Cyclic Ketimines as Superior Electrophiles for NHC-Catalyzed Homoenolate Additions with Broad Scope and Low Catalyst Loadings

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Supporting Information

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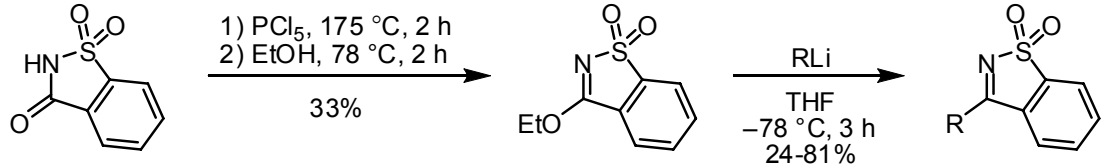
General Methods.

All reactions utilizing air- or moisture-sensitive reagents were performed in dried glassware under an atmosphere of nitrogen. CH_2Cl_2 was distilled from CaH_2. THF and Et_2O were distilled from Na/benzophenone. All aldehydes were purified by distillation or sublimation prior to use. DBU was distilled from CaH_2. Triazolium salt **1** is commercially available from Sigma-Aldrich. Other reagents were used without further purification. Thin layer chromatography (TLC) was performed on EMD precoated plates (silica gel 60 F_{254}, Art 5715) and were visualized by fluorescence quenching under UV light and by staining with phosphomolybdic acid or potassium permanganate, respectively. Column chromatography was performed on EMD Silica Gel 60 (230–400 Mesh) using a forced flow of 0.5–1.0 bar. ^{1}H NMR (500 MHz) and ^{13}C NMR (100 MHz) were measured on a Bruker Avance AVII-500 spectrometer. Chemical shifts are expressed in parts per million (ppm) with respect to the residual solvent peak. Coupling constants are reported as Hertz (Hz), signal shapes and splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; C_q, quaternary carbon. Infrared (IR) spectra were recorded on a JASCO FT/IR-4100 spectrophotometer and are reported as wavenumber (cm^{-1}).

General Procedures for the Preparation of the Cyclic Sulfonyl Ketimines S3.

The ketimines were prepared according to modified literature procedures, the ones used for table 1, entries 1, 8, 9, 10 and 11 are known compounds.[1]



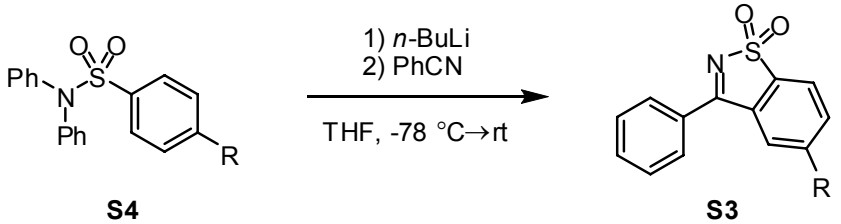
General Procedure 1:[1a]

3-Ethoxy-l,2-benzisothiazole 1,1-dioxide (S2). Saccharin (**S1**, 52.0 g, 0.284 mol) and PCl_5 (71.8 g, 0.345 mol) were gently heated until the reaction mixture became an oil, then the

[1] (a) For entries 1, 10 and 11 see: Davis, F. A.; Towson, J. C.; Vashi, D. B.; ThimmaReddy, R.; McCauley, J. P., Jr.; Harakal, M. E.; Gosciniak, D. J. *J. Org. Chem.* **1990**, *55*, 1254-1261. (b) For entry 8 see: Hellwinkel, D.; Karle, R. *Synthesis*, **1989**, 394-395. (c) For entry 9 see: Abramovitch, R. A.; Smith, E. M.; Humber, M.; Purtschert, B.; Srinivasan, P. C.; Singer, G. M. *J. Chem Soc. Perkin Trans. 1*, **1974**, *22*, 2589-2594.

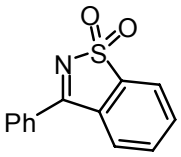
temperature was raised to 175 °C for additional 1.5 h. The side product $POCl_3$ was removed under reduced pressure, and the crude 3-chloro-1,2-benzisothiazole 1,l-dioxide was treated with absolute EtOH (400 mL). The reaction mixture was refluxed for 1 h, then cooled to room temperature. The precipitated product was collected by filtration and washed with ice-cold EtOH. The mother liquor was cooled in an ice bath to obtain more precipitate. The solids were combined and dried to give *O*-ethylsaccharin (**S2**, 23.7 g, 33%) as colorless fine-crystalline material. m.p. 216.0–219.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=1.54 (t, J=7.0 Hz, 3H), 4.67 (q, J=7.0 Hz, 2H), 7.68–7.72 (m, 1H), 7.74–7.78 (m, 2H), 7.88 (d, J=7.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=14.4, 68.6, 122.2, 123.6, 127.5, 133.7, 134.3, 143.9, 169.5. The analytical data is consistent with the literature.[1a]

Cyclic Sulfonyl Ketimines S3. The required organolithium reagent (RLi, 1.2 equiv) was prepared from the corresponding bromides and *n*-BuLi in THF at –78 °C. A suspension of 3-ethoxy-l,2-benzisothiazole 1,1-dioxide (**S2**, 1.0 equiv) was added via cannula at –78 °C. The reaction mixture was stirred for 1 h at –78 °C and warmed to room temperature over 2 h. The reaction was quenched by addition of sat aq NH_4Cl solution. The reaction mixture was extracted with EtOAc, washed with sat aq NaCl solution and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the crude product was purified by silica gel chromatography (hexanes/EtOAc).

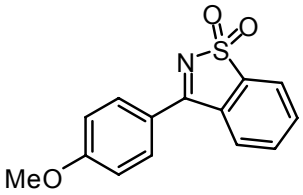


S4 **S3**

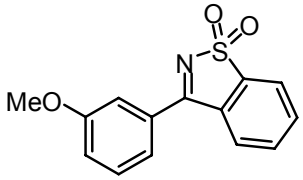
General Procedure 2:[1b] A solution of the corresponding *N*,*N*-diphenylbenzenesulfonamide **S4** (1.0 equiv) in THF was *ortho*-lithiated with *n*-BuLi (1.1 equiv) at –78 °C for 1 h. Benzonitrile (1.1 equiv) was added to the reaction mixture at –78 °C, which was then warmed to room temperature slowly. The reaction was quenched by addition of sat aq NH_4Cl solution. It was extracted with EtOAc, washed with sat aq NaCl solution, and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the crude product was purified by silica gel chromatography (CH_2Cl_2).



3-Phenyl-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 1, and table 2). Prepared according to General Procedure 1. It was purified by recrystallization from EtOAc as a colorless solid in 58% yield. R_f=0.60 (hexanes/EtOAc 1:1); 166.0–167.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.61 (d, J=7.5 Hz, 2H), 7.68–7.81 (m. 3H), 7.91 (d, J=8.0 Hz, 1H), 7.98 (d, J=7.5 Hz, 2H), 8.02 (d, J=7.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=123.2, 126.8, 129.4, 129.7, 130.6, 130.7, 133.6, 133.8, 141.2, 171.2; Spectral data is consistent with published data.[1a]

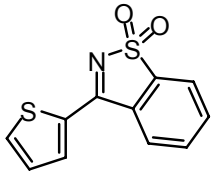


3-(4-Methoxyphenyl)-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 2). Prepared according to General Procedure 1 as a colorless solid in 31% yield. R_f=0.40 (hexanes/EtOAc 1:1); m.p. 210.0–211.5°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=3.93 (s, 3H), 7.09 (d, J=12.0 Hz, 2H), 7.72–7.78 (m, 2H), 7.94–7.97 (m, 1H), 7.98–8.02 (m, 1H), 8.02 (d, J=12.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=56.0, 115.1 (2C), 123.2, 123.3, 126.9, 131.2 (2C), 132.3, 133.5, 133.8, 141.7, 164.5, 170.2; IR (thin film): $\tilde{\nu}$=1604, 1505, 1319 s, 1256, 1161 s, 1134, 1023, 962, 844, 785, 750; HRMS (ESI): *m/z*: calcd for $C_{14}H_{12}NO_3S$: 274.0538; found: 274.0511 $[M+H]^+$.

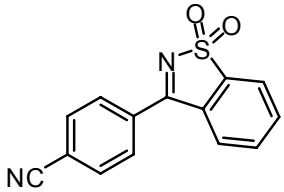


3-(3-Methoxyphenyl)-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 3). Prepared according to General Procedure 1 as a colorless solid in 81% yield. R_f=0.60 (hexanes/EtOAc 1:1); m.p. 173.0–174.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=3.91 (s, 3H), 7.21–7.25 (m, 1H), 7.47–7.55 (m, 3H), 7.73–7.82 (m, 2H), 7.92 (d, J=7.5 Hz, 1H), 8.02 (d, J=7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=56.0, 114.5, 120.1, 122.2, 123.4, 127.0, 130.6, 130.9, 131.9, 133.8, 134.0, 141.4, 160.5, 171.3; IR (thin film): $\tilde{\nu}$=1597, 1530, 1485, 1469, 1452, 1428, 1329 s, 1303, 1243, 1174 s,

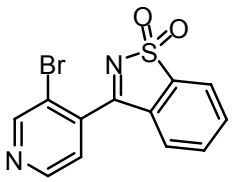
1160, 1144, 1037, 864, 848, 809, 783, 777, 750, 740, 695, 642; HRMS (ESI): *m/z*: calcd for $C_{14}H_{12}NO_3S$: 274.0538; found: 274.0533 $[M+H]^+$.



3-(Thiophen-2-yl)-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 4). Prepared according to General Procedure 1 as a colorless solid in 70% yield. R_f=0.40 (hexanes/EtOAc 1:1); m.p. 206.5–208.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.32–7.36 (m, 1H), 7.78–7.82 (m, 2H), 7.87–7.89 (m, 1H), 8.00–8.03 (m, 1H), 8.18–8.22 (m, 1H), 8.22–8.24 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=123.2, 125.9, 129.2, 130.5, 133.6, 133.8, 134.0, 135.3, 135.7, 141.4, 163.1; IR (thin film): $\tilde{\nu}$=1532, 1493, 1418, 1317, 1305, 1166, 1129, 913, 857, 799, 773, 743, 725, 663; HRMS (ESI): *m/z*: calcd for $C_{11}H_8NO_2S_2$: 248.9918; found: 248.9937 $[M+H]^+$.

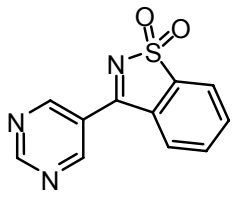


3-(4-Cyanophenyl)-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 5). Prepared according to General Procedure 1 as a colorless solid in 24% yield. R_f=0.30 (hexanes/EtOAc 1:1); m.p. 245.0–247.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.78–7.82 (m, 2H), 7.83–7.87 (m, 1H), 7.92 (d, *J*=8.0 Hz, 2H), 8.01 (d, *J*=7.5, 1H), 8.08 (d, *J*=8.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=117.1, 117.8, 123.9, 126.4, 130.0, 130.3 (2C), 133.2 (2C), 134.3, 134.3, 134.7, 141.3, 169.9; IR (thin film): $\tilde{\nu}$=2230 $_{CN}$, 1613, 1564, 1531, 1498, 1489, 1338 s, 1311, 1298, 1286, 1173 s, 968, 783, 778, 773, 748, 735, 728; HRMS (ESI): *m/z*: calcd for $C_{14}H_7N_2O_2S$: 267.0228; found: 267.0219 $[M-H]^-$.

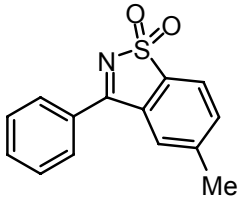


3-(3-Bromopyridin-4-yl)-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 6). Prepared according to General Procedure 1 as a colorless solid in 35% yield. For the preparation of the

required organolithium reagent, see literature.[2] R_f=0.20 (hexanes/EtOAc 1:1); m.p. 120.5–122.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.39 (d, J=7.5 Hz, 1H), 7.46 (d, J=5.0 Hz, 1H), 7.68–7.74 (m, 1H), 7.77–7.84 (m, 1H), 8.02 (d, J=7.5 Hz, 1H), 7.78 (d, J=9.0 Hz, 1H), 8.97 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=118.9, 123.6, 123.9, 126.5, 129.8, 134.4, 134.6, 139.7, 134.0, 149.2, 135.4, 169.9; IR (thin film): $\tilde{\nu}$=1550, 1396, 1343 s, 1308, 1267, 1175 s, 1090, 1023, 843, 783, 764, 750, 729, 706, 668; HRMS (ESI): *m/z*: calcd for $C_{12}H_8BrN_2O_2S$: 321.9412; found: 321.9427 $[M+H]^+$.

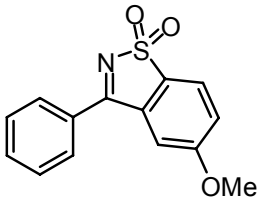


3-(Pyrimidin-5yl)-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 7). Prepared according to General Procedure 1 as a colorless solid in 42% yield. R_f=0.20 (hexanes/EtOAc 1:1); m.p. 196.5–197.5°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.82–7.86 (m, 2H), 7.87–7.92 (m, 1H), 8.08 (d, J=7.6 Hz, 1H), 9.35 (s, 2H), 9.51 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=124.1, 125.6, 126.0, 129.6, 134.6, 134.7, 140.9, 157.3 (2C), 162.0, 167.0; IR (thin film): $\tilde{\nu}$=1575, 1557, 1527, 1420, 1349, 1334 s, 1306, 1196, 1175 s, 961, 804, 789, 750, 715, 705, 763, 669, 631; HRMS (ESI): *m/z*: calcd for $C_{11}H_8N_3O_2S$: 246.0259; found: 246.0259 $[M+H]^+$.

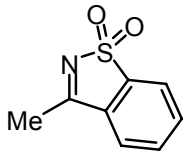


5-Methyl-3-phenyl-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 8). Prepared according to General Procedure 2 as a colorless solid in 36% yield. R_f=0.60 (CH_2Cl_2); m.p. 184.5–185.5°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.53 (s, 3H), 7.57 (d, J=7.5 Hz, 1H), 7.61 (t, J=8.0 Hz, 2H), 7.65 (s, 1H), 7.70 (t, J=7.5 Hz, 1H), 7.88 (d, J=8.0, 1H), 7.76 (d, J=8.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=22.2, 123.2, 127.4, 129.5 (2C), 129.8 (2C), 130.9, 131.4, 133.6, 134.2, 138.7, 145.2, 171.5. Spectral data is consistent with published data.[1b]

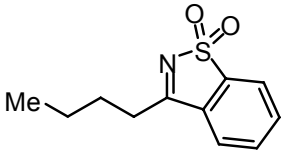
[2] Gribble, G. W.; Saulnier, M.G. *Tetrahedron Lett.* **1980**, *21*, 4137-4140.



5-Methoxy-3-phenyl-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 9). Prepared according to General Procedure 2 as a colorless solid in 58% yield. R_f=0.20 (hexanes/EtOAc 7:3); m.p. 133.0–134.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=3.93 (s, 3H), 7.21 (dd, J=2.0, 8.0 Hz, 1H), 7.30 (d, J=2.0 Hz, 1H), 7.59–7.63 (m, 2H), 7.67–7.71 (m, 1H), 7.92 (d, J=8.5 Hz, 1H), 7.93–7.96 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=56.7, 113.2, 117.7, 124.7, 129.6 (2C), 129.7 (2C), 130.8, 132.7, 133.3, 133.6, 164.3, 170.9; IR (thin film): $\tilde{\nu}$=1580, 1536, 1447, 1330 s, 1309, 1283, 1240, 1230, 1171, 1146, 1135, 973, 795, 773, 739, 698; HRMS (ESI): *m/z*: calcd for $C_{14}H_{12}NO_3S$: 274.0538; found: 274.0525 $[M+H]^+$. Spectral data is consistent with published data.[1c]



3-Methyl-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 10). Prepared according to General Procedure 1 as a colorless solid in 77% yield. R_f=0.40 (hexanes/EtOAc 1:1); 213.0–213.5°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.67 (s, 3H), 7.68–7.70 (m, 1H), 7.73–7.76 (m, 2H), 7.91–7.93 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=17.7, 122.5, 124.2, 131.7, 133.7, 134.1, 139.8, 173.3.

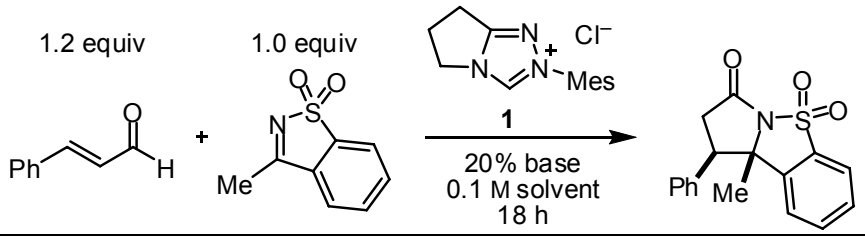


3-(*n*-Butyl)-1,2-benzisothiazole 1,1-dioxide (for table 1, entry 11). Prepared according to General Procedure 1 as a colorless solid in 79% yield. R_f=0.60 (hexanes/EtOAc 1:1); 95.0–96.0°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=0.98 (t, J=7.0 Hz, 3H), 1.47–1.54 (m, 2H), 1.82–1.89 (m, 2H), 2.96 (t, J=7.5 Hz, 2H), 7.68–7.75 (m, 3H), 7.89 (t, J=3.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=14.1, 22.6, 27.7, 31.1, 122.7, 124.3, 131.6, 133.8, 134.2, 140.0, 176.7. Spectral data is consistent with published data.[1a]

Optimization of the γ-lactam forming reaction conditions.

The crude products were analyzed by NMR spectroscopy and the conversion of the imine was determined by integration of the prominent signal for the methyl group in the starting material (δ=2.67 ppm) and in the product (δ=1.60).

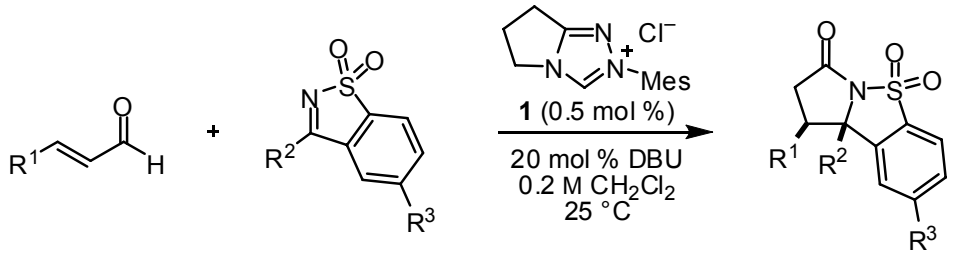
Table S-1. Optimization of the NHC-catalyzed annulation of cinnamaldehyde with a cyclic sulfonyl ketimine.



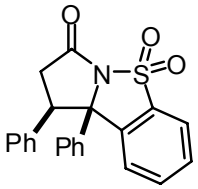
entry	mol-% catalyst	base	solvent	T (°C)	% conversion
1	15 (IMes)[a]	DBU	*t*BuOH	60	66
2	15	DBU	*t*BuOH	40	22
3	15	DBU	toluene	40	24
4	15	DBU	MeCN	40	50
5	15	DBU	CH_2Cl_2	40	>99
6	15	DBU	THF	40	82
7	15	DBU	THF	25	74
8	15	DBU	EtOAc	25	68
9	15	DBU	1,2-dichloroethane	25	83
10	15	DBU	CH_2Cl_2	25	>99
11	15	10% DBU	CH_2Cl_2	25	62
12	15	NEt_3	CH_2Cl_2	25	36
13	15	DIPEA	CH_2Cl_2	25	23
14	0.5	DBU	CH_2Cl_2	25	>99
15	0.1	DBU	CH_2Cl_2	25	38
16	0	DBU	CH_2Cl_2	25	0
17	0.5	DBU	0.2 M CH_2Cl_2	25	>99

[a] IMes = 1,3-Bis(2,4,6-trimethylphenyl)imidazol-2-ylidene.

General Procedure for the Annulation of α,β-unsaturated Aldehydes and Cyclic Sulfonyl Ketimines.

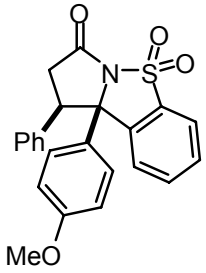


An oven-dried vial with a Teflon® coated screw cap and stir bar was charged with the cyclic sulfonyl imine (0.20 mmol, 1.0 equiv) and purged with nitrogen. The α,β-unsaturated aldehyde (0.24 mmol, 1.2 equiv), dry CH_2Cl_2 (0.9 mL) and a solution of the triazolium precatalyst **1** (1.0 µmol, 0.5 mol %) in dry CH_2Cl_2 (0.1 mL) were added. Finally, DBU (0.04 mmol, 0.2 equiv) was added, and the sealed vial was placed into an oil bath at 25 °C. After 16 to 24 hours ~ 50 µL of the reaction mixture was diluted with $CDCl_3$ to confirm complete conversion and to determine the diastereomeric ratio by ^{1}H NMR spectroscopy. The reaction mixture was directly applied onto a silica gel column (100:1 m/m silica gel/expected product) and eluted with hexanes/CH_2Cl_2/acetone (25:50:1→15:50:1 v/v/v) to give pure product.

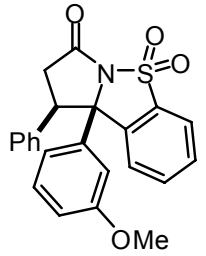


***rac*-(*1R*,9bR**)-1,9b-Diphenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 1). Prepared according to the General Procedure as a colorless solid in 89% yield. A concentrated solution of the purified product in MeOH at room temperature for 24 h gave single crystals for x-ray crystallography. R_f=0.29 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 253–253.5°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.90 (dd, J=7.5, 17.0 Hz, 1H, 2-H^a), 3.11 (dd, J=13.5, 17.0 Hz, 1H, 2-H^b), 4.16 (dd, J=7.5, 14.0 Hz, 1H, 1-H), 6.85 (d, J=7.5 Hz, 2H), 7.16 (d, J=7.5 Hz, 2H), 7.24–7.33 (m, 5H), 7.38 (t, J=7.5 Hz, 1H), 7.61–7.65 (m, 1H), 7.74 (d, J=3.5 Hz, 2H), 7.80 (d, J=8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=39.3 (C-2), 54.1 (C-1), 75.2 (C-9b), 122.2, 124.6, 127.1 (2C), 128.4 (2C), 128.6 (2C), 128.7, 128.9, 129.8 (2C), 130.1, 133.9, 134.3 (C_q), 135.2 (C_q), 135.9 (C_q), 141.5 (C_q), 169.8 (C-3); IR (thin film): $\tilde{\nu}$=3090, 3062, 3036, 3008, 2925, 2854, 1747 s, 1601, 1584, 1496, 1465, 1452, 1445, 1417, 1346 s, 1313, 1287, 1248 s, 1215, 1178 s, 1138, 1102, 1081, 1065, 1033, 1013, 1001, 975, 949, 917, 894, 881, 867, 808, 772,

759, 735 s, 703 s, 682, 660, 643, 633, 619, 603, 587, 571; HRMS (ESI): *m/z*: calcd for $C_{22}H_{17}NNaO_3S$: 398.0827; found: 398.0844 $[M+Na]^+$.

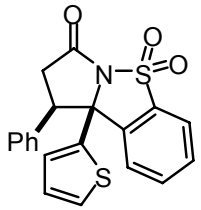


***rac*-(*1R*,9bR**)-9b-(4-Methoxyphenyl)-1-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*] isothiazol-3-one 5,5-dioxide** (table 1, entry 2). Prepared according to the General Procedure as a colorless solid in 85% yield. R_f=0.20 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. dec. >255°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.85 (dd, J=7.5, 17.0 Hz, 1H, 2-H^a), 3.07 (dd, J=14.0, 17.0 Hz, 1H, 2-H^b), 3.76 (s, 3H, OCH_3), 4.09 (dd, J=7.0, 13.5 Hz, 1H, 1-H), 6.74 (d, J=8.9 Hz, 2H), 6.86 (d, J=7.3 Hz, 2H), 7.03 (d, J=8.9 Hz, 2H), 7.28 (t, J=7.5 Hz, 2H), 7.35 (t, J=7.3 Hz, 1H), 7.57 (t, J=7.6 Hz, 1H), 7.64 (d, J=7.6 Hz, 1H), 7.68 (t, J=7.5 Hz, 1H), 7.76 (d, J=7.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=39.3 (C-2), 54.0 (C-1), 55.3 (OCH_3), 74.9 (C-9b), 113.6 (2C), 122.1, 124.3, 127.1 (C_q), 128.3 (2C), 128.5 (2C), 128.8, 129.8 (3C), 133.8, 134.3 (C_q), 135.7 (C_q), 141.6 (C_q), 159.7 (C_q), 169.7 (C-3); IR (thin film): $\tilde{\nu}$=3063, 2934, 2838, 1746 s, 1609, 1577, 1511, 1466, 1455, 1415, 1344 s, 1313, 1300, 1254 s, 1214, 1177 s, 1138, 1098, 1065, 1031, 958, 895, 831, 796, 768, 736, 702; HRMS (ESI): *m/z*: calcd for $C_{23}H_{20}NO_4S$: 406.1113; found: 406.1097 $[M+H]^+$.

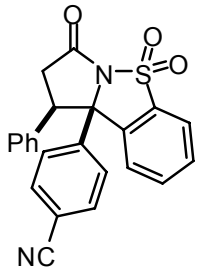


***rac*-(*1R*,9bR**)-9b-(3-Methoxyphenyl)-1-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*] isothiazol-3-one 5,5-dioxide** (table 1, entry 3). Prepared according to the General Procedure. Purification using hexanes/CH_2Cl_2/acetone (25:50:1 v/v/v) as the eluent afforded the product as a colorless solid in 96% yield. R_f=0.13 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 240–241°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.86 (dd, J=7.5, 17.0 Hz, 1H, 2-H^a), 3.10 (dd, J=13.5, 17.0 Hz,

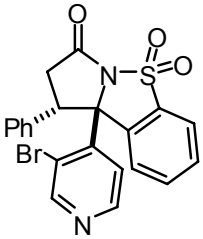
1H, 2-H^{b}), 3.62 (s, 3H, OCH_3), 4.11 (dd, *J*=7.5, 14.0 Hz, 1H, 1-H), 6.59 (s, 1H), 6.75 (dd, *J*=1.0, 8.2 Hz, 1H), 6.80 (dd, *J*=2.0, 8.2 Hz, 1H), 6.87 (d, *J*=7.7 Hz, 2H), 7.15 (t, *J*=8.2 Hz, 1H), 7.28 (t, *J*=7.7 Hz, 2H), 7.36 (t, *J*=7.2 Hz, 1H), 7.59 (dt, *J*=1.5, 7.5 Hz, 1H), 7.66–7.72 (m, 2H), 7.76 (d, *J*=7.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=39.3 (C-2), 54.2 (C-1), 55.3 (OCH_3), 75.1 (C-9b), 113.4, 114.1, 119.4, 122.2, 124.6, 128.6 (2C), 129.0, 129.5, 129.8 (2C), 130.1, 133.9, 134.5 (C_q), 136.0 (C_q), 136.8 (C_q), 141.4 (C_q), 159.4 (C_q), 169.7 (C-3); IR (thin film): $\tilde{\nu}$=3063, 2938, 2835, 1746 s, 1602, 1584, 1492, 1466, 1455, 1432, 1344 s, 1314, 1294, 1245 s, 1213, 1177 s, 1138, 1107, 1086, 1065, 1050, 950, 796, 767, 734, 703, 663; HRMS (ESI): *m/z*: calcd for $C_{23}H_{20}NO_4S$: 406.1113; found: 406.1126 $[M+H]^+$.



***rac*-(*1R*,9bS**)-1-Phenyl-9b-(thiophen-2-yl)-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 4). Prepared according to the General Procedure. Purification using hexanes/CH_2Cl_2/acetone (25:50:1 v/v/v) as the eluent afforded the product as a colorless solid in 90% yield. R_f=0.25 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 213–215°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.90 (dd, *J*=7.0, 17.0 Hz, 1H, 2-H^{a}), 3.33 (dd, *J*=14.0, 17.0 Hz, 1H, 2-H^{b}), 4.06 (dd, *J*=7.0, 13.5 Hz, 1H, 1-H), 6.74 (dd, *J*=1.0, 3.6 Hz, 1H), 6.90 (dd, *J*=3.7, 4.9 Hz, 1H), 6.93 (d, *J*=7.3 Hz, 2H), 7.23 (dd, *J*=1.0, 5.1 Hz, 1H), 7.31 (t, *J*=7.7 Hz, 2H), 7.37 (t, *J*=7.3 Hz, 1H), 7.56 (d, *J*=7.9 Hz, 1H), 7.62 (t, *J*=7.4 Hz, 1H), 7.71 (t, *J*=7.5 Hz, 1H), 7.78 (d, *J*=7.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=38.9 (C-2), 54.2 (C-1), 73.9 (C-9b), 122.3, 124.1, 126.7, 127.1, 127.4, 128.7 (2C), 129.1, 129.5 (2C), 130.4, 134.0 (C_q), 134.2, 135.4 (C_q), 140.0 (C_q), 140.5 (C_q), 169.7 (C-3); IR (thin film): $\tilde{\nu}$=3064, 3033, 2926, 1752 s, 1582, 1497, 1467, 1455, 1431, 1415, 1345 s, 1314, 1281, 1249 s, 1213, 1177 s, 1135, 1095, 1080, 1065, 1032, 1008, 958, 939, 917, 897, 861, 836, 793, 768, 735, 701; HRMS (ESI): *m/z*: calcd for $C_{20}H_{15}NNaO_3S_2$: 404.0391; found: 404.0410 $[M+Na]^+$.

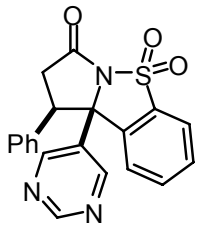


***rac*-(*1R*,9bR**)-9b-(4-Cyanophenyl)-1-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 5). Prepared according to the General Procedure as a colorless solid in 83% yield. R_f=0.14 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. >280°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.92 (dd, J=7.5, 17.0 Hz, 1H, 2-H^a), 3.03 (dd, J=13.5, 17.0 Hz, 1H, 2-H^b), 4.20 (dd, J=7.5, 13.5 Hz, 1H, 1-H), 6.85 (d, J=7.4 Hz, 2H), 7.25 (m, 2H), 7.31 (t, J=7.5 Hz, 2H), 7.39 (t, J=7.4 Hz, 1H), 7.51 (d, J=8.4 Hz, 2H), 7.65 (t, J=7.4 Hz, 1H), 7.71–7.77 (m, 2H), 7.80 (d, J=7.8 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ=38.2 (C-2), 52.0 (C-1), 74.5 (C-9b), 111.1, 118.2, 121.9, 125.1, 127.8 (2C), 128.3 (2C), 128.4, 129.7 (2C), 130.7, 132.0 (2C), 134.5, 134.9, 135.0, 140.1, 141.3, 170.1 (C-3); IR (thin film): $\tilde{\nu}$=3065, 2924, 2230, 1752 s, 1607, 1582, 1502, 1469, 1455, 1406, 1344 s, 1316, 1245, 1210, 1177 s, 1138, 1099, 1067, 1019, 969, 943, 904, 835, 759, 736, 701, 662; HRMS (ESI): *m/z*: calcd for $C_{23}H_{16}N_2NaO_3S$: 423.0779; found: 423.0775 $[M+Na]^+$.

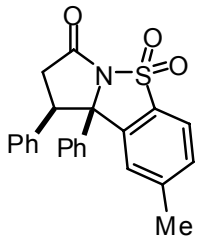


***rac*-(*1R*,9bR**)-9b-(3-Bromopyridin-4-yl)-1-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*] isothiazol-3-one 5,5-dioxide** (table 1, entry 6). Prepared according to the General Procedure using 5 mol % catalyst **1** and CH_2Cl_2/acetone (50:1 v/v) as the eluent as a sticky, colorless solid in 77% yield. R_f=0.10 (CH_2Cl_2/acetone 50:1); m.p. >280°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.84 (d, J=17.7 Hz, 1H, 2-H^a), 3.06 (dd, J=7.8, 17.8 Hz, 1H, 2-H^b), 5.35 (d, J=7.7 Hz, 1H, 1-H), 7.16 (d, J=7.0 Hz, 1H), 7.21 (t, J=7.1 Hz, 2H), 7.28–7.33 (m, 2H), 7.36 (t, J=7.9 Hz, 1H), 7.41 (t, J=7.6 Hz, 1H), 7.64 (d, J=7.7 Hz, 1H), 8.07 (d, J=5.2 Hz, 1H), 8.14 (d, J=8.0 Hz, 1H), 8.65 (d, J=5.3 Hz, 1H), 8.92 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=40.8 (C-2), 46.5 (C-1), 79.0 (C-9b), 117.7 (C_q), 122.0, 123.9, 126.7, 127.5 (2C), 128.5, 129.2 (2C), 130.7, 133.5, 134.8 (C_q), 136.4

(C_q), 138.2 (C_q), 147.9 (C_q), 150.3, 155.5, 171.0 (C-3); IR (thin film): $\tilde{\nu}$=3035, 1752 s, 1574, 1496, 1466, 1455, 1394, 1344 s, 1313, 1287, 1231, 1210, 1177 s, 1138, 1102, 1066, 1021, 946, 830, 765, 736, 701; HRMS (ESI): *m/z*: calcd for $C_{21}H_{15}BrN_2NaO_3S$: 476.9884; found: 476.9923 [*M*+Na]$^+$.

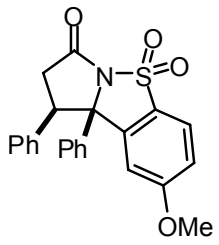


***rac*-(*1R*,9bR**)-1-Phenyl-9b-(5-pyrimidinyl)-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 7). Prepared according to the General Procedure using 5 mol % catalyst **1** and CH_2Cl_2/acetone (50:1→20:1→9:1 v/v) as the eluent as a colorless solid in 68% yield. R_f=0.45 (CH_2Cl_2/acetone 9:1); m.p. >280°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.96 (dd, *J*=7.8, 17.2 Hz, 1H, 2-H^a), 3.05 (dd, *J*=13.3, 17.2 Hz, 1H, 2-H^b), 4.26 (dd, *J*=7.8, 13.3 Hz, 1H, 1-H), 6.92 (d, *J*=7.3 Hz, 2H), 7.37 (t, *J*=7.8 Hz, 2H), 7.43 (tt, *J*=1.2, 7.4 Hz, 1H), 7.68 (ddd, *J*=0.8, 8.1, 15.9 Hz, 2H), 7.78 (dt, *J*=1.1, 7.8 Hz, 1H), 7.83 (d, *J*=7.8 Hz, 1H), 8.47 (d, *J*=2.5 Hz, 2H), 9.13 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=38.7 (C-2), 53.6 (C-1), 72.0 (C-9b), 122.7, 123.9, 129.4 (2C), 129.8 (2C), 129.89, 129.92 (C_q), 131.0, 133.0 (C_q), 134.6, 136.0 (C_q), 139.9 (C_q), 155.2 (2C), 158.6, 168.9 (C-3); IR (thin film): $\tilde{\nu}$=3089, 3062, 3035, 3008, 2924, 1756 s, 1574, 1558, 1499, 1469, 1451, 1420, 1347 s, 1313, 1289, 1244 s, 1219, 1177 s, 1154, 1141, 1119, 1093, 1083, 1066, 1059, 1042, 1032, 1013, 969, 952, 892, 804, 770, 748, 736, 725, 702, 663, 645; HRMS (ESI): *m/z*: calcd for $C_{20}H_{16}N_3O_3S$: 378.0912; found: 378.0915 [*M*+H]$^+$.

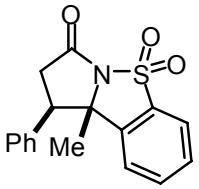


***rac*-(*1R*,9bR**)-8-Methyl-1,9b-diphenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 8). Prepared according to the General Procedure using hexanes/CH_2Cl_2/acetone (25:50:1 v/v/v) as the eluent as a colorless solid in 96% yield. R_f=0.21 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. >280°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.51 (s, 3H,

CH_3), 2.85 (dd, *J*=7.3, 16.9 Hz, 1H, 2-H^a), 3.05 (dd, *J*=13.8, 16.9 Hz, 1H, 2-H^b), 4.11 (dd, *J*=7.2, 13.7 Hz, 1H, 1-H), 6.82 (d, *J*=7.4 Hz, 2H), 7.13 (d, *J*=7.5 Hz, 2H), 7.20–7.30 (m, 5H), 7.33–7.39 (m, 2H), 7.45 (s, 1H), 7.63 (d, *J*=8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=22.4 (CH_3), 39.4 (C-2), 54.1 (C-1), 75.0 (C-9b), 122.0, 124.8, 127.1 (2C), 128.4 (2C), 128.5 (2C), 128.7, 128.9, 129.9 (2C), 130.9, 133.3 (C_q), 134.5 (C_q), 135.4 (C_q), 141.8 (C_q), 145.1 (C_q), 169.8 (C-3); IR (thin film): $\tilde{\nu}$=3060, 3031, 2894, 1746 s, 1595, 1496, 1454, 1447,1413, 1388, 1345 s, 1310, 1249, 1227, 1176 s, 1151, 1117, 1080, 1067, 1033, 1003, 974, 962, 829, 802, 770, 736, 703, 669; HRMS (ESI): *m/z*: calcd for $C_{23}H_{20}NO_3S$: 390.1164; found: 390.1148 [*M*+H]$^+$.

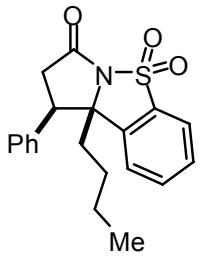


***rac*-(*1R*,9bR**)-8-Methoxy-1,9b-diphenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 9). Prepared according to the General Procedure using hexanes/CH_2Cl_2/acetone (25:50:1 v/v/v) as the eluent as a colorless solid in 98% yield. R_f=0.10 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. dec. >230°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.85 (dd, *J*=7.3, 17.0 Hz, 1H, 2-H^a), 3.05 (dd, *J*=13.8, 16.9 Hz, 1H, 2-H^b), 3.90 (s, 3H, CH_3), 4.12 (dd, *J*=7.2, 13.7 Hz, 1H, 1-H), 6.83 (d, *J*=7.5 Hz, 2H), 7.05 (dd, *J*=2.0, 8.7 Hz, 1H), 7.10–7.14 (m, 3H), 7.20–7.30 (m, 5H), 7.34 (t, *J*=7.3 Hz, 1H), 7.68 (d, *J*=8.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=39.3 (C-2), 54.1 (C-1), 56.2 (OCH_3), 74.7 (C-9b), 110.5, 115.1, 123.8, 127.1 (2C), 128.0, 128.4 (2C), 128.5 (2C), 128.8, 129.0, 129.9 (2C), 134.4 (C_q), 135.2 (C_q), 143.7 (C_q), 163.9 (C_q), 169.7 (C-3); IR (thin film): $\tilde{\nu}$=3060, 3033, 2939, 2841, 1745 s, 1594, 1495, 1480, 1455, 1446, 1428, 1340 s, 1288, 1250 s, 1214, 1179 s, 1146, 1103, 1072, 1020, 961, 864, 825, 802, 769, 753, 732, 703; HRMS (ESI): *m/z*: calcd for $C_{23}H_{20}NO_4S$: 406.1113; found: 406.1118 [*M*+H]$^+$.

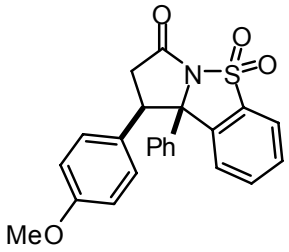


***rac*-(*1R*,9bS**)-9b-Methyl-1-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 10). Prepared according to the General Procedure using 5 mol % catalyst **1**

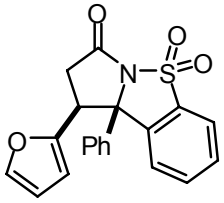
and hexanes/CH_2Cl_2/acetone (25:50:1→0:50:1 v/v/v) as the eluent as a colorless solid in 72% yield. Small single crystals were obtained by slow evaporation of the solvent from a solution of 4.4 mg purified product in 1.5 mL CH_2Cl_2. R_f=0.44 (CH_2Cl_2/acetone 50:1); m.p. >280°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=1.60 (s, 3H), 2.90 (dd, J=7.4, 17.0 Hz, 1H, 2-H^a), 3.32 (dd, J=13.8, 17.0 Hz, 1H, 2-H^b), 3.79 (dd, J=7.4, 13.8 Hz, 1H, 1-H), 7.15 (dd, J=1.7, 6.7 Hz, 1H), 7.36–7.39 (m, 2H), 7.42–7.50 (m, 3H), 7.59–7.65 (m, 2H), 7.81 (dd, J=1.3, 6.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=24.1 (CH_3), 39.1 (C-2), 52.2 (C-1), 71.1 (C-9b), 122.2, 123.6, 129.0, 129.2 (2C), 129.4 (2C), 130.2, 134.1, 134.5 (C_q), 135.2 (C_q), 141.8 (C_q), 169.6 (C-3); IR (thin film): $\tilde{\nu}$=2925, 1735 s, 1677, 1598, 1580, 1499, 1469, 1448, 1381, 1338 s, 1326, 1310, 1280, 1256, 1221, 1176 s, 1158, 1143, 1120, 1077, 1052, 1025, 998, 917, 899, 768, 752, 735, 703; HRMS (ESI): *m/z*: calcd for $C_{17}H_{16}NO_3S$: 314.0851; found: 314.0858 [M+H]$^+$.



***rac*-(*1R*,9bS**)-9b-*n*-Butyl-1-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 1, entry 11). Prepared according to the General Procedure using 5 mol % catalyst **1** and hexanes/CH_2Cl_2/acetone (25:50:1) as the eluent as a colorless solid in 78% yield. R_f=0.27 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 88–89°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=0.48–0.55 (m, 1H), 0.72 (t, J=7.4 Hz, 3H, CH_3), 1.05–1.15 (m, 1H), 1.17–1.29 (m, 1H), 1.40–1.53 (m, 2H), 2.10–2.15 (m, 1H), 2.88 (dd, J=7.3, 17.0 Hz, 1H, 2-H^a), 3.38 (dd, J=14.1, 17.0 Hz, 1H, 2-H^b), 3.78 (dd, J=7.3, 14.0 Hz, 1H, 1-H), 7.07 (d, J=7.1 Hz, 1H), 7.32 (d, J=7.0 Hz, 2H), 7.43–7.47 (m, 3H), 7.61–7.67 (m, 2H), 7.81 (d, J=7.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=13.9, 22.7, 25.3, 35.4, 39.0, 53.8 (C-1), 75.0 (C-9b), 122.3, 123.7, 128.9, 129.0 (2C), 129.5 (2C), 130.3, 134.1, 134.2 (C_q), 135.5 (C_q), 139.4 (C_q), 171.1 (C-3); IR (thin film): $\tilde{\nu}$=3063, 3033, 2957, 2931, 2871, 1748 s, 1601, 1582, 1499, 1469, 1455, 1420, 1370, 1337 s, 1315, 1266, 1249, 1240, 1217, 1174 s, 1156, 1138, 1096, 1056, 1030, 997, 955, 938, 912, 894, 811, 769, 737, 703, 674, 657, 642, 627, 619, 601; HRMS (ESI): *m/z*: calcd for $C_{20}H_{21}NNaO_3S$: 378.1140; found: 378.1149 [M+Na]$^+$.

