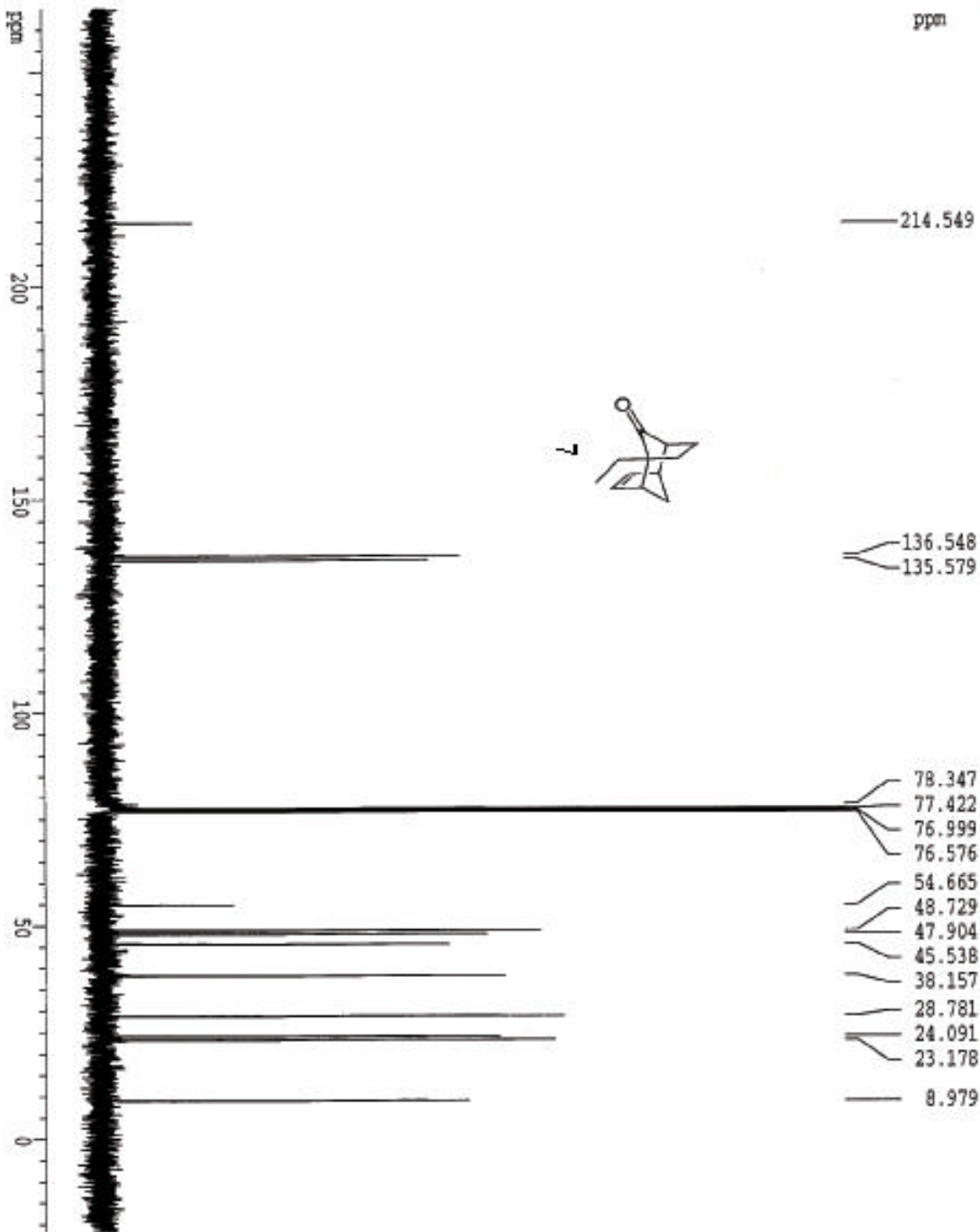
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 PL1 0.00 dB

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 LB 0.30 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
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 CY 12.50 cm
 FILP 12.000 ppm
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 F2P -0.500 ppm
 F2 -150.07 Hz
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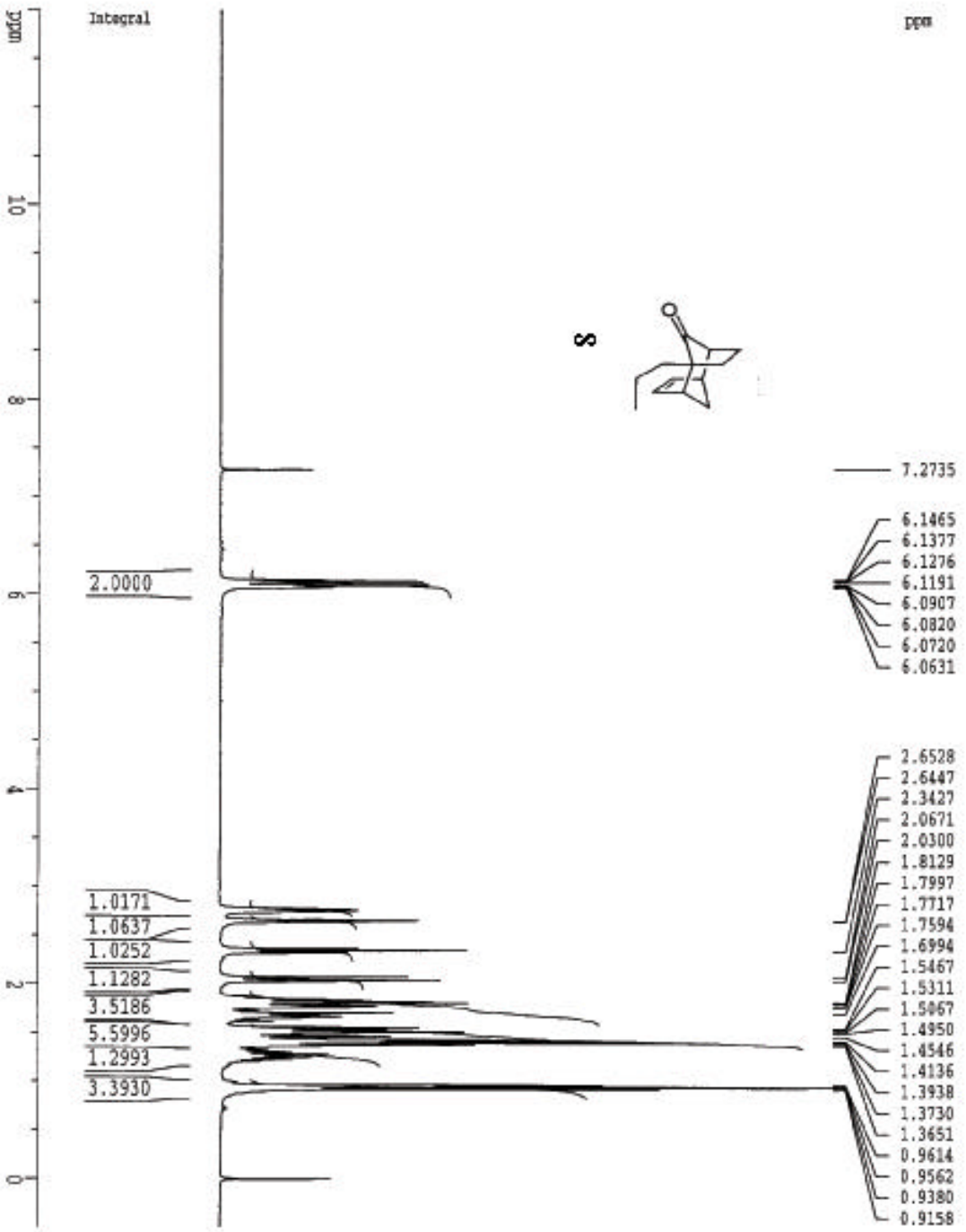
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 NS 708
 DS 4

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 FIDRES 0.330277 Hz
 AQ 1.5139316 sec
 RG 32764
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 DE 6.00 usec
 TE 300.0 K
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 P112 24.50 dB
 CHPROG2 waltz16

REPRO2 100.00 usec
 SFO2 300.1315007 MHz
 NUC2 13C
 P12 0.00 dB
 D1 1.00000000 sec
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 NUC1 13C
 P11 6.00 dB

F2 - Processing Parameters
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ID MSN plot parameters
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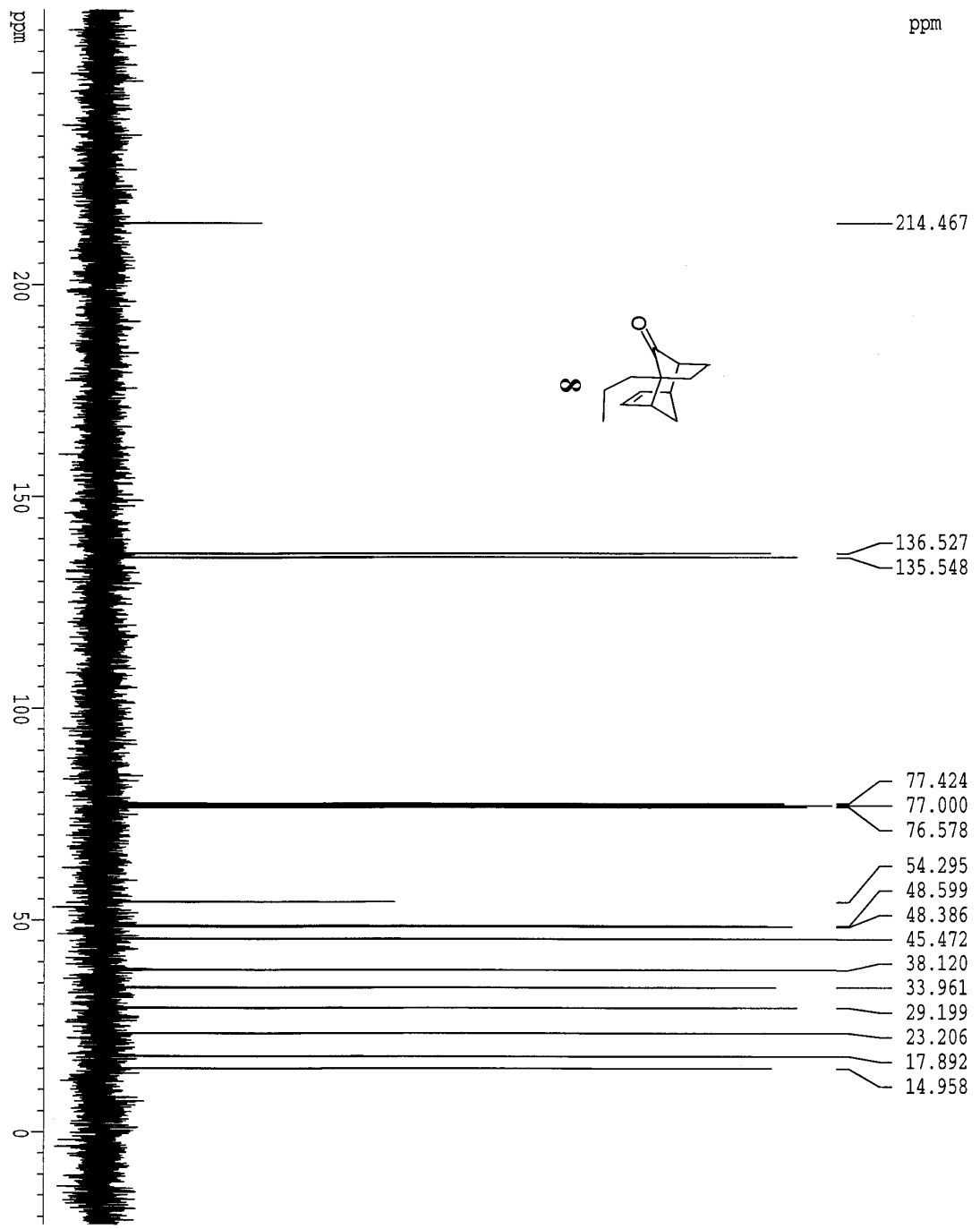
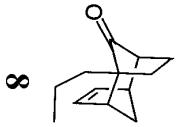


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 DS 2
 SWH 6172.839 Hz
 FIDRES 0.186380 Hz
 AQ 2.6542580 sec
 RG 128
 DW 81.000 usec
 DE 6.00 usec
 GE 300.0 K
 D1 1.00000000 sec
 P1 7.50 usec
 DE 6.00 usec
 SFO1 300.1317708 MHz
 NUC1 1H
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F2 - Processing parameters
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 NAME sw-111-53-A1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020408
 Time 21.48

