

Supporting Information

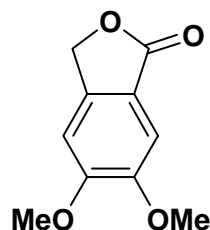
Synthesis of Crispine-A analogues *via* an intramolecular Schmidt reaction

*Ajoy Kapat, Ponminor SenthilKumar and Sundarababu Baskaran,**

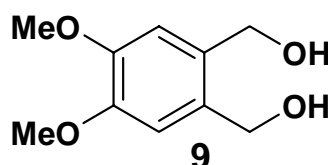
*Department of Chemistry, Indian Institute of Technology Madras,
Chennai-600 036, India*

Corresponding Author E-mail: sbhaskar@iitm.ac.in

Experimental Section.....	1 – 15
Single crystal X-ray analysis	10
NMR Spectra for selected compounds.....	16 - 42

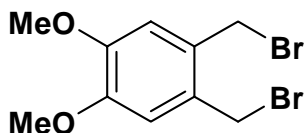


5,6-dimethoxyisobenzofuran-1(3H)-one ^1H NMR [400 MHz, CDCl_3] δ 7.27 (s, 1H), 6.87 (s, 1H), 5.19 (s, 2H), 3.96 (s, 3H), 3.93 (s, 3H), ^{13}C NMR [100 MHz, CDCl_3] δ 171.4, 154.8 150.4, 141.0, 117.6, 103.4, 69.1, 56.3, 56.2; MS (ESI) $\text{C}_{10}\text{H}_{11}\text{O}_4$ ($\text{M}+\text{H}$) $^+$ 195.

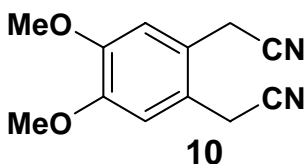


1,2-Bis(hydroxymethyl)-4,5-dimethoxybenzene (9): To a stirred solution of LAH (430 mg, 11.34 mmol) in dry THF (20 ml) at 0 °C was slowly added a solution of 5,6-dimethoxyisobenzofuran-1(3H)-one (2 g, 10.306 mmol) and stirred at 0 °C for 15 mins. The reaction mixture was then heated to reflux for 4h, cooled to 0 °C, quenched with moist Na_2SO_4 and filtered. The filtrate was then concentrated under reduced pressure to give the corresponding diol (**9**) (1.92 g, 94% yield). The crude product was taken for further reaction without purification. (IR (Neat): 3460, 3337, 2922, 1607, 1511, 1460, 1103, 754 cm^{-1} ; ^1H NMR [400 MHz, CDCl_3] δ 6.89 (s, 2H), 4.66 (s, 4H), 3.89 (s,

6H), 3.08 (bs, 1H), 1.76 (bs, 1H), ^{13}C NMR [100 MHz, CDCl_3] δ 148.5, 132.0, 113.2, 63.8, 56.0; MS (ESI) $\text{C}_{10}\text{H}_{14}\text{O}_4$ ($\text{M}+\text{Na}$) $^+$ 221.

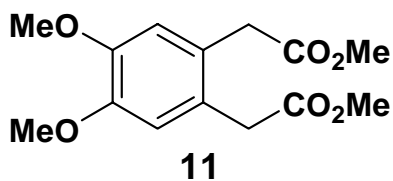


1,2-Bis(bromomethyl)-4,5-dimethoxybenzene: To a suspension of diol (**9**) (2 g, 10.10 mmol) in benzene (20 ml) was slowly added PBr_3 (2.06 ml, 22 mmol) and stirred at 50 °C for 1h then cooled to rt and stirred for 24h. The reaction mixture was then basified with saturated Na_2CO_3 solution (PH = 9). Organic layer was washed with water and dried over anhydrous Na_2SO_4 , concentrated under reduced pressure and purified by recrystallization to afford the corresponding **1,2-bis(bromomethyl)-4,5-dimethoxybenzene** (3.01 g, 92% yield). IR (neat): 2955, 1605, 1522, 1460, 1358, 1277, 1204, 1128, 1000, 871, 603 cm^{-1} ; ^1H NMR [400 MHz, CDCl_3] δ 6.84 (s, 2H), 4.63 (s, 4H), 3.89 (s, 6H); ^{13}C NMR [100 MHz, CDCl_3] δ 149.5, 129.0, 113.7, 56.0, 30.5.



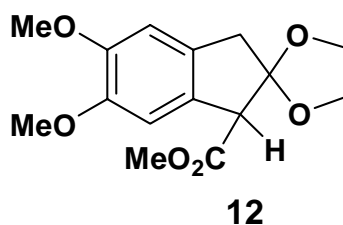
2,2'-(4,5-dimethoxy-1,2-phenylene)diacetonitrile (10): To a stirred solution of NaCN (3.16 g, 64.51 mmol) in dry DMSO (50 ml) was slowly added a solution of 1,2-bis(bromomethyl)-4,5-dimethoxybenzene (9.5 g, 29.321

mmol) at 90 °C. The reaction mixture was stirred at 90 °C for additional 3h. Then quenched with water and extracted with chloroform. Organic layer was dried over anhydrous Na₂SO₄, concentrated under reduced pressure and purified by column chromatography over silica gel using gradient elution with 10 – 20 % EtOAc in hexane to yield the corresponding dicyano compound (**10**) (5.71 g, 90% yield). IR (neat): 2959, 2941, 2837, 2250, 1609, 1525, 1417, 1272, 1180, 1089, 873, 756 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.90 (s, 2H), 3.90 (s, 6H), 3.70 (s, 4H); ¹³C NMR [100 MHz, CDCl₃] δ 149.3, 120.2, 116.9, 112.8, 56.1, 21.0; MS (ESI) C₁₂H₁₂N₂O₂ (M+Na)⁺ 239.



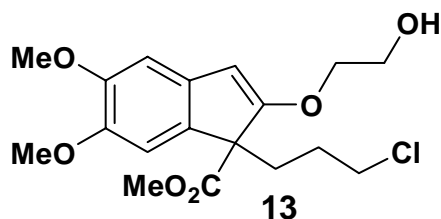
Dimethyl 2,2'-(4,5-dimethoxy-1,2-phenylene)diacetate (11a): To a solution of dicyano compound (**10**) (2.12 g, 8.62 mmol) in methanol (15 ml), thionyl chloride was slowly added (4.13 ml, 56.96 mmol) and heated to reflux for 2 days. Reaction mixture was diluted with EtOAc and washed with water. Organic layer was dried over anhydrous Na₂SO₄, concentrated and purified by column chromatography over silica gel using gradient elution with 10 – 20 % EtOAc in hexane to yield the corresponding diester (**11**) (2.86 g, 94% yield). IR (neat): 2952, 2851, 1729, 1520, 1273, 1192, 1009, 754 cm⁻¹; ¹H NMR

[400 MHz, CDCl₃] δ 6.76 (s, 2H), 3.85 (s, 6H), 3.67 (s, 6H), 3.62 (s, 4H); ¹³C NMR [100 MHz, CDCl₃] δ 171.7, 148.3, 125.2, 114.1, 55.9, 51.8, 38.2, 29.60; MS (ESI) C₁₄H₁₈O₆ (M+Na)⁺ 305.



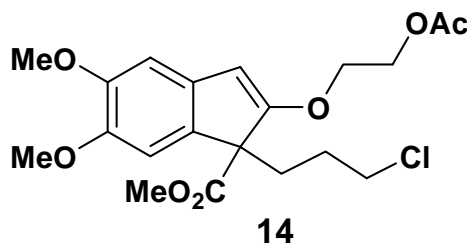
Methyl 5',6'-dimethoxy-1',3'-dihydrospiro[[1,3]dioxolane-2,2'-indene]-1'-carboxylate (12): To a stirred solution of β-ketoester (**7**) (100 mg, 0.378 mmol), triethyl orthoformate (251 μl, 1.51 mmol) and ethylene glycol (212 μl, 3.77 mmol) in dry DCM (10 ml) added catalytic amount of PTSA (7 mg, 0.03 mmol) and the reaction mixture was stirred for about 3 days. Reaction mixture was then diluted with DCM, washed with saturated NaHCO₃ followed by brine and extracted with DCM. Organic layer was dried over anhydrous Na₂SO₄, conc. and purified by column chromatography over silica gel using gradient elution with 10 – 20 % EtOAc in hexane to yield the corresponding ethylene ketal (**12**) (53%). IR (neat): 2957, 2836, 1728, 1508, 1466, 1257, 1180, 1031, 857, 572 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.77 (s, 1H), 6.74 (s, 1H), 4.01-4.11 (m, 4H), 3.86 (s, 3H), 3.84 (s, 3H), 3.73 (s, 3H), 3.73 (s, 3H), 3.43 (d, *J* = 16 Hz, 1H), 3.06 (d, *J* = 16 Hz, 1H); ¹³C NMR [100 MHz,

CDCl₃] δ 171.0, 149.4, 148.5, 132.3, 129.4, 117.9, 108.3, 107.7, 65.4, 64.5, 59.3, 56.0, 55.9, 52.0, 42.9; MS (ESI) C₁₅H₁₈O₆ (M+Na)⁺ 317.



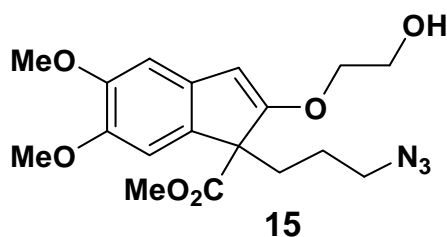
Methyl 1-(3-chloropropyl)-2-(2-hydroxyethoxy)-5,6-dimethoxy-1H-indene-1-carboxylate (13): To a suspension of NaH (14 mg, 0.35 mmol) in dry DMF (3 ml) at 0 °C was slowly added a solution of ethylene ketal (**12**) (100 mg, 0.325 mmol) in dry DMF (3 ml) and stirred at 0 °C for 5 min. Then into this added 1-chloro-3-iodopropane (52 μ l, 0.487 mmol) and stirred at 0 °C for 30 min. The reaction mixture was then quenched, washed with water and extracted with EtOAc. Organic layer was dried over anhydrous Na₂SO₄, concentrated under reduced pressure and purified by column chromatography over silica gel using gradient elution with 10 – 20 % EtOAc in hexane to yield the alkylated product (**13**) (87.3 mg, 70% yield). IR (neat): 3513, 2951, 2835, 1727, 1607, 1491, 1454, 1312, 1213, 1075, 1032, 761 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.86 (s, 1H), 6.72 (s, 1H), 5.66 (s, 1H), 4.15-4.10 (m, 4H), 3.87 (s, 3H), 3.86 (s, 3H), 3.67 (s, 3H), 3.42-3.37 (m, 2H), 2.32 (t, *J* = 8 Hz,

1H), 1.46-1.25 (m, 2H); ¹³C NMR [100 MHz, CDCl₃] δ 172.6, 164.3, 149.4, 146.1, 136.2, 129.9, 107.2, 104.0, 101.2, 71.5, 60.7, 60.4, 56.6.

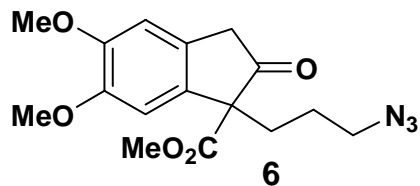


Methyl 1-(3-chloropropyl)-2-(2-hydroxyethoxy)-5,6-dimethoxy-1H-indene-1-carboxylate (14): To a stirred solution of alkylated compound (13) (9 mg, 0.024 mmol) in dry DCM (1 ml), acetic anhydride (3.47 μl, 0.0364 mmol) and triethyl amine (3.23 μl, 0.0243 mmol) was added followed by catalytic amount DMAP and stirred at rt for 2h. The reaction mixture was then diluted with DCM and washed with water. Organic layer was dried over anhydrous Na₂SO₄, conc. under reduced pressure and purified by column chromatography over silica gel using gradient elution with 10-15 % EtOAc in hexane to yield the acetylated compound (**14**) (7 mg, 70% yield). IR (neat): 2952, 1731, 1608, 1491, 1455, 1316, 1232, 1058, 761 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.83 (s, 1H), 6.73 (s, 1H), 5.64 (s, 1H), 4.41-4.39 (m, 2H) 4.20-4.13 (m, 2H), 3.87 (s, 3H), 3.86 (s, 3H), 3.63 (s, 3H), 3.41-3.36 (m, 2H), 2.32-2.27 (m, 2H), 2.09 (s, 3H), 1.29-1.25 (m, 2H); ¹³C NMR [100 MHz,

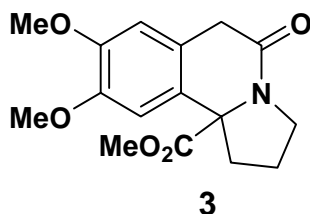
CDCl₃] δ 172.4, 170.8, 164.8, 149.5, 146.2, 136.1, 130.4, 107.1, 104.2, 100.9, 68.09, 62.1, 61.1, 56.6, 56.1, 52.6, 44.9, 30.5, 26.6, 20.7; MS (ESI) C₂₀H₂₅ClO₇ (M+H)⁺ 413.



Methyl 1-(3-azidopropyl)-2-(2-hydroxyethoxy)-5,6-dimethoxy-1H-indene-1-carboxylate (15): To a solution of alkylated compound (**13**) (70 mg, 0.0189 mmol) in DMF (2 ml) was added NaN₃ (13.5 mg, 0.020 mmol) and stirred at 60 °C for 24h. Reaction mixture was then diluted with EtOAc, washed with water. Organic layer was dried, conc. and purified by column chromatography over silica gel using gradient elution with 10 – 20 % EtOAc in hexane to yield the corresponding azido compound (**15**) (59 mg, 83% yield). IR (neat): 3498, 2935, 2094, 1727, 1607, 1491, 1455, 1309, 1214, 1966, 762 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.85 (s, 1H), 6.73 (s, 1H), 5.67 (s, 1H), 4.11-3.91 (m, 4H), 3.87 (s, 3H), 3.86 (s, 3H), 3.67 (s, 3H), 3.18-3.14 (m, 2H), 2.27-2.23 (m, 2H), 1.29-1.25 (m, 2H); ¹³C NMR [100 MHz, CDCl₃] δ 172.5, 164.5, 149.7, 146.3, 136.3, 130.1, 107.6, 104.4, 100.2, 71.6, 62.3, 60.6, 56.7, 56.1, 52.6, 51.2, 30.3, 22.7.; MS (ESI) C₁₈H₂₃N₃O₆ (M+Na)⁺ 400.

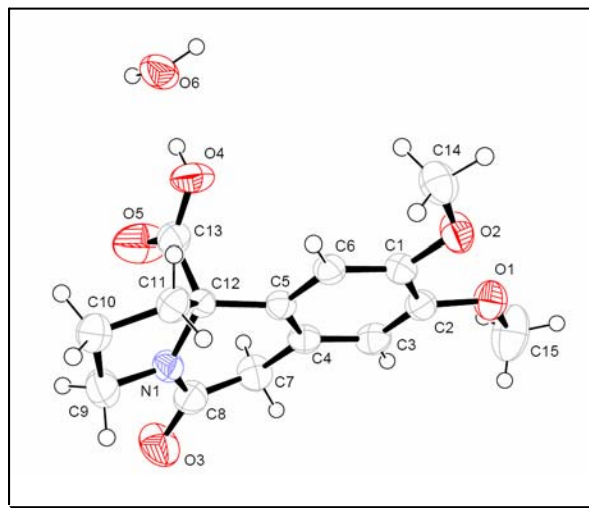
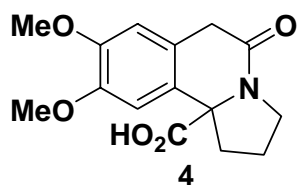


Methyl 1-(3-azidopropyl)-5,6-dimethoxy-2-oxo-2,3-dihydro-1H-indene-1-carboxylate (6): To a stirred solution of azide (**15**) (488 mg, 1.294 mmol) in methanol (10 ml) was added Dowex activated using 1N HCl and heated to reflux for 20h. The reaction mixture was then filtered, concentrated under reduced pressure and the residue was purified by column chromatography over silica gel using gradient elution with 10 – 20 % EtOAc in hexane to yield the corresponding keto azide (**6**) (349 mg, 81% yield). IR (neat): 2913, 2095, 1613, 1494, 1454, 1286, 1164, 1032, 763 cm^{-1} ; ^1H NMR [400 MHz, CDCl_3] δ 6.87 (s, 1H), 6.76 (s, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 3.76 (d, $J = 22.4$ Hz, 1H), 3.65 (s, 3H), 3.44 (d, $J = 22.4$ Hz), 3.24-3.16 (m, 2H), 2.28-2.19 (m, 2H), 1.31-1.26 (m, 2H); ^{13}C NMR [100 MHz, CDCl_3] δ 212.2, 170.8, 149.9, 145.5, 131.6, 129.1, 107.7, 106.4, 64.6, 56.1, 56.0, 52.8, 51.1, 43.4, 31.0, 23.7.



