

Supporting Information

**The Intramolecular, Stereoselective Addition of
Sulfoximine Carbanions to α , β -Unsaturated Esters**

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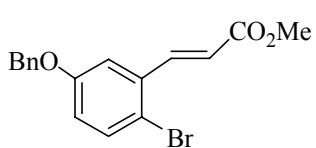
General information:

All reactions were carried out under an atmosphere of nitrogen in flame-dried glassware. THF was distilled over sodium-benzophenone before use. Toluene was distilled over CaH₂. 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 nm silica gel 60-F plates.

Melting points were measured with a Fisher-Johns melting point apparatus. Infrared spectra were recorded on a Perkin Elmer 1600 series FT-IR spectrometer. Optical rotations were measured on a Jasco DIP-370 digital polarimeter. ¹H NMR were recorded on a Bruker ARX-250 (250 MHz), DRX-300 (300 MHz), DRX-500 (500 MHz) spectrometer and are reported in ppm (δ) from tetramethylsilane (TMS: δ 0.0 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, ddd = doublet of doublet of doublet), coupling constants (Hz), and integration. ¹³C NMR spectra were recorded on a Bruker ARX-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 (CDCl₃: δ 77.0 ppm).

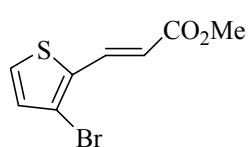
2-Bromo-3-methoxy-5-methylbenzaldehyde,¹ 3-bromothiophene-2-carbaldehyde,² 4-bromothiophene-3-carbaldehyde,³ 1-bromonaphthalene-2-carbaldehyde,⁴ 2-bromo-1-methyl-1H-indole-3-carbaldehyde,⁵ 3-bromofuran-2-carbaldehyde,⁶ 2-bromo-pyridine-3-carbaldehyde⁷ and cis-methyl o-bromocinnamate, trans-methyl o-bromocinnamate⁸ were synthesized by the literatures.

General procedure for synthesizing bromocinnamates (Procedure A):



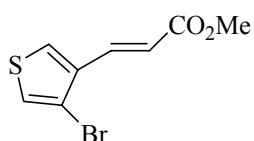
Procedure A: A mixture of the ylide Ph₃P=CHCOOMe (5.06 g, 15.1 mmol) and 5-Benzylxy-2-bromobenzaldehyde (4.0 g, 13.75 mmol) in CH₂Cl₂ (70 mL) was heated under reflux for 16 hr. After cooling, the reaction mixture was filtered. Removal of the solvent from the filtrate and crystallization from hexane and EtOAc afforded 3.36 g (70.5%) of a colorless solid, mp: 86-87 °C; IR: 3096, 3068, 2945, 1703, 1580, 1474, 1274, 1172 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.0 (d, J = 16.1 Hz, 1H), 7.48 (d, J = 8.8 Hz, 1H), 7.44-7.34 (m, 5H), 7.19 (d, J = 3.0 Hz, 1H), 6.87 (dd, J = 3.0, 8.8 Hz, 1H), 6.34 (d, J = 16.1 Hz, 1H), 5.05 (s, 2H), 3.82 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 166.6, 158.1, 143.1, 136.1, 135.0, 133.9, 128.6, 128.2, 127.4, 120.7, 118.3, 116.1, 113.7, 70.3, 51.8; Anal. Calcd for C₁₇H₁₅BrO₃: C, 58.81; H, 4.35. Found: C, 58.95; H, 4.50.

General procedure for synthesizing bromocinnamates (Procedure B):

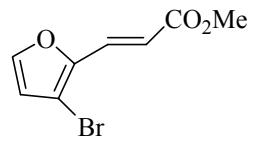


Procedure B: To 10 mL of THF in 50 mL round bottomed flask was added methyl diethylphosphonoacetate (424 μ L, 2.3 mmol). After stirring at 0 °C for 5min, 2.0 M n-butyllithium (1.15 mL, 2.3 mmol) was added dropwise. After 10 min, 3-bromothiophene-2-carbaldehyde (441 mg, 2.3 mmol) was added dropwise. The

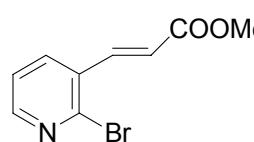
reaction mixture was warmed to room temperature, stirred for 4 hr, then quenched by ice water (10 mL). The mixture was extracted with toluene (3×10 mL), washed with water, dried over MgSO₄, filtered, and concentrated. The crude product was purified by flash chromatography (10-14% EtOAc/Hexanes) to afford a colorless solid 500 mg (88%); mp: 71-72 °C; IR: 3109, 2946, 1728, 1629, 1270, 1192; cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.82 (d, *J* = 15.8 Hz, 1H), 7.32 (d, *J* = 5.3 Hz, 1H), 7.00 (d, *J* = 5.3 Hz, 1H), 6.27 (d, *J* = 15.8 Hz, 1H), 3.79 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 166.6, 135.1, 134.0, 131.3, 127.7, 118.2, 115.9, 51.7; HRMS calcd for (C₈H₇BrO₂S)₂Na [M₂ + Na]⁺ 516.8572; Found 516.8596.



Procedure B: colorless solid, 88.2% yield; mp: 40-41 °C; IR: 3101, 2953, 1707, 1634, 1270, 1184 cm⁻¹; ¹H NMR (250 MHz, CDCl₃): δ 7.65 (d, *J* = 16.1 Hz, 1H), 7.58 (d, *J* = 3.3 Hz, 1H), 7.30 (d, *J* = 3.3 Hz, 1H), 6.44 (d, *J* = 16.1 Hz, 1H), 3.80 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 166.8, 136.2, 135.3, 125.1, 124.1, 119.3, 112.3, 51.6; HRMS calcd for C₈H₇BrO₂SNa [M + Na]⁺ 268.9242; Found 268.9250.



Procedure B: colorless solid; 87.3% yield; mp: 62-64 °C; IR: 3121, 2998, 2945, 1703, 1642, 1258 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.50-7.44 (m, 2H), 6.54-6.53 (m, 1H), 6.36 (d, *J* = 15.9 Hz, 1H), 3.79 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 166.6, 147.6, 144.4, 127.7, 116.7, 115.6, 105.3, 51.4; HRMS calcd for C₈H₇BrO₃Na [M + Na]⁺ 252.9471, found 252.9480.



Procedure B: colorless solid; mp: 97-98 °C; IR: 3072, 2990, 1715, 1634, 1188 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.36 (dd, *J* = 1.9, 4.6 Hz, 1H), 7.93 (d, *J* = 15.6 Hz, 1H), 7.89 (dd, *J* = 1.8, 7.7 Hz, 1H), 7.34 (dd, *J* = 4.7, 8.2 Hz, 1H), 6.43 (d, *J* = 16.0 Hz, 1H), 3.84 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 165.9, 150.6, 143.9, 140.9, 135.4, 131.7, 122.9, 122.4, 51.8; HRMS calcd for C₉H₈BrNO₂Na [M + Na]⁺ 263.9631; Found 263.9643.

General procedure for coupling reaction:

(*R,E*)-7: A 100 mL round bottomed flask equipped with a reflux condenser was charged with Pd(OAc)₂ (144.6 mg, 0.644 mmol), rac-BINAP (601.6 mg, 0.97 mmol), and toluene (60 mL). *E*-methyl o-bromocinnamate (3.1 g, 12.88 mmol) was added, followed by the R-sulfoxmine (2.4 g, 1.54 mmol), and cesium carbonate (5.88 g, 18.03 mmol). The reaction mixture was heated in an oil bath at 110 °C-115 °C for 44 hr. The solution was cooled and diluted with dichloromethane, filtered through a pad of Celite and concentrated in vacuo, to give a brown oil. Purification of the product by flash chromatography (66% Et₂O/Hexanes) afforded a pale yellow semisolid 3.69 g (91%); IR: 2947, 2927, 1710, 1623, 1589, 1475, 1444, 1315, 1269, 1186, 1167 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.38 (d, *J* = 16.2 Hz, 1H), 7.94-7.91 (m, 2H), 7.61-7.48 (m, 4H), 7.06-7.01 (m, 2H), 6.88-6.83 (m, 1H), 6.50 (d, *J* = 16.2 Hz, 1H), 3.82 (s, 3H), 3.29 (s, 3H); ¹³C NMR (75 Hz, CDCl₃): δ 168.0, 144.9, 142.5, 139.0, 133.3, 130.7, 129.5, 128.3, 128.0,

127.5, 122.4, 121.6, 116.8, 51.4, 46.2; Anal. Calcd for C₁₇H₁₇NO₃S: C, 64.74; H, 5.43; N, 4.44. Found: C, 64.90; H, 5.69; N, 4.51. [α]²⁵_D = 270.93 (c 1.08, CHCl₃).

(R,Z)-7: colorless liquid, 71% yield; IR: 3061, 3015, 1718, 1589 cm⁻¹; ¹H NMR (250 MHz, CDCl₃): δ 7.95-7.92 (m, 2H), 7.62-7.42 (m, 5H), 7.02-7.00 (m, 2H), 6.90-6.86 (m, 1H), 6.00 (d, J = 12.3 Hz, 1H), 3.67 (s, 3H), 3.20 (s, 3H); ¹³C NMR (62.5 Hz, CDCl₃): δ 167.1, 143.7, 142.4, 139.3, 133.2, 130.2, 129.7, 129.5, 128.4, 121.9, 121.14, 118.5, 51.1, 45.7; HRMS calcd for C₁₇H₁₇NO₃SNa [M + Na]⁺ 338.0821; Found 338.0806; [α]²⁵_D = 76.12 (c 1.13, CHCl₃).

(S, E)-8: yellow semi solid, 93.4% yield; IR: 3062, 3027, 2949, 2925, 1711, 1621, 1482, 1160; ¹H NMR (300 MHz, CDCl₃): δ 8.34 (d, J = 16.2 Hz, 1H), 7.94-7.91 (m, 2H), 7.59-7.50 (m, 3H), 7.40-7.30 (m, 5H), 7.10 (d, J = 3.0 Hz, 1H), 7.01 (d, J = 8.8, 1H), 6.74 (dd, J = 3.0, 8.8 Hz, 1H), 6.46 (d, J = 16.2 Hz, 1H), 4.96 (s, 2H), 3.82 (s, 3H), 3.26 (s, 3H); ¹³C NMR (75 Hz, CDCl₃): δ 168.0, 153.7, 142.4, 139.2, 138.6, 136.9, 133.3, 129.5, 128.9, 128.5, 128.4, 127.9, 127.4, 123.8, 118.1, 117.1, 112.8, 70.3, 51.6, 45.9; Anal. Calcd for C₂₄H₂₃NO₄S: C, 68.39, H, 5.50, N, 3.32. Found: C, 68.11; H, 5.65; N, 3.28; [α]²⁵_D = -178.06 (c 0.93, CHCl₃).

(S, E)-9: pale yellow viscous oil, 77.6% yield; IR: 3106, 3057, 3019, 2942, 1710, 1608, 1383;cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.41 (d, J = 15.7 Hz, 1H), 7.90-7.86 (m, 2H), 7.57-7.49 (m, 3H), 7.01 (d, J = 5.3 Hz, 1H), 6.67 (d, J = 5.3 Hz, 1H), 6.10 (d, J = 15.7 Hz, 1H), 3.74 (s, 3H), 3.23 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 167.9, 145.7, 139.1, 135.9, 133.4, 129.5, 128.1, 126.8, 123.8, 123.7, 112.3, 51.2, 45.8; HRMS calcd for C₁₅H₁₅NO₃S₂Na [M + Na]⁺ 344.0385; Found 344.0393; [α]²⁵_D = -517.81 (c 3.1, CHCl₃).

(R, E)-10: pale yellow oil; 82.7% yield; IR: 3096, 3060, 3019, 2917, 1703, 1625, 1437 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.88-7.85 (m, 2H), 7.78 (d, J = 16.1 Hz, 1H), 7.56-7.45 (m, 3H), 7.35 (d, J = 3.3 Hz, 1H), 6.68 (d, J = 16.1 Hz, 1H), 6.38 (d, J = 3.3 Hz, 1H), 3.76 (s, 3H), 3.22 (s, 3H); ¹³C-NMR (75 MHz, CDCl₃): δ 168.1, 142.1, 138.3, 137.5, 133.3, 132.5, 129.5, 128.4, 125.5, 116.5, 108.3, 51.4, 45.3; HRMS calcd for C₁₅H₁₅NO₃S₂Na [M + Na]⁺ 344.0385; Found 344.0440; [α]²⁵_D = 128.45 (c 3.81, CHCl₃).

(S, E)-11: pale yellow semi solid, 96% yield; IR: 3137, 3117, 3056, 3023, 2945, 2929, 1695, 1613, 1654, 1433, 1258; ¹H NMR (250 MHz, CDCl₃): δ 7.87-7.85 (m, 2H), 7.67 (d, J = 15.7 Hz, 1H), 7.58-7.46 (m, 3H), 7.11 (d, J= 1.9 Hz 1H), 6.11 (d, J = 15.7 Hz, 1H), 6.10 (d, J = 2.0 Hz, 1H), 3.72 (s, 3H), 3.23 (s, 3H); ¹³C NMR (62.5 MHz, CDCl₃): δ 168.2, 143.9, 141.4, 138.8, 135.1, 133.5, 129.5, 129.1, 128.1, 110.0, 108.9, 51.2, 45.6; HRMS calcd for C₁₅H₁₅NO₄SNa [M + Na]⁺ 328.0614; Found 328.0628; [α]²⁵_D = -515.71 (c 3.54, CHCl₃).

(S, E)-12: pale yellow oil, 86.4% yield; IR: 3060, 3015, 2941, 2929, 1716, 1421, 1315; ¹H NMR (250 MHz, CDCl₃): δ 8.09 (d, J = 16.2 Hz, 1H), 7.98-7.93 (m, 3H), 7.65 (dd, J = 1.7, 7.7 Hz 1H), 7.56-7.46 (m, 3H), 6.69 (dd, J= 4.8, 7.6 Hz, 1H), 6.56 (d, J = 16.2 Hz, 1H), 3.75 (s, 3H), 3.35 (s, 3H); ¹³C NMR (62.5 MHz, CDCl₃): δ 167.5, 157.6, 148.9,

141.3, 139.9, 135.9, 132.8, 129.2, 127.4, 121.2, 118.4, 116.1, 51.4, 45.4; HRMS calcd for $C_{16}H_{16}N_2O_3SNa$ [M + Na]⁺ 339.0774; Found 339.0762; $[\alpha]^{25}_D = -119.91$ (c 4.5, CHCl₃).

General procedure for the intramolecular conjugate addition (Procedure C):

(R, R)-13: To 5 mL THF in 50 mL round bottomed flask was added diisopropylamine (111 μ L, 0.79 mmol). After stirring at -20 °C for 5 min, 2.23 M n-butyllithium (354 μ L, 0.79 mmol) was added dropwise. After 30 min, the temperature was raised to 0 °C for 10 min, then LDA solution was added dropwise to **(R, E)-7** (130 mg, 0.395 mmol) in THF (5 mL) at -20 °C. The mixture was stirred for 1hr, quenched with water, diluted with ether (10mL), washed with brine, extracted with ether (3 \times 5 mL), washed with water (5 mL), dried over MgSO₄, filtered, and concentrated. The crude product was purified by flash chromatography (66% Et₂O/Hexanes) to afford a pale yellow semi solid 119 mg (92%): IR: 3061, 3024, 2951, 1738, 1599, 1477, 1446, 1111 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.09-8.05 (m, 2H), 7.70-7.55 (m, 3H), 7.27-7.24 (m, 1H), 7.15-7.12 (m, 2H), 6.95-6.90 (m, 1H), 3.91-3.83 (m, 1H), 3.64 (s, 3H), 3.57 (dd, J = 4.3, 12.7 Hz, 1H), 3.26 (dd, J = 11.3, 12.7 Hz, 1H), 2.99 (dd, J = 5.5, 16.2 Hz, 1H), 2.74 (dd, J = 8.2, 16.2 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃): δ 171.4, 144.9, 138.8, 133.8, 129.4, 128.8, 128.7, 125.2, 124.2, 124.1, 120.9, 51.9, 51.8, 36.4, 31.1; Anal. Calcd for C₁₇H₁₇NO₃S: C, 64.74; H, 5.43; N, 4.44. Found: C, 64.58; H, 5.64; N, 4.30; $[\alpha]^{25}_D = -16.24$ (c 1.17, CHCl₃).

(R, S)-13: Following previous procedure to afford a colorless liquid, 89% yield; IR: 2954, 1729, 1471, 1448 cm⁻¹; ¹H NMR (500 MHz, CDCl₃): δ 8.04-8.02 (m, 2H), 7.68-7.65 (m, 1H), 7.59-7.56 (m, 2H), 7.25-7.22 (m, 1H), 7.12-7.07 (m, 2H), 6.94-6.90 (m, 1H), 3.85-3.82 (m, 1H), 3.73 (dd, J = 4.2, 13.2 Hz, 1H), 3.71 (s, 3H), 3.28 (dd, J = 9.8, 17.2 Hz, 1H), 3.22 (dd, J = 5.6, 13.2 Hz, 1H), 2.86 (dd, J = 5.6, 17.2 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 173.1, 145.2, 140.0, 134.7, 130.2, 129.6, 129.6, 128.8, 124.9, 124.2, 121.8, 52.7, 51.8, 38.6, 34.4; HRMS calcd for C₁₇H₁₇NO₃SNa [M + Na]⁺ 338.0821; Found 338.0810; $[\alpha]^{25}_D = 50.67$ (c 1.05, CHCl₃).

(S, S)-14: **(S, E)-8** in THF was added 2.0 equiv. LDA at -78 °C, stirred for 30 min and then quenched following previous procedure to afford a pale yellow semi solid, yield 90.7%; IR: 3064, 3035, 2953, 2921, 1723, 1478, 1282, 1217 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.08-8.05 (m, 2H), 7.69-7.55 (m, 3H), 7.45-7.32 (m, 5H), 7.07 (d, J = 8.7 Hz, 1H), 6.89 (dd, J = 2.8, 8.7 Hz, 1H), 6.80 (d, J = 2.9 Hz, 1H), 3.86-3.80 (m, 1H), 3.62 (s, 3H), 3.57 (dd, J = 4.4, 12.8 Hz, 1H), 3.28 (dd, J = 10.3, 12.8 Hz, 1H), 2.94 (dd, J = 5.4, 16.2 Hz, 1H), 2.72 (dd, J = 8.4, 16.2 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃): δ 171.4, 153.3, 139.0, 138.5, 137.2, 133.8, 129.4, 128.9, 128.5, 127.9, 127.5, 125.2, 124.7, 114.8, 112.9, 70.6, 52.0, 51.9, 36.5, 31.6; Anal. Calcd for C₂₄H₂₃NO₄S: C, 68.39; H, 5.50; N, 3.32. Found: C, 68.50; H, 5.67; N, 3.38. $[\alpha]^{25}_D = -24.96$ (c 2.46, CHCl₃).

General procedure for the intramolecular conjugate addition (Procedure D):

(S, R)-15: To 5 mL THF in 25 mL round bottomed flask was added **(S, E)-9** (250 mg, 0.78 mmol) at -78 °C. After stirring 5min, 1.0 M LiHMDS (1.56 mL, 1.56 mmol) was added dropwise. After stirring for 30 min, the reaction mixture was quenched with

CH_3OH , washed with brine, extracted with CHCl_3 (3×10 mL), washed with water, dried over MgSO_4 , filtered, and concentrated. The crude product was purified by flash chromatography (66% $\text{Et}_2\text{O}/\text{Hexanes}$) to afford a pale yellow semi solid, 91.3% yield; IR: 3068, 2941, 1732, 1523, 1384, 1241 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.10-8.09 (m, 2H), 7.73-7.67 (m, 1H), 7.63-7.56 (m, 2H), 7.12 (dd, $J = 1.1, 5.2$ Hz, 1H), 6.84 (d, $J = 5.2$ Hz, 1H), 4.09 -3.99 (m, 1H), 3.71 (s, 3H), 3.66 (dd, $J = 4.9, 11.5$ Hz, 1H), 3.05 (dd, $J = 4.6, 16.2$ Hz, 1H), 2.78 (dd, $J = 11.5, 13.4$ Hz, 1H), 2.66 (dd, $J = 9.6, 16.2$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3): δ 170.7, 143.1, 136.4, 134.3, 129.4, 129.3, 125.5, 121.8, 113.3, 52.0, 50.8, 39.1, 29.2; HRMS calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_3\text{S}_2\text{Na} [\text{M} + \text{Na}]^+$ 344.0385; Found 344.0381; $[\alpha]^{25}_D = -12.14$ (c 1.68, CHCl_3).

(*R, R*)-**16**: Following previous procedure to afford a colorless solid, 93% yield; mp: 136-138°C; IR: 3105, 3060, 2998, 2949 1732, 1446, 1237 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.10-8.06 (m, 2H), 7.71-7.66 (m, 1H), 7.61-7.56 (m, 2H), 6.99 (dd, $J = 1.6, 3.3$ Hz, 1H), 6.62 (d, $J = 3.3$ Hz, 1H), 4.01- 3.94 (m, 1H), 3.69 (s, 3H), 3.55 (dd, $J = 4.3, 11.8$ Hz, 1H), 3.07 (dd, $J = 5.0, 16.0$ Hz, 1H), 2.90 (dd, $J = 11.8, 13.4$ Hz, 1H), 2.72 (dd, $J = 8.3, 16.0$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3): δ 171.1, 142.7, 137.4, 134.0, 129.3, 129.1, 127.1, 118.5, 107.8, 51.9, 51.0, 37.4, 29.5; HRMS calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_3\text{S}_2\text{Na} [\text{M} + \text{Na}]^+$ 344.0385; Found 344.0406; $[\alpha]^{25}_D = 40.52$ (c 2.68, CHCl_3).

(*S, S*)-**17**: To 17 mL THF in 50 mL round bottomed flask was added 1.0 M LiHMDS (531 μL , 0.53 mmol) at -50 °C for 5 min. (*S, E*)-**11** (81 mg, 0.26 mmol) in THF (10 mL) was added dropwise over 1 hr. After stirring for 4hr, the reaction was quenched with CH_3OH , washed with brine, extracted with CHCl_3 (3×10 mL), washed with water, dried over MgSO_4 , filtered, and concentrated. The crude product was purified by flash chromatography (66% $\text{Et}_2\text{O}/\text{Hexanes}$) to afford a pale yellow liquid 66 mg (84.7%); IR: 2949, 2929, 2851, 1736, 1433, 1213 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3): δ 8.13-8.11 (m, 2H), 7.73-7.70 (m, 1H), 7.62-7.59 (m, 2H), 7.24-7.23 (m, 1H), 6.34 (d, $J = 2.0$ Hz, 1H), 4.04-4.02 (m, 1H), 3.71 (s, 3H), 3.66 (dd, $J = 5.7, 11.5$ Hz, 1H), 3.21 (dd, $J = 4.6, 16.5$ Hz, 1H), 2.84 (dd, $J = 11.5, 12.7$ Hz, 1H), 2.56 (dd, $J = 9.6, 16.5$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 171.2, 140.9, 136.0, 134.4, 132.4, 129.7, 129.4, 129.3, 108.8, 52.6, 52.0, 35.6, 29.0. HRMS calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_4\text{SNa} [\text{M} + \text{Na}]^+$ 328.0614; Found 328.0619; $[\alpha]^{25}_D = 28.97$ (c 2.23, CHCl_3).

(*S, S*)-**18**: To 19 mL THF (degassing by N_2) in 50 mL round bottomed flask was added 1.0 M LiHMDS (876 μL , 0.88 mmol) at -30°C for 5min. (*S, E*)-**12** (91.7 mg, 0.29 mmol) in THF (10 mL) was added dropwise over 1hr. After stirring for 3hr, the mixture was quenched with CH_3OH , washed with brine, extracted with CHCl_3 (3×15 mL). The combined CHCl_3 extracts were washed with water, dried over MgSO_4 , filtered, and concentrated. The crude product was purified by flash chromatography (EtOAc) to afford a colorless liquid 76.5% yield; IR: 3060, 2949, 2921, 1728, 1417, 1286 cm^{-1} ; ^1H NMR (500 MHz, CDCl_3): δ 8.32-8.30 (m, 1H); 8.15-8.13 (m, 2H), 7.71-7.68 (m, 1H), 7.62-7.58 (m, 2H), 7.46-7.44 (m, 1H), 6.88 (dd, $J = 4.9, 7.6$ Hz, 1H), 3.97-3.93 (m, 1H), 3.68 (s, 3H), 3.60 (dd, $J = 4.8, 12.5$ Hz, 1H), 3.15 (t, $J = 12.6$ Hz, 1H), 3.03 (dd, $J = 5.3, 16.3$ Hz, 1H), 2.81 (dd, $J = 7.7, 16.3$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 171.1, 156.4, 148.5,

137.5, 134.2, 133.4, 129.4, 129.0, 119.2, 116.6, 52.0, 51..0, 35.8, 30.3; HRMS calcd for $C_{16}H_{16}N_2O_3SNa$ [M + Na]⁺ 339.0774; Found 339.0776; $[\alpha]^{25}_D = 28.65$ (c 1.85, CHCl₃).

19 (Procedure A): colorless solid, 60% yield; mp: 91-92 °C; IR: 3084, 3051, 2949, 2917, 1703, 1625, 1572, 1433, 1278, 1176 cm⁻¹; ¹H NMR (500 MHz, CDCl₃): δ 8.09 (d, *J* = 15.9 Hz, 1H), 7.02 (s, 1H), 6.72 (s, 1H), 6.36 (d, *J* = 15.9 Hz, 1H), 3.89 (s, 3H), 3.81 (s, 3H), 2.34 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 166.9, 156.1, 143.6, 138.2, 135.5, 120.7, 120.3, 113.9, 111.7, 56.4, 51.8, 21.4; Anal. Calcd for C₁₂H₁₃BrO₃: C, 50.55; H, 4.60. Found: C, 50.70; H, 4.74.

(R, E)-20: pale yellow semi solid, yield 53%; IR: 3060, 3015, 2945, 1719, 1621, 1466, 1303 cm⁻¹; H NMR (500 MHz, CDCl₃): δ 8.41 (d, *J* = 16.2 Hz, 1H), 7.95 (d, *J* = 7.2 Hz, 2H), 7.57-7.46 (m, 3H), 6.98 (s, 1H), 6.57 (s, 1H), 6.42 (d, *J* = 16.2 Hz, 1H), 3.75 (s, 3H), 3.44 (s, 3H), 3.14 (s, 3H), 2.23 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 167.3, 151.7, 142.6, 142.1, 131.9, 131.3, 130.7, 129.4, 128.5, 126.6, 119.1, 116.4, 113.8, 54.7, 50.9, 46.0, 20.6; Anal. Calcd for C₁₉H₂₁NO₄S: C, 63.49; H, 5.89; N, 3.90. Found: C, 63.69; H, 5.81; N, 3.77; $[\alpha]^{25}_D = 91.56$ (c 1.35, CHCl₃).

(R, R)-21: pale colorless solid, yield 36%; mp: 117-119 °C; IR: 3056, 2990, 2945, 1732, 1564, 1462, 1247 cm⁻¹; ¹H NMR (500 MHz, CDCl₃): δ 8.10-8.08 (m, 2H), 7.65-7.62 (m, 1H), 7.57-7.54 (m, 2H), 6.71 (s, 1H), 6.57 (s, 1H), 3.80-3.75 (m, 1H), 3.60 (s, 3H), 3.54 (dd, *J* = 4.5, 13.2 Hz, 1H), 3.34 (dd, *J* = 9.7, 13.2 Hz, 1H), 2.92 (dd, *J* = 5.6, 16.3 Hz, 1H), 2.72 (dd, *J* = 8.6, 16.3 Hz, 1H), 2.31 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 171.5, 152.3, 139.3, 133.5, 131.5, 130.3, 129.2, 128.9, 125.2, 118.0, 111.7, 55.9, 52.5, 51.7, 36.5, 31.8, 21.3; Anal. Calcd for C₁₉H₂₁NO₄S: C, 63.49; H, 5.89; N, 3.90. Found: C, 63.66; H, 5.81; N, 3.87; $[\alpha]^{25}_D = -15.96$ (c 1.09, CHCl₃).

22 (Procedure B): colorless solid, yield 81.6%; mp: 94-96 °C; IR: 3056, 2990, 2949, 1719, 1274, 1237; ¹H NMR (500 MHz, CDCl₃): 8.39-8.36 (m, 2H), 7.79-7.76 (m, 1H), 7.64-7.55 (m, 3H), 6.48 (d, *J* = 15.9 Hz, 1H), 3.58 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): 167.7, 144.9, 135.7, 133.3, 132.8, 129.0, 128.9, 128.9, 128.8, 128.5, 127.6, 124.6, 121.9, 52.7; HRMS calcd for C₁₄H₁₁BrO₂Na [M + Na]⁺ 312.9835; Found 312.9852.

(S, S)-23: A 100 mL round bottomed flask equipped with a reflux condenser was charged with Pd(OAc)₂ (26.6 mg, 0.12 mmol), rac-BINAP (111 mg, 0.18 mmol), and 25 mL toluene. *E*-3-(1-Bromo-naphthalen-2-yl)-acrylic acid methyl ester (690 mg, 2.37 mmol) was added, followed by the S-sulfoximine(441 mg, 2.84 mmol), and cesium carbonate(1.08 g, 3.32 mmol). The reaction mixture was heated in an oil bath at 110°C-115 °C for 44 hr. The solution was cooled and diluted with dichloromethane, filtered through a pad of Celite and concentrated in vacuo, to give a brown oil. Purification of the product by flash chromatography (75% Et₂O/Hexanes) afforded a colorless solid 521.7 mg (60.5%); Mp: 53-55°C; IR: 3056, 2950, 2251, 1733, 1372, 1262 cm⁻¹; ¹H NMR (250 MHz, CDCl₃): δ 8.66-8.62 (m, 1H), 8.14-8.10 (m, 2H), 7.78-7.41 (m, 7H), 7.27-7.24 (m, 1H), 4.04-3.93 (m, 1H), 3.65 (dd, *J* = 4.6, 12.8 Hz, 1H), 3.63 (s, 3H), 3.35 (dd, *J* = 10.6, 12.8 Hz, 1H), 3.03 (dd, *J* = 5.4, 16.2 Hz, 1H), 2.78 (dd, *J* = 8.4, 16.2 Hz, 1H); ¹³C NMR (62.5 MHz, CDCl₃): δ 171.6, 141.4, 139.3, 133.8, 133.7, 129.4, 129.2, 128.8, 127.2,

126.2, 125.3, 124.3, 123.3, 120.3, 117.8, 51.9, 51.8, 36.7, 31.7; HRMS calcd for $C_{21}H_{19}NO_3SNa$ [M + Na]⁺ 388.0978; Found 388.0985; $[\alpha]^{25}_D = 155.05$ (c 1.05, CHCl₃).

24 (Procedure B): colorless solid, yield 95%; mp: 100-102 °C; IR: 3076, 3002, 2949, 2868, 2835, 1715, 1621, 1172 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.79 (d, *J* = 16.1 Hz, 1H), 7.74-7.71 (m, 1H), 7.12-7.19 (m, 3H), 6.46 (d, *J* = 16.1 Hz, 1H), 3.80 (s, 3H), 3.57 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 168.1, 137.3, 137.0, 124.9, 122.8, 121.5, 121.1, 119.3, 113.5, 110.9, 109.7, 51.2, 31.6; HRMS calcd for $C_{13}H_{12}BrNO_2Na$ [M + Na]⁺ 315.99434; Found 315.9960.

(*S, S*)-**25:** pale yellow liquid, yield 81.5%; IR: 3056, 2945, 2921, 2246, 1732, 1466, 1225 cm⁻¹; ¹H NMR (250 MHz, CDCl₃): δ 8.08-8.05 (m, 2H), 7.73-7.56 (m, 3H), 7.39-7.35 (m, 1H), 7.22-7.19 (m, 1H), 7.08-7.00 (m, 2H), 4.13-4.05 (m, 1H), 3.72-3.64 (m, 1H), 3.68 (s, 3H), 3.65 (s, 3H), 3.41 (dd, *J* = 3.8, 16.2 Hz, 1H), 3.13 (dd, *J* = 10.4, 12.2 Hz, 1H), 2.40 (dd, *J* = 10.6, 16.2 Hz, 1H); ¹³C NMR (62.5 MHz, CDCl₃): δ 171.9, 142.9, 137.1, 134.4, 133.8, 129.5, 128.9, 125.6, 119.3, 118.5, 116.6, 108.4, 87.1, 52.5, 51.7, 37.7, 28.4, 27.6; HRMS calcd for $C_{20}H_{20}N_2O_3SNa$ [M + Na]⁺ 391.10867; Found 391.1089; $[\alpha]^{25}_D = -89.14$ (c 1.16, CHCl₃).

26 (Procedure B): colorless solid, yield 82%; mp: 162-164 °C; IR: 3080, 3003, 2949, 1695, 1617, 1486, 1254 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.98 (d, *J* = 15.9 Hz, 1H), 7.06 (s, 1H), 7.04 (s, 1H), 6.23 (d, *J* = 15.9 Hz, 1H), 6.02 (s, 2H), 3.81 (s, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 167.0, 150.0, 147.9, 142.9, 127.6, 118.5, 117.8, 113.1, 106.4, 102.2, 51.7; HRMS calcd for $C_{11}H_9BrO_4Na$ [M + Na]⁺ 306.9576; Found 306.9580.

(*R, E*)-**27:** pale yellow semi solid, 60% yield; IR: 3060, 3019, 2945, 2896, 1703, 1613, 1474, 1301, 1221; ¹H NMR (500 MHz, CDCl₃): δ 8.36 (d, *J* = 16.1 Hz, 1H), 7.93-7.91 (m, 2H), 7.60-7.51 (m, 3H), 6.95 (s, 1H), 6.66 (s, 1H), 6.25 (d, *J* = 16.1 Hz, 1H), 5.83 (dd, *J* = 1.2, 16.4 Hz, 2H), 3.80 (s, 3H), 3.27 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 168.3, 149.9, 143.0, 142.0, 140.7, 139.0, 133.4, 129.6, 128.3, 121.3, 114.0, 105.4, 103.8, 101.2, 51.4, 46.0; HRMS calcd for $C_{18}H_{17}NO_5SNa$ [M + Na]⁺ 382.0720, found 382.0719; $[\alpha]^{25}_D = 257.02$ (c 2.08, CHCl₃).

(*R, R*)-**28:** pale yellow solid, yield 87.8%; mp: 137-139 °C; IR: 3060, 2998, 2945, 2888, 1732, 1482, 1241 cm⁻¹; ¹H NMR (500 MHz, CDCl₃): δ 8.06-8.05 (m, 2H), 6.68-6.64 (m, 1H), 6.79-6.75 (m, 2H), 6.68 (s, 1H), 6.63 (s, 1H), 5.90 (dd, *J* = 1.3, 6.5 Hz, 2H), 3.70-3.76 (m, 1H), 3.62 (s, 3H), 3.53 (dd, *J* = 4.5, 13.0 Hz, 1H), 3.31 (dd, *J* = 10.1, 13.0 Hz, 1H), 2.87 (dd, *J* = 5.7, 16.3 Hz, 1H), 2.70 (dd, *J* = 8.1, 16.3 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 171.4, 147.5, 142.0, 139.5, 138.9, 133.7, 129.3, 128.7, 116.5, 105.5, 105.4, 100.8, 52.4, 51.8, 36.7, 31.5; HRMS calcd for $C_{18}H_{17}NO_5SNa$ [M + Na]⁺ 382.0720; Found 382.0731; $[\alpha]^{25}_D = -2.74$ (c 0.95, CHCl₃).

