Supporting Information

An efficient palladium-benzimidazolyl phosphine complex for the Suzuki-Miyaura coupling of aryl mesylates: facile ligand synthesis and metal complex characterization

Kin Ho Chung, Chau Ming So*, Shun Man Wong, Chi Him Luk, Chak Po Lau and Fuk Yee Kwong*

State Key Laboratory of Chirosciences and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Hong Kong.
E-mail: bccmso@inet.polyu.edu.hk, bcfyk@inet.polyu.edu.hk

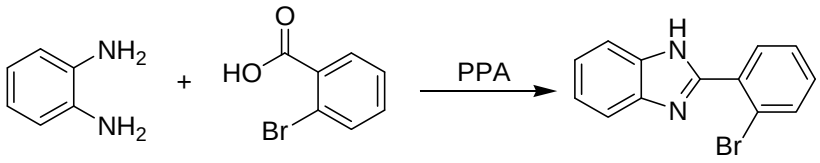
Table of Contents

1. General considerations.

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All Suzuki-Miyaura reactions were performed in Rotaflo® (England) resealable screw cap Schlenk flask (approx. 20 mL volume) in the presence of Teflon coated magnetic stirrer bar (4 mm × 10 mm). Toluene and tetrahydrofuran (THF) were distilled from sodium and sodium benzophenone ketyl under nitrogen, respectively.[1] *N,N*-Dimethylformamide (DMF) was distilled under calcium hydride under reduced pressure. Toluene and dioxane were distilled from sodium under nitrogen. *t*-Butanol was refluxing with sodium and distilled from Calcium hydrides under nitrogen. Chlorodiphenylphosphine was distilled under vacuum prior to use. New bottle of *n*-butyllithium was used (*Note*: since the concentration of *n*-BuLi from old bottle may vary, we performed titration prior to use). K_2CO_3 and K_3PO_4 and $K_3PO_4 \cdot H_2O$ were purchased from Fluka. Thin layer chromatography was performed on Merck precoated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Büchi Melting Point B-545 instrument. ^{1}H NMR spectra were recorded on a Bruker (400 MHz) spectrometer. Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). ^{31}P NMR spectra were referenced to 85% H_3PO_4 externally. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a HP 5989B Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a Brüker APEX 47e FT-ICR mass spectrometer (ESIMS). GC-MS analysis was conducted on a HP 5973 GCD system using a HP5MS column (30 m × 0.25 mm). The

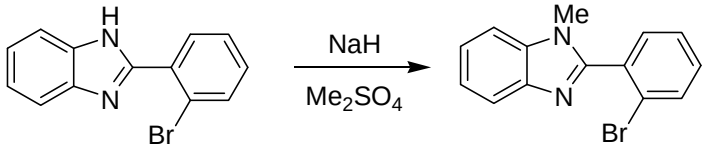
products described in GC yield were accorded to the authentic samples/dodecane calibration standard from HP 6890 GC-FID system. Compounds described in the literature were characterized by comparison of their ^{1}H, and/or ^{13}C NMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