Methyl 8,9-dimethoxy-5-oxo-1,2,3,5,6,10b-hexahydropyrrolo[2,1-a]isoquinoline-10b-carboxylate (3): In a clean flame dried RB flask, ketoazide (**15**) (364 mg, 1.04 mmol) was taken and dried azeotropically with dry benzene. Into this added DCM (5 ml) and cooled to -5 °C. Triflic acid (139 μ l, 1.57 mmol) was slowly added and stirred at -5 °C for 15min. Reaction mixture was then diluted with DCM and washed with water. Organic layer was dried over anhydrous Na₂SO₄ concentrated under reduced pressure and purified by column chromatography over silica gel using gradient elution with 30 – 40 % EtOAc in hexane to yield the corresponding cyclized product (**3**) (180.69 mg, 54% yield). IR (neat): 2953, 1731, 1650, 1518, 1433, 1411, 1254, 1217, 1133, 805, 628 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.77 (s, 1H), 6.55 (s, 1H), 3.83 (s, 3H), 3.80 (s, 3H), 3.70 (d, *J* = 19.2 Hz, 1H), 3.59 (s, 3H), 3.58-3.56 (m, 1H), 3.41 (d, *J* = 18.8 Hz, 1H), 3.05-3.02 (m, 1H), 2.05-1.97 (m, 2H), 1.88-1.81 (m, 2H); ¹³C NMR [100 MHz, CDCl₃] δ 172.1, 168.1, 149.4, 148.1, 126.0, 125.1, 110.0, 108.6, 71.6, 56.2, 56.0, 53.1, 44.7, 37.6, 36.2, 21.5; HRMS (ESI) calcd for C₁₆H₁₉NO₅ (M+H)⁺: 306.134; found: 306.1350.

Single Crystal X-Ray Analysis of Hydroxy analogue of Crispine A (4):



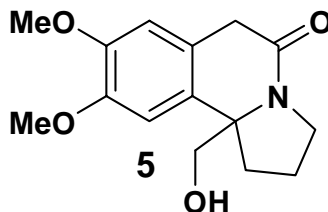
To a solution of ester (**3**) (40 mg, 0.125 mmol) in dioxane : water (3:1) (3 ml), KOH was added and stirred at rt for 5h. Then diluted with water and neutralized (PH = 6) with 1N HCl and extracted with EtOAc. Organic layers were dried over anhydrous Na₂SO₄, concentrated under reduced pressure and purified by recrystallisation from EtOAc:Hexane (1:5) (5 mg/mL) afforded suitable size and quality crystals for x-ray diffraction in the form of pale yellow needles. CCDC Number: CCDC 663178

Table 1. Crystal data and structure refinement for ajoy.

Identification code	ajoy
Empirical formula	C ₁₅ H ₁₉ N O ₆
Formula weight	309.31
Temperature	298(2) K
Wavelength	0.71073 Å

Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.3243(9) Å alpha = 90 deg. b = 10.6834(10) Å beta = 90 deg. c = 13.6598(12) Å gamma = 90 deg.
Volume	1506.7(2) Å ³
Z, Calculated density	4, 1.364 Mg/m ³
Absorption coefficient	0.106 mm ⁻¹
F(000)	656
Crystal size	0.25 x 0.22 x 0.22 mm
Theta range for data collection	2.42 to 28.46 deg.
Limiting indices	-13 ≤ h ≤ 9, -12 ≤ k ≤ 14, -17 ≤ l ≤ 14
Reflections collected / unique	19002 / 3594 [R(int) = 0.0738]
Completeness to theta = 25.00	100.0 %
Absorption correction	None
Max. and min. transmission	0.9771 and 0.9740
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3594 / 3 / 214
Goodness-of-fit on F ²	0.740
Final R indices [I > 2σ(I)]	R1 = 0.0481, wR2 = 0.1125
R indices (all data)	R1 = 0.1352, wR2 = 0.1597

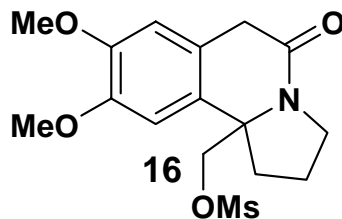
Absolute structure parameter	-0.3(19)
Extinction coefficient	0.009(3)
Largest diff. peak and hole	0.151 and -0.167 e.A ⁻³



10b-(hydroxymethyl)-8,9-dimethoxy-1,2,3,10b-tetrahydropyrrolo[2,1-

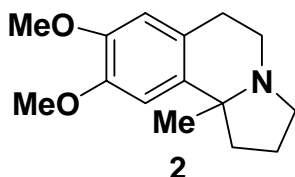
a]isoquinolin-5(6H)-one (5): To a suspension of LAH (7.5 mg, 0.19 mmol) in dry THF (2 ml) at 0 °C, a solution of ester (**3**) (55 mg, 0.18 mmol) in dry THF (2 ml) was slowly added and stirred at 0 °C for 8h. Reaction mixture was then quenched with moist Na₂SO₄. The solid was filtered, washed with EtOAc. Filtrate was concentrated under reduced pressure and purified by column chromatography over silica gel using gradient elution with 30–50 % EtOAc in hexane to yield the corresponding alcohol (**5**) (4.8 mg, 70 % yield). IR (neat): 3385, 2940, 1618, 1514, 1452, 1298, 1214, 1065, 765 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.67 (s, 1H), 6.64 (s, 1H), 3.88 (s, 3H), 3.86 (s, 3H), 3.78 (d, *J* = 19.2 Hz, 1H), 3.86-3.59 (m, 4H), 3.43 (d, *J* = 19.2 Hz, 1H), 2.60 (bs, 1H), 2.55-2.54 (m, 1H), 2.11-2.05 (m, 4H); ¹³C NMR [100 MHz, CDCl₃] δ 168.5, 148.7, 147.9, 129.4, 124.9, 110.2, 108.4, 69.3, 67.9, 60.4,

56.2, 56.0, 44.9, 37.5, 33.8, 29.6, 21.2, 21.0, 14.1; MS (ESI) C₁₅H₁₉NO₄ (M+H)⁺ 278.



(8,9-dimethoxy-5-oxo-1,2,3,5,6,10b-hexahydropyrrolo[2,1-a]isoquinolin-10b-yl)methyl methanesulfonate (16): To a solution of alcohol (**5**) (5 mg, 0.0180 mmol) in dry DCM at 0 °C was added triethyl amine (5.5 µl, 0.03969 mmol) and stirred for 10 mins. Into this slowly added methane sulfonylchloride (1.54 µl, 0.0198 mmol) and stirred at 0 °C for 20 min. The temperature was then slowly raised to rt and stirred for 6h. Reaction mixture was then diluted with DCM and washed with water. Organic layer was dried over anhydrous Na₂SO₄, conc. and purified by column chromatography over silica gel using gradient elution with 30–50 % EtOAc in hexane to yield the corresponding mesylate (**16**) (6 mg, 93 % yield). IR (neat): 2940, 1618, 1514, 1452, 1366, 1298, 1214, 1065, 765 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.68 (s, 1H), 6.65 (s, 1H), 4.15 (dd, *J* = 23.2, 10 Hz, 2H), 3.89 (s, 3H), 3.88 (s, 3H), 3.77 (d, *J* = 19.6 Hz, 1H), 3.73-3.69 (m, 1H), 3.49 (d, *J* = 19.6 Hz, 1H), 2.82 (s, 3H), 2.64-2.62 (m, 1H), 2.22-2.12 (m, 2H), 1.43-1.37 (m, 2H); ¹³C NMR

[100 MHz, CDCl₃] δ 168.1, 149.4, 148.3, 128.3, 127.8, 124.9, 110.4, 108.9, 72.4, 67.0, 56.4, 56.1, 46.2, 45.2, 37.5, 34.6, 31.5, 21.1; HRMS (ESI) calcd for C₁₆H₂₁NO₆S (M+Na)⁺: 378.0987; found: 378.0988.



Pyrrolidino[a]-1-methyl-1,2,3,4-tetrahydroisoquinoline (2):²⁶ To a stirred solution of LAH (1 mg, 0.0264 mmol) in dry THF (25 μ l) at 0 °C under argon atmosphere was slowly added a solution of Conc.H₂SO₄ (0.5 μ l) in 50 μ l of dry THF. After stirring at 0 °C for 15 min, compound (**16**) (2 mg, 0.0072 mmol) in dry THF (20 μ l) was added in one portion and the reaction was stirred at room temperature for 24 h. The reaction mixture was then cooled to 0 °C and 2 N NaOH (6 μ l) was then carefully added and the reaction mixture stirred for 15 min. The solid was collected and washed with ether. Organic layer was dried over anhydrous Na₂SO₄, conc. under reduced pressure and purified by column chromatography over deactivated silica gel using gradient elution with 30–50% methanol in DCM to yield the corresponding methyl analogue of Crispine A (**2**) in 80% yield. IR (neat) 2962, 2931, 2862, 1609, 1510, 1464, 1357, 1254, 1211, 1167, 1078, 996, 858, 770 cm⁻¹; ¹H NMR [400 MHz, CDCl₃] δ 6.65 (s, 1H), 6.53 (s, 1H), 3.86 (s, 3H), 3.84 (s, 3H), 3.22

(ddd, $J = 5.1, 11.4, 13.2$ Hz, 1H), 3.12-2.80 (m, 4H), 2.45 (ddd, $J = 15.9, 4.2, 2.6$ Hz, 1H), 2.18-2.00 (m, 2H), 1.92-1.58 (m, 2H), 1.36 (s, 3H); HRMS (ESI) calcd for $C_{15}H_{21}NO_2 (M+Na)^+$: 248.1651; found: 248.1657.

sb-ak-34
 PROTON (-5to15) CDC13 d: iitmadras 5

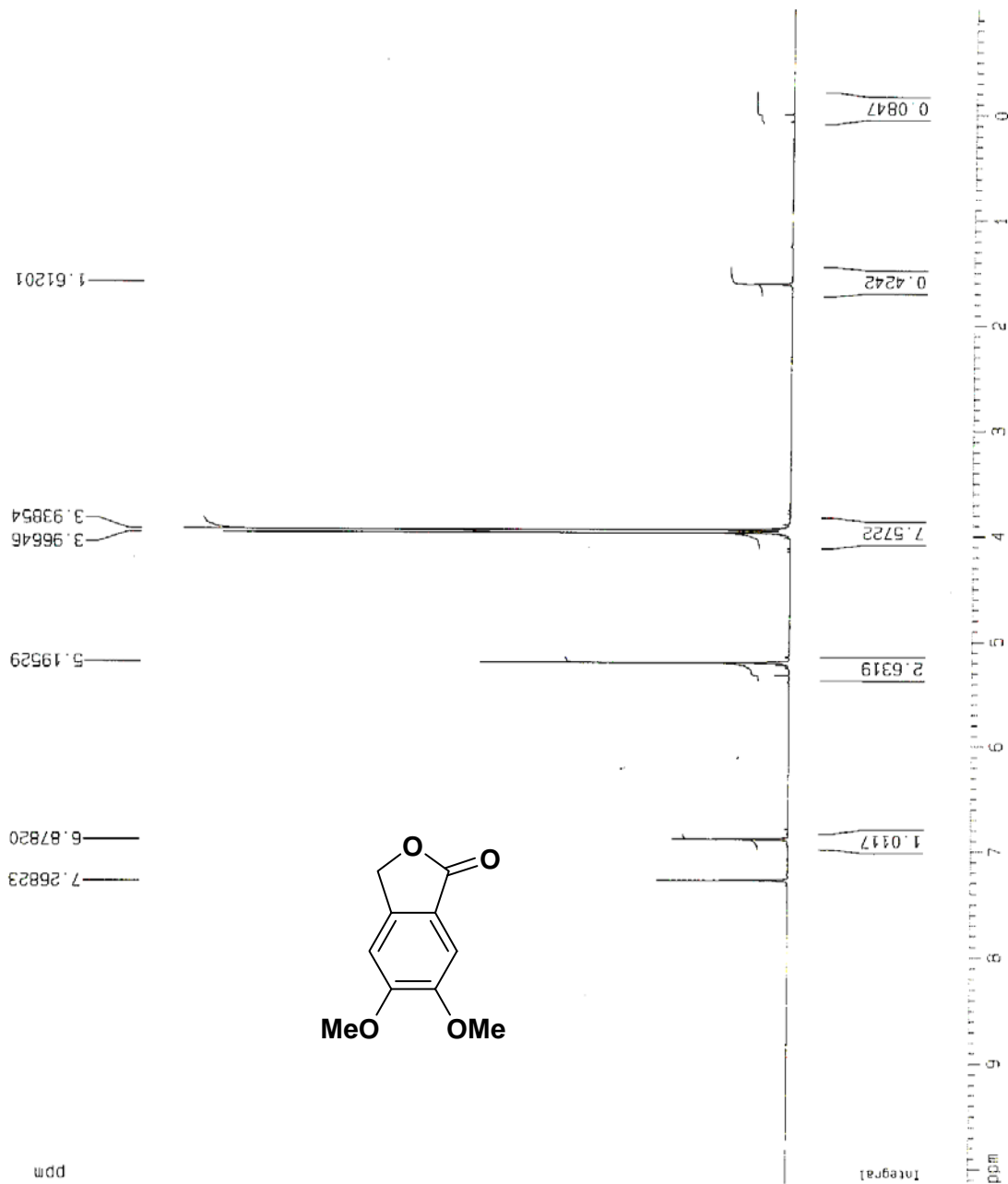
Current Data Parameters
 NAME sbak
 EXPNO 50
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050110
 Time 20.54
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 64
 DW 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NU1C1 1H
 P1 8.35 usec
 PL1 0.00 dB
 SF01 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300028 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

10 NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPHCM 0.55643 ppm/cm
 HZCM 222.54290 Hz/cm



5b-ak-2
CARBONSHORT

Current Data Parameters
 NAME sb
 EXPNO 452
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050527
 Time 18.58

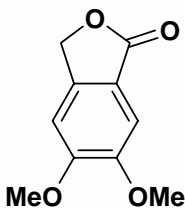
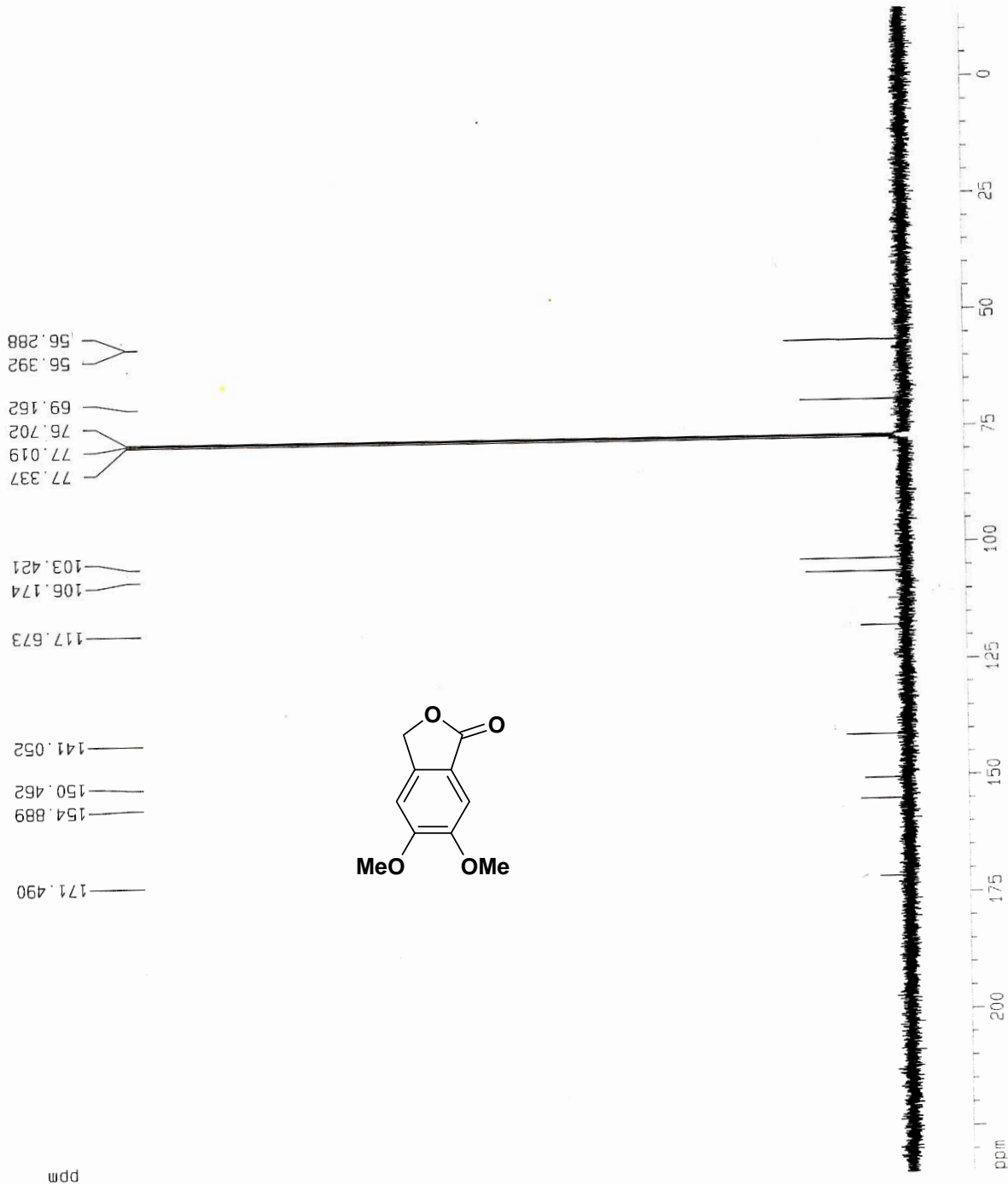
INSTRUM av400
 PROBHD 5 mm BBO BG-1H
 PULPROG zgpgc30
 TD 65536
 SOLVENT CDCl3
 NS 303
 DS 2
 SWH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 90.5
 DW 19.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 5.50 usec
 PL1 0.00 dB
 SF01 100.628364 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SF02 400.1320007 MHz

