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**Synthesis, Structure and Emission Properties of Spirocyclic
Benzofuranones and Dihydroindolones – A Domino Insertion-Coupling-
Isomerization-Diels-Alder Approach to Rigid Fluorophores**

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I. Experimental Details

General Considerations. All reactions involving palladium-copper catalysis were performed in degassed oxygen free solvents under a nitrogen atmosphere using Schlenk and syringe techniques. The catalysts $\text{Pd}(\text{Ph}_3\text{P})_2\text{Cl}_2$, and CuI were purchased reagent grade from ACROS, Aldrich, Fluka or Merck and used without further purification. Triethylamine, toluene and butyronitrile were dried and distilled according to standard procedures.¹ Column chromatography: silica gel 60 mesh 230–400 (Macherey-Nagel, Düren). TLC: silica gel plates (60 F₂₅₄ Merck, Darmstadt). Melting points (uncorrected values): Büchi Melting Point B-540. – ¹H and ¹³C NMR spectra in CDCl_3 : Bruker DRX 300, Bruker DRX 500 and Bruker AC 300. The assignments of quaternary C, CH, CH₂ and CH₃ have been made by using DEPT spectra. – IR: Bruker Vector 22 FT-IR. – UV/vis: Perkin Elmer Models Lambda 16 and Hewlett Packard HP8452 A. – Fluorescence: Perkin Elmer LS-55. – MS: Jeol JMS-700 and Finnigan TSQ 700. – Elemental analyses were carried out in the Microanalytical Laboratories of the Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg.

1. Synthesis of 2-iodophenyl phenyl propynoate **1**

In a heat gun dried and nitrogen filled Schlenk flask 20.9 g (95.0 mmol) of 2-iodo phenol were dissolved in 80 mL of THF, cooled to 0 °C and treated with 3.80 g (95.0 mmol) of sodium hydride (60 % (w/w) in white oil). Then, 4.20 g (86.4 mmol) of phenyl propynoyl chloride were added to the immediately formed suspension and the resulting solution was stirred at 45 °C over night. For work up 150 mL of water was added, the organic layer was separated and the aqueous phases were extracted with 80 mL (3 times) of diethyl ether. The combined organic phases were dried with MgSO₄, filtered and, finally, the solvents were removed in vacuum. Column chromatography on silica (hexane/ethyl acetate, 10:1) afforded 20.4 g (68 %) of **1** as colorless crystals. Mp.: 64 °C. ¹H NMR (CDCl₃, 300 MHz): δ 7.03 (m, 1 H), 7.20 (dd, *J* = 6.3, 9.6 Hz, 1 H), 7.42 (m, 3 H), 7.51 (m, 1 H), 7.88 (dd, *J* = 6.6, 9.6 Hz, 1 H). ¹³C NMR (CDCl₃, 75 MHz): δ 80.1 (C_{quat}), 89.4 (C_{quat}), 90.1 (C_{quat}), 119.1 (C_{quat}), 123.0 (CH), 128.1 (CH), 128.7 (CH), 129.6 (CH), 131.2 (CH), 133.3 (CH), 139.7 (CH), 150.6 (C_{quat}), 151.4 (C_{quat}). EI MS (70 eV, *m/z* (%)): 348 (M⁺, 6), 221 (M⁺ – I, 83), 191 (9), 165 (6), 129 (M⁺ – C₅H₄IO, 100), 101 (C₈H₅, 8), 75 (9). IR (KBr): $\tilde{\nu}$ = 3050 cm⁻¹ (w), 2231 (m), 2202 (m), 1726 (m), 1487 (w), 1463 (w), 1442 (w), 1285 (w), 1195 (w), 1140 (m), 760 (w), 730 (w), 688 (w), 601 (w). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 250 nm (1430), 266 (18400), 322 nm (1400). Anal. calcd. for C₁₅H₉IO₂ (348.1): C 51.75, H 2.61, I 36.45; found: C 51.78, H 2.71, I 36.45.

2. Synthesis of propargyl allyl ethers 2

Synthesis of propargyl allyl ether according to *Williamson's* protocol (Procedure A)

In a heat gun dried and nitrogen flushed two-necked round bottom flask with a condenser and nitrogen inlet tube 1.0 equiv. of the corresponding propargyl alcohol were dissolved in THF and cooled to 0 °C. Then, 1.0 equivalents of sodium hydride (60 % (w/w) in white oil) were added portion wise until the hydrogen evolution ceased. Subsequently, 1.1 equiv. of the desired allyl bromide derivatives were injected by syringe and the resulting reaction solution was then heated to reflux over night. For work up the reaction solution was cooled to rt. then treated with 100 mL of a saturated aqueous solution of NaCl, the organic layer was transfused and the aqueous phase was extracted three times with a 50 mL of diethylether. The combined ethereal extracts were dried with MgSO₄, filtered and subsequently the solvents were removed in vacuum.

Synthesis of propargyl allyl ether according to a modified *Williamson's* protocol (Procedure B)

In a heat gun dried and nitrogen filled two-necked round bottom flask with a condenser and nitrogen inlet tube 1.0 equivalents of the corresponding propargyl alcohol were dissolved in THF and cooled to -60 °C (dry ice). At this temperature 1.0 equiv. of *n*-BuLi (2.5 M, in Hexane) were slowly injected by syringe. The resulting solution was kept at this temperature for 30 min and subsequently treated with 1.1 equiv. of prenyl bromide and 10 % DMSO. Within 5 h the reaction solution was allowed to warm to 0 °C and it was finally kept for a another hour at rt. For work up the solution was treated with 50 mL of a saturated aqueous solution of NH₄Cl, the organic layer was separated and the aqueous phase was extracted three times with 50 mL of diethyl ether and finally it was washed 5 times with 250 mL of a saturated aqueous solution of NH₄Cl to remove DMSO. The combined organic phases were dried with MgSO₄, filtered and concentrated in vacuum.

Synthesis of propargyl allyl ether according to a modified *Williamson's* protocol (Procedure C)

In a heat gun dried and nitrogen filled two-necked round bottom flask with a condenser and nitrogen inlet tube 1.1 equiv. of ethynyl magnesium bromide (0.5 M in THF) were cooled to 0 °C and treated with 1.0 equiv. of the corresponding propargyl alcohol dissolved in a small amount of THF. Subsequently, the resulting solution was stirred for 30 min at this temperature and for another hour at rt. Finally, the mixture was cooled again to 0 °C. Now 1.2 equiv. of prenyl bromide were injected and the solution was allowed to warm to rt over night. For work up the solution was treated with 50 mL of a saturated aqueous solution of NH₄Cl, the organic layer was transferred, the aqueous phase was extracted three times with 50 mL of diethyl ether and the combined organic phases were finally washed 5 times with 250 mL of a saturated aqueous solution of NH₄Cl. After drying with MgSO₄ and filtration the solvents were removed in vacuum.

4-(1-Allyloxy-prop-2-ynyl)-benzonitrile (2a)

In a heat gun dried and nitrogen filled two neckedround bottom flask with a condenser and nitrogen inlet tube 50 mL (25.0 mmol) of ethynyl magnesium bromide (0.5 M in THF) was cooled to 0 °C and treated with 3.00 g (22.9 mmol) of 4-formyl-benzonitrile, dissolved in a small amount of THF. Subsequently, the solution was stirred for 1 h at rt and then 2/3 of the solvent was removed in vacuum. The remainder was transferred to 22.0 mL (250 mmol) of allyl bromide and 11.3 g (75.5 mmol) of NaI suspended in 80 mL of DMF. The mixture was stirred at 40 °C for 5 d. For work up the solvent and excess allyl bromide was removed in vacuum and the remainder dissolved in CH₂Cl₂ and treated with a 50 mL of water. The organic layer was separated and the aqueous layer extracted with diethyl ether. The combined organic phases were dried with MgSO₄, submitted to filtration and finally liberated from the solvents. After column chromatography on silica gel (hexane/ethyl acetate (3:1) 1.17 g (26 %) of the desired propargyl ether was obtained as a brown oil. ¹H NMR (CDCl₃, 300 MHz): δ 2.69 (d, J = 2.2 Hz, 1 H), 4.19

(m, $J \approx 12.5$ Hz, 2 H), 5.24 (d, $J = 2.2$ Hz, 1 H), 5.25 (qd, $J = 1.5$, 10.3 Hz, 1 H), 5.34 (qd, $J = 1.5$, 17.2 Hz, 1 H), 5.94 (dddd, $J = 5.3$, 6.2, 10.3, 17.2 Hz, 1 H), 7.61–7.67 (m, 4 H). ^{13}C NMR (CDCl_3 , 75 MHz): δ 69.4 (CH), 69.5 (CH_2), 80.3 (C_{quat}), 112.2 (C_{quat}), 118.3 (CH_2), 118.5 (C_{quat}), 127.8 (CH), 132.2 (CH), 133.5 (CH), 143.3 (C_{quat}). EI MS (70 eV, m/z (%)): 197 (M^+ , 7), 156 ($\text{M}^+ - \text{C}_3\text{H}_5$, 20), 140 ($\text{M}^+ - \text{C}_3\text{H}_5\text{O}$, 100). HRMS calcd. for $\text{C}_{13}\text{H}_{11}\text{NO}$: 197.0841; found: 197.0819. IR (film): $\tilde{\nu} = 3292$ cm^{-1} (s), 2863 (m), 2230 (s), 2115 (w), 1663 (m), 1295 (m), 1063 (s), 931 (m). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 240 nm (15100), 280 (2300).

1-(1-Allyloxy-prop-2-ynyl)-2-fluoro-benzene (2b)

According to procedure A and after column chromatography on silica gel (hexane/ethyl acetate, 3:1) 2.91 g (79 %) of **2b** were obtained as a yellow oil. ^1H NMR (CDCl_3 , 300 MHz): δ 2.63 (d, $J = 2.2$ Hz, 1 H), 4.19 (m, $J \approx 12.5$ Hz, 2 H), 5.25 (qd, $J = 1.5$, 10.3 Hz, 1 H), 5.35 (qd, $J = 1.6$, 17.3 Hz, 1 H), 5.51 (d, $J = 2.2$ Hz, 1 H), 5.96 (dddd, $J = 5.4$, 6.2, 10.3, 17.2 Hz, 1 H), 7.06 (dd, $J = 1.2$, 8.3 Hz, 1 H), 7.19 (ddd, $J = 1.3$, 7.6, 8.9 Hz, 1 H), 7.30 (dd, $J = 1.9$, 8.1 Hz, 1 H), 7.70 (ddd, $J = 1.7$, 7.5, 9.0 Hz, 1 H). ^{13}C NMR (CDCl_3 , 75 MHz): δ 63.9 (CH), 69.7 (CH_2), 75.2 (CH), 80.8 (C_{quat}), 115.6 (CH), 118.0 (CH_2), 124.3 (CH), 124.3 (CH), 129.1 (CH), 129.1 (CH), 133.8 (CH), 161.8 (C_{quat}). EI MS (70 eV, m/z (%)): 190 (M^+ , 10), 162 ($\text{M}^+ - \text{C}_2\text{H}_4$, 26), 133 ($\text{M}^+ - \text{C}_3\text{H}_5\text{O}$, 100), 123 (46), 113 (16), 95 ($\text{C}_6\text{H}_4\text{F}$, 17), 75 (11). HRMS calcd. for $\text{C}_{12}\text{H}_{11}\text{FO}$: 190.0794; found: 190.0786. IR (film): $\tilde{\nu} = 3300$ cm^{-1} (s), 3082 (m), 2862 (m), 1665 (m), 1491 (s), 1100 (s), 1064 (w), 759 (s). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 246 nm (2400), 280 (800).

1-(1-Allyloxy-prop-2-ynyl)-4-methoxy-benzene (2c)

According to procedure A and after column chromatography on silica gel (hexane/ethyl acetate, 3:1) 1.67 g (77 %) of **2c** were obtained as a yellow oil. ^1H NMR (CDCl_3 , 250 MHz): δ 2.64 (d, $J = 2.2$ Hz, 1 H), 3.81 (s, 3 H), 4.13 (m, $J = 12.4$ Hz, 2 H), 5.17 (d, $J = 2.2$ Hz, 1 H), 5.22 (qd, $J = 1.4$, 10.3 Hz, 1 H), 5.33 (qd, $J = 1.6$, 17.2 Hz, 1 H), 5.95 (dddd, $J = 5.5$, 6.6, 10.3, 17.1 Hz, 1 H), 6.90 (d, $J = 8.8$ Hz, 2 H), 7.45 (d, $J = 8.8$ Hz, 2 H). ^{13}C NMR (CDCl_3 , 75 MHz): δ 55.3

(CH₃), 69.0 (CH₂), 69.9 (CH), 75.3 (CH), 81.8 (C_{quat}), 113.9 (CH), 117.7 (CH₂), 128.8 (CH), 130.4 (C_{quat}), 134.2 (CH), 159.8 (C_{quat}). EI MS (70 eV, *m/z* (%)): 202 (M⁺, 23), 160 (M⁺ – C₃H₆, 43), 145 (M⁺ – C₃H₅O, 100), 135 (OCC₆H₄OCH₃⁺, 53). HRMS calcd. for C₁₃H₁₄O₂: 202.0994; found: 202.0981. IR (film): $\tilde{\nu}$ = 3288 cm⁻¹ (s), 2950 (m), 2838 (m), 1724 (m), 1611 (s), 1250 (s), 1059 (m), 929 (w). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 274 nm (5500), 282 (4800).

1-(1-Allyloxy-prop-2-ynyl)-4-ethoxy-benzene (2d)

According to procedure A and after column chromatography on silica gel (hexane/ethyl acetate, 3:1) 1.71 g (71 %) of **2d** were obtained as a yellow oil. ¹H NMR (CDCl₃, 300 MHz): δ 1.41 (t, *J* = 7.0 Hz, 3 H), 2.65 (d, *J* = 2.2 Hz, 1 H), 4.03 (q, *J* = 7.0 Hz, 2 H), 4.14 (m, *J* $\approx$ 12.5 Hz, 2 H), 5.17 (d, *J* = 2.2 Hz, 1 H), 5.23 (qd, *J* = 1.3, 10.3 Hz, 1 H), 5.36 (qd, *J* = 1.6, 17.2 Hz, 1 H), 5.95 (dddd, *J* = 5.4, 6.1, 10.4, 17.2 Hz, 1 H), 6.90 (d, *J* = 8.8 Hz, 2 H), 7.44 (d, *J* = 8.8 Hz, 2 H). ¹³C NMR (CDCl₃, 75 MHz): δ 14.7 (CH₃), 63.3 (CH₂), 68.8 (CH₂), 69.8 (CH), 75.3 (CH), 81.8 (C_{quat}), 114.1 (CH), 117.4 (CH₂), 128.7 (CH), 130.2 (C_{quat}), 134.0 (CH), 159.1 (C_{quat}). EI MS (70 eV, *m/z* (%)): 216 (M⁺, 22), 174 (M⁺ – C₃H₆, 27), 159 (M⁺ – C₃H₅O, 85), 131 (100), 121 (27). HRMS calcd. for C₁₄H₁₆O₂: 216.1150; found: 216.1158. IR (film): $\tilde{\nu}$ = 3289 cm⁻¹ (s), 2981 (m), 2931 (m), 1724 (m), 1512 (s), 1249 (m), 1116 (w), 923 (w). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 274 nm (1400), 282 (1200), 296 (800).

[4-(1-Allyloxy-prop-2-ynyl)-phenyl]-dimethylamine (2e)

According to procedure A and after column chromatography on silica gel (hexane/ethyl acetate, 3:1) 1.10 g (80 %) of **2e** were obtained as a yellow oil. ¹H NMR (CDCl₃, 250 MHz): δ 2.63 (d, *J* = 2.2 Hz, 1 H), 2.97 (s, 6 H), 4.12 (m, *J* $\approx$ 12.4 Hz, 2 H), 5.15 (d, *J* = 2.2 Hz, 1 H), 5.22 (qd, *J* = 1.6, 10.3 Hz, 1 H), 5.33 (qd, *J* = 1.6, 17.2 Hz, 1 H), 5.96 (dddd, *J* = 5.6, 6.0, 10.4, 17.3 Hz, 1 H), 6.73 (d, *J* = 8.9 Hz, 2 H), 7.39 (d, *J* = 8.9 Hz, 2 H). ¹³C NMR (CDCl₃, 75 MHz): δ 40.5 (CH₃), 68.7 (CH₂), 70.2 (CH), 74.9 (CH), 82.2 (C_{quat}), 112.2 (CH), 117.4 (CH₂), 125.8 (C_{quat}), 128.5 (CH), 134.4 (CH), 150.7 (C_{quat}). EI MS (70 eV, *m/z* (%)): 215 (M⁺, 25), 173 (M⁺ – C₃H₆,

7), 158 ($M^+ - C_3H_5O$, 100), 142 (12), 115 (4). HRMS calcd. for $C_{14}H_{17}NO$: 215.1310; found: 215.1306. IR (film): $\tilde{\nu} = 3286\text{ cm}^{-1}$ (s), 2857 (m), 2806 (w), 1614 (s), 1524 (s), 1353 (m), 1058 (s), 927 (m). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 270 nm (18400), 298 (3500), 340 (700).

1-(1-But-2-enyloxyprop-2-ynyl)-4-ethoxy-benzene (2f)

According to procedure A and after column chromatography on silica gel (hexane/ethyl acetate, 3:1) 2.54 g (57 %) of **2f** were obtained as a yellow oil. 1H NMR ($CDCl_3$, 300 MHz): δ 1.41 (t, $J = 7.1$ Hz, 3 H), 1.72 (qd, $J = 1.2, 6.1$ Hz, 3 H), 2.62 (d, $J = 2.2$ Hz, 1 H), 4.10 (m, $J = 12.5$ Hz, 2 H), 4.03 (q, $J = 7.0$ Hz, 2 H), 5.14 (d, $J = 2.2$ Hz, 1 H), 5.54–5.85 (m, 2 H), 6.89 (d, $J = 8.8$ Hz, 2 H), 7.43 (d, $J = 8.9$ Hz, 2 H); additional signals for the minor isomer (Z-isomere): δ 1.24 (3 H), 1.68 (3 H), 2.64 (1 H), 3.97–4.21 (4 H), 5.16 (1 H), 5.54–5.85 (2 H), 6.89 (2 H), 7.43 (2 H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 14.7 (CH_3), 17.7 (CH_3), 63.4 (CH_2), 68.7 (CH_2), 69.6 (CH), 75.1 (CH), 82.0 (C_{quat}), 114.4 (CH), 127.0 (CH), 128.7 (CH), 130.3 (CH), 130.4 (C_{quat}), 159.0 (C_{quat}). EI MS (70 eV, m/z (%)): 230 (M^+ , 100), 215 ($M^+ - CH_3$), 201 ($M^+ - C_2H_5$, 92), 187 ($M^+ - C_3H_7$, 41), 149 (52), 121 ($C_6H_4OC_2H_5^+$, 26). HRMS calcd. for $C_{15}H_{18}O_2$: 230.1307; found: 230.1318. IR (film): $\tilde{\nu} = 2980\text{ cm}^{-1}$ (m), 2934 (m), 1657 (m), 1599 (s), 1249 (s), 1091 (w), 922 (w). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 242 nm (9900), 282 (12700).

2-{1-[(E)-But-2-enyl]oxy}-prop-2-ynyl-thiophene (2g)

According to procedure A and after column chromatography on silica gel (hexane/ethyl acetate, 3:1) 1.08 g (23 %) of **2g** were obtained as a yellow oil. 1H NMR ($CDCl_3$, 250 MHz): δ 1.74 (qd, $J = 1.2, 6.2$ Hz, 3 H), 2.66 (d, $J = 2.2$ Hz, 1 H), 4.10 (m, $J = 12.5$ Hz, 2 H), 5.45 (d, $J = 2.2$ Hz, 1 H), 5.55–5.87 (m, 2 H), 6.98 (dd, $J = 1.5, 8.6$ Hz, 1 H), 7.18 (td, $J = 2.0, 8.5$ Hz, 1 H), 7.32 (dd, $J = 1.2, 8.4$ Hz, 1 H); additional signals for the minor isomer (Z-isomer): δ 1.70 (3 H), 2.68 (1 H), 4.23 (2 H), 5.47 (1 H), 5.55–5.87 (2 H), 6.98 (1 H), 7.18 (1 H), 7.32 (1 H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 17.7 (CH_3), 63.0 (CH_2), 65.3 (CH), 74.9 (CH), 81.0 (C_{quat}), 126.2 (CH), 126.2 (CH), 126.3 (CH), 126.4 (CH), 130.5 (CH), 141.7 (C_{quat}). EI MS (70 eV, m/z (%)): 192

(M^+ , 4), 177 ($M^+ - CH_3$, 19), 121 ($M^+ - C_4H_7O$, 100), 109 ($M^+ - C_4H_3S$, 5), 55 (C_4H_7 , 10). HRMS calcd. for $C_{11}H_{12}OS$: 192.0609; found: 192.0609. IR (film): $\tilde{\nu} = 3291\text{ cm}^{-1}$ (s), 2939 (w), 2916 (w), 2857 (m), 2115 (w), 1450 (m), 1293 (m), 1039 (s), 705 (s). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 238 nm (7800), 280 (600).

1-Methoxy-4-[1-(3-methyl-but-2-enyloxy)-prop-2-ynyl]-benzene (2h)

According to procedure C and after column chromatography on silica gel (hexane/ethyl acetate, 7:1) 4.37 g (70 %) of **2h** were obtained as a yellow oil. 1H NMR ($CDCl_3$, 250 MHz): δ 1.68 (s, 3 H), 1.76 (s, 3 H), 2.63 (d, $J = 2.2$ Hz, 1 H), 3.80 (s, 3 H), 4.11 (m, $J = 11.3$ Hz, 2 H), 5.14 (d, $J = 2.2$ Hz, 1 H), 5.38 (m, 1 H), 6.89 (d, $J = 8.8$ Hz, 2 H), 7.45 (d, $J = 8.6$ Hz, 2 H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 17.9 (CH_3), 25.6 (CH_3), 55.1 (CH_3), 64.2 (CH_2), 69.5 (CH), 74.9 (CH), 81.9 (C_{quat}), 113.6 (CH), 120.3 (CH), 128.6 (CH), 130.5 (C_{quat}), 137.8 (C_{quat}), 159.5 (C_{quat}). EI MS (70 eV, m/z (%)): 230 (M^+ , 2), 215 ($M^+ - CH_3$, 35), 161 ($M^+ - C_5H_9$, 30), 145 ($M^+ - C_5H_9O$, 100), 135 ($OCC_6H_4OCH_3^+$, 57). HRMS calcd. for $C_{15}H_{18}O_2$: 230.1307; found: 230.1277. IR (film): $\tilde{\nu} = 3287\text{ cm}^{-1}$ (s), 2970 (m), 2934 (m), 2838 (m), 1721 (w), 1619 (m), 1250 (m), 839 (w). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 260 nm (4200), 274 (3900), 282 (3100).

1-Diethoxymethyl-4-[1-(3-methyl-but-2-enyloxy)-prop-2-ynyl]-benzene (2i)

According to procedure C and after column chromatography on silica gel (hexane/ethyl acetate, 7:1) 4.29 g (71 %) of **2i** were obtained as a yellow oil. 1H NMR (300 MHz, $CDCl_3$): δ 1.21 (t, $J = 7.1$ Hz, 6 H), 1.66 (d, $J = 0.9$ Hz, 3 H), 1.73 (d, $J = 0.9$ Hz, 3 H), 2.62 (d, $J = 2.2$ Hz, 1 H), 3.50–3.59 (m, 4 H), 4.11 (m, 2 H), 5.17 (d, $J = 2.2$ Hz, 1 H), 5.36 (m, 1 H), 5.49 (s, 1 H), 7.48 (m, 4 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 15.0 (CH_3), 17.9 (CH_3), 25.7 (CH_3), 60.8 (CH_2), 64.5 (CH_2), 69.7 (CH), 75.3 (CH), 81.7 (C_{quat}), 101.1 (CH), 120.3 (CH), 126.7 (CH), 127.1 (CH), 138.0 (C_{quat}), 138.3 (C_{quat}), 139.2 (C_{quat}). EI MS (70 eV, m/z (%)): 302 (M^+ , 1), 273 ($M^+ - C_2H_5$, 10), 257 ($M^+ - OC_2H_5$, 35), 247 ($M^+ - CHC(CH_3)_2$, 45), 199 ($M^+ - CH(OC_2H_5)_2$, 25), 179 ($C_6H_5CH(OC_2H_5)_2^+$, 100). HRMS calcd. for $C_{19}H_{26}O_3$: 302.1882; found: 302.1899. IR (film):

$\tilde{\nu} = 2975 \text{ cm}^{-1}$ (s), 2931 (m), 2880 (m), 1723 (m), 1445 (w), 1374 (w), 1335 (w), 1209 (m), 1112 (m), 1055 (s). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 252 nm (9400), 290 (2500).

1-Chloro-4-[1-(3-methyl-but-2-enyloxy)-prop-2-ynyl]-benzene (2j)

According to procedure C and after column chromatography on silica gel (hexane/ethyl acetate, 7:1) 5.24 g (50 %) of **2j** were obtained as a brown oil which solidifies at -18°C . ^1H NMR (300 MHz, CDCl_3): δ 1.70 (s, 3 H), 1.76 (s, 3 H), 2.65 (d, $J = 2.2$ Hz, 1 H), 4.14 (m, 2 H), 5.16 (d, $J = 2.2$ Hz, 1 H), 5.38 (m, 1 H), 7.34 (m, 2 H), 7.47 (m, 2 H). ^{13}C NMR (75 MHz, CDCl_3): δ 17.9 (CH_3), 25.6 (CH_3), 64.6 (CH_2), 69.1 (CH), 75.5 (CH), 81.3 (C_{quat}), 120.0 (CH), 128.4 (CH), 128.5 (CH), 134.0 (C_{quat}), 136.8 (C_{quat}), 138.2 (C_{quat}). EI MS (70 eV, m/z (%)): 235 (M^+ (^{37}Cl), 1), 233 (M^+ (^{35}Cl), 1), 219 ($\text{M}^+ - \text{CH}_3$, 18), 165 ($\text{M}^+ - \text{CH}_2\text{CHC}(\text{CH}_3)_2$, 17), 149 ($\text{M}^+ - \text{OCH}_2\text{CHC}(\text{CH}_3)_2$, 100). HRMS calcd. for $\text{C}_9\text{H}_6\text{Cl}$: 149.0158; found: 149.0149. IR (film): $\tilde{\nu} = 3299 \text{ cm}^{-1}$ (s), 3240 (s), (S), 2965 (s), 2932 (s), 2910 (s), 2864 (s), 2110 (s), 1904 (m), 1492 (m), 1446 (m), 1051 (s), 1014 (s), 804 (s). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 260 nm (500), 266 (500), 276 (300), 298 (100), 324 (100).

[1-(3-Methyl-but-2-enyloxy)-prop-2-ynyl]-benzene (2k)

According to procedure B and after column chromatography on silica gel (hexane/ethyl acetate, 7:1) 6.15 g (77 %) of **2k** were obtained as a yellow oil. ^1H NMR (300 MHz, CDCl_3): δ 1.70 (s, 3 H), 1.78 (s, 3 H), 2.65 (d, $J = 2.2$ Hz, 1 H), 4.16 (m, 2 H), 5.21 (d, $J = 2.2$ Hz, 1 H), 5.41 (m, 1 H), 7.30–7.42 (m, 3 H), 7.54 (m, 2 H). ^{13}C NMR (75 MHz, CDCl_3): δ 17.9 (CH_3), 25.6 (CH_3), 64.5 (CH_2), 69.9 (CH), 75.2 (CH), 81.7 (C_{quat}), 120.3 (CH), 127.2 (CH), 128.2 (CH), 128.3 (CH), 138.0 (C_{quat}), 138.2 (C_{quat}). EI MS (70 eV, m/z (%)): 200 (M^+ , 1), 131 ($\text{M}^+ - \text{CH}_2\text{CHC}(\text{CH}_3)_2$, 27), 115 ($\text{M}^+ - \text{OCH}_2\text{CHC}(\text{CH}_3)_2$, 100), 85 ($\text{OCH}_2\text{CHC}(\text{CH}_3)_2^+$, 21), 77 (C_6H_5^+ , 12), 69 ($\text{CH}_2\text{CHC}(\text{CH}_3)_2^+$, 25). HRMS calcd. for $\text{C}_{14}\text{H}_{16}\text{O}$: 200.1201; found: 200.1213. IR (film): $\tilde{\nu} = 3291 \text{ cm}^{-1}$ (S), 2973 (w), 2932 (m), 2913 (m), 2860 (m), 2112 (w), 1669 (m), 1494 (m),

1451 (s), 1057 (s) 1029 (s), 757 (m), 741 (m). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 250 nm (400), 258 (500), 413 (400).

2-[1-(3-Methyl-but-2-enyloxy)-prop-2-ynyl]-thiophene (2I)

According to procedure B and after column chromatography on silica gel (hexane/ethyl acetate, 7:1) 4.83 g (87 %) of **2I** were obtained as a yellow oil. ¹H NMR (300 MHz, CDCl₃): δ 1.70 (s, 3 H), 1.77 (s, 3 H), 2.66 (d, J = 2.2 Hz, 1 H), 4.15 (m, 2 H), 5.39 (m, 1 H), 5.45 (dd, J = 1.1, 2.2 Hz, 1 H), 6.97 (dd, J = 3.4, 5.1 Hz, 1 H), 7.19 (m, 1 H), 7.31 (dd, J = 1.5, 5.1 Hz, 1 H). ¹³C NMR (75 MHz, CDCl₃): δ 18.0 (CH), 25.8 (CH₃), 64.2 (CH₂), 65.4 (CH), 74.9 (CH), 81.1 (C_{quat}), 120.1 (CH), 126.2 (CH), 126.3 (CH), 126.4 (CH), 138.4 (C_{quat}), 141.8 (C_{quat}). EI MS (70 eV, m/z (%)): 206 (M⁺, 4), 191 (M⁺ – CH₃, 84), 137 (M⁺ – CH₂CHC(CH₃)₂, 76), 121 (M⁺ – OCH₂CHC(CH₃)₂, 100), 69 (CH₂CHC(CH₃)₂⁺, 29), HRMS calcd. for C₁₂H₁₄OS: 206.0765; found: 206.0786. IR (film): $\tilde{\nu}$ = 2973 cm⁻¹ (w), 2931 (w), 2913 (w), 2859 (w), 2115 (w), 1673 (w), 1438 (m), 1377 (w), 1294 (m), 1231 (m), 1056 (s), 1039 (s), 704 (s). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 286 nm (400), 302 (300), 344 (100).

3. General procedure for the preparation of alkynoyl *ortho*-iodo amides **4**

In a heat gun dried and nitrogen filled Schlenk flask 1.1 equiv. of the corresponding terminal acetylene were dissolved in THF and cooled to $-78\text{ }^{\circ}\text{C}$ with dry ice (for experimental details see Table 1). At this temperature 1.0 equiv. of *n*-BuLi (2.5 *M* in hexane) were slowly added by syringe, then, the solution was stirred for 30 min and subsequently treated with 1.0 equiv. of 1-iodo-2-isocyanato benzene, dissolved in a small amount of THF and allowed to warm up to $-40\text{ }^{\circ}\text{C}$ within 2 h. At this temperature 1.1 equiv. of the corresponding electrophile dissolved in a small amount of THF were added and the solution was allowed to warm to rt over night. For work up a saturated aqueous solution of NH_4Cl was added, the organic layer was separated and the aqueous phases were extracted three times with diethyl ether. The combined organic phases were dried with MgSO_4 , filtered and, finally, the solvents were removed in vacuum. Column chromatography on silica (hexane/ethyl acetate) afforded the alkynoyl *ortho*-iodo amides **4** as solid products.

Table 1. Experimental details for the synthesis of alkynoyl *ortho*-iodo amides **4**

Entry	Terminal acetylene 1	1-Iodo-2-isocyanato benzene	Electrophile	Alkynoyl <i>ortho</i> -iodo amides 4
1	13.5 mL (0.11 mol) of phenyl acetylene	25.0 g (0.10 mol)	21.0 g (0.11 mol) of <i>p</i> -tosyl chloride	28.6 g (57 %) of 4a
2	12.0 mL (0.11 mol) of 1-hexyne	25.0 g (0.10 mol)	21.0 g (0.11 mol) of <i>p</i> -tosyl chloride	39.0 g (79 %) of 4b
3	5.10 mL (35 mmol) of tris(isopropyl)silyl acetylene	7.84 g (33.0 mmol)	7.80 g (36.5 mmol) of <i>p</i> -tosyl chloride	11.3 g (59 %) of 4c
4	6.94 g (55.0 mmol) of <i>p</i> -methoxy phenyl acetylene	12.3 g (50.0 mmol)	4.30 ml (55.0 mmol) of methyl sulfonyl chloride	11.5 g (48 %) of 4d
5	4.49 g (33.0 mmol) of <i>p</i> -methoxy phenyl acetylene	7.35 g (30.0 mmol)	6.29 g (33.0 mmol) of <i>p</i> -tosyl chloride	14.0 g (88 %) of 4e
6	7.83 g (33.0 mmol) of <i>N</i> -methyl 3-ethynyl phenothiazine	7.35 g (30.0 mmol)	6.29 g (33.0 mmol) of <i>p</i> -tosyl chloride	5.70 g (30 %) of 4f
7	5.80 mL (55.0 mmol) of phenyl acetylene	12.3 g (50.0 mmol)	5.05 g (55.0 mmol) of acetanhydride	18.4 g (94 %) of 4h
8	5.80 mL (55.0 mmol) of phenyl acetylene	12.3 g (50.0 mmol)	0.30 ml (55.0 mmol) of methyl iodide	17.2 g (95 %) of 4i

***N*-(2-Iodo-phenyl)-4-methyl-*N*-(3-phenyl-propynoyl)-benzenesulfonamide (4a)**

According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 1:1) 28.6 g (57 %) of **4a** were obtained as a colorless solid, Mp. 141°C. ¹H NMR (300 MHz, CDCl₃): δ 2.47 (s, 3 H), 7.05 (d, *J* = 7.0 Hz, 2 H), 7.22–7.24 (m, 2 H), 7.38 (m, 4 H), 7.42 (dd, *J* = 1.8, 7.7 Hz, 1 H), 7.50 (dt, *J* = 1.1, 7.4 Hz, 1 H), 8.03 (dd, *J* = 1.1, 8.1 Hz, 1 H), 8.10 (d, *J* = 8.5 Hz, 2 H). ¹³C NMR (75 MHz, CDCl₃): δ 21.7 (CH₃), 81.8 (C_{quat}), 93.4 (C_{quat}), 102.6 (C_{quat}), 119.0 (C_{quat}), 128.6 (CH), 129.3 (CH), 129.4 (CH), 130.0 (CH), 130.1 (CH), 131.3 (CH), 131.6 (CH), 132.9 (CH), 135.6 (C_{quat}), 139.6 (C_{quat}), 140.2 (CH), 145.6 (C_{quat}), 151.9 (C_{quat}). EI MS (70 eV, *m/z* (%)): 501 (M⁺, 2), 374 (M⁺ – I, 100), 346 (M⁺ – SO₂C₆H₄CH₃, 14), 318 (25), 311 (42). HRMS calcd. for C₂₂H₁₆INO₃S: 500.9896; found: 500.9892. IR (KBr): $\tilde{\nu}$ = 3059 cm⁻¹ (w), 2217 (s), 1936 (w), 1680 (s), 1371 (s), 1296 (s), 1160 (s), 703 (m), 581 (m). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 234 nm (23800), 274 (20200), 296 (17100). Anal. calcd. for C₂₂H₁₆INO₃S (481.4): C 52.71, H 3.22, I 25.31, N 2.79, S 6.40; found: C 52.73, H 3.35, I 25.28, N 2.93, S 6.57.

***N*-Hept-2-ynoyl-*N*-(2-iodo-phenyl)-4-methyl-benzenesulfonamide (4b)**

According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 1:1) 39.0 g (79 %) of **4b** were obtained as a colorless solid, Mp. 106 °C. ¹H NMR (300 MHz, CDCl₃): δ 0.73 (t, *J* = 7.1 Hz, 3 H), 1.01 (m, 2 H), 1.12 (m, 2 H), 2.04 (dt, *J* = 2.9, 6.6 Hz, 2 H), 2.45 (s, 3 H), 7.16 (tt, *J* = 0.7, 8.1 Hz, 1 H), 7.35 (d, *J* = 8.1 Hz, 3 H), 7.44 (t, *J* = 7.5 Hz, 1 H), 7.96 (d, *J* = 8.1 Hz, 1 H), 8.05 (d, *J* = 8.1 Hz, 2 H). ¹³C NMR (75 MHz, CDCl₃): δ 13.1 (CH₃), 18.2 (CH₂), 21.3 (CH₂), 21.5 (CH₃), 28.8 (CH₂), 74.3 (C_{quat}), 97.1 (C_{quat}), 102.3 (C_{quat}), 128.9 (CH), 129.1 (CH), 129.8 (CH), 130.9 (CH), 131.3 (CH), 135.5 (C_{quat}), 139.4 (C_{quat}), 140.0 (C_{quat}), 145.3 (C_{quat}), 151.6 (C_{quat}). EI MS (70 eV, *m/z* (%)): 481 (M⁺, 12), 381 (23), 372 (M⁺ – COC₂H₉, 78), 354 (M⁺ – I), 331 (27), 326 (M⁺ – SO₂C₆H₄CH₃, 5). IR (KBr): $\tilde{\nu}$ = 3069 cm⁻¹ (w), 2954 (m), 2933 (m), 2874 (w), 2224 (s), 1602 (s), 1595 (m), 1464 (m), 1255 (m), 1233 (m), 1175 (s), 704 (s), 660 (s), 579 (s). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 238 nm (21900),

268 (2300), 274 (1800), 284 (900). Anal. calcd. for $C_{20}H_{20}INO_3S$ (481.4): C 49.91, H 4.19, I 26.36, N 2.91, S 6.66; found: C 49.95, H 4.17, I 26.51, N 2.96, S 6.61.

***N*-(2-Iodo-phenyl)-4-methyl-*N*-(3-triisopropylsilanyl-propynoyl)-benzenesulfonamide (**4c**)**

According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 1:1) 11.3 g (59 %) of **4c** were obtained as a colorless solid, Mp. 123 °C. 1H NMR (300 MHz, $CDCl_3$): δ 0.85 (m, 21 H), 2.46 (s, 3 H), 7.14 (ddd, $J = 2.1, 6.9, 8.0$ Hz, 1 H), 7.36 (d, $J = 8.4$ Hz, 2 H), 7.40 (d, $J = 2.1$ Hz, 1 H), 7.43 (dd, $J = 1.3, 6.9$ Hz, 1 H), 7.95 (dd, $J = 1.3, 8.0$ Hz, 1 H), 8.07 (d, $J = 8.4$ Hz, 2 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 10.7 (CH), 18.3 (CH_3), 21.7 (CH_3), 97.1 (C_{quat}), 99.3 (C_{quat}), 102.4 (C_{quat}), 129.2 (CH), 129.3 (CH), 130.1 (CH), 131.3 (CH), 131.6 (CH), 135.5 (C_{quat}), 139.3 (C_{quat}), 140.3 (CH), 145.6 (C_{quat}), 151.0 (C_{quat}). EI MS (70 eV, m/z (%)): 581 (M^+ , 1), 538 ($M^+ - CH(CH_3)_2$, 93), 486 (100), 454 ($M^+ - I$, 21), 411 (23), 410 (93). HRMS calcd. for $C_{22}H_{25}INO_3SSi$: 538.0369; found: 538.0352. IR (KBr): $\tilde{\nu} = 2944\text{ cm}^{-1}$ (m), 2865 (m), 2155 (w), 1683 (s), 1464 (m), 1372 (m), 1356 (w), 1280 (w), 1247 (m), 1220 (s), 1211 (s), 1172 (s), 1085 (m), 762 (m), 660 (s), 584 (s), 547 (m). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 240 nm (23000), 276 (2000), 284 (1000). Anal. calcd. for $C_{25}H_{32}INO_3SSi$ (581.6): C 51.63, H 5.55, I 21.82, N 2.41, S 5.51; found: C 51.62, H 5.55, I 21.69, N 2.52, S 5.55.

***N*-(2-Iodo-phenyl)-*N*-[3-(4-methoxy-phenyl)-propynoyl]-methanesulfonamide (**4d**)**

According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 1:1) 11.5 g (48 %) of **4d** were obtained as a colorless solid, Mp. 144 °C. 1H NMR ($CDCl_3$, 300 MHz): δ 3.72 (s, 3 H), 3.79 (s, 3 H), 6.77 (d, $J = 9.0$ Hz, 2 H), 7.01 (m, 2 H), 7.21–7.27 (m, 1 H), 7.48–7.56 (m, 2 H), 8.01 (m, 1 H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 43.7 (CH_3), 55.4 (CH_3), 81.3 (C_{quat}), 95.8 (C_{quat}), 101.9 (C_{quat}), 110.5 (C_{quat}), 114.3 (CH), 129.5 (CH), 131.5 (CH), 132.4 (CH), 135.1 (CH), 138.6 (C_{quat}), 140.0 (CH), 153.4 (C_{quat}), 162.0 (C_{quat}). EI MS (70 eV, m/z (%)): 455 (M^+ , 15), 328 ($M^+ - I$, 100). HRMS calcd. for $C_{17}H_{14}NO_4S$: 328.0644; found: 328.0652. IR (KBr): $\tilde{\nu} = 2841\text{ cm}^{-1}$ (w), 2192 (s), 1670 (s), 1601 (s), 1510 (s), 1465 (m),

1442 (m), 1355 (s), 1294 (m), 1258 (s), 1156 (s), 1023 (m), 964 (s), 838 (m), 766 (m). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 308 nm (24400), 316 (23100). Anal. calcd. for C₁₇H₁₄INO₄S (455.3): C 44.85, H 3.10, N 3.08, S 7.04; found: C 45.01, H 3.14, N 2.96, S 7.12.

***N*-(2-Iodo-phenyl)-*N*-[3-(4-methoxy-phenyl)-propynoyl]-4-methyl-benzenesulfonamide (4e)**

According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 1:1) 14.0 g (88 %) of **4e** were obtained as a colorless solid, Mp. 156 °C. ¹H NMR (CDCl₃, 300 MHz): δ 2.46 (s, 3 H), 3.77 (s, 3 H), 6.74 (d, J = 8.8 Hz, 2 H), 6.98 (d, J = 8.8 Hz, 2 H), 7.22 (m, 1 H), 7.36 (d, J = 8.4 Hz, 2 H), 7.42 (dd, J = 1.8, 7.9 Hz, 1 H), 7.49 (m, 1 H), 8.03 (dd, J = 1.3, 8.0 Hz, 1 H), 8.09 (d, J = 8.4 Hz, 2 H). ¹³C NMR (CDCl₃, 75 MHz): δ 21.7 (CH₃), 55.3 (CH₃), 81.5 (C_{quat}), 94.6 (C_{quat}), 102.7 (C_{quat}), 110.8 (C_{quat}), 114.2 (CH), 129.2 (CH), 129.3 (CH), 129.9 (CH), 131.2 (CH), 131.6 (CH), 134.9 (CH), 135.7 (C_{quat}), 139.7 (C_{quat}), 140.2 (CH), 145.5 (C_{quat}), 152.1 (C_{quat}), 161.7 (C_{quat}). EI MS (70 eV, m/z (%)): 531 (M⁺, 6), 404 (M⁺ – I, 44), 159 (OCC₂C₆H₄OCH₃⁺, 100). HRMS calcd. for C₂₃H₁₈INO₄S: 531.0001; found: 531.0044. IR (KBr): $\tilde{\nu}$ = 2977 cm⁻¹ (w), 2887 (w), 2194 (s), 1677 (s), 1601 (s), 1510 (s), 1464 (m), 1365 (m), 1291 (m), 1255 (s), 1158 (s), 1086 (m), 1023 (m), 704 (s). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 310 nm (25300). Anal. calcd. for C₂₃H₁₈INO₄S (531.4): C 51.99, H 3.41, N 2.64; found: C 51.88, H 3.44, N 2.62.

***N*-(2-Iodo-phenyl)-4-methyl-*N*-[3-(10-methyl-10*H*-phenothiazin-3-yl)-propynoyl]-benzenesulfonamide (4f)**

According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 1:1) 5.70 g (30 %) of **4f** were obtained as a yellow-green fluorescent solid, Mp. 203 °C (dec.). ¹H NMR (CDCl₃, 300 MHz): δ 2.46 (s, 3 H), 3.30 (s, 3 H), 6.59 (d, J = 8.5 Hz, 1 H), 6.67 (d, J = 1.9 Hz, 1 H), 6.77 (dd, J = 0.8, 8.1 Hz, 1 H), 6.87 (dd, J = 1.9, 8.4 Hz, 1 H), 6.94 (dt, J = 1.1, 7.5 Hz, 1 H), 7.07 (dd, J = 1.5, 7.6 Hz, 1 H), 7.15 (ddd, J = 1.6, 8.1, 8.9 Hz, 1 H), 7.25 (m, 1 H), 7.36 (d, J = 8.1 Hz, 2 H), 7.41 (dd, J = 1.7, 7.9 Hz, 1 H), 7.50 (dt, J = 1.4, 7.5 Hz, 1 H),

8.03 (dd, $J = 1.4, 7.9$ Hz, 1 H), 8.09 (d, $J = 8.4$ Hz, 2 H). ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.7 (CH_3), 35.5 (CH_3), 82.5 (C_{quat}), 94.0 (C_{quat}), 102.7 (C_{quat}), 112.2 (C_{quat}), 113.7 (CH), 114.5 (CH), 122.2 (C_{quat}), 123.3 (CH), 123.5 (C_{quat}), 127.1 (CH), 127.7 (CH), 129.3 (CH), 129.3 (CH), 129.9 (CH), 131.0 (CH), 131.2 (CH), 131.6 (CH), 133.0 (CH), 135.7 (C_{quat}), 139.7 (C_{quat}), 140.2 (CH), 144.3 (C_{quat}), 145.5 (C_{quat}), 148.2 (C_{quat}), 152.0 (C_{quat}). EI MS (70 eV, m/z (%)): 636 (M^+ , 100), 452 (55), 372 (25), 354 (95), 264 (72). HRMS calcd. for $\text{C}_{29}\text{H}_{21}\text{IN}_2\text{O}_3\text{S}$: 636.0038; found: 636.0063. IR (KBr): $\tilde{\nu} = 3063\text{ cm}^{-1}$ (w), 2966 (w), 2844 (w), 2193 (s), 1677 (s), 1597 (m), 1573 (m), 1464 (s), 1373 (m), 1338 (m), 1311 (m), 1247 (m), 1189 (s), 1167 (s), 1143 (s), 1086 (m), 704 (s). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 240 nm (29100), 280 (20800), 296 (17200). Anal. calcd. for $\text{C}_{29}\text{H}_{21}\text{IN}_2\text{O}_3\text{S} \cdot 0.2\text{ H}_2\text{O}$ (640.1): C 54.41, H 3.37, N 4.38; found: C 54.16, H 3.36, N 4.31.

Acetic acid 2-{4-[(2-iodo-phenyl)-(3-phenyl-propynoyl)-sulfamoyl]-phenoxy}-ethyl ester (4g)

In a heat gun dried and nitrogen filled Schlenk flask 5.21 g (15.0 mmol) of 3-phenyl propynoic acid (2-iodo-phenyl)-amide were dissolved in 80 mL of THF and cooled to $-0\text{ }^\circ\text{C}$. At this temperature 400 mg (16.5 mmol) of sodium hydride (60 % (w/w) in white oil) were added portionwise. Then the solution was allowed to warm to rt, stirred for another hour and, finally, cooled to $0\text{ }^\circ\text{C}$ again. Subsequently, 4.60 g (16.5 mmol) of acetic acid 2-(4-chlorosulfonyl-phenoxy)-ethyl ester dissolved in 20 mL of THF were added dropwise and the solution was allowed to reach rt over night. For work up a saturated aqueous solution of NH_4Cl was added, the organic layer was separated and the aqueous phases were extracted three times with diethyl ether. The combined organic phases were dried with MgSO_4 , filtered and, finally, the solvents were removed in vacuum. Column chromatography on silica gel (hexane/ethyl acetate, 1:1) afforded 4.39 g (50 %) of **4g** as a beige solid, Mp. $68\text{ }^\circ\text{C}$. ^1H NMR (CDCl_3 , 300 MHz): δ 2.12 (s, 3 H), 4.29 (m, 2 H), 4.74 (m, 2 H), 7.05 (m, 2 H), 7.08 (s, 2 H), 7.22–7.28 (m, 3 H), 7.35–7.41 (m, 1 H), 7.46 (dd, $J = 1.8, 7.8$ Hz, 1 H), 7.49–7.54 (m, 1 H), 8.04 (dd, $J = 1.3, 7.9$ Hz, 1 H), 8.18 (d, $J = 8.9$ Hz, 2 H). ^{13}C NMR (CDCl_3 , 75 MHz): δ 20.8 (CH_3), 62.2 (CH_2), 66.3 (CH_2), 81.7

(C_{quat}), 93.3 (C_{quat}), 102.4 (C_{quat}), 114.3 (CH), 119.0 (C_{quat}), 128.4 (CH), 129.3 (CH), 130.3 (C_{quat}), 130.9 (CH), 131.3 (CH), 131.7 (CH), 132.4 (CH), 132.9 (CH), 140.2 (CH), 139.6 (C_{quat}), 152.0 (C_{quat}), 163.1 (C_{quat}), 170.8 (C_{quat}). EI MS (70 eV, *m/z* (%)): 589 (M⁺, 2), 462 (M⁺ – I, 37), 329 (100), 219 (99), 129 (OCC₂C₆H₅⁺, 100). HRMS calcd. for C₂₅H₂₀INO₆S: 589.0056; found: 589.0012. IR (KBr): $\tilde{\nu}$ = 2954 cm⁻¹ (w), 2204 (s), 1744 (s), 1679 (s), 1578 (s), 1464 (m), 1369 (m), 1269 (s), 1168 (s), 586 (s). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 288 nm (23600). Anal. calcd. for C₂₅H₂₀INO₆S (589.4): C 50.95, H 3.42, I 21.53, N 2.38, S 5.44; found: C 50.98, H 3.43, I 21.79, N 2.38, S 5.51.

***N*-(2-Iodo-phenyl)-*N*-(3-phenyl-propynoyl)-acetamide (4h)**

According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 2:1) 18.4 g (94 %) of **4h** were obtained as a colorless crystalline solid, Mp. 121 °C. ¹H NMR (CDCl₃, 300 MHz): δ 2.70 (s, 3 H), 7.11 (m, 2 H), 7.20 (m, 1 H), 7.25–7.30 (m, 2 H), 7.36–7.39 (m, 2 H), 7.50 (m, 1 H), 7.99 (dd, *J* = 1.3, 7.9 Hz, 1 H). ¹³C NMR (CDCl₃, 75 MHz): δ 27.4 (CH₃), 95.2 (C_{quat}), 101.0 (C_{quat}), 119.3 (C_{quat}), 128.5 (CH), 129.4 (CH), 130.6 (CH), 130.9 (CH), 131.0 (CH), 133.1 (CH), 133.0 (C_{quat}), 139.7 (CH), 154.0 (C_{quat}), 155.6 (C_{quat}), 171.5 (C_{quat}). EI MS (70 eV, *m/z* (%)): 389 (M⁺, 24), 346 (M⁺ – OCCH₃, 16), 262 (M⁺ – I, 22), 220 (92), 129 (OCC₂C₆H₅, 100). HRMS calcd. for C₁₇H₁₂INO₂: 388.9913; found: 388.9906. IR (KBr): $\tilde{\nu}$ = 3035 cm⁻¹ (w), 2202 (s), 1718 (s), 1676 (s), 1466 (m), 1305 (m), 1282 (s), 1223 (s), 1016 (m), 755 (m), 731 (m). UV/Vis (CH₂Cl₂): λ_{max} (ϵ) 276 nm (20200), 286 (187000). Anal. calcd. for C₁₇H₁₂INO₂ (389.2): C 52.46, H 3.11, I 32.61, N 3.60; found: C 52.62, H 3.11, I 32.56, N 3.59.

3-Phenyl-propynoic acid (2-iodo-phenyl)-methyl-amide (4i)

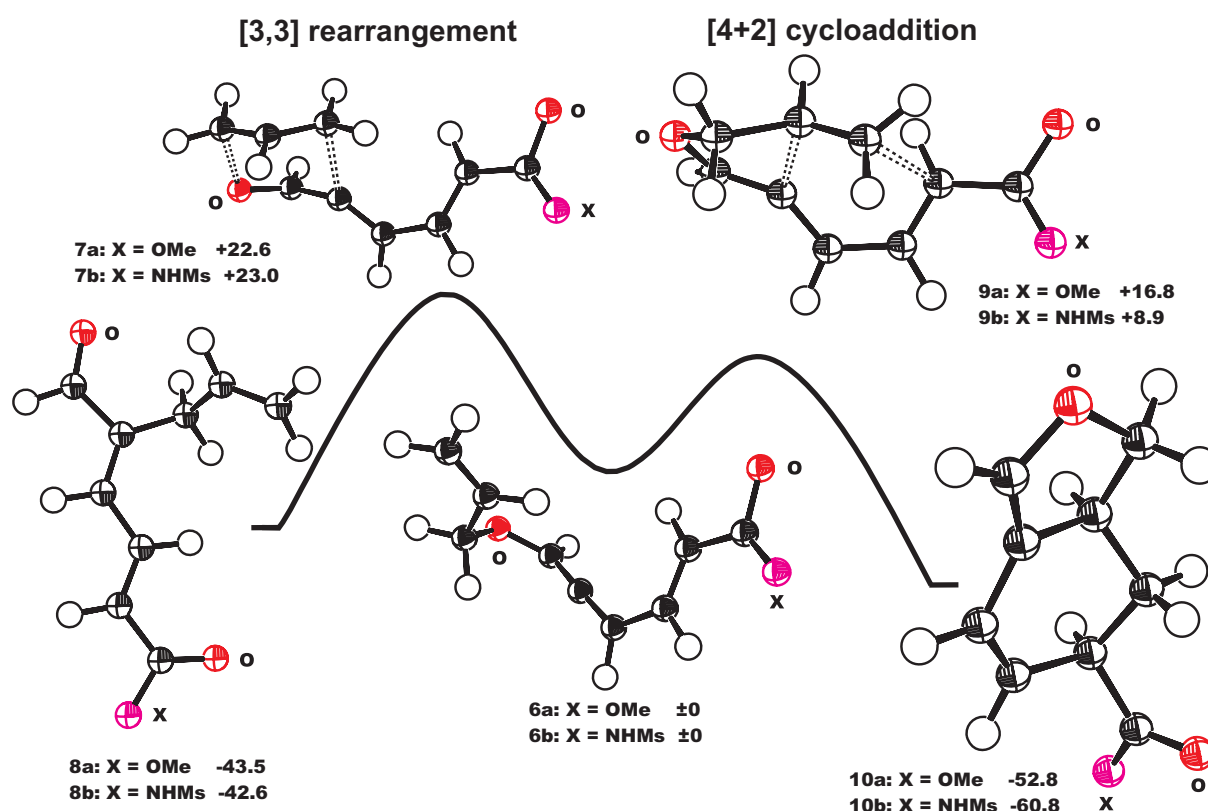
According to the general procedure and column chromatography on silica gel (hexane/ethyl acetate, 3:1) 17.2 g (95 %) of **4i** were obtained as a beige solid, Mp. 154 °C. ¹H NMR (CDCl₃, 300 MHz): δ 3.29 (3 H), 7.06 (m, 2 H), 7.13 (m, 1 H), 7.21 (m, 2 H), 7.29 (m, 1 H), 7.36–7.48

(m, 2 H), 7.95 (m, 1 H). ^{13}C NMR (CDCl_3 , 75 MHz): δ 35.1 (CH_3), 82.3 (C_{quat}), 90.5 (C_{quat}), 99.6 (C_{quat}), 120.1 (C_{quat}), 128.2 (CH), 129.5 (CH), 129.7 (CH), 129.9 (CH), 130.0 (CH), 132.4 (CH), 139.7 (CH), 145.4 (C_{quat}), 154.3 (C_{quat}). EI MS (70 eV, m/z (%)): 361 (M^+ , 3), 234 ($\text{M}^+ - \text{I}$, 100). HRMS calcd. for $\text{C}_{16}\text{H}_{12}\text{INO}$: 360.9964; found: 361.0001. IR (KBr): $\tilde{\nu}$ = 2983 cm^{-1} (w), 2968 (w), 2213 (s), 1629 (s), 1575 (m), 1490 (m), 1468 (m), 1418 (m), 1371 (s), 1313 (m), 1241 (w), 1131 (m), 1017 (m), 754 (s). UV/Vis (CH_2Cl_2): λ_{max} (ϵ) 236 nm (21700), 260 (19500). Anal. calcd. for $\text{C}_{16}\text{H}_{12}\text{INO}$ (361.2): C 53.21, H 3.35, N 3.88; found: C 53.08, H 3.37, N 3.93.

II. Computational Studies on the Concluding Pericyclic Steps: *Diels-Alder* vs. *Claisen* pathway

General considerations: All calculations in this publication were carried out on an AMD Opteron 64bit architecture cluster using Gaussian 03 x86-Linux-G03 Revision B.03.²

Geometry optimizations and transition state calculations were carried out using the Becke Three Parameter Hybrid Functionals [RB3LYP/6-31+G(d,p)], which have the form devised by *Becke* in 1993.³ Single point energy calculation were carried out using the *Møller-Plesset* correlation energy correction truncated at second-order [RMP2/6-311++G(2d,2p)//RB3LYP/6-31+G(d,p)].⁴



Scheme 1. Energy profile of the modeled pericyclic reactions.

Table 1. Relative single point energies of the structures **6**, **8** and **10** and the corresponding transition states **7** and **9** calculated on the MP2 level of theory [RMP2/6-311++G(2d,2p)//RB3LYP/6-31+G(d,p)] (energies are given in kcal/mol).

Allyloxy enallene 6	Claisen product 8	TS _[3,3] 7	Diels-Alder product 10	TS _[4+2] 9	Δ [TS _[4+2] (7)–TS _[3,3] (9)]
0 ^a (6a)	–43.50 (8a)	22.60 (7a) ^b	–52.10 (10a)	16.80 (9a) ^c	–5.80 [(7a)–(9a)]
0 ^a (6b)	–42.60 (8b)	23.00 (7b) ^d	–60.00 (10b)	8.90 (9b) ^e	–14.10 [(7b)–(9b)]

^aEnergies are set to 0 kcal/mol. Imaginary frequencies from the DFT geometry optimizations that verify transition states: ^bi508.05 cm^{–1}, ^ci463.57 cm^{–1}, ^di508.78 cm^{–1}, ^ei456.06 cm^{–1}.

Vinyl allenyl allyl ether 6a

ATOM	X	Y	Z
C	0.56655700	-2.04082500	-0.60154100
C	1.50184500	-1.62452700	0.23489200
H	0.80196600	-2.85644200	-1.28754100
C	2.39667500	-1.23333200	1.11488800
H	2.44308700	-1.68093900	2.10508600
C	-0.79216200	-1.49605000	-0.71295900
H	-1.40548800	-1.89267400	-1.51963300
C	-1.34600900	-0.56537300	0.08808900
H	-0.80719500	-0.13125000	0.92479900
C	-2.73078700	-0.10602900	-0.13807100
O	-3.48032800	-0.48638300	-1.02127000
O	-3.08623500	0.82262000	0.78553800
C	-4.42263400	1.34216700	0.66813000
H	-4.52710800	2.06079200	1.48062500
H	-5.15492500	0.53705000	0.76756900
H	-4.55870300	1.83058800	-0.30003800
O	3.36894400	-0.28449700	0.96906100
C	3.46585600	0.37820700	-0.31009300
H	4.48717800	0.76449100	-0.34603500
H	3.34227800	-0.37327400	-1.10204300
C	2.47147200	1.49365600	-0.46166500
H	1.41899800	1.21952700	-0.42180100
C	2.82188700	2.76694600	-0.66030300
H	2.07907000	3.54833000	-0.79008000
H	3.86560400	3.07084800	-0.70575000

Energy MP2 = -612.4326014 Hartree

Claisen Transition State 7a

ATOM	X	Y	Z
C	0.70504100	1.72896900	0.07425100
C	1.70413400	0.94151500	-0.32201300
H	0.95644600	2.77775400	0.24961900
C	2.97915900	0.86279600	-0.82787400
H	3.07329800	0.93559700	-1.92443600
C	-0.68886100	1.38311900	0.34578600
H	-1.20359300	1.99859500	1.08249400
C	-1.41338700	0.42291400	-0.26192300
H	-1.00692400	-0.19004200	-1.05926700
C	-2.82452300	0.19398000	0.10952000
O	-3.45368400	0.80189300	0.95821100
O	-3.35980100	-0.80918100	-0.63255100
C	-4.73797100	-1.12118500	-0.36109700
H	-5.37195300	-0.25377900	-0.56114000
H	-4.86305300	-1.42155900	0.68215400
H	-4.98717300	-1.94307400	-1.03184400
O	4.00409700	0.44507000	-0.15677900
C	3.89522600	-1.38487600	0.21484900
H	3.98615600	-1.72681900	-0.81180500
H	4.80638700	-1.45304100	0.79814400
C	2.64383600	-1.44231000	0.85294700
H	2.60743200	-1.28282800	1.92773800
C	1.48642300	-1.27875200	0.11355700

H	0.52115000	-1.21900800	0.60347000
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H	1.46247000	-1.56107400	-0.93419300
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Energy MP2 = -612.3966394 Hartree

Imaginary frequencies: i508.05 cm⁻¹

Claisen Product 8a

ATOM	X	Y	Z
C	0.79262700	-1.08813100	-0.10025000
H	0.66074200	-2.08165500	-0.53100300
C	2.06306400	-0.68958700	0.17464900
C	-0.41716200	-0.32856700	0.12074100
H	-0.34868200	0.67034900	0.54268800
C	-1.64613800	-0.80004000	-0.17873300
H	-1.79413100	-1.78652700	-0.60875800
C	-2.85500600	0.01604200	0.06855300
C	3.13897000	-1.65088100	-0.15232100
H	2.79749900	-2.61128100	-0.59352100
C	2.47496000	0.64181600	0.76348900
H	3.29658900	0.45005000	1.46531600
H	1.65289900	1.08843400	1.32923000
C	2.95957800	1.61264200	-0.29217100
H	3.82201700	1.28705600	-0.87148100
C	2.41081200	2.80661100	-0.52972800
H	2.80775600	3.46908200	-1.29330800
H	1.55184700	3.16707000	0.03233700
O	-2.87049100	1.13647900	0.54669200
O	4.32676200	-1.44295800	0.03517300

O	-3.97031300	-0.65134800	-0.30930700
C	-5.21553800	0.04576100	-0.11399100
H	-5.98748100	-0.63504700	-0.47093700
H	-5.22371600	0.97605100	-0.68700900
H	-5.36000900	0.27502800	0.94455000

Energy MP2 = -612.5018894 Hartree

Diels-Alder Transition State 9a

ATOM	X	Y	Z
C	1.75354900	0.75905300	-0.57155600
C	-0.48434100	1.65837200	-0.10902800
C	0.35226400	-0.96153400	1.28717100
C	-1.16347700	0.46772000	-0.24816300
C	1.43531300	-1.01375500	0.42582500
C	0.89613700	1.80768900	-0.36266500
H	-1.01121400	2.48498200	0.36105100
H	0.37223500	-0.36255200	2.19365100
H	-0.77424900	-0.29099400	-0.91046100
H	1.32452700	-1.69755900	-0.41874300
H	1.33511300	2.77955200	-0.13834500
H	-0.49196800	-1.62963300	1.17346800
C	2.99526600	0.44190500	-0.96150500
H	3.50620200	0.78607600	-1.85481700
O	3.66886100	-0.52456300	-0.28570600
C	2.88509900	-0.90952100	0.86313900
H	3.00794400	-0.16979400	1.66356600
H	3.29033500	-1.87306600	1.18050800

C	-2.55106100	0.35519500	0.25840300
O	-3.31263500	-0.70360800	-0.15138600
O	-3.04546400	1.13824400	1.04578000
C	-2.88934300	-1.58041000	-1.20089800
H	-2.65620200	-1.02852800	-2.11711800
H	-3.73773700	-2.24040500	-1.38583200
H	-2.02751700	-2.18696600	-0.90075800

Energy MP2 = -612.4058345 Hartree

Imaginary frequencies: i463.57 cm⁻¹

Diels-Alder Product 10a

ATOM	X	Y	Z
C	-1.78161900	0.82619200	-0.13332500
C	0.59250100	1.28408100	-0.34875300
C	-0.19151000	-1.08515800	0.18307900
C	0.96609500	-0.06365300	0.26755600
C	-1.49042600	-0.43233200	0.66608500
C	-0.68700200	1.67066700	-0.54134200
H	1.40073100	1.93355700	-0.67368600
H	-0.29762200	-1.40844900	-0.85693600
H	1.21240200	0.09169500	1.32773600
H	-1.37956000	-0.16207300	1.72896000
H	-0.89667800	2.61913200	-1.03071500
H	0.05916400	-1.97264300	0.77541800
C	-3.10655300	0.87826300	-0.36151700
H	-3.71040000	1.63511200	-0.84669400
O	-3.80086500	-0.20567700	0.10337200

C	-2.80062400	-1.21079500	0.45894000
H	-2.72578300	-1.91031400	-0.38394200
H	-3.16789300	-1.73696300	1.34117500
C	2.21523300	-0.60975300	-0.43437200
O	3.43087600	-0.10967200	-0.07621800
O	2.17634300	-1.43350500	-1.31852100
C	3.61403300	0.74542700	1.06194700
H	3.00712500	1.65267900	1.00004700
H	4.66971100	1.01804400	1.04572300
H	3.39720000	0.21341900	1.99406200

Energy MP2 = -612.5155524 Hartree

Vinyl allenyl allyl ether 6b

ATOM	X	Y	Z
C	0.10811600	-1.05404300	0.04769200
H	0.53373700	-0.45127700	0.84687900
C	0.86942300	-1.93232800	-0.63435800
H	0.38087700	-2.51235900	-1.41467900
C	-1.32540500	-0.89388100	-0.28440800
O	-1.90733400	-1.51145400	-1.16825300
N	-1.99891800	0.01795100	0.53111300
H	-1.50457400	0.53693200	1.24936200
S	-3.54504400	0.69490700	0.20030300
O	-3.78497400	1.53332300	1.38038400
O	-3.56251000	1.26906800	-1.14191500
C	-4.62246200	-0.74164200	0.23173200
H	-5.62397100	-0.37074300	0.00465900

H	-4.58393600	-1.17868400	1.22983600
H	-4.26936300	-1.43347600	-0.53354800
C	2.29987900	-2.18381400	-0.42873700
C	3.08721100	-1.51488900	0.39658200
H	2.72669300	-2.98941600	-1.02831200
C	3.85851400	-0.88893500	1.25822300
H	3.94760800	-1.23882400	2.28440300
O	4.63317700	0.21502100	1.05487600
C	4.66861100	0.77220700	-0.27900000
H	5.59074300	1.35685800	-0.30754400
H	4.74850500	-0.05460900	-0.99782900
C	3.48068300	1.64025900	-0.58046200
H	2.50800700	1.15245300	-0.59796500
C	3.57512000	2.94521100	-0.84832200
H	2.70041300	3.54210500	-1.08857000
H	4.53339100	3.46033200	-0.84372300

Energy MP2 = -1140.4283888 Hartree

Claisen-Transition State 7b

ATOM	X	Y	Z
C	2.32021100	1.81803200	-0.02732400
C	3.19521900	0.88109300	-0.39450600
C	2.71173000	-1.25400900	0.19683400
C	4.43988100	0.61801700	-0.91506900
C	3.85899500	-1.51199400	0.92493100
C	0.90136400	1.67438000	0.28407000
C	5.08979000	-1.65893200	0.26140500

C	0.04083400	0.78733100	-0.25571200
C	-1.37777700	0.77110400	0.16936400
H	0.48576100	2.38685000	0.99552400
H	1.77498900	-1.04408100	0.70097900
H	0.36244000	0.09251800	-1.02713500
H	2.71141300	2.83146300	0.08835100
H	2.62644200	-1.60257900	-0.82758500
H	5.10915300	-2.07817400	-0.74009100
H	6.00037000	-1.80320500	0.83146500
H	4.51739500	0.62544900	-2.01539400
H	3.87117200	-1.27913900	1.98663400
O	-1.84782300	1.48376500	1.04805200
O	5.42033000	0.11150900	-0.24046300
N	-2.17758500	-0.11793000	-0.55179300
H	-1.78183800	-0.70365900	-1.27941900
S	-3.75844300	-0.62721300	-0.10532600
O	-4.14241700	-1.49241100	-1.22662600
O	-3.75093300	-1.13441100	1.26356100
C	-4.69768600	0.90288400	-0.15269600
H	-5.71287800	0.64203700	0.15303800
H	-4.68196200	1.28456100	-1.17386000
H	-4.23289300	1.59382000	0.55130100

Energy MP2 = -1140.3917746 Hartree

Imaginary frequencies: i508.78 cm⁻¹

Claisen Product 8b

ATOM	X	Y	Z
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C	-3.94338200	-1.96368800	-0.04829800
H	-3.34906100	-2.88815900	0.10971600
O	-5.16201400	-1.99453500	-0.00625000
C	-3.15134600	-0.73856800	-0.30390800
C	-1.79916900	-0.88120300	-0.30168600
H	-1.39721700	-1.88009100	-0.12759800
C	-3.91317600	0.55050600	-0.51881900
H	-4.81996800	0.30470500	-1.08552100
H	-3.32798800	1.25353200	-1.11777700
C	-4.32170700	1.20186500	0.78533000
H	-4.95679100	0.60090100	1.43430900
C	-3.96785200	2.43454300	1.15761200
H	-3.34126700	3.06680200	0.53195200
H	-4.30228200	2.85795300	2.10012700
C	-0.82852700	0.16844600	-0.51015400
H	-1.17448000	1.18074900	-0.69836500
C	0.50552100	-0.04963300	-0.48116100
H	0.91587900	-1.03901800	-0.30891300
C	1.43679000	1.07310900	-0.72566500
O	1.08513100	2.18481600	-1.09754500
N	2.81300600	0.85005500	-0.53540700
H	3.39558400	1.65530000	-0.75156000
S	3.69286700	-0.43162600	0.16765600
O	3.08495300	-1.70015400	-0.23560500
O	5.08688800	-0.11057600	-0.13506200
C	3.42699700	-0.22764300	1.93975300
H	3.80643900	0.75049900	2.23689200

H	3.98873800	-1.02591500	2.42921700
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H	2.36093700	-0.32444400	2.15055100
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Energy MP2 = -1140.4963243 Hartree

Diels-Alder Transition State 9b

ATOM	X	Y	Z
C	-3.25214600	0.92460100	0.15093800
C	-0.88324200	1.54146800	-0.02921900
C	-1.65920500	-1.42543000	-0.45311800
C	-0.40379800	0.48887900	0.72116100
C	-2.90662200	-1.11526400	0.05977400
C	-2.26007600	1.79139200	-0.22384900
H	-1.43017300	-1.28284200	-1.50648500
H	-1.01956700	0.05862500	1.49893900
H	-3.05480700	-1.37336900	1.11008600
H	-0.20255800	2.14312900	-0.62920000
H	-0.92549100	-1.96177000	0.13540000
H	-2.52106600	2.59202500	-0.91536900
C	-4.57578000	0.79585300	0.30747100
H	-5.23592500	1.47906400	0.83207800
O	-5.17664600	-0.35968800	-0.07093400
C	-4.20002700	-1.19659500	-0.72740500
H	-4.06003500	-0.86243500	-1.76273800
H	-4.62709200	-2.20189000	-0.71522800
C	0.99537000	0.02812600	0.81377500
O	1.33964400	-0.82576000	1.62663800
N	1.92833100	0.60761800	-0.05137700

H	1.63323300	1.25264700	-0.77570300
S	3.46107000	-0.07363300	-0.42550600
O	4.02169400	0.90038400	-1.36982400
O	3.31307100	-1.47691900	-0.80457500
C	4.32938200	0.01647700	1.14374700
H	3.75491000	-0.56012500	1.86916900
H	4.41535600	1.06538400	1.42825600
H	5.31254700	-0.42481100	0.96845800

Energy MP2 = -1140.4141775 Hartree

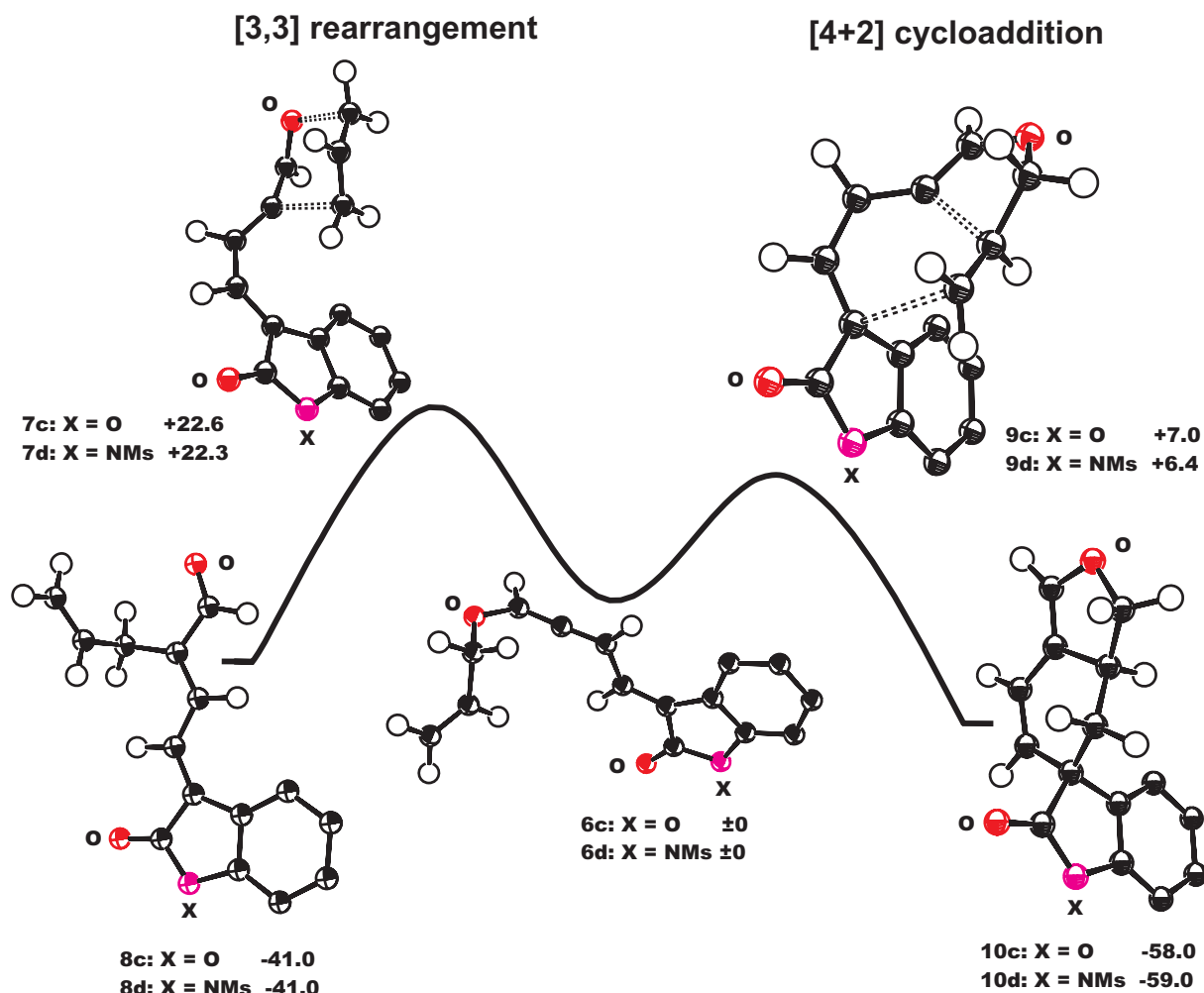
Imaginary frequencies: i456.06 cm⁻¹

Diels-Alder Product 10b

ATOM	X	Y	Z
C	2.87298900	0.79559100	0.26619500
C	0.58257800	0.98211100	1.04368100
C	1.31018200	-1.09551900	-0.25236500
C	0.13061000	-0.18433700	0.16580400
C	2.46187800	-0.23128600	-0.77533200
C	1.86185900	1.41253200	1.08713200
H	1.63851900	-1.66925000	0.62011000
H	-0.34089000	0.20634900	-0.74325200
H	2.12416700	0.29506400	-1.68235300
H	-0.16384300	1.45369600	1.67811000
H	0.96667200	-1.80811800	-1.01080200
H	2.13870800	2.21885700	1.76264600
C	4.21480500	0.89513500	0.24738500
H	4.88181200	1.54759700	0.79725200

O	4.83154900	0.03079600	-0.61421300
C	3.80934700	-0.92398400	-1.04107100
H	3.92855300	-1.82621800	-0.42729300
H	4.00452100	-1.16288700	-2.08730900
C	-0.91300900	-0.99149300	0.93358500
O	-0.63597800	-1.86168300	1.73832300
N	-2.27056200	-0.64991400	0.77660100
H	-2.90115000	-1.22224300	1.33505600
S	-3.11244200	0.13770000	-0.49011400
O	-4.49912400	-0.29127500	-0.29992400
O	-2.40919000	-0.07606300	-1.75622300
C	-2.98997800	1.88452100	-0.07019300
H	-1.94040300	2.18125500	-0.07284500
H	-3.44763700	2.03605800	0.90770100
H	-3.54166000	2.42221700	-0.84402800

Energy MP2 = -1140.5240378 Hartree



Scheme 2. Expanded models for the gas phase computations of concluding pericyclic step.

Table 2. Relative single point energies of the structures **6**, **8** and **10** and the corresponding transition states **7** and **9** calculated on the MP2 level of theory [RMP2/6-311++G(2d,2p)//RB3LYP/6-31+G(d,p)] (energies are given in kcal/mol).^[Fehler! Textmarke nicht definiert.]