INSTRUM dtx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30

TD 65536
 SOLVENT CDCl3
 NS 117
 DS 4

SWH 21645.021 Hz
 FIDRES 0.330277 Hz
 AQ 1.5139316 sec

RG 32768
 DW 23.100 usec
 DE 6.00 usec
 TE 300.0 K

D11 0.03000000 sec
 PL12 24.50 dB
 CPDPRG2 waltz16

PCPD2 100.00 usec
 SFO2 300.1315007 MHz
 NUC2 1H

PL2 0.00 dB
 D1 1.00000000 sec
 P1 7.75 usec

DE 6.00 usec
 SFO1 75.4769164 MHz
 NUC1 13C

PL1 6.00 dB

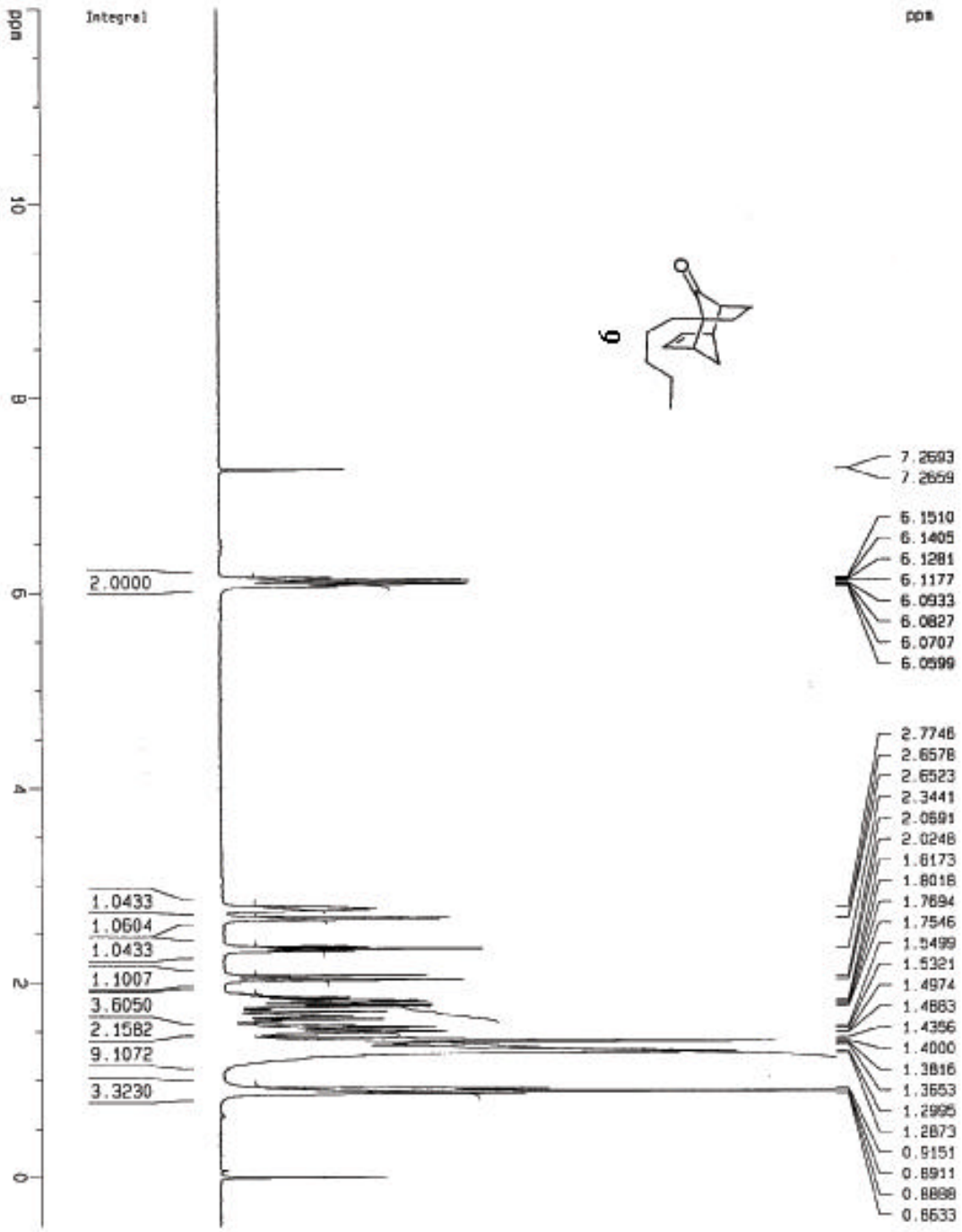
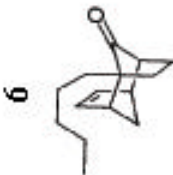
F2 - Processing parameters
 SI 32768
 SF 75.4677518 MHz

WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm

F1P 264.844 ppm
 F1 19987.16 Hz
 F2P -21.968 ppm
 F2 -1657.86 Hz

PPMCM 14.34058 ppm/cm
 HZCM 1082.25098 Hz/cm

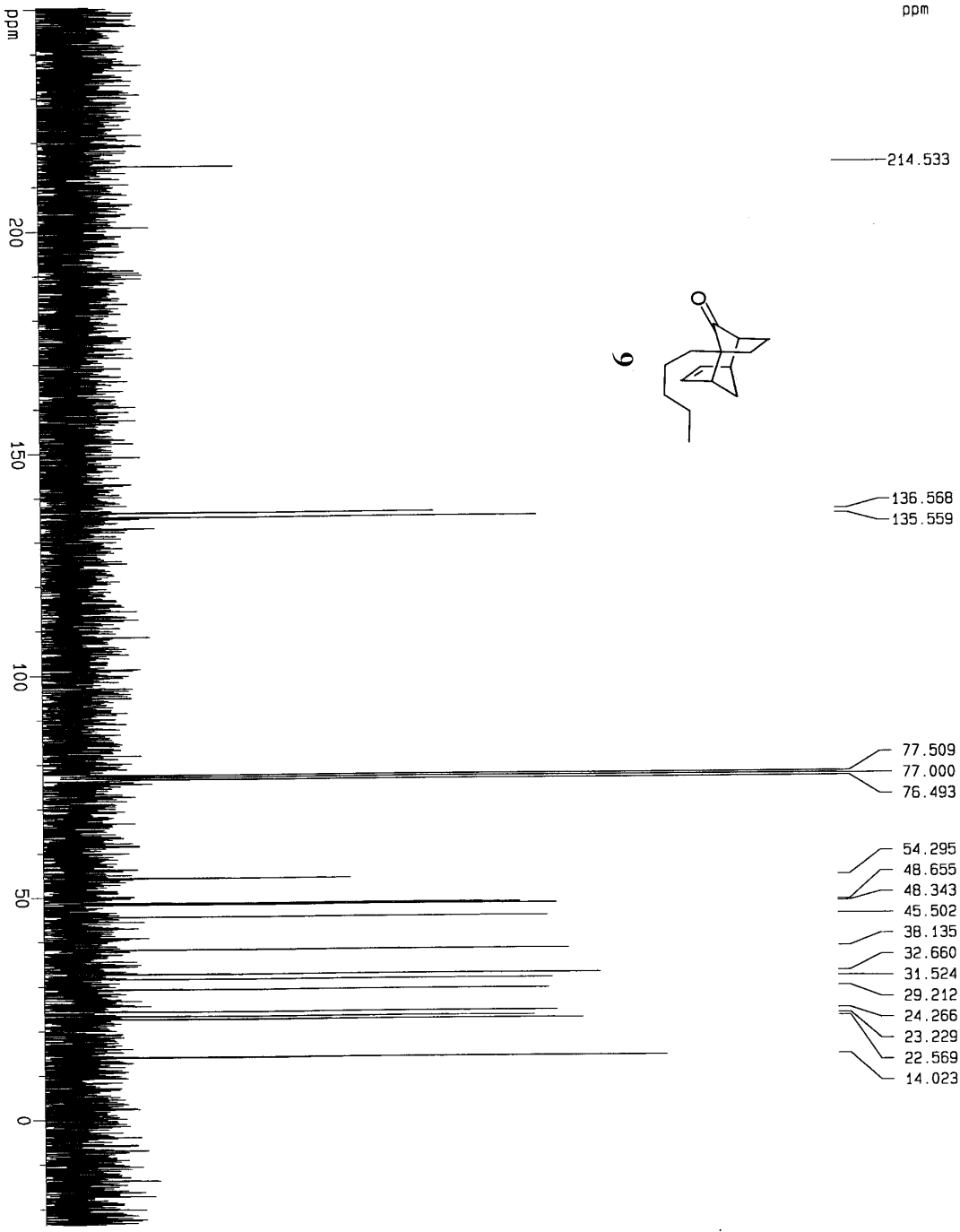


Current Data Parameters
 NAME SW-III-60-A2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020413
 Time 23.32
 INSTRUM 400250
 PULPROG 5 PR OMP 1H
 TD 16380
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5209.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457778 sec
 RG 715
 QW 95.000 u88
 DE 137.14 u58
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.70 u88
 SFO1 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300056 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

3D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FXP 12.000 ppm
 F1 3001.56 Hz
 F2 -0.500 ppm
 F3 -129.07 Hz
 PPMX0 0.82500 ppm
 HZXM 156.33129 Hz/



Current Data Parameters
 NAME SW-III-60-A2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

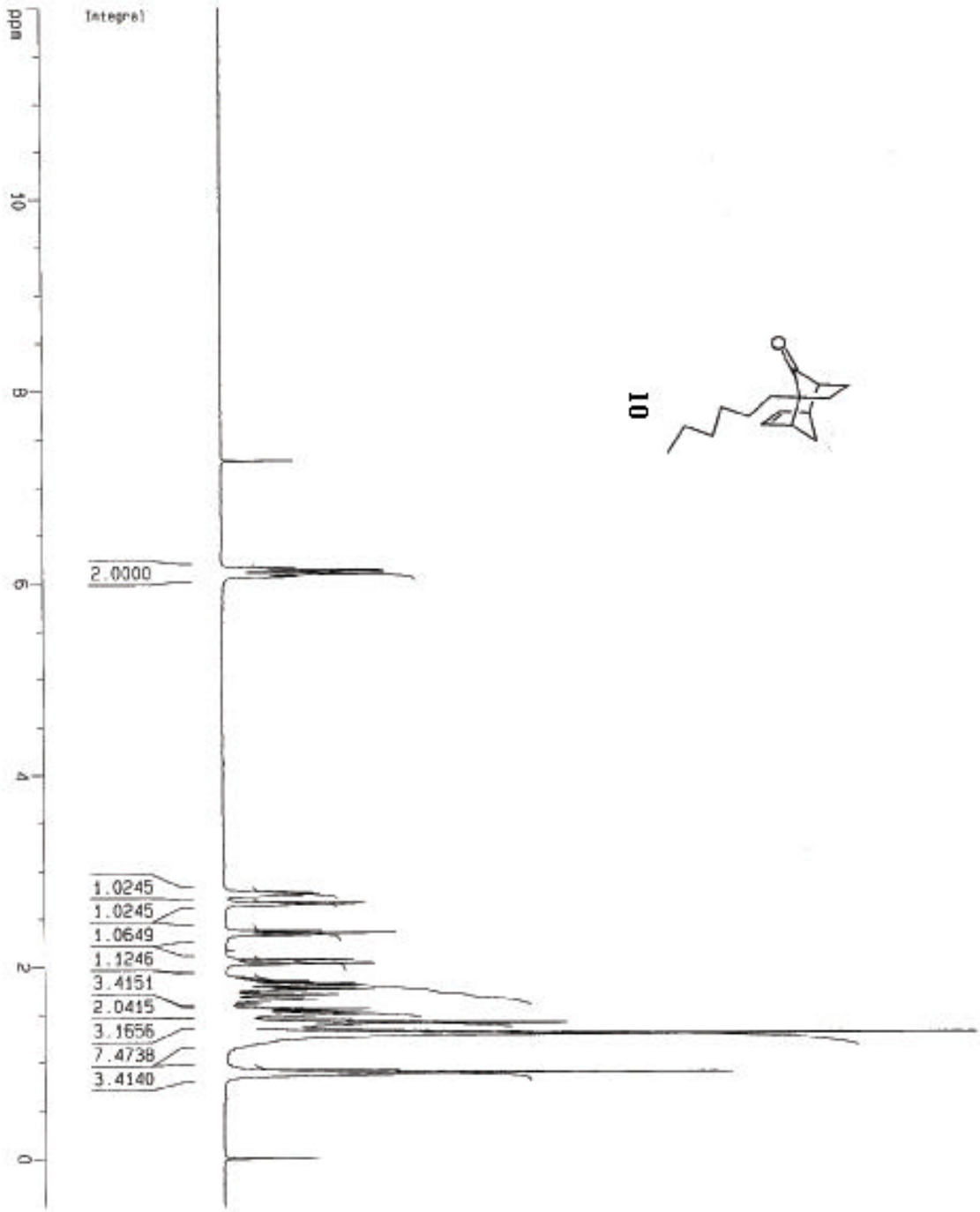
Date_ 20020413
 Time 23.34
 INSTRUM arx250
 PROBRD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 105
 DS 4
 SMH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DM 29.000 use
 DE 41.43 use
 TE 300.0 K
 D12 0.00002000 sec
 D15 23.00 dB
 CPDPRG waitz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 5.35 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters

SI 32768
 SF 62.8952408 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 CY 18.00 cm
 F1P 250.405 ppm
 F1 15749.28 Hz
 F2P -23.724 ppm
 F2 -1492.10 Hz
 PPKCM 13.70643 ppm
 HZCM 862.06891 Hz/

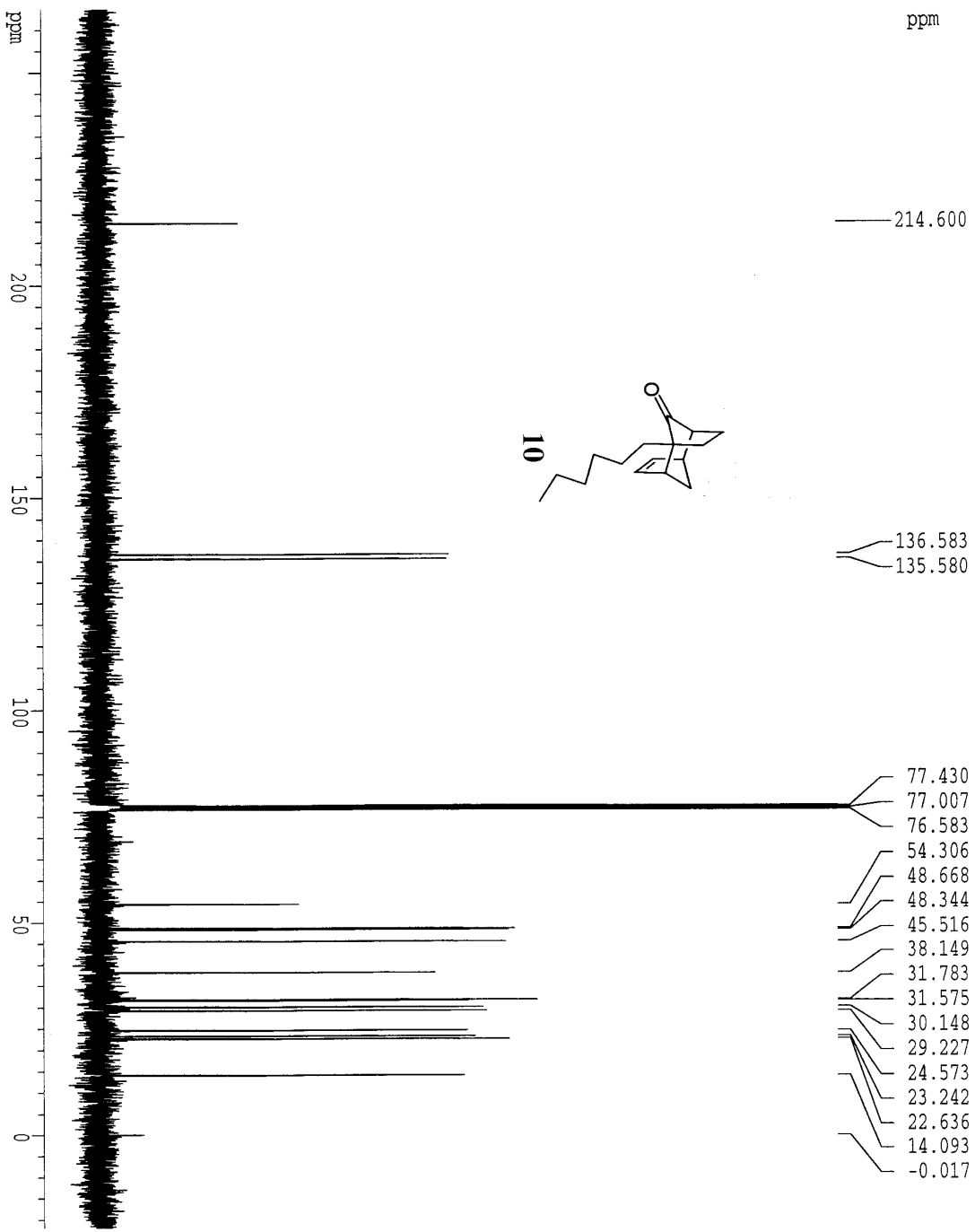


Current Data Parameters
 NAME SW-11-74-A2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011026
 Time 0.37
 INSTRUM ark250
 PROBNM 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 715
 CW 98.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.00000000 sec
 P1 E. 70 use
 SFO1 250.1315021 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300049 MHz
 WDM EN
 SSB 0
 LB 0.20 Hz
 BB 0
 PC 1.50

1D NMR plot parameters
 CK 20.00 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 FWHM 0.62500 ppm
 HZCN 156.33125 Hz/

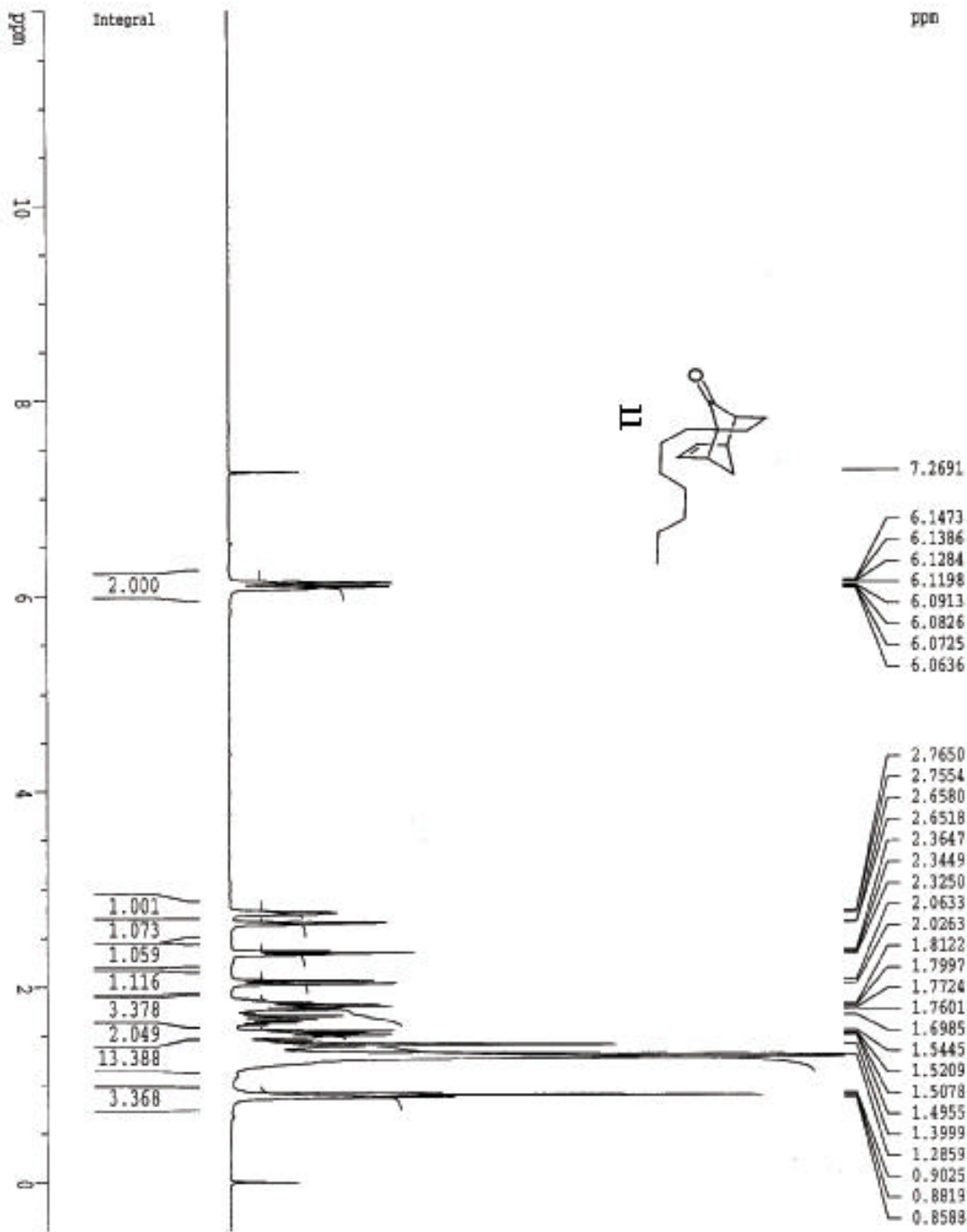


Current Data Parameters
 NAME SW-IT-67-A3
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20010115
 Time 16.28
 INSTRUM dirx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgdc30
 TD 65536
 SOLVENT CDC13
 NS 767
 DS 4
 SWH 21645.021 Hz
 FIDRES 0.330277 Hz
 AQ 1.5139316 sec
 RG 32768
 DW 23.100 usec
 DE 6.00 usec
 TE 300.0 K
 D11 0.03000000 sec
 PL12 24.50 dB
 CPDPRG2 waltz16
 PCPD2 100.00 usec
 SFO2 300.1315007 MHz
 NUC2 1H
 PL2 0.00 dB
 D1 1.00000000 sec
 P1 7.75 usec
 DE 6.00 usec
 SFO1 75.4769164 MHz
 NUC1 13C
 PL1 6.00 dB

F2 - Processing parameters
 SI 32768
 SF 75.4677498 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 20.00 cm
 F1P 264.870 ppm
 F1 19989.14 Hz
 F2P -21.942 ppm
 F2 -1655.88 Hz
 DPVCM 14.34058 ppm/cm
 HZCM 1082.25110 Hz/cm



Current Data Parameters
 NAME sw-II-117-A2
 EXPRNO 1
 PROCNO 1

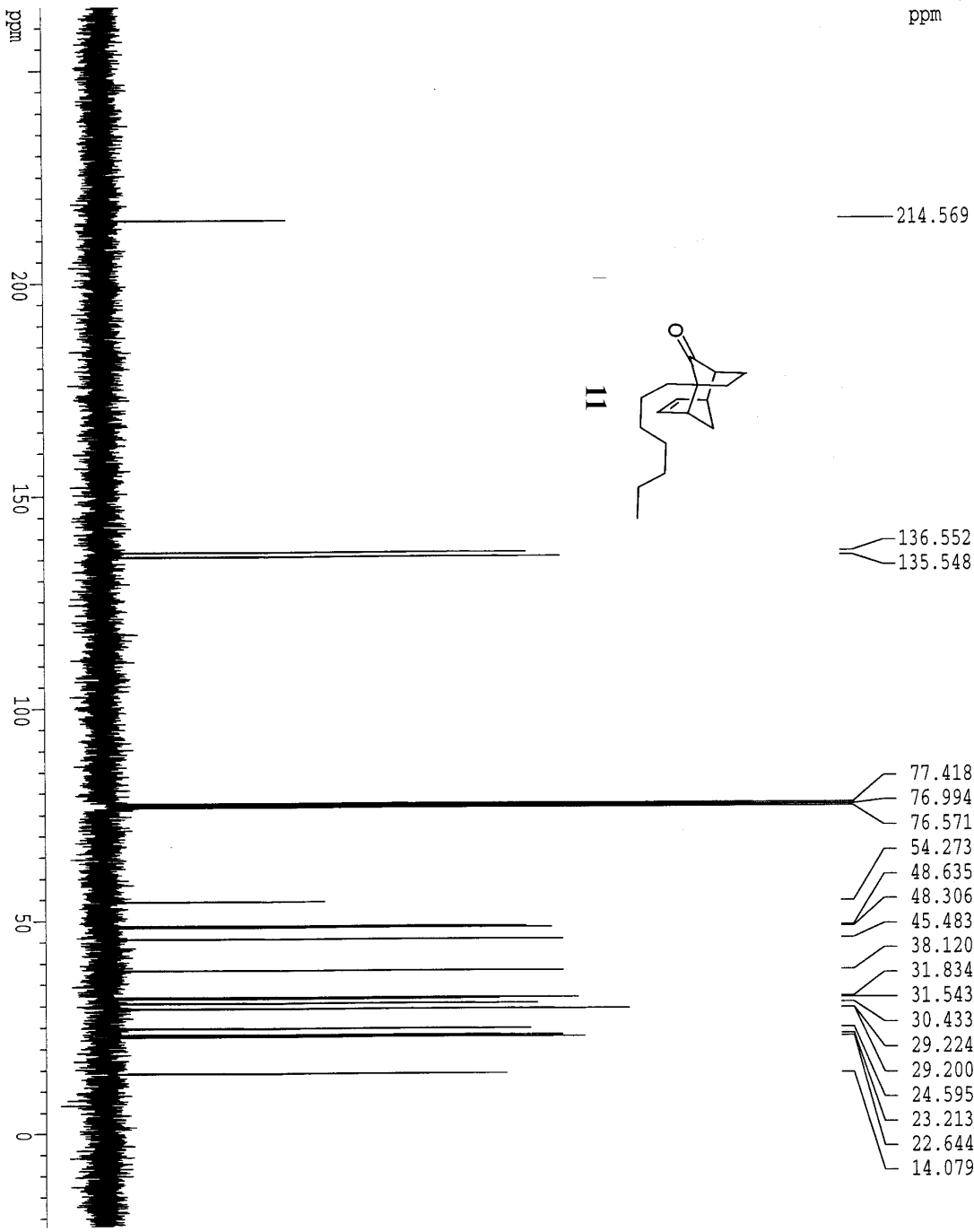
F2 - Acquisition Parameters
 Date_ 20011229
 Time 16.56
 INSTRUM drx300
 PROBNM 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLC/SMT CDC13
 NS 16
 DS 2