F2 - Processing parameters
 SI 131072
 SF 100.6127690 MHz
 NDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 14.00 cm
 F1P 234.849 ppm
 F1 23628.84 Hz
 F2P -14.877 ppm
 F2 -1496.79 Hz
 -PNUC 12.48630 ppm/cm
 -HZCM 1256.28137 Hz/cm



50-ak-expt-5
PROTON (5to15)

Current Data Parameters
 NAME sbak
 EXPNO 4
 PROCNO 1

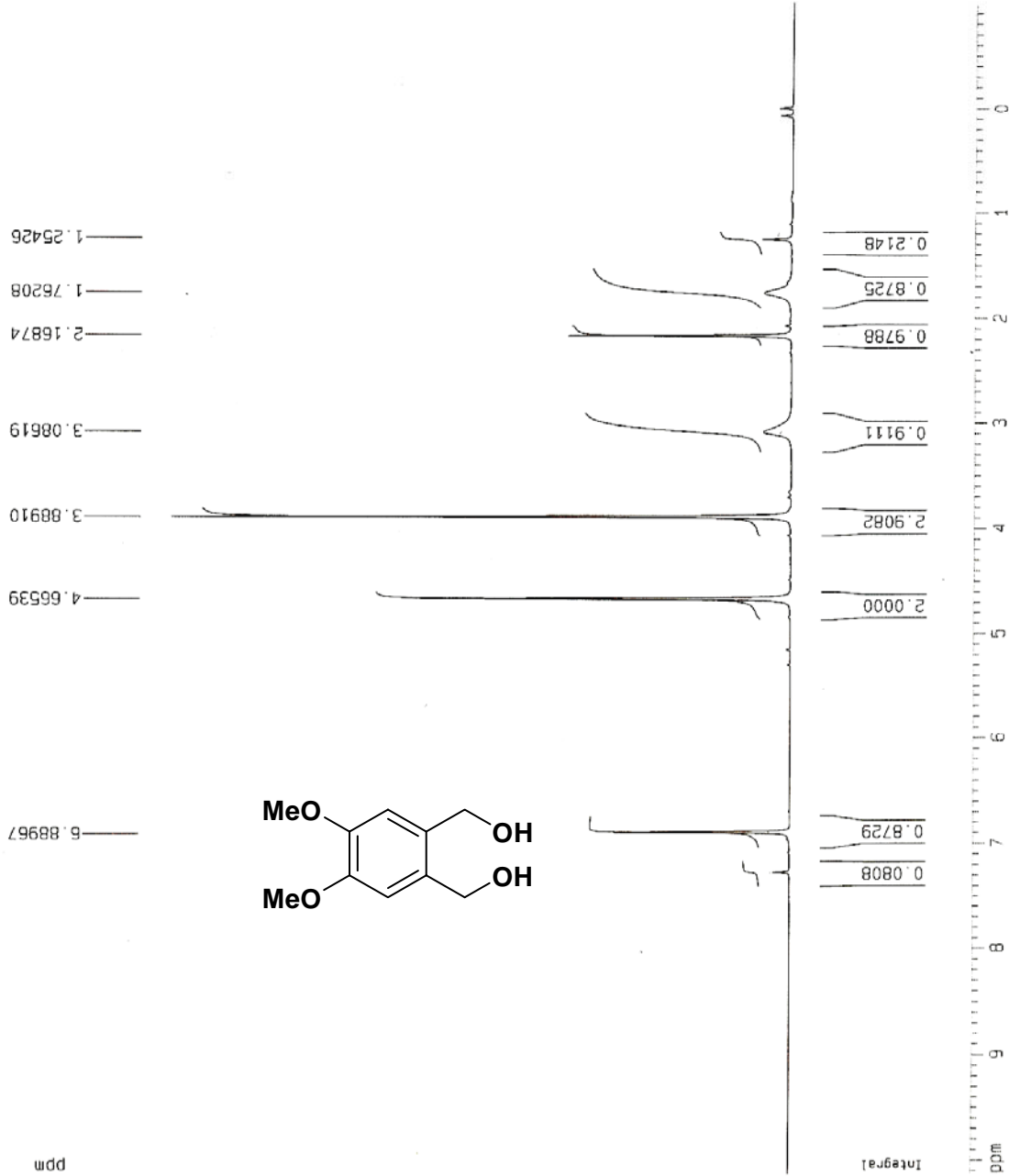
F2 - Acquisition Parameters

Date_ 20050608
 Time 13.16
 INSTRUM av400
 PROBD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 6369.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 64
 DM 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 8.35 usec
 PL1 0.00 dB
 SF01 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300049 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

10 NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.55643 ppm/cm
 HZCM 222.64290 Hz/cm



sb-ek-expt-5
CARBONSHORT

Current Data Parameters
NAME sbak
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters

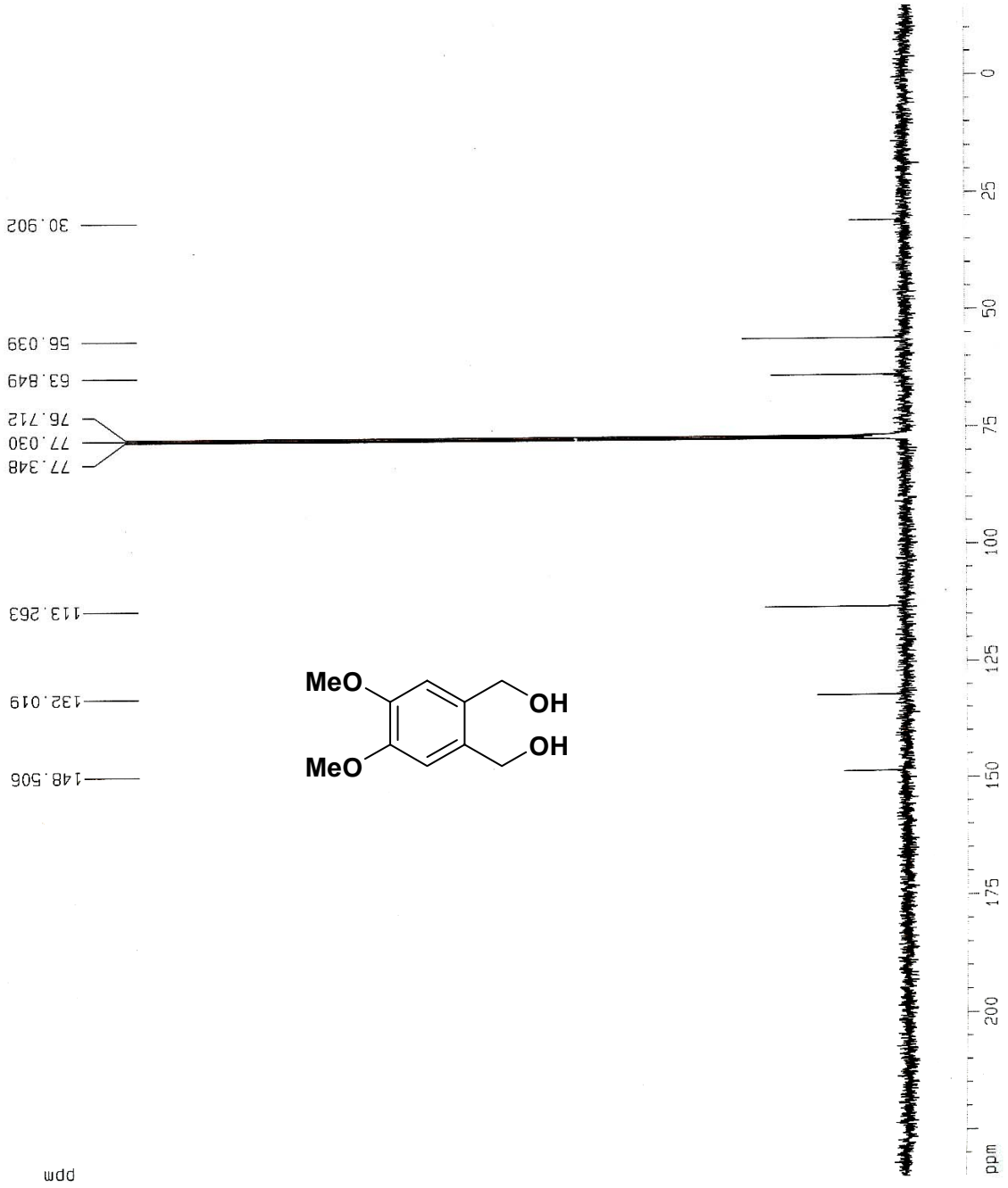
Date_ 20050608
Time 13.20
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT cdc13
NS 215
DS 2
SMH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 1448.2
DM 19.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 5.50 usec
PL1 0.00 dB
SF01 100.6236354 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 18.00 dB
SF02 400.1320007 MHz

F2 - Processing parameters
SI 131072
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 14.00 cm
F1P 234.849 ppm
F1 23628.84 Hz
F2P -14.877 ppm
F2 -1496.79 Hz
PPMCM 12.46630 ppm/cm
HZCM 1256.28137 Hz/cm



x50-ak-exp1-7
 PROTON (-5to15)

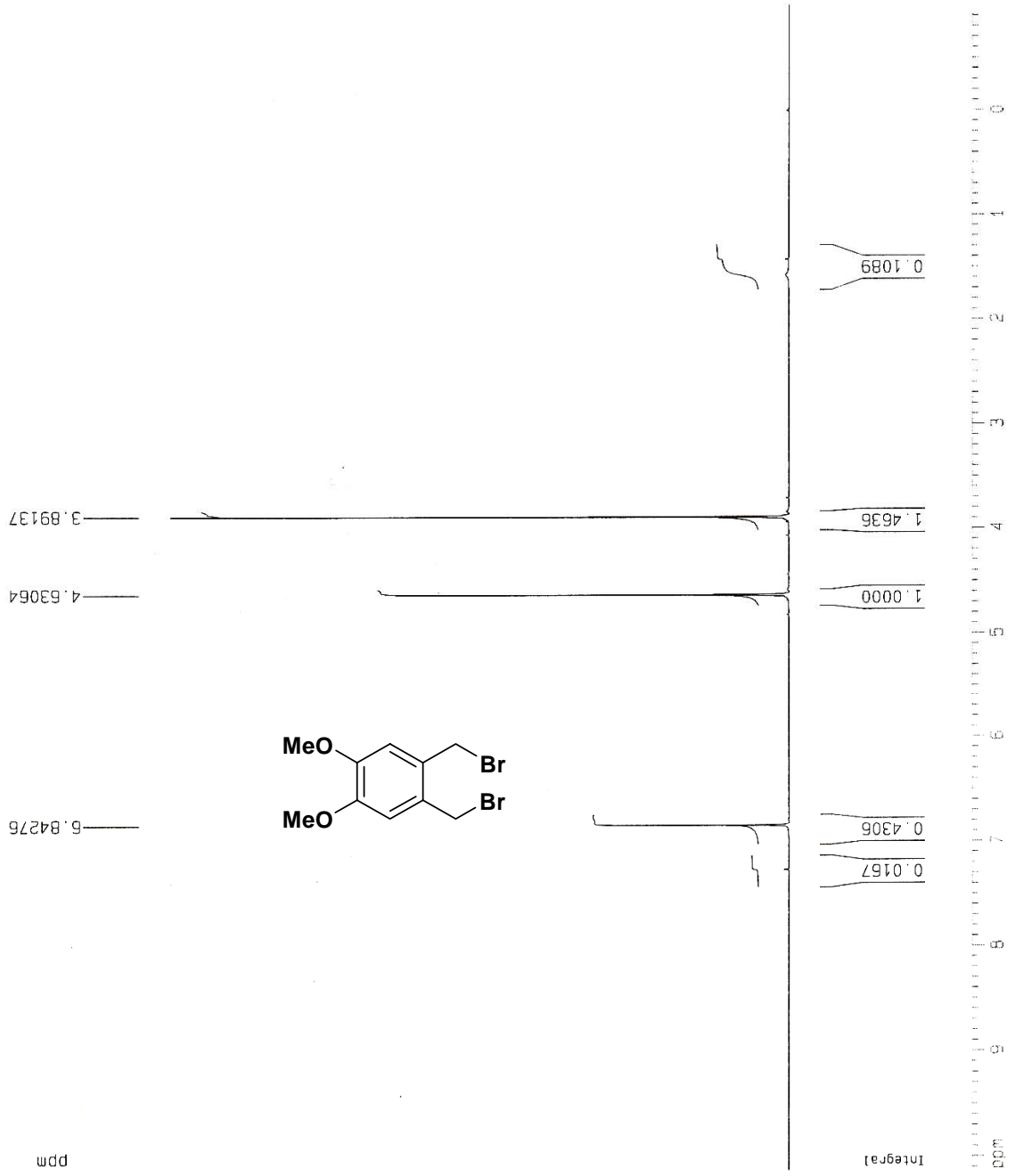
Current Data Parameters
 NAME sbak
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050708
 Time 11.01
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TO 32768
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 64
 DW 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

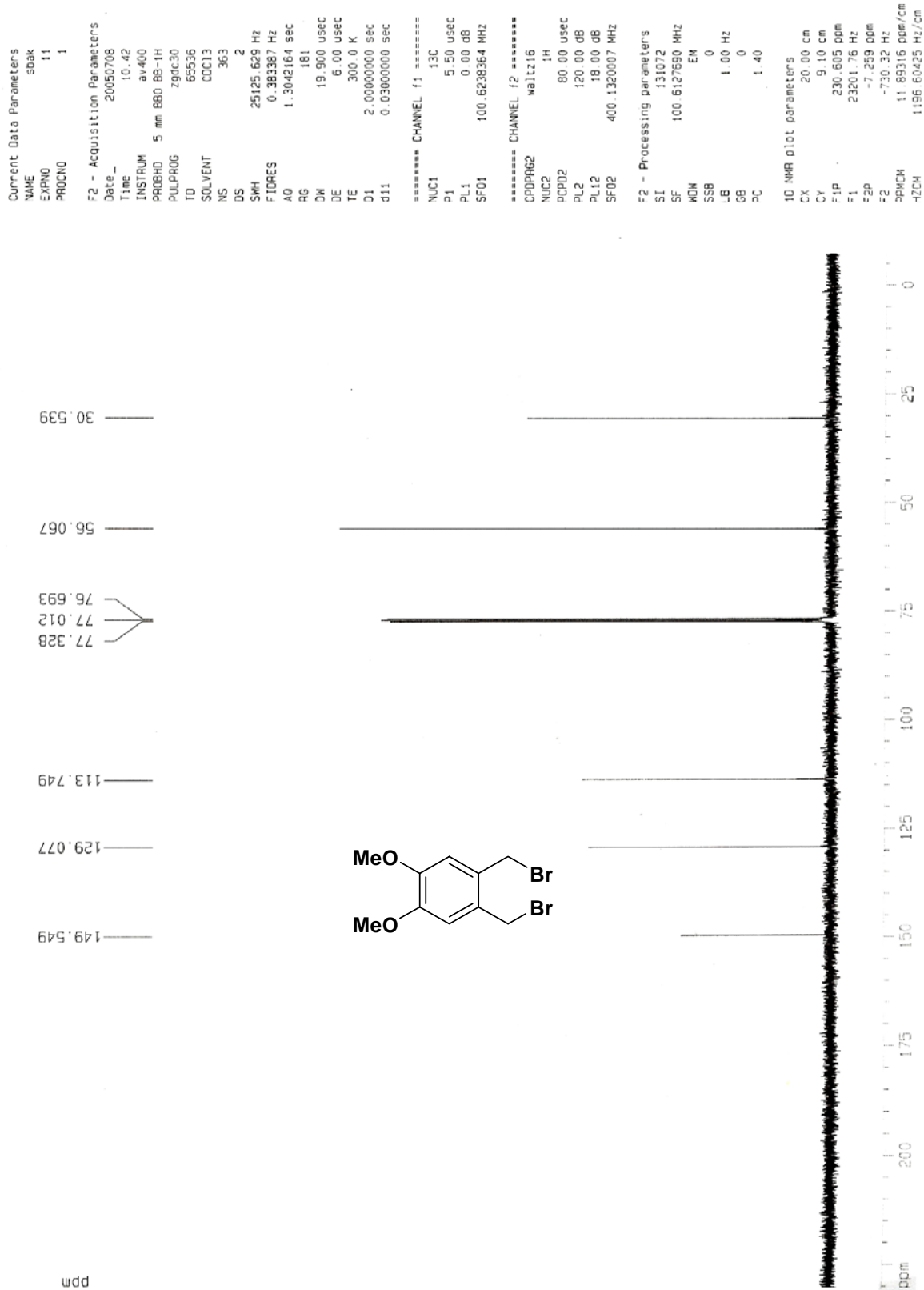
***** CHANNEL f1 *****
 NUC1 1H
 P1 8.35 usec
 PL1 0.00 dB
 SF01 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.55643 ppm/cm
 HZCM 222.64290 Hz/cm