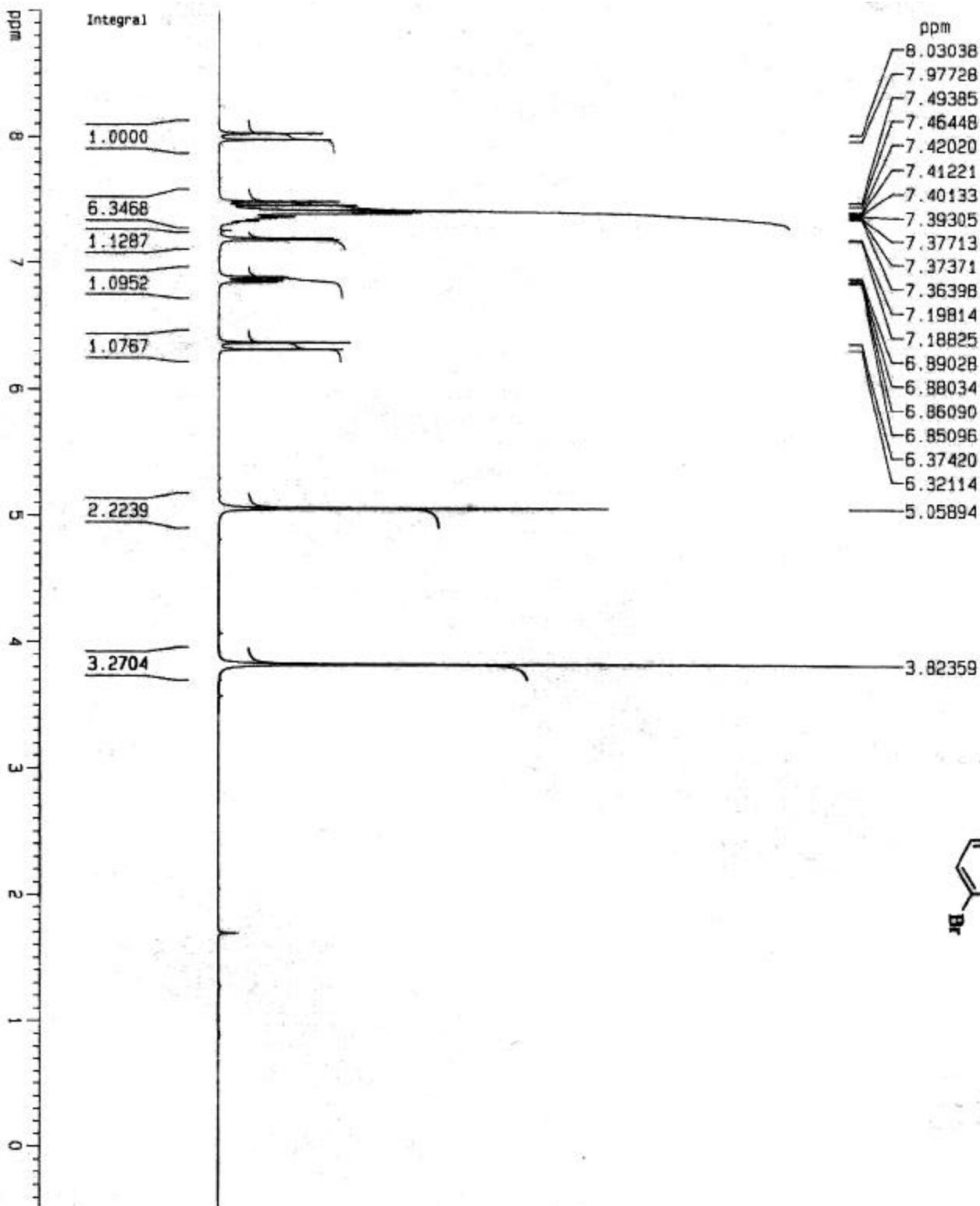
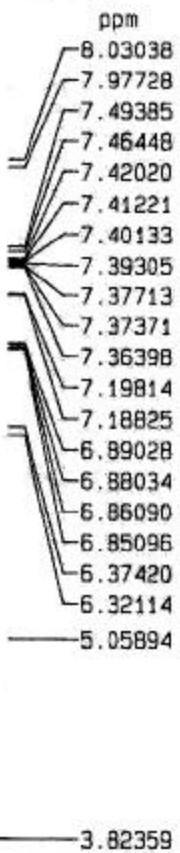
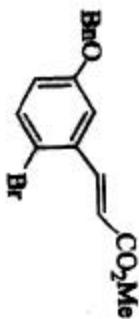
(1) Hiroya K.; Tadao K. *J. Chem. Soc., Perkin Trans. 1*, **1998**, 203.

(2) Lance S. F.; Brian I.; and Kevin A. S. *J. Chem. Soc., Perkin Trans. 1*, **1997**, 3465.

(3) Gronowitz P.; Moses A. B. *Arki. Kemi* **1961**, 17, 165.

- (4) Melvin S. N.; Alvin. K. *J. Org. Chem.* **1949**, 14, 375.
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- (7) Atsushi N.; Yoshinori K.; Takao S. *Synthesis*, **1999**, 306.
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1H NMR



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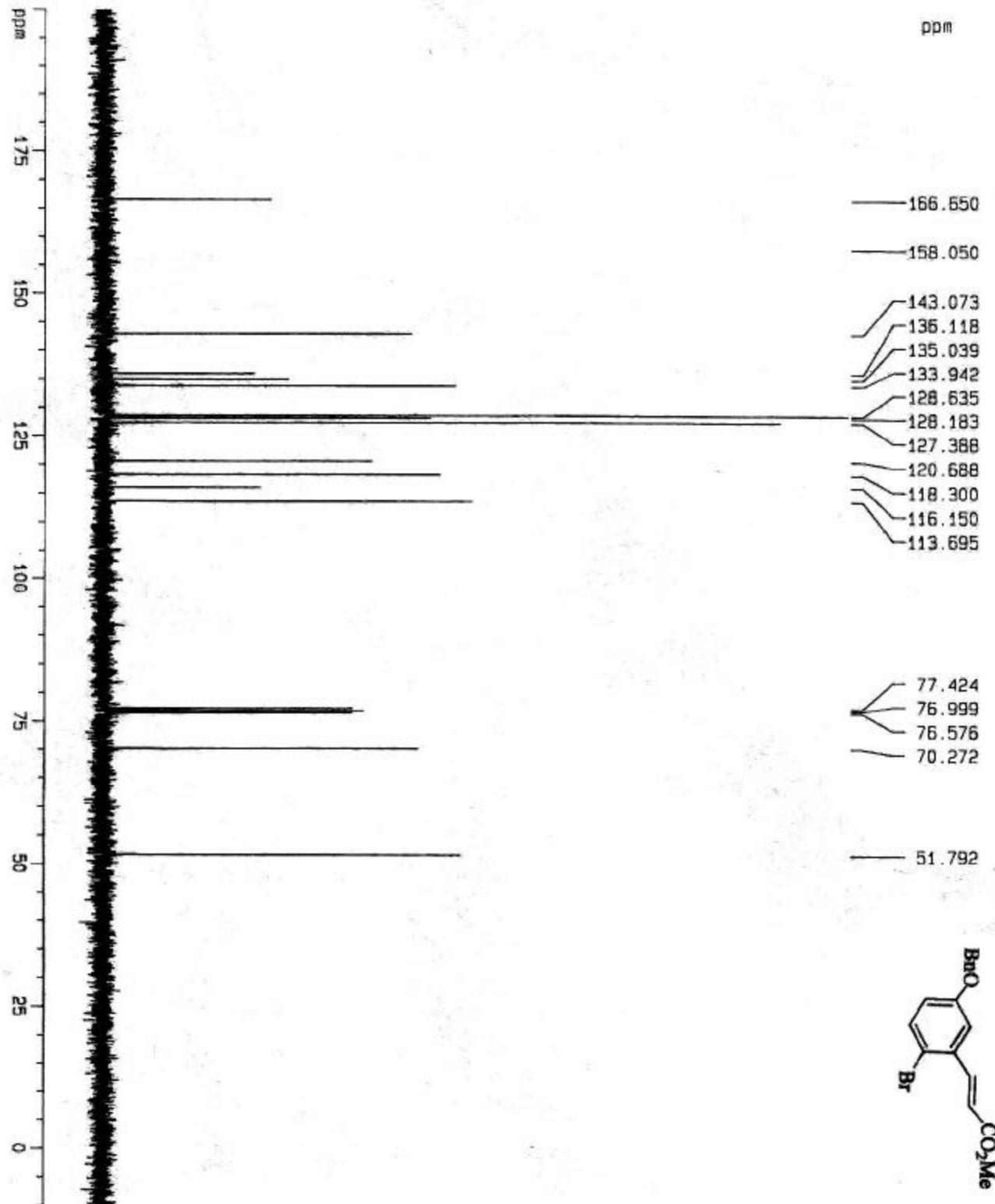
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¹³C NMR



Current Date Parameters
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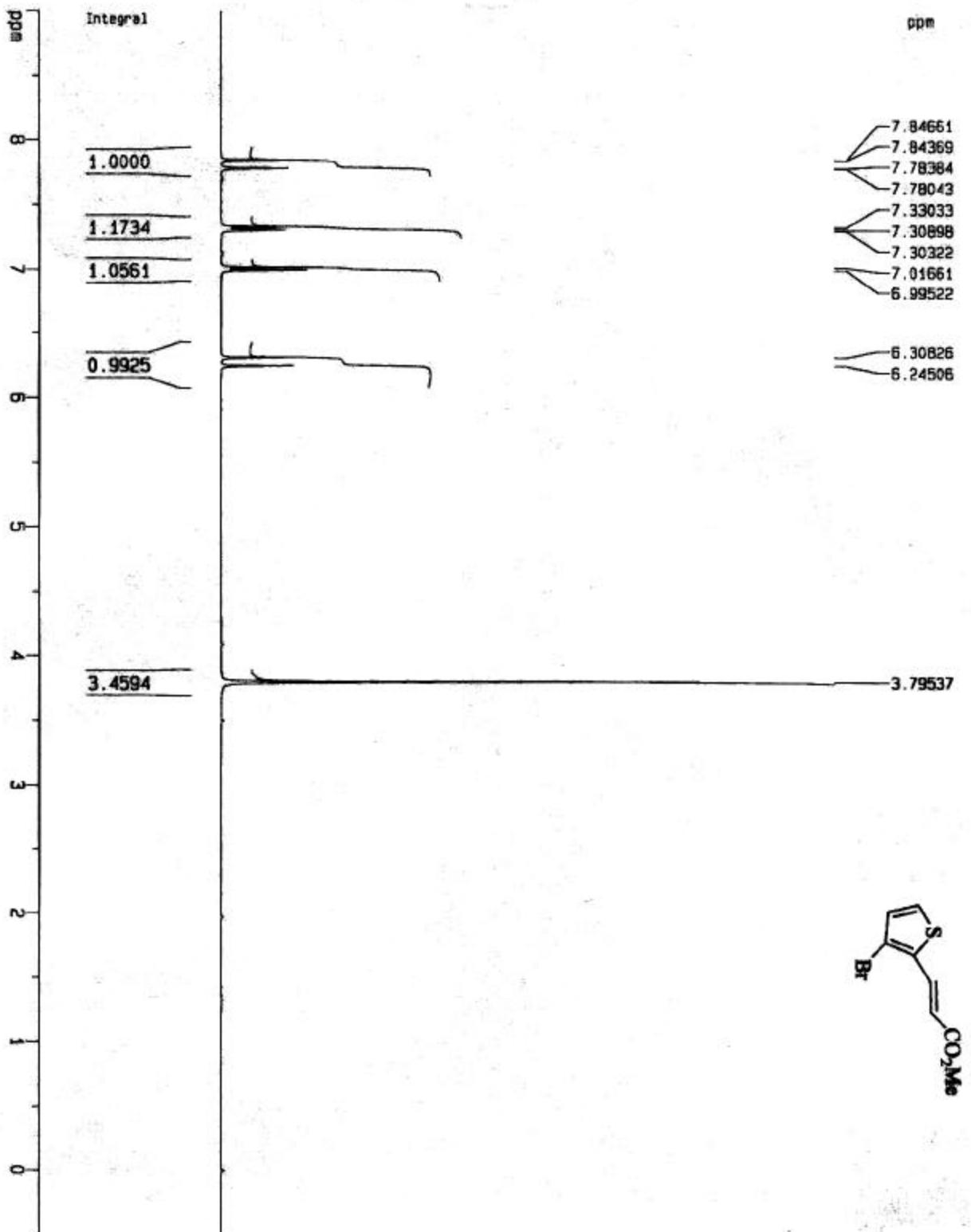
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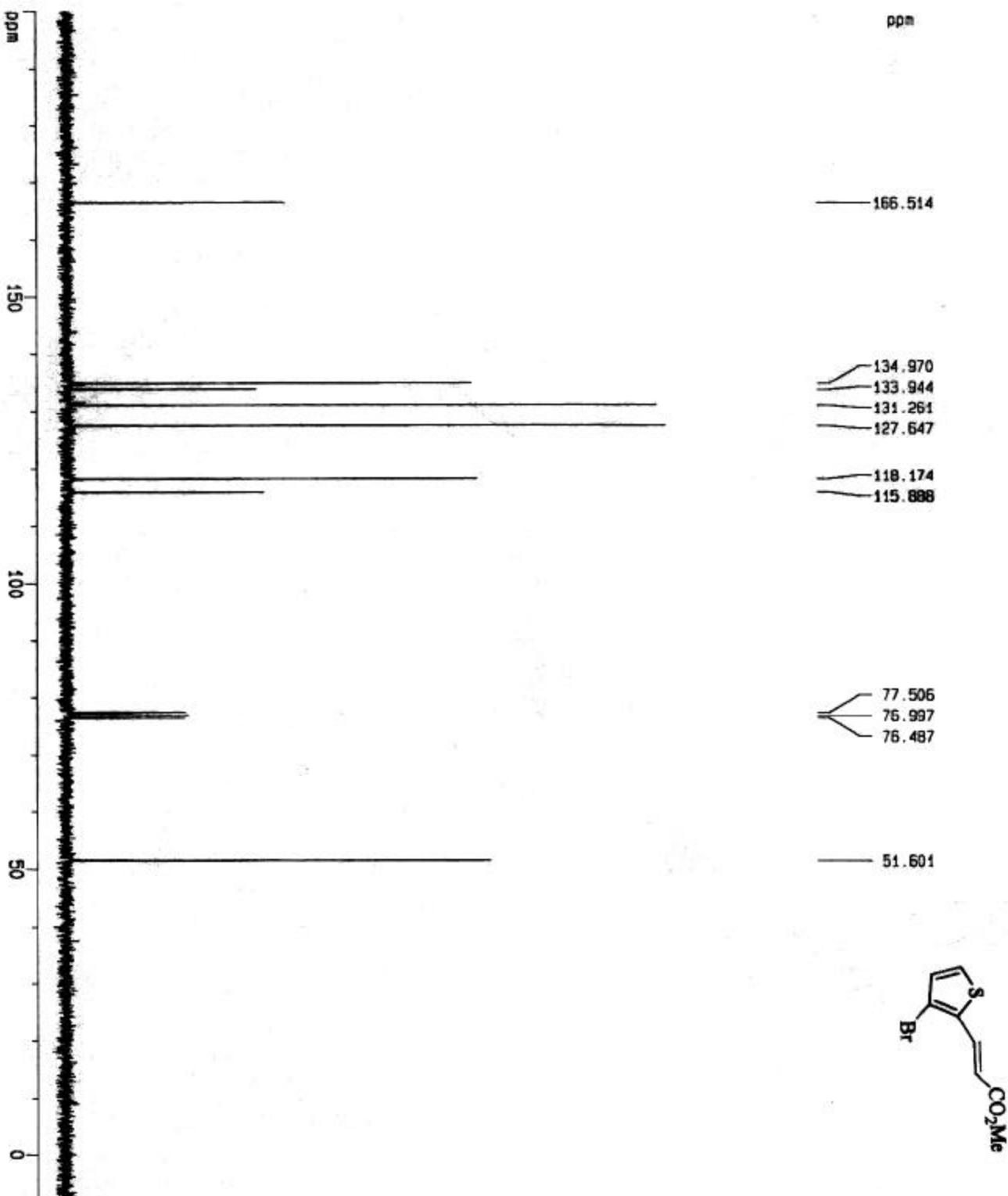


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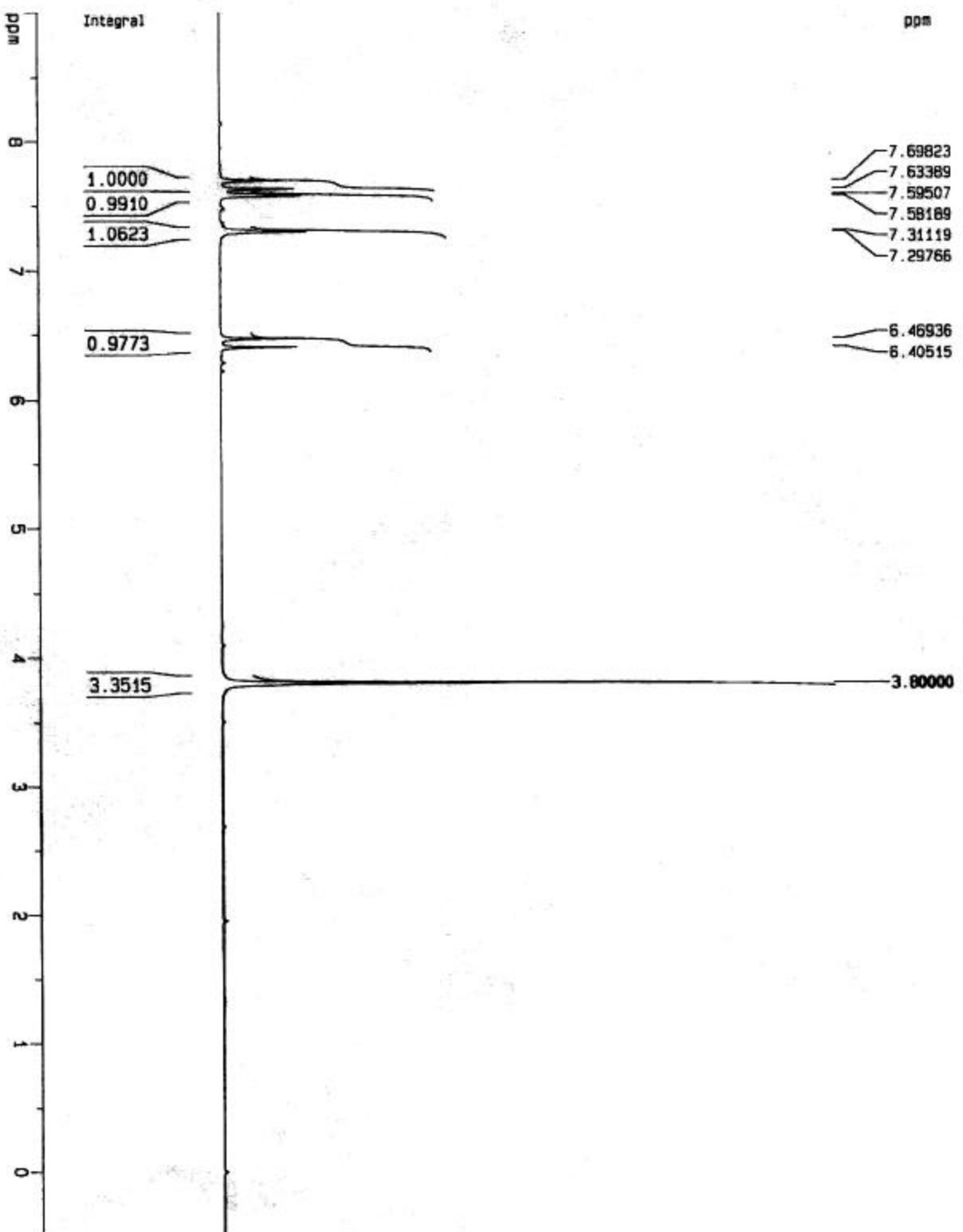
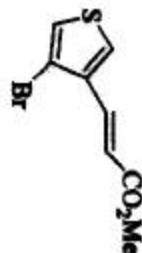
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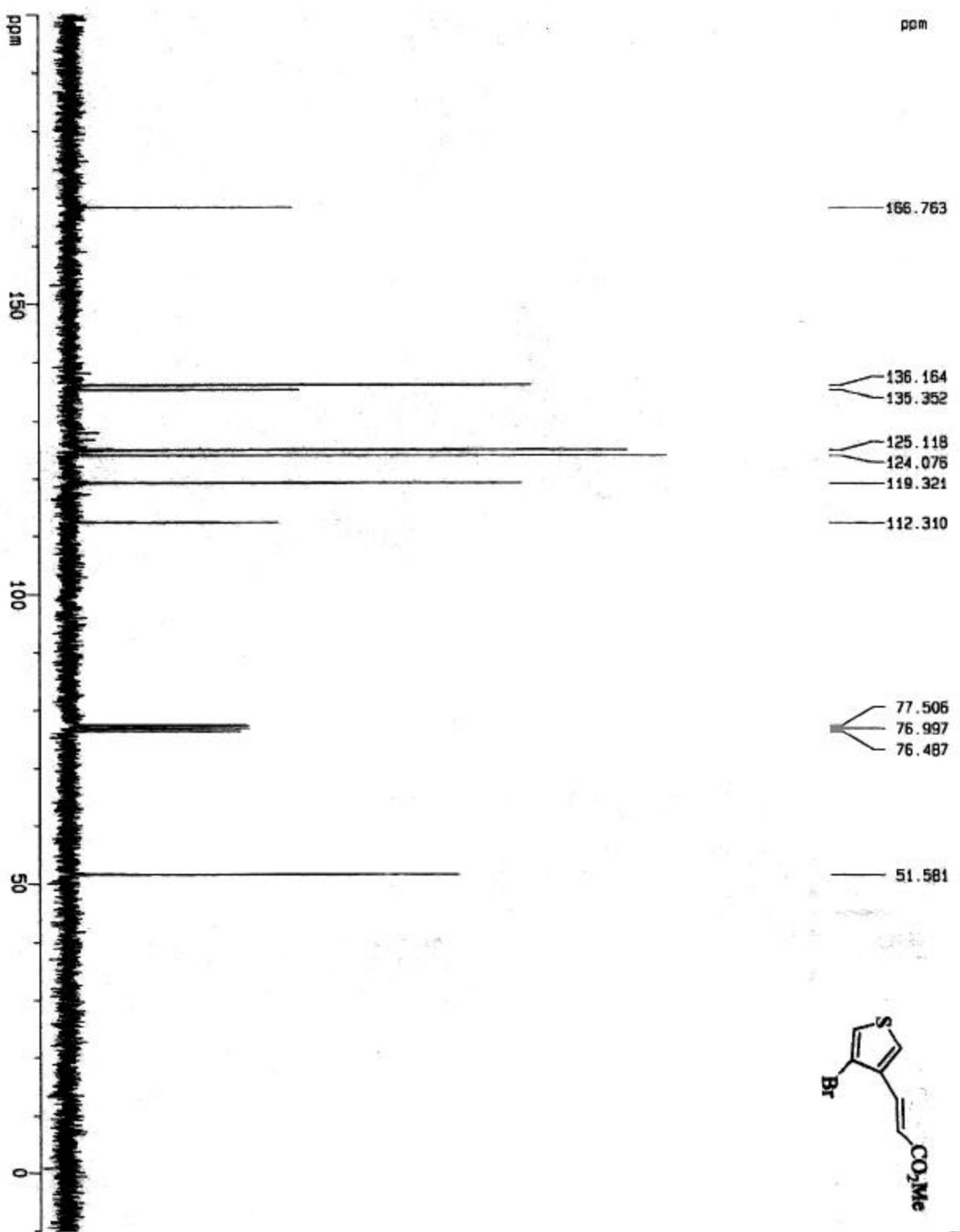
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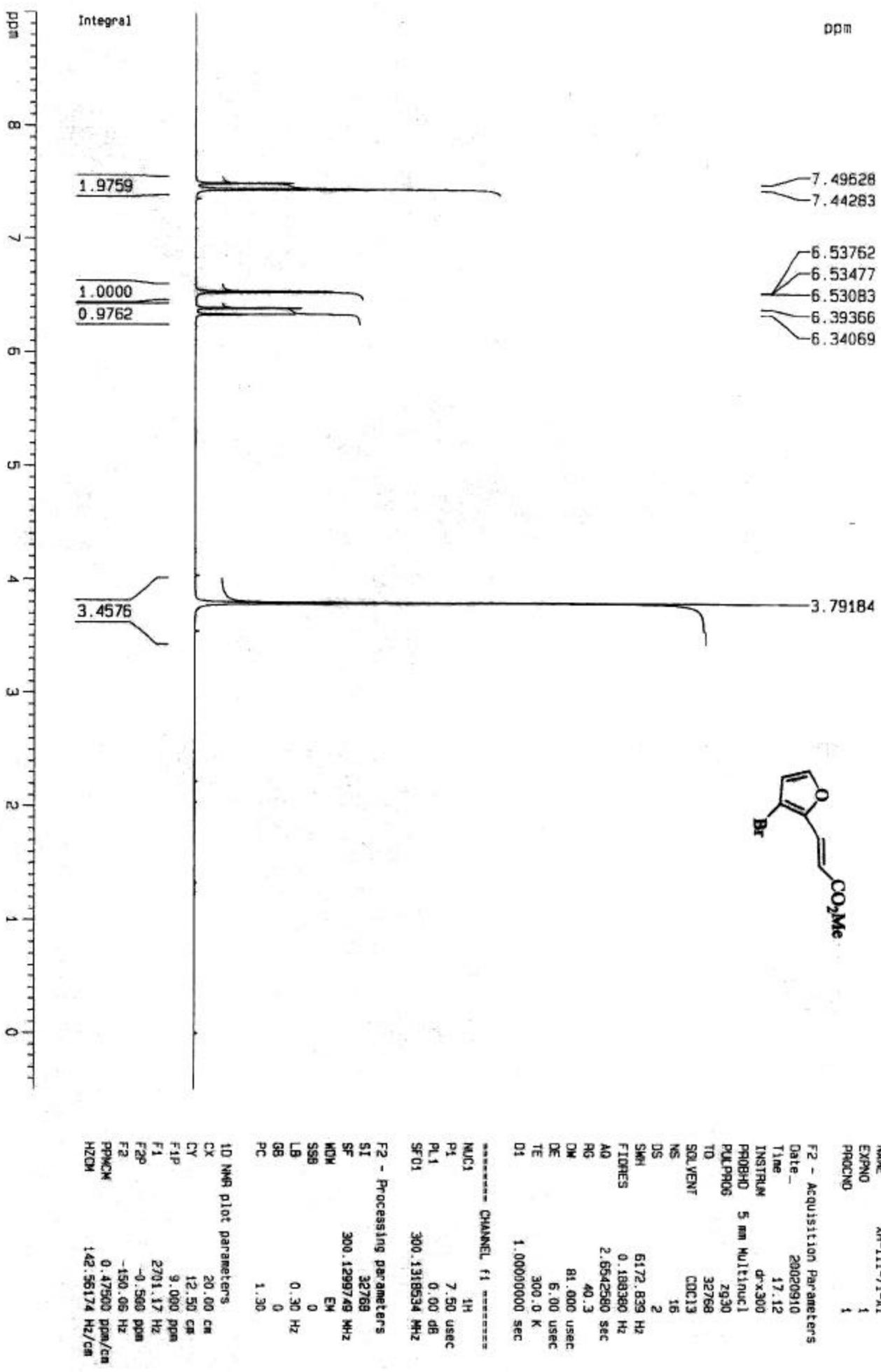
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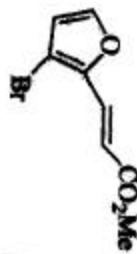
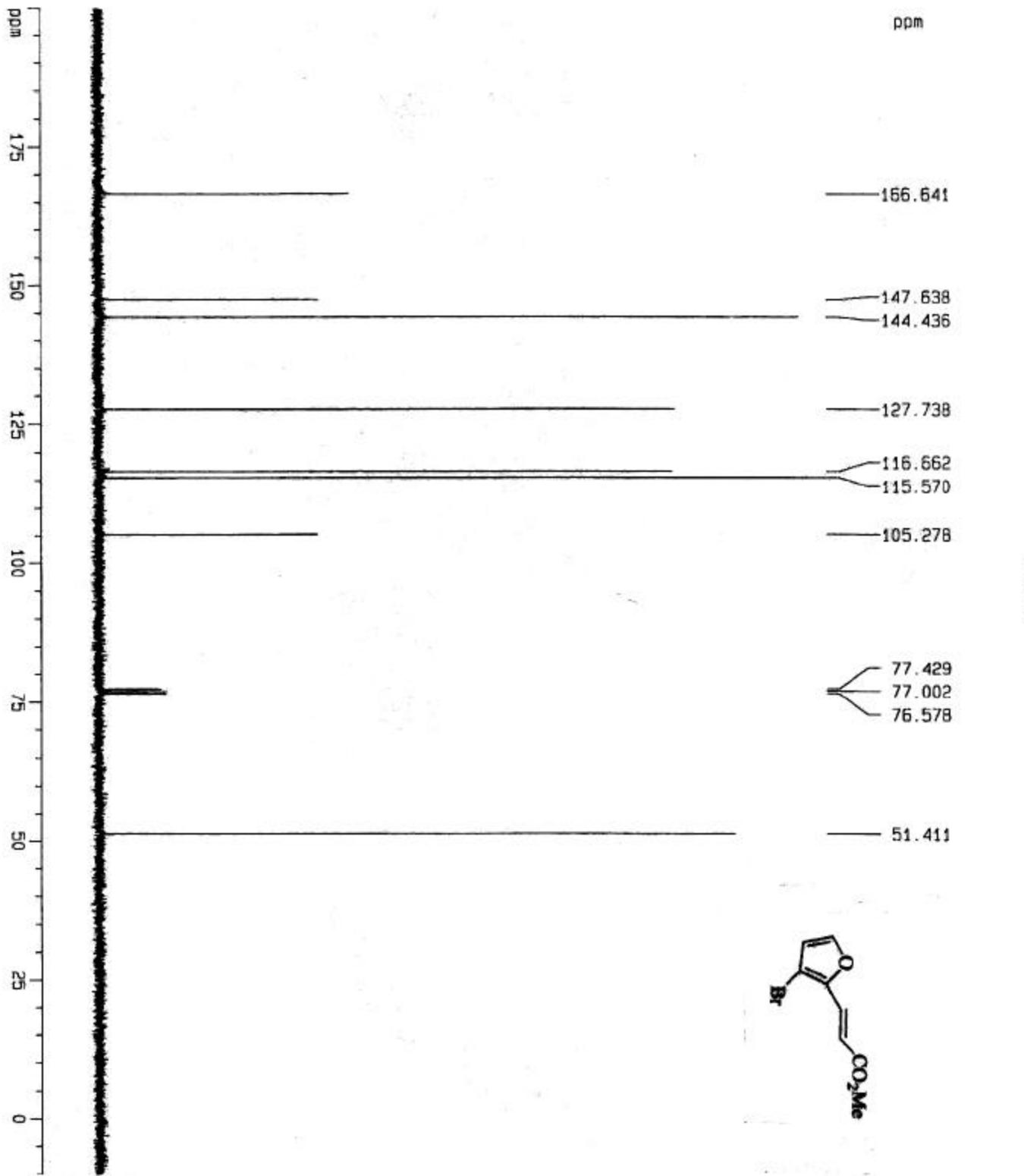
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 Cx 20.00 cm
 Cy 10.00 cm
 F1P 200.000 pp
 F1 12579.05 Hz
 F2P -10.000 pp
 F2 -628.95 Hz
 PPMCM 10.50000 pp
 HZCM 660.40009 Hz

1H NMR

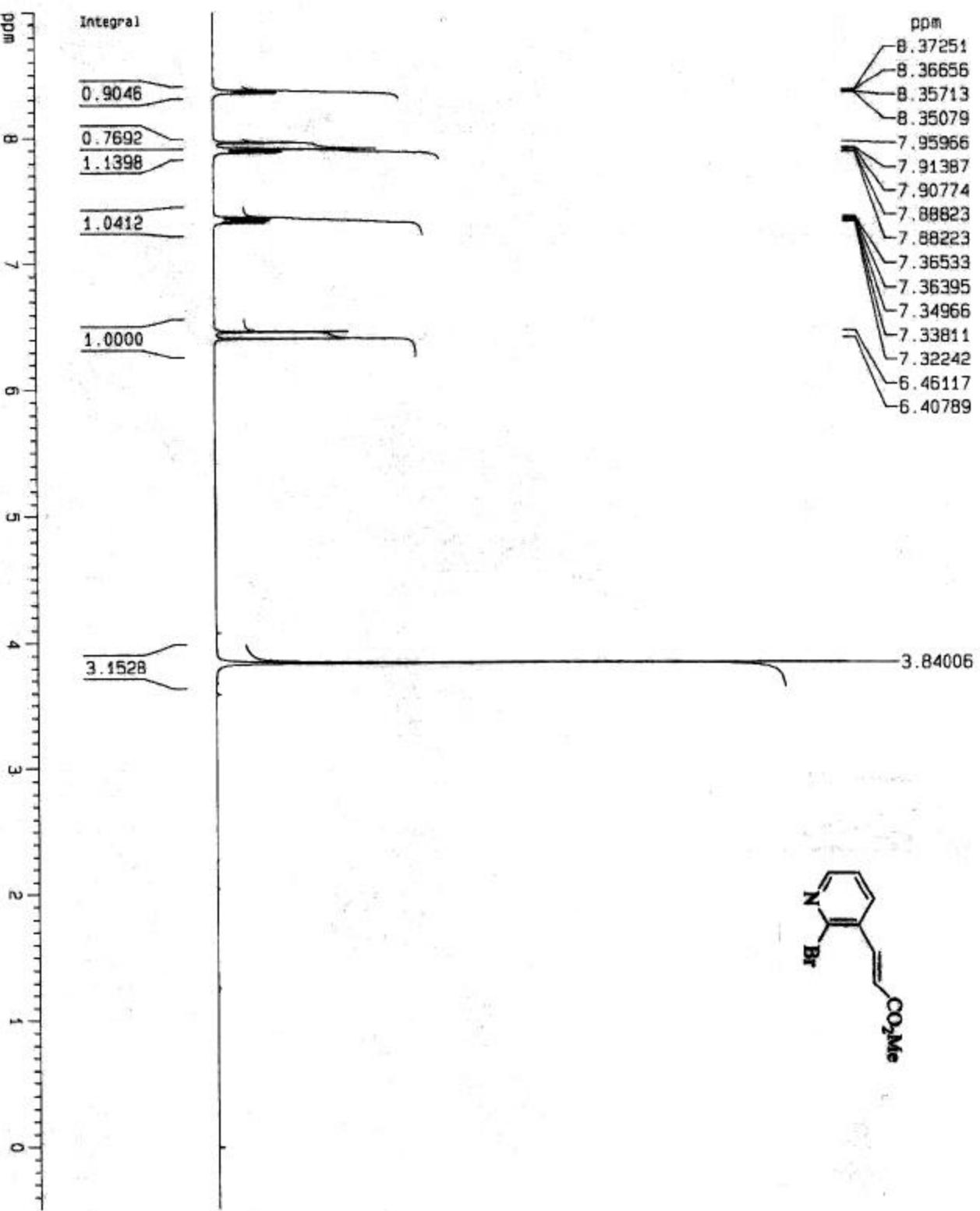
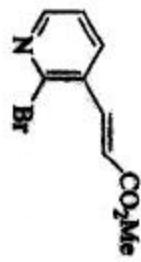




Current Data Parameters	
NAME:	XH-III-71-A1
EXPO:	2
PROCNO:	1
F2 - Acquisition Parameters	
Date:	20020510
Time:	17.19
INSTRUM:	drx100
PROBOD:	5 mm Multinucl
PULPROG:	zg0630
TD:	65536
SOLVENT:	CDCl3
NS:	128
D5:	4
SWH:	18850.141 Hz
FTDRES:	0.287630 Hz
AD:	1.738924 sec
RG:	32768
DM:	26.525 usec
DE:	37.89 usec
TE:	300.0 K
D1:	1.0000000 sec
d11:	0.0300000 sec
***** CHANNEL f1 *****	
NUC1:	13C
P1:	7.75 usec
PL1:	6.00 dB
SF01:	75.4760107 MHz
***** CHANNEL f2 *****	
NUC2:	1H
PPD02:	100.00 usec
PL2:	120.00 dB
PL12:	24.50 dB
SF02:	300.1312005 MHz
F2 - Processing Parameters	
SI:	32768
SF:	75.4677657 MHz
MDW:	EW
SSB:	0
LB:	1.00 Hz
GB:	0
PC:	1.40
1D NMR plot parameters	
CX	20.00 cm
CY	12.50 cm
CP	200.000 pps
F1	15093.5 Hz
F2P	-10.000 ppm
F2	-754.58 Hz
PPMCH	10.50000 ppm/cm
HZCM	792.41150 Hz/cm

1H NMR

ppm
 8.37251
 8.36656
 8.35713
 8.35079
 7.95966
 7.91387
 7.90774
 7.88823
 7.88223
 7.36533
 7.36395
 7.34966
 7.33811
 7.32242
 6.46117
 6.40789