Allyloxy enallene 6	Claisen product 8	TS _[3,3] 7	Diels-Alder product 10	TS _[4+2] 9	Δ [TS _[4+2] (7)–TS _[3,3] (9)]
0 ^a (6c)	–41.00 (8c)	22.60 (7c) ^a	–58.00 (10c)	7.00 (9c) ^b	–15.60 [(7c)-(9c)]
0 ^a (6d)	–41.00 (8d)	22.30 (7d) ^c	–59.00 (10d)	6.40 (9d) ^d	–15.90 [(7d)-(9d)]

^aEnergies are set to 0 kcal/mol. Imaginary frequencies from the DFT geometry optimizations that verify transition states: ^bi505.64 cm^{–1}, ^ci456.88 cm^{–1}, ^di503.87 cm^{–1}, ^ei455.57 cm^{–1}.

Vinyl allenyl allyl ether 6d

ATOM	X	Y	Z
H	-0.46967900	3.18926500	0.04014400
C	0.53327200	2.81287100	0.20217400
C	3.16978500	1.87801100	0.63685200
C	0.82915300	1.45676700	0.02771600
C	1.54407800	3.69703300	0.58709300
C	2.84415600	3.23070500	0.79975700
C	2.15436700	1.00907100	0.25185600
H	1.31574400	4.74985200	0.71957300
H	3.62455100	3.92448400	1.09733100
H	4.17644200	1.52155600	0.80245700
C	0.01788800	0.30540500	-0.36118300
C	0.93170900	-0.87662800	-0.36701400
N	2.20348700	-0.40377200	0.03708600
S	3.63490900	-1.37631900	-0.14908600
O	3.75956100	-1.75784200	-1.55230100
O	4.70795600	-0.63633400	0.51911000
C	3.22927400	-2.82654300	0.83127400
H	2.33133800	-3.27952400	0.41225000
H	3.08989400	-2.51132100	1.86574200
H	4.09510900	-3.48577100	0.73860000
O	0.67006400	-2.03810100	-0.63438800
C	-1.28505500	0.11345200	-0.69673700
H	-1.55966500	-0.90889700	-0.94956300
C	-2.34479400	1.10039900	-0.76804000
C	-3.58879700	0.79214200	-1.11015100

H	-2.10834400	2.13592700	-0.53152400
C	-4.79699600	0.48452900	-1.52676000
H	-5.04237500	0.51109100	-2.58614700
O	-5.88367000	0.12212400	-0.78687600
C	-5.71902700	0.04050000	0.64634700
H	-5.06683000	0.86258300	0.97134400
H	-6.71939800	0.20306600	1.05436900
C	-5.17780600	-1.29121400	1.07982900
H	-4.20313500	-1.57274400	0.68589400
C	-5.82200200	-2.10939800	1.91572700
H	-5.39415900	-3.05764500	2.22672200
H	-6.79895100	-1.85580400	2.32179700

Energy MP2 = -1369.7123044 Hartree

Claisen Transition State 7d

ATOM	X	Y	Z
C	-2.46447900	-1.19990600	-1.54989400
C	-3.36263600	-0.49563800	-0.86263500
C	-2.87646300	-0.16305300	1.33207500
C	-4.62787000	0.03759600	-0.82096400
C	-3.98624500	-0.79890500	1.85738300
C	-1.06426100	-1.46933800	-1.24191000
C	-5.25184200	-0.19745200	1.74250700
C	-0.07946300	-0.64373900	-0.80698400
C	1.26669500	-1.23597900	-0.52885700
C	4.50426400	-1.42578600	-0.65705400
H	-0.74059900	-2.49421500	-1.42814100

H	-2.83925700	-1.74000800	-2.42404200
H	-2.85314300	0.91791600	1.24765000
H	-5.32904400	0.88558800	1.74272200
H	-6.13463600	-0.71599400	2.09857200
H	-4.75106900	1.04535800	-1.25266400
H	-3.93902200	-1.86662800	2.05615600
H	4.59295300	-0.83063200	-1.56636600
H	5.48803700	-1.63834500	-0.23297900
H	-1.90803100	-0.65089200	1.32387400
H	3.92697700	-2.33632300	-0.81387000
N	2.11392700	-0.16046600	-0.17112400
O	3.45264100	-1.23519600	1.78526600
O	-5.58568800	-0.42977500	-0.08745000
O	1.61118300	-2.40423400	-0.59792100
O	4.30267700	0.87741400	0.66184000
S	3.65943200	-0.43590600	0.58149400
C	0.04833700	0.79592100	-0.58227600
C	0.90593100	3.40849600	-0.10550400
C	-0.84545900	1.85879200	-0.74329300
C	1.38222900	1.06852800	-0.19500300
C	1.82593600	2.36387800	0.05123000
C	-0.41127700	3.16535100	-0.50606000
H	-1.86559800	1.66652200	-1.05272800
H	2.84652500	2.55753500	0.34939100
H	-1.10211600	3.99352600	-0.63026900
H	1.23272800	4.42608300	0.08619900

Energy MP2 = -1369.6767672 Hartree

Imaginary frequencies: i503.87 cm⁻¹

Claisen Product 8d

ATOM	X	Y	Z
H	-0.83633300	2.99408600	0.12647200
C	0.21017900	2.72109700	0.18816800
C	2.95816400	2.05805200	0.36449800
C	0.61416800	1.38495400	0.07884600
C	1.16808100	3.71847500	0.37891700
C	2.52339000	3.38592200	0.46374000
C	1.99445800	1.07441200	0.17300600
H	0.85670600	4.75483200	0.46106300
H	3.26186300	4.16808000	0.61089300
H	4.00691000	1.80641400	0.43282500
C	-0.11921700	0.14112000	-0.12144900
C	0.90319700	-0.95441300	-0.14857000
N	2.15761300	-0.34103100	0.06050300
S	3.65115600	-1.20130600	-0.21145800
O	3.65653200	-1.69179700	-1.58534000
O	4.71072700	-0.31253900	0.26906700
C	3.49077800	-2.58683900	0.92079200
H	2.60451900	-3.15479700	0.63995600
H	3.42684500	-2.19325800	1.93561000
H	4.40341400	-3.17181900	0.78727900
O	0.71975200	-2.15099300	-0.29561800
C	-1.42817200	-0.20242500	-0.27880000
H	-1.60305800	-1.26859100	-0.40375400

C	-2.56987600	0.66901200	-0.30185700
C	-3.86586700	0.26500900	-0.43656200
H	-2.39708400	1.73803800	-0.21153500
C	-4.89036000	1.33493300	-0.45221300
H	-4.49647600	2.36468300	-0.31605300
O	-6.08410500	1.14575300	-0.61194100
C	-5.72317900	-2.18627700	1.30714500
H	-5.80356600	-2.63848500	2.29136400
H	-6.64407500	-2.06345800	0.74272100
C	-4.54457700	-1.79454900	0.81788500
H	-3.64464300	-1.91923200	1.42044000
C	-4.34654000	-1.16349700	-0.54591500
H	-3.63048400	-1.75710100	-1.12649600
H	-5.29734500	-1.16459200	-1.08611300

Energy MP2 = -1369.7789262 Hartree

Diels-Alder Transition State 9d

ATOM	X	Y	Z
H	-2.13667100	1.72431800	-1.19801600
C	-1.13497700	1.91506000	-0.83180500
C	1.49642200	2.42107800	0.09016500
C	-0.23383100	0.85674300	-0.67449900
C	-0.73164000	3.21440200	-0.51178400
C	0.56385600	3.45853400	-0.04604300
C	1.08367500	1.13302300	-0.23341100
H	-1.42991600	4.03767000	-0.62773700
H	0.86633300	4.47074800	0.20485700

H	2.50457600	2.61542500	0.42815700
C	1.02487400	-1.13945200	-0.76279100
N	1.83746200	-0.08131100	-0.27226900
S	3.32741300	-0.39814600	0.55929100
O	3.93789800	0.91058800	0.80552100
O	3.05129600	-1.30476200	1.67161000
C	4.28190200	-1.26439700	-0.69187000
H	4.43563700	-0.58696100	-1.53237600
H	3.72825200	-2.15782200	-0.97930300
H	5.23085800	-1.51159200	-0.21108300
O	1.41104500	-2.28386700	-0.94847300
C	-0.33156700	-0.56808300	-0.98066300
C	-1.28068600	-1.33953700	-1.63646300
H	-0.89294200	-2.24838100	-2.09447300
C	-1.48679500	-1.08719700	1.44507400
H	-0.54359000	-0.61926300	1.69464400
H	-1.51270000	-2.17387800	1.45807700
C	-2.63100900	-0.33563700	1.24036700
H	-2.49460100	0.74354700	1.30818800
C	-2.67922600	-1.21177000	-1.59193100
H	-3.24166800	-1.95680500	-2.15421200
C	-3.37214300	-0.49450200	-0.64416000
C	-4.59863000	-0.04896000	-0.33635300
H	-5.28972700	0.45630000	-1.00351800
C	-4.00419500	-0.76933100	1.73031700
H	-4.17758500	-0.47774400	2.76821300
H	-4.14393500	-1.85105700	1.61634800

O	-5.00015700	-0.06756600	0.95816200
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Energy MP2 = -1369.7021325 Hartree

Imaginary frequencies: i455.57 cm⁻¹

Diels-Alder Product 10d

ATOM	X	Y	Z
H	1.67369900	2.61241400	0.46508000
C	0.61040700	2.51323800	0.27055500
C	-2.17524000	2.26428400	-0.15372700
C	0.01840400	1.25512700	0.23028300
C	-0.18163800	3.65200100	0.07702700
C	-1.55517100	3.52064100	-0.13821800
C	-1.36796200	1.14544000	0.03725000
H	0.27349600	4.63726800	0.10146300
H	-2.16558700	4.40619100	-0.28755300
H	-3.24114100	2.16864100	-0.30486000
C	-0.59783300	-1.03898600	0.35563200
N	-1.73163800	-0.24028300	0.11919000
S	-3.25638600	-0.94844600	-0.35127000
O	-4.22454500	0.14983200	-0.34684300
O	-3.03699100	-1.74132300	-1.55686800
C	-3.61000300	-2.04289700	1.02968100
H	-3.70560500	-1.43669800	1.93103700
H	-2.80144200	-2.76918400	1.10297800
H	-4.56020000	-2.52014100	0.78005500
O	-0.61311800	-2.24644300	0.49168800
C	0.64561400	-0.12127200	0.39137900

C	1.38377300	-0.27959600	1.71129000
H	0.77279400	-0.28385700	2.60977100
C	1.53042300	-0.55529800	-0.82820300
H	1.04697300	-0.23376300	-1.75711900
H	1.57271000	-1.65031600	-0.82913200
C	2.94910300	0.00436300	-0.70474200
H	2.90976600	1.10080500	-0.78291900
C	2.72410500	-0.40856200	1.80650000
H	3.18203700	-0.55024900	2.78281000
C	3.55816600	-0.38102700	0.63111400
C	4.85094700	-0.69169000	0.42442700
H	5.63192000	-0.96392300	1.12356200
C	4.00964600	-0.54725600	-1.67370700
H	4.22496000	0.09267500	-2.53036900
H	3.75566600	-1.55714400	-2.02153000
O	5.23679800	-0.65289600	-0.88754400

Energy MP2 = -1369.8064064 Hartree

Vinyl allenyl allyl ether 6c

ATOM	X	Y	Z
H	-1.50102100	-2.40917800	0.09590800
C	-2.33028600	-1.72282600	0.22434400
C	-4.54162800	0.02590400	0.57525300
C	-2.18252400	-0.35020100	-0.01097600
C	-3.57522000	-2.21285500	0.63188400
C	-4.66587600	-1.35062700	0.80513000
C	-3.29949900	0.48476200	0.17315300

H	-3.69653800	-3.27570200	0.81568300
H	-5.62361200	-1.75224100	1.12168300
H	-5.37406000	0.70882500	0.70312000
C	-1.09368700	0.52544900	-0.43285000
C	-1.68057300	1.90168100	-0.47290600
O	-1.17705600	2.95706100	-0.76319400
C	0.21352100	0.35198200	-0.75873800
H	0.76003900	1.24982500	-1.04019200
C	0.95604800	-0.89337900	-0.77435800
C	2.24256900	-0.96022700	-1.08969500
H	0.43038400	-1.81013800	-0.51147000
C	3.49728300	-1.02065200	-1.47708200
H	3.74895100	-1.15653200	-2.52656700
O	4.62530800	-0.94833100	-0.71434400
C	4.45842000	-0.76895900	0.71004100
H	3.60128200	-1.37160300	1.04011100
H	5.36869700	-1.17958500	1.15317200
C	4.28877000	0.67474300	1.08573700
H	3.42629500	1.19001800	0.66748800
C	5.12274500	1.32402500	1.90187600
H	4.96081700	2.36320000	2.17172800
H	5.99414400	0.83554300	2.33276600
O	-3.01772100	1.81060200	-0.09350000

Energy MP2 = -802.5117386 Hartree

Claisen Transition State 7c

ATOM	X	Y	Z
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C	-1.29187500	-1.37278500	-1.32954100
C	-2.09909300	-0.39961500	-0.90918200
C	-1.84147700	0.22046300	1.25869500
C	-3.21757900	0.35971700	-1.15348000
C	-3.11824300	-0.09313700	1.68692200
C	-0.02559500	-1.83330800	-0.77104100
C	-4.20297700	0.70389800	1.27972900
C	1.03622400	-1.12283200	-0.31576700
C	2.21688500	-1.86058500	0.24221000
H	0.11143600	-2.91500400	-0.75886300
H	-1.65942700	-1.98018200	-2.16142000
H	-1.58029000	1.24583800	1.02130200
H	-4.04955800	1.76529100	1.10972300
H	-5.21354700	0.43087200	1.56126000
H	-3.06971200	1.27813600	-1.74637100
H	-3.32360800	-1.09888600	2.04484200
H	-1.00472100	-0.43341100	1.47809000
O	-4.33876700	0.21936600	-0.52244900
O	2.38991700	-3.04043700	0.41184100
C	1.41297200	0.28823500	-0.28360400
C	2.82225600	2.68788600	-0.00025600
C	0.82207700	1.48680100	-0.70001100
C	2.71016300	0.33076600	0.25643600
C	3.43527300	1.49906700	0.41636000
C	1.53642100	2.68074200	-0.55767800
H	-0.17172300	1.48899400	-1.13185000
H	4.43409000	1.48275100	0.83804800

H	1.08685700	3.61465400	-0.88050300
H	3.35611200	3.62709900	0.10802000
O	3.18778700	-0.92368200	0.58547900

Energy MP2 = -802.4757866 Hartree

Imaginary frequencies: i505.64 cm⁻¹

Claisen Product 8c

ATOM	X	Y	Z
H	-1.18897000	-2.33724900	0.18347700
C	-2.07796700	-1.71748800	0.19505000
C	-4.44517200	-0.14437100	0.24648000
C	-2.00224400	-0.32868600	0.01925700
C	-3.32801200	-2.30951600	0.39253000
C	-4.49539100	-1.53380500	0.41726800
C	-3.19564500	0.41721000	0.05268300
H	-3.39470000	-3.38403800	0.52938600
H	-5.45601100	-2.01512800	0.57266100
H	-5.33744200	0.47119400	0.26442800
C	-0.93422500	0.63527400	-0.20534800
C	-1.61429200	1.97025400	-0.28931100
O	-1.14855800	3.06672500	-0.46301200
C	0.41956400	0.57446900	-0.34062000
H	0.91108700	1.53218300	-0.49443500
C	1.23570700	-0.60696500	-0.30353800
C	2.59501200	-0.63474800	-0.41290600
H	0.73266500	-1.56345500	-0.18356700
C	3.23137300	-1.97153900	-0.36722000

H	2.53124400	-2.81977400	-0.21026100
O	4.42635400	-2.17305800	-0.50046100
C	5.09664100	1.15613600	1.31708000
H	5.29901800	1.59282600	2.29069200
H	5.93929800	0.72244800	0.78453500
C	3.86491800	1.14892400	0.80262000
H	3.04122900	1.57816200	1.37325700
C	3.50170300	0.56652700	-0.54885000
H	3.01828300	1.33480600	-1.16373700
H	4.41335100	0.25141900	-1.06414700
O	-2.98040500	1.76965200	-0.12819500

Energy MP2 = -802.5783113 Hartree

Diels-Alder Transition State 9c

ATOM	X	Y	Z
H	-0.30912400	1.63353800	-1.33275300
C	0.64442800	1.56018100	-0.82306500
C	3.16379600	1.38408200	0.48155100
C	1.12499700	0.31839400	-0.38939200
C	1.41611100	2.70430400	-0.59174300
C	2.65375200	2.62016500	0.05985200
C	2.38394800	0.26730400	0.23738900
H	1.04992500	3.67087300	-0.92402900
H	3.23455000	3.52136500	0.23125400
H	4.13064200	1.29464900	0.96450000
C	1.78508000	-1.88988900	0.04900800
O	1.90565300	-3.08764600	0.12854800

C	0.66946600	-1.06321300	-0.50043100
C	-0.34358300	-1.68592800	-1.21354200
H	-0.16620700	-2.73485000	-1.44610400
C	-0.97509800	-0.77929900	1.68213600
H	0.00947400	-0.53088800	2.05618600
H	-1.32058400	-1.79700800	1.84471200
C	-1.79435600	0.18693900	1.12154600
H	-1.35737100	1.18389800	1.06574100
C	-1.62985000	-1.18989700	-1.48598000
H	-2.28849500	-1.85414200	-2.04477400
C	-2.22063900	-0.13974000	-0.82145000
C	-3.29201100	0.66687500	-0.86070600
H	-3.67713900	1.19338900	-1.72801900
C	-3.29586900	0.24085800	1.36510400
H	-3.54176200	0.76792500	2.28925400
H	-3.73274500	-0.76492000	1.37880100
O	-3.89240200	1.01429700	0.30420800
O	2.76522600	-1.02548100	0.54019000

Energy MP2 = -802.4994974 Hartree

Imaginary frequencies: i456.88 cm⁻¹

Diels-Alder Product 10c

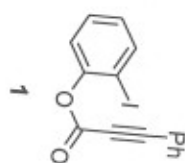
ATOM	X	Y	Z
H	0.49756100	-2.26291800	0.70514500
C	1.39117200	-1.72933500	0.39621300
C	3.75622600	-0.34261600	-0.33508600
C	1.35062800	-0.36295900	0.13152300

C	2.61299000	-2.40702300	0.27778400
C	3.77763300	-1.72159900	-0.08681100
C	2.53151600	0.29376900	-0.21259000
H	2.65677900	-3.47285400	0.47914200
H	4.71586300	-2.26163700	-0.17049500
H	4.65033800	0.20876200	-0.60455600
C	1.01448200	1.95684800	-0.16474700
O	0.60056600	3.08068700	-0.24400300
C	0.22651900	0.65968400	0.15770000
C	-0.43352900	0.77357900	1.52427200
H	0.17405900	1.19099700	2.32214400
C	-0.82757400	0.48206700	-0.98516600
H	-0.31351400	0.20663200	-1.91271500
H	-1.31082500	1.45340700	-1.14069400
C	-1.88497000	-0.55373300	-0.59594600
H	-1.40358900	-1.53958900	-0.51062800
C	-1.70290800	0.38761000	1.77202200
H	-2.12216000	0.52779500	2.76566300
C	-2.51969600	-0.18918100	0.73385600
C	-3.83598100	-0.45634800	0.65319100
H	-4.61779400	-0.38334400	1.39896800
C	-3.13271000	-0.65878700	-1.49003600
H	-3.11711600	-1.48258200	-2.20486400
H	-3.33449500	0.28352200	-2.01615700
O	-4.24757100	-0.89451900	-0.57599600
O	2.34476800	1.65632400	-0.40100300

Energy MP2 = -802.6041378 Hartree

- ¹ *Organikum*, 21st ed.; Becker, H. G. O.; Beckert, R.; Domschke, G.; Fanghänel, E.; Habicher, W. D.; Metz, P.; Pavel, D.; Schwetlick, K. Wiley-VCH, Weinheim, New York, Chichester, Brisbane, Singapore, Toronto, **2001**.
- ² Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision B.03, *Gaussian, Inc., Wallingford CT*, **2004**.
- ³ Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
- ⁴ a) Møller, C.; Plesset, M. S. *Phys. Rev.* **1934**, *46*, 618. b) Head-Gordon, M.; Pople, J. A.; Frisch, M. J. *Chem. Phys. Lett.* **1988**, *153*, 503. c) Frisch, M. J.; Head-Gordon, M.; Pople, J. A. *Chem. Phys. Lett.* **1990**, *166*, 275. d) Frisch, M. J.; Head-Gordon, M.; Pople, J. A. *Chem. Phys. Lett.* **1990**, *166*, 281. e) Head-Gordon, M.; Head-Gordon, T.; *Chem. Phys. Lett.* **1994**, *220*, 122. f) Saebo, S.; Almlöf, J. *Chem. Phys. Lett.* **1989**, *154*, 83.

D'Souza DS-8 in CDCl3



Current Data Parameters
NAME: m19012ae
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20020912
Time: 7.56

INSTRUM: spect
PROBHD: 5 mm BBI 1H-BB
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 5462.456 Hz
FIDRES: 0.167311 Hz
AQ: 2.9864915 sec
RG: 71.8
OR: 91.200 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec

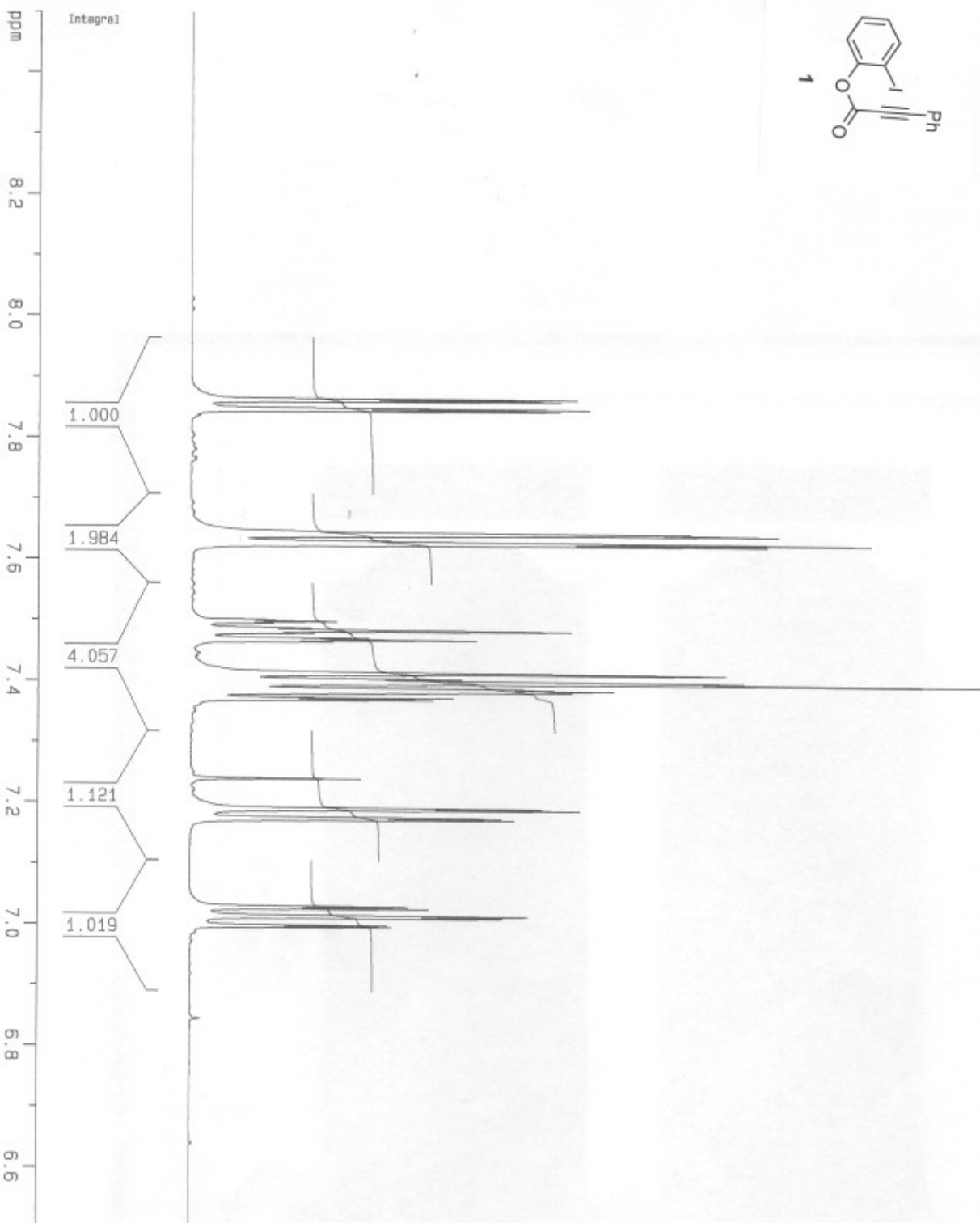
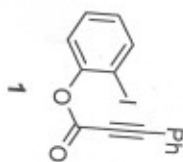
===== CHANNEL f1 =====
NUC1: 1H
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 500.1362738 MHz

F2 - Processing parameters
SI: 16384
SF: 500.1300232 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 13.00 cm
FIP: 8.500 ppm
F1: 4251.11 Hz
F2P: -0.300 ppm
F2: -150.04 Hz
PPMCK: 0.44000 ppm/cm
HZCM: 220.05722 Hz/cm



D'Souza DS-8 in CDCl3



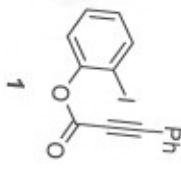
Current Data Parameters
NAME: MISO1296
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20020912
Time: 7.56
INSTRUM: spect
PROBHD: 5 mm BBI 1H-90
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 5482.456 Hz
FIDRES: 0.167311 Hz
AQ: 2.9894915 sec
RG: 71.8
DM: 91.200 usec
DE: 5.00 usec
TE: 300.0 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.00 usec
PL1: 0.00 dB
SFO1: 500.1322738 MHz

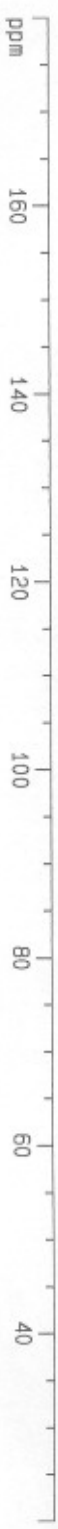
F2 - Processing parameters
SI: 16384
SF: 500.1300232 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 13.00 cm
F1P: 8.500 ppm
F1: 4251.11 Hz
F2P: 6.500 ppm
F2: 3250.85 Hz
PPMCK: 0.10000 ppm/cm
HZCM: 50.01300 Hz/cm



ppm

- D'Souza DS-8 in CDCl₃
- 151.411
 - 150.639
 - 139.672
 - 133.320
 - 131.181
 - 129.579
 - 128.672
 - 128.145
 - 122.979
 - 119.099
 - 90.116
 - 89.426
 - 80.146
 - 77.275
 - 77.241
 - 77.021
 - 76.987
 - 76.767
 - 76.733



Current Data Parameters
NAME: D'Souza DS-8
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030312
Time: 8.58
INSTRUM: spect
PROBHD: 5 mm BBI 1H-5B
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 1600
DS: 2
SWH: 30894.197 Hz
FIDRES: 0.470950 Hz
AQ: 1.0817382 sec
RG: 5792.8
DN: 16.200 ussec
DE: 8.00 ussec
TE: 300.0 K
D1: 1.00000000 sec
d11: 0.03000000 sec
d12: 0.00020000 sec

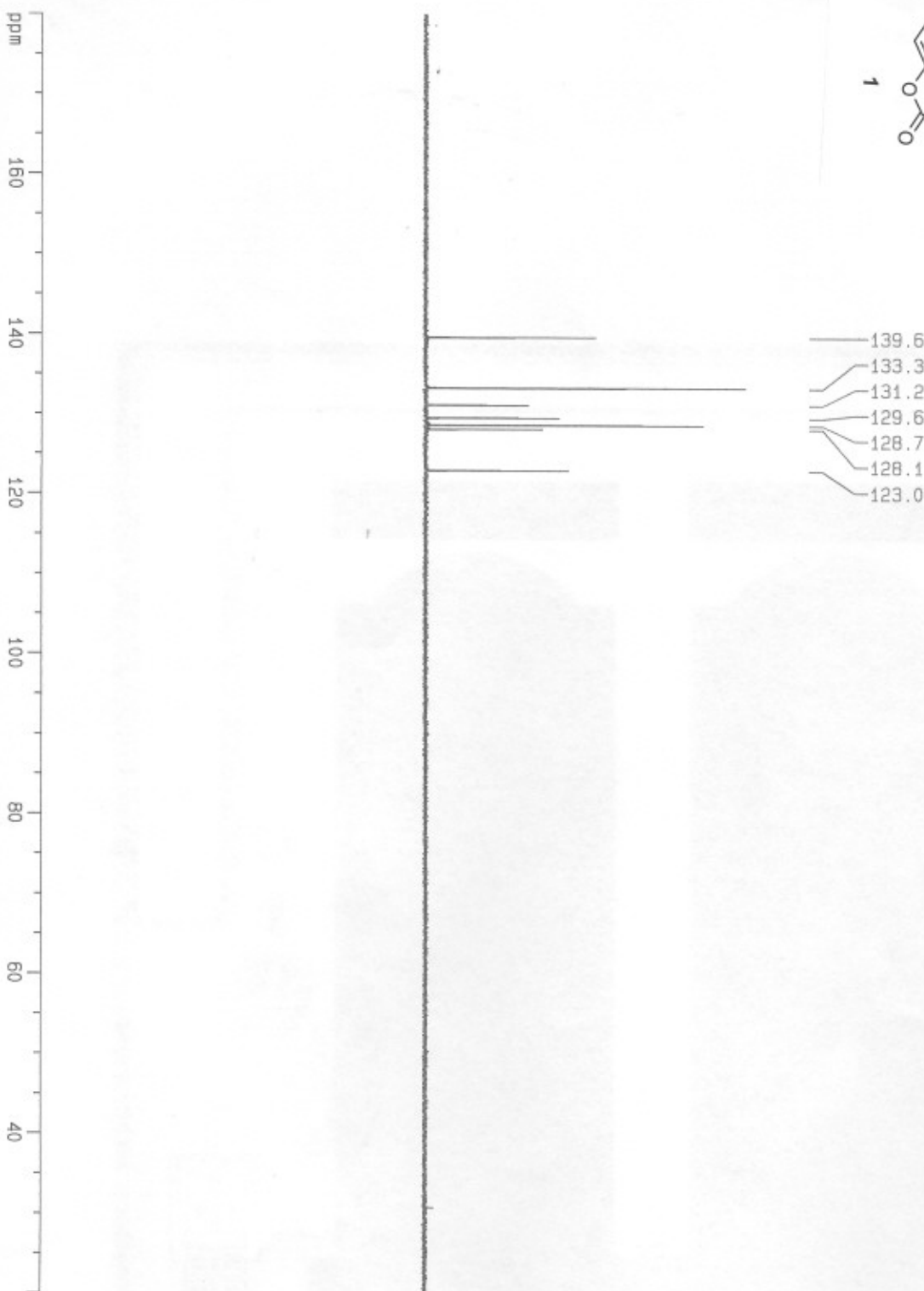
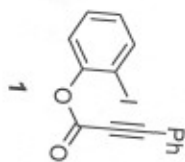
CHANNEL f1
NUC1: 13C
P1: 11.50 ussec
PL1: -3.00 dB
SFO1: 125.7713172 MHz

CHANNEL f2
NUC2: 1H
PCPG2: 100.00 ussec
PL2: 0.00 dB
PL12: 20.40 dB
PL13: 20.00 dB
SFO2: 500.1322003 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577956 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 10.00 cm
F1P: 180.000 Dps
F1: 22636.40 Hz
F2P: 20.000 Dps
F2: 2515.16 Hz
FREQM: 6.00000 Dps/cm
HZCM: 1005.05236 Hz/cm

D. Souza DS-8 in CDCl3



Current Data Parameters
NAME: mmo12se
EXPNO: 3
PROCNO: 1

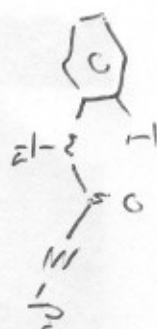
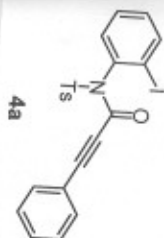
F2 - Acquisition Parameters
Date_: 20120912
Time: 10.03
INSTRUM: spect
PROBHD: 5 mm BBI 1H-8B
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 800
DS: 2
SWH: 2777.777 Hz
FIDRES: 0.42395 Hz
AQ: 1.179090 sec
RG: 1825.5
ZM: 18.000 cm/s
DE: 6.00 usec
TE: 300.0 K
CHRG2: 145.000000 sec
O1: 4.0000000 sec
O2: 0.0044639 sec
O3: 0.0002000 sec
DELTA: 0.0001464 sec

CHANNEL f1
NUC1: 13C
P1: 11.50 usec
PL1: 23.00 dB
SFO1: 125.769000 MHz

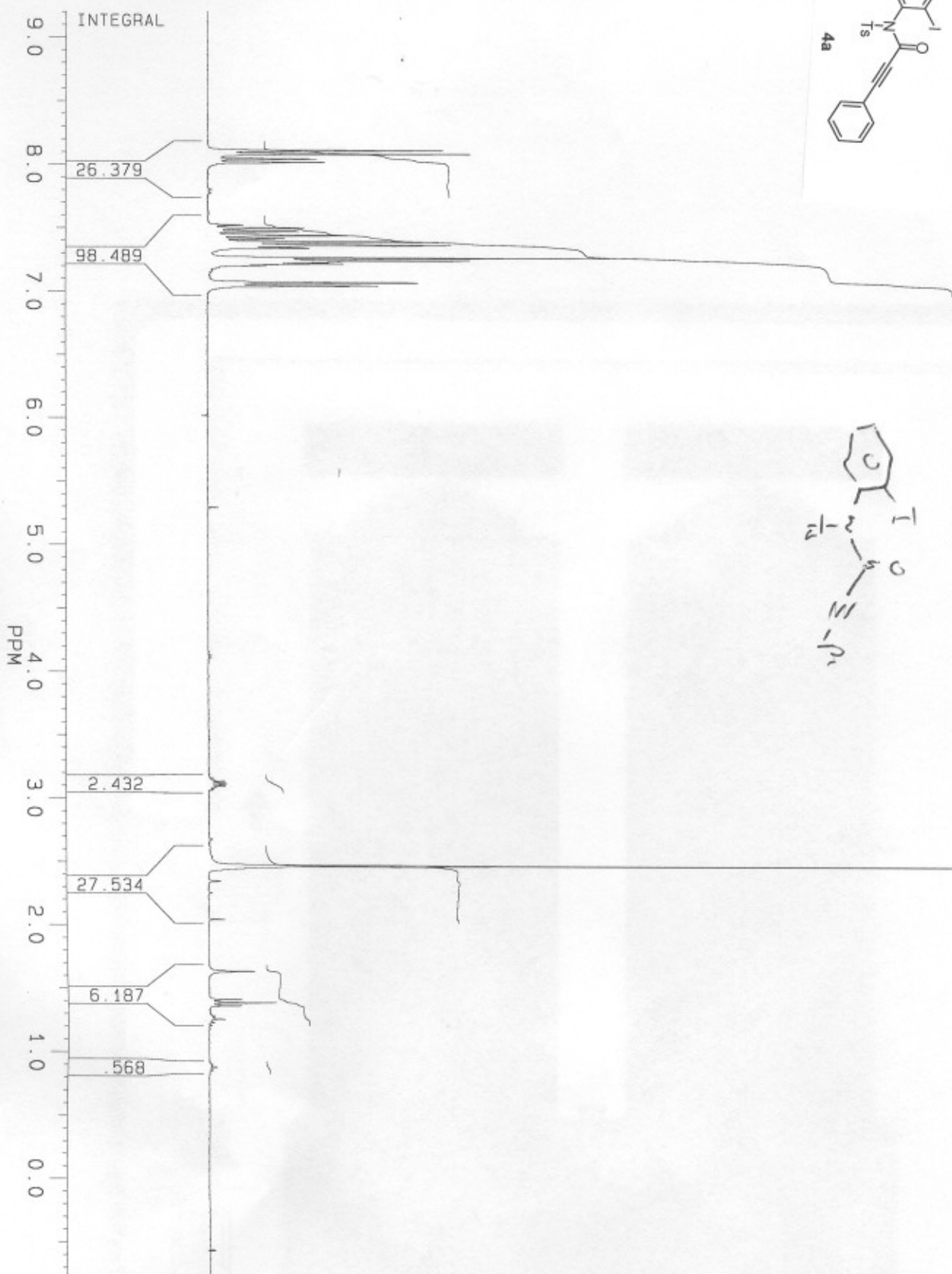
CHANNEL f2
CPDPRG2: zgpg30
NUC2: 1H
P2: 9.50 usec
PL2: 19.00 dB
SFO2: 500.132200 MHz

F2 - Processing parameters
SI: 32768
SF: 125.757702 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
F1P: 100.000 ppm
F2P: 22636.40 Hz
F2: 25115.18 Hz
P2MCM: 8.00000 ppm/cm
HZCM: 1005.00236 Hz/cm



DS-203 IN CDCL3 D"SOUZA



NO1905.104
AU PROG:
X00. AU
DATE 19-11-3

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SM 6024.096
HZ/PT .368

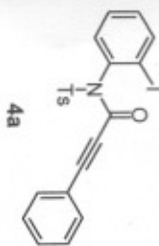
PW 0.0
RD 0.0
AQ 2.720
RG 20
NS 16
TE 297

FW 7600
O2 3200.000
DP 63L PD

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 .800P
HZ/CW 136.427
PPM/CW .455
SR 3369.88



N019.002	
AU PROG:	
X02.AU	
DATE 19-11-3	
SF	75.469
SY	75.0
01	6141.605
SI	65536
TD	65536
SW	18518.519
HZ/PT	.565
PW	0.0
RD	0.0
AG	1.769
RG	400
NS	920
TE	297
FW	23200
02	4588.000
DP	18H CPD
LB	1.000
GB	0.0
CX	22.00
CY	0.0
F1	200.005P
F2	-4.055P
HZ/CM	700.003
PPM/CM	9.275
SR	-1402.20



DS-203 IN CDCL3 D'SOUZA

140.238
132.879
131.619
131.300
130.923
129.952
129.382
129.289
128.468

21.755



NO19.003
AU PROG:
DEPT: AUR
DATE 19-11-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 200
NS 228
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 5.00
F1 200.005P
F2 -4.055P
HZ/CM 700.003
PPM/CM 9.275
SR -1402.20





NO1905.116
AU PROG:
X00.AU
DATE 20-11-3

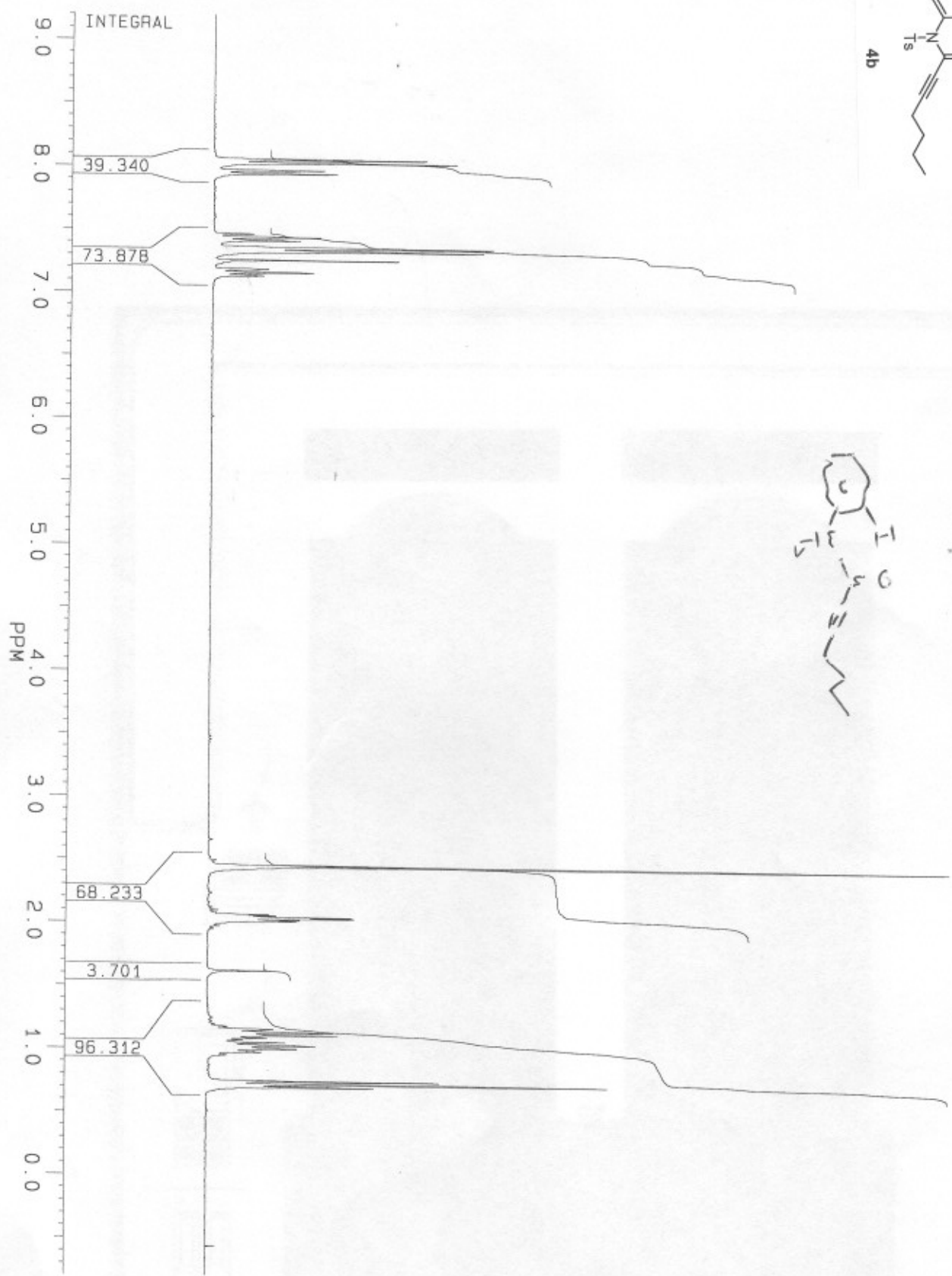
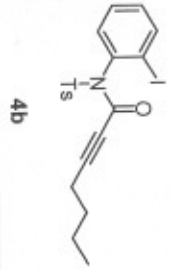
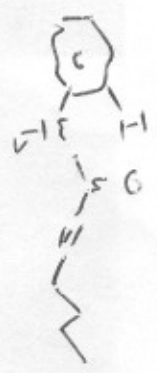
SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PW 0.0
RD 0.0
AQ 2.720
RG 10
NS 16
TE 297

FW 7600
D2 3200.000
DP 63L P0

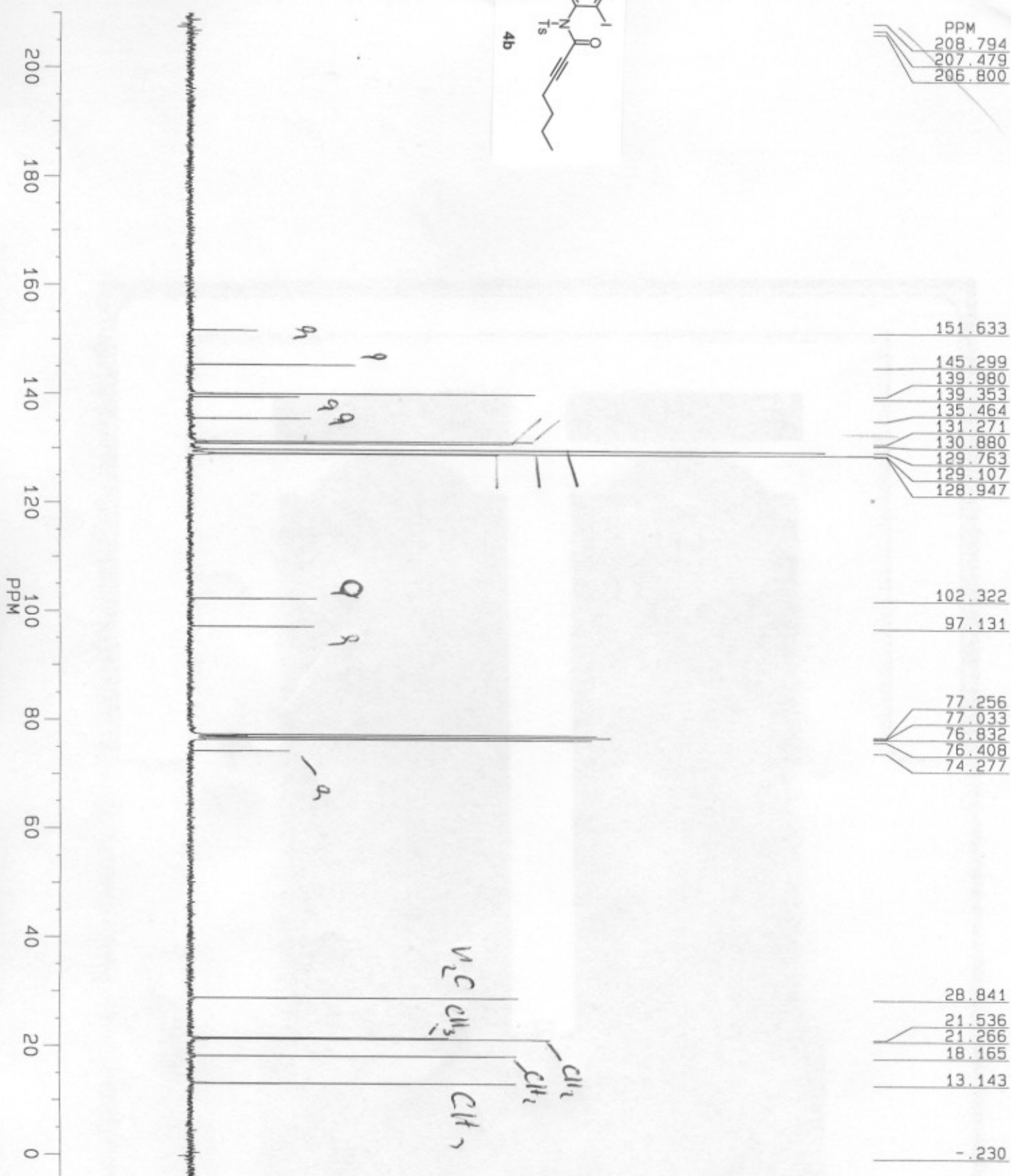
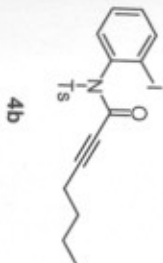
LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 .800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88

DS-159 IN CDCL3 D'SOUZA



DS-159 IN CDCL₃ D²SOUZA

PPM
208.794
207.479
206.800



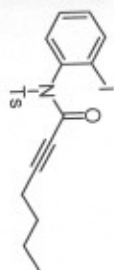
NO191S.108
AU PROG:
X02.AU
DATE 20-11-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AG 1.769
RG 320
NS 2000
TE 297

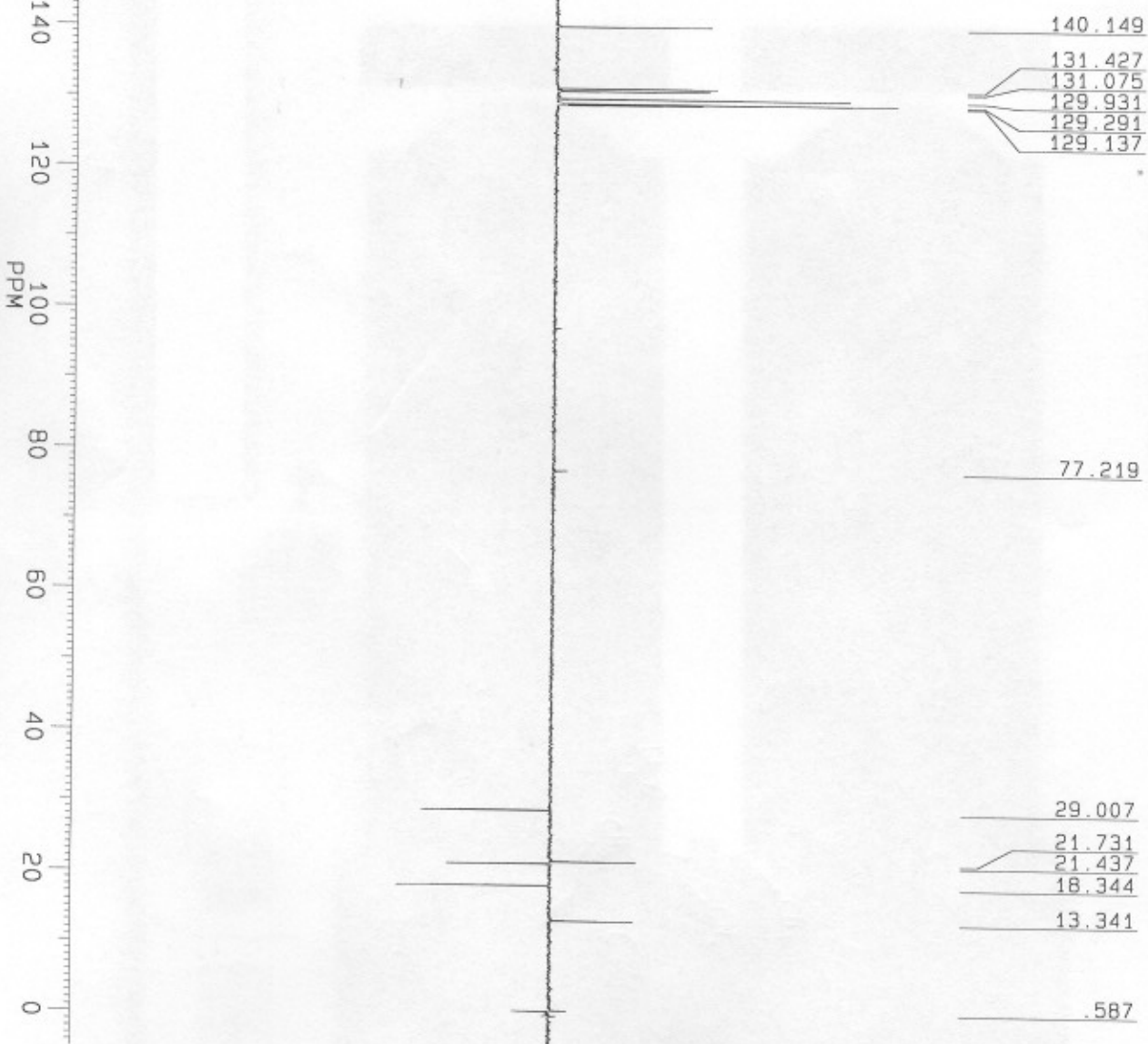
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O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 13.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89



4b

DS-159 IN CDCL3 D"SOUZA



NO192S.108
AU PROG:
X09. AU
DATE 20-11-3

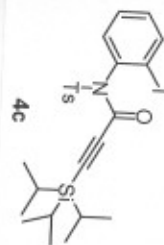
SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 1000
TE 297

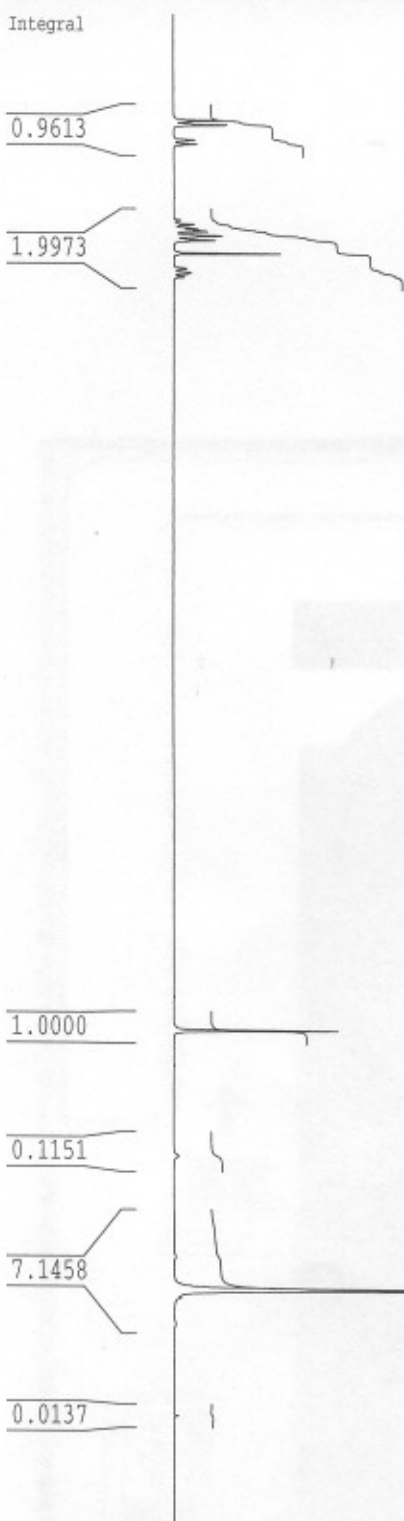
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O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 5.00
F1 210.002P
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HZ/CW 737.534
PPM/CW 9.773
SR -1401.63

D'Souza DS_239 CDCl3



ppm



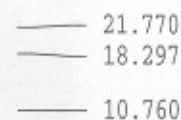
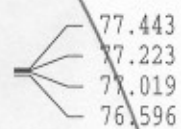
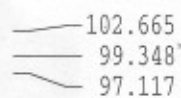
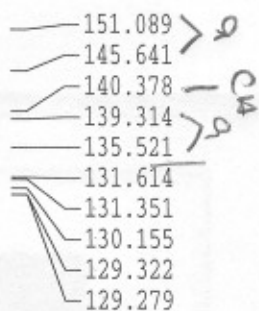
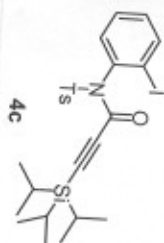
Current Data Parameters
NAME ap23muso
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 8:41
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PROBHD 5 mm TBI 1H/3
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 90.5
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

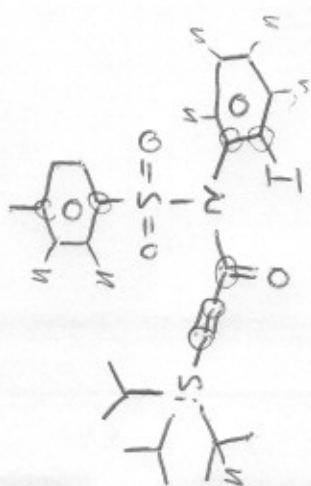
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PL1 0.00 dB
SFO1 300.1316507 MHz

F2 - Processing parameters
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SF 300.1300120 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FLP 8.728 ppm
F1 2619.54 Hz
F2P -0.619 ppm
F2 -185.71 Hz
PRCM 0.46734 ppm/cm
H2CM 140.26207 Hz/cm



16 C-14 to -e



CH₃ : 2
CH₂ : 0
CH : 7
Quart : 7

-CH



Current Data Parameters
NAME ap23muso
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040423
Time 10.14
INSTRUM spect
PROBHD 5 mm TBI 1H/3
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1632
DS 2
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 2048
RW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

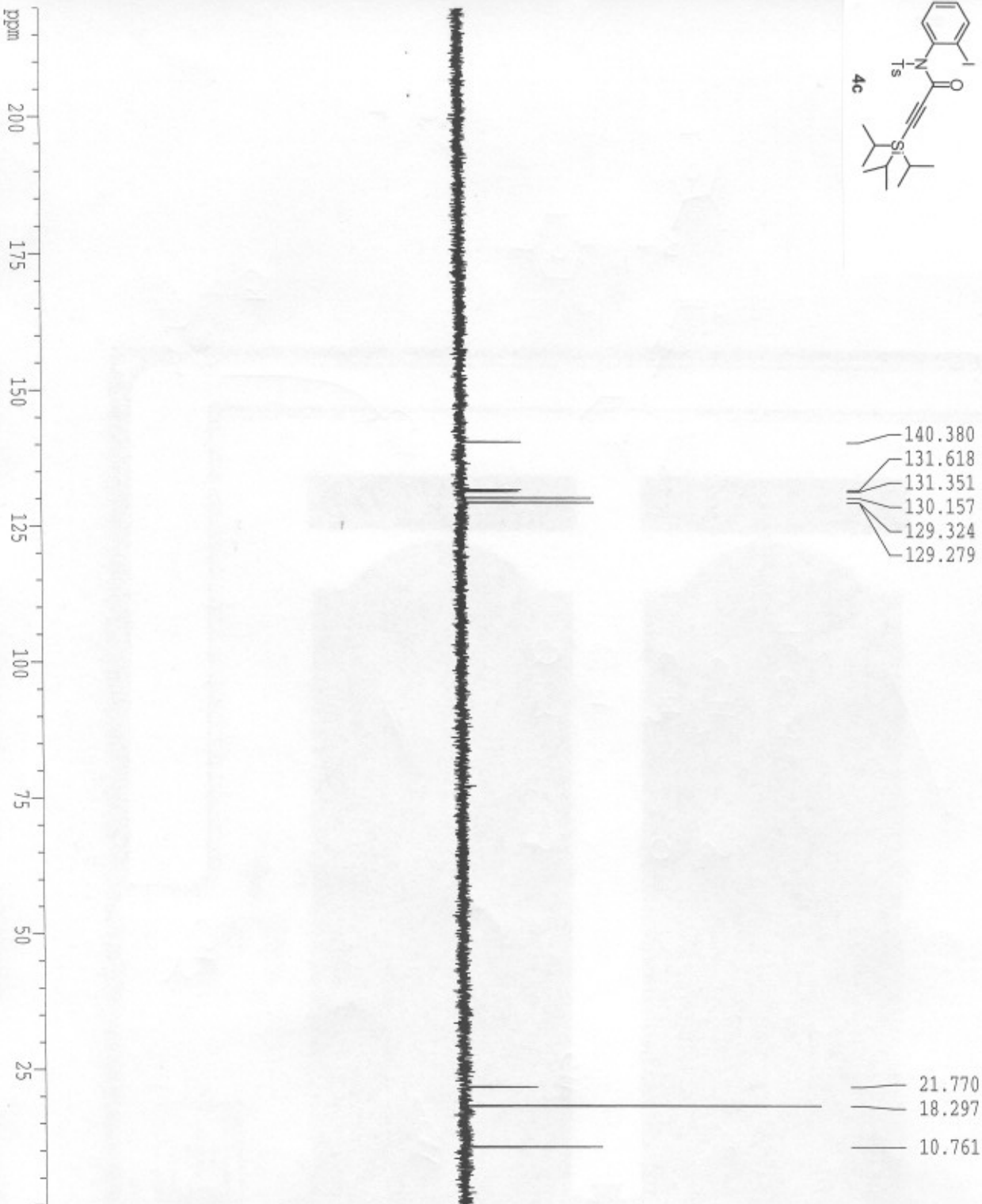
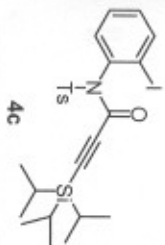
===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 -6.00 dB
SFO1 75.4752160 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 24.00 dB
PL13 26.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 75.4677504 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.50

ID NMR plot parameters
CX 20.00 cm
FLP 200.000 ppm
F1 15093.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCK 10.00000 ppm/cm
HZCM 754.67749 Hz/cm

D'Souza DS_239 CDCl3



Current Data Parameters
NAME aplinuso
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040423

Time 8.51
INSTRUM spect
PROBHD 5 mm TBI 1H/3
PULPROG 32768
TD 32768
SOLVENT CDCl3
NS 224

DS 8
SMH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec

RG 2048
DM 22.050 usec
DE 6.00 usec

TE 300.0 K
D1 2.00000000 sec
D2 0.00345000 sec
D12 0.00002000 sec

DELTA 0.00001401 sec

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

NUC1 13C
P1 11.00 usec
P2 22.00 usec
PL1 -6.00 dB

SFO1 75.4752160 MHz

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

CEPRG2 waltz16

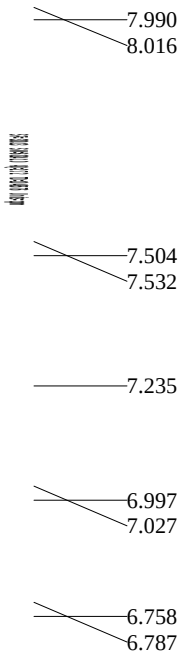
NUC2 1H
P3 8.50 usec
P4 17.00 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 24.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters

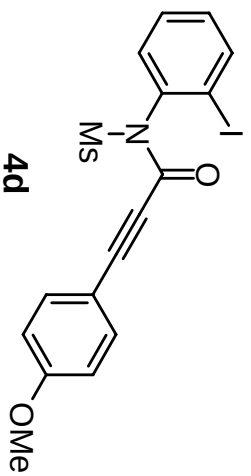
SI 32768
SF 75.4677503 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

ID NMR plot parameters

CX 20.00 cm
PLP 220.000 ppm
F1 16602.90 Hz
P2P 0.000 ppm
F2 0.00 Hz
PEWCH 11.00000 ppm/cm
HZCN 830.14526 Hz/cm

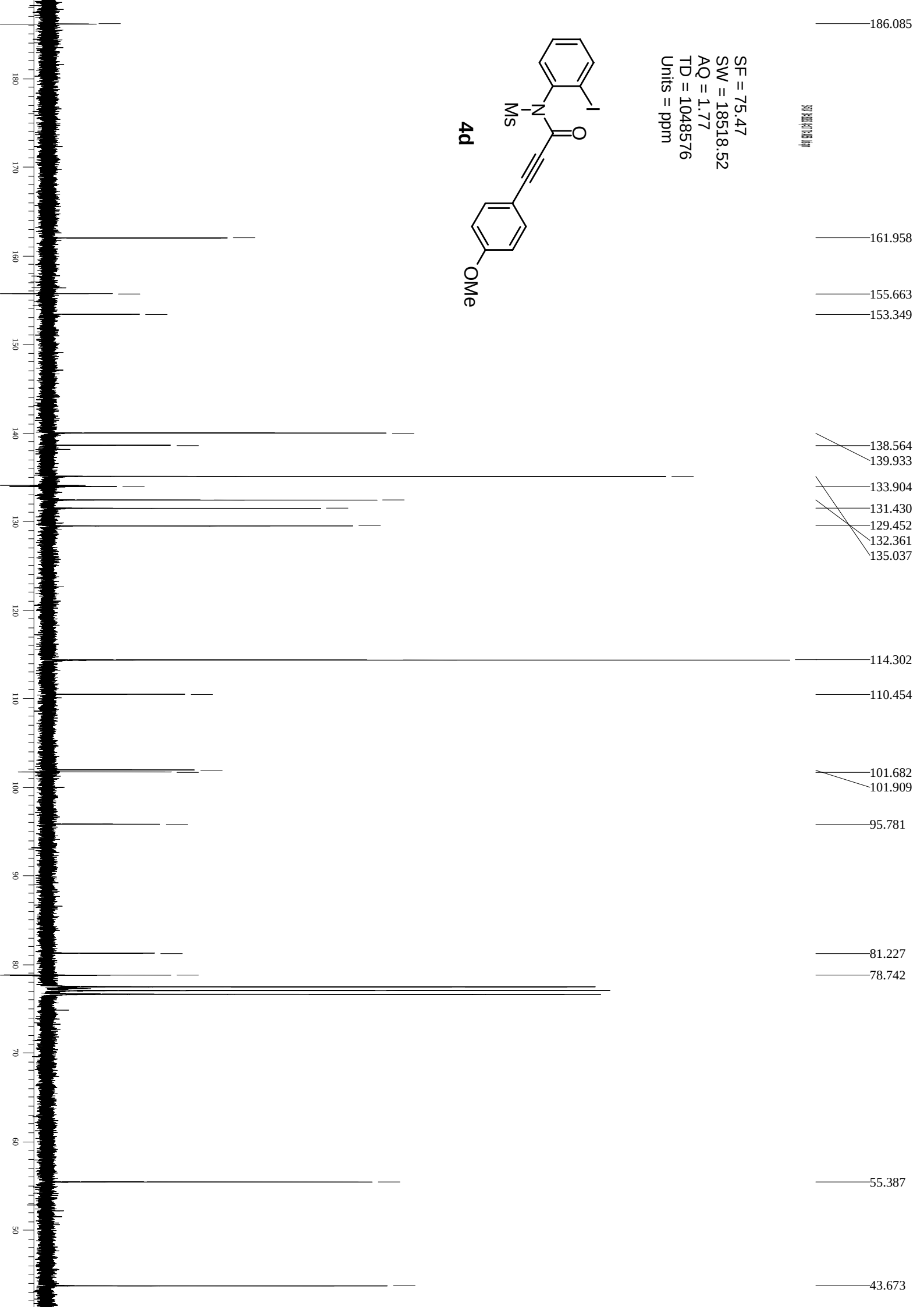
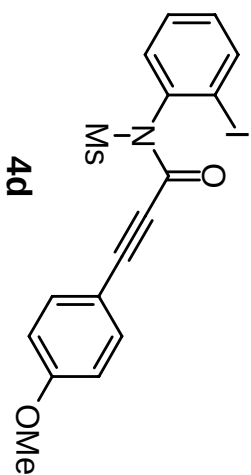


SF = 300.13
SW = 6024.10
AQ = 2.72
TD = 1048576
Units = ppm

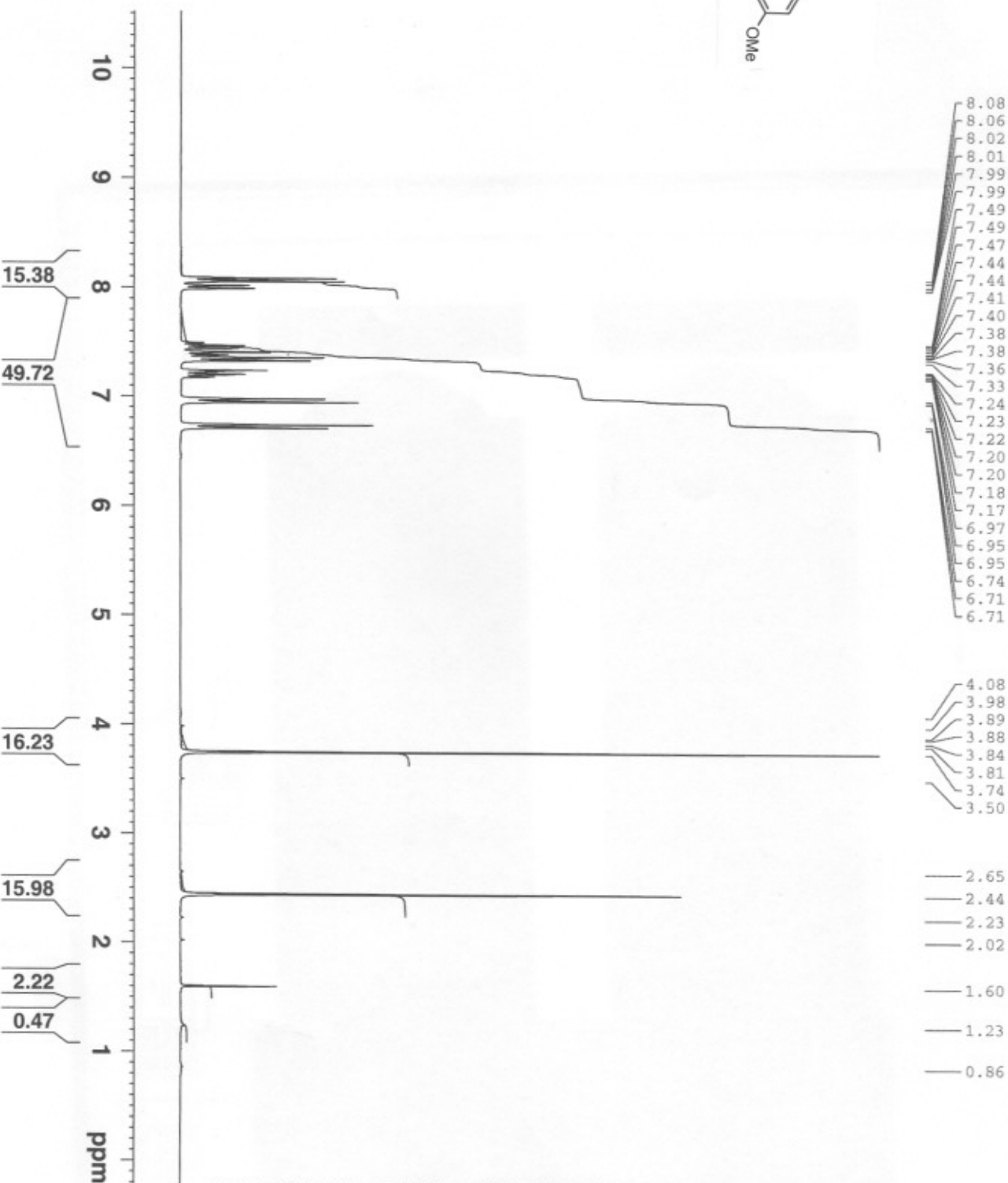
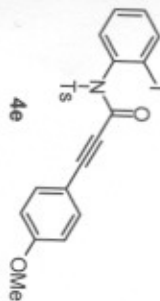


SPIN ECHO 129.00 MHz

SF = 75.47
SW = 18518.52
AQ = 1.77
TD = 1048576
Units = ppm



DS-602 MU in CDCL3 D'Souza



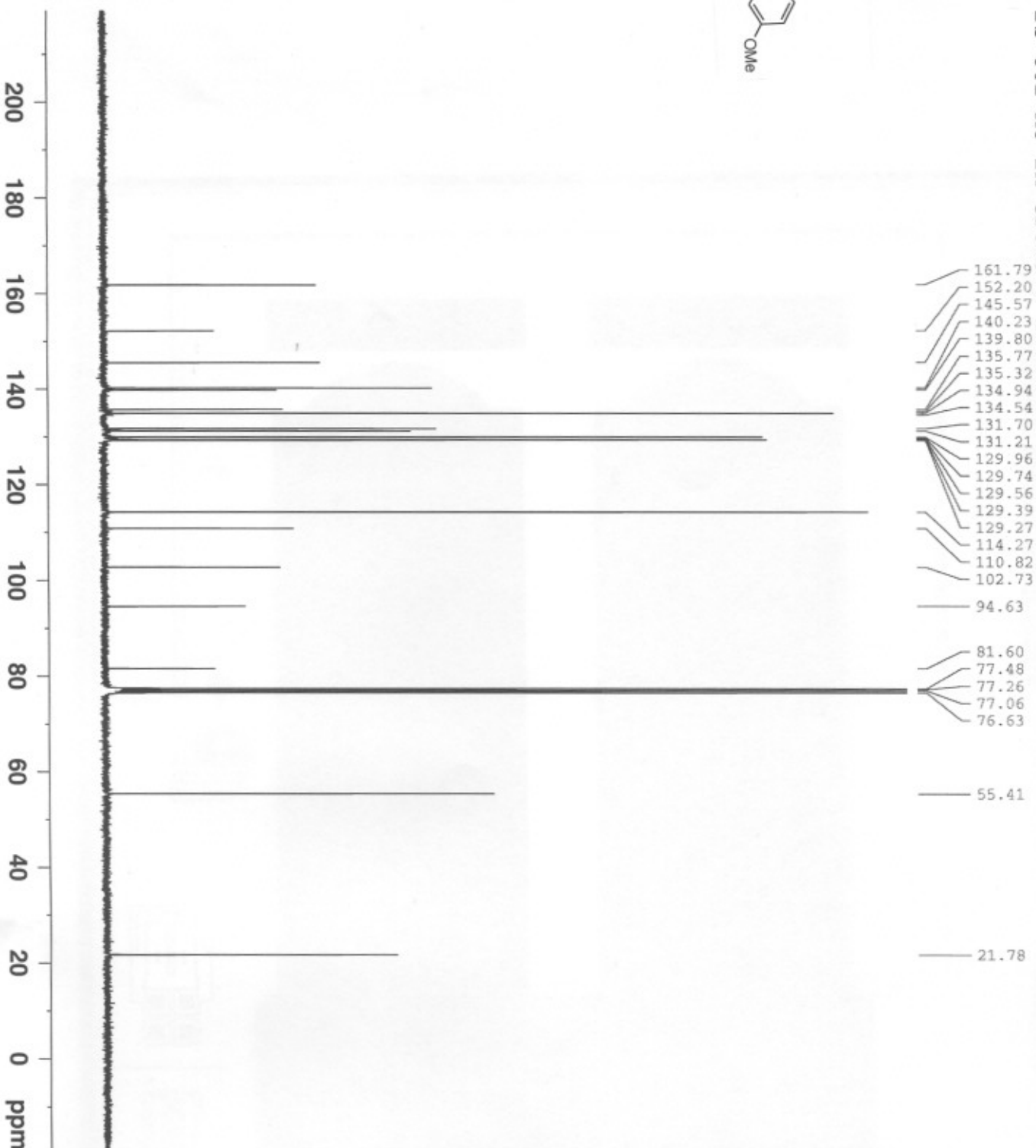
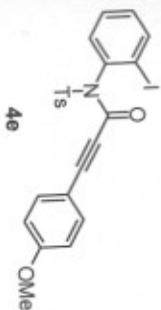
Current Data Parameters
NAME mudsjn23
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060625
Time 20.41
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 362
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz
F2 - Processing Parameters
SI 32768
SF 300.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 6.00



DS-602 MU in CDCL3 D'Souza



Current Data Parameters
NAME mudsjn23
EXPNO 2
PROCNO 1

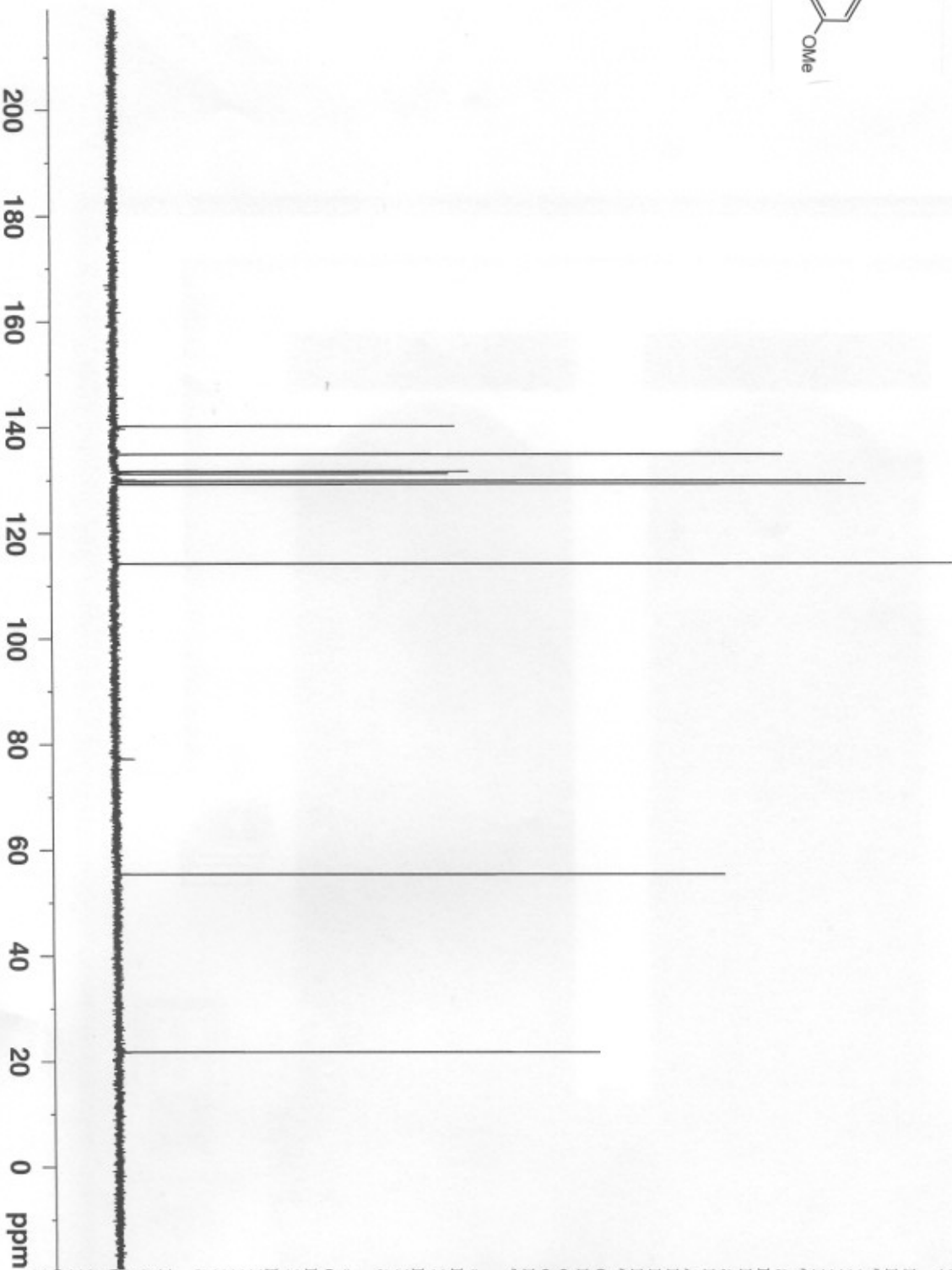
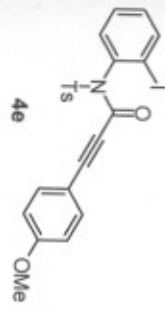
F2 - Acquisition Parameters
Date_ 20060626
Time 1.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DS-602 MU in CDCL3 D"Souza



Current Data Parameters
NAME mudsjn23
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 3.11

INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 2000

DS 4
SMH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384

DW 27.800 usec
DE 6.00 usec
TE 300.0 K

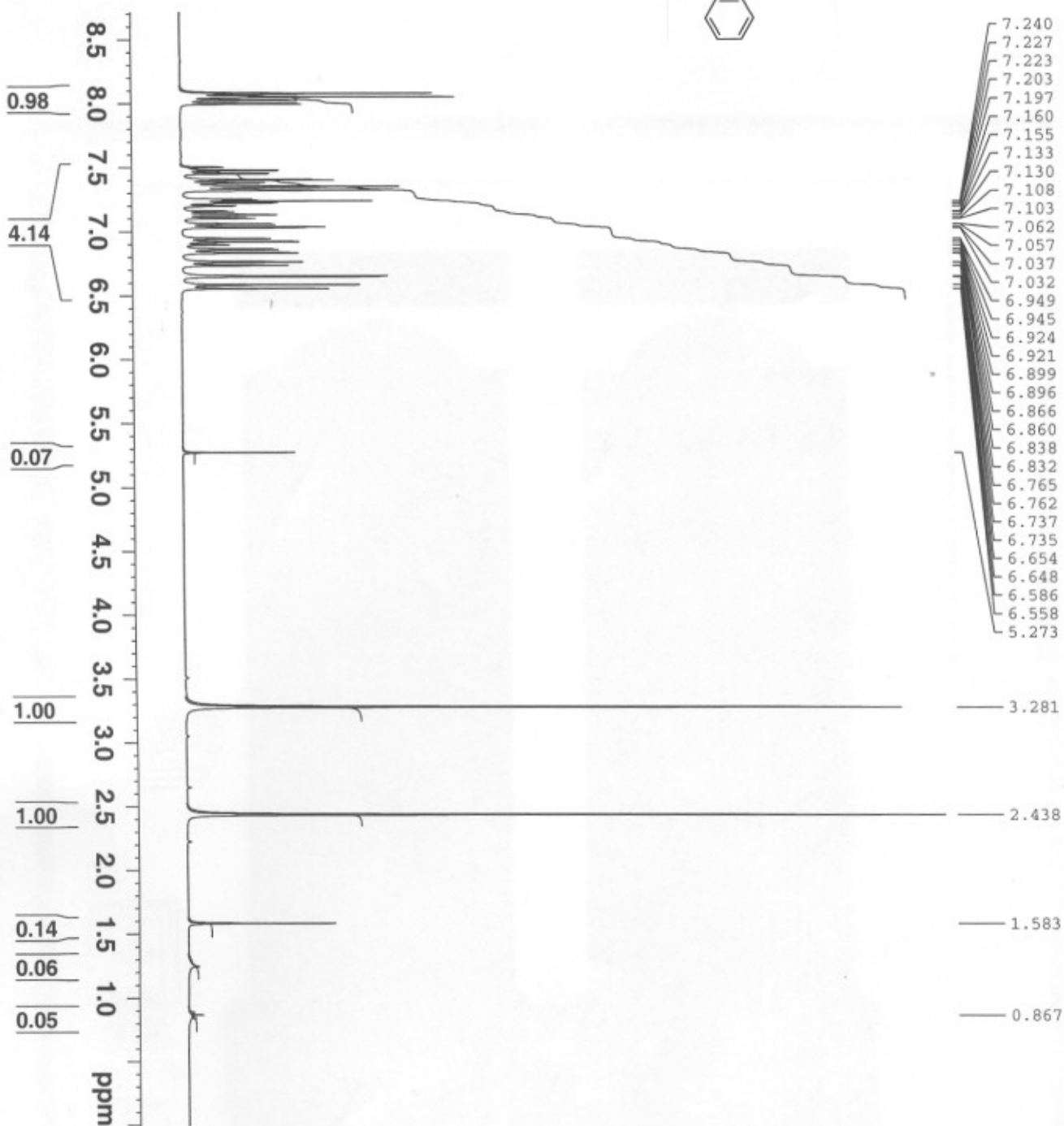
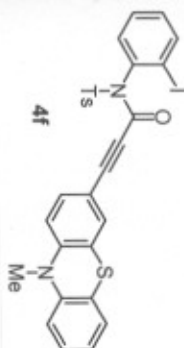
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

D'Souza DS_476MU CDCl3



Current Data Parameters
NAME jn09muso
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060612
Time 4.09

INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zg30

TD 16384
SOLVENT CDCl3

NS 16
DS 2
SWH 5707.763 Hz

FIDRES 0.348374 Hz
AQ 1.4352884 sec

RG 203.2
DW 87.600 use

DE 6.00 use
TE 300.0 K

D1 2.00000000 sec
MCREST 0.00000000 sec

MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 use

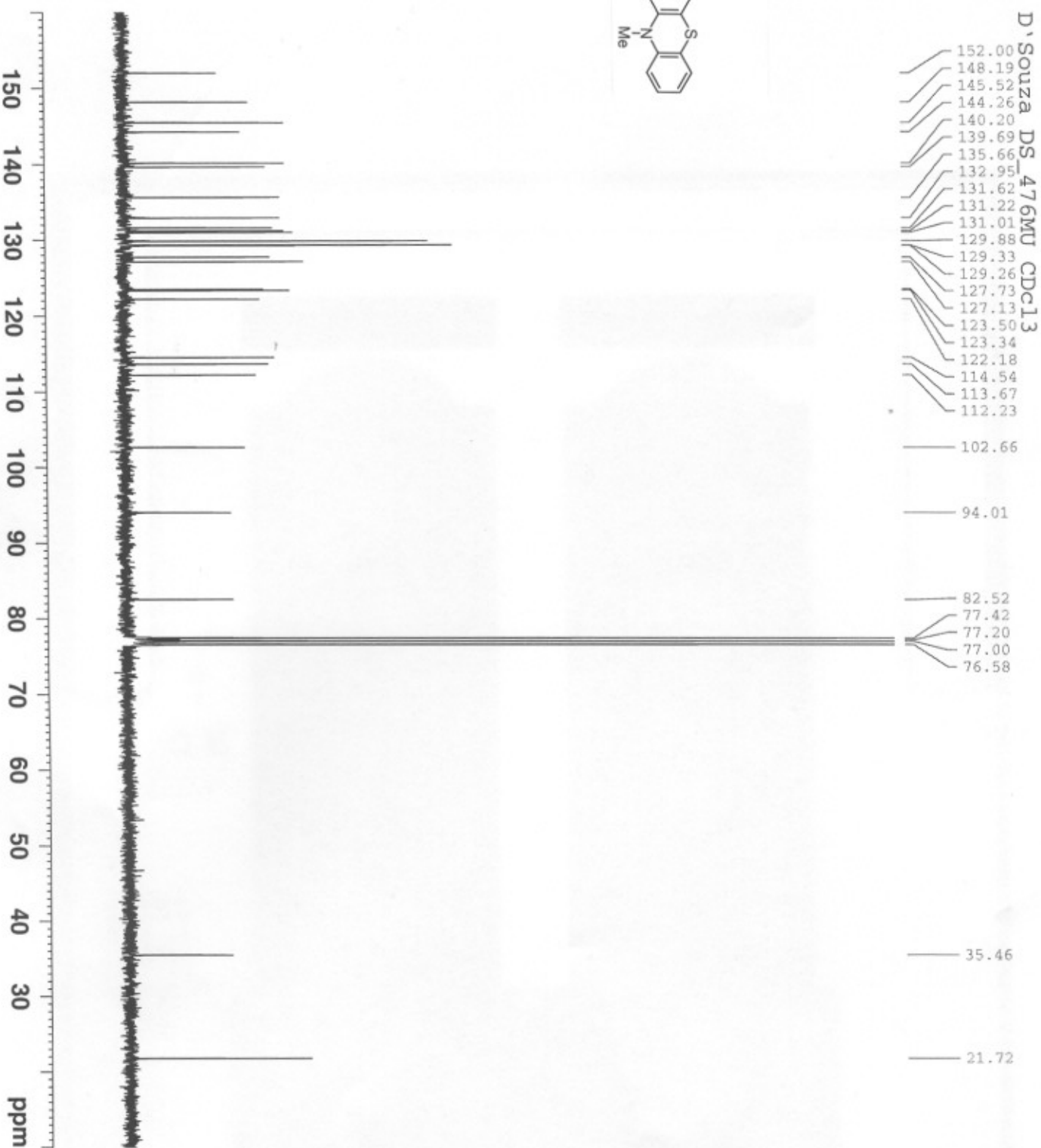
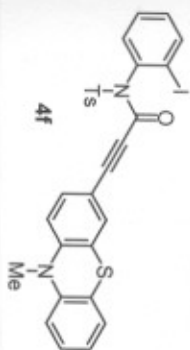
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768

SF 300.1300123 MHz
WDW EM

SSB 0
LB 0.10 Hz

GB 0
PC 1.00



```

Current Data Parameters
NAME          jn09muso
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20060612
Time          5.43
INSTRUM       spect
PROBHD        5 mm TBI 1H/31
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            2000
DS            4
SMH           22675.736 Hz
FIDRES        0.692009 Hz
AQ            0.7225844 sec
RG            8192
DE            22.050 usec
TE            300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            20.00 usec
PL1           0.00 dB
SFO1          75.4752658 MHz

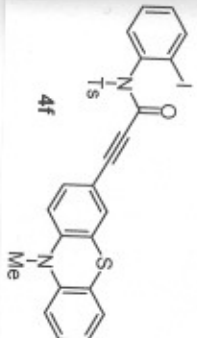
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         100.00 usec
PL2           0.00 dB
PL12          20.00 dB
PL13          120.00 dB
SFO2          300.1316507 MHz

F2 - Processing parameters
SI            32768
SF            75.4677545 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            2.00
  
```


D'Souza DS-476MU CDCl₃

140.20
132.95
131.62
131.22
131.01
129.88
129.33
129.26
127.73
127.13
123.34
114.54
113.67

35.46
21.72



150 140 130 120 110 100 90 80 70 60 50 40 30 ppm



Current Data Parameters
NAME jn09muso
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060612
Time 4.08
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG dept135b
TD 32768
SOLVENT CDCl₃
NS 1000
DS 8
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 7298.2
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 1.50000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00002546 sec
MCREST 0.00000000 sec
MCWERK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 20.00 usec
P2 40.00 usec
PL1 0.00 dB
SFO1 75.4730017 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.00 usec
P4 20.00 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 75.4677545 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

DS-510 MU in CDCL3 D'Souza

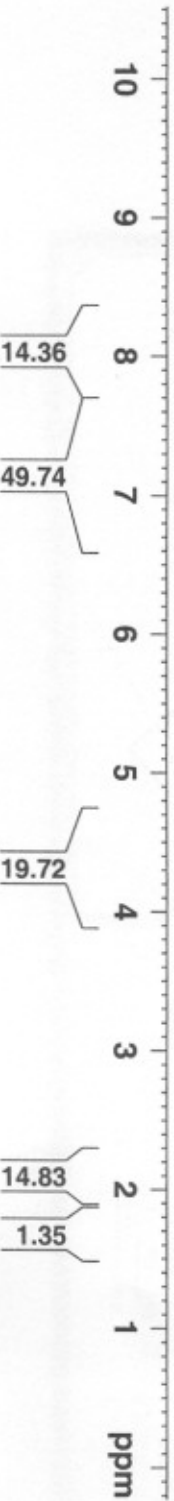
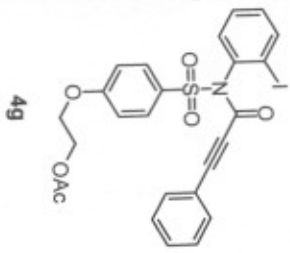


Current Data Parameters
NAME musook21
EXPNO 1
PROCNO 1

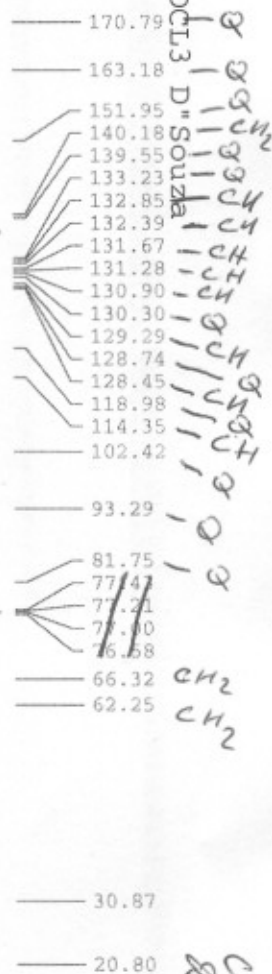
F2 - Acquisition Parameters
Date_ 20051021
Time 20.21
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 287.4
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.20
8.19
8.18
8.17
8.16
8.15
8.06
8.05
8.03
8.03
7.54
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.47
7.47
7.45
7.44
7.41
7.39
7.38
7.38
7.36
7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.23
7.22
7.22
7.08
7.06
7.05
7.04
4.49
4.48
4.46
4.30
4.28
4.27
2.18
2.14
2.14
2.14
2.14
2.13
2.12
2.12
2.11
2.11
2.11
2.11
2.10
2.10
2.10
2.09
2.09
1.69



DS-510 MU in CDCl₃ D² Souza



CH: 9
CH₂: 2
CH₃: 1

Current Data Parameters
NAME musook21
EXPNO 2
PROCNO 1

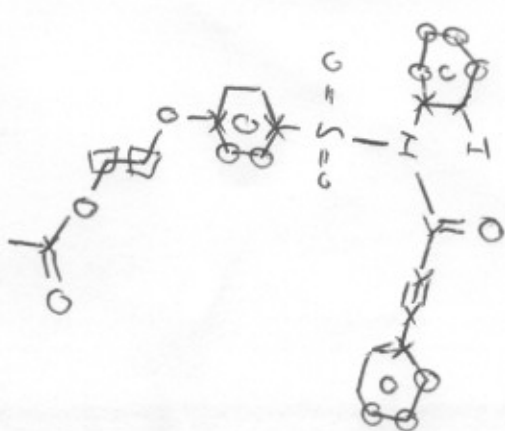
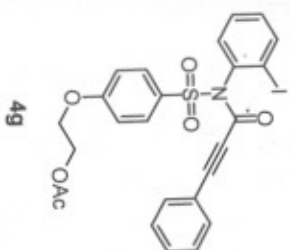
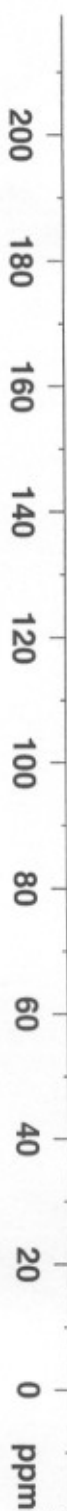
F2 - Acquisition Parameters

Date_ 20051021
Time 22.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 2400
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing Parameters
SI 32768
SF 75.4677545 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



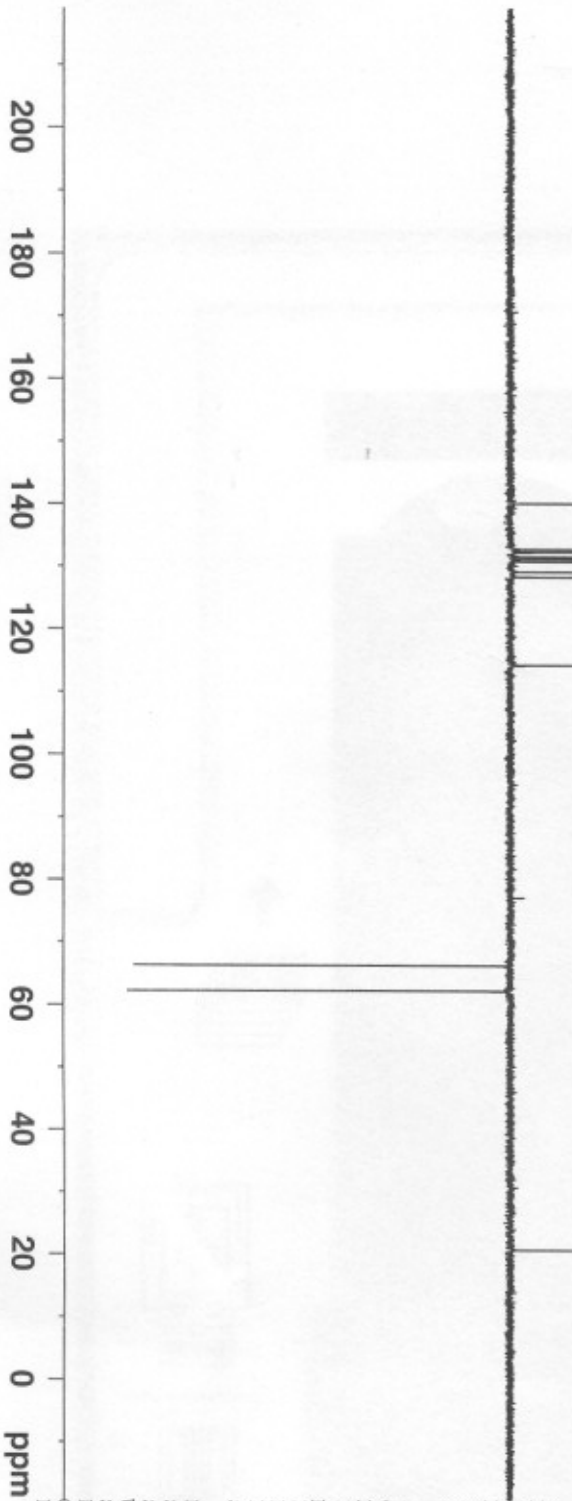
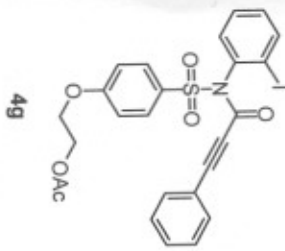
DS-510 MU in CDCL3 D'Souza

140.19
132.85
132.39
131.67
131.30
130.91
129.30
128.45
114.35

77.21
66.31
62.26

20.81

CH



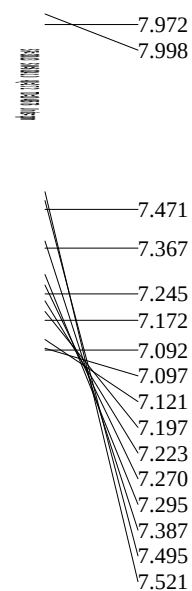
Current Data Parameters
NAME musook21
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051022
Time 0.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

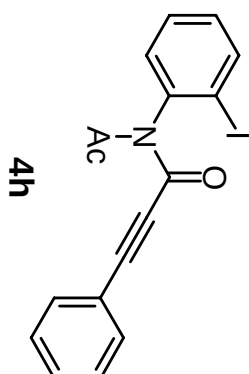
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
PL3 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

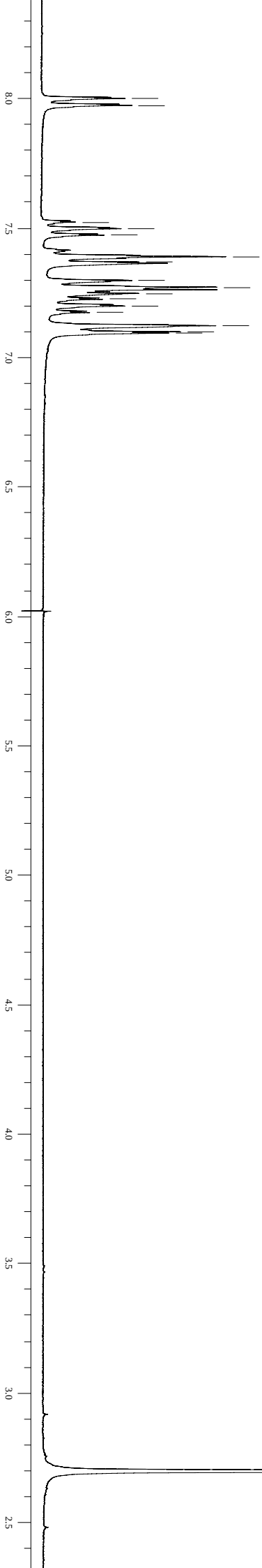
F2 - Processing parameters
SI 32768
SF 75.4677545 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

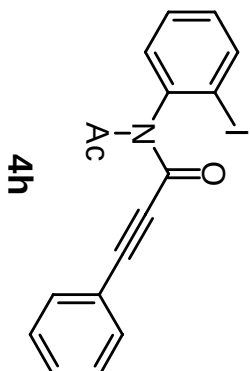


SF = 300.13
SW = 6024.10
AQ = 2.72
TD = 1048576
Units = ppm



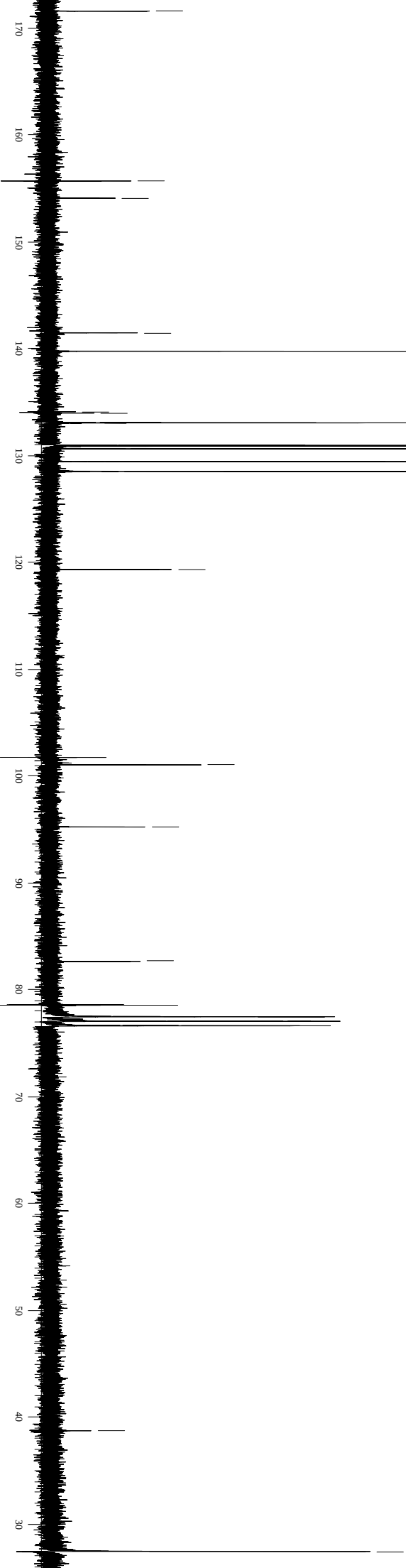
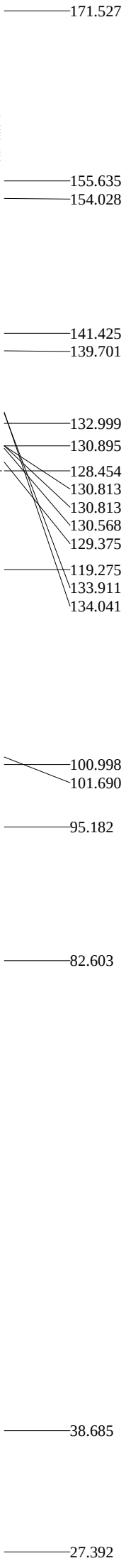
2.699

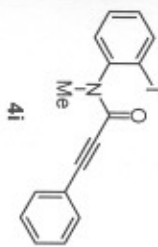




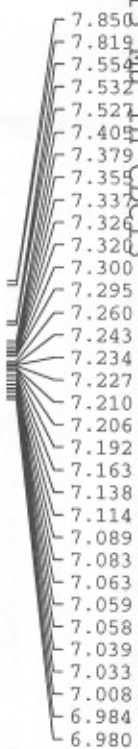
SF = 75.47
SW = 18518.52
AQ = 1.77
TD = 1048576
Units = ppm

100.00000000000000





DS_115_Mn_in_CDCl3



3.483
3.216
3.194

1.722

Current Data Parameters
NAME j131dsnu
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

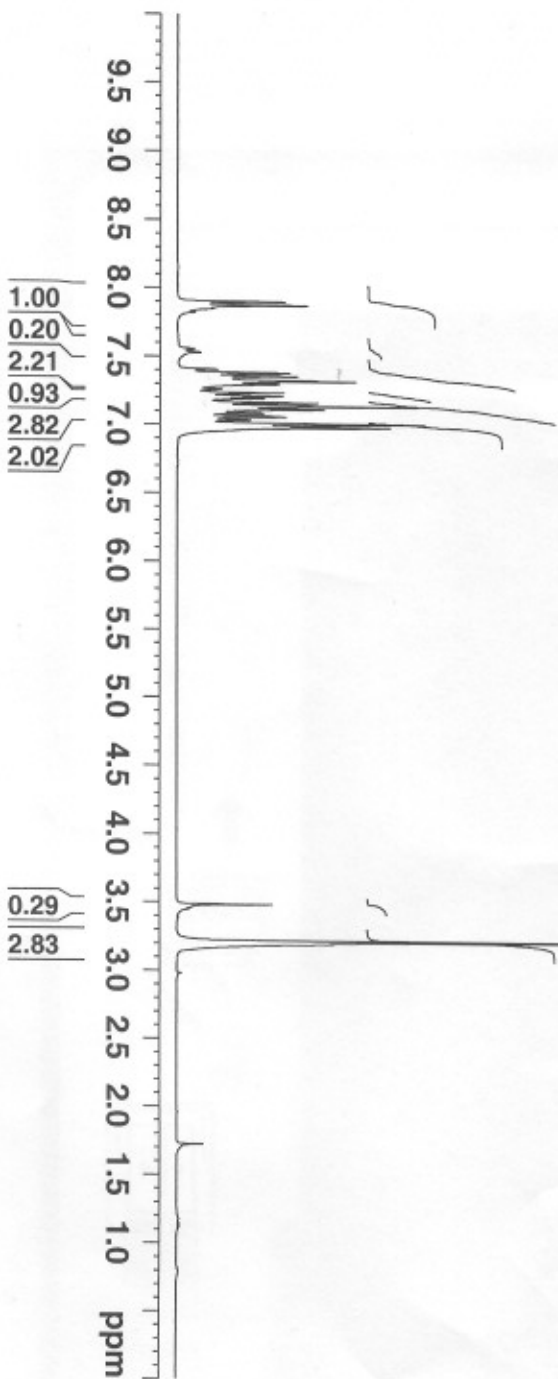
Date_ 20060731
Time 10.32
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SMH 3591.954 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 90.5
DW 139.200 use
DE 6.00 use
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

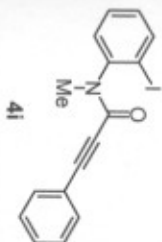
===== CHANNEL f1 =====

NUC1 1H
P1 10.00 use
PL1 0.00 dB
SFO1 300.1315007 MHz

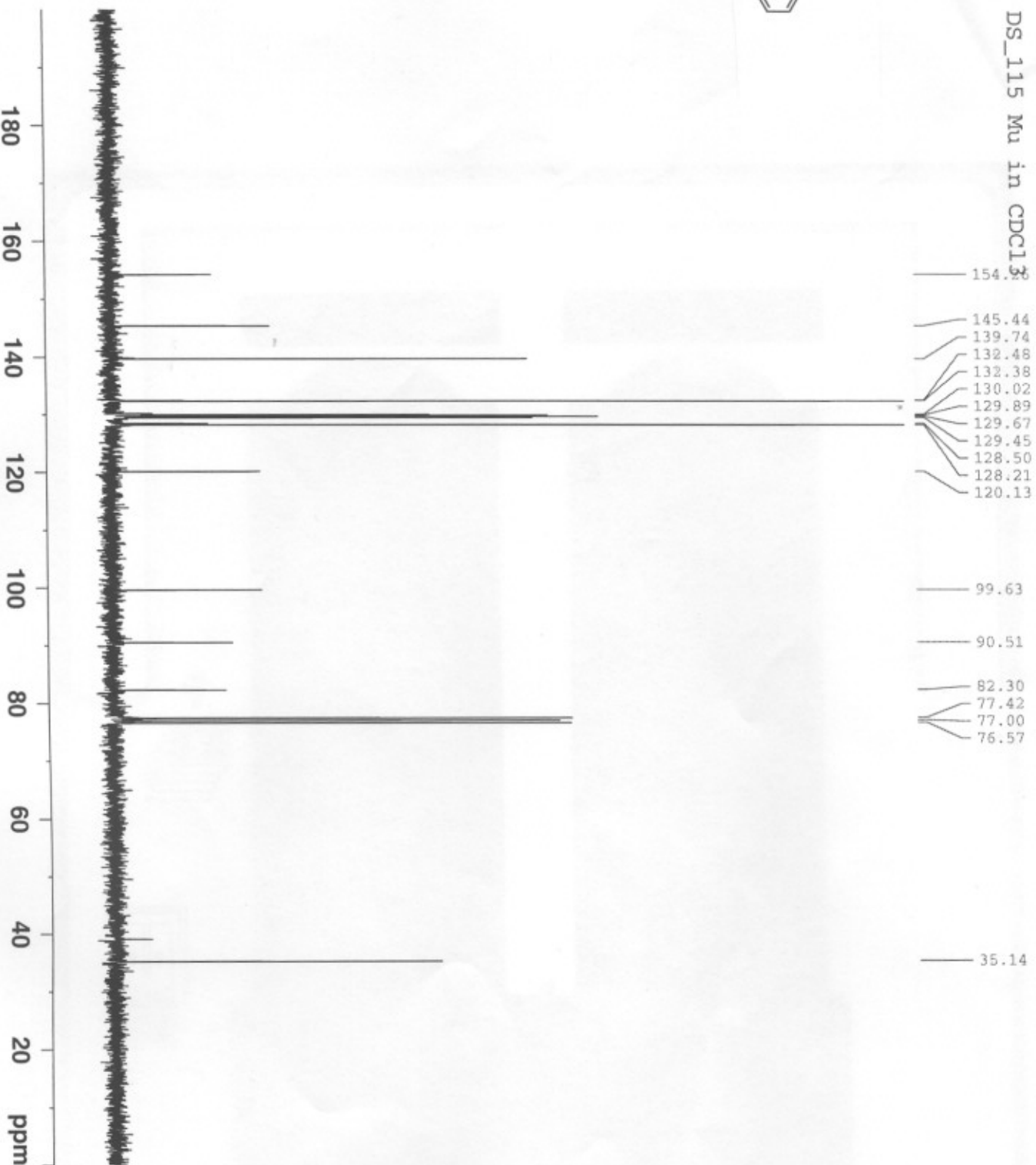
F2 - Processing Parameters

SI 32768
SF 300.1300273 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00





DS_115 Mu in CDCl₃



Current Data Parameters
NAME j131dsu
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060731
Time 13.09
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 467
DS 4
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 4096
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
MCREST 0.0000000 sec
MCWRR 0.0150000 sec

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

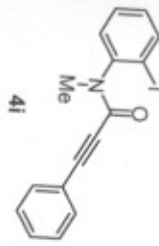
NUC1 13C
P1 20.00 usec
PL1 0.00 dB
SFO1 75.4752658 MHz

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

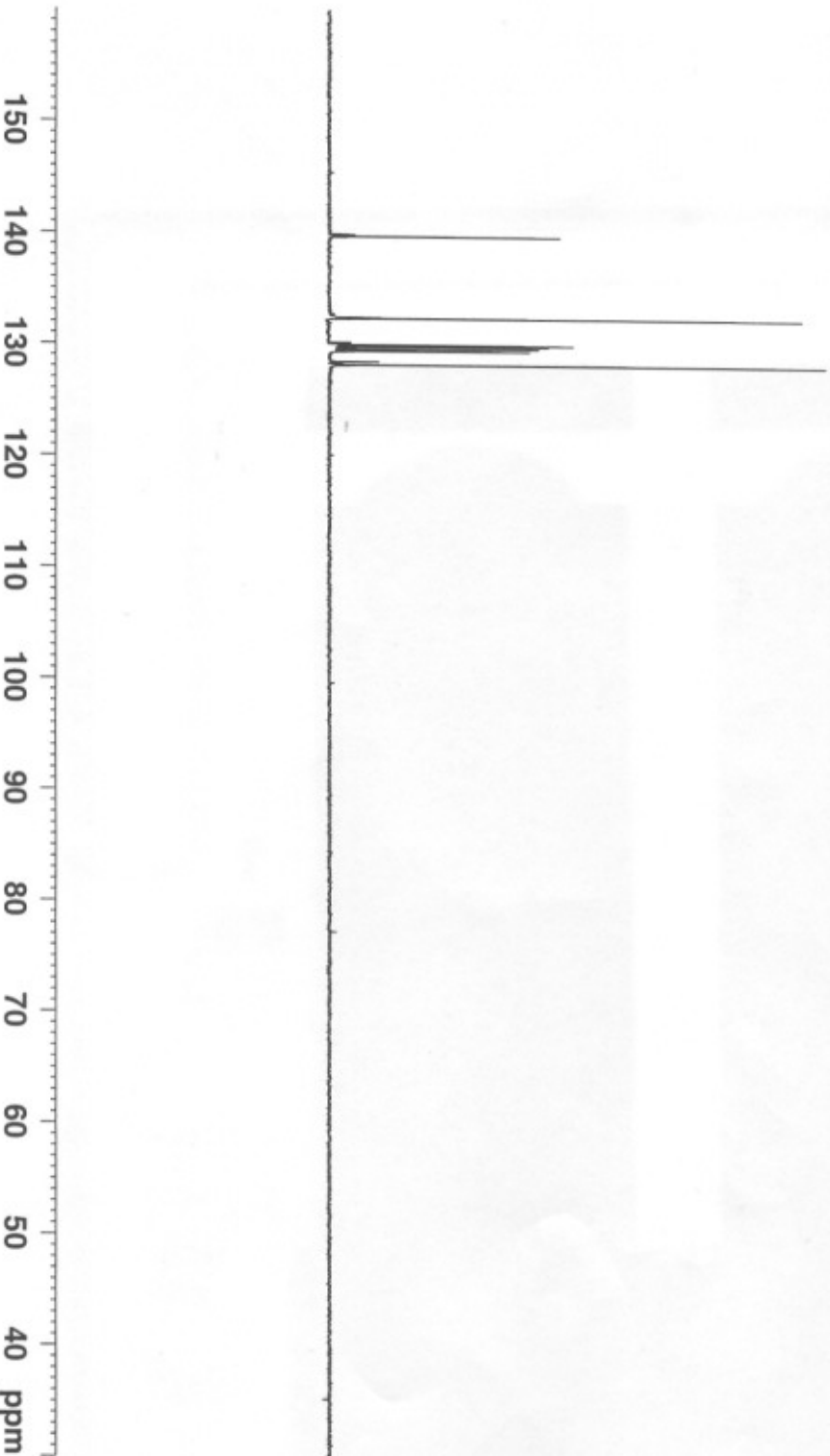
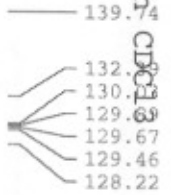
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 24.00 dB
PL13 26.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters

SI 32768
SF 75.4677573 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



DS_115 Mu in CDCl₃



Current Data Parameters
NAME j131dsmu
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060731
Time 13.05

INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG dept135
TD 32768
SOLVENT CDCl₃
NS 91
DS 8

SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 4096

DW 22.050 usec
DE 6.00 usec
TE 300.0 K

CNST2 145.0000000

D1 2.00000000 sec

d2 0.00344828 sec

d12 0.00002000 sec

DELTA 0.00002546 sec

MCREST 0.00000000 sec

MCWRK 0.01500000 sec

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

NUC1 13C

P1 20.00 usec

P2 40.00 usec

PL1 0.00 dB

SFO1 75.4730017 MHz

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

CPDPRG2 waltz16

NUC2 1H

P3 7.50 usec

P4 15.00 usec

PCPD2 100.00 usec

PL2 0.00 dB

PL12 20.00 dB

SFO2 300.1316507 MHz

F2 - Processing parameters

SI 32768

SF 75.4677571 MHz

WDW EM

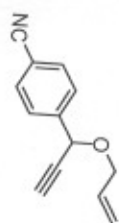
SSB 0

LB 1.00 Hz

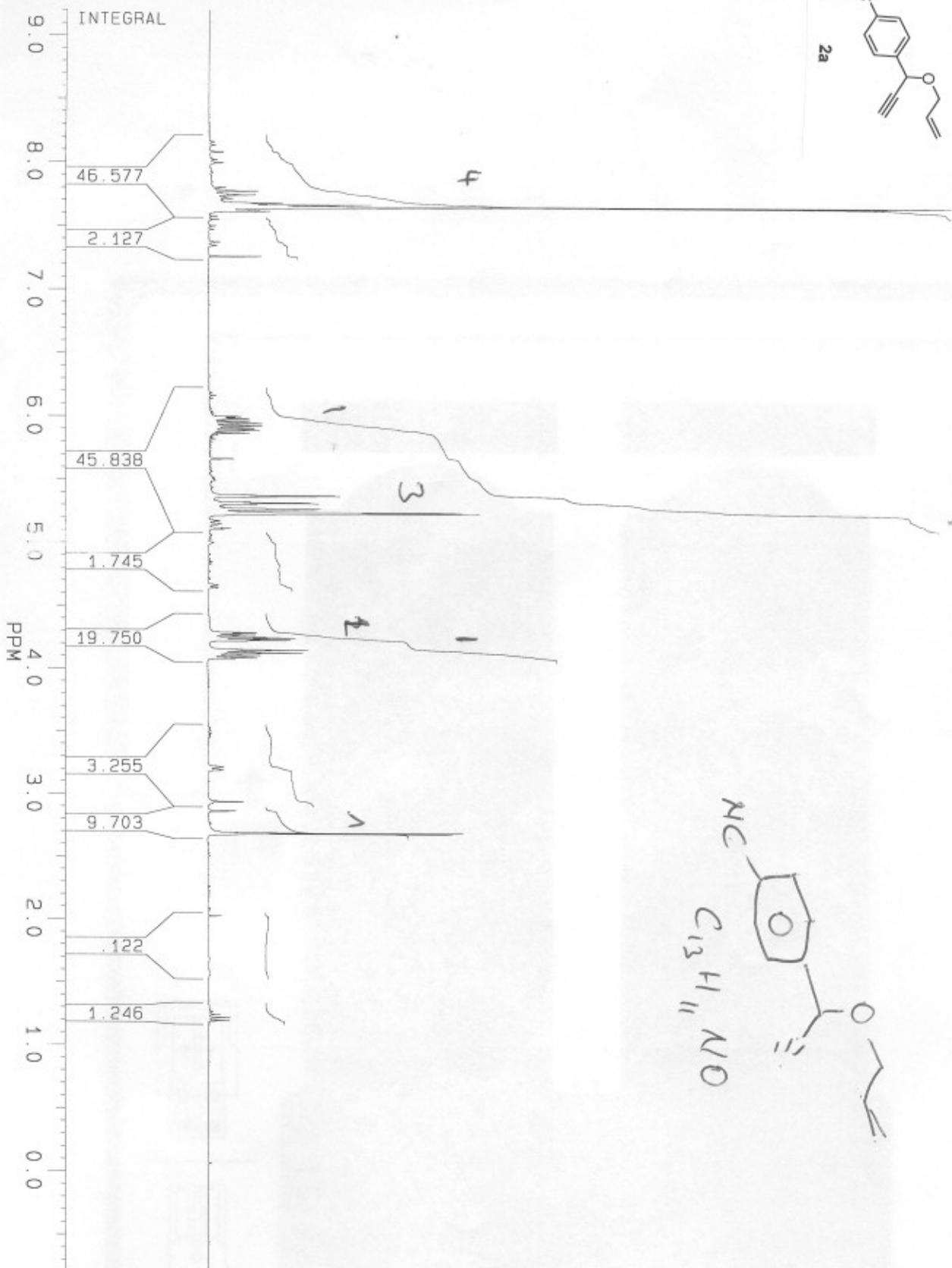
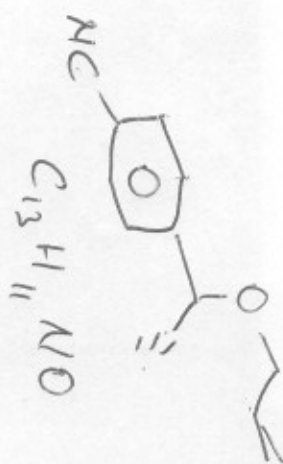
GB 0

PC 1.00

97845



DS-82 IN CDCL3 D'SOUZA



JAE2205.104
AU PROG:
X00.AU
DATE 22-1-3

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

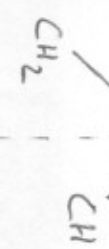
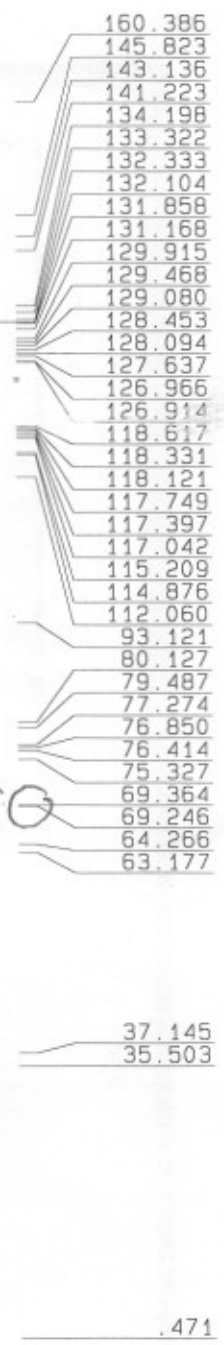
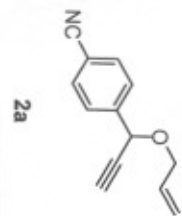
PM 0.0
RD 0.0
AQ 2.720
RG 4
NS 16
TE 297

FW 7600
O2 3200.000
DP 63L PO

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 -.800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88

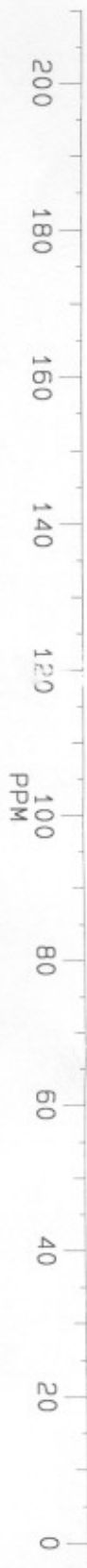
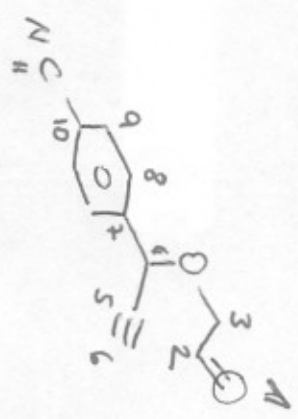
DS-82 IN CDCL3 D"SOUZA

PPM



C₁₃H₁₁N₂

11.51165



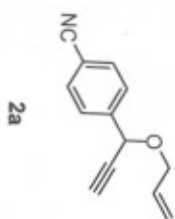
JJA221S.104
AU PROG:
X02.AU
DATE 22-1-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 1000
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 13.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89



DS-82 IN CDCL3 0" SOUZA

133.453
132.496
132.272
132.023
131.335
129.636
128.357
127.796
127.121
127.066
118.329
117.581

80.257
76.595

69.521
69.377

35.650



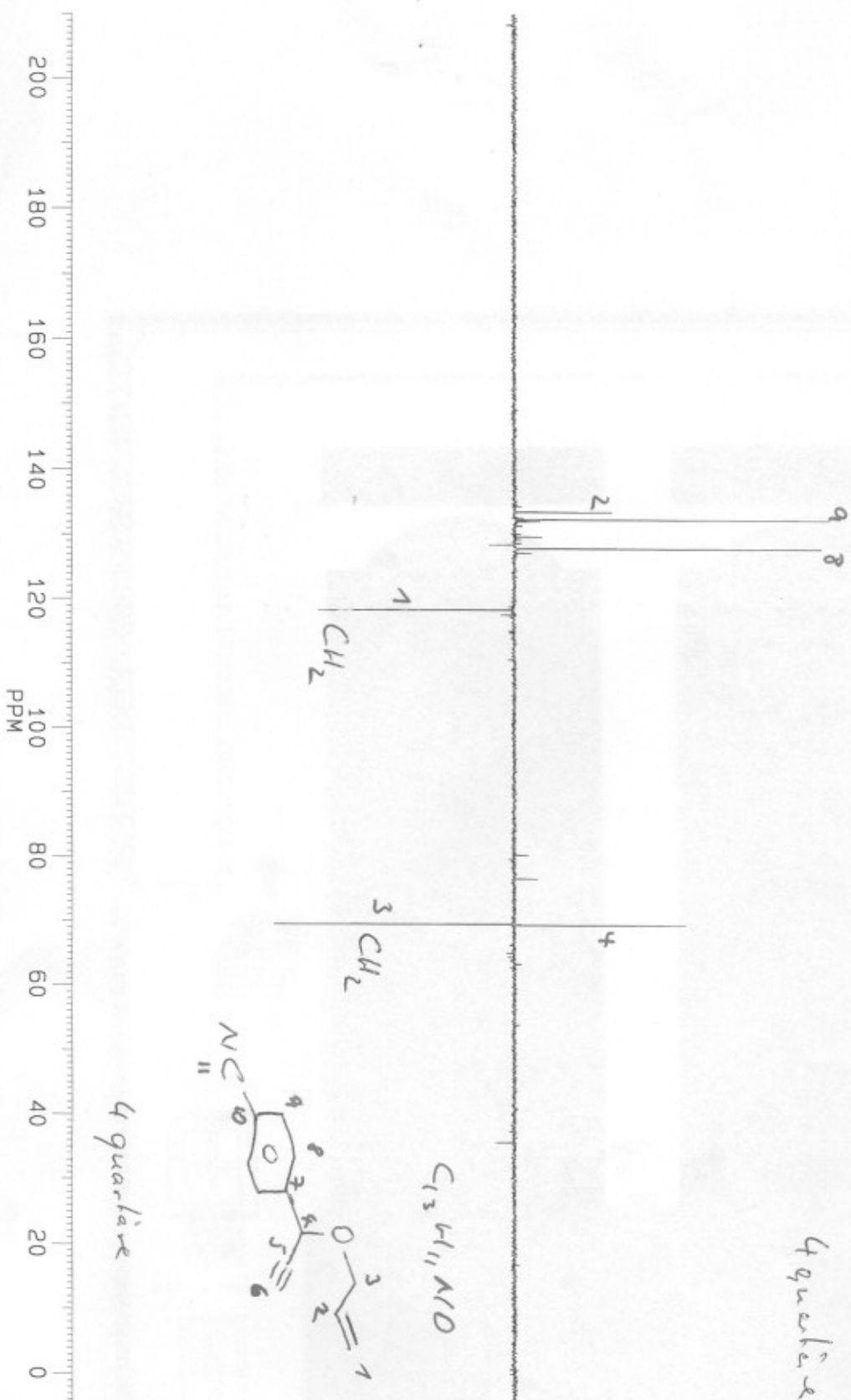
JAE225.104
AU PROG:
X09.AU
DATE 22-1-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 600
TE 297

FW 23200
O2 4588.000
DP 18H D0

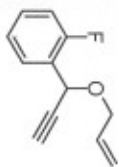
LB 1.000
GB 0.0
CX 22.00
CY 5.00
F1 210.002P
F2 -4.998P
HZ/CM 737.534
PPM/CM 9.773
SR -1399.94



4 quarte

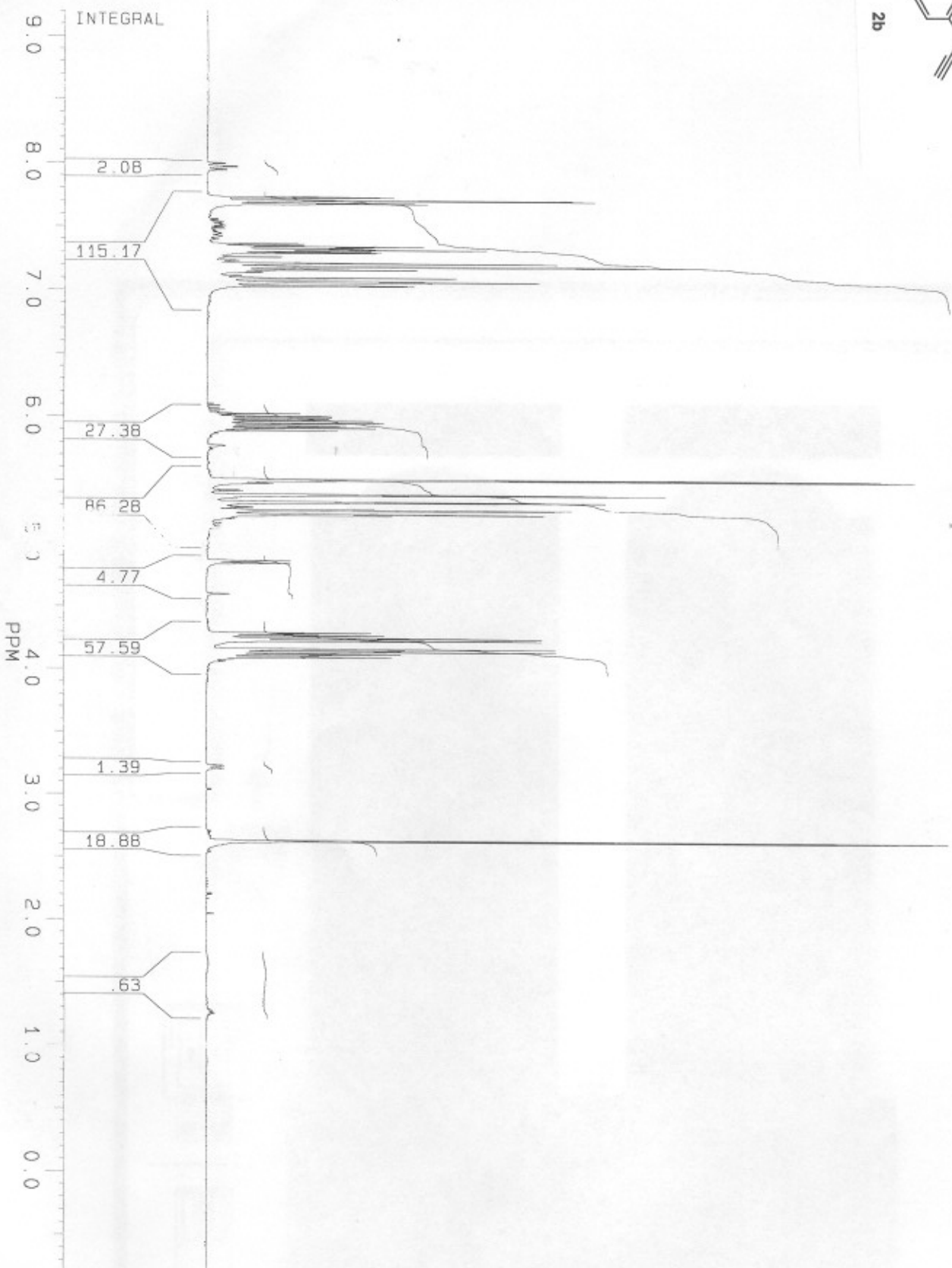
C13 H11 N1 O

4 quarte



2b

OS-90 IN CDCL3 D"SOUZA



JAZ805.111
AU PROG:
X00 .AU
DATE 29-1-3

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

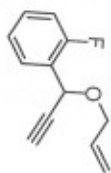
PM 0.0
RD 0.0
AQ 2.720
RG 4
NS 16
TE 297

FW 7600
O2 3200.000
DP 63L P0

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 .800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88

87200

DS-90 IN CDCL3 D" SOUZA

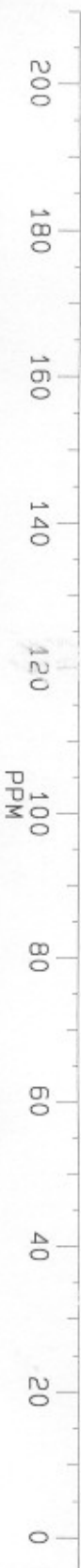


2b

161.771
158.476
134.528
134.411
133.821
132.108
131.853
130.351
130.240
129.129
129.085
125.653
125.476
124.317
124.270
123.933
123.880
118.308
118.036
117.108
116.812
115.547
115.263
80.755
77.426
77.003
76.578
75.236
69.709
65.748
63.935
63.871
34.700
1.326
.668
.000

CH₂

CDCl₃



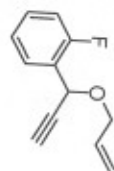
JA281S.111
AU PROG:
X02.AU
DATE 29-1-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PM 0.0
RD 0.0
AQ 1.769
RG 320
NS 400
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 13.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1402.45

DS-90 IN CDCL₃ D²SOUZA

2b

134.389
133.621
131.933
130.201
130.090
128.955
128.911
124.159
124.112
118.158
117.933
115.383
115.100

75.100
69.546
65.592
63.733
63.669

1.145



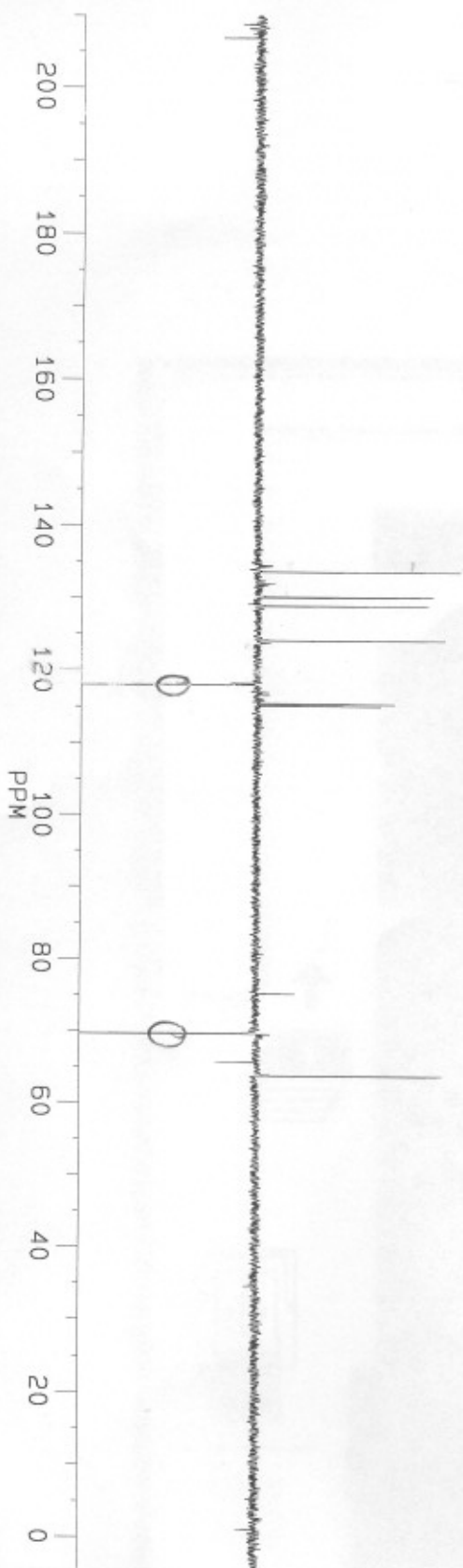
JA2825.111
AU PROG:
X09.AU
DATE 29-1-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 280
TE 297

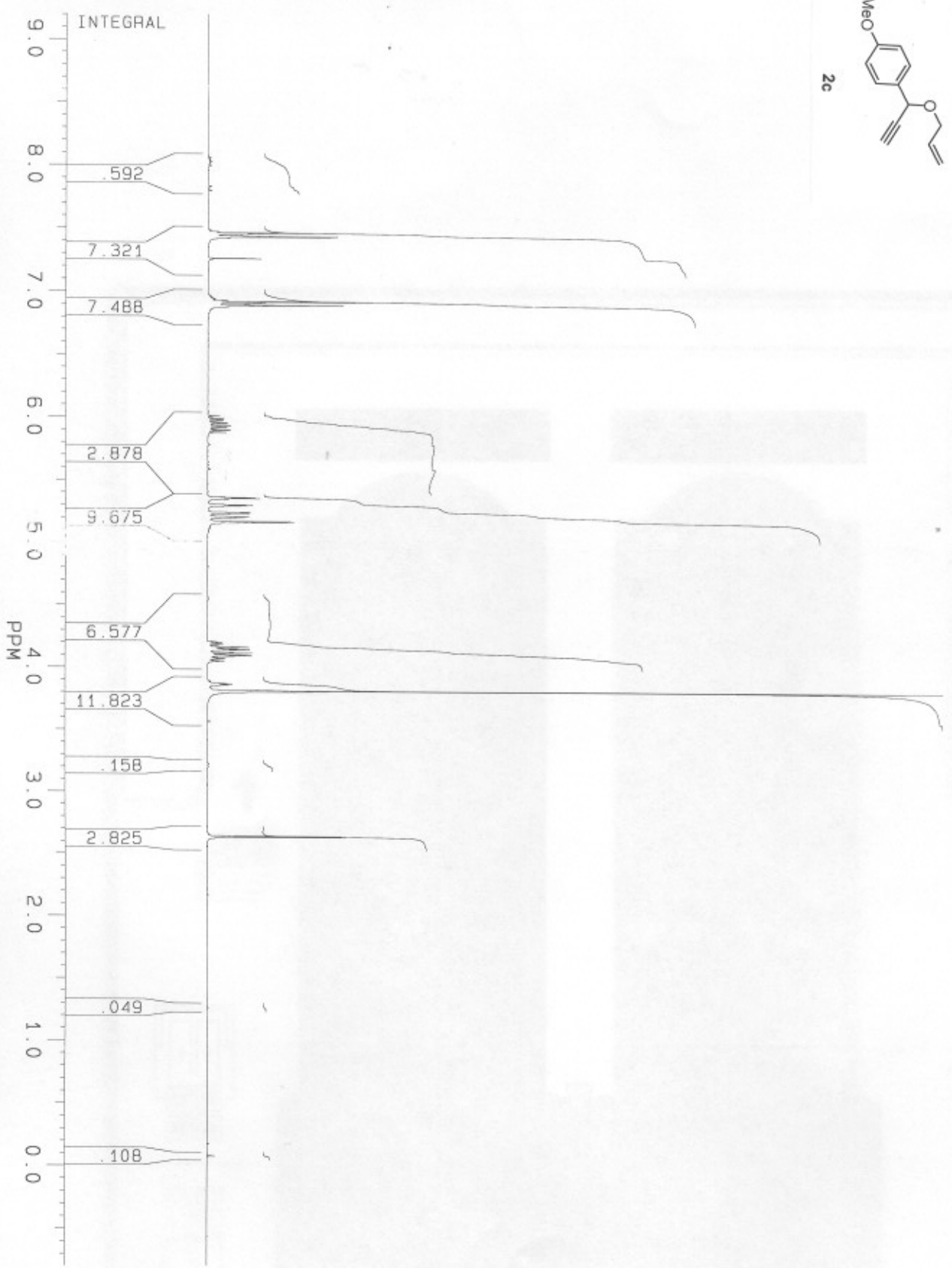
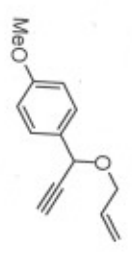
FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 8.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89



87008

DS-31 IN CDCL3 D"SOUZA



DE1705.109
AU PROG:
X00.AU
DATE 17-12-2

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PM 0.0
RD 0.0
AQ 2.720
RG 4
NS 16
TE 297

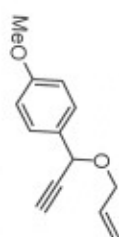
FW 7600
O2 3200.000
DP 63L P0

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 .800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88

DS-31 IN CDCL3 D'SOUZA

PPM

159.571

133.989
132.087
131.758
130.186
128.574117.522
113.679
113.534
113.27981.593
77.238
77.017
76.815
76.391
75.143
69.739
68.76855.226
55.088

2c

200
180
160
140
120
100
80
60
40
20
0
PPM



DE171S.109
AU PROG:
X02.AU
DATE 17-12-2

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PM 0.0
RD 0.0
AQ 1.769
RG 320
NS 400
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 13.00
F1 210.005P
F2 -4.995P
H2/CM 737.534
PPM/CM 9.773
SR -1388.89

DS-31 IN CDCL3 D'SOUZA

PPM

133.967

128.591

117.591

113.673

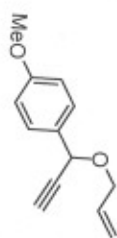
75.178

69.724

68.786

55.100

-1.183



2c



DE1725.109

AU PROG:

X09.AU

DATE 17-12-2

SF 75.469

SY 75.0

O1 6141.605

SI 65536

TD 65536

SW 18518.519

HZ/PT .565

PW 0.0

PD 0.0

AQ 1.769

RG 320

NS 200

TE 297

FW 23200

O2 4588.000

DP 18H D0

LB 1.000

GB 0.0

CX 22.00

CY 8.00

F1 210.005P

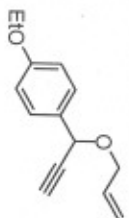
F2 -4.995P

HZ/CM 737.534

PPM/CM 9.773

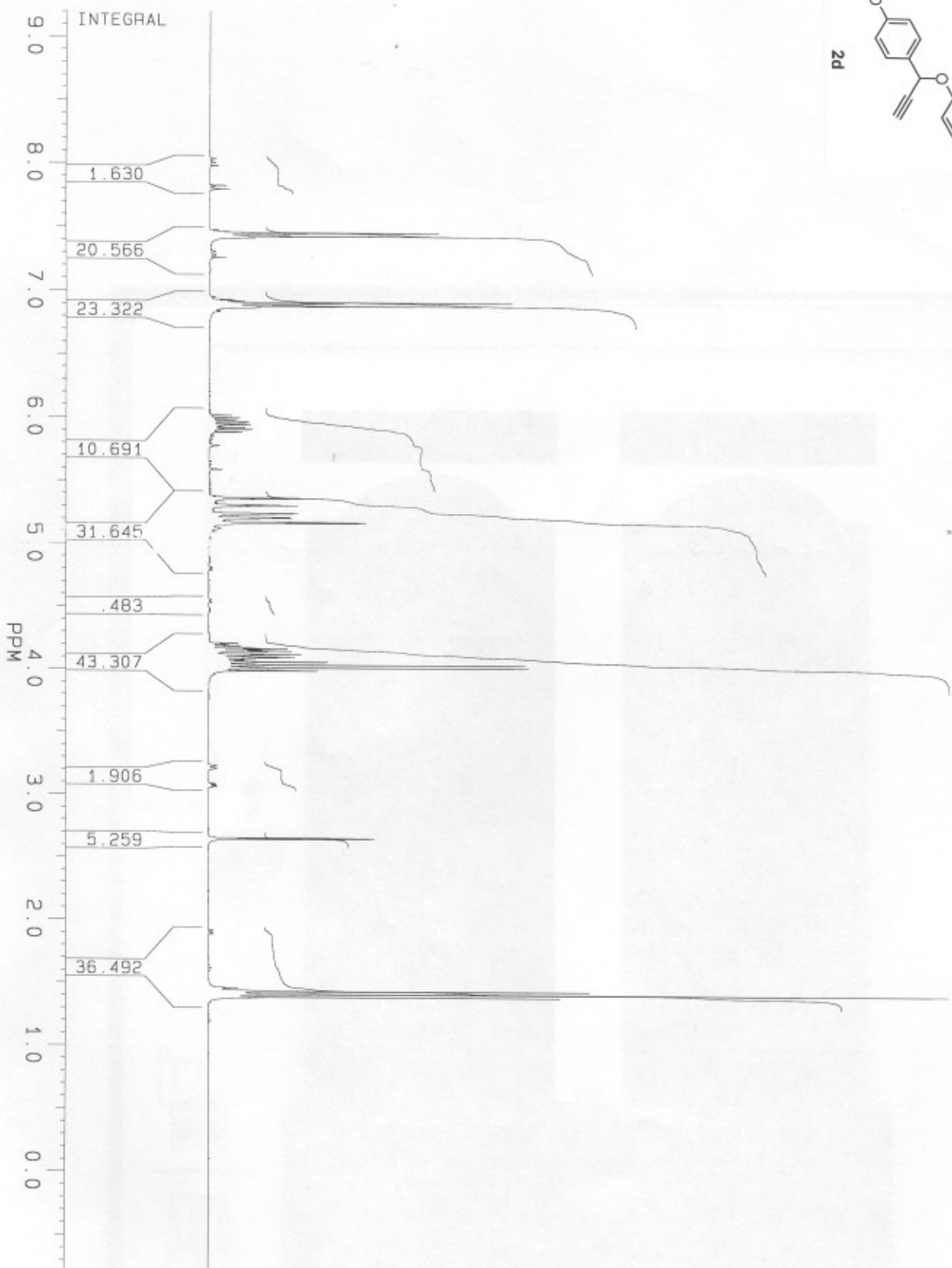
SR -1388.89





2d

DS-51 IN CDCL3 D" SOUZA



DE170S.107
 AU PROG:
 X00.AU
 DATE 17-12-2

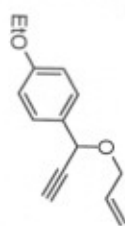
SF 300.133
 SY 210.0
 O1 5173.724
 S1 32768
 TD 32768
 SW 6024.096
 HZ/PT .368

PW 0.0
 RD 0.0
 AQ 2.720
 RG 2
 NS 16
 TE 297

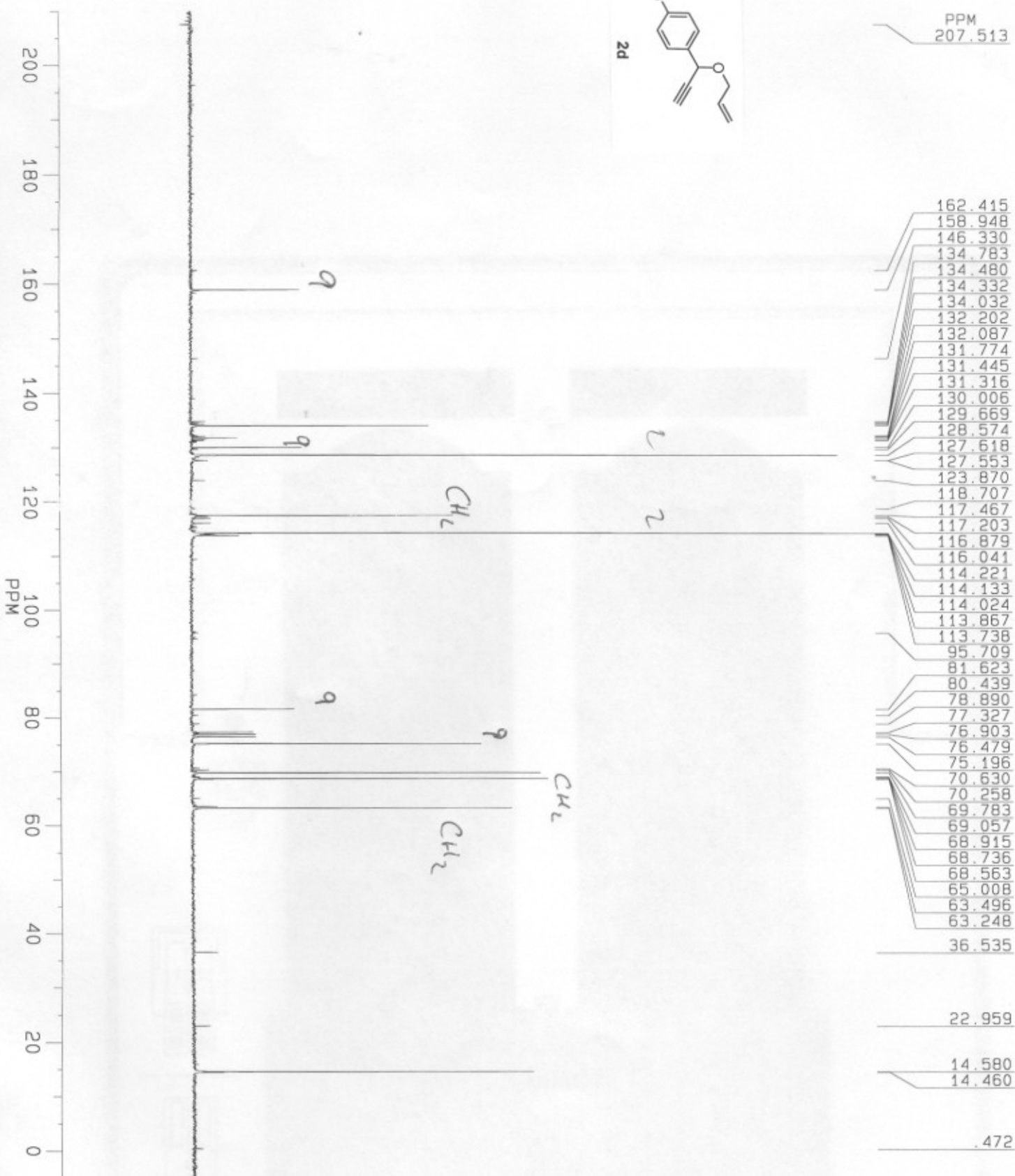
FW 7600
 O2 3200.000
 DP 63L PD

LB .100
 GB 0.0
 CX 22.00
 CY 13.00
 F1 9.200P
 F2 .800P
 HZ/CM 136.427
 PPM/CM .455
 SR 3369.88

37000

PPM
207.513

2d



DE171S.107
AU PROG:
X02.AU
DATE 17-12-2

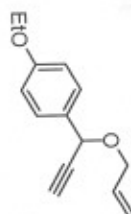
SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 400
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 13.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89

PPM
208.164
207.494



2d

134.011
132.051
131.795
131.453
131.330
128.723
128.591
127.558
123.971
117.532
117.269
116.911
116.055
114.206
114.116
114.011
113.855
113.727

81.602
75.230
70.248
69.980
69.769
69.060
68.916
68.752
68.579
65.029
63.501
63.243

36.537

22.973
14.596
14.542
14.477
14.354



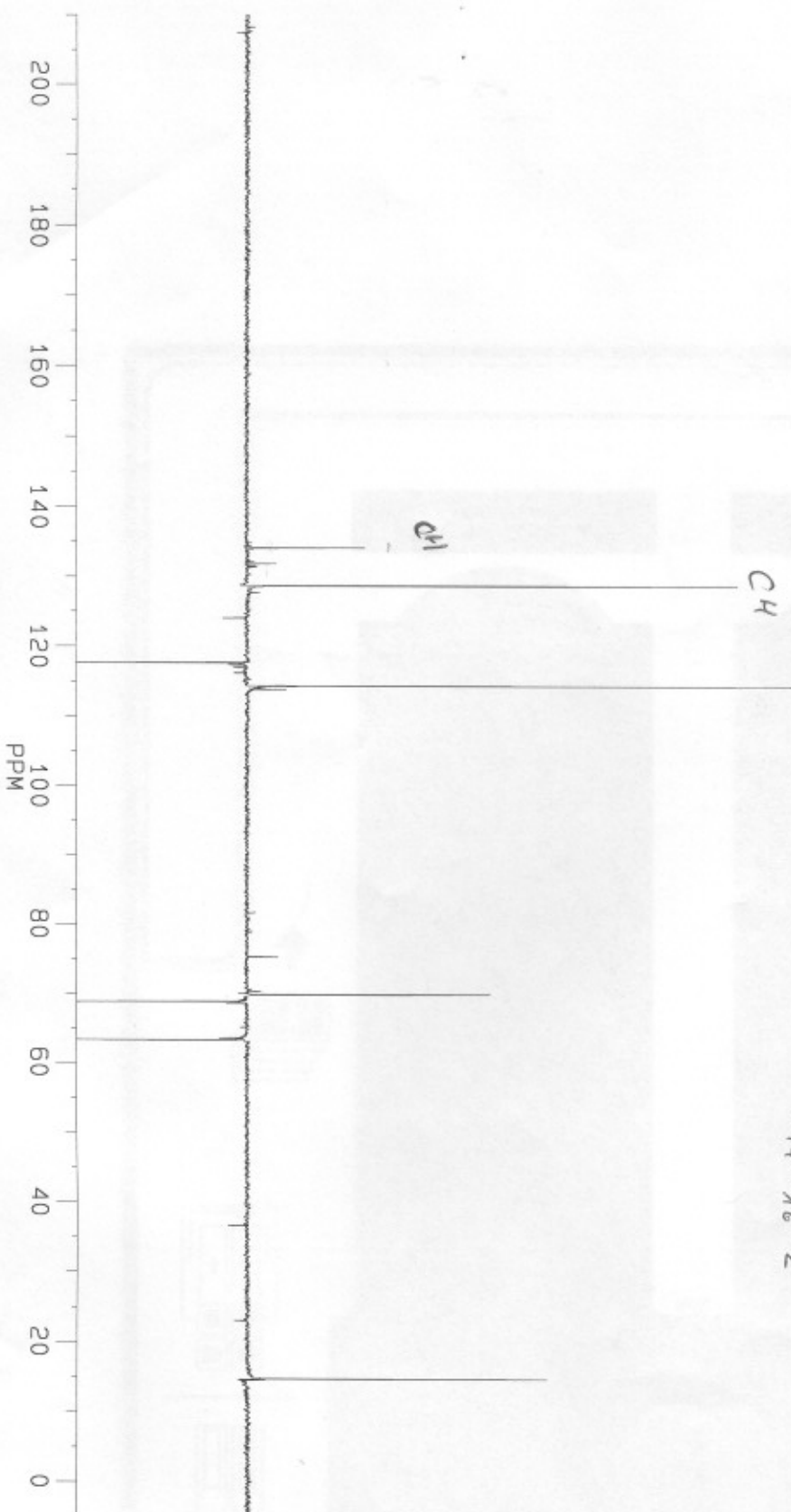
DE172S.107
AU PROG:
X09.AU
DATE 17-12-2

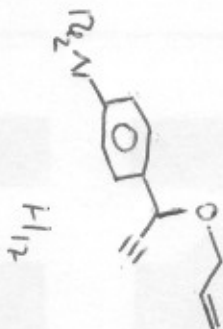
SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 200
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 8.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89





ppm

-7.29076
-7.25562

-6.62806
 -6.59271

-5.24264
-5.03302
-5.02433

-4.00122
 -3.99590
 -3.99040

-2.84688
-2.51334
-2.50456

Current Data Parameters	
NAME	DS_B3
EXPNO	10
PROCNO	1

```

F2 - Acquisition Parameters
Date_ 20030116

```

INSTAUM
PADBD
PULPADG
TD
SOLVENT

COC13

SMH	2762.431 HZ
FIDRES	0.084303 HZ
AQ	5.9310579 sec

DM	181.000 usec
DE	258.57 usec
TE	300.0 K
D1	2.00000000 sec
P1	8.50 usec
SFO1	250.1340034 MHz
NUCLEUS	¹ H

F2 - Processing Parameters	
SI	32768
SF	250.1328830 MHz
MDM	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

10 NMR plot parameters	
CX	22.00 cm
F1P	10.096 ppm
F1	2525.29 Hz
F2P	-0.948 ppm
F2	-237.14 Hz
PPMCM	0.50199 ppm/cm
HZCM	125.56506 Hz/cm

DS-83 IN CDCL₃ AK PROF MUELLER

PPM

150.718

134.423

128.496

125.751

117.417

112.216

82.183

77.423

77.202

77.000

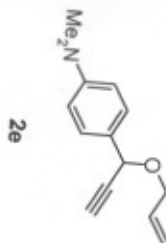
76.576

74.851

70.163

68.655

40.465

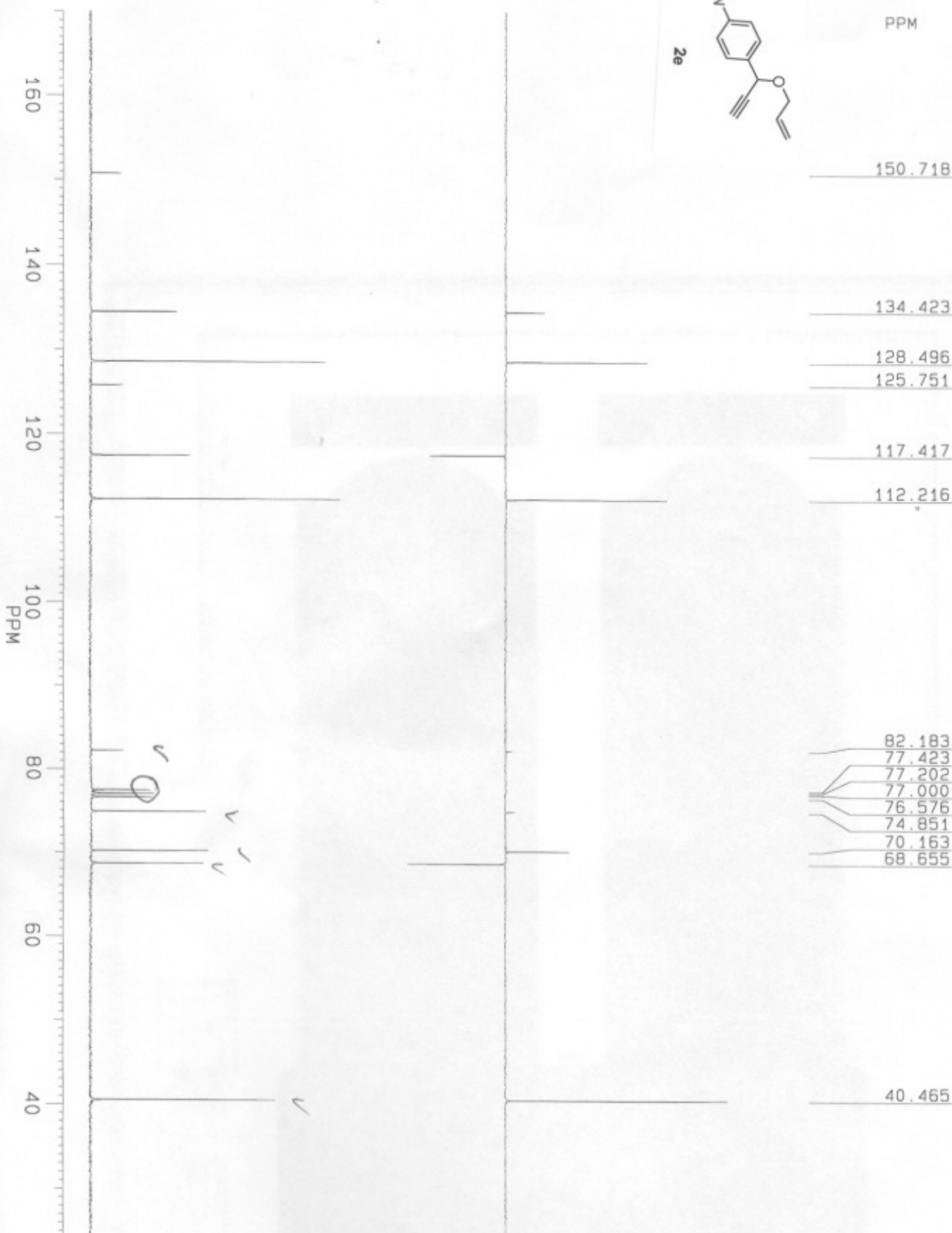
JA17.001 / 442
DATE 17-1-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 2.5
RD 1.000
AQ 1.769
RG 320
NS 720
TE 297