5b-ak-expt-7
CARBONSHORT



SB/AK/10
 PROTON (-5to15)

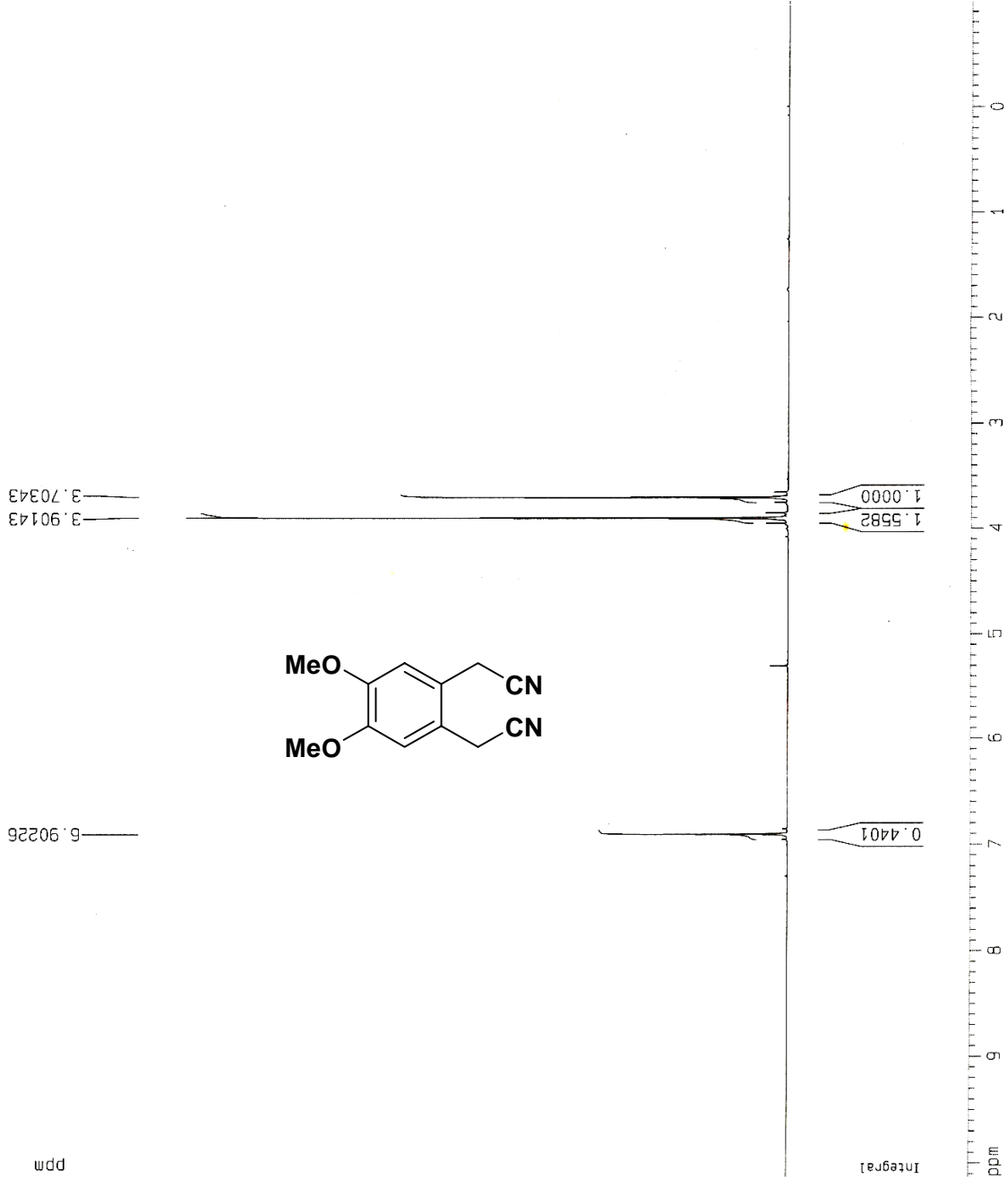
Current Data Parameters
 NAME sbak
 EXPNO 18
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050722
 Time 17:25
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 22.6
 DW 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.35 usec
 PL1 0.00 dB
 SF01 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1299951 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.55643 ppm/cm
 HZCM 222.64290 Hz/cm



SB/AK/10
CARBONSHORT

Current Data Parameters
 NAME sbak
 EXPNO 16
 PROCNO 1

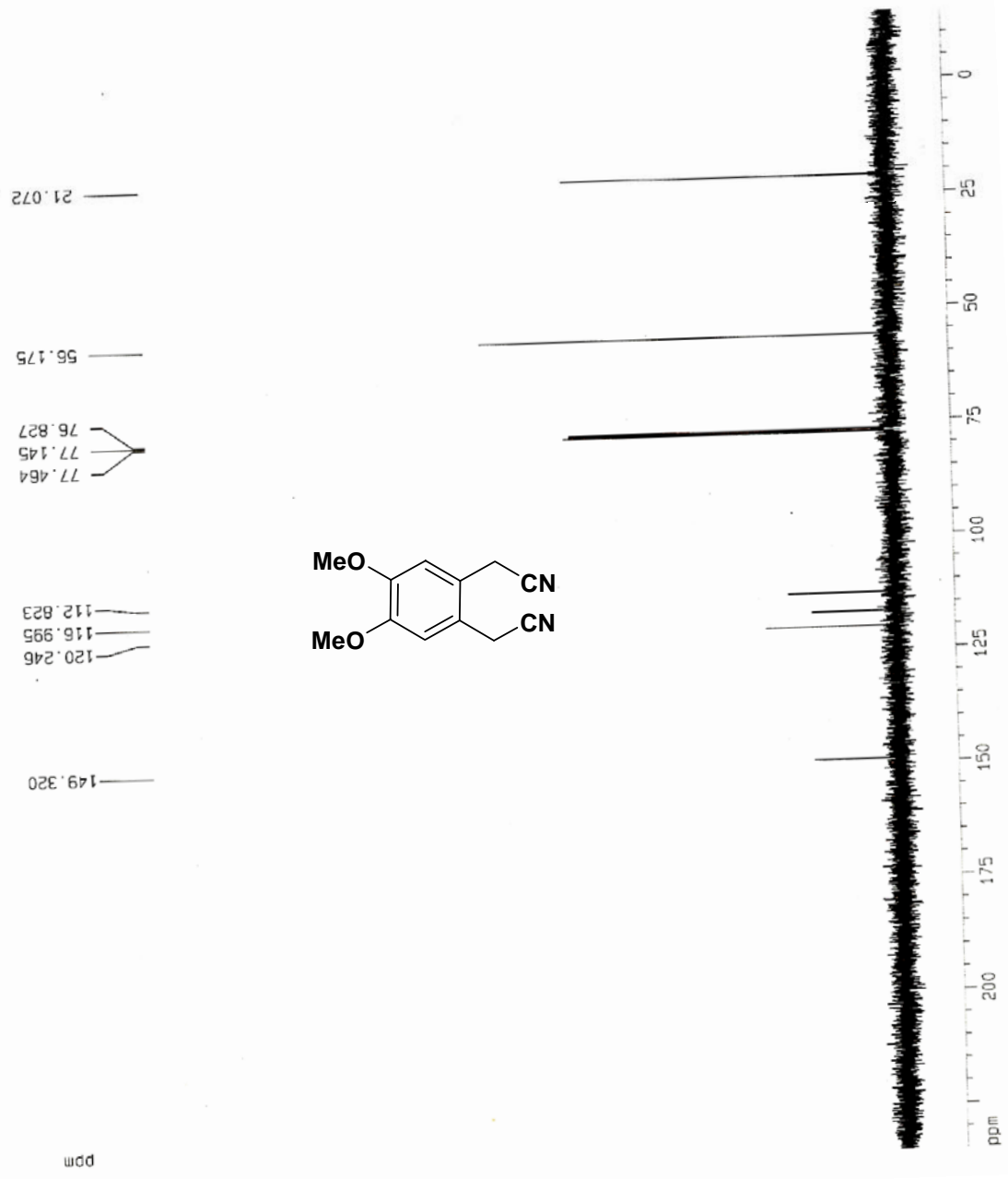
F2 - Acquisition Parameters
 Date_ 20050722
 Time 17.20
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TO 65535
 SOLVENT CDCl3
 NS 40
 DS 2
 SMH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 6502
 DN 19.900 USEC
 DE 6.00 USEC
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 5.50 usec
 PL1 0.00 dB
 SF01 100.6238364 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 18.00 dB
 SF02 400.1320007 MHz

F2 - Processing parameters
 SI 131072
 SF 100.6127650 MHz
 NDM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 6.92 cm
 F1P 234.849 ppm
 F1 23628.84 Hz
 F2P -14.877 ppm
 F2 -1496.79 Hz
 PPMCM 12.48630 ppm/cm
 HZCM 1255.28137 Hz/cm



sbak-275
 PROTON (-5to15)

Current Data Parameters
 NAME sb2
 EXPNO 628
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20070609
 Time 11.25
 INSTRUM av400
 PROBH0 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT COC13
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 57
 DM 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

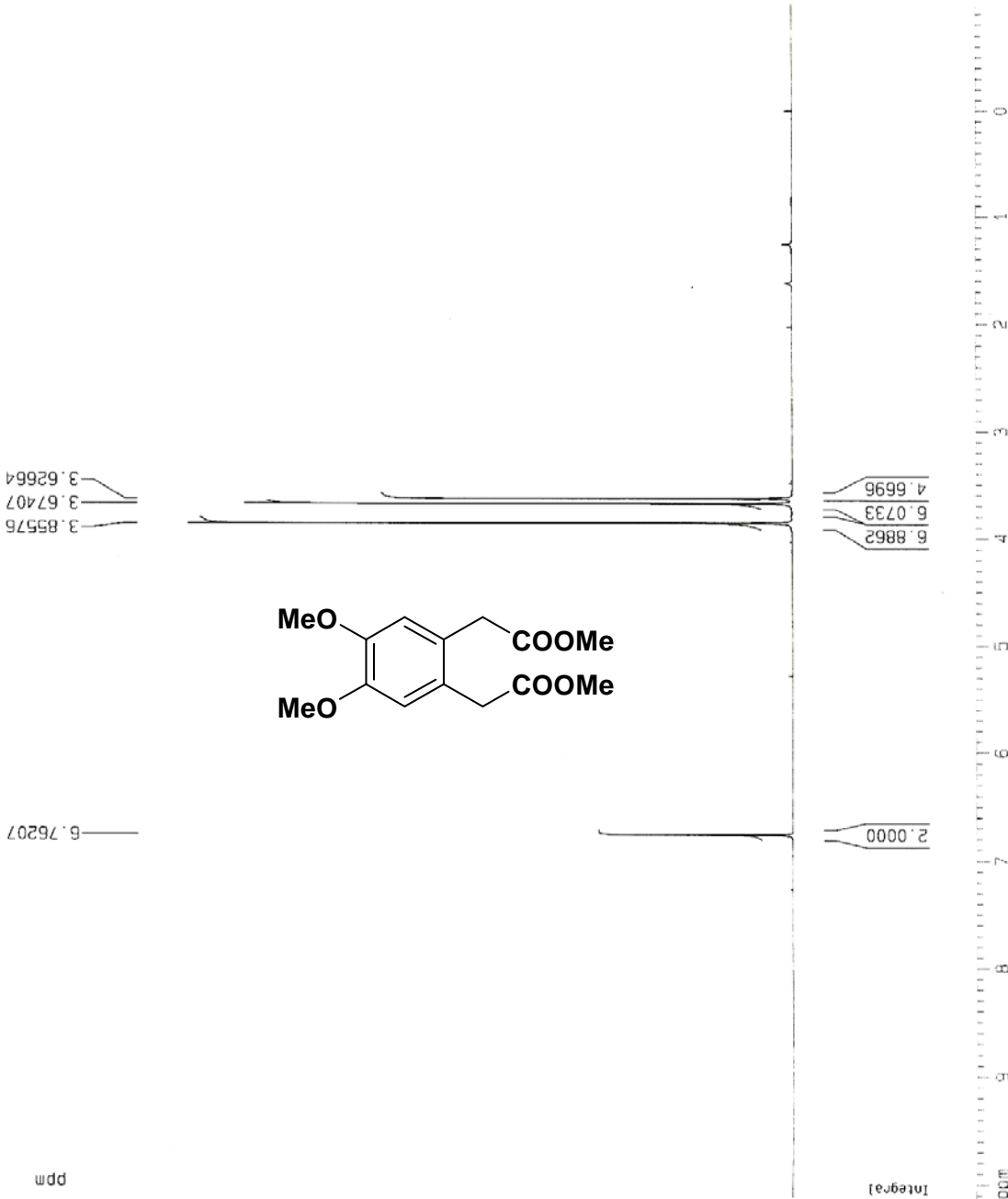
***** CHANNEL f1 *****
 NUC1 1H
 P1 11.00 usec
 PL1 3.00 dB
 SF01 400.1319460 MHz

F2 - Processing parameters

SI 16384
 SF 400.1300055 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

1D NMR plot parameters

CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.55643 ppm/cm
 HZCM 222.64290 Hz/cm



sbak-275
CARBONSHORT

Current Data Parameters
 NAME sb2
 EXPNO 629
 PROCNO 1

F2 - Acquisition Parameters

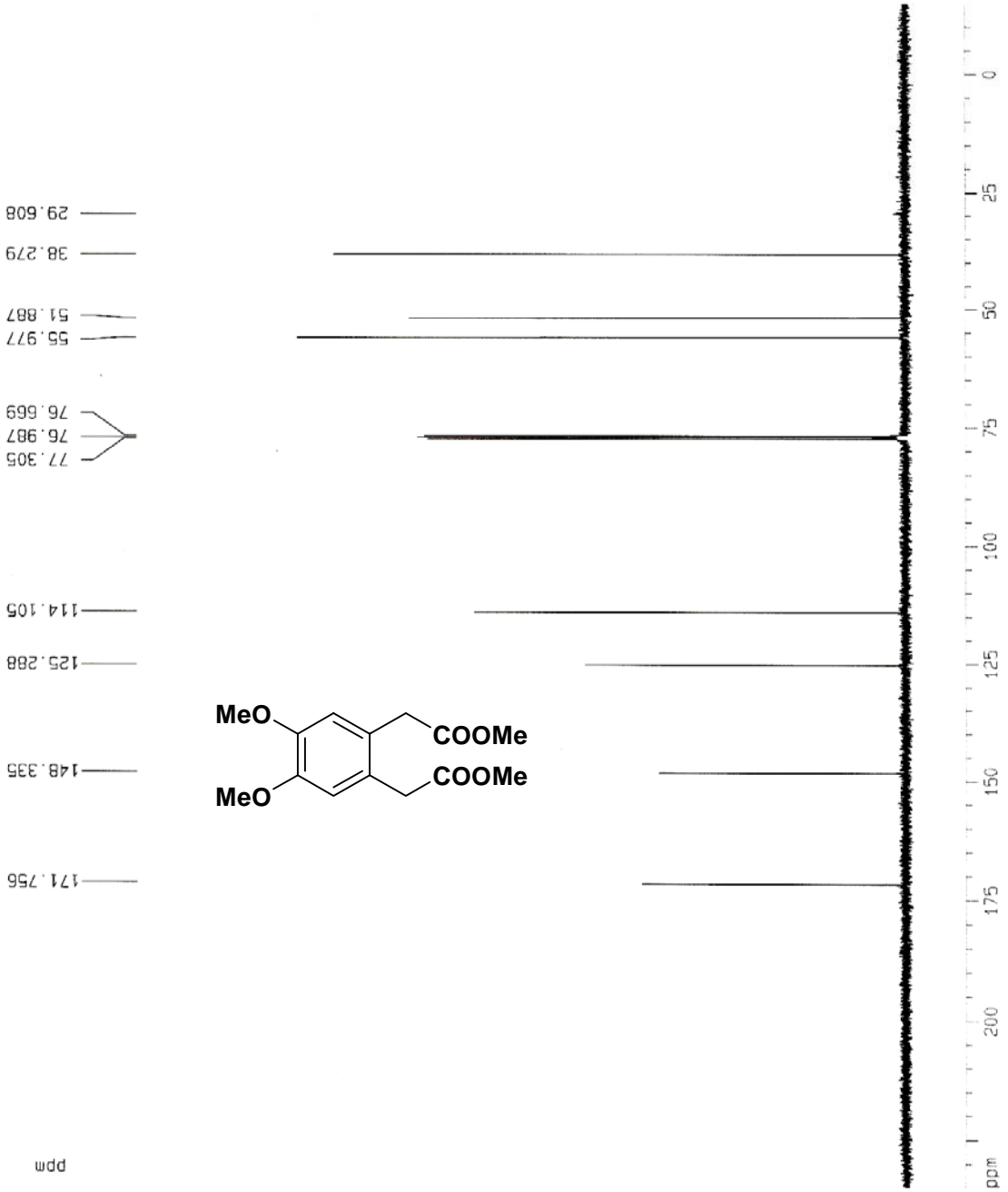
Date_ 20070609
 Time 11:55
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TO 85556
 SOLVENT CDCl3
 NS 512
 DS 2
 SWH 25125.629 Hz
 FIDRES 0.383387 Hz
 AQ 1.3042164 sec
 RG 1149.4
 DM 19.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 100.6238364 MHz