SMF 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 256
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K

DL 1.00000000 sec
 PL 7.50 usec
 DE 6.00 usec
 SFO1 300.1317708 MHz
 PROC1 1H
 P11 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1306034 MHz
 WDM KM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.50

ID NAME plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3601.56 Hz
 F2P -0.500 ppm
 F2 -150.07 Hz
 PPM2CN 0.62500 ppm/cm
 HZCN 387.58125 Hz/cm



Current Data Parameters
 NAME sw-11-117-A2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011229
 Time 16.38

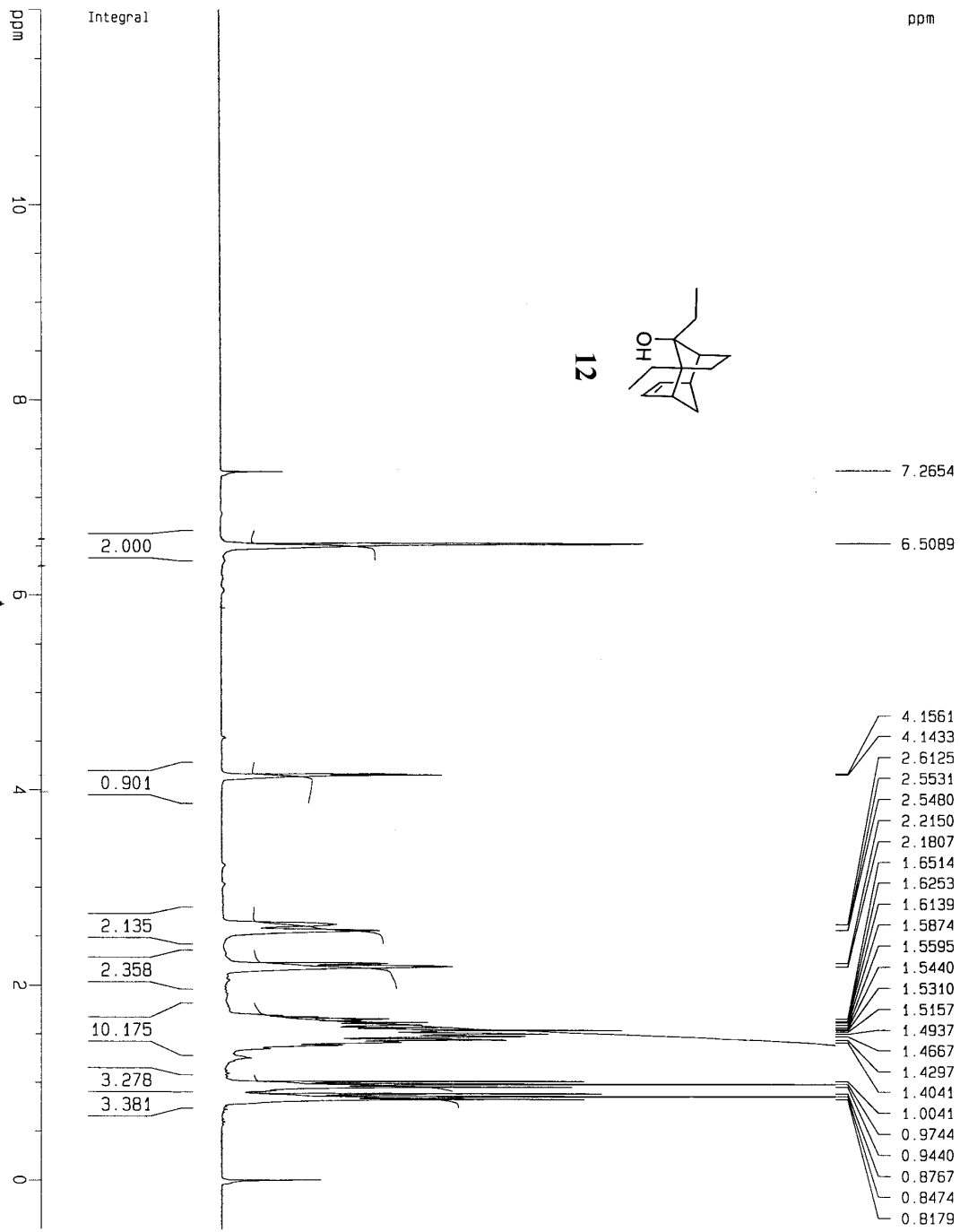
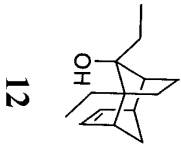
INSTRUM dx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 166
 DS 4

SMH 21645.021 Hz
 FIDRES 0.330277 Hz
 AQ 1.5139316 sec
 RG 32768
 DM 23.100 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.03000000 sec
 D11 24.50 dB
 PL12

CPDPRG2 waltz16
 PCPD2 100.00 usec
 SFO2 300.1315007 MHz
 NUC2 1H
 PL2 0.00 dB
 DI 1.00000000 sec
 P1 7.75 usec
 DE 6.00 usec
 SFO1 75.4769164 MHz
 NUC1 13C
 PL1 6.00 dB

F2 - Processing parameters
 SI 32768
 SF 75.4677518 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

ID NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 264.844 ppm
 F1 19987.16 Hz
 F2P -21.968 ppm
 F2 -1657.86 Hz
 PPMCM 14.34058 ppm/cm
 HZCM 1082.25098 Hz/cm



Current Data Parameters
 NAME sw-111-36-A1
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters
 Date_ 20020308
 Time 13.33
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 715
 DW 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.0000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300065 MHz
 MDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 PPMCM 0.62500 ppm
 HZCM 156.33125 Hz/

Current Data Parameters

NAME sw-III-36-A1
 EXPNO 2
 PROCNO 2

F2 - Acquisition Parameters

Date_ 20020308
 Time 13.35
 INSTRUM srx250
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 106
 DS 4
 SMH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DM 29.000 use
 DE 41.43 use
 TE 300.0 K
 D12 0.0002000 sec
 DL5 23.00 dB
 CPDPRG waltz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 5.35 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

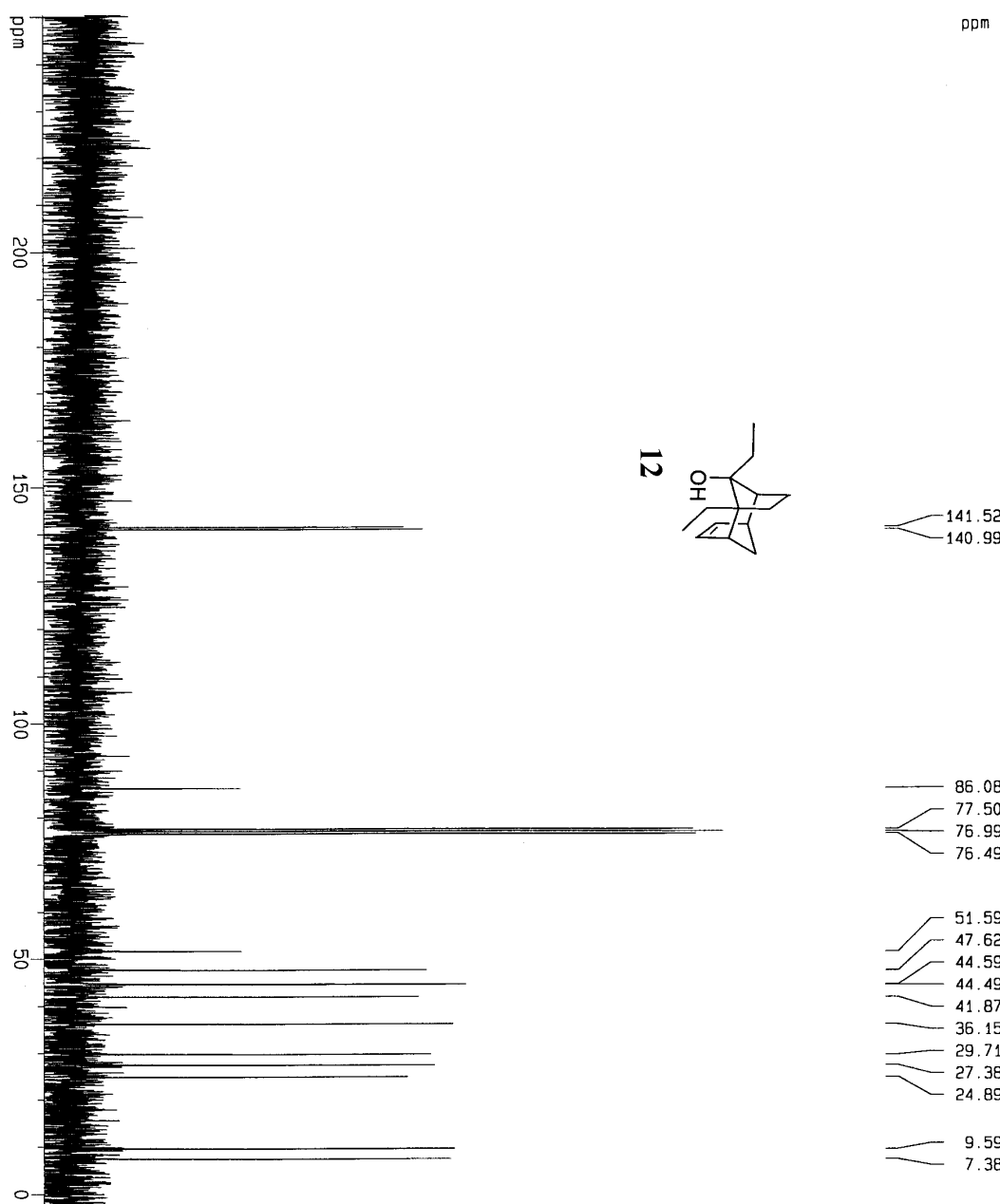
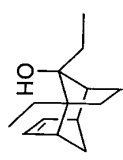
F2 - Processing parameters

SF 62.8952408 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

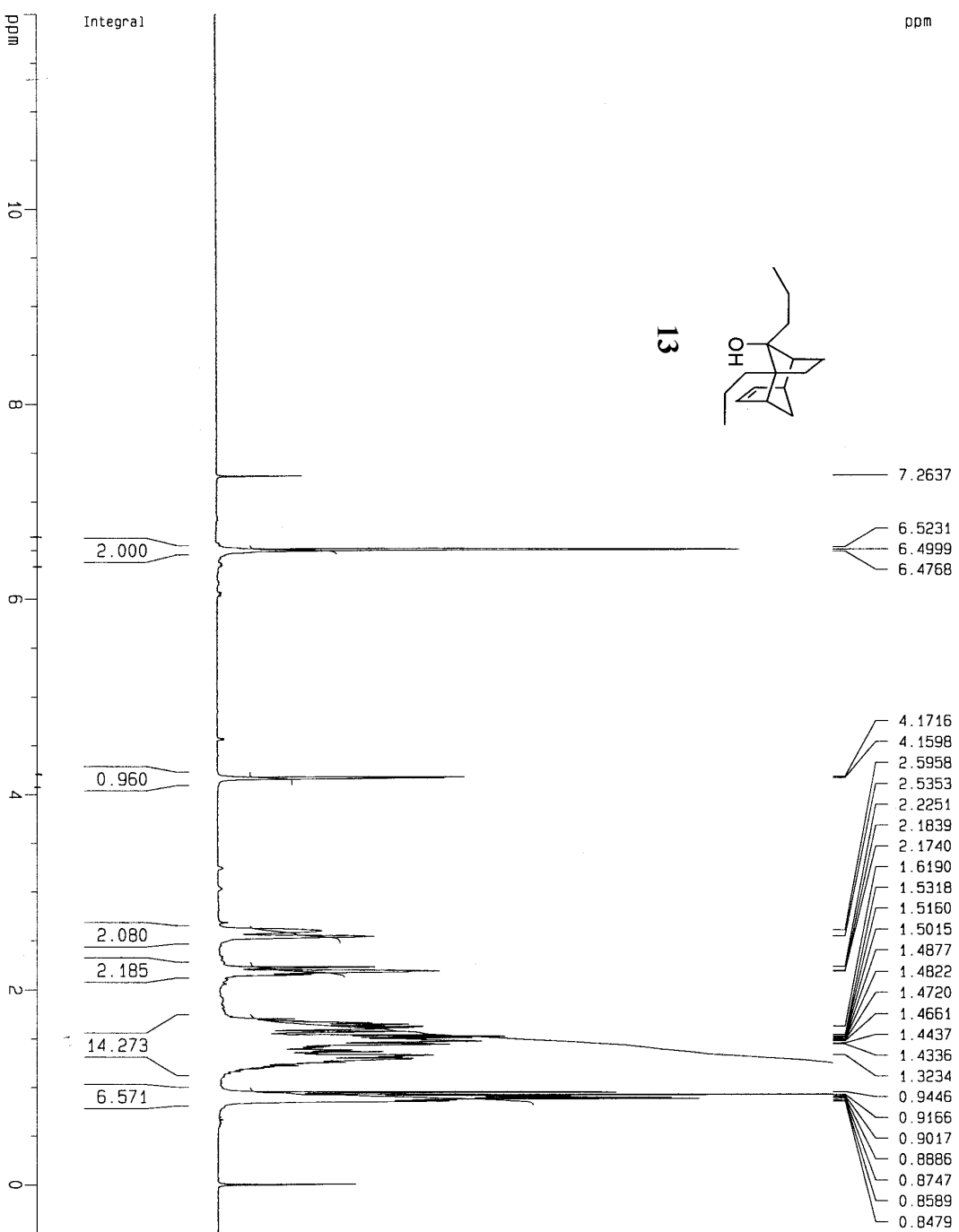
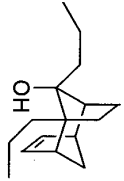
1D NMR plot parameters

