

SUPPORTING INFORMATION

Title: Intermolecular [4+2] Cycloadditions of a Reactive Cyclopentadienone

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General Information:

All reactions were carried out in oven dried nitrogen stream cooled glassware. Toluene was distilled over CaH_2 and stored over 4\AA molecular sieves and used for a month. THF was freshly distilled over sodium-benzophenone and methylene chloride was over CaH_2 .

Chromatographic separation was performed on Silicycle ultra pure silica gel (230-400 mesh) and also on 60 \AA mesh from Aldrich. Analytical thin layer chromatography was done on silica gel with UV indicator from Sigma-Aldrich.

Melting points were determined with a Fisher-Johns melting point apparatus and are uncorrected. Infrared spectra were recorded on a Perkin Elmer 1600 series FT-IR spectrometer. ^1H -NMR were recorded on a Bruker ARS-250 (250 MHz), DRX-300 (300 MHz), and DRX-500 (500 MHz) spectrometer and are reported in ppm (δ) from tetramethylsilane (TMS: $\delta = 0.0\text{ppm}$). Data are reported according to the following sequence: chemical shift, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet, dd=doublet of doublet, ddd=doublet of doublet of doublet, bm=broad multiplet), coupling constants in Hz, and integration. ^{13}C -NMR spectra were performed on a Bruker ARS-250 (62.5 MHz), DRX-300 (75 MHz), and DRX-500 (125 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with solvent resonance as the internal standard (CDCl_3 : δ 77 ppm).

Compounds **DA-17**¹ and **DA-18**¹ are reported in the literature.

Experimental : General procedure

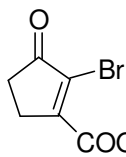
Diels-Alder reactions in THF: Bromo-enone ester **11** was taken into a 10mL flask equipped with a stir bar and a condenser. A solution of this compound was made in THF in 0.10-0.04 M concentration. Desired amount of diene and triethylamine were added into this solution and heated to gentle reflux under nitrogen atmosphere. Reaction was monitored by TLC. Usually a pale yellow color reaction mixture was obtained when the reaction was complete. After completion of the reaction, THF was removed under vacuum. The crude product was dissolved in dichloromethane, washed with 1×5mL 1M HCl, 1×5mL water, 1×5mL brine, dried over MgSO_4 and concentrated. Purification of

this crude product by flash chromatography on silica gel with 15-25% EtOAC/hexanes gave the desired Diels-Alder adduct.

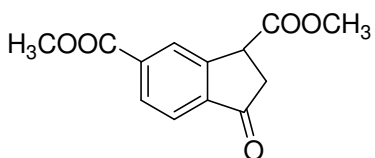
Diels-Alder reactions in toluene: Reactions were usually carried out in 20-40mg scale of compound **11** and reproducible. Into a 10mL flask enone ester **11** was taken and a solution of this was made in toluene in 0.04 M concentration. Desired amount of diene and triethylamine were added into this solution and heated to reflux under nitrogen atmosphere at bath temperature 120-130°C. Reaction was monitored by TLC. A nice light yellow color was an indicative of a successful reaction. After completion of the reaction, toluene was removed under vacuum. Purification of this crude product by flash chromatography on silica gel with 15-20% EtOAC/hexanes provided the desired product.

Diels-Alder reaction with Danishefsky diene: A solution of Bromo-enone-ester **11** (8.1mg, 0.037mmol) and Et₃N.HBr (0.007 mmol, 20 mol%) was made in d₆-benzene under nitrogen atmosphere. Danishefsky diene (0.185mmol) and Et₃N (0.111 mmol) were added to the reaction mixture and transferred to an NMR tube. The reaction was monitored by ¹H-NMR at 80 °C. After 5.5 hours all the SM (**11**) was consumed. The reaction mixture was cooled down to room temperature and poured into 5% HCl. The aqueous medium was extracted with EtOAC (3 × 10mL). The combined organic layers was washed with NaHCO₃ solution, brine, dried over Na₂SO₄ and concentrated. Purification by flash chromatography on silica gel with Hexanes/Et₂O (1: 2) provided 53% of the DA adduct.

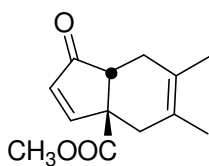
Analytical Data section:



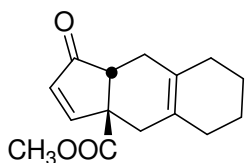
(**11**) White solid, mp 66-67 °C, IR (neat) 3000, 2970, 2361, 2333, 1718 cm^{-1} ; $^1\text{H-NMR}$ (300 MHz, CDCl_3): δ 2.63-2.66 (m, 2H), 2.88-2.91 (m, 2H), 3.92 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 28.3, 32.6, 52.4, 130.9, 157.5, 163.8, 201.3; HRMS calculated for $\text{C}_7\text{H}_7\text{BrO}_3^+$ 217.957307 amu, found 217.9597 amu.



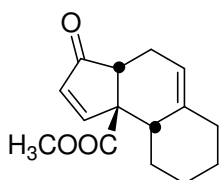
(**14**) Solid, mp 98-99°C, IR (neat) 3020, 2400, 1724, 1615, 1523, 1437, 1301, 1255, 1210 cm^{-1} ; $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 2.94-3.00 (dd, J = 19.1, 8.2 Hz, 1H), 3.20-3.26 (dd, J = 19.2, 3.7 Hz, 1H), 3.82 (s, 3H), 3.97 (s, 3H), 4.36-4.39 (dd, J = 8.1, 3.6, 1H), 7.80-7.81 (d, J =8.1 Hz, 1H), 8.31-8.34 (dd, J = 8.1, 1.6, 1H), 8.4 (d, J =1.5Hz, 1H), 8.34-; ^{13}C NMR (125 MHz, CDCl_3) δ 39.7, 43.5, 52.5, 52.9, 125.4, 126.8, 131.2, 135.7, 136.6, 155.0, 165.9, 171.5, 202.9; HRMS calculated for $\text{C}_{13}\text{H}_{12}\text{O}_5\text{Na}^+$ 271.057693 amu, found 271.05614 amu.



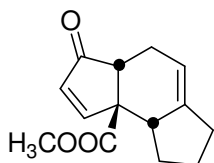
(**DA-15**) White solid, mp 60-61 °C, 73% yield, IR (neat) 2987, 2952, 2858, 1715, 1437, 1294, 1220, 1132 cm^{-1} ; $^1\text{H-NMR}$ (500 MHz, CDCl_3) δ : 1.59 (s, 3H), 1.64 (s, 3H), 2.17-2.20 (d, J = 14.7 Hz, 1H), 2.22-2.28 (bm, 1H), 2.34-2.40 (dd, J = 14.7, 3.1 Hz, 1H), 2.3-2.6 (bd, J = 14.7 Hz, 1H), 2.85-2.90 (dd, J = 6.1, 3.1, 1H), 3.75 (s, 3H), 6.14-6.14 (d, J =5.6 Hz, 1H), 7.44-7.45 (d, J = 5.6 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 19.18, 19.22, 31.0, 37.5, 48.3, 52.6, 56.9, 124.0, 128.2, 134.4, 163.4, 174.2, 210.1; HRMS calculated for $\text{C}_{13}\text{H}_{16}\text{O}_3\text{Na}^+$ 234.099163 amu, observed mass 243.09964 amu



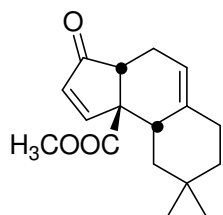
(DA-16) Oil, 82% yield, IR (neat) 2930, 715, 1436, 1252 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3): δ 1.45-1.55 (m, 4H), 1.67-2.50 (m, 4H), 2.25-2.35 (m, 2H), 2.86-2.90 (dd, J = 12, 6.6Hz, 1H), 3.75 (s, 3H), 6.13-6.15 (d, J = 5.6 Hz, 1H), 7.44-7.46 (d, J = 5.6 Hz, 1H) ; ^{13}C -NMR (125 MHz, CDCl_3) δ 22.8, 22.9, 29.63, 30.3, 30.2, 36.4, 48.2, 52.6, 56.8, 126.6, 130.7, 134.1, 163.5, 174.2, 210.1; HRMS calculated for ($\text{C}_{15}\text{H}_{18}\text{O}_3 + \text{O}_2 + \text{Na}^+$) 301.104643 amu, found 301.10599 amu.



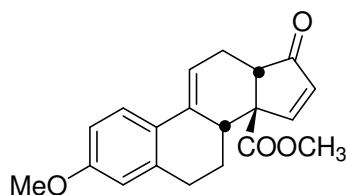
(DA-19) Oil, 77% yield in Toluene, 63% in THF , IR (neat) 2936, 2867, 1717, 1435, 1236, cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3): δ 1.35-1.27 (m, 1H), 1.50-1.40 (m, 2H), 1.61-1.53 (m, 1H), 1.83-1.71 (m, 2H), 2.15-2.02 (m, 2H), 2.29-2.22 (m, 1H), 2.65-2.60 (ddd, J = 17.0, 6.5, 2.0 Hz, 1H), 2.73-2.68 (m, 1H), 2.76-2.73 (dd, J = 7.2, 2.1 Hz, 1H), 3.79 (s, 3H), 5.51-5.47 (m, 1H), 6.25-6.24 (d, J = 5.8Hz, 1H), 7.70-7.69 (d, J = 5.8Hz, 1H); ^{13}C -NMR (62.5 MHz, CDCl_3) δ 23.0, 23.1, 26.1, 30.9, 42.1, 49.3, 52.6, 58.6, 118.8, 134.2, 138.8, 162.1, 174.6, 209.0; HRMS calculated for $\text{C}_{15}\text{H}_{18}\text{O}_3\text{Na}^+$ 301.104643 amu, found 301.10412 amu.



(DA-20) Oil, 56% yield in Toluene, 33% yield in THF, IR (neat) 2952, 1715, 1434, 1233 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3): δ 2.02-1.96 (m, 1H), 2.24-2.08 (m, 3H), 2.68-2.63 (ddd, 14.7, 7.3, 1.9Hz, 1H), 2.83-2.82 (dd, J = 6.2, 2.0 Hz, 1H), 3.77 (s, 3H), 6.00-5.78 (m, 1H), 6.22-6.21 (d, J = 5.8Hz, 1H), 7.60-7.59 (d, J =5.8Hz, 1H); ^{13}C NMR (62.5 MHz, CDCl_3) δ 25.1, 26.2, 28.1, 31.6, 45.3, 50.0, 52.6, 59.4, 116.5, 135.6, 144.7, 161.6, 174.5, 209.9; HRMS calculated for $\text{C}_{14}\text{H}_{16}\text{O}_3\text{Na}^+$ 255.099163amu, found 287.08989 amu.



(**DA-21**) Oil, 80% yield, IR (neat), 2953, 2927, 2863, 1717, 1237 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3): δ 0.96 (s, 3H), 0.97 (s, 3H), 1.28-1.16 (m, 2H), 1.43-1.32 (m, 2H), 2.10-1.98 (m, 2H), 2.25-2.16 (m, 1H), 2.65-2.59 (ddd, J = 15.7, 7.9, 1.9 Hz, 1H), 2.73-2.70 (dd, J = 6.8, 2.0 Hz, 1H), 2.86-2.80 (m, 1H), 3.77 (s, 3H), 5.50-5.49 (b, 1H), 6.24-6.23 (5.8 Hz), 7.66-7.64 (d, J = 5.9 Hz, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 23.5, 27.5, 28.5, 30.1, 37.3, 38.4, 38.9, 49.7, 52.6, 58.8, 118.8, 134.7, 138.9, 162.1, 174.6, 209.3,



(**DA-22**) White semi solid, 80% yield, IR (neat) 3020, 2949, 2839, 1713, 1607, 1572, 1496, 1435, 1248 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3): δ 1.64-1.56 (m, 1H), 2.07-2.02 (m, 1H), 2.41-2.36 (m, 1H), 2.73-2.62 (m 2H), 2.85-2.80 (m, 2H), 3.14-3.09 (m, 1H), 3.77 (s, 3H), 3.81 (s, 3H), 6.18-6.16 (m, 1H), 6.22-6.20 (d, J = 5.8 Hz, 1H), 6.61 (dd, J = 2.61 Hz, 1H), 6.71-6.68 (dd, J = 8.6, 2.7 Hz, 1H), 7.40-7.39 (d, J = 5.7 Hz, 1H), 7.62-7.61 (d, J = 5.8 Hz, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 23.8, 25.0, 30.0, 41.5, 50.7, 52.7, 55.2, 60.0, 112.66, 112.72, 119.0, 125.0, 126.9, 135.1, 136.0, 138.7, 158.7, 161.5, 174.3, 209.6; HRMS calculated 347.125378 amu, found 347.12457 amu.

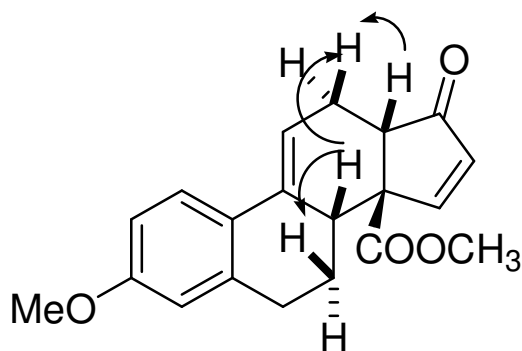
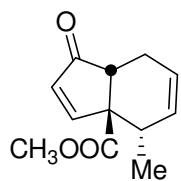
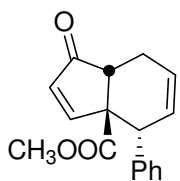


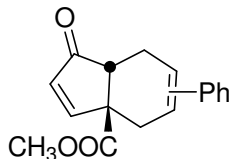
Figure 1: The nOe effect in Diels-Alder adduct **22**



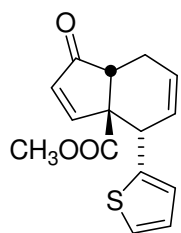
(DA-23) Oil, 13% yield; IR (neat): 3036, 2954, 2879, 2848, 1715, 1595, 1457, 1436, 1254, 1231 cm^{-1} ; $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 1.18 (d, J = 9.0 Hz, 3H), 2.19-2.25 (m, 1H), 2.64-2.69 (ddd, J = 15.0, 7.5, 2.2 Hz, 1H), 2.75-2.77 (dd, J = 7.5, 2.0 Hz, 1H), 2.80-2.85 (m, 1H), 3.77 (s, 3H), 5.42-5.45 (m, 1H), 5.81-5.86 (m, 1H), 6.25-6.26 (d, J = 5.5 Hz, 1H), 7.63-7.65 (d, J = 5.5 Hz, 1H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 15.9, 24.4, 35.5, 50.1, 52.6, 60.3, 128.0, 132.5, 135.7, 161.5, 174.4, 209.4; Elemental analysis: Expt C, 69.83%; H, 6.59% Calculated C 69.88%, H, 6.84%.



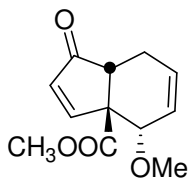
(DA-24) Oil, 66% yield; IR (neat): 3032, 2952, 2847, 1717, 1598, 1454, 1254, 1230 cm^{-1} ; $^1\text{H-NMR}$ (250 MHz, CDCl_3): δ 2.10-2.40 (m, 1H), 2.75-2.87 (m, 2H), 3.68 (s, 3H), 4.05-4.09 (q, J = 2.9 Hz, 1H), 5.87-5.93 (m, 1H), 5.99-6.04 (m, 1H), 6.20-6.23 (d, J = 5.9 Hz, 1H), 7.09-7.15 (m, 2H), 7.18-7.21 (d, J = 5.9 Hz, 1H), 7.29-7.40 (m, 3H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 24.2, 47.0, 49.5, 52.4, 61.5, 127.4, 128.5, 129.0, 129.1, 130.7, 134.8, 139.1, 162.2, 174.0, 209.0; Elemental analysis: Expt C, 75.97%; H, 6.23% Calculated C 76.10%, H, 6.01%



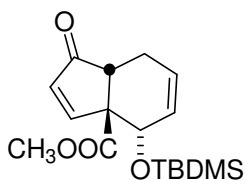
(DA-25) Oil, 80% yield, 1:1 mixture of two regeoisomers; IR (neat): 3032, 2952, 2900, 2844, 1714, 1593, 1495, 1436, 1249, 1220 cm^{-1} ; $^1\text{H-NMR}$ (250 MHz, CDCl_3): δ 2.35-3.15 (m, 5H, from each regeoisomers), 3.79 (s, 3H, from each regeoisomers), 5.9-5.97 (m, 1H from one regeoisomer), 6.15-6.23 (3H, from both isomers), 7.17-7.37 (m, 5H, from each regeoisomers), 7.47-7.52 (d, 2H, J = 5.6 Hz, from each regeoisomers); $^{13}\text{C NMR}$ (62.5 MHz, CDCl_3): δ 25.4, 27.8, 31.7, 33.7, 47.5, 48.4, 52.78, 52.83, 56.4, 56.97, 120.6, 124.3, 125.2, 125.5, 127.26, 127.3, 128.35, 128.40, 134.63, 134.9, 140.18, 140.54, 163.4, 163.9, 173.9, 173.9, 209.28, 209.8, from both the regeoisomers; HRMS calculated for $\text{C}_{17}\text{H}_{16}\text{O}_3\text{Na}^+$ to be 291.099163 amu, found 291.09932 amu.



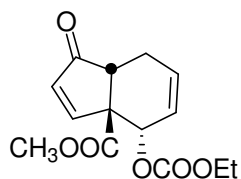
(DA-26) Oil, 78% yield; IR (neat): 3044, 2952, 2902, 2361, 2329, 1716, 1435, 1297, 1231 cm^{-1} ; ^1H -NMR (300 MHz, CDCl_3): δ 2.98-2.40 (m, 1H), 2.74-2.85 (m, 2H), 3.75 (s, 3H), 4.47-4.44 (dd, J = 5.7, 3.0 Hz, 1H), 5.89-6.06 (m, 2H), 6.26-6.24 (d, J = 5.6Hz, 1H), 6.85-6.82 (d, J = 3.6, 1H), 7.02-6.99 (q, J = 3.6Hz, 1H), 7.25-7.23 (dd, J = 5.1, 1.2 Hz, 1H), 7.32-7.29 (d, J = 5.6 Hz, 1H) ; ^{13}C NMR (75 MHz, CDCl_3): δ 24.5, 42.0, 49.6, 52.7, 61.8, 124.8, 126.1, 127.1, 129.1, 130.7, 135.47, 142.06, 162.0, 173.9, 208.8; Elemental analysis: Expt C, 65.72%; H, 4.99% Calculated C 65.67%, H, 5.14%



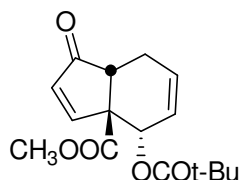
(DA-27) Oil, 84 % yield in Toluene, 52% yield in THF, IR (neat): 3046, 2952, 2829, 1716, 1593, 1437, 1256 cm^{-1} ; ^1H -NMR (CDCl_3) δ 2.22-2.17 (m, 1H), 2.69-2.63 (m, 2H), 3.47 (s, 3H), 3.81 (s, 3H), 4.48-4.47 (dd, J = 4.3, 2.2 Hz, 1H), 5.84-5.76 (m, 2H), 6.33-6.32 (d, J = 5.8 Hz, 1H), 7.73-7.72 (d, J =5.8 Hz, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 24.3, 48.4, 52.8, 58.1, 61.1, 80.0, 126.8, 129.6, 135.9, 162.4, 173.9, 208.8; HRMS (EI) calculated for $\text{C}_{12}\text{H}_{14}\text{O}_4^+$ 222.08921 amu, found 222.0779 amu.



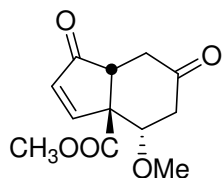
(DA-28) Oil, 79% Yield, IR (neat): 2953, 2856, 1718, 1254, 1119 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3): δ 0.08 (s, 3H), 0.10 (s, 3H), 0.92 (s, 9H), 2.23-2.18 (m, 1H), 2.67-2.62 (m, 2H), 3.77 (s, 3H), 4.85-4.84 (q, J = 4.72, 2.32 Hz, 1H), 5.61-5.58 (m, 1H), 5.76-5.71 (m, 1H), 6.32-6.31 (d, J = 5.8 Hz, 1H), 7.80-7.79 (d, J = 5.8 Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 5.4, -4.6, 17.9, 24.3, 25.6, 30.9, 48.1, 52.6, 62.5, 72.3, 125.9, 133.1, 135.8, 162.9, 174.0, 207.0; HRMS calculated for $\text{C}_{17}\text{H}_{26}\text{O}_4\text{SiNa}^+$ 345.149255 amu, found 345.14820 amu.



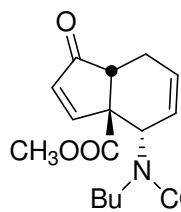
(DA-29) Oil, 72% yield; IR (neat): 2956, 2361, 1750, 1718, 1437, 1472, 1257 cm^{-1} ; $^1\text{H-NMR}$ (300 MHz, CDCl_3): δ 1.31-1.36 (t, J = 7.2Hz, 3H), 2.20-2.34 (m, 1H), 2.66-2.74 (ddd, J = 16.7, 6.9, 2.1Hz, 1H), 2.79-2.83(dd, J = 6.9, 2.1Hz, 1H), 3.78(s, 3H), 4.20-4.28 (q, J = 7.2 Hz, 2H), 5.63-5.68 (dt, J = 9.6, 2.7 Hz, 1H), 5.83-5.92 (m, 1H), 6.34 (d, J =5.7Hz, 1H), 7.72 (d, J = 5.7 Hz, 1H) ; ^{13}C NMR (125 MHz, CDCl_3) δ 14.2, 23.9, 47.4, 53.1, 60.0, 64.6, 75.4, 127.8, 128.1, 136.4, 154.4, 160.6, 172.4, 208.0; Elemental analysis: Expt C, 60.16%; H, 5.57% Calculated C 59.99%, H, 5.75%.



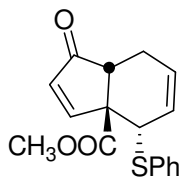
(DA-30) White Solid, mp $^{\circ}\text{C}$, 61% yield; IR (neat): 2974, 1736, 1716, 1480, 1485, 1437, 1255, 1279, 1234, 1147 cm^{-1} ; $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 1.23 (s, 9H), 2.36-2.28(m, 1H), 2.72-2.66 (ddd, J = 15.6, 7.5, 2.5Hz, 1H), 2.91-2.88(dd, J = 7.0, 2.5Hz, 1H), 3.76 (s, 3H), 5.60-5.56 (dt, J = 10.0, 2.5Hz, 1H), 5.78-5.76 (q, J = 2.5Hz, 1H), 5.91-5.86 (m, 1H), 6.34 (d, J =6.0Hz, 1H), 7.66 (d, J = 6.0Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3); 23.9, 27.0, 38.9, 47.1, 53.0, 60.2, 71.4, 128.0, 128.4, 136.1, 160.6, 172.4, 177.2, 208.1; Elemental analysis: Expt C, 65.57%; H, 6.85% Calculated C 65.74%, H, 6.90%



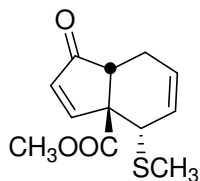
(DA-31) Oil, 53% yield, IR (neat): 3076, 2955, 2836, 1792, 1718, 1457, 1437, 1232, 1100 cm^{-1} ; $^1\text{H-NMR}$ (500MHz, CDCl_3): δ 2.18 (dd, J = 18, 10 Hz, 1H), 2.55-2.67 (m 2H), 2.78-2.95 (m, 2H), 3.42 (s, 3H), 3.83 (s, 3H), 4.34-4.28 (dd, J = 8.0, 3.4 Hz, 1H), 6.44-6.41 (d, J =5.8 Hz, 1H), 7.76-7.74 (d, J = 5.8 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 37.8, 39.8, 45.7, 53.2, 57.7, 59.0, 77.8, 134.6, 161.0, 173.0, 205.8, 206.5;



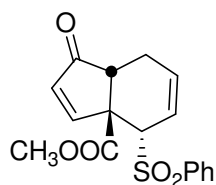
(DA-32) Oil, 84% yield, IR (neat liq) 2957, 2874, 2362, 1718, 1653, 1413, 1239 cm^{-1} ; $^1\text{H-NMR}$ (250 MHz, CDCl_3): δ 0.95-0.90 (t, $J=7.3\text{Hz}$, 3H), 1.33-1.24 (m, 2H), 1.68-1.40 (m, 2H), 2.14 (s, 3H), 2.38-2.34 (m, 1H), 2.91-2.72 (m, 3H), 3.17-3.11 (m, 1H), 3.78 (s, 3H), 5.43-5.40 (q, $J=2.7\text{ Hz}$, 1H), 5.71-5.64 (dt, $J=9.8, 3.0\text{ Hz}$, 1H), 6.03-5.96 (m, 1H), 6.23-6.21 (d, $J=5.9\text{Hz}$, 1H), 7.57-7.54 (d, $J=5.9\text{ Hz}$, 1H). $^{13}\text{C NMR}$ (62.5 MHz, CDCl_3) δ 13.6, 20.2, 21.9, 22.4, 33.4, 48.26, 48.35, 52.9, 56.6, 60.0, 125.6, 129.5, 133.5, 162.0, 171.6, 173.5, 207.9. HRMS calculated for $(\text{C}_{17}\text{H}_{23}\text{NO}_4^- \text{Na}^+)$ 328.151927amu, found 328.15191 amu.