2. Preparation of benzimidazolyl phosphine ligands L1-L3



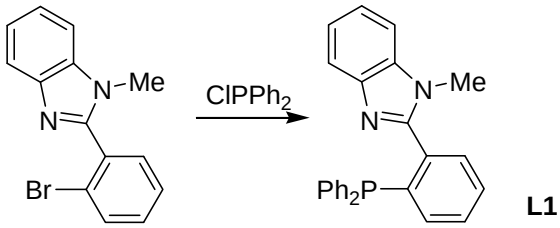
2-(2-bromophenyl)-1H-benzoimidazole was synthesized according to the literature method.[2] 2-bromobenzoic acid (100 mmol) and 1,2-phenylenediamine (100 mmol) were taken in polyphosphoric acid (~120 g) and heated to 150 ^{o}C for 6 h. The reaction mixture was poured over crushed ice and kept in a refrigerator overnight. The resulting violet solid precipitate was filtered and added to 0.5 M Na_2CO_3 solution (500 mL), stirred for 30 min and filtered. The precipitate was dissolved in methanol (300 mL), and filtered through celite. The solution was evaporated to yield a white solid. Hexane was used to further wash the product. The product was then dried under vacuum to afford 2-(2-bromophenyl)-1H-benzoimidazole (20 g, 70%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.35 (m, 3H), 7.43-7.47 (m, 1H), 7.53-7.56 (m, 1H), 7.70 (d, *J*=8.0Hz, 1H), 7.85-7.87 (m, 1H), 8.25 (d, *J*=7.6Hz, 1H), 10.52 (s, 1H); ^{13}C NMR (100 MHz, MeOD) δ 114.6, 121.7, 122.5, 127.2, 131.1, 131.7, 131.8, 133.1, 138.0, 150.7; MS (EI): *m/z* (relative intensity) 272.0 (M+, 100), 193.0 (53), 90.0 (28).

2-(2-bromophenyl)-1-methyl-1H-benzoimidazole



General procedure for methylation of 2-(2-bromophenyl)-1H-benzoimidazole: 2-(2-bromophenyl)-1H-benzoimidazole (10.9 g, 40 mmol) was dissolved in 500 ml THF in dropping funnel and added dropwisely to the 1 L THF solution contained 1.2 equiv NaH (60% in mineral oil, 1.92 g, 48 mmol) at room temperature. NaH was washed with hexane (10 ml × 3) under N_2. The mixture stirred for 1 h at room temperature. Dimethylsulfate (4.16ml, 44 mmol) was then added to the mixture dropwisely. The mixture was refluxed for 30 min and stirred at room temperature for 3 h. Solvent was removed by vacuum. EA and water was added to the mixture and the organic phase was separated. The combined organic phase was washed with brine several times and concentrated. The concentrated mixture was applied to 3 × 3cm silica pad and eluted with EA. The organic solvent was dried over Na_2SO_4 and evaporated in vacuum. The white solid of 2-(2-bromophenyl)-1-methyl-1H-benzoimidazole[3] (8.6 g, 75%) was obtained. ^{1}HNMR (400 MHz, $CDCl_3$) δ 3.66 (s, 3H), 7.34-7.49 (m, 5H), 7.55 (dd, *J*=7.4Hz, 1.6Hz, 1H), 7.72 (dd, *J*=8.0 Hz, 1.2Hz, 1H), 7.85-7.89 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.7, 109.6, 120.0, 122.3, 122.8, 123.7, 127.4, 131.3, 132.0, 132.3, 132.7, 135.4, 142.7, 152.4; MS (EI): *m/z* (relative intensity) 286.0 (M+, 100), 207.1 (93), 103.1 (22), 77.0 (43).

1-methyl-2-(2-(diphenylphosphino)phenyl)-1H-benzoimidazole (L1)