Current Data Parameters
 NAME XH-III-70-A1
 EXPNO 1
 PRODNO 1

F2 - Acquisition Parameters

Date_ 20050910

Time_ 17.27

INSTRUM dnx300

PROBHD 5 mm Multinucl

PULPROG 2930

TD 32768

SOLVENT CDCl₃

NS 16

DS 2

SWH 0.188380 Hz

FIDRES 2.6542580 sec

AQ 64

RG 81.000 usec

DW 6.00 usec

DE 300.0 K

TE 1.0000000 sec

D1

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

NUC1 ¹H

P1 7.50 usec

PL1 0.00 dB

SF01 300.1319534 MHz

F2 - Processing parameters

SI 32768

SF 300.1299732 MHz

WDW EW

SSB 0

LB 0.30 Hz

GB 0

PC 1.30

1D NMR plot parameters

CX 20.00 cm

CY 12.50 cm

F1P 9.000 ppm

F1 2701.17 Hz

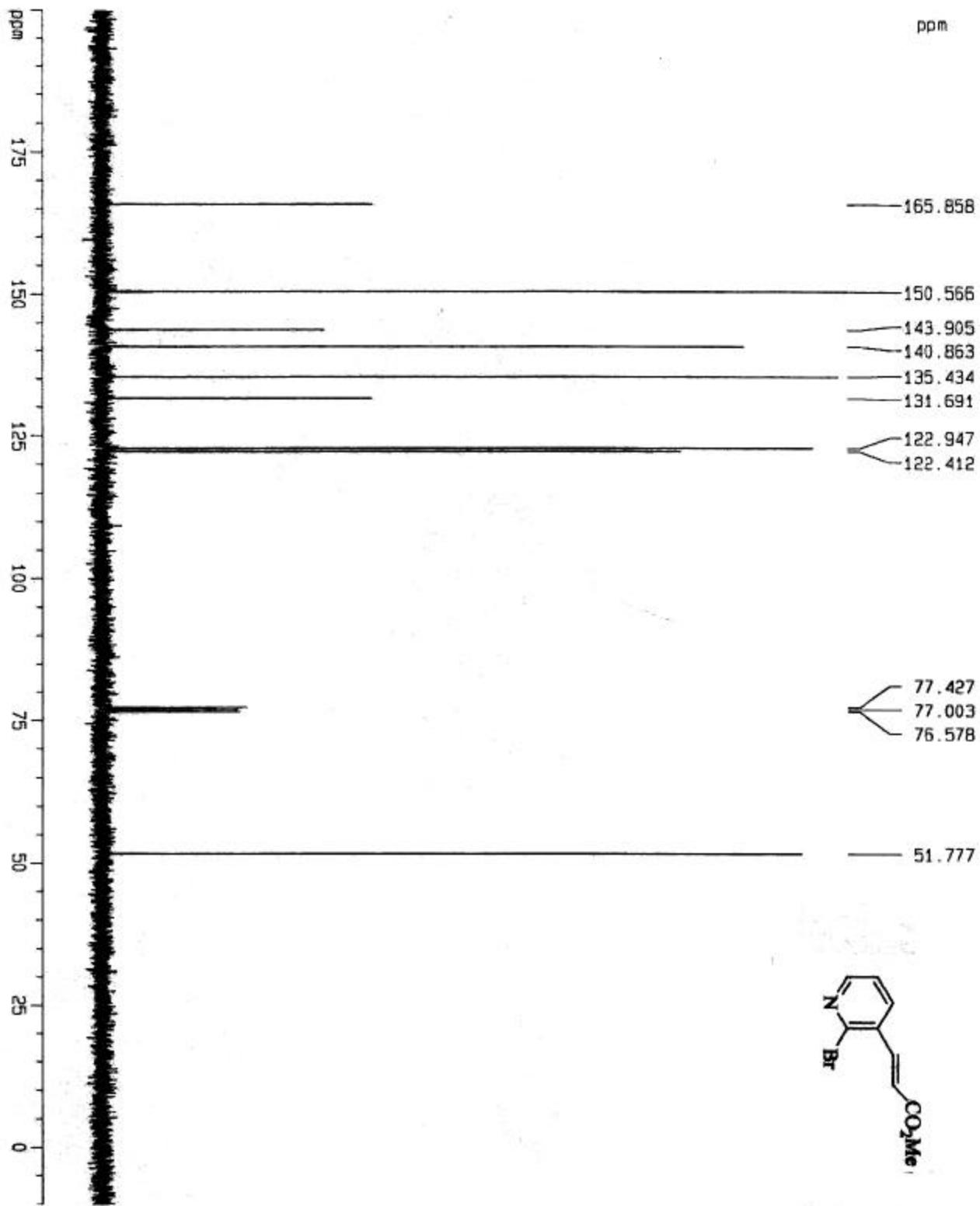
F2P -0.500 ppm

F2 -150.06 Hz

PPMCM 0.47500 ppm/cm

HZCM 142.58174 Hz/cm

¹³C NMR



Current Data Parameters
NAME NH-III-70-A1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date 20020610
Time 17.33
INSTRUM drx300
PROBHD 5 mm Multinuc
PULPROG zgpc30
TD 66536
SOLVENT CDCl₃
NS 134
DS 4
SWH 16850.141 Hz
FIDRES 0.287630 Hz
AQ 1.7385924 sec
RG 32768
DM 26.525 usec
DE 37.69 usec
TE 300.0 K
D1 1.0000000 sec
d1 0.0300000 sec

CHANNEL f2

NUC1 ¹³C
P1 7.75 usec
PL1 6.00 dB
SF01 75.4760107 MHz

CHANNEL f1

OPPRG2 waltz16
NUC2 ¹H
PCP02 100.00 usec
PL2 120.00 dB
PL12 24.50 dB
SF02 300.1312005 MHz

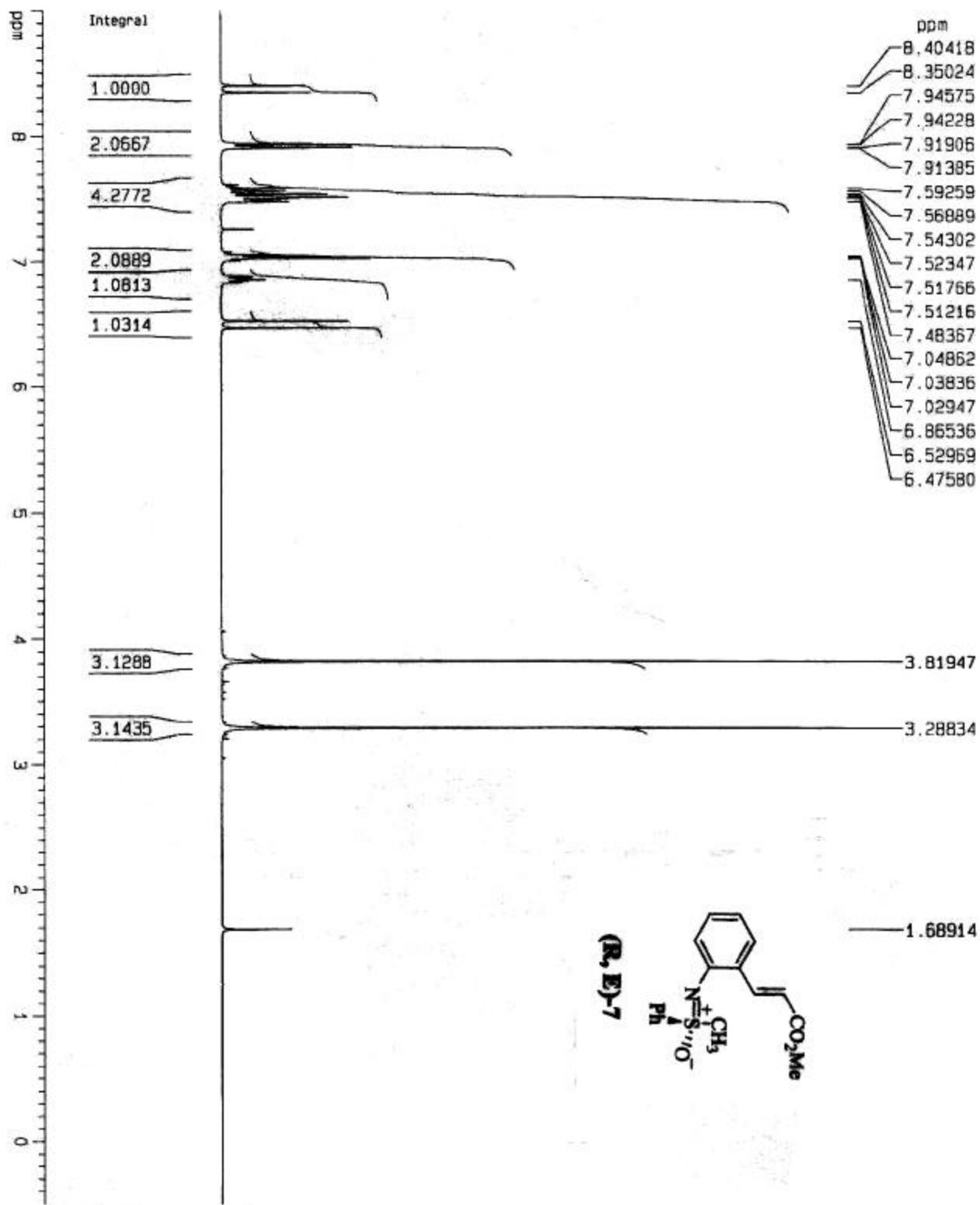
F2 - Processing parameters

SI 32768
SF 75.4677634 MHz
NDH EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

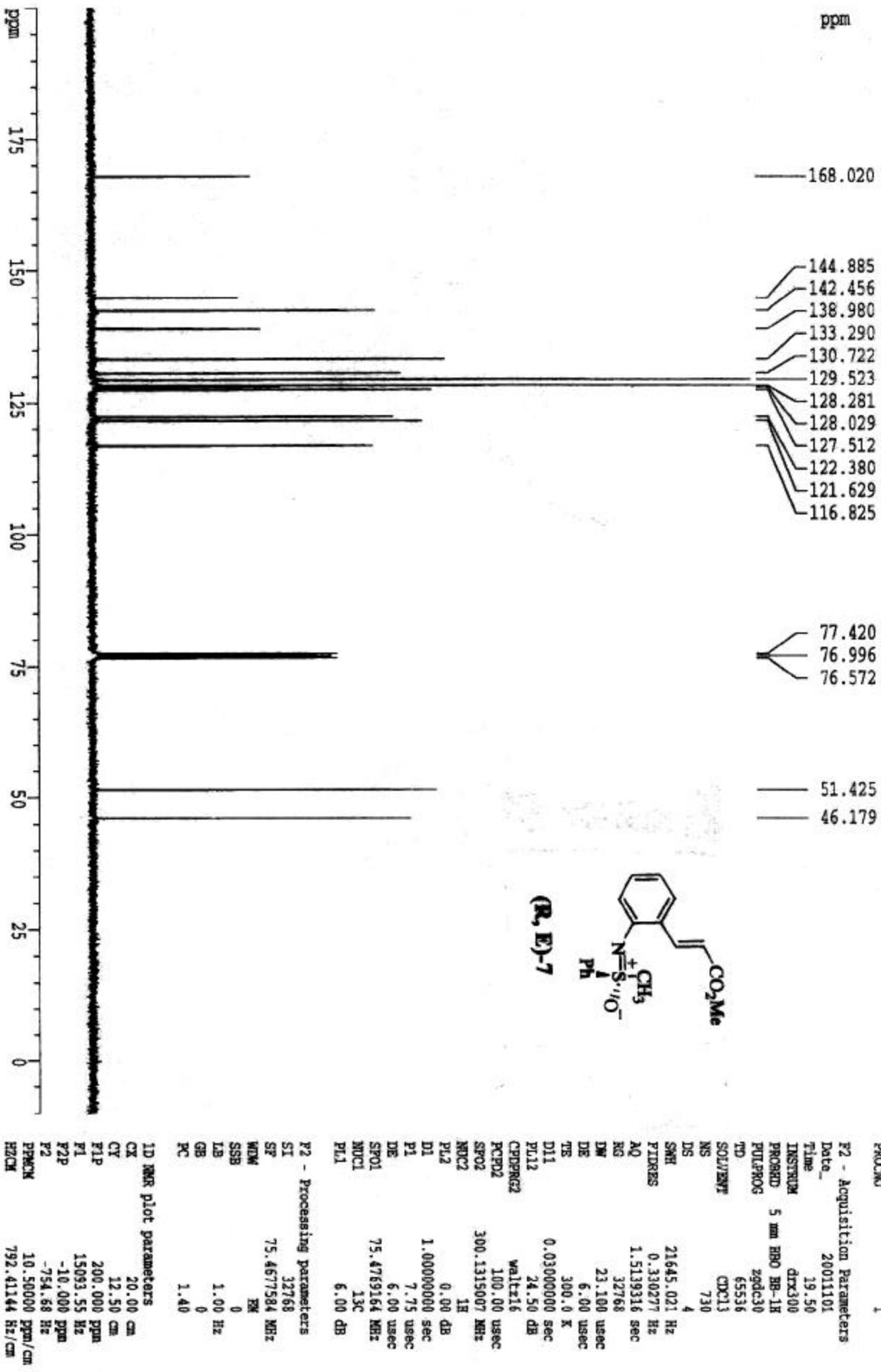
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.00 ppm
F1 15093.55 Hz
F2P -10.00 ppm
F2 -754.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 792.41±50 Hz/cm

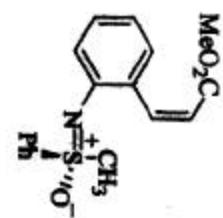
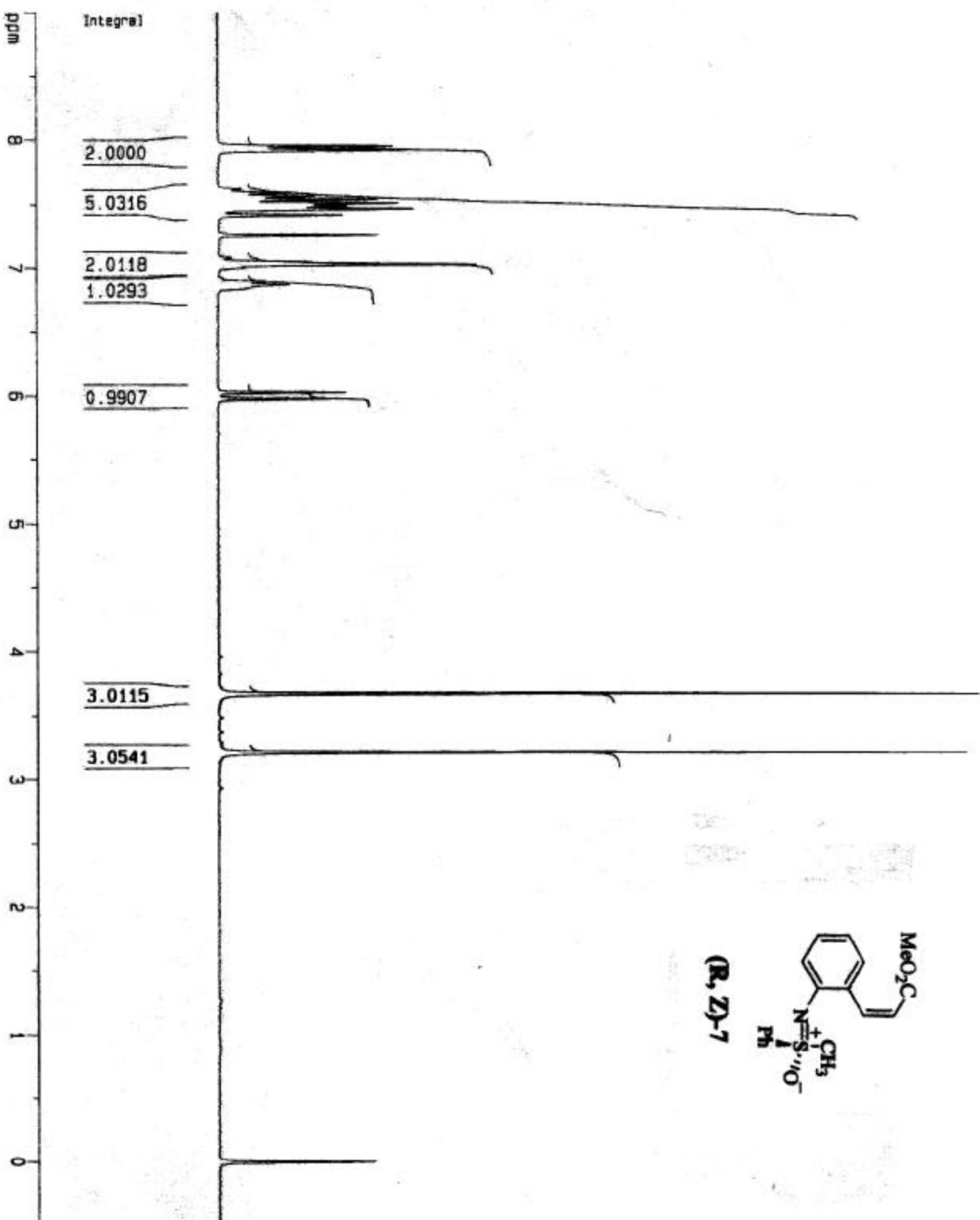
1H NMR

S-20



Current Data Parameters	
NAME	XH-I-60
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date	20020804
Time	16.59
INSTRUM	drx300
PROBHD	5 mm Multinucl
PULPROG	zg30
ID	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FORES	0.188380 Hz
AQ	2.654250 sec
R6	287.4
DM	81.00 usec
DE	6.00 usec
TE	300.0 K
D1	1.0000000 sec
----- CHANNEL f1 -----	
NJCI	1H
P1	7.50 usec
PL1	0.00 dB
SF01	300.1318534 MHz
SI	32768
SF	300.1300062 MHz
MDM	EN
SSB	0
LB	0.30 Hz
GB	0
PC	1.30
F2 - Processing parameters	
CX	20.00 cm
CY	12.50 cm
F1P	9.0000 ppm
F1	2701.17 Hz
F2P	-0.500 ppm
F2	-180.06 Hz
PPMDD	0.47500 ppm/cm
HZCM	142.56175 Hz/cm





Current Data Parameters
 NAME XH-IV-91-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date 20030213

Time 14.22

INSTRUM apx250

PROBHD 5 mm QNP 1H

PULPROG 2930

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SWH 5208.333 Hz

AQ 0.158946 Hz

TDRES 3.1457779 sec

RG 4096

DW 96.000 use

DE 137.14 use

TE 300.0 K

D1 1.0000000 sec

P1 8.70 use

SFO1 250.1315321 MHz

NUCLEUS 1H

F2 - Processing parameters

SI 16384

SF 250.1299836 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

CP 9.000 ppm

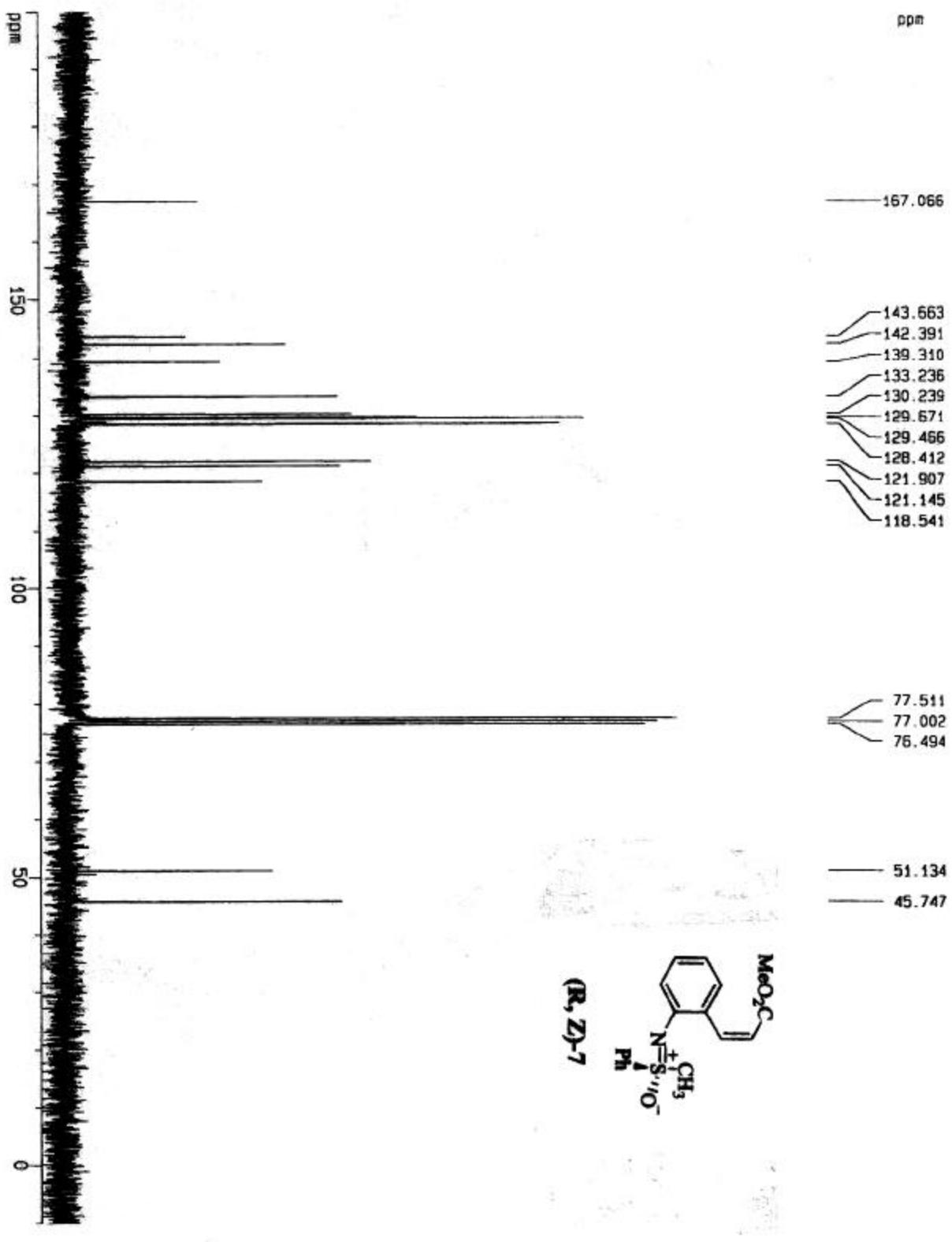
F1P 2251.17 Hz

F1 -0.500 ppm

F2P -125.06 Hz

F2 -0.47500 ppm

PPMCM 118.81174 Hz

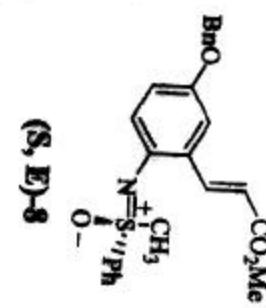
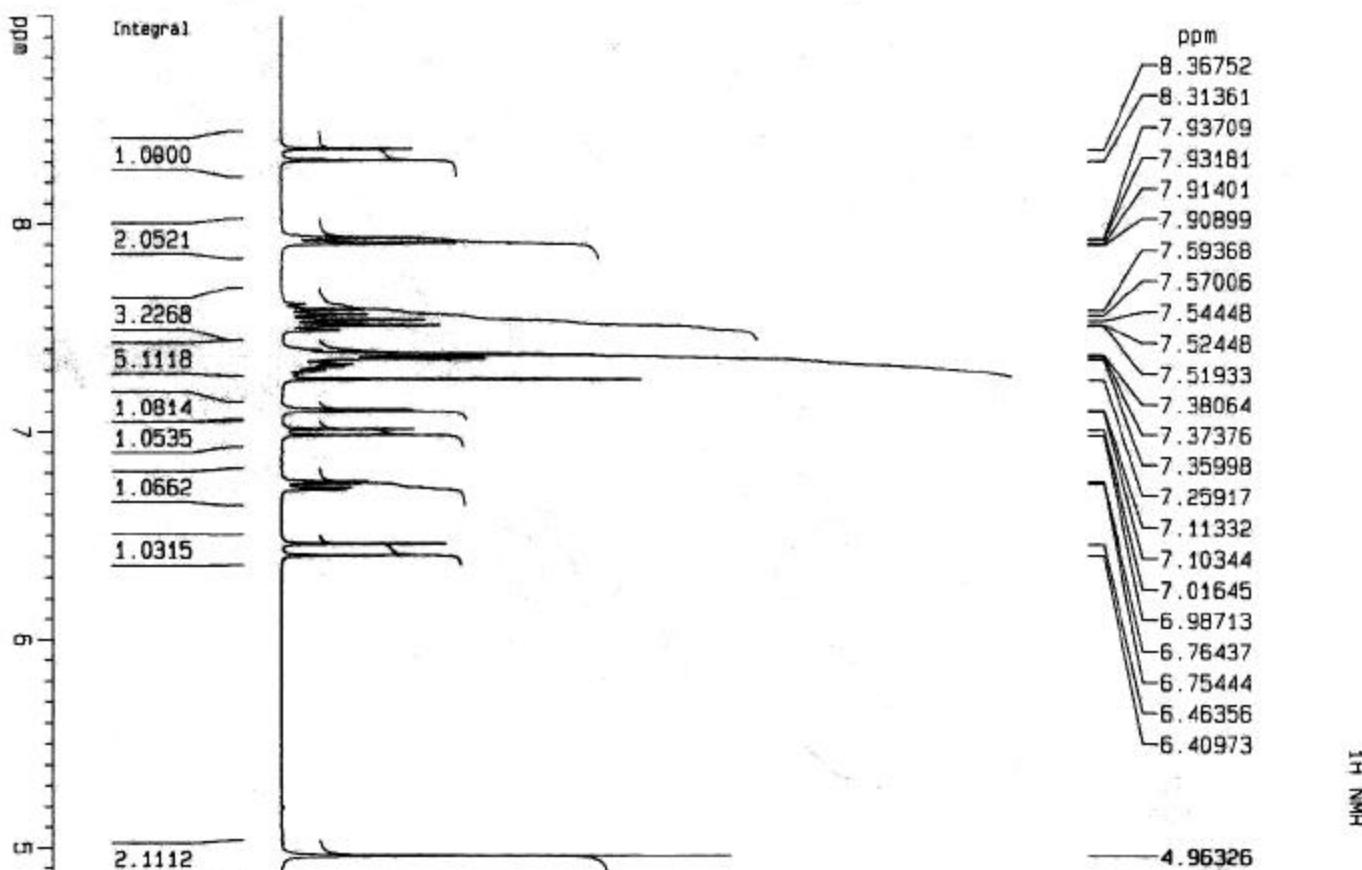


Current Data Parameters
 NAME XH-IV-91-A1
 EXPNO 2
 PROCN 1

F2 - Acquisition Parameters
 Date 2030211
 Time 21:51
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zgdc30
 TD 36864
 SOLVENT CDCl3
 NS 338
 DS 4
 SWH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DW 29.000 usec
 DE 41.43 usec
 TE 300.0 K
 D12 0.00002000 sec
 D1 23.00 dB
 D12 0.0000000 sec
 D1 1.0000000 sec
 P1 5.35 usec
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.0300000 sec

F2 - Processing parameters
 ST 32768
 SF 62.8952459 MHz
 MDW EH
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

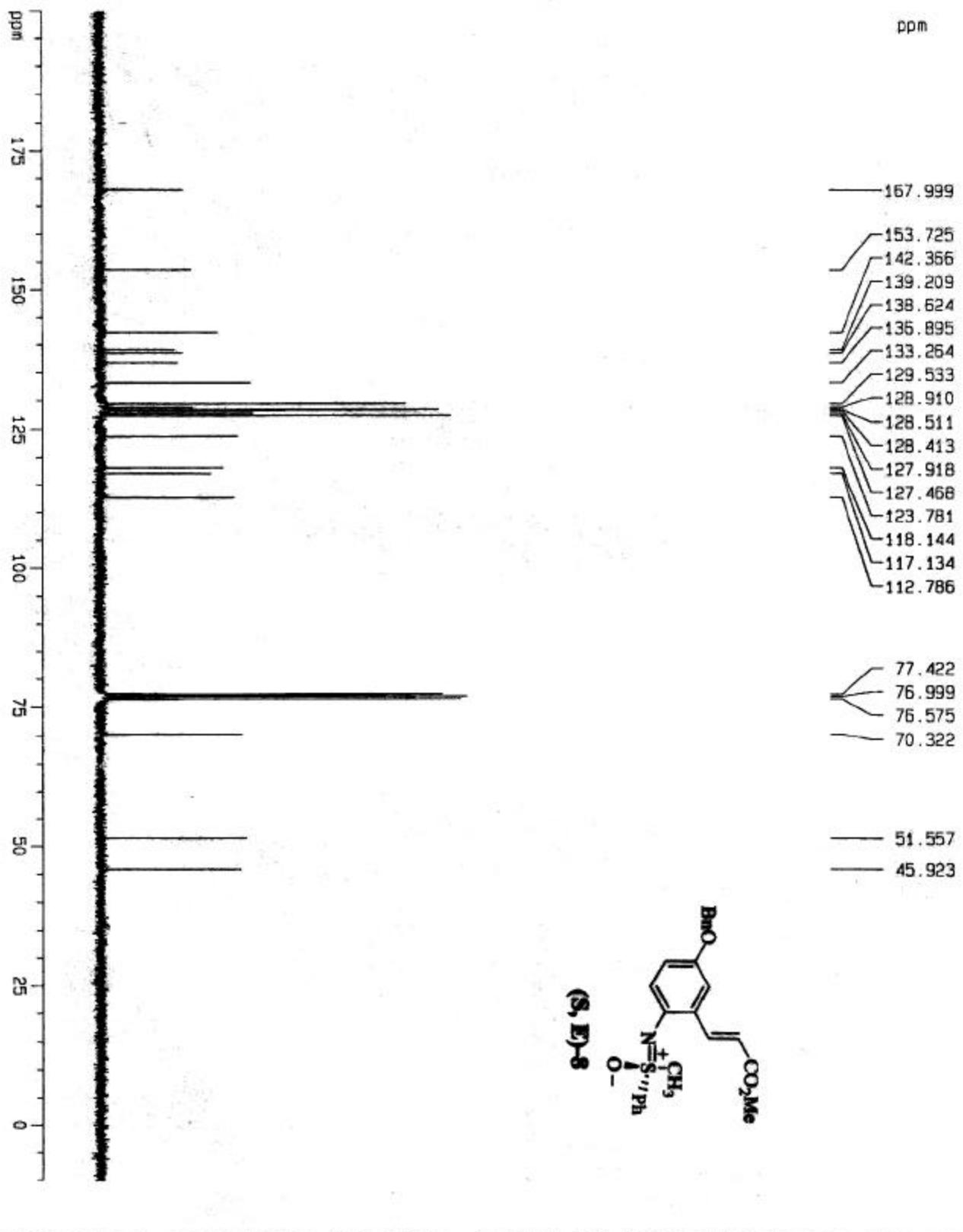
1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 200.000 ppm
 F1 12579.05 Hz
 F2P -10.000 ppm
 F2 -628.95 Hz
 AP1CK 10.50000 ppm
 HZM 660.40009 Hz



Current Data Parameters	
NAME	XH-I-94-1
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
DATE	20020829
TIME	12:36
INSTRUM	drx300
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
MS	16
DS	2
SWH	5172.839 Hz
FORES	0.188360 Hz
AB	2.6542560 SEC
B61	812.7
DW	81.000 usec
DE	6.00 usec
TE	300.0 K
D1	1.0000000 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.50 usec
PL1	0.00 dB
SF01	300.1318534 MHz
F2 - Processing parameters	
S1	32768
SF	300.1300665 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	9.000 ppm
F1	2701.17 Hz
F2P	1.600 ppm
F2	480.21 Hz
PPMCM	0.37000 ppm/cm
Hz/cm	111.04810 Hz/cm

¹³C NMR



Current Data Parameters

NAME	XH-I-94-1
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date	20020804
Time	21:30
INSTRUM	drx300
PROBHD	5 mm Multinucl
PULPROG	Zgdc30
TD	65536
SQ SOLVENT	CDCl ₃
NS	520
DS	4
SWH	1883.2 Hz
FOIDRES	0.287352 Hz
A9	1.740136 sec
RG	32768
DW	26.556 usec
DE	6.00 usec
TE	300.0 K
D1	1.0000000 sec
d1	0.03000000 sec

CHANNEL f1

NUC1	¹³ C
P1	7.75 usec
PL1	6.00 dB
SF01	75.4760107 MHz

CHANNEL f2

NUC2	¹ H
PCP02	Wait216
NUC2	¹ H
PCP02	100.00 usec
PL2	120.00 dB
PL12	24.50 dB
SF02	300.1312005 MHz

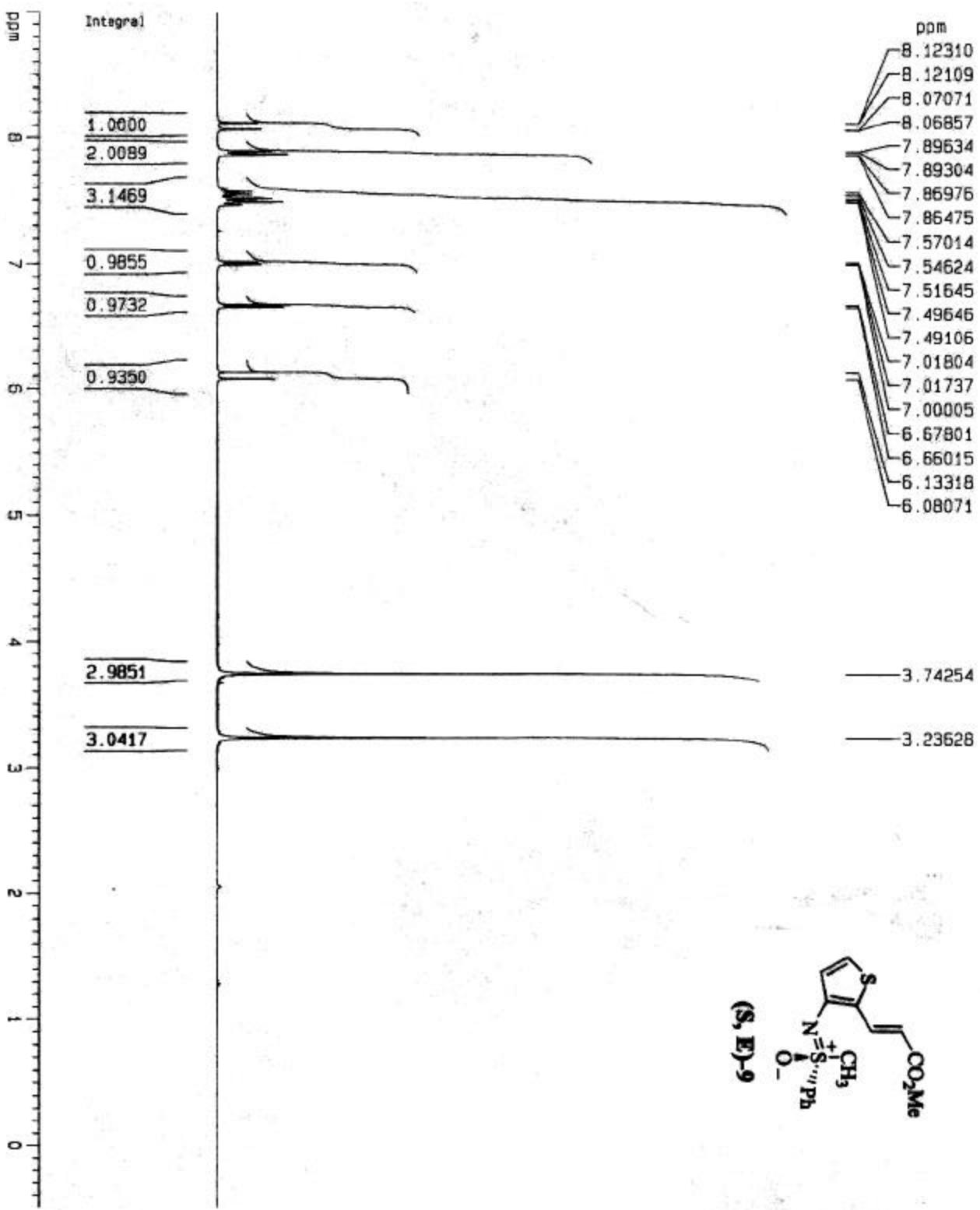
F2 - Processing parameters

S1	32768
SF	75.4677536 MHz
WDW	EN
SSB	0
LB	1.00 Hz
PC	0
TC	1.40

1D NMR pick parameters

CX	20.00 cm
CY	5.00 cm
FIp	200.000 ppm
F1	15093.55 Hz
F2p	-10.000 ppm
F2	-754.68 Hz
PPMCH	10.50000 ppm/cm
HZCM	792.41136 Hz/cm

1H NMR



Current Data Parameters
NAME XH-III-5d
EXPRO 1
PROCNO 1

F2 - Acquisition Parameters

Date 20020813
Time 14.23
INSTRUM drx300
PROBHD 5 mm Multinucl
PULPROG 2930
TD 32768