(DA-33) Oil, 84% yield; IR (neat) 3053, 2952, 2847, 1717, 1585, 1479, 1438, 1300, 1233 cm^{-1} ; $^1\text{H-NMR}$ (300 MHz, CDCl_3): δ 2.42-2.27 (m, 1H), 2.73-2.63 (m, 1H), 2.81-2.76 (dd, $J=5.3, 2.9$, 1H), 3.63 (s, 3H), 4.47-4.44 (m, 1H), 5.83-5.77 (m, 1H), 5.94-5.88 (m, 1H), 6.33-6.32 (d, $J=5.8\text{ Hz}$, 1H), 7.46-7.25 (m, 5H), 7.77-7.74 (d, $J=5.8\text{ Hz}$, 1H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 23.8, 49.7, 49.9, 52.8, 60.6, 127.5, 129.3, 129.9, 130.2, 131.9, 134.4, 135.9, 139.1, 161.5, 173.2, 208.2; HRMS calculated for $(\text{C}_{17}\text{H}_{16}\text{O}_3\text{S} + \text{O} + \text{Na})^+$ 339.066148 amu, observed 339.06514 amu.



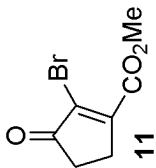
(DA-34) Oil 67% yield; IR (neat): 3042, 2953, 2920, 2847, 1716, 1594, 1435, 1232 cm^{-1} ; $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ 2.16 (s, 3H), 2.26-2.33 (m, 1H), 2.62-2.67 (ddd, $J=19.2, 6.5, 3.0\text{ Hz}$, 1H), 2.76-2.78 (dd, $J=7.5, 3.0\text{ Hz}$, 1H), 3.79 (s, 3H), 3.92-3.94 (m, 1H), 5.74-5.77 (m, 1H), 5.89-5.92 (m, 1H), 6.3 (d, $J=5.5\text{Hz}$, 1H), 7.72 (d, $J=5.5\text{ Hz}$, 1H); $^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 16.1, 23.8, 47.6, 49.8, 52.9, 60.8, 129.0, 130.1, 135.5, 161.7, 173.55, 208.3; Elemental analysis: Expt C, 60.27%; H, 5.76% Calculated C 60.48%, H, 5.92%.



White solid, mp 160-161°C, 74% Yield, IR (neat) cm^{-1} ; ^1H -NMR (300 MHz, CDCl_3): δ 2.15-2.05 (m, 1H), 2.81-2.67 (m, 2H), 5.84-5.78 (dt, $J = 3.1$ Hz, 1H), 6.09-6.00 (m, 1H), 6.42-6.39 (d, $J = 5.8$ Hz, 1H), 7.73-7.56 (m, 3H), 7.96-7.92 (m, 2H), 7.96-7.92 (m, 2H), 8.13-8.01 (d, $J = 5.8$ Hz, 1H); ^{13}C NMR (62.5 MHz, CDCl_3) δ 23.9, 50.1, 53.6, 57.6, 65.5, 121.4, 128.4, 129.5, 131.9, 134.2, 135.9, 139.0, 160.6, 173.1, 206.7. X-Ray crystallography data on this compound is provided.

Reference:

1. Hirao, K; Yamashita, A; Ando, A.; Ijima, H.; Yamamoto, Y.; Hamada, T. and Yonemitsu, O *J. Chem. Research (S)*, **1987**, 162-163.



Current Data Parameters
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 EXPNO 1
 PROCNO 1

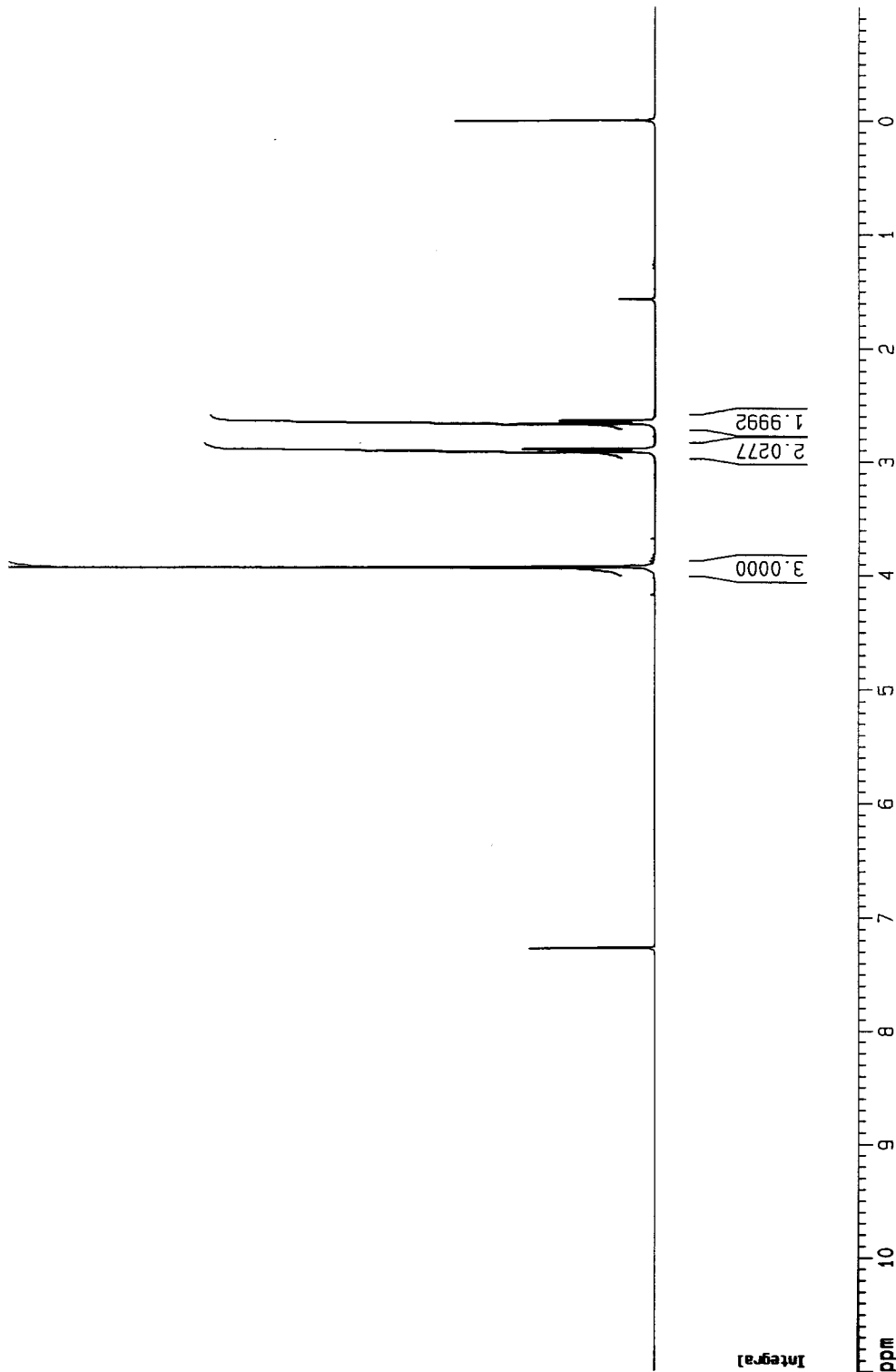
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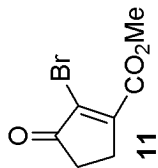
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 INSTRUM drx300
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 2
 SMH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 1024
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 7.05 usec
 PL1 0.00 dB
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F2 - Processing parameters
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 SF 300.1300047 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.30

1D NMR plot parameters
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 CY 12.50 cm
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 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07799 Hz/cm





Current Data Parameters
 NAME NG-3-013d-300
 EXPNO 2
 PROCNO 1

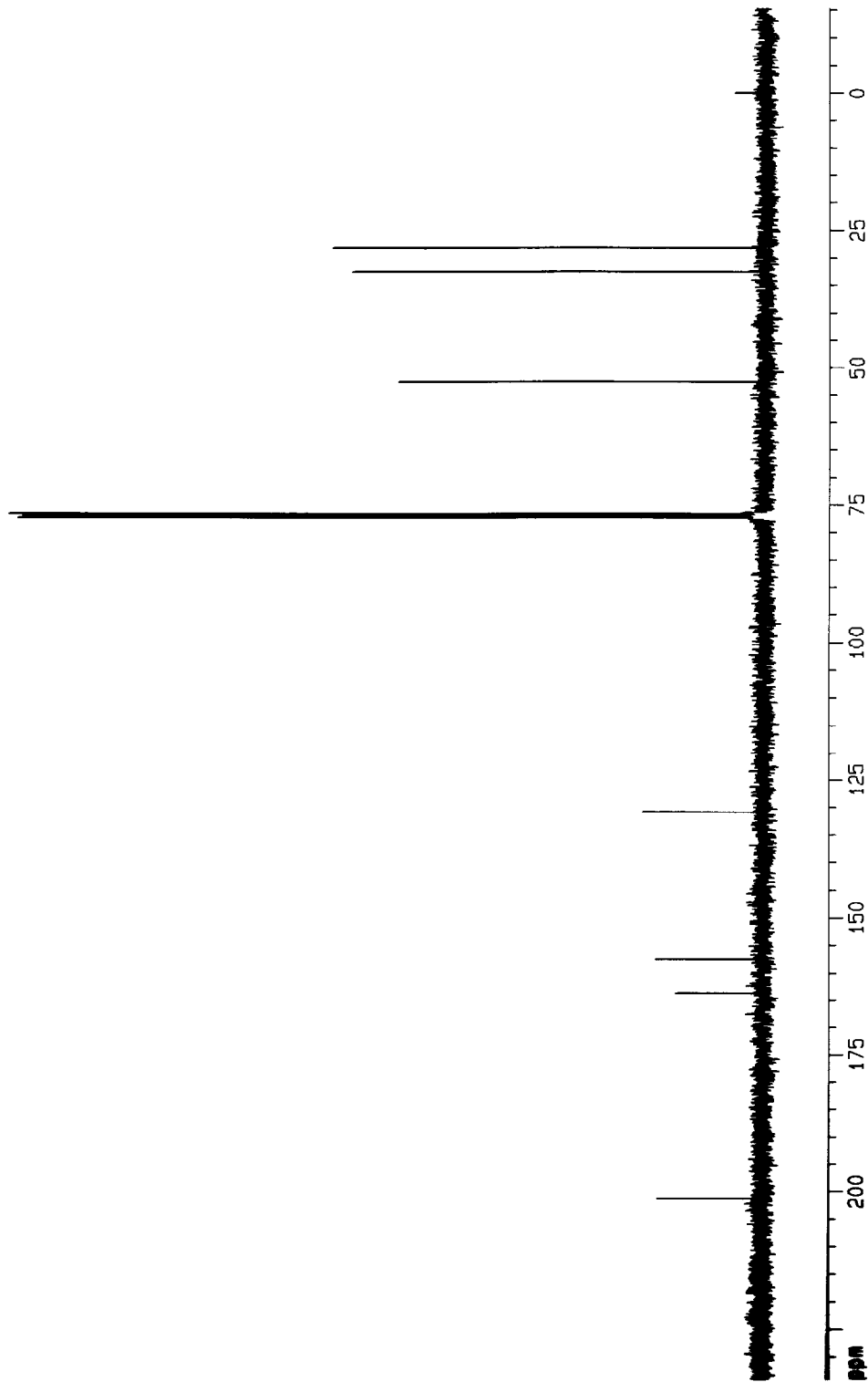
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 PROBD 5 mm Multinuc1
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 TD 65536
 SOLVENT CDCl3
 NS 572
 DS 4
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 22528
 DW 26.550 usec
 DE 6.00 usec
 TE 297.1 K
 D1 1.29999995 sec
 d11 0.03000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 5.00 dB
 SF01 75.4760107 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 25.60 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677514 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 11.00 cm
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 F1 17675.51 Hz
 F2P -15.329 ppm
 F2 -1156.88 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61957 Hz/cm





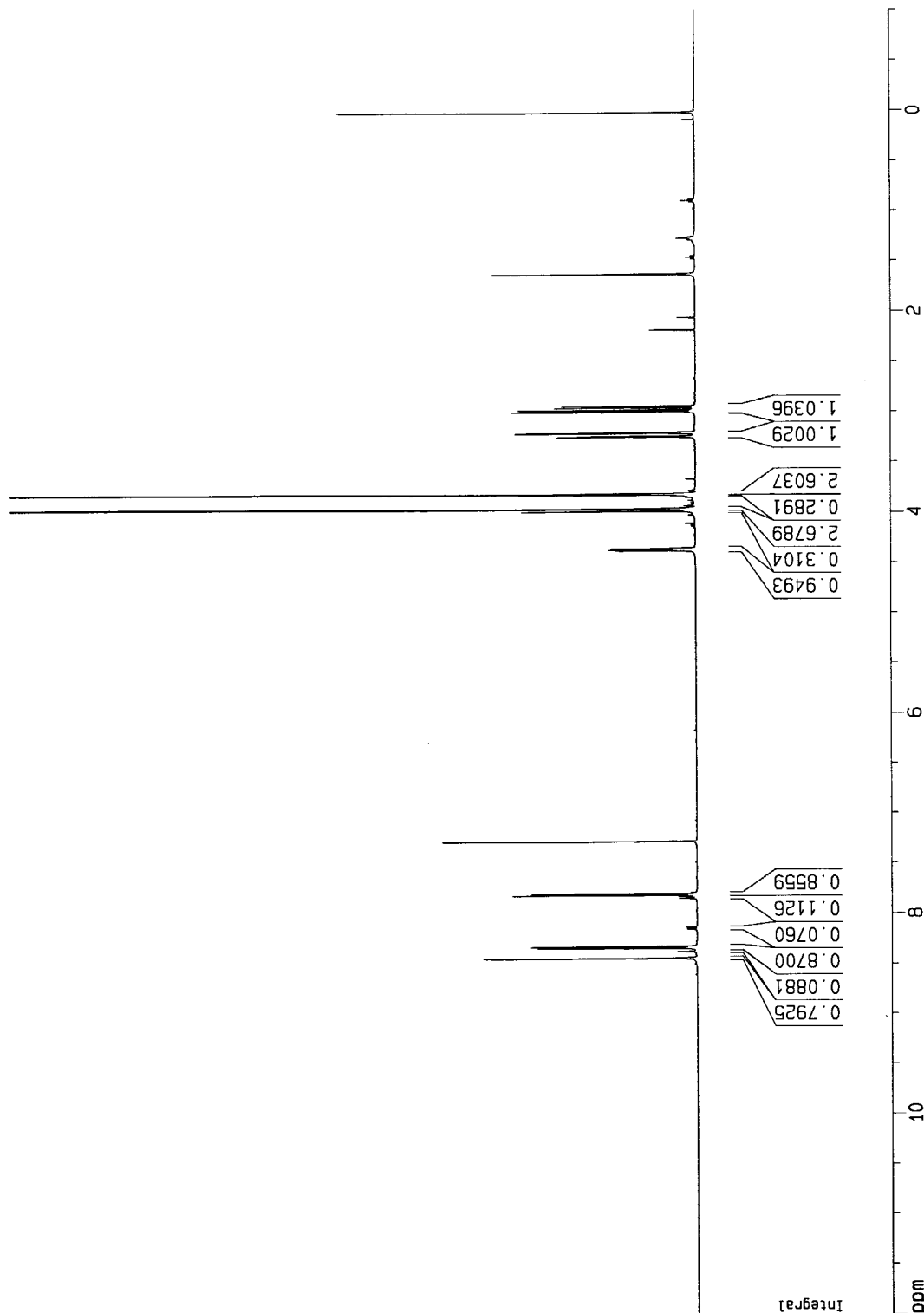
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EXPNO	1
PROCNO	1

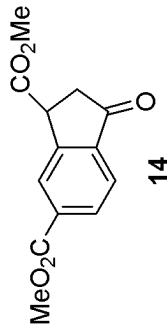
[illegible]

	1H
NUC1	
P1	13.25 usec
PL1	-3.00 dB
SFO1	500.1330885 MHz

SI	32768
SF	500.130000 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.40

CX	20.00 cm
CY	30.00 cm
F1P	12.000 ppm
F1	5001.56 Hz
F2P	-1.000 ppm
F2	-500.13 Hz
PPMCM	0.65000 ppm/cr
HZCM	325.08450 Hz/cm





Current Data Parameters
 NAME MG-IV-048b-500
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

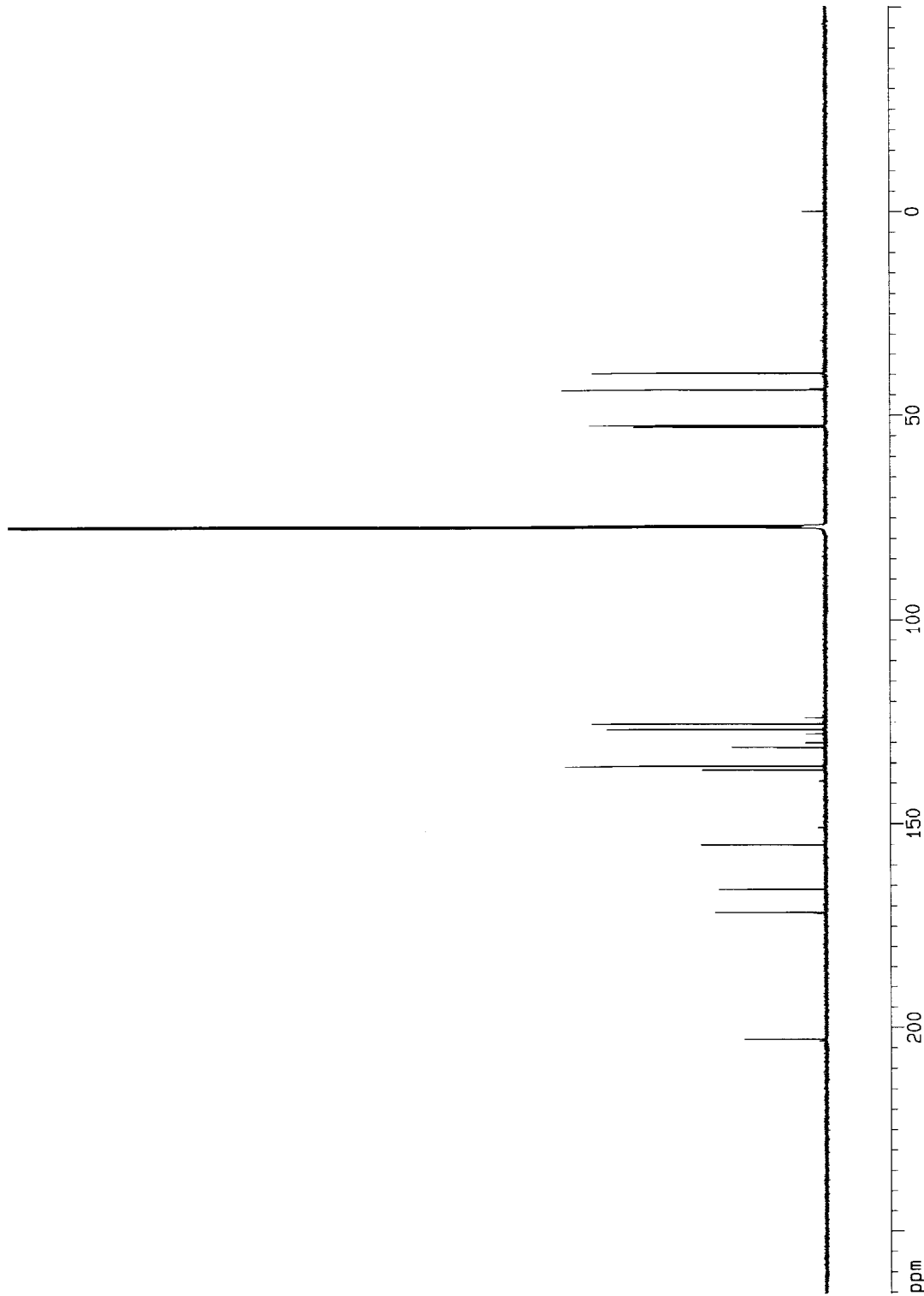
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 Time 17.12
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 PROBH0 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8310
 DS 4
 SWH 39681.812 Hz
 FIDRES 0.605496 Hz
 AQ 0.8258188 sec
 RG 16384
 DM 12.600 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

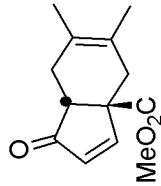
===== CHANNEL f1 =====
 NUC1 13C
 P1 8.10 usec
 PL1 3.00 dB
 SF01 125.7713108 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 88.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577935 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 24.00 cm
 F1P 265.258 ppm
 F1 33358.26 Hz
 F2P -50.284 ppm
 F2 -6323.55 Hz
 PPMCM 15.77708 ppm/cm
 HZCM 1984.09045 Hz/cm





DA-15

Current Data Parameters
 NAME MG-2-034a-500
 EXPNO 1
 PROCNO 1

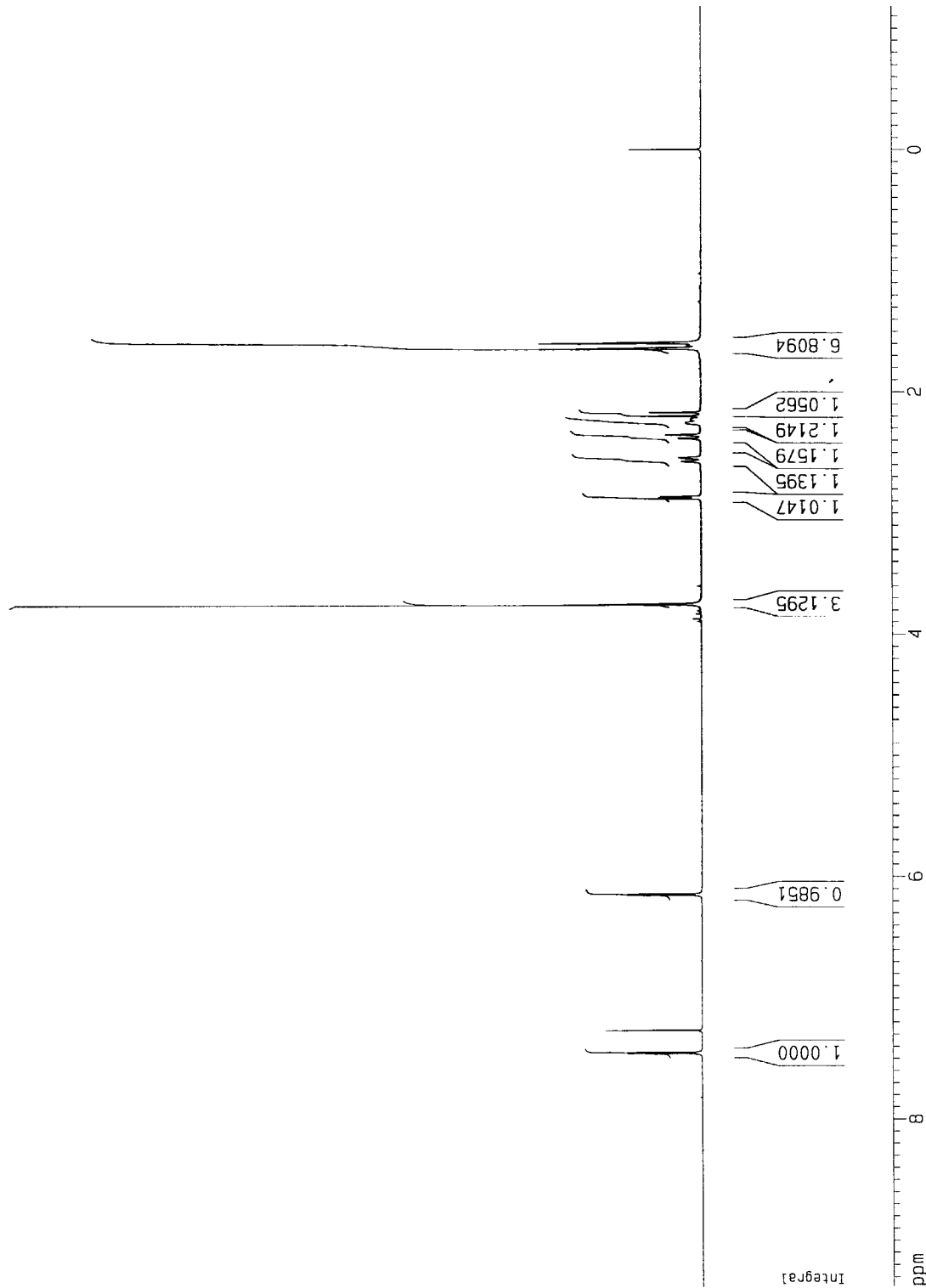
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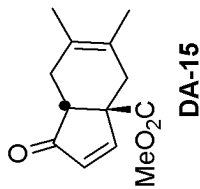
Date_ 20031220
 Time 12.05
 INSTRUM DRX500
 PROBHD 5 mm Multinuc1
 PULPROG zg30
 TD 57344
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.180151 Hz
 AQ 2.7754996 sec
 RG 114
 DW 48.400 usec
 DE 6.00 usec
 TE 296.7 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.25 usec
 PL1 -3.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300093 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 9.379 ppm
 F1 4690.87 Hz
 F2P -1.182 ppm
 F2 -590.93 Hz
 PPMCM 0.52804 ppm/cr
 HZCM 264.08994 Hz/cm