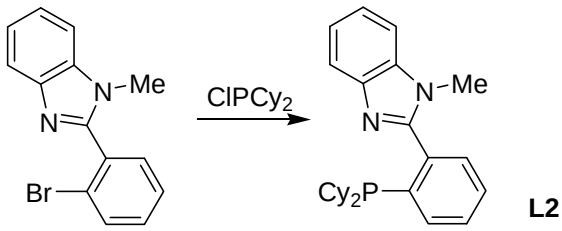


L1

General procedure for ligand synthesis: 2-(2-bromophenyl)-1-methyl-benzoimidazole (0.86 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 °C in dry ice/acetone bath. Titrated *n*-BuLi (3.0 mmol) was added dropwisely by syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodiphenylphosphine (0.55 mL, 3.0 mmol) was added. The reaction was allowed to warm to room temperature and stirred for 5 h. Solvent was removed under reduced pressure. DCM and water was added to the mixture and the organic phase was separated. The combined organic phase was washed with brine several times and concentrated. The concentrated mixture was applied to 2 × 10 cm silica pad and eluted with 200ml EA:Hexane (1:9). This fraction was discarded and further eluted with EA: Hexane (4:6). The collected solvent was removed under vacuum and the solid product was further purified by washing with small amount of cold diethyl ether. The product was then dried under vacuum. White solid of 2-(2-(dicyclohexylphosphino)phenyl)-1-methyl-benzoimidazole **(L1)** (0.95g, 80%) were obtained. Melting point. 174.2-176.2°C; ^{31}P NMR (161MHz, CD_2Cl_2) δ -11.7; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 3.46 (s, 3H), 7.25-7.38 (m, 14H), 7.49-7.55 (m, 3H), 7.72-7.74 (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 30.5, 109.3, 119.5, 121.7, 122.2, 128.1, 128.2, 128.5, 129.5, 130.4, 130.5, 133.5, 133.7, 133.8, 135.4, 136.0, 136.3, 136.6, 136.7, 139.5, 139.7, 142.7, 153.1 (unresolved complex C-P splittings were observed); IR (cm^{-1}): 3051.12, 1613.13, 1478.90, 1462.03, 1424.04,

1377.53, 1327.71, 1282.58, 1244.50, 1148.55, 1125.98, 1093.06, 1027.09, 1005.94, 773.97, 745.88, 695.76, 521.56, 493.47, 469.17; MS (EI): *m/z* (relative intensity) 392.1 (M+, 2), 315.1 (100), 223.0 (22), 207.0 (26); HRMS: calcd. for $C_{26}H_{21}N_2PH^+$: 393.1521, found 393.1524.

1-methyl-2-(2-(dicyclohexylphosphino)phenyl)-1H-benzoimidazole (L2)

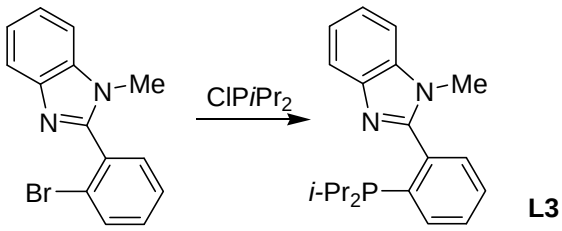


L2

General procedures for the synthesis of ligand **L1** were followed. 2-(2-bromophenyl)-1-methyl-benzoimidazole (2.86 g, 10.0 mmol), *n*-BuLi (10.0 mmol), chlorodicyclohexylphosphine (2.20 mL, 10.0 mmol), and 40 mL THF were used to afford 1-methyl-2-(2-(dicyclohexylphosphino)phenyl)-1H-benzoimidazole (**L2**) (2.85 g, 70%) as a white solid. Small amount of cool hexane instead of diethyl ether was used for washing the products. Melting point. 155.7-158.1 ºC; ^{31}P NMR (161MHz, CD_2Cl_2) δ -8.07; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 1.10-1.31(m, 10H), 1.67-1.78 (m, 10H), 1.91-1.94 (m, 2H), 3.56 (s, 3H), 7.30-7.37 (m, 2H), 7.43-7.61 (m, 4H), 7.71-7.79 (m, 2H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 26.3, 27.1, 27.1, 27.2, 29.2, 29.3, 30.0, 30.2, 30.6, 30.7, 33.6, 33.7, 109.4, 119.3, 121.5, 122.0, 128.5, 128.8, 130.5, 1306, 132.6, 132.7, 135.3, 137.0, 137.2, 138.8, 139.1, 142.9, 154.6, 154.6(unresolved complex C-P splittings were observed); IR (cm^{-1}): 3049.23, 2922.74, 2846.49, 1444.05, 1420.25, 1380.93, 1323.98, 1279.02, 1236.37, 1179.81, 1150.92, 1121.29, 1041.62, 1001.29, 885.48, 849.19, 773.73, 746.94, 526.06, 457.22; MS (EI): *m/z* (relative intensity) 404.2 (M+, 0), 321.1

(100), 238.0 (39), 223.0 (28), 55.1 (7); HRMS: calcd. for $C_{26}H_{33}N_2PH^+$: 405.2460, found 405.2445.