CX 20.00 cm
 CY 10.00 cm
 F1P 250.405 ppm
 F1 15749.28 Hz
 F2P -23.724 ppm
 F2 -1492.10 Hz
 PPKCM 13.70643 ppm
 HZCM 862.06891 Hz/

- 141.524
- 140.999
- 86.083
- 77.508
- 76.999
- 76.492
- 51.594
- 47.620
- 44.596
- 44.495
- 41.874
- 36.151
- 29.710
- 27.387
- 24.893
- 9.595
- 7.382



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Current Data Parameters
 NAME Sw-III-34-A1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

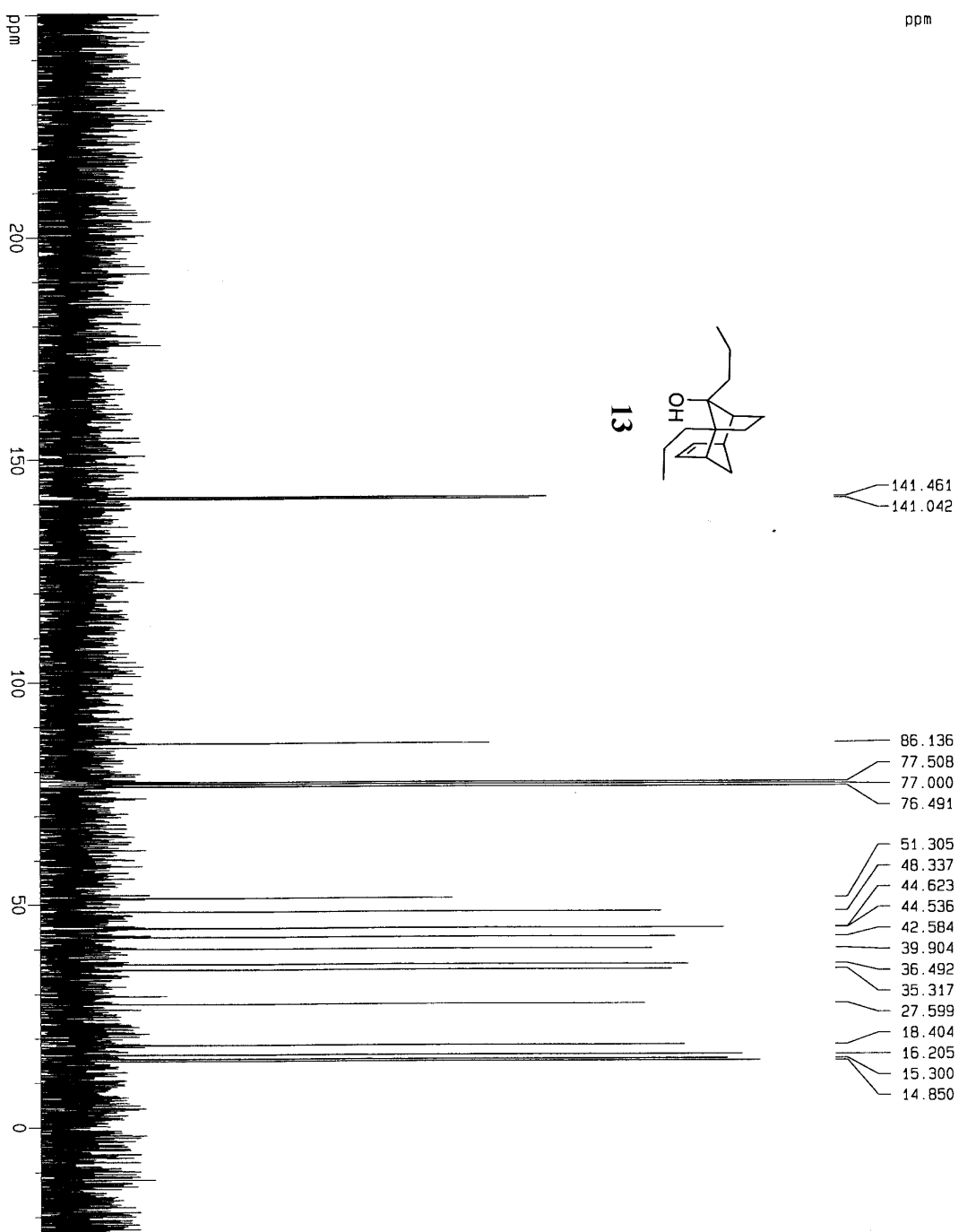
Date_ 20020306
 Time 16.18
 INSTRUM arx250
 PROBHD 5 mm GNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 715
 DE 96.000 use
 TE 137.14 use
 D1 300.0 K
 D1 1.00000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters

SI 16384
 SF 250.1300062 MHz
 MDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters

CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 PPMCM 0.62500 ppm
 HZCM 156.33125 Hz



Current Data Parameters
 NAME sw-III-34-A1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

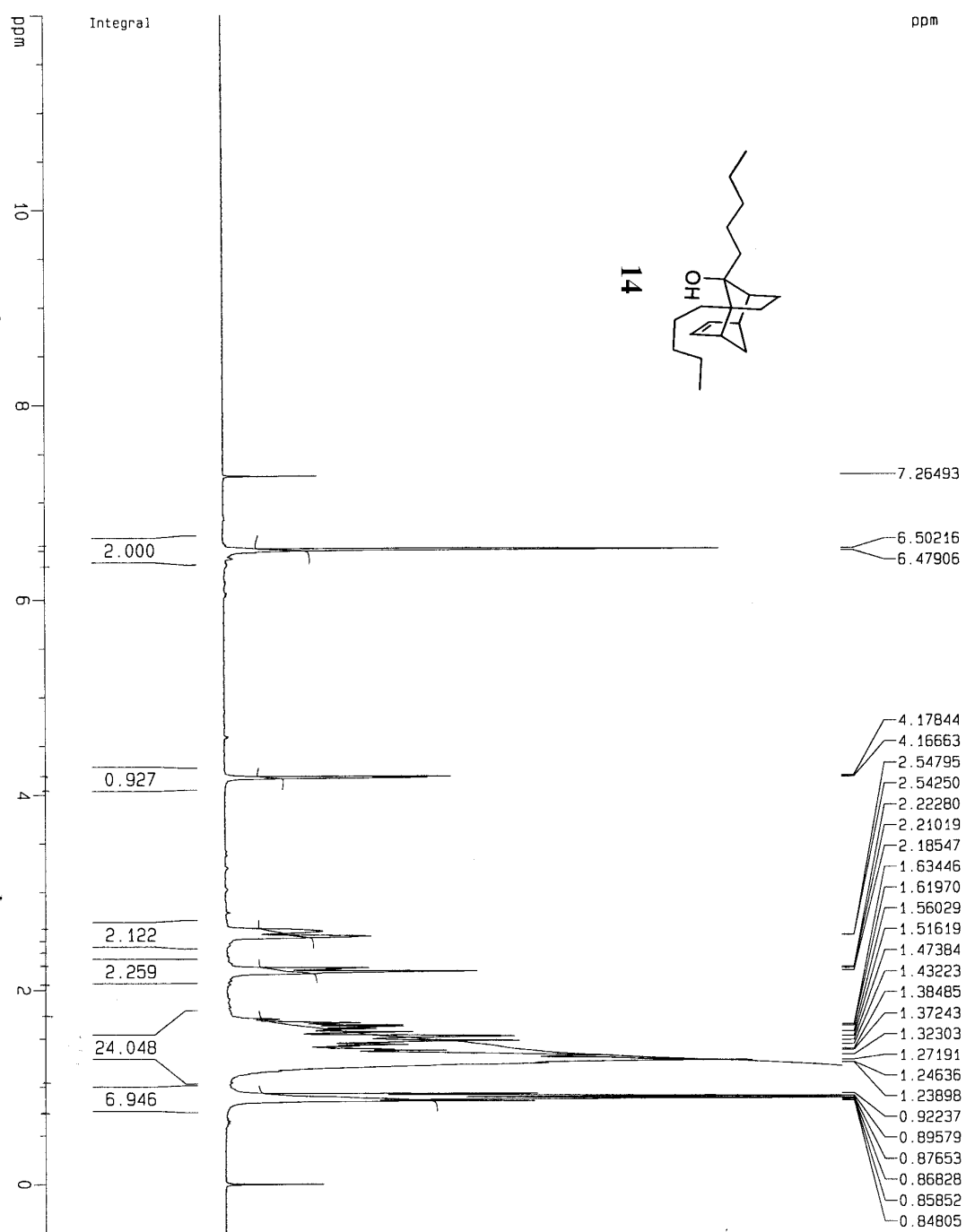
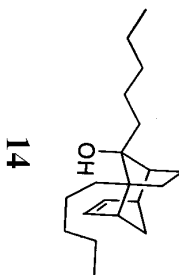
Date_ 20020306
 Time 16.21
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 111
 DS 4
 SMH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DW 29.000 use
 DE 41.43 use
 TE 300.0 K
 D12 0.00002000 sec
 DL5 23.00 dB
 CPOPRG Waltz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 5.35 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters

SI 32768
 SF 62.8952408 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 CY 20.00 cm
 F1P 250.405 ppm
 F1 15749.28 Hz
 F2P -23.724 ppm
 F2 -1492.10 Hz
 PPMCM 13.70643 ppm
 HZCM 862.06991 Hz/



Current Data Parameters
 NAME SW-III-32-A1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020305
 Time 13.33
 INSTRUM apr250
 PROBHD 5 mm GNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 512
 DM 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300062 MHz
 WDM EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 PPMCM 0.62500 ppm
 HZCM 156.33125 Hz/

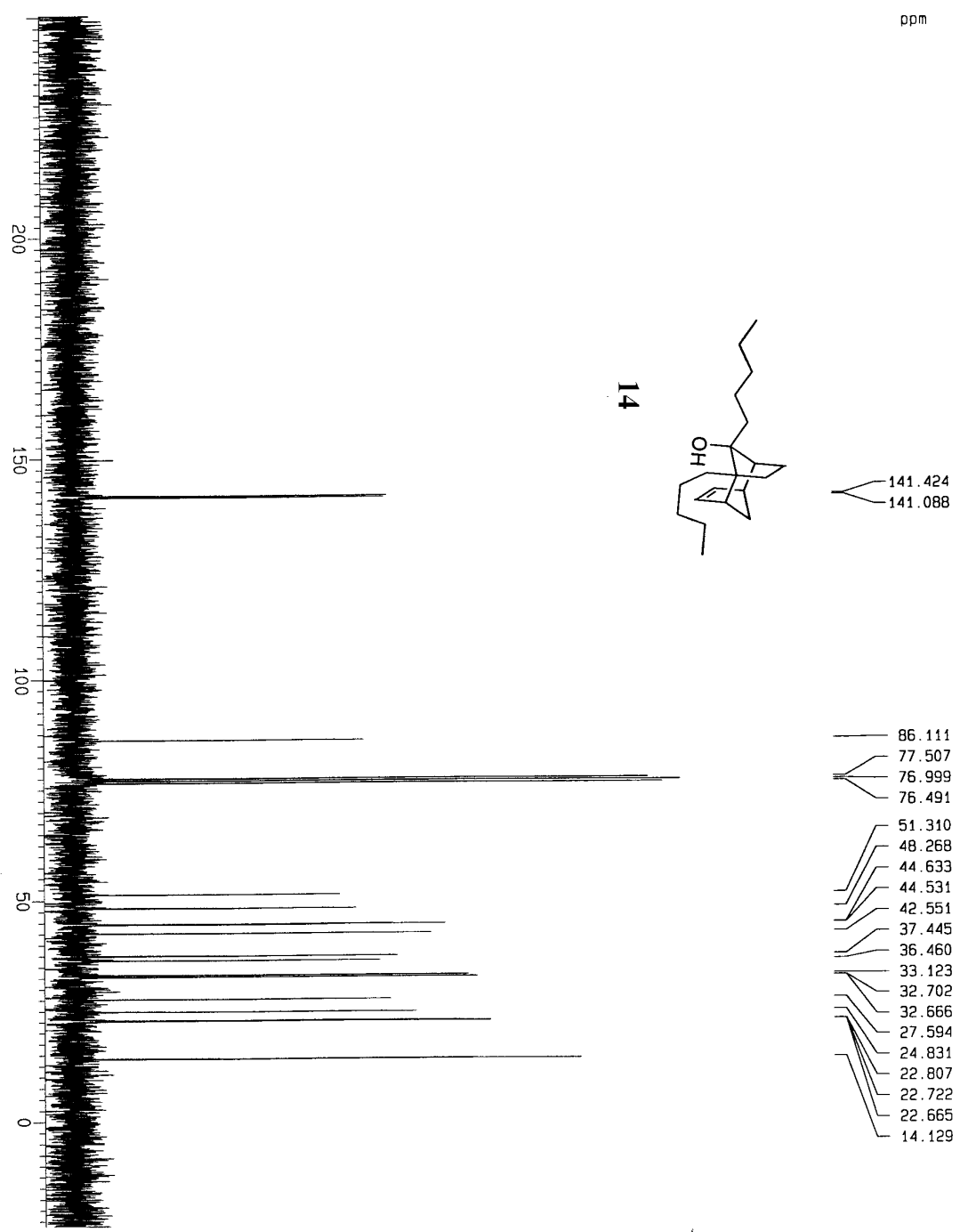
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 NAME sw-III-32-A1
 EXPNO 2
 PROCNO 1