Current Data Parameters
 NAME MG-2-034a-500
 EXPNO 2
 PROCNO 1

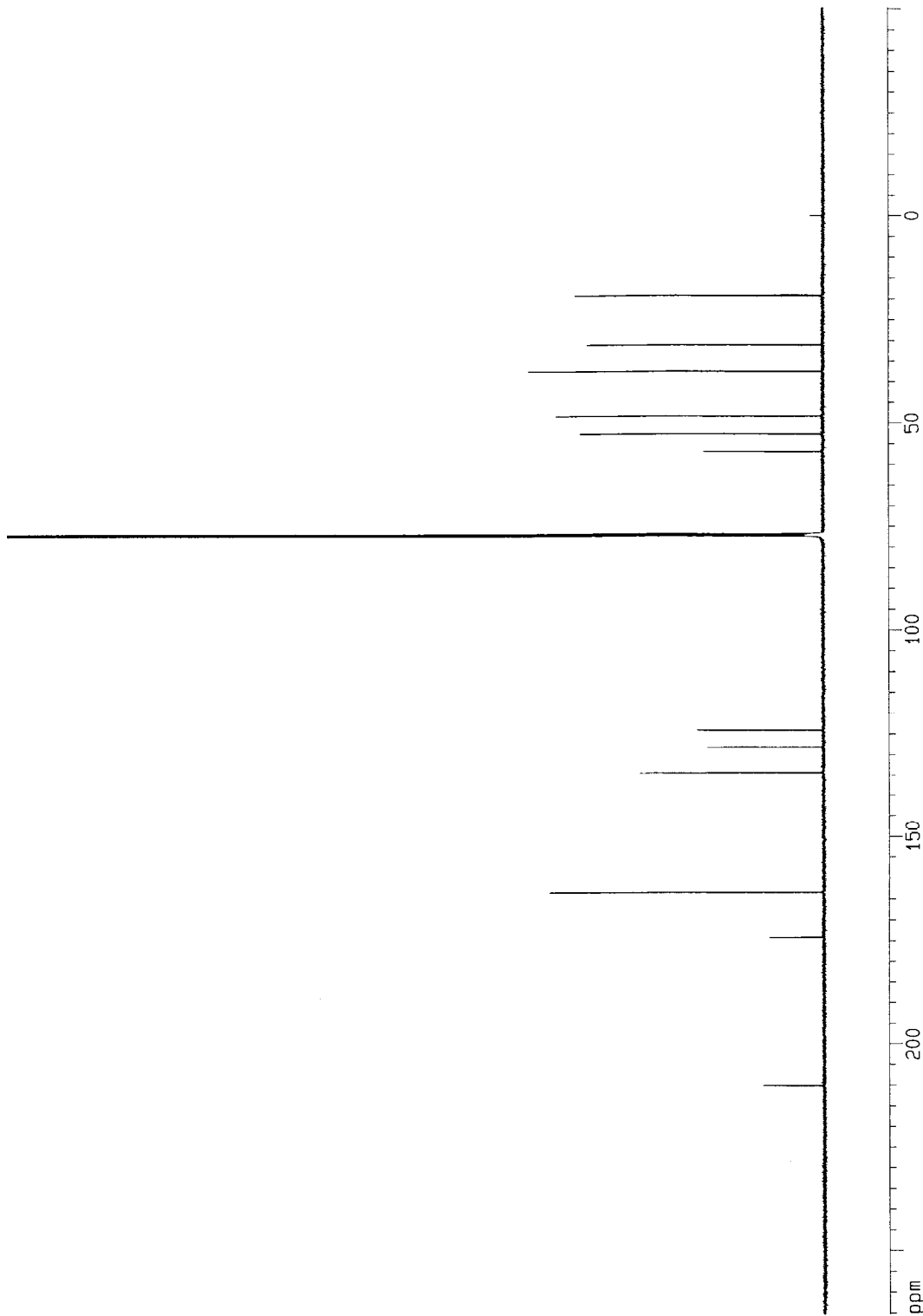
F2 - Acquisition Parameters
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 Time 12.07
 INSTRUM DRX500
 PROBHD 5 mm Multinuc1
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 4994
 DS 4
 SWH 39681.812 Hz
 FIDRES 0.605496 Hz
 AQ 0.8258188 sec
 RG 16384
 DM 12.600 usec
 DE 5.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

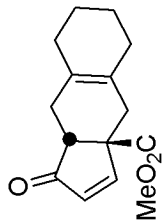
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 P1 8.10 usec
 PL1 3.00 dB
 SF01 125.7713108 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 88.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577935 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 15.00 cm
 F1P 265.258 ppm
 F1 33358.26 Hz
 F2P -50.284 ppm
 F2 -6323.55 Hz
 PPMCM 15.77708 ppm/cm
 HZCM 1984.09045 Hz/cm





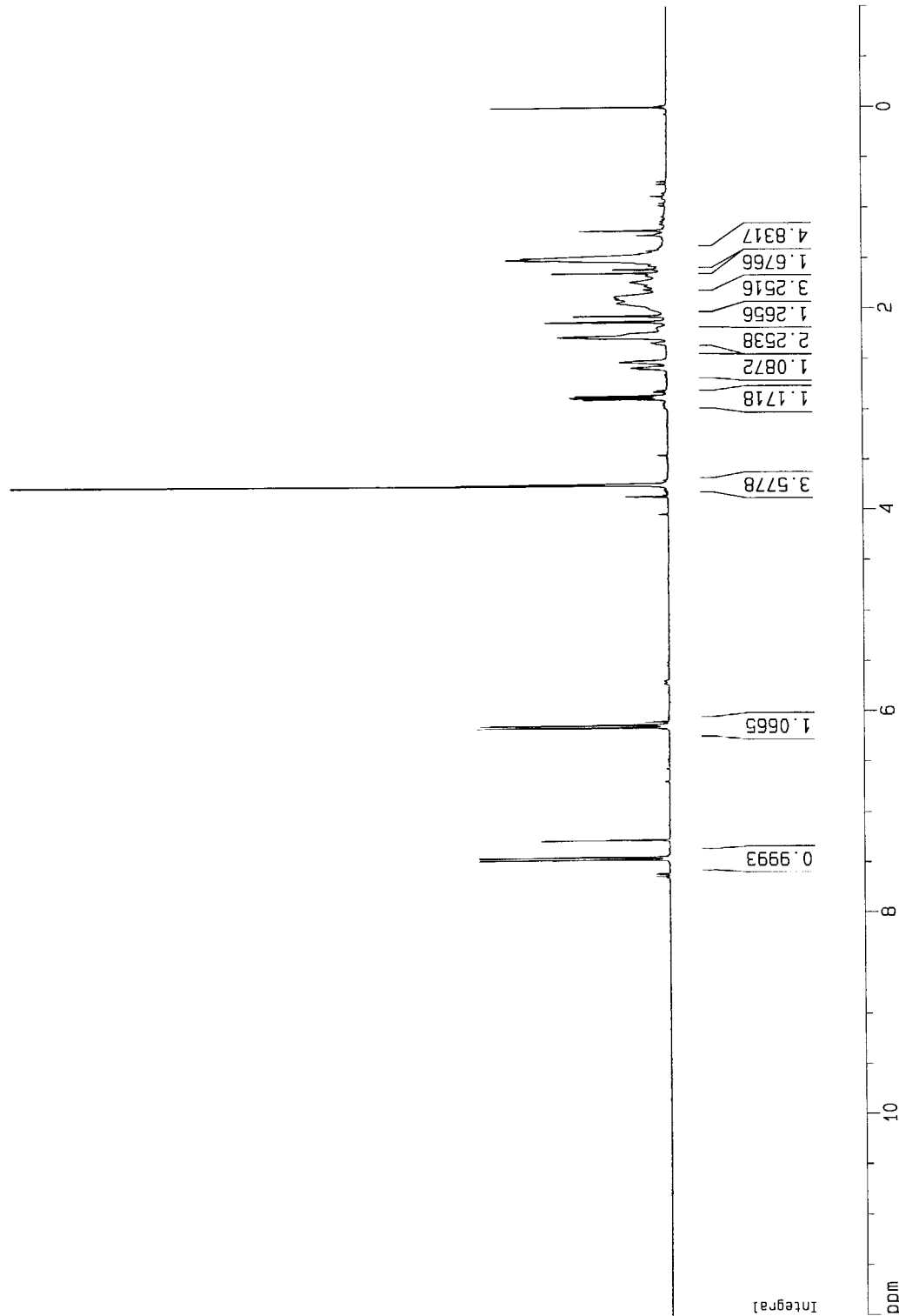
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 PROCNO 1

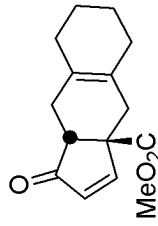
F2 - Acquisition Parameters

Date_ 20050401
 Time 0.52
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 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 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 250.1300043 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 30.00 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -1.000 ppm
 F2 -250.13 Hz
 PPMCM 0.65000 ppm
 HZCM 162.58450 Hz/





DA-16

Current Data Parameters
 NAME MG-4-015a-500
 EXPNO 2
 PROCNO 1

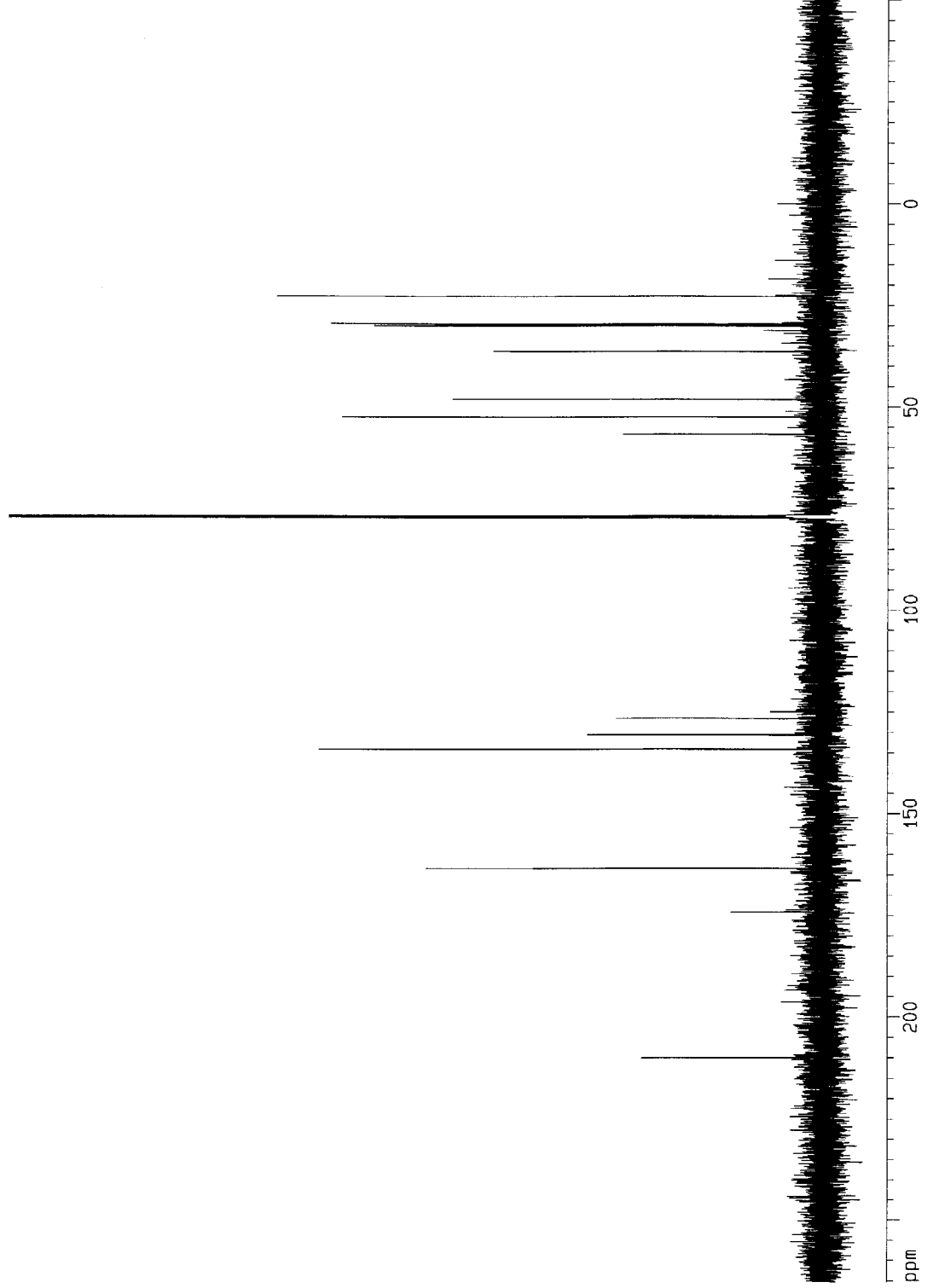
F2 - Acquisition Parameters
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 Time 1.25
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 PROBHD 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 182
 DS 4
 SWH 39661.812 Hz
 FIDRES 0.1605496 Hz
 AQ 0.8258188 sec
 RG 16384
 DW 12.600 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

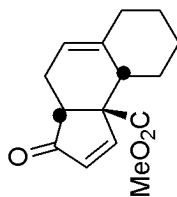
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 P1 8.10 usec
 PL1 3.00 dB
 SF01 125.7713108 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 88.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 SF02 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

1D NMR plot parameters
 CX 20.00 cm
 CY 35.00 cm
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 F2P -50.274 ppm
 F2 -6322.34 Hz
 PPMCM 15.77708 ppm/cm
 HZCM 1984.09033 Hz/cm





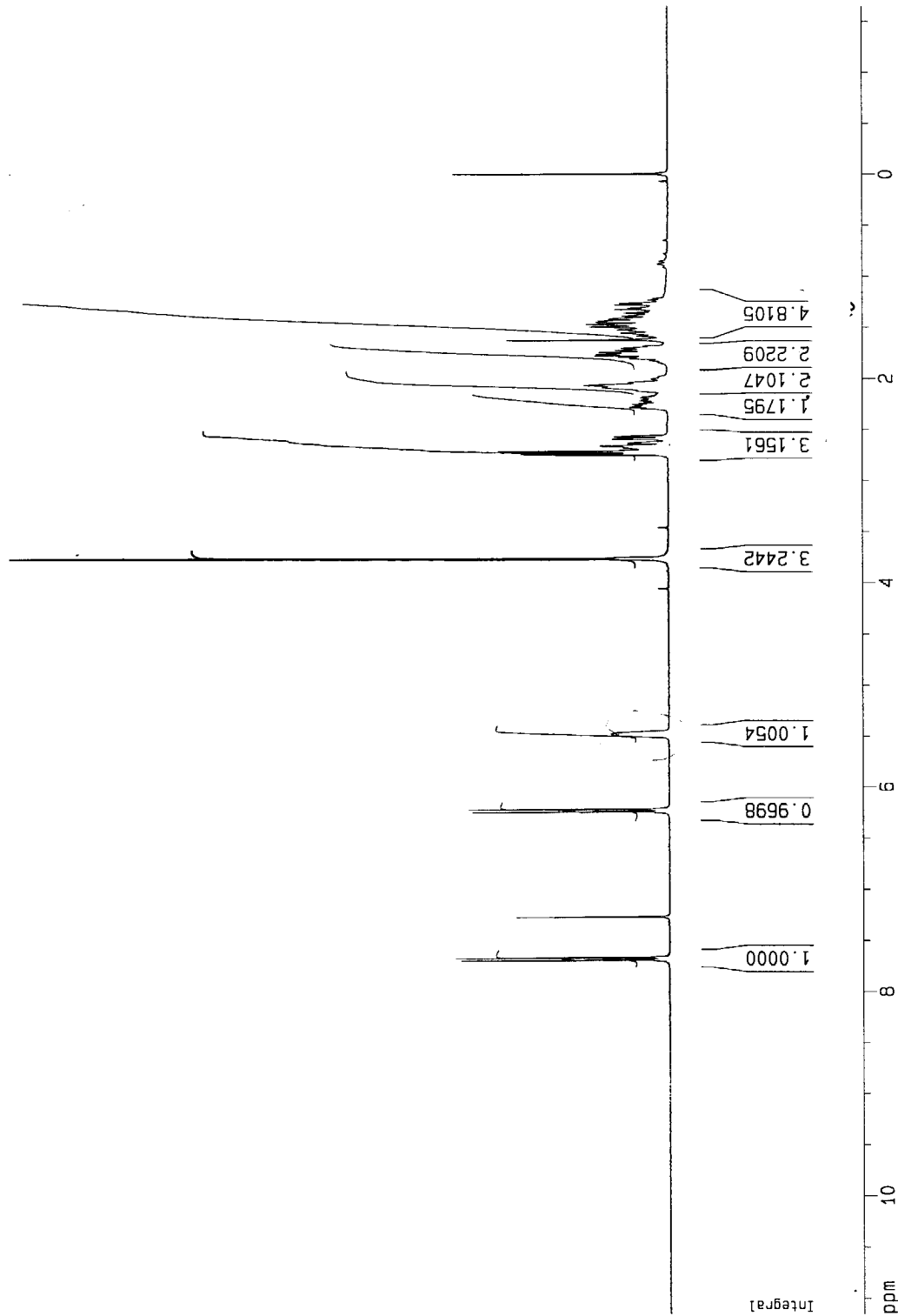
DA-19

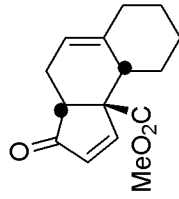
Current Data Parameters
 NAME MG-2-110a-250
 EXPNO 1
 PROCNO 1

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 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1430
 DW 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 250.1300055 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 30.00 cm
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 F2P -1.647 ppm
 F2 -412.05 Hz
 PPMCM 0.64010 ppm
 HZCM 160.10803 Hz/





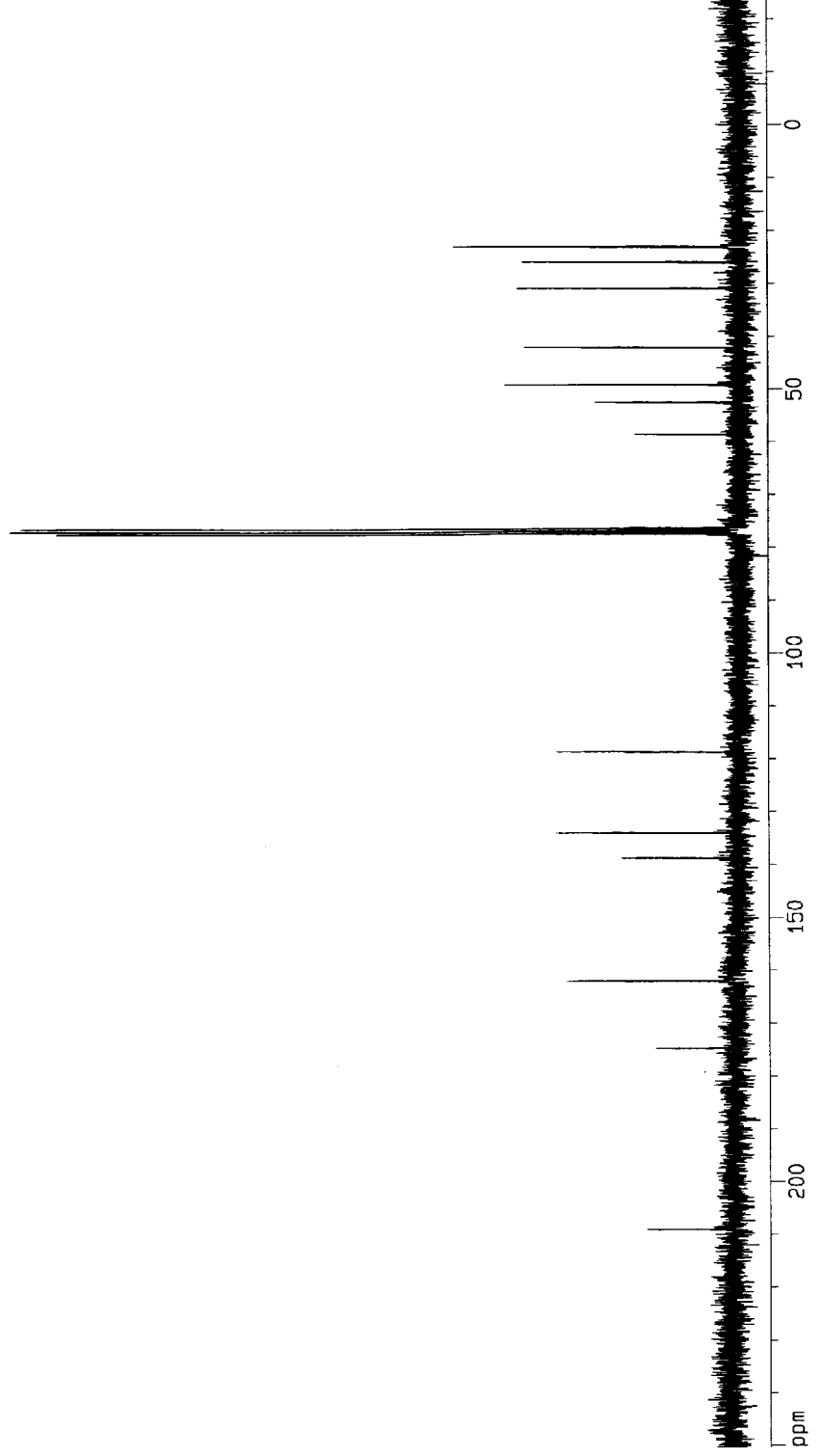
DA-19

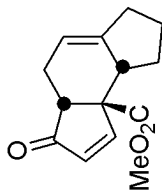
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
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 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TO 36864
 SOLVENT CDCl₃
 NS 722
 DS 4
 SWH 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
 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
 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
 PPKCM 13.70643 ppm
 HZCM 862.06891 Hz/





DA-20

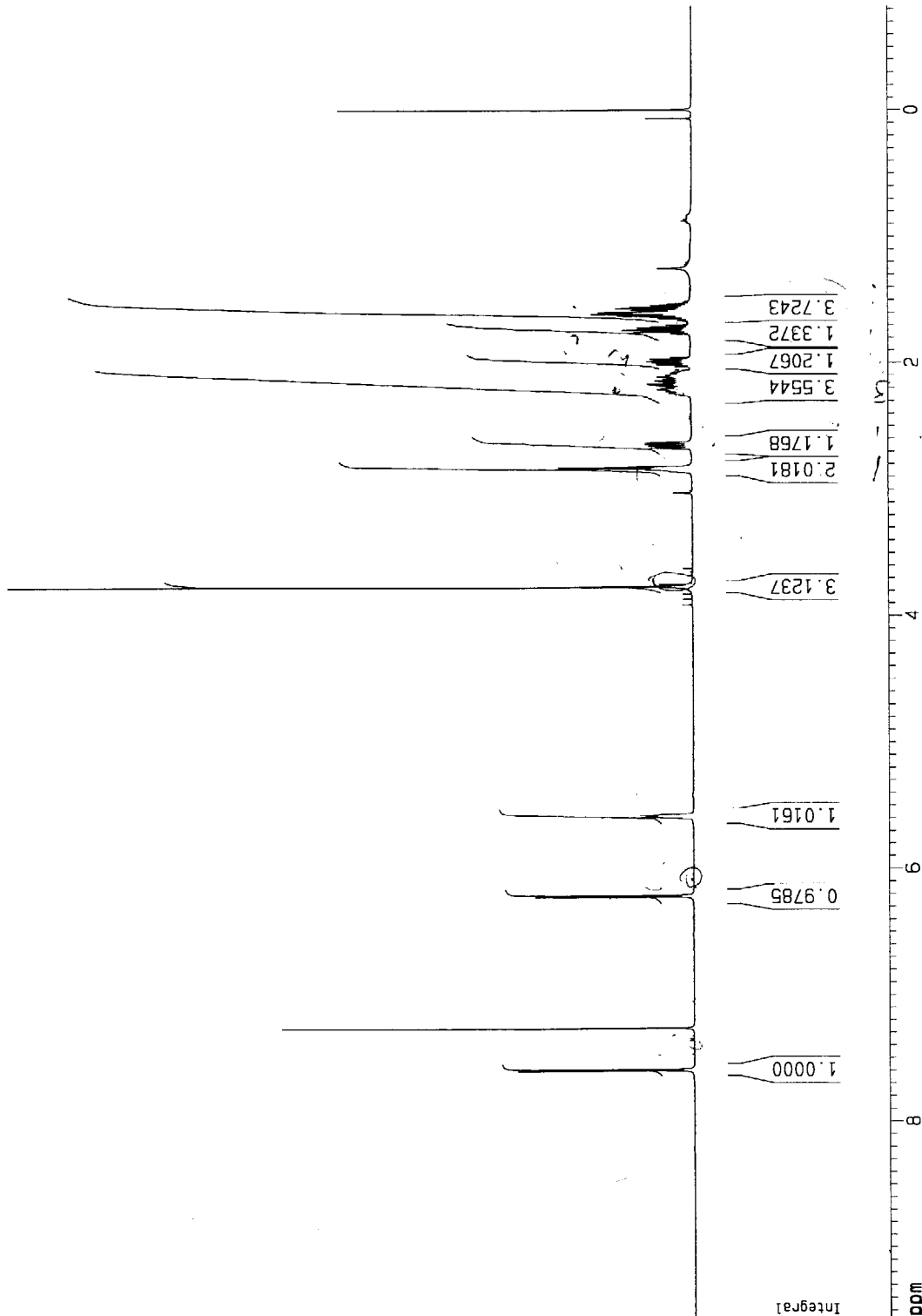
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 EXPNO 1
 PROCNO 1