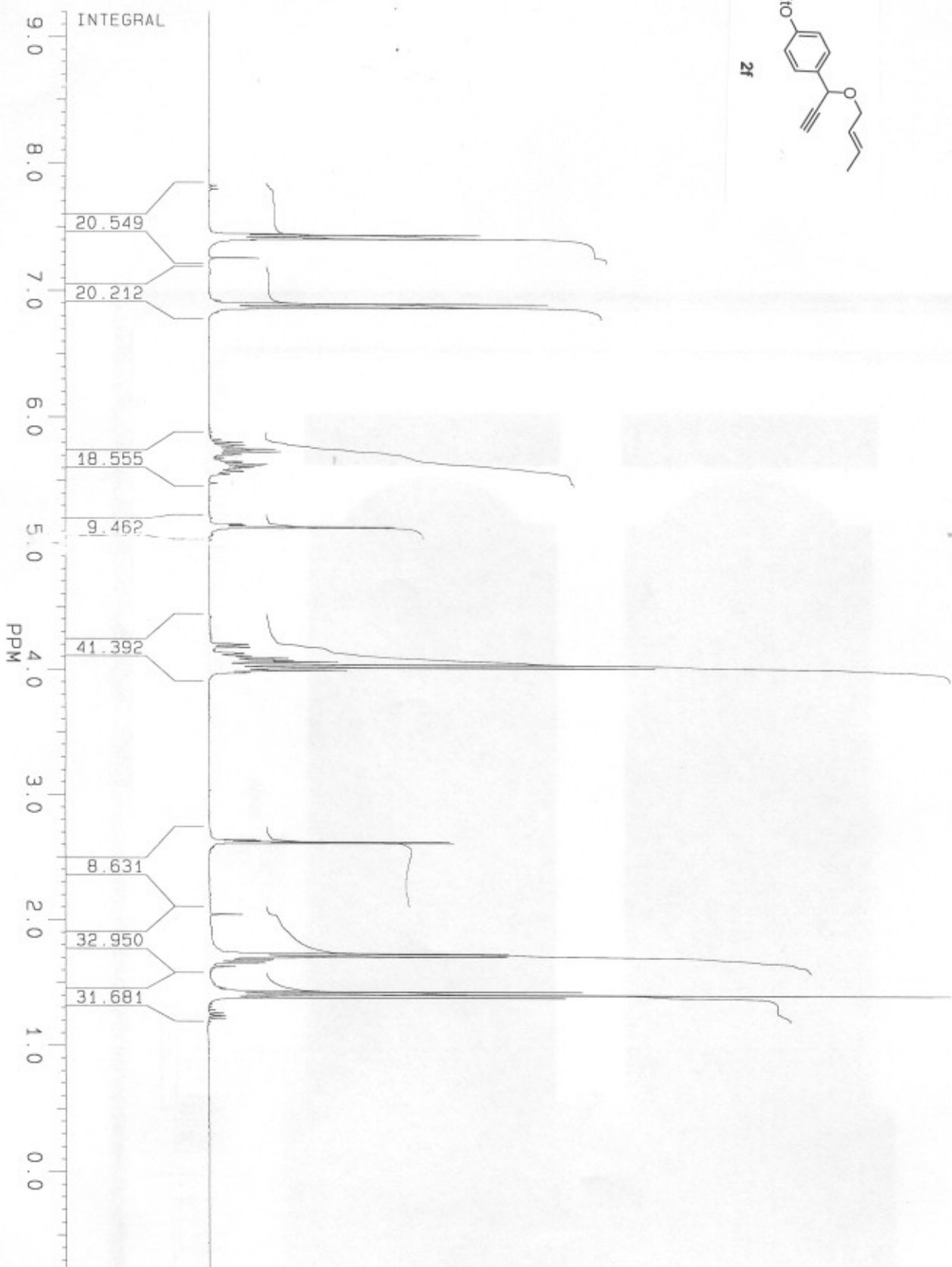
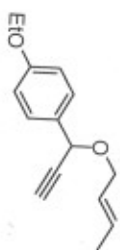
FW 23200
O2 4588.000
DP 18H CPD

LB 1.000
GB 0.0
CX 22.00
CY 4.50
F1 169.999P
F2 24.244P
HZ/CM 499.995
PPM/CM 6.625
SR -1399.94



67512

DS-89 IN CDCL3 D"SOUZA



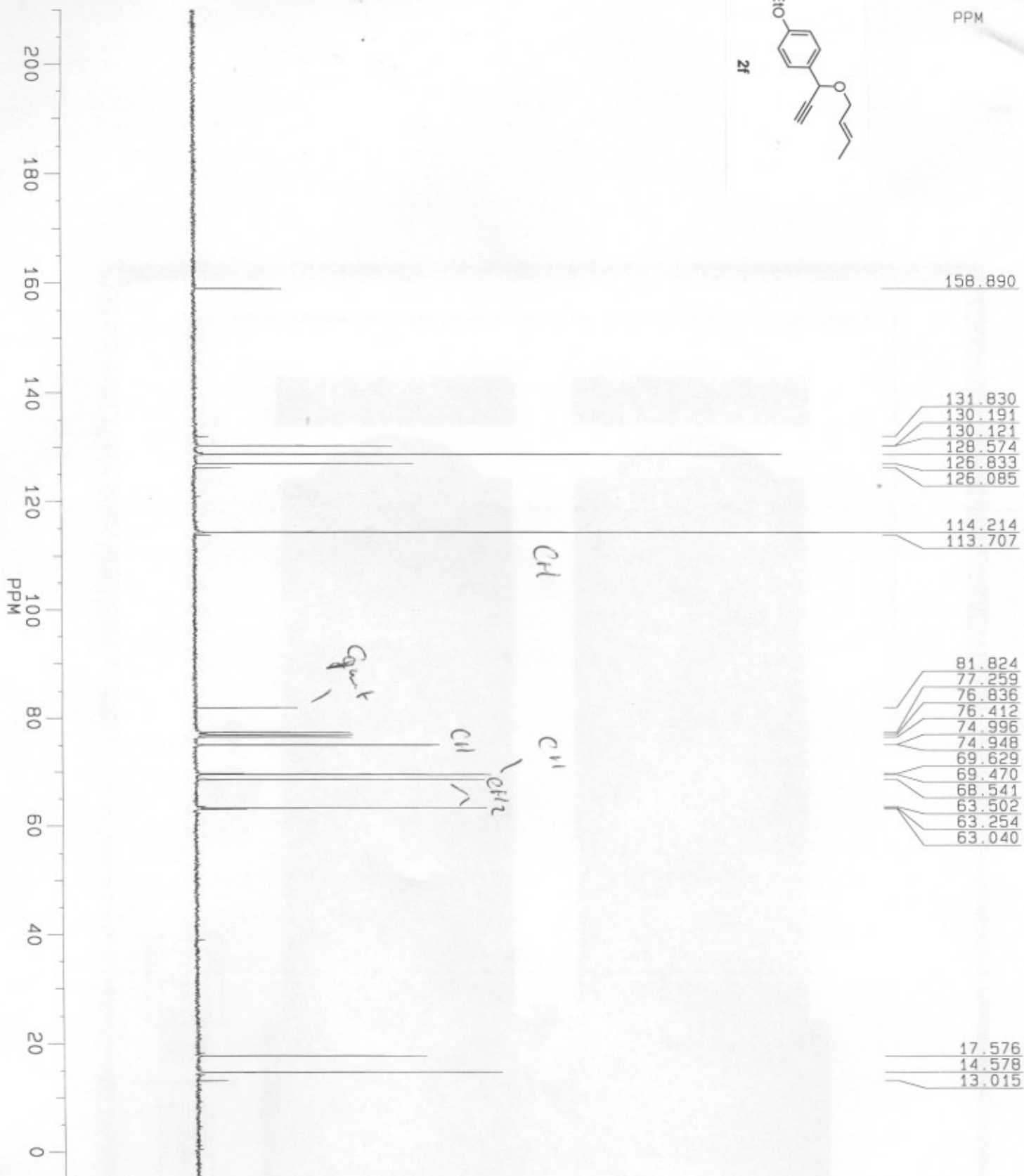
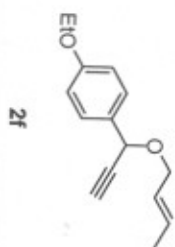
JJA240S.112
AU PROG:
X00.AU
DATE 25-1-3

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PM 0.0
RD 0.0
AQ 2.720
RG 4
NS 16
TE 297

FW 7600
O2 3200.000
DP 63L PD

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 -.800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88



JA2415.112
AU PROG:
X02. AU
DATE 25-1-3

SF	75.469
SY	75.0
O1	6141.605
SI	65536
TD	65536
SW	18518
HZ/PT	.519
	.565

PW	0.0
RD	0.0
AG	1.769
RG	320
NS	800
TE	297

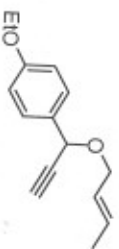
FW	23200
O2	4588.000
DP	18H DO

LB	1.000
GB	0.0
CX	22.00
CY	13.00
F1	210.005P
F2	-4.995P
HZ/CM	737.534
PPM/CM	9.773
SR	-1388.89

DS-89 IN CDCL3 D"SOUZA

37872

PPM



130.209
128.593
126.801
126.051

114.198
113.696

81.803
74.985
69.614
69.456
68.562
63.248
63.037

17.619
14.595
13.046



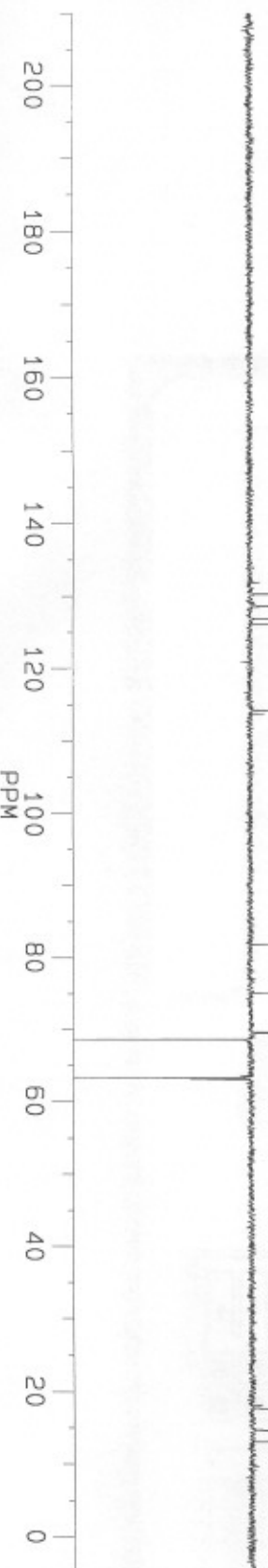
JN2425.112
AU PROG:
X09. AU
DATE 25-1-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 400
TE 297

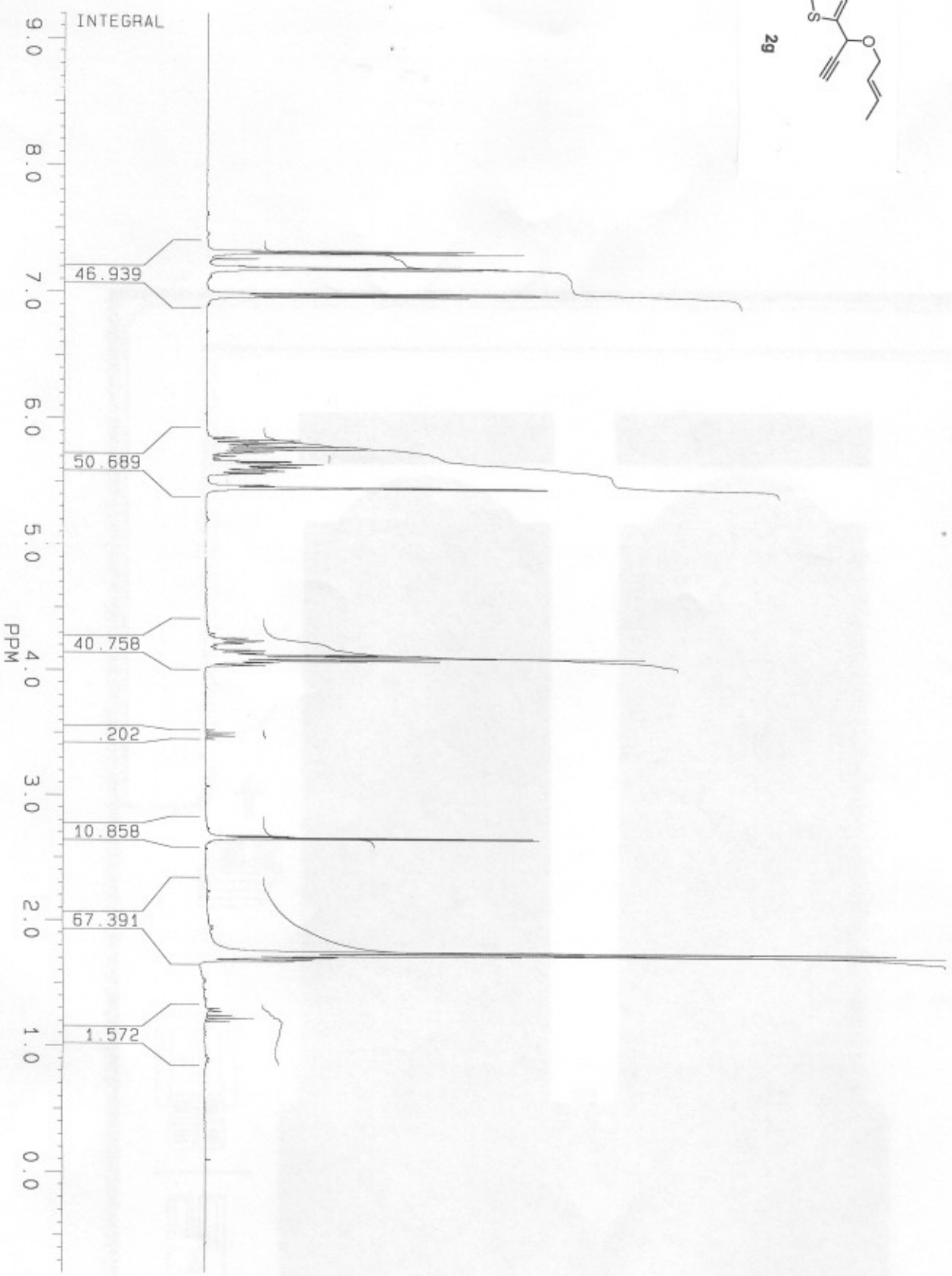
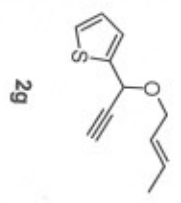
FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 8.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89



37703

DS-69 IN CDCL3 D"SOUZA



DE1705.103
 AU PROG:
 X00.AU
 DATE 17-12-2

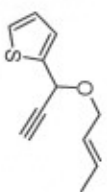
B
 H
 N
 R

SF 300.133
 SY 210.0
 O1 5173.724
 SI 32768
 TD 32768
 SW 6024.096
 HZ/PT .368

PM 0.0
 RD 0.0
 A0 2.720
 RG 4
 NS 16
 TE 297

FW 7600
 O2 3200.000
 DP 63L P0

LB .100
 GB 0.0
 CX 22.00
 CY 13.00
 F1 9.200P
 F2 -800P
 HZ/CM 136.427
 PPM/CM .455
 SR 3369.88



29

PPM

141.721

130.531
129.063
126.669
126.387
126.281
126.230
126.168
125.876

80.961
77.426
77.001
76.577
74.935

68.456
65.534
65.345
62.965

17.693

13.140

DS-69 IN CDCL3 D" SOUZA



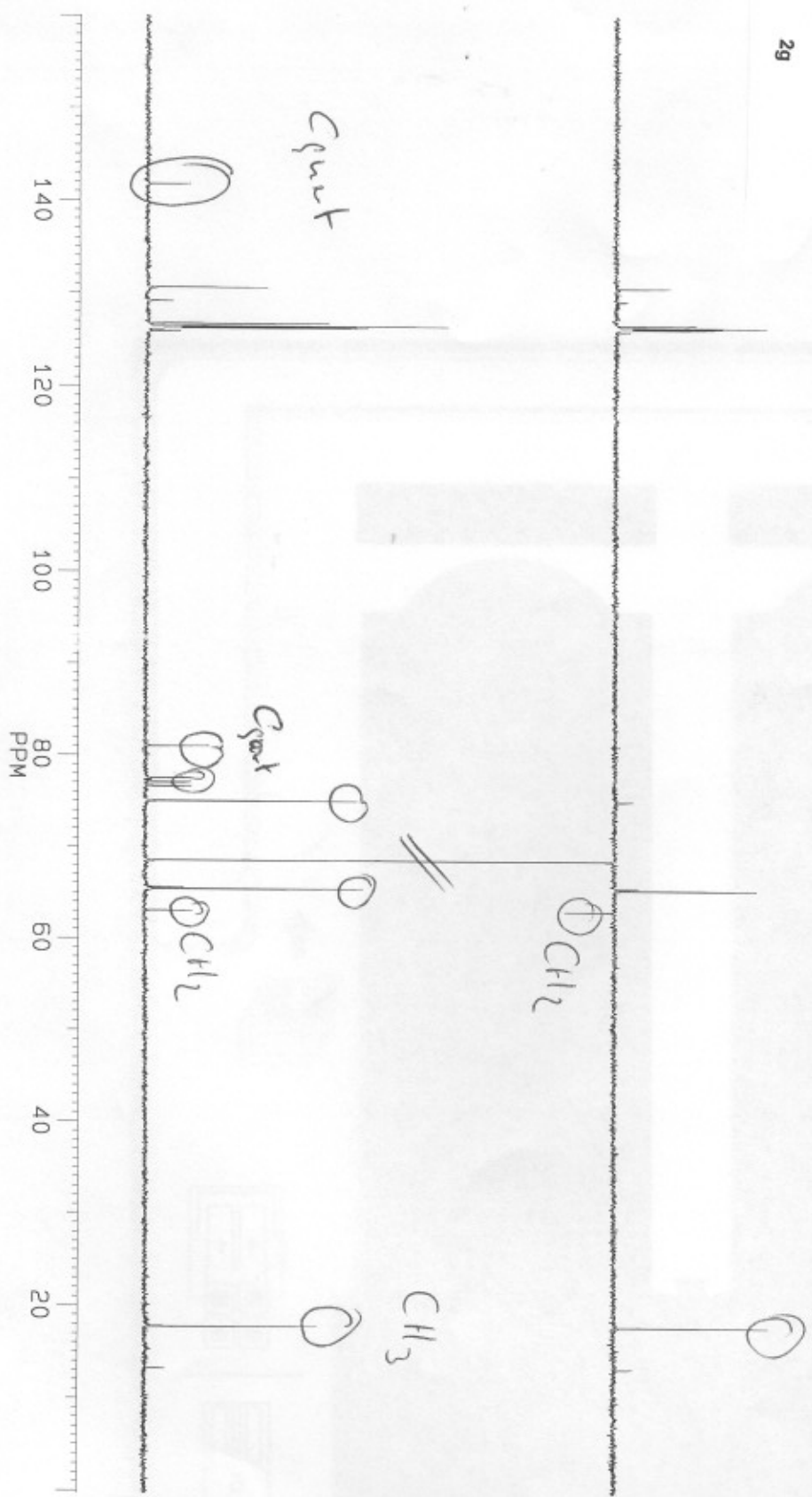
DE17.002 / 03
AU PRD:
X02. AU
DATE 17-12-2

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PM 0.0
RD 0.0
AQ 1.769
RG 320
NS 128
TE 297

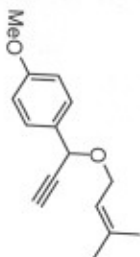
FW 23200
O2 4588.000
DP 18H CPD

LB 1.000
GB 0.0
CX 22.00
CY 4.50
F1 160.002P
F2 -325P
HZ/CM 549.984
PPM/CM 7.288
SR -1398.81

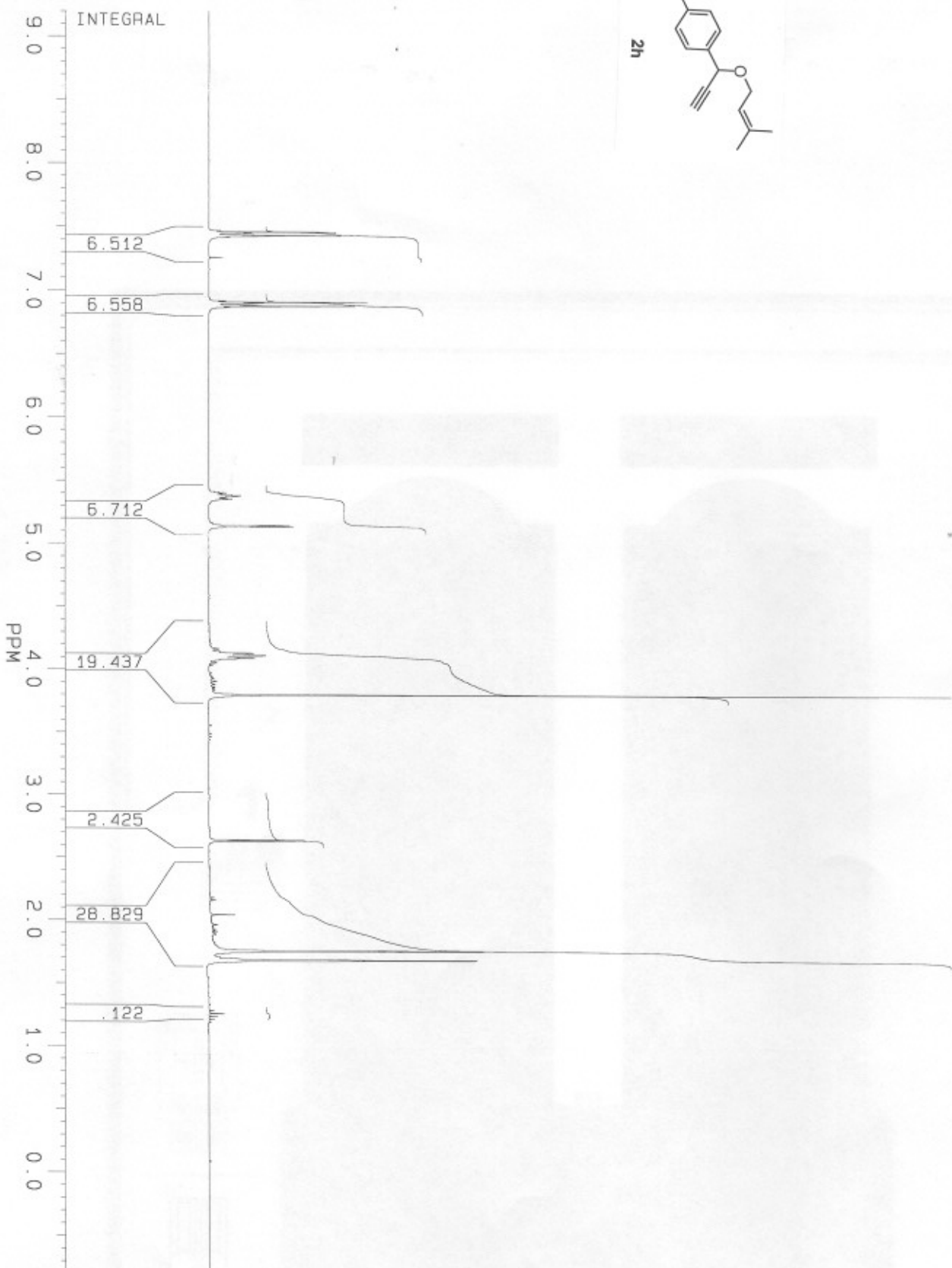


87700

DS-72 IN CDCL3 D"SOUZA



2h



DE170S.111
AU PROG:
X00.AU
DATE 18-12-2

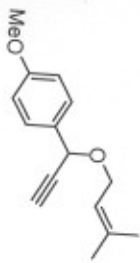
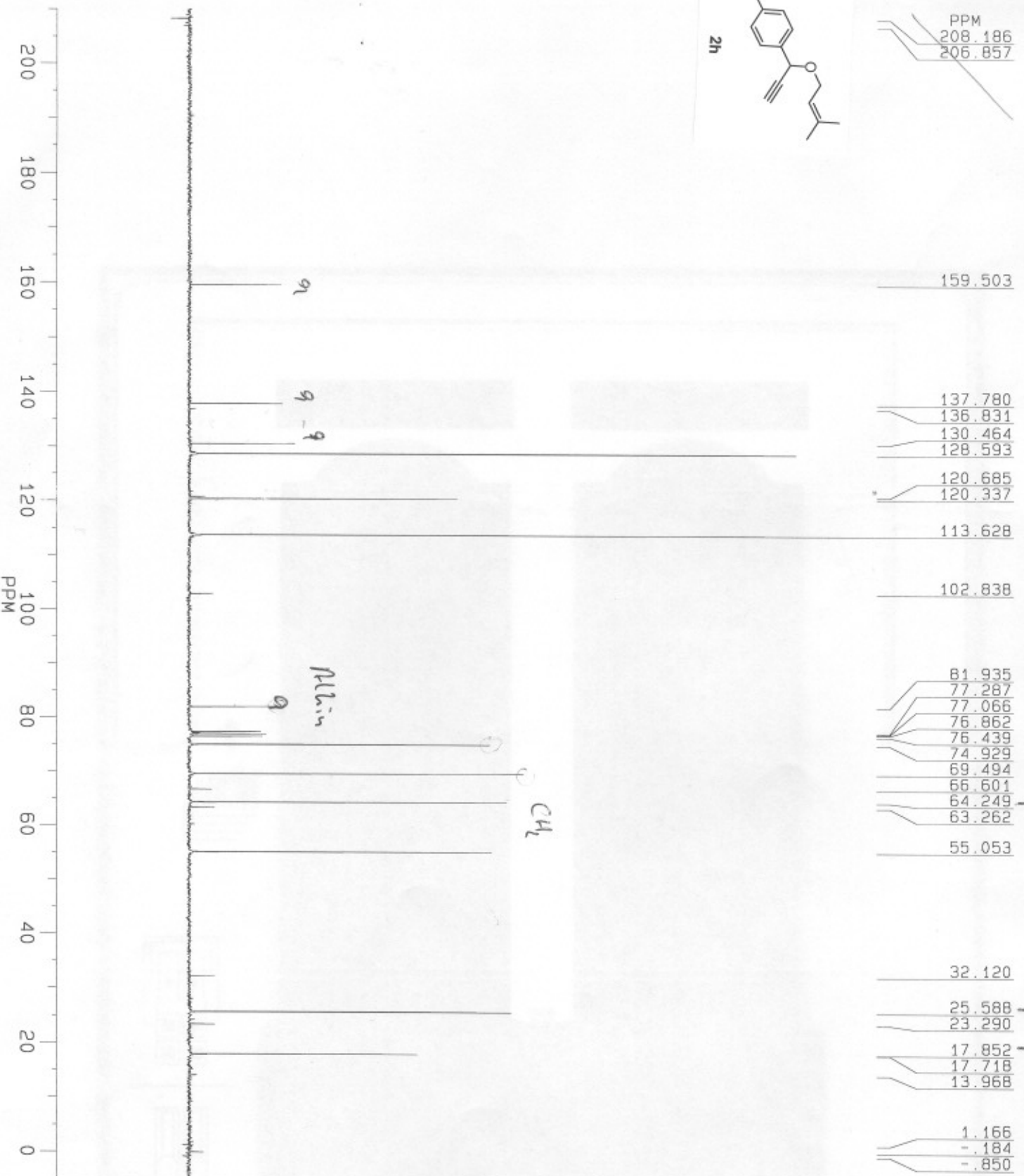
SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PW 0.0
RD 0.0
AQ 2.720
RG 2
NS 16
TE 297

FW 7600
O2 3200.000
DP 63L P0

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 .800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88

DS-72 IN CDCL3 D"SOUZA


 PPM
 208.186
 206.857

 DE171S.111
 AU PROG:
 X02.AU
 DATE 18-12-2

 SF 75.469
 SY 75.0
 O1 6141.605
 SI 65536
 TD 65536
 SW 18518.519
 HZ/PT .565

 PW 0.0
 RD 0.0
 AQ 1.769
 RG 320
 NS 560
 TE 297

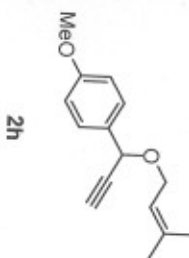
 FW 23200
 O2 4588.000
 DP 18H D0

 LB 1.000
 GB 0.0
 CX 22.00
 CY 13.00
 F1 210.005P
 F2 -4.995P
 HZ/CM 737.534
 PPM/CM 9.773
 SR -1388.89

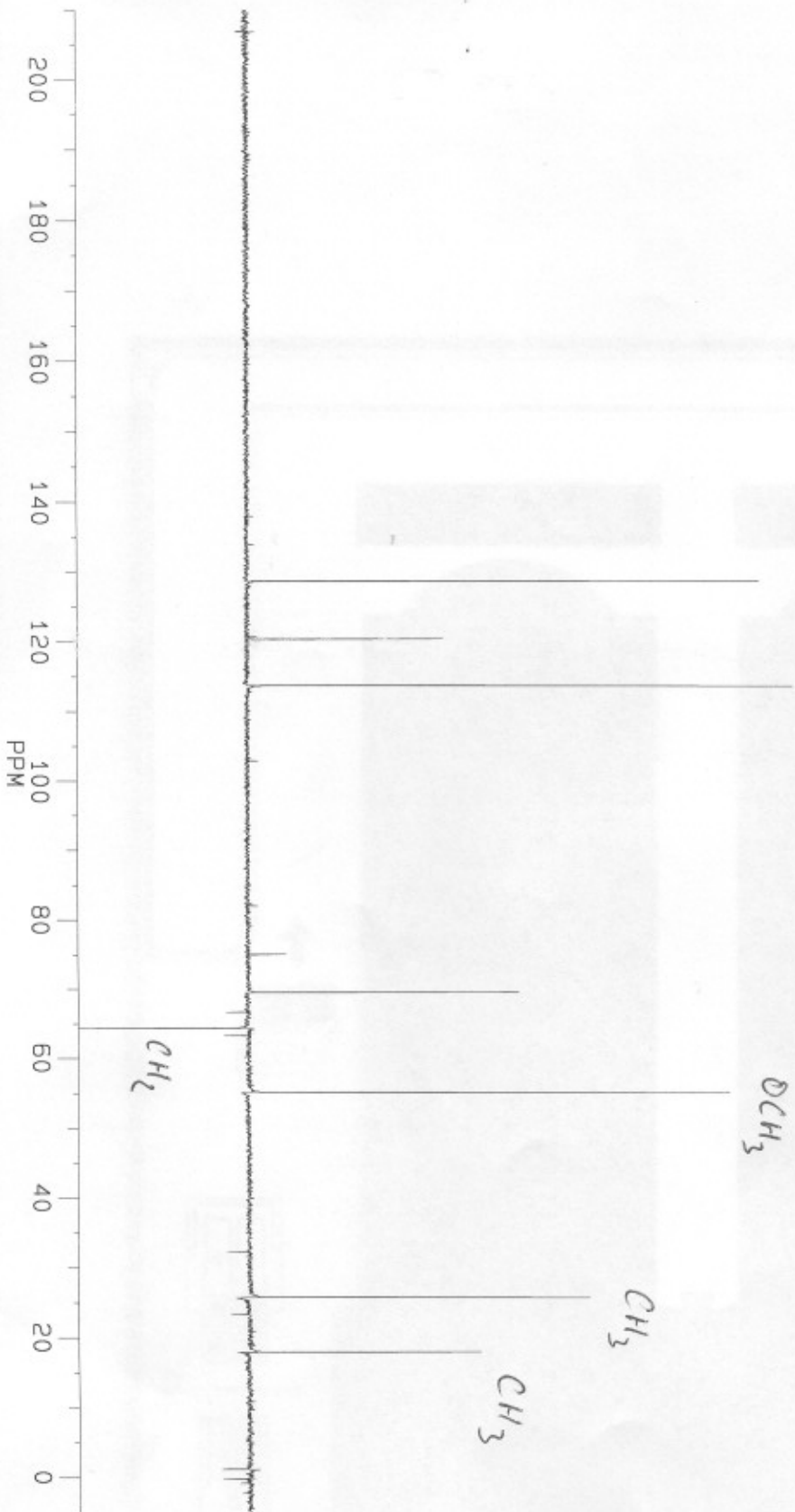
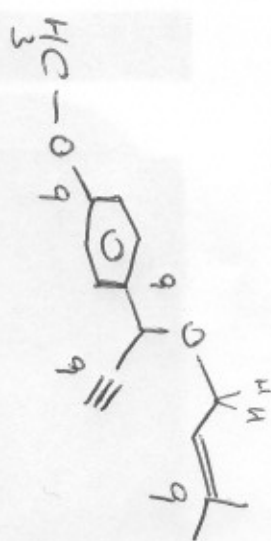
DS-72 IN CDCL3 D" SOUZA

32200

PPM
206.877



128.613
120.638
120.302
113.621
102.840
81.915
74.966
69.486
66.619
64.249
63.264
55.062
32.126
25.625
25.573
23.292
17.875
1.160
-.187
-.831



DE1725.111
AU PROG:
X09.AU
DATE 18-12-2

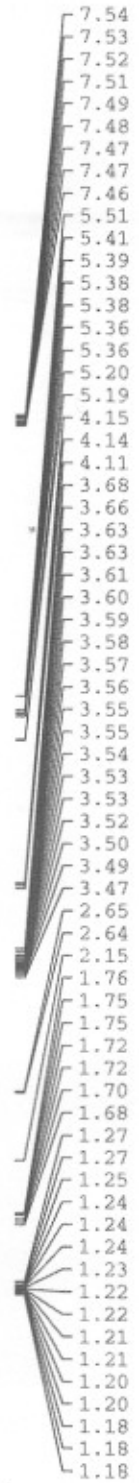
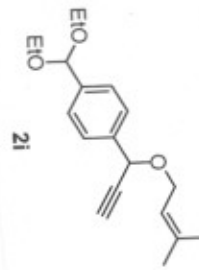
SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 320
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 8.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89

DS-642 MU in CDCL3 D'Souza



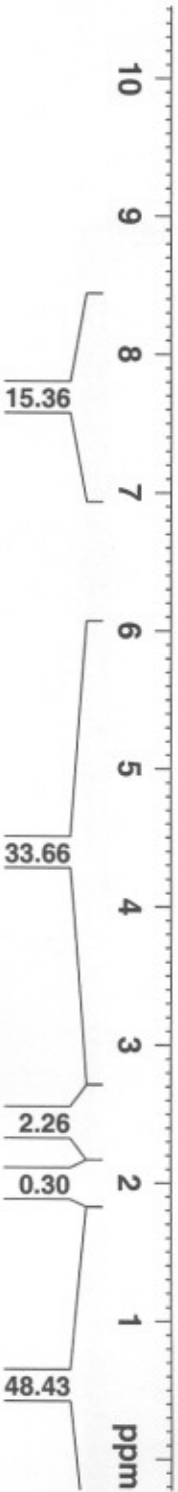
Current Data Parameters
NAME mudsau07
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

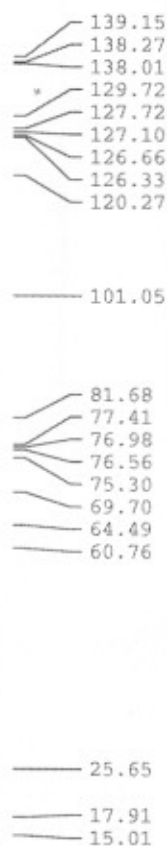
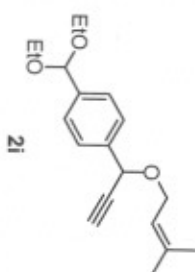
Date_ 20060807
Time 15.02
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 35.9
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DS-642 MU in CDCL3 D"Souza



Current Data Parameters
 NAME mudsau07
 EXPNO 2
 PROCNO 1

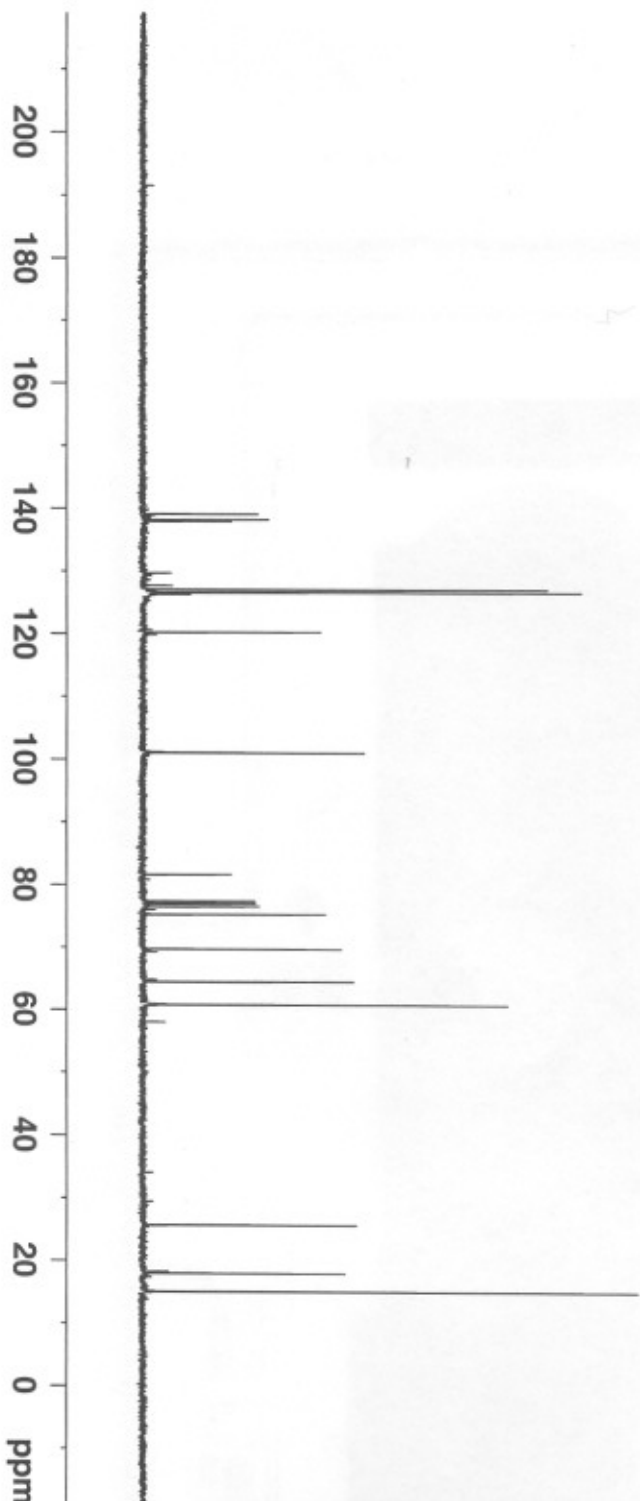
F2 - Acquisition Parameters
 Date_ 20060807
 Time 15.05

INSTRUM spect
 PROBD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 176
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 18390.4
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

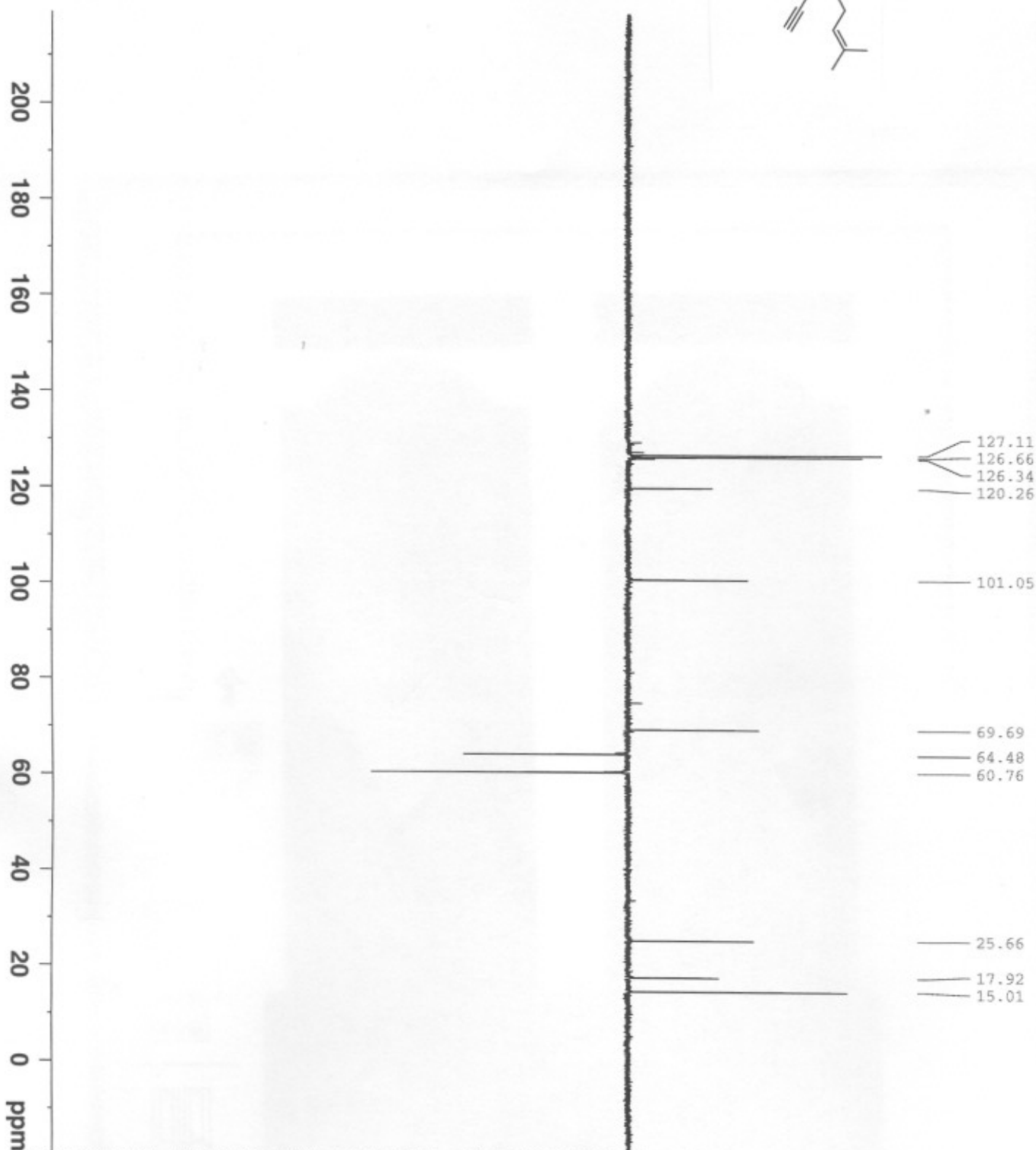
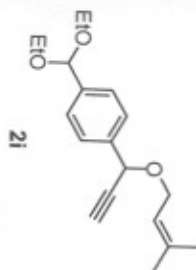
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.00 usec
 PL1 1.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.20 dB
 PL12 16.22 dB
 PL13 17.00 dB
 SFO2 300.1312005 MHz

F2 - Processing Parameters
 SI 32768
 SF 75.4677601 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 6.00



DS-642 MU in CDCL3 D'Souza



Current Data Parameters
NAME mudsau07
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060807
Time 14.58

INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 48

DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DM 27.800 usec
DE 6.00 usec
TE 300.0 K

CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.0002000 sec
DELTA 0.0001528 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing Parameters
SI 32768
SF 75.4677601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 5.00

40466

DS-199 IN CDCL3 D'SOUZA



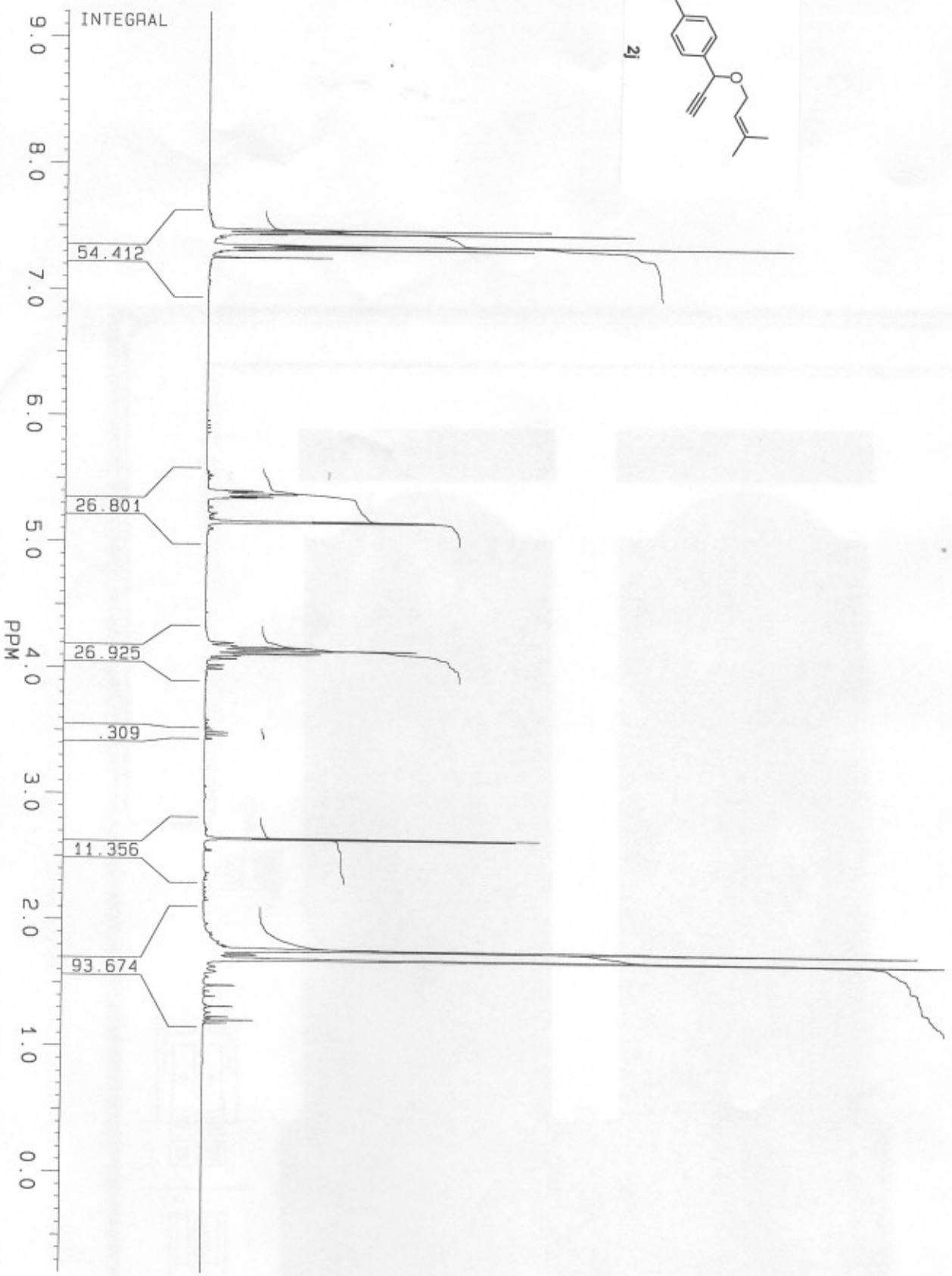
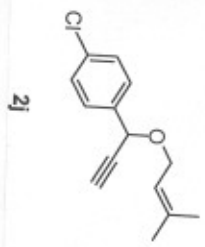
AP1605.103
AU PROG:
X00.AU
DATE 16-4-4

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PW 0.0
RD 0.0
AQ 2.720
RG 4
NS 16
TE 297

FW 7600
O2 3200.000
DP 63L P0

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 -.800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88



DS-1914 IN CDCL3 D'SOUZA

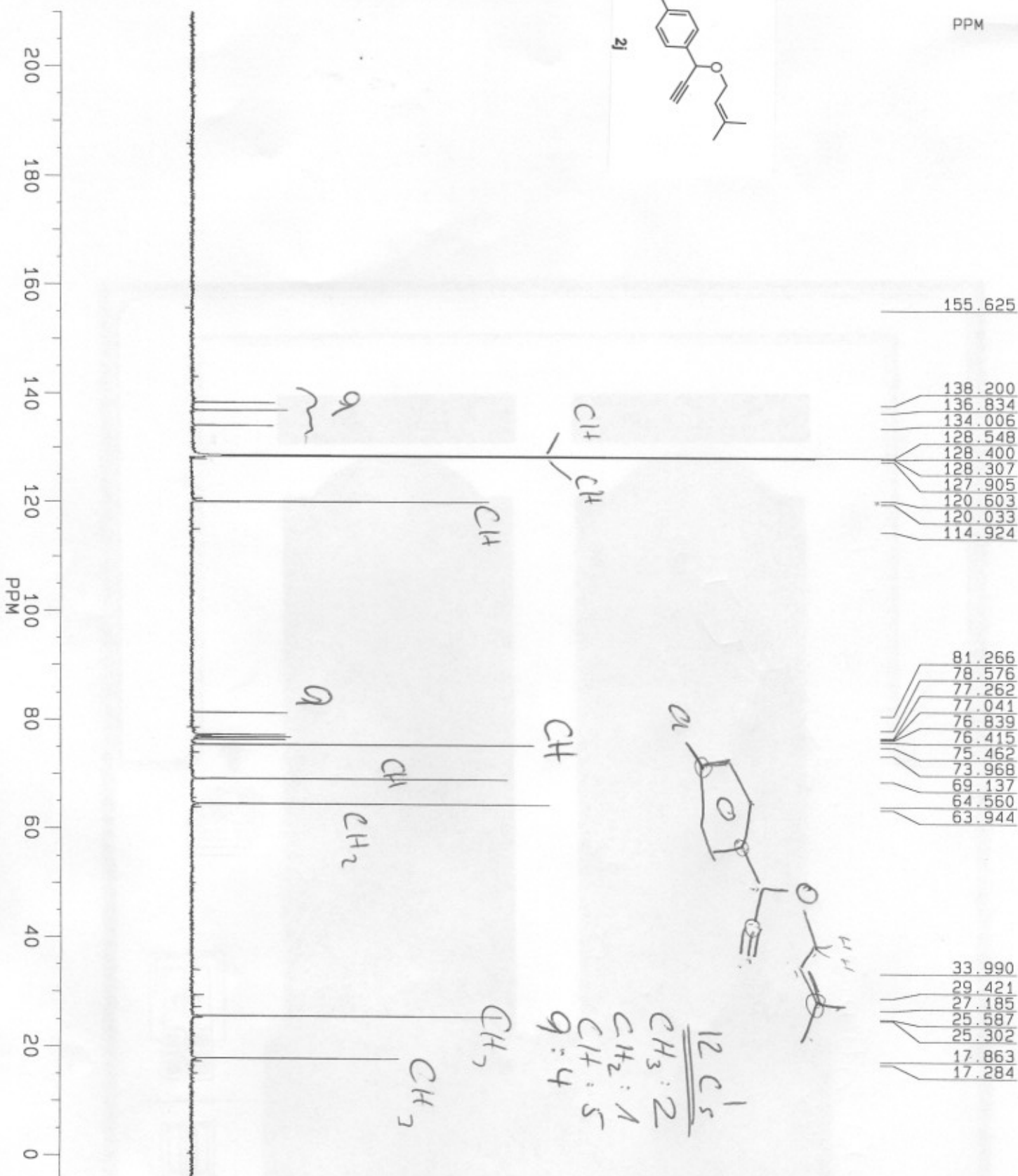
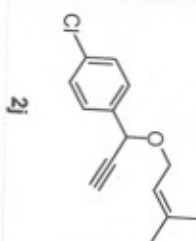
PPM

155.625

138.200
136.834
134.006
128.548
128.400
128.307
127.905
120.603
120.033
114.924

81.266
78.576
77.262
77.041
76.839
76.415
75.462
73.968
69.137
64.560
63.944

33.990
29.421
27.185
25.587
25.302
17.863
17.284

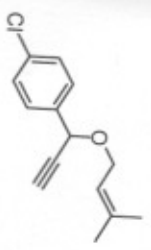


AP161S.103
AU PROG:
X02.AU
DATE 16-4-4

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PM 0.0
RD 0.0
AQ 1.769
RG 400
NS 800
TE 297

FW 23200
O2 4588.000
DP 18H D0
LB 1.000
GB 0.0
CX 22.00
CY 13.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89



PPM

DS-190 IN CDCL3 D'SOUZA

128.729
128.575
120.163

75.661
69.288
64.719

25.783
18.047



AP1625.103
AU PROG:
X09.AU
DATE 16-4-4

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 400
NS 320
TE 297

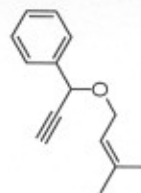
FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 5.00
F1 210.002P
F2 -4.998P
HZ/CM 737.534
PPM/CM 9.773
SR -1401.07

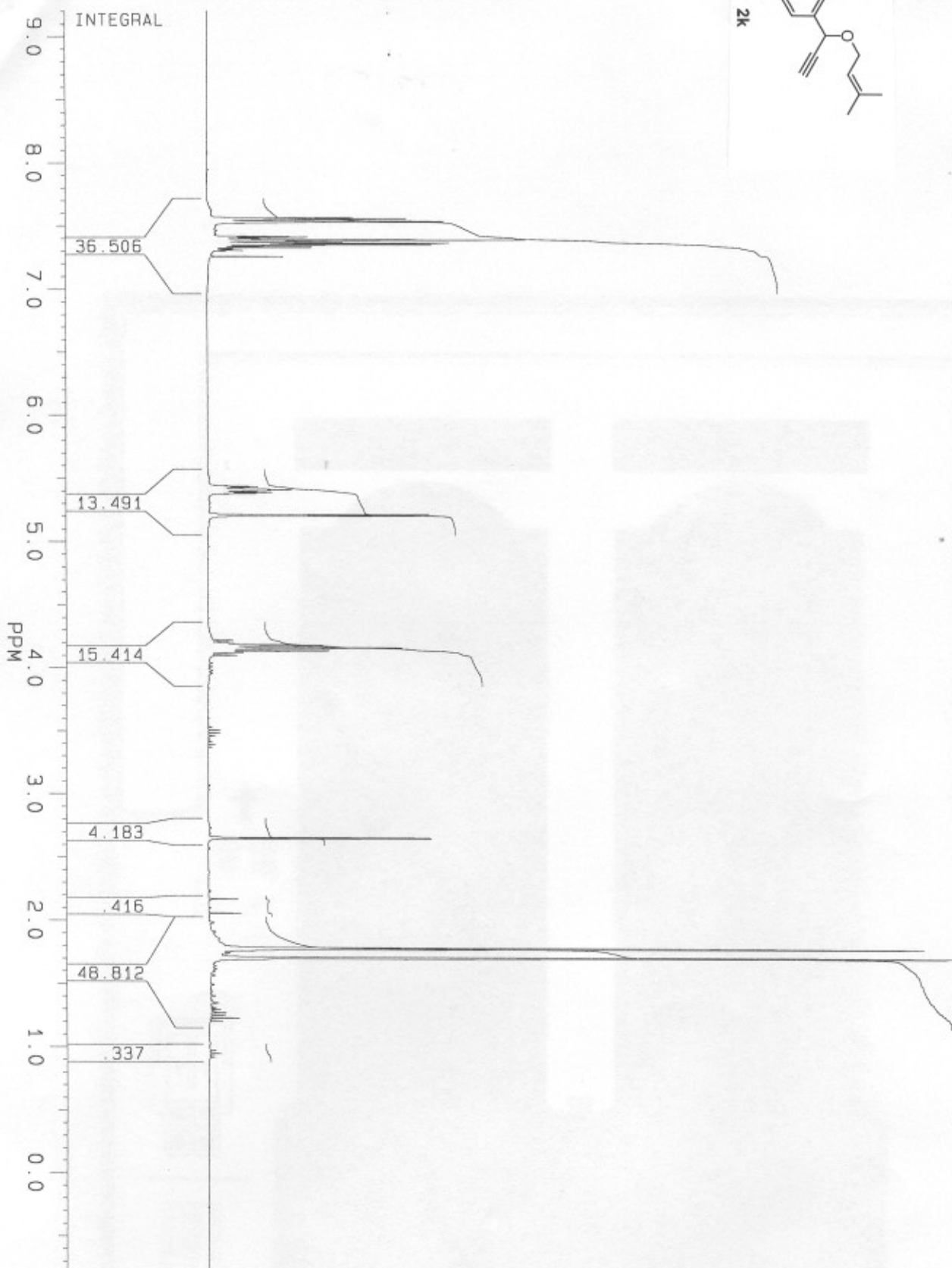


30726

DS-221 IN CDCL3 D'SOUZA



2k



DE0805.106
AU PROG:
X00.AU
DATE 9-12-3

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PW 0.0
RD 0.0
AQ 2.720
RG 2
NS 16
TE 297

FW 7500
O2 3200.000
DP 63L P0

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 .800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88

$$\begin{array}{l} 39 \\ 1 \text{ CH}_2 \end{array}$$
$$2 \text{ CH}_3$$

	81.732
	77.304
	77.079
	76.877
	76.453
	75.170
	69.912
	64.474

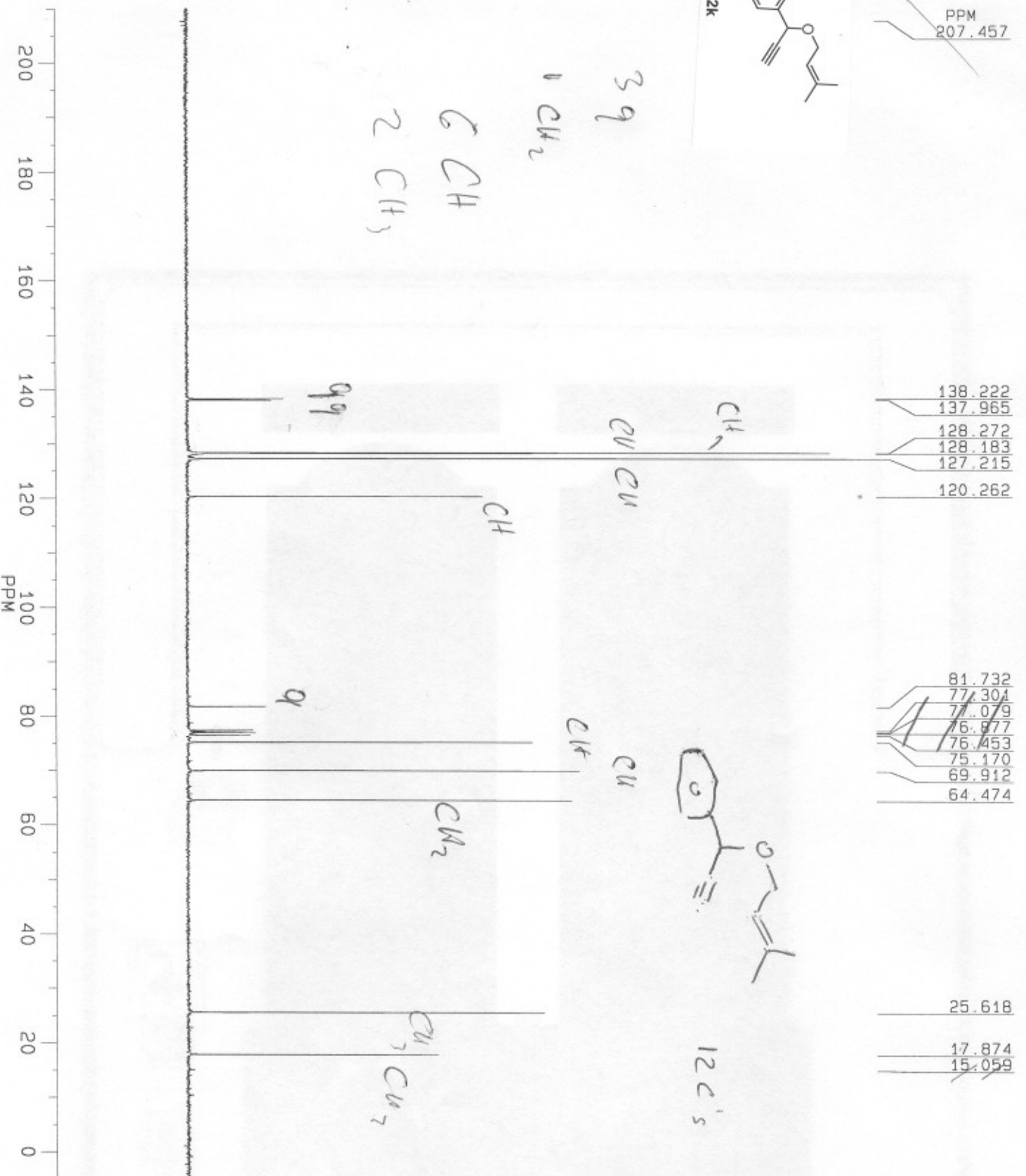
$$\begin{array}{r} 17.874 \\ 15.059 \\ \hline \end{array}$$
CC(=O)C(C)C1=CC=CC=C1

12c's

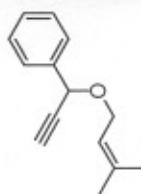


SF	75.469
SY	75.0
O1	6141.605
SI	65536
TD	65536
SW	18518
HZ/PT	.519
	.565

PM	0.0
RD	0.0
AQ	1.769
RG	320
NS	600
TE	297
FW	23200
O2	4588.000
DP	18H D0
LB	1.000
G8	0.0
CX	22.00
CY	13.00
F1	210.005P
F2	-4.995P
HZ/CM	737.534
PPM/CM	9.773
SR	-1388.89



PPM
206.791



2k

138.042

128.293

128.210

127.230

120.227

81.711

78.746

75.207

69.903

64.472

25.653

17.896



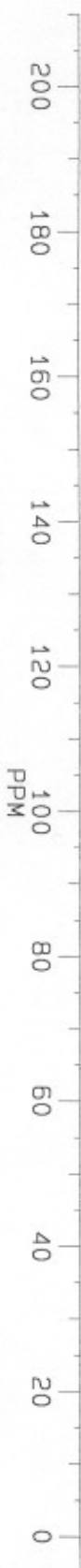
DE0825.106
AU PROG:
X09.AU
DATE 9-12-3

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PW 0.0
RD 0.0
AQ 1.769
RG 320
NS 400
TE 297

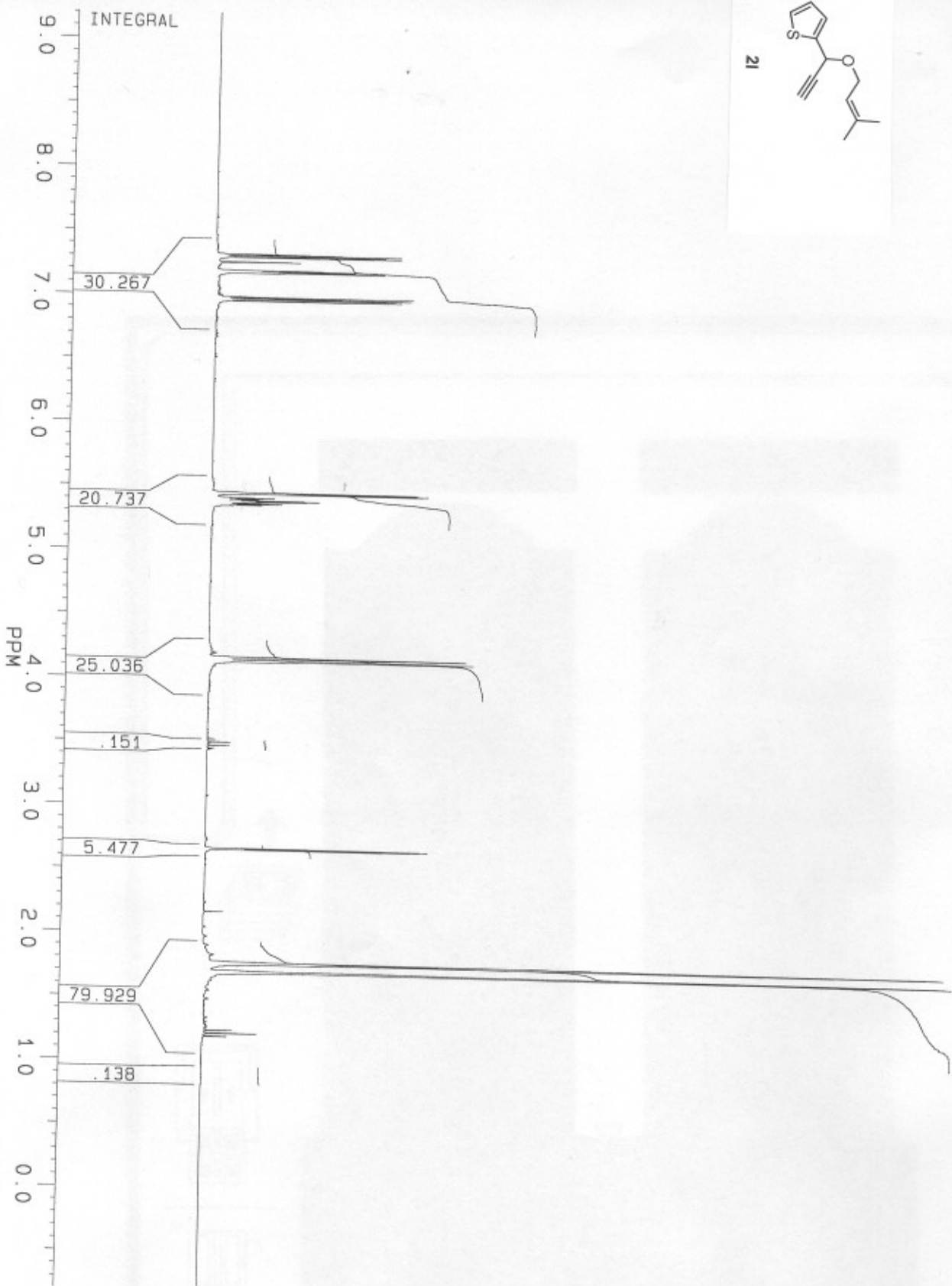
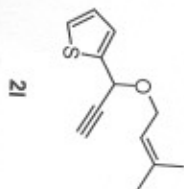
FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 8.00
F1 210.005P
F2 -4.995P
HZ/CM 737.534
PPM/CM 9.773
SR -1388.89



40528

DS-236 IN CDCL3 D'SOUZA



AP1905.119
AU PROG:
X00.AU
DATE 20-4-4

SF 300.133
SY 210.0
O1 5173.724
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PW 0.0
RD 0.0
AQ 2.720
RG 4
NS 16
TE 297

FW 7600
O2 3200.000
DP 63L P0

LB .100
GB 0.0
CX 22.00
CY 13.00
F1 9.200P
F2 .800P
HZ/CM 136.427
PPM/CM .455
SR 3369.88

DS-236 IN CDCL3 D"SOUZA

PPM

141.849
138.401

126.392
126.307
126.177

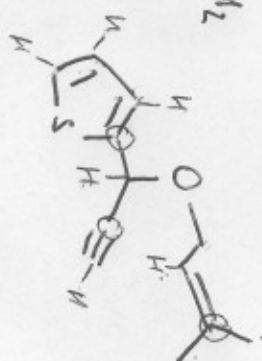
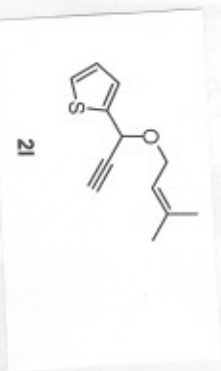
120.131

81.104
78.781
77.420
77.203
76.996
76.573
74.851

65.373
64.164

25.750

18.016



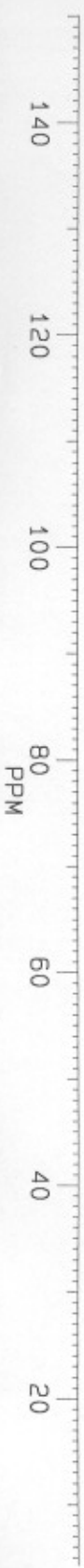
AP191S.119
AU PROG:
X02. AU
DATE 20-4-4

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

PM 0.0
RD 0.0
AQ 1.769
RG 400
NS 400
TE 297

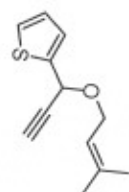
FW 23200
O2 4588.000
DP 18H DO

LB 1.000
GB 0.0
CX 22.00
CY 0.0
F1 150.005P
F2 4.250P
HZ/CM 499.995
PPM/CM 6.625
SR -1399.94



DS-236 IN CDCL3 D'SOUZA

21



PPM

134.019

126.408

126.343

126.217

120.097

74.888

65.356

64.158

25.785

18.038



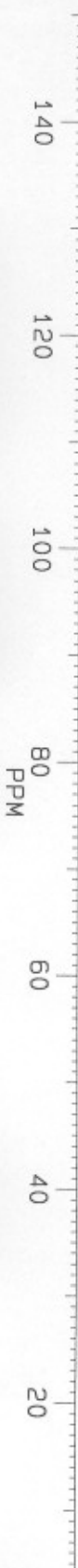
AP192S.119
AU PROG:
X09.AU
DATE 20-4-4

SF 75.469
SY 75.0
O1 6141.605
SI 65536
TD 65536
SW 18518.519
HZ/PT .565

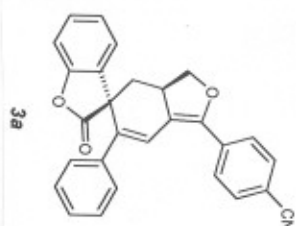
PW 0.0
RD 0.0
AQ 1.769
RG 400
NS 200
TE 297

FW 23200
O2 4588.000
DP 18H D0

LB 1.000
GB 0.0
CX 22.00
CY 5.00
F1 150.005P
F2 4.250P
HZ/CM 499.995
PPM/CM 6.625
SR -1399.94



D'Souza DS-92 in CDCl₃



Current Data Parameters
NAME: mds05re
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030205
Time: 7.39

INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zg30
TD: 32768
SOLVENT: CDCl₃

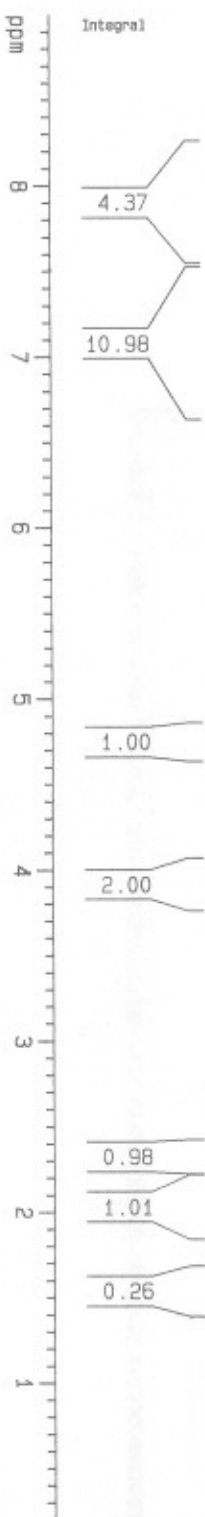
NS: 16
DS: 4
SWH: 5482.456 Hz
FIDRES: 0.167314 Hz
AQ: 2.9884915 sec

RG: 128
DM: 91.200 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.10 usec
PL1: 0.00 dB
SFO1: 500.1322738 MHz

F2 - Processing parameters
SI: 16384
SF: 500.1300232 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 13.00 cm
FAP: 9.000 ppm
F1: 4501.17 Hz
F2P: 0.200 ppm
F2: 100.03 Hz
PPHCK: 0.44000 ppm/cm
HZCH: 220.05722 Hz/cm



ppm

177.782

152.422
149.849
139.721
135.241
134.779
132.324
132.307
129.540
128.619
127.915
127.505
126.583
124.679
124.565
122.553
118.561
113.730
112.053
111.394

6
D'Souza
DS-9211h
CDCl₃

77.261
77.007
76.753
74.595

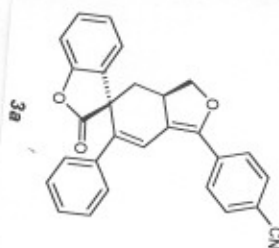
CH₂

53.280

q

38.596
38.331

CH₂
-CH



180
160
140
120
100
80
60
40

q
-CH

CH₂

q

CH₂

-CH

Current Data Parameters
NAME: macofcra
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030205
Time: 7.58

INSTRUM: spect
PROBHD: 5 mm TBC 1H/13
PULPROG: zgpg30
TO: 65536
SOLVENT: CDCl₃
NS: 2400
DS: 2
SWH: 30564.187 Hz
FIDRES: 0.479550 Hz
AQ: 1.0617332 sec
RG: 5732.6
DM: 18.200 usec
DE: 6.00 usec
TE: 300.2 K
D1: 1.00000000 sec
d11: 0.03000000 sec
d12: 0.00020000 sec

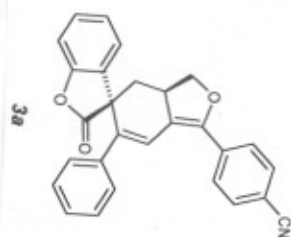
===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
SFO1: 125.7713172 MHz

===== CHANNEL f2 =====
CPROG2: waltz16
NUC2: 1H
PC2P2: 100.00 usec
PL2: 0.00 dB
PL12: 25.00 dB
PL13: 25.00 dB
SFO2: 500.1325000 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577556 MHz
KON: EN
SBB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

10 NMR plot parameters
CX: 20.00 cm
CY: 12.00 cm
FAP: 185.000 ppm
F1: 24522.77 Hz
F2: 20.000 ppm
F3: 2015.16 Hz
PRCH: 875000 ppm/cm
HCH: 5100.38086 Hz/cm

D'Souza DS-92 in CDCl3



ppm

132.3
129.5
128.6
127.9
127.5
126.6
124.7
124.5
122.5
111.4

74.6

38.6
38.3

ppm 180 160 140 120 100 80 60 40

Current Data Parameters
NAME: DS-92
EXPNO: 3
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030205
Time: 9.20
INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 400
DS: 2
SWH: 30064.197 Hz
FIDRES: 0.470000 Hz
AQ: 1.0617182 sec
RG: 11500.0
DM: 16.330 uSAC
DE: 0.00 uSAC
TE: 300.2 K
CHRG2: 1.45, 0.000000 sec
D1: 4.0000000 sec
D2: 0.00344628 sec
D12: 0.0000000 sec
DELTA: 0.0001354 sec

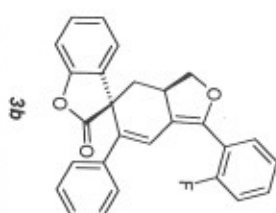
CHANNEL f1
NUC1: 13C
P1: 10.40 uSAC
PL1: 20.00 uSAC
PL1: 0.00 dB
SFO1: 125.7713172 MHz

CHANNEL f2
CPDPRG2: waltz16
NUC2: 1H
P2: 10.10 uSAC
P3: 20.20 uSAC
P4: 100.00 uSAC
P5: 0.00 dB
P6: 20.00 dB
SFO2: 500.1362900 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577882 MHz
RG: 0
KHM: 0
SSB: 0
LB: 1.00 Hz
BB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
F1P: 198.000 ppm
F1: 24522.77 Hz
F2P: 20.000 ppm
F2: 2515.18 Hz
FREQM: 8.75000 ppm/cm
HZCM: 1100.38066 Hz/cm

D'Souza DS-57 in CDCl₃



Current Data Parameters
NAME mds257a
EXPNO 1
PROCNO 1

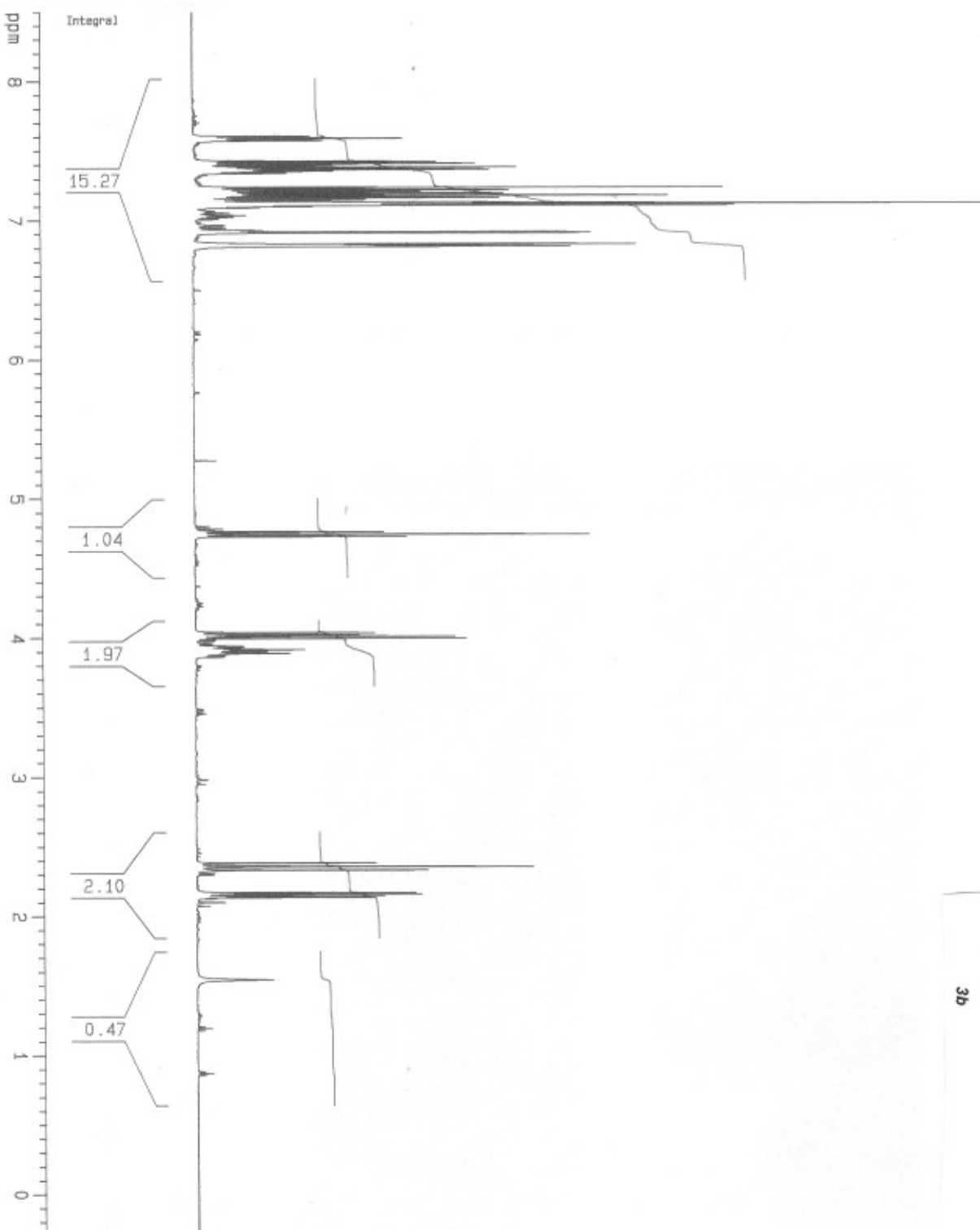
F2 - Acquisition Parameters
Date_ 20030129
Time 7.42

INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 4
SWH 5482.456 Hz
FIDRES 0.167311 Hz
AQ 2.9884915 sec
RG 128
RW 91.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 ¹H
P1 10.10 usec
PL1 0.00 dB
SFO1 500.132738 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 8.500 ppm
F1 4251.11 Hz
F2P -0.300 ppm
F2 -150.04 Hz
PPMCH 0.44000 ppm/cm
HZCM 220.05722 Hz/cm



ppm

178.193

160.423

158.421

152.370

147.384

140.044

132.839

132.429

130.972

130.906

130.186

130.163

129.309

128.461

128.067

127.451

126.687

126.463

124.860

124.478

124.233

124.208

123.429

123.361

118.542

118.432

116.363

116.186

112.982

111.234

77.249

76.995

76.741

74.937

53.257

39.100

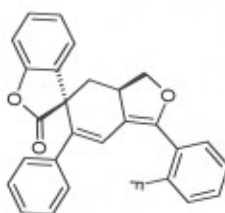
37.874

D'Souza

DS-57

1H CDCl3

3b



Current Data Parameters
NAME: 20030129
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030129
Time: 8.20
INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 2000
DS: 2
SWH: 30864.187 Hz
FIDRES: 0.470260 Hz
AQ: 1.0017082 sec
RG: 5782.8
CH: 16.1200 umsc
DE: 8.00 umsc
TE: 300.2 K
O1: 1.00000000 sec
d11: 0.03000000 sec
d12: 0.00020000 sec

CHANNEL: F1
NUC1: 13C
P1: 10.40 umsc
PL1: 0.00 dB
SFO1: 125.7713172 MHz

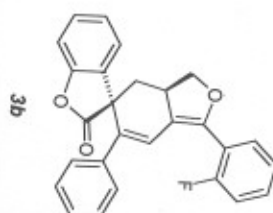
CHANNEL: F2
NUC2: 1H
P2: 100.00 umsc
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 500.132500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577558 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

50 MHz plot parameters
CX: 20.00 cm
CY: 12.00 cm
F1P: 180.000 ppm
F1: 23083.86 Hz
F2P: 25315.16 Hz
F2: 0.50100 ppm/cm
P1: 0.50100 ppm/cm
H2CH: 1068.94128 Hz/cm

ppm 180 160 140 120 100 80 60 40

D'Souza DS-57 in CDCl₃



74.9

39.1
37.9

Current Data Parameters
NAME: DS-57
EXPNO: 3
PROCNO: 1

F2 - Acquisition Parameters

Date_: 2003/12/29
Time: 9.08
INSTRUM: spect
PROBHD: 5 mm T1H 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 400
DS: 2
SWH: 22777.777 Hz
FIDRES: 0.452650 Hz
AQ: 1.1785800 sec
RG: 1622.3
DN: 16.000 usec
DE: 6.00 usec
TE: 300.2 K
D1: 4.00000000 sec
D12: 0.00344828 sec
d12: 0.00025000 sec
DELTA: 0.0001324 sec

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

NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
RF1: 125.765000 MHz

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

NUC2: 1H
P2: 10.10 usec
PL2: 0.00 dB
RF2: 500.132500 MHz

F2 - Processing parameters

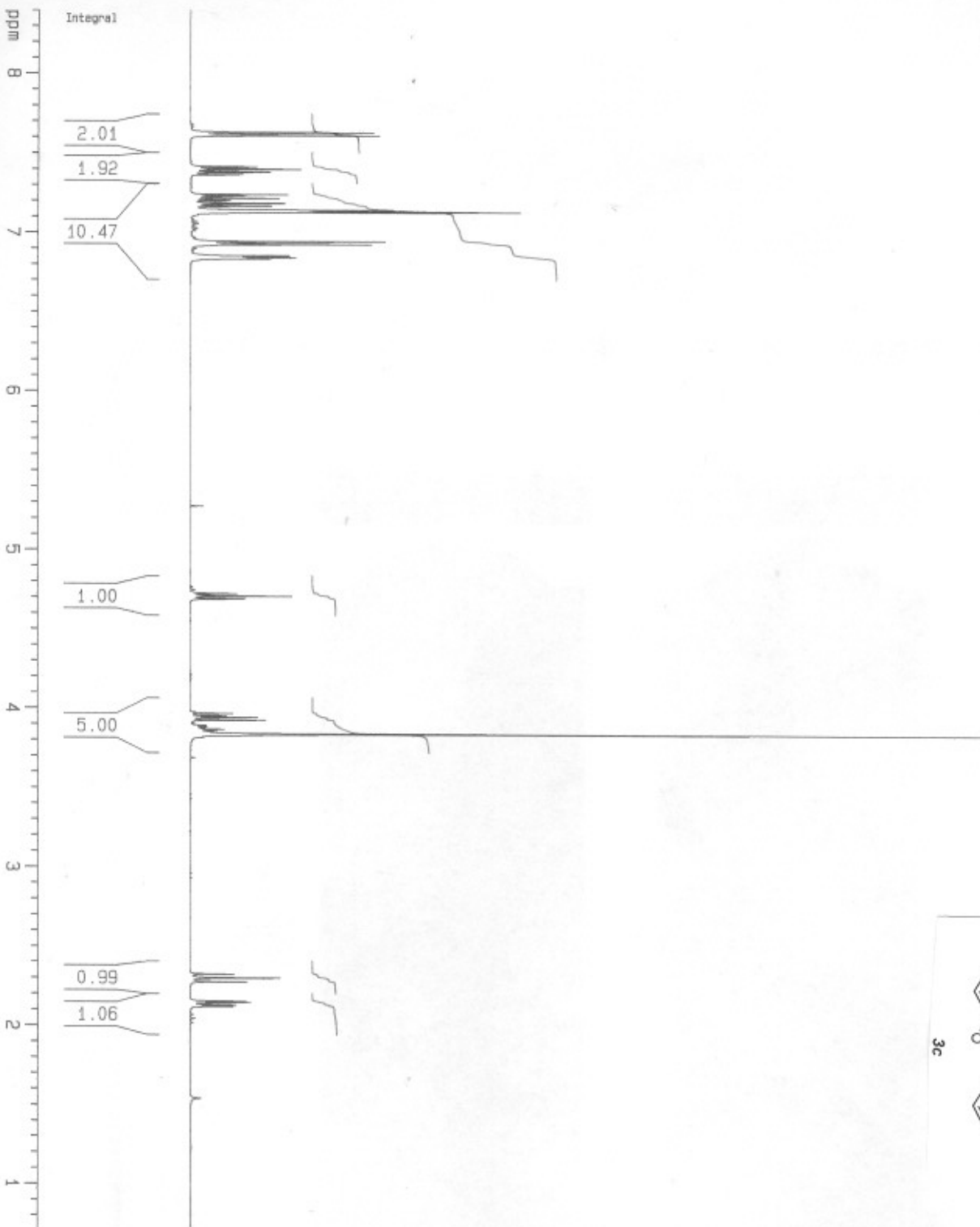
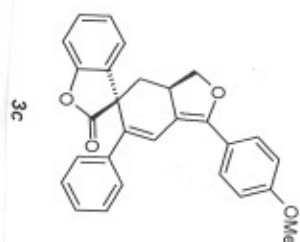
SI: 32768
SF: 125.7577802 MHz
RGW: EN
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

10 NMR plot parameters

CX: 20.00 cm
CY: 5.00 cm
F1P: 100.000 ppm
F1: 22893.98 Hz
F2P: 20.000 ppm
F2: 2515.16 Hz
PPMCK: 8.50000 ppm/cm
PCDK: 1088.94128 Hz/cm

ppm 180 160 140 120 100 80 60 40

O'Souza DS-36 in CDCl₃



Current Data Parameters

NAME	DS-36
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20030121
Time	9.45
INSTRUM	spect
PROBHD	5 mm TBI 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	16
DS	4
SWH	5482.455 Hz
FIDRES	0.157311 Hz
AQ	2.9884915 sec
RG	114
DW	91.200 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

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

NAC1	1H
P1	10.10 usec
PL1	0.00 dB
SFO1	500.1362736 MHz

F2 - Processing parameters

SI	16384
SF	500.1300232 MHz
MDM	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	13.00 cm
F1P	8.400 ppm
F1	4501.08 Hz
F2P	0.700 ppm
F2	350.09 Hz
PRNCH	0.38500 ppm/cm
HZCM	192.55006 Hz/cm

ppm

178.290

160.286

152.422

152.363

140.318

133.113

131.510

129.227

128.770

128.514

127.310

126.410

124.953

124.438

123.743

123.189

114.045

111.207

108.952

D'Souza DS-36 in CDCl3

77.254

77.000

76.746

74.463

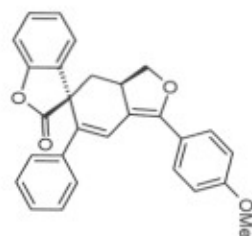
55.318

53.175

38.833

37.954

3c



Current Data Parameters
NAME 3c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030121
Time 8.00

INSTRUM spect
PROBHD 5 mm TBI H-13
PULPROG zgpg30

TD 65536
FIDRES 0.0000000
SOLVENT CDCl3

NS 2000
DS 2
SWH 30864.197 Hz

FT/RES 0.470950 Hz
AQ 1.0617332 sec

RG 5792.6
DM 16.200 usec

DE 6.00 usec
TE 300.2 K

D1 1.00000000 sec
d11 0.03000000 sec

d12 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.40 usec
PL1 0.00 dB
SFO1 125.7713172 MHz

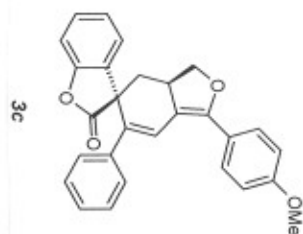
===== CHANNEL f2 =====
CPDPRG2 zgpg30
NUC2 1H
P2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 500.1325500 MHz

F2 - Processing parameters
SI 32768
SF 125.757705 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.00 cm
F1P 196.000 usec
F1 23893.98 Hz
F2P 20.000 usec
F2 2515.16 Hz
PPIPCM 8.20000 usec/cm
H2O 1098.94181 Hz/cm

ppm 180 160 140 120 100 80 60 40

D'Souza DS-36 in CDCl3



ppm

180
160
140
120
100
80
60
40

129.2
128.8
128.5
127.3
126.4
124.8
124.4
123.7
114.0
111.2
74.4
55.3
38.8
37.9

Current Data Parameters
NAME: mds231e
EXPNO: 3
PROCNO: 1

F2 - Acquisition Parameters
Date_: 2003121
Time: 9.16
INSTRUM: spect
PROBHD: 5 mm TBI 51/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 500
DS: 2
SWH: 27777.777 Hz
FIDRES: 0.423655 Hz
AQ: 1.175892 sec
RG: 1665.5
DM: 18.000 umsc
DE: 6.00 umsc
TE: 300.0 K
DVTG: 145.000000 sec
D1: 4.0000000 sec
d2: 0.00344826 sec
d12: 0.0000000 sec
DELTA: 0.0001324 sec

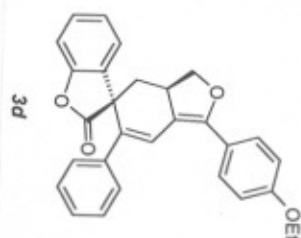
===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 umsc
PC: 20.00 umsc
PL1: 0.00 dB
SFO1: 125.769000 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
P2: 10.10 umsc
PC: 20.20 umsc
PCPD2: 100.00 umsc
PL2: 0.00 dB
PL12: 20.00 dB
SFO2: 500.132500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577562 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
RC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
F1P: 195.000 50%
F1: 23893.88 Hz
F2P: 20.000 50%
F2: 2515.16 Hz
PPH2CH: 8.50000 ppm/cm
HZCH: 1008.94128 Hz/cm

D'Souza DS-70 in CDCl₃



Current Data Parameters
NAME mds221a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030122
Time 13.47

INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃

DS 16
NS 4
SMH 5482.456 Hz
FIDRES 0.167311 Hz
AQ 2.9884915 sec
RG 101.6
DM 91.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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

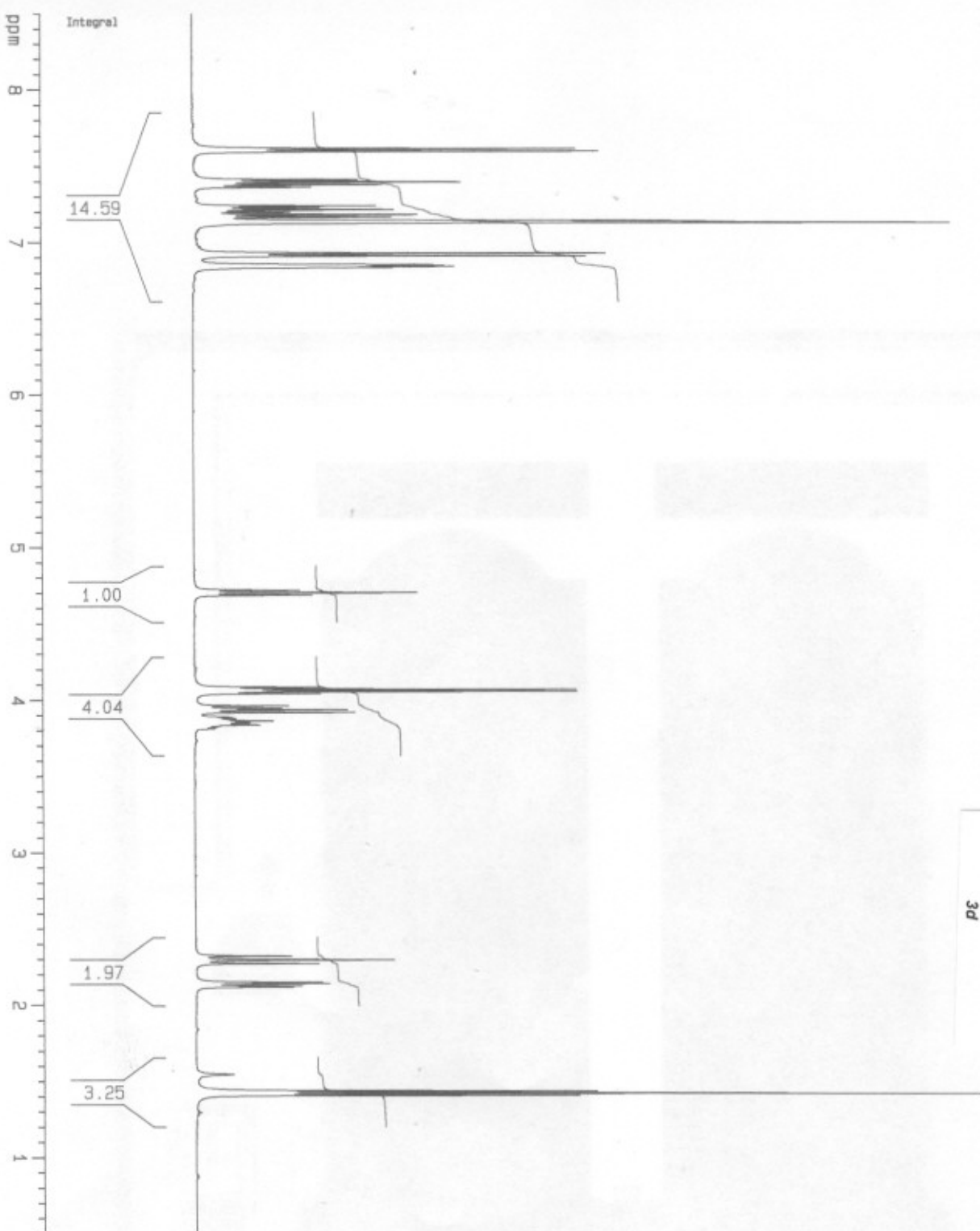
MUC1 1H
P1 10.10 usec
PL1 0.00 dB
GFO1 500.1322738 MHz

F2 - Processing parameters

SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
CY 13.00 cm
F1P 8.500 ppm
F1 4251.11 Hz
F2P 0.500 ppm
F2 250.07 Hz
PPMCK 0.40000 ppm/cm
HZCM 200.05202 Hz/cm



ppm

178.300

159.693

152.500

152.363

140.339

133.128

131.425

129.220

128.762

128.509

127.295

126.418

124.860

124.435

123.790

123.002

114.546

111.200

108.862

77.256

77.002

76.748

74.452

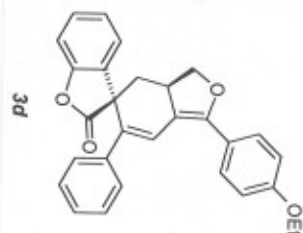
63.525

53.175

38.828

37.962

14.751



3d

Current Data Parameters
NAME: 3d
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters

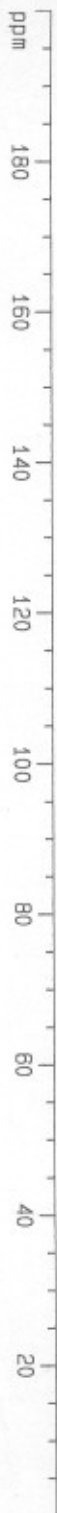
Date_: 2003/12/22
Time: 14.42
INSTRUM: spect
PROBHD: 5 mm TBI 5H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 2000
DS: 2
SWH: 30964.187 Hz
FIDRES: 0.470920 Hz
AQ: 1.0617382 sec
RG: 512.0
GB: 16.250
DE: 6.00 umic
TE: 300.0 K
D1: 1.00000000 sec
d11: 0.03000000 sec
d12: 0.00000000 sec

CHANNEL F1
NUC1: 13C
P1: 10.40 umic
PL1: 0.00 dB
SFO1: 125.7713172 MHz

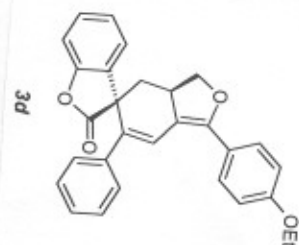
CHANNEL F2
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 umic
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 500.132500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.767055 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 25.00 cm
CY: 12.00 cm
F1P: 200.000 000
F1: 25151.56 Hz
F2P: 0.000 000
F2: 0.00 Hz
PNUC1: 13C
PCNUC1: 125.767055 MHz



D'Souza DS-70 in CDCl3



ppm

180
160
140
120
100
80
60
40
20

129.2
128.7
128.5
127.3
126.4
124.8
124.4
123.8
114.5
111.2
74.4
63.5
38.8
37.9
14.7

Current Data Parameters
NAME mus221a
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030122
Time 18.13
INSTRUM spect
PROBHD 5 mm TBI 5H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 2
SWH 27777.777 Hz
FIDRES 0.42385 Hz
AQ 1.178980 sec
RG 11628.0
WDW 18.000 usec
DE 15.40 usec
TE 300.0 K
DENSITY 1.45000000
D1 4.00000000 sec
d2 0.00344828 sec
d12 0.00055500 sec
DELTA 0.00001324 sec

CHANNEL F1

NUC1 13C
P1 10.40 usec
PL1 0.00 dB
RG1 125.769500 MHz

CHANNEL F2

CPDPRG2 waltz16
NUC2 1H
P2 10.10 usec
PL2 0.00 dB
RG2 500.132500 MHz

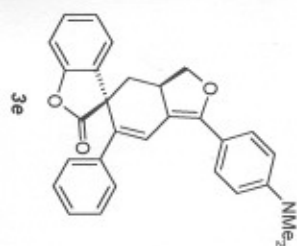
F2 - Processing parameters

SF 32758
SF 125.7677682 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
CY 5.00 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCH 10.00000 ppm/cm
H2CH 1257.57800 Hz/cm

D'Souza DS-84 in CDCl₃



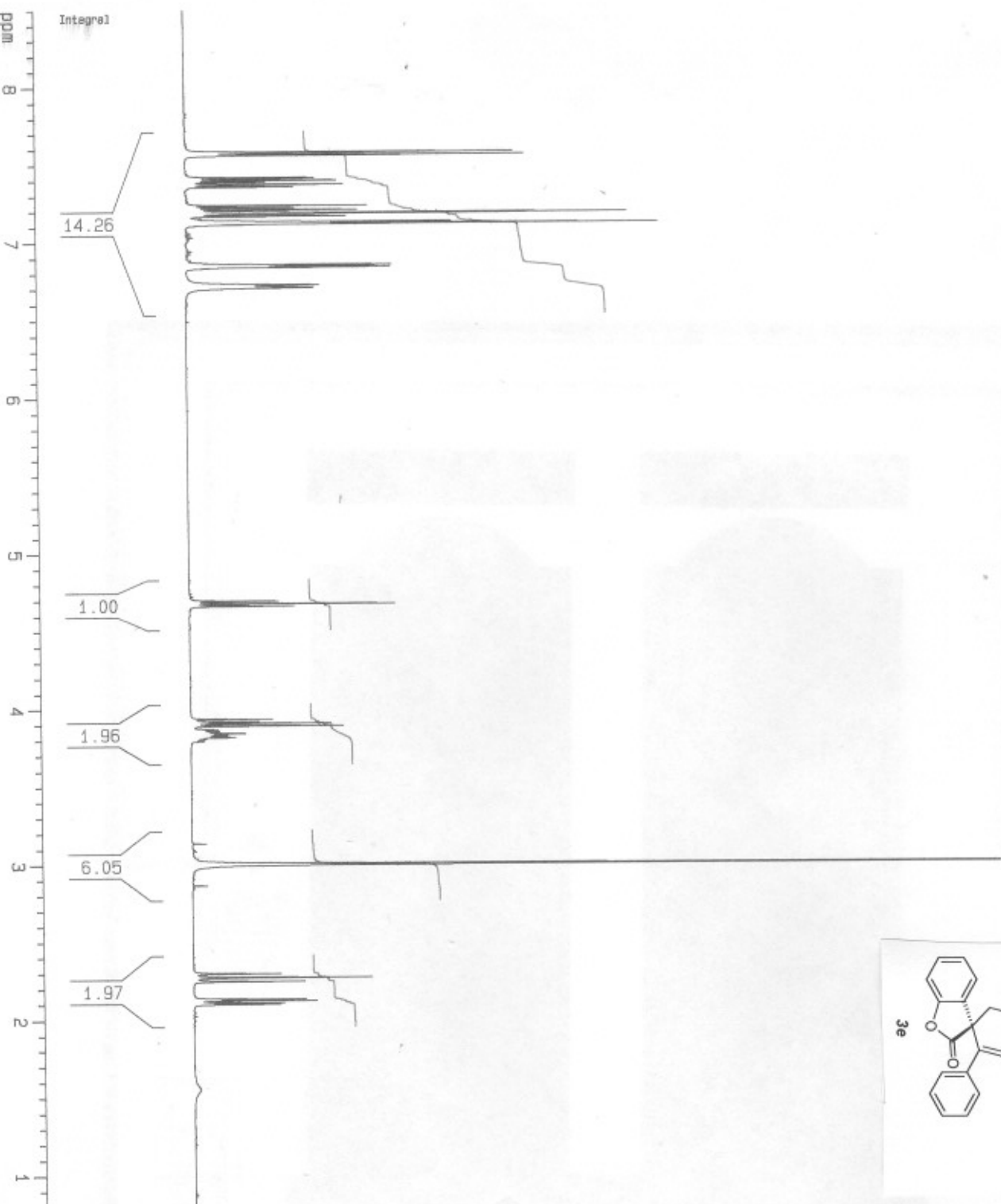
Current Data Parameters
NAME mudo77e
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030206
Time 17.00
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 4
SWH 5482.455 Hz
FIDRES 0.167311 Hz
AQ 2.9884915 sec
RG 90.5
RW 91.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

CHANNEL f1
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SF01 500.132739 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 42.88 cm
F1P 8.300 ppm
F1 4261.11 Hz
F2P 0.800 ppm
F2 400.10 Hz
PPM0M 0.38600 ppm/cm
HZCM 192.550006 Hz/cm

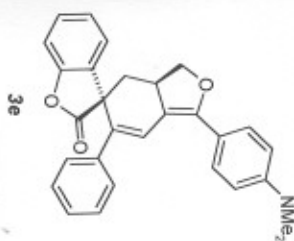


ppm

178.504

153.406
152.329
150.770140.566
133.428
129.995
129.119
128.492
128.482
127.055
126.276
124.930
124.403
124.286
111.822
111.141
107.538p. Souza DS-84 in CDCl₃77.268
77.014
76.759
74.308

53.115

40.235
38.890
37.681

ppm 180 150 140 120 100 80 60 40

q

q q

q q

q q

q q

q q

q q

q q

q q

q q

q q

q q

q q

q q

CH₂

q

C-

-CH

CH₂

24

Current Data Parameters
NAME: mds071e
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030308
Time: 19.28
INSTRUM: spect
PROBHD: 5 mm TBI 5H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 4000
DS: 2
SWH: 27777.777 Hz
FIDRES: 0.423855 Hz
AQ: 1.1795960 sec
RG: 5792.8
CH: 18.000 umsc
DE: 8.00 umsc
TE: 300.2 K
D1: 1.00000000 sec
d11: 0.03000000 sec
d12: 0.00020000 sec

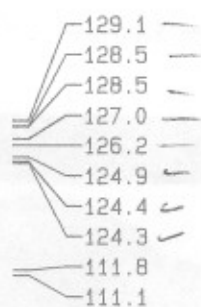
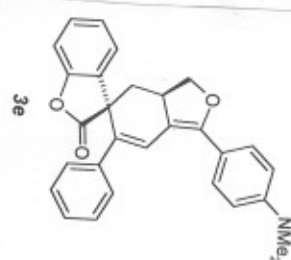
CHANNEL f1
NUC1: 13C
P1: 10.40 umsc
PL1: 0.00 dB
SFO1: 125.7703714 MHz

CHANNEL f2
NUC2: 1H
P2: 100.00 umsc
PL2: 0.00 dB
PL3: 20.00 dB
PL13: 20.00 dB
SFO2: 500.1325000 MHz

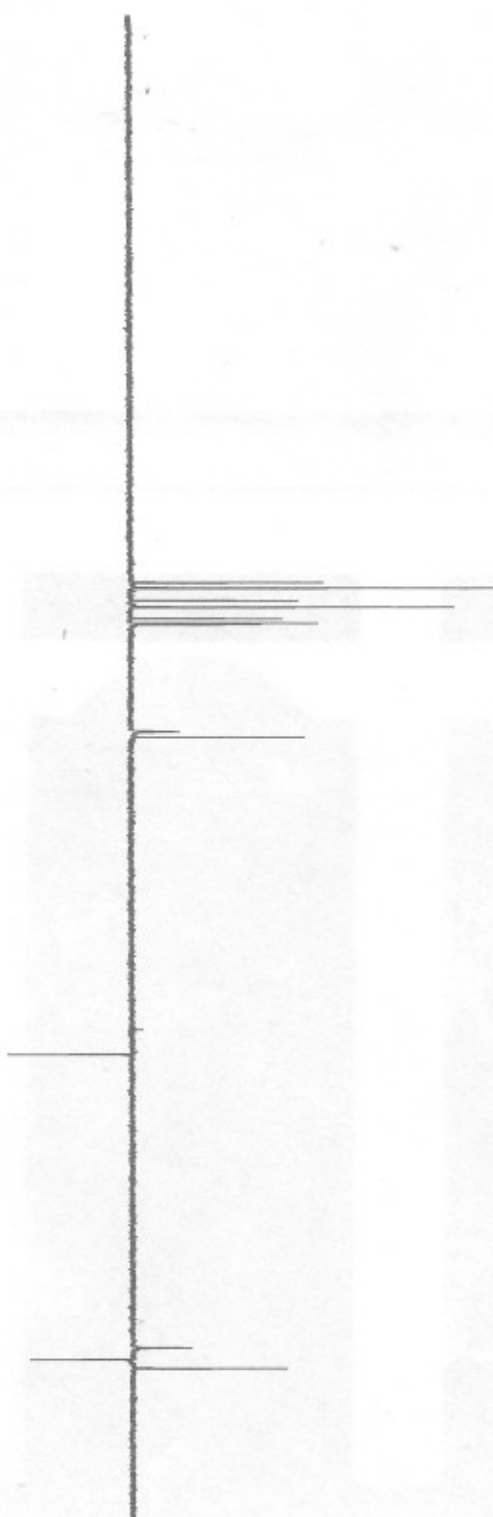
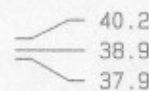
F2 - Processing parameters
SI: 32768
SF: 125.7577265 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 18.28 cm
F1P: 195.000 DDM
F1: 24632.77 Hz
F2P: 20.000 DDM
F2: 2515.16 Hz
SFWDW: 8.73500 DDM/Hz
WDW: 1100.38588 Hz/Hz

D'Souza DS-84 in CDCl3



74.3



Current Data Parameters
NAME mod071e
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030208
Time 21.45
INSTRUM spect
PROBHD 5 mm TSI 1H/13
PULPROG zgpg30
TD 65536
TO 65536
SOLVENT CDCl3
NS 1900
DS 2
SWH 27777.777 Hz
FIDRES 0.42805 Hz
AQ 1.179580 sec
RG 1625.5
DM 16.000 umsec
DE 6.00 umsec
TE 300.0 K
DMSI2 145.000000 sec
D1 4.00000000 sec
d2 0.00344828 sec
d12 0.0002900 sec
DELTA 0.0001324 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.40 umsec
SFO 125.760314 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 10.10 umsec
SFO2 500.132500 MHz

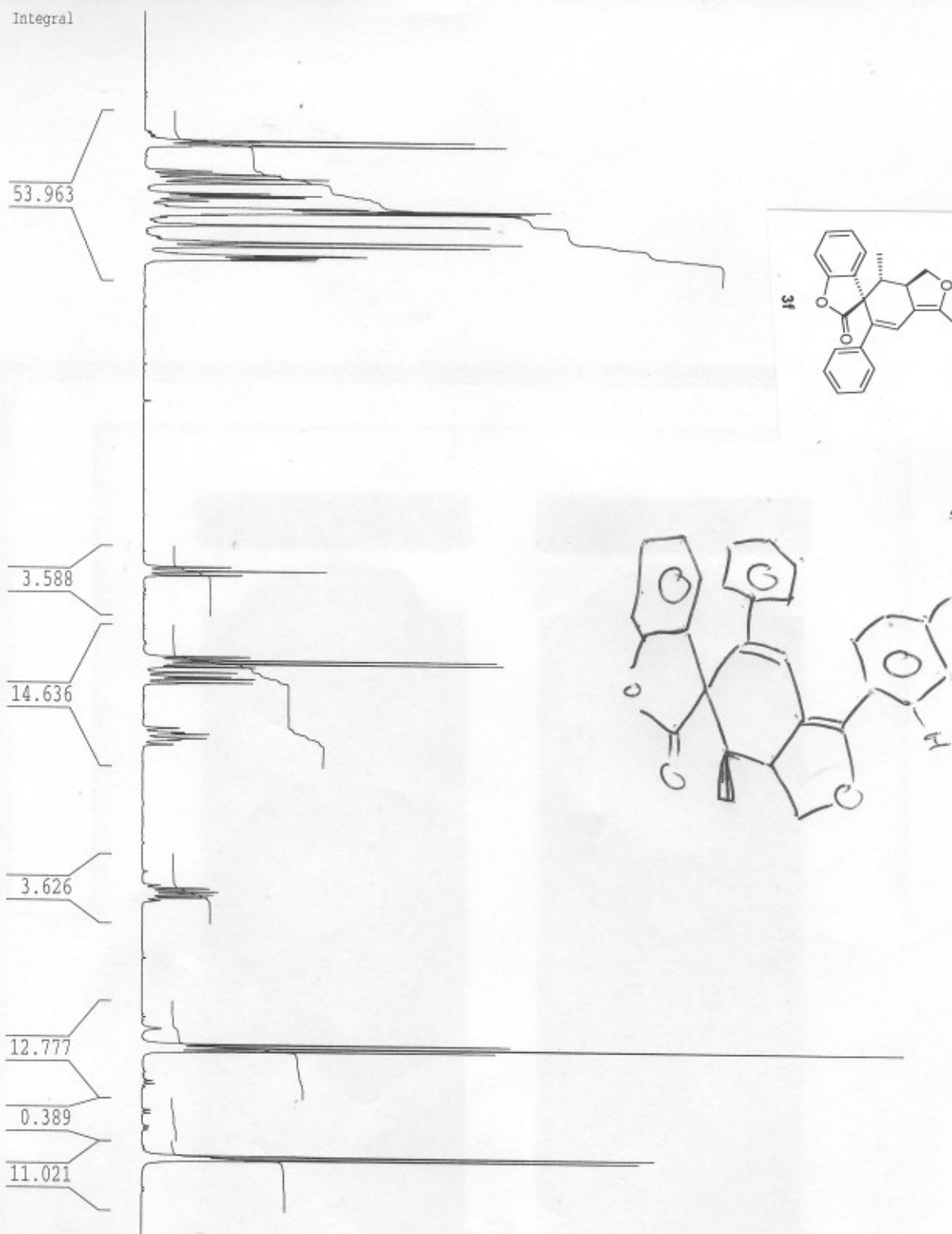
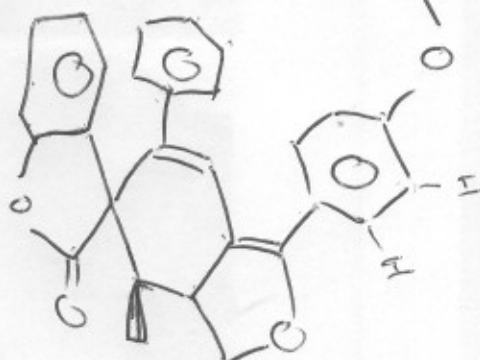
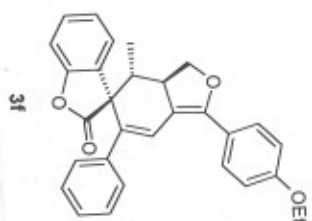
F2 - Processing parameters
SI 32768
SF 125.757582 MHz
KCN 64
SFO 500.132500 MHz
LB 1.00 Hz
GB 0
PC 1.00

1D 1H/13C plot parameters
CX 20.00 cm
CY 1.00 cm
F1P 155.000 ppm
F1 2652.77 Hz
F2P 20.000 ppm
F2 2515.18 Hz
P1P104 8.75000 ppm/cm
HZ04 1100.38988 Hz/cm

ppm 180 160 140 120 100 80 60 40

D Souza DS_Spiro-40Et-Crotyl CDCl3

109



Current Data Parameters
NAME felimso
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030211
Time 17.41

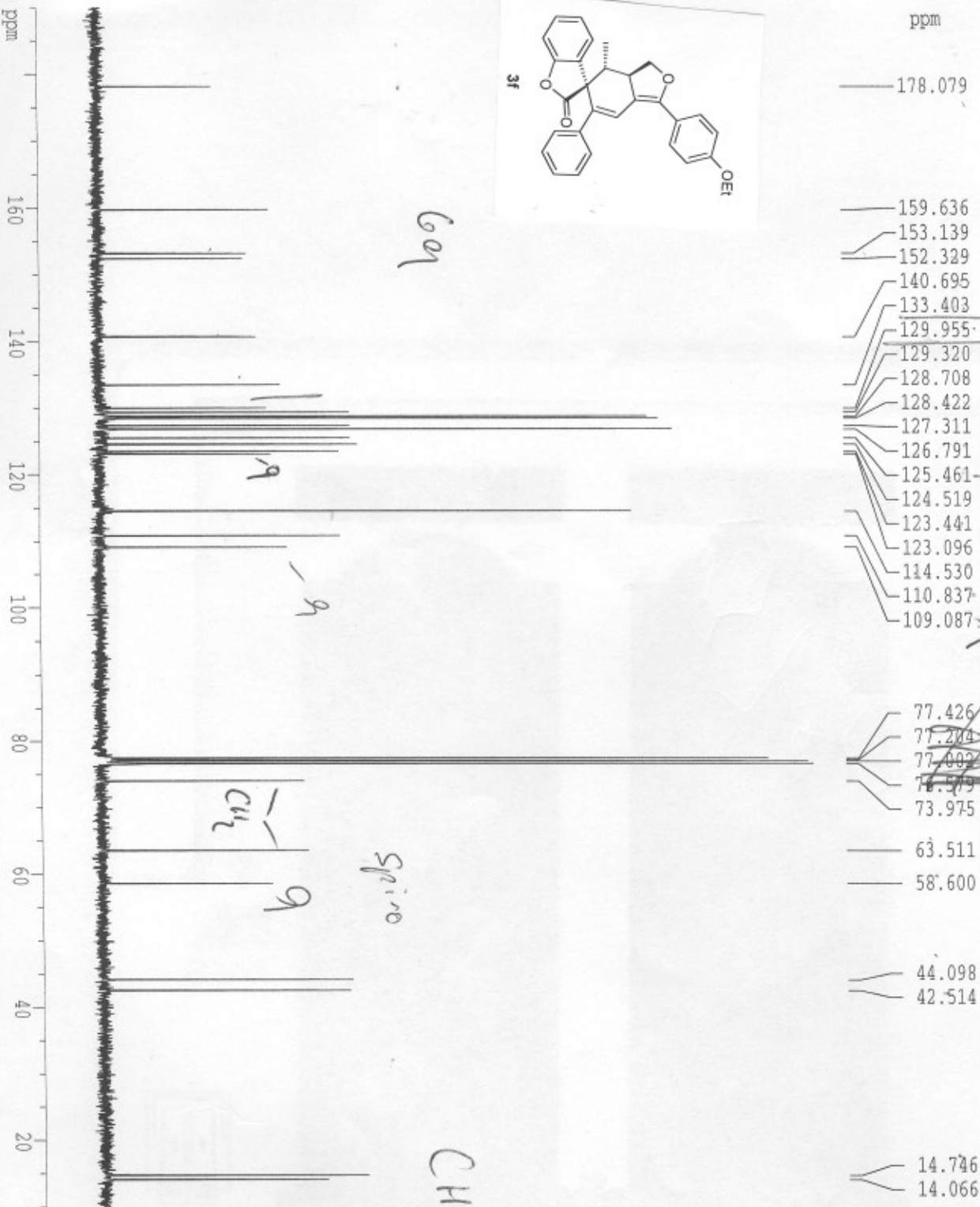
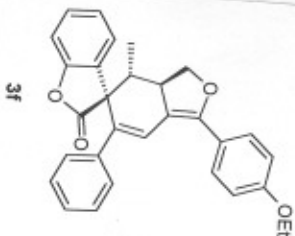
INSTRUM spect
PROBHD 5 mm TBI 1H/3
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2

SMF 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 90.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 300.1300389 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.417 ppm
F1 2526.28 Hz
F2P 0.038 ppm
F2 11.42 Hz
PPMCM 0.41896 ppm/cm
HZCM 125.74303 Hz/cm



D Souza DS_Spiro-40Et-Crotyl CDCl3

178.079	
159.636	
153.139	
152.329	
140.695	
133.403	
129.955	
129.320	
128.708	
128.422	
127.311	
126.791	
125.461	
124.519	
123.441	
123.096	
114.530	
110.837	
109.087	
77.426	
77.204	
77.002	
76.579	
73.975	
63.511	
58.600	
44.098	
42.514	
14.746	
14.066	

Current Data Parameters
NAME felluso
EXNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030211
Time 19.31

INSTRUM spect
PROBHD 5 mm TBI 1H/3
PULPROG zgpg30

TD 32768
SOLVENT CDCl3
NS 2400

DS 2
SMH 22675.736 Hz
FIDRES 0.692009 Hz

AQ 0.7225844 sec
RG 5792.6
DM 22.050 usec

DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 -6.00 dB
SFO1 75.4752160 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec

PL2 0.00 dB
PL12 24.00 dB
PL13 26.00 dB
SFO2 300.1316507 MHz

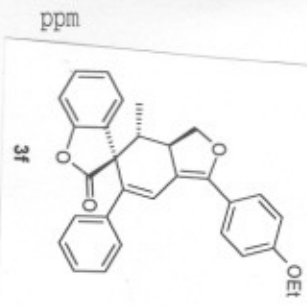
F2 - Processing parameters
SI 32768

SF 75.4677520 MHz
MCM EM
SSB 0

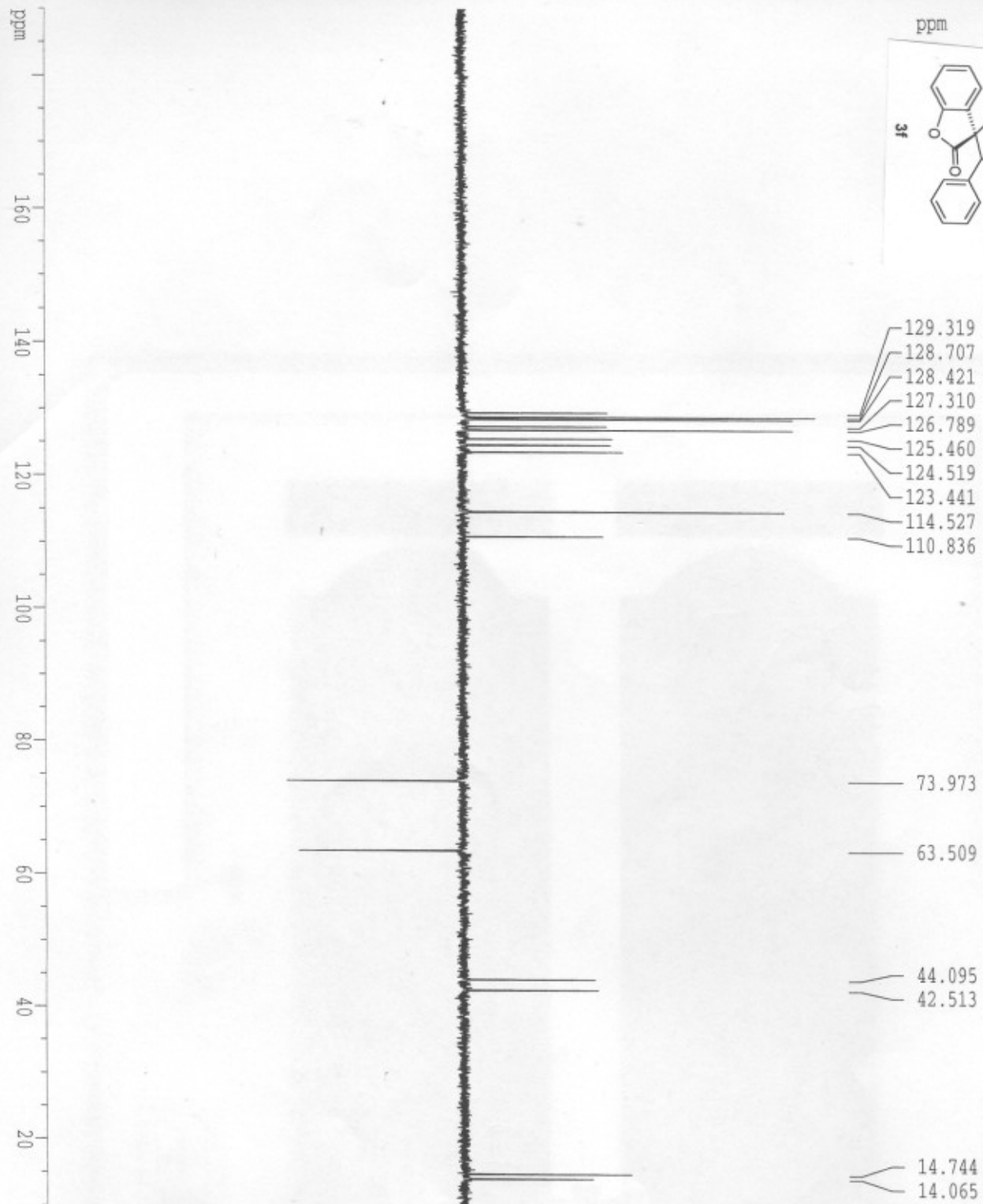
LB 1.00 Hz
GB 0
PC 0.50

ID NMR plot parameters

CX 20.00 cm
F1P 190.000 ppm
F1 14338.87 Hz
F2P 10.000 ppm
F2 754.68 Hz
PPMCM 9.00000 ppm/cm
HZCM 679.20978 Hz/cm



D Souza DS_Spiro-40Et-Crotyl CDCl3



```

Current Data Parameters
NAME          felinuso
EXPNO         12
PROCNO        1

F2 - Acquisition Parameters
Date_         20030211
Time          20.08
INSTRUM       spect
PROBHD        5 mm TBI 1H/3
PULPROG       dept135
TD            32768
SOLVENT       CDCl3
NS            800
DS            8
SMH           22675.736 Hz
FIDRES        0.692009 Hz
AQ            0.7225844 sec
RG            7298.2
DE            22.050 usec
TE            300.0 K
D1            2.00000000 sec
D2            0.00345000 sec
D12           0.00002000 sec
DELTA         0.00001401 sec

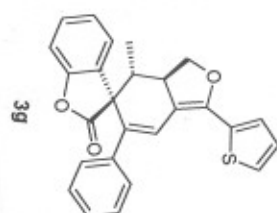
===== CHANNEL f1 =====
NUC1          13C
P1            11.00 usec
P2            22.00 usec
PL1           -6.00 dB
SFO1          75.4752160 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
P3            8.50 usec
P4            17.00 usec
PCPD2         100.00 usec
PL2           0.00 dB
PL12          24.00 dB
SFO2          300.1316507 MHz

F2 - Processing parameters
SI            32768
SF            75.4677521 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00

ID NMR plot parameters
CX            20.00 cm
PIF           190.000 ppm
F1            14338.87 Hz
F2            10.000 ppm
F3            754.68 Hz
FPMCM         9.00000 ppm/cm
HZCM          679.20978 Hz/cm
  
```

D'Souza DS



Current Data Parameters
NAME mds037e
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030131
Time 8.12

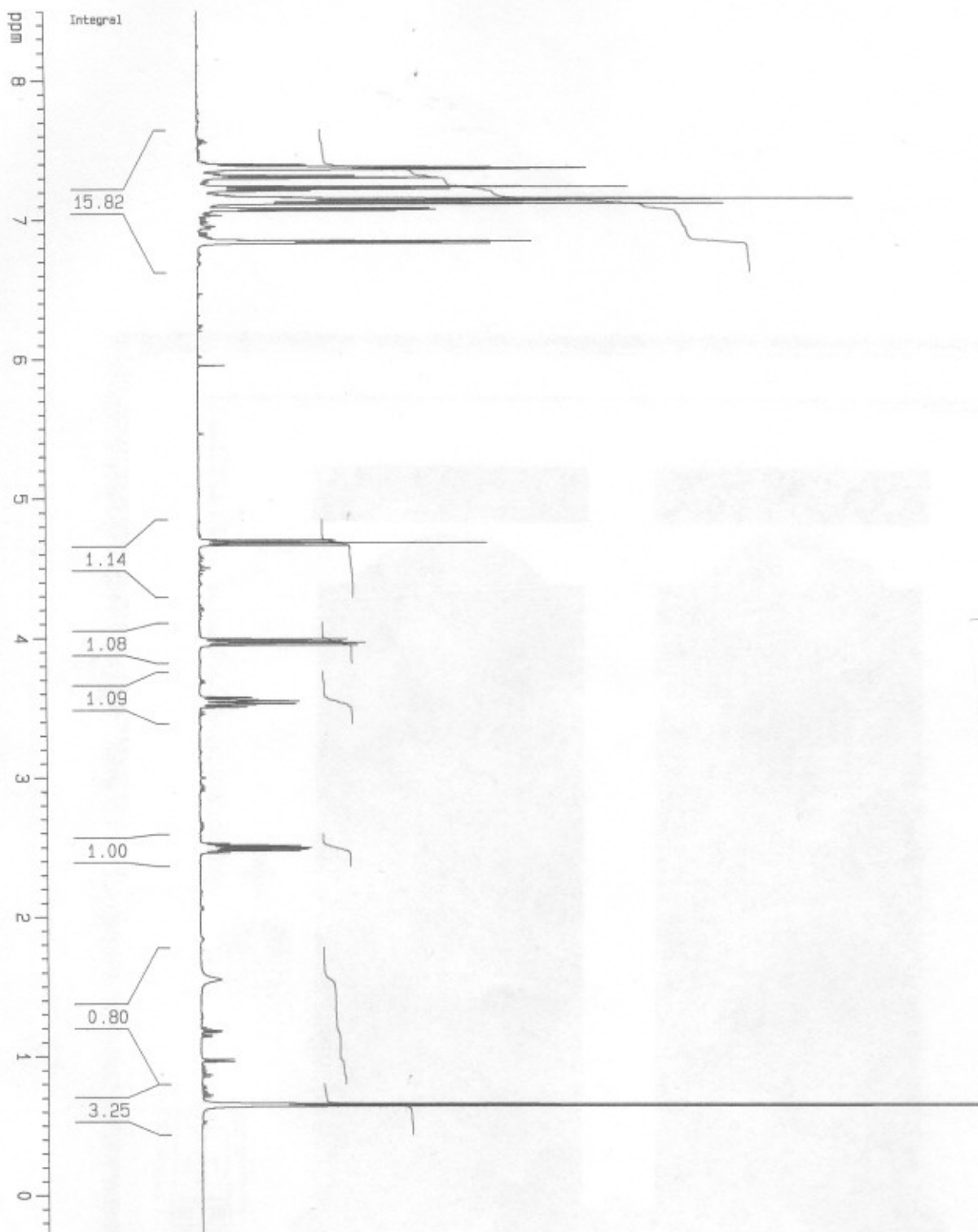
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4

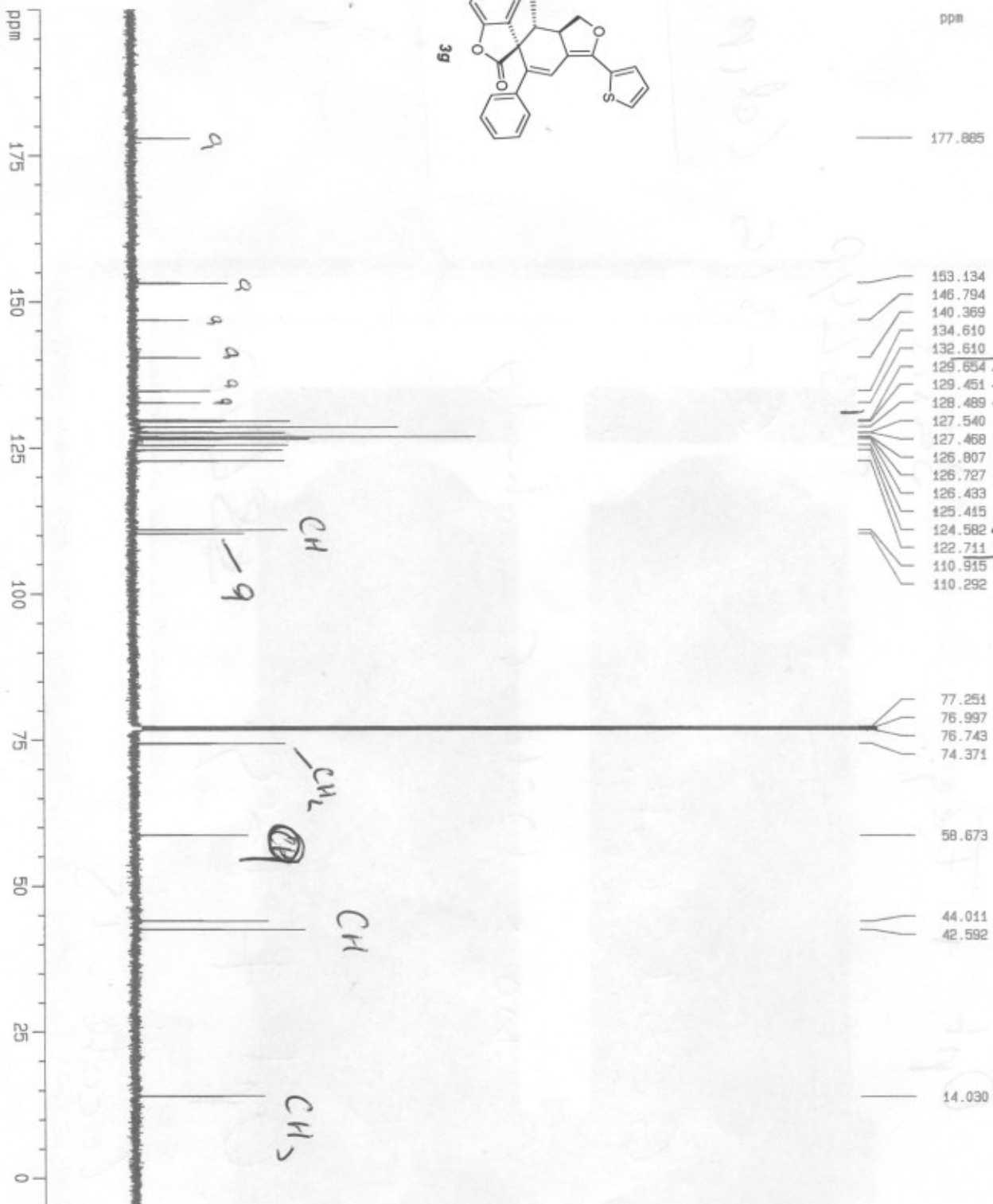
SWH 5482.456 Hz
FIDRES 0.167314 Hz
AQ 2.9864915 sec
RG 143.7
OW 91.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SFO1 500.1322738 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDM EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 8.500 ppm
F1 4251.11 Hz
F2P -0.300 ppm
F2 -150.04 Hz
PRNCH 0.44000 ppm/cm
HZCH 220.05722 Hz/cm





Current Data Parameters

NAME	VALUE	UNITS
EXPNO	2	
PROCNO	1	

F2 - Acquisition Parameters

NAME	VALUE	UNITS
DATE_	20030311	
TIME	8.22	
INSTRUM	800MC	
PROBHD	5 mm TBI 1H/13	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
RG	4000	
DG	2	
SWH	30864.187 Hz	
FIDRES	0.470660 Hz	
AQ	1.0617332 sec	
RG	5792.6	
SW	18,200 MHz	
DE	5.00 MHz	
TE	300.0 K	
OL	1.00000000 sec	
dl1	0.00000000 sec	
dl2	0.00000000 sec	

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

NAME	VALUE	UNITS
NUC1	13C	
PC1	10.40 MHz	
PL1	0.00 dB	
PR1	125.7713172 MHz	

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

NAME	VALUE	UNITS
CHRGPRG2	waitz15	
NUC2	1H	
PCPRG2	100.00 MHz	
PL2	0.00 dB	
PR2	20.00 MHz	
PR13	20.00 MHz	
PR22	500.1322500 MHz	

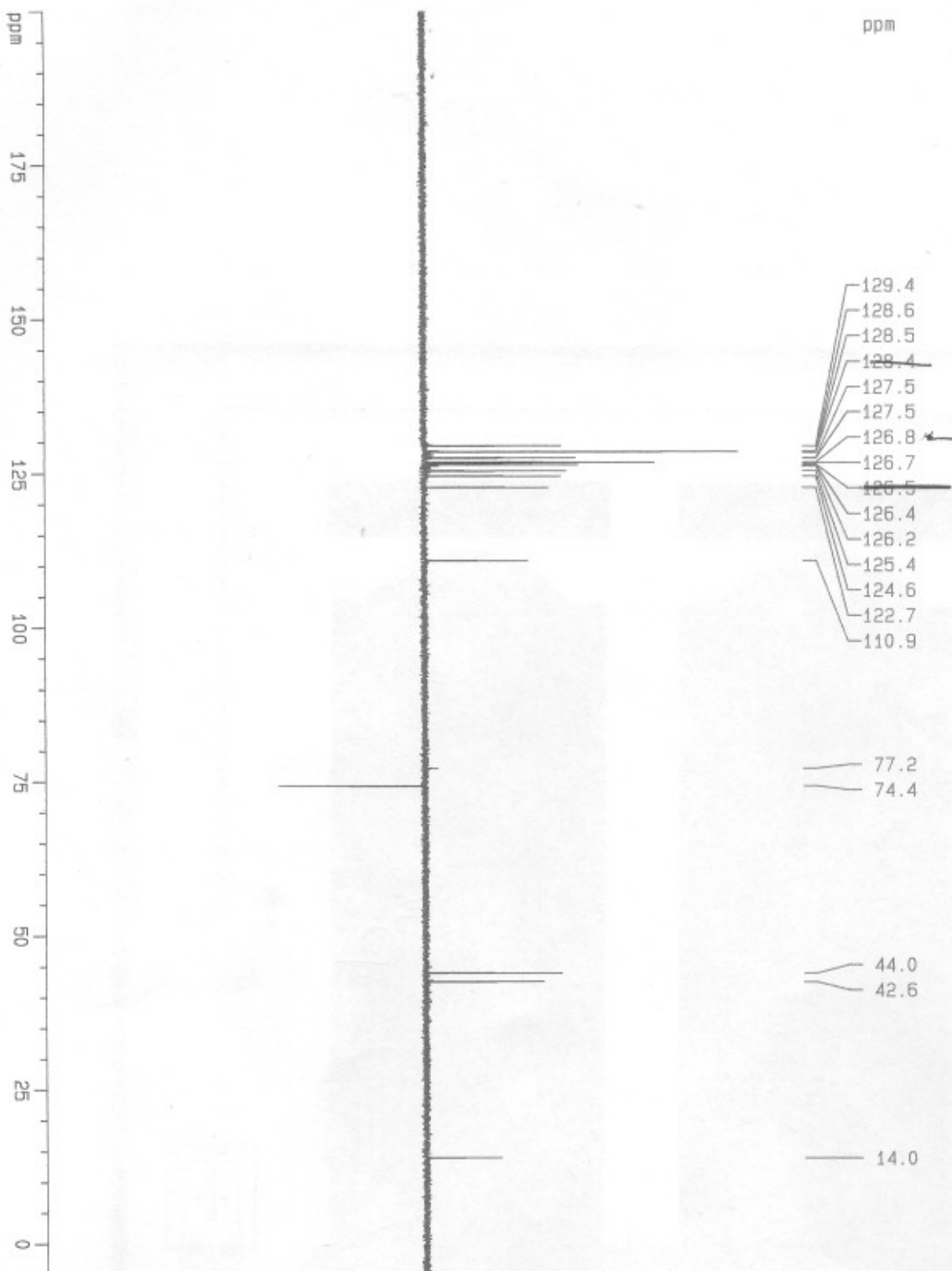
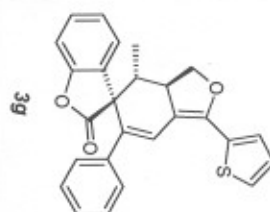
F2 - Processing parameters

NAME	VALUE	UNITS
SI	32768	
GF	125.757956 MHz	
MDW	EM	
SB	0	
LB	1.00 Hz	
GB	0	
PC	1.00	

10 NMR plot parameters

NAME	VALUE	UNITS
CH	20.00 MHz	
CK	15.14 MHz	
F1P	200.000 MHz	
F1	200.000 MHz	
F2P	500.132 MHz	
F2	500.132 MHz	
PRMCM	10.25000 MHz/cm	
HZCM	1259.01756 Hz/cm	

D'Souza DS-74 in CDCl3



Current Data Parameters
NAME DS-74
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030131
Time 10.52
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1300
DS 2
SWH 30064.167 Hz
FIDRES 0.470220 Hz
AQ 1.0617322 sec
RG 1865.0
IN 16.200 umsc
DE 0.00 umsc
TE 300.0 K
CHRG2 1.40, 0.000000
D1 4.00000000 sec
G2 0.00344828 sec
G12 0.00020000 sec
DELTA 0.00001324 sec

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

NUC1 13C
P1 10.40 umsc
SE 20.00 umsc
PL1 0.00 dB
SFO1 125.7713172 MHz

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

CPDPRG2 HLLH218
NUC2 1H
P2 10.10 umsc
SE 20.00 umsc
PL2 0.00 dB
SFO2 500.1326250 MHz

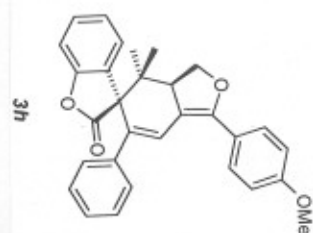
F2 - Processing parameters

SI 32768
SF 125.7577962 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

10 MHz plot parameters

CX 20.00 cm
CY 5.00 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PCPDCH 10.25000 ppm/cm
HZCM 1289.01798 Hz/cm

D'Souza DS-75 in CDCl3



Current Data Parameters
NAME mud31ja
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030130
Time 7.42

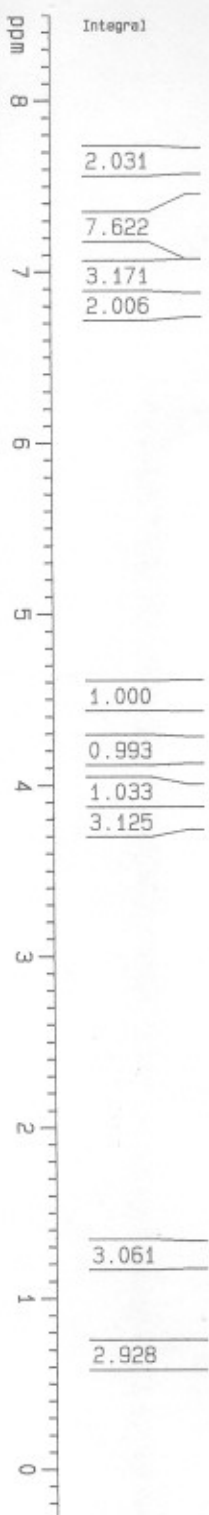
INSTRUM spect
PROBHD 5 mm TBI HV/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4

SWH 5492.456 Hz
FIDRES 0.167311 Hz
AQ 2.9864915 sec
RG 90.5
RW 91.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SFO1 500.1322736 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 8.500 ppm
F1 4251.11 Hz
F2P -0.300 ppm
F2 -150.04 Hz
PPMCM 0.44000 ppm/cm
HZCM 220.05722 Hz/cm



ppm

175.628

160.273

153.020

141.194

132.903

131.685

129.241

128.770

126.484

127.161

126.246

125.998

124.091

123.332

122.573

114.030

110.492

108.061

77.257

77.003

76.749

70.072

61.758

55.340

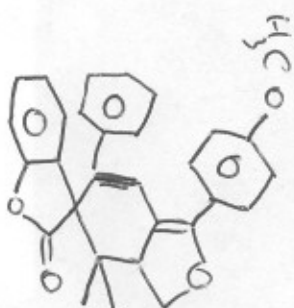
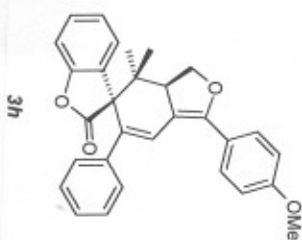
47.737

39.430

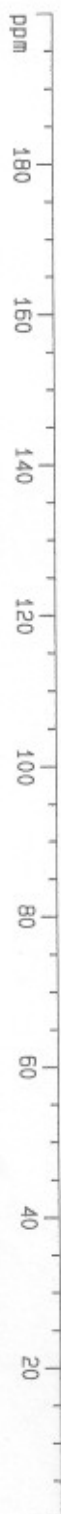
22.505

16.566

P. Souza | DS-751 | in CDCl3

C₃₀H₂₆O₄

Σ 26



Current Data Parameters
NAME mad3114
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030130
Time 10.36
INSTRUM spect
PROBHD 5 mm TBI JY/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3000
DS 2
SWH 30684.197 Hz
FIDRES 0.472955 Hz
AQ 1.6817325 sec
RG 3728.0
DM 16.700 umsc
DE 9.00 umsc
TE 300.2 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00000000 sec

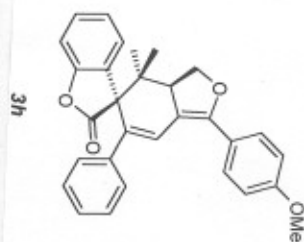
CHANNEL f1
NUC1 13C
P1 10.40 umsc
PL1 0.00 dB
SFO1 125.7713172 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 umsc
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 500.1362500 MHz

F2 - Processing parameters
SI 32768
SF 125.7577556 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

10 MHz plot parameters
CX 20.00 cm
CY 12.00 cm
F1P 200.000 ppm
F1 25151.96 Hz
F2P 0.000 ppm
F2 0.00 Hz
FTMCH 10.00000 ppm/cm
HZCH 1257.57500 Hz/cm

D'Souza DS-75 in CDCl₃



129.2
128.7
128.5
127.1
126.2
126.0
124.1
122.5
114.0
110.5

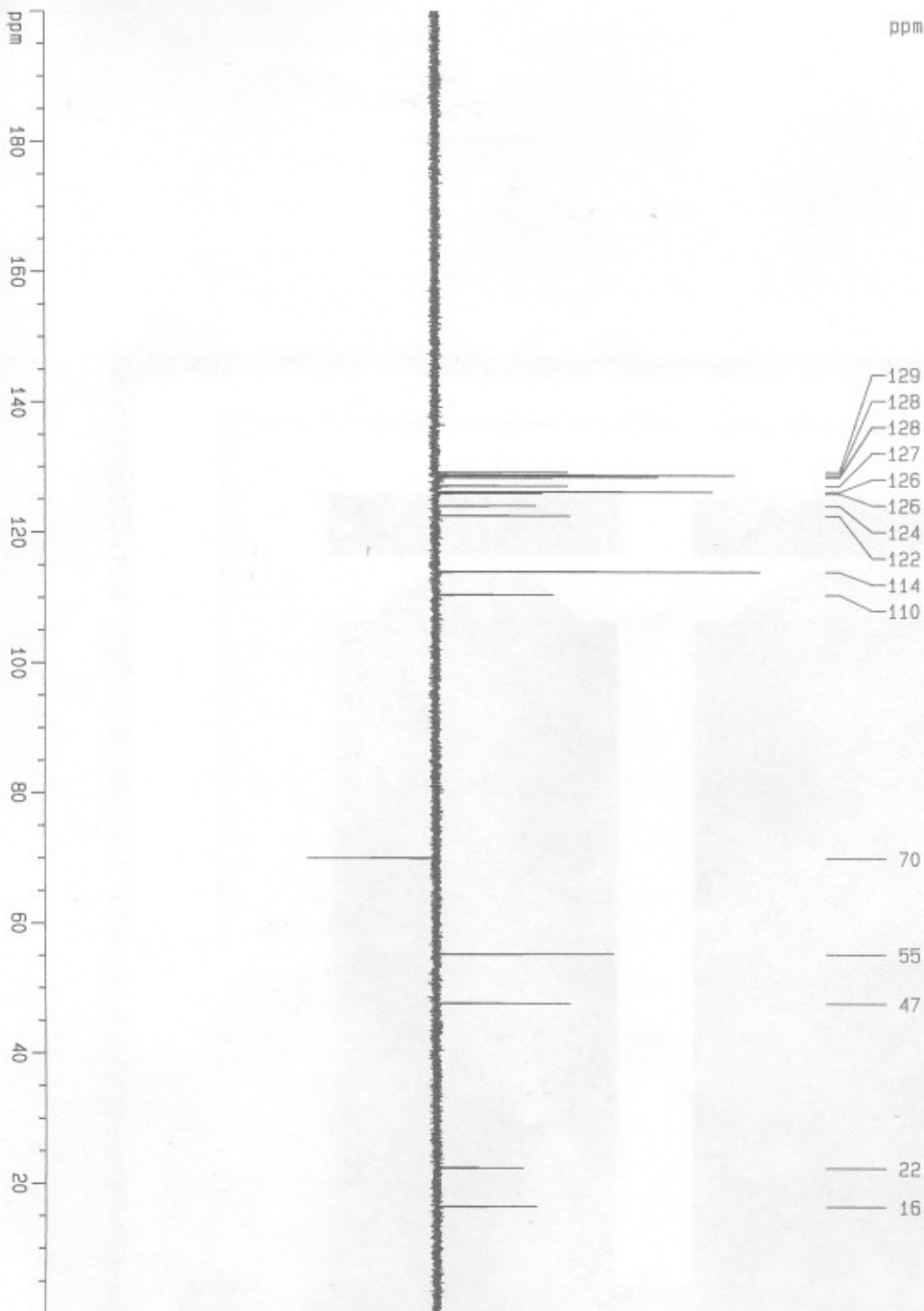
70.0

55.3

47.7

22.5

16.5



Current Data Parameters
NAME DS-75
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030130
Time 8.04
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TO 60000
SOLVENT CDCl₃
NS 400
DS 2
FIDRES 31152.548 Hz
AQ 0.470332 Hz
RG 1.0516028 Hz
IN 1600.15
DE 16.000 uS
TE 300.0 K
DELTA 1.45.0000000
DELT2 4.000000000 sec
DE 0.00344828 sec
DELT 0.000000000 sec
DELTA 0.00001324 sec

CHANNEL F1

NUC1 13C
P1 10.40 uS
P2 20.80 uS
PL1 0.00 dB
SFO1 125.7712189 MHz

CHANNEL F2

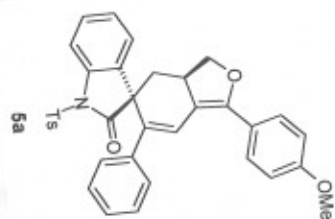
CPDPRG2 waltz16
NUC2 1H
P3 10.10 uS
P4 20.20 uS
PCPD2 100.00 uS
PL2 0.00 dB
SFO2 500.1322500 MHz

F2 - Processing parameters

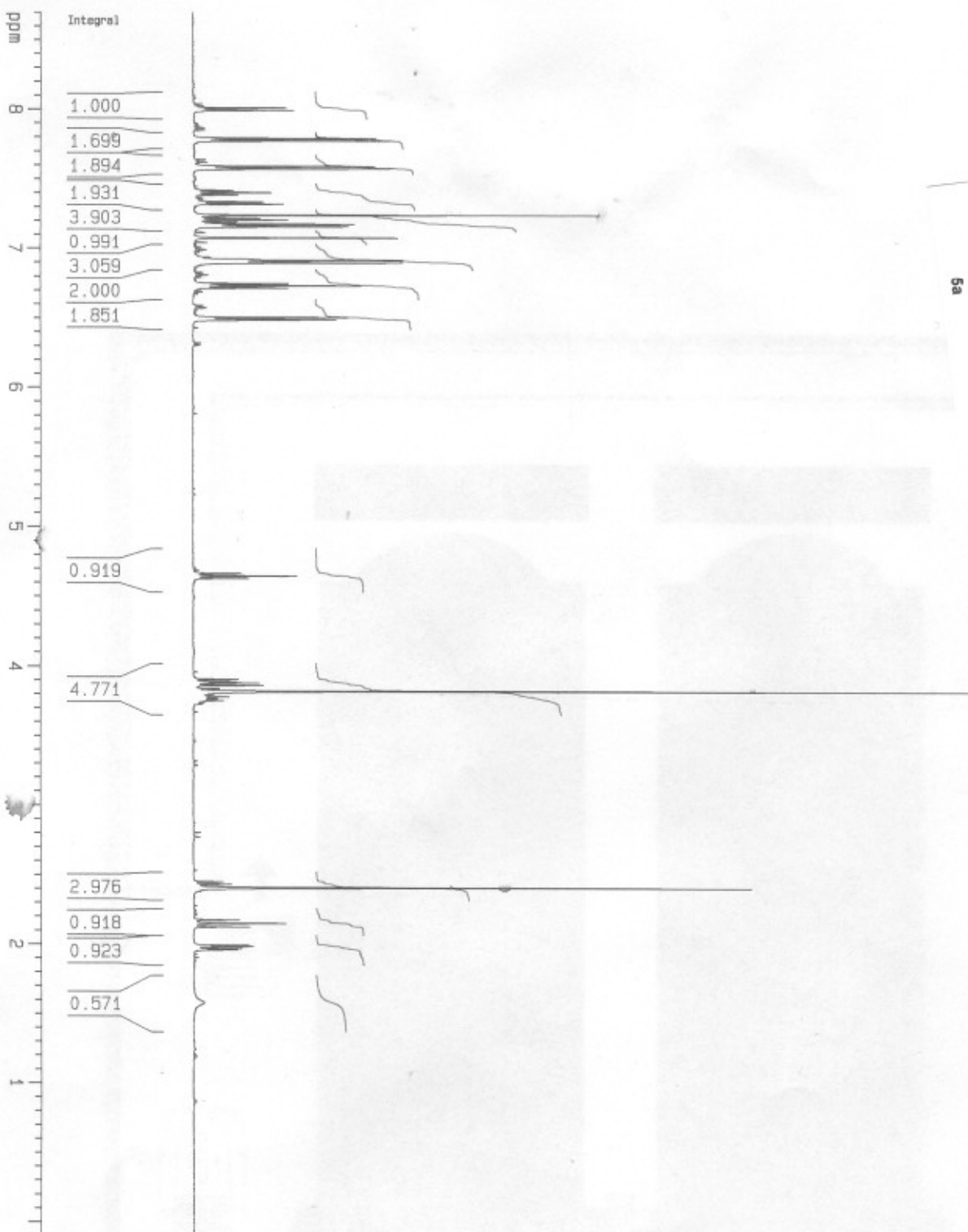
SF 320765
F2 125.7677992 MHz
RGW 0
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

10 NMR plot parameters

CX 20.00 cm
CY 5.00 cm
FAP 200.000 200
F1 25151.56 Hz
F2P 0.000 200
F2 0.00 Hz
PPMCM 10.00000 200/cm
HDCM 1257.57900 Hz/cm



D'Souza DS-209 in CDCl₃



Current Data Parameters

NAME	muso2mo
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20031125
Time	12.55
INSTRUM	spect
PROBHD	5 mm 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	16
DS	4
SWH	5492.456 Hz
FIDRES	0.167311 Hz
AQ	2.9884915 sec
RG	101.6
DM	91.200 usec
DE	6.00 usec
TE	299.0 K
D1	1.00000000 sec

CHANNEL f1

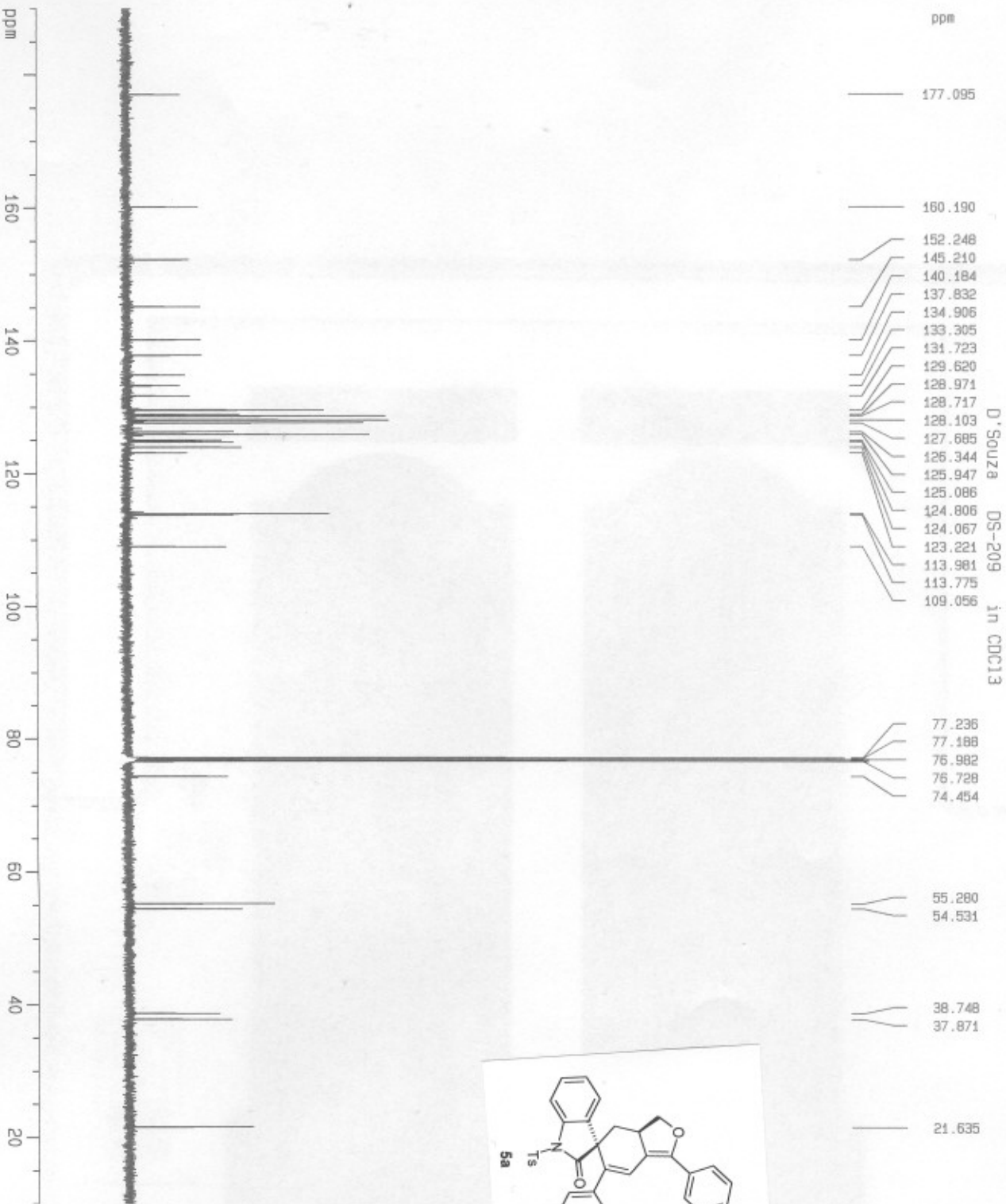
NUC1	1H
P1	10.10 usec
PL1	0.00 dB
SFO1	500.1322820 MHz