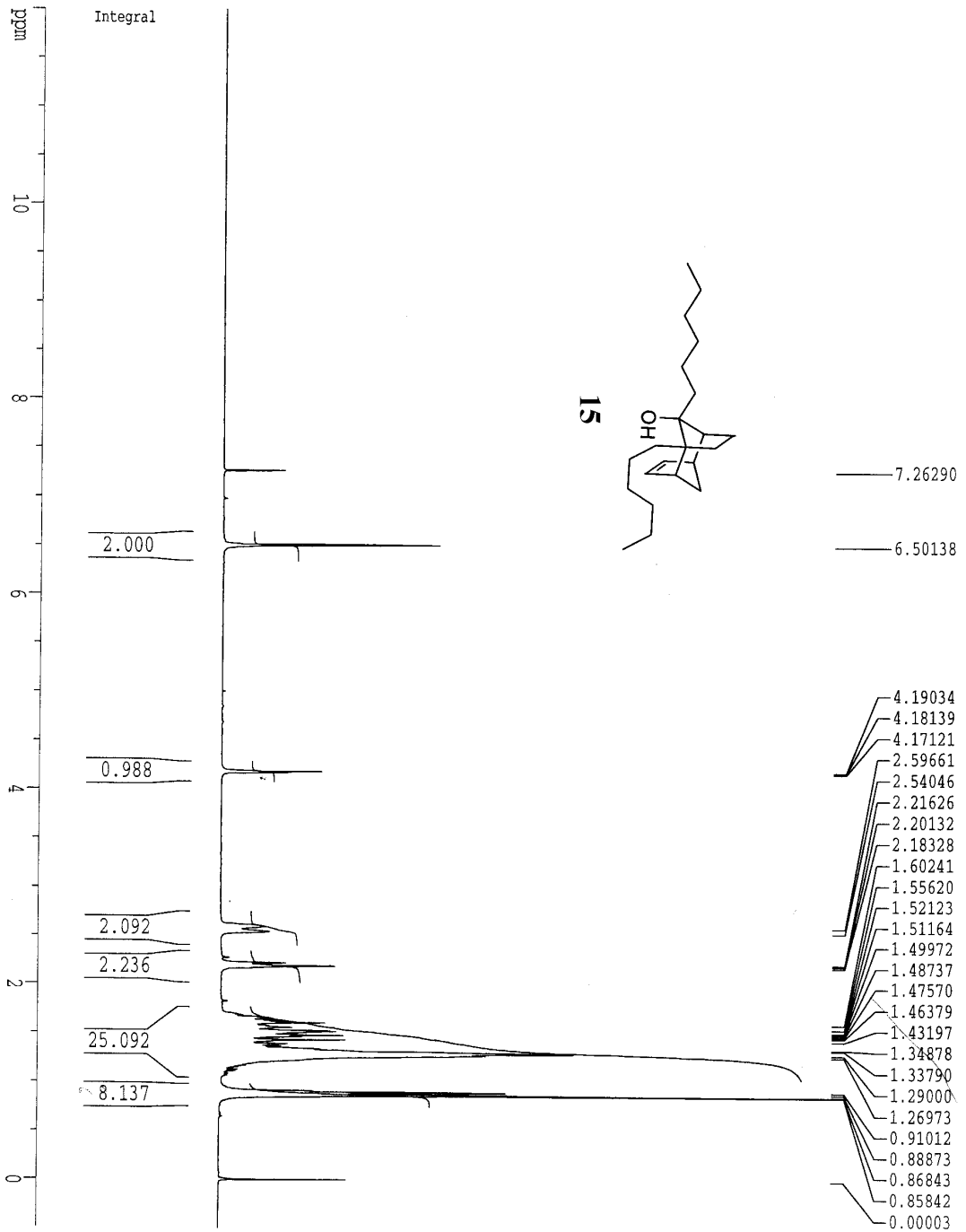
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 Date_ 20020305
 Time 13.36
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 138
 DS 4

SMH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DM 29.000 use
 DE 41.43 use
 TE 300.0 K
 D12 0.00002000 sec
 DL5 23.00 dB
 CPDPRG Waitz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 5.35 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters
 SI 32768
 SF 62.8952408 MHz
 MDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 250.405 ppm
 F1 15749.28 Hz
 F2P -23.724 ppm
 F2 -1492.10 Hz
 PPMICM 13.70643 ppm
 HZCM 862.06891 Hz/





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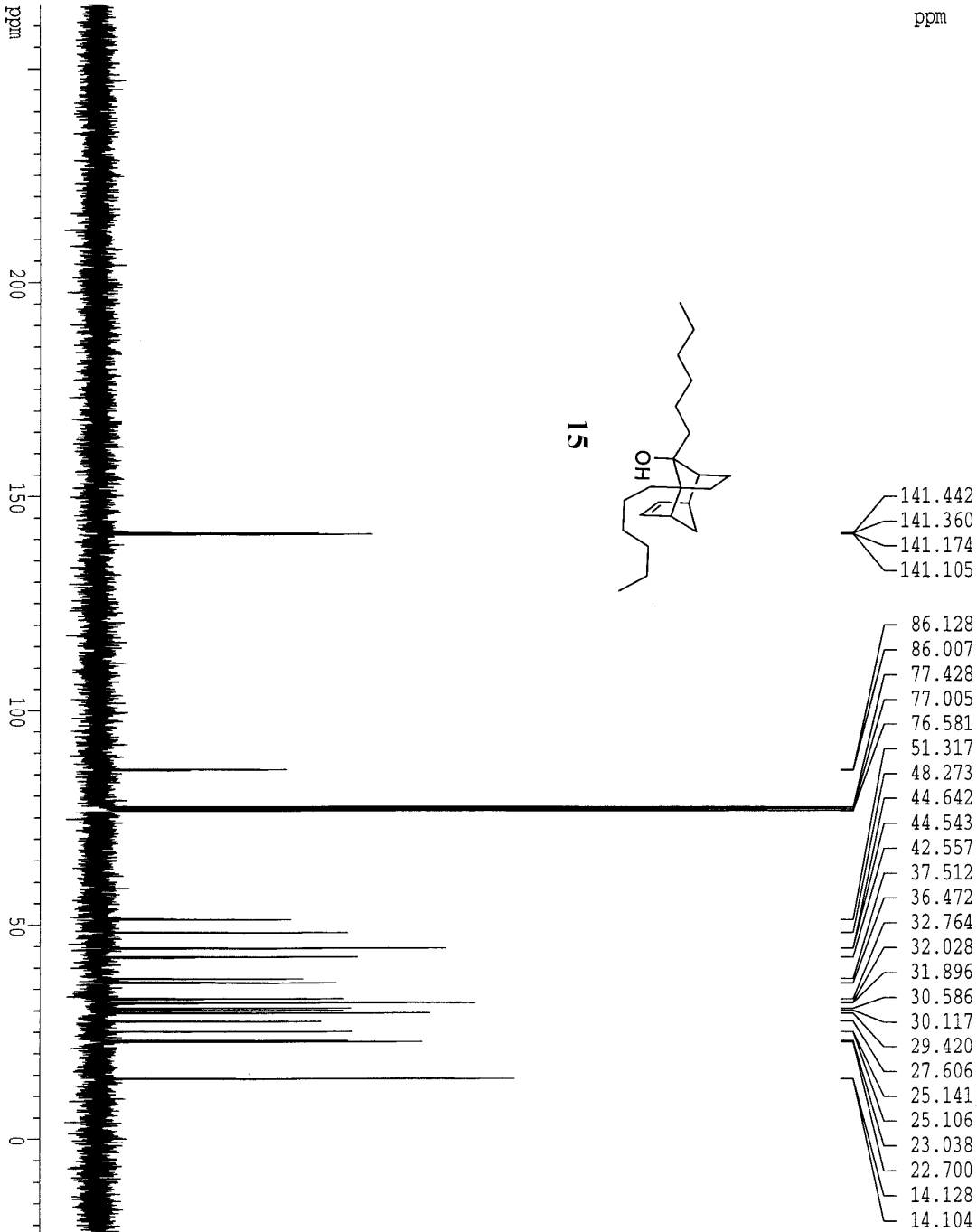
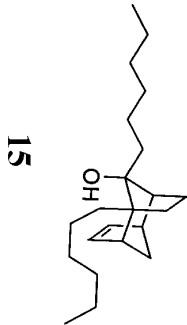
Current Data Parameters
 NAME sw-II-67-A1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011015
 Time 16.04
 INSTRUM dtx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2

SMH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 128
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 7.50 usec
 DE 6.00 usec
 SFO1 300.1317708 MHz
 NUQC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300053 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 FIP 12.000 ppm
 F1 3601.56 Hz
 F2P -0.500 ppm
 F2 -150.07 Hz
 PPMCM 0.62500 ppm/cm
 HZCM 187.58125 Hz/cm



Current Data Parameters
 NAME sw-II-67-A1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011015
 Time 16.07