SOLVENT CDCl3
NS 2
DS 16
SWH 0.188380 Hz
FIDRES 2.6542560 sec
AQ 64

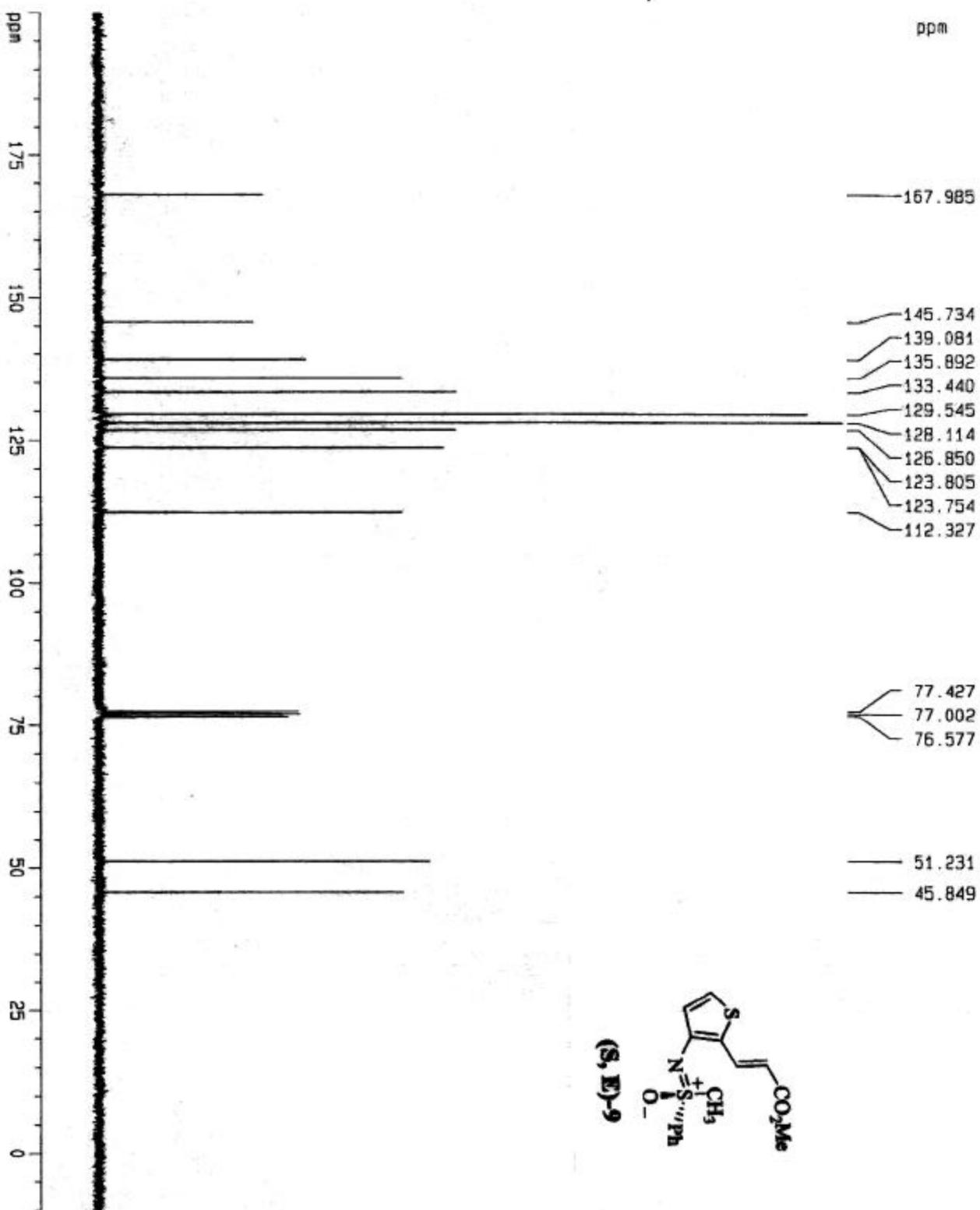
RG 81.000 usec
D1 6.00 usec
DE 300.0 K
TE 1.0000000 SEC
P1 7.50 usec
SF 300.1300058 MHz
MW EM
SSB D
LB 0.30 Hz
GB 0
PC 1.30

F2 - Processing parameters

S1 32768
SF 300.1300058 MHz
MW EM
SSB D
LB 0.30 Hz
GB 0
PC 1.30

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 9.000 ppm
F1 2701.17 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCH 0.47500 ppm/cm
HZCM 142.55175 Hz/cm

13C NMR



Current Data Parameters
NAME XH-III-54
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20020813

Time 14.29

INSTRUM dtx300

PROBOD 5 mm Multinuc1

PULPROG zgdc30

TD 65536

SOLVENT CDCl3

N5 149

D5 4

DS 18832.578 Hz

SWH 0.287362 Hz

TDRES 1.7400136 sec

A9 32768

RG 26.550 usec

DM 6.00 usec

DE 300.0 K

TE 0.0000000 sec

D1 0.03000000 sec

T1 7.75 usec

P1 6.00 dB

R1 75.4760107 MHz

SW01

===== CHANNEL f2 =====

NUC1 13C

PI 100.00 usec

P1 120.00 dB

P2 24.50 dB

P12 300.1312005 MHz

SWP02

NUC2 1H

PCPD02

P1 100.00 usec

P2 120.00 dB

P12 24.50 dB

P12 300.1312005 MHz

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

NUC1 1H

PI 32768

P1 75.4677623 MHz

PCPD01

NUC2 1H

PCPD02

P1 200.000 ppm

P2 15933.55 Hz

P12 -10.000 ppm

P12 -754.68 Hz

P12 10.50000 ppm/cm

PCPD03

NUC1 1H

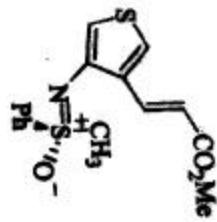
PCPD04

P1 792.41150 Hz/cm

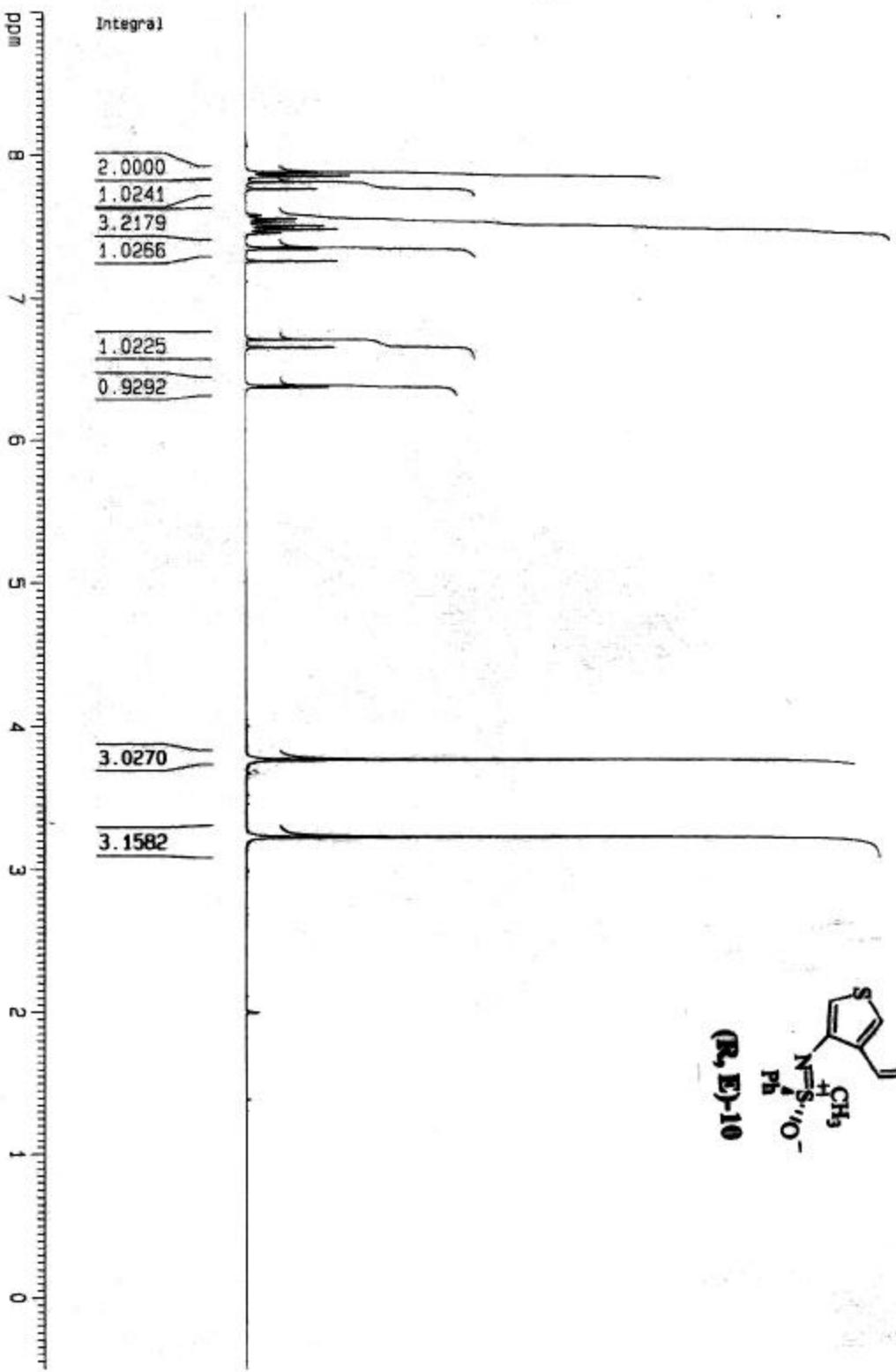
¹H NMR

ppm
 7.88443
 7.88073
 7.87533
 7.85750
 7.85243
 7.81614
 7.76259
 7.55889
 7.53476
 7.50483
 7.48507
 7.47957
 7.35739
 7.34653
 7.26018
 6.71512
 6.66157
 6.38814
 6.37726

3.76527
 3.22774



(R,E)-10



Current Data Parameters
 NAME XH-III-79-A1
 EXPNO 1
 PROJNO 1

F2 - Acquisition Parameters
 Date 20000924
 Time 16:26

INSTRUM

5 mm

Multinucl

PULPROG

zg30

TD

32768

SOLVENT

CDCl₃

DS

2

NS

16

SWH

0.188389 Hz

AQ

2.6542580 sec

RG

64

DW

81.000 usec

DE

6.00 usec

TE

300.0 K

D1

1.0000000 sec

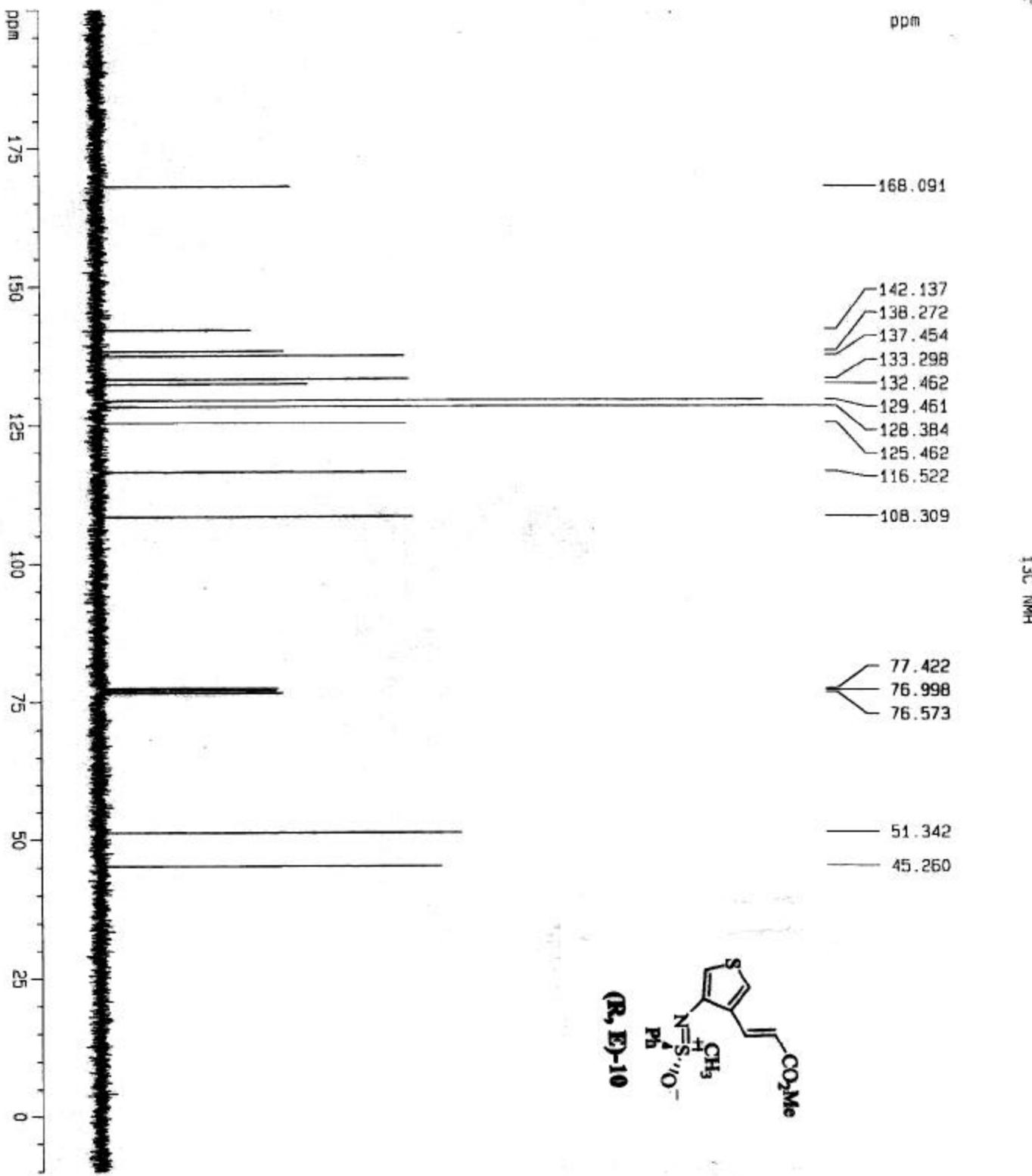
***** CHANNEL f1 *****

NUC1 1H
 P1 7.50 usec
 PL1 0.00 dB
 SF 300.1300058 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.30

F2 - Processing parameters

SI 32768
 SF 300.1300058 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.30

1D NMR plot: parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 9.000 ppm
 F1 2701.17 Hz
 F2P -0.500 ppm
 F2 -150.06 Hz
 FWHM 0.47500 ppm/cm
 HZCM 142.56175 Hz/cm



Current Data Parameters

NAME	XH-III-79-A1
EXPTD	2
PROCNO	1

F2 - Acquisition Parameters

Date 20000924

Time 16.32

INSTRUM drx300

PROBHD 5 mm Multinucl

PULPROG zgdc30

TD 65536

SOLVENT DDC13

NS 199

DS 4

SWH 18850.141 Hz

FTRES 0.287630 Hz

AD 1.7383924 sec

RG 32768

DW 26.525 usec

DE 37.89 usec

TE 300.0 K

DI 1.00000000 sec

DT 0.03000000 sec

SC 11

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

NUC1 13C

PA 7.75 usec

PL1 6.00 dB

SP01 75.4760107 MHz

===== CHANNEL f2 =====

NUC2 1H

PA2 100.00 usec

PL2 120.00 dB

PL1,2 24.50 dB

SP02 300.1312005 MHz

F2 - Processing parameters

SI 32768

SF 75.4677623 MHz

MW EN

SSB 0

LB 1.00 Hz

GS 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 12.50 cm

CP 200.000 ppm

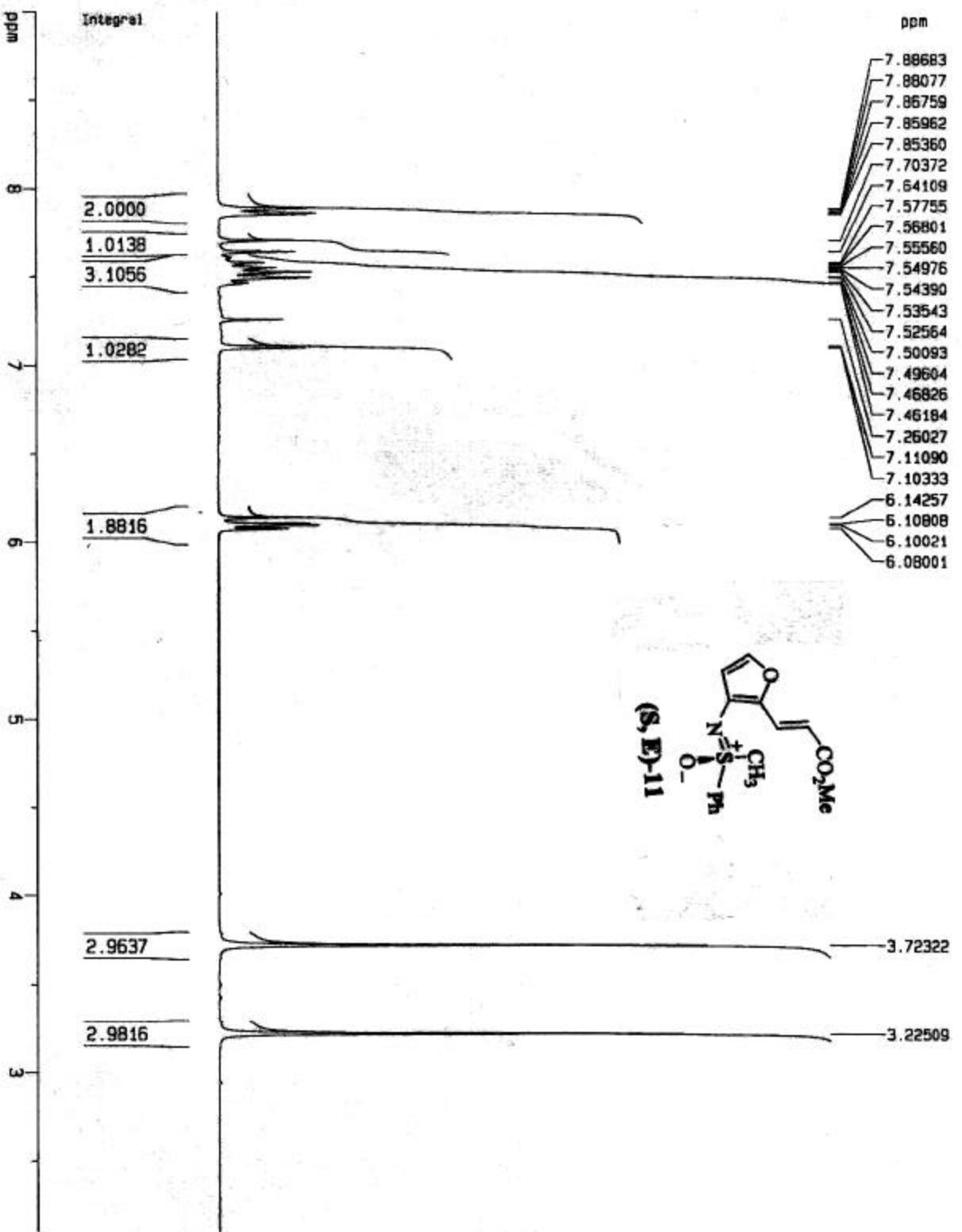
F1 15093.55 Hz

F2 -19.000 ppm

F3 -754.68 Hz

PPMCH 10.50000 ppm/cm

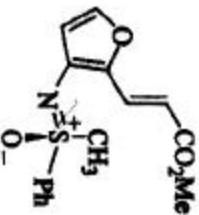
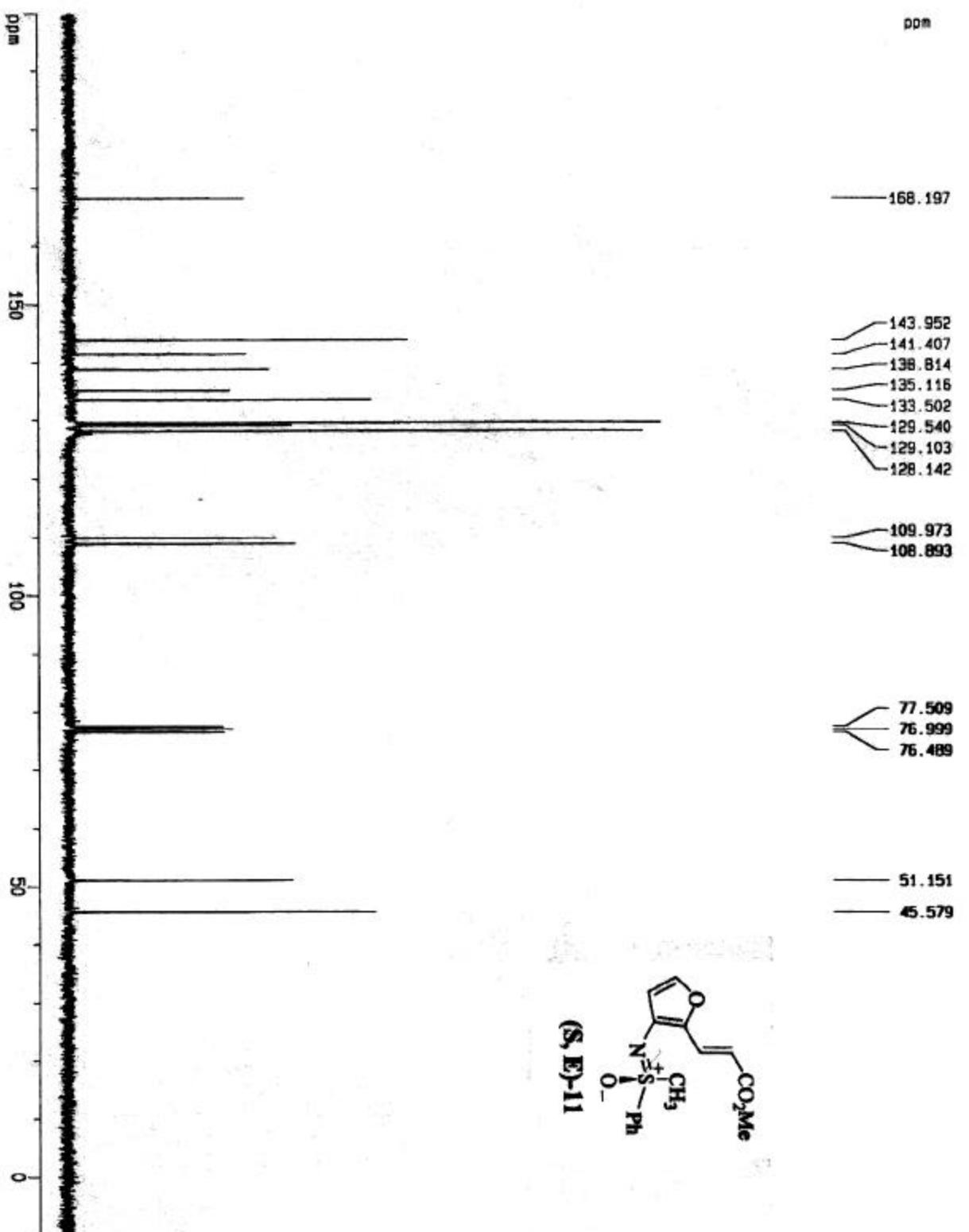
HZCM 792.41150 Hz/cm



Current Data Parameters
 NAME XH-III-73-A1
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date 20200913
 Time 15.22
 INSTRUM arx250
 PROBOD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT DDC13
 NS 16
 DS 2
 SWH 5208.333 Hz
 FIDRES 0.156946 Hz
 AQ 3.1457779 sec
 PG 360
 DM 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.0000000 sec
 P1 8.70 use
 SFO1 250.1315321 MHz
 NUCLEUS 1H

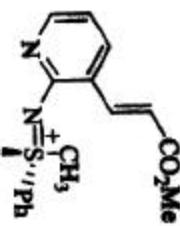
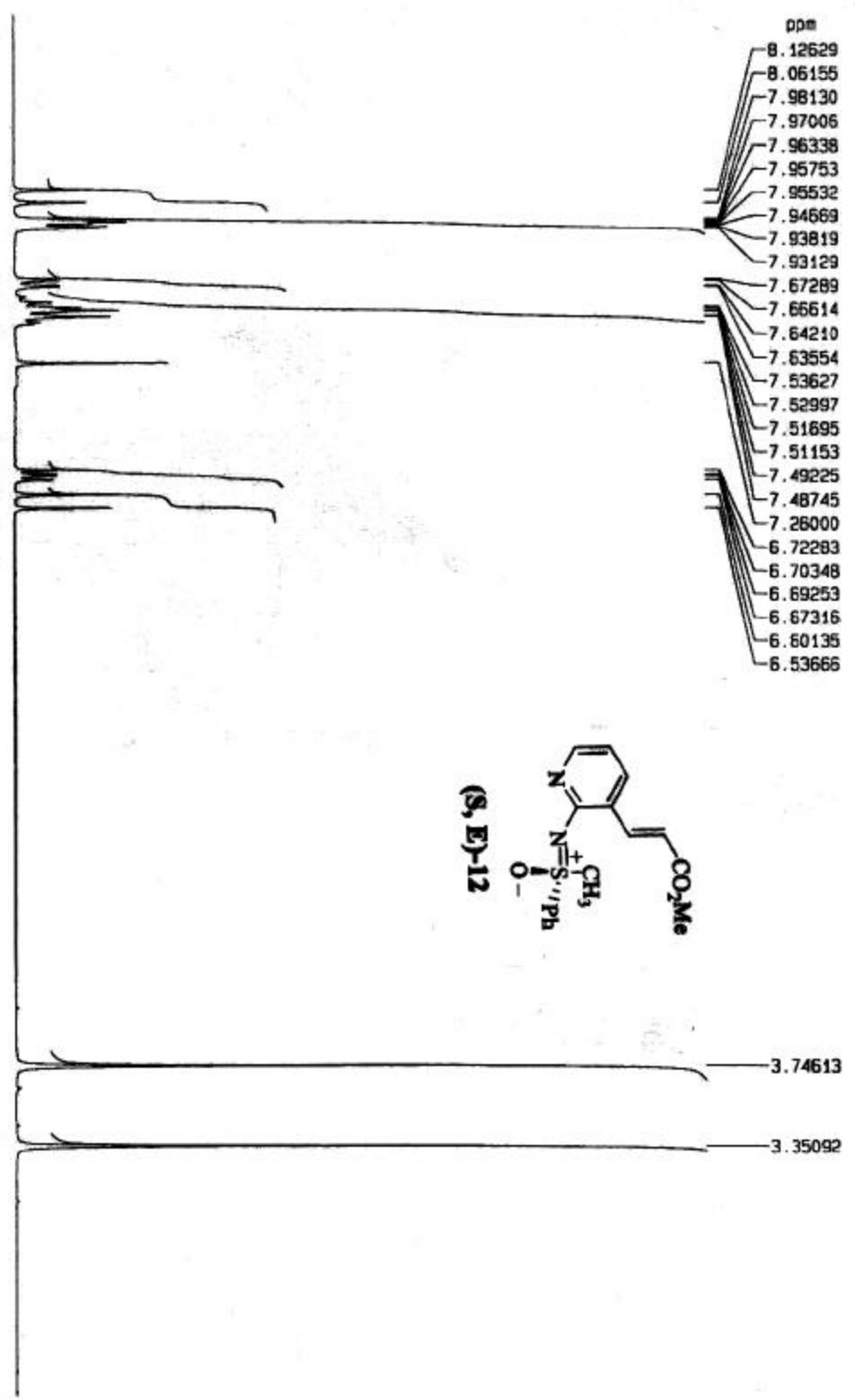
F2 - Processing parameters
 ST 16384
 SF 250.1300073 MHz
 MDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 9.000 ppm
 F1 2251.17 Hz
 F2P 2.100 ppm
 F2 525.27 Hz
 F2PPMCH 0.34500 ppm
 HZCM 86.29485 Hz/



Current Data Parameters
 NAME XH-III-73-A1
 EXPNO 2
 PROBNO 1
 F2 - Acquisition Parameters
 Date 20020913
 Time 15.28
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zgdc30
 TD 36864
 SOLVENT CDCl3
 NS 212
 DS 4
 SWH 17241.379 Hz
 R1 29.000 use
 DE 0.467702 Hz
 AQ 1.0591050 sec
 RG 22800
 D1 300.0 K
 TE 0.00002000 sec
 D12 23.00 dB
 D1 103.00 use
 P1 1.00000000 sec
 P1 5.35 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec
 F2 - Processing parameters
 SI 32768
 SF 62.8952503 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 200.000 ppm
 F1 12579.05 Hz
 F2P -10.000 ppm
 F2 -628.95 Hz
 PPMCH 10.50000 ppm
 HZCM 650.40009 Hz /



Current Data Parameters
 NAME XH-III-72-A1
 EXPND 1
 PROCN0 1

F2 - Acquisition Parameters

Date 20020913

Time 15.05

INSTRUM anx250

PROBD 5 mm QNP 1H

PULPROG 2930

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SWH 5208.333 Hz

FRAMES 0.158946 Hz

AQ 3.1457779 sec

R6 360

DW 96.000 use

DE 137.14 use

TE 300.0 K

D1 1.0000000 sec

P1 8.70 use

SFO1 250.1315321 MHz

NUCLEUS ¹H

F2 - Processing parameters

SI 15384

SF 250.1300073 MHz

MWD EM

SSB 0

LB 0.20 Hz

GB 0

PC 1.50

1D NMR plot parameters

CX 20.00 cm

CY 8.00 cm

F1P 9.000 ppm

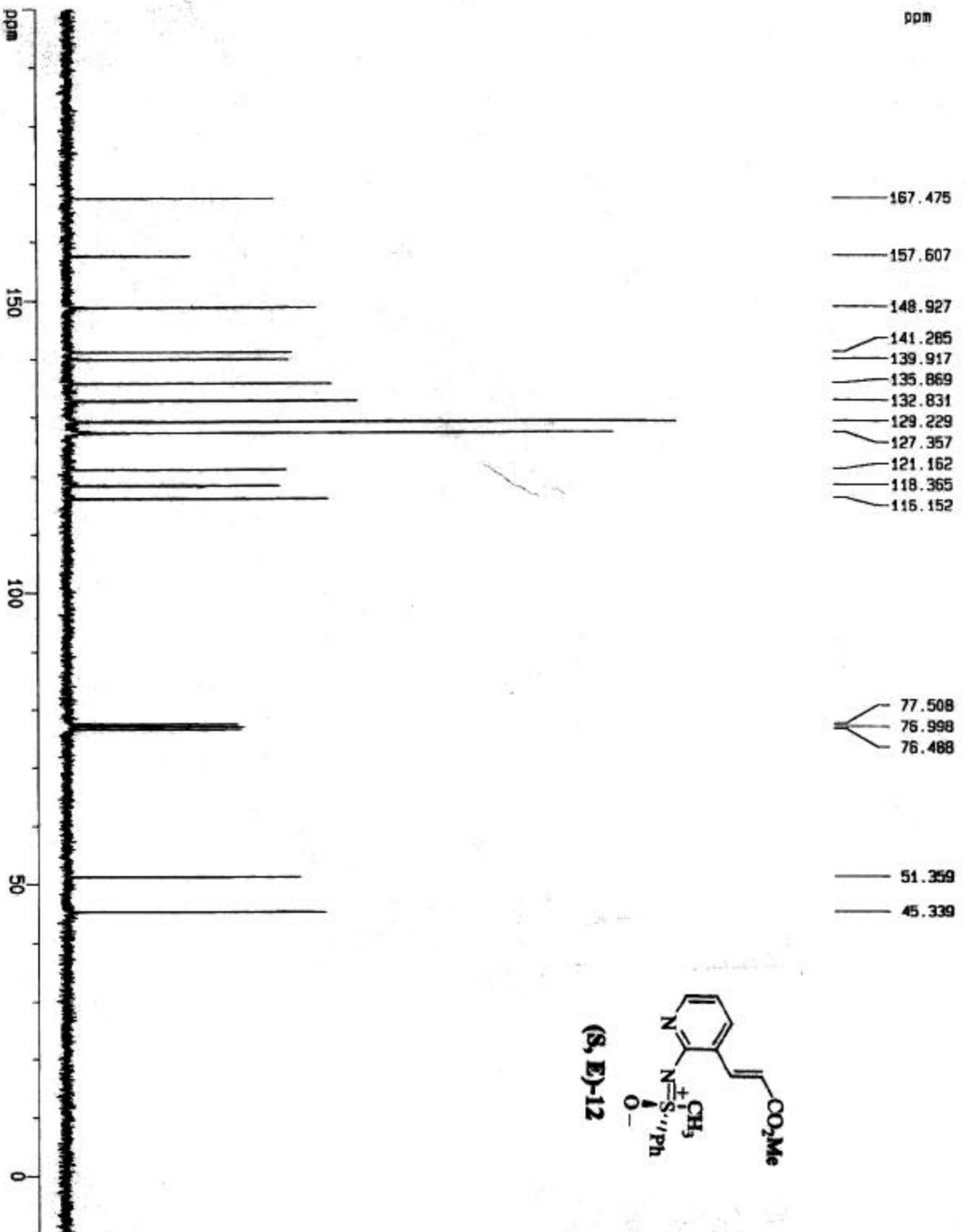
F1 2251.17 Hz

F2P 2.100 ppm

F2 525.27 Hz

PPMCH 0.34500 ppm

H2CM 86.29485 Hz/



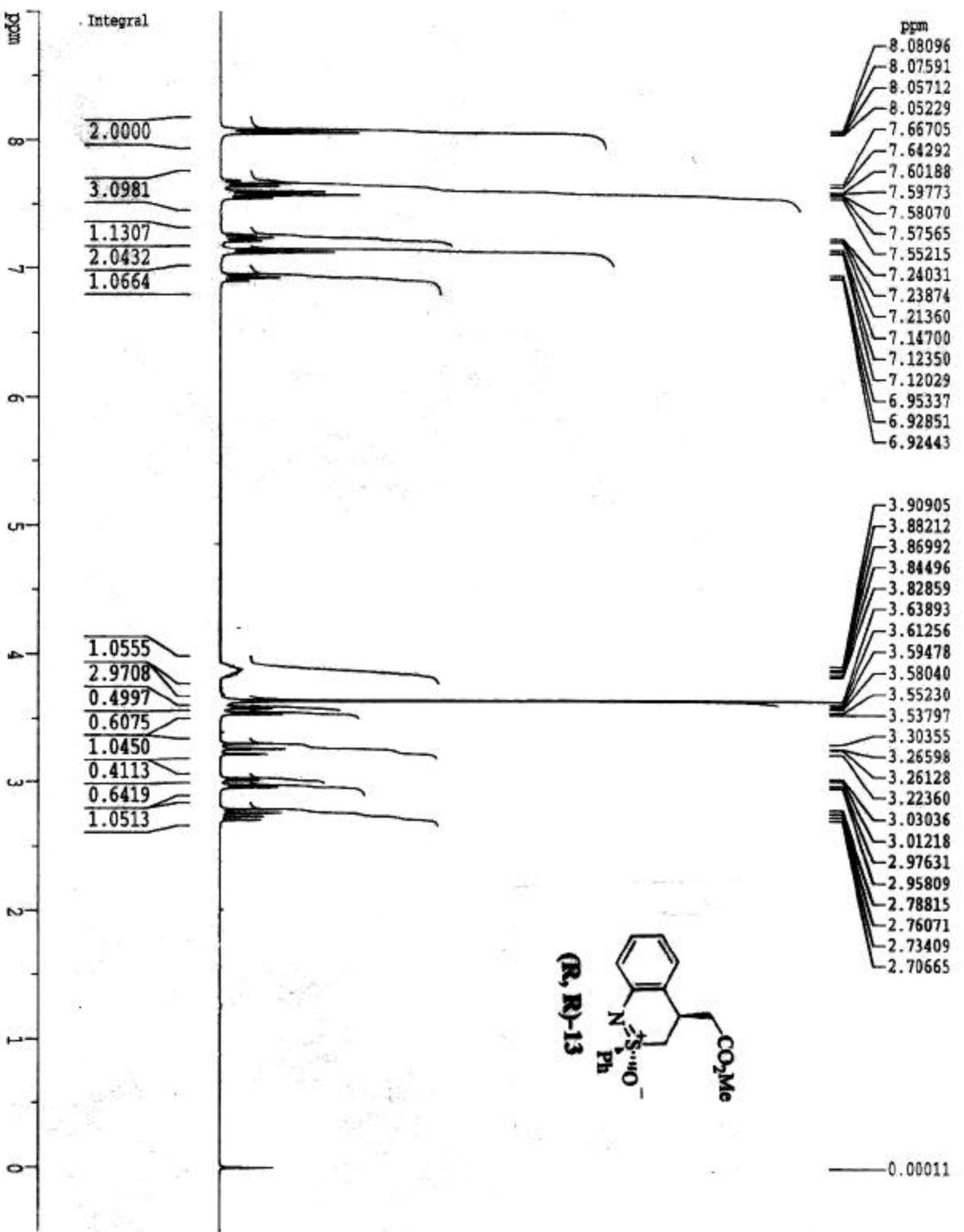
Current Data Parameters
 NAME XH-III-72-A1
 EXPNO 2
 PROCNO 1
 S-33

F2 - Acquisition Parameters	
Date	20020913
Time	15.14
INSTRUM	brx250
PROBOD	5 mm QNP 1H
PULPROG	zgdc30
TD	36864
SOLVENT	CDCl3
NS	250
DS	4
SWH	17241.379 Hz
ETR	0.467702 Hz
AQ	1.0591060 sec
RG	22800
DW	29.000 use
DE	41.43 use
TE	300.0 K
D1	0.00002000 sec
D1.5	23.00 dB
CPDPRG	Waltz15
P31	103.00 use
D1	1.0000000 sec
P1	5.35 use
SF01	62.9023694 MHz
NUCLEUS	13C
D11	0.03000000 sec