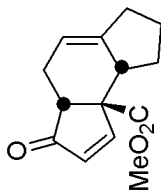
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 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 57344
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.180151 Hz
 AQ 2.7754996 sec
 RG 161.3
 DW 48.400 usec
 DE 6.00 usec
 TE 296.7 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.25 usec
 PL1 -3.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300109 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 30.00 cm
 F1P 9.549 ppm
 F1 4775.63 Hz
 F2P -0.820 ppm
 F2 -410.00 Hz
 PPMCM 0.51843 ppm/cm
 HZCM 259.28125 Hz/cm





DA-20

Current Data Parameters
 NAME MG-2-111a-250
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

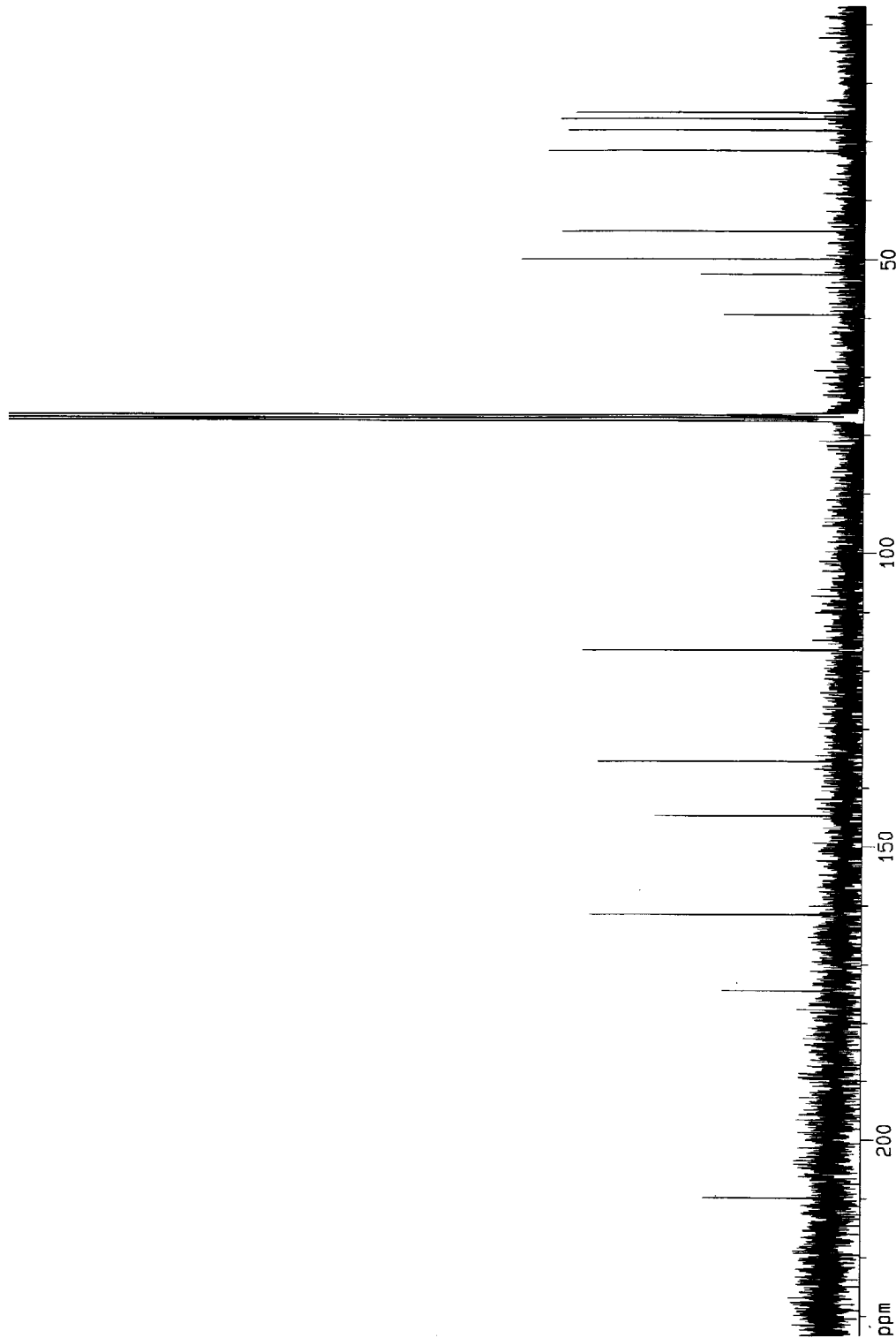
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 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 2007
 DS 4
 SWH 17241.379 Hz
 FIDRES 0.487702 Hz
 AQ 1.0691060 sec
 RG 22800
 DW 29.000 usec
 DE 41.43 usec
 TE 300.0 K
 D12 0.0002000 sec
 DL5 23.00 dB
 CPOPRG waltz16
 P31 103.00 usec
 D1 1.0000000 sec
 P1 5.35 usec
 SF01 52.9023694 MHz
 NUCLEUS 13C
 D11 0.0300000 sec

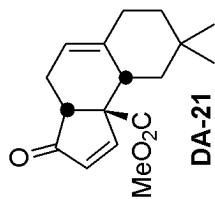
F2 - Processing parameters

SI 32768
 SF 52.8952403 MHz
 WDW 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 233.411 ppm
 F1 14680.45 Hz
 F2P 6.889 ppm
 F2 433.28 Hz
 PPMCM 11.32611 ppm
 HZCM 712.35852 Hz/





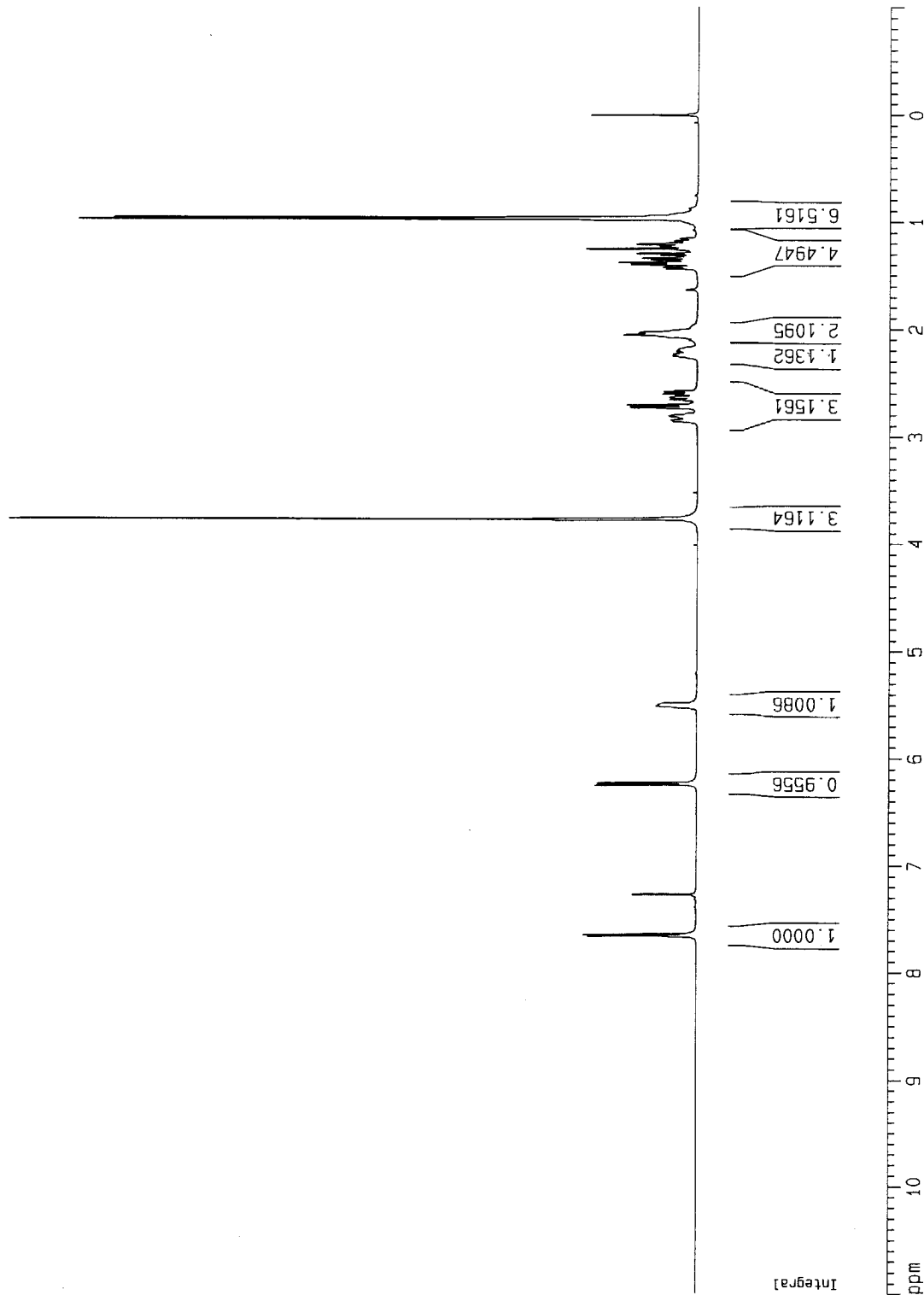
Current Data Parameters
 NAME MG-3-073a-300
 EXPNO 1
 PROCNO 1

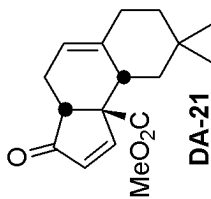
F2 - Acquisition Parameters
 Date_ 20050124
 Time 15.56
 INSTRUM drx300
 PROBHD 5 mm Multinuc1
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 2
 SMH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 228.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 7.05 usec
 PL1 0.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300022 MHz
 NDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.30

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07800 Hz/cm





Current Data Parameters
 NAME MG-3-073a-300
 EXPNO 2
 PROCNO 1

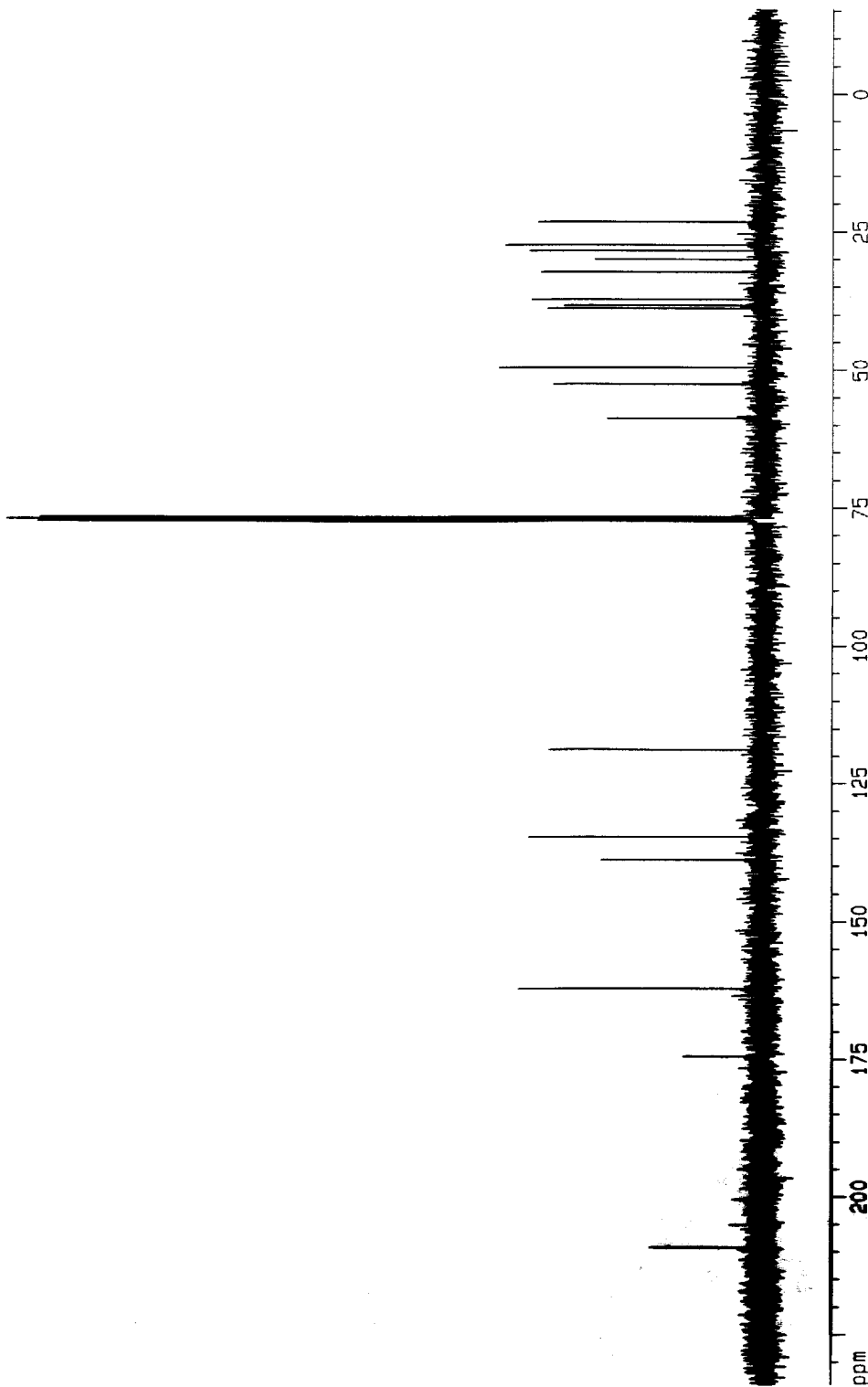
F2 - Acquisition Parameters
 Date_ 20050124
 Time 15:58
 INSTRUM drx300
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TO 65536
 SOLVENT COC13
 NS 158
 DS 4
 SMH 18832.353 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 22528
 DN 26.550 usec
 DE 6.00 usec
 TE 297.1 K
 D1 1.25999995 sec
 d11 0.03000000 sec
 D31 0.00000000 sec

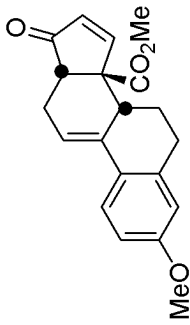
===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 8.50 usec
 PL1 5.00 dB
 SF01 75.4760107 MHz

===== CHANNEL f2 =====
 CHUPRG2 waitz16
 NUC2 ¹H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 25.60 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677508 MHz
 ADW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 11.00 cm
 F1P 234.220 ppm
 F1 17676.09 Hz
 F2P -15.322 ppm
 F2 -1156.30 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61957 Hz/cm





DA-22

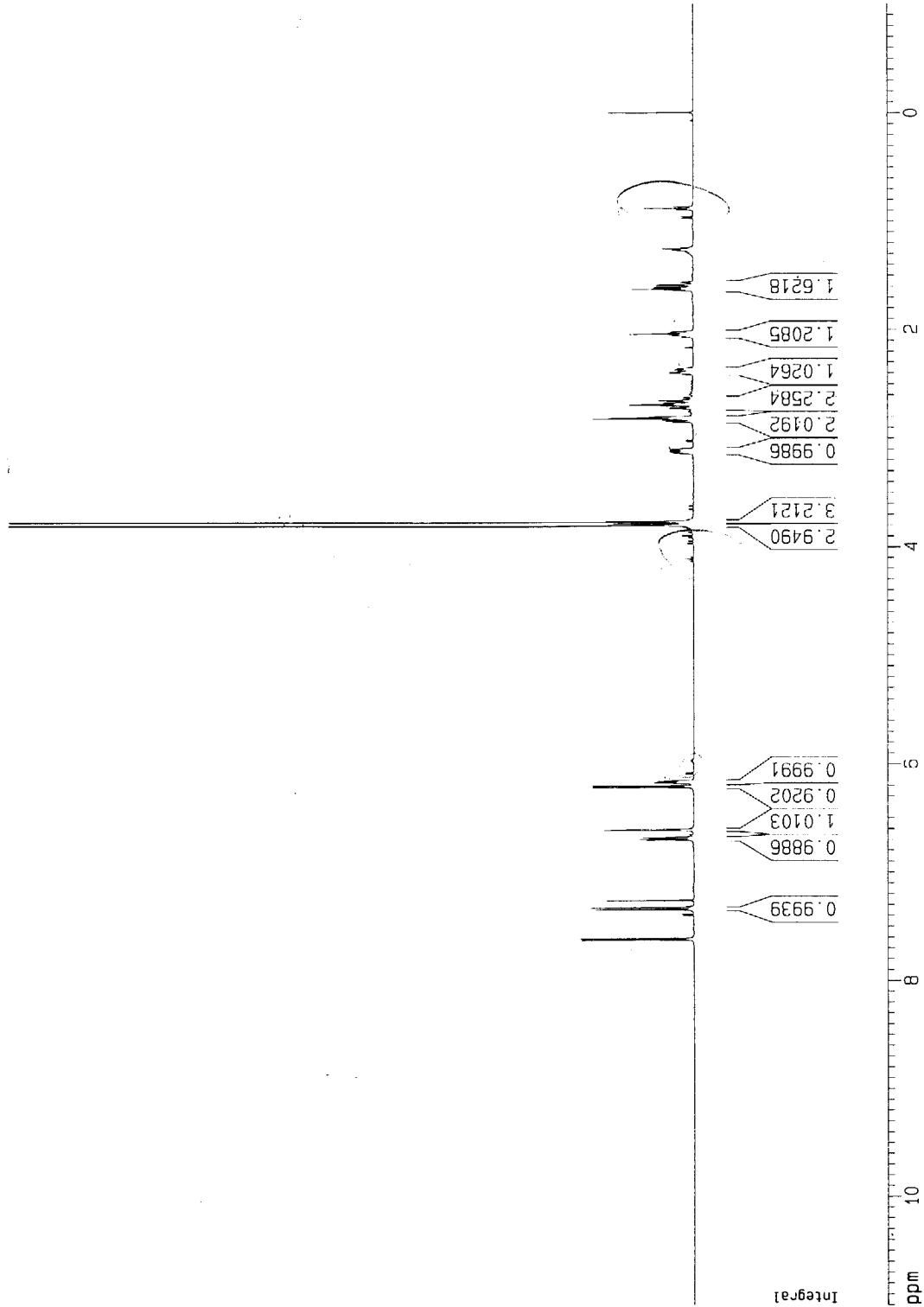
Current Data Parameters
 NAME MG-3-061a-500
 EXPNO 1
 PROCNO 1

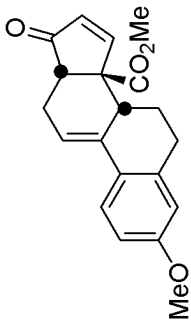
F2 - Acquisition Parameters
 Date_ 20041102
 Time 20.39
 INSTRUM DRX500
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 57344
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.180151 Hz
 AQ 2.7754996 sec
 RG 101.6
 DW 48.400 usec
 DE 6.00 usec
 TE 296.7 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.25 usec
 PL1 -3.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300125 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 15.00 cm
 F1P 11.000 ppm
 F1 5501.43 Hz
 F2 -1.000 ppm
 F2 -500.13 Hz
 PPMCM 0.60000 ppm/cr
 HZCM 300.07800 Hz/cm





DA-22

Current Data Parameters
 NAME NG-3-050a-300
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20041101
 Time 22.58
 INSTRUM drx300
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 78
 DS 4
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 22528
 DN 26.550 usec
 DE 6.00 usec
 TE 297.1 K
 O1 1.29999995 sec
 d11 0.03000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 5.00 dB
 SF01 75.4760107 MHz

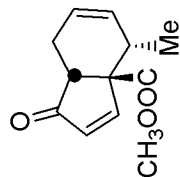
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 25.60 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677514 MHz
 WDW 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 234.213 ppm
 F1 17675.51 Hz
 F2P -15.329 ppm
 F2 -1156.88 Hz
 PPMCH 12.47711 ppm/cm
 HZCH 941.61957 Hz/cm



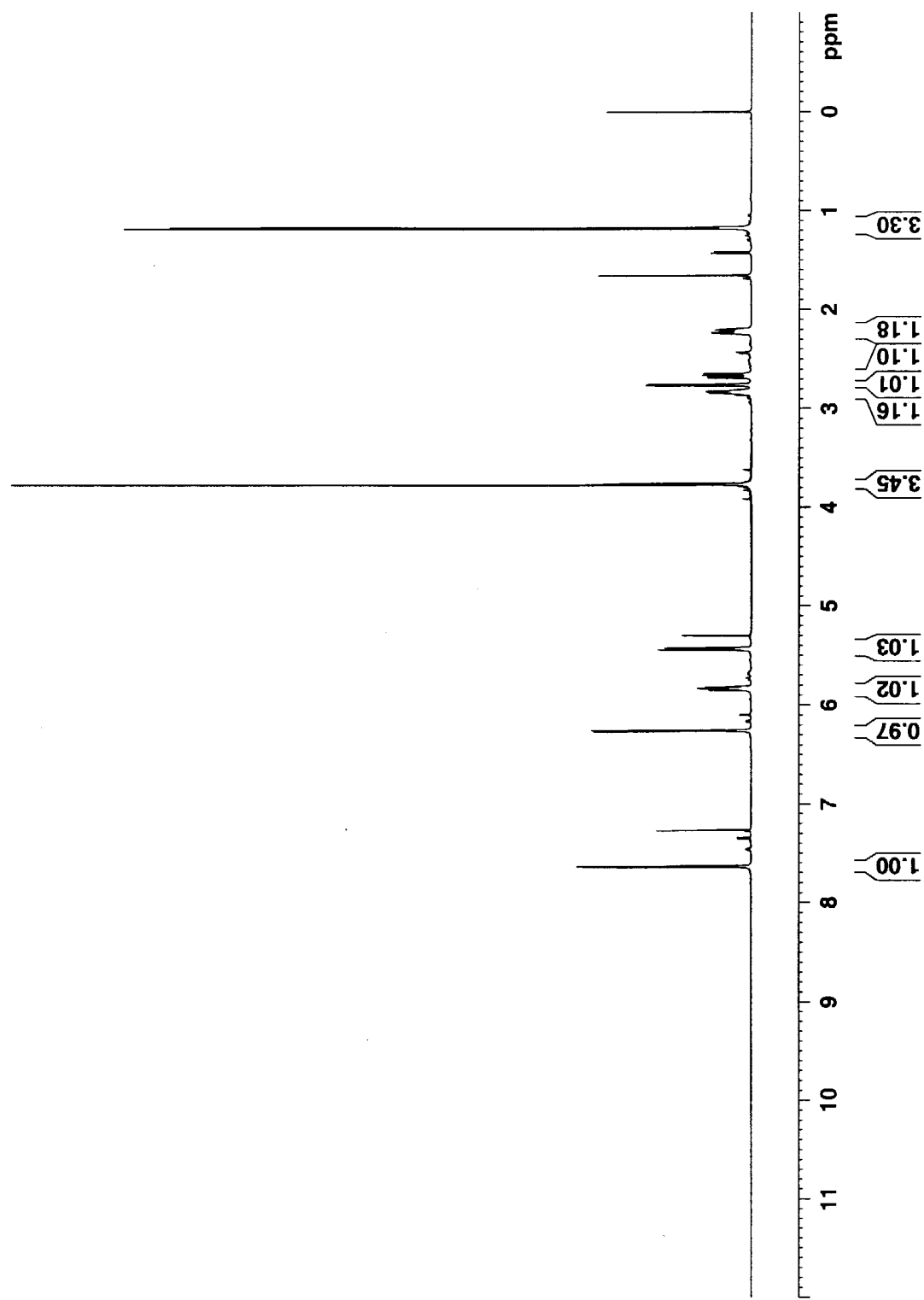


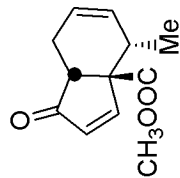
Current Data Parameters
 NAME MG-V-84a-A3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060210
 Time 22.43
 INSTRUM DRX500
 PROBHD 5 mm Multinucl
 PULPROG zg30pad
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 114
 DW 48.400 use
 DE 6.00 use
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.50 use
 PL1 0.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300071 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40