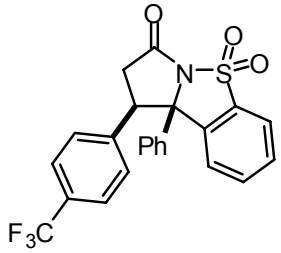


***rac*-(*1R*,9bR**)-1-(4-Methoxyphenyl)-9b-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*] isothiazol-3-one 5,5-dioxide** (table 2, entry 1). Prepared according to the General Procedure as a colorless solid in 95% yield. R_f=0.22 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 175–176°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.82 (dd, J=7.2, 16.9 Hz, 1H, 2-H^a), 3.00 (dd, J=13.9, 16.9 Hz, 1H, 2-H^b), 3.82 (s, 3H, OCH_3), 4.07 (dd, J=7.2, 13.8 Hz, 1H, 1-H), 6.72 (d, J=8.6 Hz, 2H), 6.78 (d, J=8.6 Hz, 2H), 7.15 (d, J=7.5 Hz, 2H), 7.22–7.30 (m, 3H), 7.56–7.60 (m, 1H), 7.67–7.72 (m, 2H), 7.76 (d, J=7.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=39.5 (C-2), 53.6 (C-1), 55.5 (OCH_3), 75.2 (C-9b), 113.9 (2C), 122.2, 124.6, 126.1 (C_q), 127.2 (2C), 128.4 (2C), 128.7, 130.0, 130.9 (2C), 133.8, 135.3 (C_q), 136.0 (C_q), 141.5 (C_q), 160.0 (C_q), 169.8 (C-3); IR (thin film): $\tilde{\nu}$=3062, 3004, 2960, 2934, 2838, 1747 s, 1611, 1583, 1515 s, 1496, 1464, 1451, 1444, 1428, 1344 s, 1309, 1295, 1254 s, 1215, 1177 s, 1138, 1113, 1102, 1080, 1066, 1033, 957, 833, 819, 775, 762, 735, 699, 660, 646, 633; HRMS (ESI): *m/z*: calcd for $C_{23}H_{20}NO_4S$: 406.1113; found: 406.1069 $[M+H]^+$.

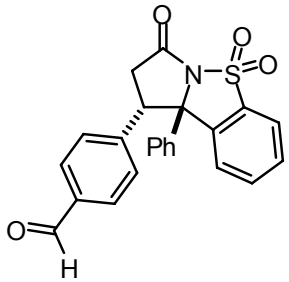


***rac*-(*1R*,9bS**)-1-(2-Furyl)-9b-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 2, entry 2). Prepared according to the General Procedure as a colorless solid in 98% yield. R_f=0.37 (hexanes/CH_2Cl_2/acetone 15:50:1); m.p. 266–267°C (with dec.); ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.87 (dd, J=7.5, 16.9 Hz, 1H, 2-H^a), 3.06 (dd, J=13.7, 16.8 Hz, 1H, 2-H^b), 4.23 (dd, J=7.4, 13.6 Hz, 1H, 1-H), 6.00 (d, J=3.2 Hz, 1H), 6.31 (dd, J=1.9, 3.2 Hz, 1H), 7.16–7.19 (m, 2H), 7.19–7.24 (m, 3H), 7.44 (d, J=1.3 Hz, 1H), 7.61 (t, J=7.6 Hz, 1H), 7.76 (d, J=7.8 Hz, 1H), 7.79 (dt, J=1.0, 7.8 Hz, 1H), 8.21 (d, J=7.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=36.7 (C-2), 47.1 (C-1), 75.1 (C-9b), 110.2, 111.1, 122.1, 125.2, 125.8 (2C), 128.56 (2C), 128.59, 130.2, 134.2, 135.90 (C_q), 135.91 (C_q), 141.1 (C_q), 142.8, 148.8 (C_q), 169.0 (C-3);

IR (thin film): $\tilde{\nu}$=3063, 2922, 1747 s, 1595, 1497, 1467, 1451, 1416, 1344 s, 1247, 1179 s, 1139, 1103, 1079, 1066, 1007, 977, 963, 937, 885, 858, 774, 757, 735, 703, 666, 640; HRMS (ESI): *m/z*: calcd for $C_{20}H_{15}NNaO_4S$: 388.0619; found: 388.0577 [*M*+Na]$^+$.

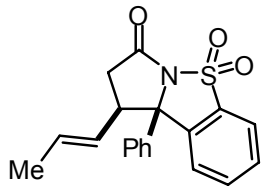


***rac*-(*1R*,9bR**)-9b-Phenyl-1-(4-trifluoromethylphenyl)-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*] isothiazol-3-one 5,5-dioxide** (table 2, entry 3). Prepared according to the General Procedure using hexanes/CH_2Cl_2/acetone (25:50:1) as the eluent as a colorless solid in 89% yield. R_f=0.30 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 278°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.90 (dd, *J*=7.4, 16.9 Hz, 1H, 2-H^a), 3.07 (dd, *J*=13.6, 16.9 Hz, 1H, 2-H^b), 4.19 (dd, *J*=7.4, 13.6 Hz, 1H, 1-H), 6.93 (d, *J*=8.1 Hz, 2H), 7.15 (d, *J*=7.7 Hz, 2H), 7.24–7.28 (m, 2H), 7.30–7.34 (m, 1H), 7.51 (d, *J*=8.2 Hz, 2H), 7.61 (d, *J*=7.5 Hz, 1H), 7.64 (d, *J*=7.7 Hz, 1H), 7.73 (t, *J*=7.7 Hz, 1H), 7.78 (d, *J*=7.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=39.4 (C-2), 53.7 (C-1), 75.0 (C-9b), 122.4, 123.9 (q, *J*=270 Hz, CF_3), 124.4, 125.5 (q, *J*=3.6 Hz, 2C, F_3CCCH), 127.0 (2C), 128.7 (2C), 129.1, 130.2 (2C), 130.3, 131.2 (q, *J*=32.5 Hz, F_3CC), 134.0, 134.9 (C_q), 136.1 (C_q), 138.7 (C_q), 141.1 (C_q), 169.1 (C-3); IR (thin film): $\tilde{\nu}$=3073, 2925, 2853, 1753 s, 1619, 1597, 1582, 1496, 1465, 1451, 1445, 1427, 1348 s, 1326 s, 1248, 1215, 1178 s, 1138, 1113, 1069 s, 1034, 1017, 1002, 952, 896, 882, 867, 859, 841, 815, 771, 763, 746, 735, 700, 683, 658, 646, 633, 612; HRMS (ESI): *m/z*: calcd for $C_{23}H_{16}F_3NNaO_3S$: 466.0701; found: 466.0668 [*M*+Na]$^+$.

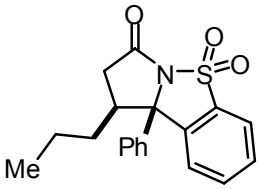


***rac*-(*1R*,9bS**)-4-(9b-Phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-on-1-yl)benzaldehyde *S*,*S*-dioxide** (table 2, entry 4). Prepared according to the General Procedure using hexanes/CH_2Cl_2/acetone (25:50:1→0:50:1 v/v/v) as the eluent as a tan solid in 55% yield.

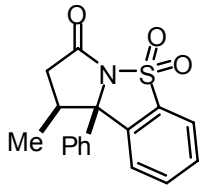
R_f=0.45 (CH_2Cl_2/acetone 50:1); m.p. 265°C (with dec.); ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.80 (d, J=17.5 Hz, 1H, 2-H^a), 3.20 (dd, J=7.6, 17.5 Hz, 1H, 2-H^b), 4.45 (d, J=7.5 Hz, 1H, 1-H), 7.22–7.25 (m, 1H), 7.27–7.33 (m, 2H), 7.36–7.41 (m, 3H), 7.48 (t, J=8.2 Hz, 2H), 7.54–7.57 (m, 1H), 7.69 (d, J=8.3 Hz, 2H), 7.85 (d, J=8.1 Hz, 2H), 9.86 (s, 1H, CHO); ^{13}C NMR (125 MHz, $CDCl_3$): δ=40.8 (C-2), 52.7 (C-1), 78.3 (C-9b),121.8, 125.1 (2C), 125.4, 128.5 (2C), 129.1, 129.7 (2C), 130.0, 130.4 (2C), 133.6, 134.4 (C_q), 136.0 (C_q), 137.9 (C_q), 141.1 (C_q), 145.4 (C_q), 171.2 (C-3), 191.5 (CHO); IR (thin film): $\tilde{\nu}$=3061, 3035, 2923, 2839, 2747, 1748 s, 1703 s, 1649, 1608, 1577, 1493, 1469, 1451, 1428, 1412, 1392, 1341 s, 1314, 1284, 1250, 1233, 1213, 1197, 1174 s, 1137, 1115, 1101, 1080, 1067, 1033, 1017, 1000, 968, 958, 948, 846, 823, 760, 735, 700, 670, 653; HRMS (ESI): *m/z*: calcd for $C_{23}H_{18}NO_4S$: 404.0957; found: 404.0962 $[M+H]^+$.



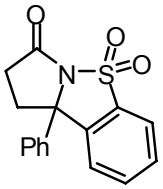
***rac*-(*1R*,9bR**)-9b-Phenyl-1-(1-propenyl)-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 2, entry 5). Prepared according to the General Procedure using 5 mol % catalyst **1** as a colorless solid in 75% yield. The configuration of the alkene was predominantly *trans*. R_f=0.17 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. dec. >210°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=1.76 (dd, J=1.6, 6.6 Hz, 3H, CH_3), 2.63 (d, J=10.2 Hz, 2H, 2-H_2), 3.43 (q, J=9.9 Hz, 1H, 1-H), 5.04 (ddd, J=1.6, 9.3, 15.2 Hz, 1H, 1-CH), 5.80 (qd, J=6.6, 15.2 Hz, 1H, C*H*CH_3), 7.35 (t, J=7.3 Hz, 1H), 7.41 (t, J=7.2 Hz, 2H), 7.53 (d, J=7.7 Hz, 2H), 7.58 (t, J=7.5 Hz, 1H), 7.70–7.76 (m, 2H), 7.85 (d, J=7.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=18.2 (CH_3), 39.2 (C-2), 51.7 (C-1), 74.1 (C-9b), 122.1, 124.0, 126.7 (2C), 127.4, 128.7, 128.8 (2C), 130.0, 131.3, 133.9, 135.7 (C_q), 136.0 (C_q), 141.9 (C_q), 170.0 (C-3); IR (thin film): $\tilde{\nu}$=3089, 3061, 3025, 2915, 2855, 1747 s, 1595, 1496, 1465, 1451, 1415, 1378, 1347 s, 1313, 1248 s, 1206, 1178 s, 1139, 1105, 1080, 1065, 965, 948, 838, 768, 734, 699, 664, 654, 642, 625; HRMS (ESI): *m/z*: calcd for $C_{19}H_{17}NNaO_3S$: 362.0827; found: 362.0838 $[M+Na]^+$.



***rac*-(*1R*,9bS**)-9b-Phenyl-1-(1-propyl)-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 2, entry 6). Prepared according to the General Procedure using 2.0 equiv enal, 5 mol % catalyst **1** and hexanes/CH_2Cl_2/acetone (25:50:1) as the eluent as a colorless solid in 96% yield. R_f=0.24 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 228°C (with dec.); ^{1}H NMR (500 MHz, $CDCl_3$): δ=0.88 (t, J=7.3 Hz, 3H, CH_3), 0.88–0.97 (m, 1H), 1.18–1.34 (m, 2H), 1.73–1.79 (m, 1H), 2.48 (dd, J=12.8, 16.9 Hz, 1H, 2-H^a), 2.76 (dd, J=7.7, 16.9 Hz, 1H, 2-H^b), 2.82–2.89 (m, 1H, 1-H), 7.30–7.34 (m, 1H), 7.36–7.40 (m, 2H), 7.44–7.47 (m, 2H), 7.59 (dt, J=1.0, 7.7 Hz, 1H), 7.72 (d, J=7.8 Hz, 1H), 7.77 (dt, J=1.1, 7.6 Hz, 1H), 7.89 (d, J=7.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=14.1, 21.2, 34.2, 38.5, 47.2 (C-1), 75.0 (C-9b), 122.3, 124.1, 126.6 (2C), 128.7, 128.9 (2C), 130.2, 133.9, 136.0 (C_q), 136.4 (C_q), 141.9 (C_q), 170.5 (C-3); IR (thin film): $\tilde{\nu}$=3062, 2959, 2931, 2872, 1747 s, 1597, 1583, 1496, 1466, 1451, 1419, 1346 s, 1312, 1244 s, 1206, 1179 s, 1140, 1100, 1080, 1065, 1033, 965, 938, 834, 767, 735, 700, 663, 632; HRMS (ESI): *m/z*: calcd for $C_{19}H_{19}NNaO_3S$: 364.0983; found: 364.0993 [M+Na]$^+$.

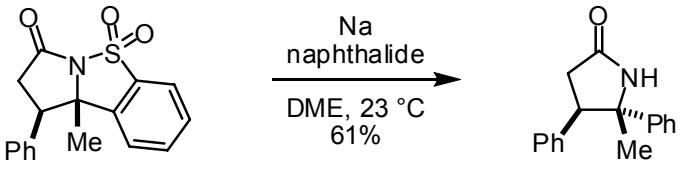


***rac*-(*1R*,9bS**)-1-Methyl-9b-phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 2, entry 7). Prepared according to the General Procedure using 2.0 equiv enal and 5 mol % catalyst **1** as a colorless solid in 78% yield. R_f=0.25 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. dec. >250°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=1.11 (d, J=6.8 Hz, 3H, CH_3), 2.49 (dd, J=12.9, 17.0 Hz, 1H, 2-H^a), 2.69 (dd, J=7.6, 17.0 Hz, 1H, 2-H^a), 2.95–3.03 (m, 1H, 1-H), 7.34–7.36 (m, 1H), 7.41 (t, J=8.0 Hz, 2H), 7.47–7.50 (m, 2H), 7.60 (t, J=7.8 Hz, 1H), 7.74–7.78 (m, 2H), 7.86 (d, J=7.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=16.5 (CH_3), 40.4, 42.3, 75.2 (C-9b), 122.3, 123.9, 126.6 (2C), 128.7, 129.0 (2C), 130.1, 133.8, 135.4 (C_q), 136.4 (C_q), 141.9 (C_q), 170.4 (C-3); IR (thin film): $\tilde{\nu}$=2981, 2887, 1745 s, 1599, 1496, 1468, 1450, 1419, 1387, 1342 s, 1244, 1219, 1176 s, 1141, 1100, 1081, 1063, 1032, 1000, 961, 952, 836, 769, 755, 733, 700, 674, 656; HRMS (ESI): *m/z*: calcd for $C_{17}H_{16}NO_3S$: 314.0851; found: 314.0849 [M+H]$^+$.



***rac*-9b-Phenyl-1,2-dihydrobenzo[*d*]pyrrolo[1,2-*b*]isothiazol-3-one 5,5-dioxide** (table 2, entry 8). Prepared according to the General Procedure using 5 mol % catalyst **1** and initially 1.5 equiv of enal. An additional portion (1.5 equiv) of enal was added after 6.5 h, which drove the reaction to completion within 21 h total reaction time. The product was obtained as a colorless solid in 80% yield. R_f=0.16 (hexanes/CH_2Cl_2/acetone 25:50:1); m.p. 176–177°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=2.60–2.74 (m, 3H), 3.11–3.16 (m, 1H), 7.34 (t, *J*=7.3 Hz, 1H), 7.42 (t, *J*=7.3 Hz, 2H), 7.54 (dt, *J*=0.9, 7.9 Hz, 1H), 7.59 (d, *J*=7.9 Hz, 1H), 7.66 (dt, *J*=1.1, 7.8 Hz, 1H), 7.69–7.72 (m, 2H), 7.75 (d, *J*=7.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=33.5 (CH_2), 37.0 (CH_2), 74.1 (C-9b), 122.2, 123.9, 125.3 (2C), 128.8, 129.4 (2C), 130.2, 134.5, 134.6 (C_q), 140.1 (C_q), 141.6 (C_q), 171.8 (C-3); IR (thin film): $\tilde{\nu}$=3062, 2925, 1752 s, 1493, 1468, 1451, 1341 s, 1288, 1252, 1228 s, 1181 s, 1160, 1140, 1100, 1066, 961, 766, 733, 699, 659, 630, 608; HRMS (ESI): *m/z*: calcd for $C_{16}H_{14}NO_3S$: 300.0694; found: 300.0681 $[M+H]^+$.

Deprotection of the Annulation Product.



S5

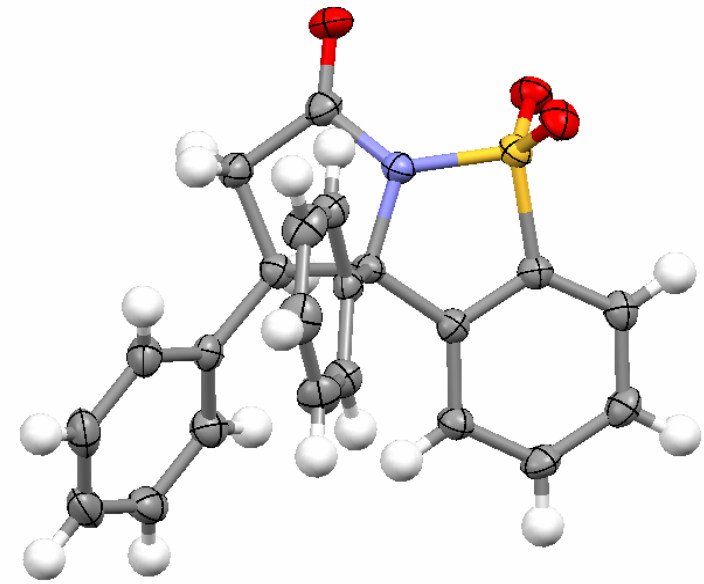
***rac*-(*4R*,5S**)-5-Methyl-4,5-diphenylpyrrolidin-2-one** (eq 2). Sodium metal (138 mg, 6.0 mmol) was weighed in hexanes and added to a solution of naphthalene (846 mg, 6.6 mmol) in dry DME (20 mL). It was stirred for 4 h at 23 °C during which the metal slowly dissolved to give a 0.3 M solution of sodium naphthalide.

The reagent solution (1.5 mL, 0.45 mmol, 6.0 equiv) was transferred with a syringe into a Schlenk flask, diluted with DME (1 mL) and the solid lactam **S5** (23.5 mg, 0.075 mmol, 1.0 equiv) was added in one portion. After 90 seconds the reaction was quenched with 5% aqueous NaH_2PO_4 (3 mL) and extracted with EtOAc (3 x 10 mL). The combined organic layers were washed with brine (10 mL) and dried with $MgSO_4$. The solvents were evaporated and the

residue was purified by column chromatography (3 g silica gel, hexanes/acetone 3:1→1.5:1 v/v) to give the product (11.4 mg, 61%) as a colorless solid. R_f=0.28 (hexanes/acetone 2:1); m.p. 178–179°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ=1.28 (s, 3H), 2.72 (dd, J=8.3, 16.9 Hz, 1H, 3-H^a), 2.85 (dd, J=9.4, 17.0 Hz, 1H, 3-H^b), 3.65 (t, J=8.9 Hz, 1H, 4-H), 6.02 (s, br, 1H, NH), 7.01–7.04 (m, 2H), 7.27–7.32 (m, 3H), 7.32–7.36 (m, 3H), 7.37–7.41 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ=23.6 (CH_3), 35.8 (C-3), 54.2 (C-4), 65.0 (C-5), 125.5 (2C), 127.67, 127.69, 128.51 (2C), 128.53 (2C), 128.8 (2C), 137.6 (C_q), 145.7 (C_q), 176.5 (C-2); IR (thin film): $\tilde{\nu}$=3209, 3086, 3061, 3030, 2972, 2931, 2872, 1693 s, 1601, 1583, 1496, 1454, 1446, 1420, 1378, 1359, 1305, 1282, 1252, 1228, 1186, 1155, 1145, 1082, 1073, 1028, 909, 768, 759, 733, 729, 721, 698 s , 651; HRMS (ESI): *m/z*: calcd for $C_{17}H_{17}NNaO$: 274.1208; found: 274.1211 $[M+Na]^+$.

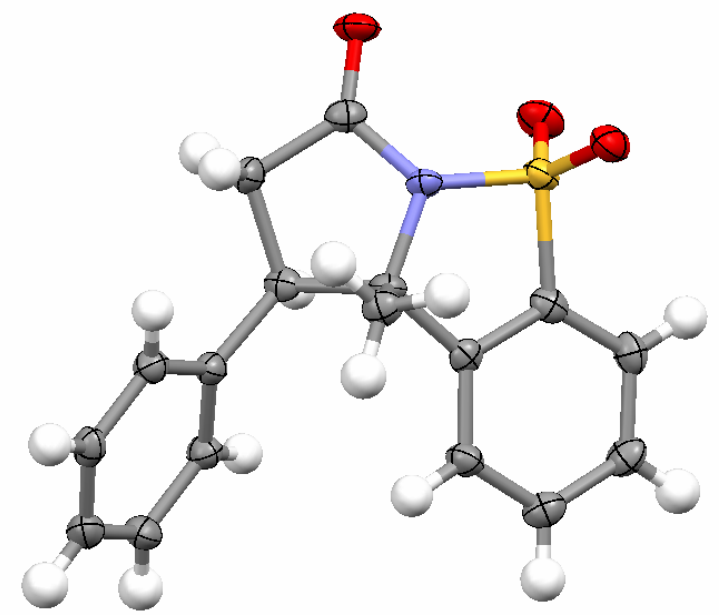
Determination of the relative configuration by x-ray analysis.

The relative configuration of two γ-lactam compounds was determined by x-ray crystallography (figure S-1 and S-2). The configuration of the other reaction products were assigned by analogy according to the specific ^{1}H NMR signals of the lactam methylene and methine protons. See the corresponding CIF files for further information.



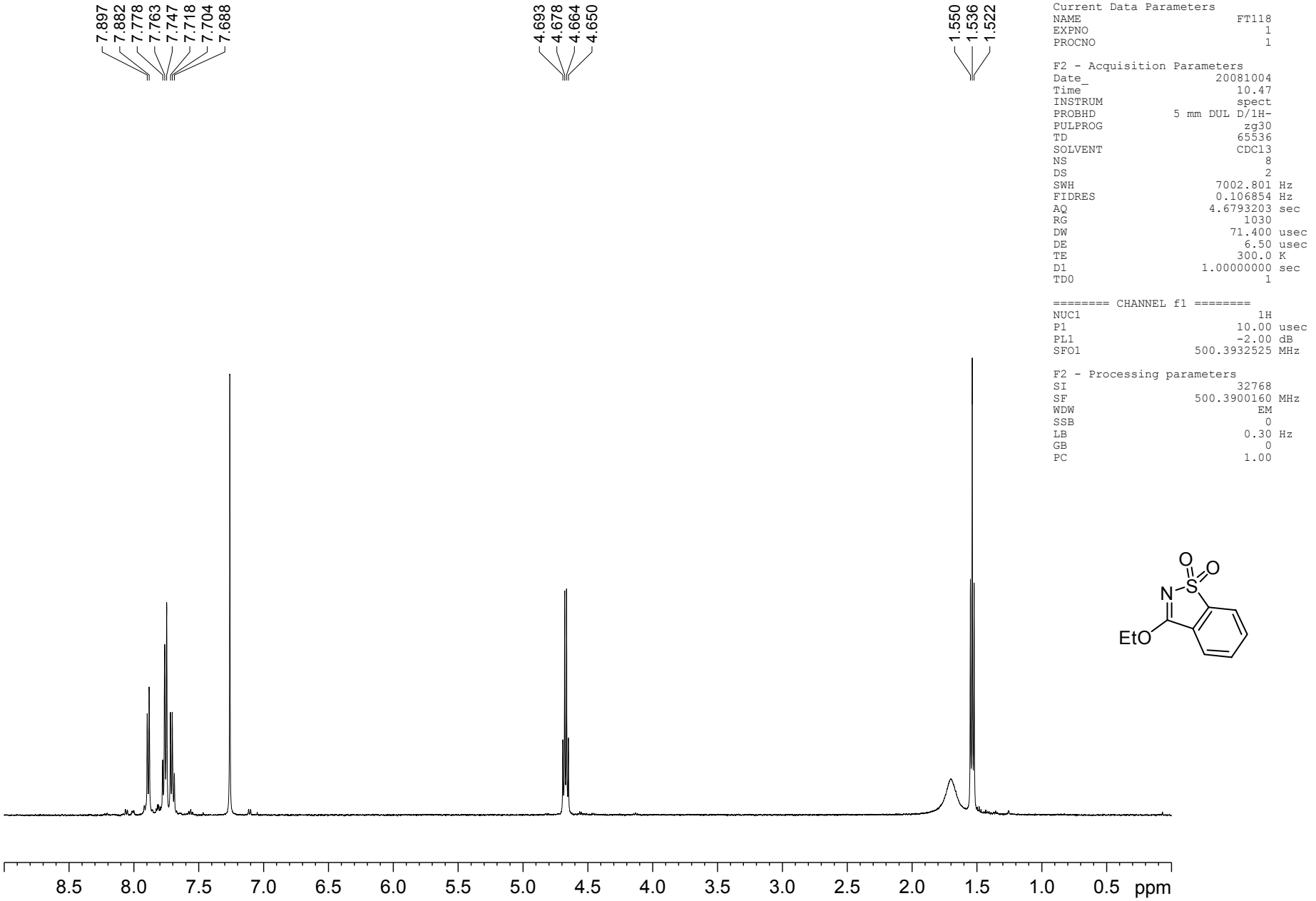
Crystal Data: $C_{17}H_{15}NSO_3$, M = 313.37, orthorhombic, $P2_12_12_1$, a = 7.2823(5) Å, b = 8.0024(6) Å, c = 24.632(2) Å, V = 1435.4(2) Å^3, Z = 4, D_{calcd} = 1.450 g/cm^3, 9538 collected reflections, 9538 unique (R_{int} = 0.0000), R_1 = 0.0480, wR_2 = 0.1215 (for all unique).

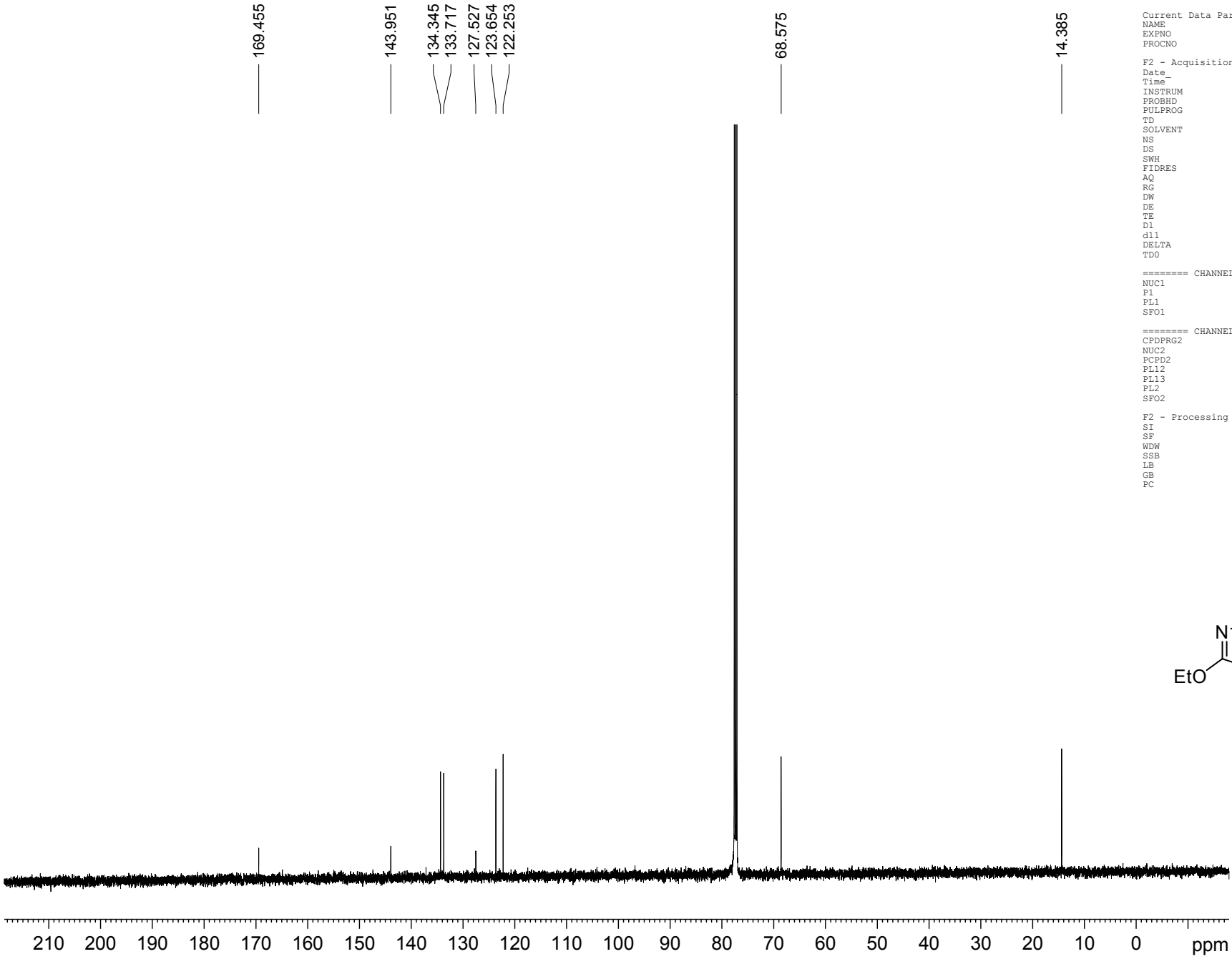
Figure S-1. ORTEP representation of the diphenyl substituted γ-lactam (table 1, entry 1).



Crystal Data: $C_{22}H_{17}NSO_3$, M = 375.44, monoclinic, $P2_1/c$, a = 16.6026(13) Å, b = 17.9592(13) Å, c = 12.9034(10) Å, β = 108.505(2)°, V = 3648.5(5) Å^3, Z = 8, D_{calcd} = 1.367 g/cm^3, 23317 collected reflections, 6411 unique (R_{int} = 0.0311), R_1 = 0.0562, wR_2 = 0.1098 (for all unique).

Figure S-2. ORTEP representation of the methyl phenyl substituted γ-lactam (table 1, entry 10).


7.897
7.882
7.778
7.763
7.747
7.718
7.704
7.688
4.693
4.678
4.664
4.650
1.550
1.536
1.522
Current Data Parameters
NAME FT118
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20081004
Time 10.47
INSTRUM spect
PROBHD 5 mm DUL D/1H-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 1030
DW 71.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.00 dB
SFO1 500.3932525 MHz
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
S
EtO
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

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Current Data Parameters
NAME                         FT118
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PROCNO                           1

F2 - Acquisition Parameters
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PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                           1407
DS                              4
SWH                     29761.904 Hz
FIDRES                   0.454131 Hz
AQ                       1.1010548 sec
RG                            456
DW                         16.800 usec
DE                          6.50 usec
TE                          298.3 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                          13C
P1                         10.00 usec
PL1                         0.00 dB
SFO1                  125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                          1H
PCPD2                      60.00 usec
PL12                       13.56 dB
PL13                      120.00 dB
PL2                        -2.00 dB
SFO2                  500.3920016 MHz

F2 - Processing parameters
SI                            32768
SF                    125.8231236 MHz
WDW                              EM
SSB                               0
LB                             1.00 Hz
GB                                0
PC                             1.40
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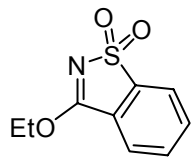

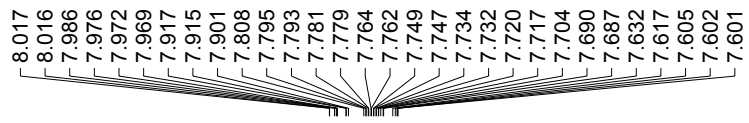

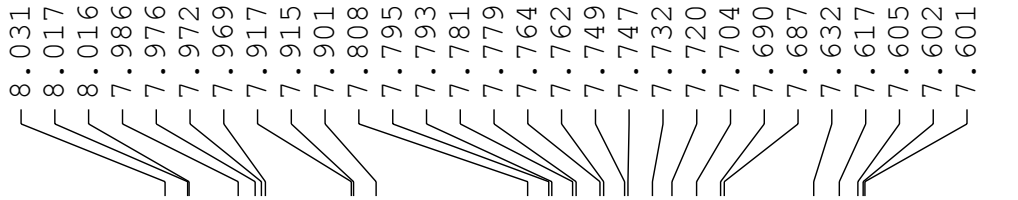

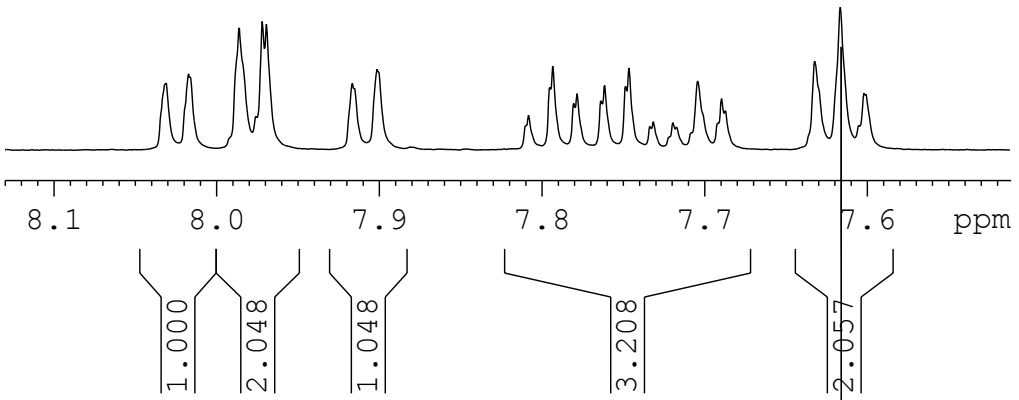


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NAME                         FT474
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PROCNO                           1

F2 - Acquisition Parameters
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Time                         18.16
INSTRUM                      spect
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PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                               8
DS                               2
SWH                    7002.801 Hz
FIDRES                 0.106854 Hz
AQ                     4.6793203 sec
RG                            1150
DW                       71.400 usec
DE                        6.50 usec
TE                         298.3 K
D1                    1.00000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                            1H
P1                         10.76 usec
PL1                         0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                           32768
SF                    500.3900169 MHz
WDW                             EM
SSB                              0
LB                            0.30 Hz
GB                               0
PC                            1.00
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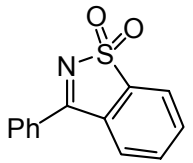
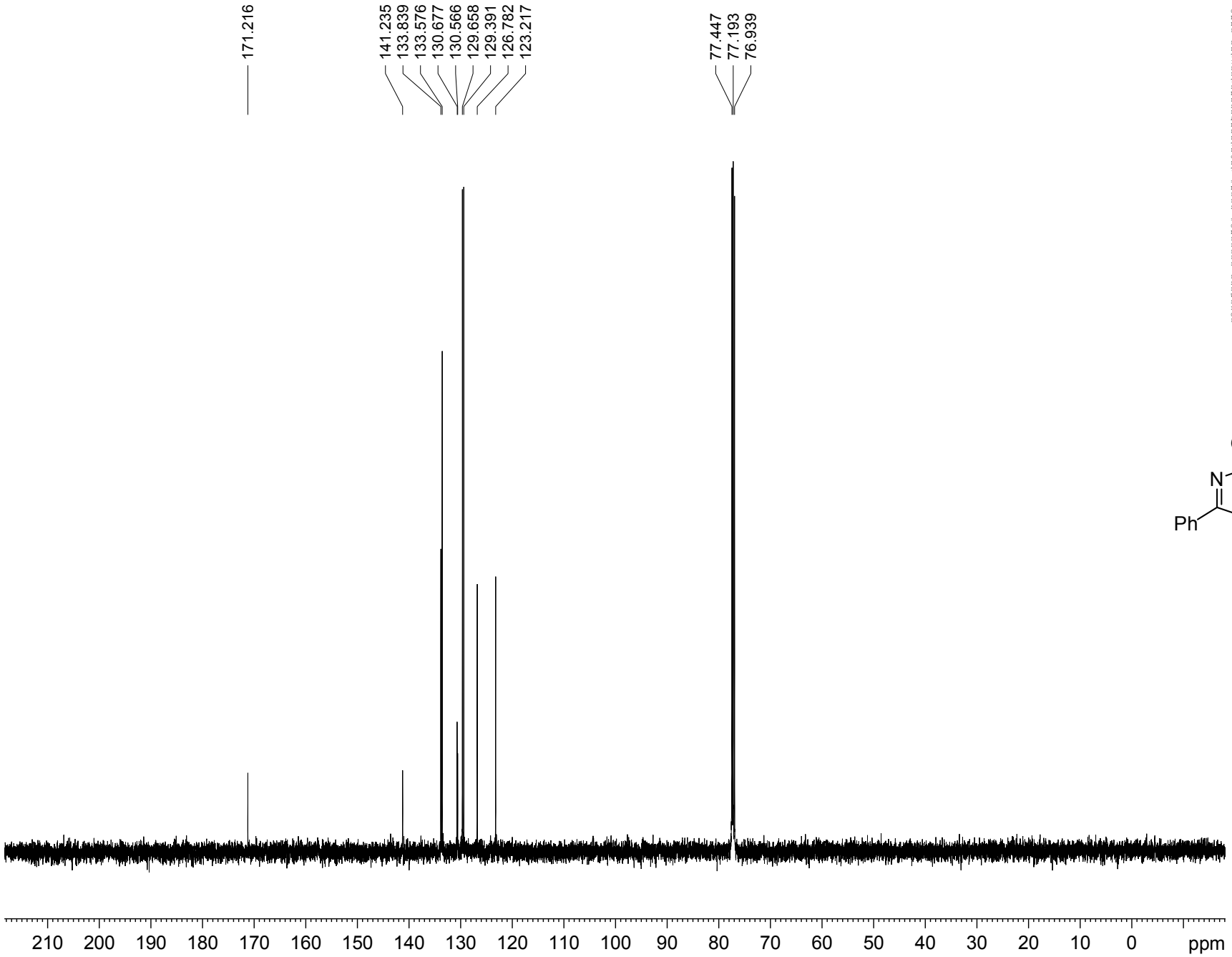
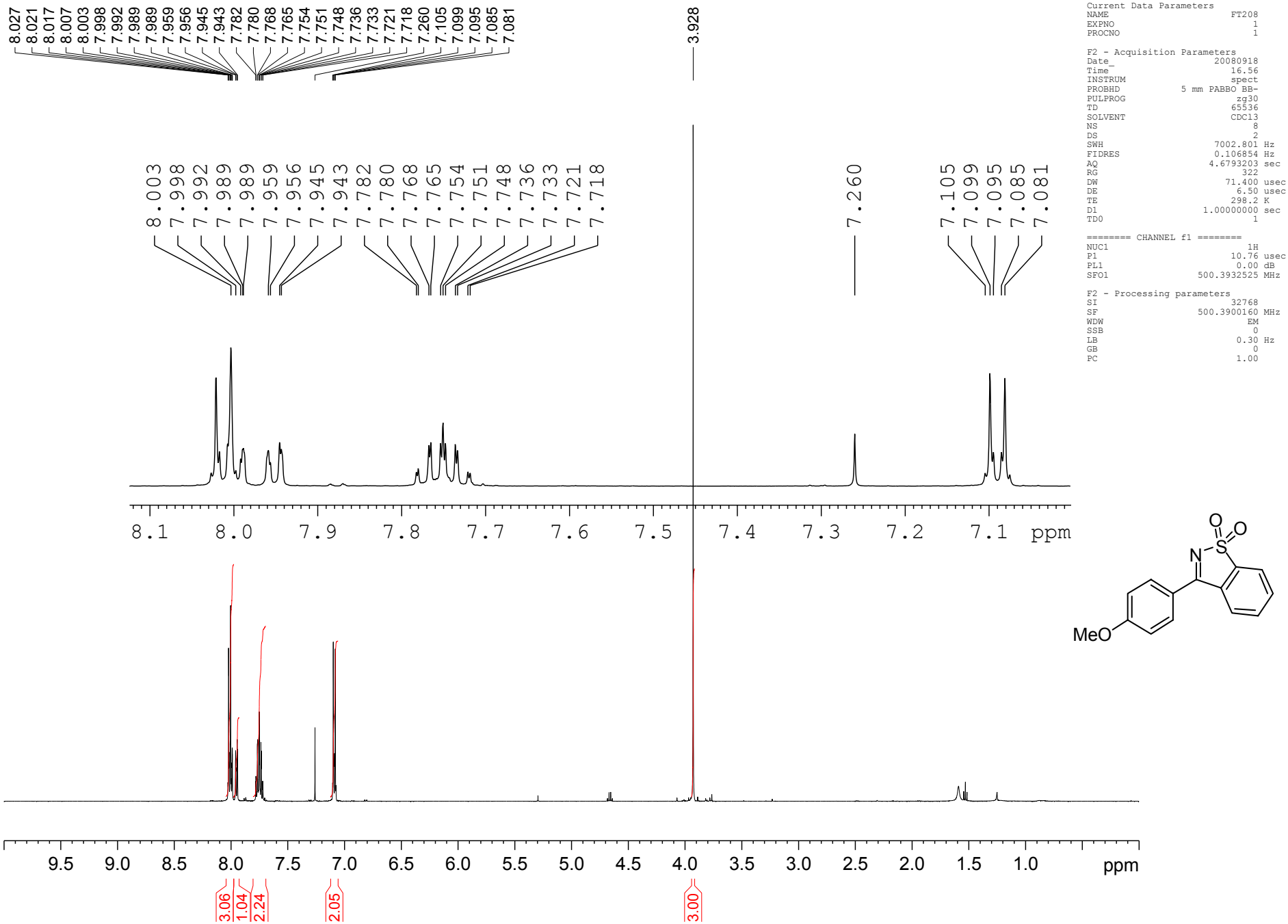