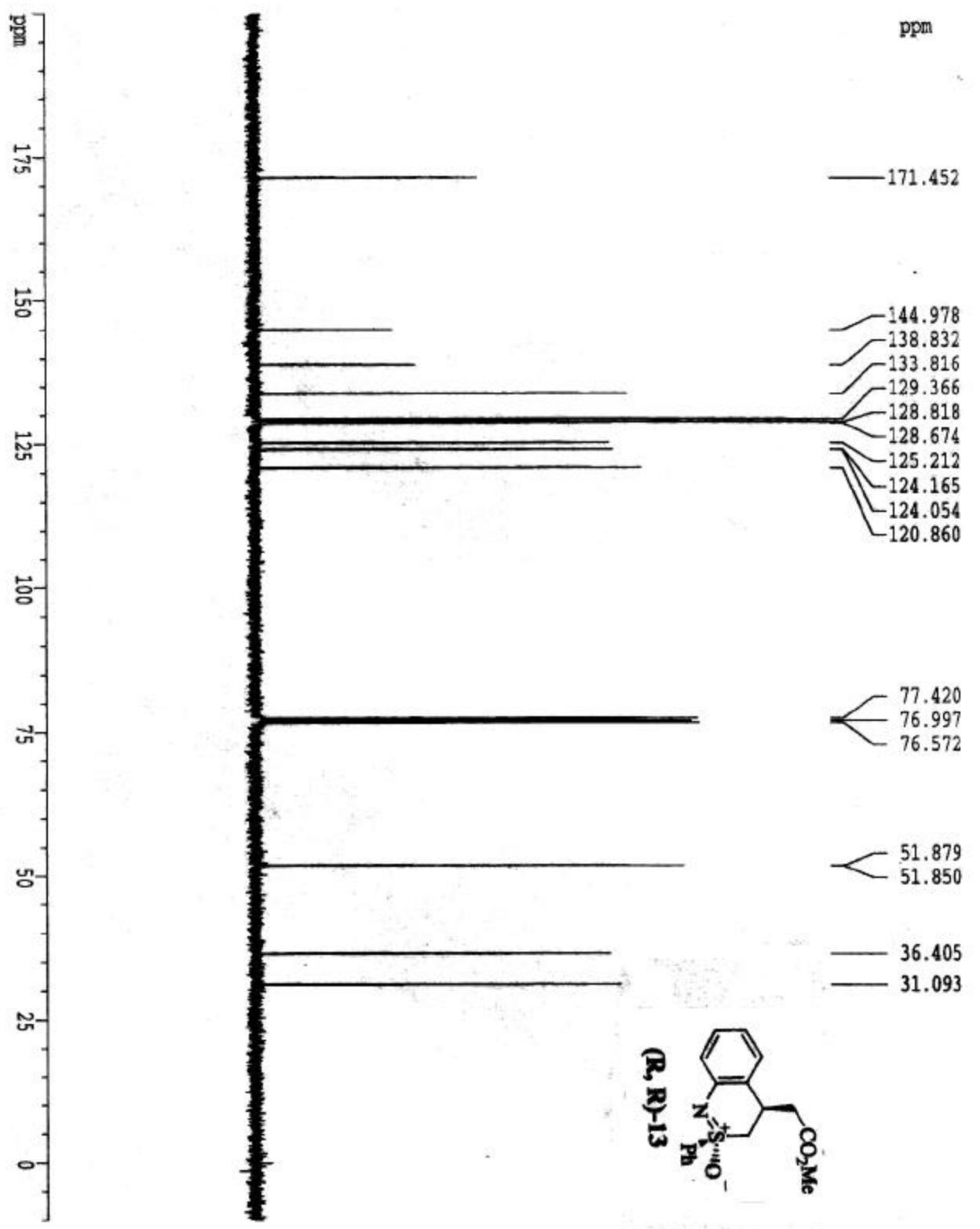
F2 - Processing parameters	
SI	32768
SF	62.8952693 MHz
DM	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	200.000 ppm
F1	12579.05 Hz
F2P	-10.000 ppm
F2	-528.95 Hz
PPCM	10.50000 ppm
HZCM	650.40015 Hz /



Current Data Parameters	
NAME	XH-I-27-1
EXPNO	1
PROCNO	
F2 - Acquisition Parameters	
Date_	2001/03/0
Time	11.55
INSTRUM	drx300
PROBOD	5 mm BBO BB-1M
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	16
DS	2
AQ	
RG	128
DW	81.000 usec
DR	6.00 usec
TR	2.6542580 sec
TE	300.0 K
DI	1.0000000 sec
P1	7.50 usec
DR	6.00 usec
SW1	6172.839 Hz
SW2	0.188380 Hz
FO1	300.1317708 MHz
NUC1	1H
PL1	0.00 dB
F2 - Processing parameters	
ST	16384
SP	300.1300056 MHz
WDW	EM
SSB	0
LB	0
GB	0.30 Hz
PC	1.50
1D NMR plot parameters	
CX	20.00 cm
CY	12.50 cm
FLP	9.000 ppm
F1	2701.17 Hz
F2P	-0.500 ppm
F2	-150.07 Hz
PPCM	0.47500 ppm/cm
HZCM	142.56175 Hz/cm



F2 - Processing parameters

SI	32768
SP	75.4677557 MHz
NDW	1000
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
FLP	200,000 pps
P1	15033.55 Hz
F2P	-10.00 ppm
F2	-754.68 Hz
PPM/CM	10.50000 Hz/cm
HZ/CM	792.4114 Hz/cm

Current Data Parameters

NAME	XH-I-27-1
EXPO	2
PROCNO	1

F2 - Acquisition Parameters

Date_ 20011030

Time 12.04

INSTRUM dtx300

PROBD 5 mm BBO BB-1H

PULPROG zgdc30

TD 6536

SOLVENT CDCl3

NS 4

SWH 21645.021 Hz

EDD 0.330277 Hz

AQ 1.5139316 sec

RG 32768

DM 23.100 usec

DR 6.00 usec

TE 300.0 K

D1 0.03000000 sec

PL12 24.50 dB

CPDPRG2 waltz16

PCP2 100.00 usec

SR02 300.1315007 MHz

NUC2 1H

PL2 1.00000000 sec

D1 7.75 usec

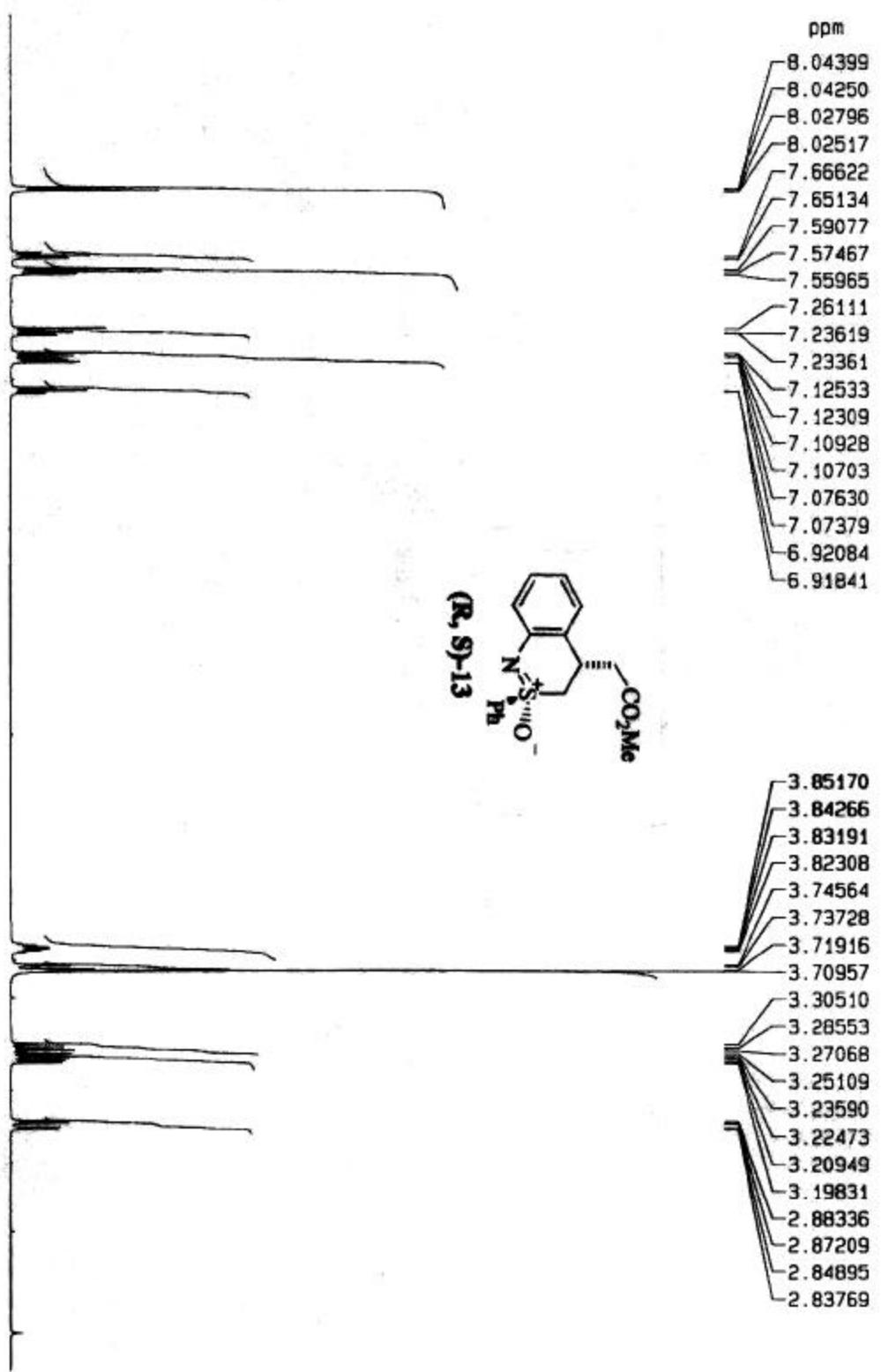
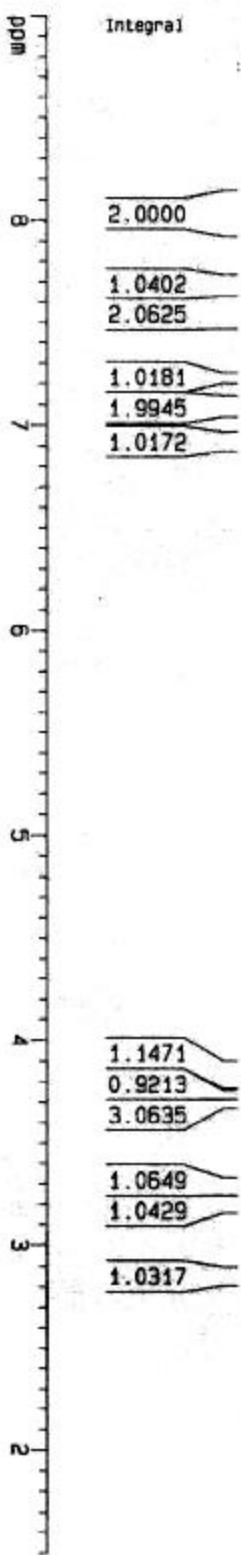
P1 6.00 usec

DE 75.4769164 MHz

SFO1 13C

NUC1 6.00 dB

PL1



Current Data Parameters

NAME XH-IV-98-A1

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date 20030214

Time 10.37

INSTRUM DRX500

PROBOD 5 mm Multinuci

PULPROG zg30

TD 57344

SOLVENT CDCl₃

NS 16

DS 2

SWH 10330.578 Hz

FIDRES 0.180151 Hz

AQ 2.7754996 sec

R6 64

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 500.1300128 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 9.000 ppm

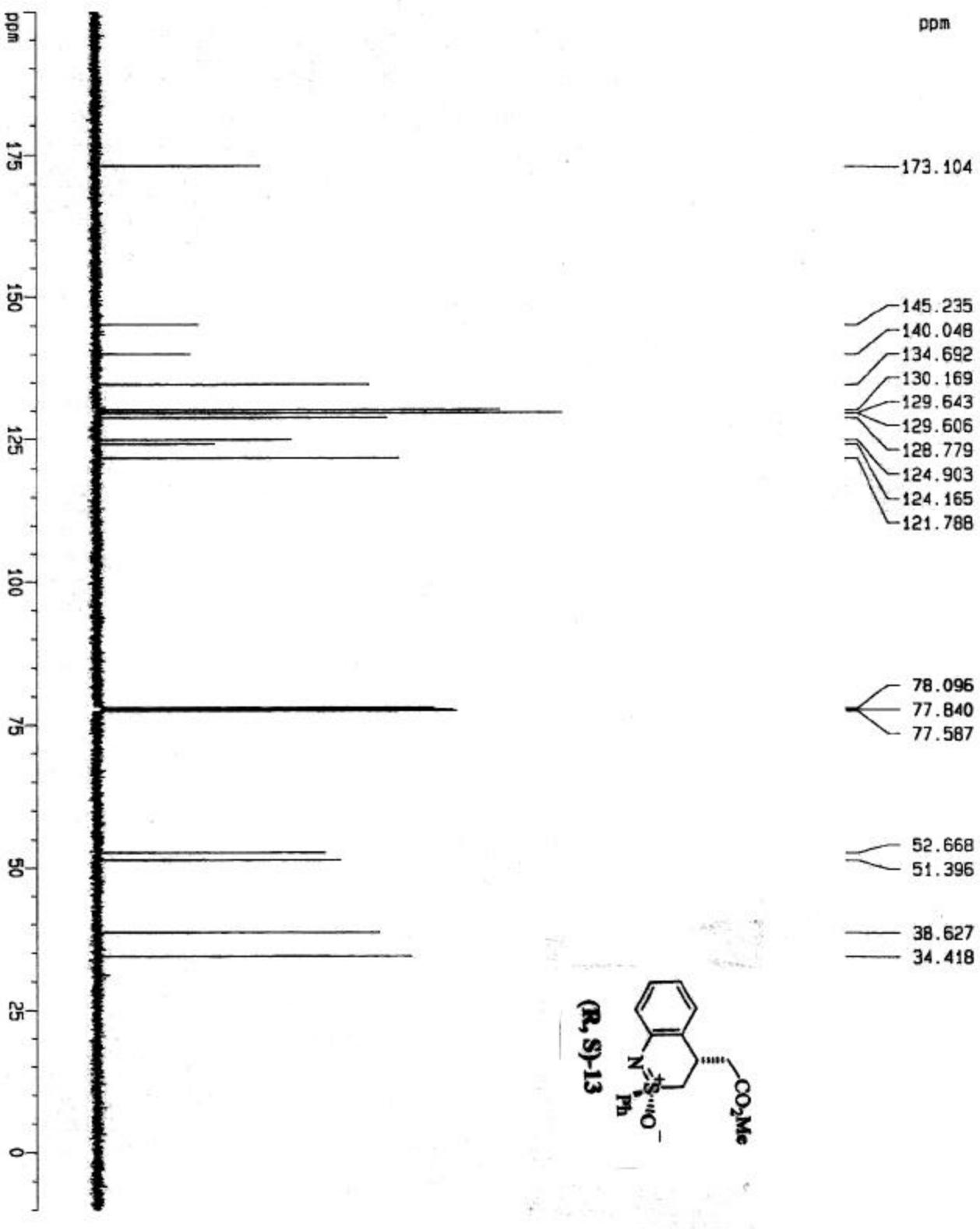
F1 4501.17 Hz

F2P 1.500 ppm

F2 750.20 Hz

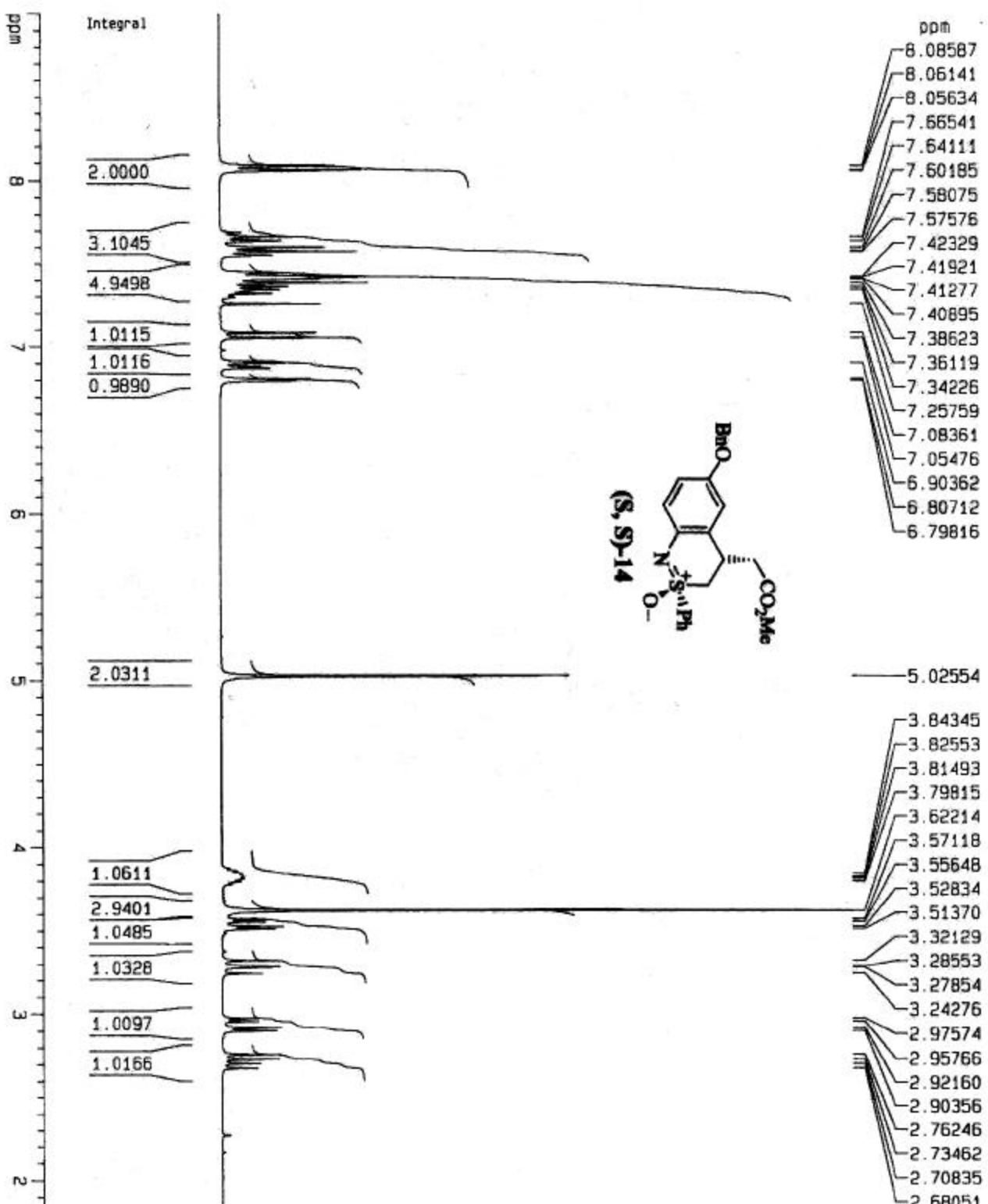
PPMCH 0.37500 ppm/c

HZCM 187.54675 Hz/c

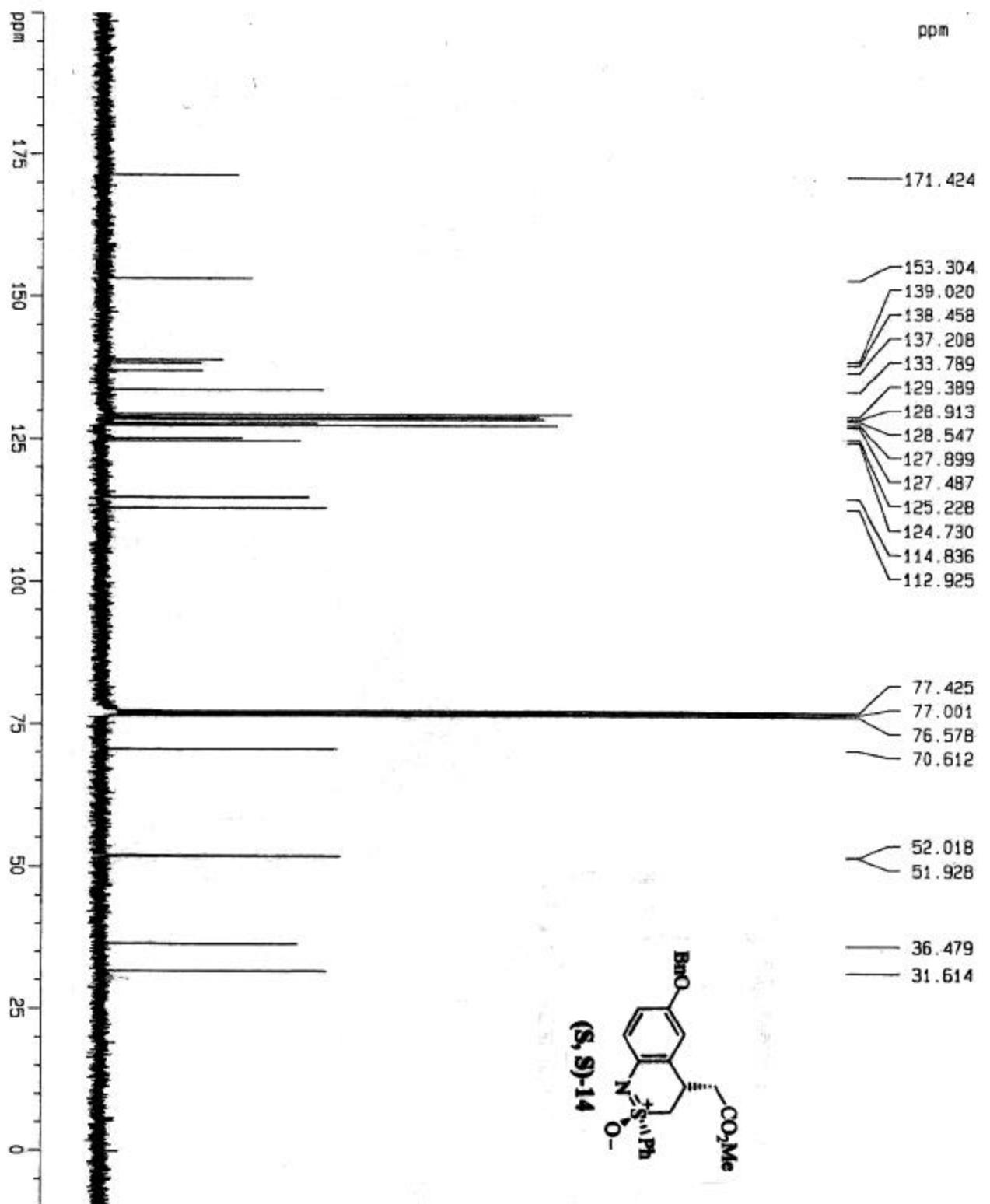


Current Data Parameters	
NAME	XH-IV-9B-A1
EXPO	2
PROCNO	1
F2 - Acquisition Parameters	
Date	2003/21/14
Time	10:41
INSTRUM	DNP300
PROBHD	5 mm Multincl
PULPROJ	299.030
TD	65536
SOLVENT	DCD13
NS	154
DG	4
SWH	39681.812 Hz
FIDRES	0.605496 Hz
AQ	0.82581081 sec
RG	16384
DW	12.600 usec
DE	6.00 usec
TE	256.0 K
D1	1.0000000 sec
d11	0.03000000 sec
CHANNEL f1	
NUC1	13C
P1	7.90 usec
PL1	3.00 dB
SF01	125.7713108 MHz
CHANNEL f2	
CPDPFG2	500.1320006 MHz
NUC2	1H
PCPDP2	88.00 usec
PL2	0.00 dB
PL12	21.00 dB
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
1D NMR plot parameters	
CK	20.00 cm
CY	8.00 cm
F1P	200.000 ppm
F1	25151.54 Hz
F2P	-10.000 ppm
F2	-1257.58 Hz
PPMCM	10.50000 ppm/cm
HZCM	1320.45581 Hz/cm

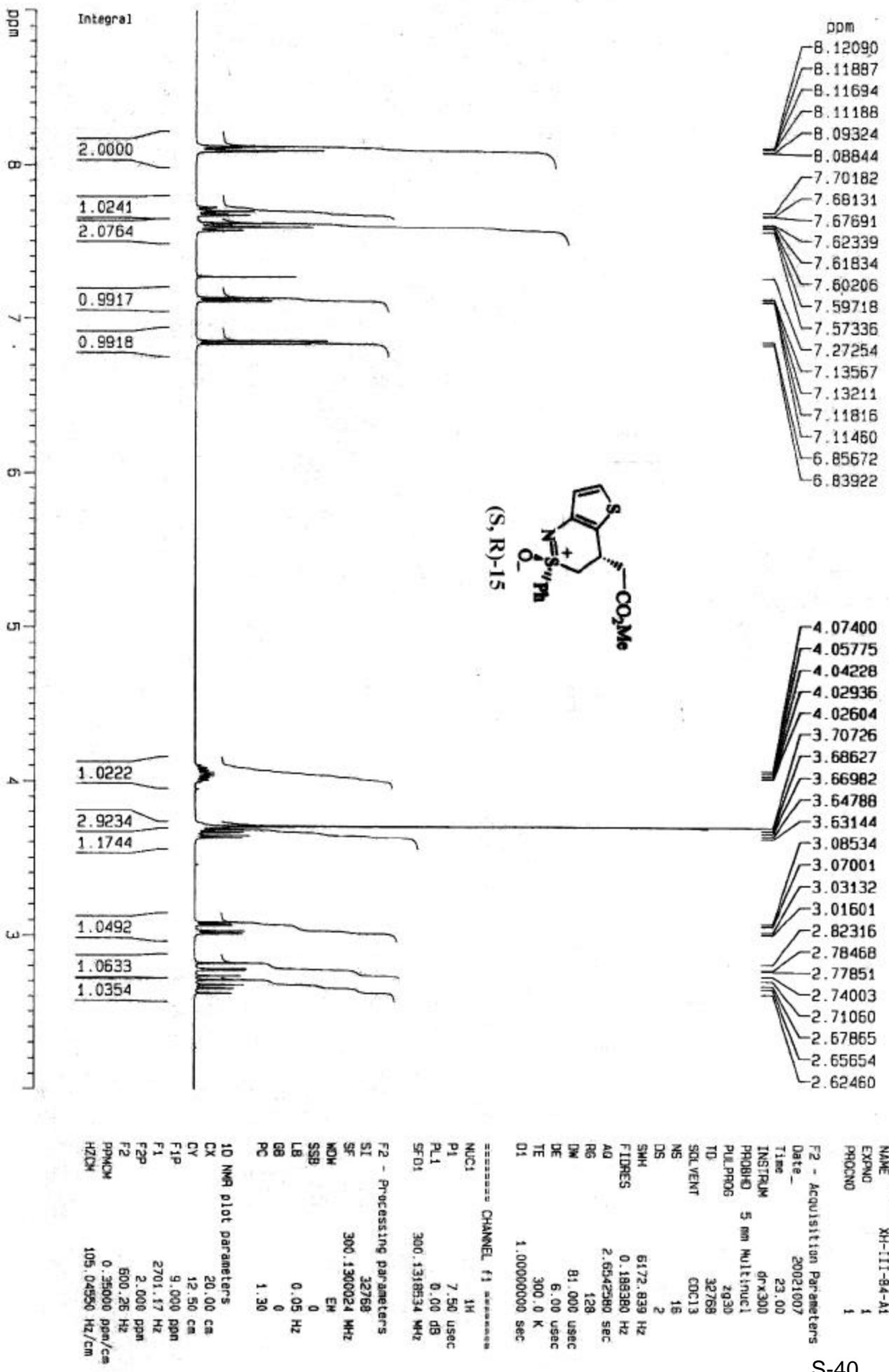
1H NMR

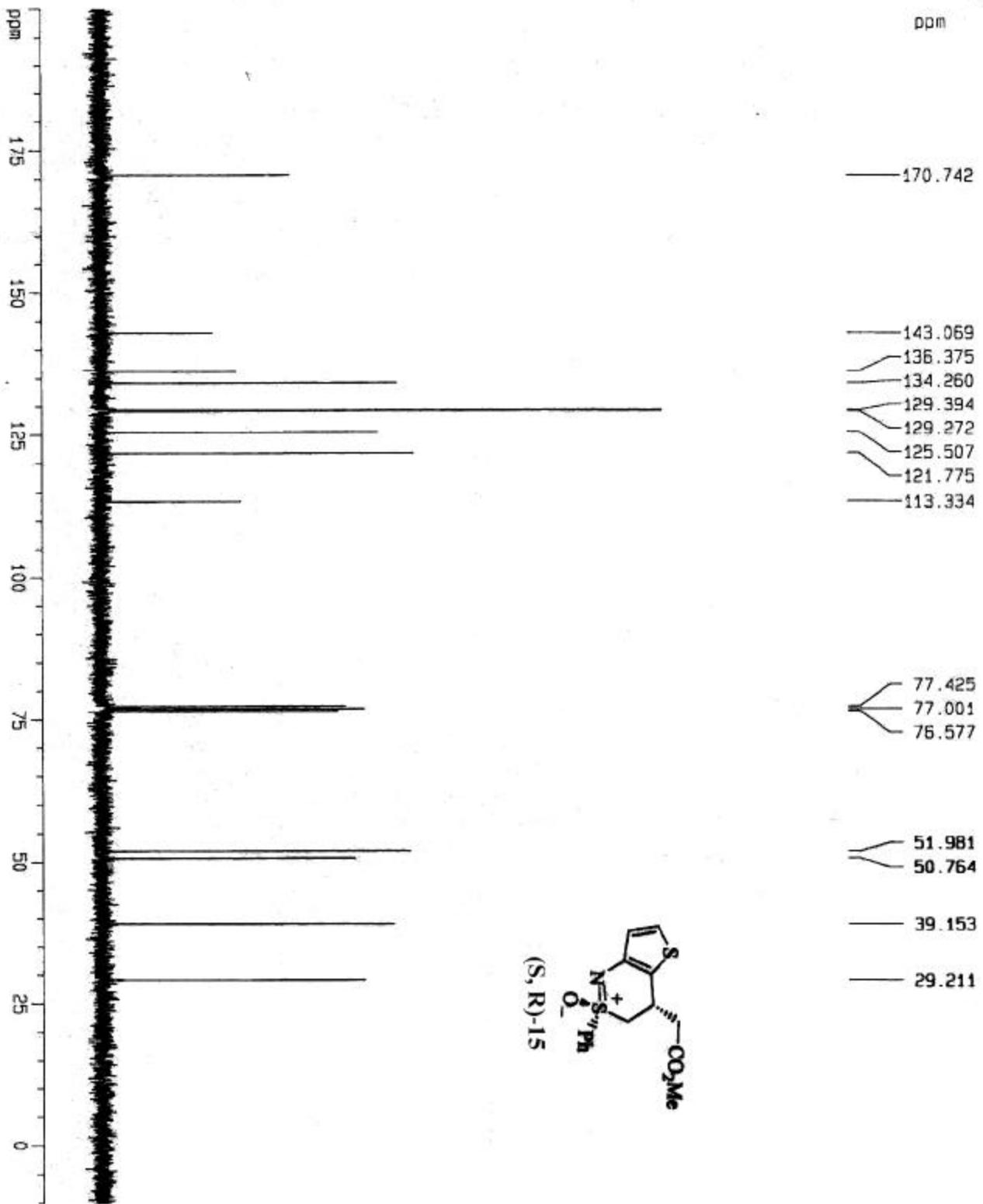


Current Data Parameters	
NAME	XH-1-100-A1
EXPO	1
PRODNO	1
F2 - Acquisition Parameters	
Date	20020901
Time	16.13
INSTRUM	drx300
PROBHD	5 mm Multinuc
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
RG	0.188380 Hz
FORES	2.6542580 sec
AQ	362
DW	81.000 usec
DE	5.00 usec
TE	300.0 K
DT	1.0000000 sec
***** CHANNEL f1 *****	
NUC1	1H
P1	7.50 usec
PL1	0.00 dB
SF01	300.1319534 MHz
F2 - Processing parameters	
SI	32768
SF	300.1300069 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	9.000 ppm
F1	2701.17 Hz
F2P	1,800 ppm
F2	540.23 Hz
PPMCM	0.360000 ppm/cm
HZCM	108.04581 Hz/cm



Current Data Parameters	
NAME	XH-I-100-A1
EXPO.	2
PRGNO	1
F2 - Acquisition Parameters	
Date	20020901
Time	16.21
INSTRUM	dr-300
PROBHD	5 mm Multinuc1
PULPROG	Zgdc30
TD	65536
SOLVENT	CDCl3
NS	6191
DS	4
SWH	18850.141 Hz
FORES	0.28630 Hz
RG	1.7389924 sec
DM	32758
DE	26.525 usec
TE	37.89 usec
PL1	300.0 K
D1	1.0000000 sec
SI	0.0300000 sec
***** CHANNEL f1 *****	
NUC1	13C
P1	7.75 usec
PL1	6.00 dB
SFO1	75.4760107 MHz
***** CHANNEL f2 *****	
CPDPG2	Mult16
NUC2	1H
PCP02	100.00 usec
PL2	120.00 dB
PL12	24.50 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677519 MHz
MDW	EH
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
1D NMR plot parameters	
CX	20.00 cm
CY	8.00 cm
F1P	200.000 ppm
F1	15053.55 Hz
F2P	-10.000 Hz
F2	-754.68 Hz
PPMCM	105000 ppm/cm
HZCM	792.41138 Hz/cm





F2 - Acquisition Parameters

NAME	XH-III-84-A1
DATE	20021007
TIME	23:02
INSTRUM	drx300
PROBID	5 mm MultiIncl
PULPROG	290E30
TD	65536
SOLVENT	CDCl ₃
NS	305
D1	4
SWH	18000.141 Hz
FLDRES	0.287630 Hz
A1	1.738394 sec
R1	32768
DE	26.525 usec
TE	37.89 usec
D1	300.0 K
d11	1.0000000 sec
DS	0.0300000 sec

===== CHANNEL 12 =====

CPDPK62	Waitz16
NUC1	13C
P1	7.75 usec
PL1	6.00 dB
SFO1	75.4760107 MHz

===== CHANNEL 11 =====

CPDPK62	Waitz16
NUC1	1H
PCP02	100.00 usec
PL2	120.00 dB
PL12	24.50 dB
SFO2	300.1312005 MHz

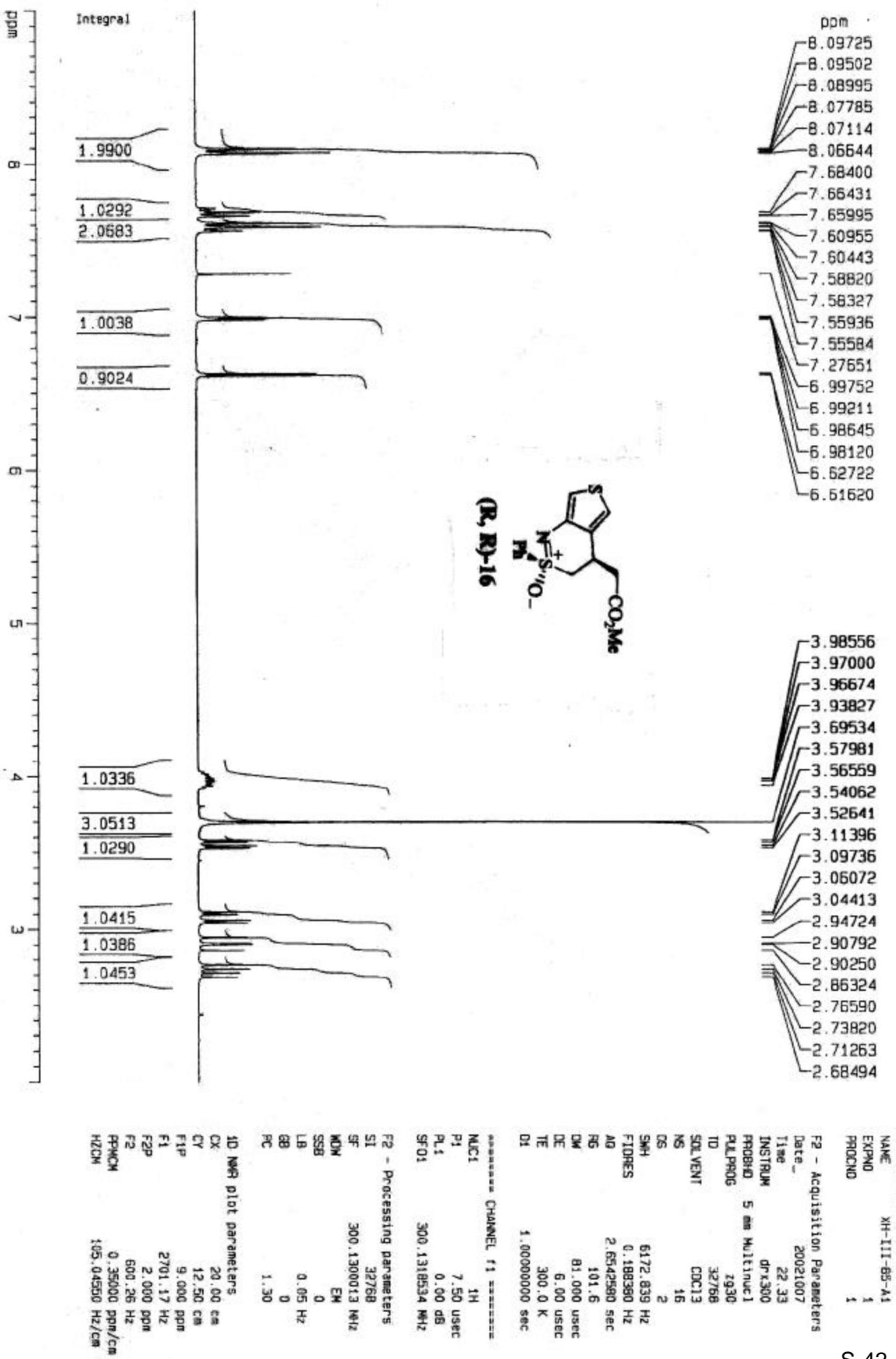
F2 - Processing parameters

SI	32768
SF	75.4677571 MHz
WDW	EN
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