***** CHANNEL f2 *****
 CPROG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 20.23 dB
 PL13 16.00 dB
 SFO2 400.1320007 MHz

F2 - Processing parameters
 SI 131072
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 9.94 cm
 F1P 234.849 ppm
 F1 23628.84 Hz
 F2P -14.877 ppm
 F2 -1498.79 Hz
 PPMCM 12.46630 ppm/cm
 HZCM 1256.28137 Hz/cm



sd-ak-241
PROTON (~5to15)

```

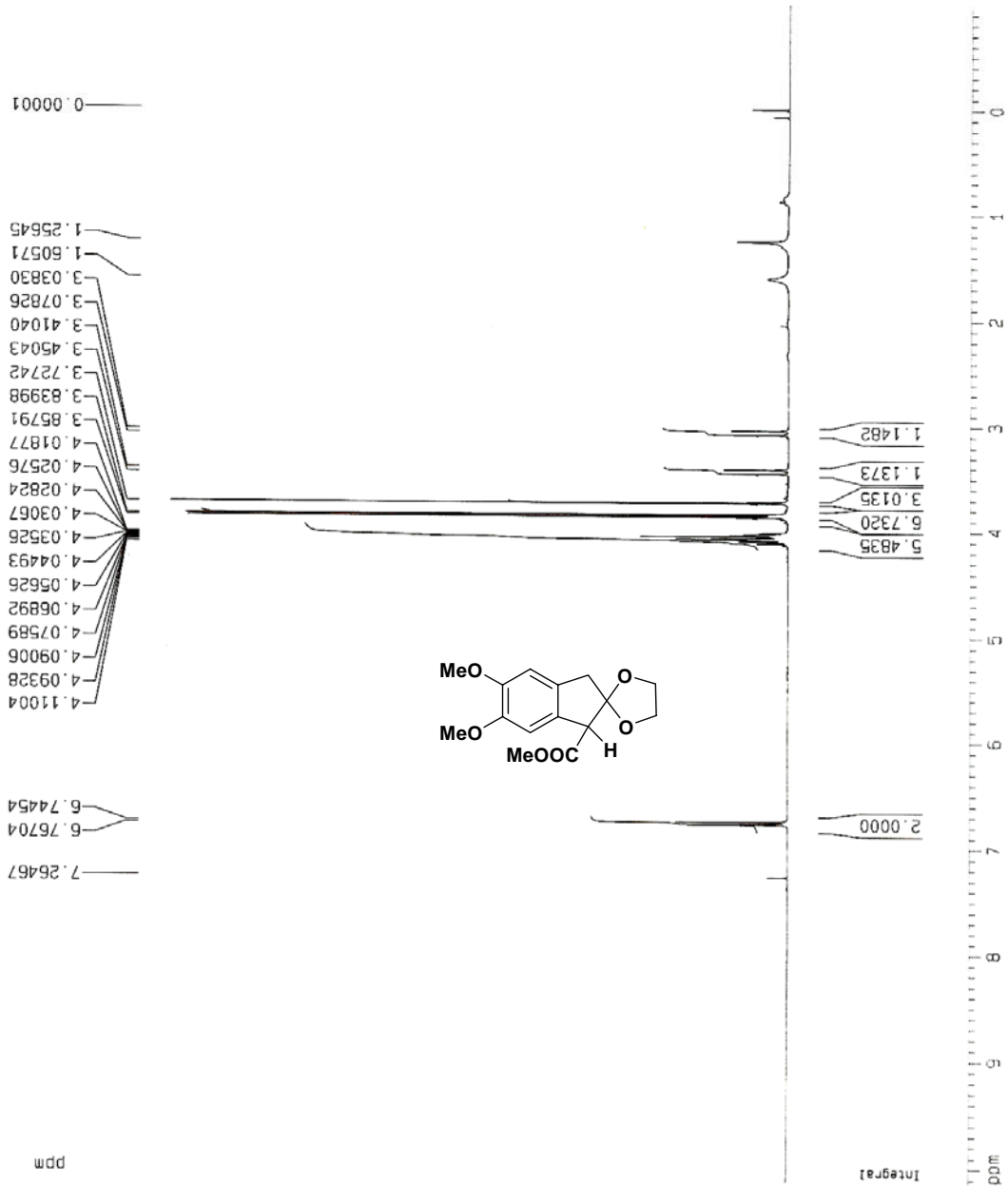
Current Data Parameters
NAME      sb1
EXPNO    1088
PROCNO   1

F2 - Acquisition Parameters
Date_    20070304
Time     17.20
INSTRUM  av400
PROBHD   5 mm BBO BB-1H
PULPROG  zg
TO       32768
SOLVENT  CDCl3
NS       16
DS       0
SWH      8389.262 Hz
FIDRES   0.256020 Hz
AQ       1.9530228 sec
RG       90.5
DM       59.600 usec
DE       5.00 usec
TE       300.0 K
D1       2.00000000 sec

***** CHANNEL f1 *****
NUC1     1H
P1       11.25 usec
PL1      -3.00 dB
SFO1     400.1319460 MHz

F2 - Processing parameters
SI       16384
SF       400.1300070 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       3.00

ID NMR plot parameters
CX       20.00 cm
CY       10.00 cm
F1P      10.129 ppm
F1       4052.73 Hz
F2P      -1.000 ppm
F2       -400.13 Hz
PPMCH    0.55643 ppm/cm
HZCHK    222.64290 Hz/cm
    
```



50-ak-241
CARBONSHORT

```

Current Data Parameters
NAME          SD1
EXPNO        1089
PROCNO       1

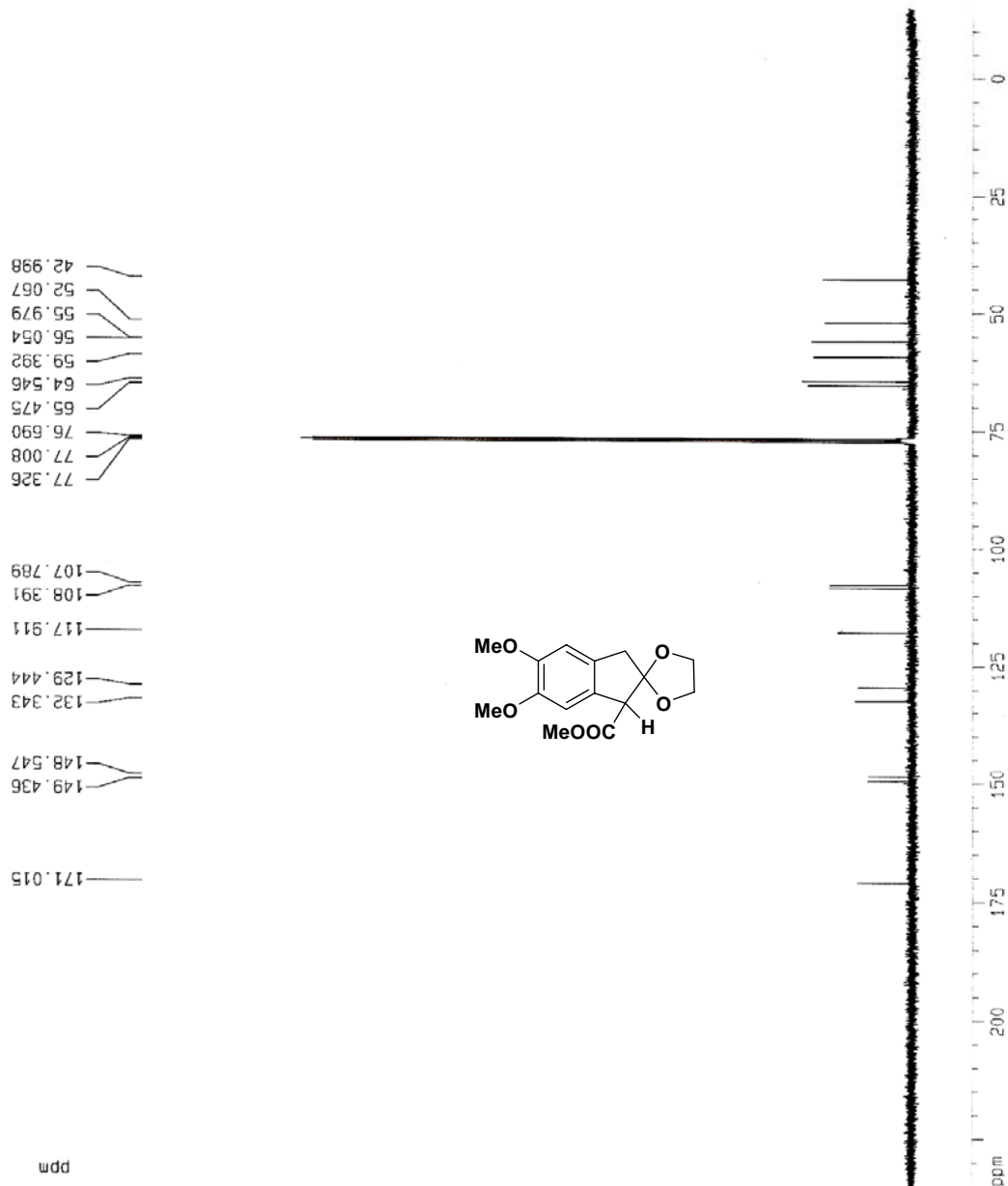
F2 - Acquisition Parameters
Date_        20070304
Time         17.22
INSTRUM      sv400
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           512
DS           2
SWH           25125.025 Hz
FIDRES       0.383387 Hz
AQ           1.3042164 sec
RG           1149.4
DW           19.900 usec
DE           6.00 usec
TE           300.0 K
D1           2.0000000 sec
d11          0.0300000 sec
d12          0.0002000 sec

***** CHANNEL f1 *****
NUC1          13C
P1           14.00 usec
PL1          -4.00 dB
SFO1         100.6238364 MHz

***** CHANNEL f2 *****
CPDPRG2      waltz16
NUC2          1H
PCPD2        100.00 usec
PL2          -3.00 dB
PL12         15.98 dB
PL13         16.00 dB
SFO2         400.1320007 MHz

F2 - Processing parameters
SI           131072
SF           100.6127650 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

10 NMR plot parameters
CX           20.00 cm
CY           9.84 cm
FIP          234.849 00MHz
F1           23628.84 Hz
F2P          -14.877 ppm
F2           -1496.79 Hz
PPMCM        12.48630 ppm/cm
AQCM         1256.28137 Hz/cm
  
```



sb-ak-260
 PROTON (-5to15)

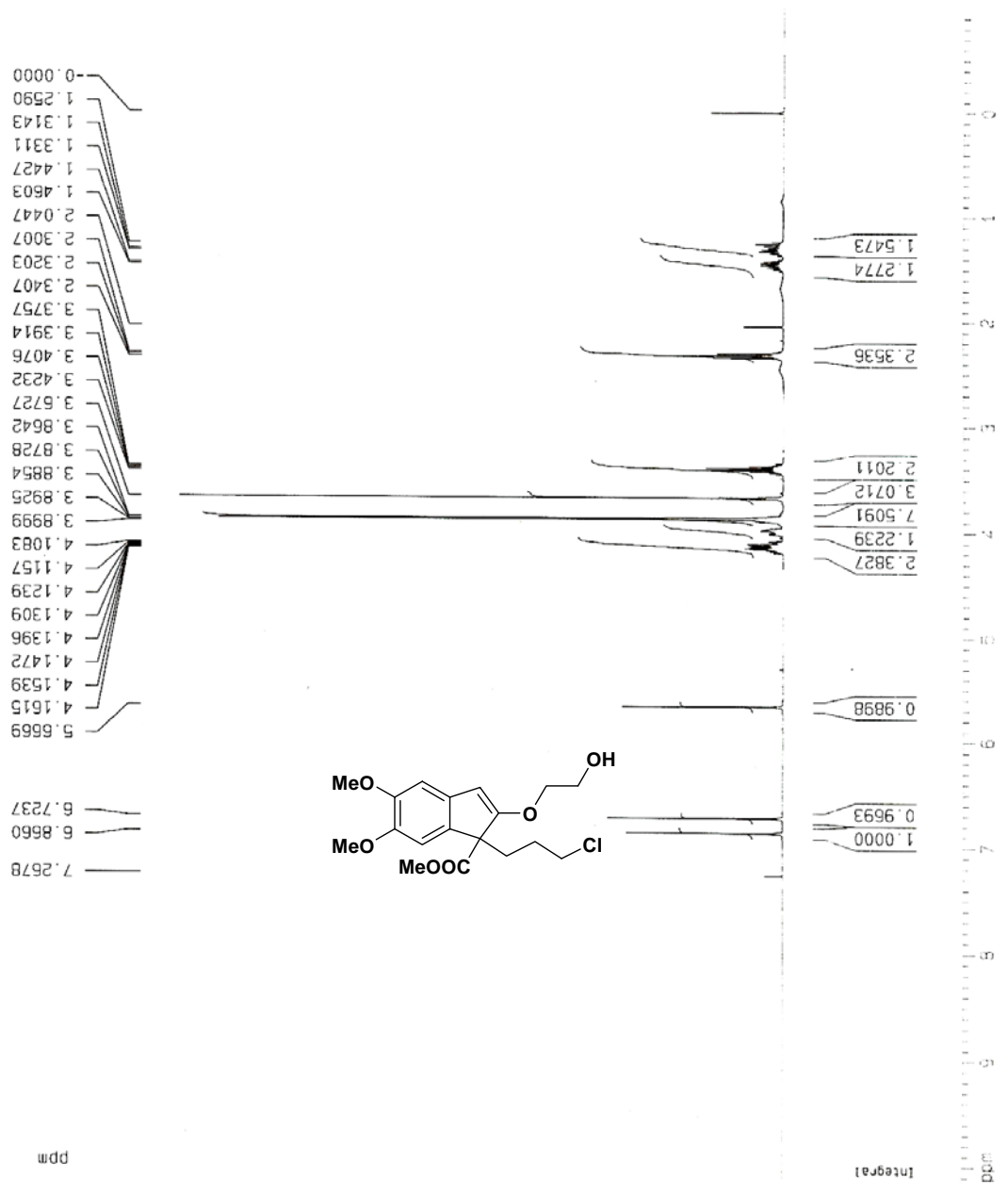
Current Data Parameters
 NAME S02
 EXPNO 122
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070408
 Time 16.26
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SMH 899.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 64
 DW 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 3.00 dB
 SF01 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300058 MHz
 NDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PP4CM 0.55643 ppm/cm
 RZCM 222.64290 Hz/cm



sb-ak-260
CARBONSHORT

```

Current Data Parameters
NAME          SB2
EXPNO        123
PROCNO       1

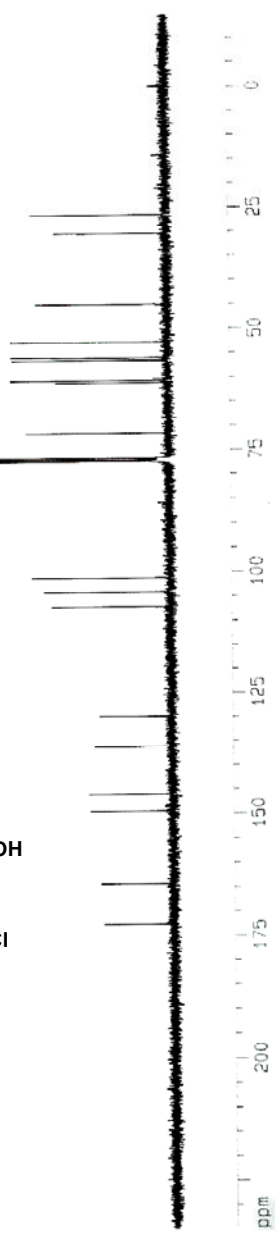
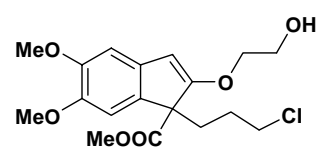
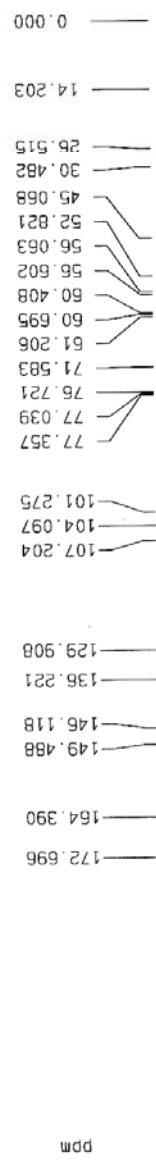
F2 - Acquisition Parameters
Date_        20070408
Time         23.15
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           512
DS           2
SWH          25125.629 Hz
FIDRES       0.383387 Hz
AQ           1.3042164 sec
RG           14586.5
DM           19.900 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          0.00 dB
SFO1         100.6236364 MHz

***** CHANNEL f2 *****
CPDPRG2      waltz16
NUC2         1H
PCPD2        80.00 USEC
PL2          3.00 dB
PL12         20.23 dB
PL13         16.00 dB
SFO2         400.1320007 MHz

F2 - Processing parameters
SI           131072
SF           100.6127670 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

ID NMR plot parameters
CX           20.00 cm
CY           9.54 cm
FIP          234.849 ppm
F1           2628.64 Hz
F2           -14.877 ppm
F3           -1456.79 Hz
SFOCM        12.48630 ppm/cm
+TCM         1256.28137 Hz/cm
  