1-methyl-2-(2-(diisopropylhexylphosphino)phenyl)-1H-benzoimidazole (L3)



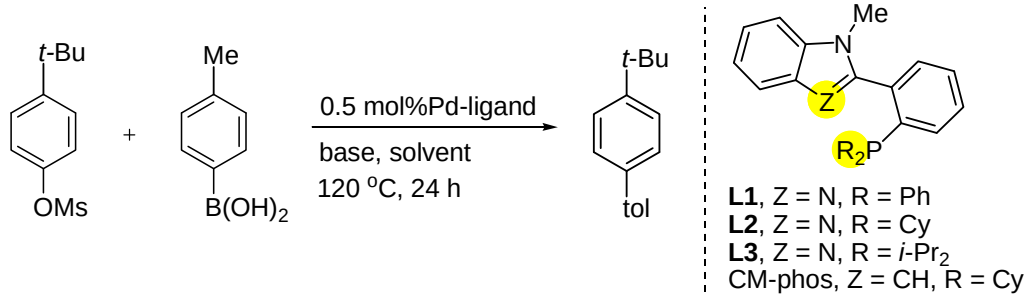
L3

General procedures for the synthesis of ligand **L1** were followed. 2-(2-bromophenyl)-1-methyl-benzoimidazole (0.86 g, 3.0 mmol), *n*-BuLi (3.0 mmol), chlorodiisopropylphosphine (0.47 mL, 3.0 mmol) were used to afford 1-methyl-2-(2-(diisopropylphosphino)phenyl)-1H-benzoimidazole (**L2**) (0.802 g, 83%) as a white solid. Small amount of cool hexane instead of diethyl ether was used for washing the products. Melting point. 147.7-149.7 ºC; ^{31}P NMR (161MHz, CD_2Cl_2) δ 0.45; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 1.02-1.09 (m, 12H), 2.14-2.18 (m, 2H), 3.59 (s, 3H), 7.31-7.38 (m, 2H), 7.44- 7.46 (m, 1H), 7.50-7.63 (m, 3H), 7.71-7.73 (m, 1H), 7.78-7.80 (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 19.1, 19.2, 19.5, 19.6, 23.6, 23.8, 30.5, 30.6, 109.3, 119.3, 121.5, 122.1, 128.6, 128.9, 130.5, 130.6, 132.2, 132.3, 135.2, 137.4, 137.6, 138.5, 138.8, 142.9, 154.4, 154.5 (unresolved complex C-P splittings were observed); IR (cm^{-1}): 2959.77, 2941.70, 2859.58, 1441.13, 1421.73, 1382.81, 1325.73, 1279.50, 1239.22, 1150.84, 1119.29, 1032.32, 1002.00, 881.61, 775.91, 749.74, 653.87, 609.59, 596.19, 515.71; MS (EI): *m/z* (relative intensity) 324.2 (M+, 0), 281.1 (100), 238.0 (56), 223.0 (38), 207.0 (48); HRMS: calcd. for $C_{20}H_{25}N_2PH^+$: 325.1834, found 325.1822.

3. General procedures/data for initial ligand and reaction conditions screening

General procedure for screening: $Pd(OAc)_2$ (1.15 mg, 0.05 mmol), Ligand **L,** 4-*tert*-butylphenyl mesylate (1.0 mmol), *p*-tolylboronic acid (2 mmol) and base (3 mmol) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. The tube was evacuated and flushed with nitrogen (3 cycles). Solvent (3.0 mL) was added with continuous stirring at room temperature for 5 minutes. The tube was then placed into a preheated oil bath (120 ^{o}C) and stirred for 24 h. After completion of reaction, the reaction tube was allowed to cool to room temperature. Ethyl acetate (~10 mL), dodecane (227 μL, internal standard) and water were added. The organic layer was subjected to GC analysis. The GC yield obtained was previously calibrated by authentic sample/dodecane calibration curve.