INSTRUM dx300
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30

TD 65536
 SOLVENT CDCl3
 NS 278

DS 4
 SWH 21645.021 Hz
 FIDRES 0.330277 Hz

AQ 1.5139316 sec
 RG 32768
 DW 23.100 usec

DE 6.00 usec
 TE 300.0 K
 D11 0.03000000 sec

PL12 24.50 dB
 CPDPRG2 waltz16
 PCPD2 100.00 usec

SFO2 300.1315007 MHz
 NUC2 1H
 PL2 0.00 dB

D1 1.00000000 sec
 P1 7.75 usec
 DE 6.00 usec

SFO1 75.4769164 MHz
 NUC1 13C
 PL1 6.00 dB

F2 - Processing parameters
 SI 32768
 SF 75.4677498 MHz

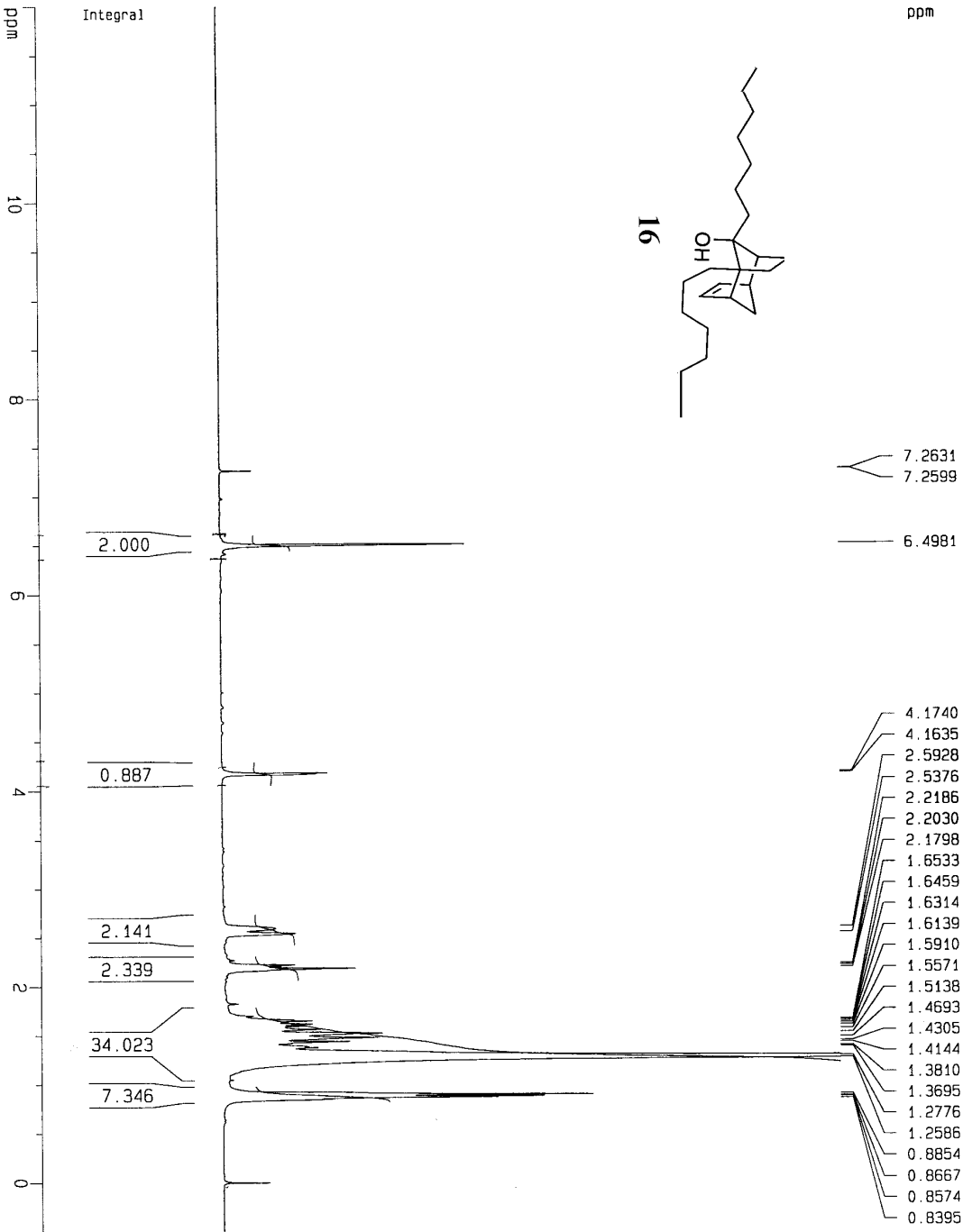
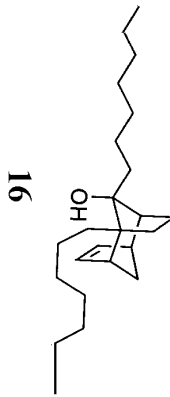
WDW EM
 SSB 0
 LB 1.00 Hz

GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm

F1P 264.870 ppm
 F1 19989.14 Hz
 F2P -21.942 ppm

F2 -1655.88 Hz
 PPRCM 14.34058 ppm/cm
 HZCM 1082.25110 Hz/cm



Current Data Parameters
 NAME sw-III-38-A1
 EXPNO 1
 PROCNO 2

F2 - Acquisition Parameters

Date_ 20020308
 Time 13.43
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 256
 DM 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

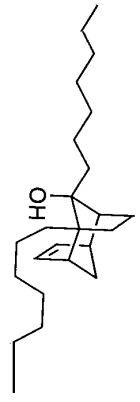
F2 - Processing parameters

SI 16384
 SF 250.130066 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters

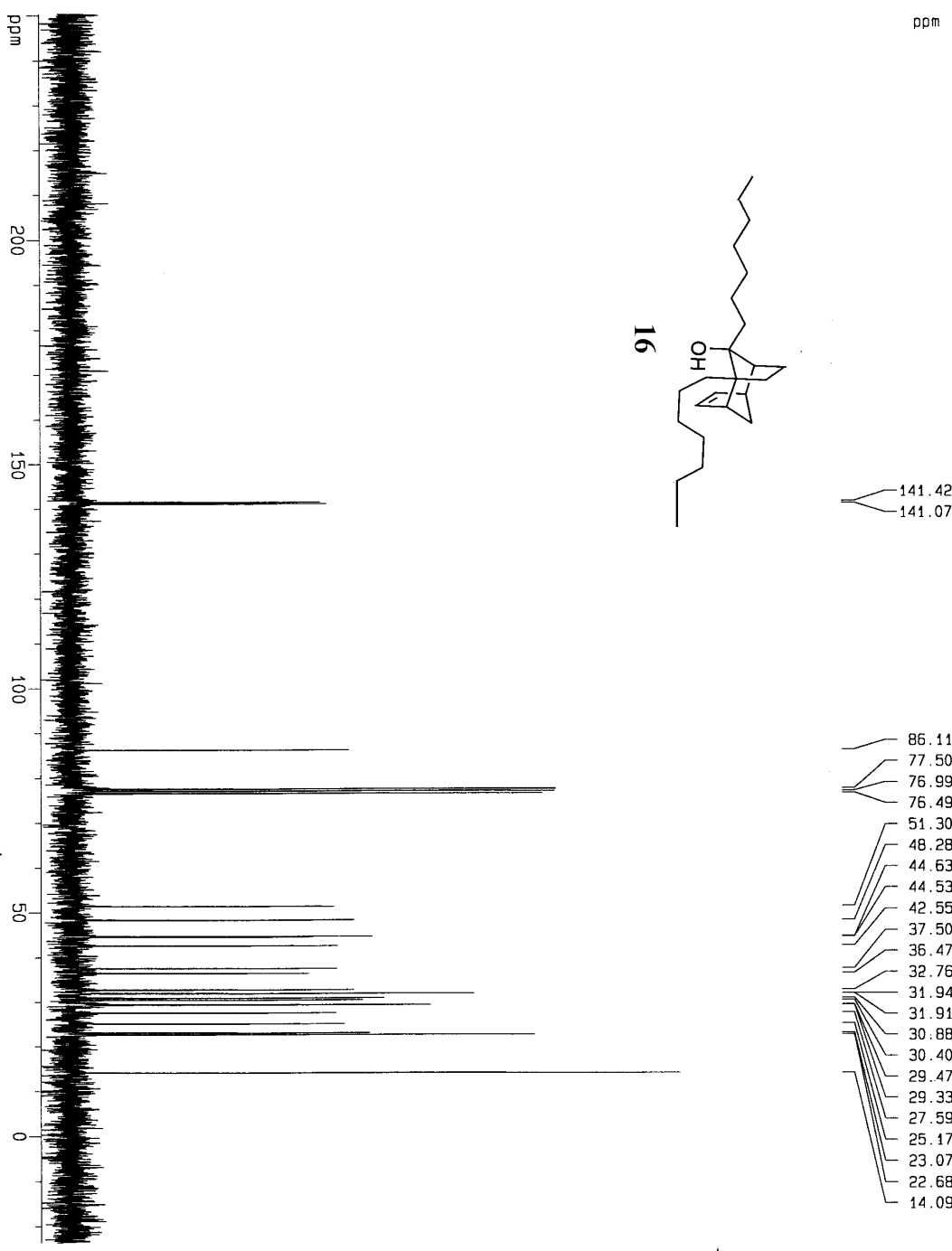
CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 PPKCM 0.62500 ppm
 HZCM 156.33125 Hz/

16



141.428
141.073

86.112
77.508
76.999
76.491
51.309
48.280
44.634
44.530
42.556
37.507
36.470
32.763
31.945
31.916
30.886
30.407
29.472
29.331
27.598
25.178
23.073
22.681
14.096



Current Data Parameters
NAME sw-111-38-A1
EXPNO 2
PROCNO 2

F2 - Acquisition Parameters
Date_ 20020308
Time 13.45
INSTRUM srx250
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 36864
SOLVENT CDCl3
NS 223
DS 4
SWH 17241.379 Hz
FIDRES 0.467702 Hz
AQ 1.0691060 sec
RG 22800
DM 29.000 use
DE 41.43 use
TE 300.0 K
D12 0.00002000 sec
DL5 23.00 dB
CPDPRG waliz16
P31 103.00 use
D1 1.00000000 sec
P1 5.35 use
SF01 62.9023694 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters
SI 32768
SF 62.8952408 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 250.405 ppm
F1 15749.28 Hz
F2P -23.724 ppm
F2 -1492.10 Hz
PPKCK 13.70643 ppm
HZCM 862.06891 Hz/

Current Data Parameters
 NAME SW-VI-76-A1A
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030604
 Time 22.08

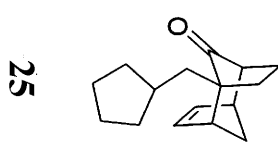
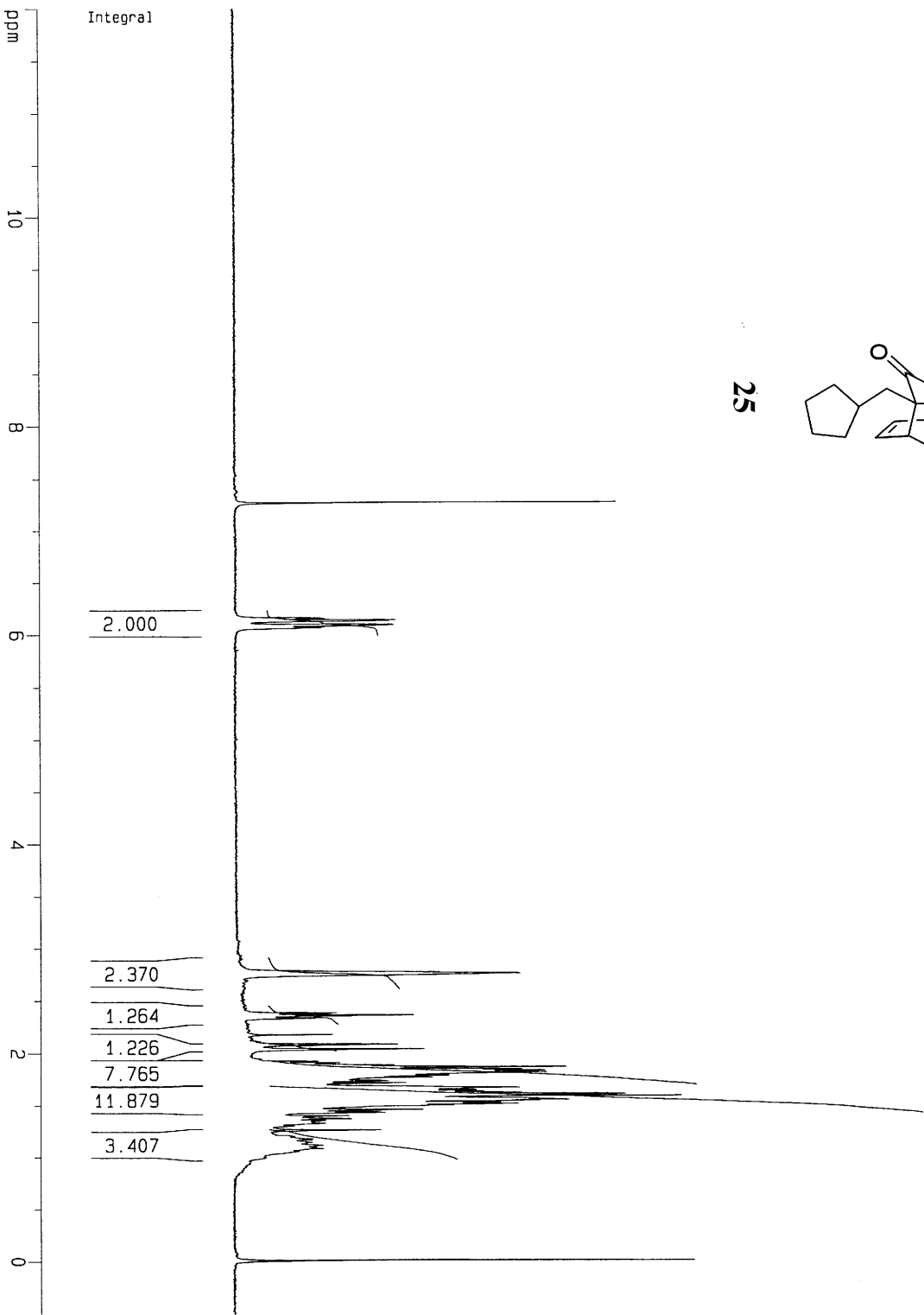
INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2

SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1024

DW 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.0000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300049 MHz
 MDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 7.00 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 PPMCM 0.62500 ppm
 HZCM 156.33125 Hz/



Current Data Parameters
 NAME SW-VI-76-A1A
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030601
 Time 22.09