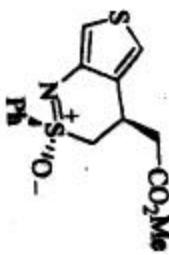
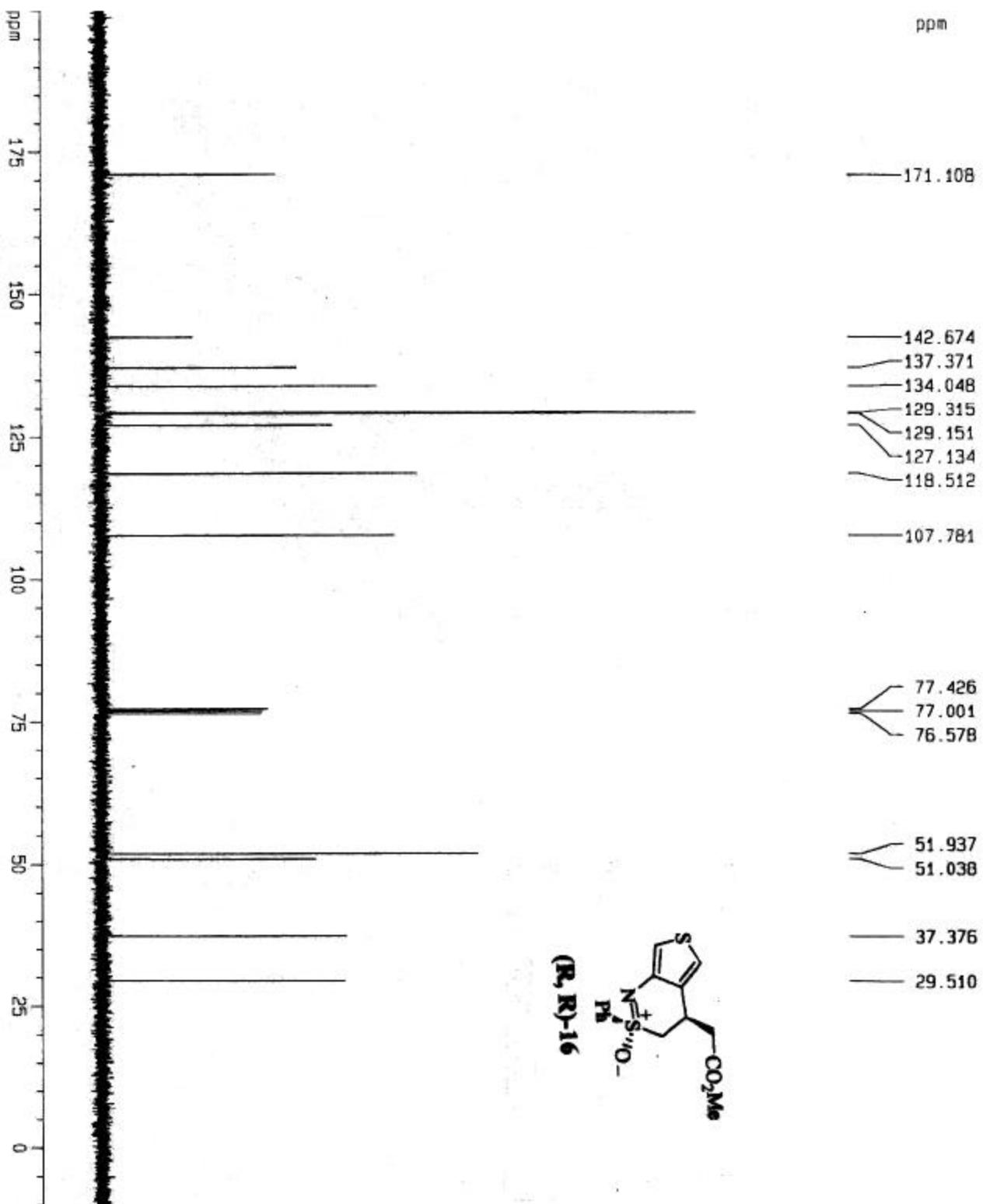
1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
Flip	200.000 ppm
F1	150.9355 Hz
F2	-10.000 ppm
F2P	-754.68 Hz
PPMCH	10.50000 ppm/
HZCM	792.41144 Hz/c

1H NMR



¹³C NMR



Current Data Parameters
NAME NH-111-85-A1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 2002/06/7
Time 22:38
INSTRUM drx300
PROBHD 5 mm Multinucl
PULPROG zgpc30
TD 65536
SOLVENT DCl/3
NS 374
DS 4
SWH 16650.141 Hz
FIDRES 0.287650 Hz
AQ 1.7383924 sec
RG 32768
DM 26.505 usec
DE 37.89 usec
TE 300.0 K
D1 1.0000000 sec
d11 0.0300000 sec

CHANNEL f1

NUC1	¹³ C
P1	7.75 usec
PL1	6.00 dB
SF01	75.4760107 MHz

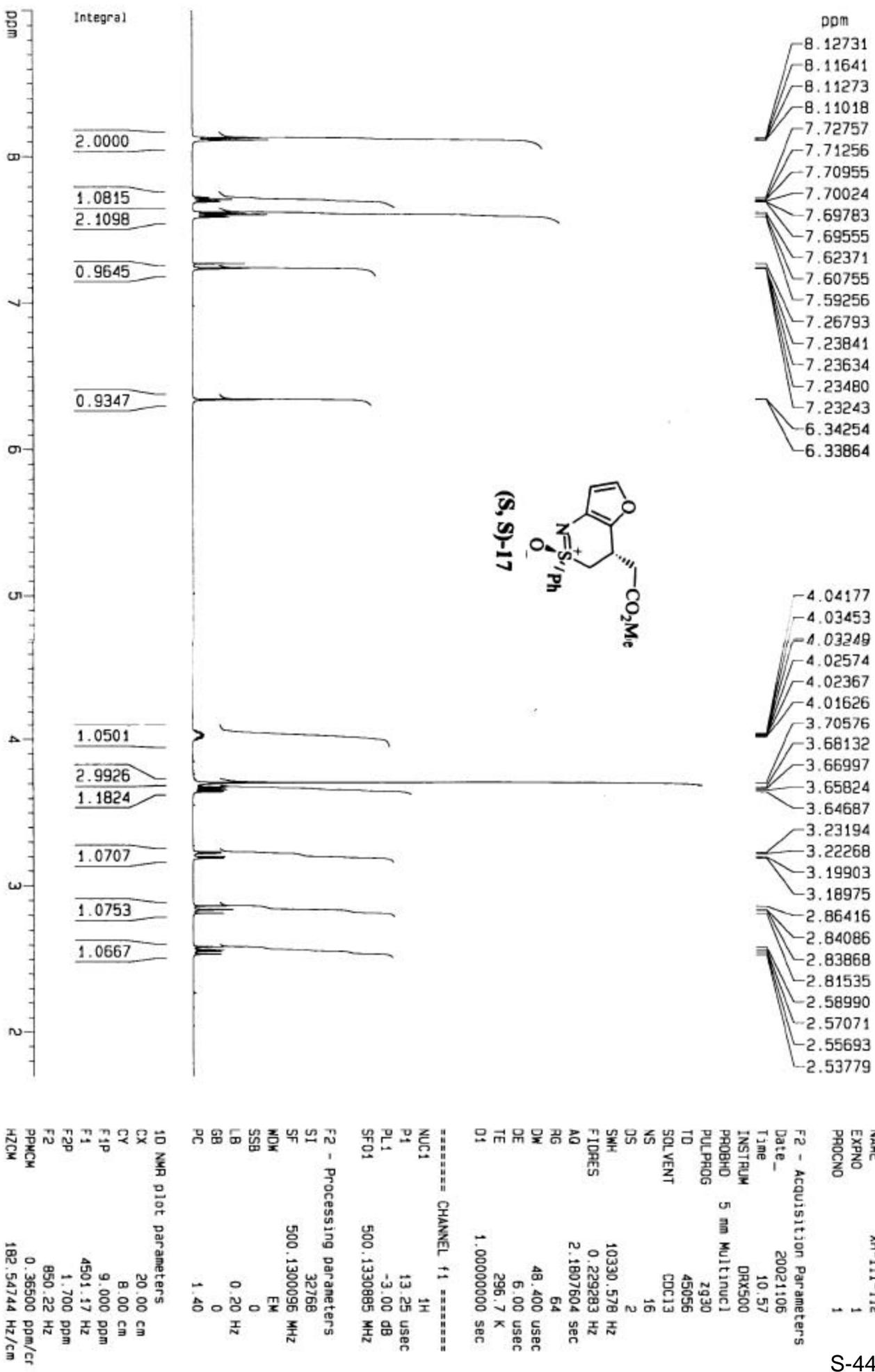
CHANNEL f2

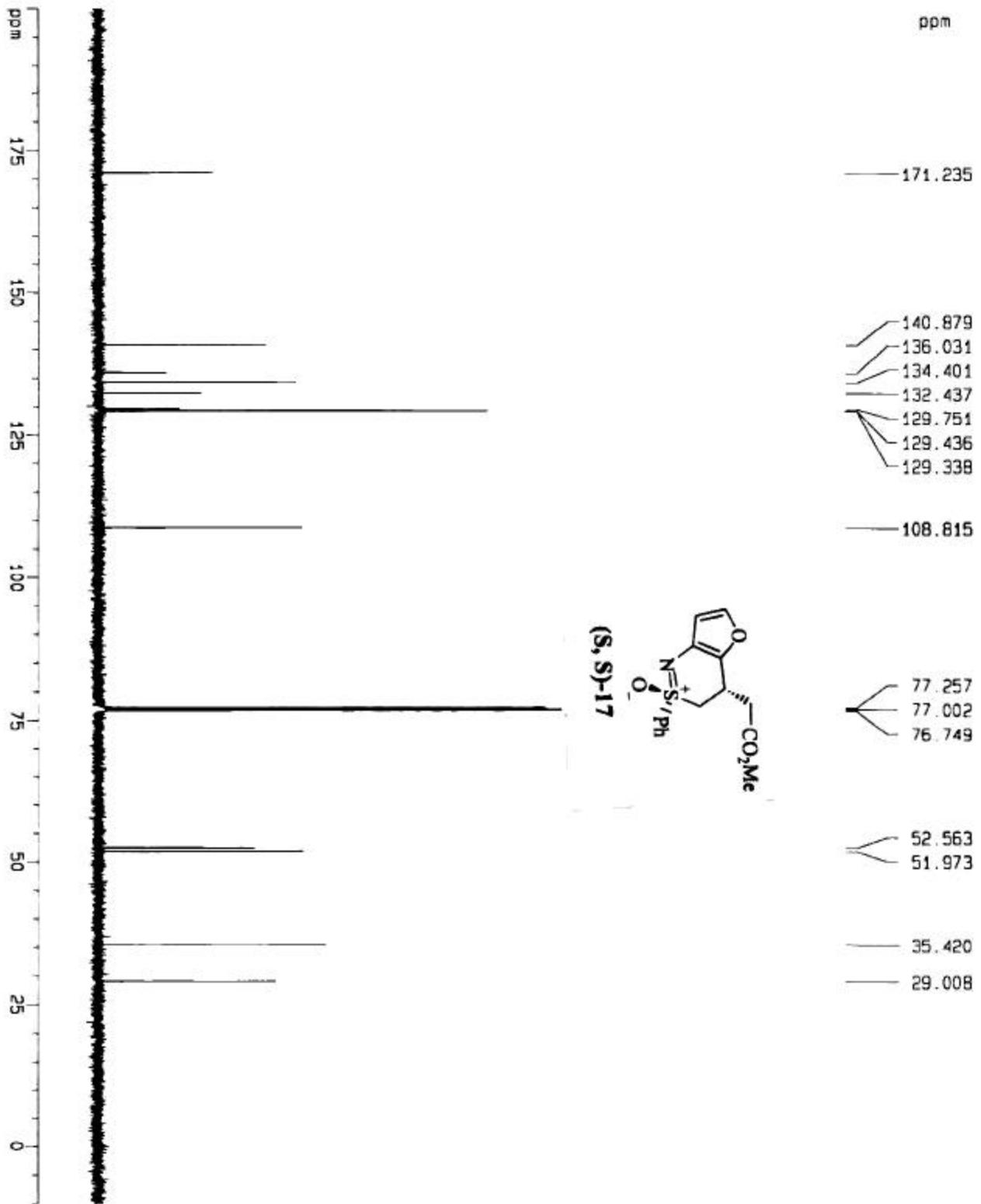
OPRF1G2	mult16
NUC2	¹ H
PCP02	100.00 usec
PL2	120.00 dB
PL12	24.50 dB
SF02	300.1312005 MHz

F2 - Processing parameters

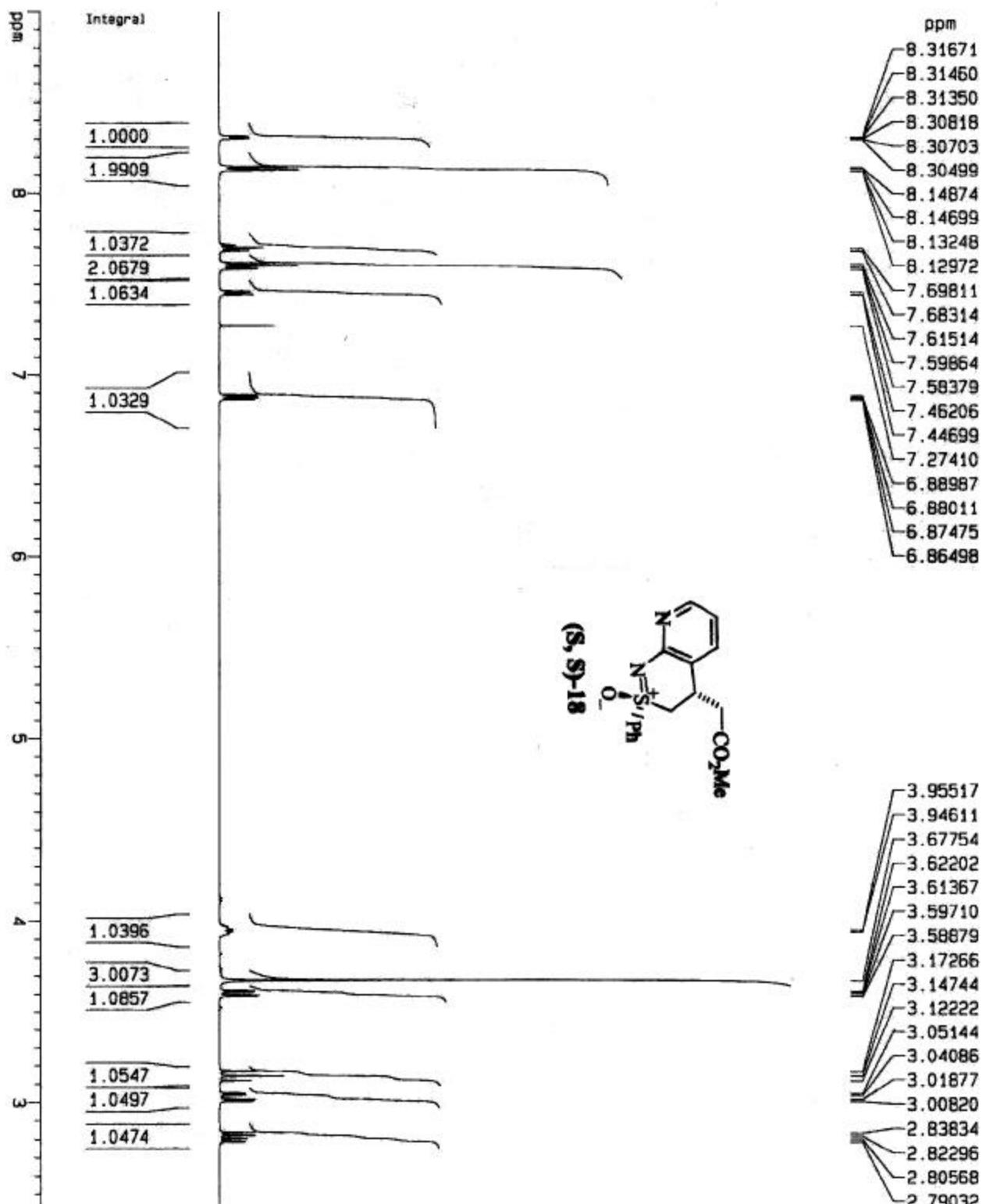
SI	32768
SF	75.4677594 MHz
NUW	EW
SSB	0
LB	0.30 Hz
GB	0
PC	1.40

1D NMR plot parameters	
CX	20.00 cm
CY	10.00 cm
CP	200.000 ppm
F1	{5993.55 Hz
F2	-10.000 ppm
F2	-754.68 Hz
PPMCH	10.50000 ppm/cm
PPCM	792.4114 Hz/cm

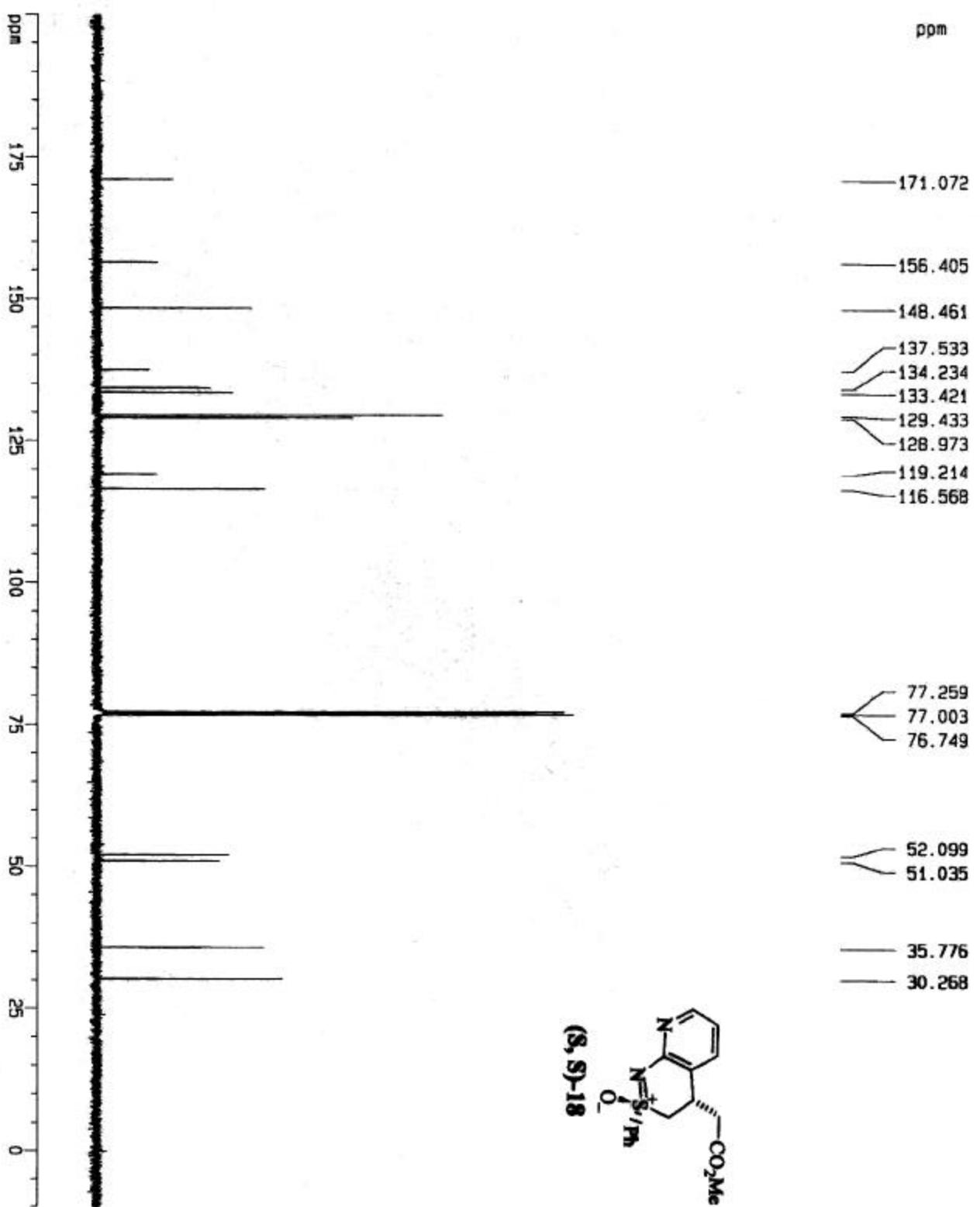




Current Data Parameters	
NAME	XH-III-112
EXPNO	2
PROCNO	1
F2 - Acquisition Parameters	
Date	2002/10/05
Time	11.03
INSTRUM	DRA500
P1	90.00
PR1	5 mm Multinucl
PULPROG	zgoc30
TD	65536
SOLVENT	CDC13
NS	222
DS	4
SWH	30681.812 Hz
ETOT	0.650495 Hz
RG	0.6258188 sec
GS	16.384
DW	12.500 usec
DE	6.00 usec
TE	298.0 K
DM	1.0000000 sec
DT	0.0300000 sec
----- CHANNEL f1 -----	
N1	13C
P1	7.90 usec
PL1	3.00 dB
SP1	125.7713108 MHz
SW1	500.1320005 MHz
----- CHANNEL f2 -----	
NUC2	1H
PCP2	88.00 usec
PL2	0.00 dB
PL12	21.00 dB
SG12	500.1320005 MHz
F2 - Processing parameters	
SI	32768
SF	125.7577947 MHz
MON	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
1D NMR dist parameters	
CX	20.00 cm
CY	8.00 cm
F1P	200.000 ppm
F1	25151.56 Hz
F2P	-10.000 ppm
F2	-1257.58 Hz
PPMCH	10.50000 ppm/cm
HZCM	1360.45691 Hz/cm



Current Data Parameters	
NAME	XH-III-134-2
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date_	2021105
Time	11.10
INSTRUM	DRX500
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	45056
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	10330.578 Hz
FIRES	2.229283 Hz
AQ	2.1807604 sec
RG	64
DW	48.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.0000000 sec
CHANNEL f1	
NUC1	¹ H
P1	13.25 usec
PL1	-3.00 dB
SF01	500.1330885 MHz
F2 - Processing parameters	
SI	32768
SF	500.1300065 MHz
KDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.40
1D NMR plot parameters	
CX	20.00 cm
CY	8.00 cm
F1P	9.000 ppm
F1	4501.17 Hz
F2P	2.400 ppm
F2	1200.31 Hz
PPCM	0.33000 ppm/ Hz/cm
HCZM	165.04289 Hz/cm



Current Data Parameters

NAME	XH-III-134-2
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date	2002106
Time	11.14
INSTRUM	DRX500
PROBHD	5 mm Multinucl
POLARBG	zgpc30
TD	65536
SOLVENT	ODC13
NS	348
DS	4
SWH	26681.812 Hz
ETRATES	0.655496 Hz
AQ	0.828188 sec
RG	16384
DW	12.600 usec
DE	6.00 usec
TE	298.0 K
D1	1.000000 sec
d11	0.0300000 sec

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

NUC1	13C
P1	7.90 usec
PL1	3.00 dB
SP01	125.7713108 MHz

===== CHANNEL f2 =====

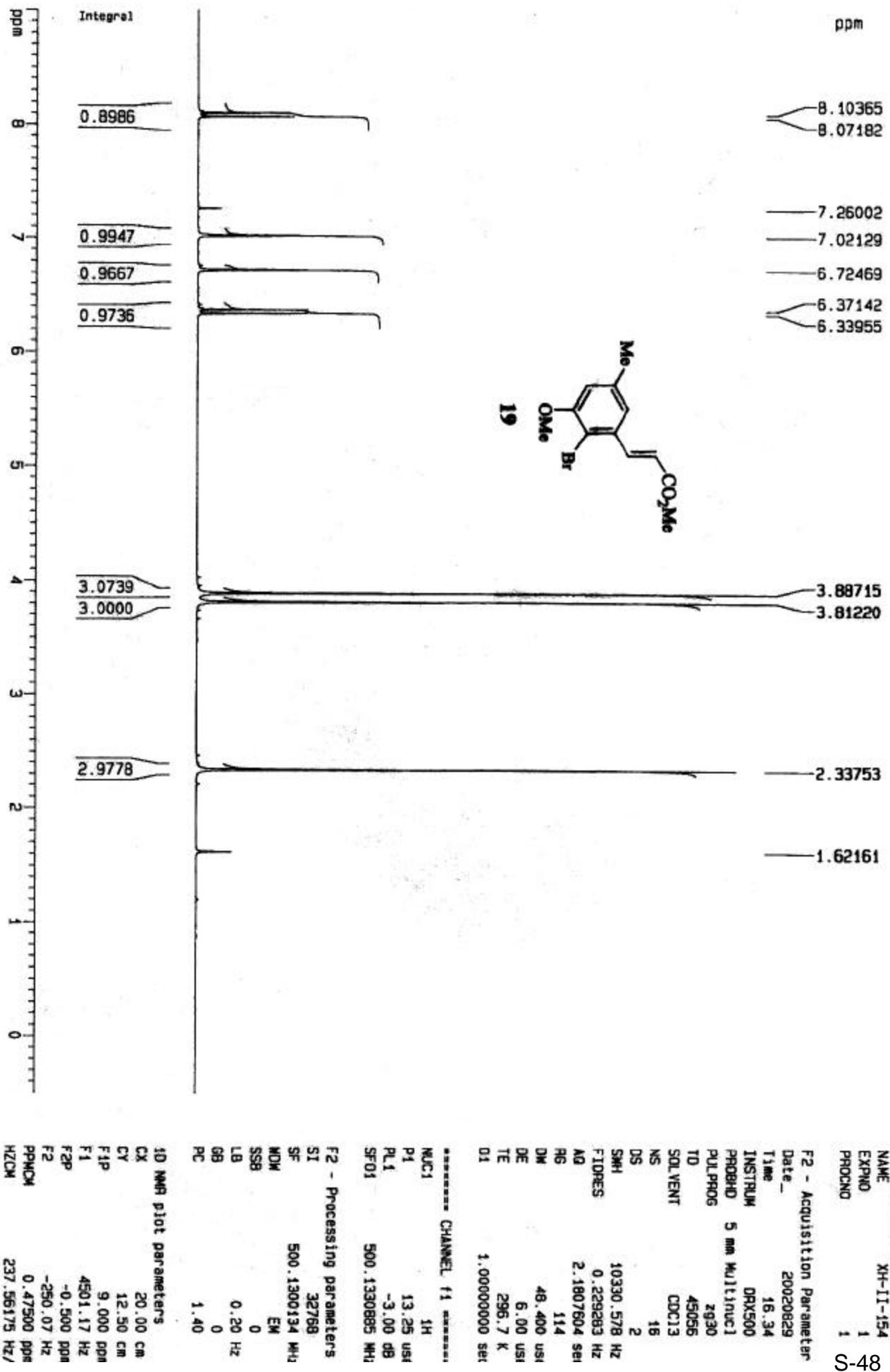
CPDPR2	Waltz16
NUC2	1H
PCPD2	BB.00 usec
PL2	0.00 dB
PL12	21.00 dB
SP02	500.1320005 MHz

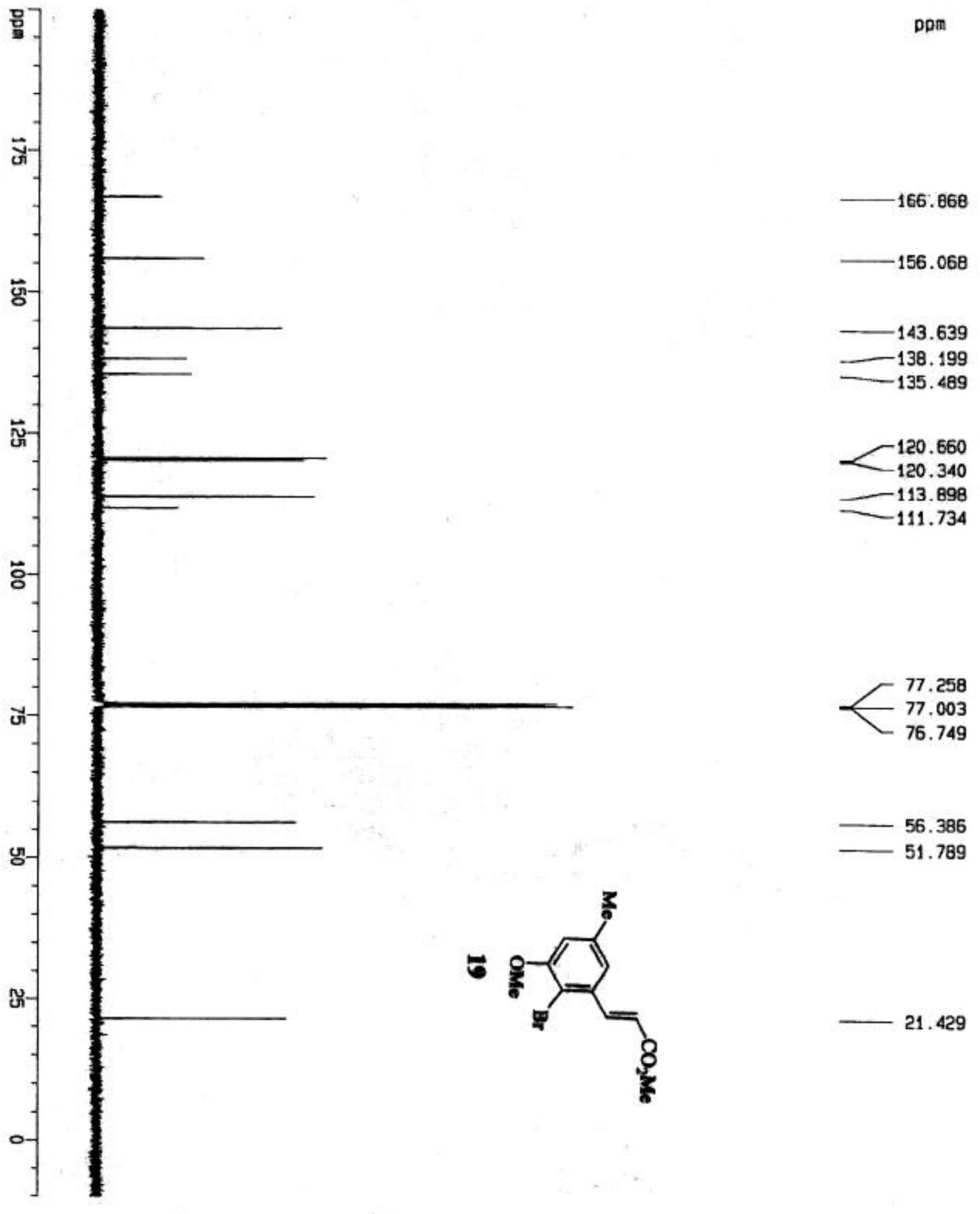
F2 - Processing parameters

SI	32768
SF	125.757959 MHz
NDW	EM
SSB	0
LB	1.00 Hz
OB	0
PC	1.40

10 user plot parameters

CX	20.00 cm
CY	8.00 cm
F3P	200.000 ppm
F3	25.151.56 Hz
F2P	-10.000 ppm
F2	-1257.59 Hz
PPMCH	10.50000 ppm/cm
HZCM	1320.45681 Hz/cm





Current Data Parameters
 NAME XH-II-154
 EXPND 2
 PRODNO 1

F2 - Acquisition Parameters
 Date 20020829
 Time 16.37
 INSTRNMN DRX500
 PROBHD 5 mm Multinuclei
 PULPROG 280C30
 TD 65536
 SOLVENT DDC13
 NS 270
 DS 4
 SWH 39681.812 Hz
 FIDRES 0.605496 Hz
 ACQ 0.8258188 sec
 R6 16384
 DM 12.600 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.0000000 sec
 D11 0.03000000 sec

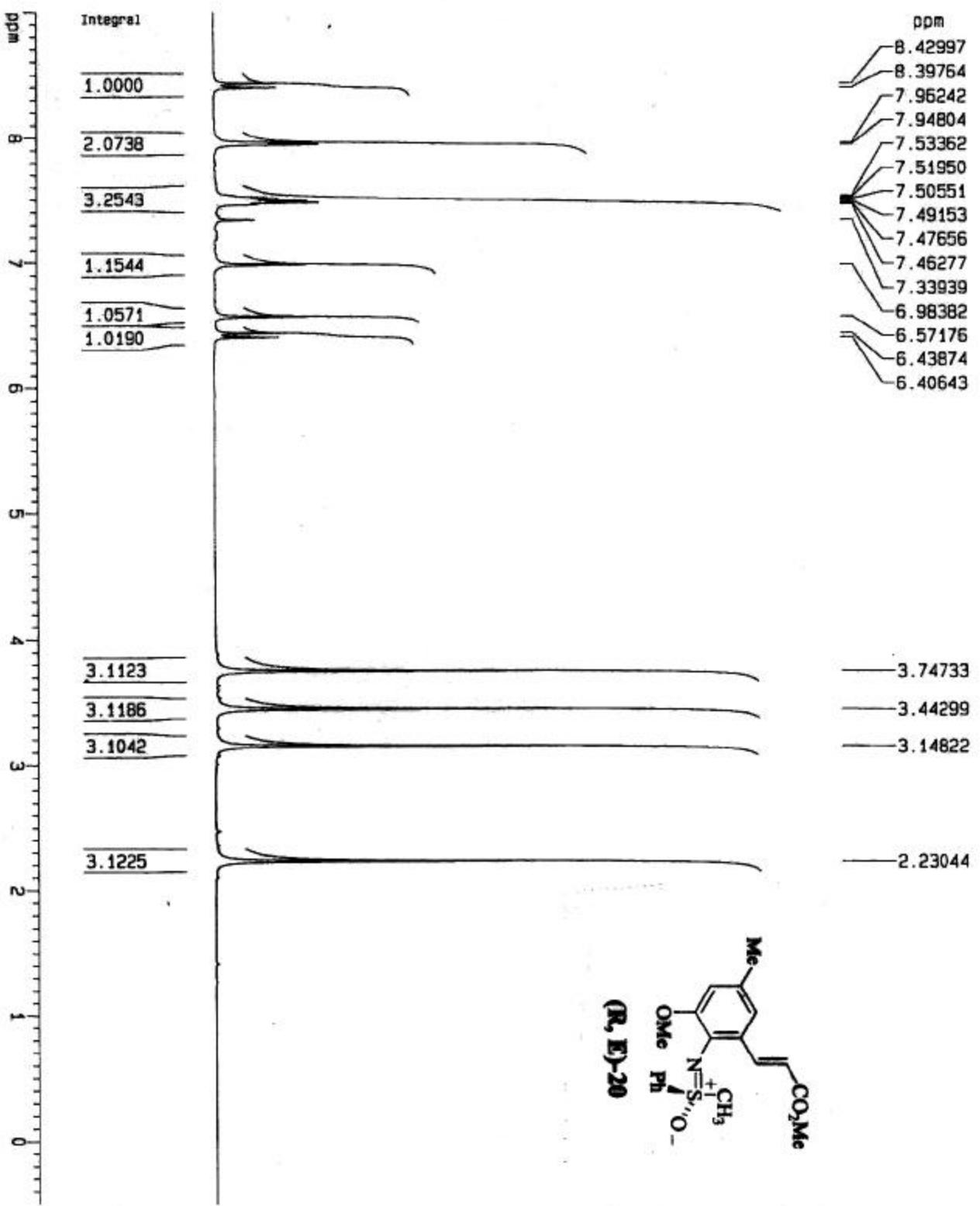
***** CHANNEL f1 *****
 NUC1 13C
 P1 8.24 usec
 PL1 3.00 dB
 SFO1 125.7713108 MHz

***** CHANNEL f2 *****
 CPDPG2 wait:15
 NUC2 1H
 P0P2 107.00 usec
 PL2 0.00 dB
 PL12 21.00 dB
 SF02 500.1320005 MHz

F2 - Processing parameters

ST 32768
 SF 125.7577847 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 200.000 ppm
 F1 25.151-.95 Hz
 -10.000 ppm
 F2P -1257.58 Hz
 F2 -1257.58 Hz
 PPMW 10.50000 ppm/cm
 HZCM 1320.45691 Hz/cm



Current Data Parameters

NAME	XH-II-155-A1
EXPND	1
PRODNO	1

F2 - Acquisition Parameters

Date	20020527
Time	18.59
INSTRUM	DRX500
PROBOD	5 mm Multinucl
PULPROG	zg30
TD	45056
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.229283 Hz
AQ	2.1807604 sec
RG	20.2
DW	48.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 5ec