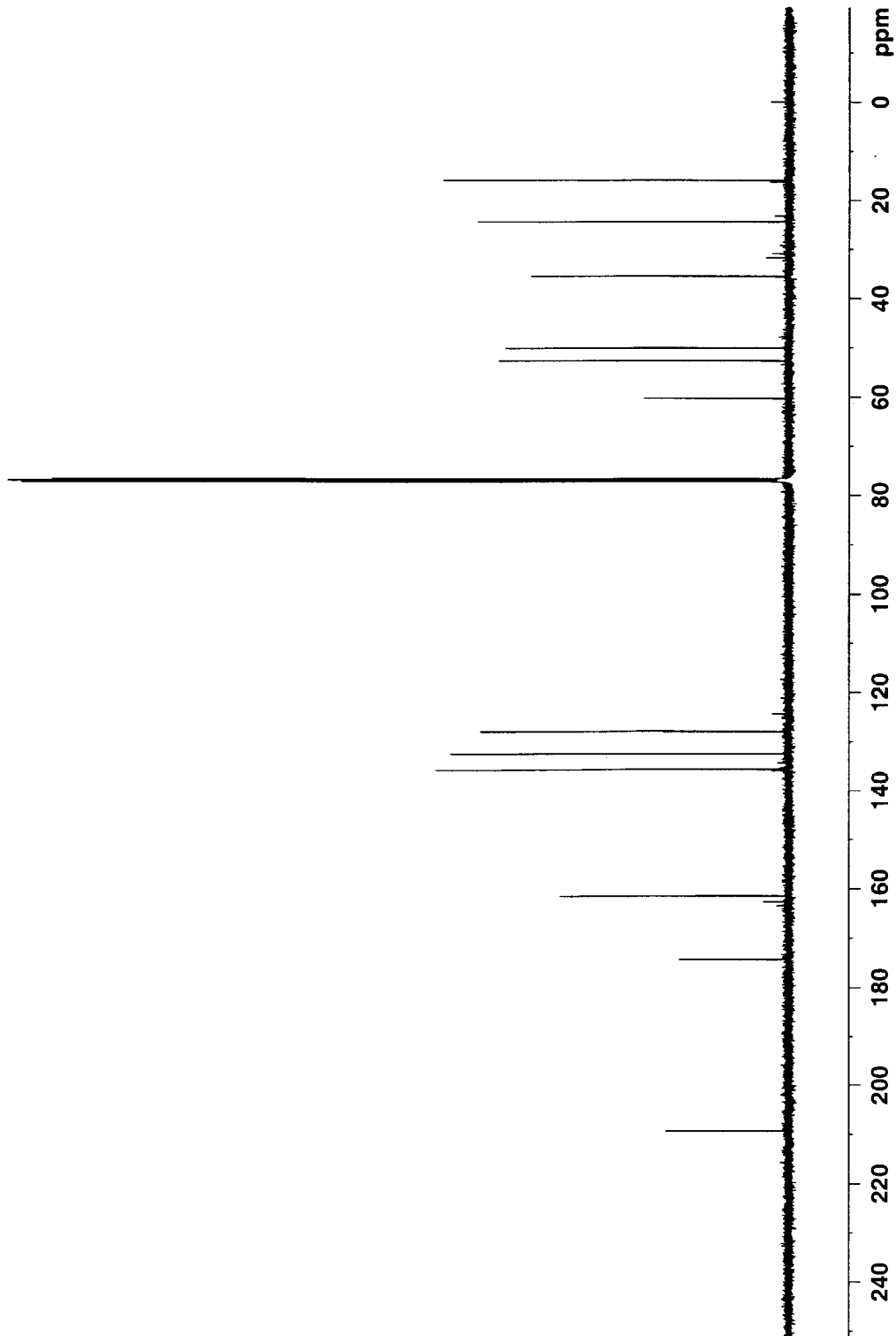
Current Data Parameters
 NAME MG-V-84a-A3
 EXPNO 2
 PROCNO 1

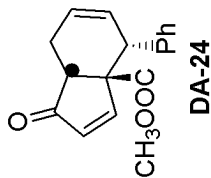
F2 - Acquisition Parameters
 Date_ 20060210
 Time 23:07
 INSTRUM DRX500
 PROBD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 428
 DS 4
 SMH 34013.605 Hz
 FIDRES 0.519006 Hz
 AQ 0.9634292 sec
 RG 32768
 DW 14.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 8.10 usec
 PL1 3.00 dB
 SFO1 125.7723786 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 P2 88.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577938 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



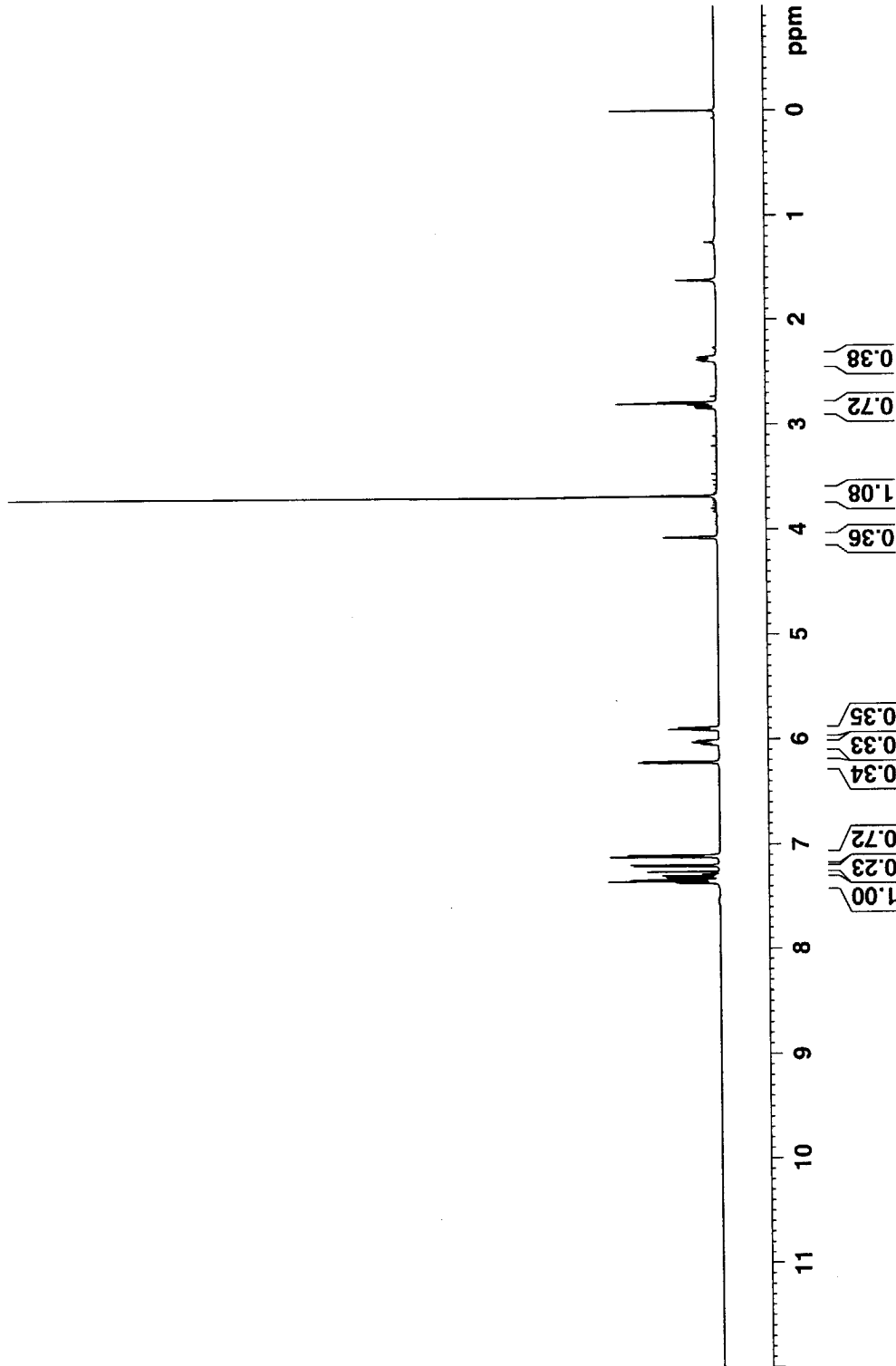


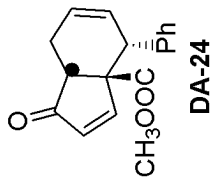
Current Data Parameters
 NAME MG-IV-77a-A3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060208
 Time 14.38
 INSTRUM DRX500
 PROBHD 5 mm Multinucl
 PULPROG zg30pad
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 128
 DW 48.400 use
 DE 6.00 use
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 11.50 use
 PL1 0.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300115 MHz
 EM 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40





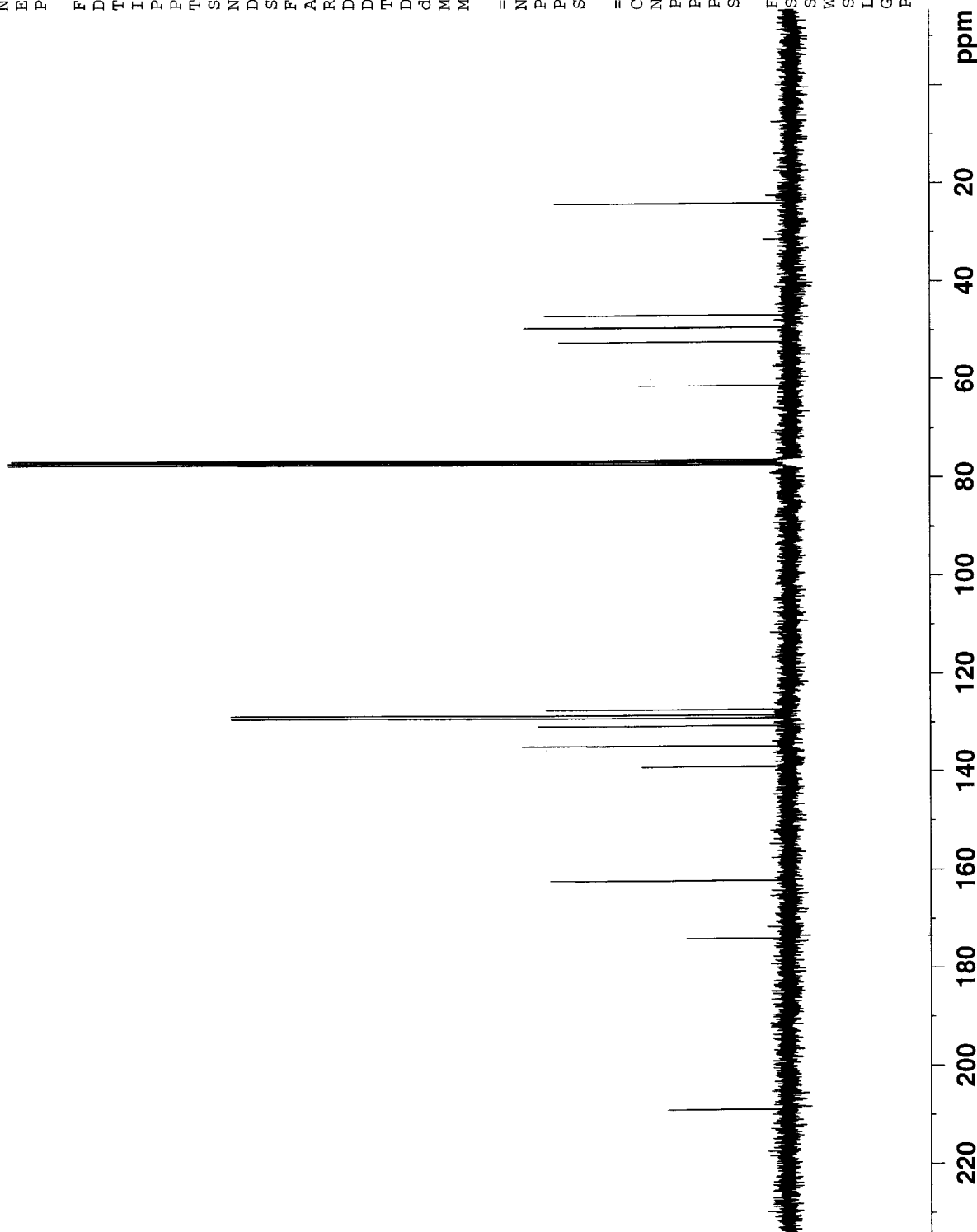
Current Data Parameters
NAME MG-IV-077b-300
EXPNO 2
PROCNO 1

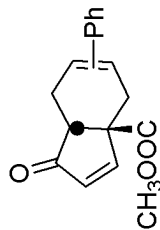
F2 - Acquisition Parameters
Date_ 20050628
Time 22.26
INSTRUM DRX300
PROBHD 5 mm Multinucl
PULPROG zgdc30
TD 65536
SOLVENT CDC13
NS 13
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 22528
DW 26.550 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 5.00 dB
SFO1 75.4760107 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 25.60 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





DA-25

Current Data Parameters
 NAME MG-4-062a-250
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050525
 Time 23.48

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

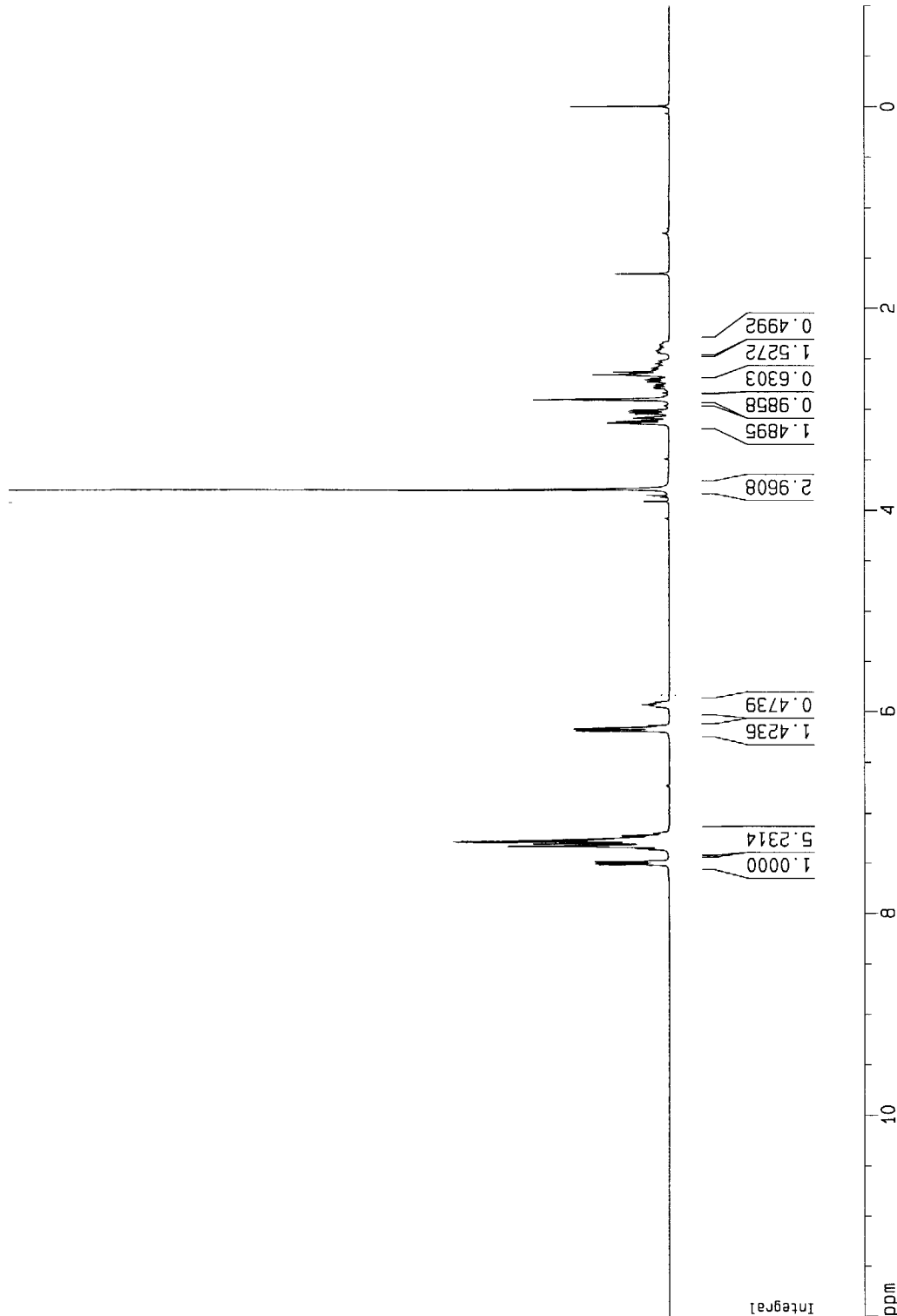
SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1024

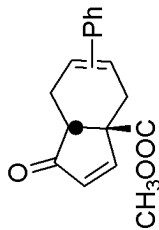
DW 96.000 use
 DE 137.14 use
 TE 300.0 K

D1 1.00000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300075 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 -1.000 ppm
 F2 -250.13 Hz
 PPMCM 0.65000 ppm
 HZCM 162.58450 Hz/





DA-25

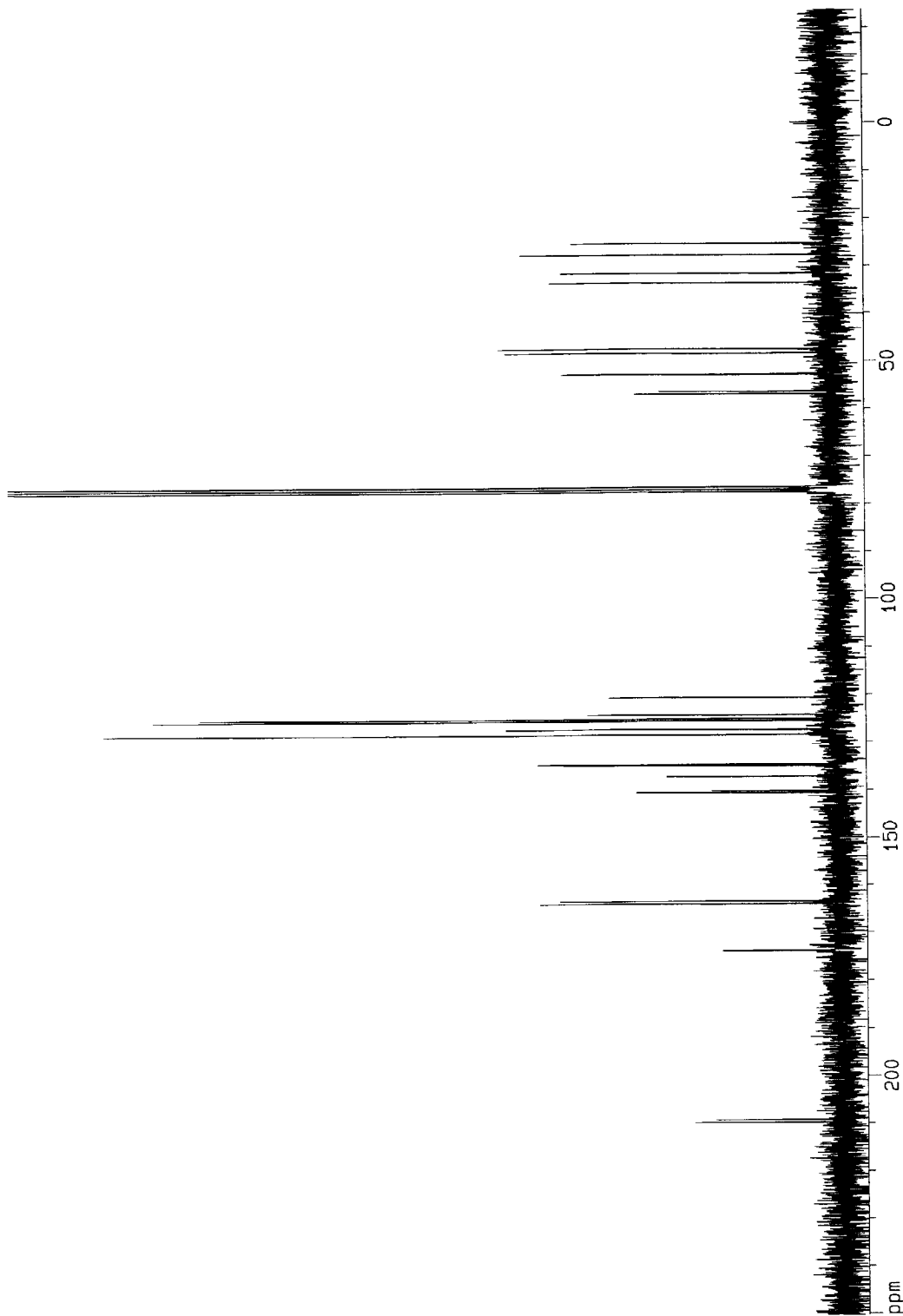
Current Data Parameters
 NAME MG-4-082a-250
 EXPNO 2
 PROCNO 1

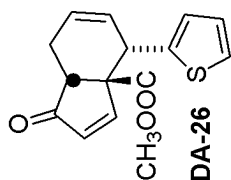
F2 - Acquisition Parameters
 Date_ 20050525
 Time 23.52

INSTRUM arx250
 PROBD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDC13
 NS 536
 DS 4
 SWH 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
 CPDPRG waltz16
 P31 103.00 use
 D1 2.00000000 sec
 P1 6.00 use
 SFO1 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters
 SI 32768
 SF 62.8952434 MHz
 WDW 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 250.363 ppm
 F1 15746.65 Hz
 F2P -23.765 ppm
 F2 -1494.73 Hz
 PPMCM 13.70643 ppm
 HZCM 662.06897 Hz/



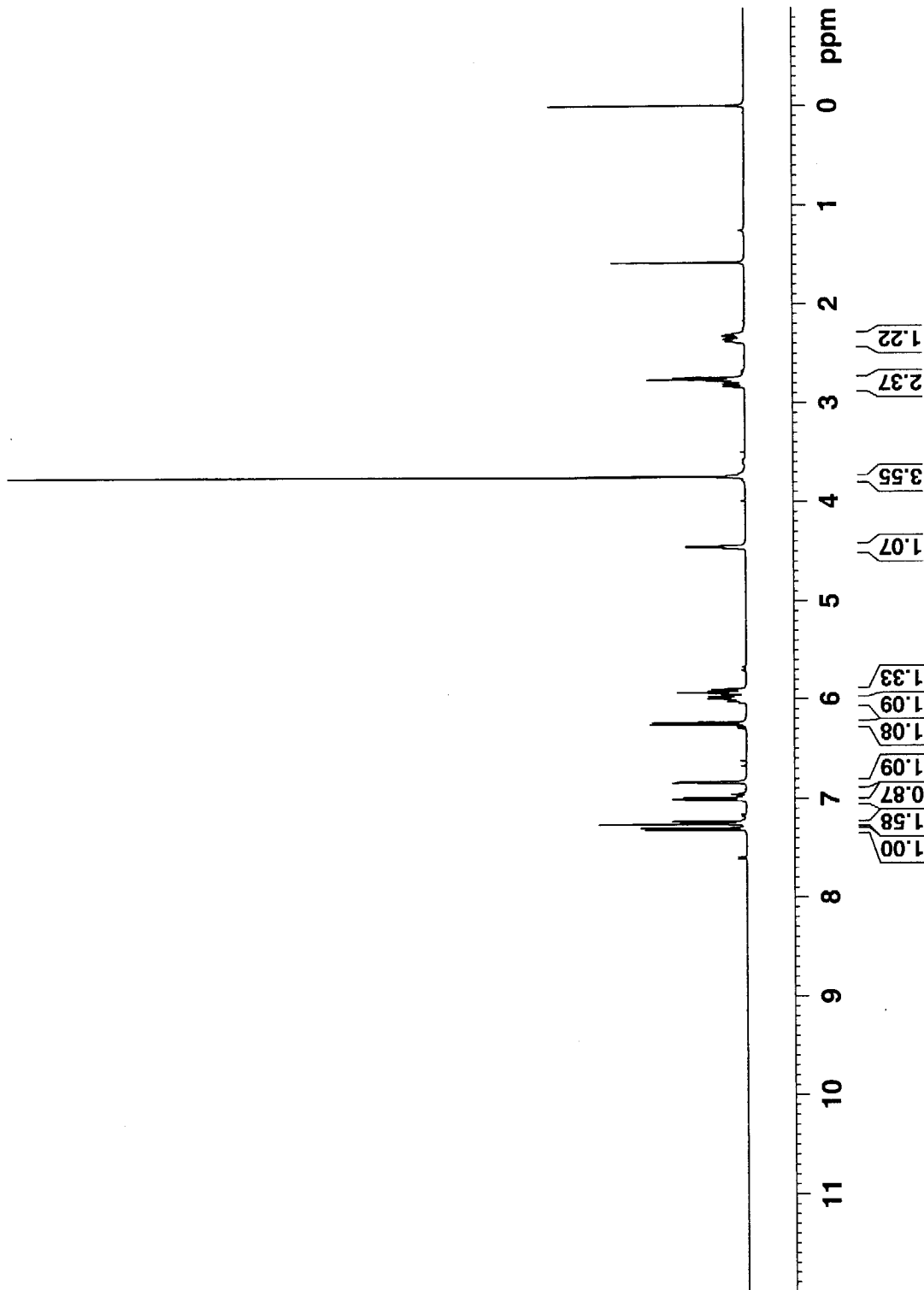


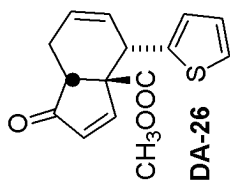
Current Data Parameters
 NAME MG-IV-142ba-A2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050908
 Time 10.58
 INSTRUM DRX300
 PROBHD 5 mm Multinucl
 PULPROG zg30pad
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 645.1
 DW 81.000 use
 DE 6.00 use
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 7.05 use
 PL1 0.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300054 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.30