F2 - Processing parameters

SI	16394
SF	500.1300232 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	13.00 cm
F1P	8.700 ppm
F1	4351.13 Hz
F2P	-0.100 ppm
F2	-50.01 Hz
PPMCM	0.44000 ppm/cm
HZCM	220.05722 Hz/cm



Current Data Parameters

NAME	DS-209
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20031126
Time	11.15
INSTRUM	BOEC
PROBHD	5 mm TBI 1H/13
PULPROG	ZGPG30
TD	65536
SOLVENT	CDCl3
NS	3000
DS	2
SWH	30854.157 Hz
FIDRES	0.470650 Hz
AQ	1.0617332 sec
RG	512.8
DM	16.200 umic
DE	8.00 umic
TE	298.0 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00000000 sec

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

NUC1	13C
P1	10.40 umic
PL1	0.00 dB
SC1	125.7713172 MHz

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

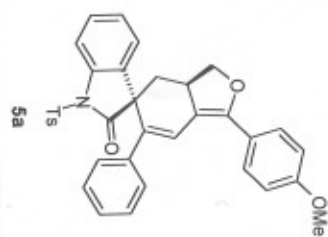
CPDPRG2	WALTZ16
NUC2	1H
PCPD2	100.00 umic
PL2	0.00 dB
PL12	20.00 dB
PL13	20.00 dB
SC2	500.1325000 MHz

F2 - Processing parameters

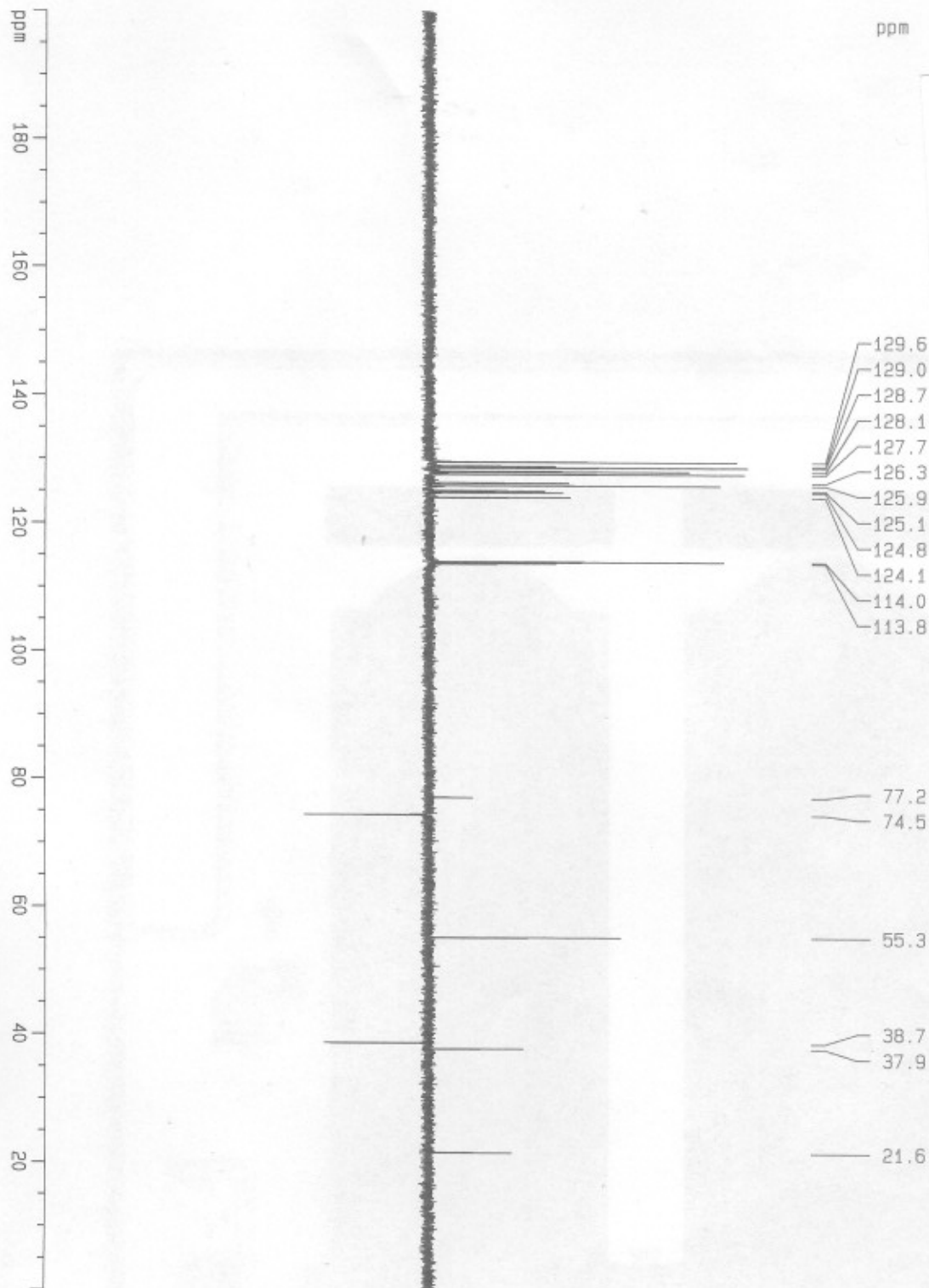
SI	32768
SF	125.7577884 MHz
KCN	EW
SSB	0
LB	1.00 Hz
BB	0
PC	1.00

10 MHz plot parameters

CX	20.00 cm
CY	13.00 cm
F1P	100.000 ppm
F1	22893.88 Hz
F2P	10.000 ppm
F2	1057.55 Hz
PRGCM	9.00000 ppm/cm
KC24	1131.05015 Hz/cm



D'Souza DS-209 in CDCl₃



Current Data Parameters
NAME: DS-209
EXPNO: 4
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20031228
Time: 15.18
INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 512
DS: 2
SWH: 30864.157 Hz
FIDRES: 0.470950 Hz
AQ: 1.0617352 sec
RG: 1825.5
CW: 18.200 usec
DE: 6.00 usec
TE: 298.2 K
CHRG2: 145.0000000 sec
D1: 4.00000000 sec
d2: 0.00344828 sec
d12: 0.00002000 sec
DELTA: 0.00001324 sec

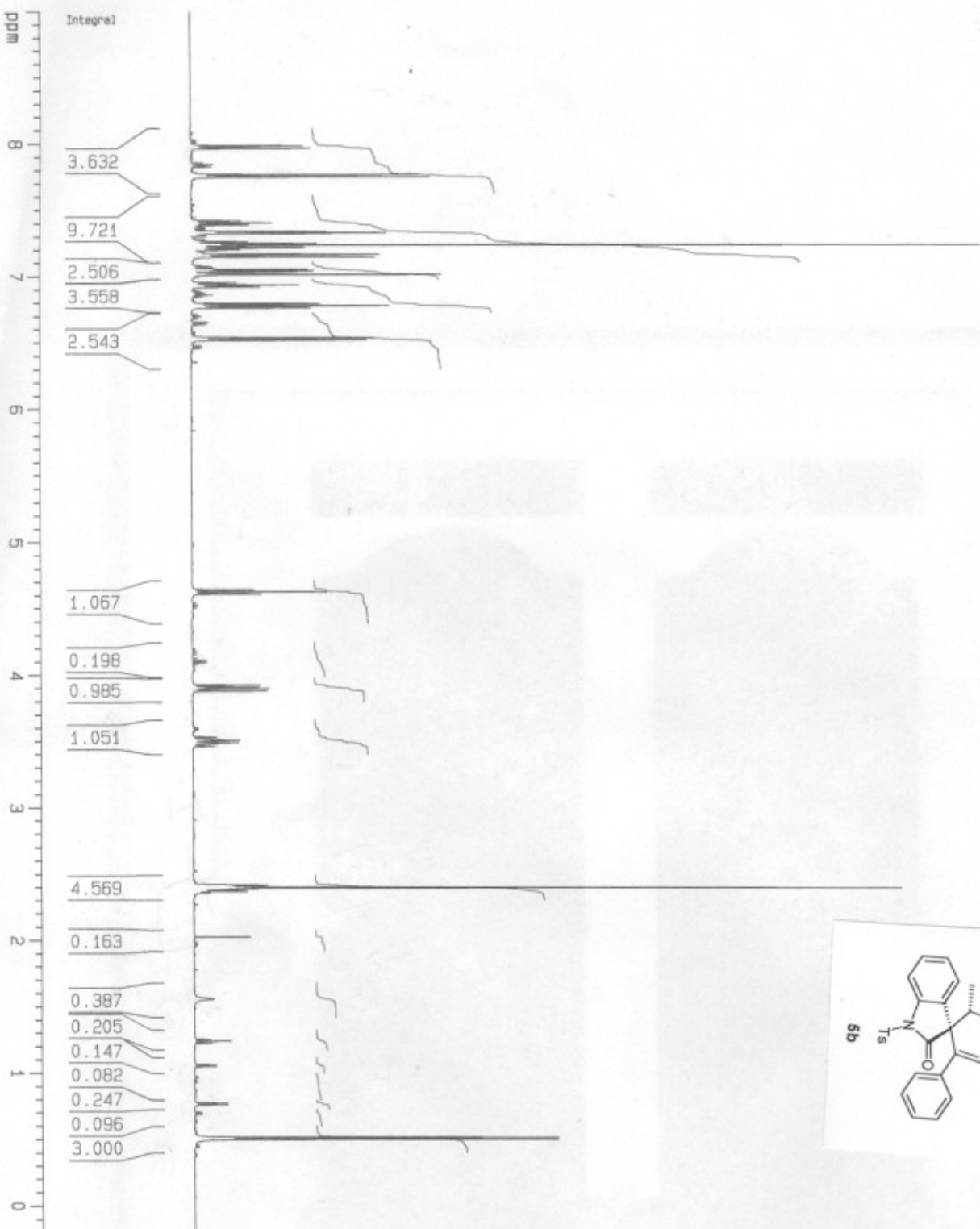
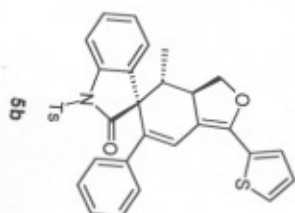
===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
PC1: 155.7713172 MHz

===== CHANNEL f2 =====
CPROG2: waltz16
NUC2: 1H
P2: 16.10 usec
PL2: 0.00 dB
PC2: 100.62 usec
PCPD2: 100.00 usec
PL2: 0.00 dB
PL2: 20.00 dB
PC2: 500.132500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577082 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

10 MHz plot parameters
CX: 20.00 cm
CY: 5.00 cm
FLP: 200.000 kHz
F1: 25151.56 Hz
F2: 0.000 kHz
F3: 0.00 Hz
FREQH: 10.00000 MHz/cm
HCHW: 1257.57894 Hz/cm

D'Souza DS-173 in CDCl3



Current Data Parameters

NAME	mus24re
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20040224
Time	15.09
INSTRUM	spect
PROBHD	5 mm 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	4
SWH	5482.456 Hz
FIDRES	0.167311 Hz
AQ	2.9894915 sec
RG	114
DW	91.200 usec
DE	5.00 usec
TE	298.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	10.10 usec
PL1	0.00 dB
SFO1	500.1322738 MHz

F2 - Processing parameters

SI	16384
SF	500.1300232 MHz
MDW	EH
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	13.00 cm
F1P	9.000 ppm
F1	4501.17 Hz
F2P	-0.200 ppm
F2	-100.03 Hz
PPMCM	0.45000 ppm/cm
HZCM	230.05981 Hz/cm

ppm

176.666

146.603
145.215
140.271
139.307
135.227
134.950
132.678
130.005
129.593
129.198
128.078
127.934
127.766
127.416
126.709
126.597
126.568
126.305
125.754
124.920
123.047
113.402
110.316

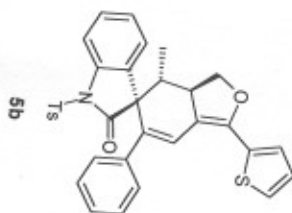
77.250
77.201
76.996
76.742
74.469

59.297

43.941
42.998

21.659

13.330



Current Data Parameters
NAME musc44g
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040224
Time 15.32

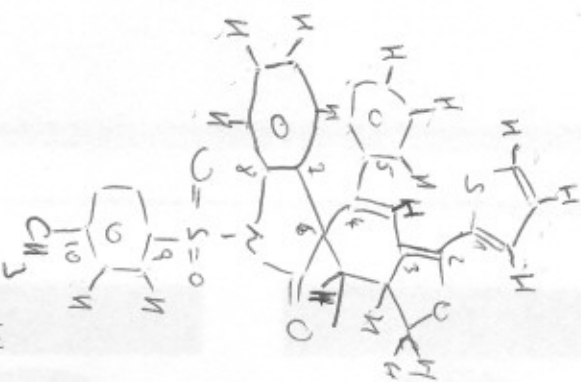
INSTRUM spect
PROBHD 5 mm TBI 51/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1800
DS 2
SWH 30864.197 Hz
FIDRES 0.470920 Hz
AQ 1.0617382 sec
RG 5782.8
DN 16.200 usac
DE 8.00 usac
TE 298.0 K
D1 1.0000000 sec
d11 0.0300000 sec
d12 0.0000000 sec

CHANNEL f1
NUC1 13C
P1 10.40 usac
PL 0.00 dB
SFO1 125.7713172 MHz

CHANNEL f2
NUC2 1H
P2 100.00 usac
PL 0.00 dB
SFO2 500.132500 MHz

F2 - Processing parameters
SI 32768
SF 125.757795 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

10 MHz plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 200.000 ppm
F1 25151.58 Hz
F2P -5.000 ppm
F2 -628.79 Hz
P1PCX 10.25500 ppm/cm
P1PCY 1280.01750 Hz/cm



29

CH : 18 15
CH2 : 1
CH3 : 22 ✓
q : 11

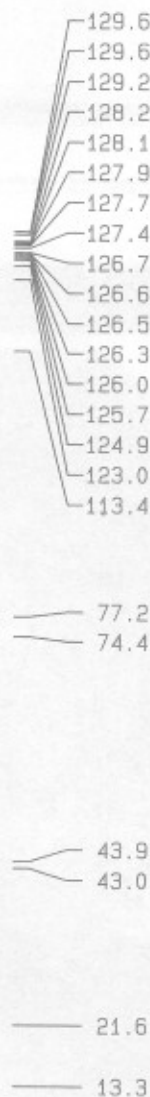
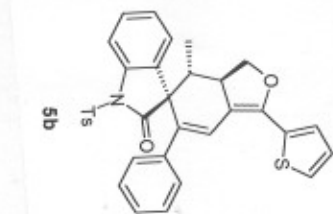
CHN
CH2
CH3
CH3

CH

q

ppm
175
150
125
100
75
50
25
0

D. Souza DS-173 in CDCl3



Current Data Parameters
NAME: musd44e
EXPNO: 3
PROCNO: 1

F2 - Acquisition Parameters
Date_: 2010/02/25
Time: 8.01

INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zgpg30

TD: 65536
SOLVENT: CDCl3

NS: 810
DS: 2

SWH: 30894.197 Hz
FIDRES: 0.470950 Hz

AQ: 1.0617332 sec
RG: 1635.5

NUC1: 13C
NUC2: 1H

DE: 15.200 uSAC
TE: 298.0 K

DW: 140.0000000 sec
DELT2: 4.000000000 sec

DE: 0.00344828 sec
DELT: 0.0002500 sec

DELTA: 0.0001364 sec

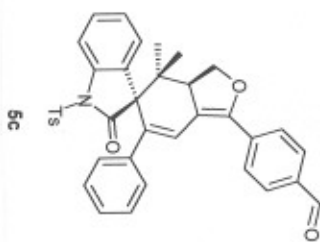
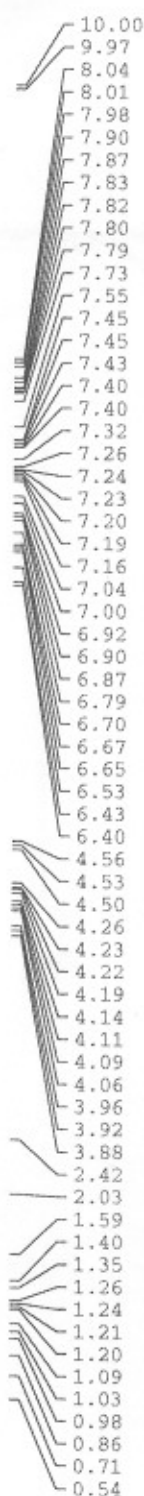
===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 uSAC
PL: 20.00 uSAC
PC: 0.00 dB
SFO1: 125.7713172 MHz

===== CHANNEL f2 =====
INSTRUM: spect
P1: 10.10 uSAC
PL: 20.20 uSAC
PC: 100.00 uSAC
SFO2: 500.1322500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577582 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
FIP: 200.000 50M
F1: 25151.98 Hz
F2: -5.000 50M
F3: -528.73 Hz
PRMCK: 10 25000 ppm/cm
KICK: 1280.01778 Hz/cm

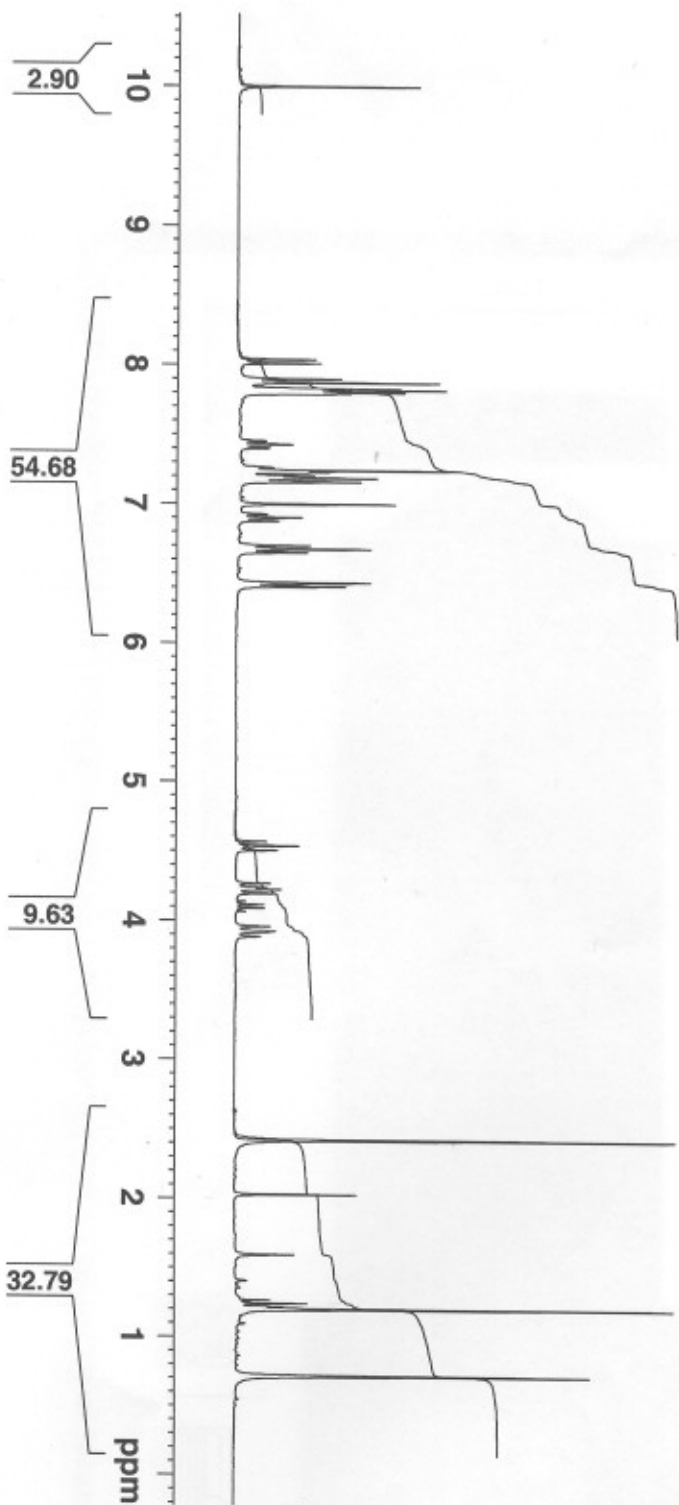
DS-645 MU in CDCL3 D"Souza



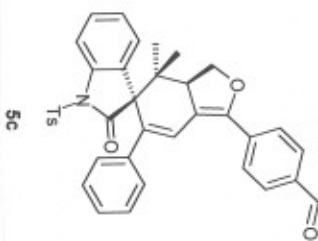
Current Data Parameters
NAME mudsau10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060810
Time 8.39
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 406.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 5.00



DS-645 MU in CDCL3 D'Souza



Current Data Parameters
NAME mudsau10
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060810
Time 8.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1320
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

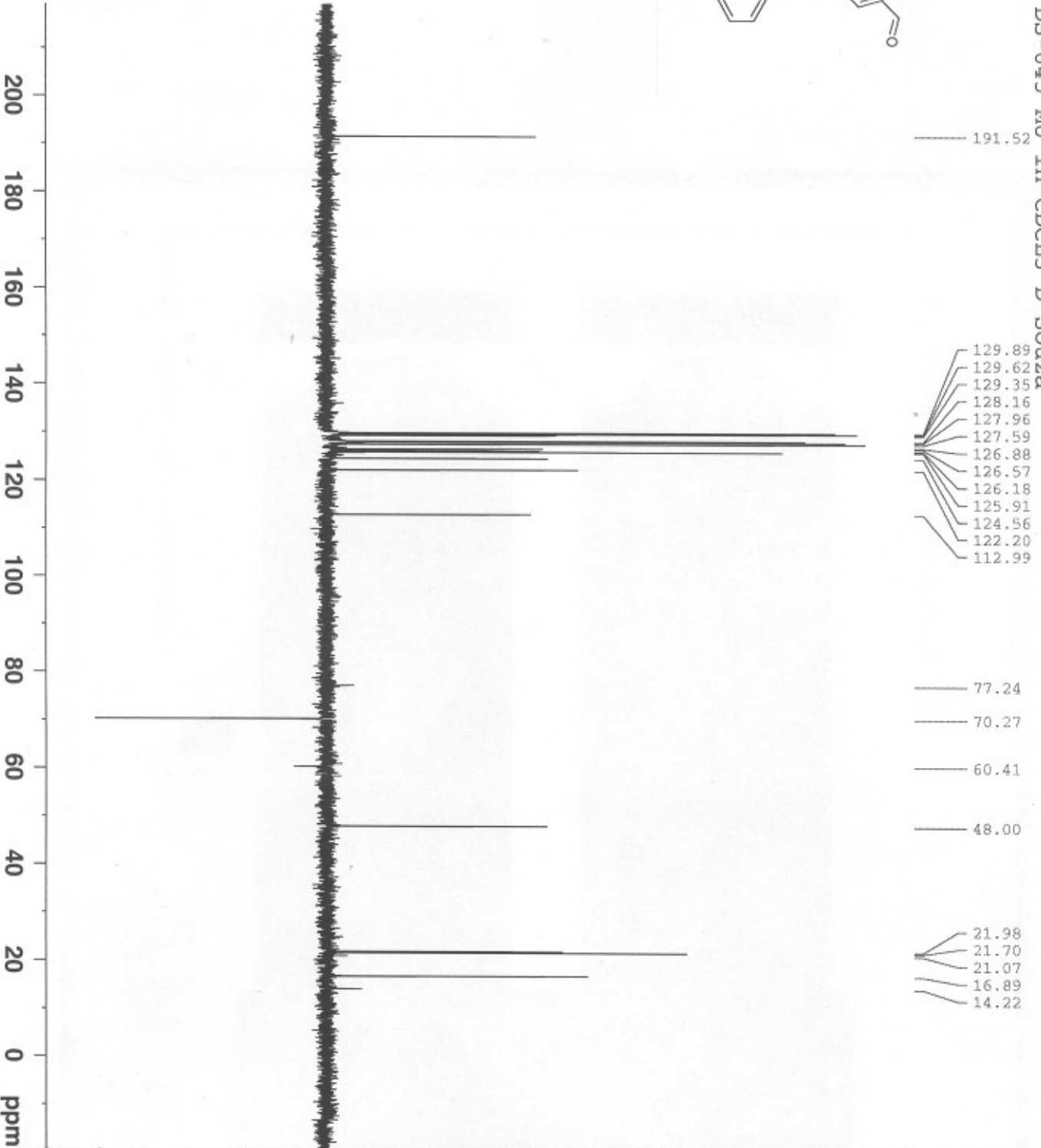
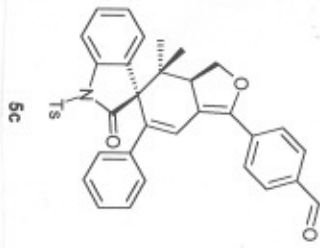
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing Parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



DS-645 MU in CDCL3 D'Souza



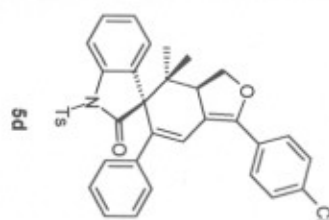
Current Data Parameters
NAME mudsau10
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060810
Time 11.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1280
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.0002000 sec
DELTA 0.0001528 sec
TDO 1

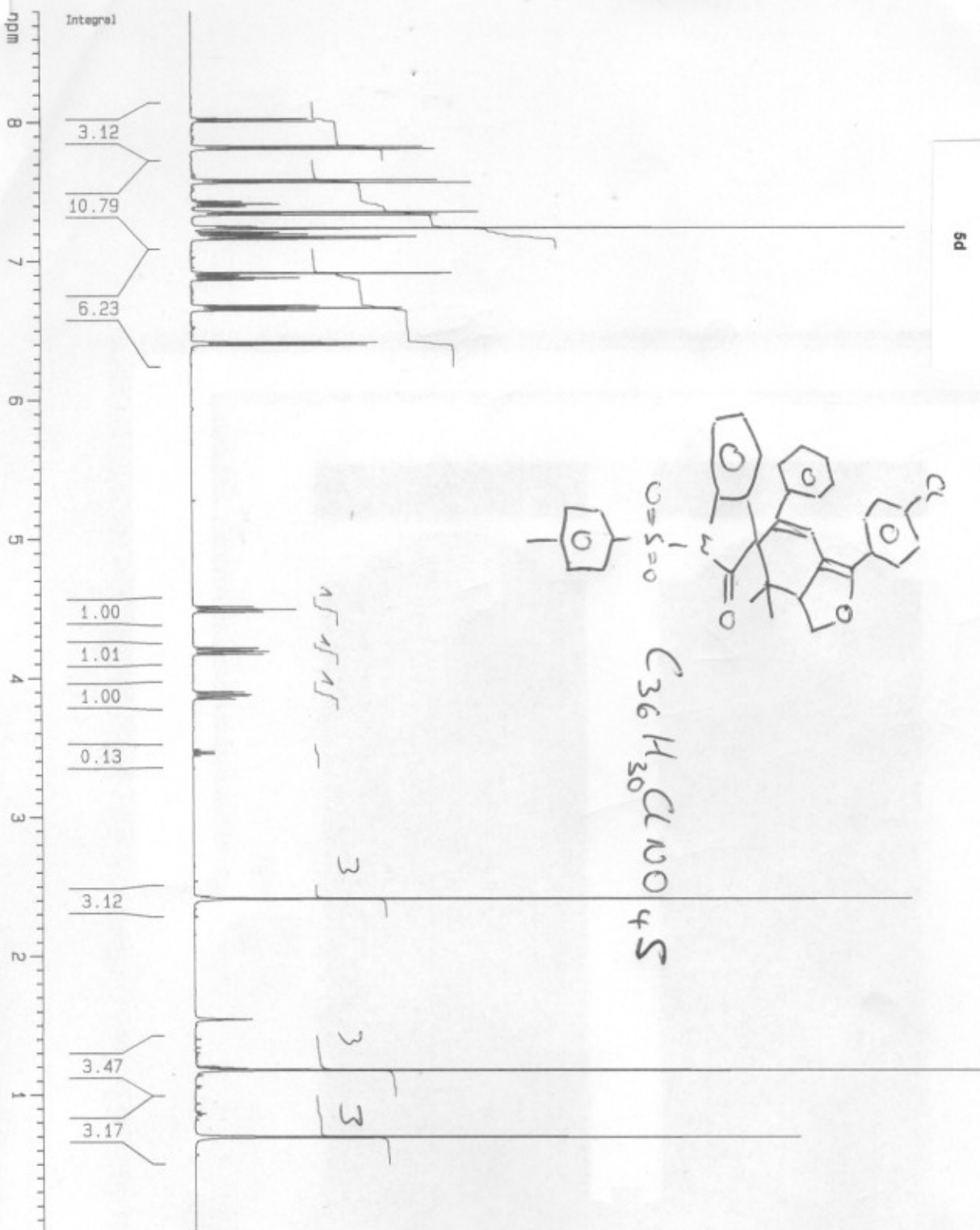
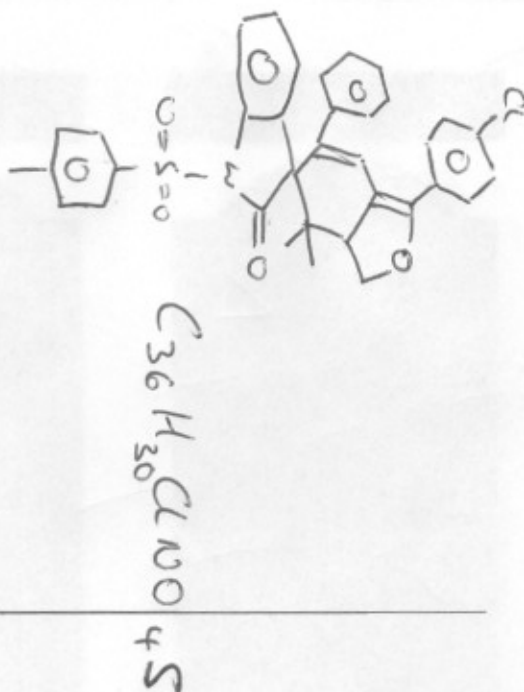
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



D'Souza DS-238 in CDCl₃



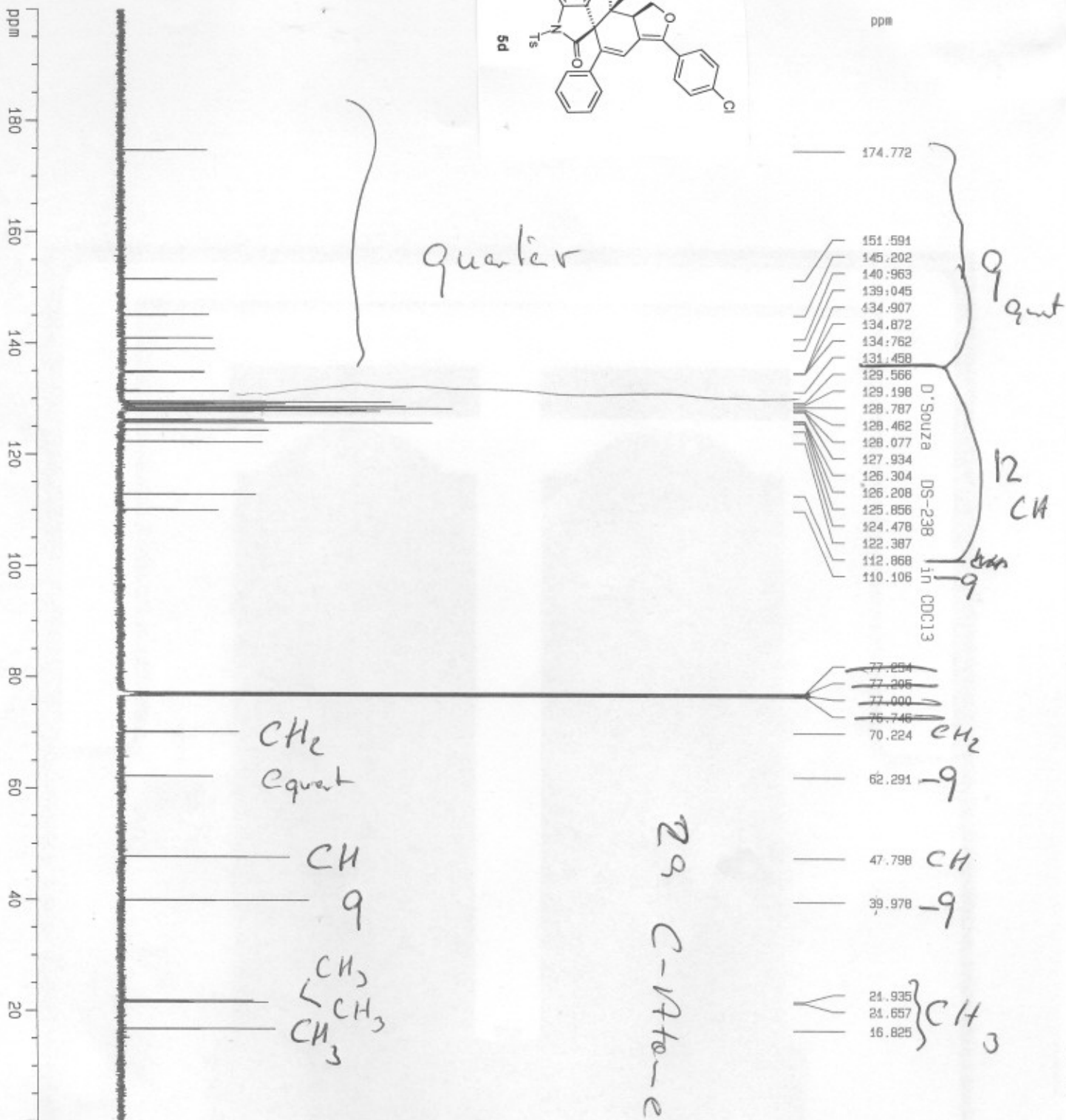
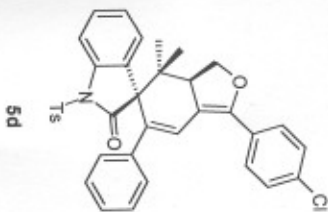
Current Data Parameters
NAME DS-238
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040429
Time 15.22
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 4
SWH 5482.455 Hz
FIDRES 0.167311 Hz
AQ 2.9884915 sec
RG 128
RW 91.200 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SFO1 500.132738 MHz

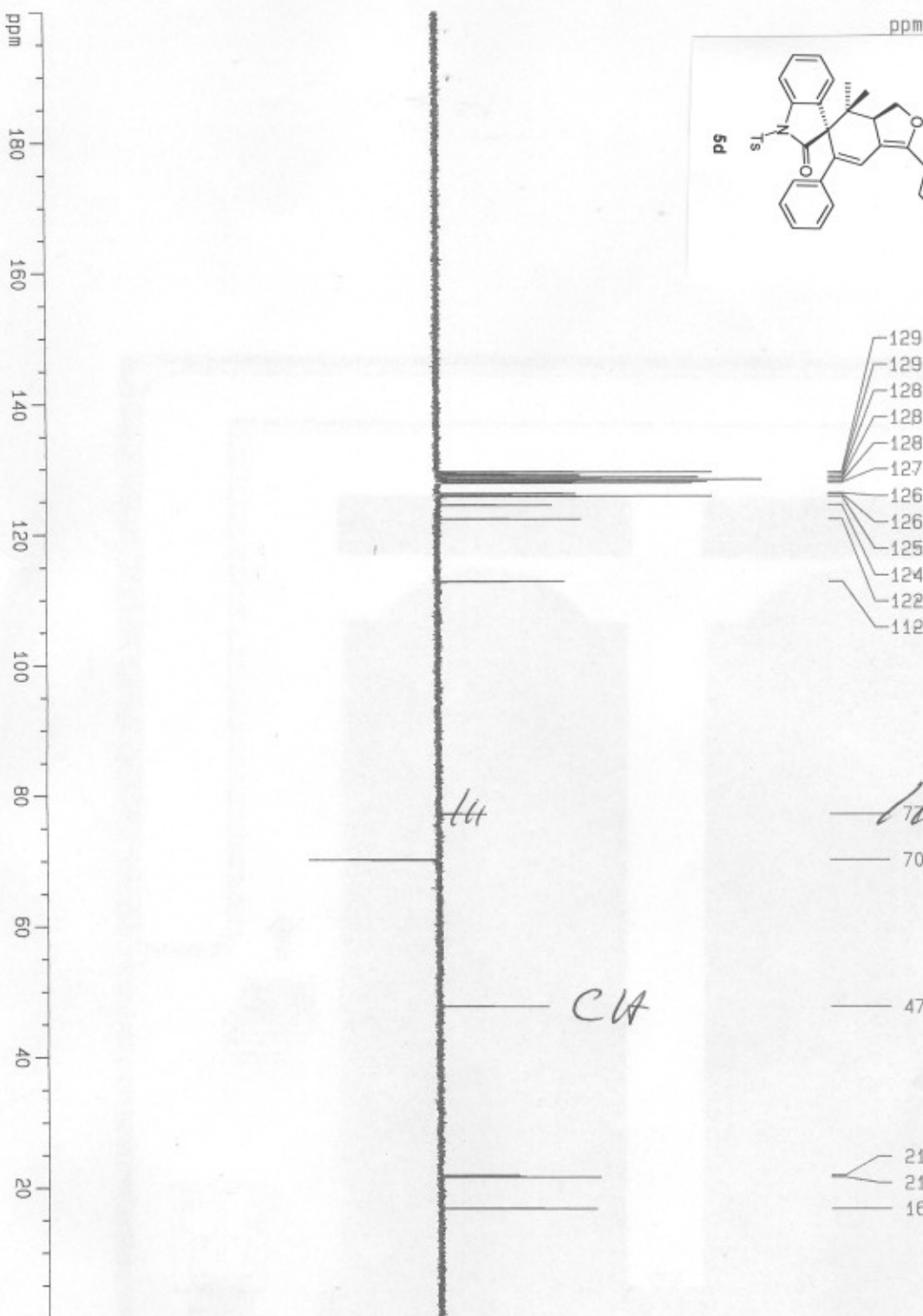
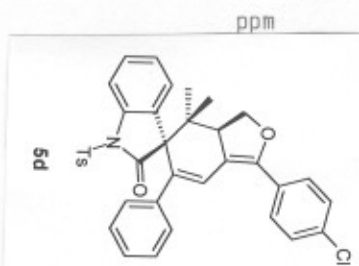
F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 20.00 cm
CY 13.00 cm
FIP 8.800 ppm
F1 4401.14 Hz
F2 0.000 ppm
F2 0.00 Hz
PPMCH 0.44000 ppm/cm
HZCM 220.05722 Hz/cm



Current Data Parameters	
NAME	6003005
EXPNO	2
PROCNO	1
F2 - Acquisition Parameters	
Date_	20040429
Time	21.23
INSTRUM	spect
PROBHD	5 mm TBI 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	2
SWH	30864.187 Hz
FIDRES	0.470550 Hz
AQ	1.0617382 sec
RG	5732.8
DM	16.200 umic
DE	6.00 umic
TE	298.0 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00050000 sec
CHANNEL f1	
NUC1	13C
PC	10.40 umic
PL1	0.00 dB
PR01	125.773172 MHz
CHANNEL f2	
NUC2	1H
PCP2	100.00 umic
PL2	0.00 dB
PL12	20.00 dB
PL13	20.00 dB
PR02	500.132200 MHz
F2 - Processing parameters	
SI	32768
GF	128.7877937 MHz
KCM	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00
10 NMR plot parameters	
EX	20.00 cm
CV	18.27 cm
F4P	200.000 000
F1	25151.56 Hz
F2P	0.000 000
F2	0.00 Hz
PRCKA	10.00000 cps/cm
PRCKB	1287.57000 Hz/cm

D'Souza DS-238 in CDCl3



129.5
129.2
128.8
128.4
128.0
127.9
126.3
126.2
125.8
124.4
122.4
112.8

CH₂ 12

70.2 CH₂

47.8 CH

21.9
21.6
16.8 CH₃

Current Data Parameters
NAME DS-238
EXPNO 3
PROCNO 1

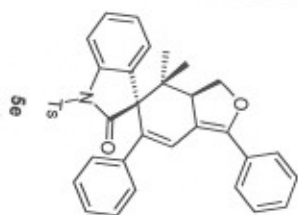
F2 - Acquisition Parameters
Date_ 20040420
Time 1.20
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
RG 2800
GB 2
SWH 30564.157 Hz
FIDRES 0.470850 Hz
AQ 1.0517352 sec
RG 1625.5
DN 16.200 usec
DE 8.00 usec
TE 298.0 K
CHGT2 145.000000 sec
D1 4.00000000 sec
d2 0.00344628 sec
d12 0.00000000 sec
DELTA 0.00001324 sec

===== CHANNEL F1 =====
NUC1 13C
P1 10.40 usec
PL1 20.80 usec
PL1 0.00 dB
SFO1 125.7713172 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
P2 10.10 usec
PL2 20.20 usec
PL2 0.00 dB
SFO2 500.1325291 MHz

F2 - Processing parameters
SI 32768
SF 125.7577682 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

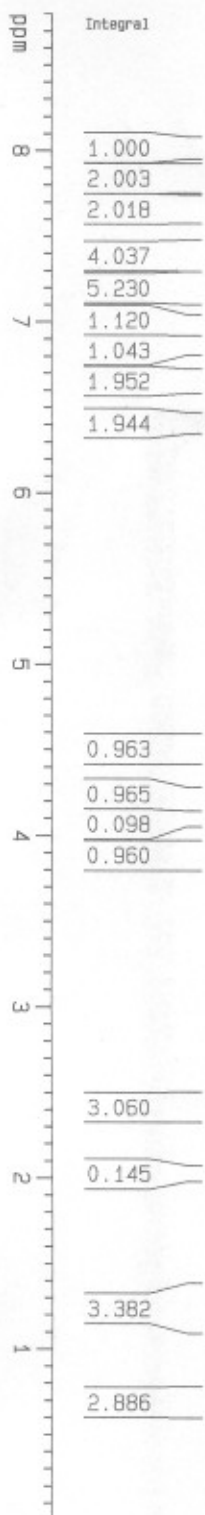
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P 0.000 ppm
F2 0.00 Hz
FREQM 10.00000 ppm/cm
HZCM 1257.57960 Hz/cm



D'Souza DS-227 in CDCl₃

C₃₀ H₃₁ N O₄ S

CH₃ 3
CH₂ 1
CH 14



Current Data Parameters
NAME: muso11de
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20031211
Time: 14.21
INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zg30
TD: 32768
SOLVENT: CDCl₃
NS: 16
DS: 4
SWH: 5482.456 Hz
FIDRES: 0.167311 Hz
AQ: 2.9864915 sec
RG: 101.5
DM: 91.200 usec
DE: 6.00 usec
TE: 298.0 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 10.10 usec
PL1: 0.00 dB
SFO1: 500.1326738 MHz

F2 - Processing parameters
SI: 16384
SF: 500.1300232 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 13.00 cm
F1P: 8.800 ppm
F1: 4401.14 Hz
F2P: 0.000 ppm
F2: 0.00 Hz
PPMCM: 0.44000 ppm/cm
HZCM: 220.05722 Hz/cm

ppm

174.855

152.819

145.133

141.070

138.993

134.916

134.139

131.616

130.725

129.592

129.525

129.084

129.001

128.508

128.000

127.908

127.242

126.242

126.126

125.889

124.431

122.794

112.778

109.535

D'Souza DS-227 in CDCl₃CH₃

77.225

77.176

76.971

76.717

70.160

CH₂

62.273

9

47.729

CH

39.915

9

21.910

21.619

16.790

CH₃

Se

Ts

10

ppm

160

140

120

100

80

60

40

20

9

9

9

4

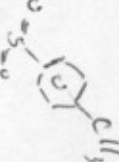
9

CH₂

9

CH

9

CH₃/CH₂CH₂ : 1CH₃ : 3

CH : 14

9 : 12

C : 30

2

Current Data Parameters
NAME: 20031212
EXPNO: 5
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20031212
Time: 5.32
INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 9600
DS: 2
SWH: 30854.197 Hz
FIDRES: 0.470500 Hz
AQ: 1.0517330 sec
RG: 67382.8
DM: 16.200 umic
DE: 6.50 umic
TE: 298.0 K
D1: 1.00000000 sec
d11: 0.03000000 sec
d12: 0.00020000 sec

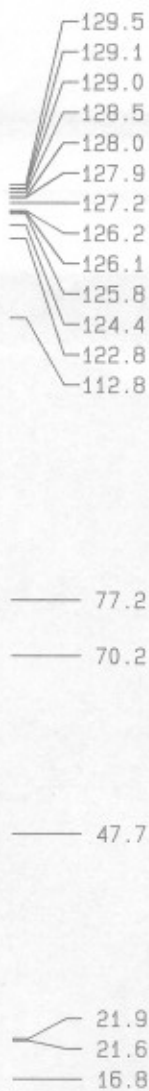
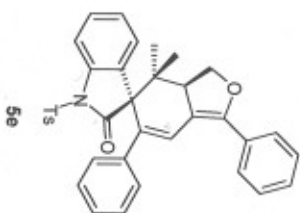
CHANNEL F1
NUC1: 13C
P1: 10.40 umic
PL1: 0.00 dB
SFO1: 125.771372 MHz

CHANNEL F2
CPDPRG2: naltz16
NUC2: 1H
P2: 190.00 umic
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 500.1362600 MHz

F2 - Processing parameters
SI: 32768
SF: 125.757764 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 13.00 cm
F1P: 150.000 ppm
F1: 23993.98 Hz
F2P: 0.000 ppm
F2: 0.00 Hz
FREQH: 9.50000 ppm/cm
H1CN: 1194.89810 Hz/cm

D'Souza DS-227 in CDCl3



Current Data Parameters
NAME: mus01108
EXPNO: 7
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20031212
Time: 7.26
INSTRUM: spect
PROBHD: 5 mm BBI 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 1180
DS: 2
SWH: 30064.187 Hz
FIDRES: 0.473650 Hz
AQ: 1.0617262 sec
RG: 1665.5
CW: 16.200 usec
DE: 0.00 usec
TE: 296.0 K
CHST2: 1.4E+000000
D1: 4.0000000 sec
d2: 0.00344698 sec
d12: 0.0002000 sec
DELTA: 0.0001324 sec

CHANNEL f1
NUC1: 13C
P1: 10.40 usec
PL1: 20.00 dB
SFO1: 125.7713172 MHz

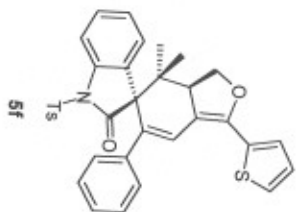
CHANNEL f2
NUC2: 1H
P2: 10.10 usec
PL2: 20.00 dB
SFO2: 500.1322000 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577982 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

10 MHz plot parameters
CX: 20.00 cm
CY: 5.00 cm
FIP: 190.000 ppm
F1: 22893.96 Hz
F2: 0.00 Hz
PPOW: 9.50000 dB/cm
H2O: 1154.59910 Hz/cm

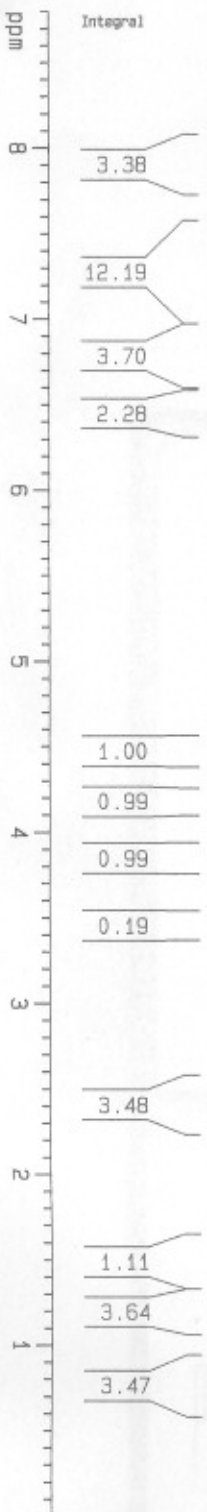
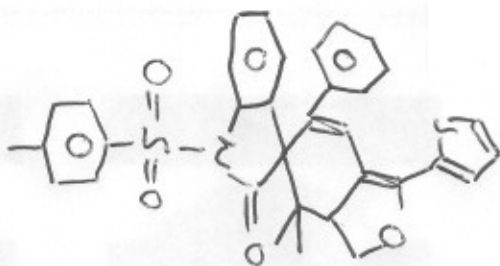
ppm

160
140
120
100
80
60
40
20



D'Souza DS-240 in CDCl3

C₃₄H₂₉N₂O₄S₂



Current Data Parameters
 NAME: DS-240
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20040429
 Time: 7.41
 INSTRUM: spect
 PROBHD: 5 mm TBI 1H/13
 PULPROG: zg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 4
 SMH: 5482.456 Hz
 FIDRES: 0.157314 Hz
 AQ: 2.9884915 sec
 RG: 143.7
 DW: 91.200 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 1.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 10.10 usec
 PL1: 0.00 dB
 SFO1: 500.1362738 MHz

F2 - Processing parameters
 SI: 16384
 SF: 500.1360232 MHz
 FIDM: EM
 SSB: 0
 LB: 0.10 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 20.00 cm
 CY: 13.00 cm
 F1P: 6.800 ppm
 F1: 4401.44 Hz
 F2P: 0.000 ppm
 F2: 0.00 Hz
 PPMCH: 0.44000 ppm/cm
 HZCH: 220.05722 Hz/cm

ppm

160

140

120

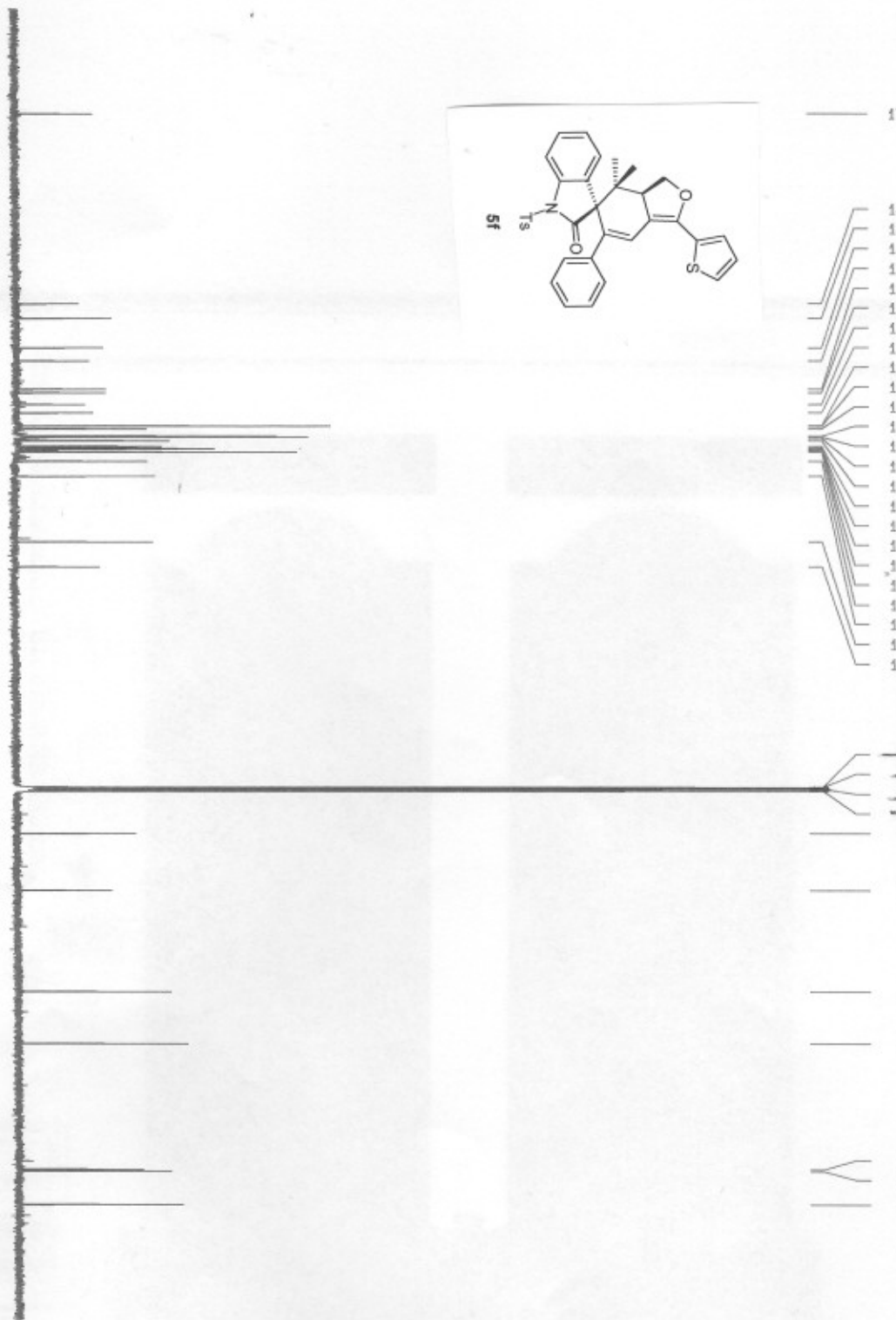
100

80

60

40

20



99

9

-CH₂

9

CH₂

9

CH₃

ppm

174.818

147.320

145.202

140.934

139.002

134.926

134.387

132.718

131.501

129.645

129.574

129.165

128.086

127.959

127.856

127.436

126.626

126.358

126.250

126.052

125.848

124.492

122.305

112.831

109.185

77.236

77.208

77.092

76.748

70.560

62.335

47.661

40.165

21.927

21.658

16.827

5f

TS

Current Data Parameters

NAME: 20040428

EXPNO: 3

PROCNO: 1

F2 - Acquisition Parameters

Date_: 20040428

Time: 22.30

INSTRUM: spect

PROBHD: 5 mm TBI 1H/13

PULPROG: zgpg30

TD: 65536

SOLVENT: CDCl3

NS: 1000

DS: 2

SWH: 30964.107 Hz

FIDRES: 0.470385 Hz

AQ: 1.081732 sec

RG: 579.2

DE: 16.200 usec

TE: 298.2 K

DE: 6.00 usec

U1: 1.0000000 sec

U2: 0.0300000 sec

U3: 0.0002000 sec

CHNCL: CHANNEL f1

NUC1: 13C

P1: 30.40 usec

PL1: 0.00 dB

SE1: 125.773172 MHz

CHNCL: CHANNEL f2

NUC2: 1H

P2: 150.00 usec

PL2: 0.00 dB

SE2: 500.132500 MHz

F2 - Processing parameters

SI: 32768

SF: 125.757707 MHz

WDW: EM

SSB: 0

LB: 1.00 Hz

GB: 0

PC: 1.00

1D NMR plot parameters

EX: 20.00 cm

CV: 18.92 cm

FLP: 180.000 ppm

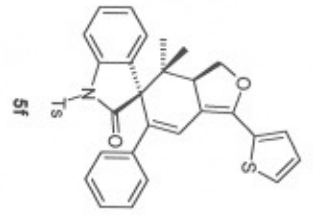
FL: 23859.98 Hz

F2P: 0.000 ppm

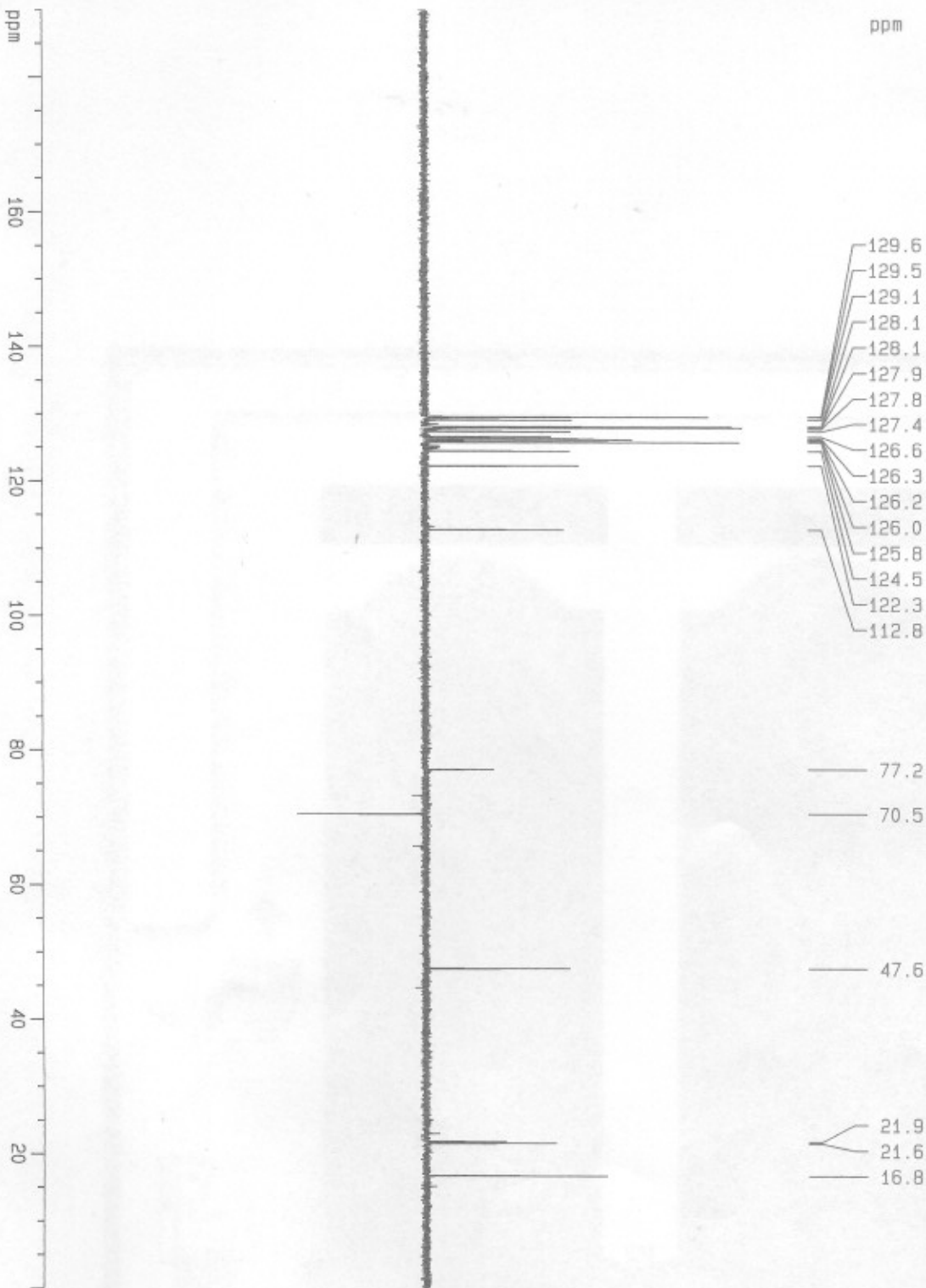
F2: 0.00 Hz

PPMCK: 9.50000 ppm/cm

PCCK: 1194.60010 Hz/cm



D'Souza DS-240 in CDCl₃



Current Data Parameters
NAME DS-240
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040229
Time 2.27
INSTRUM spect
PROBHD 5 mm BBI 5H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 2560
DS 2
SWH 30864.197 Hz
FIDRES 0.470950 Hz
AQ 1.0617352 sec
RG 1605.5
CH 16.200 umsc
DE 6.00 umsc
TE 298.2 K
CHRG2 146.0000000 sec
D1 4.00000000 sec
D2 0.00000000 sec
D12 0.00000000 sec
DELTA 0.00001584 sec

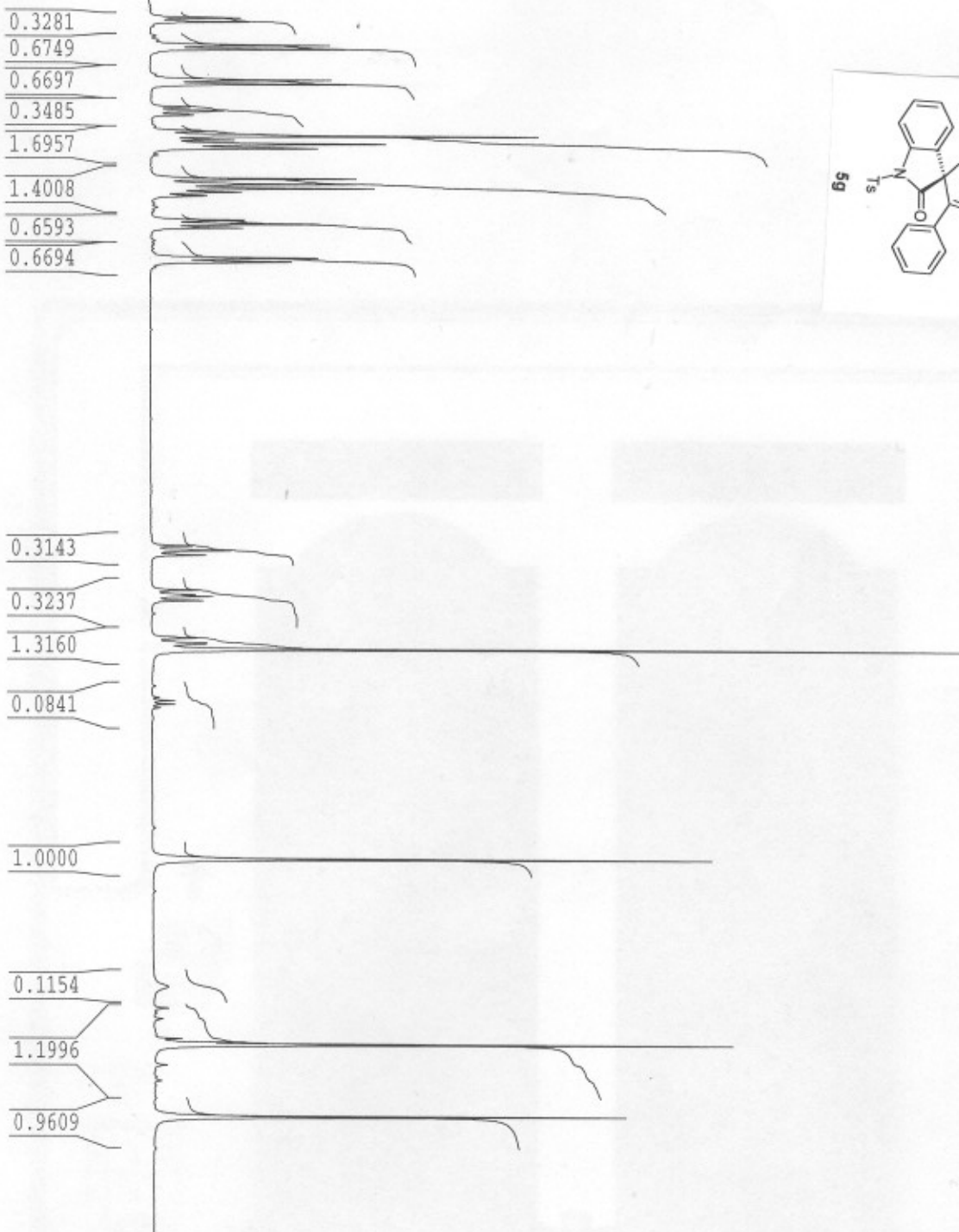
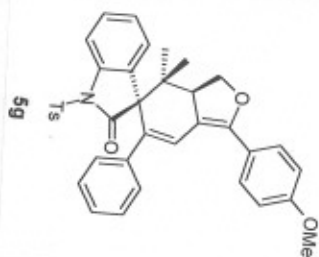
CHANNEL F1
NUC1 13C
P1 10.40 umsc
PL1 0.00 dB
SFO1 125.7713172 MHz

CHANNEL F2
NUC2 1H
P2 10.10 umsc
PL2 0.00 dB
SFO2 500.1327500 MHz

F2 - Processing parameters
SI 32768
SF 125.7677082 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

10 MHz plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 160.000 DDM
F1 22695.98 Hz
F2P 0.000 DDM
F2 0.00 Hz
PRMCM 9.50000 DDM/cm
H2CM 1194.65910 Hz/cm

DS_194 in CDCl3



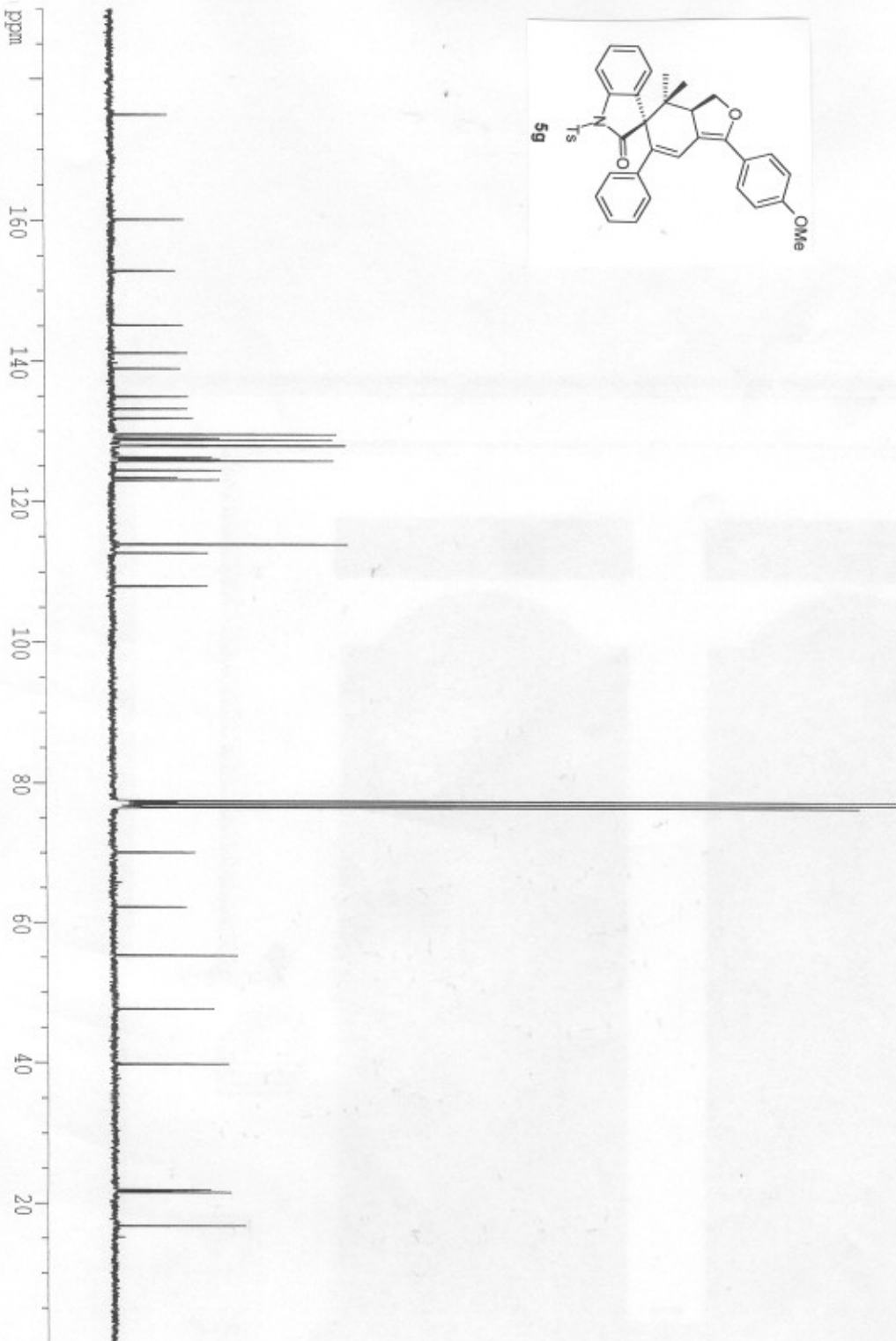
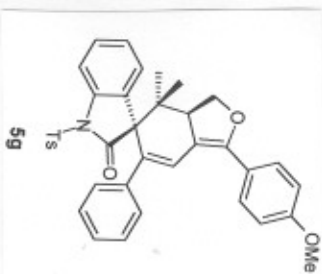
Current Data Parameters
NAME mz6musc
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040327
Time 9.16
INSTRUM spect
PROBHD 5 mm TBI 1H/3
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 181
RW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 300.1300120 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FLP 8.663 ppm
F1 2599.92 Hz
F2P -0.096 ppm
F2 -28.77 Hz
PNUCM 0.43792 ppm/cm
HSCM 131.43439 Hz/cm



ppm

174.979	9
160.199	9
152.863	9
145.134	9
141.213	9-5
138.973	9
134.970	9
133.234	9
131.817	9
129.540	9
129.038	9
128.720	9
128.008	9
127.935	9
126.284	9
126.012	9
125.808	9
124.425	9
123.385	9
123.024	9
113.981	9
112.744	9
108.030	9
77.431	9
77.201	9
76.998	9
76.574	9
70.103	CH ₂
62.234	9
55.317	CH ₃
47.697	CH
39.810	9
21.936	CH ₃
21.634	CH ₃
16.793	CH ₃

D'Souza DS_194 in CDCl₃

Current Data Parameters

NAME	m26mso
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20040327
Time	12.18
INSTRUM	spect
PROBHD	5 mm TBI 1H/3
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl ₃
NS	4000
DS	2
SWH	22675.736 Hz
FIDRES	0.692009 Hz
AQ	0.7225844 sec
RG	2048
DW	22.050 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec

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

NUC1	13C
PL	11.00 usec
PL1	-6.00 dB
SFO1	75.4752160 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	0.00 dB
PL12	24.00 dB
PL13	26.00 dB
SFO2	300.1316507 MHz

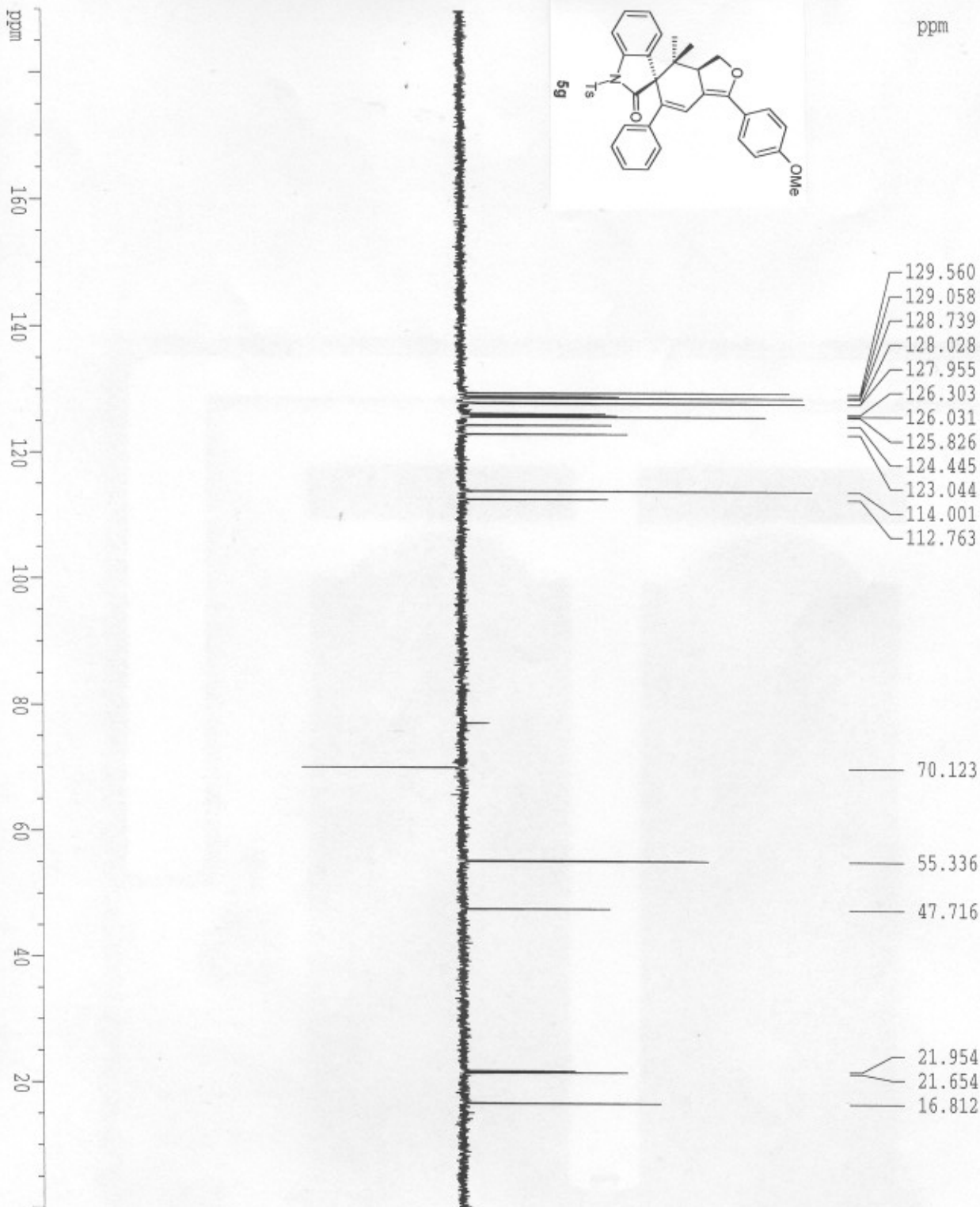
F2 - Processing parameters

SI	32768
SF	75.4677520 MHz
MDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	0.50

ID NMR plot parameters

CK	20.00 cm
PIF	190.000 ppm
F1	14338.87 Hz
F2P	0.000 ppm
F2	0.00 Hz
PPM/K	9.50000 ppm/cm
HZ/C	716.94360 Hz/cm

D'Souza DS_194 in CDCl3



Current Data Parameters

NAME	m26mso
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20040327
Time	13.50
INSTRUM	spect
PROBHD	5 mm TBI 1H/3
PULPROG	depc135
TD	32768
SOLVENT	CDCl3
NS	2000
DS	8
SWH	22675.736 Hz
FTIDRES	0.692009 Hz
AQ	0.725844 sec
RG	5792.6
TDW	22.050 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
D2	0.00345000 sec
D12	0.00002000 sec
DELTA	0.00001401 sec

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

NUC1	13C
P1	11.00 usec
P2	22.00 usec
PL1	-6.00 dB
SFO1	75.6752160 MHz

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

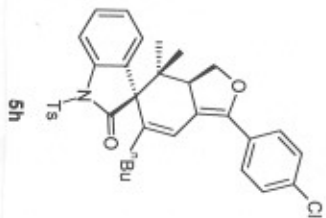
CPDPRG2	waltz16
MUFC2	1H
P3	8.50 usec
P4	17.00 usec
PCPD2	100.00 usec
PL2	0.00 dB
PL12	24.00 dB
SFO2	300.1316507 MHz

F2 - Processing parameters

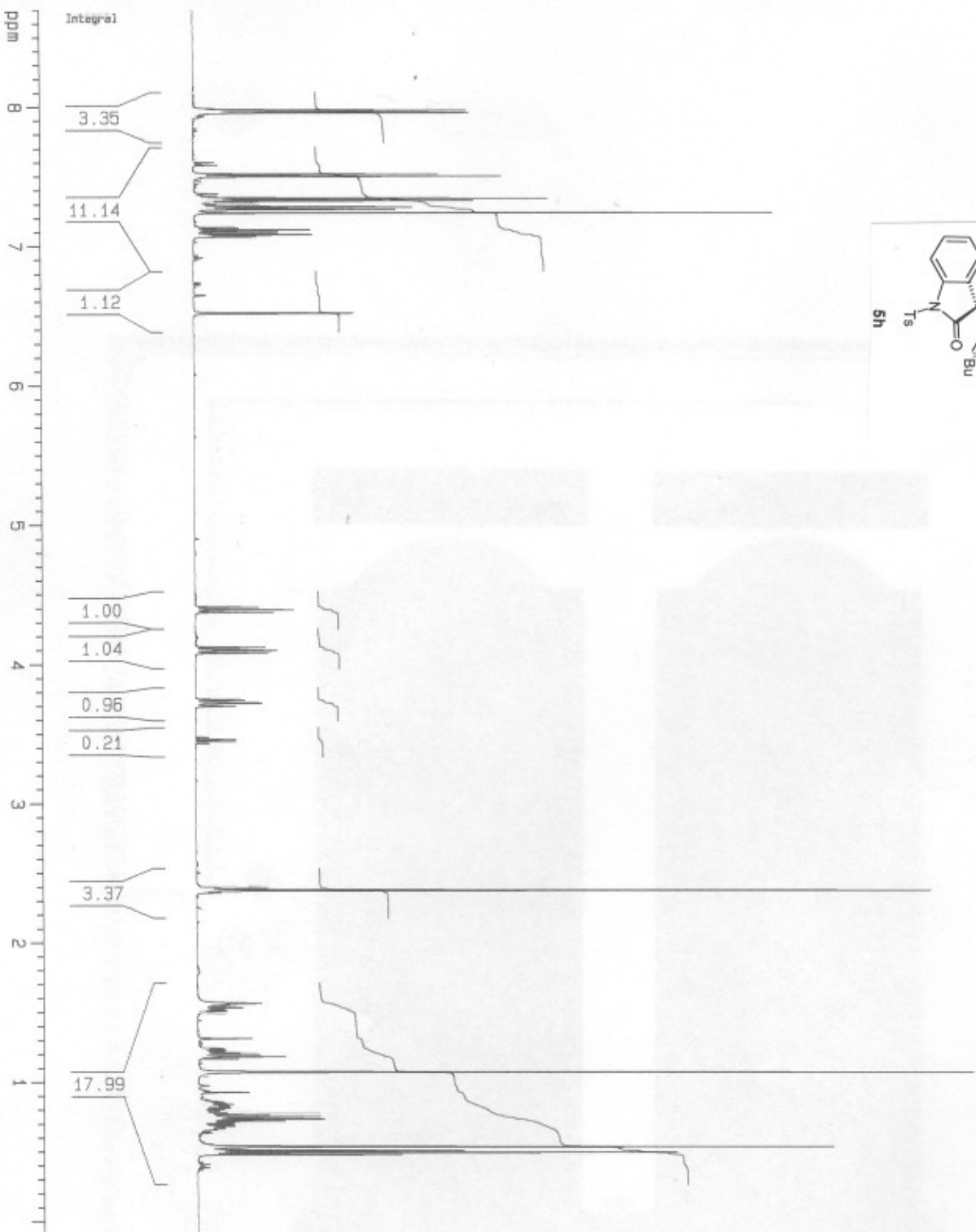
SI	32768
SF	75.4677506 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
PLP	190.000 ppm
F1	14338.87 Hz
F2P	0.000 ppm
F2	0.00 Hz
PPMCM	9.50000 ppm/cm
HZCM	716.94360 Hz/cm