```



sd-ak-261
 PR010N (-5to15) CDCl3 d: 111madras 5

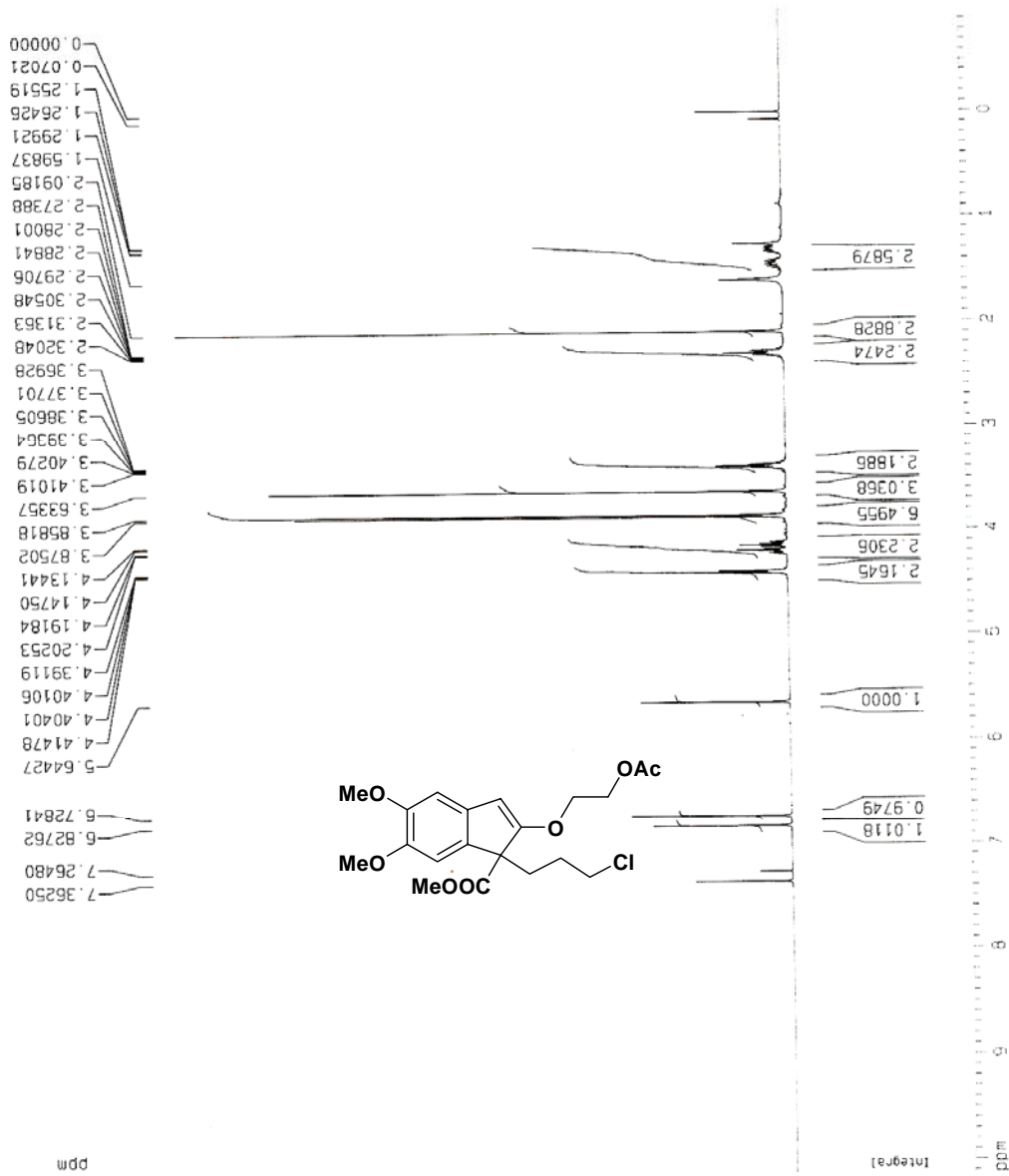
Current Data Parameters
 NAME 502
 EXPNO 168
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070413
 Time 10.28
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 128
 DM 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 11.00 usec
 PL 3.00 dB
 LF 1L
 SF01 400.1319460 MHz

F2 - Processing parameters
 IS 16384
 SF 400.1300070 MHz
 KW EM
 EN 0
 LB 0.30 Hz
 GB 0
 CB 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1 10.129 ppm
 F2 4052.73 Hz
 P1 -1.000 ppm
 P2 -400.13 Hz
 SFO1 0.55643 ppm/cm
 SFO2 222.64290 Hz/cm



stak-261
CARBONSHORT

```

Current Data Parameters
NAME          sb2
EXPNO        167
PROCNO       1

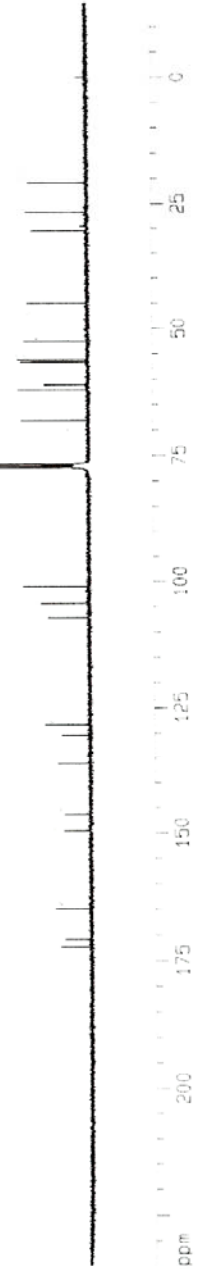
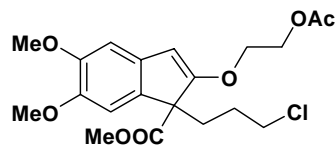
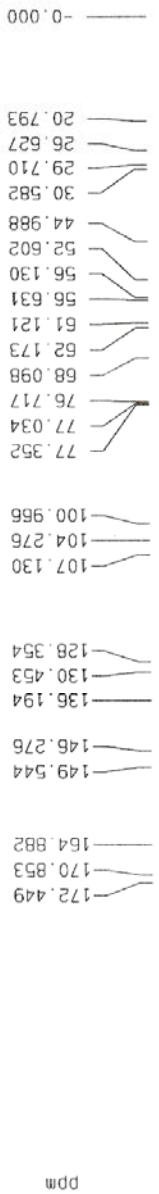
F2 - Acquisition Parameters
Date_        20070413
Time         7.08
INSTRUM      av400
PROBHD       5 mm BBO BB-H
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS            4000
DS            2
SWH           25125.629 Hz
FIDRES       0.383387 Hz
AQ            1.3042164 sec
RG            1149.4
DM            19.900 usec
DE            6.00 usec
TE            300.0 K
D1            2.0000000 sec
d11           0.0300000 sec
d12           0.0000200 sec

***** CHANNEL f1 *****
NUC1          13C
P1            11.00 usec
PL1           0.00 dB
SFO1         100.623364 MHz

***** CHANNEL f2 *****
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           3.00 dB
PL12         20.23 dB
PL13         16.00 dB
SFO2         400.1320007 MHz

F2 - Processing parameters
SI            131072
SF            100.6127637 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

1D NMR plot parameters
CX            20.00 cm
CY            9.94 cm
F1P           234.848 ppm
F1            23628.84 Hz
F2P           -14.877 ppm
F2            -1496.79 Hz
SFOCM         12.48630 ppm/cm
ZCVM          1256.28125 Hz/cm
  
```



sb-ak-263
 PROTON (-5to15) CDCl3 d: iitmadras 6

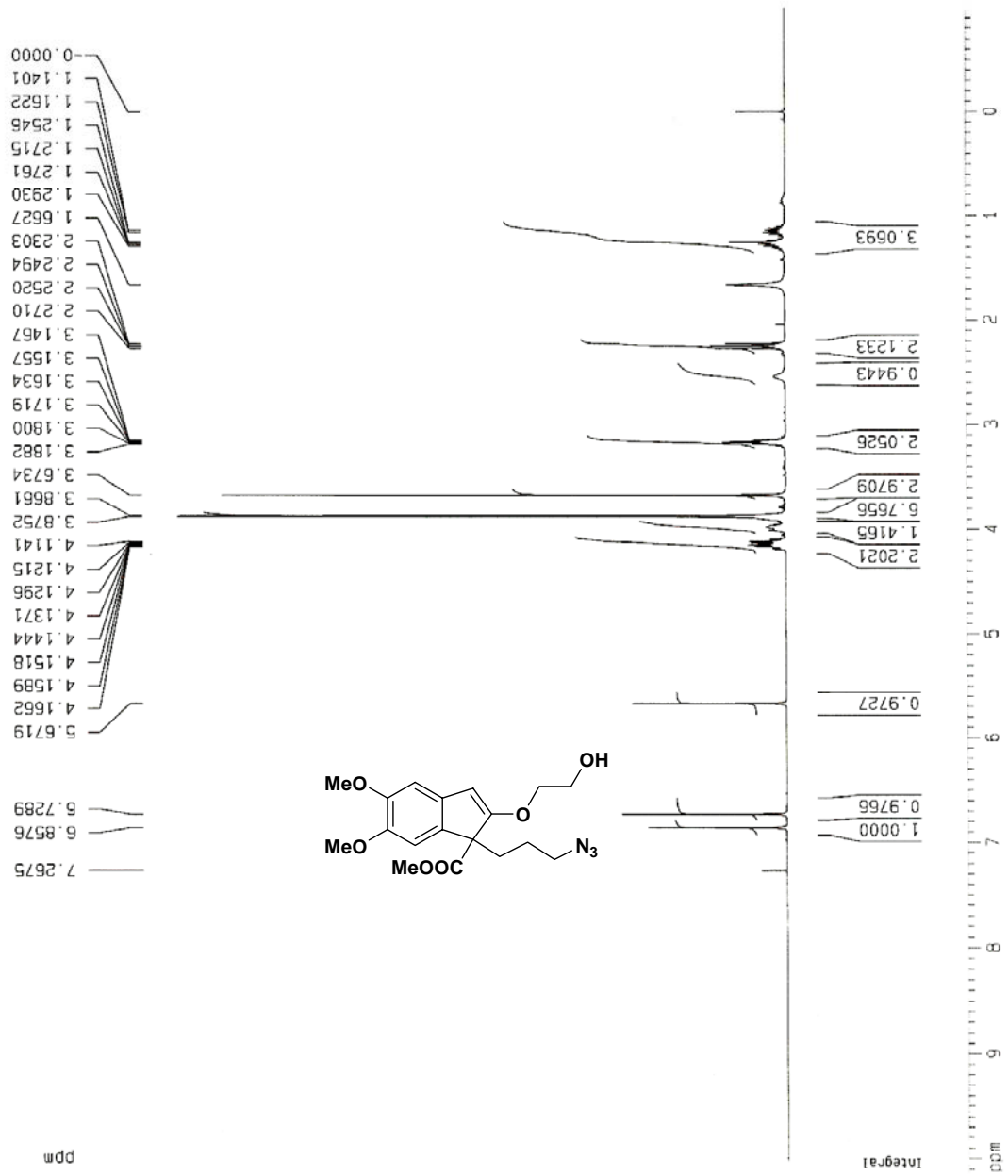
Current Data Parameters
 NAME SB2
 EXPNO 583
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070505
 Time 16.34
 INSTRUM av400
 PROBHD 5 mm BBO BB-JH
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 101.6
 DW 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 3.00 dB
 SF01 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300057 MHz
 NCM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCM 0.55643 ppm/cm
 HZCM 222.64290 Hz/cm



sb-8k-263
CARBONSHOT CDC13 d: iitmadras 1

```

Current Data Parameters
NAME          sb2
EXPNO        622
PROCNO       1

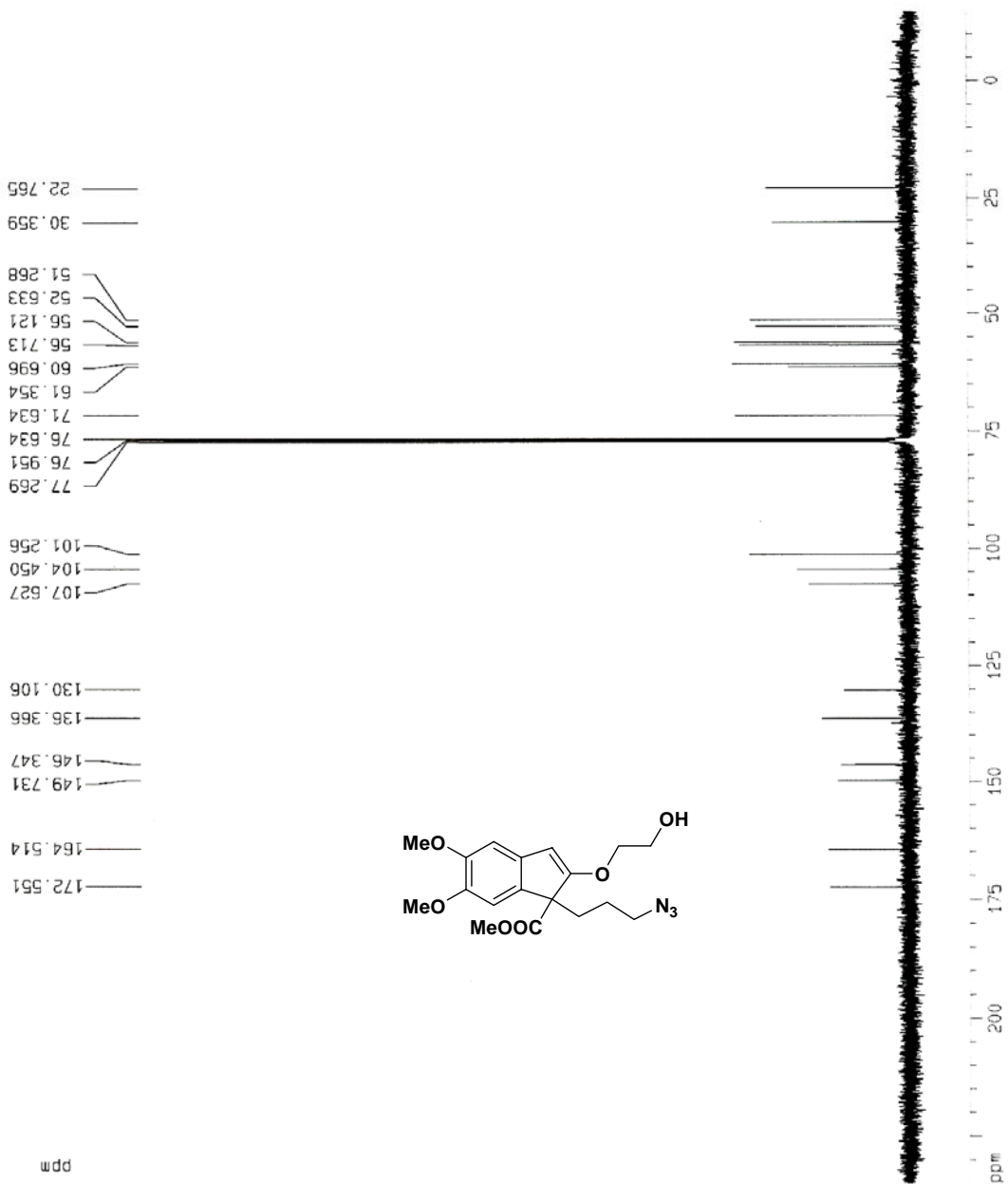
F2 - Acquisition Parameters
Date_        20070608
Time         23:11
INSTRUM     av400
PROBHD      5 mm BBO BB-1H
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           1000
DS           2
SWH          25125.629 Hz
FIDRES      0.386387 Hz
AQ           1.3042164 sec
RG           31481.4
DM           19.900 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          0.00 dB
SFO1         100.6238364 MHz

***** CHANNEL f2 *****
CFDPRG2     waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         3.00 dB
PL12        20.23 dB
PL13        16.00 dB
SFO2        400.1320007 MHz

F2 - Processing parameters
SI           131072
SF           100.6127690 MHz
RG           0
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

ID NMR plot parameters
CX           20.00 cm
CY           20.47 cm
F1P          234.849 ppm
F1           25628.84 Hz
F2P          -14.877 ppm
F2           -1495.79 Hz
PPMCH        12.48630 ppm/cm
-ZCH         1255.28137 Hz/cm
    
```



sd-ak-221
PROTON (-5t015)