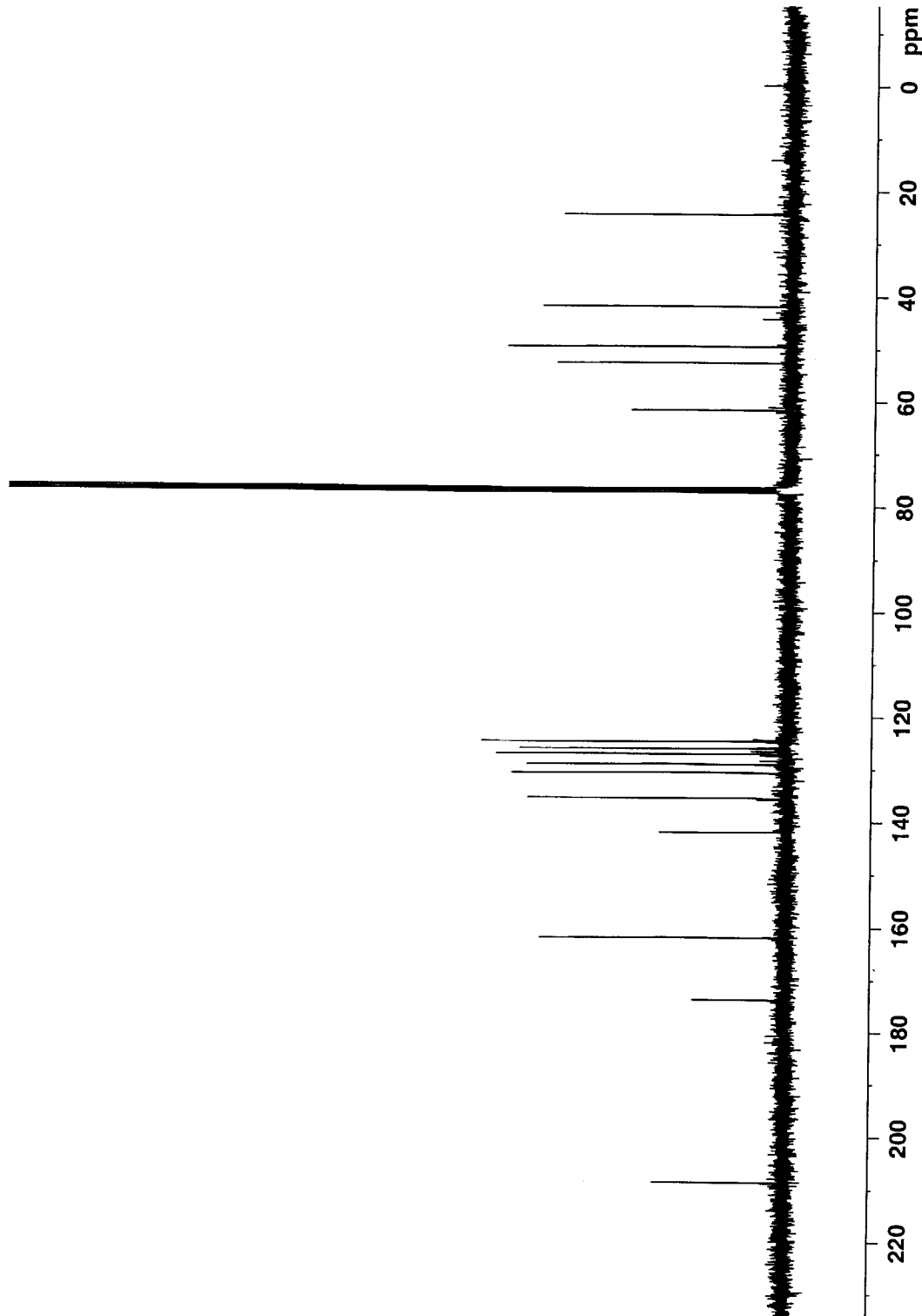
Current Data Parameters
 NAME MG-IV-142B-A2
 EXPNO 2
 PROCNO 1

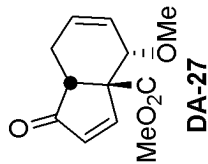
F2 - Acquisition Parameters
 Date_ 20050907
 Time 12.11
 INSTRUM DRX300
 PROBHD 5 mm Multinucl
 PULPROG zgpg30pad
 TD 65536
 SOLVENT CDC13
 NS 561
 DS 4
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 22528
 DW 26.550 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 5.00 dB
 SFO1 75.4760107 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 25.60 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32788
 SF 75.4677508 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





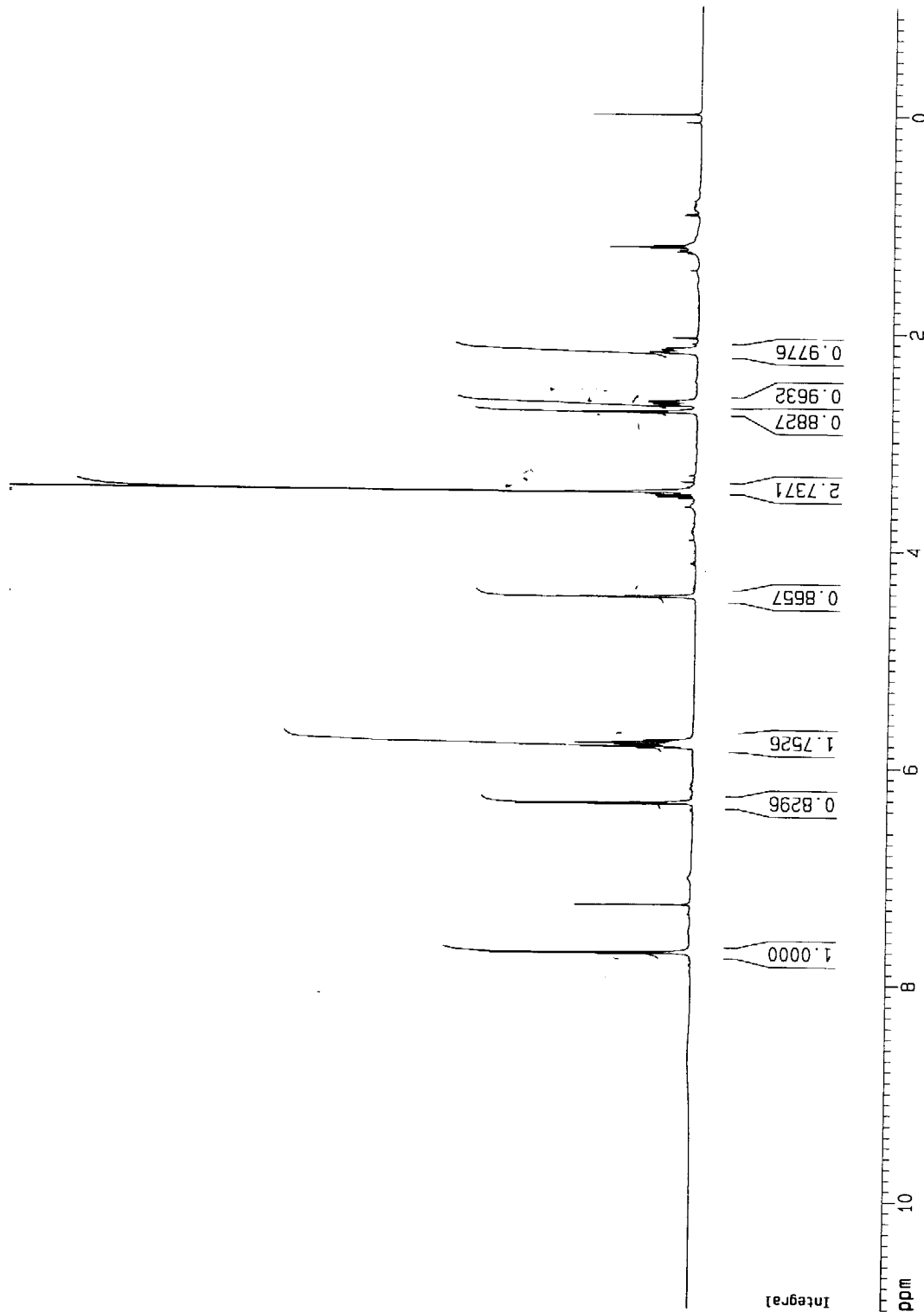
Current Data Parameters
 NAME MG-3-025a-500
 EXPNO 1
 PROCNO 1

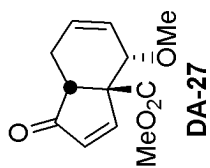
F2 - Acquisition Parameters
 Date_ 20040902
 Time 22.56
 INSTRUM DRX500
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 57344
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.180151 Hz
 AQ 2.7754996 sec
 RG 128
 DW 48.400 usec
 DE 6.00 usec
 TE 296.7 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.25 usec
 PL1 -3.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300081 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.40

1D NMR plot parameters:
 CX 20.00 cm
 CY 20.00 cm
 F1P 11.000 ppm
 F1 5501.43 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCM 0.60000 ppm/cr
 HZCM 300.07800 Hz/cm





Current Data Parameters
 NAME MG-3-025-300
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

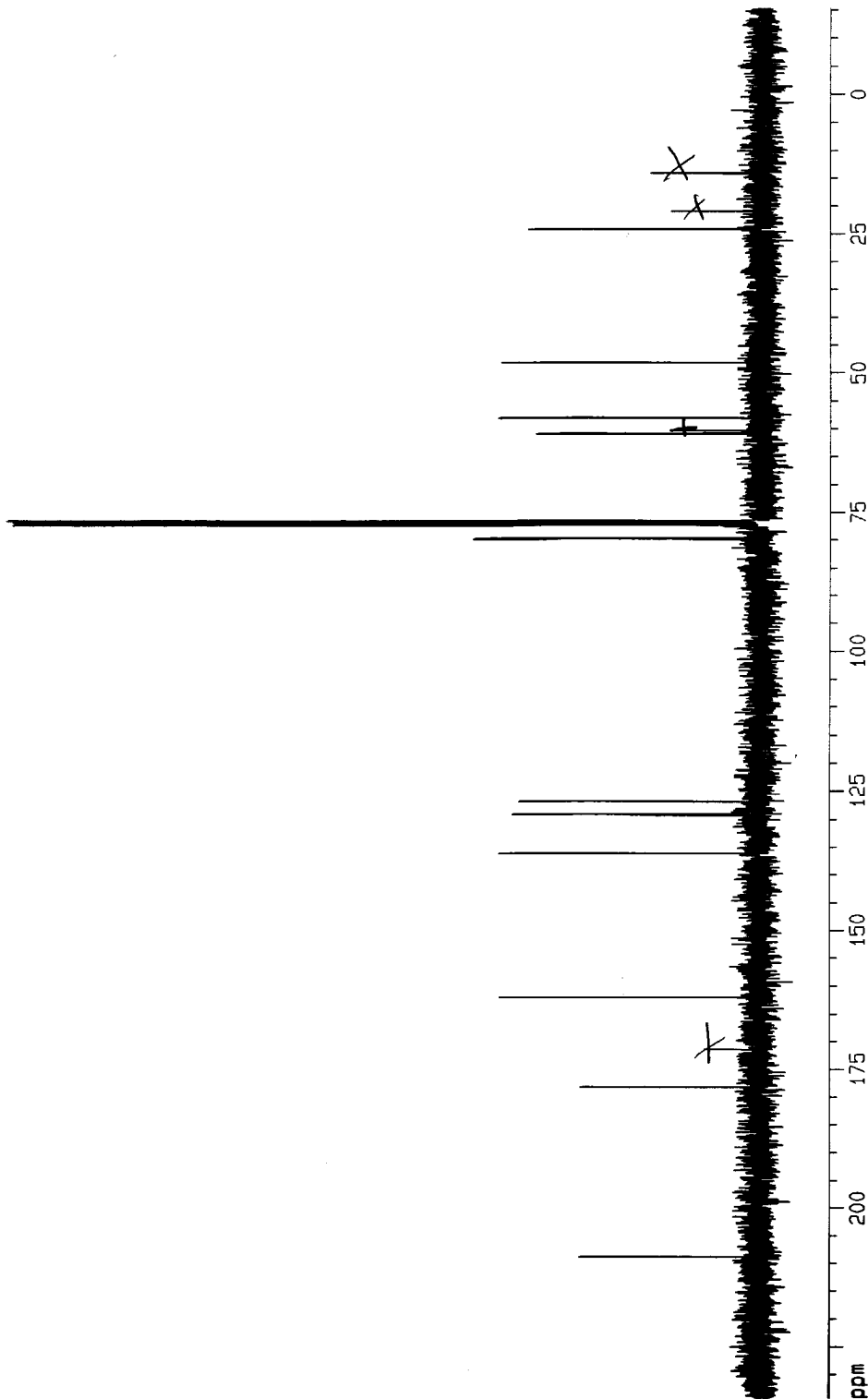
Date_ 20040902
 Time 13.20
 INSTRUM drx300
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 121
 DS 4
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 22528
 DM 26.550 usec
 DE 6.00 usec
 TE 297.1 K
 D1 1.29999995 sec
 d11 0.03000000 sec
 D31 0.00000000 sec

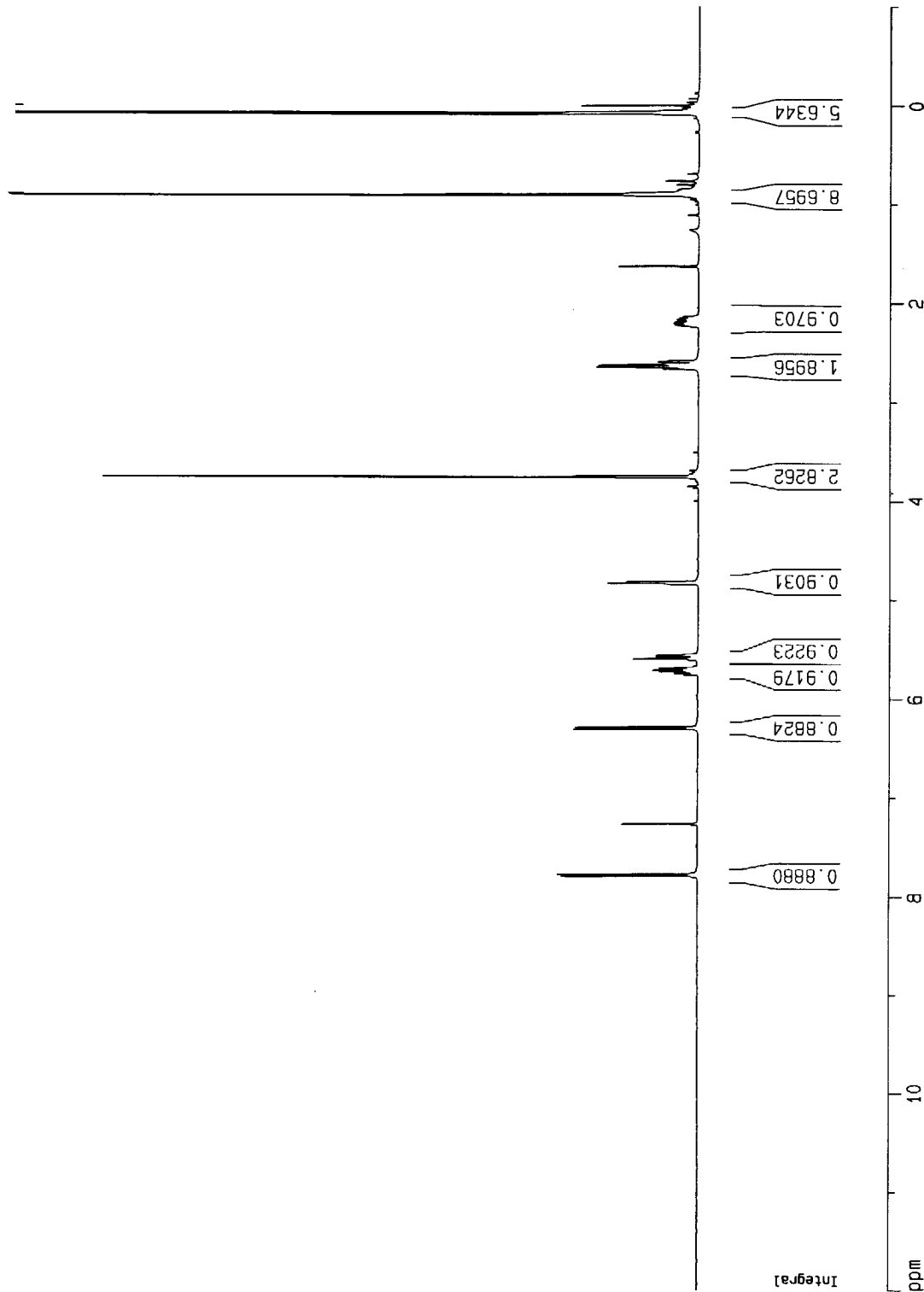
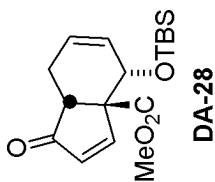
===== CHANNEL f1 =====
 NUC1 13C
 P1 8.50 usec
 PL1 5.00 dB
 SF01 75.4760107 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 25.60 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677520 MHz
 NDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 11.00 cm
 F1P 234.205 ppm
 F1 17674.94 Hz
 F2P -15.337 ppm
 F2 -1157.45 Hz
 PPMCM 12.47711 ppm/cm
 HZCM 941.61957 Hz/cm





Current Data Parameters	
NAME	MG-4-024a-300
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20050406
Time	12.38
INSTRUM	dx300
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.188380 Hz
AQ	2.6542580 sec
RG	203.2
AW	81.0000 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
D31	0.00000000 sec

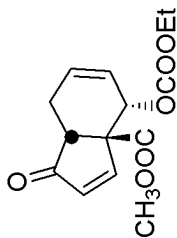
```
===== CHANNEL f1 =====
NUC1      1H
P1        7.05 usec
PL1       0.00 dB
SF01     300.1318534 MHz
```

EM	0
FSF	300.130037 MHz
SI	32768
PC	1.30
GB	0
LB	0.30 Hz
SSB	
MDW	

1D NMR plot parameters	
CX	20.00 cm
CY	40.00 cm
F1P	12.000 ppm
F1	3601.56 Hz
2P	-1.000 ppm
2	-300.13 Hz
PPMCM	0.65000 ppm/cm
HZCM	195.08450 Hz/cm



HZCM
1984.09045 Hz/cm



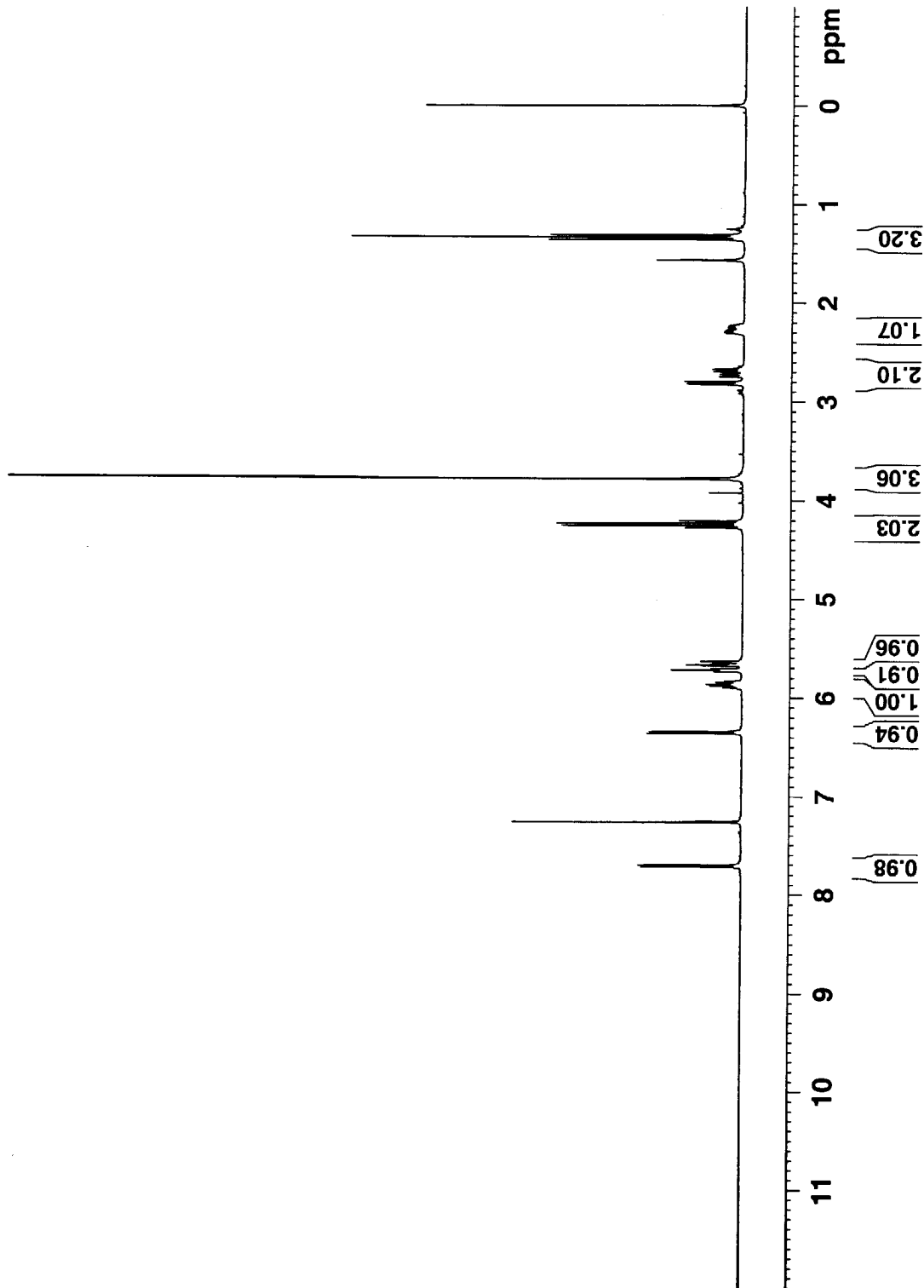
DA-29

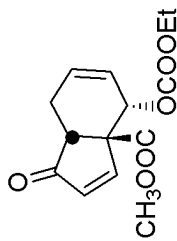
Current Data Parameters
 NAME MG-IV-135b-A2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050830
 Time 14.24
 INSTRUM DRX300
 PROBD 5 mm Multinucl
 PULPROG zg30pad
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 812.7
 DW 81.000 use
 DE 6.00 use
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 7.05 use
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300045 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.30





DA-29

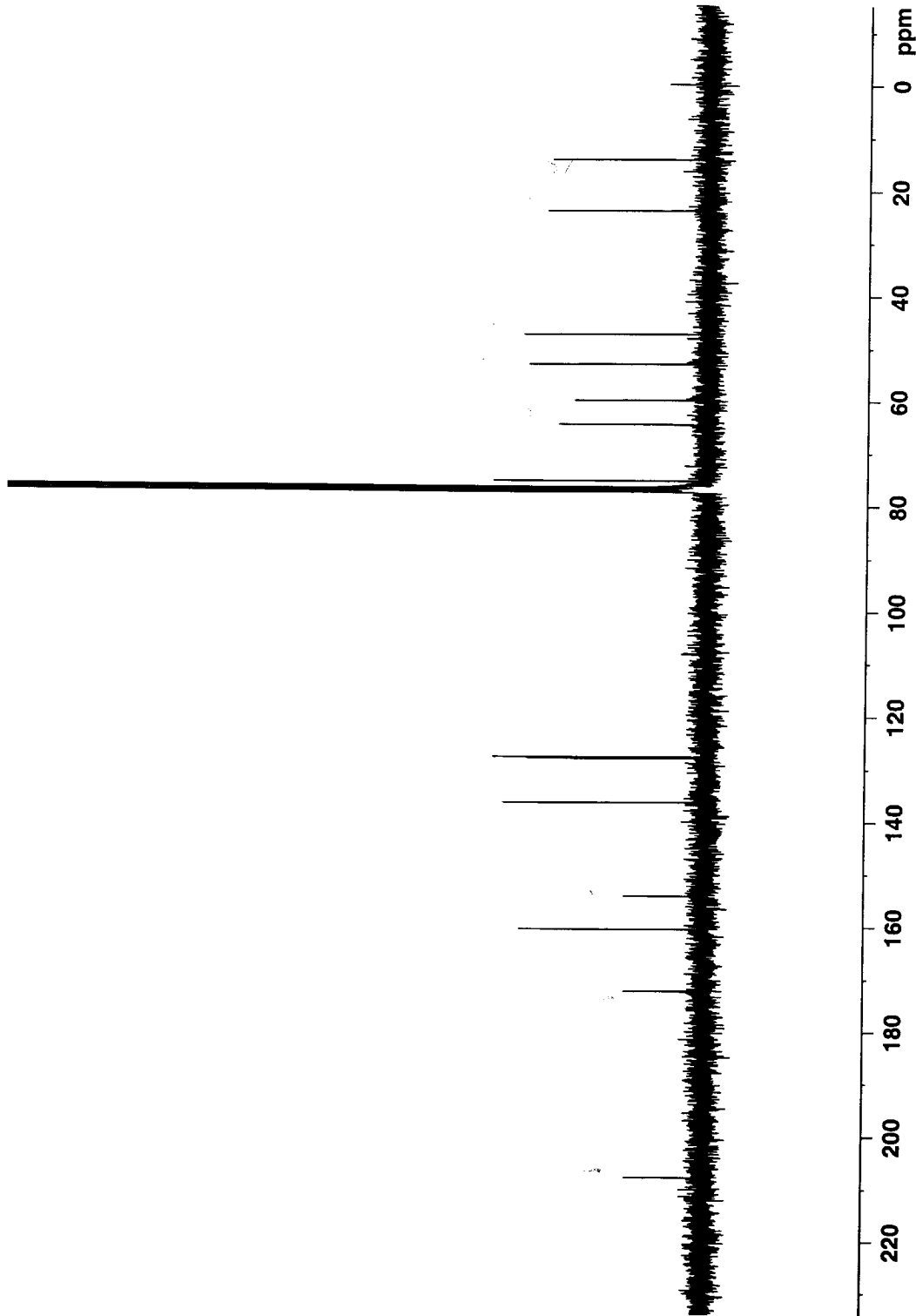
Current Data Parameters
 NAME MG-IV-135b-A2
 EXPNO 2
 PROCNO 1