D'Souza DS-237 in CDCl₃



Current Data Parameters
NAME muscodine
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040504
Time 7.45
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 4
SWH 5482.458 Hz
FIDRES 0.167311 Hz
AQ 2.5684915 sec
RG 101.6
DM 91.200 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec

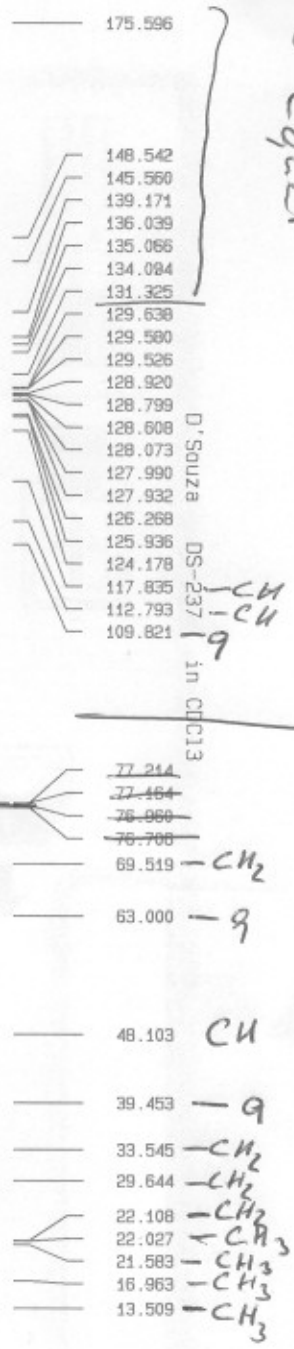
===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SFO1 500.1362736 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

13 NMR plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 9.700 ppm
F1 4351.13 Hz
F2P -0.100 ppm
F2 -50.01 Hz
PPMCK 0.44000 ppm/cm
HCM 220.05722 Hz/cm

8 Count

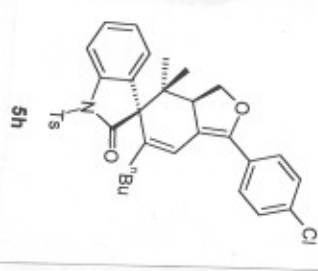
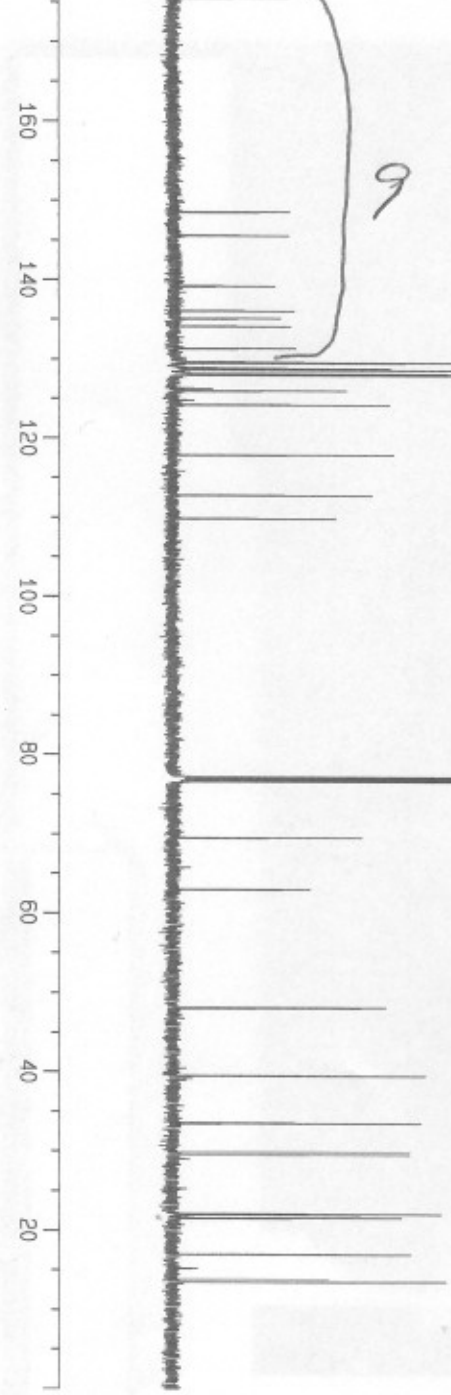
ppm



CH₃: 4
CH₂: 4
CH: 10
9: 12

9

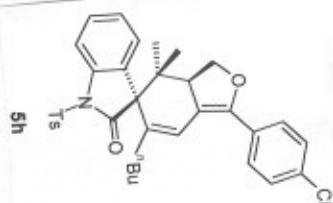
ppm



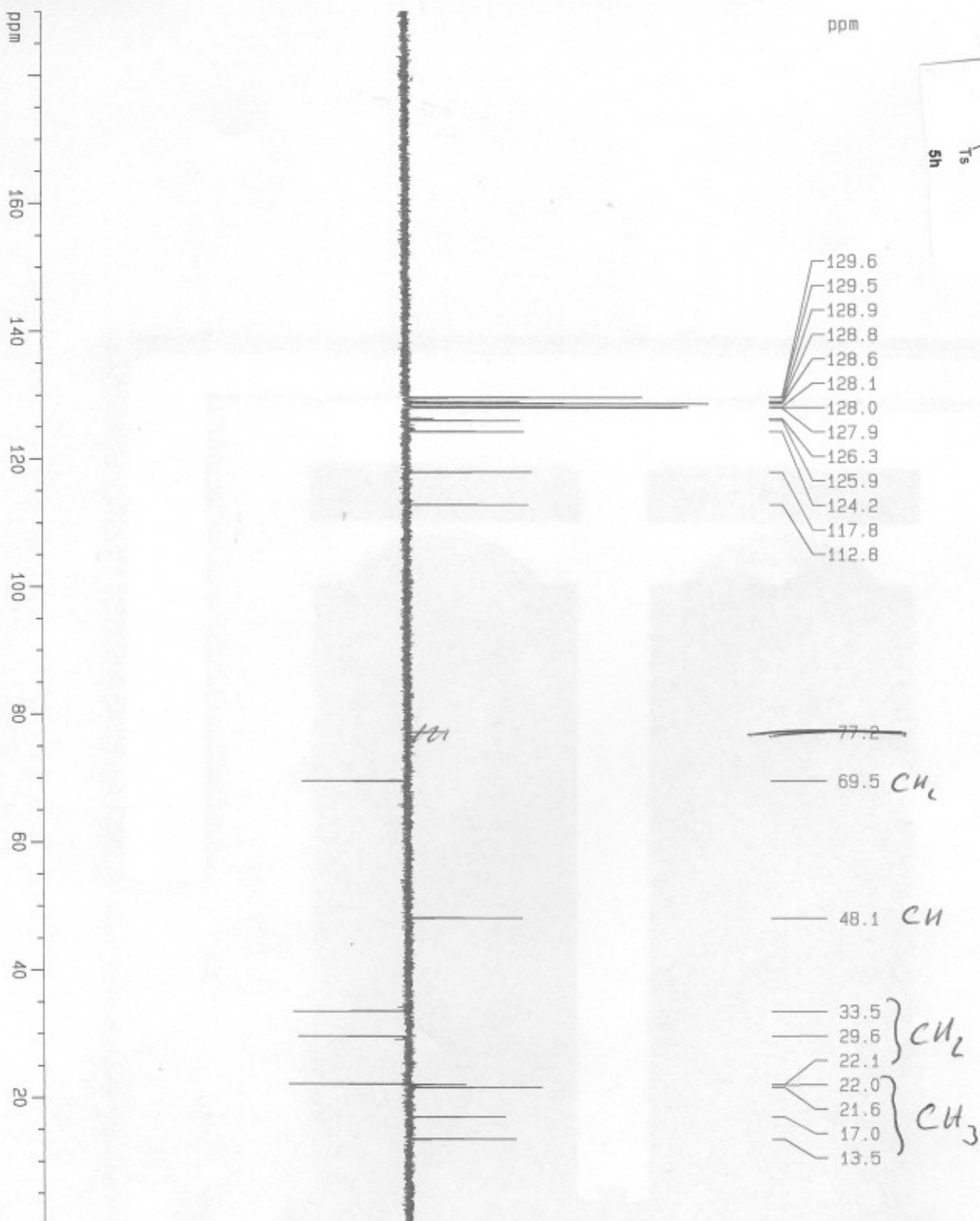
4CH₃
4CH₂
1CH
29

us 220

Current Data Parameters	Parameter	Value
NAME	5h	
EXPNO	2	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20040504	
Time	10.06	
INSTRUM	nmr	
PROBHD	5 mm TBI 1H/13	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	4000	
DS	2	
SWH	50814.187 Hz	
FIDRES	0.470561 Hz	
AQ	1.061232 sec	
RG	5792.8	
DE	18.200 umsc	
TE	5.00 umsc	
DE	398.9 K	
D1	1.0000000 sec	
D11	0.0300000 sec	
D12	0.0000000 sec	
CHNMR CHANNEL F1		
NUC1	13C	
P1	10.40 umsc	
PL1	0.00 dB	
SFO1	125.773172 MHz	
CPDPRG2	zgpg30	
NUC2	1H	
PCPD2	100.00 umsc	
PL2	0.00 dB	
PL12	20.00 dB	
PL13	20.00 dB	
SFO2	500.132500 MHz	
F2 - Processing parameters		
SI	32768	
SF	125.757784 MHz	
WID	EW	
BBB	0	
LB	1.00 Hz	
GB	0	
PC	1.00	
10 MHz plot parameters		
CA	20.00 cm	
CT	13.00 cm	
F1P	180.000 ppm	
F1	23813.38 Hz	
F2P	0.000 ppm	
F2	0.00 Hz	
PPHCK	9.150000 ppm/cm	
HZCM	1194.189110 Hz/cm	



D'Souza DS-237 in CDCl₃



Current Data Parameters
NAME: DS-237
EXPNO: 3
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20040504
Time: 10.35
INSTRUM: spect
PROBHD: 5 mm 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl₃
NS: 2
DS: 2
SWH: 30164.157 Hz
FIDRES: 0.40350 Hz
AQ: 1.081733 sec
RG: 16.620
ZM: 16.620
ZC: 0.00
TE: 298.15 K
DELTA: 1.45000000 sec
O1: 4.00000000 sec
O2: 0.00344628 sec
O3: 0.00025000 sec
O4: 0.00013584 sec

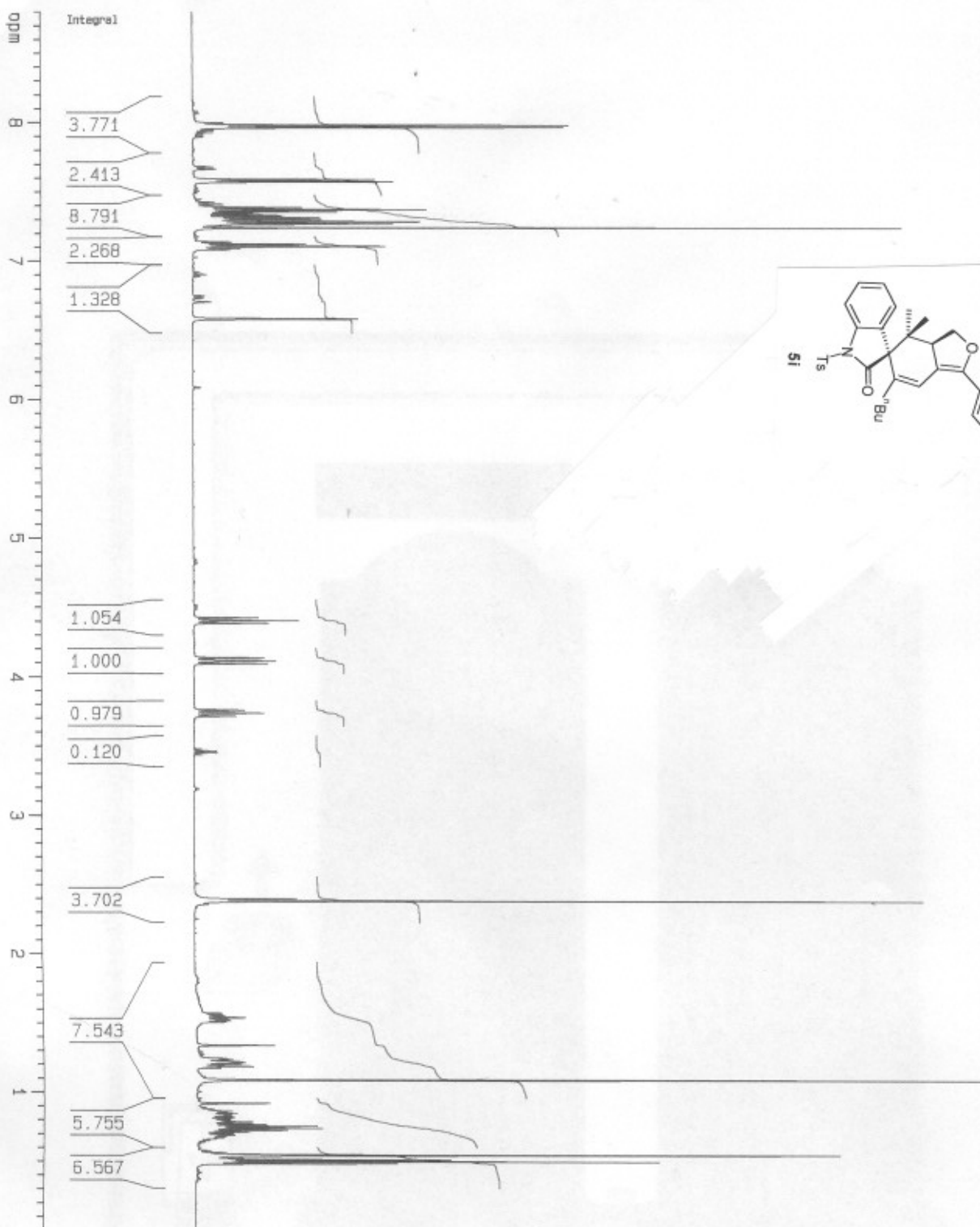
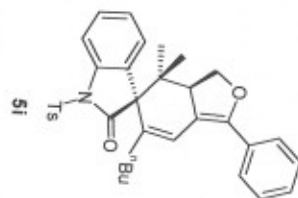
CHANNEL f1
NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
SFO1: 125.7713172 MHz

CHANNEL f2
NUC2: 1H
P2: 10.10 usec
PL2: 0.00 dB
SFO2: 500.132500 MHz

F3 - Processing parameters
SI: 32768
SF: 125.7577083 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.05

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
FLP: 190.000 DPH
F1: 22893.98 Hz
F2P: 0.000 DPH
F2: 0.00 Hz
FPMN: 9.35000 DPH/cm
H2O: 1194.58910 Hz/cm

D'Souza DS-195 in CDCl3



Current Data Parameters

NAME	DS-195
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20040422
Time	10.32
INSTRUM	nmr1
PROBHD	5 mm TBI 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	4
SWH	5492.466 Hz
FIDRES	0.167311 Hz
AQ	2.5984915 sec
RG	114
DW	91.200 usec
DE	6.00 usec
TE	298.0 K
D1	1.00000000 sec

CHANNEL f1

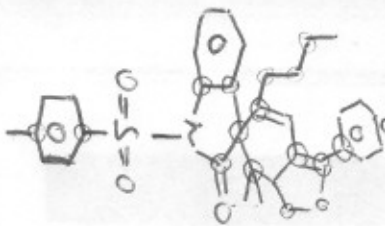
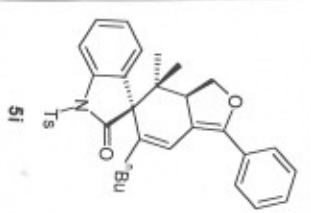
NUC1	1H
P1	10.10 usec
PL1	0.00 dB
SFO1	500.1322798 MHz

F2 - Processing parameters

SI	16384
SF	500.1300232 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	13.00 cm
F1P	8.800 ppm
F1	4401.14 Hz
F2P	0.000 ppm
F2	0.00 Hz
PPMCH	0.44000 ppm/cm
HZCM	220.05722 Hz/cm



ppm

175.762

149.771
145.562
139.202
135.883
135.316
135.145
131.563
131.232
130.016
129.720
129.614
129.557
128.763
128.476
128.424
128.329
128.043
127.983
127.356
126.919
126.052
125.175
124.590
124.200
118.270
112.779
109.291

D'Souza DS-195 in CDCl3

77.253
77.203
76.996
76.744
69.534

63.068

48.109

39.477
39.366
29.717
29.188
22.154
22.084
21.625
17.008
13.556

CH₃: 4
CH₂: 4
CH: 11
Cquad: 11

Current Data Parameters
NAME: mms2cap
EXPNO: 5
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20040423
Time: 7.45
INSTRUM: spect
PROBHD: 5 mm TBI HX/13
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 2600
DS: 4
SWH: 30554.187 Hz
FIDRES: 0.477056 Hz
AQ: 1.0617358 sec
RG: 0.792, 0
DM: 10, 200 usec
DE: 5.00 usec
TE: 298.0 K
D1: 2.00000000 sec
d11: 0.03000000 sec
d12: 0.00000000 sec

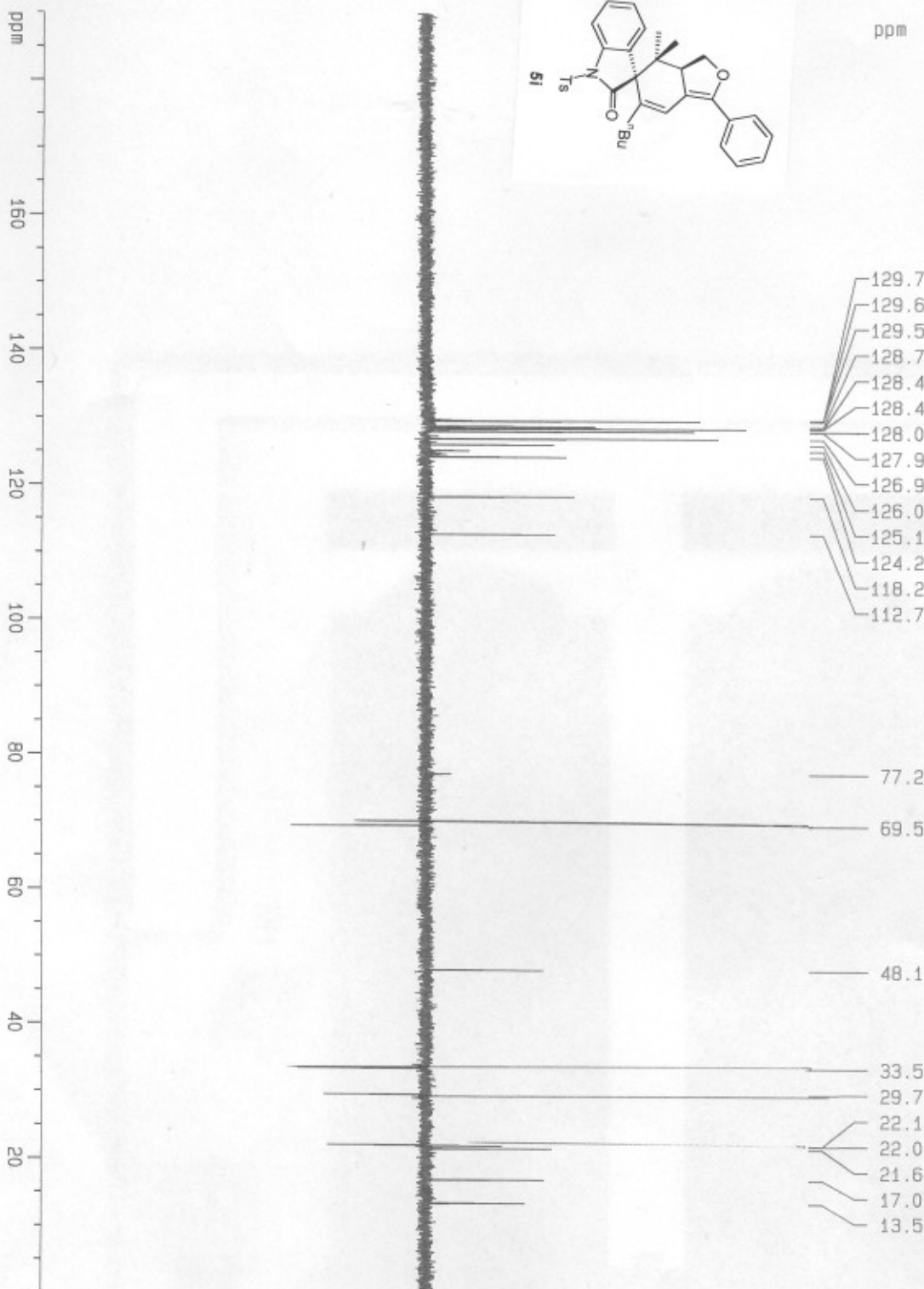
CHANNEL: f1
NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
SFO1: 125.7713172 MHz

CHANNEL: f2
NUC2: 1H
P2: 100.00 usec
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 500.132501 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577058 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 21.02 cm
F1P: 180.000 MHz
F2P: 22893.98 Hz
F2: 0.000 MHz
P2CH: 9.05000 MHz/cm
H2CH: 1504.85807 Hz/cm

D'Souza DS-195 in CDCl3



Current Data Parameters
NAME: DS-195
EXPNO: 4
PROCNO: 1

F2 - Acquisition Parameters
Date_: 200402
Time: 15.11
INSTRUM: spect
PROBHD: 5 mm TBI 51/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 720
DS: 2
SWH: 30064.197 Hz
FIDRES: 0.479550 Hz
AQ: 1.0617352 sec
RG: 1825.5
IN: 16.200 usec
DE: 6.00 usec
TE: 298.0 K
DMSD2: 146.0000000
D1: 4.00000000 sec
d2: 0.00344828 sec
d12: 0.00000000 sec
DELTA: 0.0001324 sec

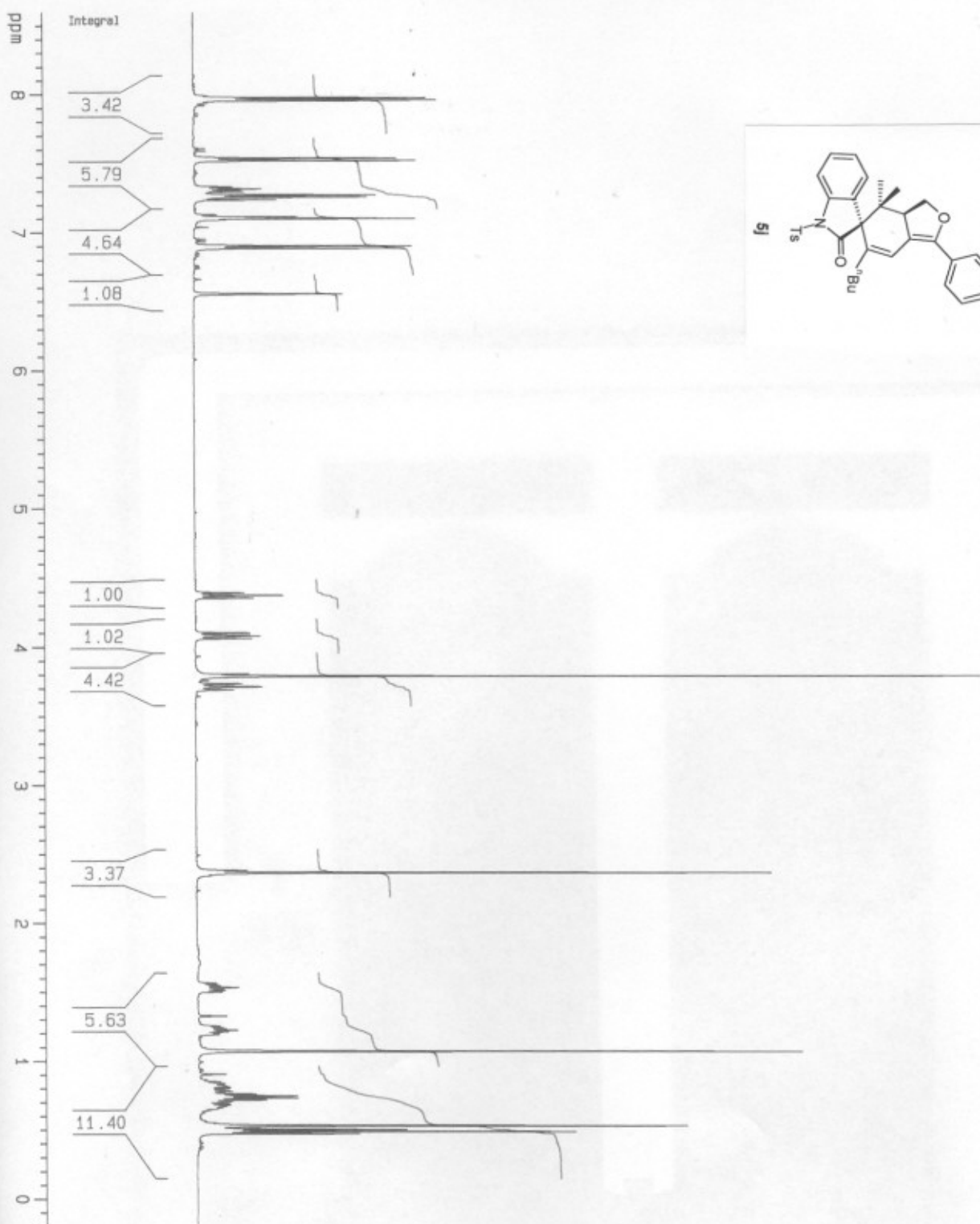
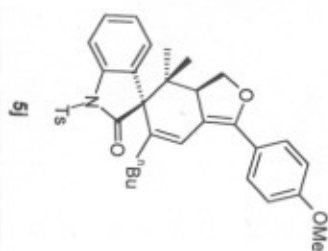
CHANNEL f1 13C
NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
SFO1: 125.7713172 MHz

CHANNEL f2 1H
NUC2: 1H
P2: 10.10 usec
PL2: 0.00 dB
SFO2: 500.136049 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7573982 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
FIDP: 190.000 ppm
F1: 22892.08 Hz
F2P: 0.000 ppm
F2: 0.00 Hz
FREQ: 9.55000 ppm/cn
ACQ: 1194.08510 Hz/cn

D'Souza DS-196 in CDCl3



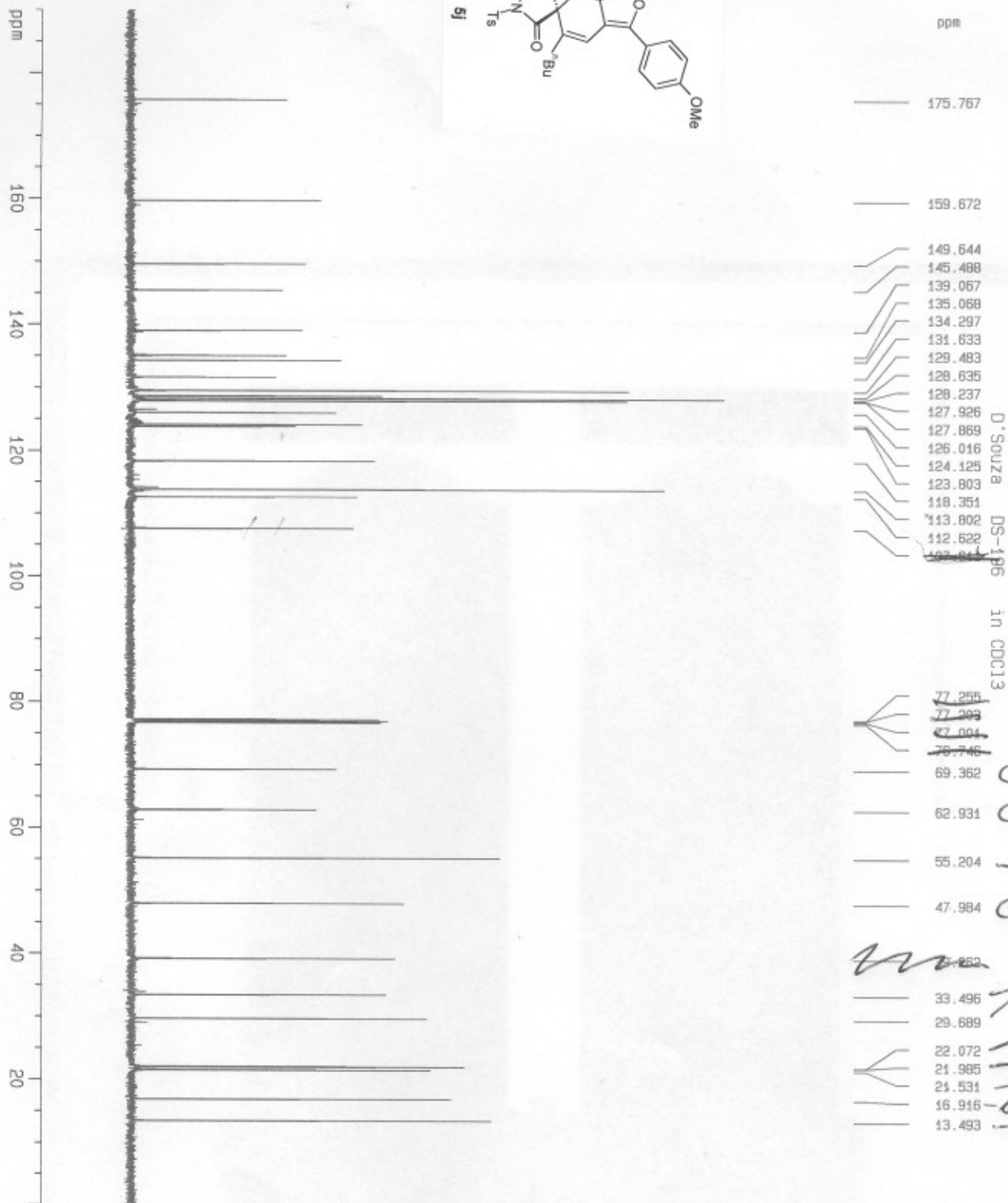
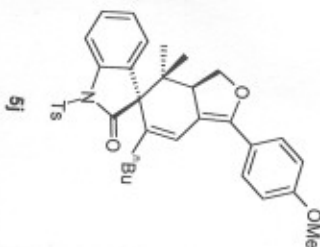
Current Data Parameters
NAME muso13m
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040513
Time 8.45
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 5482.456 Hz
FIDRES 0.167311 Hz
AQ 2.9884915 sec
RG 22.5
DM 91.200 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SF01 500.132738 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 8.600 ppm
F1 4301.12 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.44000 ppm/cm
HZCM 220.05722 Hz/cm



Current Data Parameters

NAME	VALUE	UNIT
EXPNO	2	
PROCNO	1	

F2 - Acquisition Parameters

NAME	VALUE	UNIT
DATE_	20040513	
TIME	8.51	
INSTRUM	SPYCE	
PROBHD	5 mm TBI HV13	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl ₃	
NS	1000	
DS	2	
SWH	30984.197	Hz
FIDRES	0.470650	Hz
AQ	1.2617332	sec
RG	5792.0	
DM	10.200	umax
DE	5.00	umax
TE	298.0	K
D1	1.00000000	sec
d11	0.03000000	sec
d12	0.00020000	sec

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

NAME	VALUE	UNIT
MUCL	13C	
P1	10.40	umax
PL1	0.00	dB
SE01	125.7713172	MHz

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

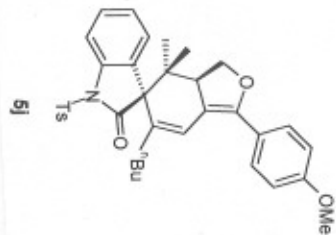
NAME	VALUE	UNIT
NUC2	13C	
PCPD2	100.00	umax
PL2	0.00	dB
PL12	20.00	dB
PL13	20.00	dB
SE02	500.1325895	MHz

F2 - Processing parameters

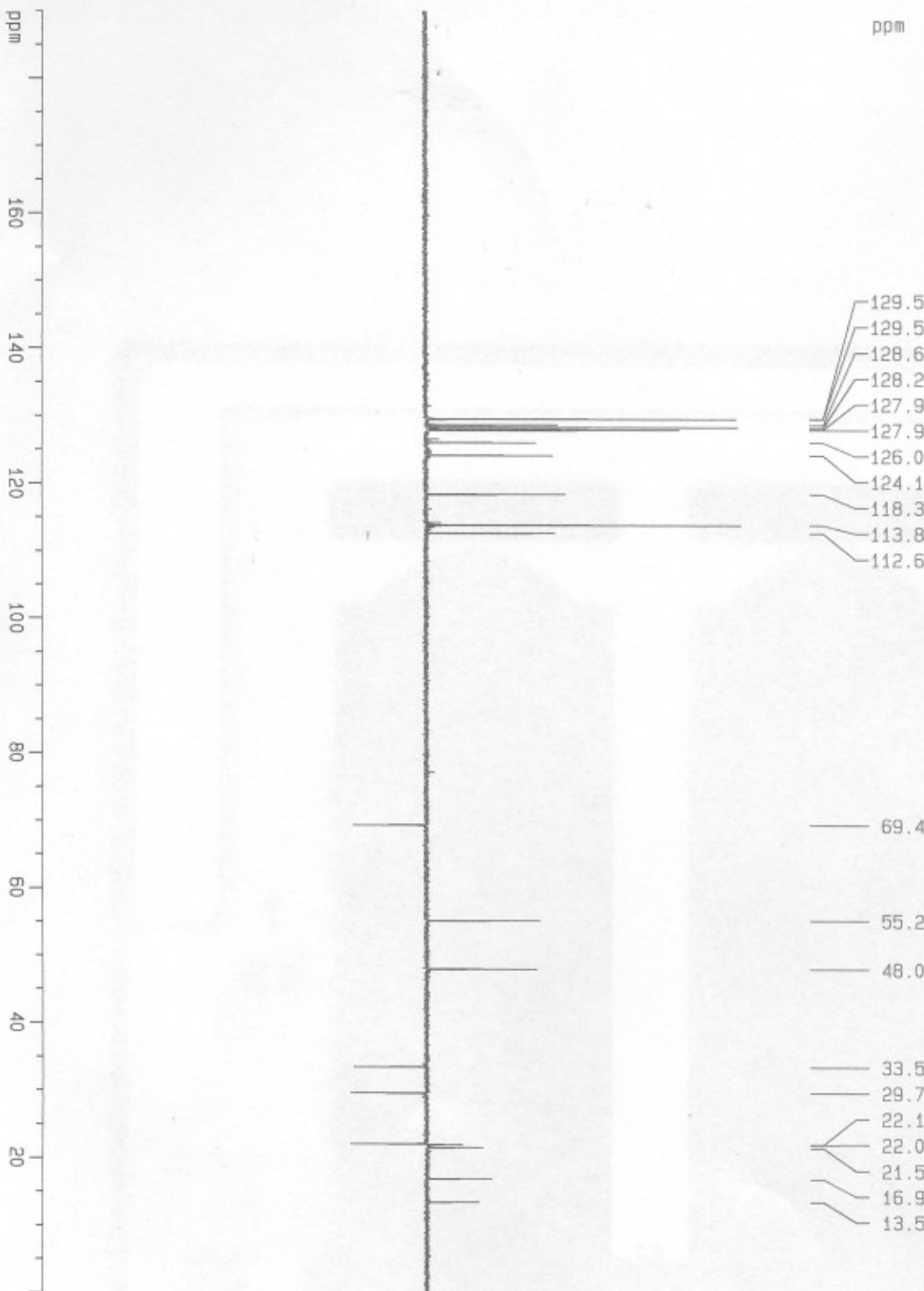
NAME	VALUE	UNIT
SI	32768	
SF	125.7578041	MHz
KOH	EX	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.00	

10 MHz 0.10t parameters

NAME	VALUE	UNIT
CX	20.00	cm
CY	9.50	cm
F1P	150.000	ppm
F1	23593.98	Hz
F2P	0.000	ppm
F2	0.00	Hz
PPMCK	9.55000	ppm/cm
KCHN	1194.88910	Hz/cm



D'Souza DS-196 in CDCl3



Current Data Parameters
NAME DS-196
EXPNO 3
PROCNO 1

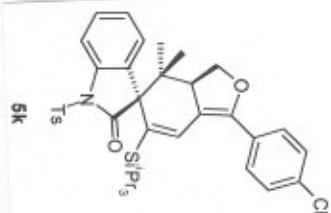
F2 - Acquisition Parameters
Date_ 20040513
Time 9.57
INSTRUM spect
PROBHD 5 mm TBI HX/13
PULPROG zgpg30
TD 65536
FIDRES 0.00135
SOLVENT CDCl3
NS 240
DS 2
SWH 30864.197 Hz
FIDRES 0.470950 Hz
AQ 1.0817132 sec
RG 1525.5
GB 16.200 umsc
DE 8.00 umsc
TE 298.0 K
CHG12 145.0000000
D1 4.0000000 sec
d2 0.0034828 sec
d12 0.0000200 sec
DELTA 0.0001304 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.40 umsc
PC 20.00 umsc
PL1 0.00 dB
SF01 125.7713172 MHz

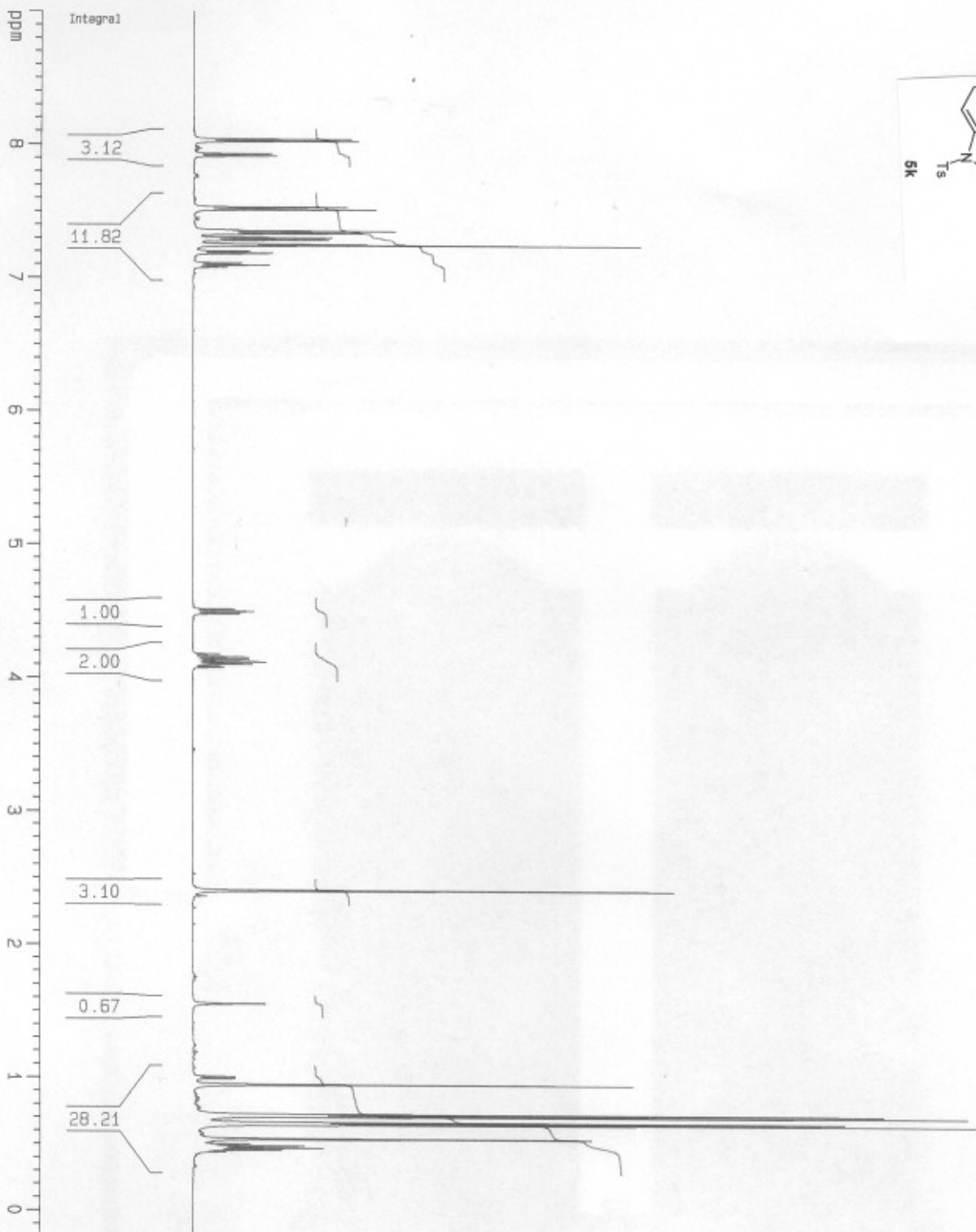
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.10 umsc
PC 20.20 umsc
PL2 0.00 dB
SF02 500.1325801 MHz

F2 - Processing parameters
SI 32768
SF 125.7578652 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 180.000 ppm
F1 23893.38 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCH 9.50000 ppm/cm
RCOM 1194.89310 Hz/cm



D'Souza DS-243 in CDCl₃



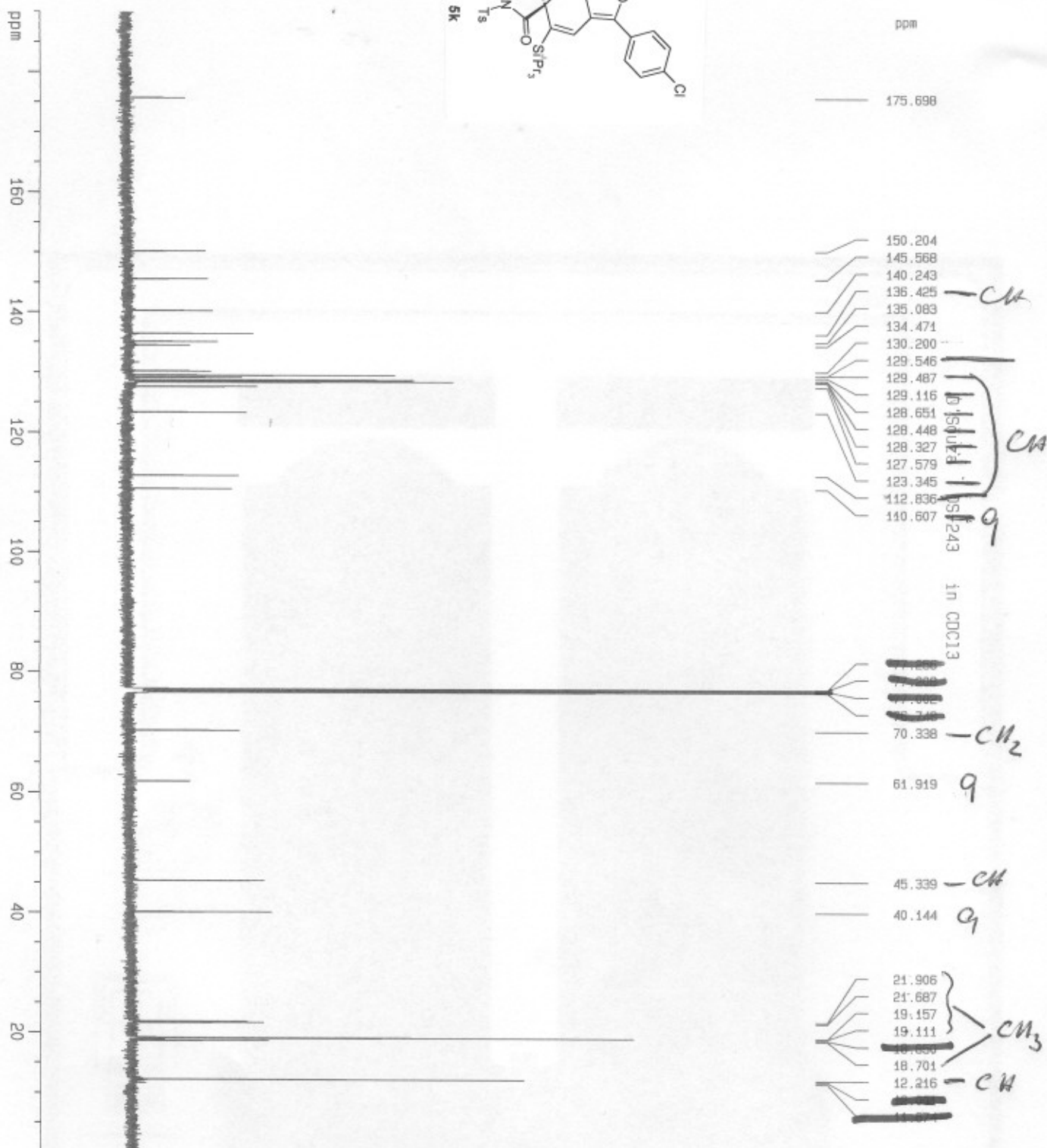
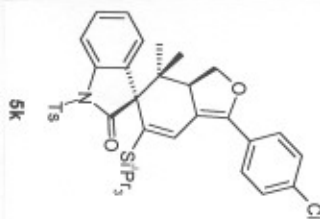
Current Data Parameters
NAME nus07na
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040507
Time 7.47
INSTRUM spect
PROBHD 5 mm TBI 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 4
SWH 6009.615 Hz
FIDRES 0.163399 Hz
AQ 2.7263477 sec
RG 90.15
DM 63.200 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec

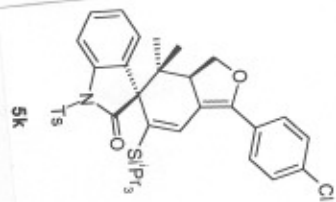
===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SF01 500.1320237 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 13.00 cm
FLP 9.000 ppm
F1 4501.17 Hz
F2 -0.200 ppm
F2 -100.03 Hz
PQMCN 0.46000 ppm/cm
HZCN 230.05981 Hz/cm



Current Date Parameters		Previous Date Parameters	
DATE	TIME	DATE	TIME
20090901	1	20090831	2
F2 - Acquisition Parameters Date: 20090901 Time: 9.24 Instrument: 5 MHz TMR H1 Preamplifier: ZPS50 Filter: 60536 ID: 60536 SOLVENT: CDCl3 NS: 3400 DS: 2 SWH: 39864.197 Hz FIDRES: 0.479305 Hz AQ: 1.0817382 sec RG: 5792.6 DE: 16.205 usec IN: 6.00 usec TE: 298.0 K D1: 1.00000000 sec d11: 0.03000000 sec d12: 0.00028000 sec			
CHANNEL F1 - 1H NUC1: 1H P1: 10.40 usec PL1: 0.00 dB SFO1: 425.7713172 MHz			
CHANNEL F2 - 13C CPDPRG2: WALTZ16 NUC2: 13C P2: 100.00 usec PL2: 0.00 dB PL12: 29.00 dB PL13: 29.00 dB SFO2: 500.1352610 MHz			
F2 - Processing parameters SI: 32768 SF: 125.7571920 MHz MDW: EN SEB: EN LB: 1.00 Hz GB: 0 PC: 1.00			
10 MHz plot parameters CX: 20.00 cm CY: 15.25 cm F1: 150.000 MHz F2: 23093.98 Hz F2P: 0.000 MHz F2R: 0.00 Hz GAMMA: 2.55000 percent GPCN: 1194.186497 Hz/cm			



D'Souza DS-243 in CDCl₃

ppm



Current Data Parameters
NAME DS-243
EXPNO 3
PROCNO 1

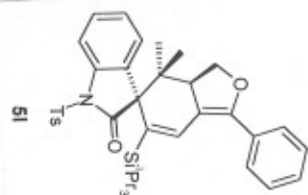
F2 - Acquisition Parameters
Date_ 20040507
Time 10.05
INSTRUM spect
PROBHD 5 mm 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 640
DS 2
SWH 30864.157 Hz
FIDRES 0.470563 Hz
AQ 1.0517352 sec
RG 1625.5
SN 16.200
SC 0.00
TE 298.0 K
CHST2 145.0000000 sec
D1 4.00000000 sec
d2 0.00344639 sec
d12 0.00020000 sec
DELTA 0.0001324 sec

CHANNEL f1 13C
NUC1 13C
P1 10.40 usec
PL1 29.00 dB
PC1 0.00 dB
SFO1 125.7713172 MHz

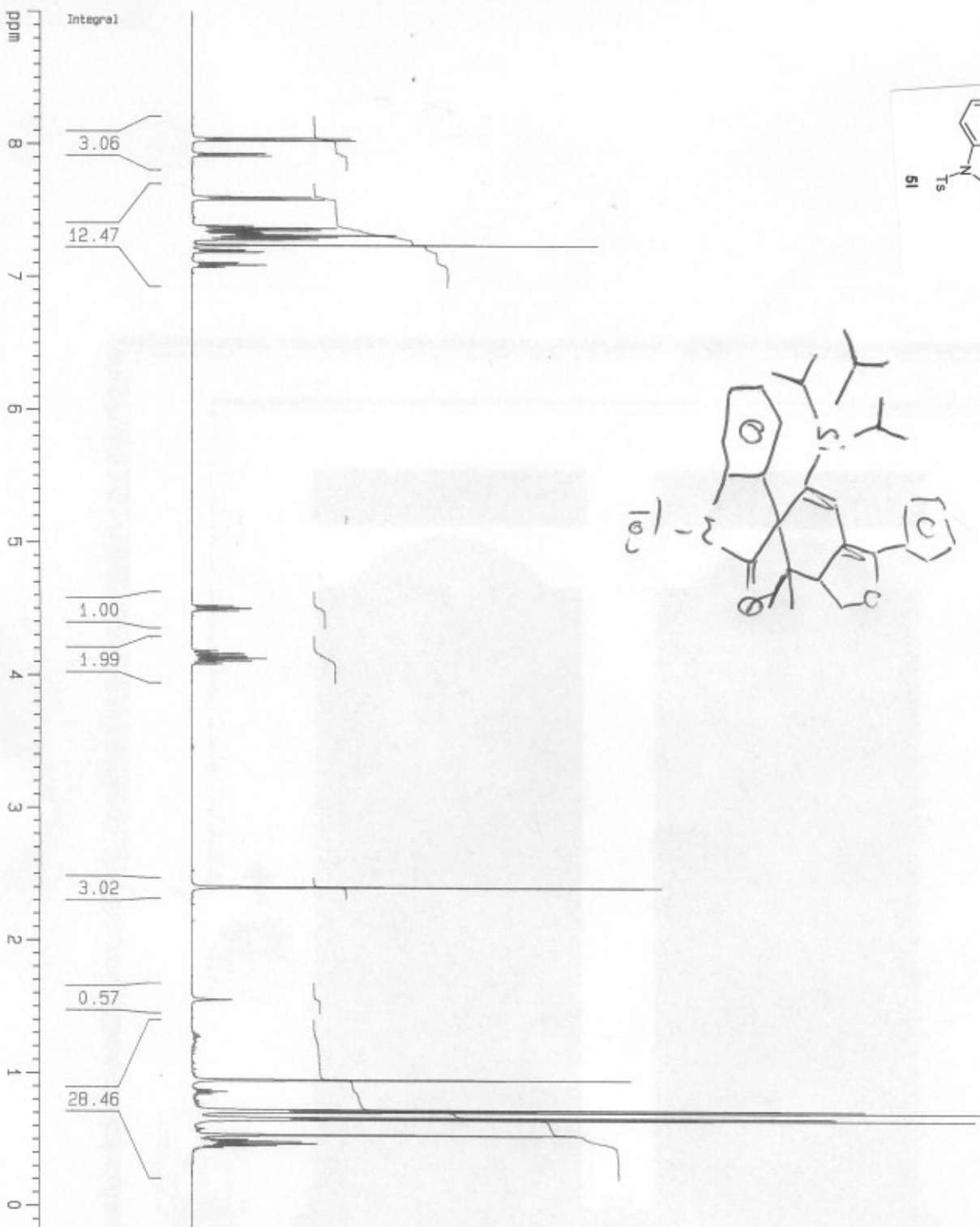
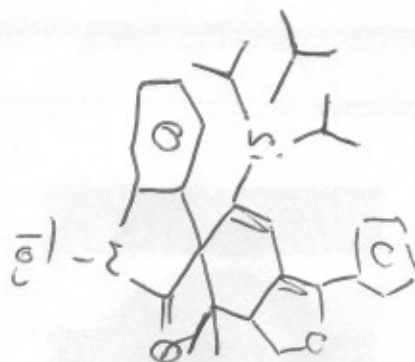
CHANNEL f2 1H
NUC2 1H
P2 10.10 usec
PL2 20.20 dB
PC2 0.00 dB
SFO2 500.1322500 MHz

F2 - Processing parameters
SI 32768
SF 125.757992 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
FLP 150.000 ppm
F1 20864.08 Hz
FRP 0.000 ppm
F2 0.00 Hz
PRMCX 9.50000 ppm/cm
HZCM 1194.09510 Hz/cm



D'Souza DS-241 in CDCl3



Current Data Parameters

NAME	EXPNO	PROCNO
DS-241	1	1

F2 - Acquisition Parameters

Date_	Time
20040506	9.45

INSTRUM spect

PROBHD 5 mm TBI HX/13

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 4

SWH 6009.645 Hz

FIDRES 0.183399 Hz

AQ 2.7263477 sec

R6 80.6

DE 63.200 usec

TE 298.0 K

D1 1.00000000 sec

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

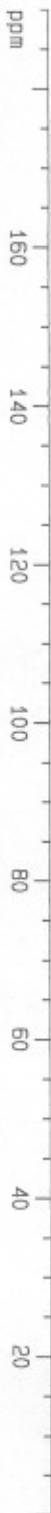
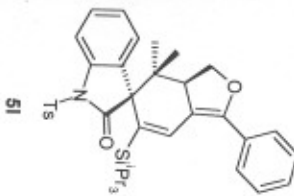
NUC1	1H
P1	10.10 usec
PL1	0.00 dB
SFO1	500.130251 MHz

F2 - Processing parameters

SI	16384
SF	500.1300232 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

10 NMR plot parameters

CX	20.00 cm
CY <td>13.00 cm</td>	13.00 cm
FAP <td>9.000 ppm</td>	9.000 ppm
F1 <td>4501.17 Hz</td>	4501.17 Hz
F2P <td>-0.200 ppm</td>	-0.200 ppm
F2 <td>-100.03 Hz</td>	-100.03 Hz
PPMCH <td>0.46000 ppm/cm</td>	0.46000 ppm/cm
HZCM <td>230.06981 Hz/cm</td>	230.06981 Hz/cm



	175.813	9
	151.411	9
	145.516	
	140.237	CH
	136.932	
	135.122	9
	131.086	
	129.653	CH
	129.472	
	129.285	9
	129.036	
	128.724	D'Souza DS-241 in CDCl3
	128.439	
	128.381	
	127.603	
	127.144	
	123.301	9
	112.786	
	110.047	

5 CH₃
2 CH
4 CH₂
2 9

Current Data Parameters
NAME: 51
EXPNO: 2
PROCNO: 1

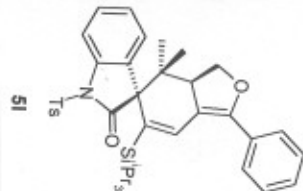
F2 - Acquisition Parameters
Date_: 20040306
Time: 10.31
INSTRUM: spect
PROBHD: 5 mm TBI HV/13
PULPROG: zgpg30
TO: 65536
SOLVENT: CDCl3
NS: 3460
DS: 2
SWH: 30854.197 Hz
FIDRES: 0.470650 Hz
AQ: 1.0617332 sec
RG: 5792.8
CW: 18.200 usec
DE: 5.00 usec
TE: 298.0 K
D1: 1.00000000 sec
d11: 0.03000000 sec
d12: 0.00000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
SFO1: 125.7713173 MHz

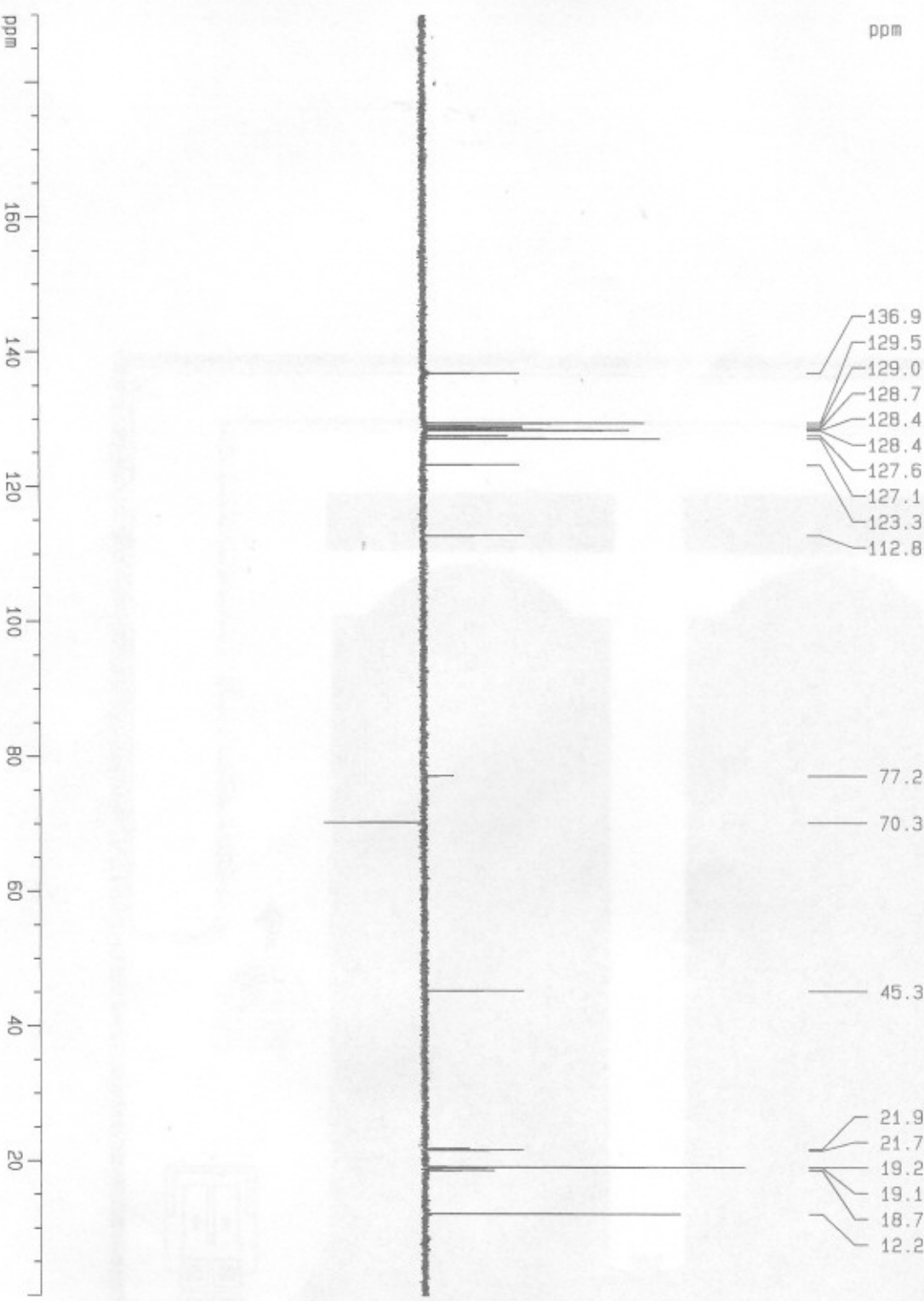
===== CHANNEL f2 =====
NAME: 51
NUC2: 1H
P2: 140.00 usec
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 500.1325500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577537 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 13.00 cm
F1P: 190.000 ppm
F1: 23833.88 Hz
F2P: 0.000 ppm
F2: 0.00 Hz
PREF: 9.50000 ppm/cm
H2O: 1194.58910 Hz/cm



D'Souza DS-241 in CDCl3



Current Data Parameters
NAME DS-241
EXPNO 3
PROCNO 1

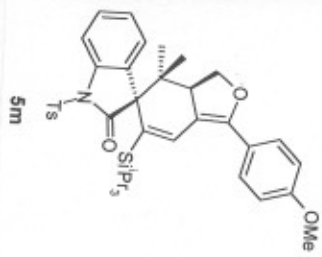
F2 - Acquisition Parameters
Date_ 20/05/06
Time 18.27
INSTRUM spect
PROBHD 5 mm TBI 5H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 2
SWH 30064.167 Hz
FIDRES 0.470950 Hz
AQ 1.0617332 sec
RG 1825.5
DM 16.200 umc
DE 6.00 umc
TE 298.0 K
CHST2 145.000000 sec
D1 4.00000000 sec
d2 0.00344828 sec
d12 0.00000000 sec
DELTA 0.00001324 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.40 umc
PC 28.80 umc
RG 0.00 dB
SFO1 125.7713172 MHz

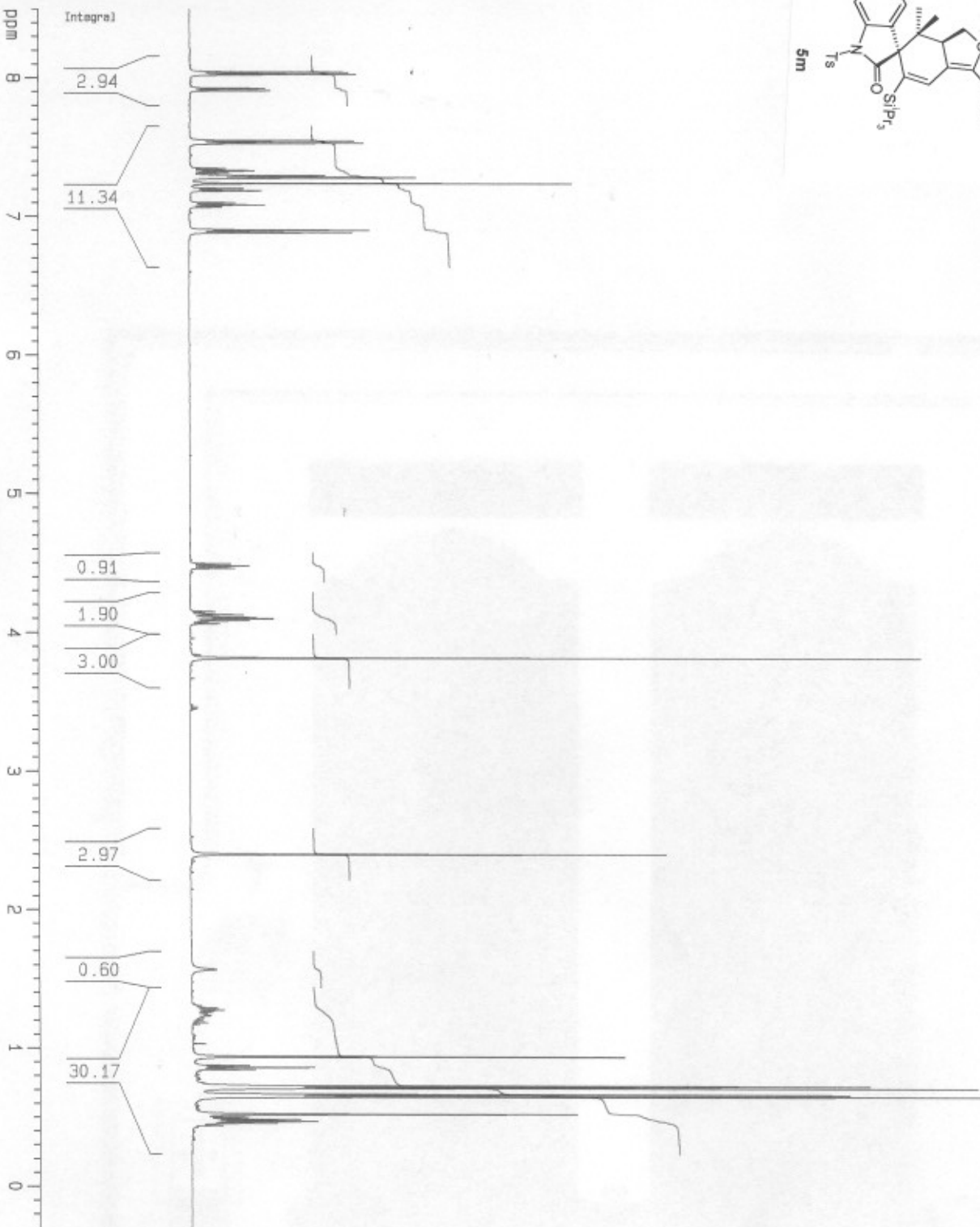
===== CHANNEL f2 =====
NUC2 1H
P2 10.10 umc
PC 20.20 umc
RG 0.00 dB
SFO2 500.1322500 MHz

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

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 150.000 500
F1 23693.98 Hz
F2P 0.000 500
F2 0.00 Hz
PRACH 9.55000 500/cm
H2O 1194.89810 Hz/cm



D'Souza DS-242 in CDCl₃



Current Data Parameters

NAME	DS-242
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20040511
Time	10.10
INSTRUM	spect
PROBHD	5 mm TBI HX/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl ₃
NS	16
DS	4
SWH	5482.406 Hz
FIDRES	0.167311 Hz
AQ	2.9894915 sec
RG	71.6
DM	91.200 usec
DE	5.00 usec
TE	298.0 K
D1	1.00000000 sec

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

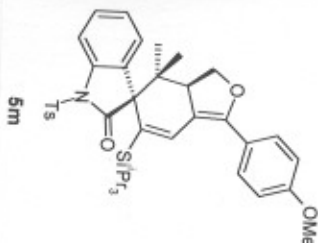
NUC1	¹ H
P1	10.10 usec
PL1	0.00 dB
SFO1	500.1322738 MHz

F2 - Processing parameters

SI	16394
SF	500.1300232 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	13.00 cm
F1P	8.500 ppm
F1	4251.11 Hz
F2P	-0.300 ppm
F2	-150.04 Hz
PPHCK	0.44000 ppm/cm
HZCM	220.05722 Hz/cm



ppm

175.921

159.965

151.456

145.487

140.236

137.167

135.150

129.783

129.461

128.986

128.561

128.448

128.038

127.614

123.751

123.270

113.843

112.758

108.622

D'Souza DS-242 in CDCl₃

77.256

77.260

77.264

76.750

70.223

CH₂

61.856

-q

55.300

CH₃

45.227

CH

39.935

-q

21.912

21.678

19.185

19.145

18.691

14.940

12.264

CH₃

CH

Current Data Parameters	Parameter	Value
NAME	DS-242	
EXPNO	3	
PROCNO	1	

F2 - Acquisition Parameters	Parameter	Value
Date_	20040511	
Time	11.04	
INSTRUM	spect	
PROBHD	5 mm 1H/13	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl ₃	
NS	4000	
DS	2	
SWH	36864.407 Hz	
FIDRES	0.47395 Hz	
AQ	1.061732 sec	
RG	3729.6	
DE	16.400 uarc	
TE	300.2 K	
D1	1.00000000 sec	
D11	0.03000000 sec	
D12	0.00000000 sec	

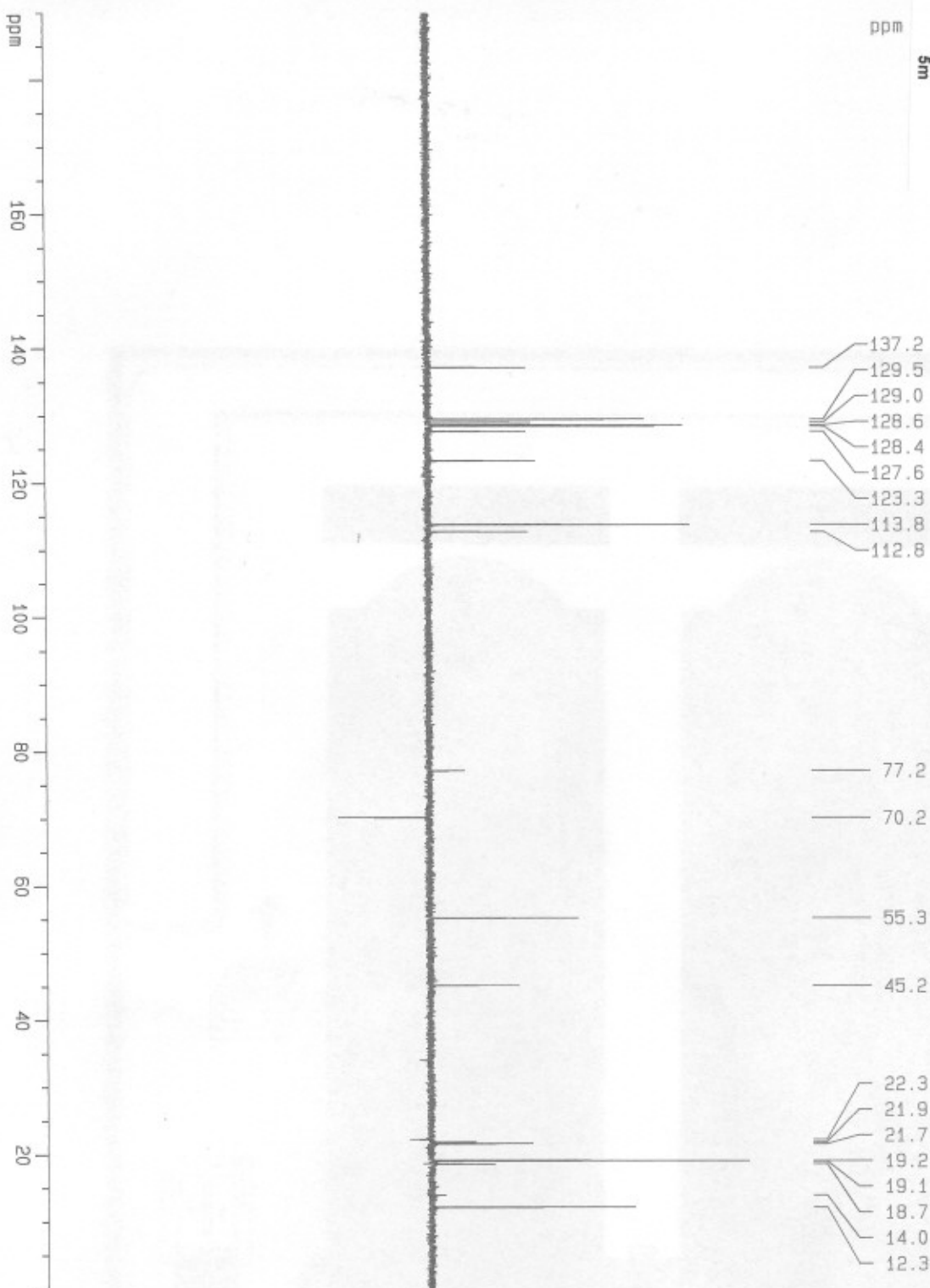
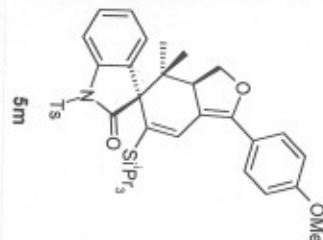
CHANNEL f1	Parameter	Value
NALC1	13C	
P1	10.40 uarc	
PL1	0.00 dB	
SFO1	125.7713172 MHz	

CHANNEL f2	Parameter	Value
NALC2	1H	
PCPD2	100.00 uarc	
PL2	0.00 dB	
PL12	20.00 dB	
PL13	20.00 dB	
SFO2	500.132500 MHz	

F2 - Processing Parameters	Parameter	Value
SI	32768	
SF	125.7577528 MHz	
WDW	EM	
SGB	0	
LB	1.00 Hz	
GB	0	
PC	1.00	

1D NMR plot parameters	Parameter	Value
EX	20.00 cm	
CV	13.00 cm	
F1P	150.000 ppm	
F1	23863.88 Hz	
F2P	0.000 ppm	
F2	0.00 Hz	
FNUC1	13C	
FNUC2	1H	

D'Souza DS-242 in CDCl3



Current Data Parameters
NAME DS-242
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040511
Time 13.13
INSTRUM spect
PROBHD 5 mm TBI 51/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 2
SWH 30564.187 Hz
FIDRES 0.470950 Hz
AQ 1.0617332 sec
RG 1625.5
RW 16.200 usec
DE 6.00 usec
TE 298.0 K
DMSD2 145.000000 sec
D1 4.00000000 sec
d2 0.00344028 sec
d12 0.00000000 sec
DELTA 0.00001324 sec

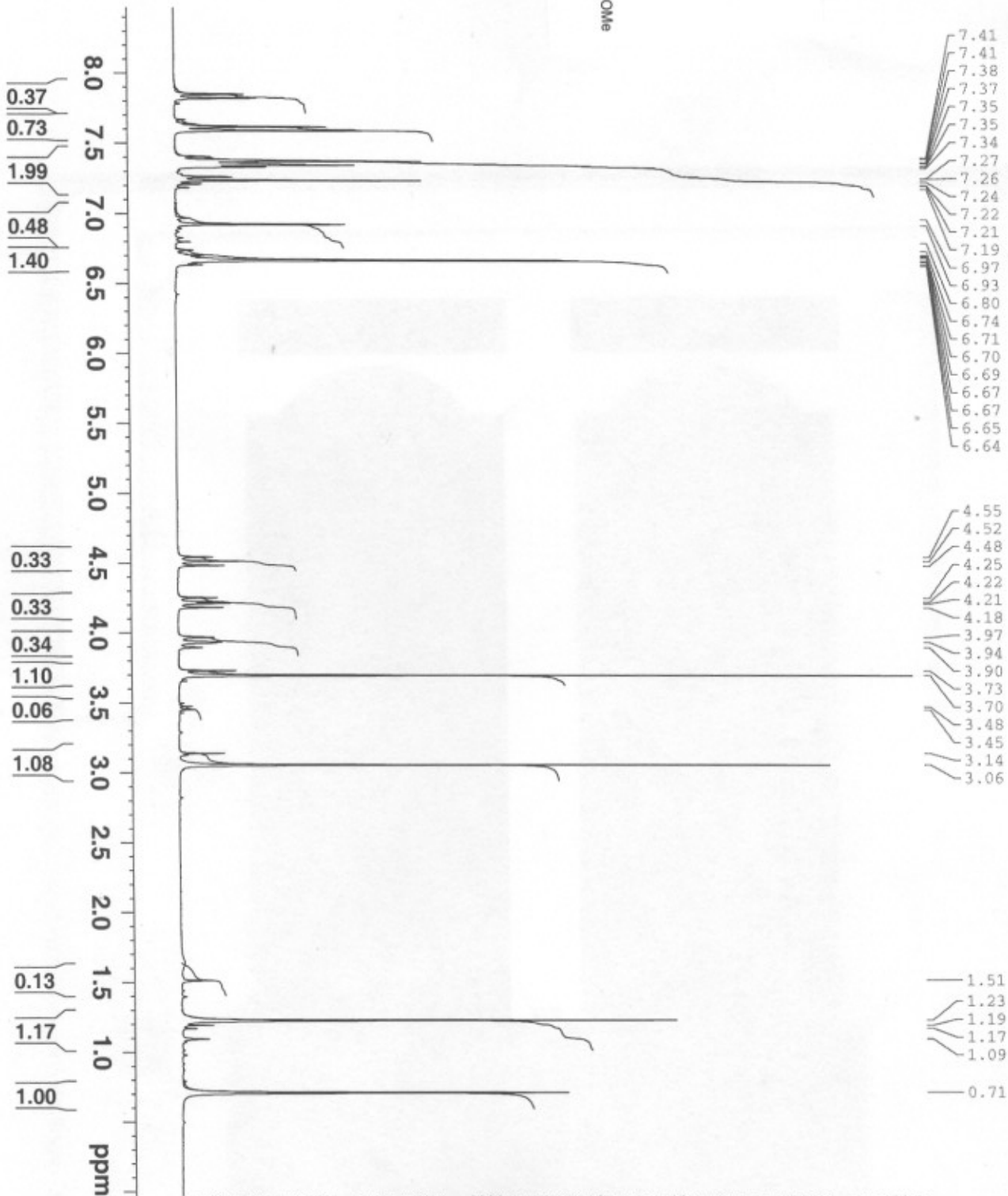
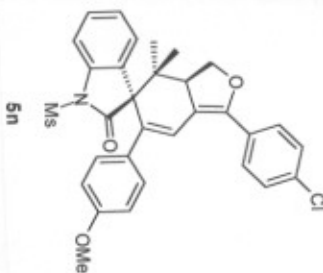
===== CHANNEL f1 =====
NUC1 13C
P1 10.40 usec
PL 20.00 usec
FL1 0.00 dB
FREQ1 125.7713172 MHz

===== CHANNEL f2 =====
CPROG2 zgpg30
NUC2 1H
P2 10.10 usec
PL 20.00 usec
PCPD2 100.00 usec
FREQ2 500.132500 MHz