171.216
141.235
133.839
133.576
130.677
130.566
129.658
129.391
126.782
123.217
77.447
77.193
76.939
Current Data Parameters
NAME FT474
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date 20080929
Time 18.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 93
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
S
N
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm




```
Current Data Parameters
NAME                         FT208
EXPNO                            1
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20080918
Time_                        16.56
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                               8
DS                               2
SWH                   7002.801 Hz
FIDRES                0.106854 Hz
AQ                    4.6793203 sec
RG                             322
DW                      71.400 usec
DE                       6.50 usec
TE                       298.2 K
D1                    1.00000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                            1H
P1                      10.76 usec
PL1                      0.00 dB
SFO1                 500.3932525 MHz

F2 - Processing parameters
SI                           32768
SF                  500.3900160 MHz
WDW                             EM
SSB                              0
LB                       0.30 Hz
GB                               0
PC                            1.00
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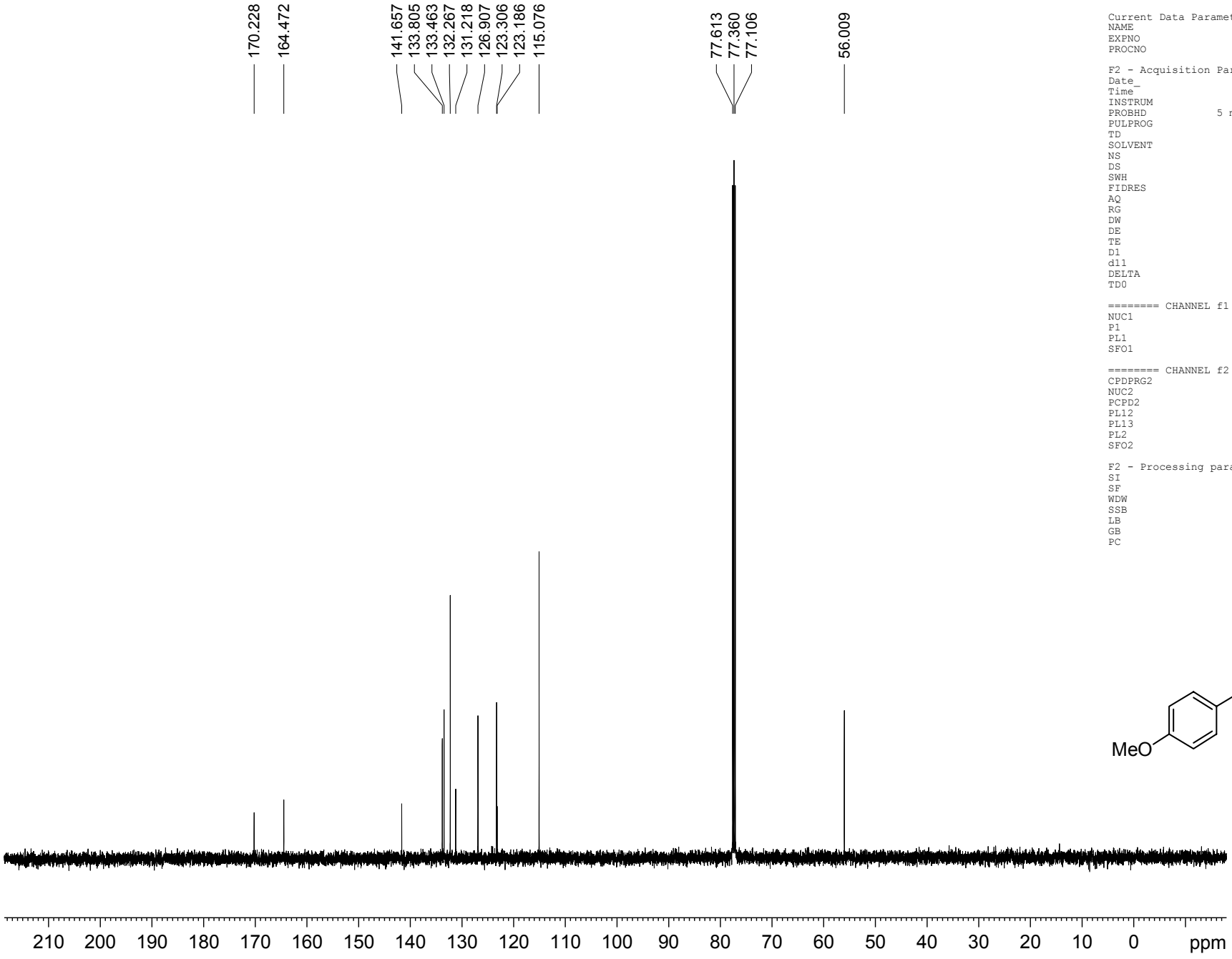


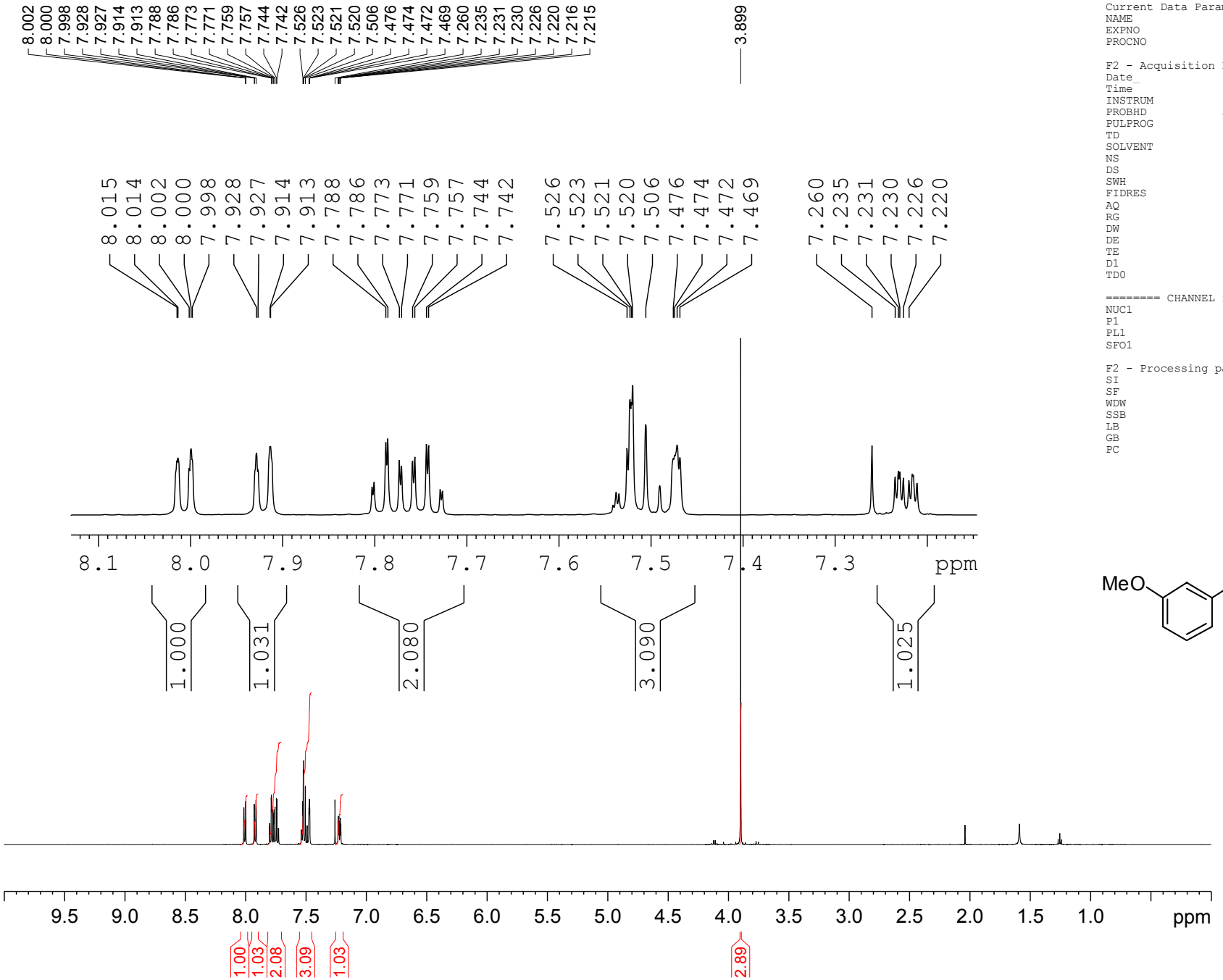

```
Current Data Parameters
NAME                                  FT208
EXPNO                                     2
PROCNO                                    1

F2 - Acquisition Parameters
Date_                              20080918
Time                                 17.02
INSTRUM                              spect
PROBHD                5 mm PABBO BB-
PULPROG                           zgpg30
TD                                 65536
SOLVENT                            CDC13
NS                                   107
DS                                     4
SWH                           29761.904 Hz
FIDRES                         0.454131 Hz
AQ                            1.1010548 sec
RG                                   456
DW                               16.800 usec
DE                                6.50 usec
TE                                298.9 K
D1                           2.00000000 sec
d11                          0.03000000 sec
DELTA                        1.89999998 sec
TD0                                    1

======== CHANNEL f1 ========
NUC1                                 13C
P1                                7.50 usec
PL1                               1.00 dB
SFO1                      125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                          waltz16
NUC2                                 1H
PCPD2                            80.00 usec
PL12                              17.43 dB
PL13                              18.43 dB
PL2                                0.00 dB
SFO2                      500.3920016 MHz

F2 - Processing parameters
SI                                 32768
SF                        125.8231264 MHz
WDW                                   EM
SSB                                    0
LB                                1.00 Hz
GB                                     0
PC                                 1.40
```

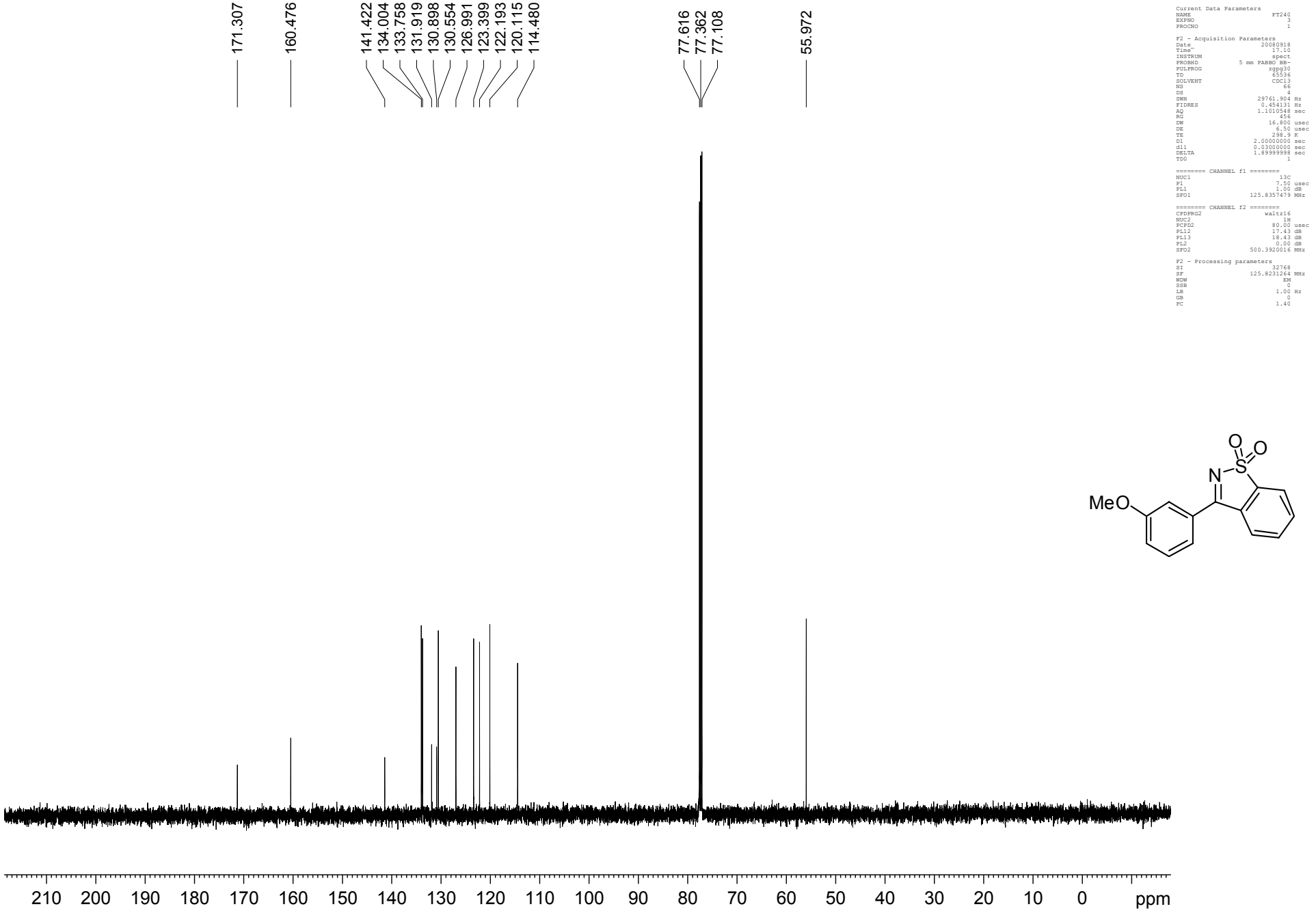



```
Current Data Parameters
NAME                         FT240
EXPNO                            2
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20080918
Time                         17.06
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                               8
DS                               2
SWH                    7002.801 Hz
FIDRES                 0.106854 Hz
AQ                     4.6793203 sec
RG                             287
DW                      71.400 usec
DE                       6.50 usec
TE                       298.3 K
D1                    1.00000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                            1H
P1                      10.76 usec
PL1                      0.00 dB
SFO1                 500.3932525 MHz

F2 - Processing parameters
SI                           32768
SF                   500.3900160 MHz
WDW                             EM
SSB                              0
LB                       0.30 Hz
GB                               0
PC                            1.00
```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134.004
133.758
131.919
130.898
130.554
126.991
123.399
122.193
120.115
114.480
77.616
77.362
77.108
55.972
Current Data Parameters
NAME FT240
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080918
Time 17.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 66
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231264 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
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S
MeO
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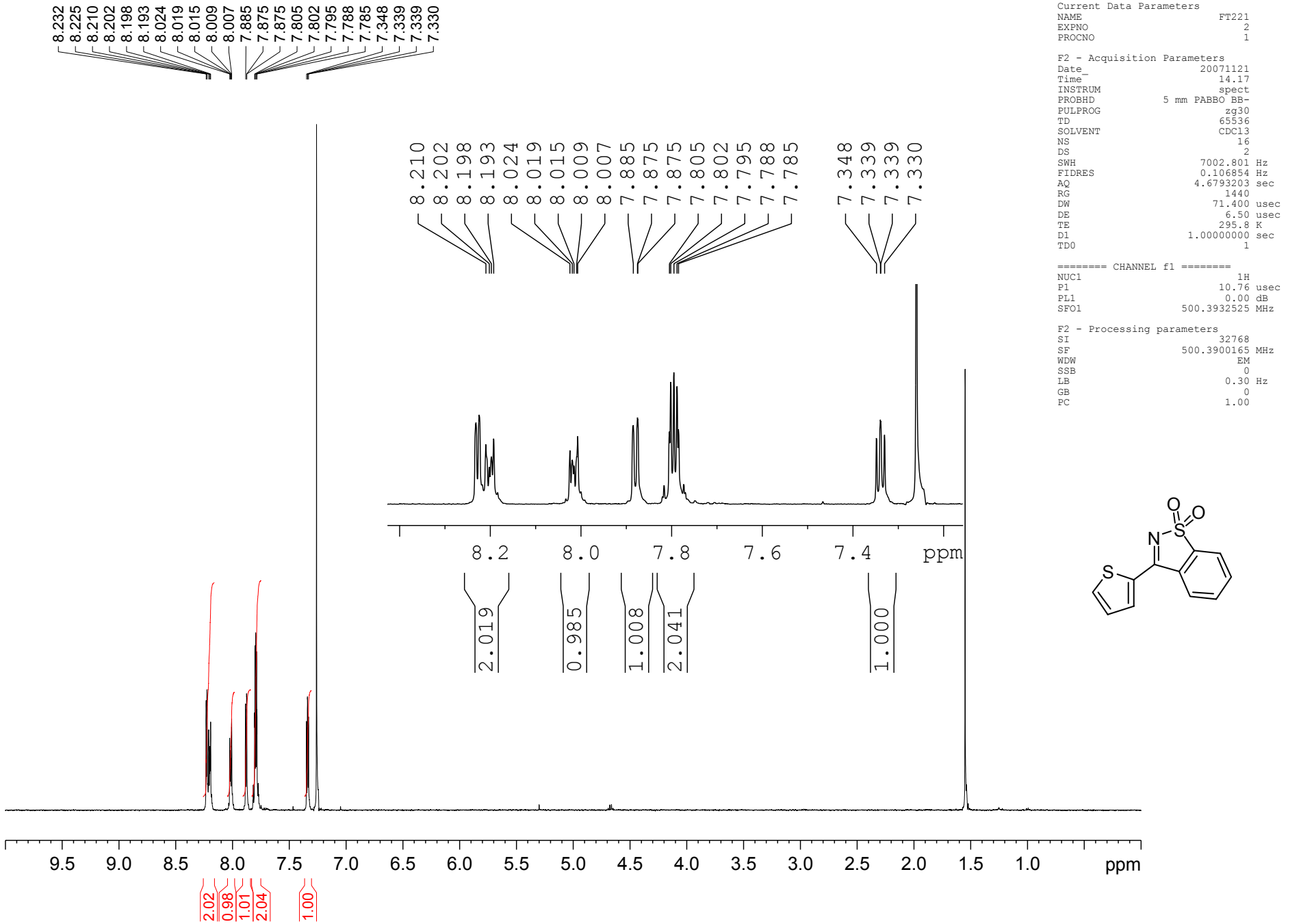


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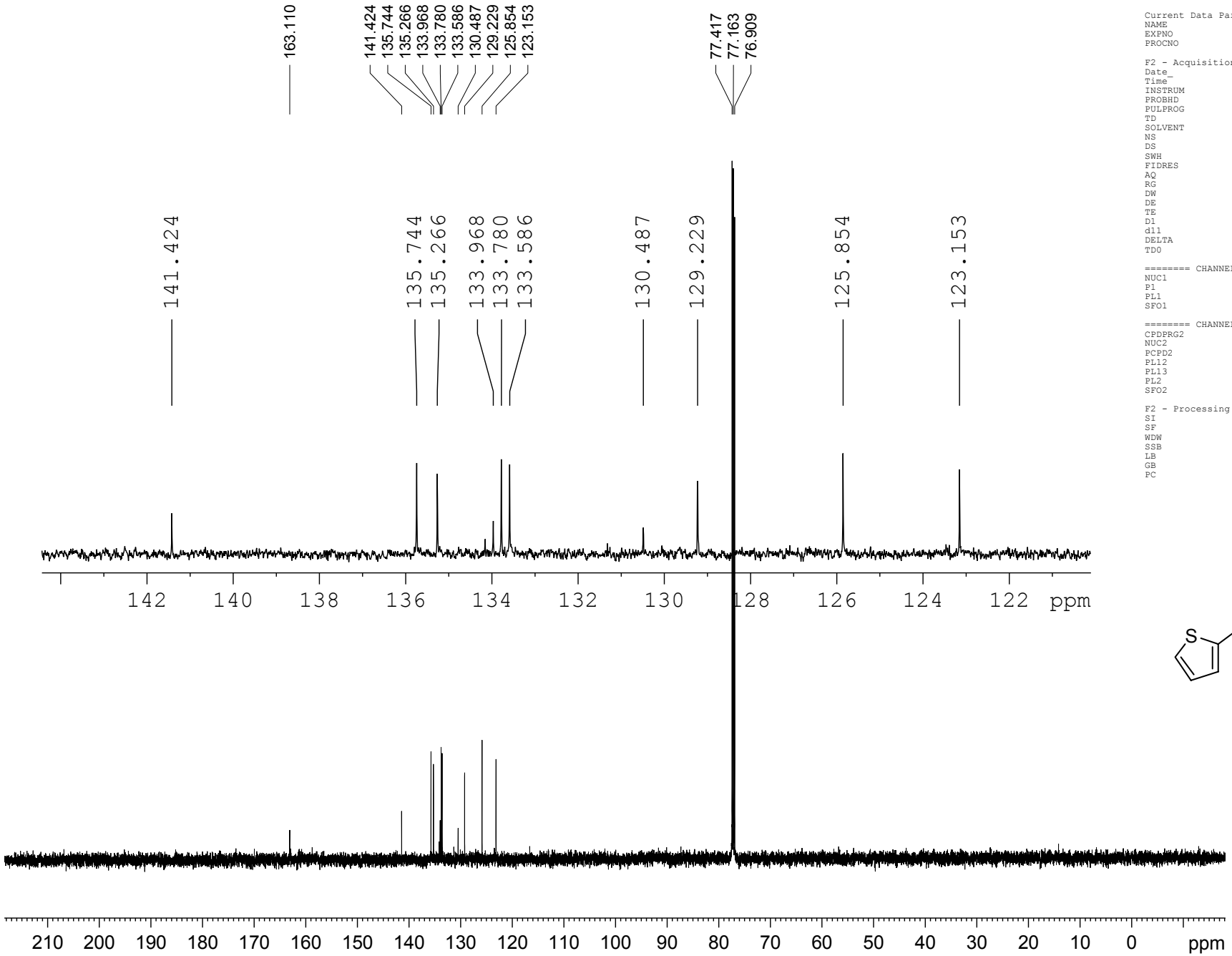
Current Data Parameters
NAME                         FT221
EXPNO                            2
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20071121
Time                         14.17
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                           1440
DW                       71.400 usec
DE                        6.50 usec
TE                         295.8 K
D1                    1.00000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                            1H
P1                       10.76 usec
PL1                       0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                           32768
SF                    500.3900165 MHz
WDW                             EM
SSB                              0
LB                        0.30 Hz
GB                               0
PC                            1.00
```

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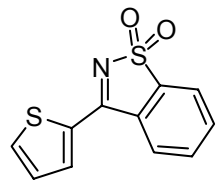
Current Data Parameters
NAME                         FT221
EXPNO                            4
PROCNO                           1

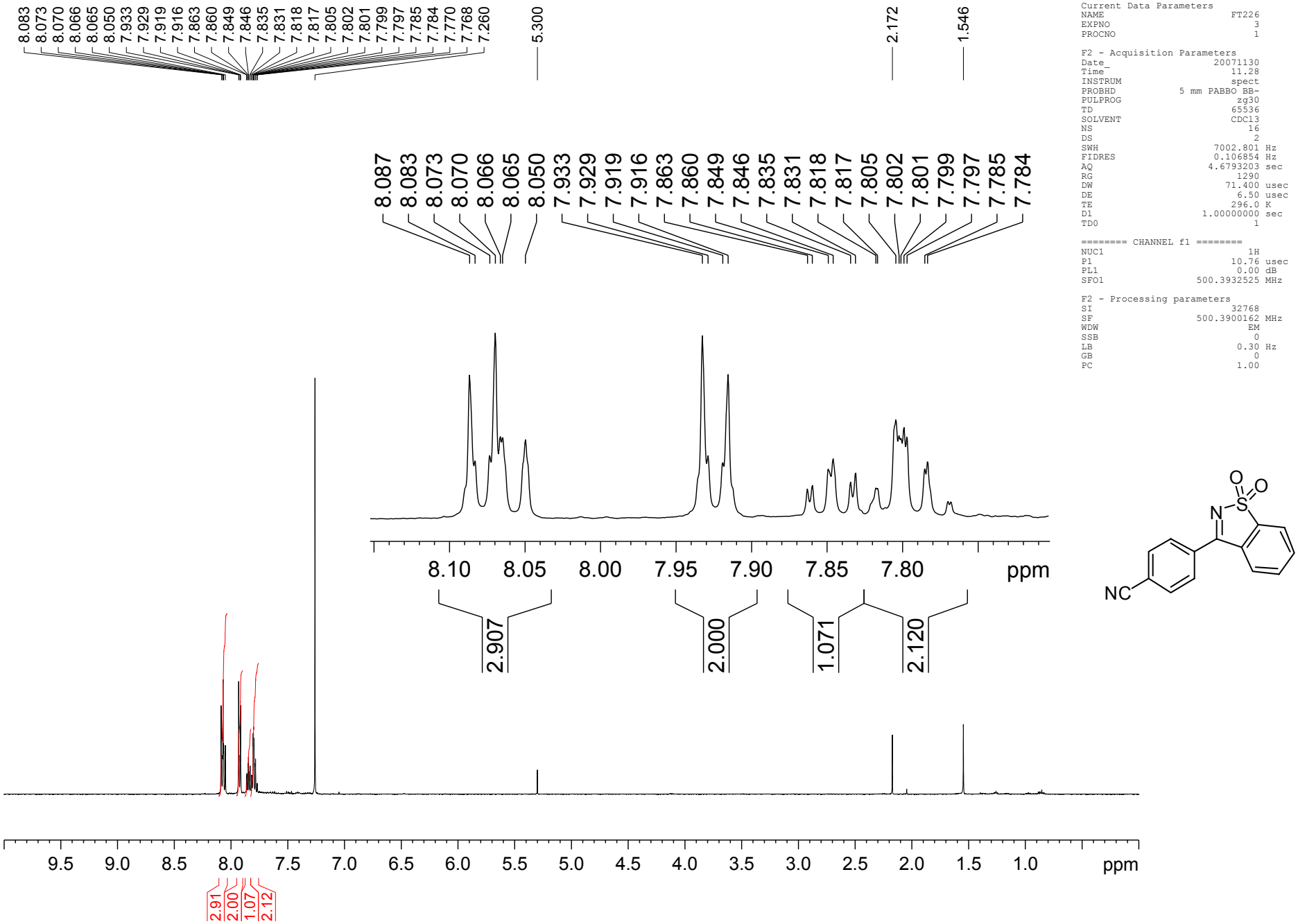
F2 - Acquisition Parameters
Date_                     20080918
Time                         17.21
INSTRUM                      spect
PROBHD            5 mm PABBO BB-
PULPROG                     zgpg30
TD                           65536
SOLVENT                      CDCl3
NS                             117
DS                               4
SWH                      29761.904 Hz
FIDRES                   0.454131 Hz
AQ                       1.1010548 sec
RG                             456
DW                        16.800 usec
DE                         6.50 usec
TE                         298.5 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                           13C
P1                        7.50 usec
PL1                       1.00 dB
SFO1                 125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                     80.00 usec
PL12                      17.43 dB
PL13                      18.43 dB
PL2                        0.00 dB
SFO2                 500.3920016 MHz

F2 - Processing parameters
SI                             32768
SF                   125.8231500 MHz
WDW                            EM
SSB                              0
LB                        1.00 Hz
GB                               0
PC                            1.40
```






```
Current Data Parameters
NAME                         FT226
EXPNO                            3
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20071130
Time                         11.28
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                           1290
DW                         71.400 usec
DE                          6.50 usec
TE                         296.0 K
D1                    1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                         10.76 usec
PL1                         0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                    500.3900162 MHz
WDW                            EM
SSB                             0
LB                          0.30 Hz
GB                              0
PC                           1.00
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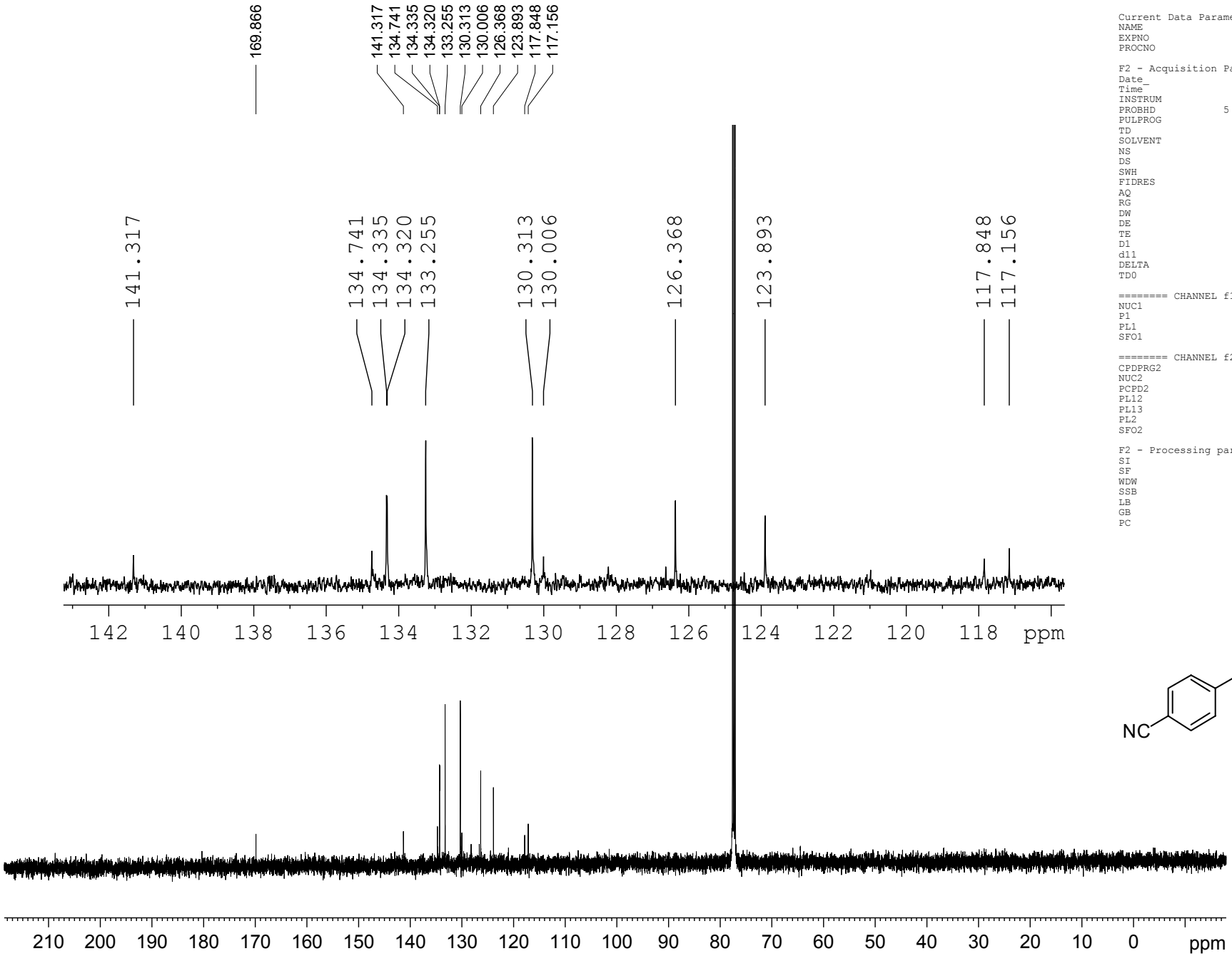


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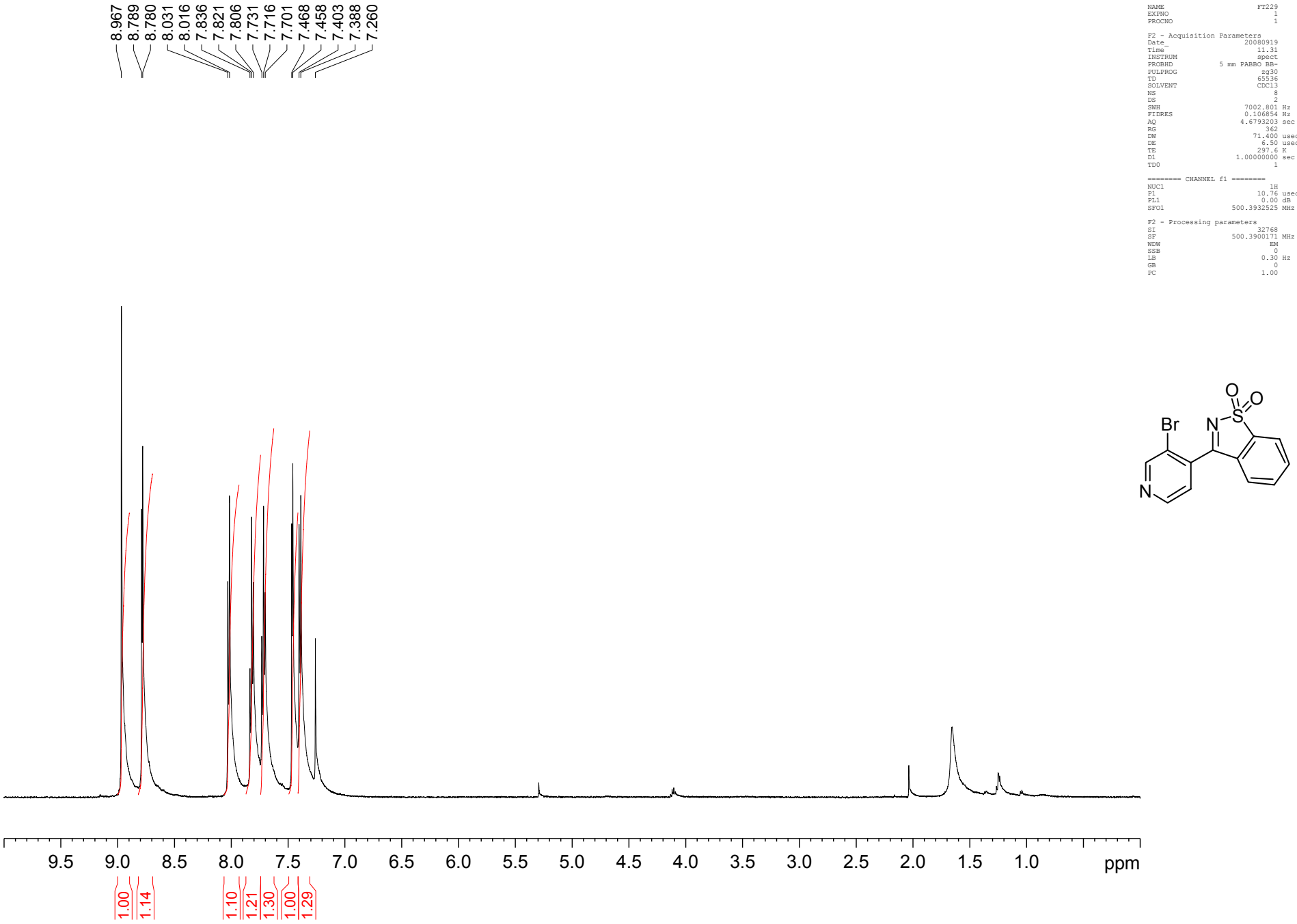
Current Data Parameters
NAME                         FT226
EXPNO                            6
PROCNO                           1

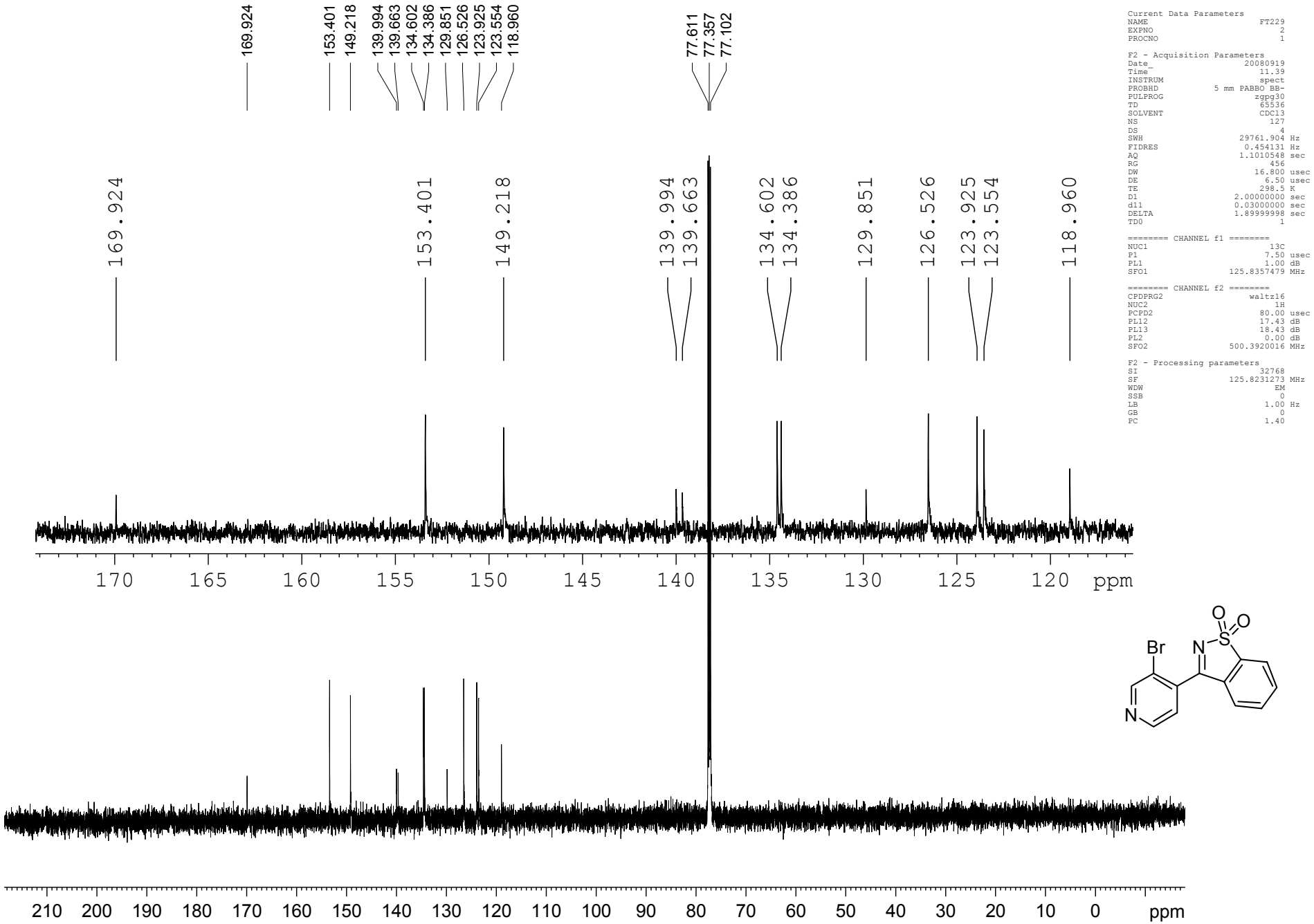
F2 - Acquisition Parameters
Date_                     20080930
Time                         15.14
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                            748
DS                              4
SWH                     29761.904 Hz
FIDRES                      0.454131 Hz
AQ                      1.1010548 sec
RG                           1030
DW                         16.800 usec
DE                          6.50 usec
TE                          298.4 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                             1

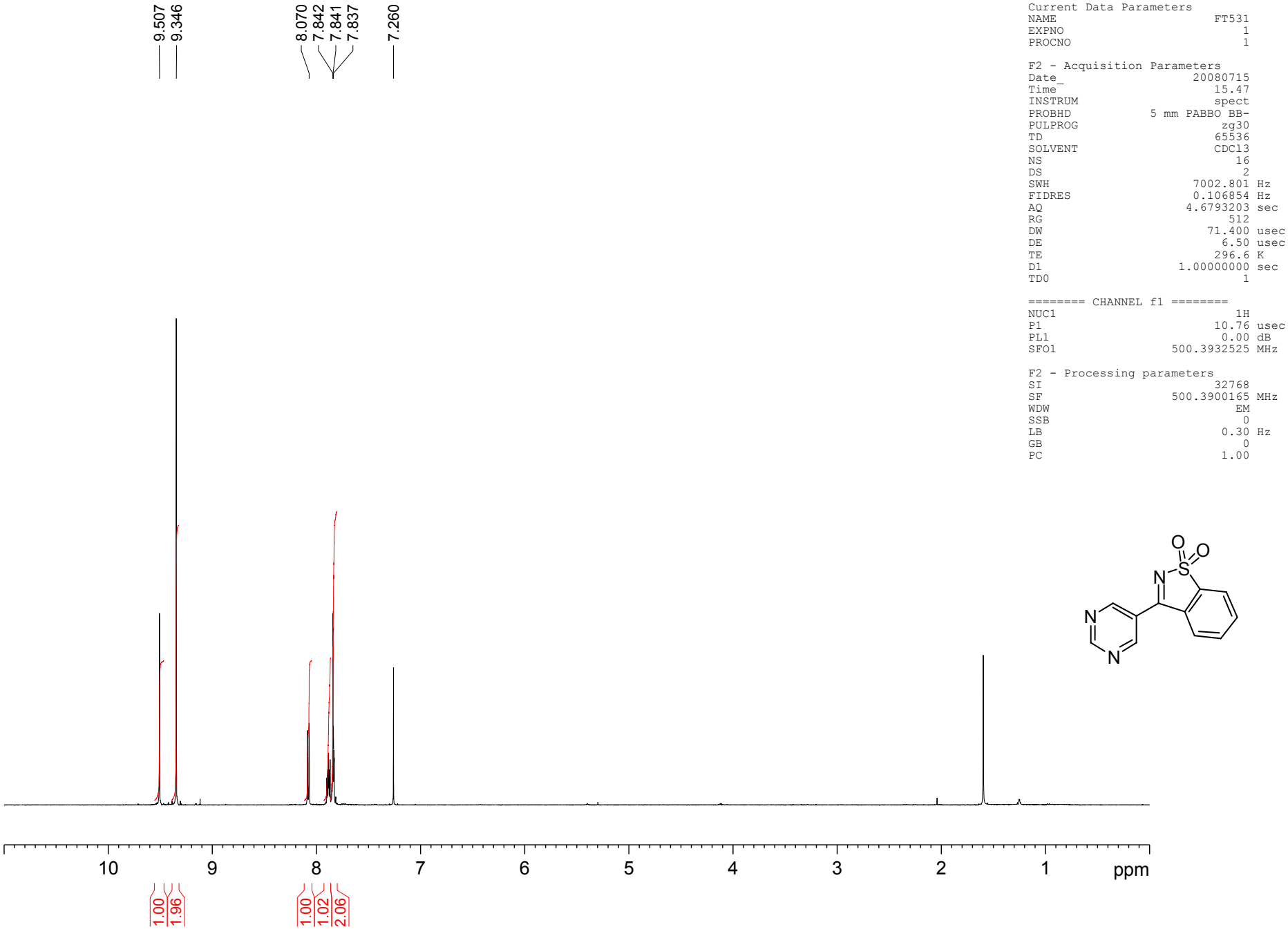
======== CHANNEL f1 ========
NUC1                          13C
P1                          7.50 usec
PL1                         1.00 dB
SFO1                125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL12                       17.43 dB
PL13                       18.43 dB
PL2                         0.00 dB
SFO2                500.3920016 MHz

F2 - Processing parameters
SI                           32768
SF                  125.8231246 MHz
WDW                             EM
SSB                              0
LB                          1.00 Hz
GB                               0
PC                          1.40
```


8.967
8.789
8.780
8.031
8.016
7.836
7.821
7.806
7.731
7.716
7.701
7.468
7.458
7.403
7.388
7.260
NAME FT229
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080919
Time_ 11.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 362
DW 71.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz
F2 - Processing parameters
SI 32768
SF 500.3900171 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
N
O
O
S
N
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.14
1.10
1.21
1.30
1.00
1.29


169.924
153.401
149.218
139.994
139.663
134.602
134.386
129.851
126.526
123.925
123.554
118.960
77.611
77.357
77.102
ppm
Br
N
O
O
S
N

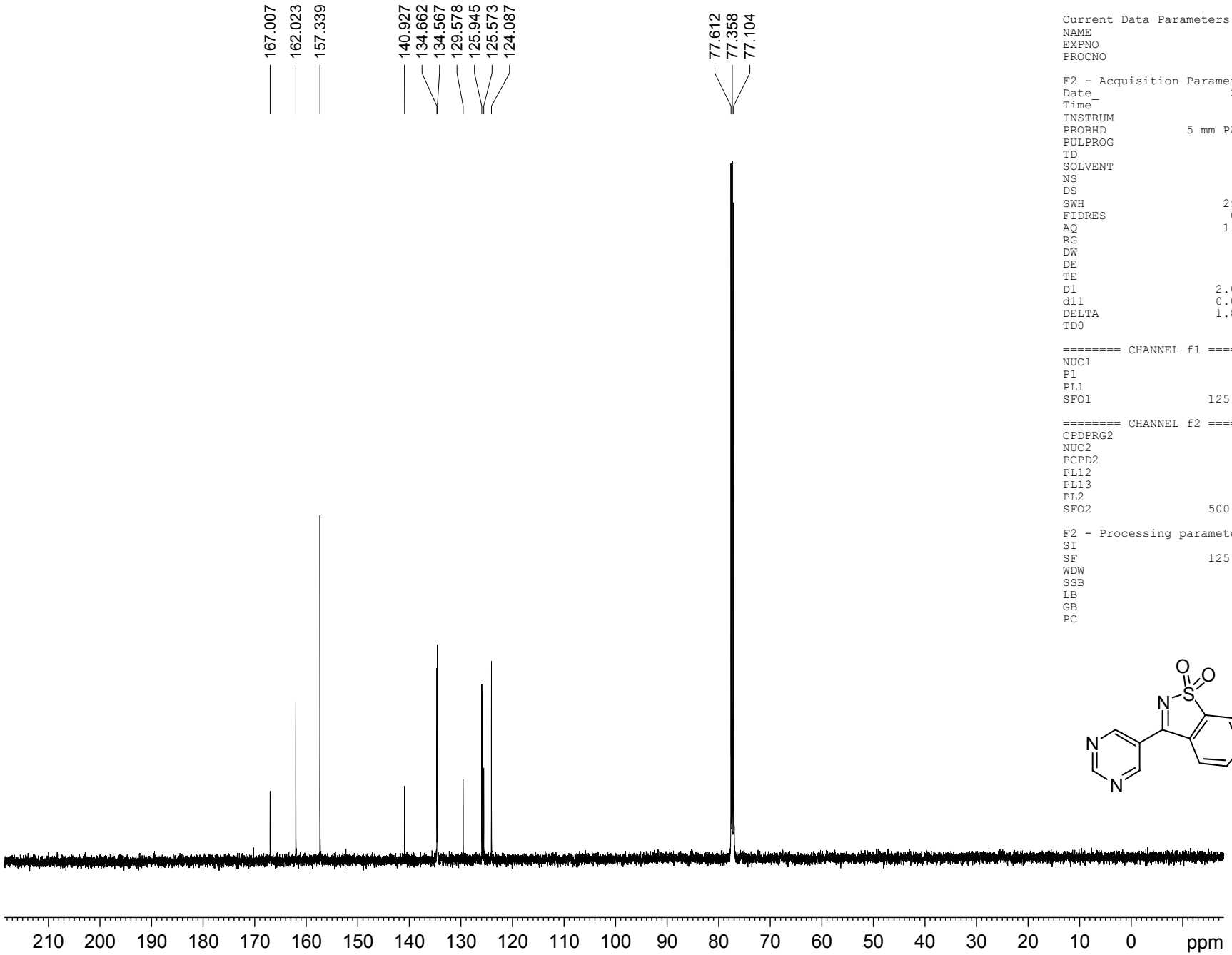