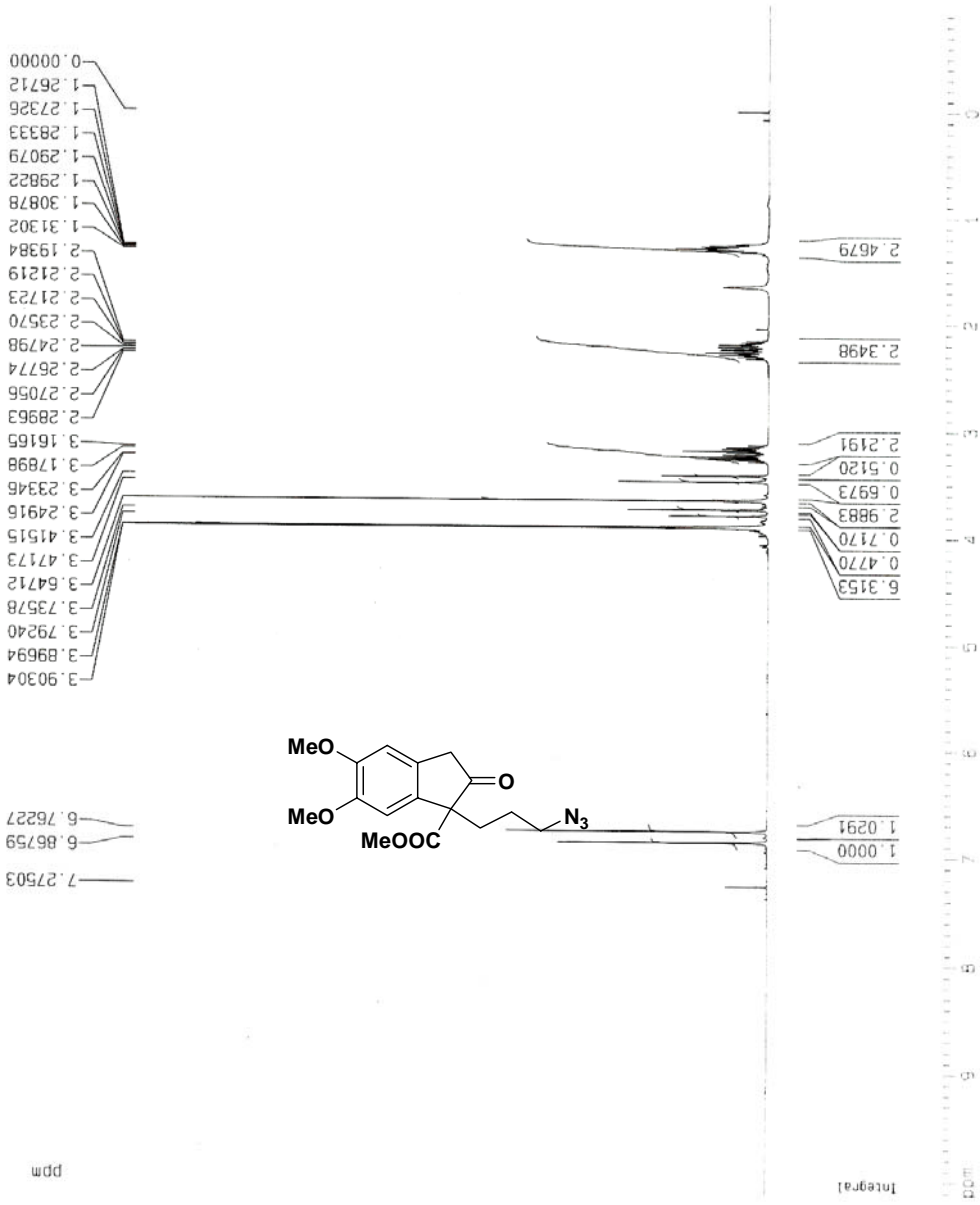
Current Data Parameters
 NAME s02
 EXPNO 80
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070403
 Time 17:53
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SMH 6389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 57
 DW 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 11.00 usec
 PL1 3.00 dB
 SFO1 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300028 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 GC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 21.46 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 SFOCM 0.55643 ppm/cm
 HZCM 222.64290 Hz/cm



sb-ak-221
CARBONSHORT

```

Current Data Parameters
NAME      sb2
EXPNO    81
PROCNO   1

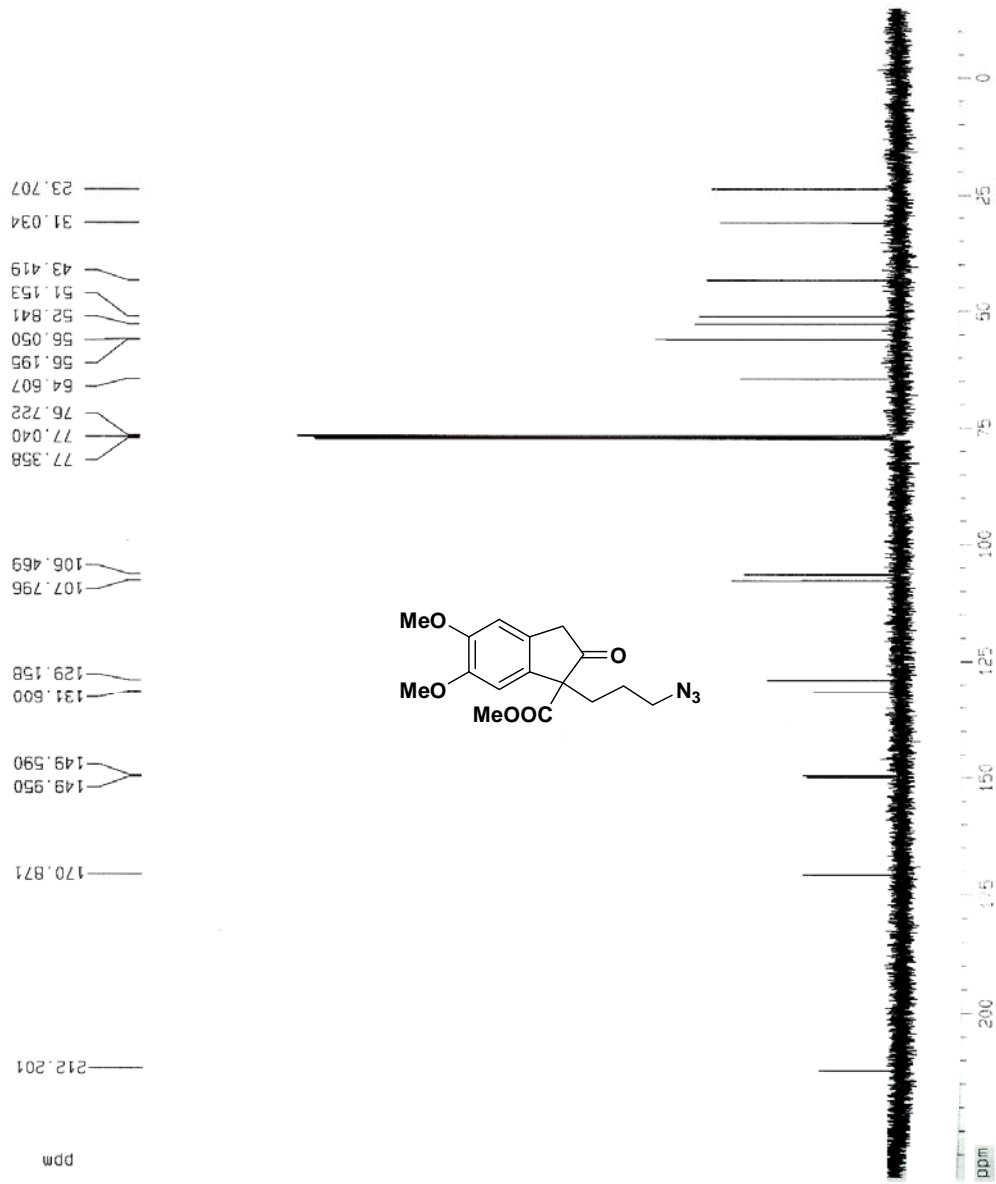
F2 - Acquisition Parameters
Date_    20070403
Time     10.00
INSTRUM  av400
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TO       69536
SOLVENT  CDCl3
NS       97
DS       2
SMA      25125.629 HZ
FIDRES   0.383387 HZ
AQ       1.3042164 SEC
RG       2896.3
DM       19.500 USEC
DE       6.00 USEC
TE       300.0 K
D1       2.00000000 SEC
d11      0.03000000 SEC
d12      0.00002000 SEC

***** CHANNEL f1 *****
NUC1     13C
P1       11.00 USEC
PL1      0.00 DB
SF01     100.628364 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 USEC
PL2      3.00 DB
PL12     20.23 DB
PL13     16.00 DB
SF02     400.1320007 MHz

F2 - Processing parameters
S1       131072
SF       100.6127650 MHz
RG       0
SSB      0
B        1.00 HZ
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 CM
CY       9.94 CM
F1P      234.849 ppm
F1       23828.84 HZ
F2P      -14.877 ppm
F2       -1496.79 HZ
RGCMH    12.48630 ppm/cm
-DCM     1256.28137 Hz/cm
  
```



sbak-226
 PROTON (-5 to 15)

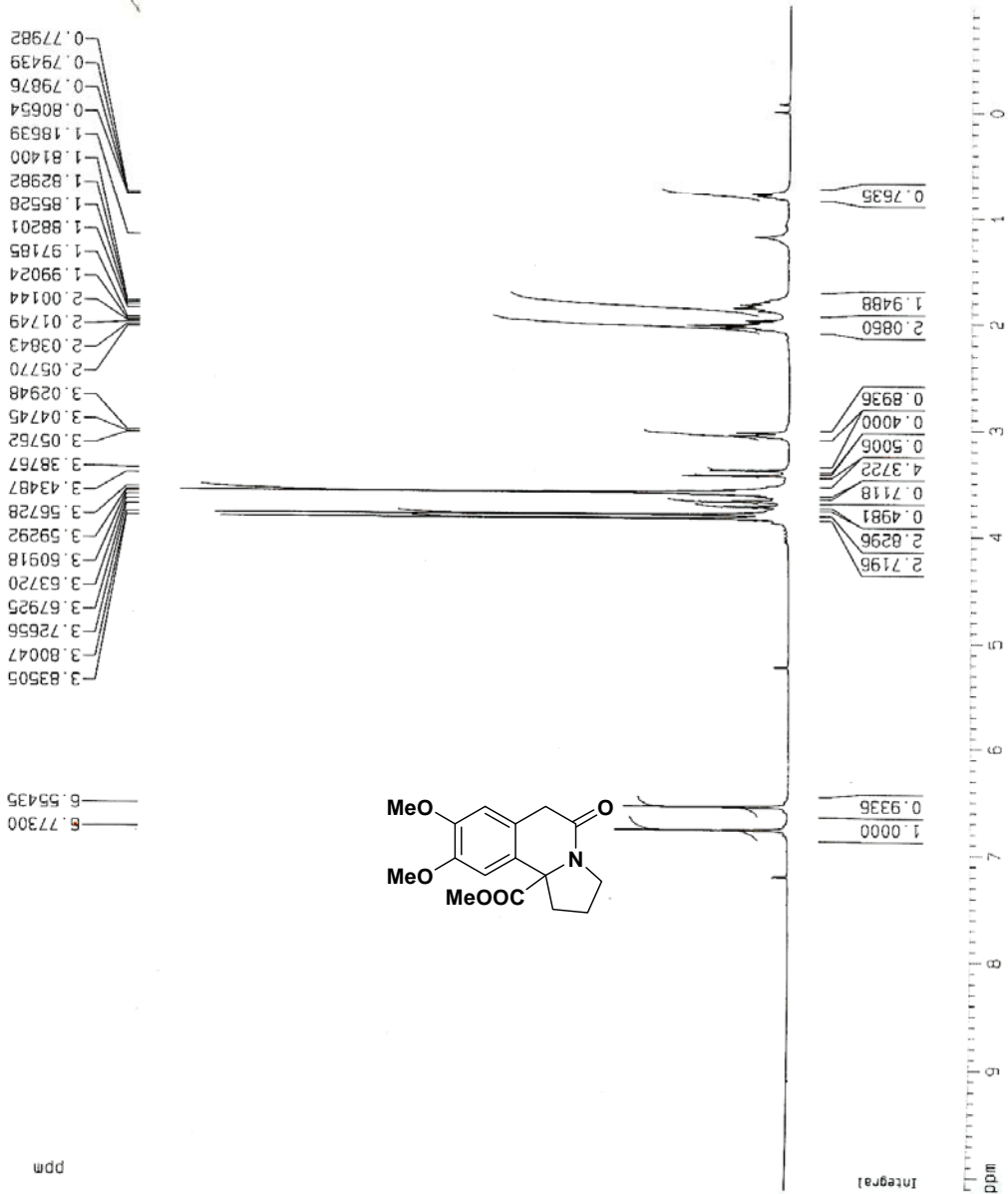
Current Data Parameters
 NAME sol
 EXPNO 964
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070202
 Time 16.50
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 71.8
 DM 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.25 usec
 PL1 -3.00 dB
 SFO1 400.1319460 MHz