F2 - Processing parameters
SI 32768
SF 125.7577930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
FID 190.000 dB
F1 23893.38 Hz
F2 0.000 dB
FZ 0.00 Hz
PFGNCH 9.50000 pps/cm
RGCM 1194.88887 Hz/cm

D'Souza DS_447 CDCl3

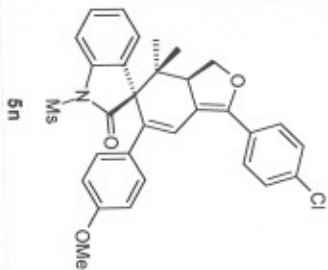


Current Data Parameters
NAME apl8musu
EXPNO 1
PROCNO 1

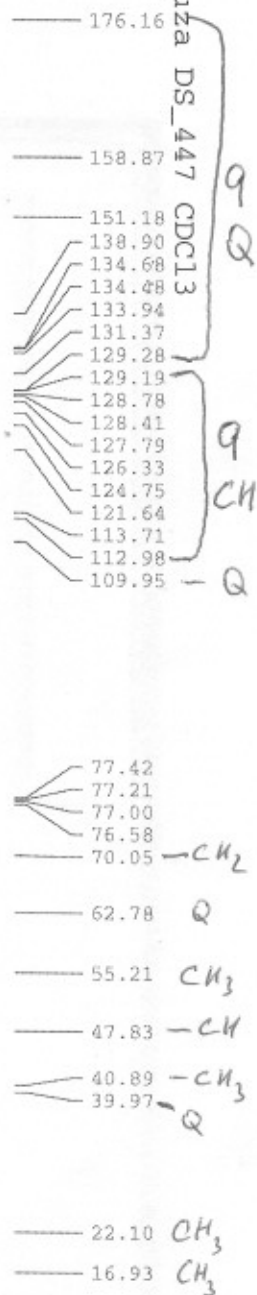
F2 - Acquisition Parameters
Date_ 20050503
Time 7.03
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5707.763 Hz
FIDRES 0.174187 Hz
AQ 2.8705268 sec
RG 114
DW 87.600 usec
DE 6.00 usec
TE 300.0 K
DI 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300123 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



D'Souza DS_447 CDC13



Current Data Parameters
NAME apl8musu
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050420
Time 7.42
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 940
DS 4
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 4096
DE 22.050 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 20.00 usec
PL1 0.00 dB
SFO1 75.4752658 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 120.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

180 160 140 120 100 80 60 40 20 ppm

D'Souza DS_447 CDCl3

129.19
128.78
128.41
127.79
126.33
124.76
121.64
113.71
112.98

70.06
55.21
47.82
40.89
22.11
16.94

Current Data Parameters
NAME apl8musu
EXPNO 3
PROCNO 1

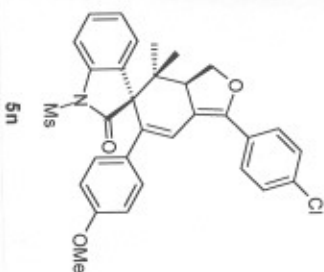
F2 - Acquisition Parameters

Date_ 20050418
Time 14.37
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG dept135
TD 32768
SOLVENT CDCl3
NS 256
DS 8
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 4096
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
CNS12 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00002546 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

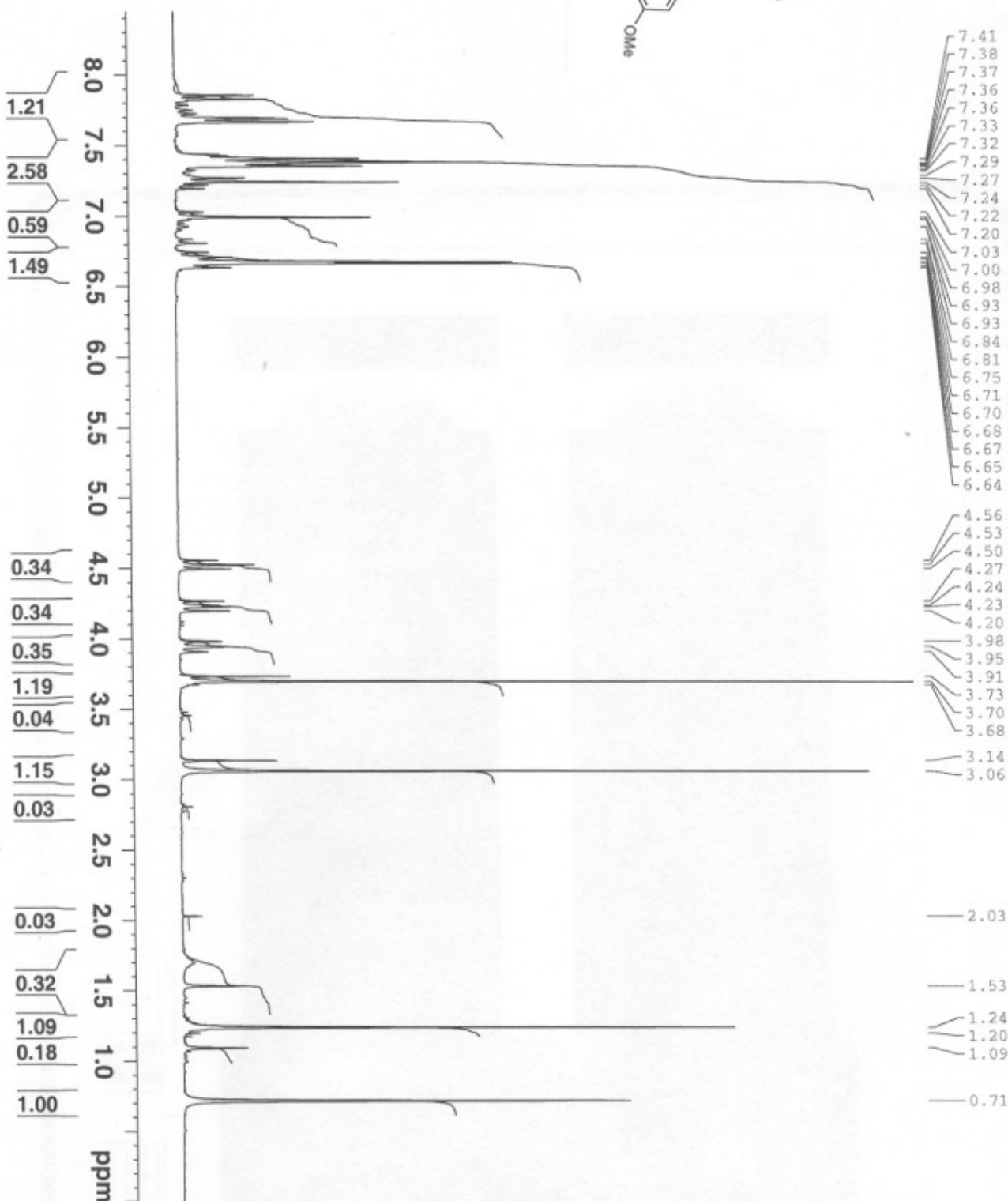
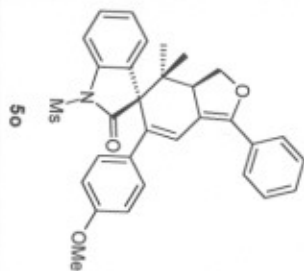
===== CHANNEL f1 =====
NUC1 13C
P1 20.00 usec
P2 40.00 usec
PL1 0.00 dB
SFO1 75.4730017 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 7.50 usec
P4 15.00 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



D-Souza DS_451 CDC13

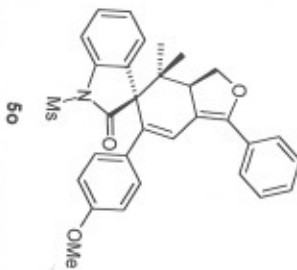


Current Data Parameters
NAME apl8muso
EXPNO 1
PROCNO 1

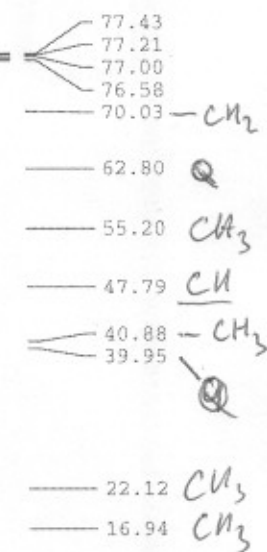
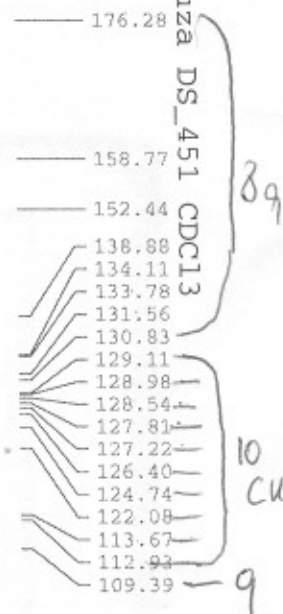
F2 - Acquisition Parameters
Date_ 20050426
Time 15.10
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 5707.763 Hz
FIDRES 0.174187 Hz
AQ 2.8705268 sec
RG 114
DW 87.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300121 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



D-Souza DS_451 CDC13



CH₃ : 4 CH : 11
CH₂ : 1 Q :

180 160 140 120 100 80 60 40 20 ppm

Current Data Parameters
NAME apl8muso
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050418
Time 18.05
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 1200
DS 4
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 4096
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 20.00 usec
PL1 0.00 dB
SFO1 75.4752658 MHz

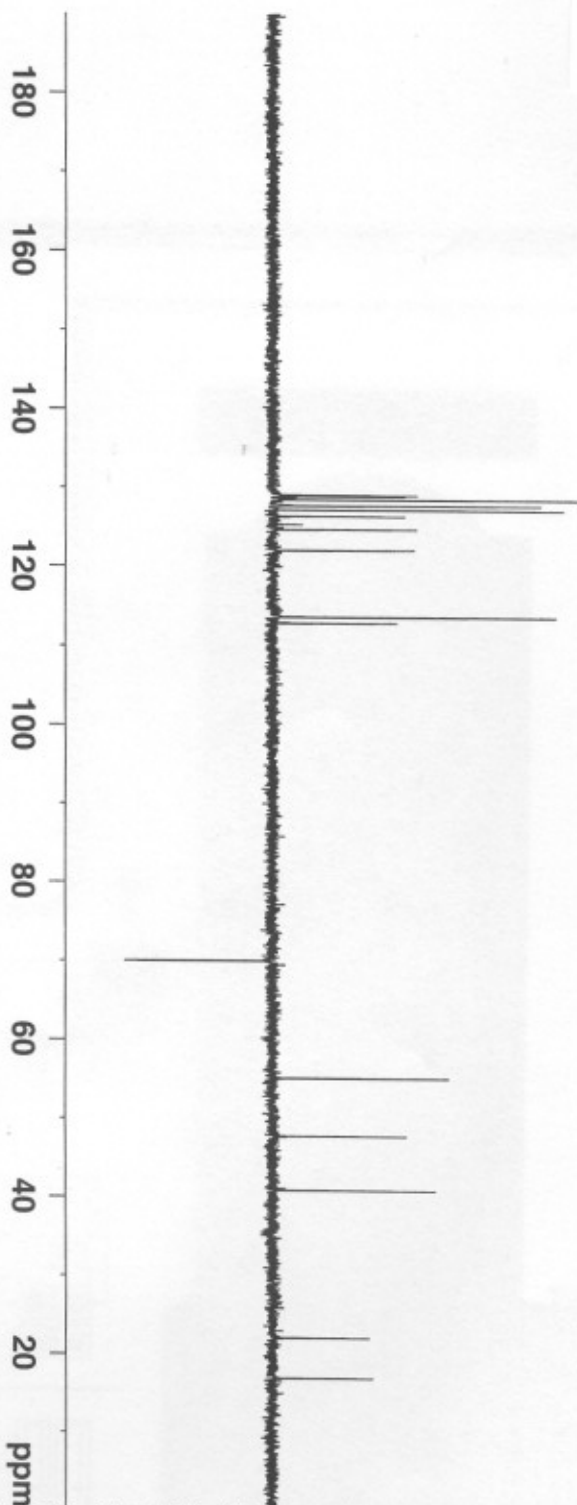
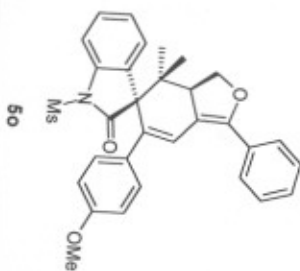
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 120.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

D'Souza DS_451 CDCl3

129.11
128.98
128.54
127.80
127.22
126.40
124.74
122.08
113.67
112.92

70.03
55.20
47.78
40.88
22.12
16.94



Current Data Parameters
NAME apl8muso
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050418
Time 14.14

INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 376
DS 8

SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 4096

DW 22.050 usec
DE 6.00 usec
TE 300.0 K

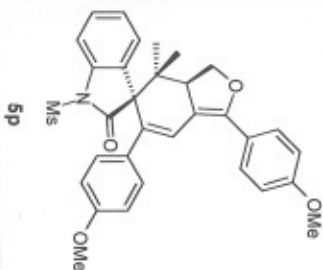
CNSTR2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00002546 sec
MCREST 0.00000000 sec
MCNTRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 20.00 usec
P2 40.00 usec
PL1 0.00 dB
SFO1 75.4730017 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 7.50 usec
P4 15.00 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

D-Souza DS_433 CDCl3



7.61
7.60
7.40
7.40
7.37
7.35
7.26
7.26
7.24
7.24
7.21
7.21
6.96
6.94
6.93
6.92
6.91
6.90
6.70
6.69
6.67
6.66
6.64
6.63

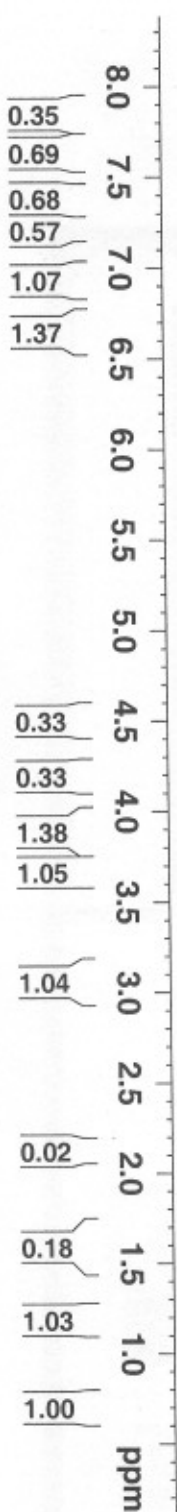
4.53
4.50
4.47
4.24
4.21
4.20
4.17
3.95
3.91
3.88
3.83
3.73
3.70
3.13
3.06

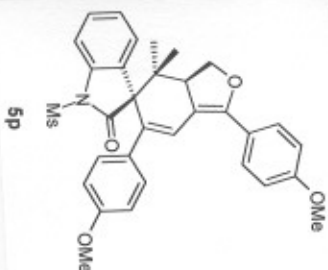
2.15
1.60
1.22
0.71

Current Data Parameters
NAME apl8musz
EXPNO 1
PROCNO 1

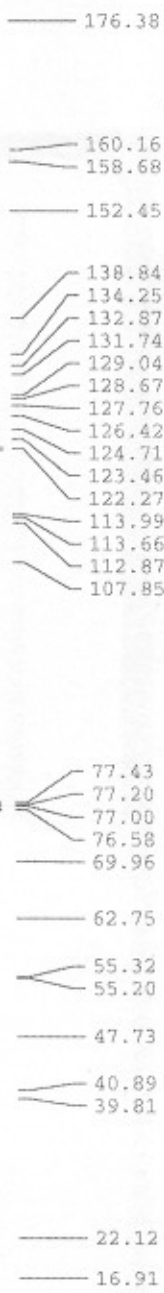
F2 - Acquisition Parameters
Date_ 20050419
Time 22.07
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5707.763 Hz
FIDRES 0.174187 Hz
AQ 2.8705268 sec
RG 114
DM 87.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWPK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz
F2 - Processing parameters
SI 32768
SF 300.1300121 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00





D-Souza DS_433 CDCl3



Current Data Parameters
 NAME apl8musz
 EXPNO 2
 PROCNO 1

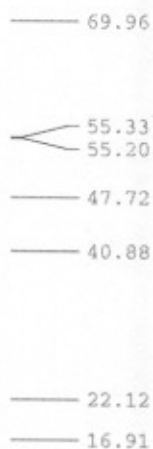
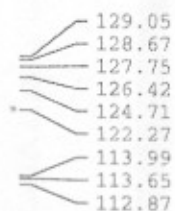
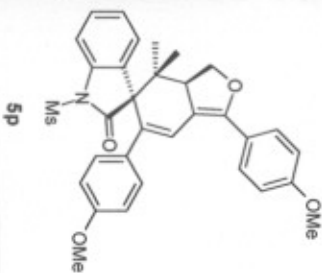
F2 - Acquisition Parameters
 Date_ 20050419
 Time 23.03
 INSTRUM spect
 PROBHD 5 mm TBI 1H/31
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1200
 DS 4
 SWH 22675.736 Hz
 FIDRES 0.692009 Hz
 AQ 0.7225844 sec
 RG 6502
 DW 22.050 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 20.00 usec
 PL1 0.00 dB
 SFO1 75.4752558 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 20.00 dB
 PL13 120.00 dB
 SFO2 300.1316507 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677524 MHz
 WTMW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

D'Souza DS_433 CDCl3



Current Data Parameters
NAME ap18musz
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050418
Time 14.57
INSTRUM spect
PROBHD 5 mm TBI 1H/31
PULPROG dept135
TD 32768
SOLVENT CDCl3
NS 360
DS 8
SWH 22675.736 Hz
FIDRES 0.692009 Hz
AQ 0.7225844 sec
RG 4096
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00002546 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

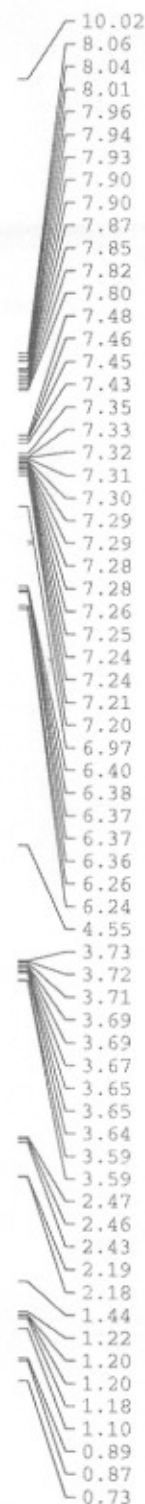
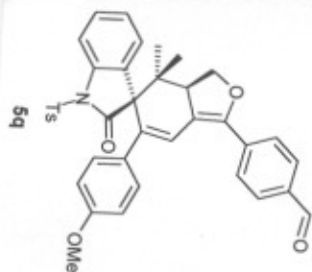
===== CHANNEL f1 =====
NUC1 13C
P1 20.00 usec
P2 40.00 usec
PL1 0.00 dB
SFO1 75.4730017 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 7.50 usec
P4 15.00 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.00 dB
SFO2 300.1316507 MHz

F2 - Processing parameters
SI 32768
SF 75.4677524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



DS-646 MU in CDCL3 D Souza



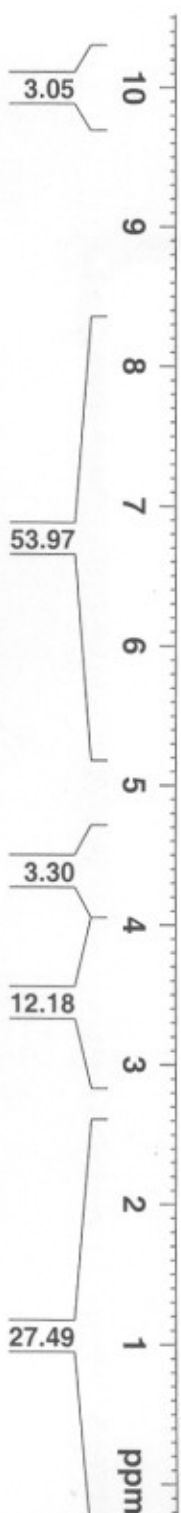
Current Data Parameters
NAME mudsde01
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061203
Time 0.25
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 228.1
RW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





DS-646 MU in CDCL3 D Souza

191.60
174.68
174.29
158.50
150.49
145.53
139.10
136.61
136.52
136.28
135.87
134.87
134.76
133.30
133.07
131.11
130.29
130.07
129.89
129.72
129.66
129.57
129.42
129.33
129.19
129.09
128.12
128.07
128.01
127.61
127.49
127.24
127.10
127.02
126.60
126.20
125.30
125.14
124.72
124.56
121.09
119.55
113.54
113.23
112.95
112.74
77.48
77.26
77.05
76.63
70.12
62.52
55.10
55.04
54.89
48.05
40.20
39.92
25.22
22.34
22.00
21.71
21.66
16.90
15.27
14.08

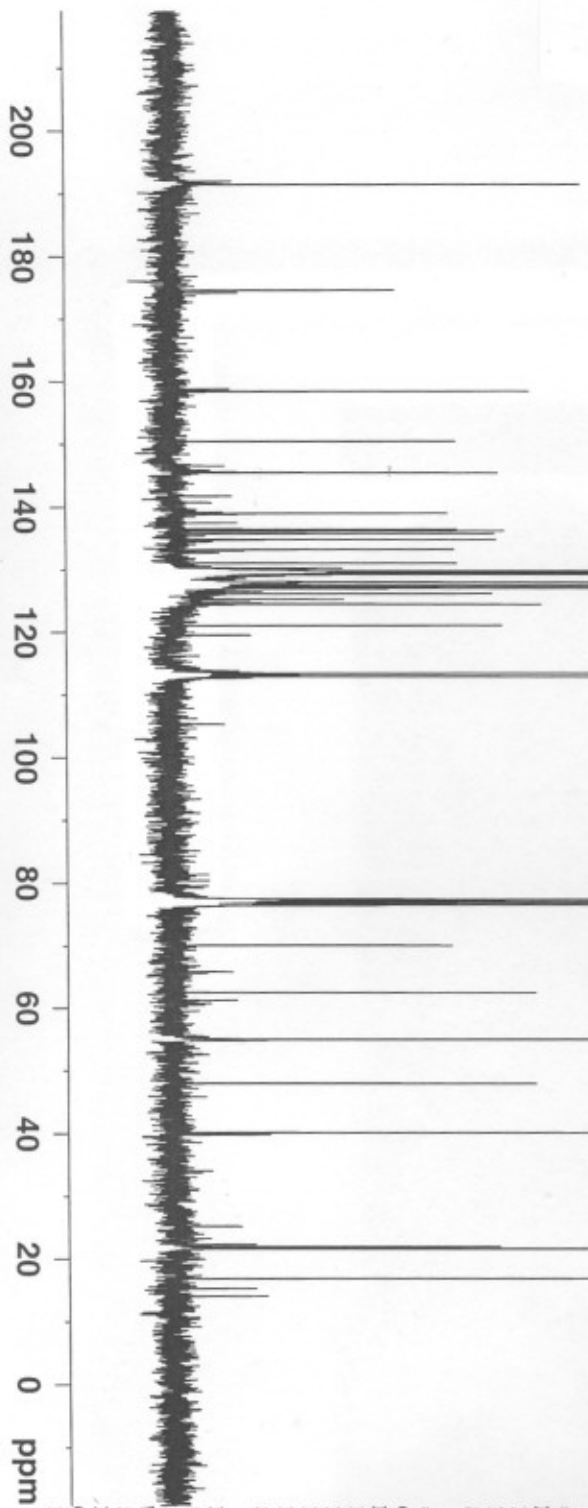
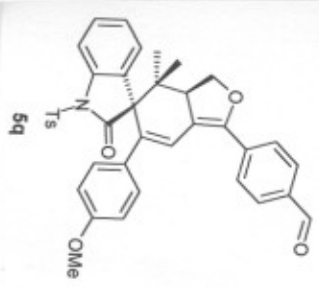
Current Data Parameters
NAME mudsde01
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061203
Time 4.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 13004
DN 27.800 usec
DE 6.00 usec
TE 300.0 K
DI 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME mudsde01
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061203
Time 6.55

INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 2000

DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384

DW 27.800 usec
DE 6.00 usec
TE 300.0 K

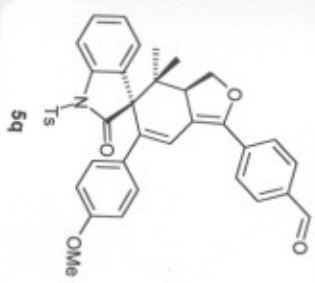
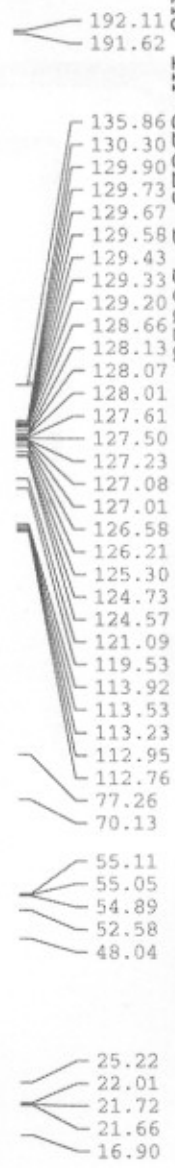
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

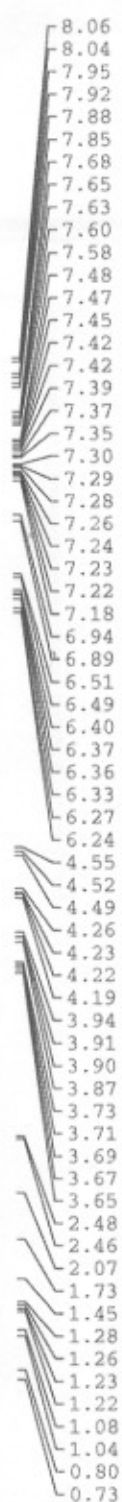
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DS-646 MU in CDCl3 D Souza



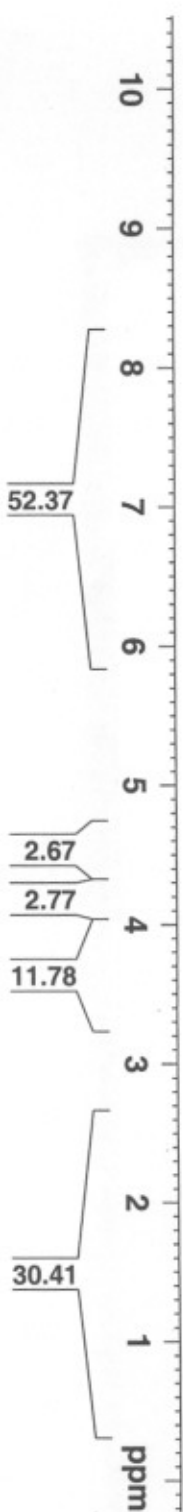
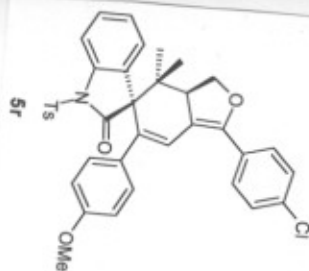
DS-606 MU in CDCL3 D'Souza



Current Data Parameters
NAME musojn23
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 8.14
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 256
RW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME musojn23
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060626
Time 8.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 828
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

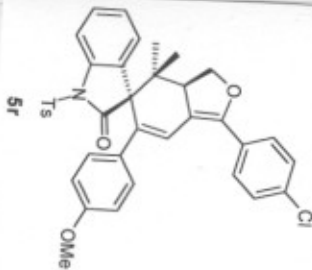
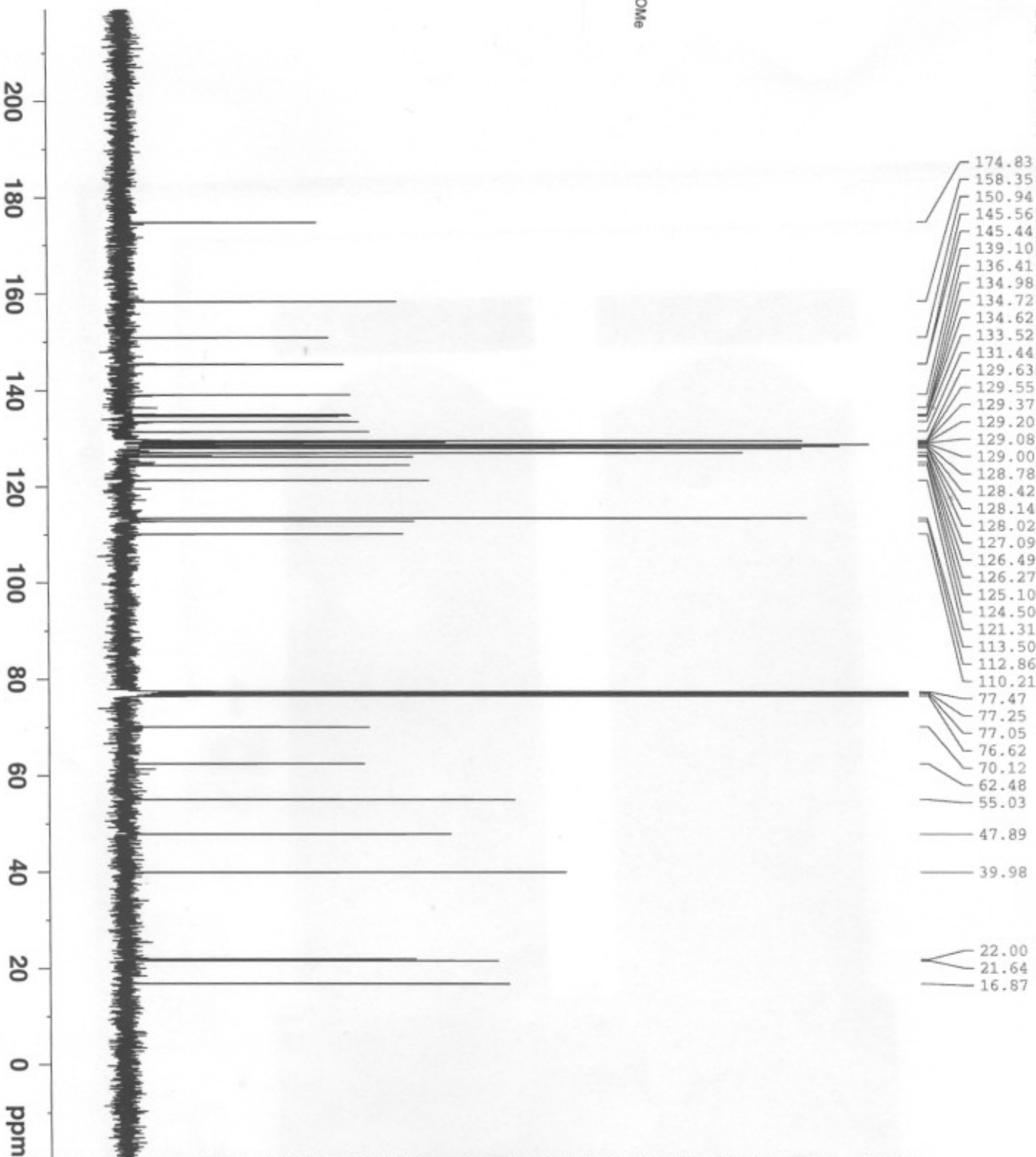
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DS-606 MU in CDCl3 D'Souza





DS-606 MU in CDCL3 D"Souza



Current Data Parameters
NAME musojn23
EXPNO 3
PROCNO 1

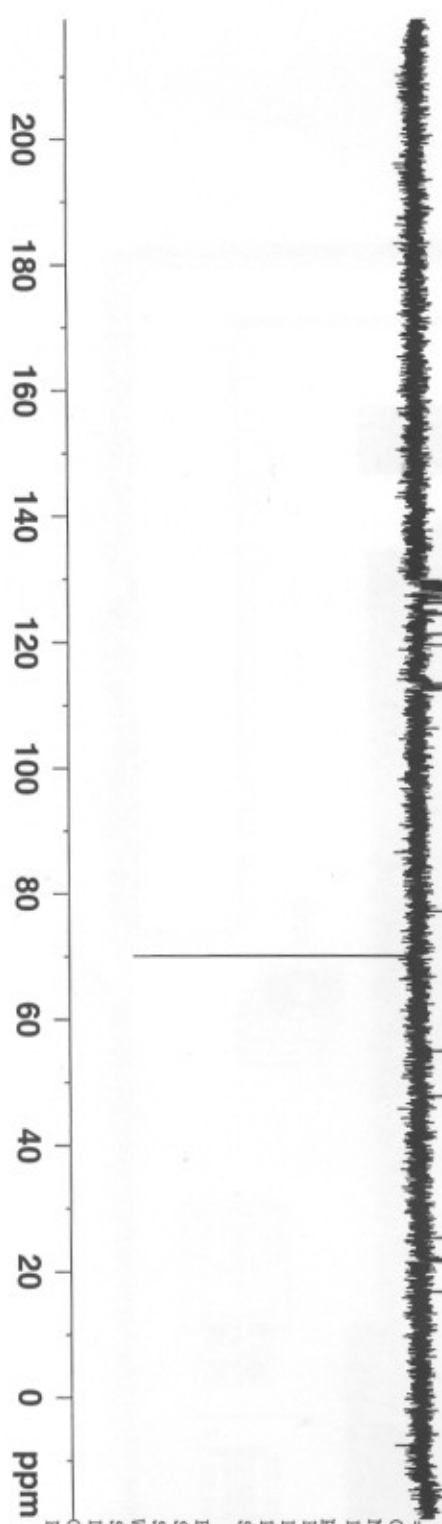
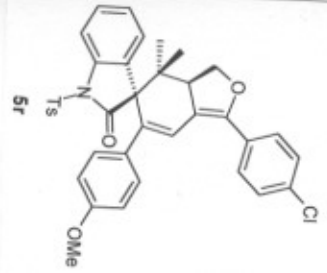
F2 - Acquisition Parameters
Date_ 20060626
Time 9.24

INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 417
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d12 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

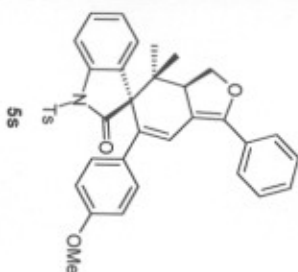
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing Parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



DS-605 MU in CDCL3 D'Souza



Current Data Parameters
NAME musujn26
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 9.42

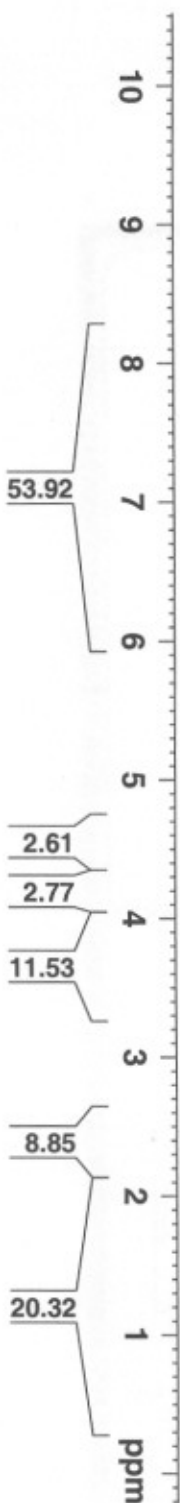
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2

SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 228.1

DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

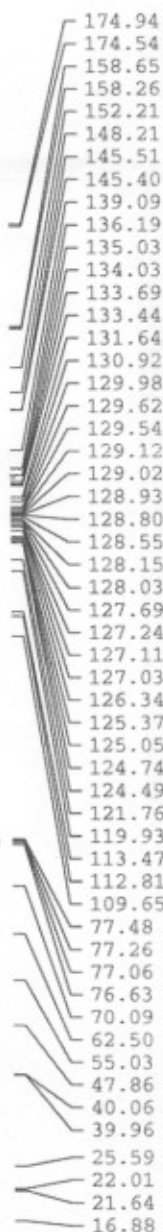
===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 6.00





DS-605 MU in CDCl3 D'Souza



Current Data Parameters
NAME musujn26
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 10.09

INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024

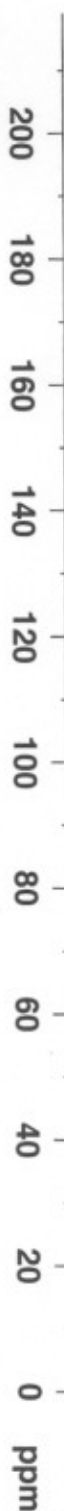
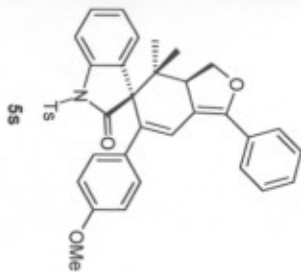
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384

DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

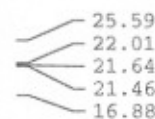
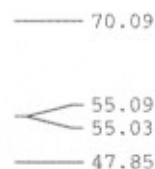
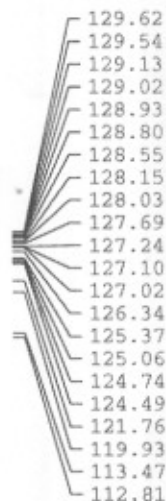
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



DS-605 MU in CDCL3 D'Souza



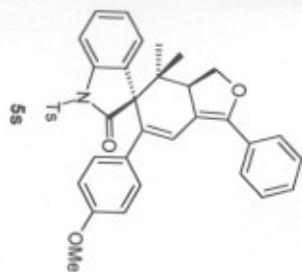
Current Data Parameters
NAME musujn26
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 11.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
CNS12 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

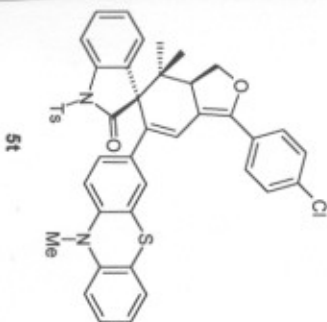
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



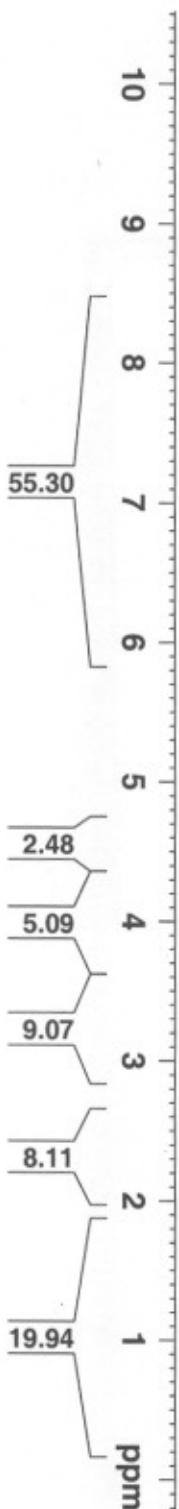
DS-608 MU in CDCL3 D"Souza



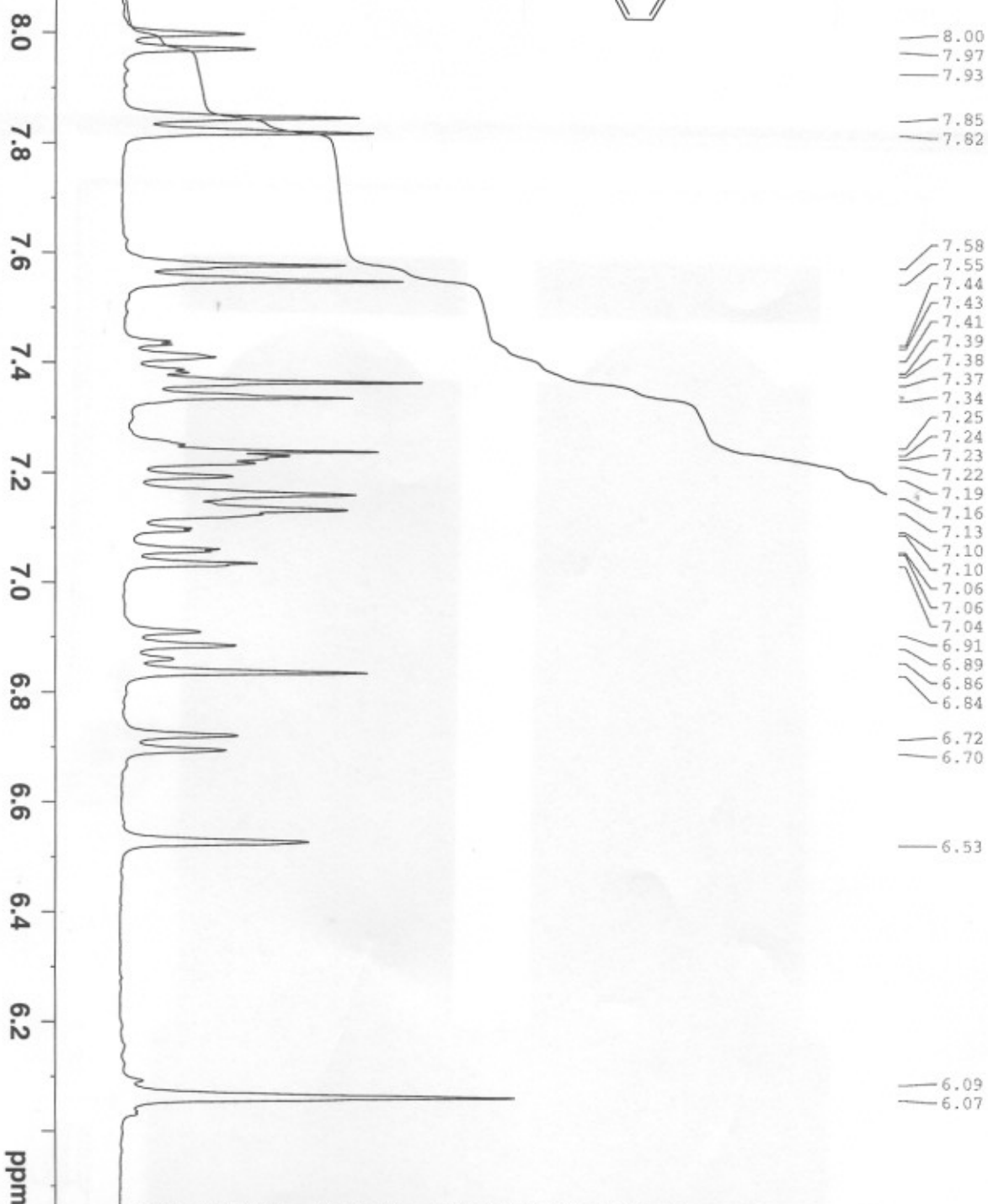
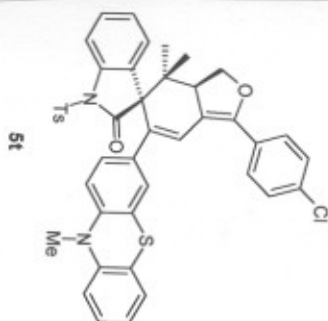
Current Data Parameters
NAME mudsjn26
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 14.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 9.00



DS-608 MU in CDCL3 D'Souza



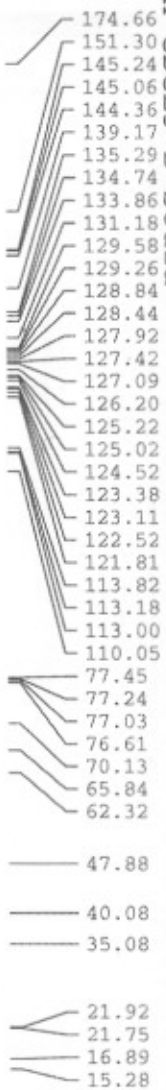
Current Data Parameters
NAME mudsjn26
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 14.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 9.00



DS-608 MU in CDCL₃ D'Souza



Current Data Parameters
NAME mudsjn26
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

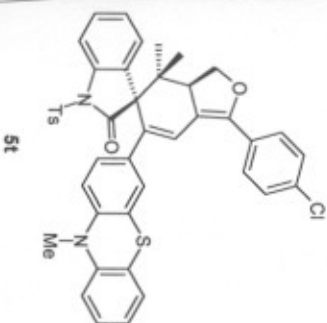
Date_ 20060626
Time 15.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 2400
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



DS-608 MU in CDCL3 D"Souza

129.60
129.27
128.84
128.45
128.08
127.92
127.43
127.10
126.20
125.21
124.98
124.53
122.53
121.80
113.83
113.18
112.99

70.14
65.86

47.86

35.09

21.92
21.77
16.89
15.29



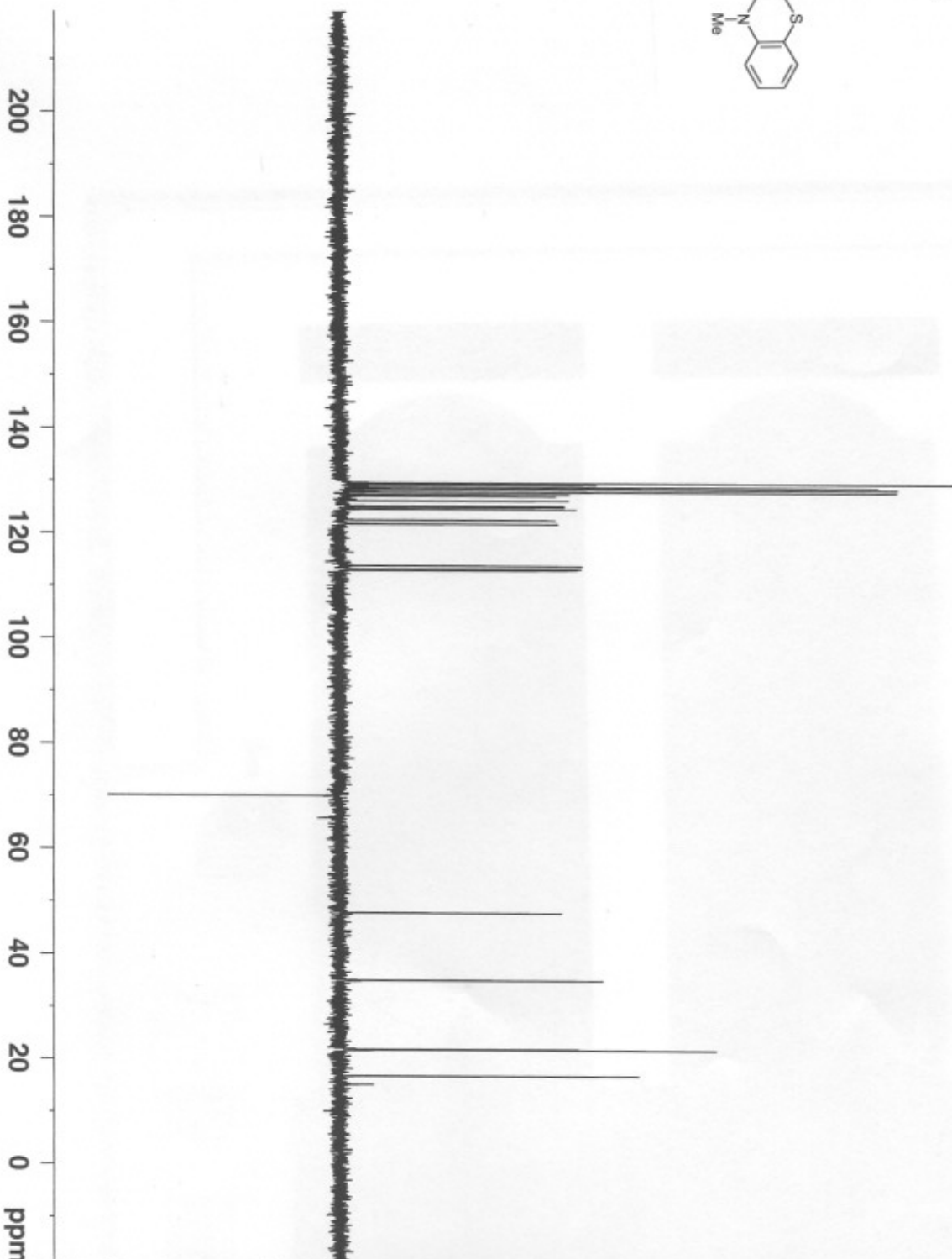
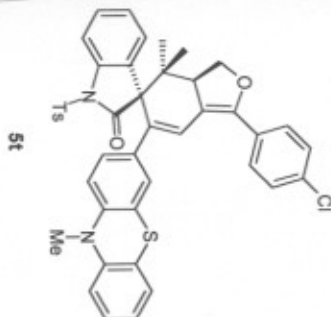
Current Data Parameters
NAME mudsjn26
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 18.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

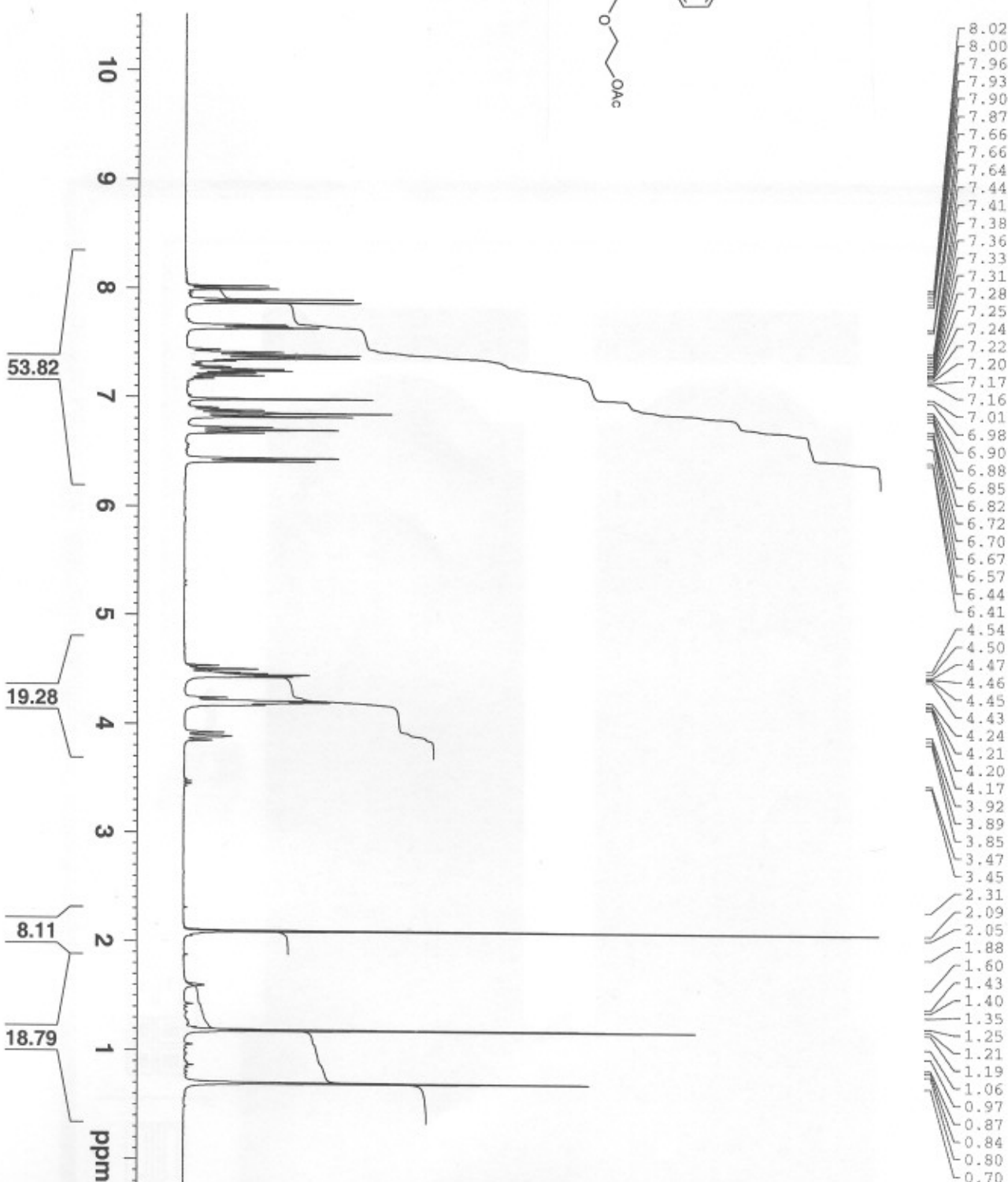
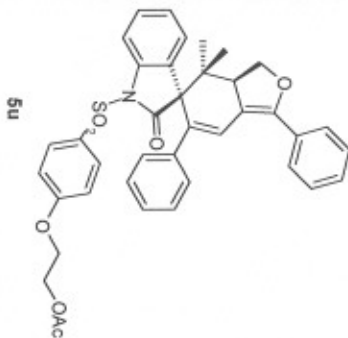
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing Parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



DS-609 MU in CDCL3 D"Souza

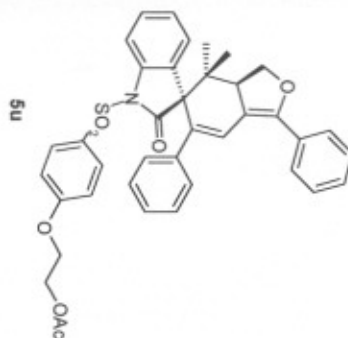


Current Data Parameters
NAME muszjn26
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 18.55
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 256
DE 81.000 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 9.00

DS-609 MU in CDCL3 D'Souza



8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 ppm

8.02
8.00
7.96
7.93
7.90
7.87

7.66
7.66
7.64

7.44
7.41
7.38
7.36
7.33
7.31
7.28
7.25
7.24
7.22
7.20
7.17
7.16

7.01
6.98

6.90
6.88
6.85
6.82

6.72
6.70
6.67

6.57

6.44
6.41



53.82

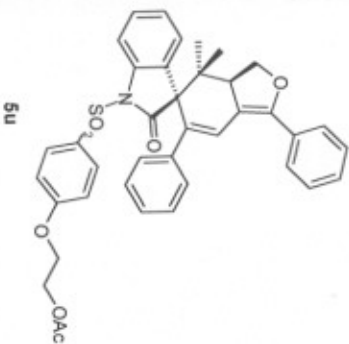
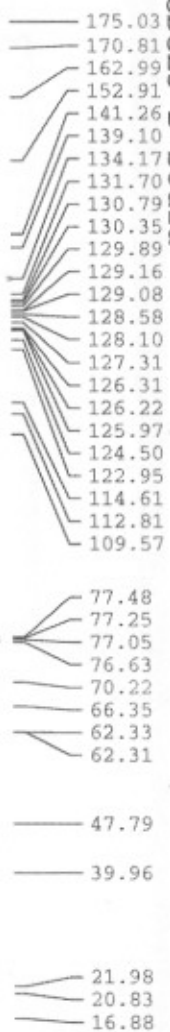
Current Data Parameters
NAME muszjn26
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 18.55
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.376760 Hz
AQ 1.3271540 sec
RG 256
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.20 dB
SFO1 300.1318534 MHz

F2 - Processing Parameters
SI 32768
SF 300.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 9.00

DS-609 MU in CDCL3 D'Souza



Current Data Parameters
NAME muszjn26
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 20.40
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DE 27.800 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

DS-609 MU in CDCL3 D"Souza

130.50
130.35
129.17
129.08
128.81
128.58
128.11
127.31
126.31
126.21
125.96
124.51
122.95
114.61
112.81

70.22
66.34
62.31

47.78

21.98
20.85
16.88



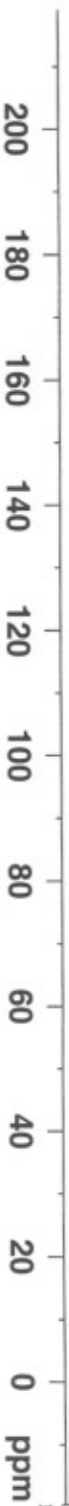
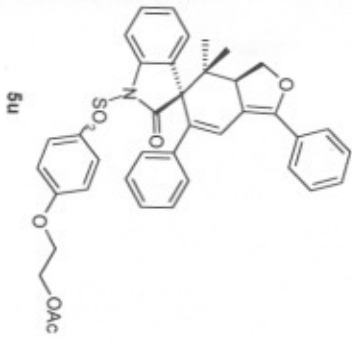
Current Data Parameters
NAME muszjn26
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060626
Time 21.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
CNS2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001528 sec
TD0 1

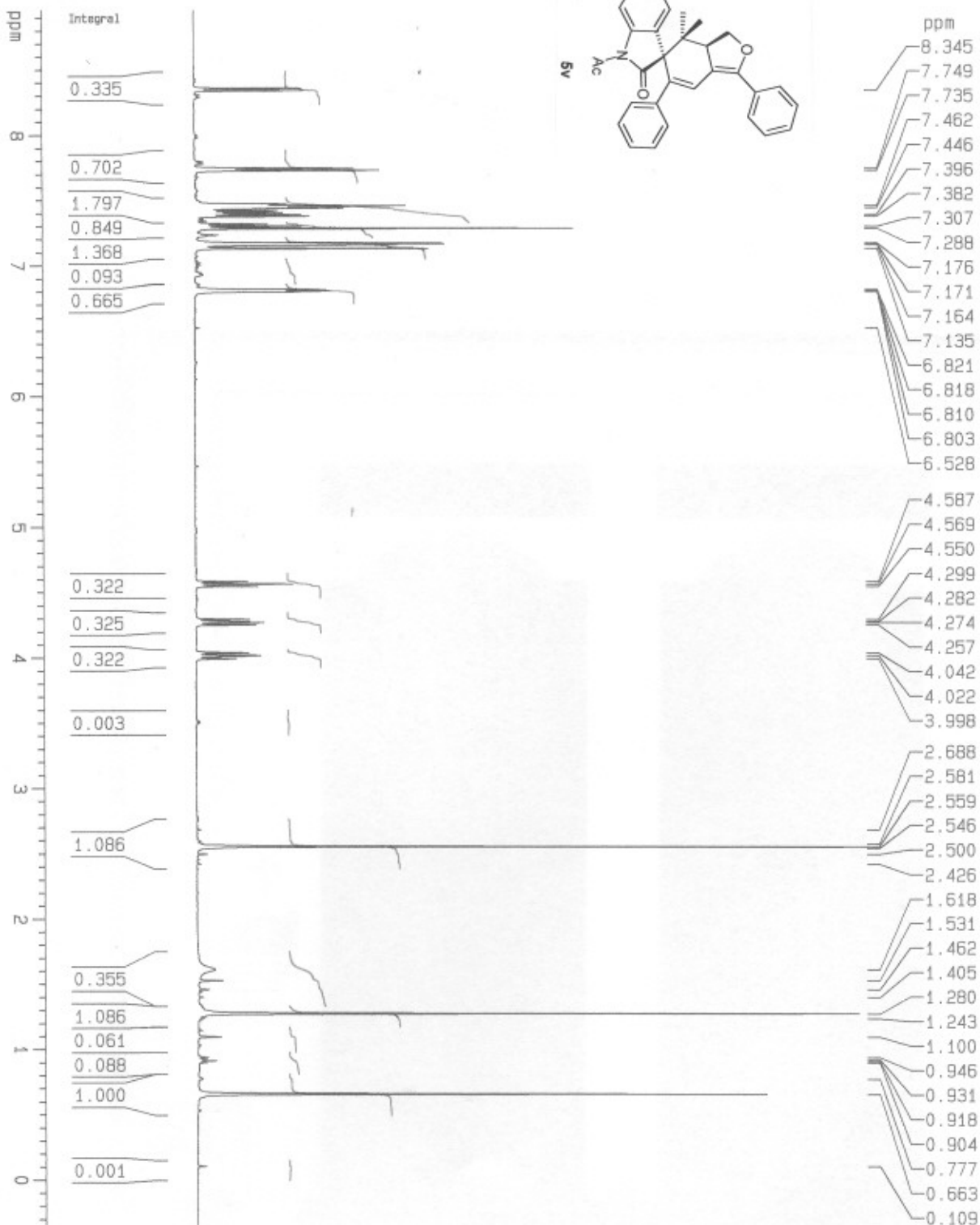
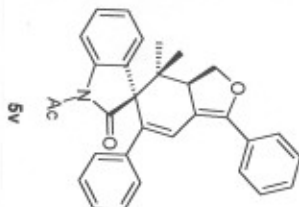
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
P2 24.00 usec
PL1 1.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.00 usec
P4 24.00 usec
PCPD2 100.00 usec
PL2 -2.20 dB
PL12 16.22 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



D'Souza DS_453MU CDCl3



Current Data Parameters

NAME DS_453MU

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20050519

Time 12.08

INSTRUM spect

PROBHD 5 mm TBI 1H/13

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SWH 8012.820 Hz

FIDRES 0.244632 Hz

AQ 2.0447731 sec

RG 128

DW 62.400 usec

DE 6.00 usec

TE 300.0 K

D1 2.00000000 sec

CHANNEL f1

NUC1 1H

P1 10.10 usec

PL1 0.00 dB

SFO1 500.1330008 MHz

F2 - Processing parameters

SF 500.1330008 MHz

SI 16384

WDW EM

SSB 0

LB 0.10 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

CY 13.00 cm

F1P 8.963 ppm

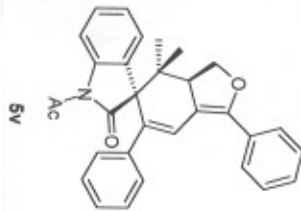
F1 4482.42 Hz

F2P -0.372 ppm

F2 -185.92 Hz

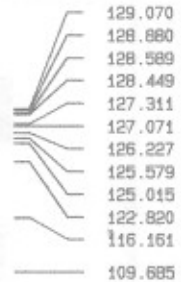
PPMCM 0.46571 ppm/cm

HZCM 233.41586 Hz/cm



5v

ppm



D'Souza DS_453Mu CDCl3



Current Data Parameters
NAME: D'Souza DS_453Mu
EXPNO: 8
PROCNO: 1

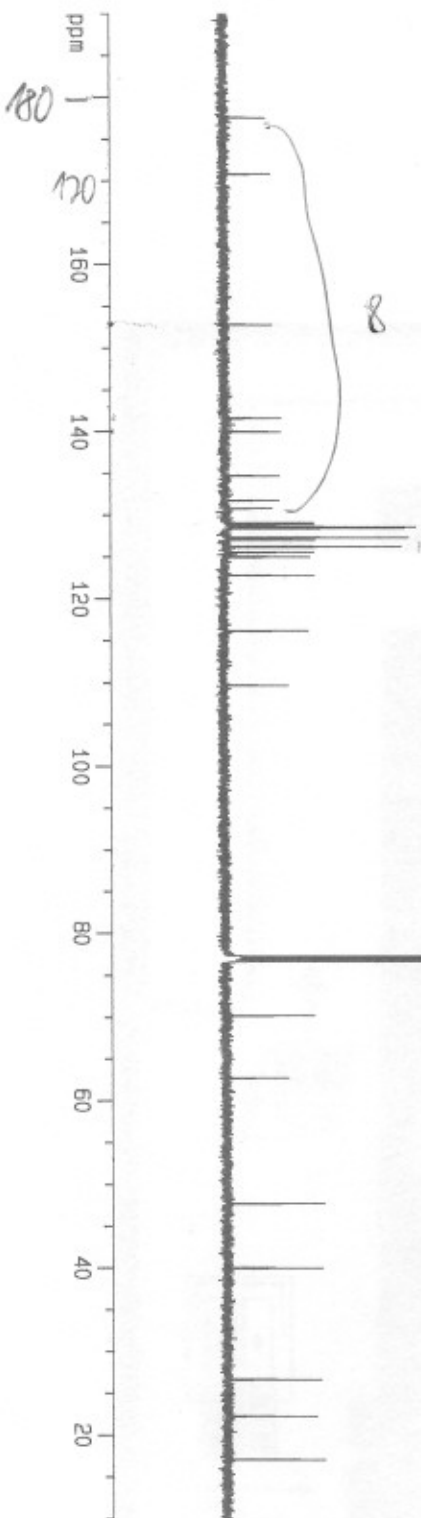
F2 - Acquisition Parameters
Date_: 20050320
Time: 7.35
INSTRUM: spect
PROBHD: 5 mm TBI HX/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 3880
DS: 2
SWH: 30854.157 Hz
FIDRES: 0.470650 Hz
AQ: 1.5617322 sec
RG: 5792.8
CW: 16.200 usec
DE: 5.00 usec
TE: 298.0 K
O1: 2.00000000 sec
d11: 0.03000000 sec
d12: 0.00020000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 usec
PL1: 0.00 dB
SFO1: 125.7713172 MHz

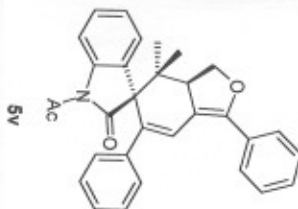
===== CHANNEL f2 =====
NAME: nutcr
NUC2: 1H
P2: 100.00 usec
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 500.132500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7571028 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 0.50

10 NMR plot parameters
CX: 20.00 cm
CY: 13.00 cm
F1P: 190.000 ppm
F1: 22893.88 Hz
F2P: 10.000 ppm
F2: 1257.88 Hz
PRGCM: 9.00000 ppm/c
MCH: 1131.82007 Hz/cm



D'Souza_DS_453MU_CDCl3



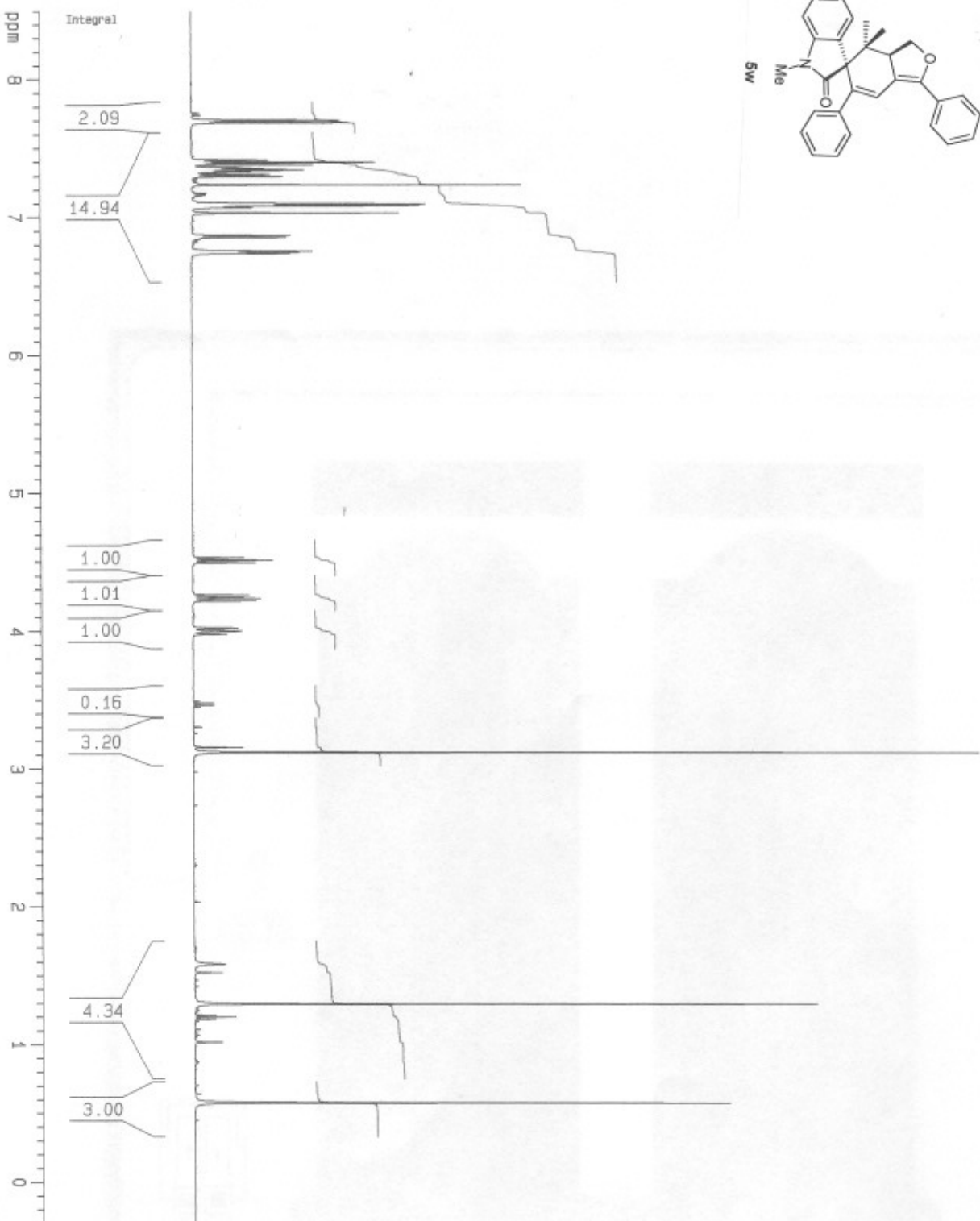
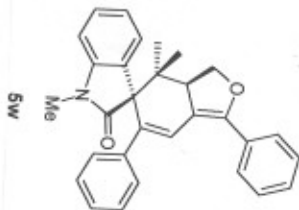
ppm

160
140
120
100
80
60
40
20

129.1
128.9
128.6
128.5
127.3
127.1
126.2
125.6
125.4
125.0
122.8
116.2
77.2
70.2
47.7
26.7
22.3
17.1

Current Data Parameters
NAME: multiSpec
EXPNO: 7
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20050520
Time: 4.17
INSTRUM: spect
PROBHD: 5 mm TBI 1H/13
PULPROG: gpg135
TD: 65536
SOLVENT: CDCl3
NS: 2000
DS: 2
SWH: 36664.197 Hz
FIDRES: 0.470950 Hz
AQ: 1.0617332 sec
RG: 1625.5
IN: 15.200 uMHC
DE: 8.00 uMHC
TE: 298.0 K
DMSD2: 145.0000000 sec
D1: 1.000000000 sec
d2: 0.00344028 sec
d12: 0.00020000 sec
DELTA: 0.00001284 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 uMHC
PC2: 20.80 uMHC
PL1: 0.00 dB
PC1: 120.773172 MHz
===== CHANNEL f2 =====
NUC2: 1H
P2: 10.10 uMHC
PC2: 20.20 uMHC
PL2: 0.00 dB
PC2: 500.132250 MHz
F2 - Processing parameters
SI: 32768
SF: 125.761920 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00
===== 1D NMR plot parameters =====
CX: 20.00 cm
CY: 5.00 cm
FAP: 150.000 ppm
F1: 228631.88 Hz
F2P: 10.000 ppm
F2: 1257.58 Hz
PPMCM: 9.00000 ppm/cm
HZCM: 1131.82007 Hz/cm

D'Souza DS.258 CDCl3



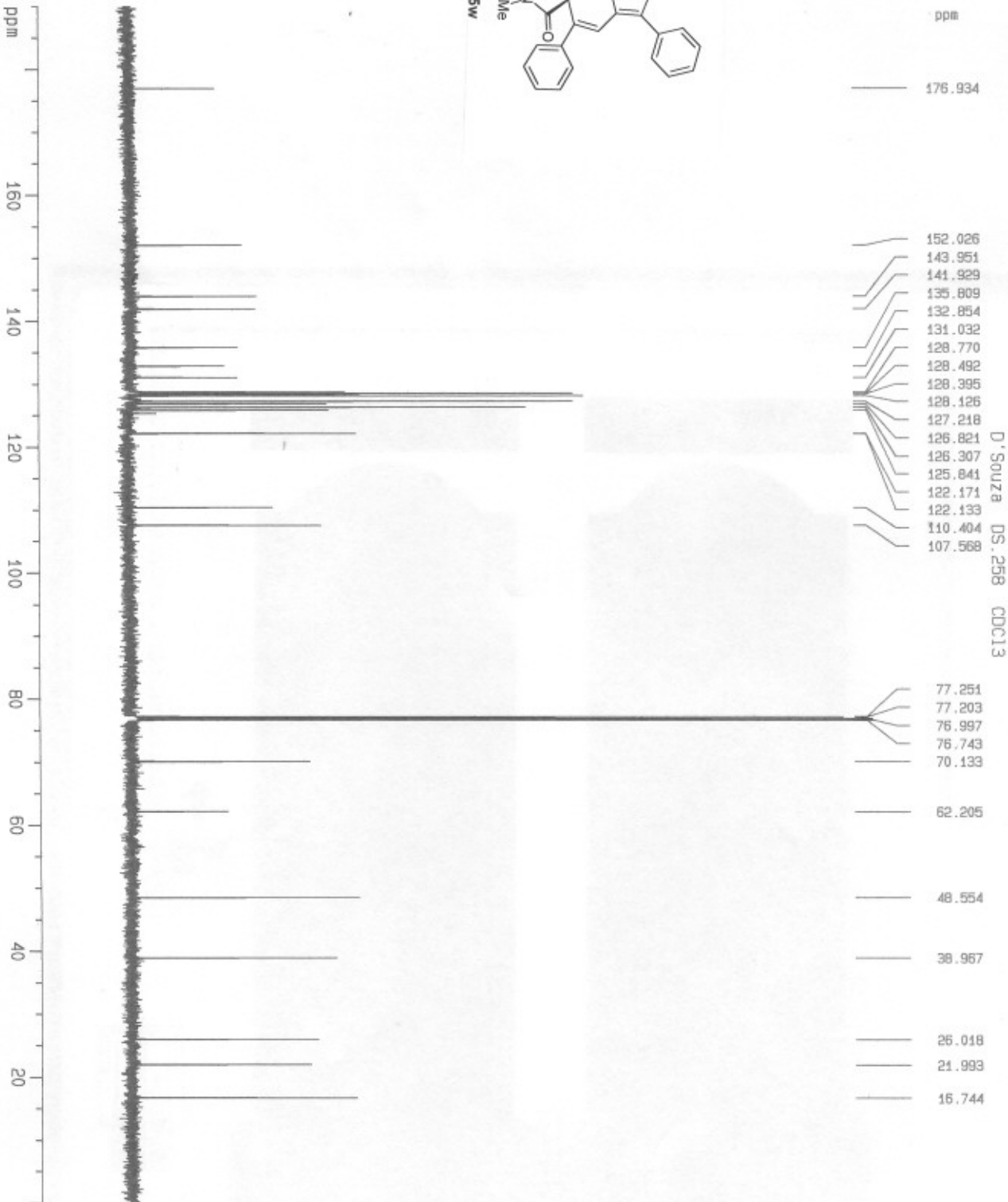
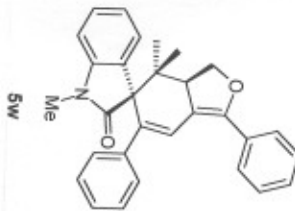
Current Data Parameters
NAME mus05j1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040705
Time 10.50
INSTRUM spect
PROBHD 5 mm TBI AV13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 5482.456 Hz
FIDRES 0.167311 Hz
AQ 2.3894915 sec
RG 80.5
OW 51.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 0.00 dB
SFO1 500.1322738 MHz

F2 - Processing parameters
SI 16384
SF 500.1300232 MHz
MCW 0
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 13.00 cm
F1P 8.500 ppm
F1 4251.11 Hz
F2P -0.300 ppm
F2 -150.04 Hz
PPMCM 0.44000 ppm/cm
HZCM 220.05722 Hz/cm



Current Data Parameters
NAME: mus0511
EXPNO: 3
PROCNO: 1

F2 - Acquisition Parameters
Date_: 2004/05
Time: 12.17
INSTRUM: spect
PROBHD: 5 mm THT V13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 4400
DS: 2
SWH: 30864.197 Hz
FIDRES: 0.470950 Hz
AQ: 1.051732 sec
RG: 5792.8
DM: 18.200 Usec
DE: 8.00 Usec
TE: 298.0 K
D1: 1.00000000 sec
d15: 0.03000000 sec
d12: 0.00020000 sec

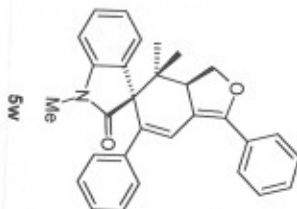
CHANNEL f1 13C
NUC1: 13C
P1: 10.40 Usec
PL1: 0.00 dB
SFO1: 125.773172 MHz

CHANNEL f2 1H
NUC2: 1H
PCPD2: 160.00 Usec
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 500.132550 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7577975 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR Plot Parameters
CX: 20.00 cm
CY: 13.00 cm
F1P: 150.000 ppm
F1: 23863.86 Hz
F2P: 0.000 ppm
F2: 0.00 Hz
PRCH: 9.50000 ppm/cm
HZCH: 1194.69910 Hz/cm

D'Souza DS.258 CDCl3



ppm



- 128.8
- 128.5
- 128.4
- 128.1
- 127.2
- 126.8
- 126.3
- 125.8
- 122.2
- 122.1
- 107.6
- 77.2
- 70.1
- 48.5
- 26.0
- 22.0
- 16.7

Current Data Parameters
NAME: DS.258
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 2004/07/05
Time: 11.04
INSTRUM: spect
PROBHD: 5 mm TBI 4H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 800
DS: 2
SWH: 30564.197 Hz
FIDRES: 0.470500 Hz
AQ: 1.061739 sec
RG: 1638.8
CH: 16.200 umsc
CTE: 8.00 umsc
TE: 298.0 K
CHRG2: 145.000000 sec
D1: 4.00000000 sec
D2: 0.00040000 sec
D12: 0.00000000 sec
DELTA: 0.00001304 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 10.40 umsc
PC: 20.00 umsc
PL1: 0.00 dB
RF01: 125.7713172 MHz

===== CHANNEL f2 =====
CPDPRG2: zgpg30
NUC2: 1H
P2: 10.10 umsc
PC: 20.00 umsc
PL2: 0.00 dB
RF02: 500.132500 MHz

F2 - Processing parameters
SI: 32768
SF: 125.767982 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
FID: 180.000 DDM
F1: 228951.98 Hz
F2: 0.000 DDM
F2: 0.00 Hz
PWCN: 9.50000 ppa/cm
HZCN: 1164.69810 Hz/cm