```
Current Data Parameters
NAME                         FT531
EXPNO                            1
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20080715
Time                         15.47
INSTRUM                      spect
PROBHD           5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDC13
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                            512
DW                       71.400 usec
DE                        6.50 usec
TE                        296.6 K
D1                     1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                       10.76 usec
PL1                       0.00 dB
SFO1                 500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                   500.3900165 MHz
WDW                            EM
SSB                             0
LB                        0.30 Hz
GB                              0
PC                           1.00
```



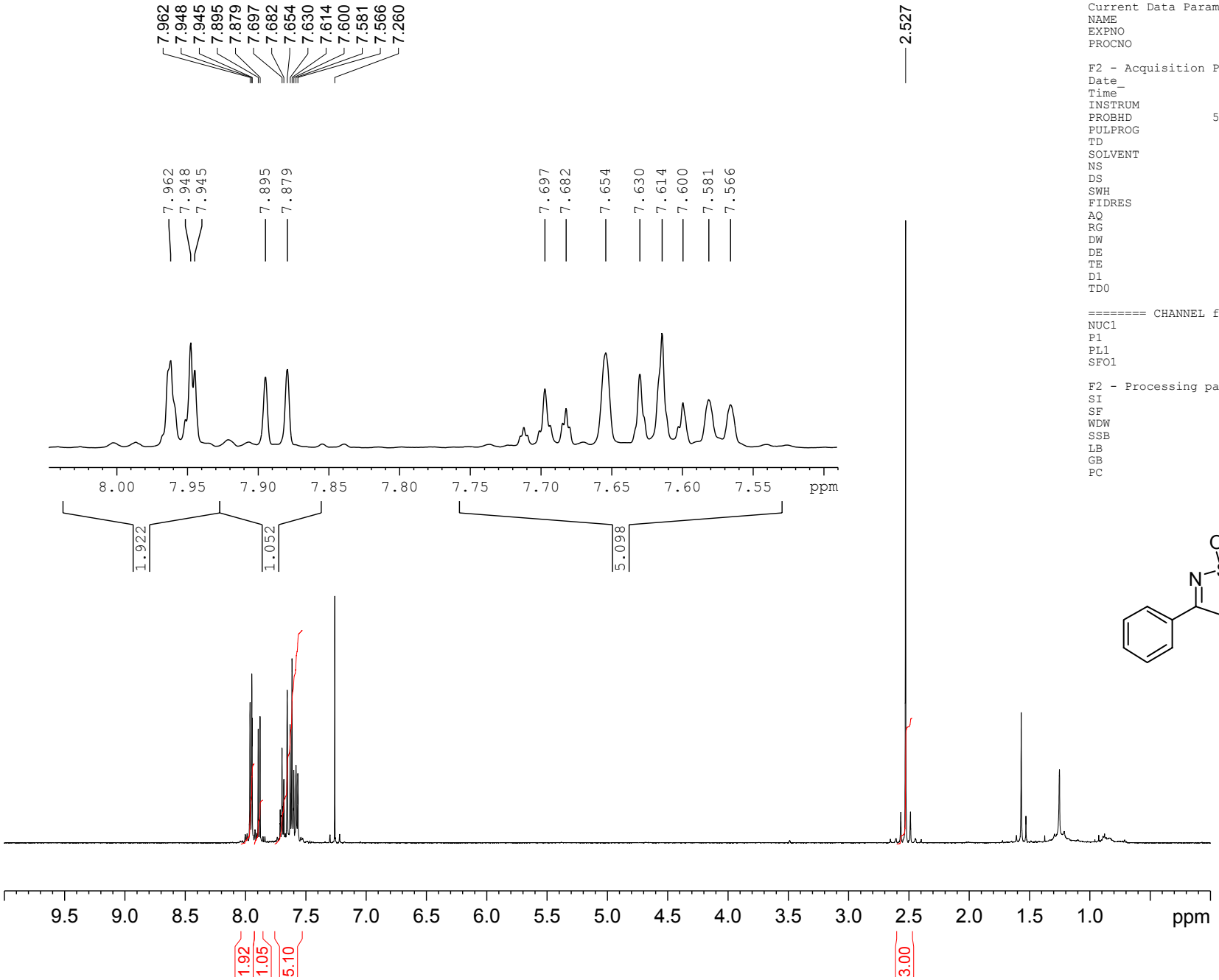

```
Current Data Parameters
NAME                          FT531
EXPNO                             3
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20080919
Time                          12.00
INSTRUM                       spect
PROBHD           5 mm PABBO BB-
PULPROG                    zgpg30
TD                          65536
SOLVENT                      CDCl3
NS                             297
DS                               4
SWH                      29761.904 Hz
FIDRES                       0.454131 Hz
AQ                           1.1010548 sec
RG                             456
DW                            16.800 usec
DE                             6.50 usec
TE                            298.7 K
D1                           2.00000000 sec
d11                          0.03000000 sec
DELTA                        1.89999998 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                            13C
P1                             7.50 usec
PL1                            1.00 dB
SFO1                   125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                    waltz16
NUC2                            1H
PCPD2                         80.00 usec
PL12                          17.43 dB
PL13                          18.43 dB
PL2                            0.00 dB
SFO2                   500.3920016 MHz

F2 - Processing parameters
SI                             32768
SF                     125.8231273 MHz
WDW                               EM
SSB                               0
LB                             1.00 Hz
GB                                0
PC                             1.40
```

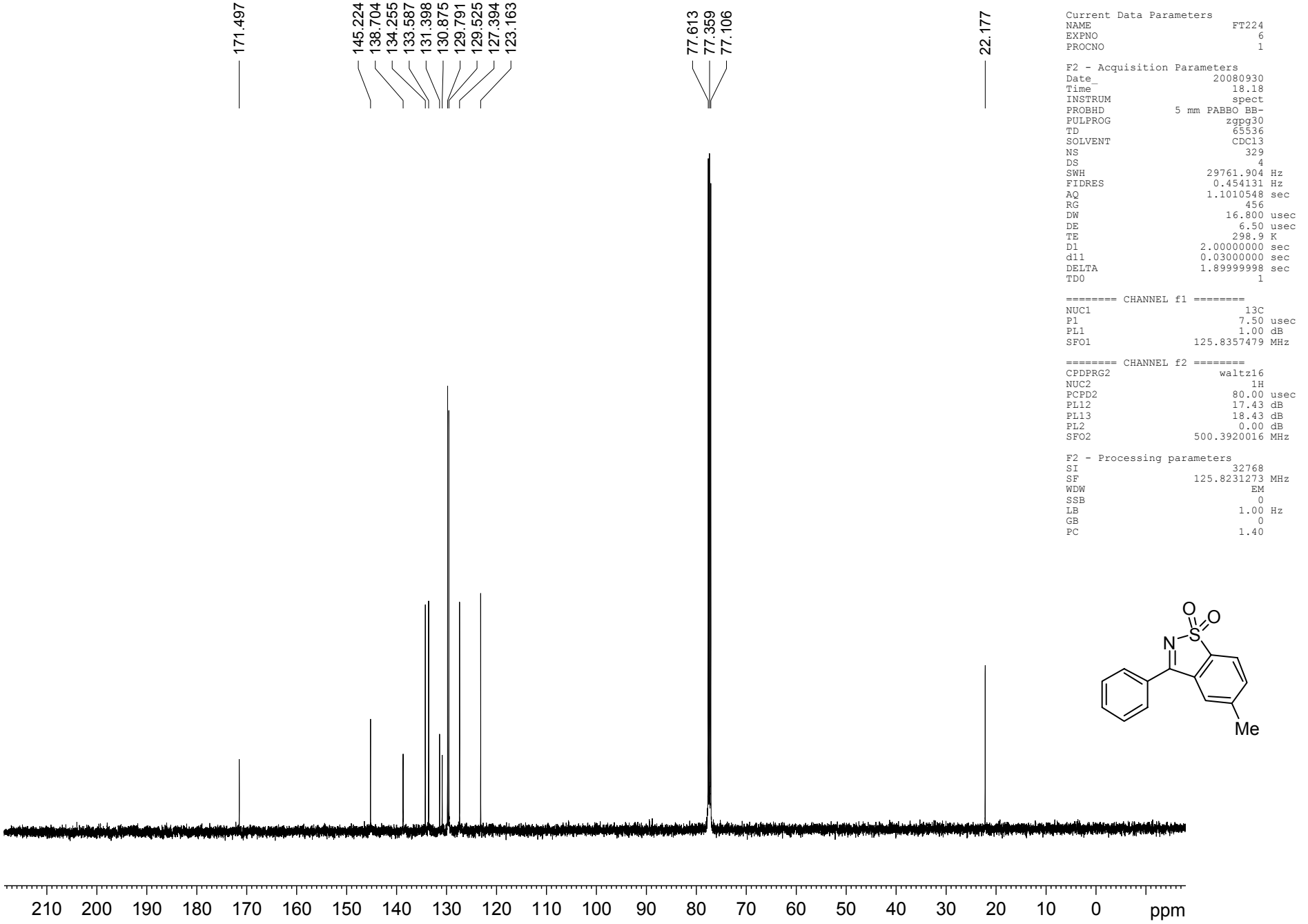


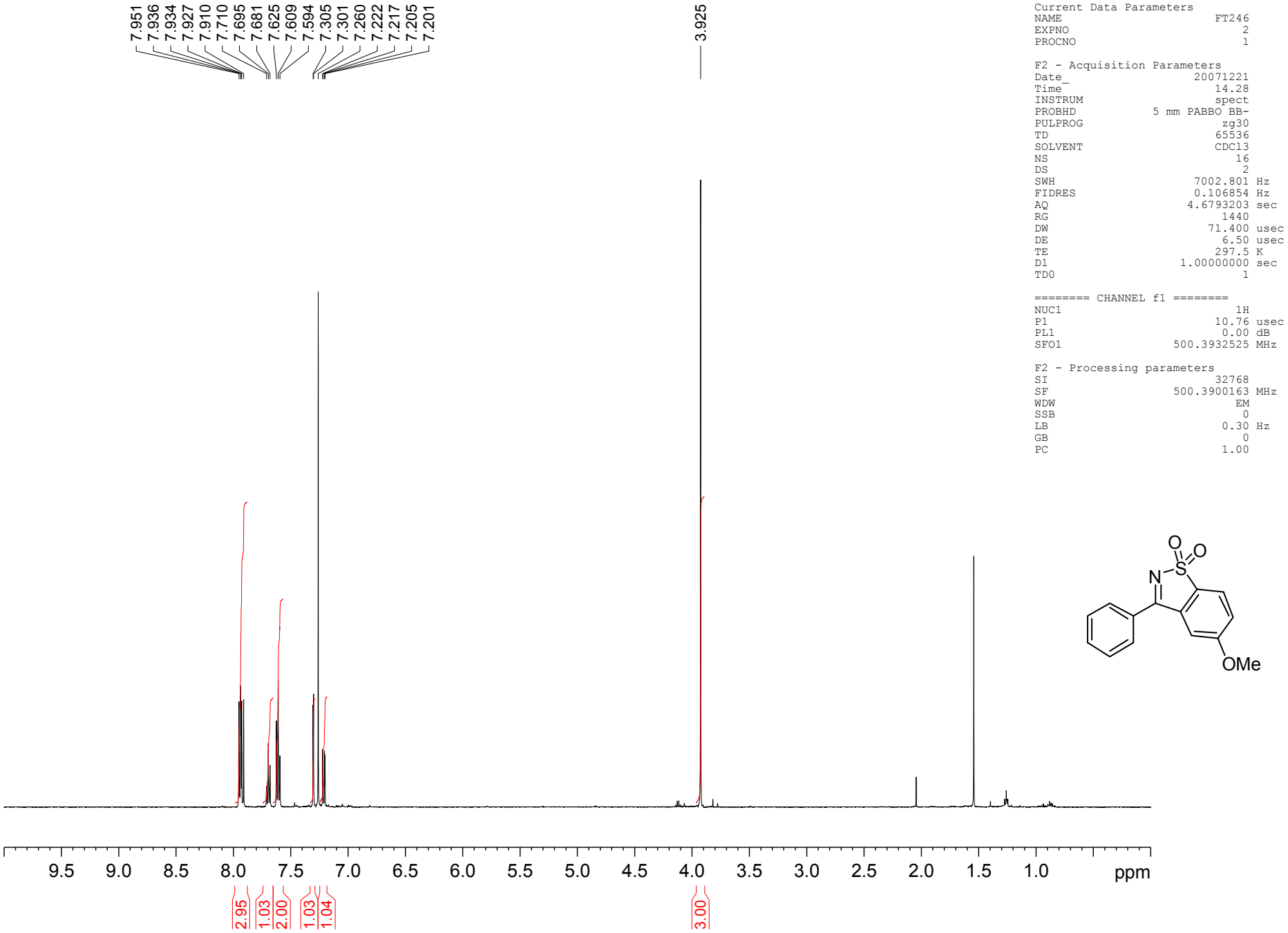

```
Current Data Parameters
NAME                         FT224
EXPNO                            3
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20071126
Time                         11.13
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                               8
DS                               2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                     4.6793203 sec
RG                             456
DW                      71.400 usec
DE                       6.50 usec
TE                       295.4 K
D1                   1.00000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                            1H
P1                       10.76 usec
PL1                       0.00 dB
SFO1                 500.3932525 MHz

F2 - Processing parameters
SI                           32768
SF                   500.3900162 MHz
WDW                             EM
SSB                              0
LB                        0.30 Hz
GB                               0
PC                            1.00
```


171.497
145.224
138.704
134.255
133.587
131.398
130.875
129.791
129.525
127.394
123.163
77.613
77.359
77.106
22.177
Current Data Parameters
NAME FT224
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080930
Time 18.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 329
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231273 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
N
S
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

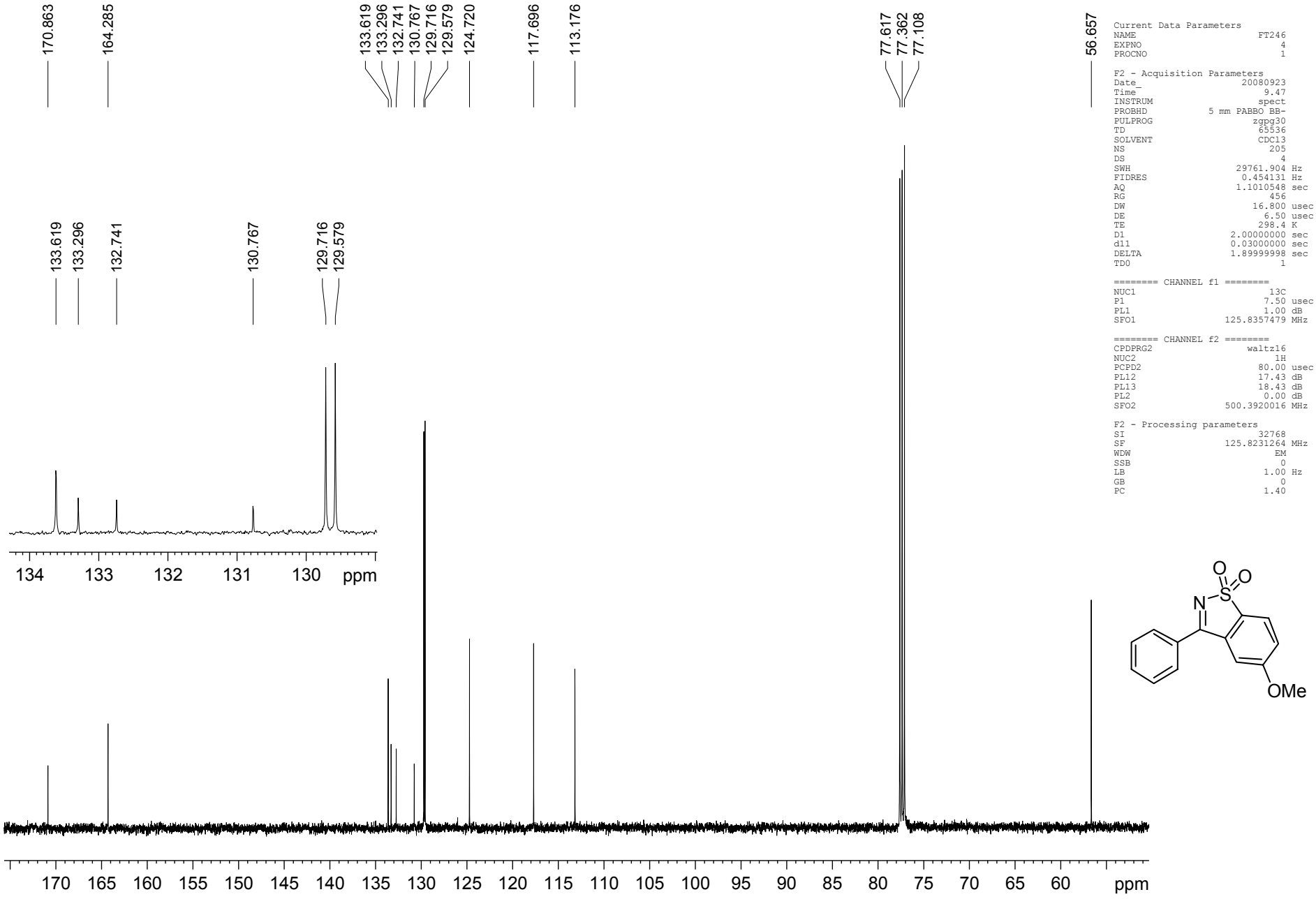


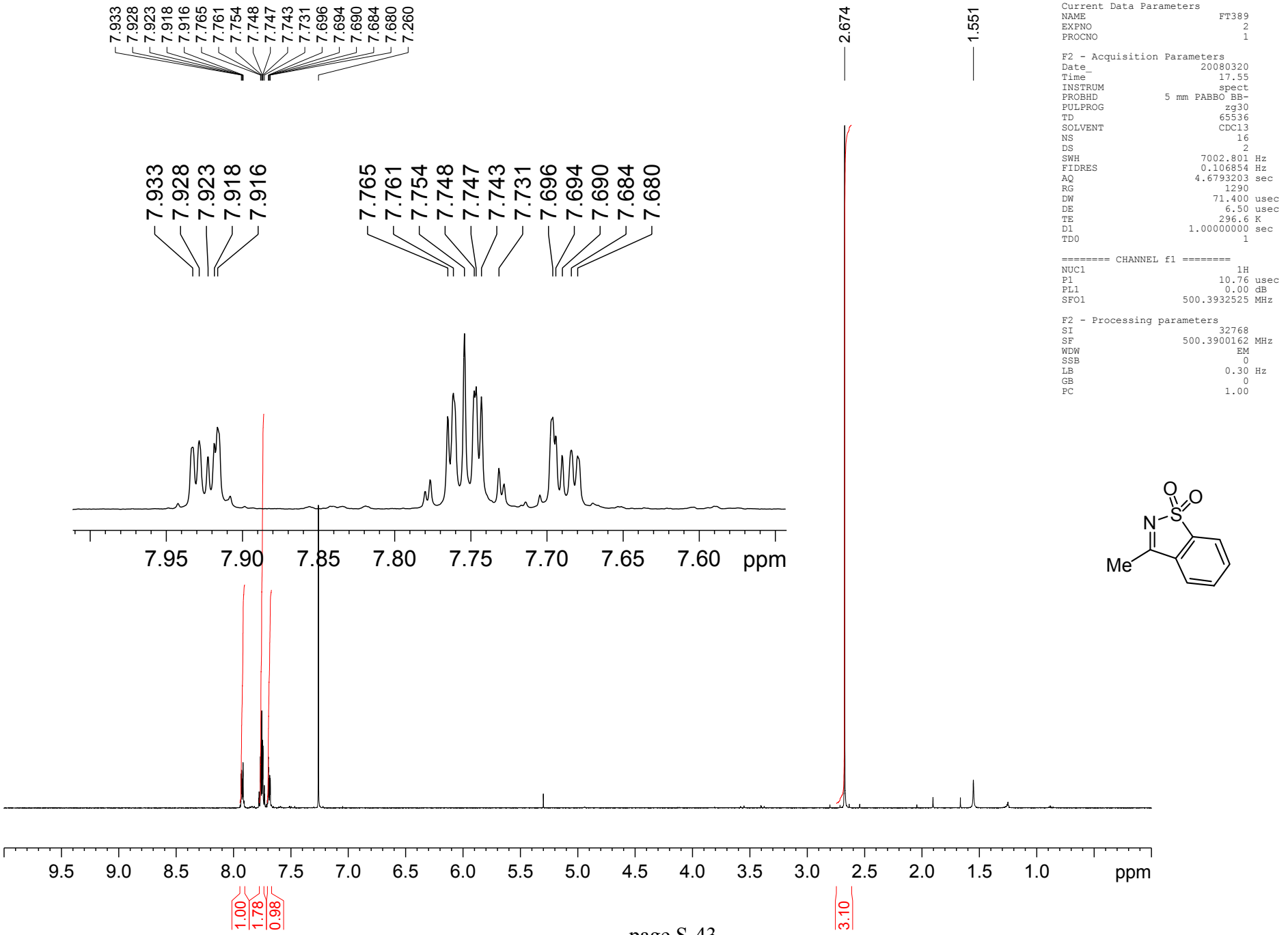

```
Current Data Parameters
NAME                         FT246
EXPNO                            2
PROCNO                           1

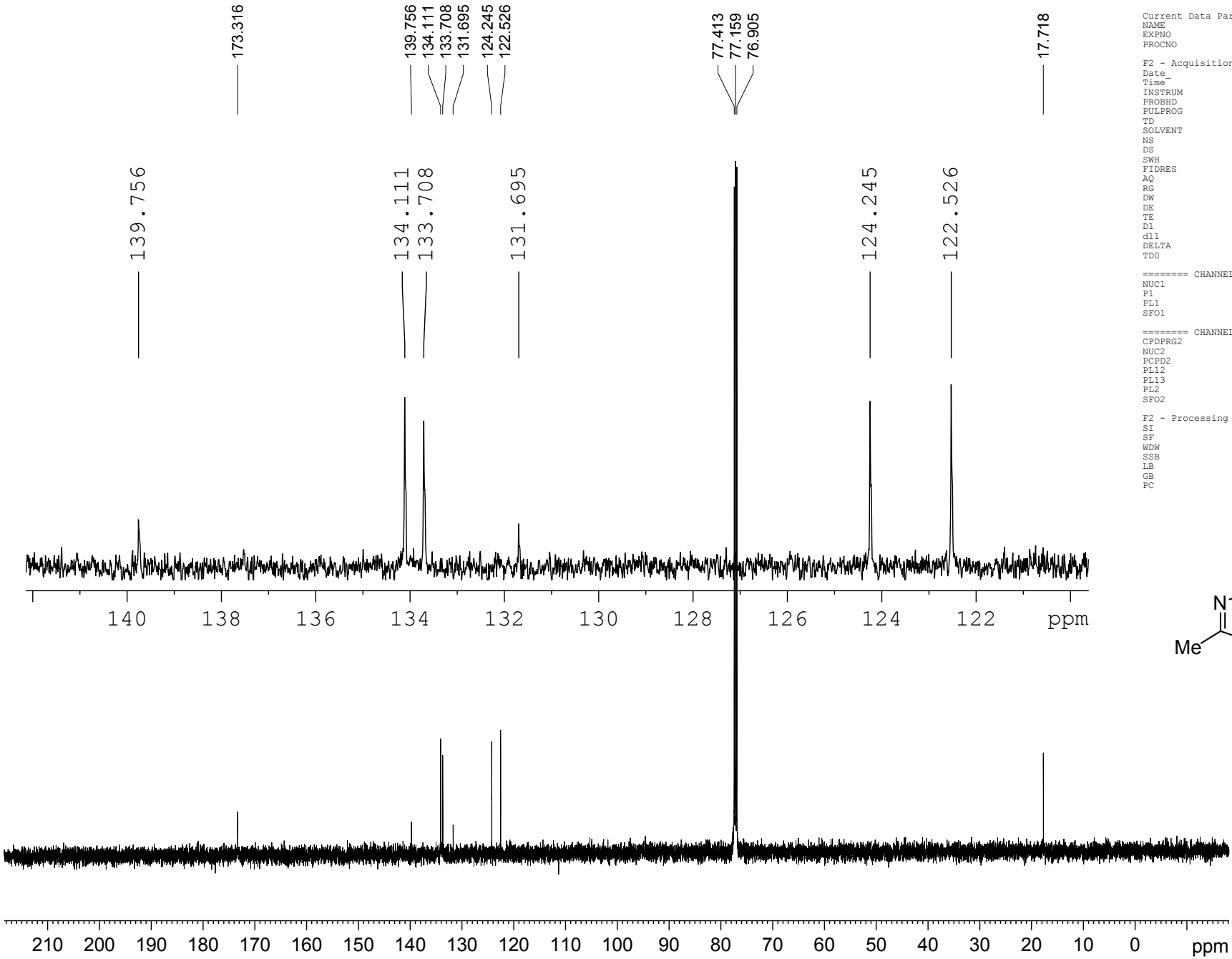
F2 - Acquisition Parameters
Date_                     20071221
Time                         14.28
INSTRUM                      spect
PROBHD           5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDC13
NS                             16
DS                              2
SWH                    7002.801 Hz
FIDRES                 0.106854 Hz
AQ                    4.6793203 sec
RG                          1440
DW                       71.400 usec
DE                        6.50 usec
TE                        297.5 K
D1                   1.00000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                            1H
P1                       10.76 usec
PL1                       0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                           32768
SF                    500.3900163 MHz
WDW                             EM
SSB                              0
LB                        0.30 Hz
GB                               0
PC                            1.00
```


170.863
164.285
133.619
133.296
132.741
130.767
129.716
129.579
124.720
117.696
113.176
77.617
77.362
77.108
56.657
Current Data Parameters
NAME FT246
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080923
Time 9.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 205
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231264 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
134 133 132 131 130 ppm
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 ppm
O
O
S
N
OMe


7.933
7.928
7.923
7.918
7.916
7.765
7.761
7.754
7.748
7.747
7.743
7.731
7.696
7.694
7.690
7.684
7.680
7.260
2.674
1.551
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
ppm
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.78
0.98
3.10
Current Data Parameters
NAME FT389
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080320
Time 17.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 1290
DW 71.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz
F2 - Processing parameters
SI 32768
SF 500.3900162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
S
Me



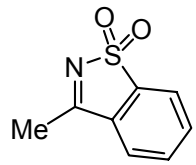

```
Current Data Parameters
NAME                         FT389
EXPNO                            4
PROCNO                           1

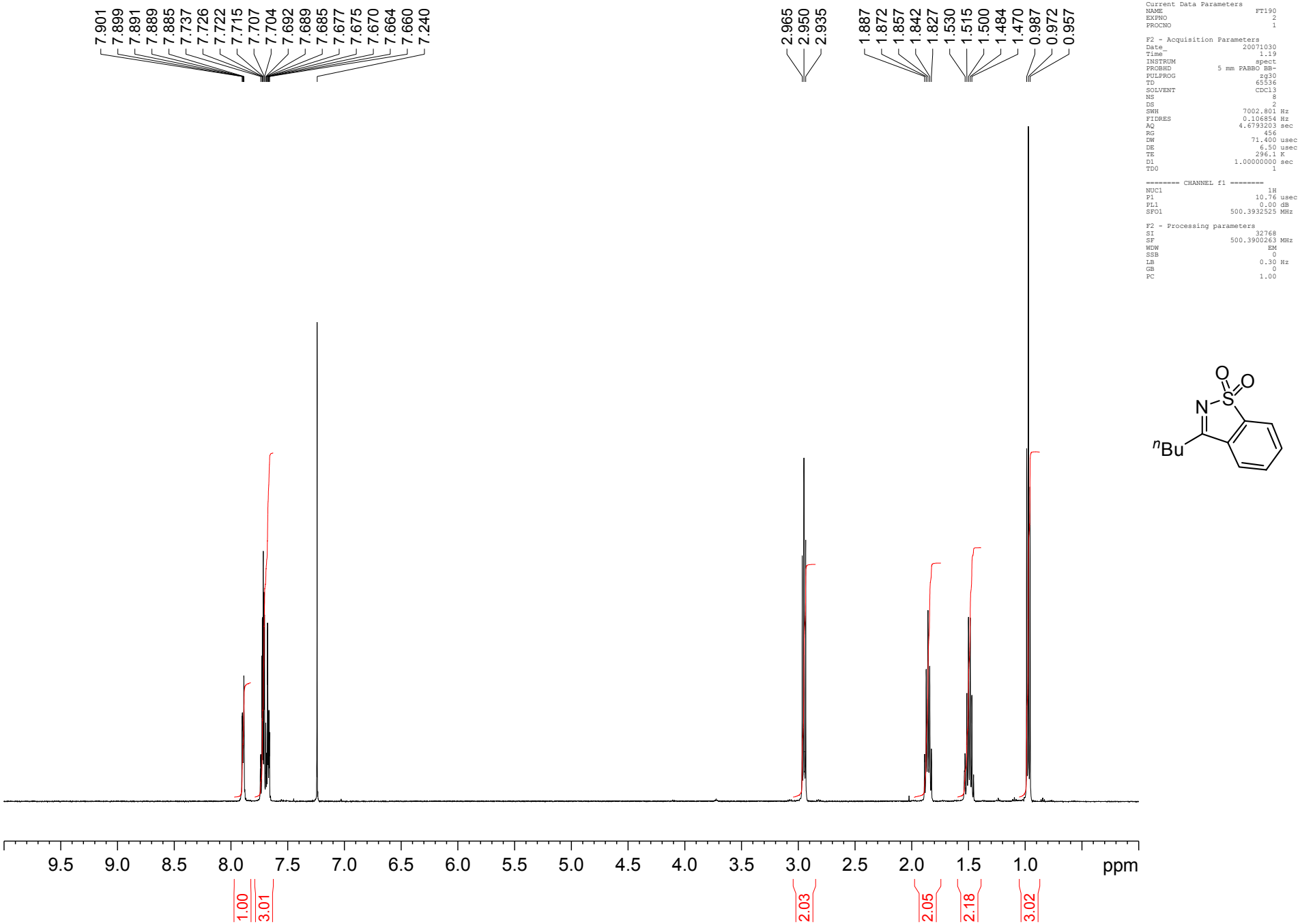
F2 - Acquisition Parameters
Date_                     20080929
Time                         18.08
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                            194
DS                              4
SWH                     29761.904 Hz
FIDRES                  0.454131 Hz
AQ                      1.1010548 sec
RG                            456
DW                         16.800 usec
DE                          6.50 usec
TE                          298.7 K
D1                      2.00000000 sec
d11                     0.03000000 sec
DELTA                   1.89999998 sec
TD0                              1

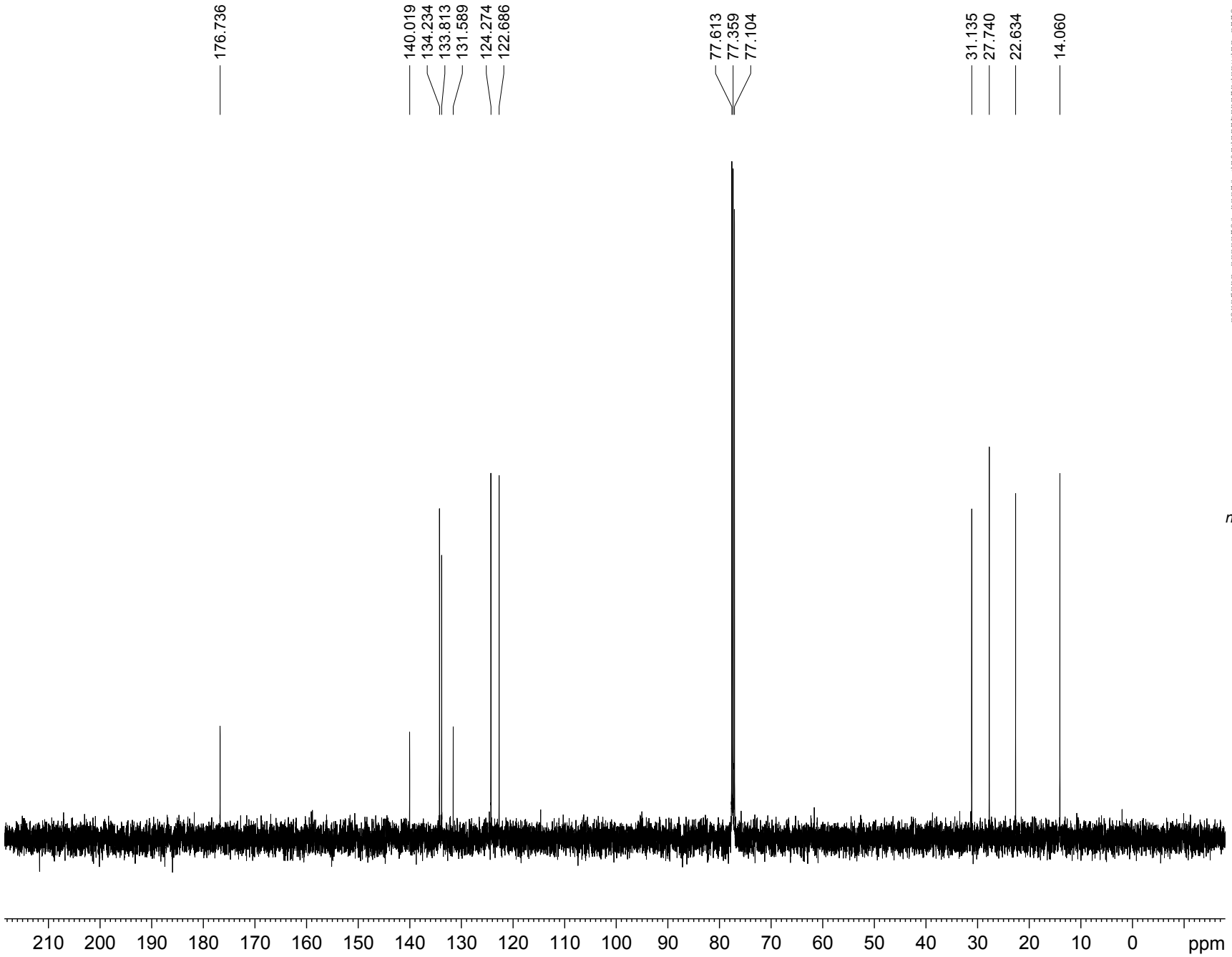
======== CHANNEL f1 ========
NUC1                           13C
P1                          7.50 usec
PL1                         1.00 dB
SFO1                  125.8357479 MHz

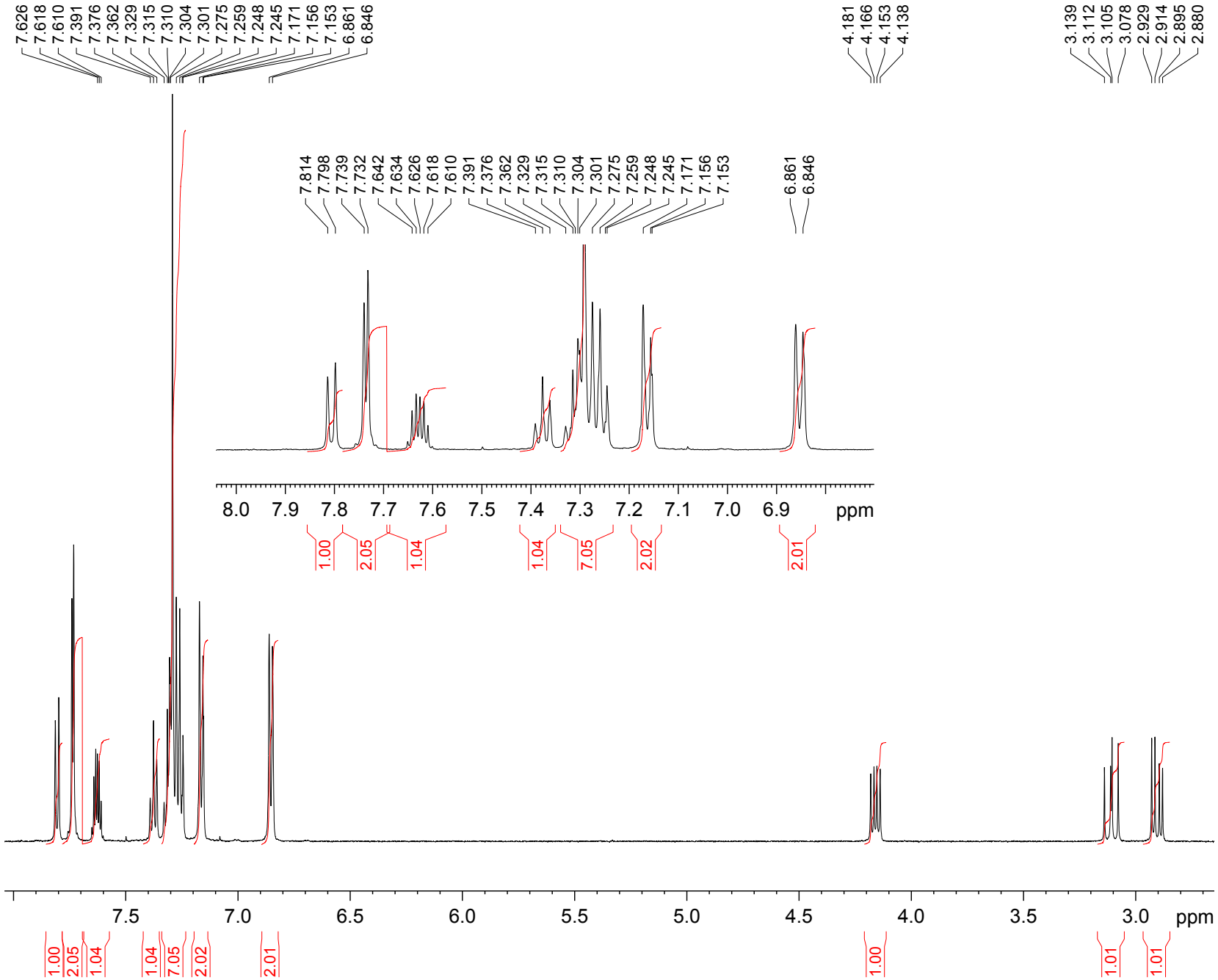
======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                      80.00 usec
PL12                       17.43 dB
PL13                       18.43 dB
PL2                         0.00 dB
SFO2                  500.3920016 MHz

F2 - Processing parameters
SI                            32768
SF                    125.8231500 MHz
WDW                              EM
SSB                               0
LB                             1.00 Hz
GB                                0
PC                             1.40
```




7.901
7.899
7.891
7.889
7.885
7.737
7.726
7.722
7.715
7.707
7.704
7.692
7.689
7.685
7.677
7.675
7.670
7.664
7.660
7.240
2.965
2.950
2.935
1.887
1.872
1.857
1.842
1.827
1.530
1.515
1.500
1.484
1.470
0.987
0.972
0.957
Current Data Parameters
NAME FT190
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071030
Time 1.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 456
DW 71.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz
F2 - Processing parameters
SI 32768
SF 500.3900263 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
S
N
nBu
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
3.01
2.03
2.05
2.18
3.02


176.736
140.019
134.234
133.813
131.589
124.274
122.686
77.613
77.359
77.104
31.135
27.740
22.634
14.060
Current Data Parameters
NAME FT190
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date 20080929
Time 18.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 17
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231309 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
S
N
nBu
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

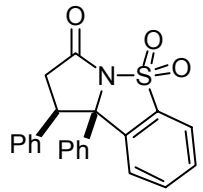


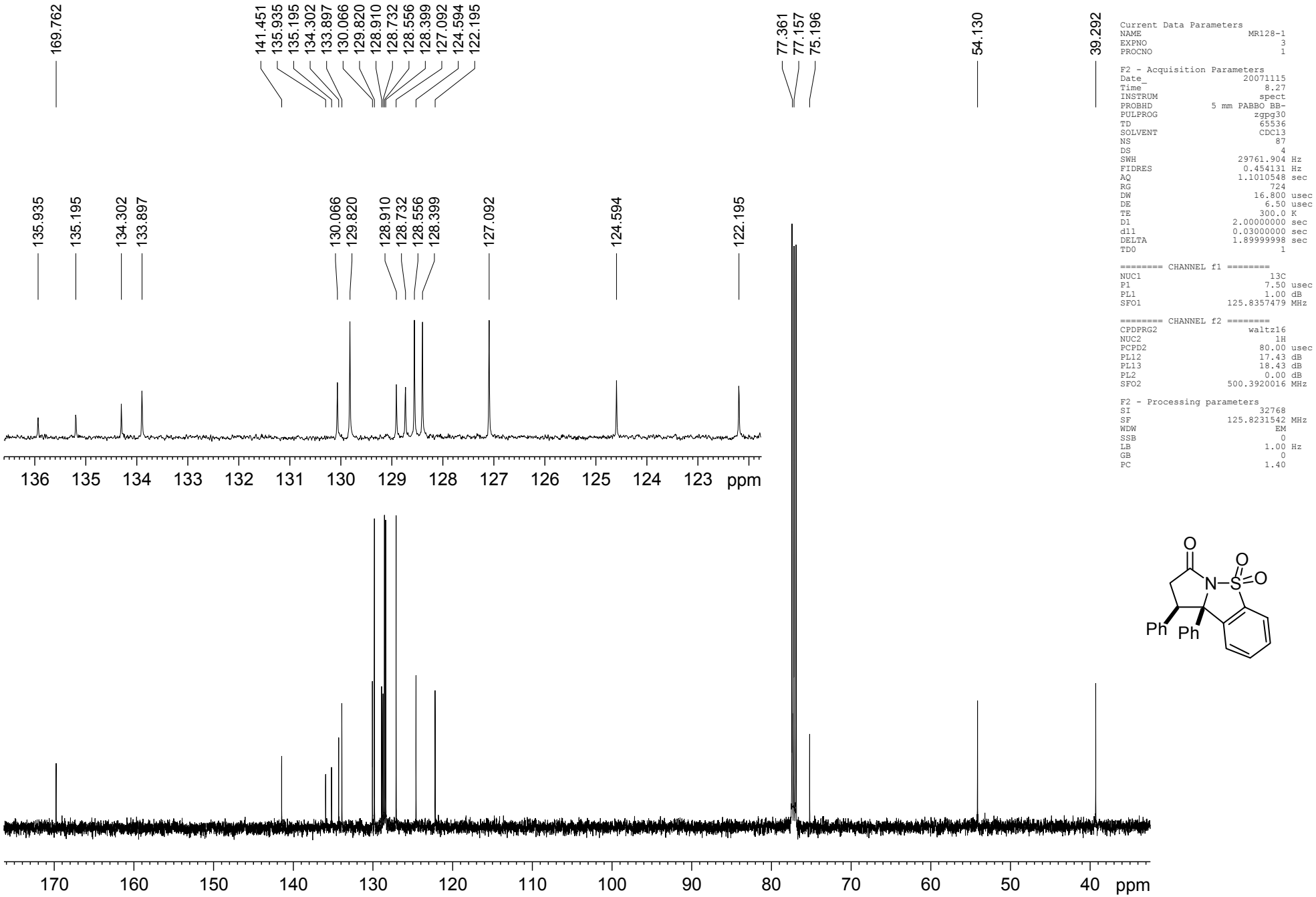