******* CHANNEL f1 *******

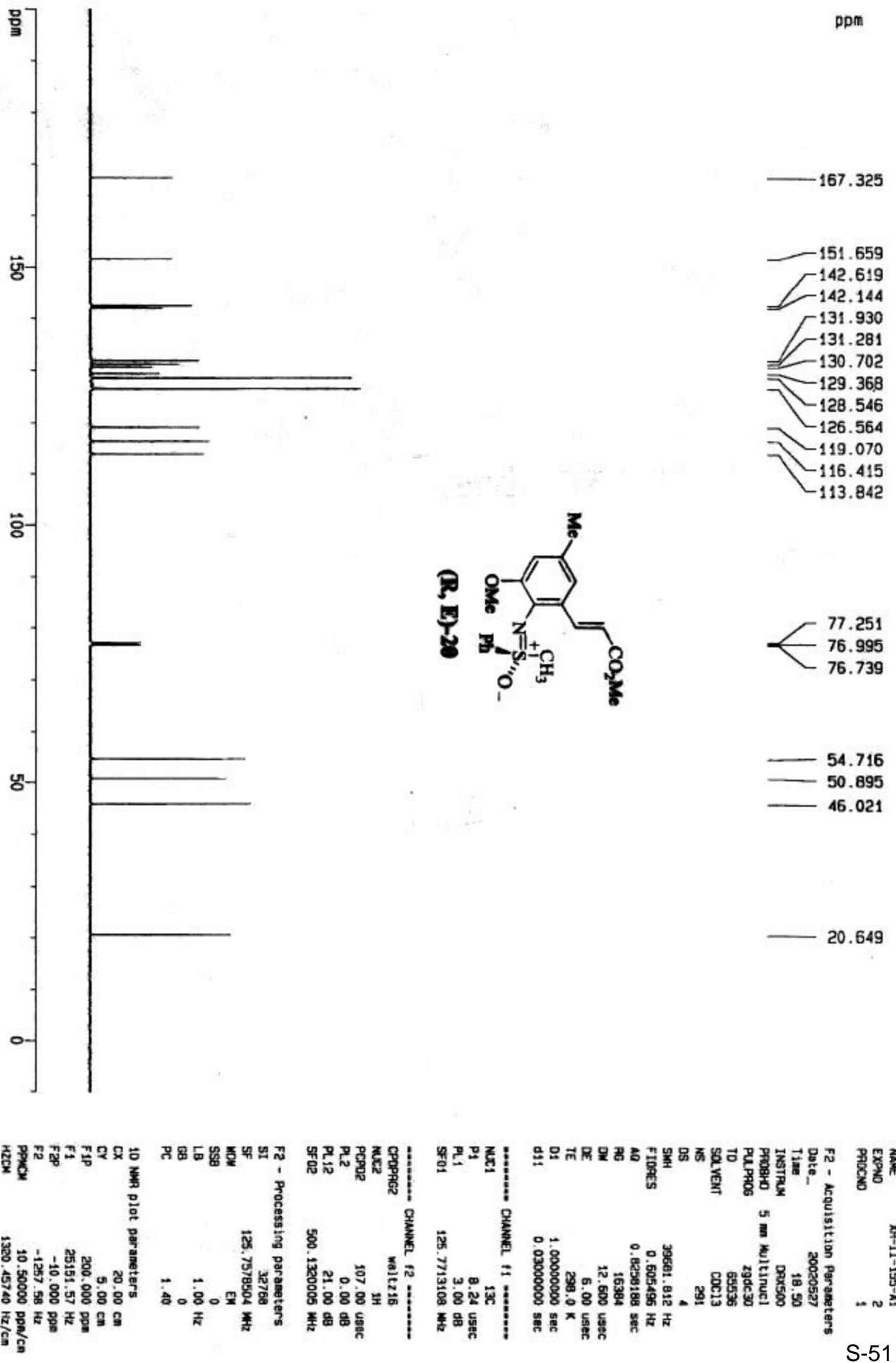
NUC1	1H
P1	13.25 usec
PL1	-3.00 dB
SFO1	500.1330885 MHz

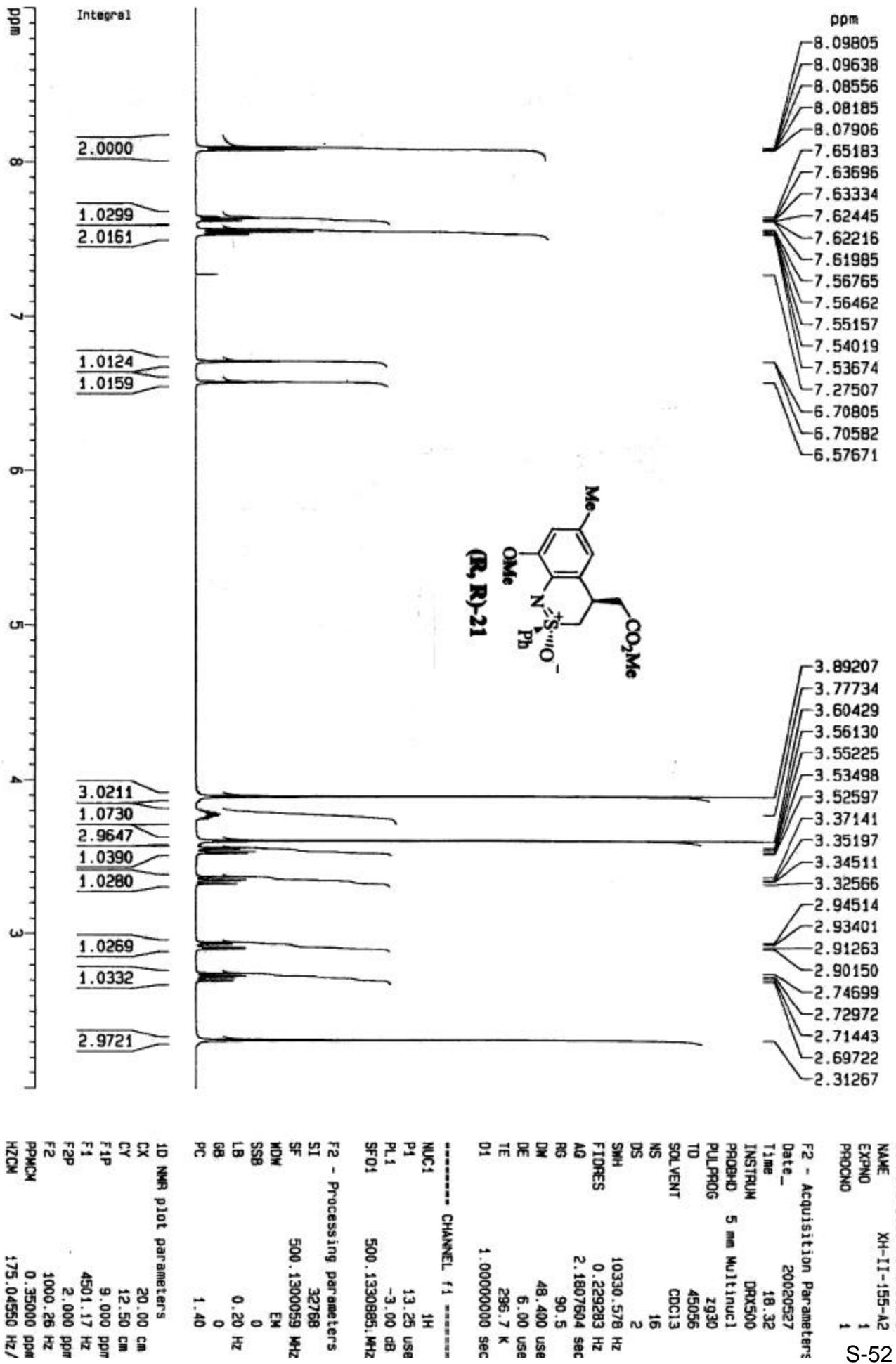
F2 - Processing parameters

SI	32768
SF	500.1299718 MHz
WDW	EN
SSB	0
LB	0.20 Hz
GB	0
PC	1.40

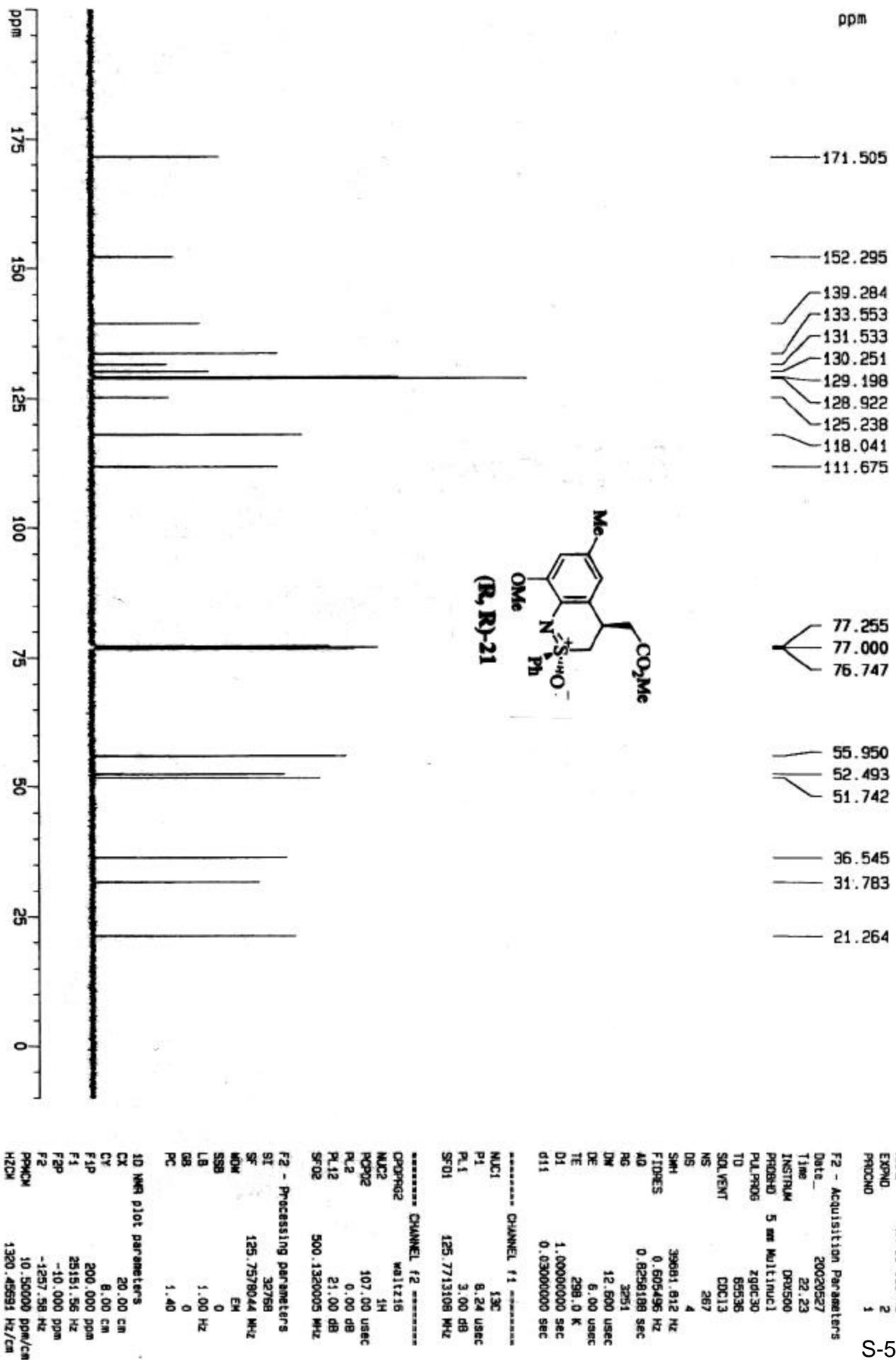
1D NMR plot parameters

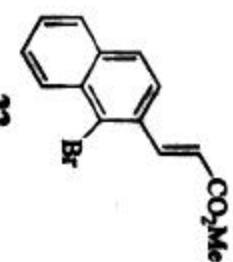
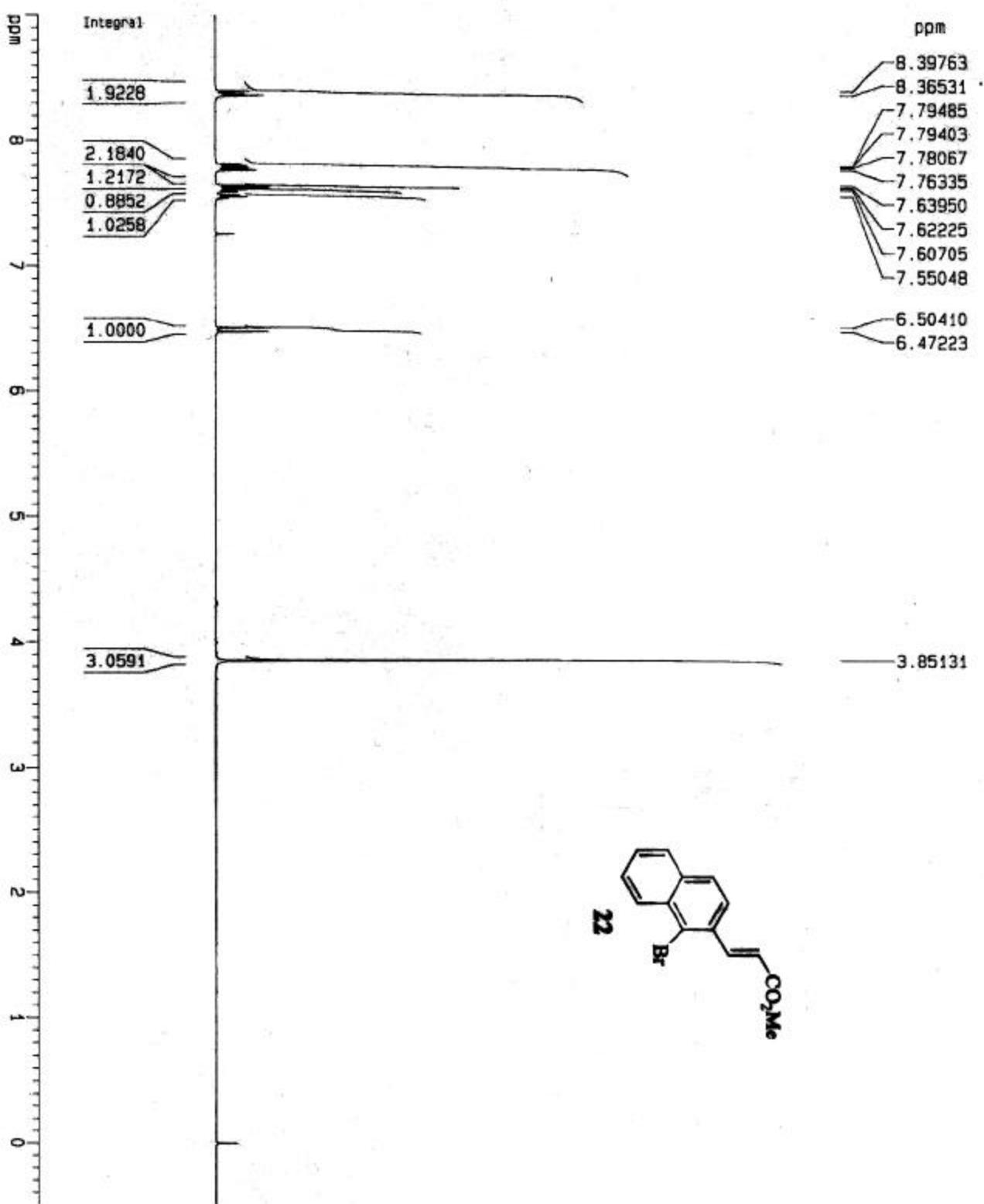
CX	20.00 cm
CY	5.00 cm
F1P	9.000 ppm
F1	4501.17 Hz
F2P	-0.500 ppm
F2	-250.06 Hz
PPMCH	0.47500 ppm/
Hz/cm	237.56174 Hz/cm





ppm





Current Data Parameters
NAME XH-III-61
EXPNO 1
PROCNO 1
S-54

F2 - Acquisition Parameters

Date 20021125

Time 11.08

INSTRUM DRX500

PROBOD 5 mm Multinucl

PULPROG zg30

TD 45056

SOLVENT CDCl3

NS 16

DS 2

SWH 10330.578 Hz

FORES 0.229683 Hz

AQ 2.1807604 sec

RG 64

DM 48.400 usec

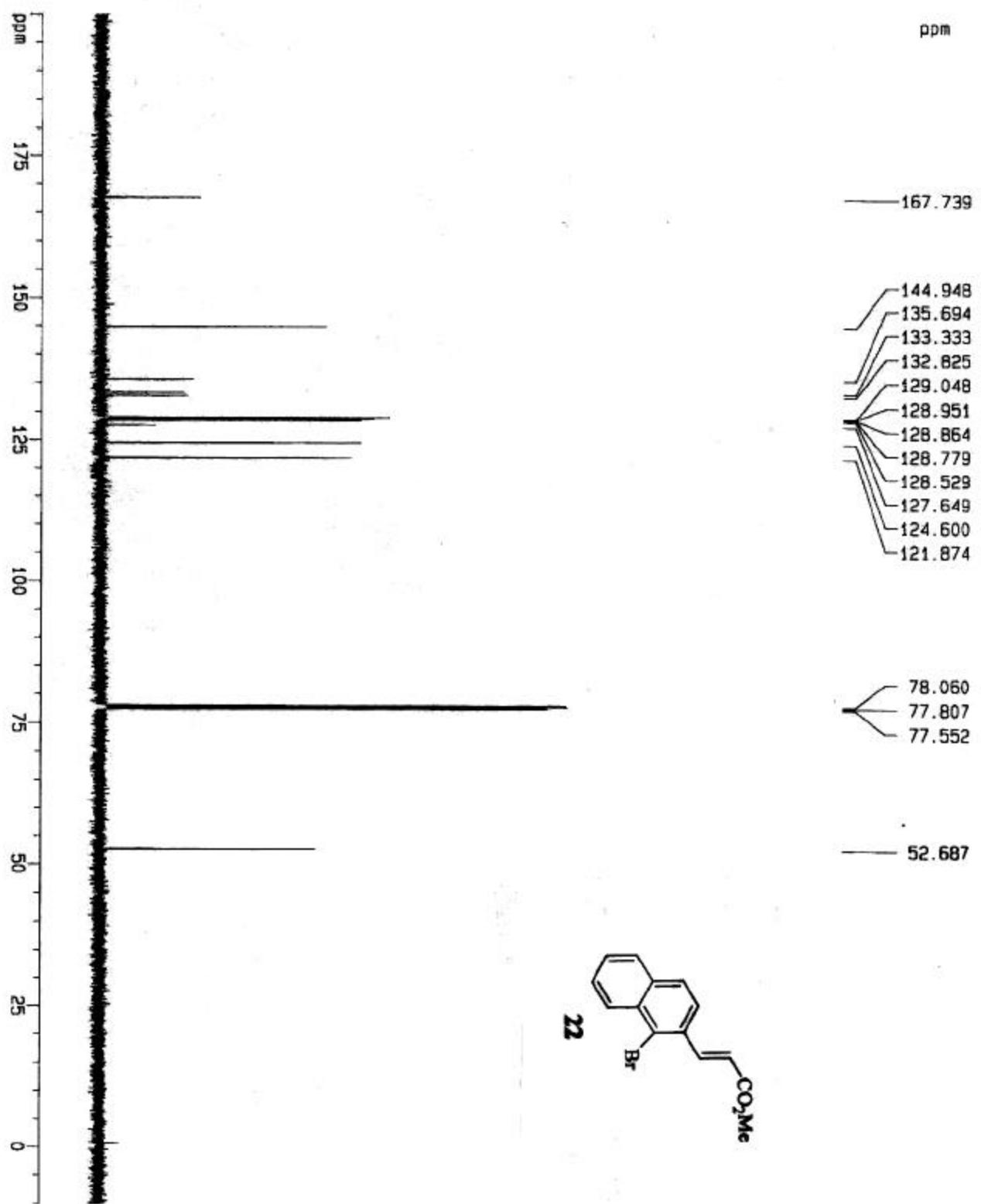
DE 6.00 usec

TE 296.7 K

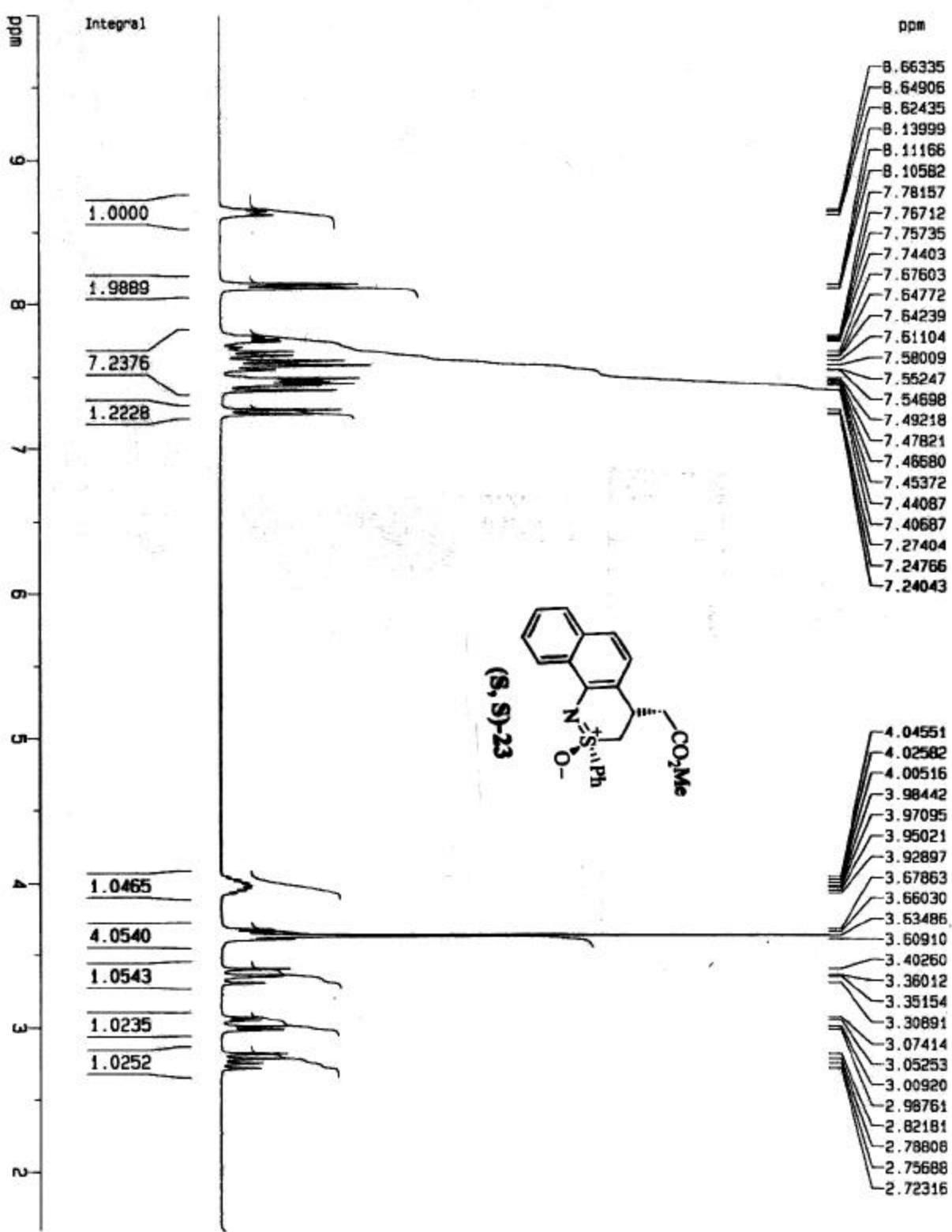
D1 1.0000000 sec

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

CX	20.00 cm
CY	6.00 cm
F1P	9.000 ppm
F1	4501.17 Hz
F2P	-0.500 ppm
F2	-250.07 Hz
PPMCM	0.47500 ppm/c
HZCM	237.56375 Hz/c



Current Data Parameters	
NAME	XH-III-51
EXPNO	2
PROBOD	1
F2 - Acquisition Parameters	
Date_	20021125
Time	41.12
INSTRUM	DRX500
PROBOD	5 mm Multinucl
PULPROG	290t30
TD	65536
SOLVENT	CDC13
NS	214
DS	4
SWH	39681.812 Hz
EDRES	0.605496 Hz
AQ	0.8258188 sec
RG	16384
DM	12.600 usec
DE	6.00 usec
TE	298.0 K
D1	1.000000 sec
d1	0.0300000 sec
CHANNEL f1	
NUC1	13C
P1	7.90 usec
PL1	3.00 dB
SF01	125.7713108 MHz
CHANNEL f2	
CPDRG2	Wal1216
NUC2	1H
PCPQP2	88.00 usec
PL2	0.00 dB
PL12	21.00 dB
SF02	500.1320005 MHz
F2 - Processing parameters	
S1	32768
SF	125.7576929 MHz
MON	EN
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
1D NMR plot parameters	
CDK	20.00 cm
CY	8.00 cm
FI	200.000 ppm
F1	25151.54 Hz
F2P	-10.000 ppm
F2	-1257.58 Hz
PPMCM	10.000 ppm/cm
HZCM	1320.48581 Hz/cm



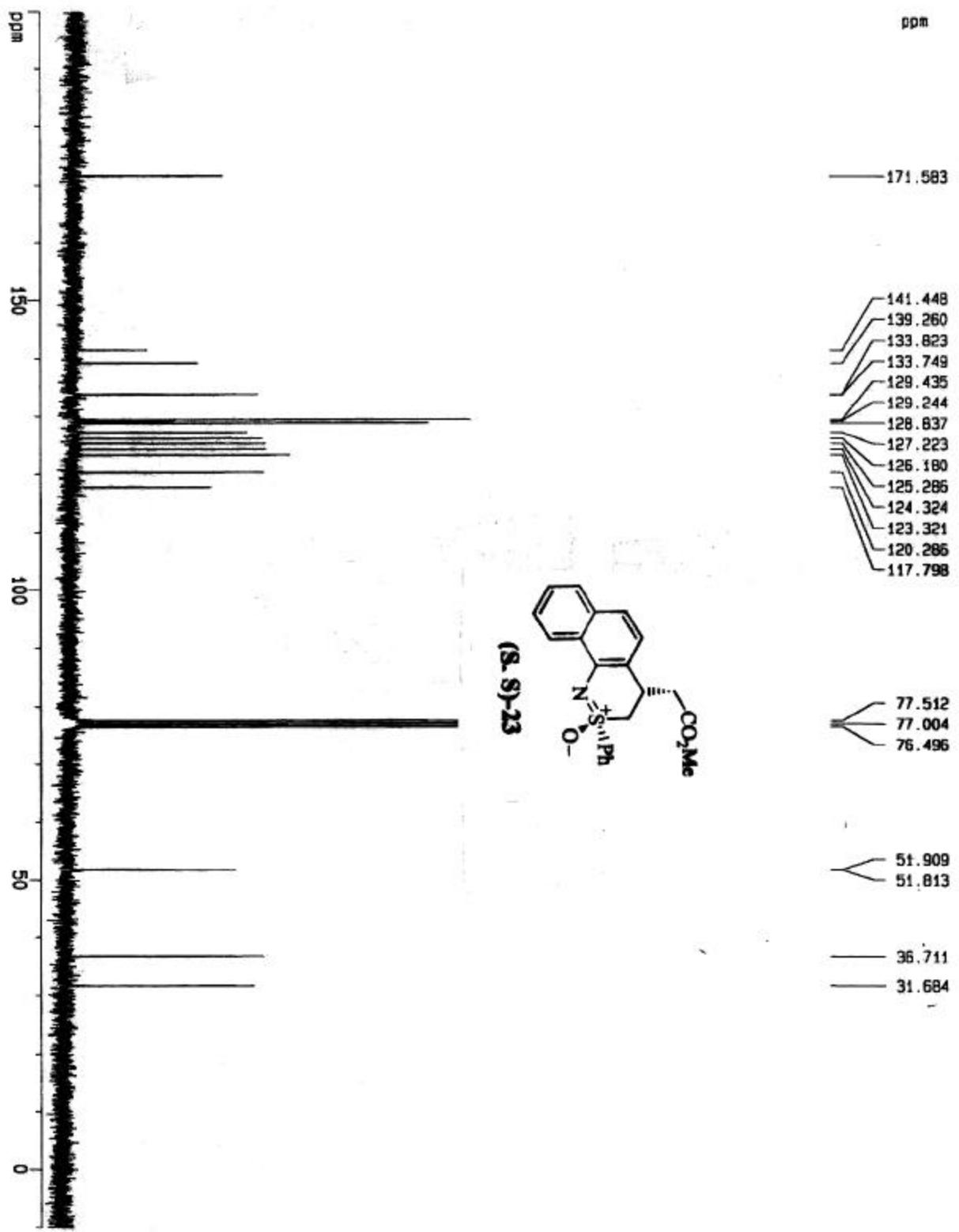
Current Data Parameters
 NAME XH-III-62
 EXPNO 1
 PROCN 1

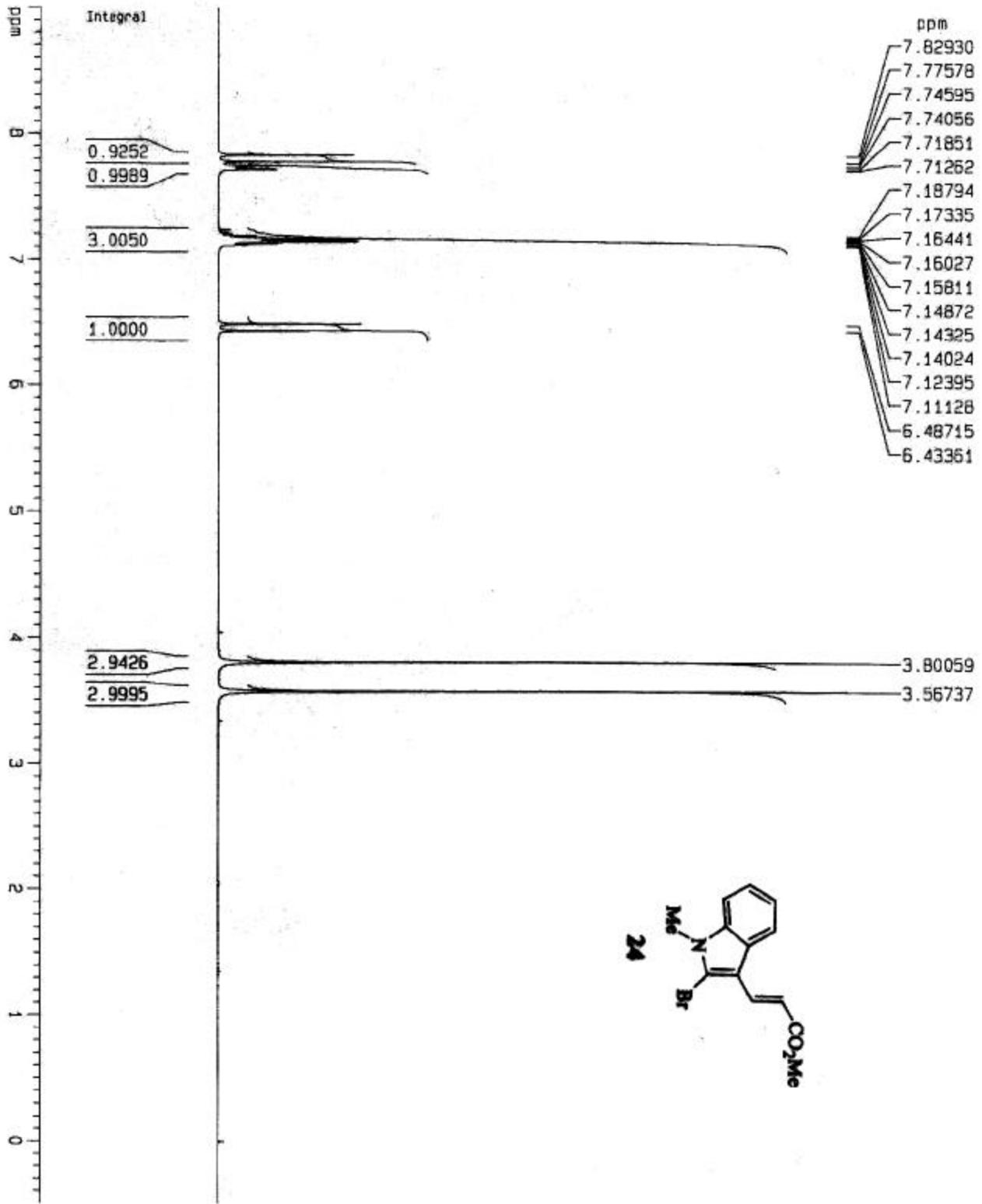
F2 - Acquisition Parameters
 Date 20020828
 Time 16.22
 INSTRUM ar250
 PROBID 5 mm QNP 1H
 PULPROG zg30
 TO 32768
 SOLVENT CUC13
 NS 16
 DS 2
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.145779 sec
 PG 1024
 DW 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.0000000 sec
 P1 8.70 use
 SFO1 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 250.1300107 MHz
 MDW 0
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 10,000 ppm
 F1 2501.30 Hz
 F2P 1.600 ppm
 F2 400.21 Hz
 PPMIN 0.42000 ppm
 HZCM 105.05460 Hz /

Current Data Parameters
 NAME XH-III-62
 EXPNO 2
 PRGNO 1
 S-57





F2 - Acquisition Parameters

Date	20021001
Time	14:39
INSTRUM	drx300
PROBOD	5 mm Multinucl
PULPROG	zg30
TD	32768
SOLVENT	CDC13
NS	16
DS	2
SWH	6172.839 Hz
FLORES	0.188380 Hz
AQ	2.6542580 sec
RG	64
DW	81.000 usec
DE	6.00 usec
TE	300.0 K
D1	1.0000000 sec

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

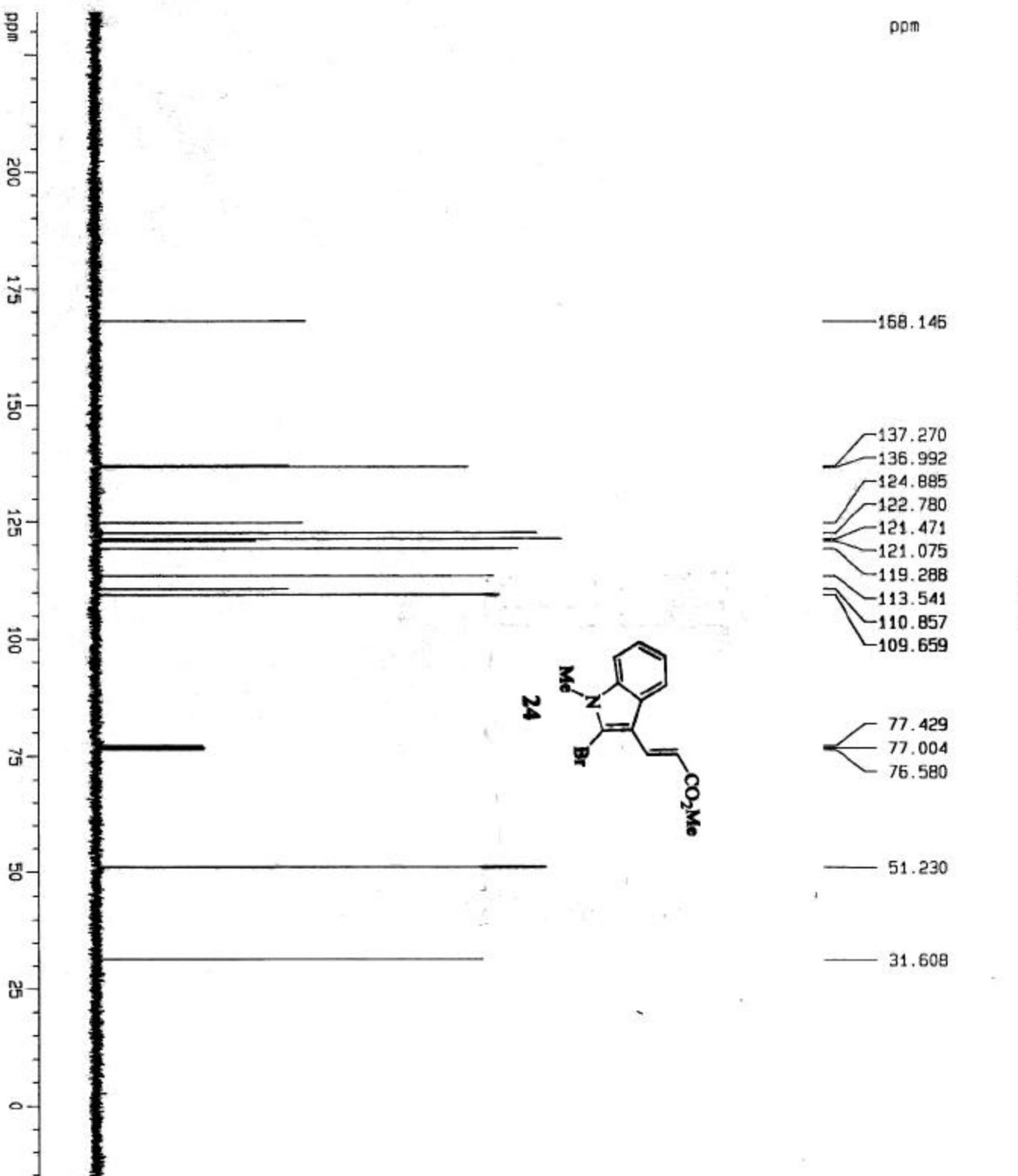
NUC1	1H
P1	7.50 usec
PL1	0.00 dB
SF01	300.1318334 MHz