F2 - Processing parameters
 SI 16364
 SF 400.1300262 MHz
 NDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 10.129 ppm
 F1 4052.73 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPHCM 0.55663 ppm/cm
 HZCM 222.64291 Hz/cm



sb-ak-226
CARBONSHORT

Current Data Parameters
NAME sb1
EXPNO 966
PROCNO 1

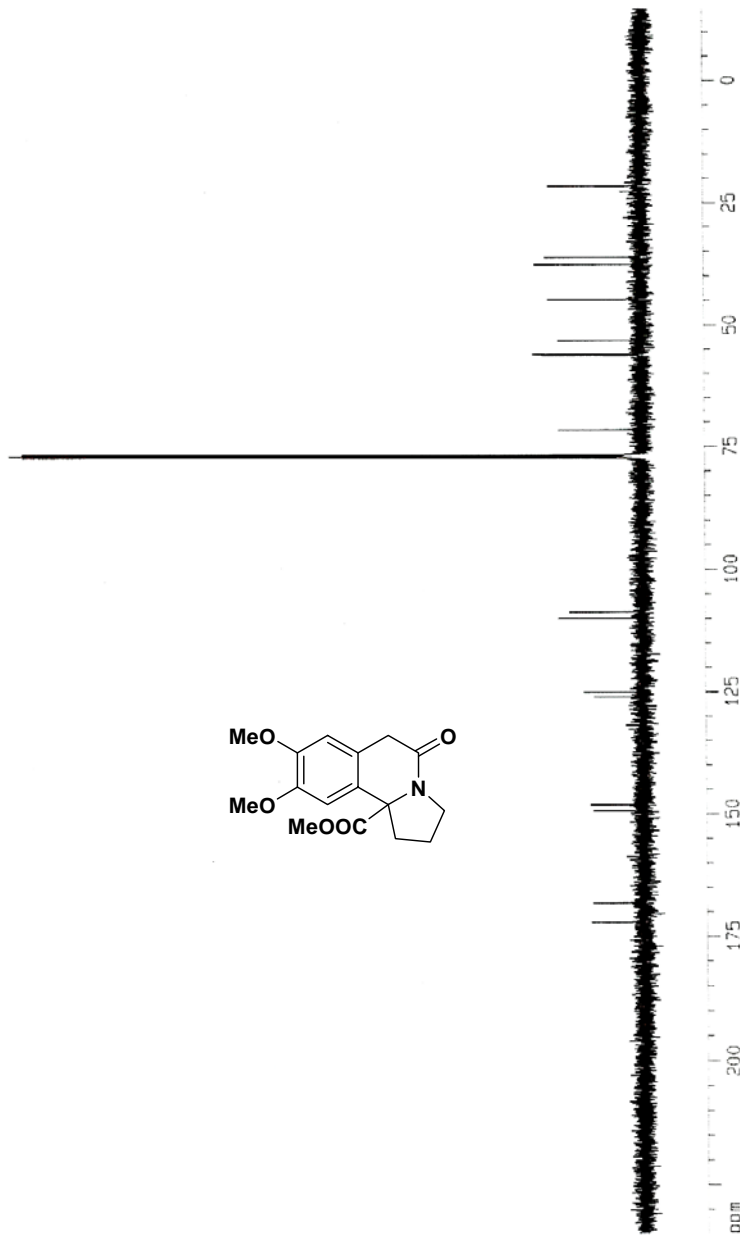
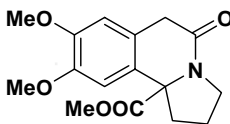
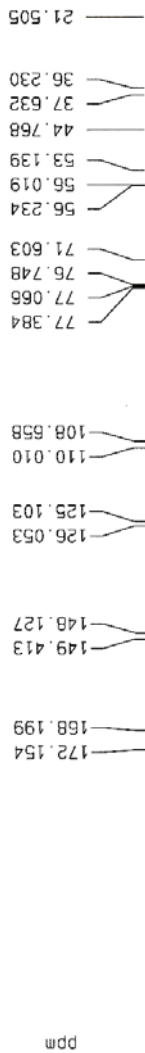
F2 - Acquisition Parameters
Date_ 20070202
Time 19.21
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 115
DS 2
SWH 25125.629 Hz
FIDRES 0.363387 Hz
AQ 1.3042164 sec
RG 1149.4
DM 19.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 14.00 usec
PL1 -4.00 dB
SF01 100.6236364 MHz

***** CHANNEL f2 *****
CFPRPG2 Waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 15.56 dB
PL13 16.00 dB
SF02 400.1320007 MHz

F2 - Processing parameters
SI 131072
SF 100.6127680 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

AD NMR plot parameters
CX 20.00 cm
CY 9.94 cm
F1 234.849 ppm
F2 23628.84 Hz
F2P -14.877 ppm
F2 -1496.79 Hz
PRMCM 12.48630 ppm/cm
F2CH 1256.28137 Hz/cm



sb-ak-235
 PROTON (-5t015)

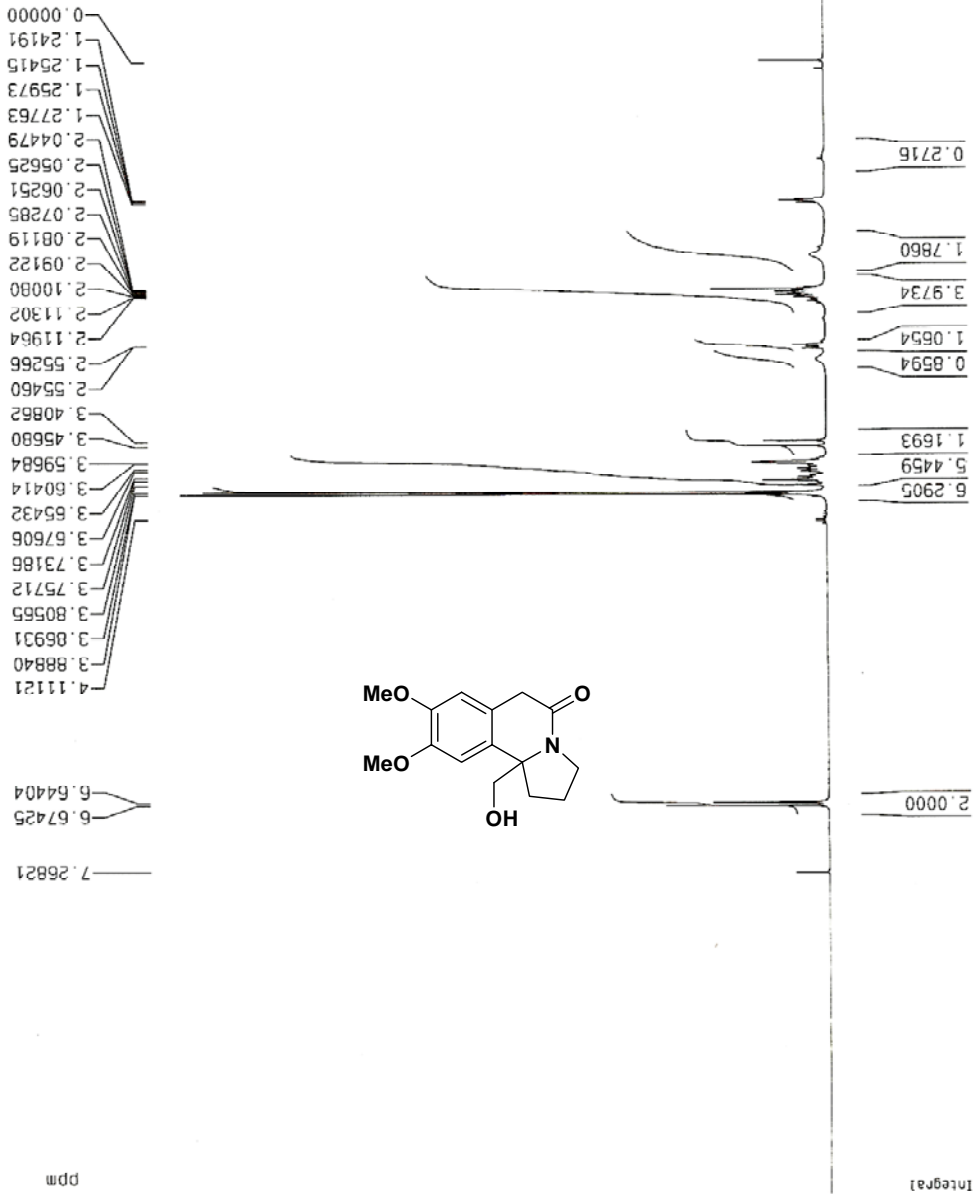
Current Data Parameters
 SBI 801
 EXPNO 1035
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070219
 Time 11:37
 INSTRUM av400
 PROBRD 5 mm BBO BB-1H
 PULPROG zg
 TO 32768
 SOLVENT CDCl3
 NS 67
 DS 0
 SWH 8369.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 101.6
 DM 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

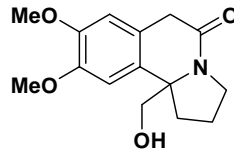
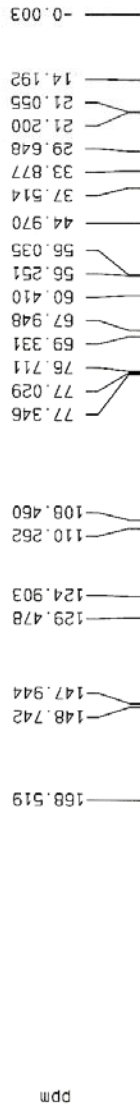
***** CHANNEL f1 *****
 NUC1 1H
 P1 11.25 usec
 PL1 -3.00 dB
 SFO1 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300056 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

ID NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 FIP 10.129 ppm
 F1 4052.73 Hz
 F2 -1.000 ppm
 FZ -400.13 Hz
 PPMCM 0.55643 ppm/cm
 HZCM 222.64290 Hz/cm



sb-ak-235
CARBONSHORT



```

Current Data Parameters
NAME          SB1
EXPNO        1031
PROCNO       1

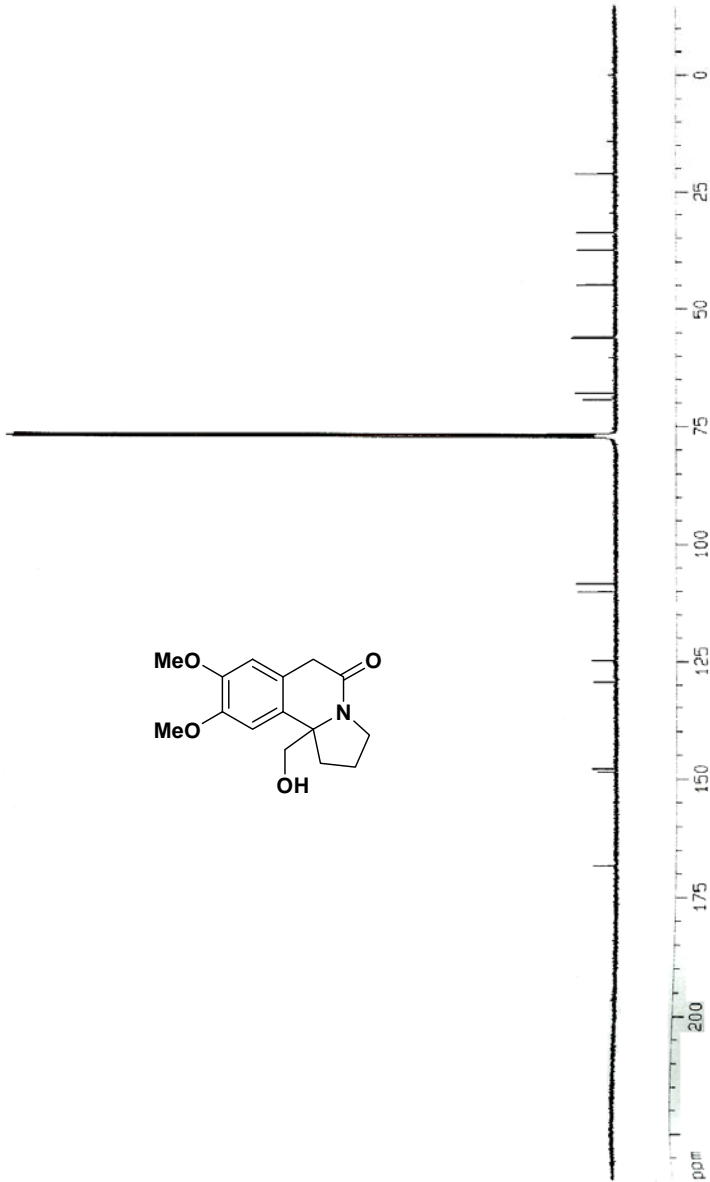
F2 - Acquisition Parameters
Date_        20070217
Time         9.04
INSTRUM     av400
PROBHD      5 mm BBO BB-1H
PULPROG     zgpg30
TD          65536
SOLVENT     CDCl3
NS          8003
DS          2
SWH         25125.629 Hz
FIDRES     0.38387 Hz
AQ         1.3042164 sec
RG         1148.4
DM         19.900 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          14.00 usec
PL1         -4.00 dB
SFO1        100.6283564 MHz

***** CHANNEL f2 *****
COPROG2     waltz16
NUC2         1H
P2          100.00 usec
PL2         -3.00 dB
PL12        15.98 dB
PL13        16.00 dB
SFO2        400.1320007 MHz

F2 - Processing parameters
SI          131072
SF          100.6127690 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

ID NMR plot parameters
CY          20.00 cm
CX          9.94 cm
F1P         234.849 ppm
F1          23626.84 Hz
F2P         -14.877 ppm
F2          -1486.79 Hz
PPHOM      12.48630 ppm/cm
AZDN       1255.28137 Hz/cm
  
```



sb-ms-ak-mesylation
 PROTON (-5to15)

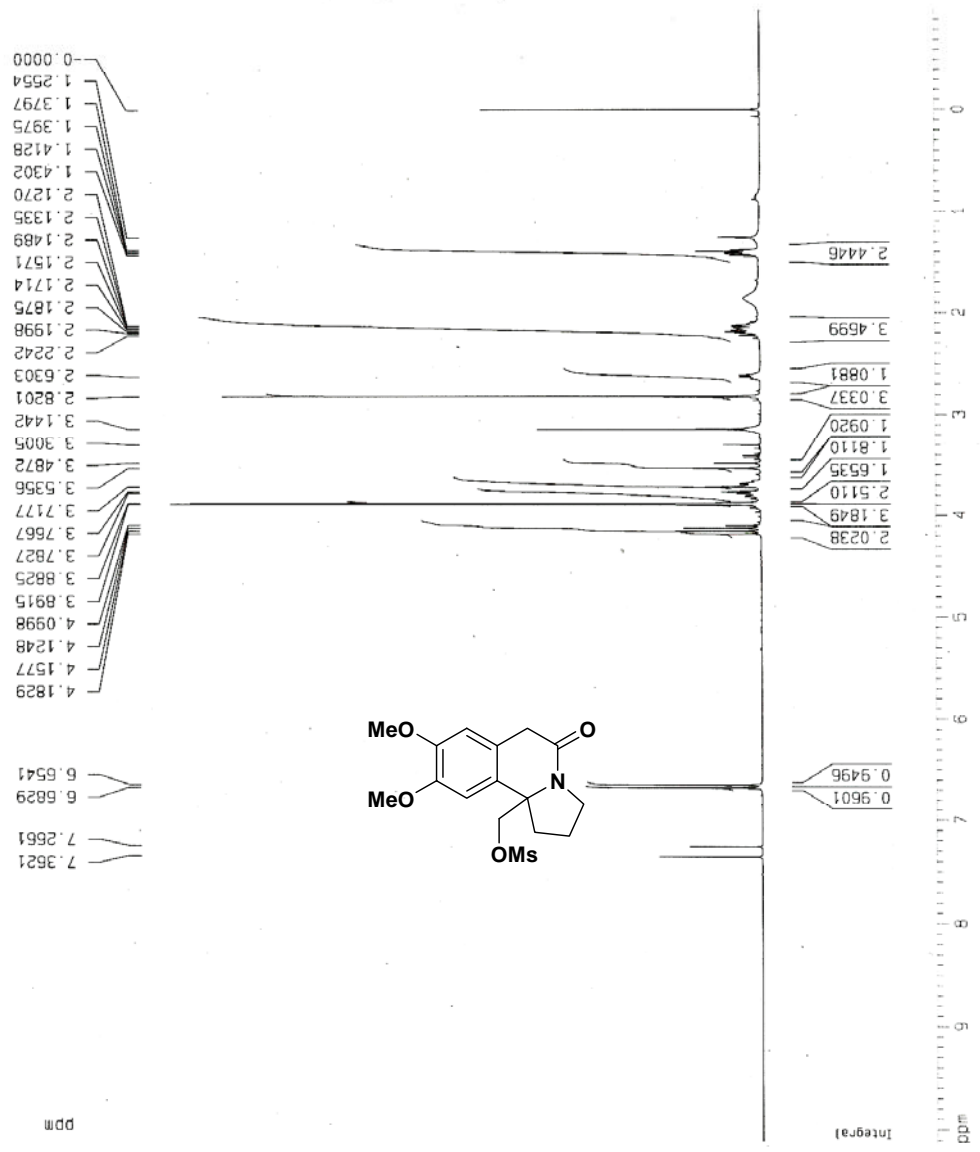
Current Data Parameters
 NAME SB2
 EXPNO 1316
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070825
 Time 9.04
 INSTRUM av400
 PROBNM 5 mm BBO BB-1H
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8389.262 Hz
 FIDRES 0.256020 Hz
 AQ 1.9530228 sec
 RG 128
 DN 59.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 11.00 usec
 PL1 3.00 dB
 SFO1 400.1319460 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300064 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 3.00

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 FIP 10.129 ppm
 F1 4052.73 Hz
 F2 -1.000 ppm
 SFO1 0.55643 ppm/cm
 SFO2 222.64290 Hz/cm



sb-ms-ak-mesylation
CARBONSHORT

Current Data Parameters
 NAME sb2
 EXPNO 1317
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070823
 Time 9:09
 INSTRUM av400
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT DMS-D6
 NS 1220
 DS 2
 SWH 26125.629 Hz
 FIDRES 0.303387 Hz
 AQ 1.30742164 sec
 RG 1149.4
 DR 19.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00020000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 100.6238364 MHz

***** CHANNEL f2 *****
 CPDPRG2 wait:16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 3.00 dB
 PL12 20.25 dB
 PL13 16.00 dB
 SFO2 400.1320007 MHz

F2 - Processing parameters
 S1 131072
 SF 100.6127650 MHz
 KDM EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 11.93 cm
 FIP 234.849 ppm
 F1 23628.84 Hz
 F2P -14.877 ppm
 F2 -1496.79 Hz
 SPMCM 12.48630 ppm/cm
 HZCM 1256.28137 Hz/cm