```
Current Data Parameters
NAME                  MR128-3crystal
EXPNO                              2
PROCNO                             1

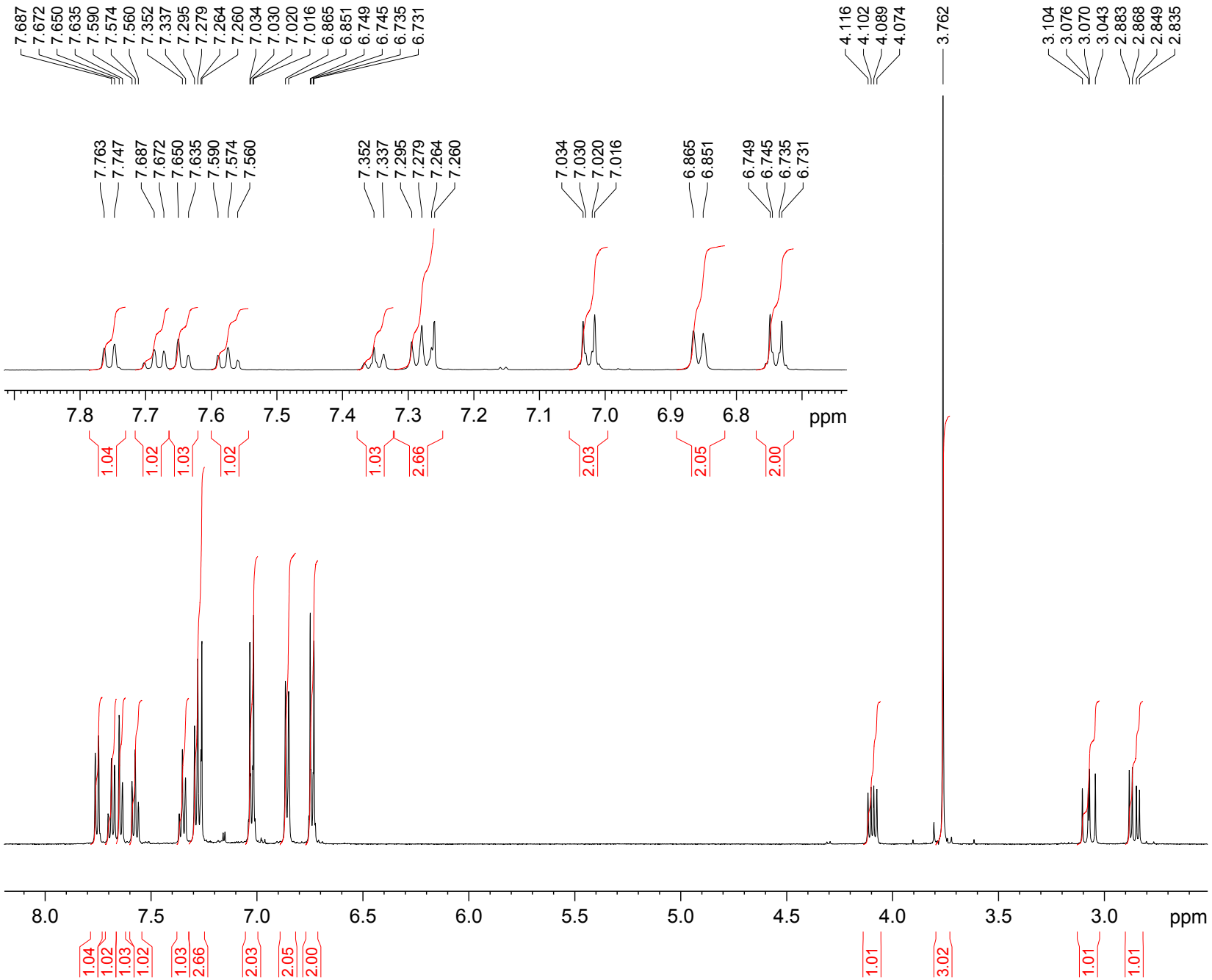
F2 - Acquisition Parameters
Date_                       20080103
Time_                           9.36
INSTRUM                        spect
PROBHD          5 mm PABBO BB-
PULPROG                         zg30
TD                             65536
SOLVENT                        CDCl3
NS                                10
DS                                 2
SWH                       7002.801 Hz
FIDRES                    0.106854 Hz
AQ                        4.6793203 sec
RG                              1150
DW                        71.400 usec
DE                         6.50 usec
TE                         298.1 K
D1                        1.00000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                              1H
P1                        10.76 usec
PL1                        0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                             32768
SF                    500.3900000 MHz
WDW                               EM
SSB                                0
LB                         0.30 Hz
GB                                 0
PC                              1.00
```




169.762
141.451
135.935
135.195
134.302
133.897
130.066
129.820
128.910
128.732
128.556
128.399
127.092
124.594
122.195
77.361
77.157
75.196
54.130
39.292
Current Data Parameters
NAME MR128-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071115
Time 8.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 87
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 724
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
N
S
O
Ph
Ph
136 135 134 133 132 131 130 129 128 127 126 125 124 123 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 ppm

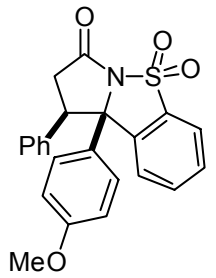


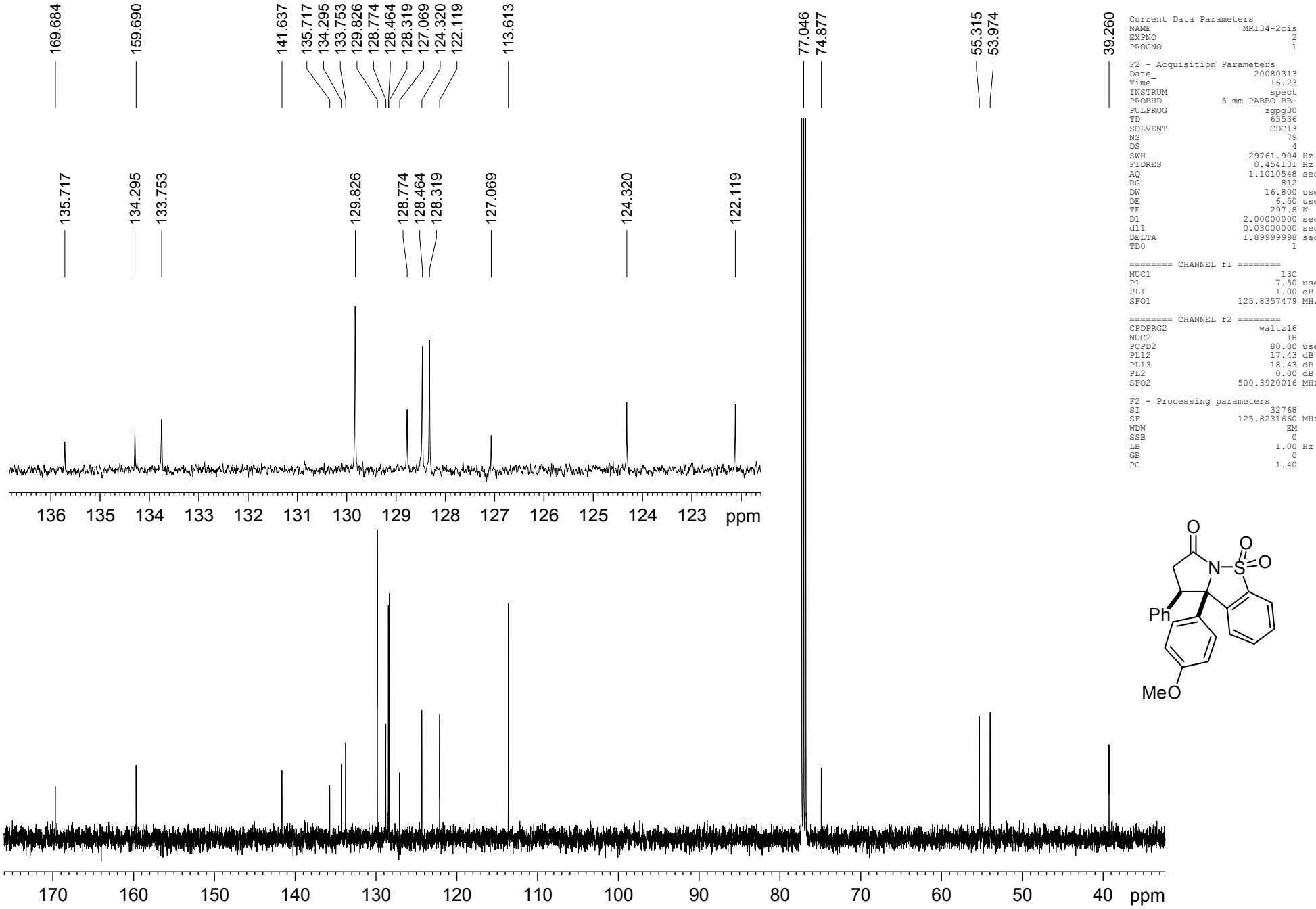

```
Current Data Parameters
NAME                   MR134-2cis
EXPNO                           3
PROCNO                          1

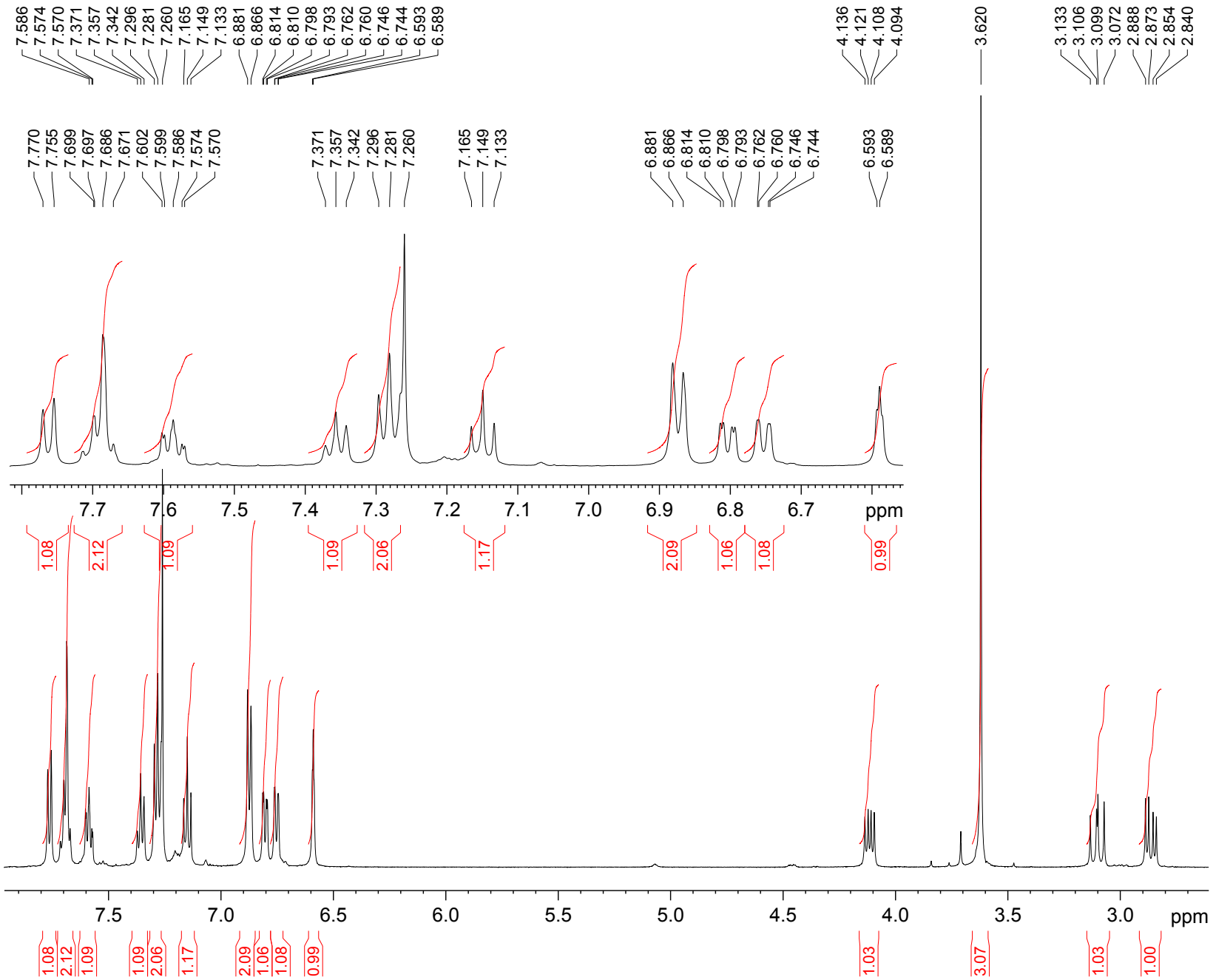
F2 - Acquisition Parameters
Date_                    20080315
Time                        15.20
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                    4.6793203 sec
RG                           406
DW                      71.400 usec
DE                       6.50 usec
TE                       296.5 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                      10.76 usec
PL1                      0.00 dB
SFO1                 500.3932525 MHz

F2 - Processing parameters
SI                         32768
SF                   500.3900160 MHz
WDW                           EM
SSB                            0
LB                       0.30 Hz
GB                             0
PC                          1.00
```




169.684
159.690
141.637
135.717
134.295
133.753
129.826
128.774
128.464
128.319
127.069
124.320
122.119
113.613
77.046
74.877
55.315
53.974
39.260
Current Data Parameters
NAME MR134-2cis
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080313
Time 16.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 79
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 812
DW 16.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231660 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
136 135 134 133 132 131 130 129 128 127 126 125 124 123 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 ppm
O
O
O
N
S
Ph
MeO

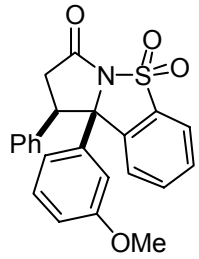


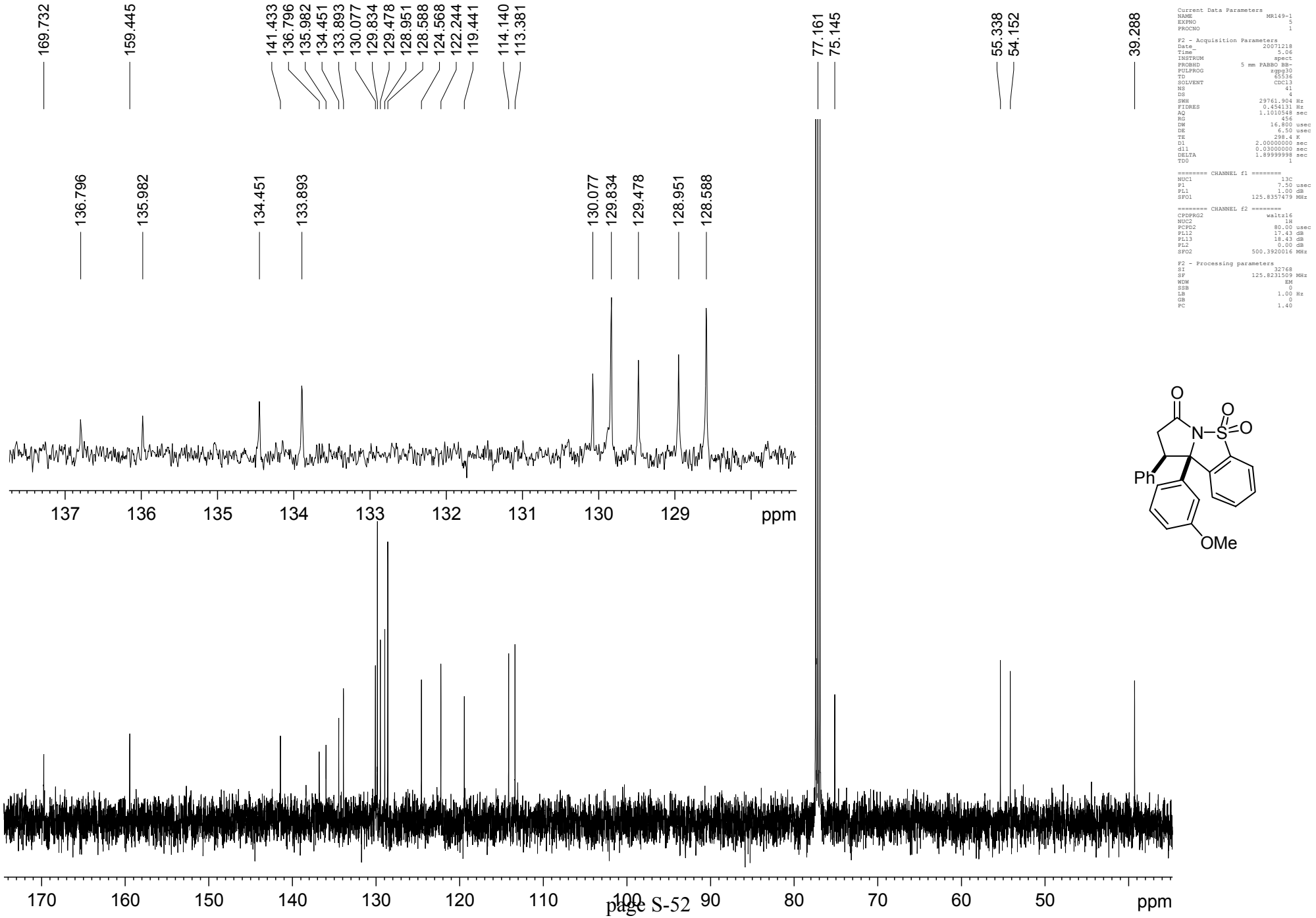

```
Current Data Parameters
NAME                      MR149-1
EXPNO                           4
PROCNO                          1

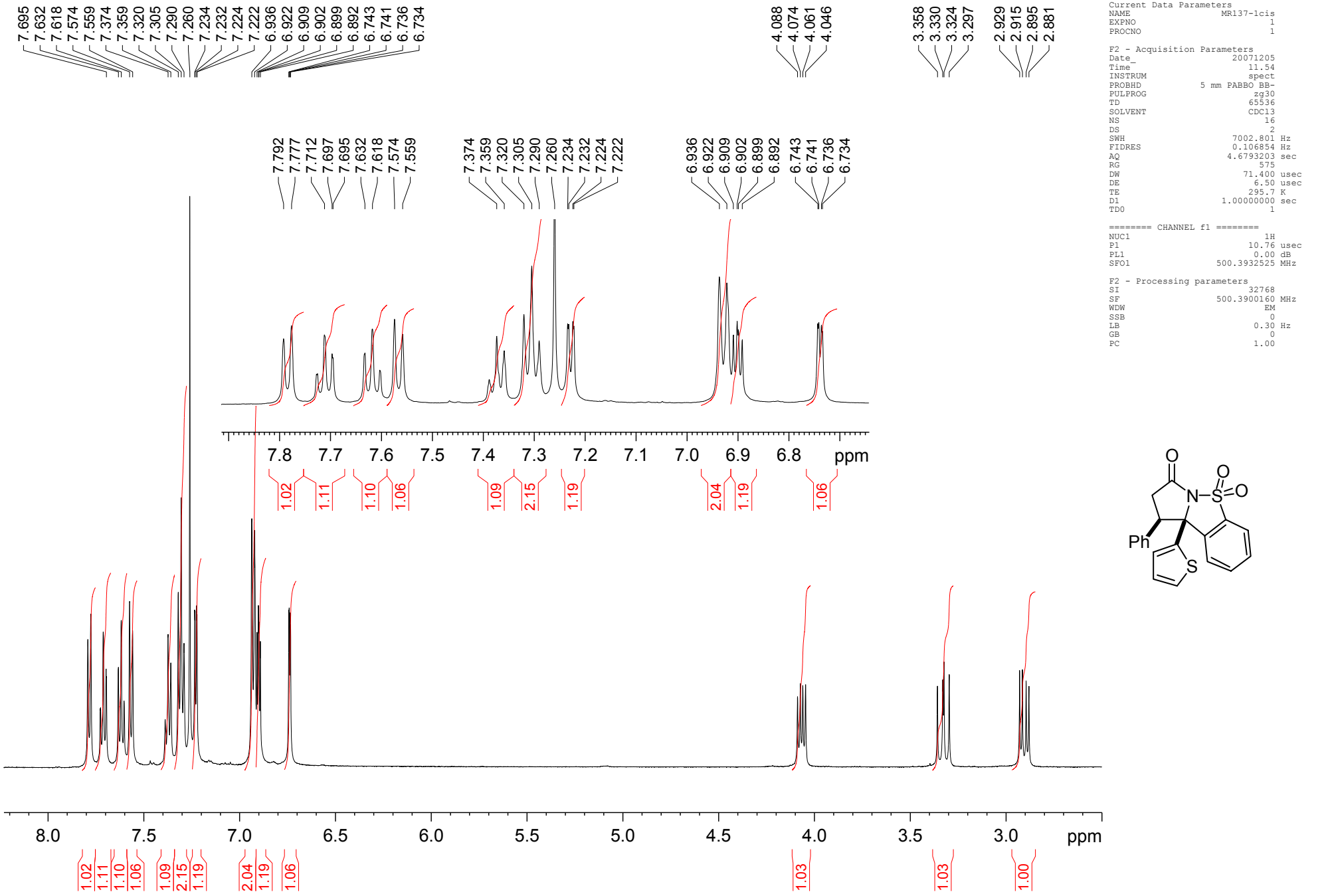
F2 - Acquisition Parameters
Date_                    20071218
Time                         5.01
INSTRUM                     spect
PROBHD  5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                            512
DW                         71.400 usec
DE                          6.50 usec
TE                         297.8 K
D1                    1.00000000 sec
TD0                             1

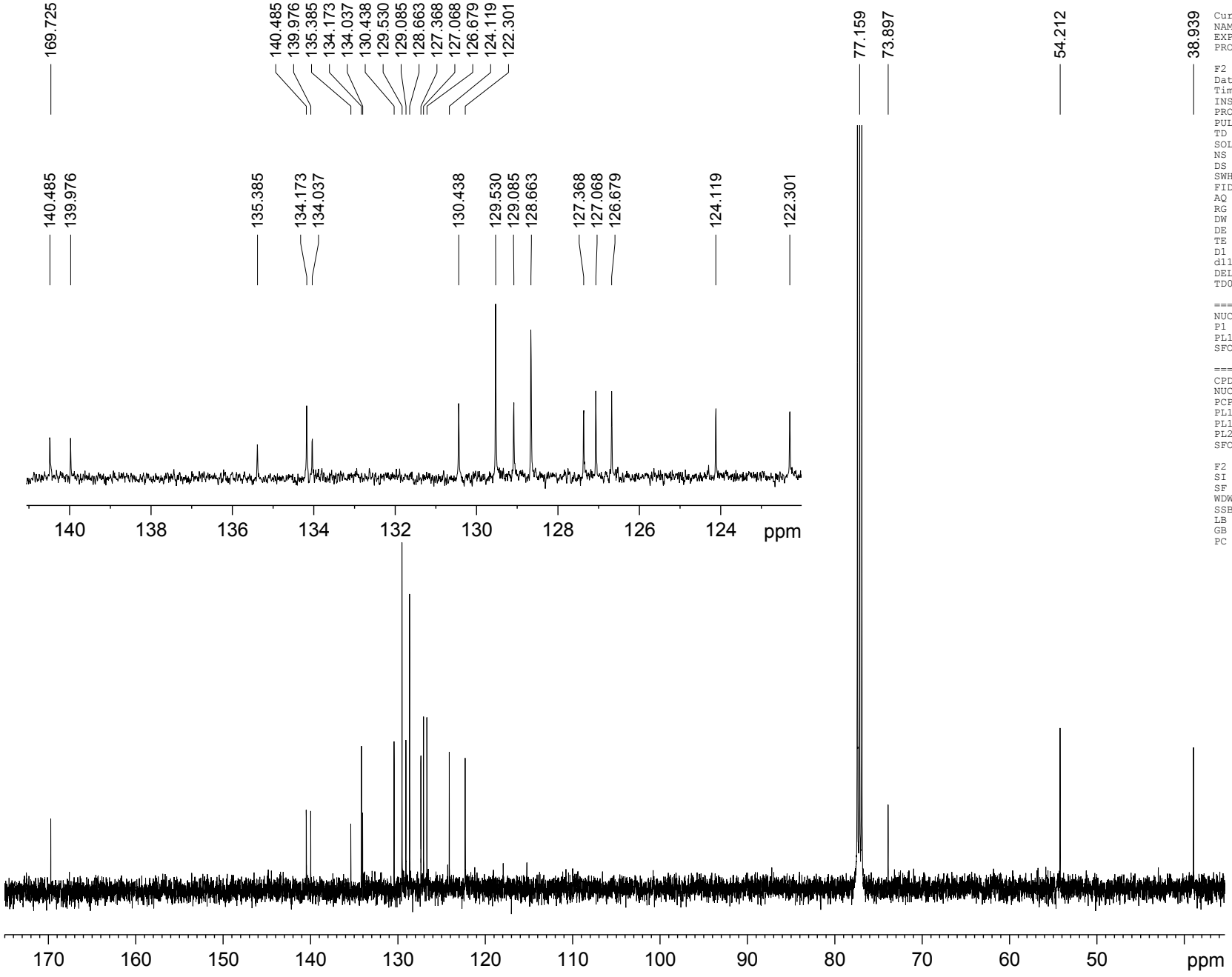
======== CHANNEL f1 ========
NUC1                           1H
P1                         10.76 usec
PL1                         0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                  500.3900160 MHz
WDW                            EM
SSB                             0
LB                          0.30 Hz
GB                              0
PC                           1.00
```




169.732
159.445
141.433
136.796
135.982
134.451
133.893
130.077
129.834
129.478
128.951
128.588
124.568
122.244
119.441
114.140
113.381
77.161
75.145
55.338
54.152
39.288
Current Data Parameters
NAME MR149-1
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071218
Time 5.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 41
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 456
DW 16.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
O
N
S
Ph
OMe
137
136
135
134
133
132
131
130
129
ppm
170
160
150
140
130
120
110
100
90
80
70
60
50
ppm


7.695 7.632 7.618 7.574 7.559 7.374 7.359 7.320 7.305 7.290 7.260 7.234 7.232 7.224 7.222 6.936 6.922 6.909 6.902 6.899 6.892 6.743 6.741 6.736 6.734
4.088 4.074 4.061 4.046
3.358 3.330 3.324 3.297
2.929 2.915 2.895 2.881
Current Data Parameters
NAME MR137-1cis
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071205
Time 11.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 575
DW 71.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.792 7.777 7.712 7.697 7.695 7.632 7.618 7.574 7.559
7.374 7.359 7.320 7.305 7.290 7.260 7.234 7.232 7.224 7.222
6.936 6.922 6.909 6.902 6.899 6.892 6.743 6.741 6.736 6.734
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm
1.02 1.11 1.10 1.06 1.09 2.15 1.19 2.04 1.19 1.06
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 ppm
1.02 1.11 1.10 1.06 1.09 2.15 1.19 2.04 1.19 1.06 1.03 1.03 1.00
O
O
N
S
O
Ph
S



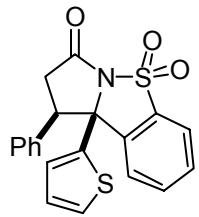

```
Current Data Parameters
NAME                  MR137-1cis
EXPNO                          2
PROCNO                         1

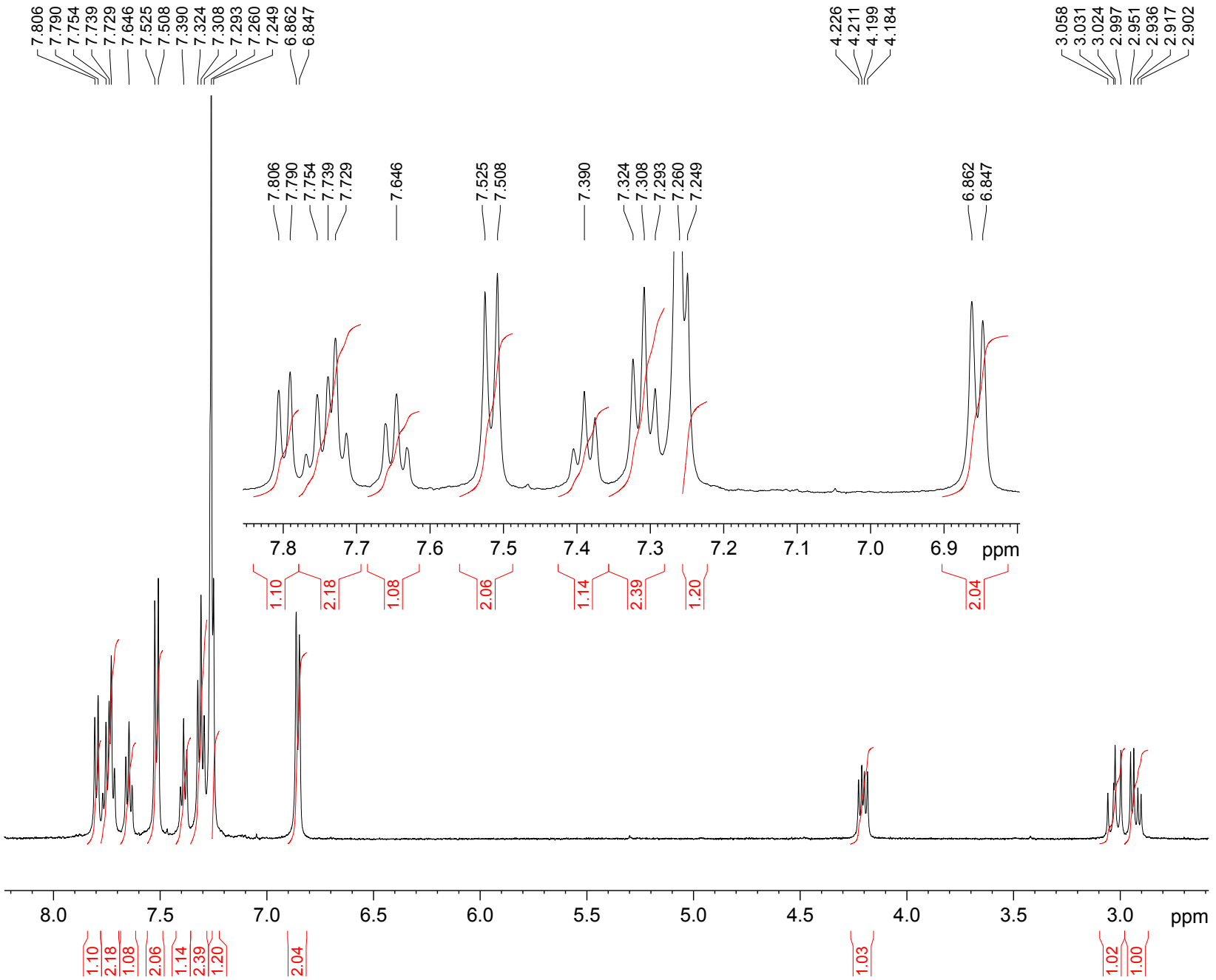
F2 - Acquisition Parameters
Date_                   20071205
Time                       11.59
INSTRUM                    spect
PROBHD      5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         155
DS                           4
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                   1.1010548 sec
RG                         456
DW                      16.800 usec
DE                       6.50 usec
TE                      297.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       7.50 usec
PL1                      1.00 dB
SFO1              125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL12                    17.43 dB
PL13                    18.43 dB
PL2                      0.00 dB
SFO2              500.3920016 MHz

F2 - Processing parameters
SI                         32768
SF                125.8231516 MHz
WDW                           EM
SSB                            0
LB                       1.00 Hz
GB                             0
PC                          1.40
```



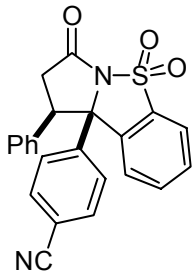


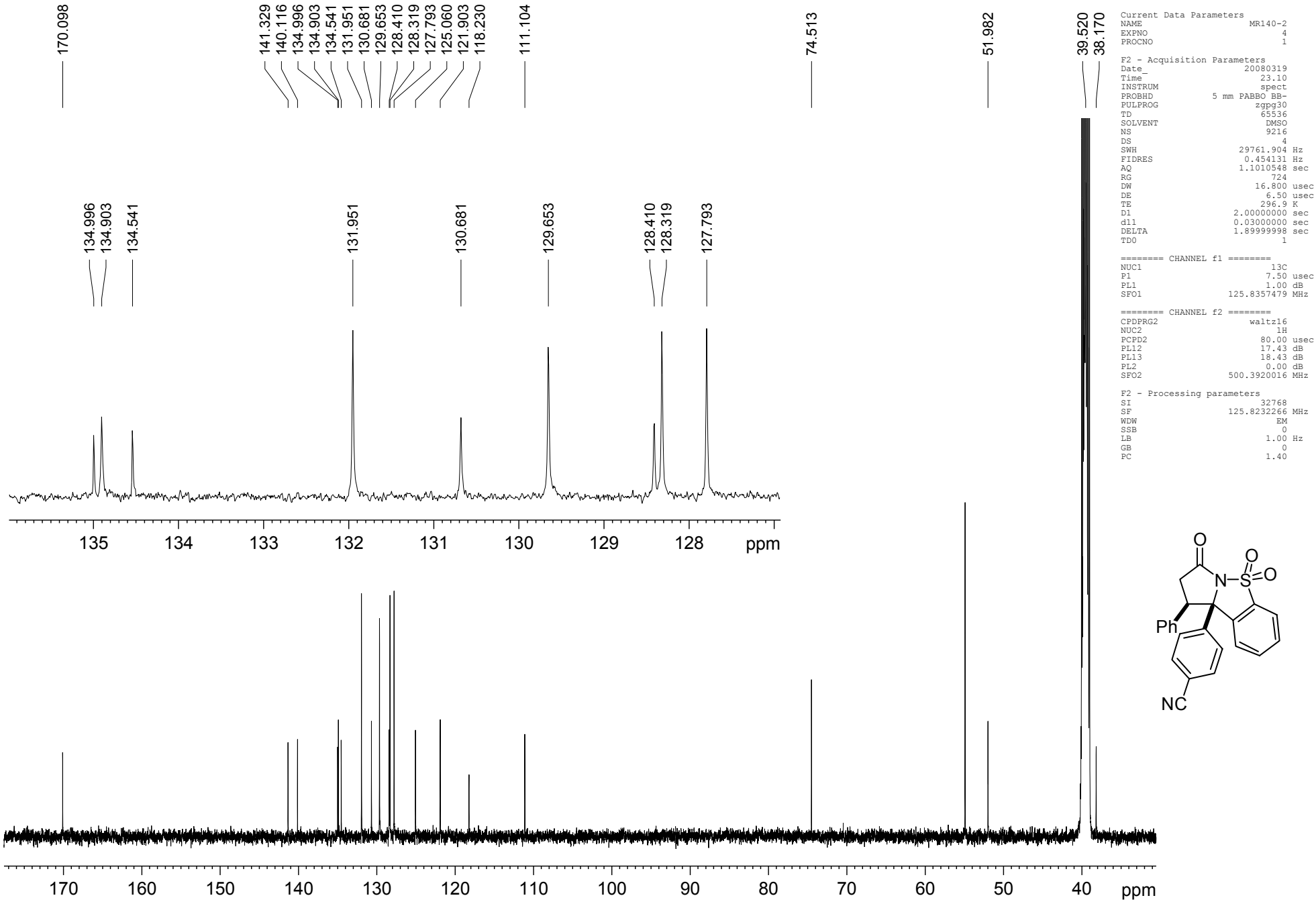

```
Current Data Parameters
NAME                  MR140-1trans
EXPNO                            1
PROCNO                           1

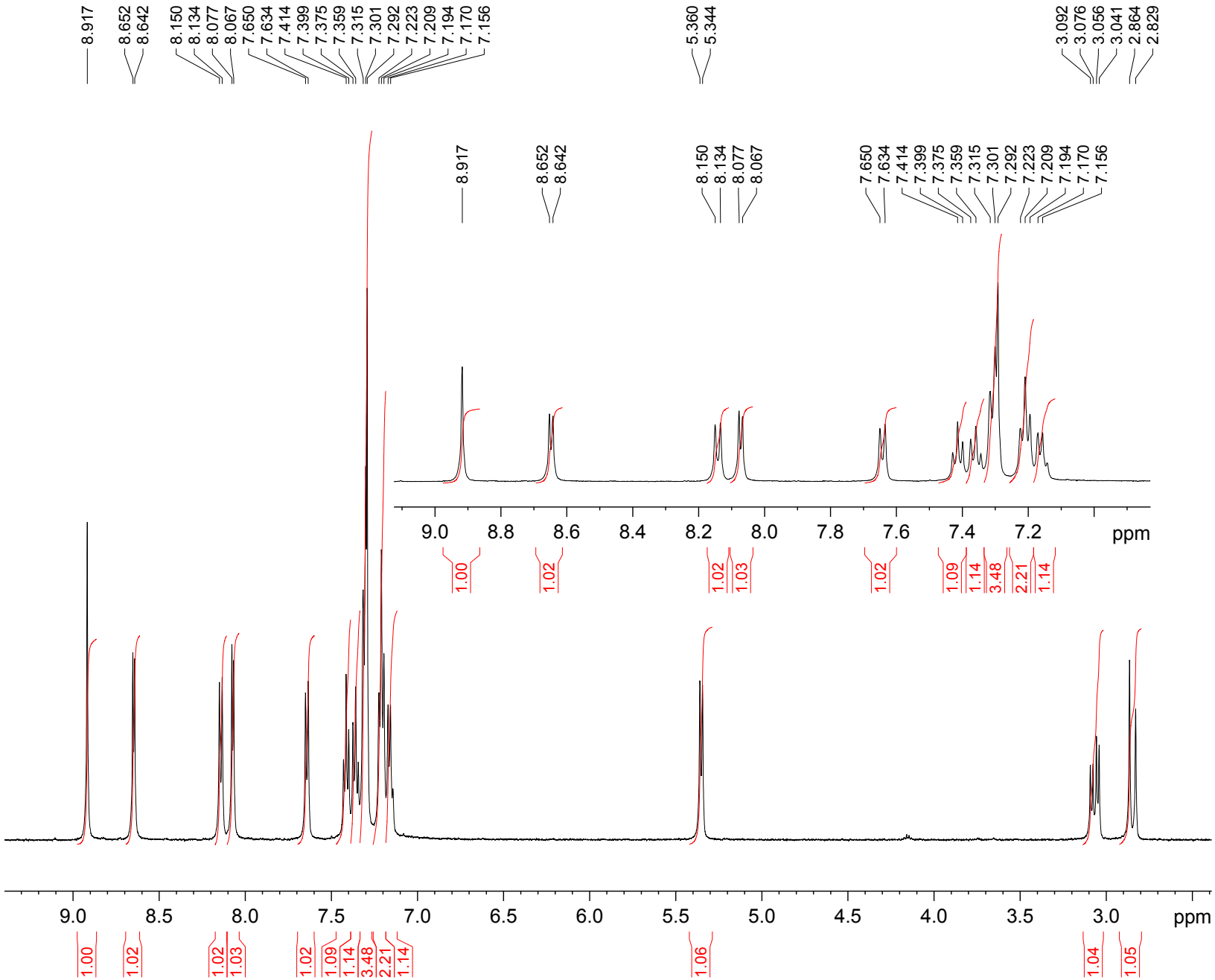
F2 - Acquisition Parameters
Date_                     20071205
Time                         13.28
INSTRUM                      spect
PROBHD       5 mm PABBO BB-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                    4.6793203 sec
RG                           1150
DW                        71.400 usec
DE                         6.50 usec
TE                         296.0 K
D1                   1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                        10.76 usec
PL1                        0.00 dB
SFO1                 500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                   500.3900160 MHz
WDW                            EM
SSB                             0
LB                         0.30 Hz
GB                              0
PC                         1.00
```




170.098
141.329
140.116
134.996
134.903
134.541
131.951
130.681
129.653
128.410
128.319
127.793
125.060
121.903
118.230
111.104
74.513
51.982
39.520
38.170
Current Data Parameters
NAME MR140-2
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080319
Time 23.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 9216
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 724
DW 16.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8232266 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
135
134
133
132
131
130
129
128
ppm
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm
O
O
N
S
O
Ph
NC

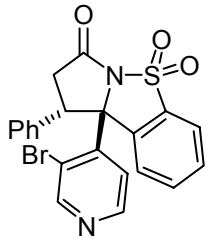


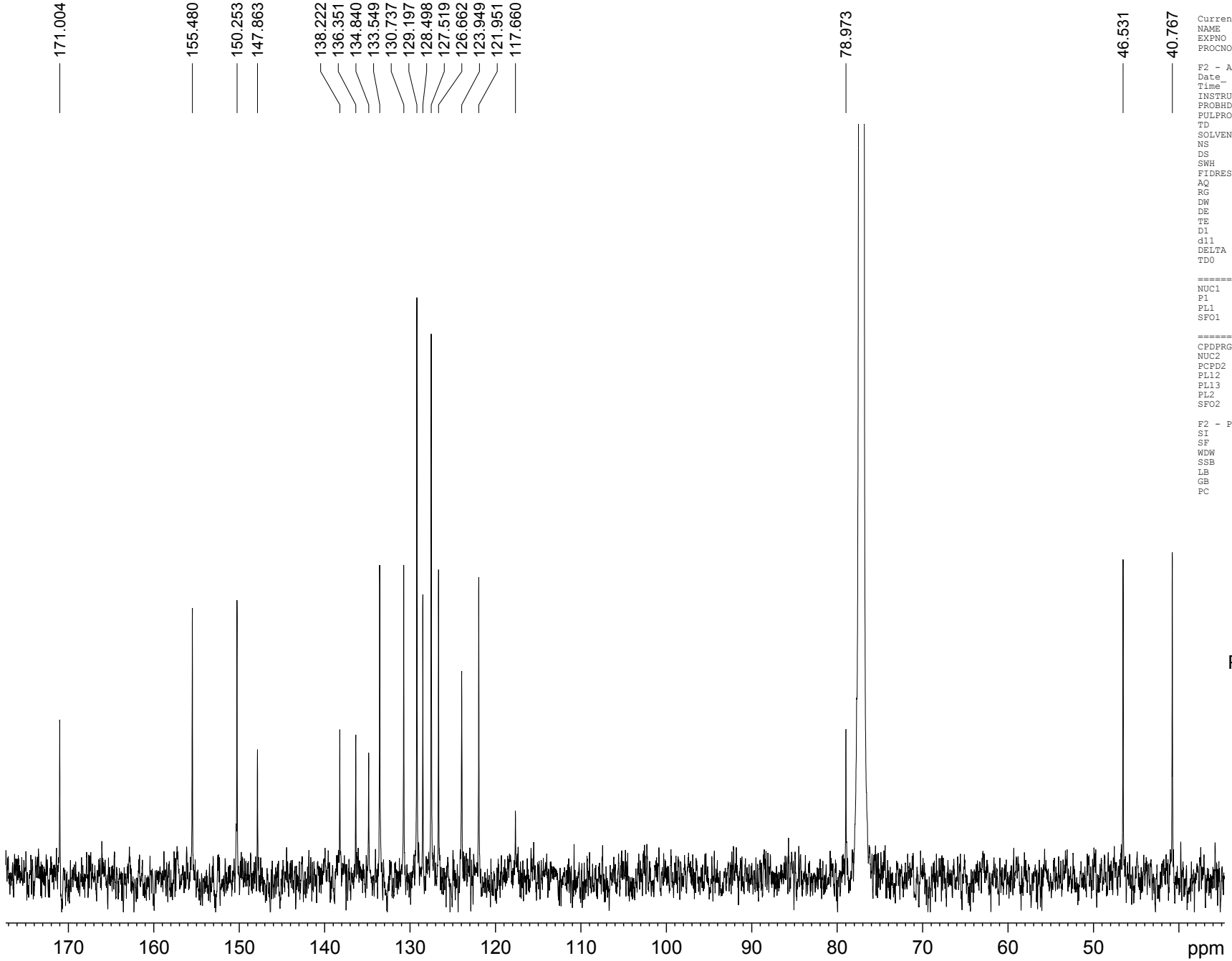