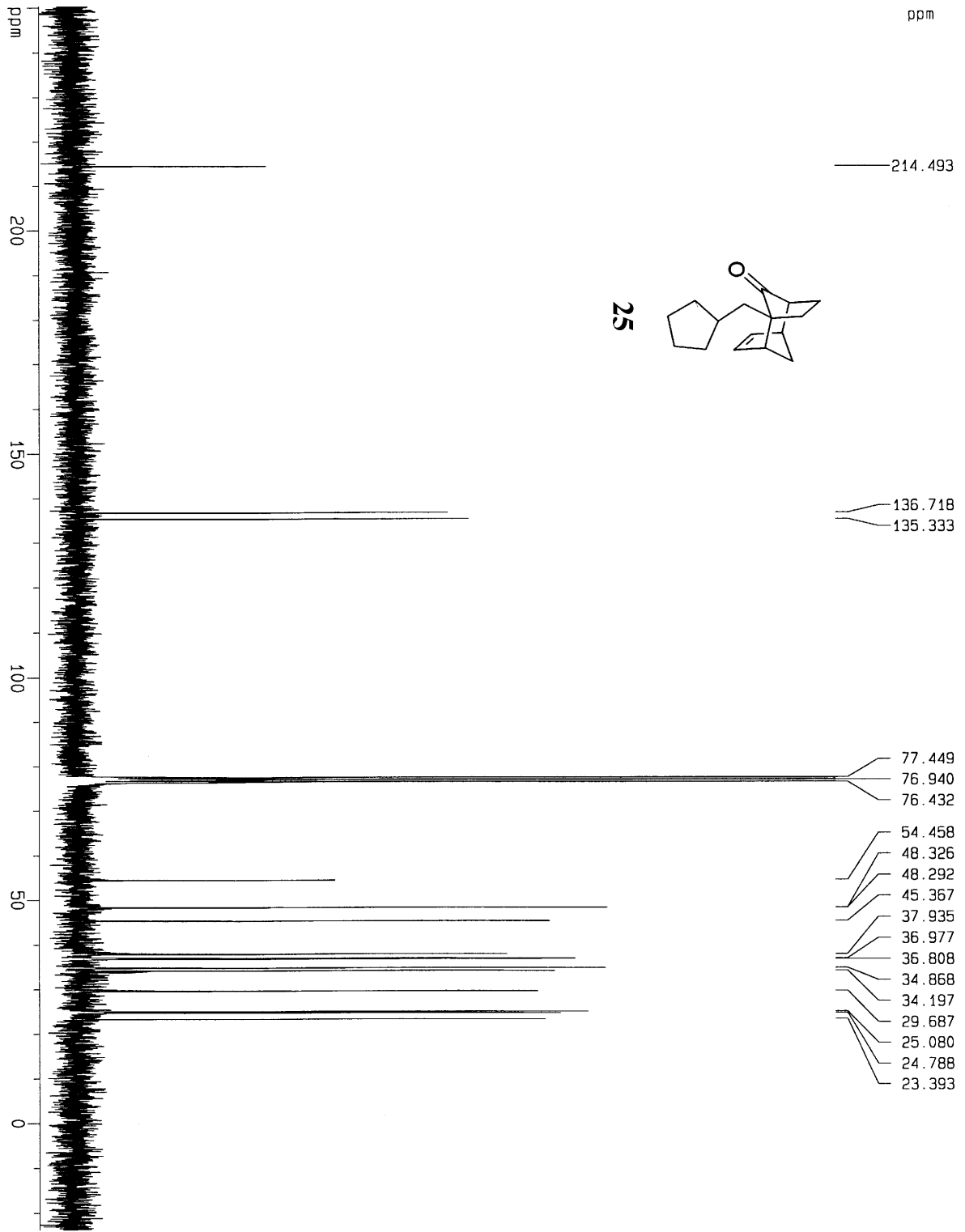
INSTRUM arx250
 PROBHD 5 mm GNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 4753
 DS 4

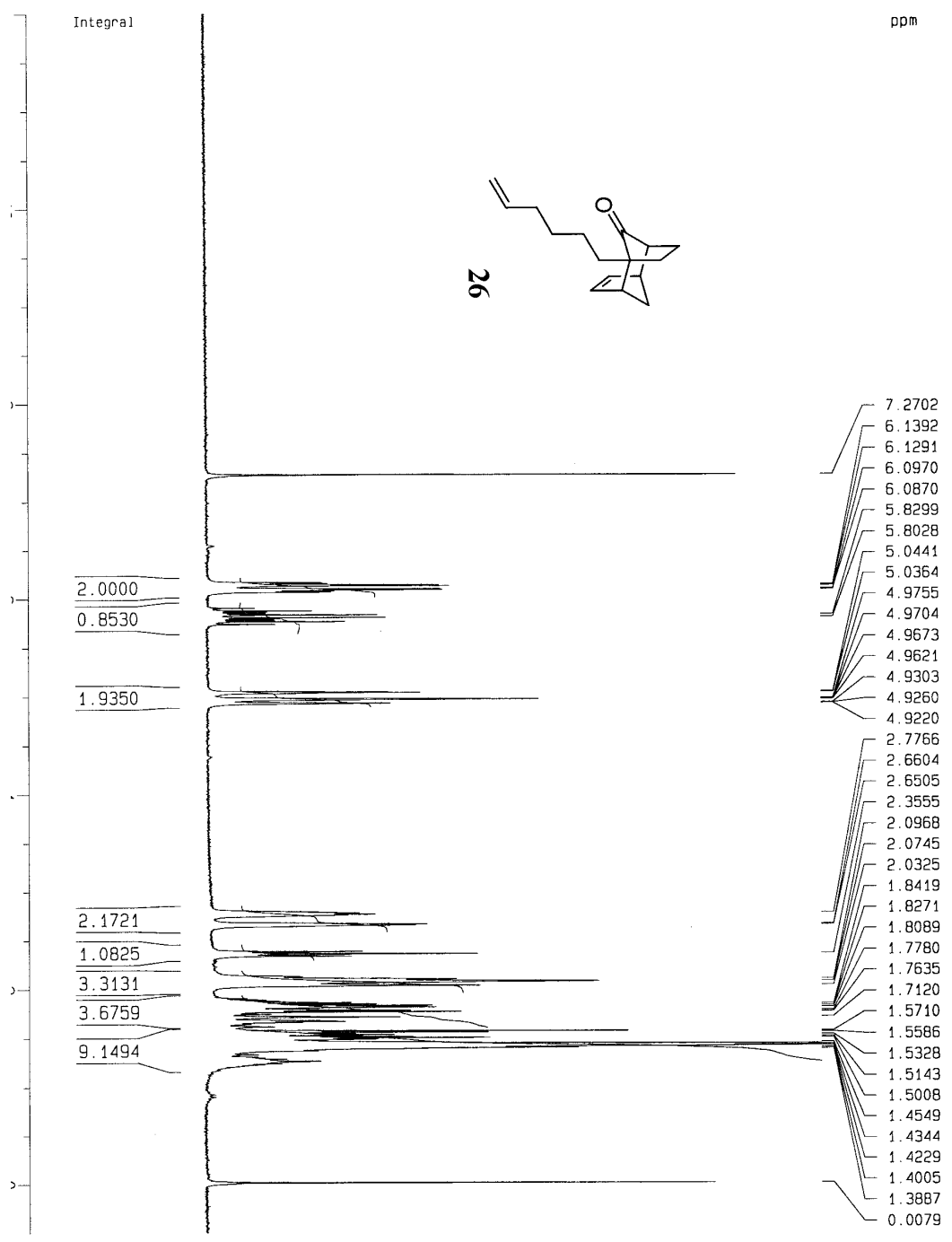
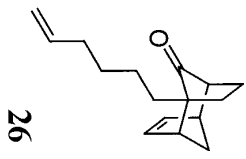
SMH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DM 29.000 use
 DE 41.43 use
 TE 300.0 K

D12 0.0000200 sec
 DL5 23.00 dB
 CPDPRG walz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 5.35 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters
 SI 32768
 SF 62.8952440 MHz
 MDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 40.00 cm
 F1P 250.354 ppm
 F1 15746.05 Hz
 F2P -23.775 ppm
 F2 -1495.33 Hz
 PPMCM 13.70643 ppm
 HZCM 862.06897 Hz/





- 7.2702
- 6.1392
- 6.1291
- 6.0970
- 6.0870
- 5.8299
- 5.8028
- 5.0441
- 5.0364
- 4.9755
- 4.9704
- 4.9673
- 4.9621
- 4.9303
- 4.9260
- 4.9220
- 2.7766
- 2.6604
- 2.6505
- 2.3555
- 2.0968
- 2.0745
- 2.0325
- 1.8419
- 1.8271
- 1.8089
- 1.7780
- 1.7635
- 1.7120
- 1.5710
- 1.5586
- 1.5328
- 1.5143
- 1.5008
- 1.4549
- 1.4344
- 1.4229
- 1.4005
- 1.3887
- 0.0079

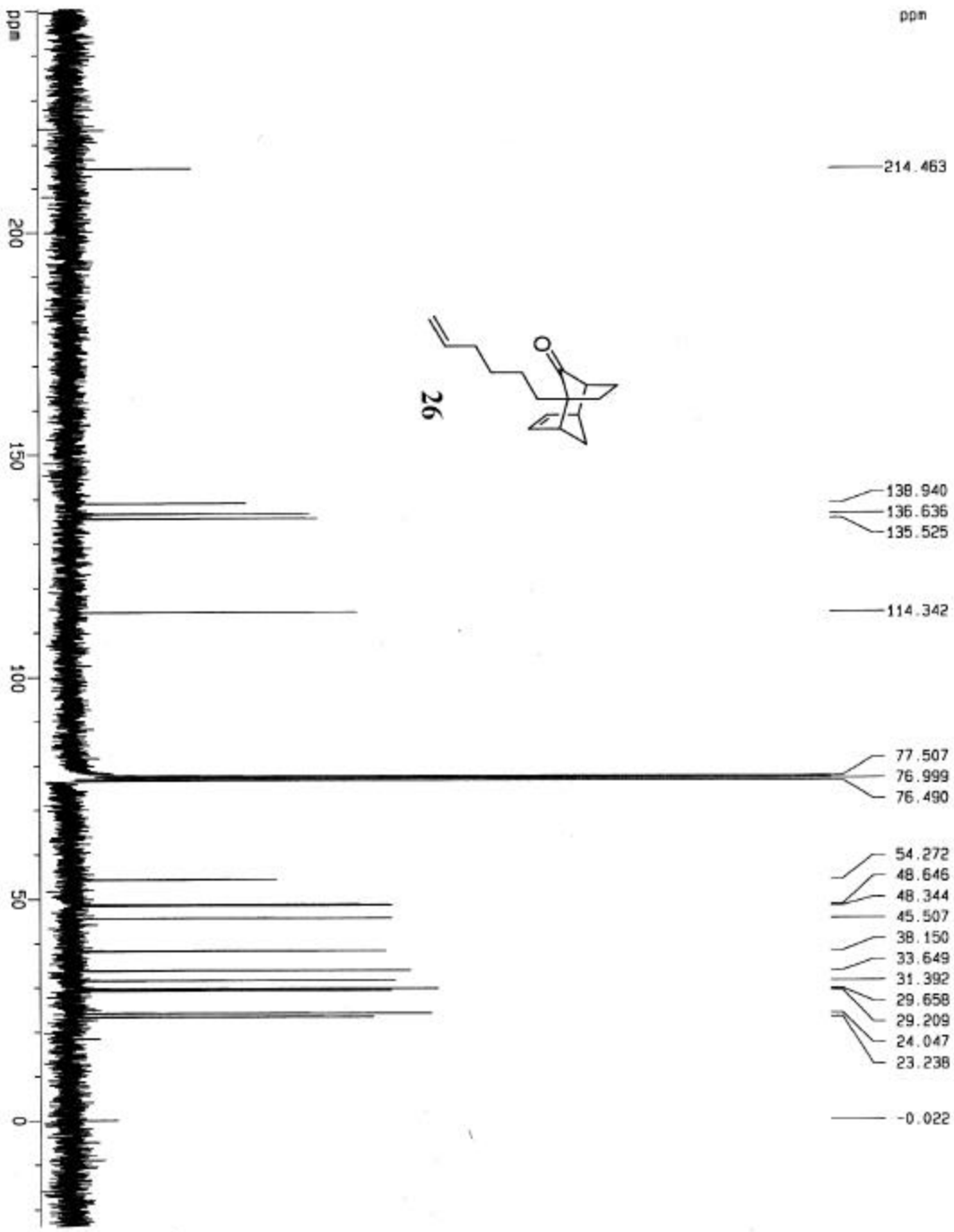
- 2.0000
- 0.8530
- 1.9350
- 2.1721
- 1.0825
- 3.3131
- 3.6759
- 9.1494

Current Data Parameters
 NAME SW-IV-64-A1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20021029
 Time 23.09
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 2048
 DW 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.70 use
 SFO1 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300049 MHz
 WDM EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -0.500 ppm
 F2 -125.07 Hz
 PPMCM 0.62500 ppm
 HZCM 156.33125 Hz/



Current Data Parameters
 NAME sw-III-107-A1
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020612
 Time 11:48

INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TO 36964
 SOLVENT CDCl3
 NS 3957
 DS 4

SMH 17241.379 Hz
 FIDRES 0.457702 Hz
 AQ 1.0591050 sec
 RG 22800
 DW 29.000 use
 DE 41.43 use
 TE 300.0 K

D12 0.00002000 sec
 DLS 23.00 dB
 OPDPRG waltz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 5.35 use

SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters
 SI 32768
 SF 62.8952403 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 30.00 cm
 F1P 250.413 ppm
 F1 15749.81 Hz
 F2P -23.715 ppm
 F2 -1491.57 Hz
 FREQM 13.70543 ppm
 HZCM 862.06891 Hz/