F2 - Processing parameters

SI	32768
SF	300.130035 MHz
KDM	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.30

10 NMR plot parameters

CX	20.00 cm
CY	12.50 cm
CP	9.000 ppm
F1	2701.17 Hz
F2	-0.500 ppm
F2PPM	-150.06 Hz
PPMCH	0.47500 ppm/cm
HzCM	142.56175 Hz/cm



13C NMR

Current Data Parameters

NAME XH-III-81-A1
EXPNO 2
PRCHNO 1

F2 - Acquisition Parameters

Date_ 20021001

Time 14.44

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 65536

SOLVENT CDCl3

NS 214

DS 4

SWH 18850.141 Hz

FORES 0.287630 Hz

TDZ 1.738324 sec

RG 32768

DM 26.525 usec

DE 37.89 usec

TE 300.0 K

D1 1.0000000 sec

D11 0.03000000 sec

CHANNEL f1 = 13C

NUC1 1H

P1 7.75 usec

PL1 6.00 dB

SP01 75.4760107 MHz

CHANNEL f2 =

CPDPB62 waltz16

NUC2 1H

P1 100.00 usec

PL2 120.00 dB

PL12 24.50 dB

SP02 300.1312005 MHz

F2 - Processing parameters

SI 32768

SF 75.4677681 MHz

MW EM

SSB 0

L6 1.00 Hz

RR 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 8.00 cm

CP 234.138 ppm

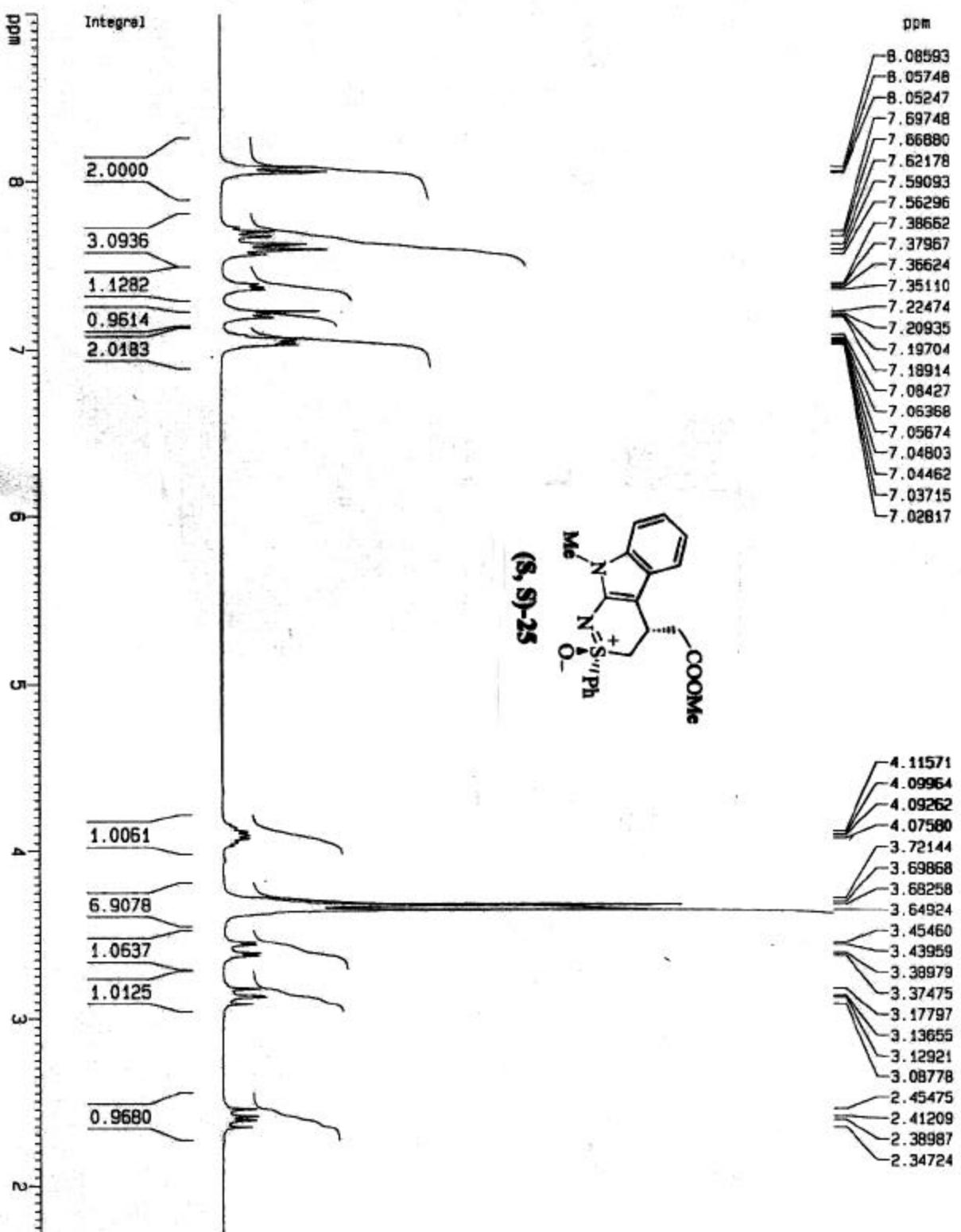
F1 17660.89 Hz

F2P -15.406 ppm

F2 -152.69 Hz

PPMCH 12.47723 ppm/cm

HZCM 941.68897 Hz/cm



Current Data Parameters

NAME	XH-III-82-A1
EXPNO	1
PROCNO	1

S-60

F2 - Acquisition Parameters

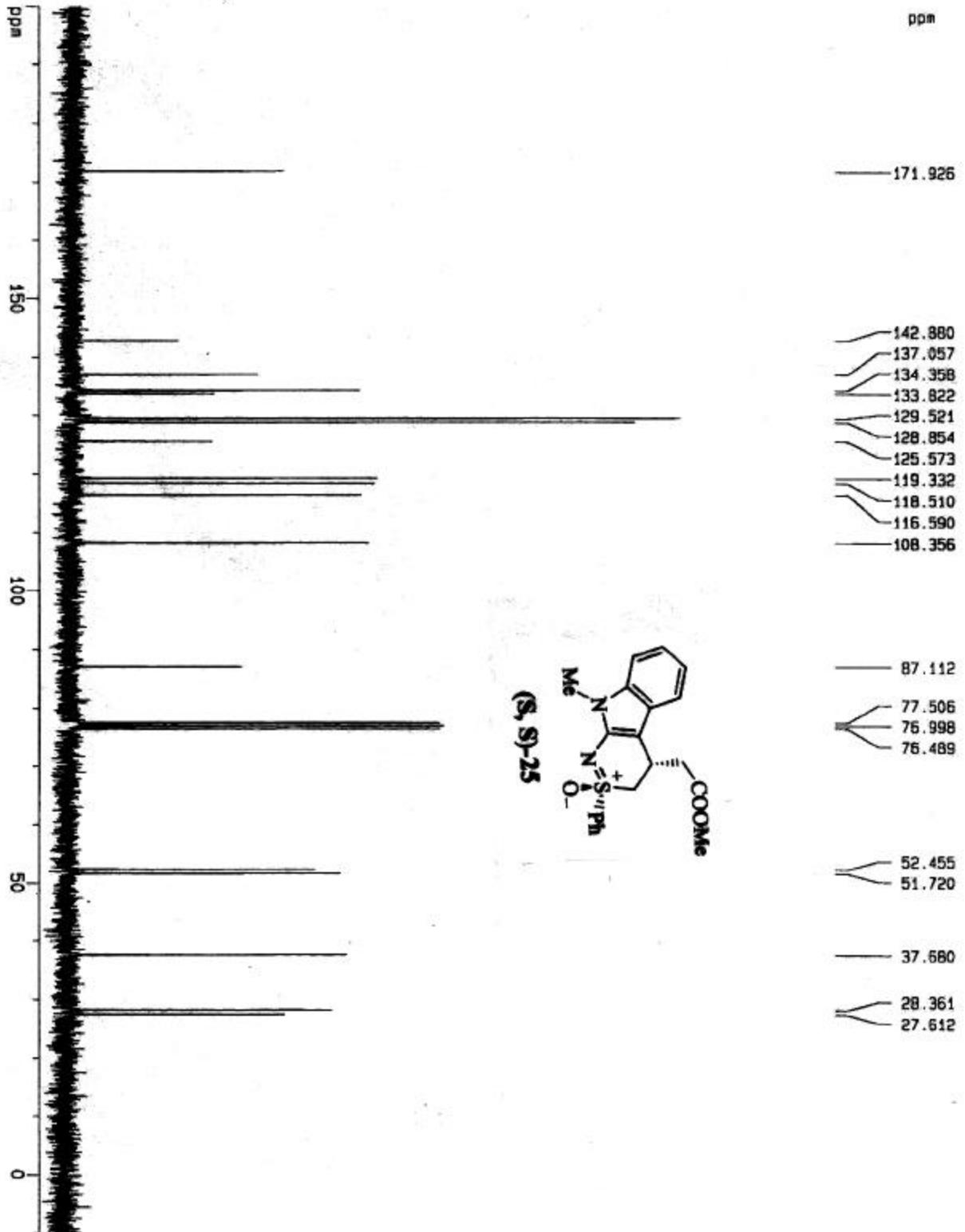
Time	20021006
Time	16.53
INSTRUM	av250
PROBHD	5 mm QNP 1H
PULPROG	2g30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	5208.333 Hz
DE	137.14 use
FIDRES	0.158946 Hz
AD	3.1457779 sec
RG	715
DW	96.000 use
TE	300.0 K
D1	1.0000000 sec
P1	6.70 use
SF01	250.1315321 MHz
NUCLEUS	1H

F2 - Processing parameters

SI	16384
SF	250.1300164 MHz
KD1	EM
SSB	0
LB	0.20 Hz
BB	0
PC	1.50

1D NMR plot parameters

CX	20.00 cm
CY	8.00 cm
F1P	9.000 ppm
F1	2251.17 Hz
F2P	1.700 ppm
F2	425.22 Hz
PPMCH	0.39500 ppm
HZCM	91.28745 Hz/



Current Data Parameters
 NAME XH-III-02-A1
 EXPNO 2
 PROCHD 1
 S-61

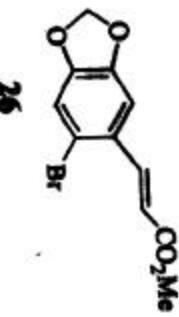
F2 - Acquisition Parameters

DATE	20021006
TIME	16.58
INSTRUM	anx250
PROBOD	5 mm QNP 1H
PULPROG	zgdc30
TD	36864
SOLVENT	CDC13
NS	386
DS	4
SWH	17241.379 Hz
FIRES	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
D5	23.00 dB
CPDPRG	Maltz16
P31	103.00 use
D1	1.0000000 sec
P1	5.35 use
SF01	62.9023694 MHz
NUCLEUS	¹³ C
D11	0.03000000 sec

F2 - Processing parameters

ST	32768
SF	62.8952471 MHz
MDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40
PPM/W	10.50000 ppm
Hz/cm	660.40009 Hz/

1H NMR



Current Data Parameters
NAME XH-III-69-A1
EXPNO 1
PROCNO 1

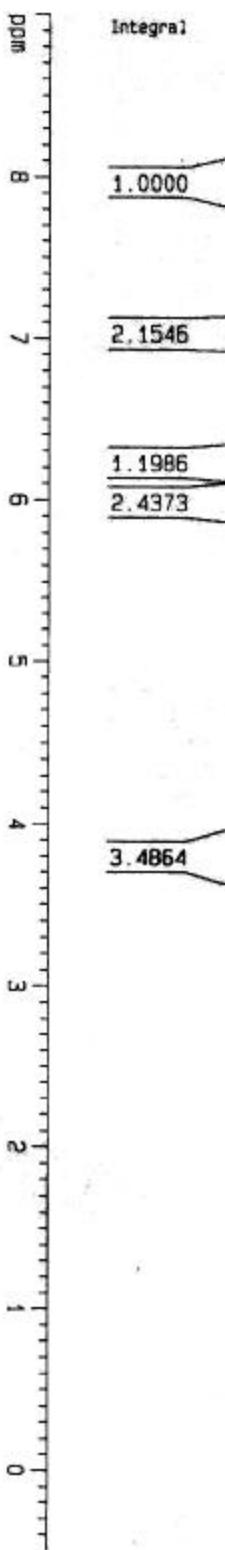
F2 - Acquisition Parameters
Date 20020910
Time 17.40
INSTRUM drx300
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542560 SEC
RG 256
DM DE 6.00 usec
TE 300.0 K
D1 1.0000000 SEC

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

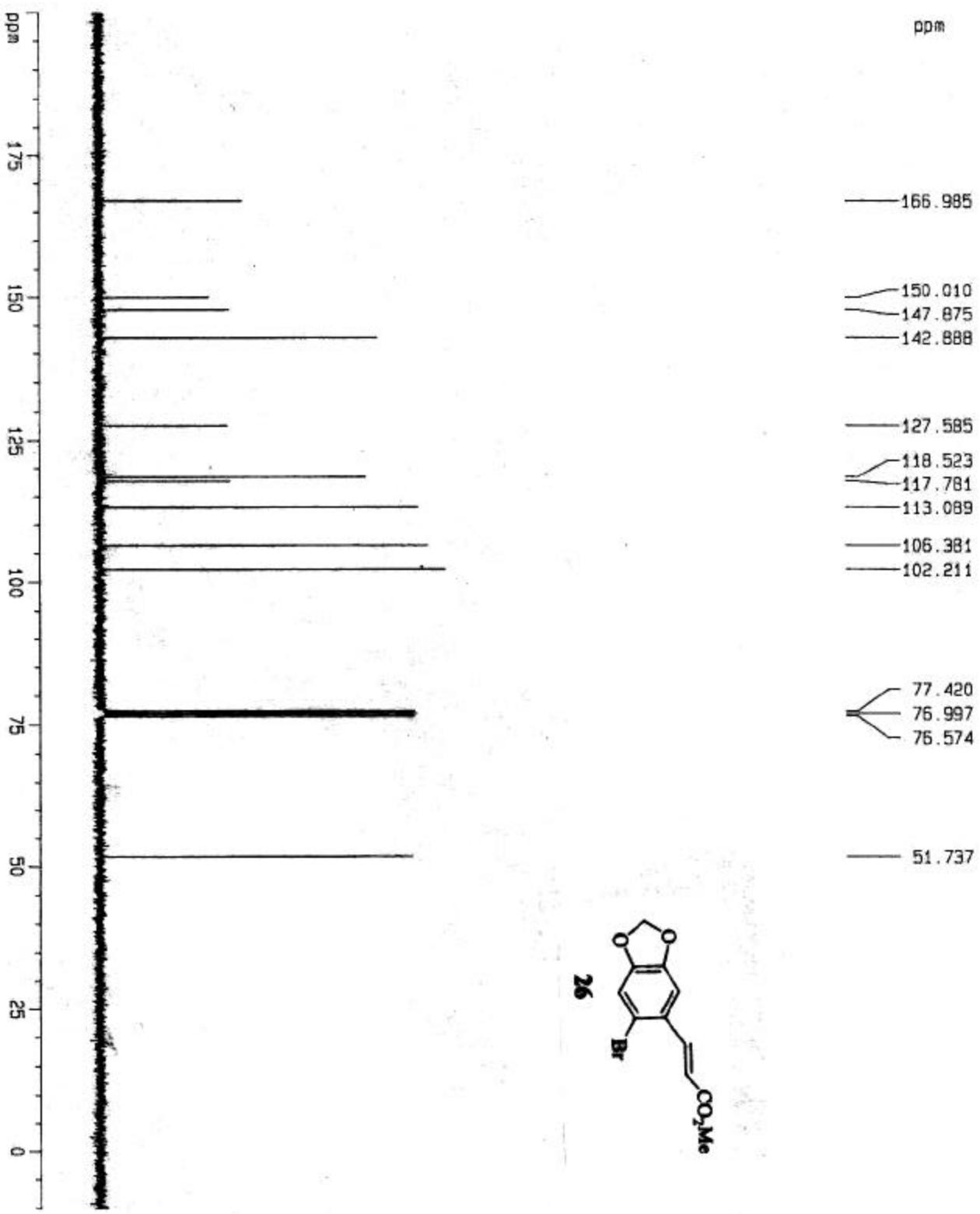
NUC1 1H
SI 32768
SF 300.1300035 MHz
NDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.30

F2 - Processing parameters

CX 20.00 cm
CY 8.00 cm
F1P 9.000 ppm
F1 2701.47 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCH 0.47500 ppm/cm
Hz/cm 142.56175 Hz/cm



¹³C NMR



Current Data Parameters	
NAME	XN-IIII-69-A1
EXPO	2
PROGNO	1
F2 - Acquisition Parameters	
Date	20020910
Time	17.45
INSTRUM	dmx300
PRGRHD	5 mm Multinucl
PULPROG	zgpc30
TD	65536
SOLVENT	CDCl ₃
NS	2731
DS	4
SWH	18850 141 Hz
FINRES	0.287630 Hz
TDZ	1.7383924 sec
RG	32768
DE	26.525 usec
TE	37.89 usec
TE	300.0 K
D1	1.0000000 sec
d11	0.0300000 sec

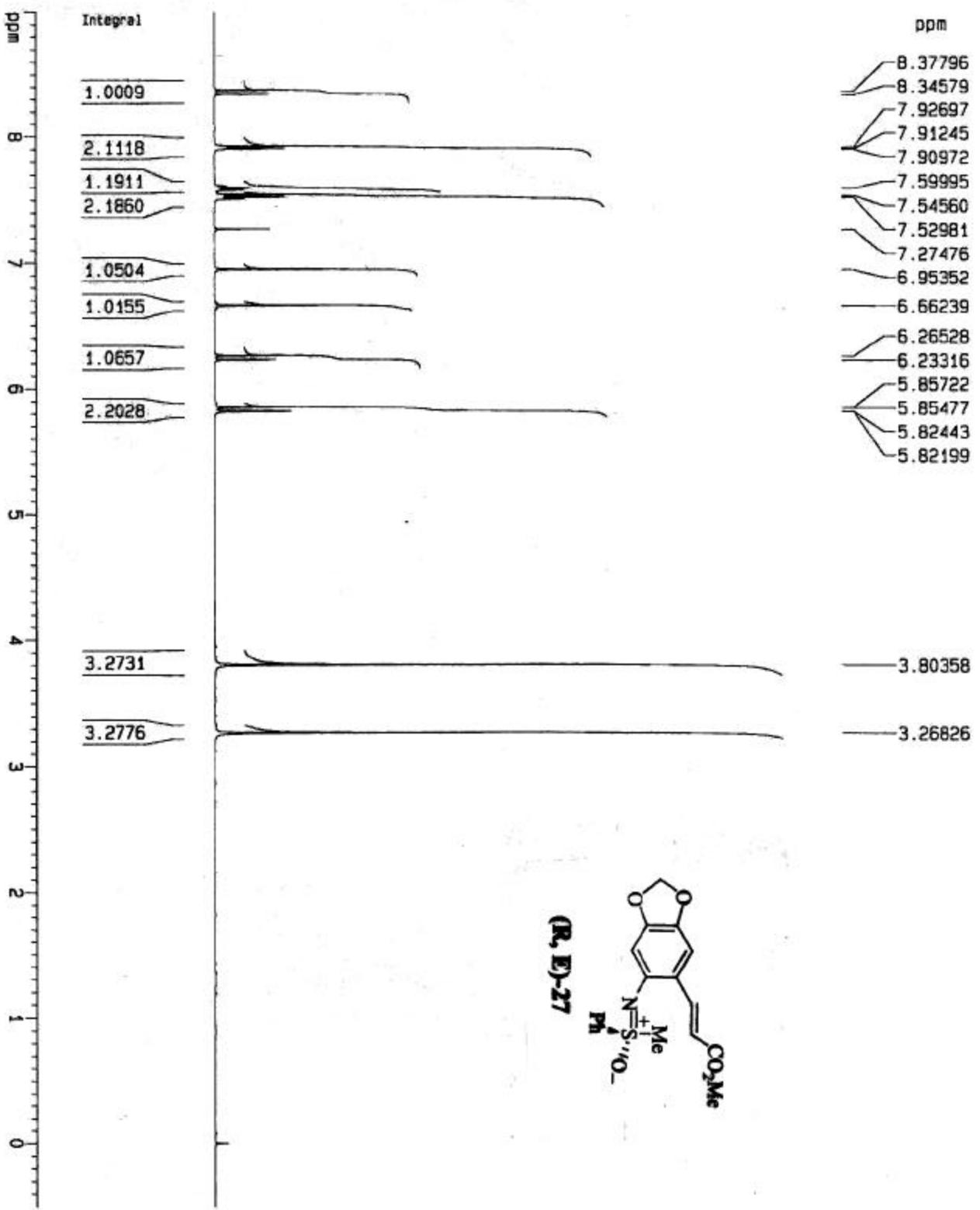
CHANNEL f1	
NUC1	¹³ C
P1	7.75 usec
PL1	5.00 dB
SF01	75.4760107 MHz

CHANNEL f2	
NUC2	¹ H
NH2	100.00 usec
PCP02	120.00 dB
PL2	24.50 dB
PL12	300.1312005 MHz
SF02	

F2 - Processing parameters	
SI	32768
SF	75.4677519 MHz
MWD	EW
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

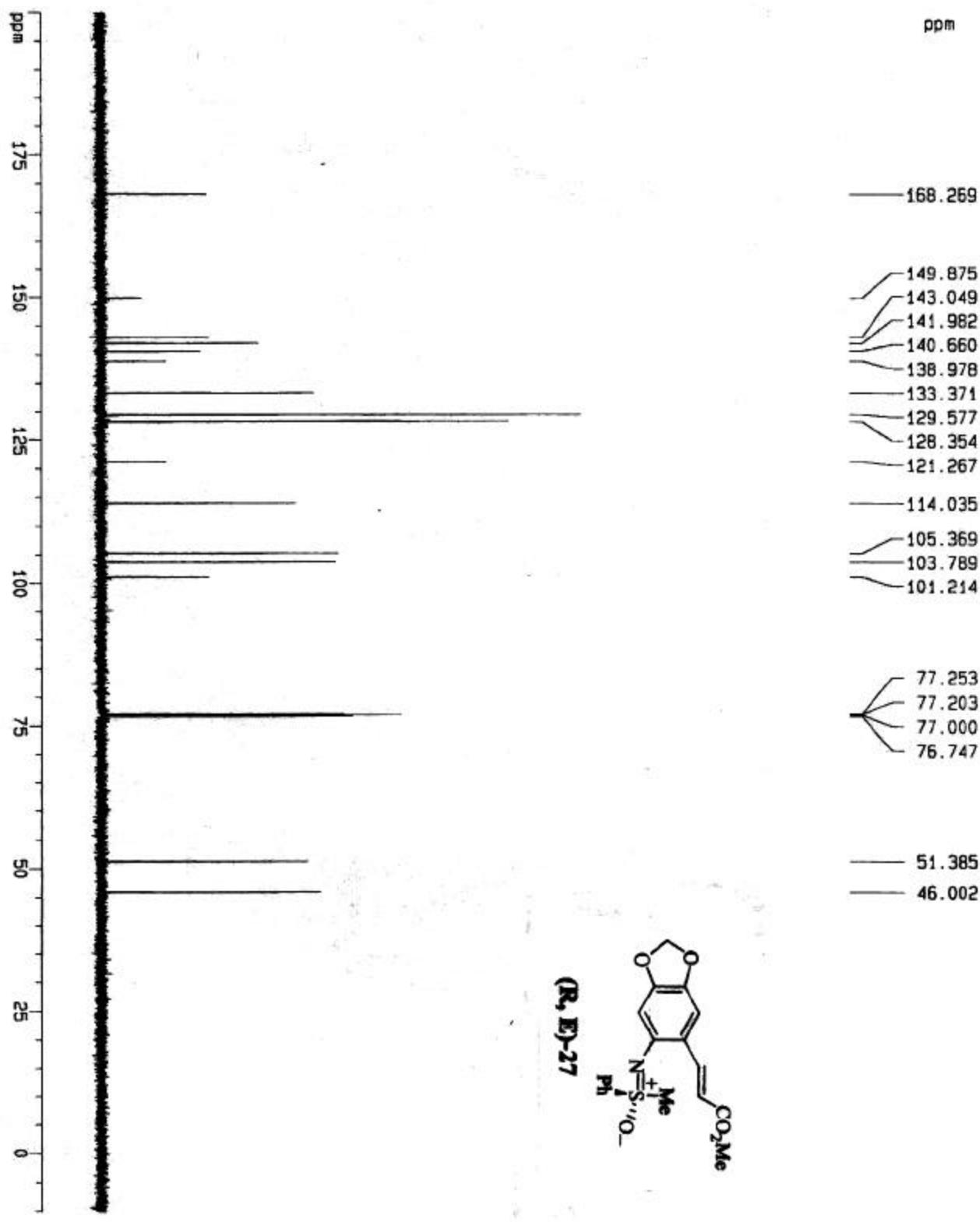
1D NMR plot parameters

CX	20.00 cm
CY	6.00 cm
F1P	200.000 ppm
F1	15983.55 Hz
F2P	-10.000 ppm
F2	-754.68 Hz
PPMCM	10.50000 ppm/cm
HZCM	792.41138 Hz/cm

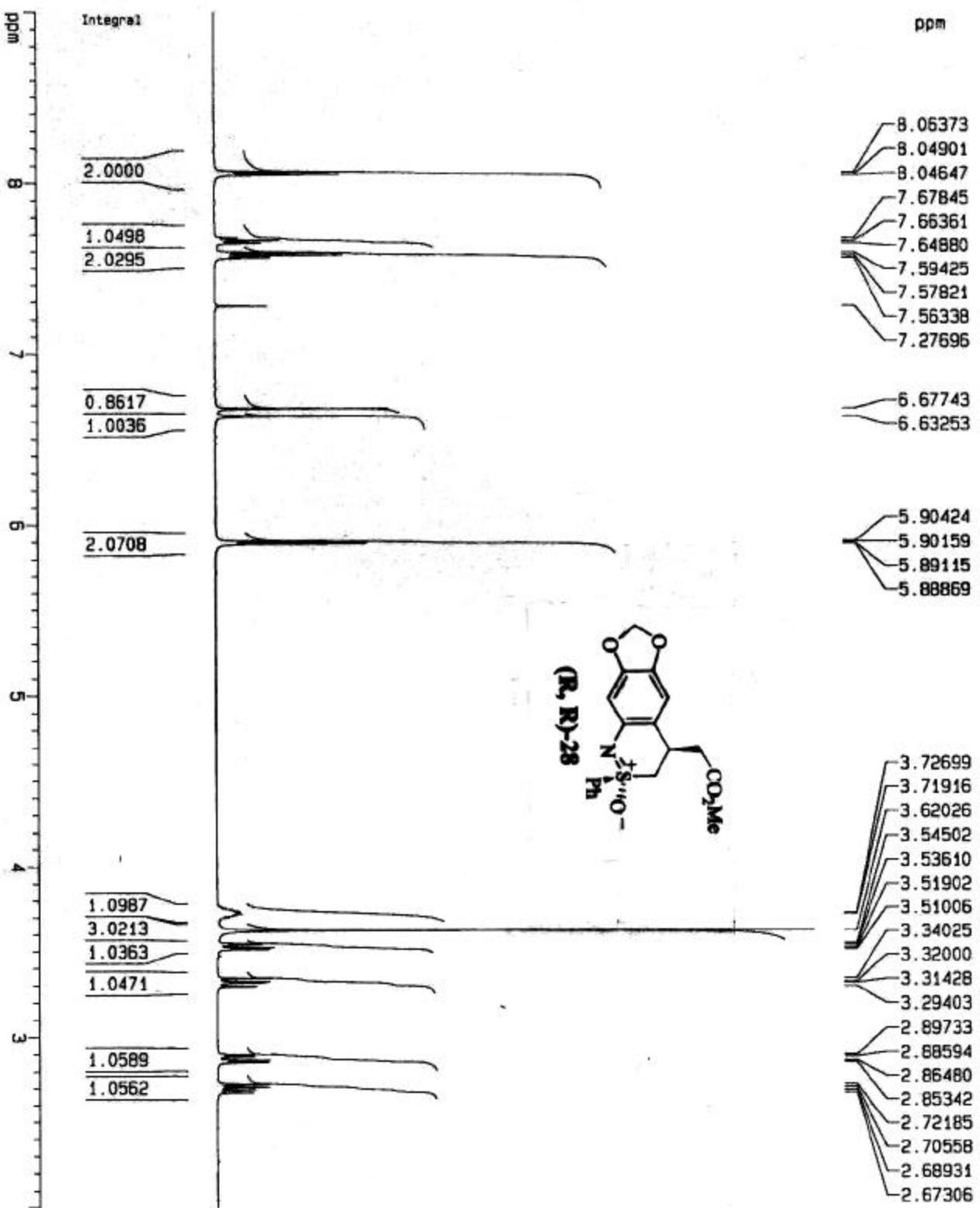


Current Data Parameters	
NAME	XH-III-74-A1
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date	20021118
Time	0.20
INSTRUM	DGX500
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	45056
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	10330.578 Hz
TDRES	0.229283 Hz
AQ	2,1807604 sec
RG	64
DW	48,400 usec
DE	6.00 usec
TE	295.7 K
D1	1.0000000 sec
***** CHANNEL f1 *****	
NUC1	¹ H
P1	13.25 usec
PL1	-3.00 dB
SFO1	500.1330885 MHz
F2 - Processing parameters	
SI	32768
SF	500.1300059 MHz
WDW	EM
SSB	0
LB	0.05 Hz
GB	0
PC	1.40

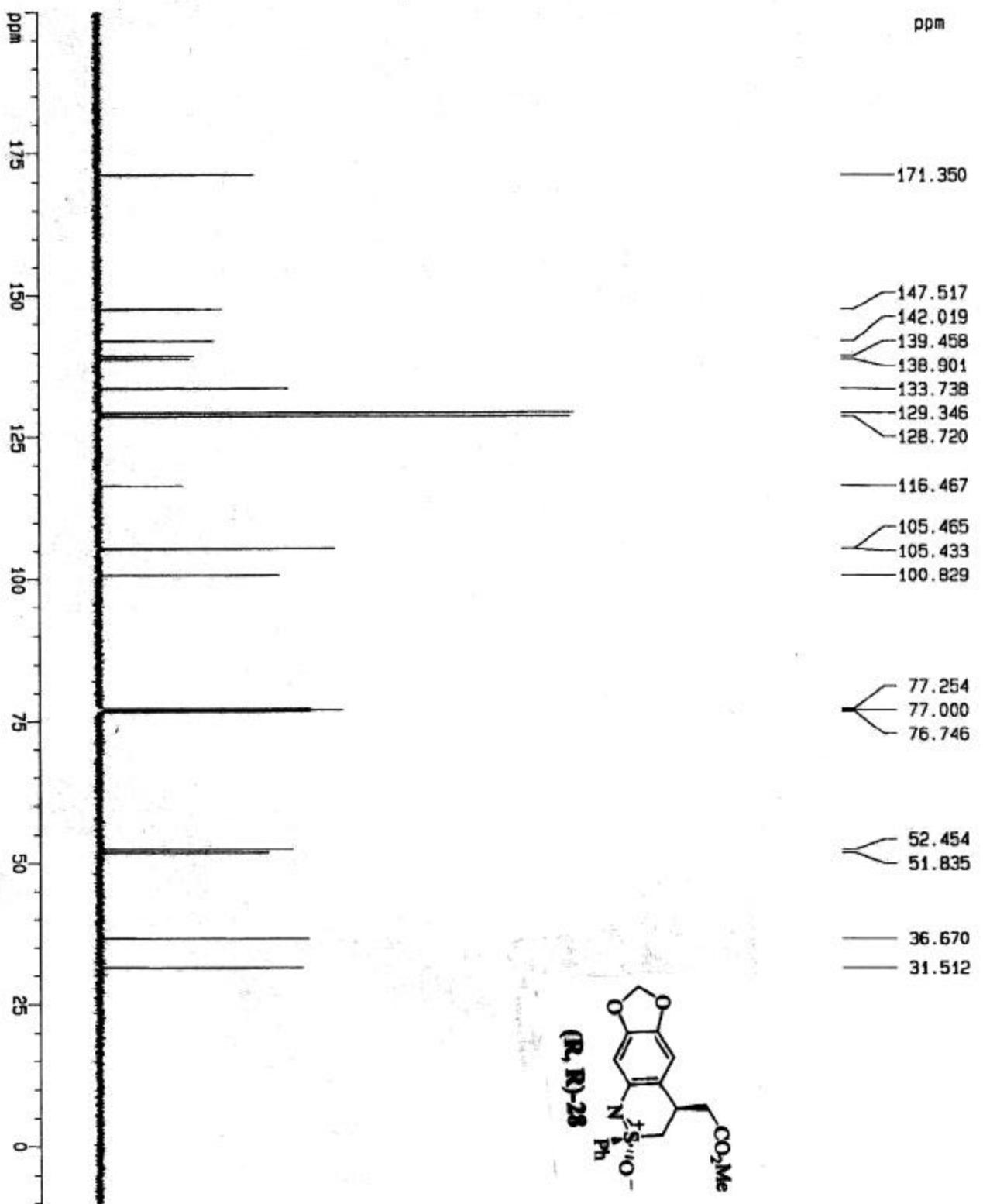
1D NMR plot parameters	
CX	20.00 cm
CY	6.00 cm
F1P	9.000 ppm
F1	4501.17 Hz
F2P	-0.500 ppm
F2	-250.07 Hz
PPCM	0.47500 ppm/
HZCM	237.56175 Hz/c



Current Data Parameters	
NAME	XI-111-7-A1
EXPO	2
PROCD	
F2 - Acquisition Parameters	
Date	20021118
Time	0.26
INSTRM	DRX500
PROBHD	5 mm Multinucl
PULPROG	zgdc30
TD	65536
SOLVENT	CDC13
NS	177
DS	4
SWH	39661.812 Hz
FLDRES	0.605496 Hz
A9	0.828168 sec
RG	16384
DW	12.600 usec
DE	6.00 usec
TE	298.0 K
D1	1.000000 sec
d11	0.0300000 sec
***** CHANNEL f1 *****	
NUC1	¹³ C
P1	7.90 usec
PL1	3.00 dB
SD1	125.7713108 MHz
***** CHANNEL f2 *****	
CPDP1	Waltz16
NUC2	¹ H
PCPD2	88.00 usec
P1.2	0.00 dB
P1.12	21.00 dB
SD2	500.1320005 MHz
F2 - Processing parameters	
SI	32768
SF	125.757995 MHz
MON	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.40
1D NMR plot parameters	
CX	20.00 cm
CY	8.00 cm
F1P	200.000 ppm
F1	25151.56 Hz
F2P	-10.000 ppm
F2	-1257.98 Hz
PPM	10.50000 ppm/cm
HECM	1320.45691 Hz/cm



Current Data Parameters	
NAME	XH-III-83-A1
EXPNO	1
PROCNO	1
	S-66
F2 - Acquisition Parameters	
DATE	20021008
TIME	15:36
INSTRUM	DRX500
PROBHD	5 mm Multinucl
PULPROG	zg30
TD	45056
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.229283 Hz
AQ	2.1807604 sec
RG	64
DW	48.400 usec
DE	6.00 usec
TE	295.7 K
D1	1.0000000 sec
----- CHANNEL f1 -----	
NUC1	¹ H
P1	13.25 usec
PL1	-3.00 dB
SF01	500.1330885 MHz
F2 - Processing parameters	
SI	32768
SF	500.1300049 MHz
NDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.40
1D NMR plot parameters	
CX	20.00 cm
CY	10.00 cm
F1P	9.000 ppm
F1	4501.17 Hz
F2P	2.000 ppm
F2	1000.26 Hz
PPMCM	0.35000 ppm/
HZCM	175.04550 Hz/c



	Current Data Parameters
NAME	XI-III-B3-A1
EXPNO	2
PROCNO	1
F2 - Acquisition Parameters	
Date	20021008
Time	15.42
INSTRUM	DR500
PROBHD	5 mm Multinucl
PULPROG	zg3630
TD	65536
SOLVENT	CDC13
NS	165
DS	4
SWH	39881.812 Hz
FORES	0.505095 Hz
AD	0.8250186 sec
RG	16384
DE	12.600 usec
TE	298.0 K
D1	1.0000000 sec
d1	0.0300000 sec
***** CHANNEL F1 *****	
NUC1	13C
P1	7.90 usec
PL1	3.00 dB
SR01	125.7713108 MHz
***** CHANNEL F2 *****	
CPDPK2	W411215
NUC2	1H
PCP02	88.00 usec
PL2	0.00 dB
PL12	21.00 dB
SR02	500.1320005 MHz
F2 - Processing parameters	
S1	32768
SF	125.757032 MHz
WDW	EW
SSB	0
L1	1.00 Hz
LB	0
GS	1.40
PC	
1D NMR plot parameters	
CX	20.00 cm
CY	8.00 cm
F1P	200.000 ppm
F1	25151.56 Hz
F2P	-10.000 ppm
F2	-1257.58 Hz
PPMCM	10.50000 ppm/cm
HZCM	1320.46591 Hz/cm