```
Current Data Parameters
NAME                  MR148-1oben
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20071215
Time                         8.56
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                     7002.801 Hz
FIDRES                 0.106854 Hz
AQ                     4.6793203 sec
RG                          1030
DW                        71.400 usec
DE                         6.50 usec
TE                        297.8 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.76 usec
PL1                        0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                         32768
SF                    500.3900000 MHz
WDW                           EM
SSB                            0
LB                         0.30 Hz
GB                             0
PC                          1.00
```





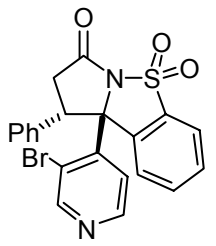

```
Current Data Parameters
NAME                  MR148-1oben
EXPNO                           4
PROCNO                          1

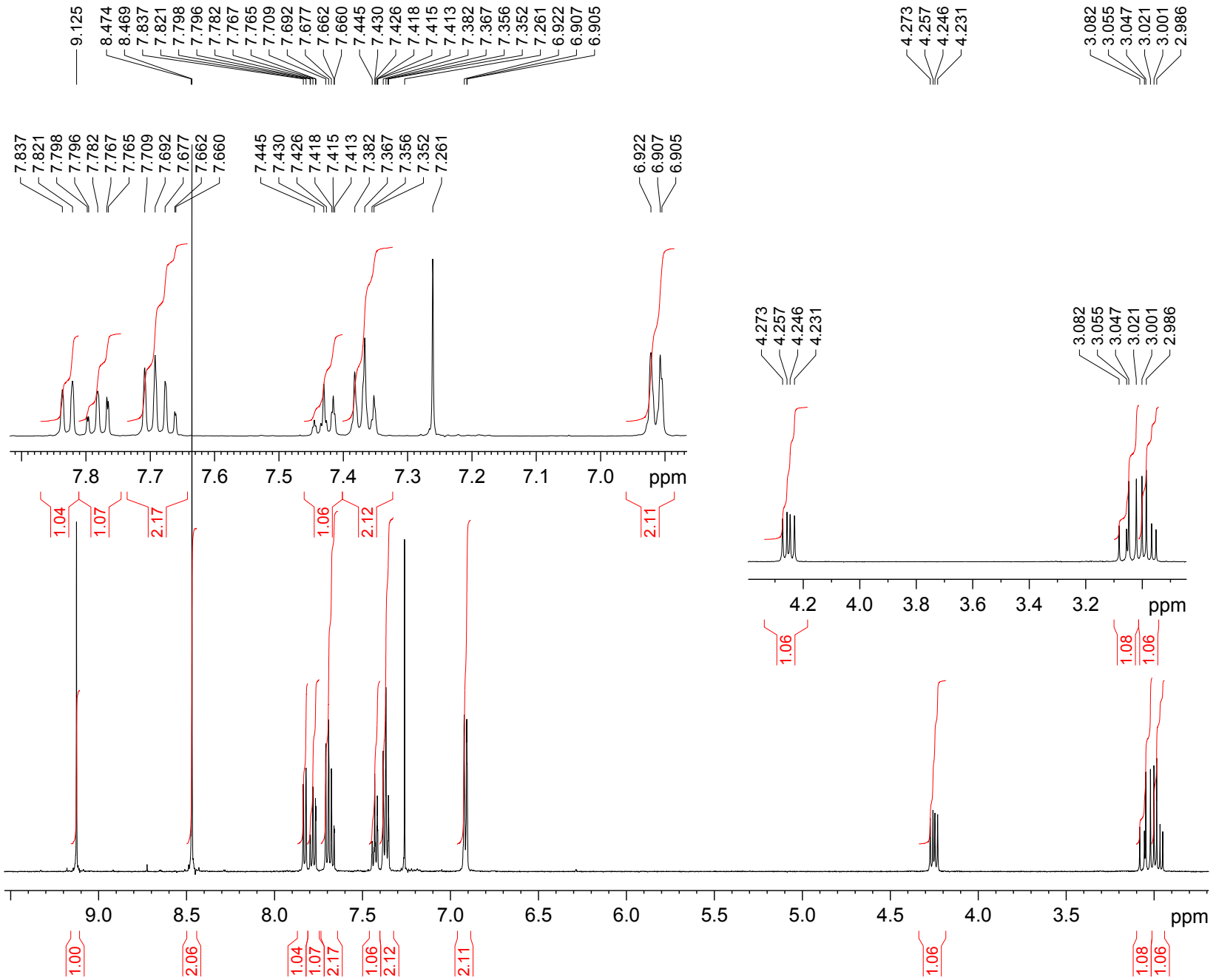
F2 - Acquisition Parameters
Date_                    20080927
Time                        23.32
INSTRUM                     spect
PROBHD          5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                          1347
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010548 sec
RG                           912
DW                        16.800 usec
DE                         6.50 usec
TE                        298.9 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                         7.50 usec
PL1                        1.00 dB
SFO1                 125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                          1H
PCPD2                     80.00 usec
PL12                      17.43 dB
PL13                      18.43 dB
PL2                        0.00 dB
SFO2                 500.3920016 MHz

F2 - Processing parameters
SI                           32768
SF                   125.8231500 MHz
WDW                             EM
SSB                              0
LB                         5.00 Hz
GB                               0
PC                            1.40
```



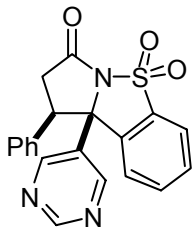


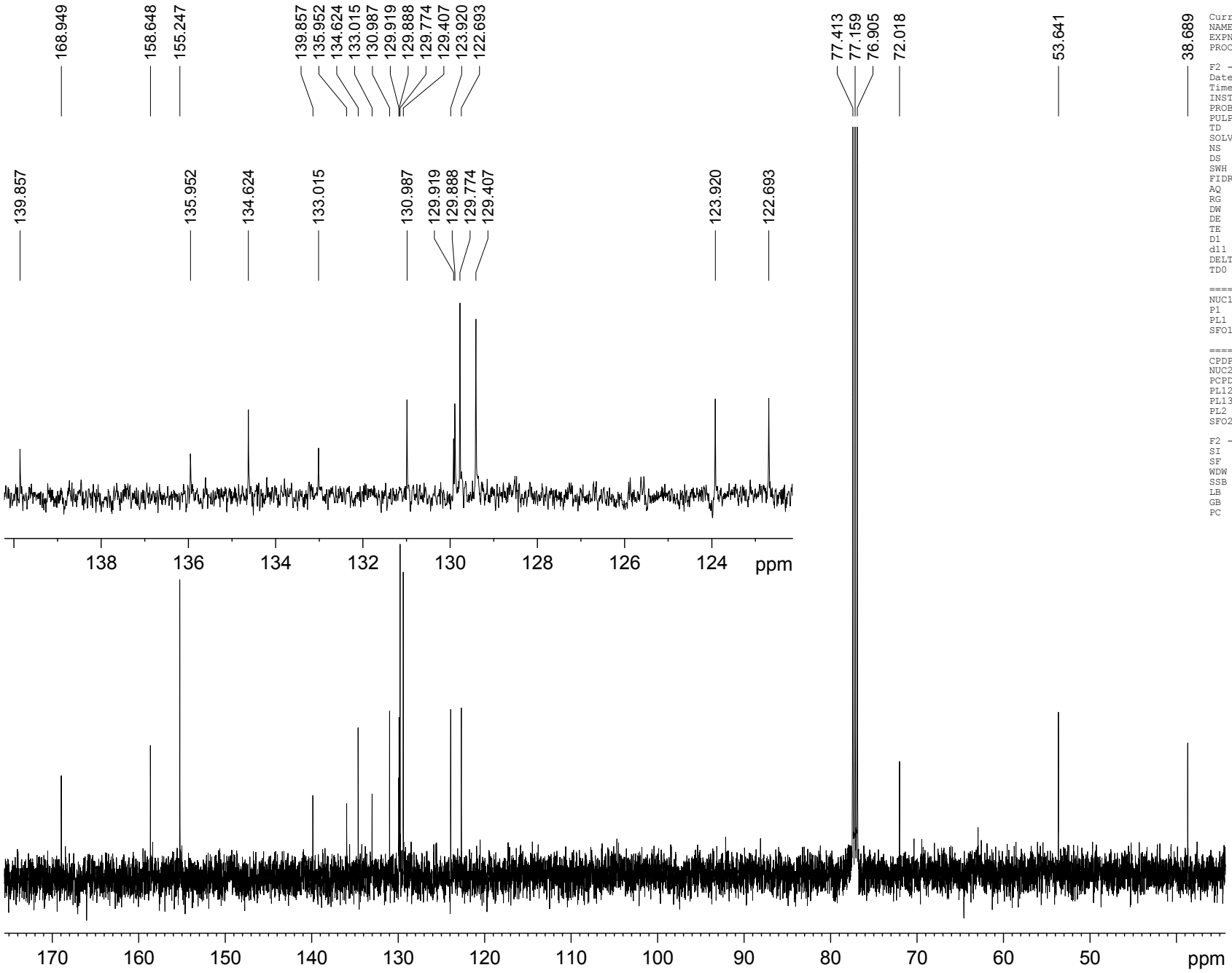

```
Current Data Parameters
NAME                      MR217-2
EXPNO                           3
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20080723
Time                        10.32
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                             16
DS                              2
SWH                   7002.801 Hz
FIDRES                0.106854 Hz
AQ                    4.6793203 sec
RG                            512
DW                     71.400 usec
DE                      6.50 usec
TE                        298.2 K
D1                  1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                     10.76 usec
PL1                     0.00 dB
SFO1                500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                  500.3900160 MHz
WDW                            EM
SSB                             0
LB                      0.30 Hz
GB                              0
PC                           1.00
```





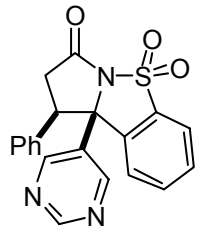

```
Current Data Parameters
NAME                   MR217-2
EXPNO                        4
PROCNO                       1

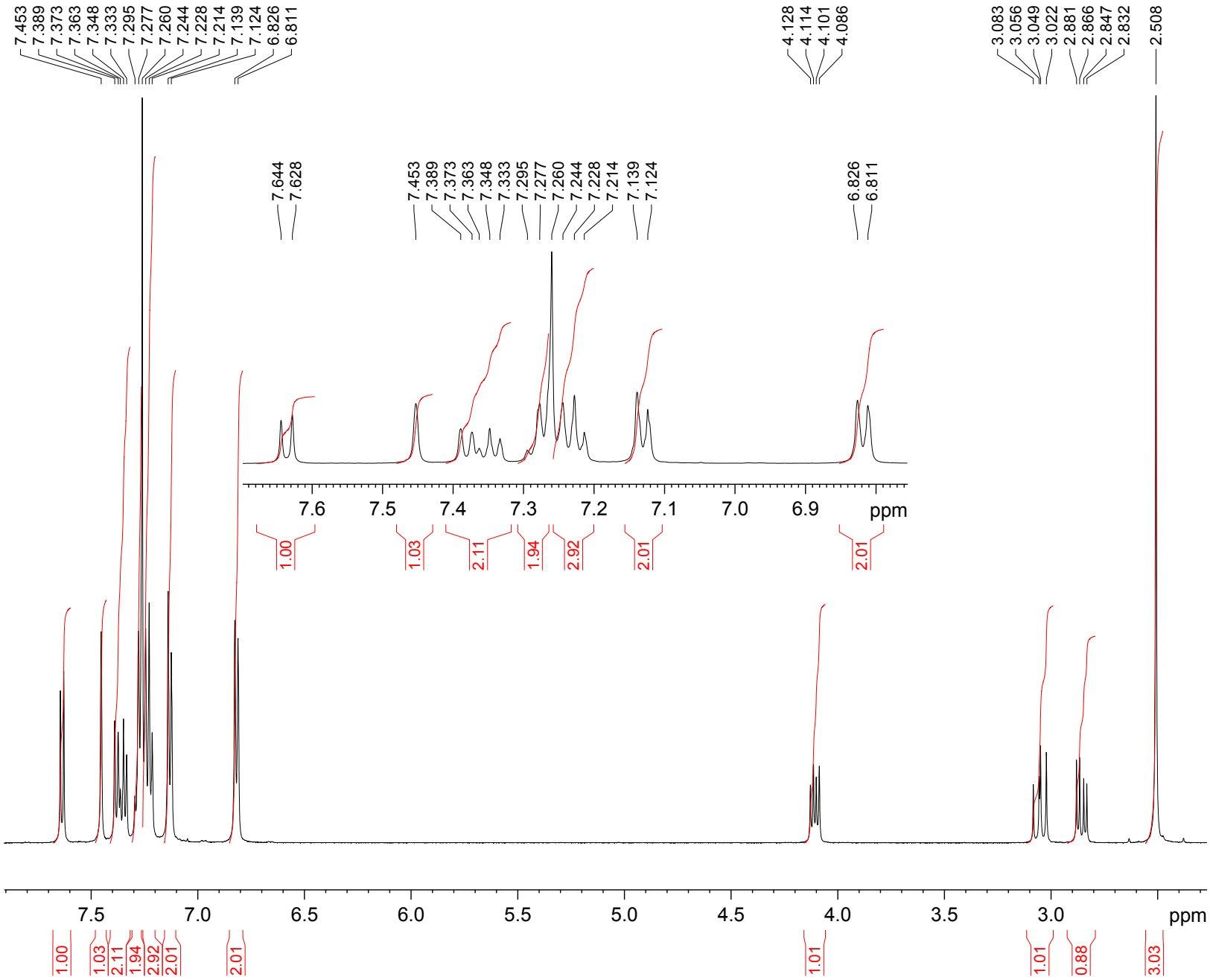
F2 - Acquisition Parameters
Date_                 20080723
Time                     10.34
INSTRUM                  spect
PROBHD  5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                         106
DS                           4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                        1030
DW                    16.800 usec
DE                     6.50 usec
TE                    298.6 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                     7.50 usec
PL1                    1.00 dB
SFO1           125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 80.00 usec
PL12                  17.43 dB
PL13                  18.43 dB
PL2                    0.00 dB
SFO2           500.3920016 MHz

F2 - Processing parameters
SI                         32768
SF             125.8231500 MHz
WDW                           EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                     1.40
```



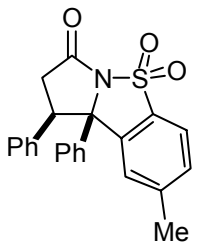


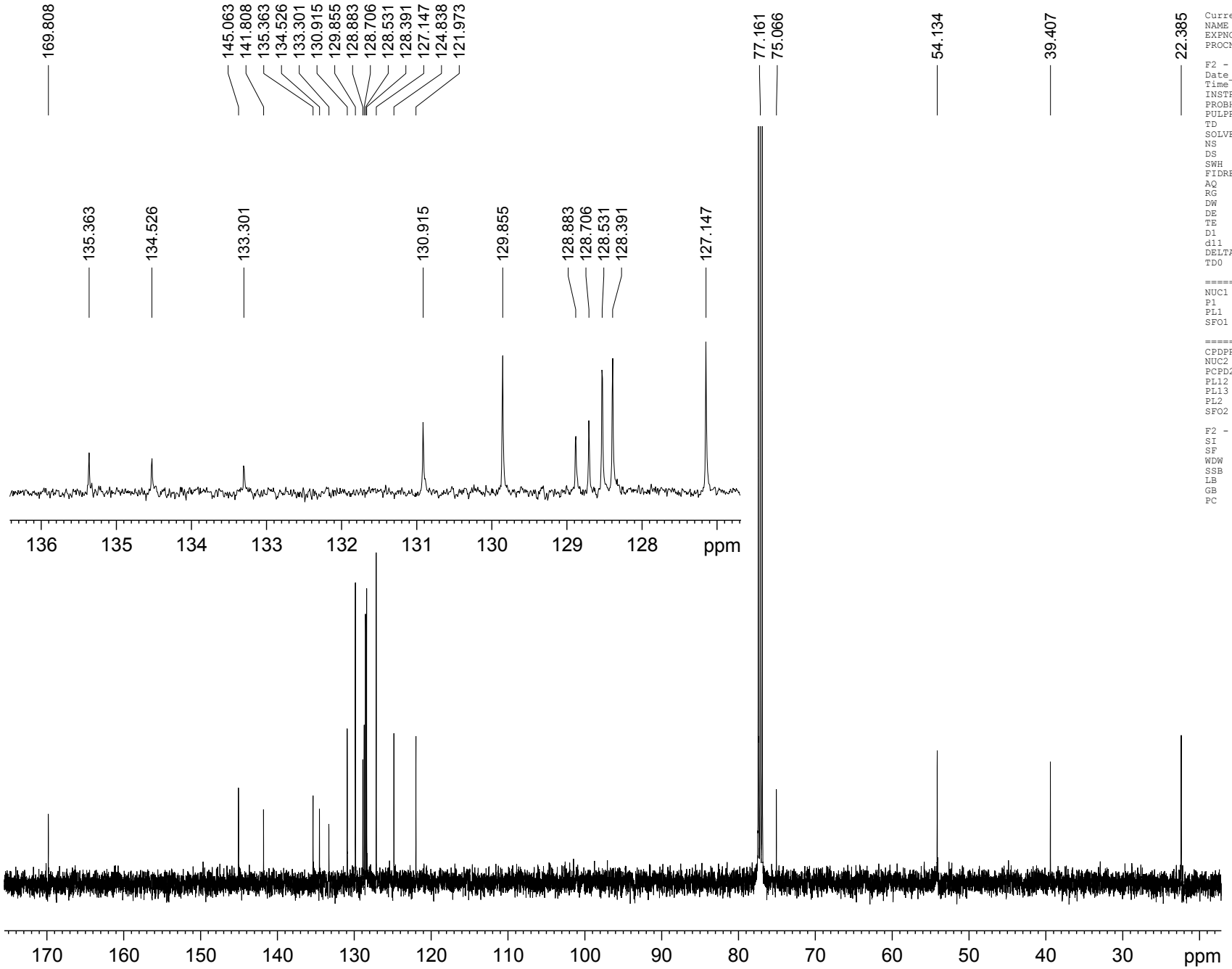

```
Current Data Parameters
NAME                  MR141-1cis
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20071205
Time                       12.08
INSTRUM                    spect
PROBHD  5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                   7002.801 Hz
FIDRES                0.106854 Hz
AQ                    4.6793203 sec
RG                          575
DW                     71.400 usec
DE                      6.50 usec
TE                      296.1 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                     10.76 usec
PL1                     0.00 dB
SFO1                500.3932525 MHz

F2 - Processing parameters
SI                        32768
SF                  500.3900161 MHz
WDW                          EM
SSB                           0
LB                     0.30 Hz
GB                            0
PC                         1.00
```





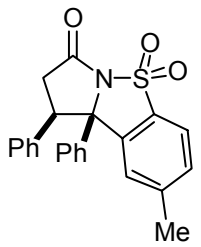

```
Current Data Parameters
NAME                  MR141-1cis
EXPNO                          2
PROCNO                         1

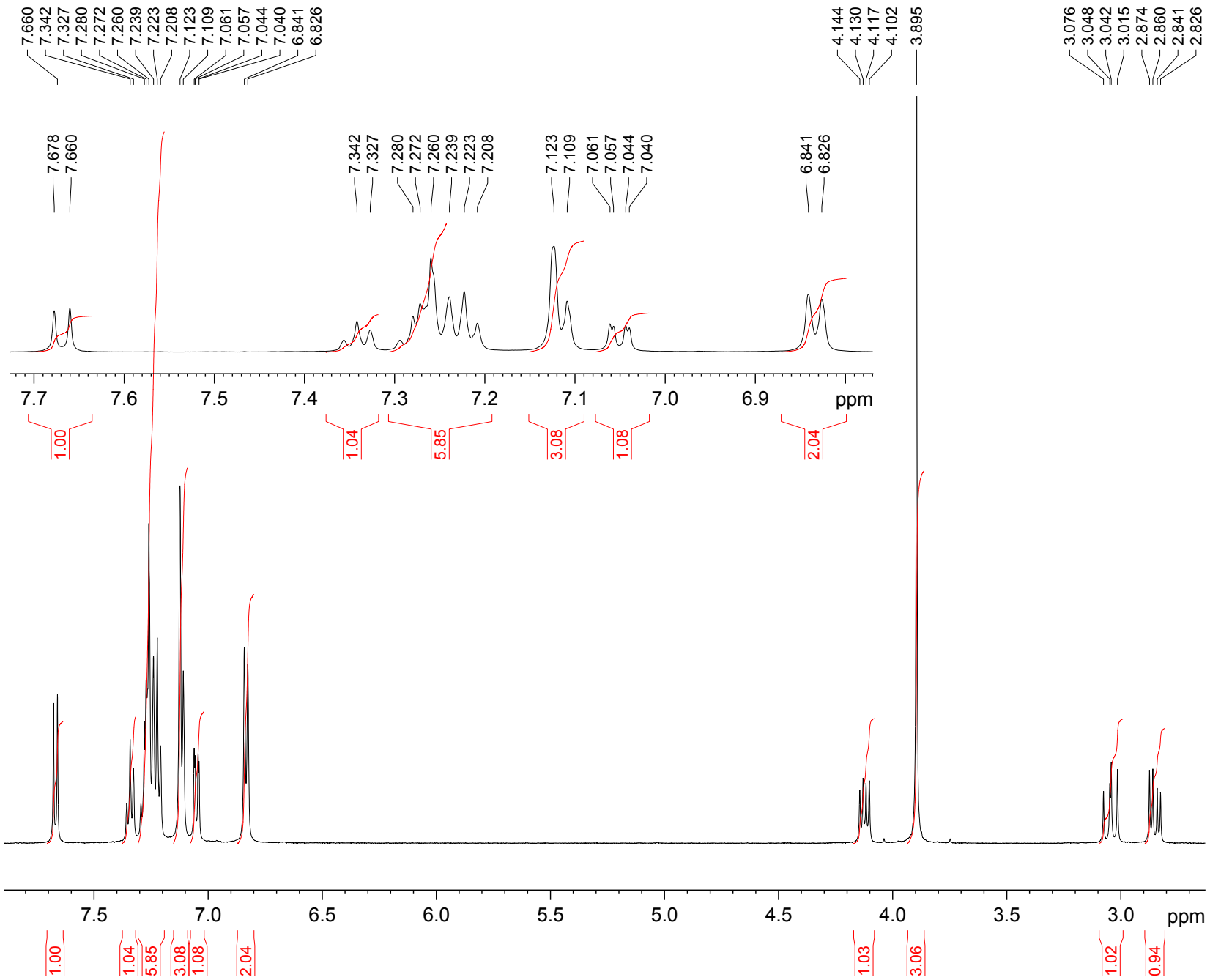
F2 - Acquisition Parameters
Date_                   20071205
Time                       12.17
INSTRUM                    spect
PROBHD  5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                           168
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010548 sec
RG                           456
DW                        16.800 usec
DE                         6.50 usec
TE                        297.3 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                         7.50 usec
PL1                        1.00 dB
SFO1                 125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                          1H
PCPD2                     80.00 usec
PL12                      17.43 dB
PL13                      18.43 dB
PL2                        0.00 dB
SFO2                 500.3920016 MHz

F2 - Processing parameters
SI                         32768
SF                   125.8231508 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                          1.40
```





Current Data Parameters

NAME	MR162-1
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

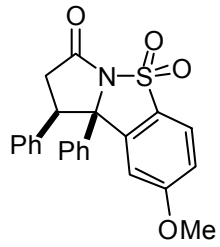
Date_	20080110
Time	8.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	10
DS	2
SWH	7002.801 Hz
FIDRES	0.106854 Hz
AQ	4.6793203 sec
RG	322
DW	71.400 usec
DE	6.50 usec
TE	297.9 K
D1	1.00000000 sec
TD0	1

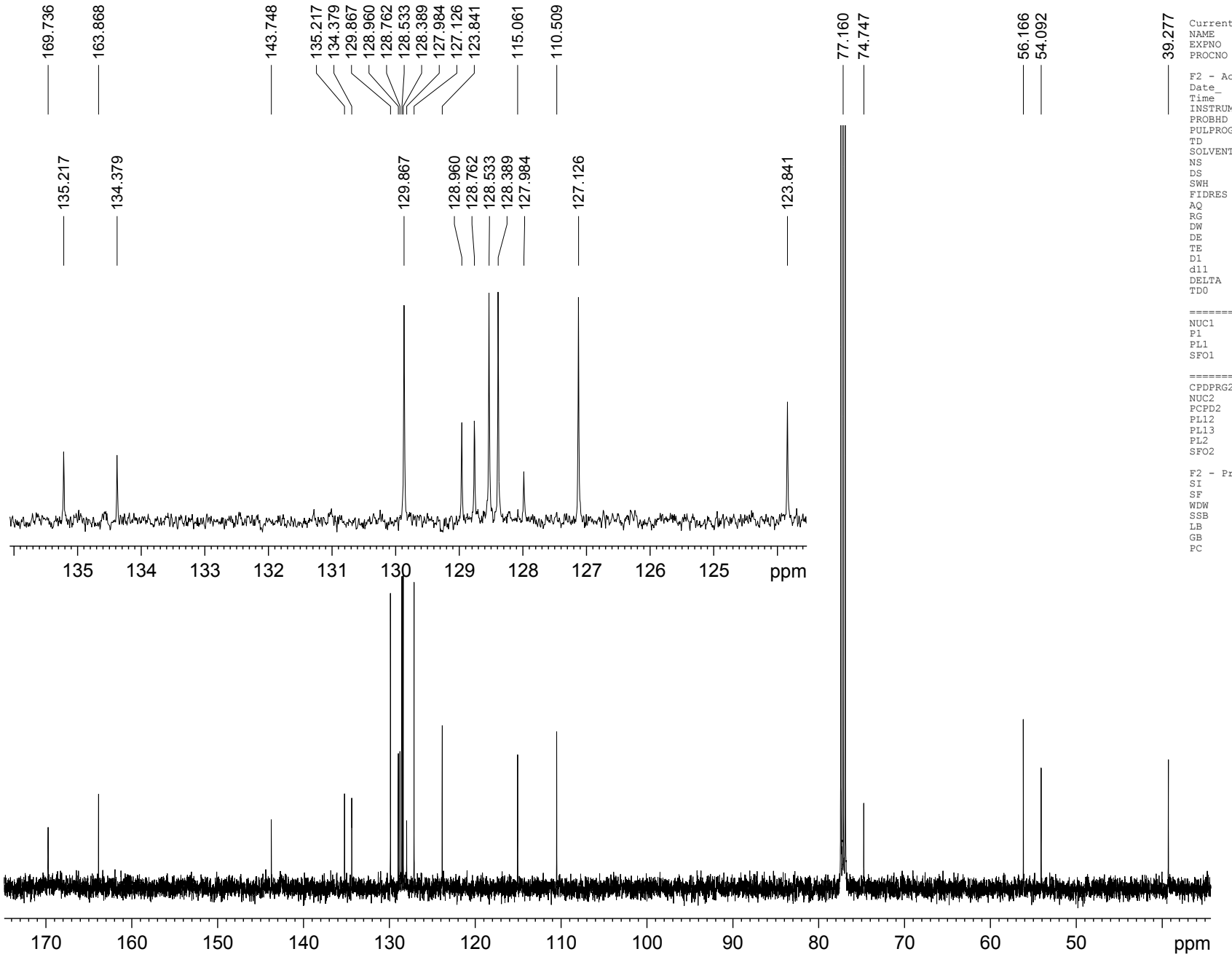
======== CHANNEL f1 ========

NUC1	1H
P1	10.76 usec
PL1	0.00 dB
SFO1	500.3932525 MHz

F2 - Processing parameters

SI	32768
SF	500.3900160 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





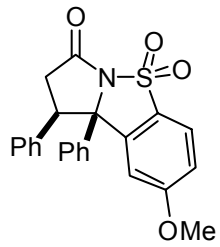

```
Current Data Parameters
NAME                      MR162-1
EXPNO                           3
PROCNO                          1

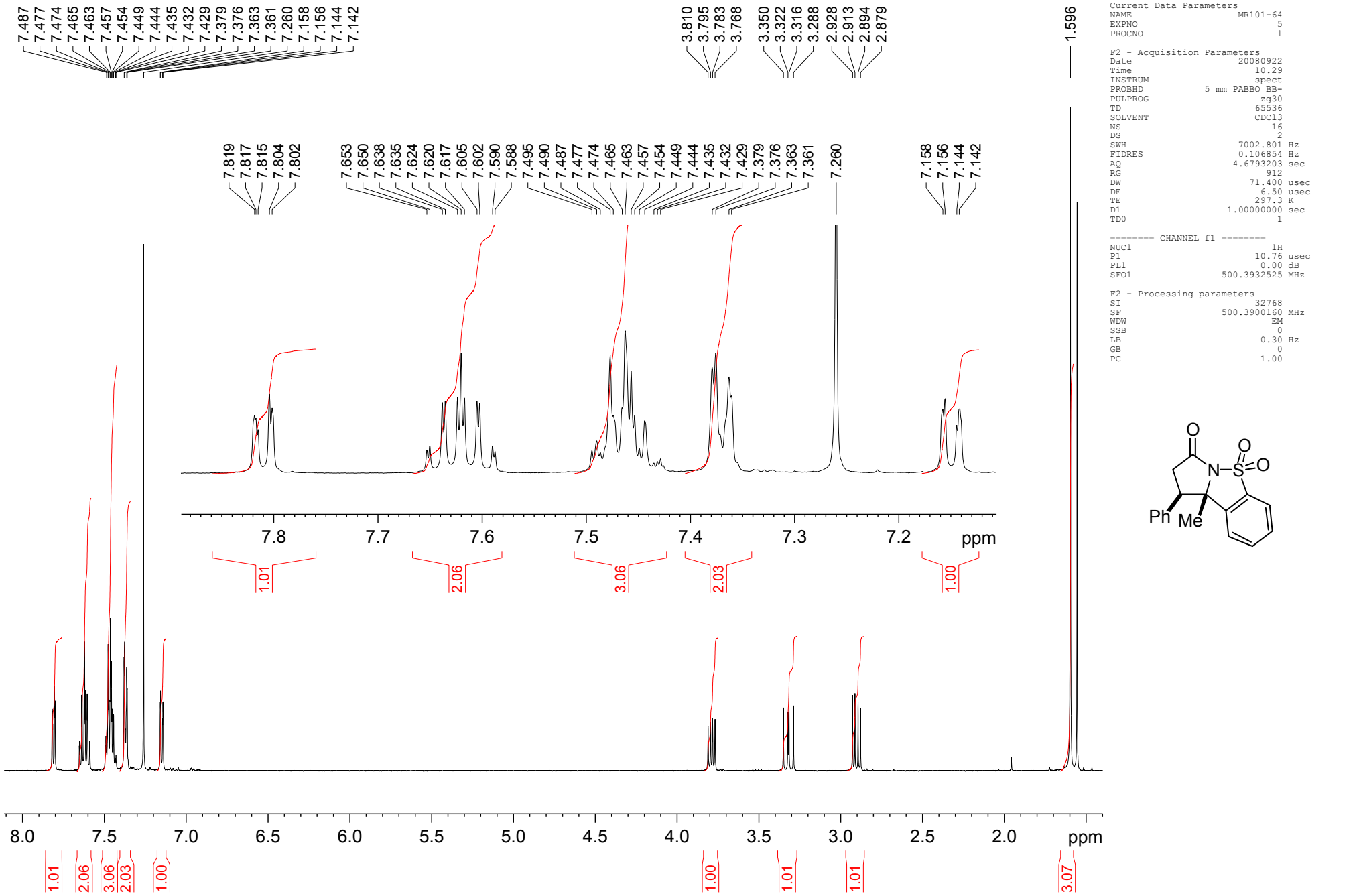
F2 - Acquisition Parameters
Date_                    20080110
Time                         8.25
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDC13
NS                           133
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010548 sec
RG                           456
DW                        16.800 usec
DE                         6.50 usec
TE                        298.7 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                        7.50 usec
PL1                       1.00 dB
SFO1                125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL12                      17.43 dB
PL13                      18.43 dB
PL2                        0.00 dB
SFO2                500.3920016 MHz

F2 - Processing parameters
SI                           32768
SF                  125.8231508 MHz
WDW                            EM
SSB                             0
LB                         1.00 Hz
GB                              0
PC                         1.40
```



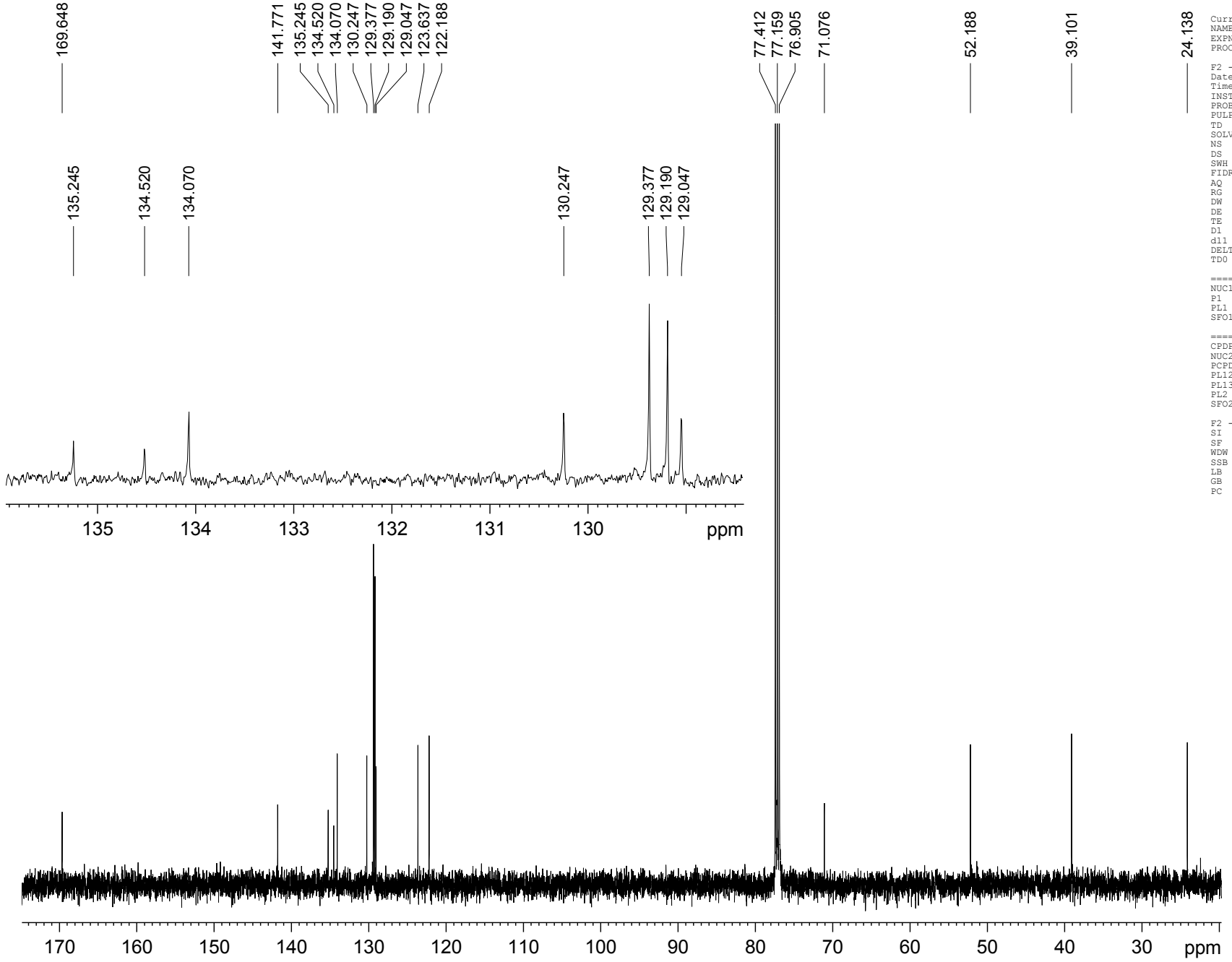



```
Current Data Parameters
NAME                   MR101-64
EXPNO                         5
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080922
Time                      10.29
INSTRUM                   spect
PROBHD  5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                 7002.801 Hz
FIDRES              0.106854 Hz
AQ                  4.6793203 sec
RG                         912
DW                    71.400 usec
DE                     6.50 usec
TE                     297.3 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                    10.76 usec
PL1                    0.00 dB
SFO1           500.3932525 MHz

F2 - Processing parameters
SI                       32768
SF             500.3900160 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                        1.00
```



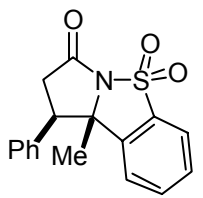

```
Current Data Parameters
NAME                  MR101-63
EXPNO                        3
PROCNO                       1

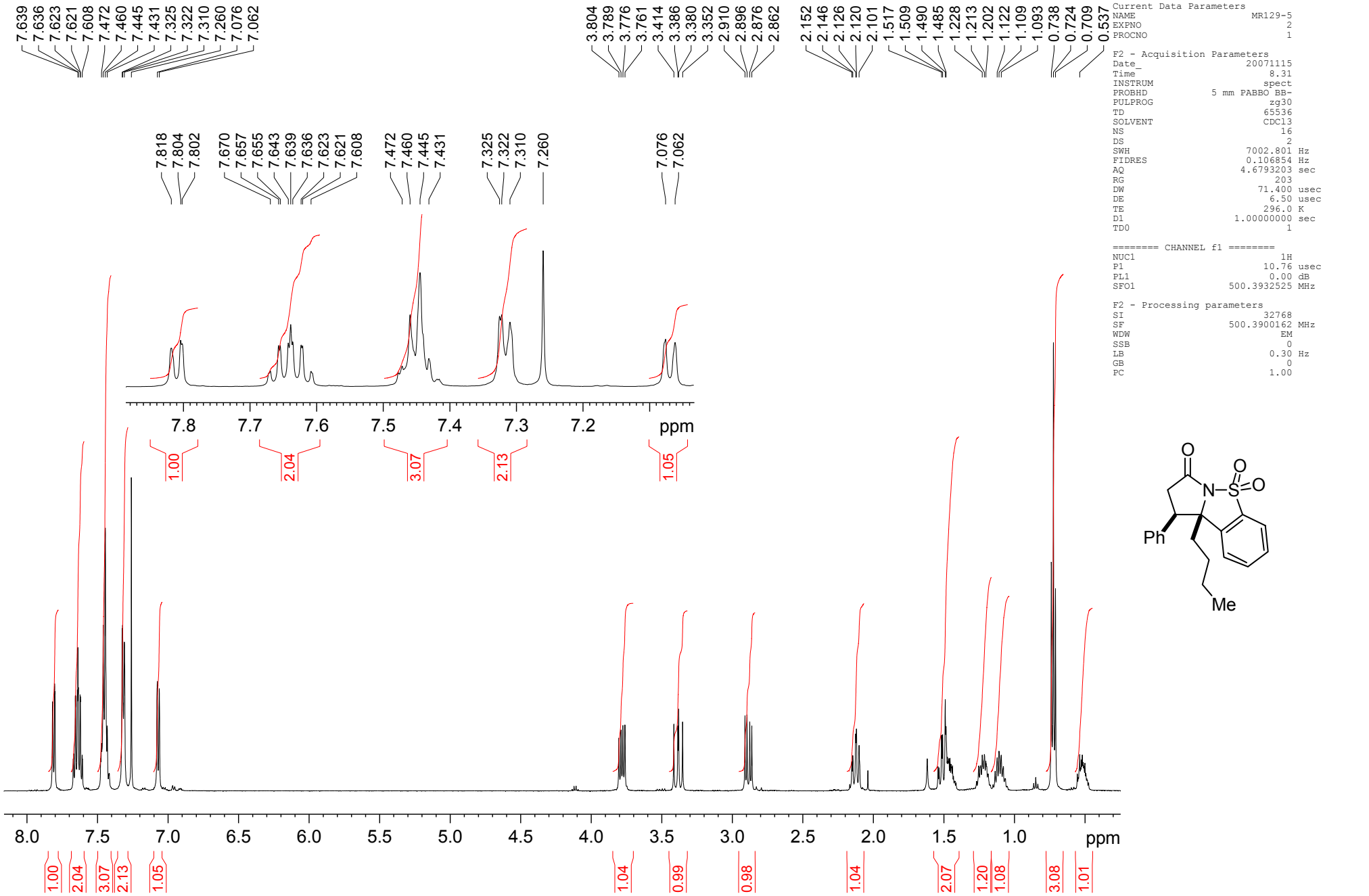
F2 - Acquisition Parameters
Date_                 20080801
Time                     18.18
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        211
DS                          4
SWH                 29761.904 Hz
FIDRES                0.454131 Hz
AQ                   1.1010548 sec
RG                         912
DW                    16.800 usec
DE                     6.50 usec
TE                     298.6 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                          1