S.Table 1 Optimization of reaction conditions



entry	ligand	M:L	solvent	base	%yield[b]
1	**L1**	1:2	*t*-BuOH	K_3PO_4	2
2	**L2**	1:2	*t*-BuOH	K_3PO_4	80
3	**L3**	1:2	*t*-BuOH	K_3PO_4	60
4	CM-phos	1:2	*t*-BuOH	K_3PO_4	20
5	**L2**	1:1	*t*-BuOH	K_3PO_4	26

6	**L2**	1:3	*t*-BuOH	K_3PO_4	74
7	**L2**	1:4	*t*-BuOH	K_3PO_4	70
8[c]	**L2**	1:2	*t*-BuOH	K_3PO_4	64
9[d]	**L2**	1:2	*t*-BuOH	K_3PO_4	58
10[e]	**L2**	1:2	*t*-BuOH	K_3PO_4	51
11	**L2**	1:2	toluene	K_3PO_4	53
12	**L2**	1:2	dioxane	K_3PO_4	25
13	**L2**	1:2	DMF	K_3PO_4	2
14	**L2**	1:2	*t*-BuOH	Cs_2CO_3	20
15	**L2**	1:2	*t*-BuOH	CsF	33
16	**L2**	1:2	*t*-BuOH	K_2CO_3	63
17	**L2**	1:2	*t*-BuOH	Na_2CO_3	43
18	**L2**	1:2	*t*-BuOH	K_3PO_4•H_2O	44

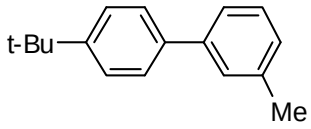
[a]Reaction conditions: 0.5 mol% of $Pd(OAc)_2$, 4-*tert*-butylphenyl mesylate (1.0 mmol), *p*-tolylboronic acid (2.0 mmol), base (3.0 mmol), solvent (3 mL), at 120 °C under N_2 for 24 h. [b]Calibrated GC yields were reported using dodecane as the internal standard. [c]$Pd_2(dba)_3$. [d] $PdCl_2$. [e]$Pd(TFA)_2$.

4. General procedures for palladium-catalyzed Suzuki coupling of aryl mesylates

General procedure for Suzuki coupling of aryl mesylates: $Pd(OAc)_2$ (1.15 mg, 0.05 mmol), Ligand **L2** (Pd:L = 1:2)**,** aryl mesylate (1.0 mmol), arylboronic acid (2 mmol) and base (3 mmol) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. The tube was evacuated and flushed with nitrogen (3 cycles). The solvent *tert*-butanol (3-5 mL) was added with continuous stirring at room temperature for 5 minutes. The tube was then placed into a preheated oil bath (120 ^{o}C) and stirred for the time period as indicated in Tables. After completion of reaction as judged by GC analysis, the reaction tube was allowed to cool to room temperature and quenched with water and diluted with EtOAc. The organic layer was separated and the aqueous layer was washed with EtOAc. The filtrate was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.

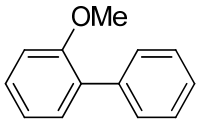
5. Characterization data for coupling products

4'-(*tert*-butyl)-3-methyl-1,1'-biphenyl (1a,b)[4]



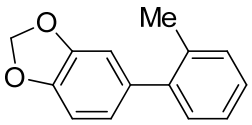
Hexane, R_f=0.55; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.53 (s, 9H), 2.57 (s, 3H), 7.30 (d, *J*=7.2 Hz, 1H), 7.45-7.49 (m, 1H), 7.55-7.63 (m, 4H), 7.69-7.71 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 31.2, 34.3, 123.9, 125.4, 126.6, 127.5, 127.6, 128.4, 137.9, 138.2, 140.9, 149.8; MS (EI): *m/z* (relative intensity) 224.1 (M^+, 33), 209.1 (100), 181.1 (15), 165.1 (12).