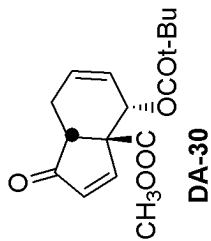
F2 - Acquisition Parameters
 Date_ 20050830
 Time 14:29
 INSTRUM DRX300
 PROBHD 5 mm Multinucl
 PULPROG zgpg30pad
 TD 65536
 SOLVENT CDC13
 NS 923
 DS 4
 SWH 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7400308 sec
 RG 22528
 DW 26.550 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.00 usec
 PL1 5.00 dB
 SFO1 75.4760107 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 100.00 usec
 PL2 120.00 dB
 PL12 25.60 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677497 MHz
 EM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



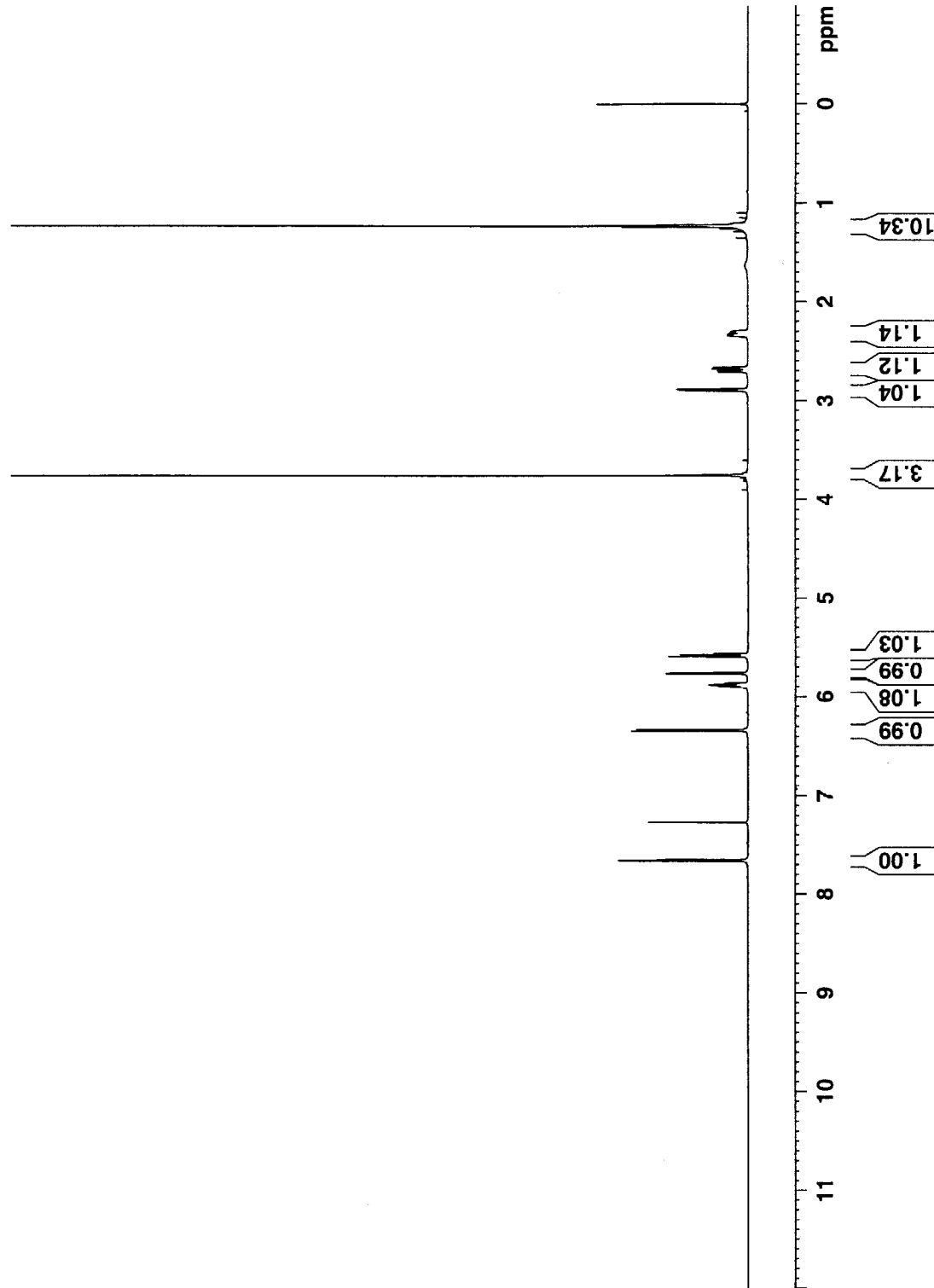


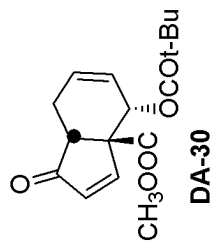
Current Data Parameters
 NAME MG-IV-136B-A3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050830
 Time 21.33
 INSTRUM DRX500
 PROBD 5 mm Multinucl
 PULPROG zg30pad
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 71.8
 DW 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.25 usec
 PL1 -3.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300087 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME MG-IV-136b-A3
 EXPNO 2
 PROCNO 1

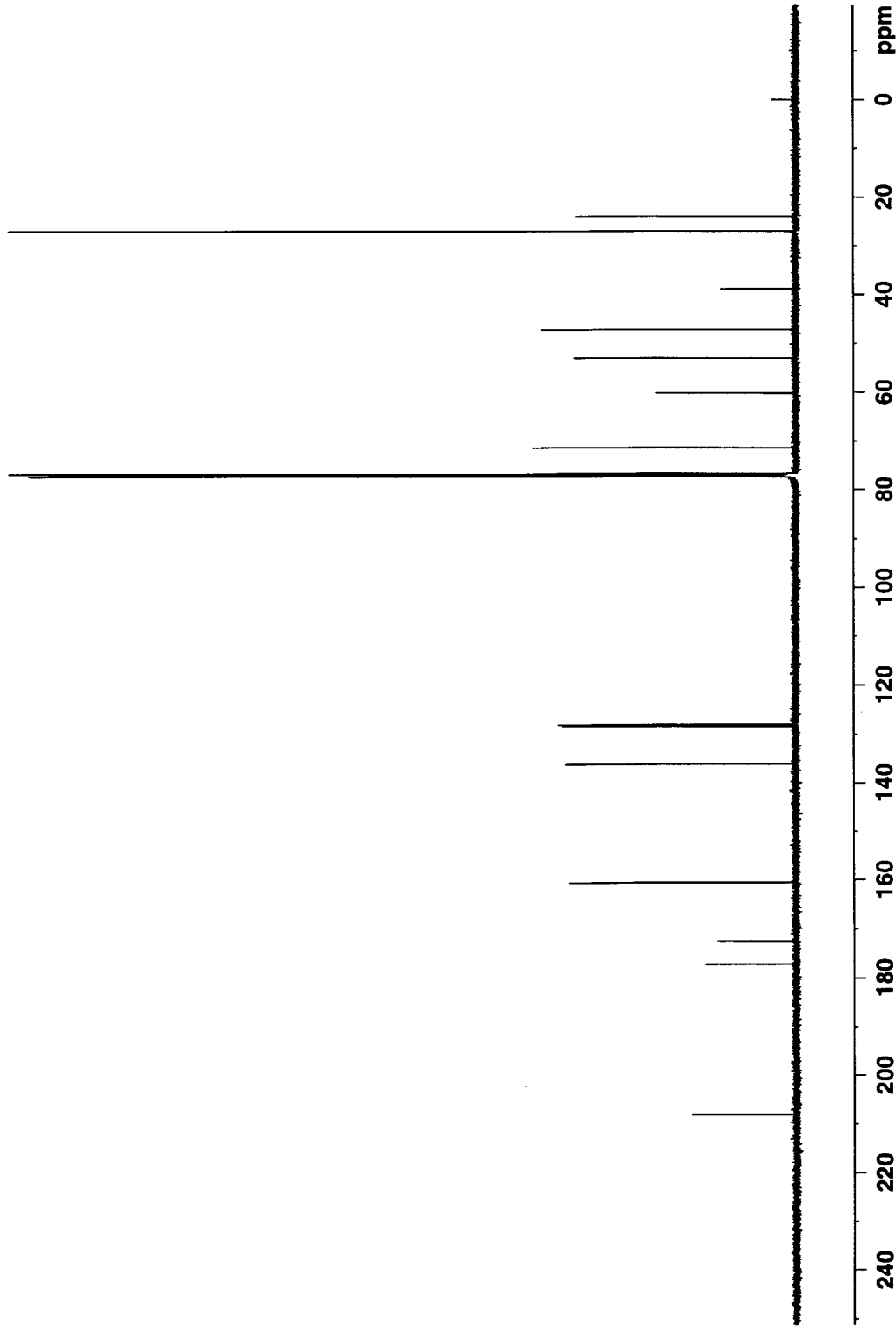
F2 - Acquisition Parameters
 Date_ 20050830
 Time 21.40

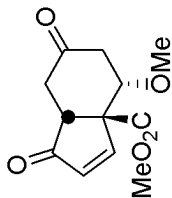
INSTRUM DRX500
 PROBHD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 831
 DS 4
 SWH 34013.605 Hz
 FIDRES 0.519006 Hz
 AQ 0.9634292 sec
 RG 32768
 DW 14.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.10 usec
 PL1 3.00 dB
 SFO1 125.7723786 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 88.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577938 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





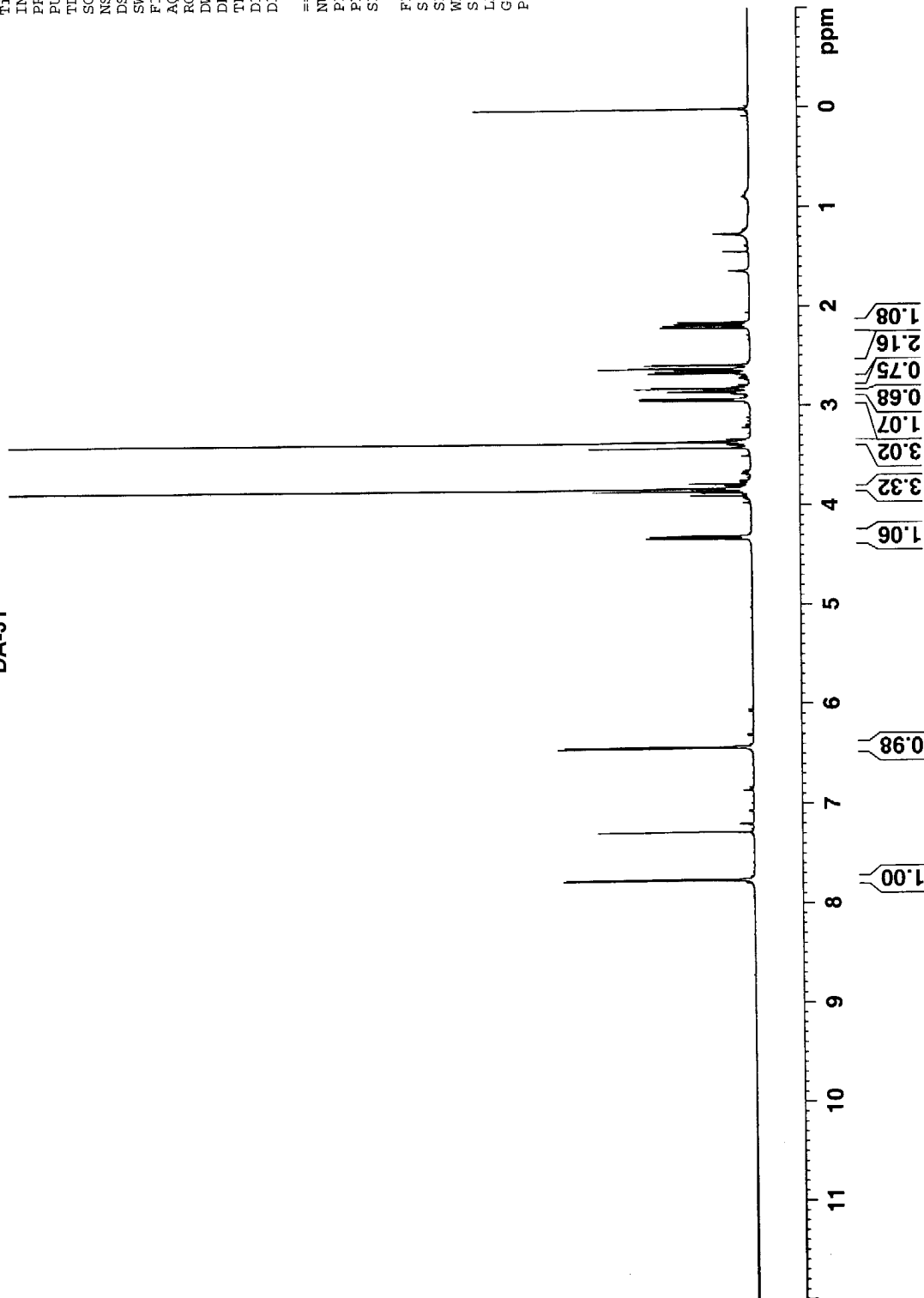
DA-31

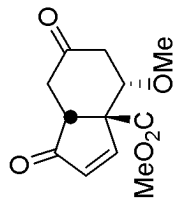
Current Data Parameters
 NAME MG-V-93b-A3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060227
 Time 14.51
 INSTRUM DRX500
 PROBD 5 mm Multinucl
 PULPROG zg30pad
 TD 65536
 SOLVENT CDCl3
 NS 6
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.50 usec
 PL1 0.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40





DA-31

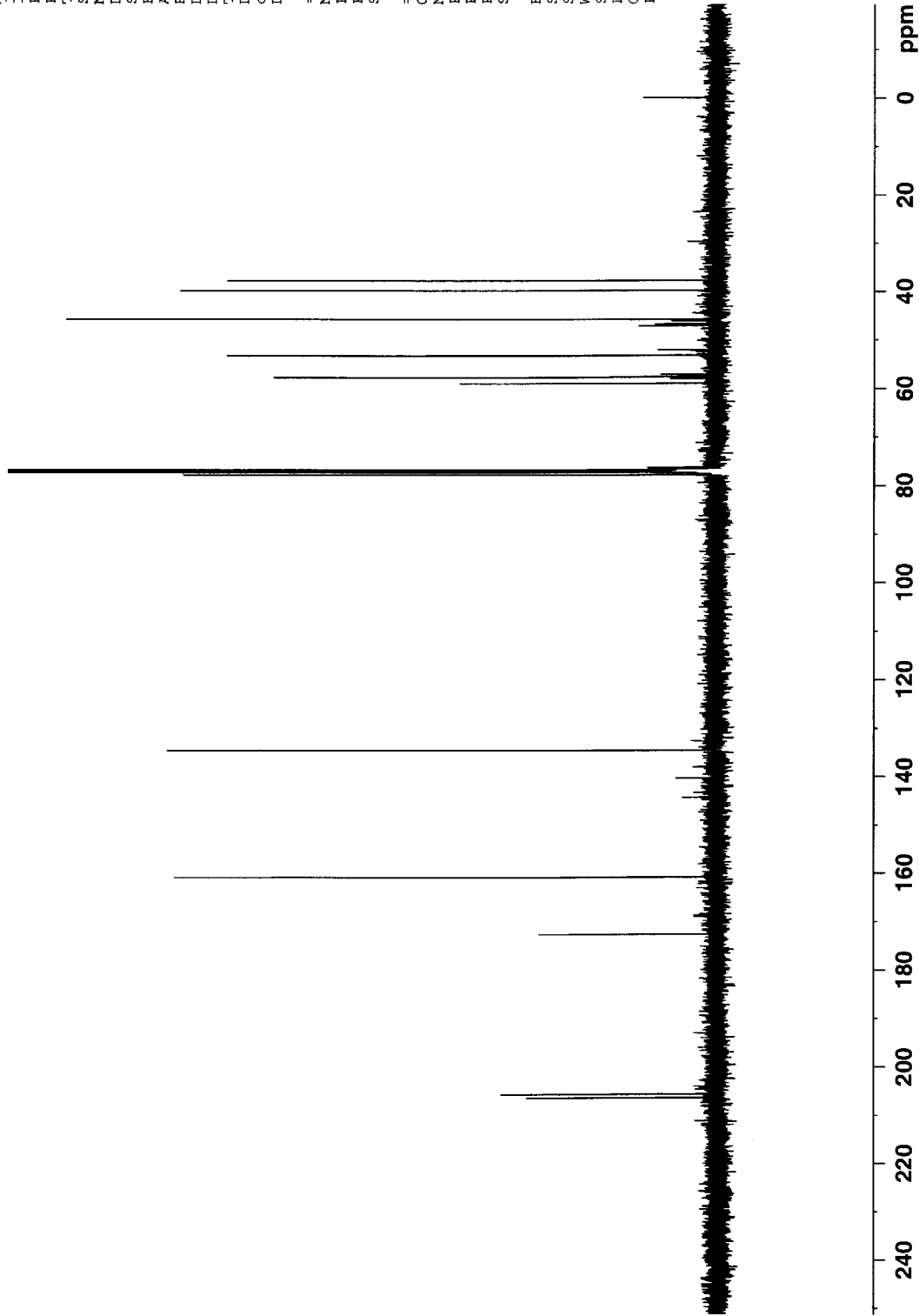
Current Data Parameters
 NAME MG-V-93b-A3
 EXPNO 2
 PROCNO 1

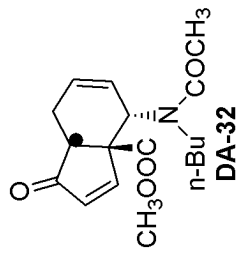
F2 - Acquisition Parameters
 Date_ 20060227
 Time 14.53
 INSTRUM DRX500
 PROBD 5 mm Multinucl
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 669
 DS 4
 SWH 34013.605 Hz
 FIDRES 0.519006 Hz
 AQ 0.9634292 sec
 RG 32768
 DW 14.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.10 usec
 PL1 3.00 dB
 SFO1 125.7723786 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 88.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577938 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



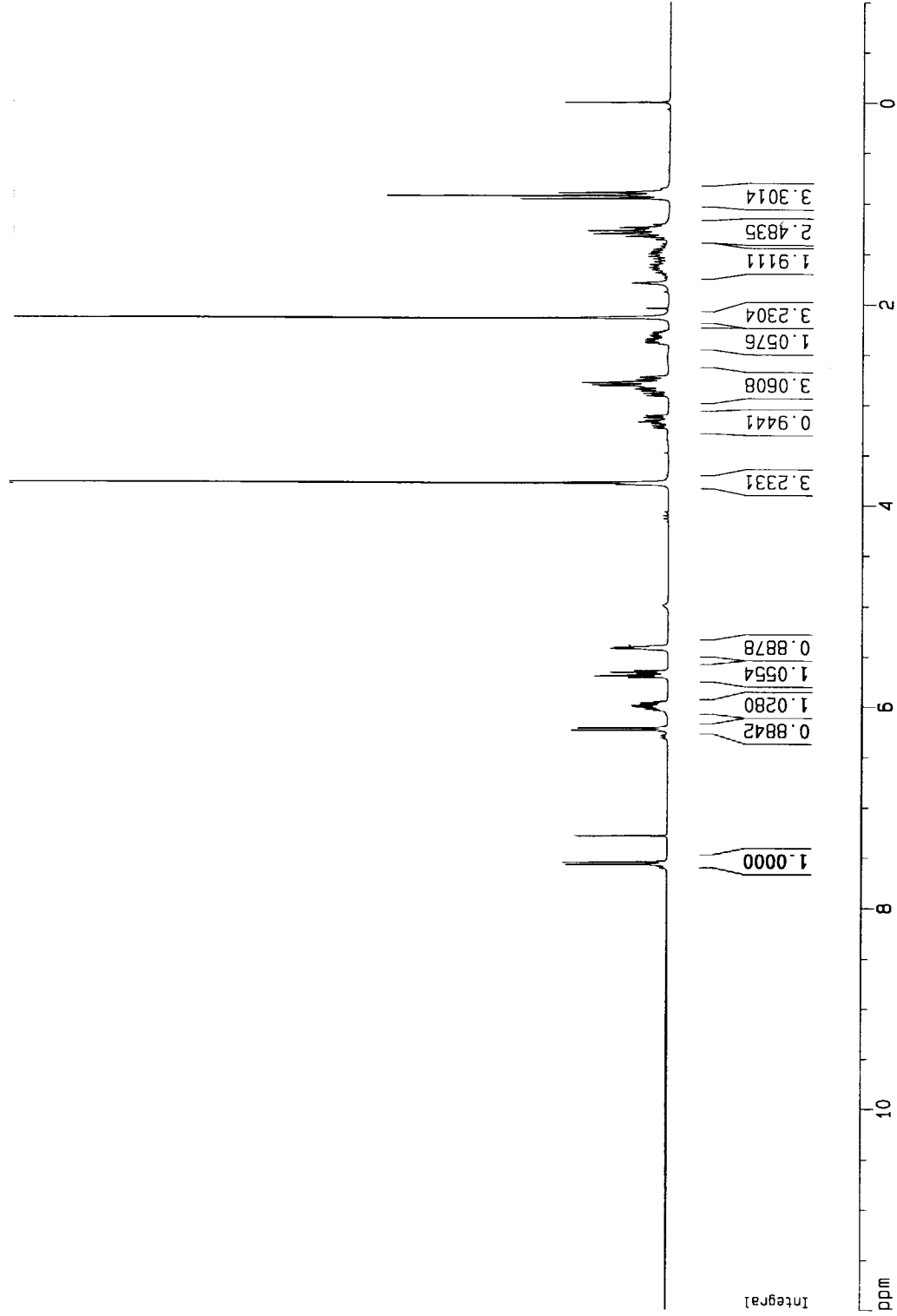


Current Data Parameters
 NAME MG-4-066b-250
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050530
 Time 23.03
 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 3.145779 sec
 RG 715
 DW 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

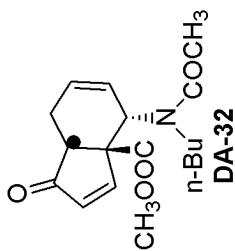
F2 - Processing parameters
 SI 16384
 SF 250.1300024 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -1.000 ppm
 F2 -250.13 Hz
 PPMCM 0.65000 ppm
 HZCM 162.58450 Hz/



Integral

ppm



Current Data Parameters
NAME MG-4-066b-250
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