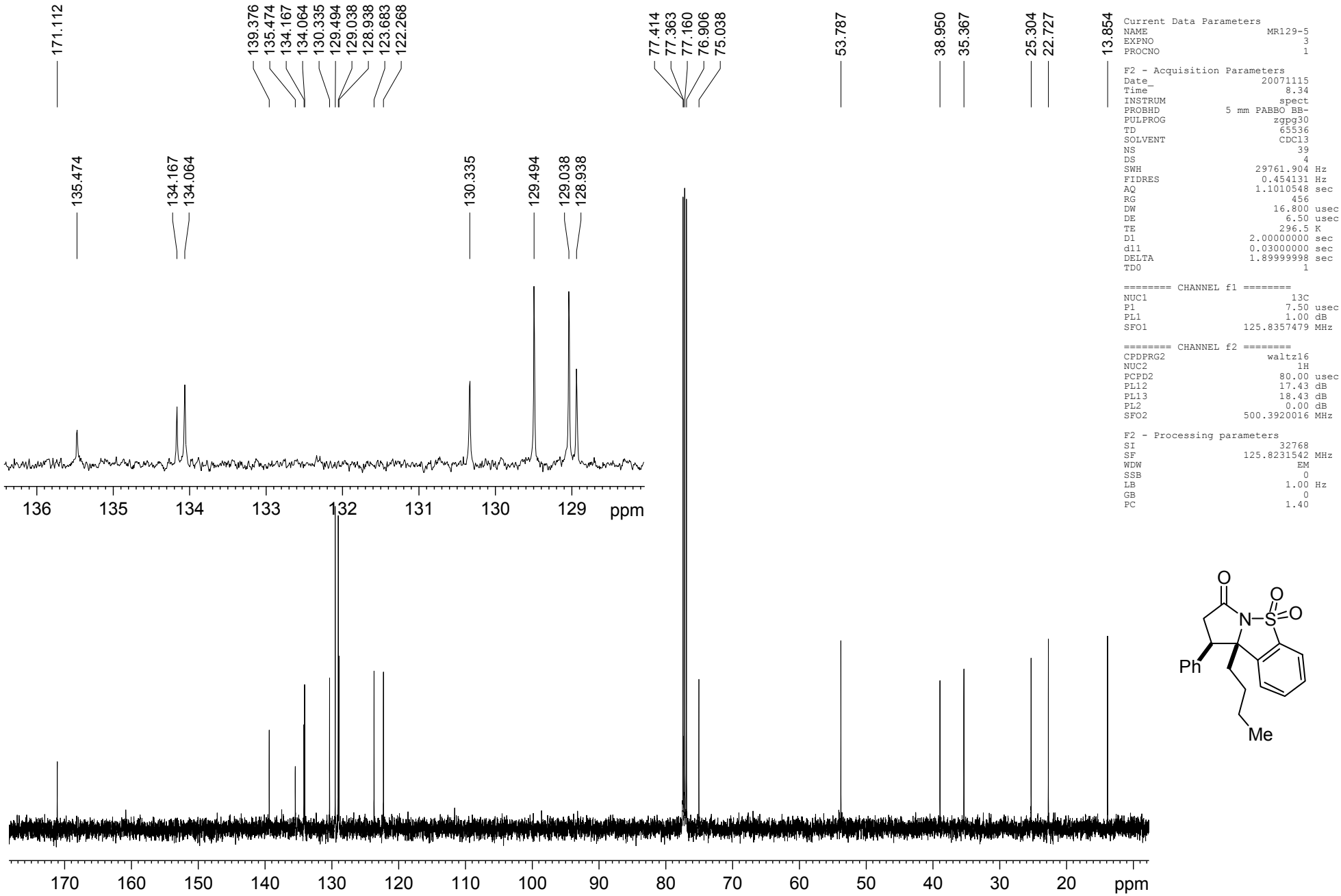
======== CHANNEL f1 ========
NUC1                       13C
P1                    7.50 usec
PL1                    1.00 dB
SFO1              125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 80.00 usec
PL12                   17.43 dB
PL13                   18.43 dB
PL2                     0.00 dB
SFO2              500.3920016 MHz

F2 - Processing parameters
SI                         32768
SF                125.8231500 MHz
WDW                           EM
SSB                            0
LB                     1.00 Hz
GB                             0
PC                          1.40
```




7.639 7.636 7.623 7.621 7.608 7.472 7.460 7.445 7.431 7.325 7.322 7.310 7.260 7.076 7.062
3.804 3.789 3.776 3.761 3.414 3.386 3.380 3.352 2.910 2.896 2.876 2.862 2.152 2.146 2.126 2.120 2.101 1.517 1.509 1.490 1.485 1.228 1.213 1.202 1.122 1.109 1.093 0.738 0.724 0.709 0.537
Current Data Parameters
NAME MR129-5
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071115
Time 8.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 203
DW 71.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz
F2 - Processing parameters
SI 32768
SF 500.3900162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.818 7.804 7.802 7.670 7.657 7.655 7.643 7.639 7.636 7.623 7.621 7.608 7.472 7.460 7.445 7.431 7.325 7.322 7.310 7.260 7.076 7.062
7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
1.00 2.04 3.07 2.13 1.05
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00 2.04 3.07 2.13 1.05 1.04 0.99 0.98 1.04 2.07 1.20 1.08 3.08 1.01
O
O
N
S
O
Ph
Me



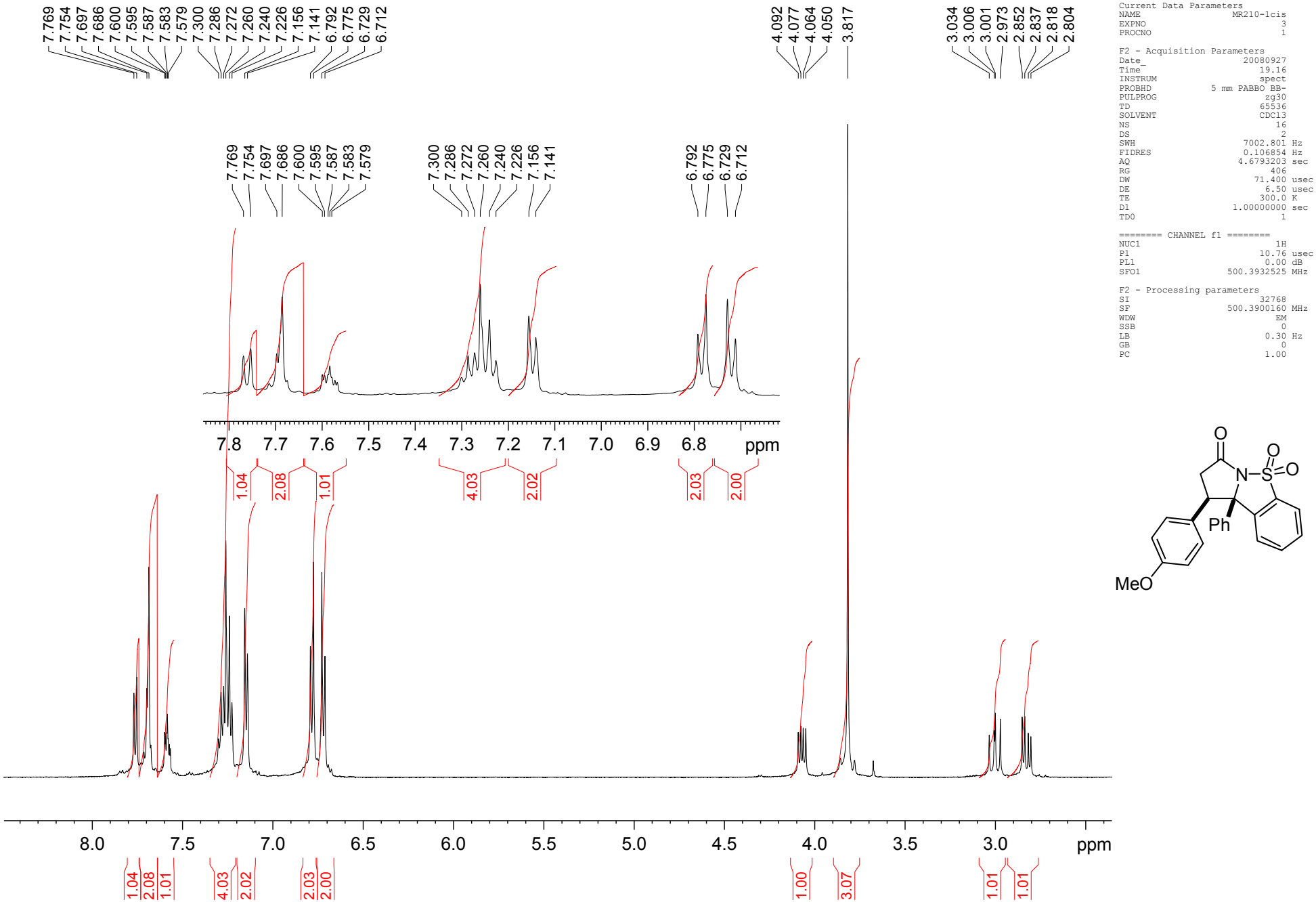

```
Current Data Parameters
NAME                      MR129-5
EXPNO                           3
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20071115
Time_                        8.34
INSTRUM                     spect
PROBHD          5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                            39
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010548 sec
RG                           456
DW                        16.800 usec
DE                         6.50 usec
TE                        296.5 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                         7.50 usec
PL1                        1.00 dB
SFO1                 125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL12                      17.43 dB
PL13                      18.43 dB
PL2                        0.00 dB
SFO2                 500.3920016 MHz

F2 - Processing parameters
SI                         32768
SF                   125.8231542 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                         1.40
```

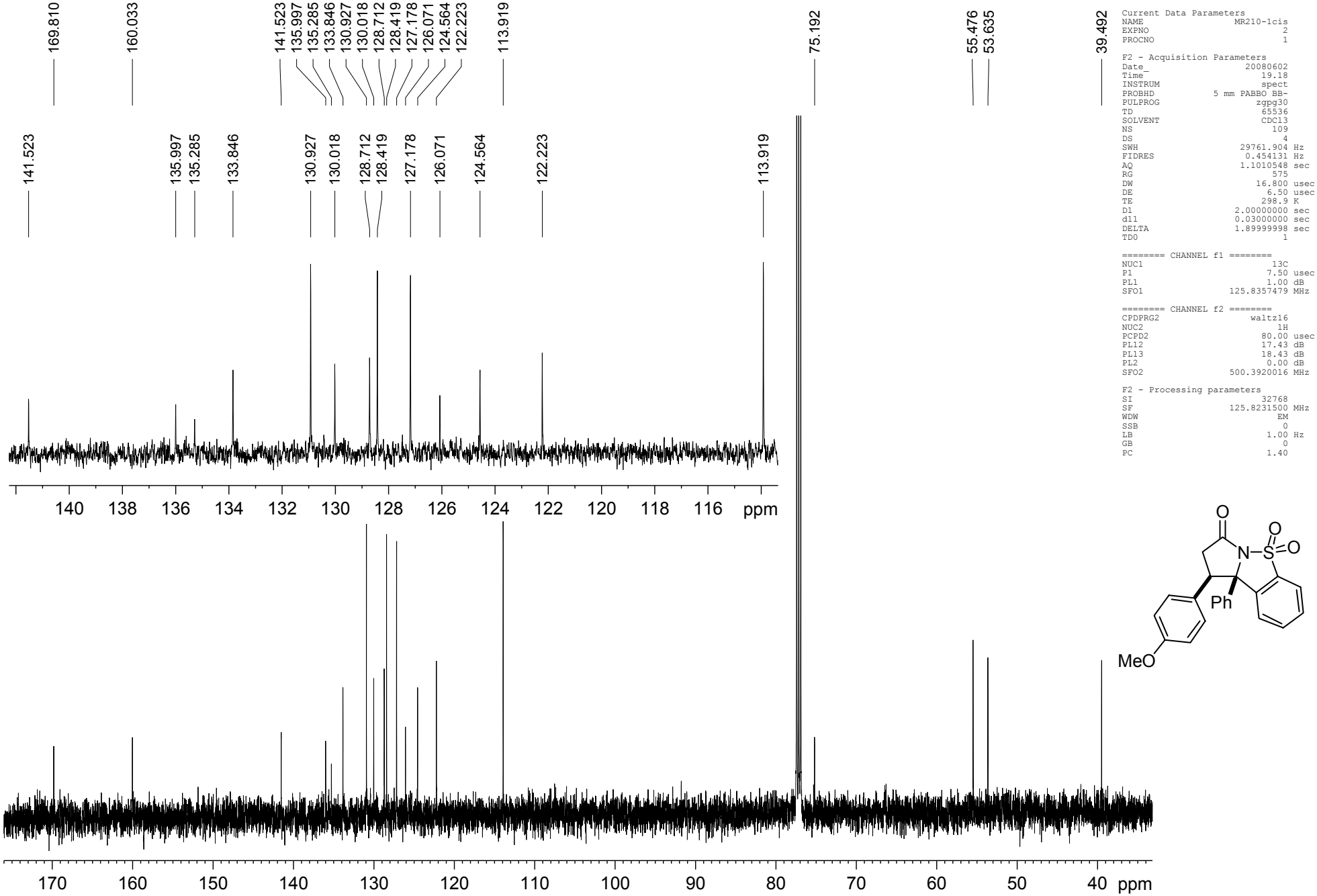



```
Current Data Parameters
NAME                  MR210-1cis
EXPNO                          3
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20080927
Time                       19.16
INSTRUM                    spect
PROBHD  5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            16
DS                             2
SWH                  7002.801 Hz
FIDRES               0.106854 Hz
AQ                   4.6793203 sec
RG                           406
DW                    71.400 usec
DE                     6.50 usec
TE                     300.0 K
D1                   1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                    10.76 usec
PL1                    0.00 dB
SFO1                500.3932525 MHz

F2 - Processing parameters
SI                         32768
SF                  500.3900160 MHz
WDW                           EM
SSB                            0
LB                     0.30 Hz
GB                             0
PC                          1.00
```



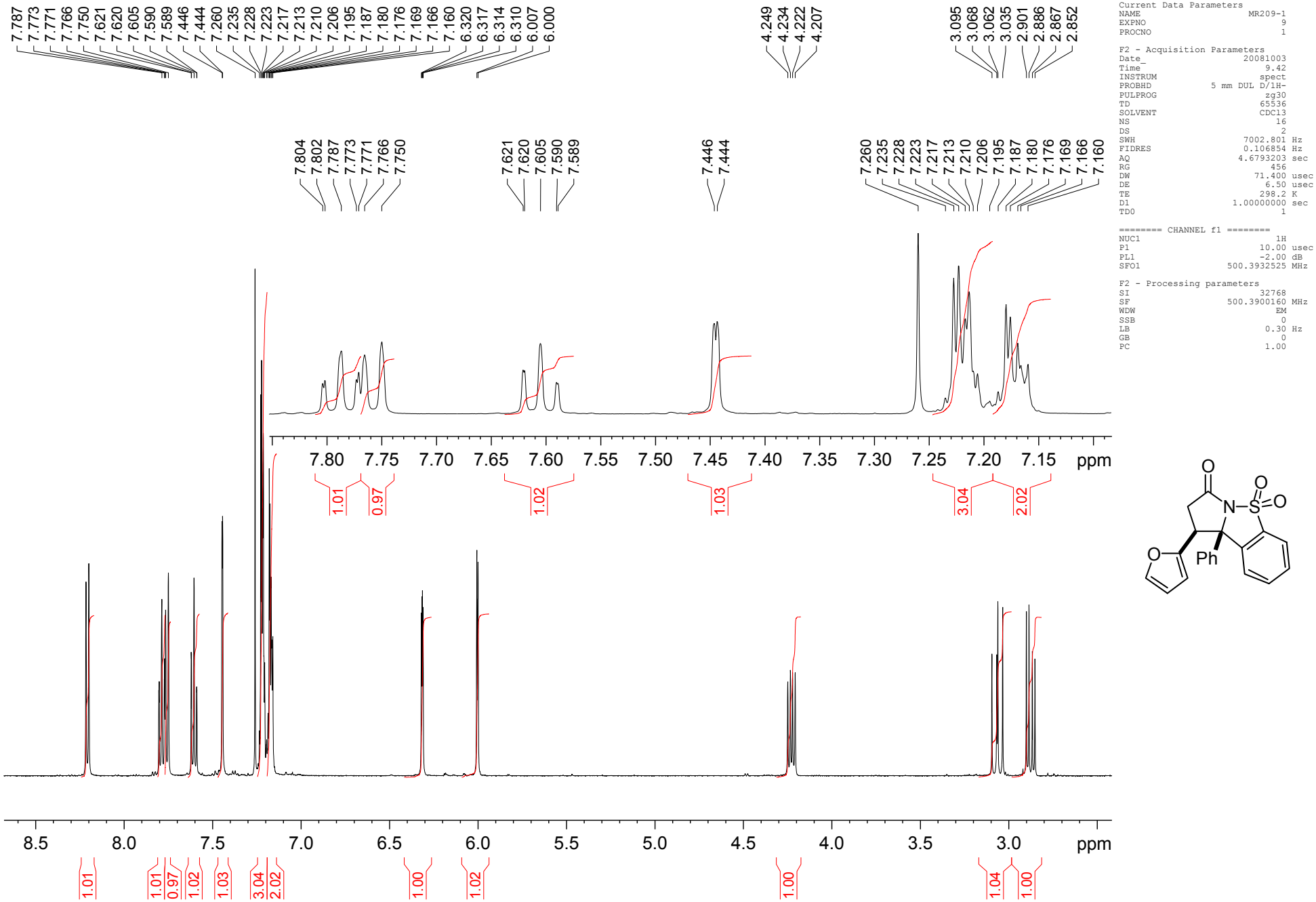
Current Data Parameters
NAME MR210-1cis
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080602
Time 19.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 109
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 575
DW 16.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 32768
SF 125.8231500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

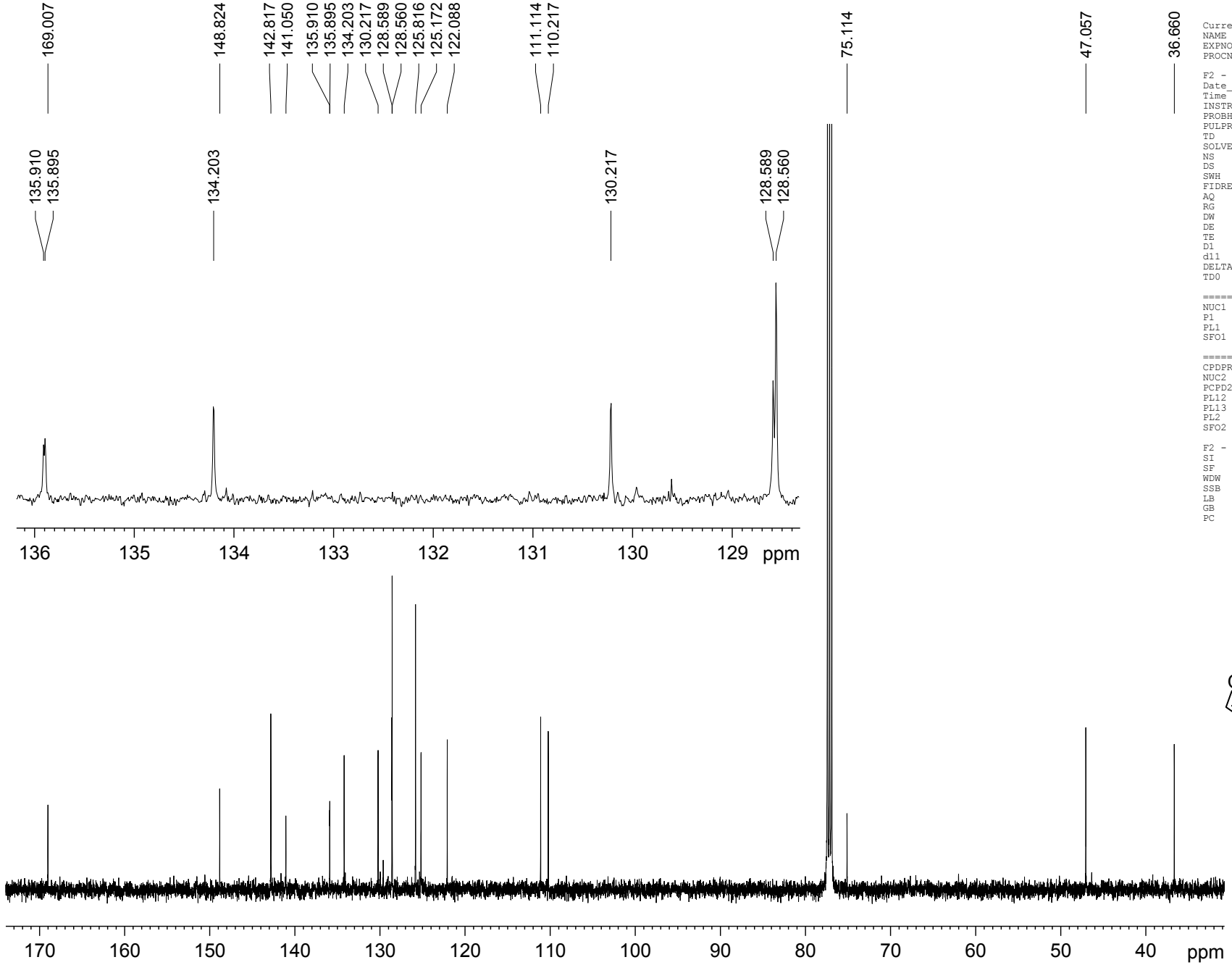



```
Current Data Parameters
NAME                      MR209-1
EXPNO                           9
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20081003
Time                         9.42
INSTRUM                     spect
PROBHD       5 mm DUL D/1H-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                           456
DW                        71.400 usec
DE                         6.50 usec
TE                        298.2 K
D1                  1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.00 usec
PL1                       -2.00 dB
SFO1                500.3932525 MHz

F2 - Processing parameters
SI                         32768
SF                  500.3900160 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```



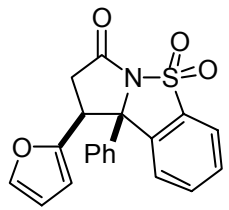

```
Current Data Parameters
NAME                      MR209-1
EXPNO                           5
PROCNO                          1

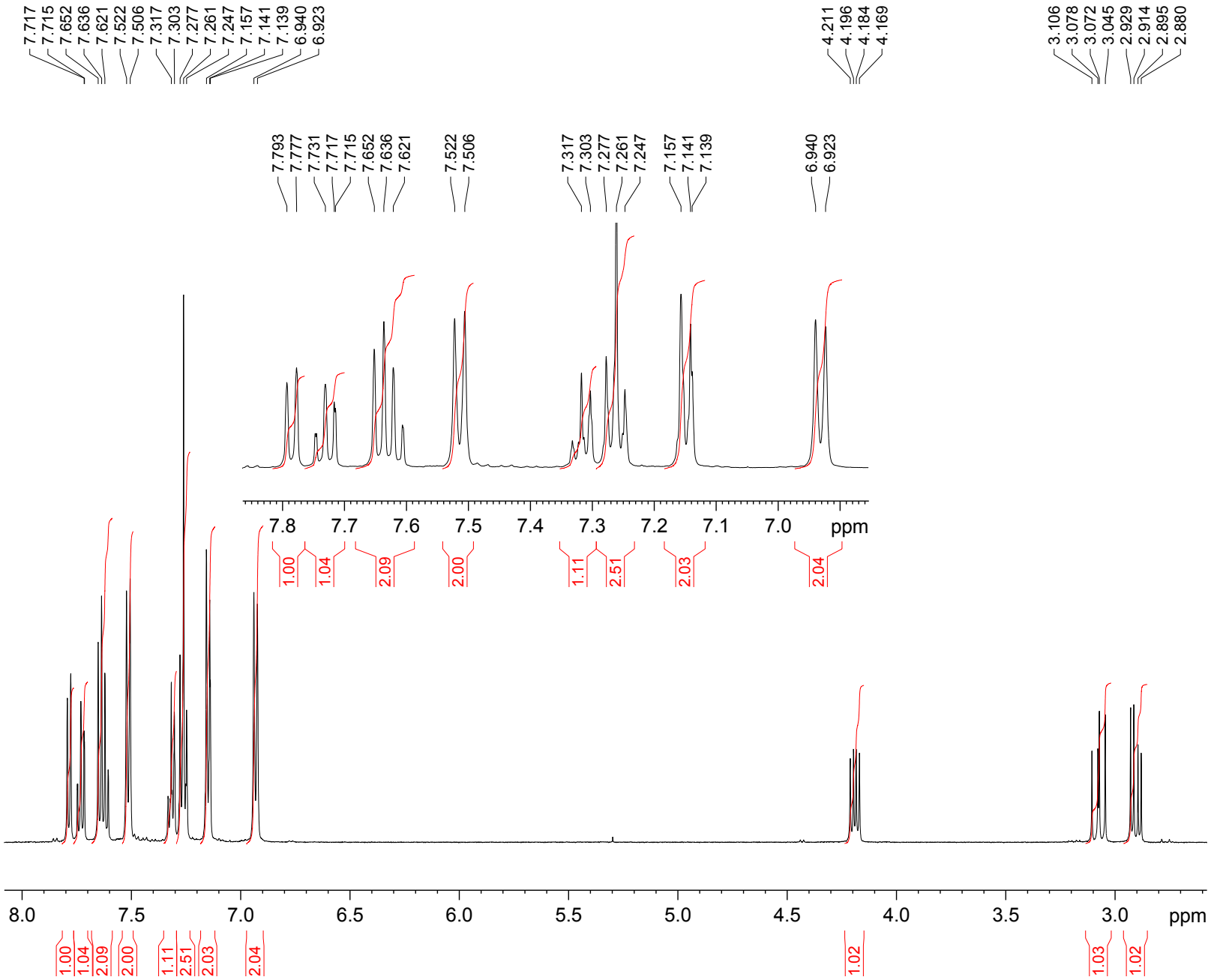
F2 - Acquisition Parameters
Date_                    20080928
Time                         1.22
INSTRUM                     spect
PROBHD          5 mm PABBO BB-
PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                            462
DS                              4
SWH                     29761.904 Hz
FIDRES                  0.454131 Hz
AQ                      1.1010548 sec
RG                            912
DW                         16.800 usec
DE                          6.50 usec
TE                         298.5 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                          13C
P1                          7.50 usec
PL1                         1.00 dB
SFO1                  125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                           1H
PCPD2                      80.00 usec
PL12                       17.43 dB
PL13                       18.43 dB
PL2                         0.00 dB
SFO2                  500.3920016 MHz

F2 - Processing parameters
SI                            32768
SF                    125.8231500 MHz
WDW                              EM
SSB                               0
LB                          1.00 Hz
GB                                0
PC                             1.40
```



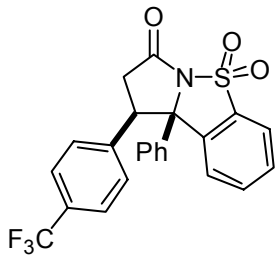


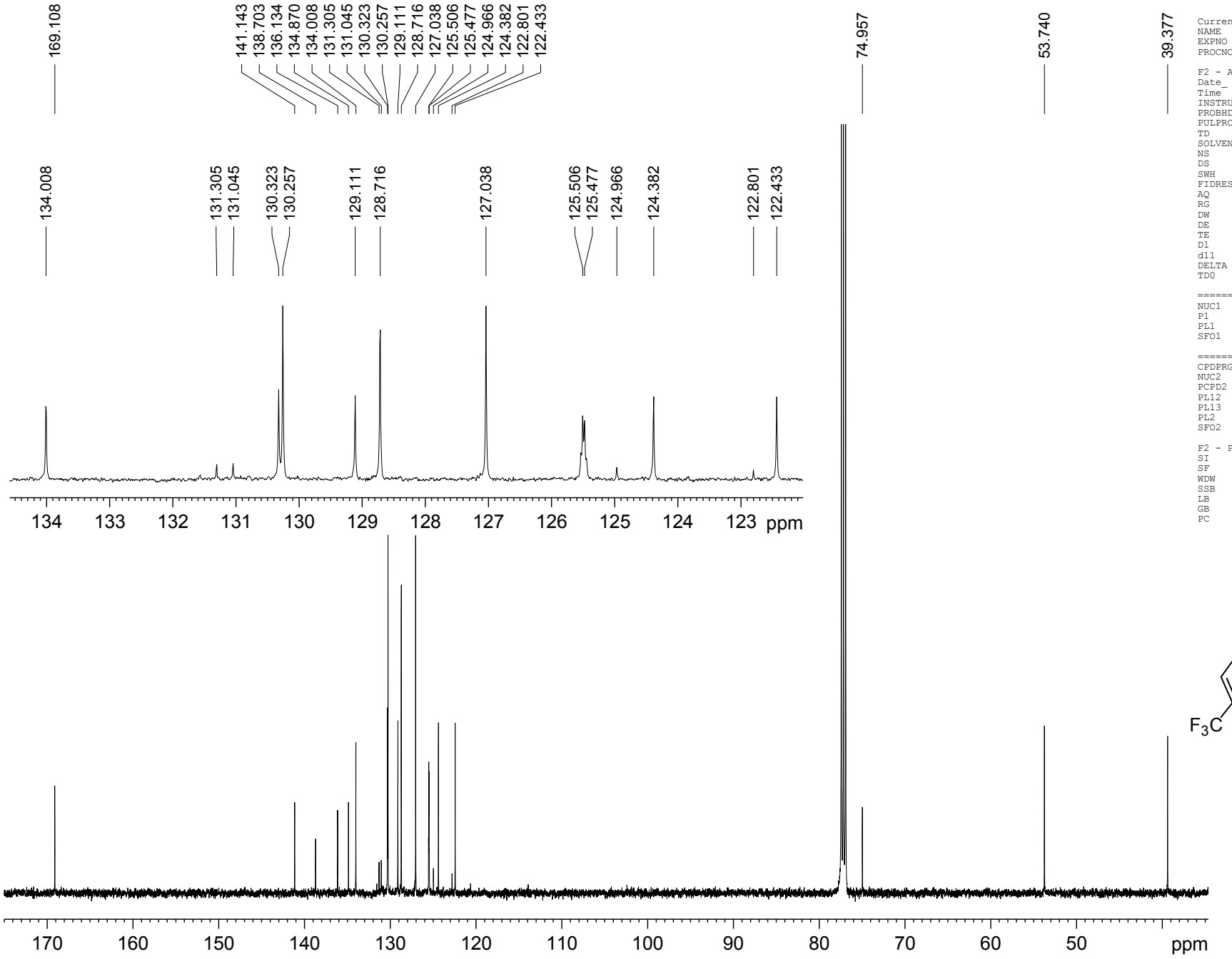

```
Current Data Parameters
NAME                      MR211-1
EXPNO                           2
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20080709
Time                        17.35
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                     4.6793203 sec
RG                            362
DW                     71.400 usec
DE                      6.50 usec
TE                        298.2 K
D1                  1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                     10.76 usec
PL1                     0.00 dB
SFO1                500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                  500.3900160 MHz
WDW                            EM
SSB                             0
LB                      0.30 Hz
GB                              0
PC                           1.00
```





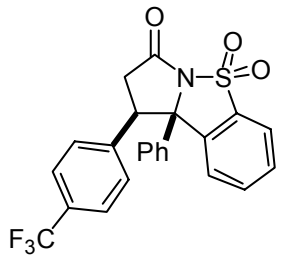

```
Current Data Parameters
NAME                      MR211-1
EXPNO                           5
PROCNO                          1

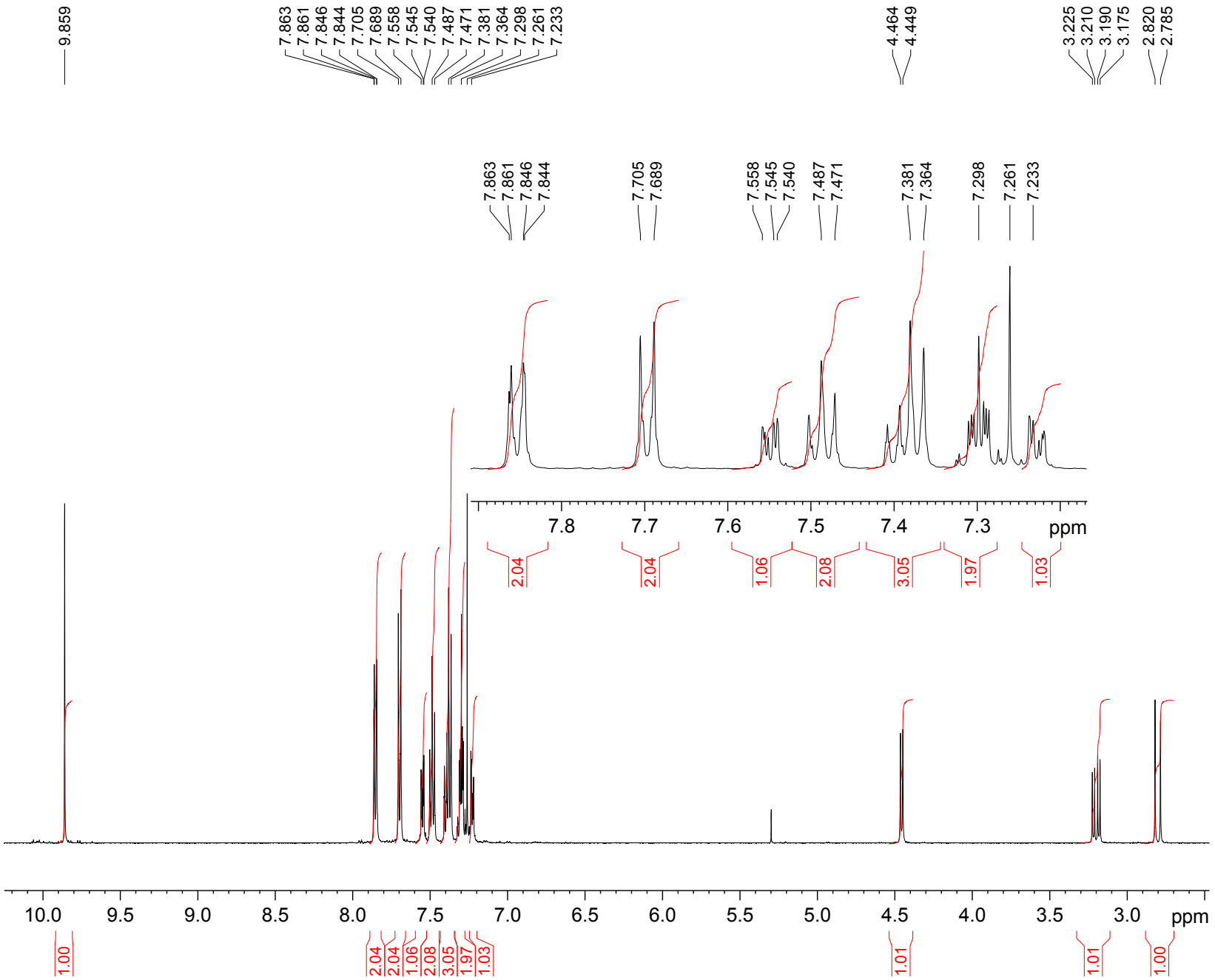
F2 - Acquisition Parameters
Date_                    20080927
Time                        20.35
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                         1571
DS                            4
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                   1.1010548 sec
RG                          912
DW                     16.800 usec
DE                      6.50 usec
TE                      298.6 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                      7.50 usec
PL1                     1.00 dB
SFO1               125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                  80.00 usec
PL12                    17.43 dB
PL13                    18.43 dB
PL2                      0.00 dB
SFO2               500.3920016 MHz

F2 - Processing parameters
SI                         32768
SF                 125.8231500 MHz
WDW                           EM
SSB                            0
LB                      1.00 Hz
GB                             0
PC                      1.40
```



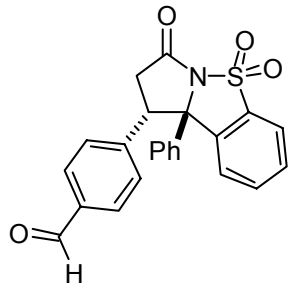


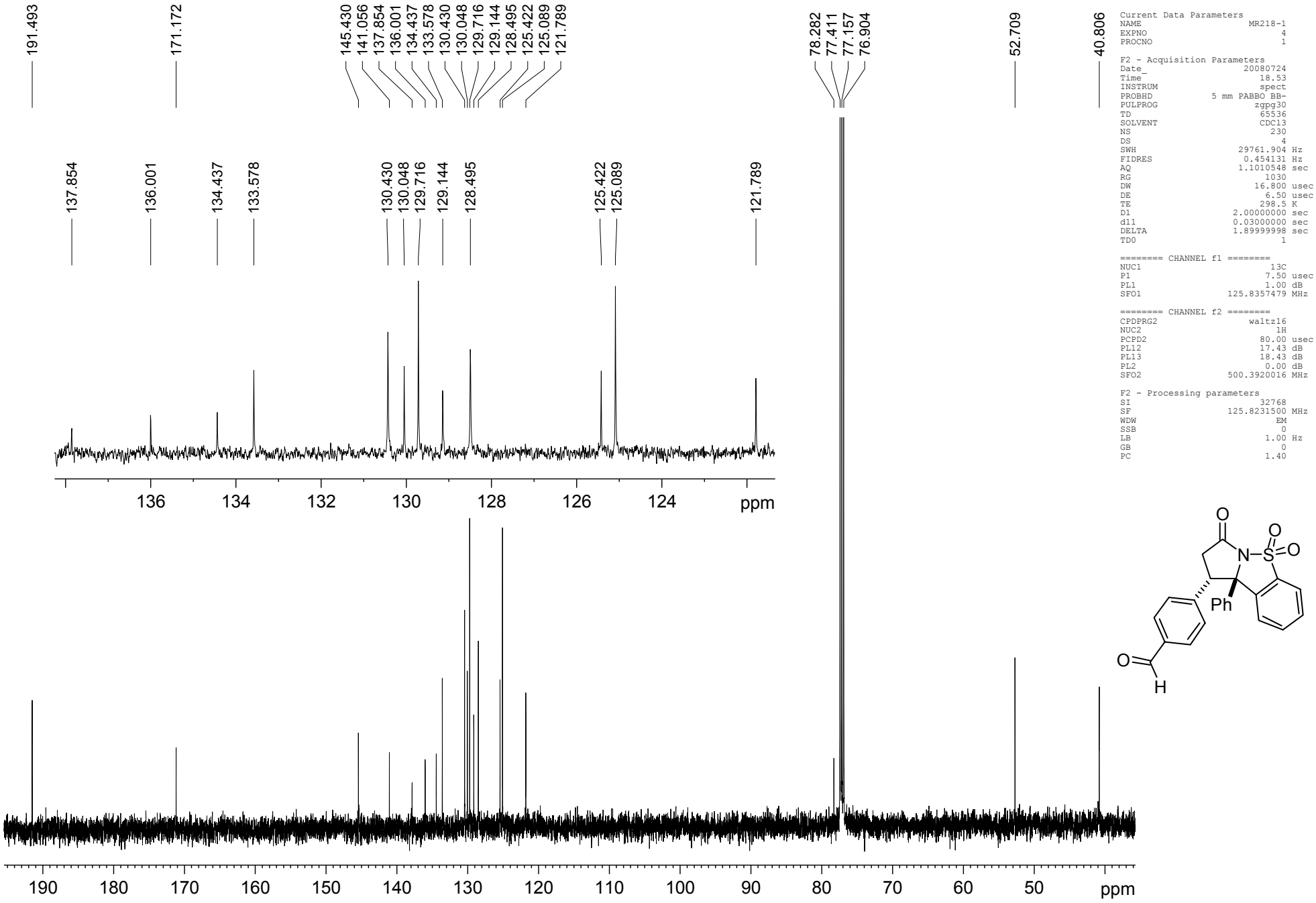

```
Current Data Parameters
NAME                      MR218-1
EXPNO                           2
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20080723
Time                        10.29
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                            645
DW                       71.400 usec
DE                        6.50 usec
TE                        298.3 K
D1                   1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                       10.76 usec
PL1                       0.00 dB
SFO1                 500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                  500.3900160 MHz
WDW                            EM
SSB                             0
LB                        0.30 Hz
GB                              0
PC                           1.00
```





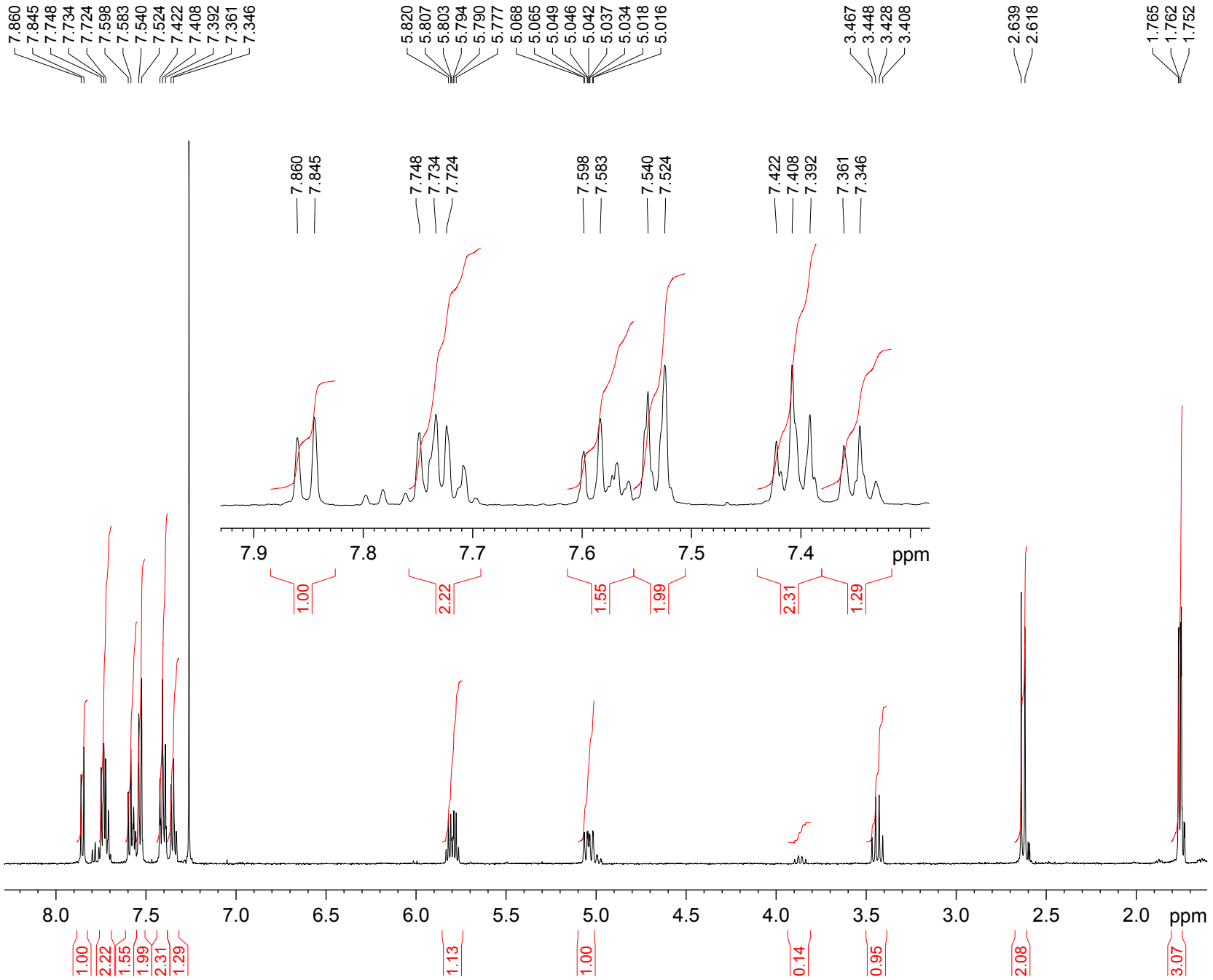

```
Current Data Parameters
NAME                      MR218-1
EXPNO                           4
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20080724
Time                        18.53
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                           230
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010548 sec
RG                          1030
DW                        16.800 usec
DE                         6.50 usec
TE                        298.5 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                         7.50 usec
PL1                        1.00 dB
SFO1                 125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL12                      17.43 dB
PL13                      18.43 dB
PL2                        0.00 dB
SFO2                 500.3920016 MHz

F2 - Processing parameters
SI                           32768
SF                 125.8231500 MHz
WDW                             EM
SSB                              0
LB                         1.00 Hz
GB                               0
PC                            1.40
```



Current Data Parameters

NAME	MR213-2
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

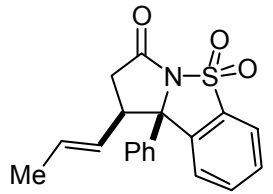
Date_	20080709
Time	17.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	14
DS	2
SWH	7002.801 Hz
FIDRES	0.106854 Hz
AQ	4.6793203 sec
RG	1030
DW	71.400 usec
DE	6.50 usec
TE	298.4 K
D1	1.00000000 sec
TD0	1

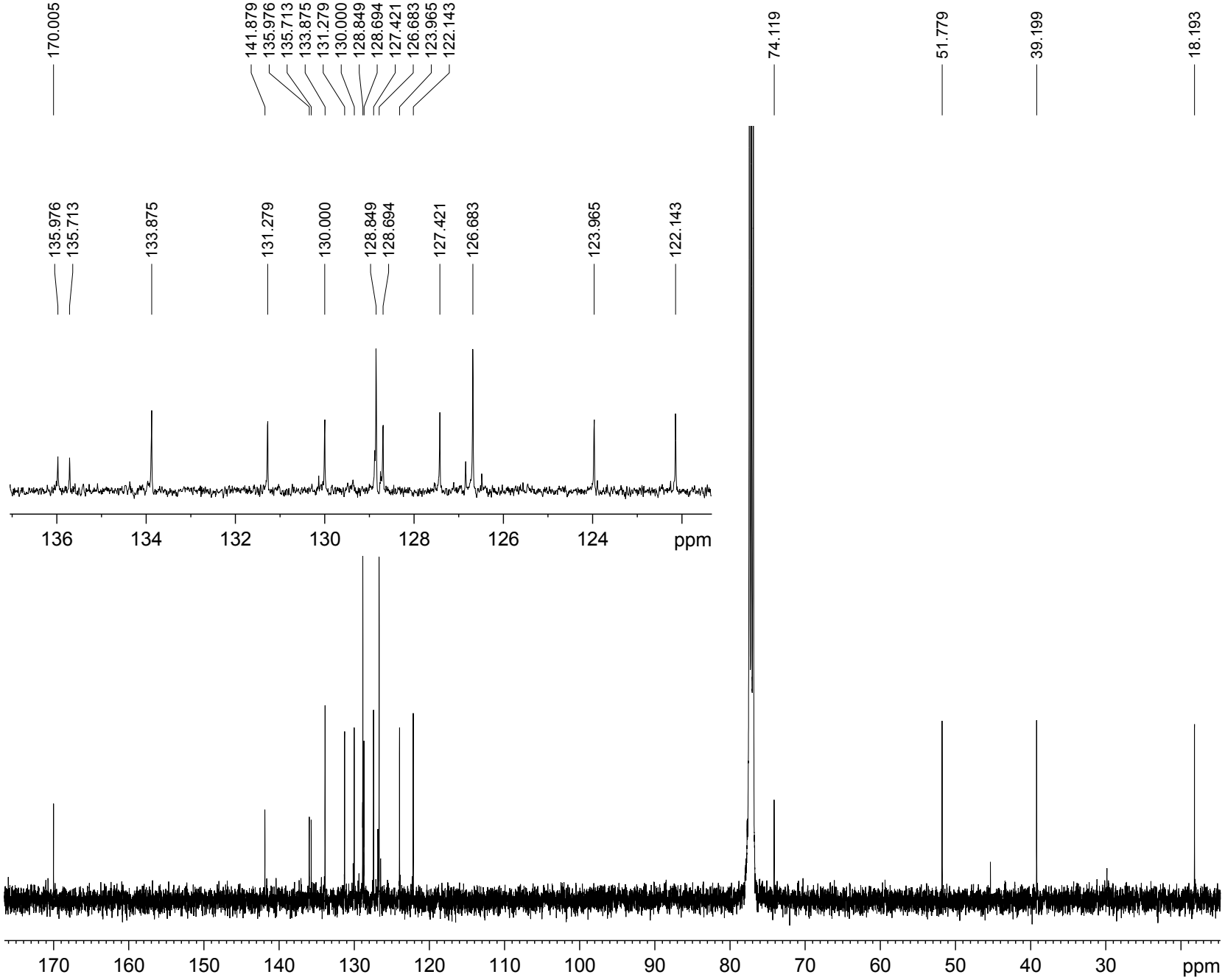
======== CHANNEL f1 ========

NUC1	1H
P1	10.76 usec
PL1	0.00 dB
SFO1	500.3932525 MHz

F2 - Processing parameters

SI	32768
SF	500.3900160 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





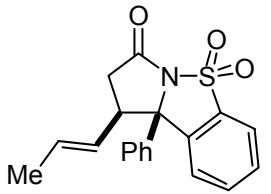

```
Current Data Parameters
NAME                      MR213-2
EXPNO                           7
PROCNO                          1

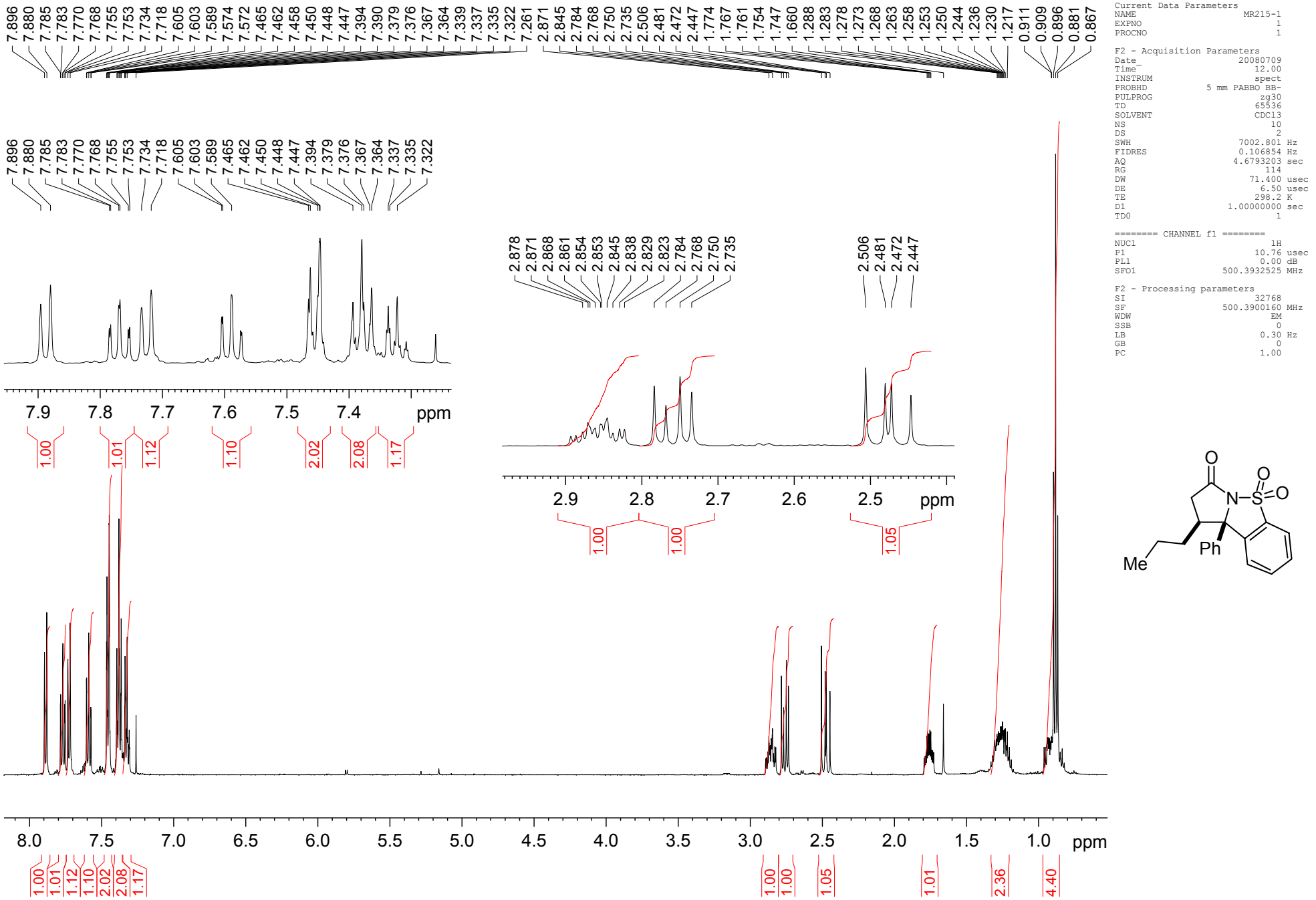
F2 - Acquisition Parameters
Date_                    20080928
Time                         1.57
INSTRUM                     spect
PROBHD          5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                          6144
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010548 sec
RG                          1030
DW                        16.800 usec
DE                         6.50 usec
TE                        298.5 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                            1

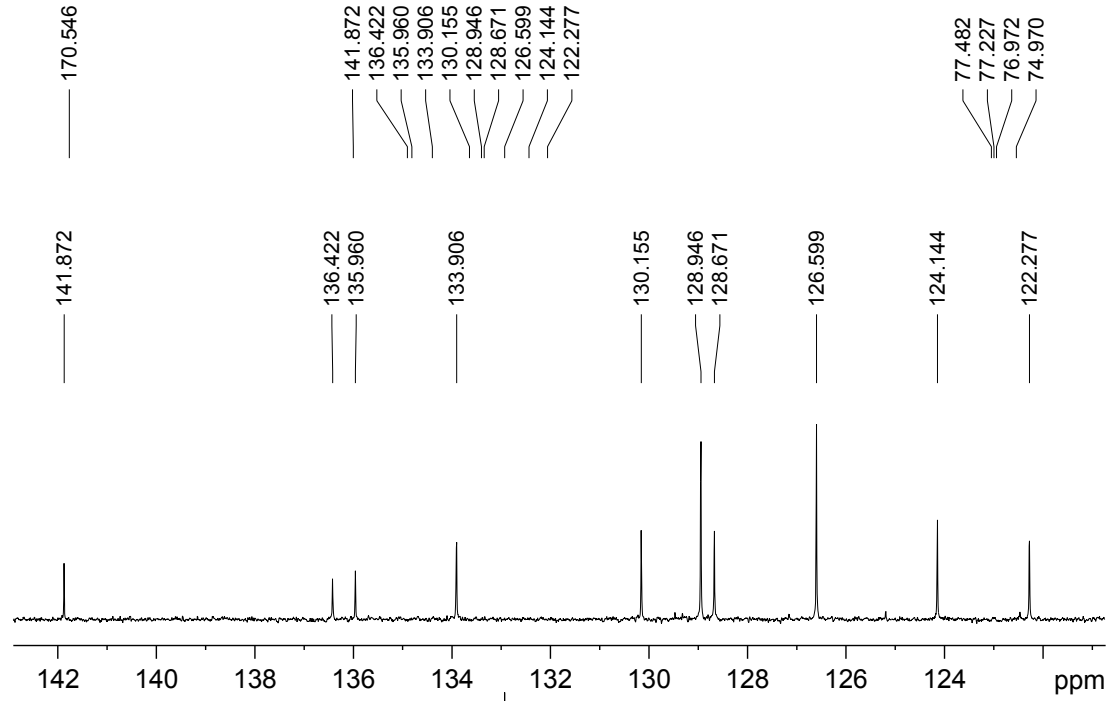
======== CHANNEL f1 ========
NUC1                         13C
P1                        7.50 usec
PL1                       1.00 dB
SFO1                125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                    80.00 usec
PL12                     17.43 dB
PL13                     18.43 dB
PL2                       0.00 dB
SFO2                500.3920016 MHz

F2 - Processing parameters
SI                           32768
SF                  125.8231500 MHz
WDW                            EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                         1.40
```




7.896 7.880 7.785 7.783 7.770 7.768 7.755 7.753 7.734 7.718 7.605 7.603 7.589 7.574 7.572 7.465 7.462 7.458 7.450 7.448 7.447 7.394 7.390 7.379 7.376 7.367 7.364 7.339 7.337 7.335 7.322 7.261 2.871 2.845 2.784 2.768 2.750 2.735 2.506 2.481 2.472 2.447 1.774 1.767 1.761 1.754 1.747 1.660 1.288 1.283 1.278 1.273 1.268 1.263 1.258 1.253 1.250 1.244 1.236 1.230 1.217 0.911 0.909 0.896 0.881 0.867
Current Data Parameters
NAME MR215-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080709
Time 12.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 7002.801 Hz
FIDRES 0.106854 Hz
AQ 4.6793203 sec
RG 114
DW 71.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.76 usec
PL1 0.00 dB
SFO1 500.3932525 MHz
F2 - Processing parameters
SI 32768
SF 500.3900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.896 7.880 7.785 7.783 7.770 7.768 7.755 7.753 7.734 7.718 7.605 7.603 7.589 7.465 7.462 7.450 7.448 7.447 7.394 7.379 7.376 7.367 7.364 7.337 7.335 7.322
2.878 2.871 2.868 2.861 2.854 2.853 2.845 2.838 2.829 2.823 2.784 2.768 2.750 2.735
2.506 2.481 2.472 2.447
7.9 7.8 7.7 7.6 7.5 7.4 ppm
1.00 1.01 1.12 1.10 2.02 2.08 1.17
2.9 2.8 2.7 2.6 2.5 ppm
1.00 1.00 1.05
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00 1.01 1.12 1.10 2.02 2.08 1.17 1.00 1.00 1.05 1.01 2.36 4.40
O O N S O Ph Me



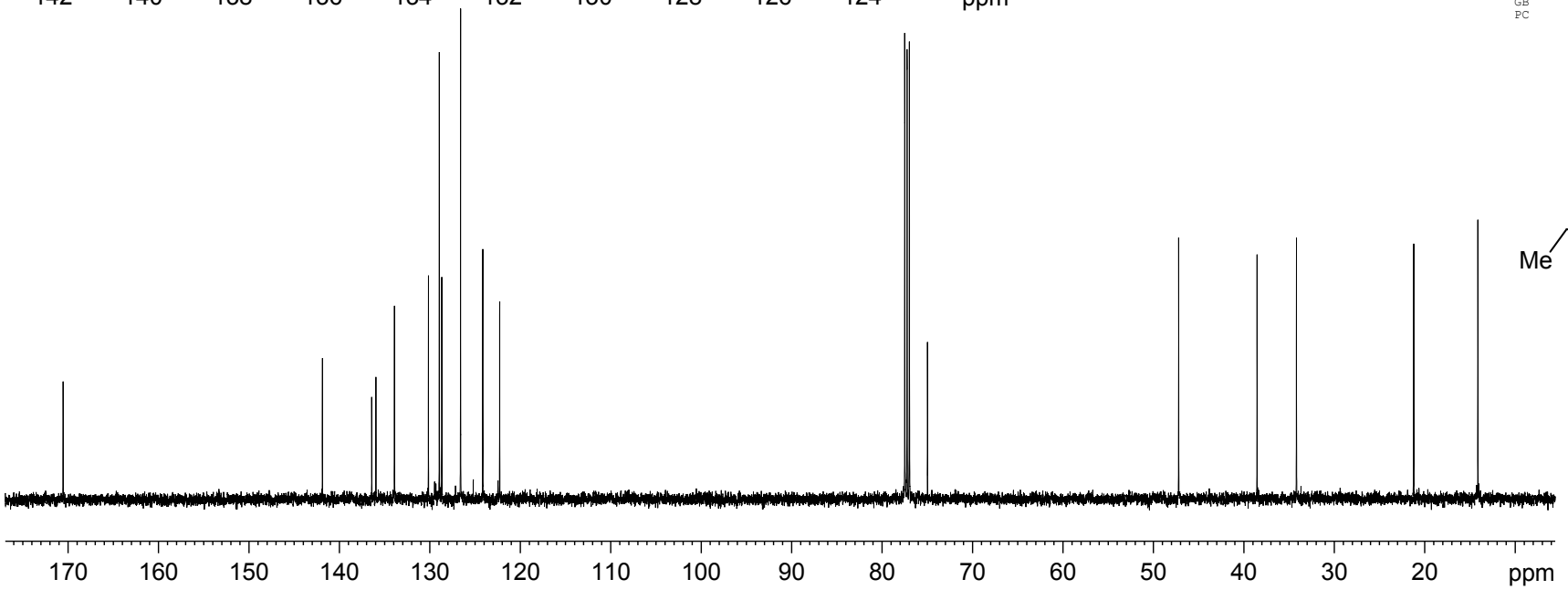

```
Current Data Parameters
NAME                       MR215-1
EXPNO                            2
PROCNO                           1

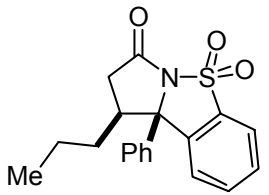
F2 - Acquisition Parameters
Date_                     20080709
Time_                        12.05
INSTRUM                      spect
PROBHD          5 mm PABBO BB-
PULPROG                     zgpg30
TD                           65536
SOLVENT                      CDCl3
NS                              60
DS                               4
SWH                      29761.904 Hz
FIDRES                       0.454131 Hz
AQ                        1.1010548 sec
RG                            1440
DW                           16.800 usec
DE                            6.50 usec
TE                           298.9 K
D1                        2.00000000 sec
d11                       0.03000000 sec
DELTA                     1.89999998 sec
TD0                              1

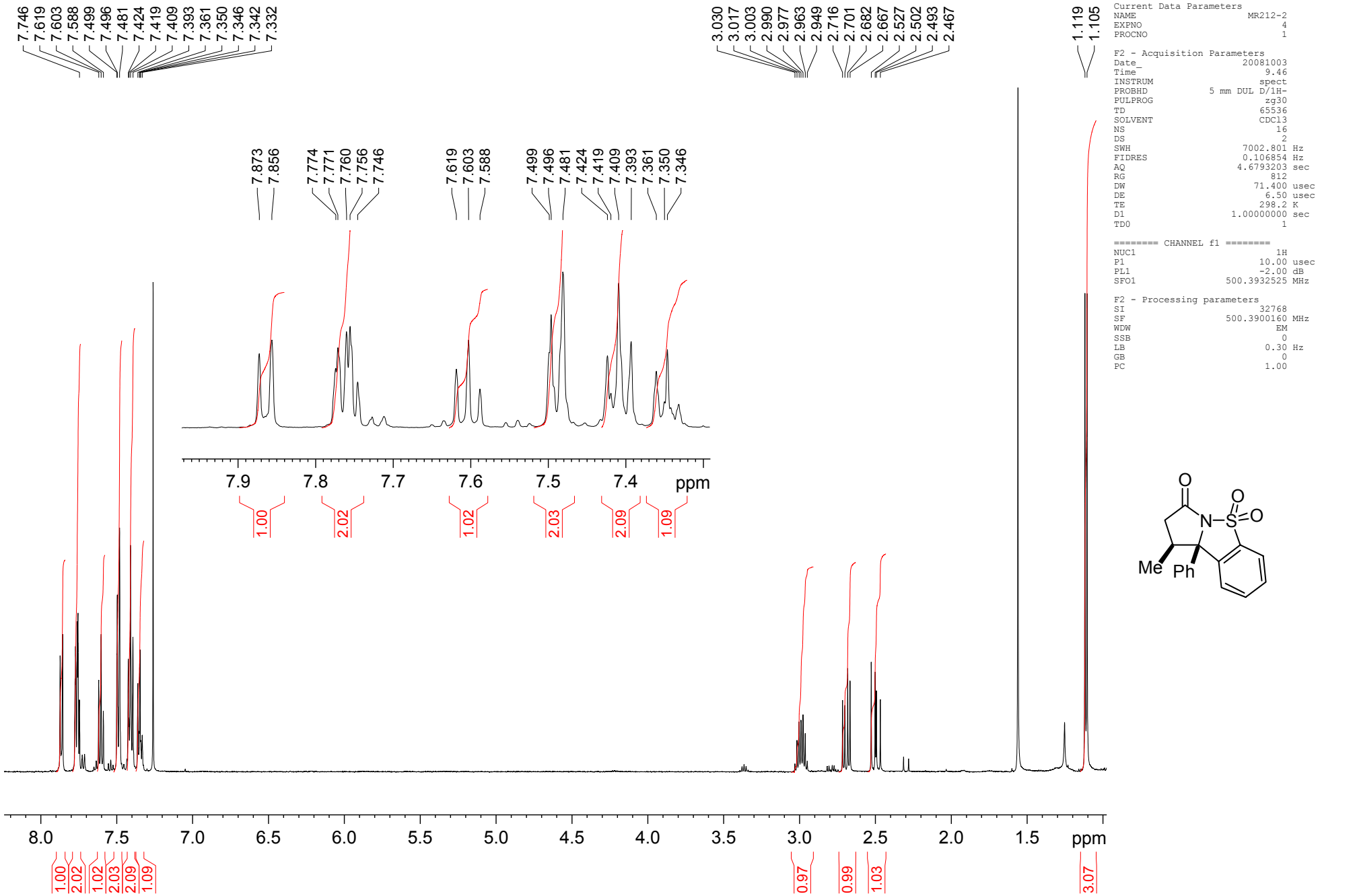
======== CHANNEL f1 ========
NUC1                           13C
P1                            7.50 usec
PL1                           1.00 dB
SFO1                  125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                    waltz16
NUC2                           1H
PCPD2                        80.00 usec
PL12                         17.43 dB
PL13                         18.43 dB
PL2                           0.00 dB
SFO2                  500.3920016 MHz

F2 - Processing parameters
SI                            32768
SF                    125.8231500 MHz
WDW                              EM
SSB                              0
LB                            1.00 Hz
GB                               0
PC                            1.40
```





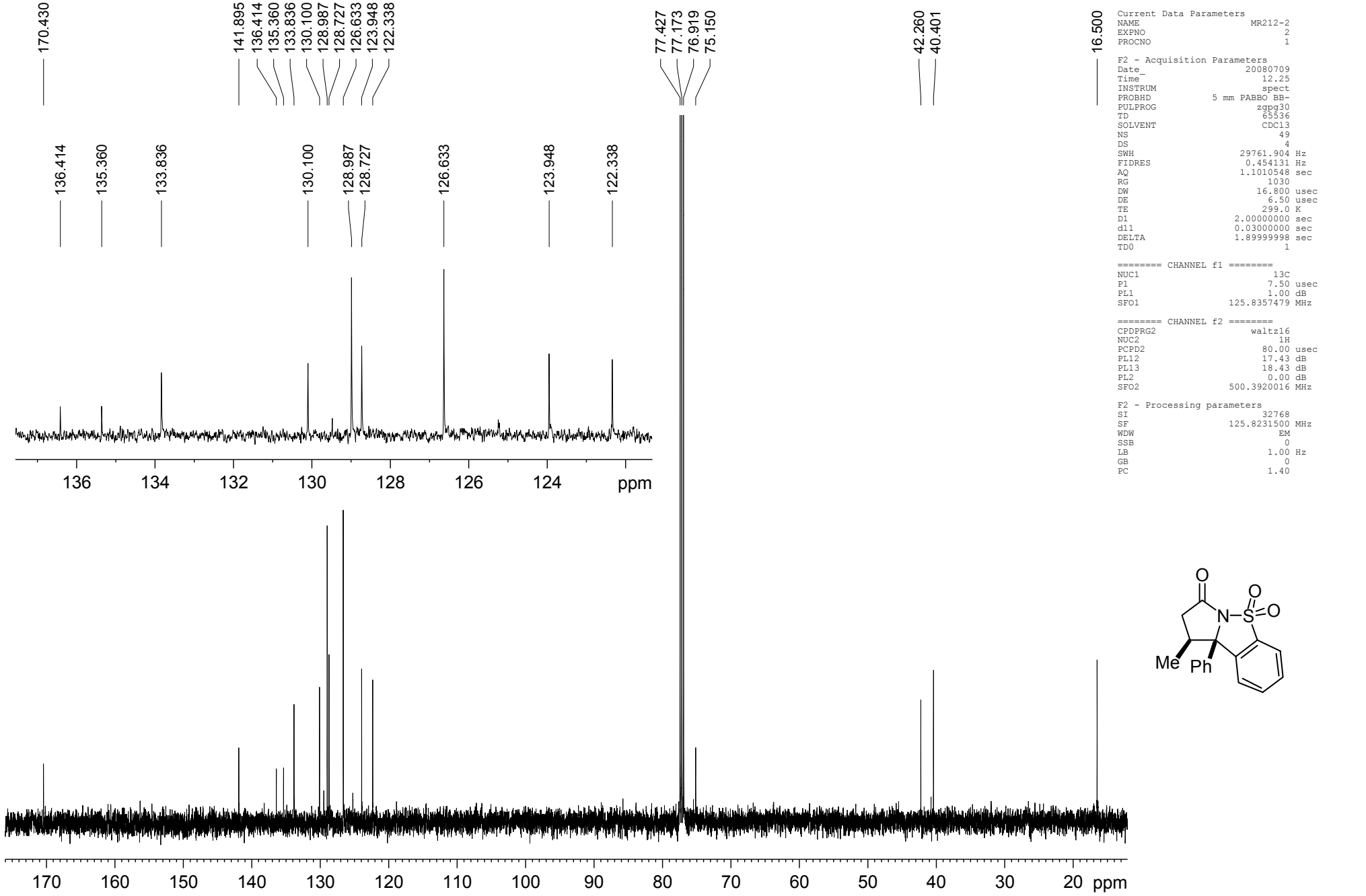


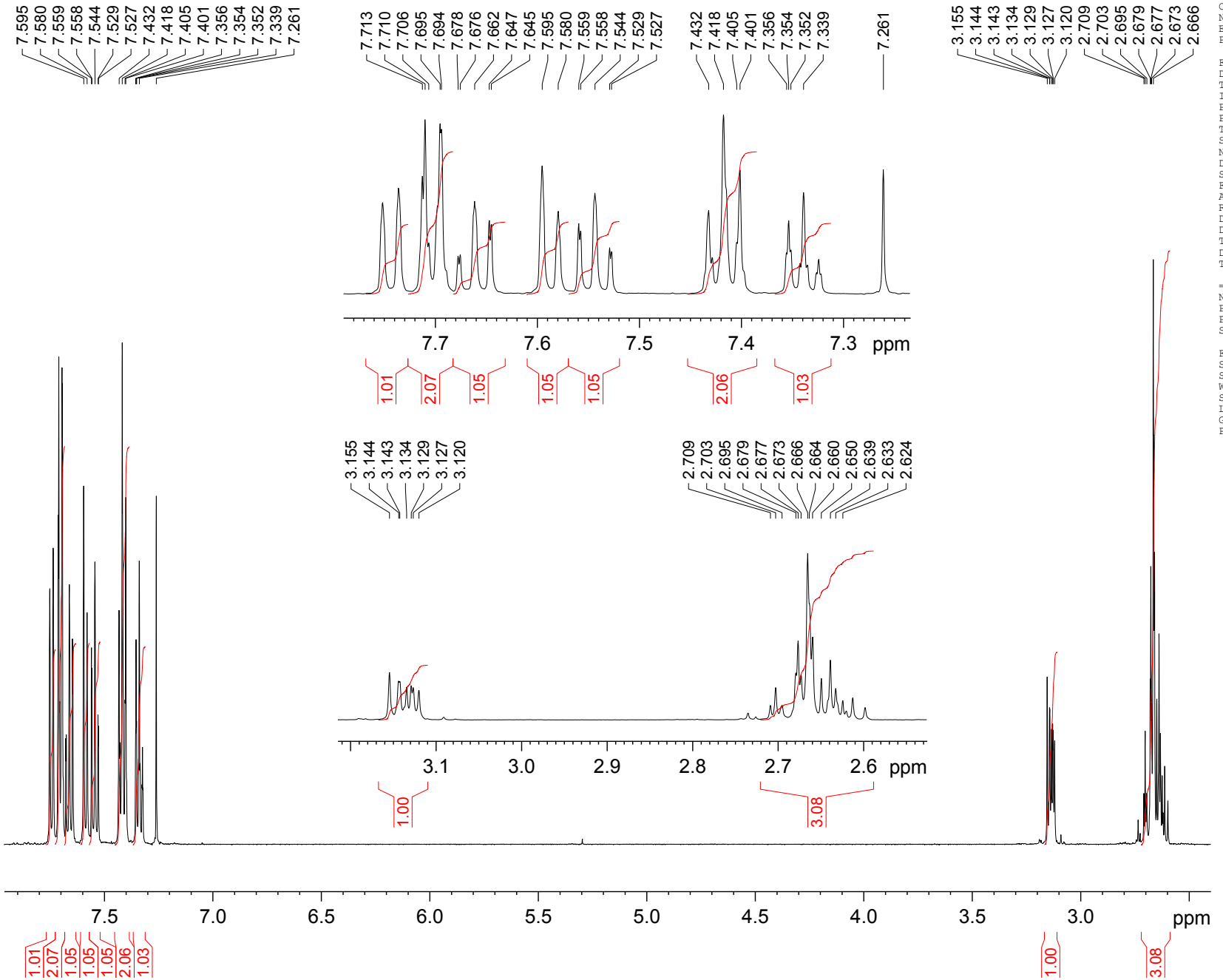

```
Current Data Parameters
NAME                      MR212-2
EXPNO                           4
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20081003
Time                         9.46
INSTRUM                     spect
PROBHD       5 mm DUL D/1H-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                     7002.801 Hz
FIDRES                 0.106854 Hz
AQ                     4.6793203 sec
RG                           812
DW                        71.400 usec
DE                         6.50 usec
TE                        298.2 K
D1                   1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.00 usec
PL1                       -2.00 dB
SFO1                500.3932525 MHz

F2 - Processing parameters
SI                         32768
SF                  500.3900160 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```


170.430
141.895
136.414
135.360
133.836
130.100
128.987
128.727
126.633
123.948
122.338
77.427
77.173
76.919
75.150
42.260
40.401
16.500
Current Data Parameters
NAME MR212-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080709
Time 12.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 49
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.50 usec
PL1 1.00 dB
SFO1 125.8357479 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 17.43 dB
PL13 18.43 dB
PL2 0.00 dB
SFO2 500.3920016 MHz
F2 - Processing parameters
SI 32768
SF 125.8231500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
136
134
132
130
128
126
124
ppm
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
O
O
N
S
O
Me
Ph

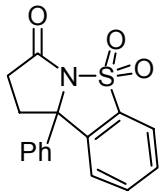


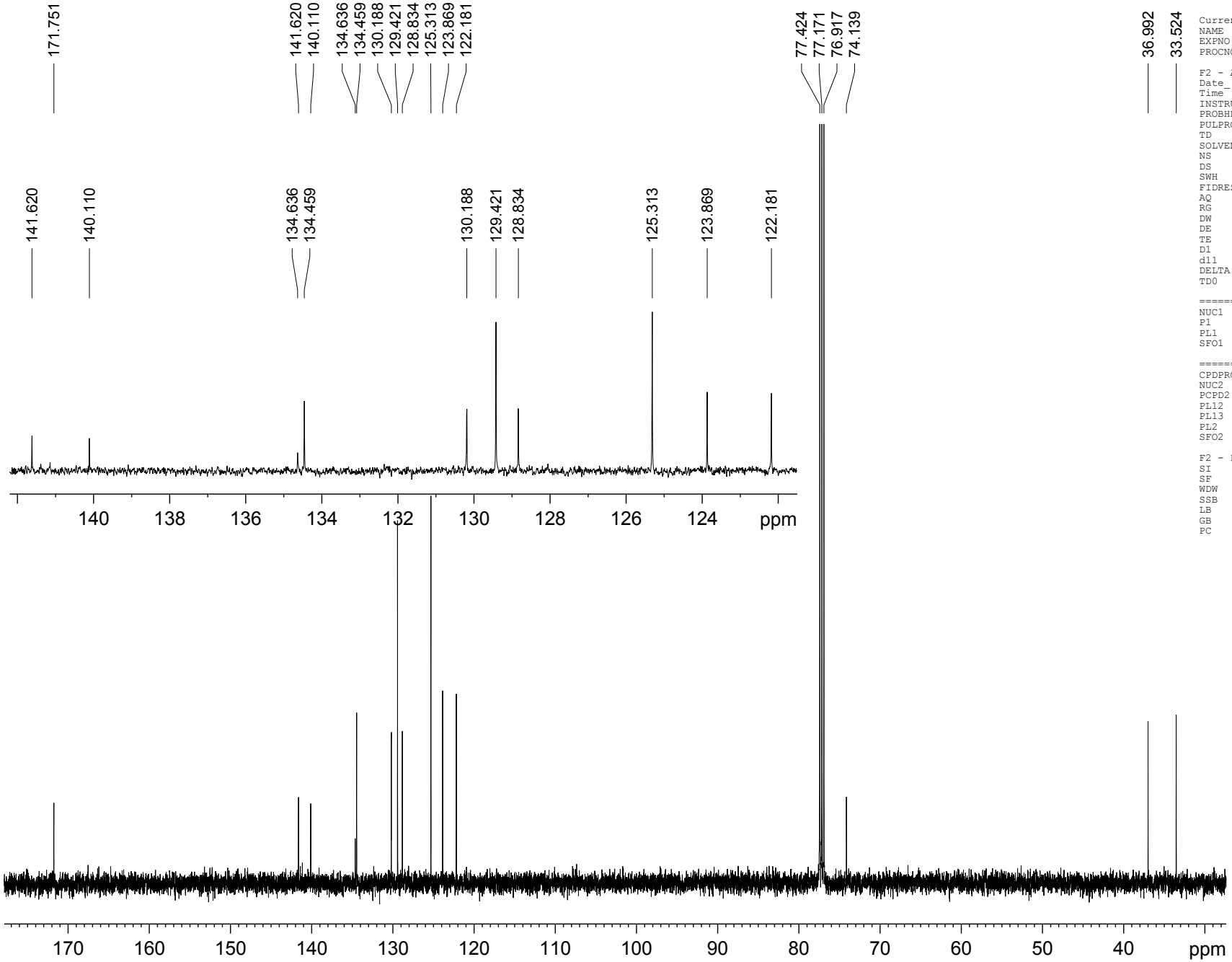

```
Current Data Parameters
NAME                      MR214-2
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20080709
Time_                       12.13
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                            362
DW                       71.400 usec
DE                        6.50 usec
TE                        298.2 K
D1                   1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                        10.76 usec
PL1                        0.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                  500.3900160 MHz
WDW                            EM
SSB                             0
LB                         0.30 Hz
GB                              0
PC                           1.00
```





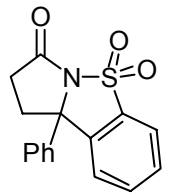

```
Current Data Parameters
NAME                      MR214-2
EXPNO                           2
PROCNO                          1

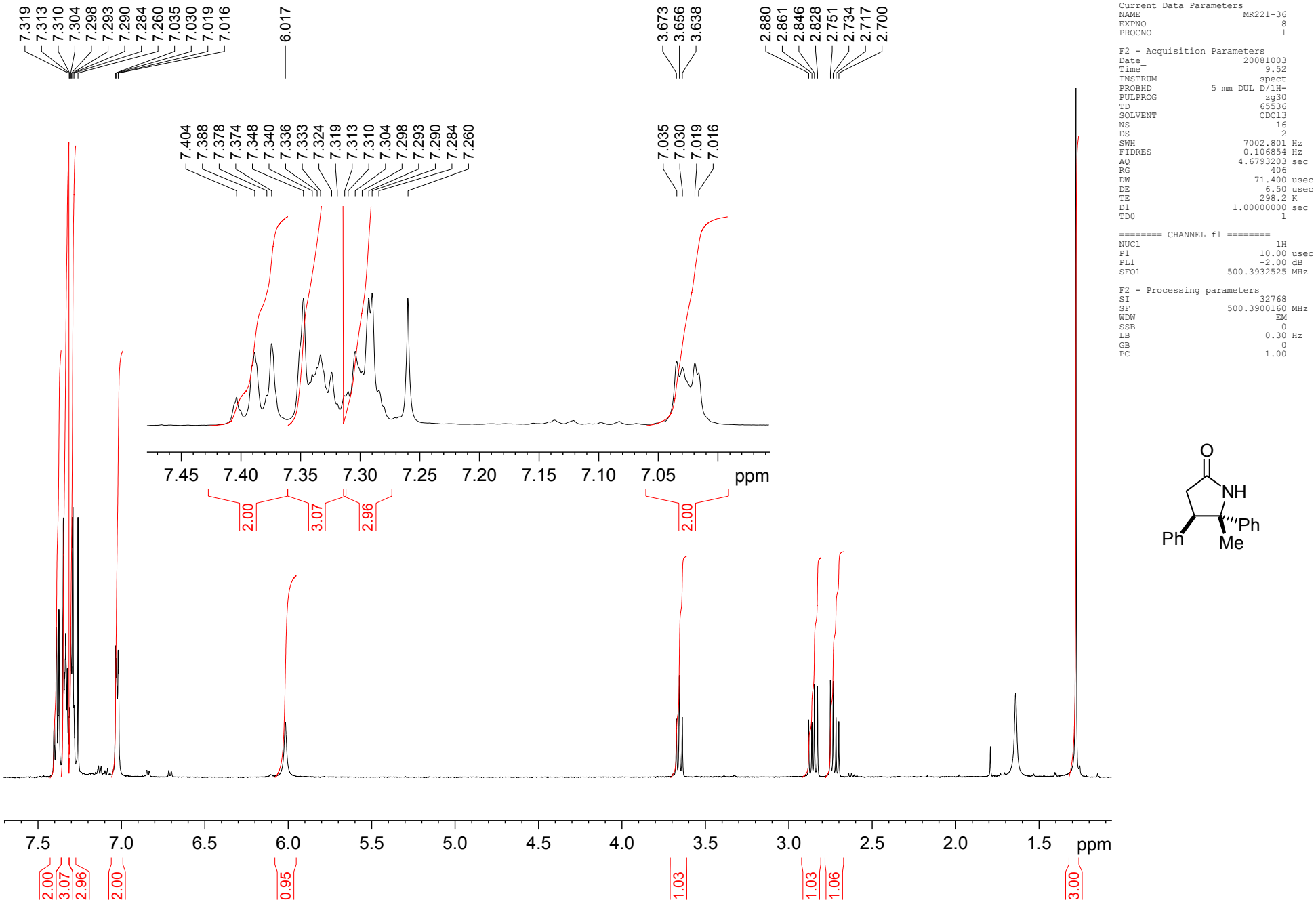
F2 - Acquisition Parameters
Date_                    20080709
Time                        12.16
INSTRUM                     spect
PROBHD       5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           76
DS                            4
SWH                   29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010548 sec
RG                         1290
DW                       16.800 usec
DE                        6.50 usec
TE                       299.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                          7.50 usec
PL1                         1.00 dB
SFO1                125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                      80.00 usec
PL12                       17.43 dB
PL13                       18.43 dB
PL2                         0.00 dB
SFO2                500.3920016 MHz

F2 - Processing parameters
SI                           32768
SF                  125.8231500 MHz
WDW                             EM
SSB                              0
LB                          1.00 Hz
GB                               0
PC                            1.40
```



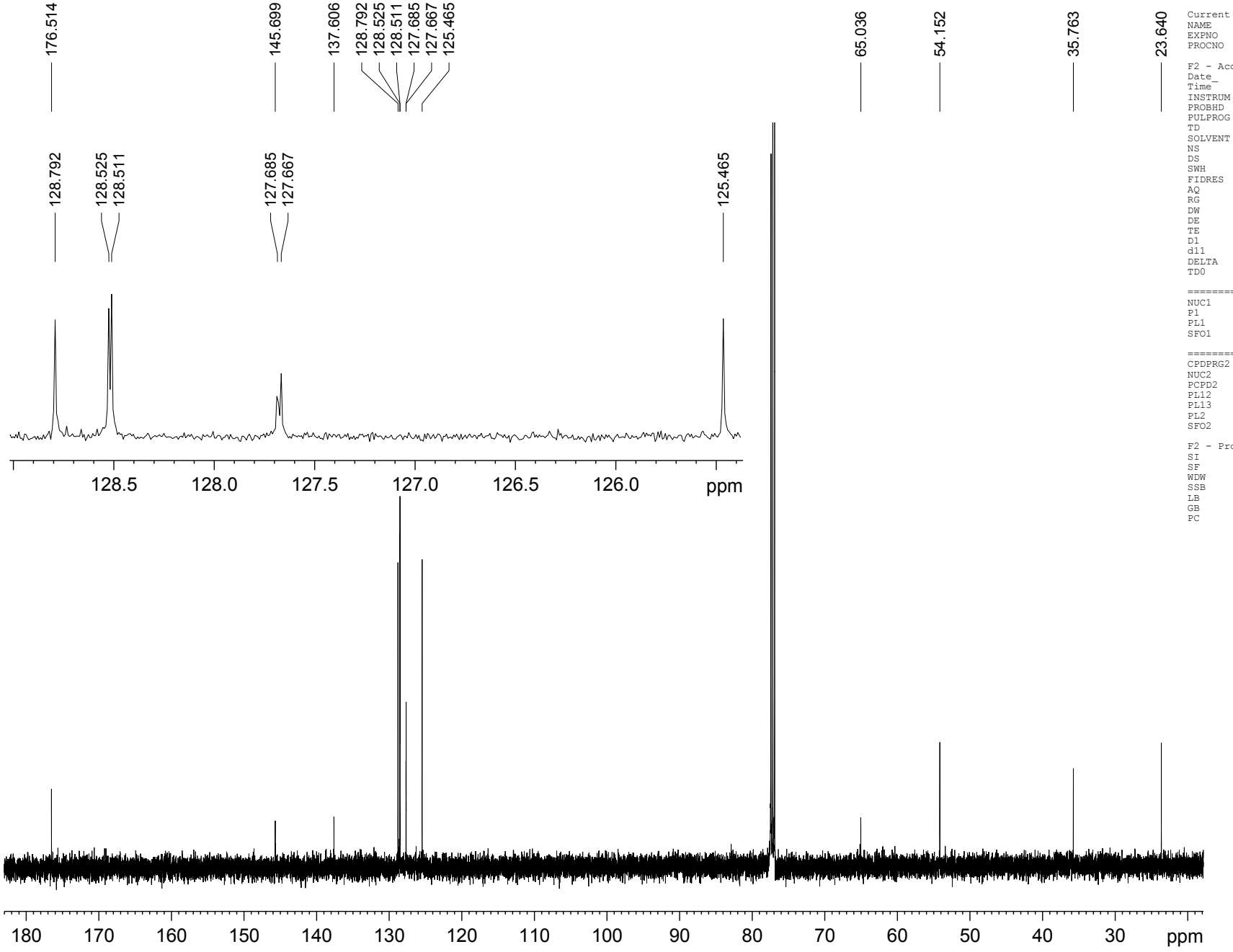



```
Current Data Parameters
NAME                      MR221-36
EXPNO                            8
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20081003
Time                          9.52
INSTRUM                      spect
PROBHD          5 mm DUL D/1H-
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                             16
DS                              2
SWH                     7002.801 Hz
FIDRES                  0.106854 Hz
AQ                      4.6793203 sec
RG                            406
DW                         71.400 usec
DE                          6.50 usec
TE                         298.2 K
D1                    1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                           1H
P1                         10.00 usec
PL1                        -2.00 dB
SFO1                  500.3932525 MHz

F2 - Processing parameters
SI                          32768
SF                    500.3900160 MHz
WDW                            EM
SSB                             0
LB                          0.30 Hz
GB                              0
PC                           1.00
```




```
Current Data Parameters
NAME                   MR221-36
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080928
Time                      18.40
INSTRUM                   spect
PROBHD  5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         255
DS                           4
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                   1.1010548 sec
RG                        1030
DW                       16.800 usec
DE                        6.50 usec
TE                       298.6 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        7.50 usec
PL1                       1.00 dB
SFO1               125.8357479 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL12                     17.43 dB
PL13                     18.43 dB
PL2                       0.00 dB
SFO2               500.3920016 MHz

F2 - Processing parameters
SI                         32768
SF                 125.8231500 MHz
WDW                           EM
SSB                            0
LB                        0.10 Hz
GB                             0
PC                         1.40
```