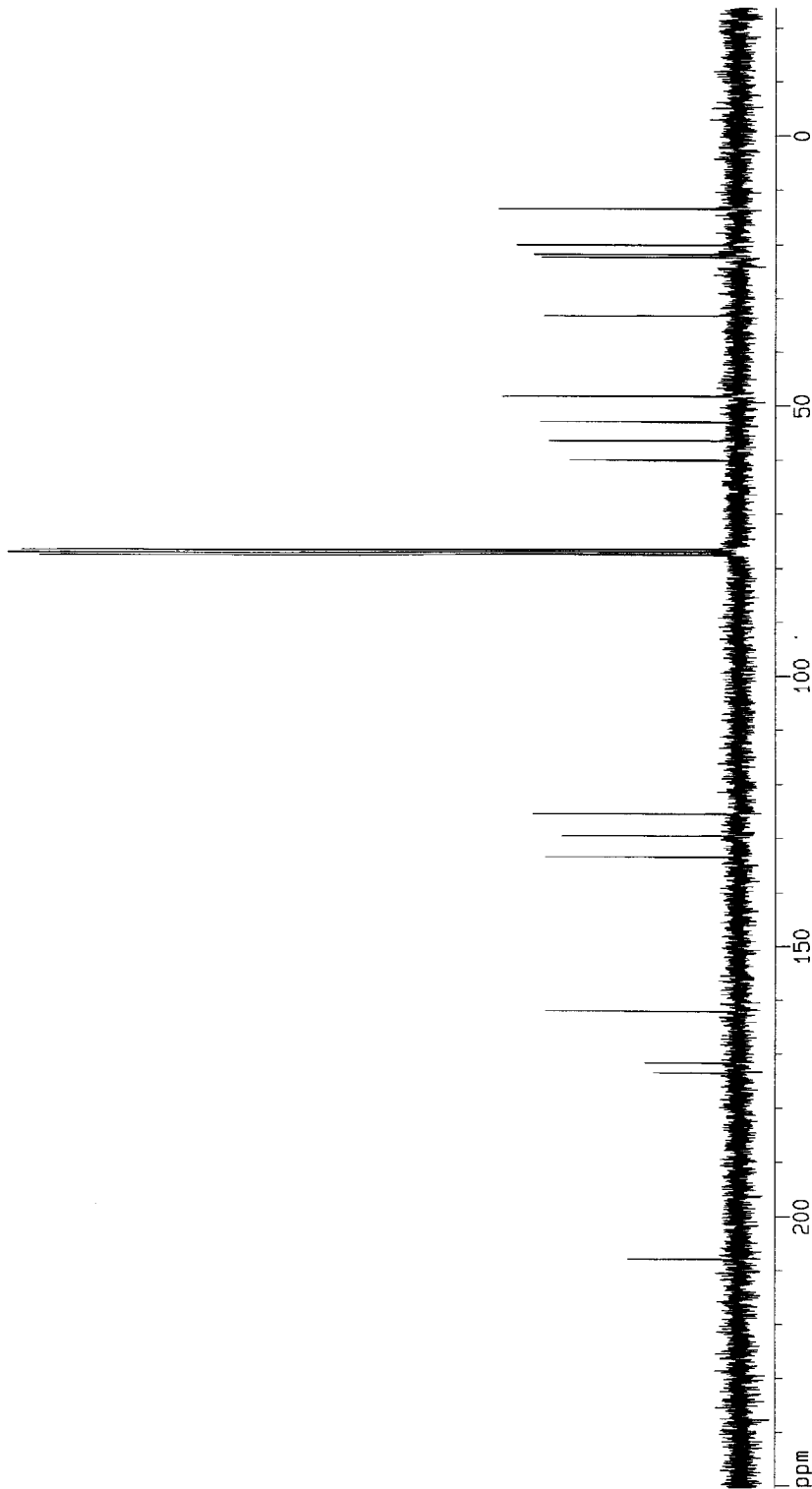
Date_ 20050530
Time 23.07
INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 36864
SOLVENT CDCl₃
NS 450
DS 4
SWH 17241.379 Hz
FIDRES 0.467702 Hz
AQ 1.0691060 sec
RG 22800
DW 29.000 use
DE 41.43 use
TE 300.0 K
D12 0.00002000 sec
DL5 23.00 dB
CPDPRG waltz16
P31 103.00 use
D1 2.00000000 sec
P1 6.00 use
SF01 62.9023694 MHz
NUCLEUS 13C
D11 0.03000000 sec

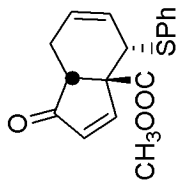
F2 - Processing parameters

SI 32768
SF 62.8952419 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 250.388 ppm
F1 45748.23 Hz
F2P -23.740 ppm
F2 -1493.15 Hz
PPMCM 13.70643 ppm
HZCM 862.06903 Hz/





DA-33

Current Data Parameters
 NAME MG-4-035a-300
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050429
 Time 14.42
 INSTRUM drx300
 PROBD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 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
 D1 1.00000000 sec
 D31 0.00000000 sec

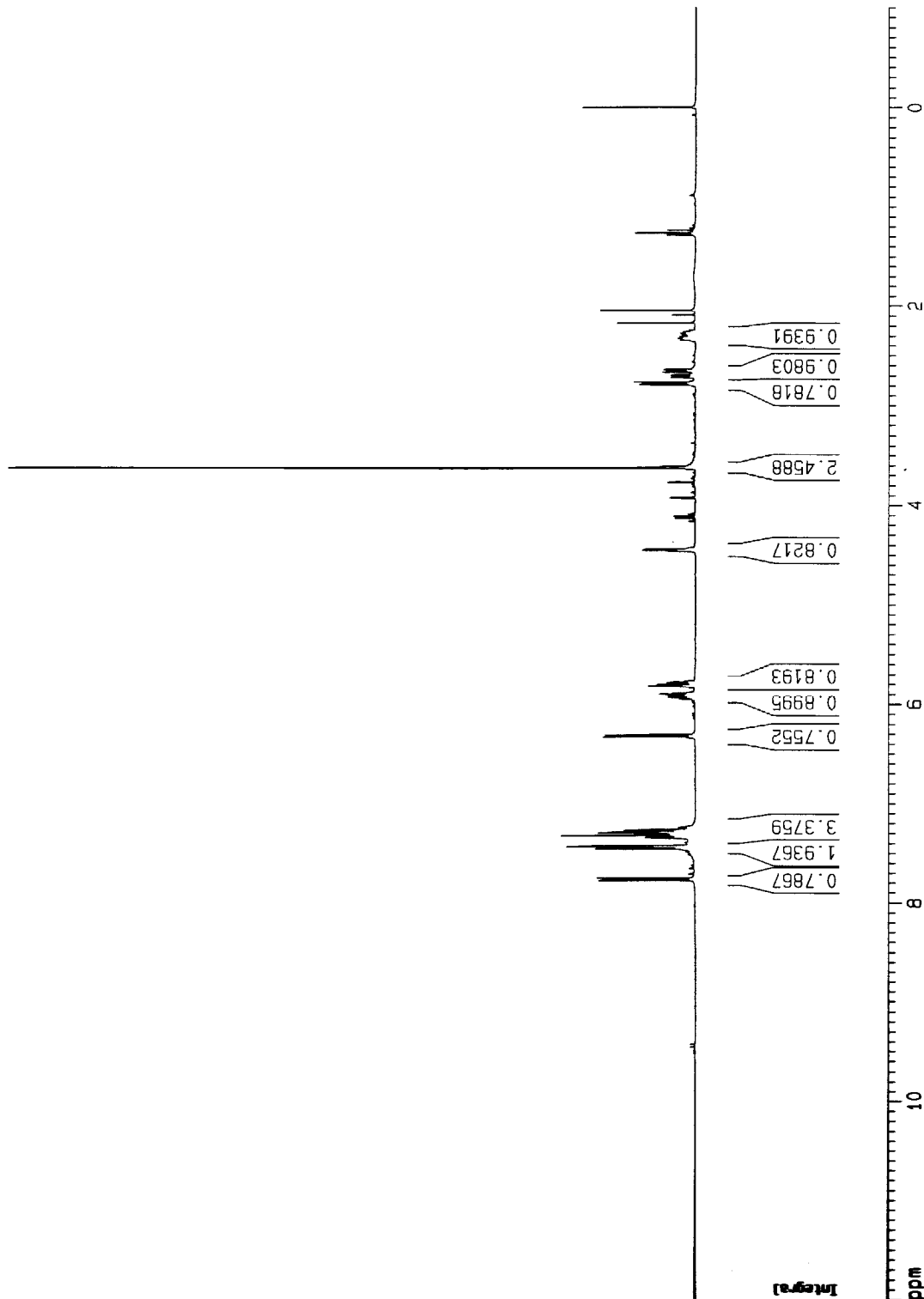
===== CHANNEL f1 =====

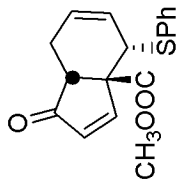
NUC1 ¹H
 P1 7.05 usec
 PL1 0.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300022 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.30

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 12.000 ppm
 F1 3601.56 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.65000 ppm/cm
 HZCM 195.08450 Hz/cm





DA-33

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Current Data Parameters
NAME      MG-4-35a-300
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20050422
Time      22.49
INSTRUM   drx300
PROBHD    5 mm Multinucl
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         321
DS         4
SWH        18832.393 Hz
FIDRES     0.287360 Hz
AQ         1.7400308 sec
RG         22528
DM         26.550 usec
DE         6.00 usec
TE         297.1 K
D1         1.79999995 sec
d11        0.03000000 sec
D31        0.00000000 sec

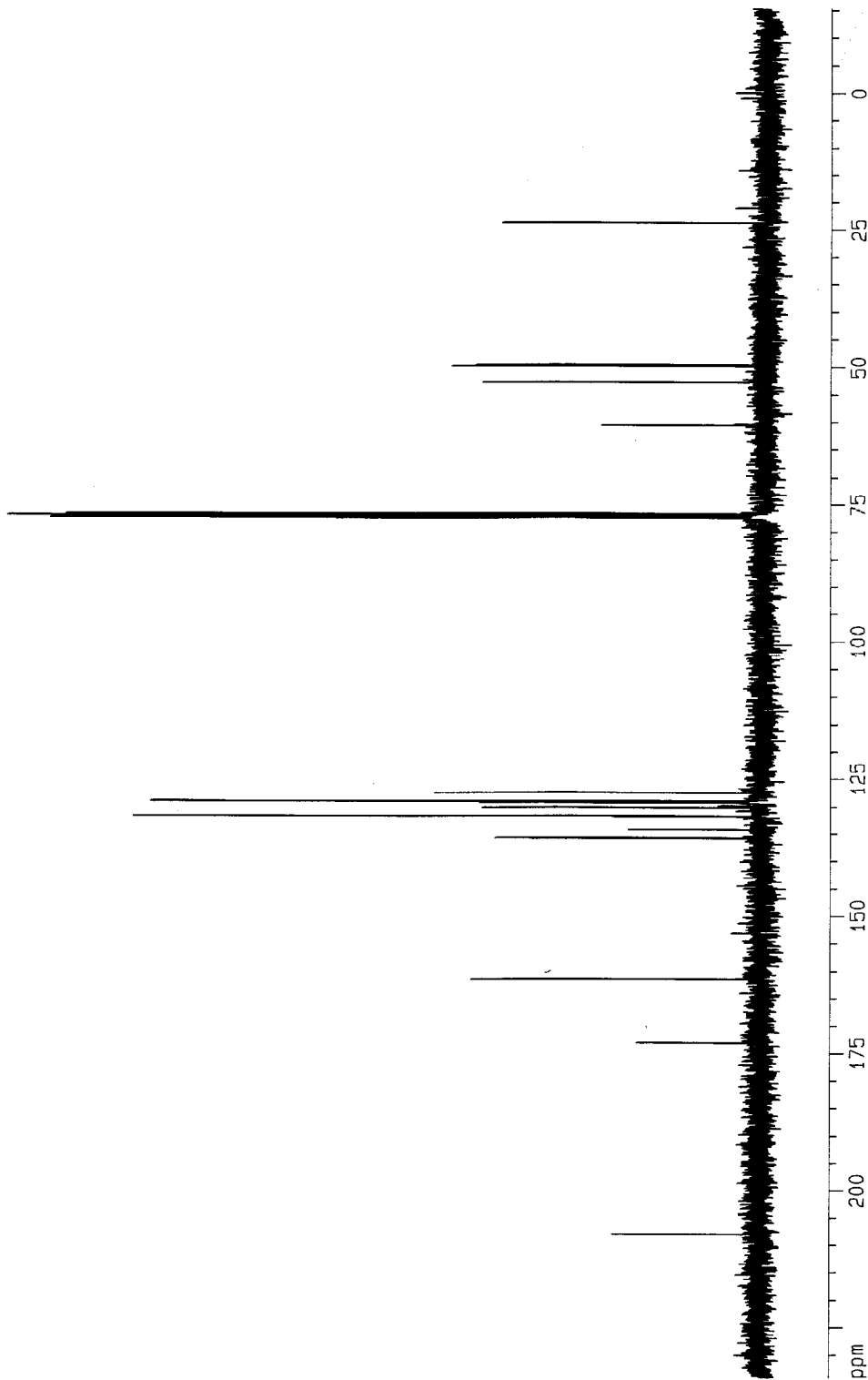
===== CHANNEL f1 =====
NUC1       13C
P1         8.50 usec
PL1        5.00 dB
SF01       75.4760107 MHz

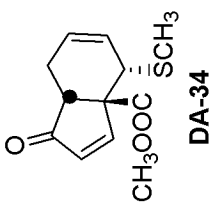
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      100.00 usec
PL2        120.00 dB
PL12       25.60 dB
SF02       300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4677508 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
CY         11.00 cm
F1P        234.220 ppm
F1         17676.09 Hz
F2P        -15.322 ppm
F2         -1156.30 Hz
PPMCM      12.47711 ppm/cm
HZCM       941.61957 Hz/cm

```



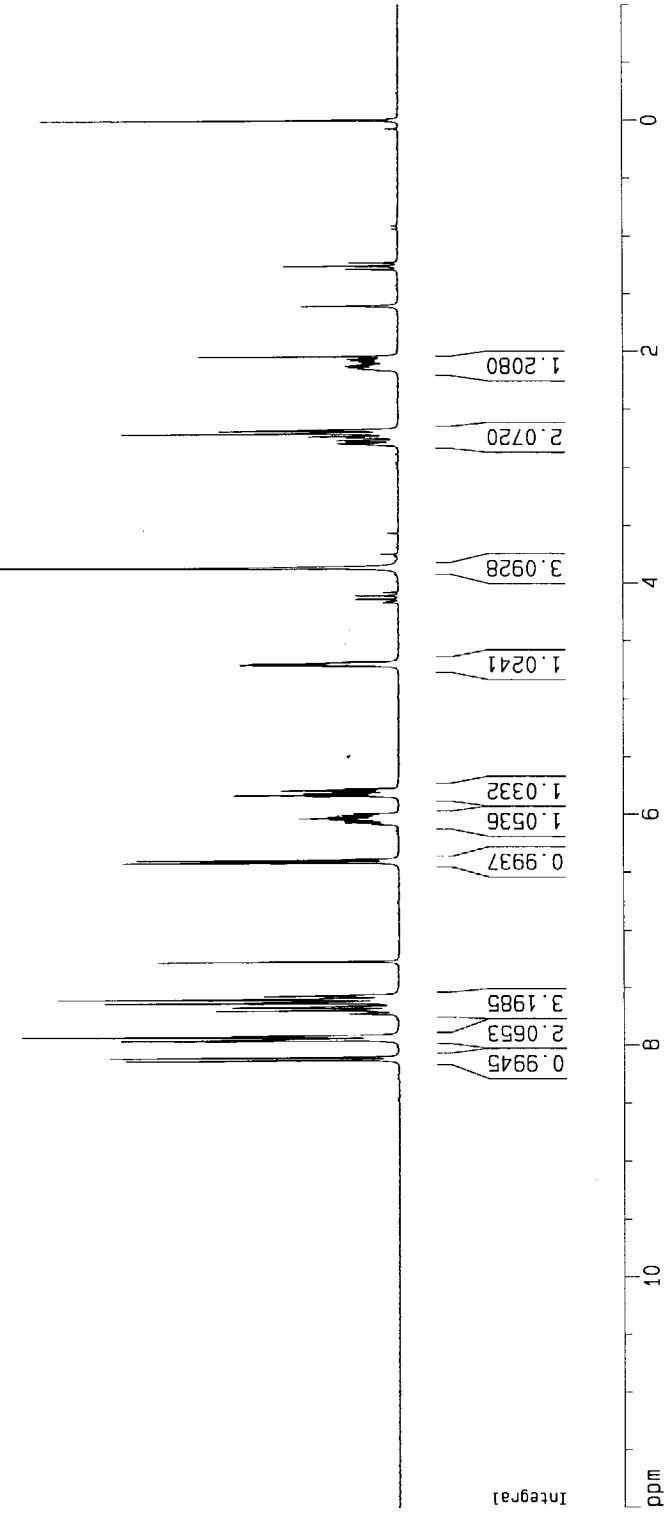


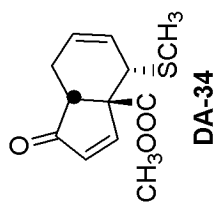
Current Data Parameters
 NAME MG-IV-046a-250
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050505
 Time 0.35
 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
 SF01 250.1315321 MHz
 NUCLEUS 1H

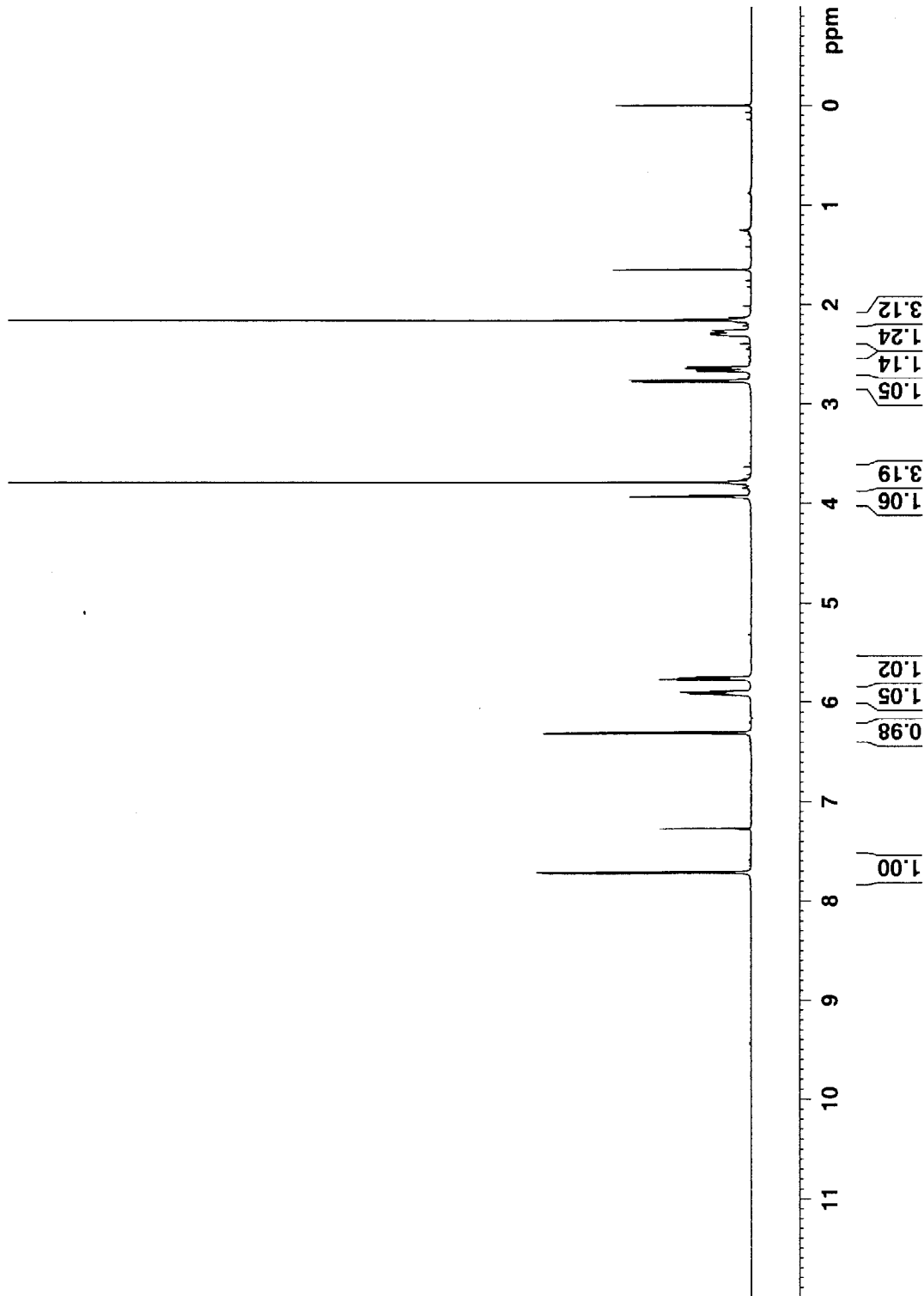
F2 - Processing parameters
 SI 16384
 SF 250.1300049 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 30.00 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -1.000 ppm
 F2 -250.13 Hz
 PPMCM 0.65000 ppm
 HZCM 162.58452 Hz/





Current Data Parameters
 NAME MG-V-83a-A3
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060210
 Time 14.09
 INSTRUM DRX500
 PROBD 5 mm Multinuc
 PULPROG zg30pad
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 114
 DW 48.400 use
 DE 6.00 use
 TE 300.0 K
 D1 1.00000000 sec
 D31 0.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 ¹H
 P1 11.50 use
 PL1 0.00 dB
 SFO1 500.1330885 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.1300068 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40



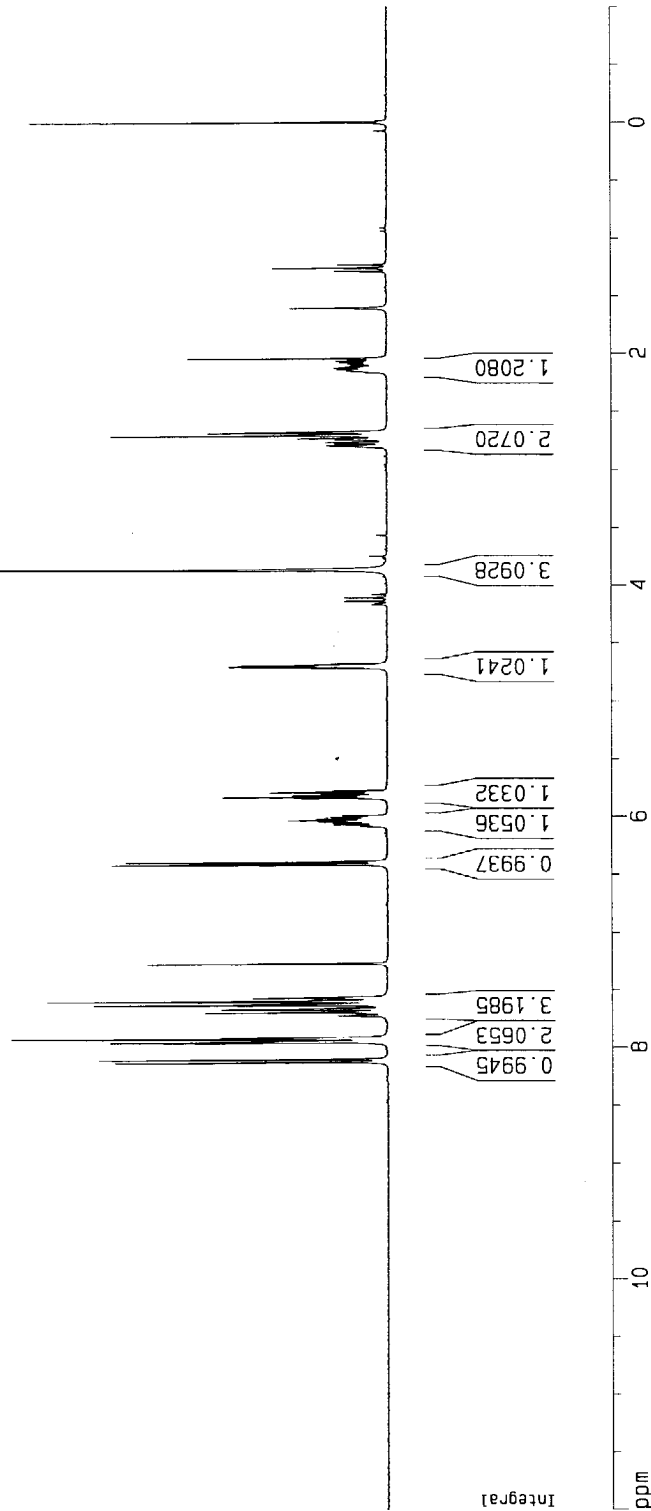
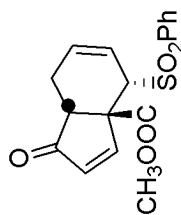
Current Data Parameters
 NAME MG-IV-046a-250
 EXPNO 1
 PROCNO 1

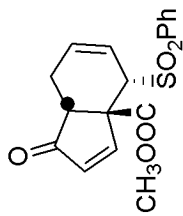
F2 - Acquisition Parameters

Date_ 20050505
 Time 0.35
 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
 SF01 250.1315321 MHz
 NUCLEUS 1H

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

1D NMR plot parameters
 CX 20.00 cm
 CY 30.00 cm
 F1P 12.000 ppm
 F1 3001.56 Hz
 F2P -1.000 ppm
 F2 -250.13 Hz
 PPMCM 0.65000 ppm
 HZCM 162.58452 Hz/





Current Data Parameters
 NAME MG-IV-046a-250
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050505
 Time 0.39
 INSTRUM arcx250
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDC13
 NS 209
 DS 4
 SWH 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
 CPDPRG waltz16
 P31 103.00 use
 D1 2.00000000 sec
 P1 6.00 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
 PPMCM 13.70643 ppm
 HZCM 862.06891 Hz/