2-methoxy-1,1'biphenyl (1c)[5]



EA:Hexane = 1:9, R_f=0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.97 (s, 3H), 7.17-7.19 (m, 1H), 7.24-7.28 (m, 1H), 7.51-7.55 (m, 3H), 7.62-7.64 (m, 2H), 7.78 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.6, 111.4, 121.0, 127.1, 128.1, 128.8, 129.7, 130.9, 131.0, 138.8, 156.7; MS (EI): *m/z* (relative intensity) 184.1 (M^+, 100), 169.1 (53), 141.1 (36), 115.1 (36).

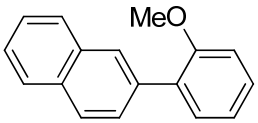
5-*o*-tolylbenzo[*d*][1,3]dioxole (1d)[6]



EA:Hexane = 1:4, R_f=0.25; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 6.10 (s, 2H), 6.94-6.95 (m, 1H), 6.99-7.01 (m, 2H), 7.38-7.40 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.4, 100.9,

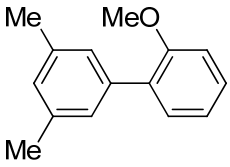
107.9, 109.7, 122.4, 125.6, 127.0, 129.7, 130.2, 135.3, 135.8, 141.5, 146.4, 147.2; MS (EI): *m/z* (relative intnsity) 212.1 (M^+, 100), 181.1 (22), 153.1 (42), 115.1 (14).

2-(2-methoxyphenyl)naphthalene (1e)[7]



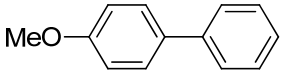
Hexane, R_f=0.55; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.04 (s, 3H), 7.26 (d, *J*=8.4 Hz, 1H), 7.40 (t, *J*=7.2 Hz, 1H), 7.63-7.67 (m, 1H), 7.78-7.80 (m, 3H), 8.09 (d, *J*=8.4 Hz, 1H), 8.17-8.20 (m, 3H), 8.35 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.3, 111.2, 120.8, 125.6, 125.8, 127.1, 127.5, 128.0, 128.6, 130.5, 131.0, 132.3, 133.3, 136.2, 156.5; MS (EI): *m/z* (relative intensity) 234.1 (M^+, 100), 219.1 (40), 202.1 (10), 191.1 (35).

2-methoxy-3',5'-dimethyl-1,1'-biphenyl (1f)[8]



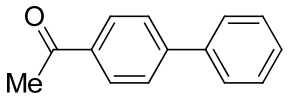
EA:Hexane = 1:9, R_f=0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.60 (s, 6H), 4.00 (s, 3H), 7.16-7.26 (m, 3H), 7.40 (s, 2H), 7.50-7.55 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 55.4, 111.0, 120.6, 127.3, 128.3, 128.6, 130.8, 130.9, 137.2, 138.4, 156.4; MS (EI): *m/z* (relative intensity) 212 (M^+, 100), 197.1 (61), 182.1 (46), 165.1 (16).

4-methoxy-1,1'biphenyl (1g)[9]



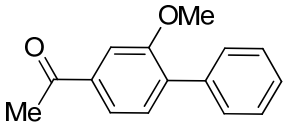
DCM, R_f=0.2; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.94 (s, 3H), 7.12 (d, J=6.8 Hz, 2H), 7.43-7.47 (m, 1H), 7.54-7.57 (t, *J*=6.8 Hz, 2H), 7.67-7.72 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.1, 114.1, 126.5, 126.6, 128.0, 128.6, 133.6, 140.7, 159.1; MS (EI): *m/z* (relative intensity) 184.1 (M^+, 100), 169.1 (50), 141.1 (46), 115.1 (34).

1-([1,1'-biphenyl]-4-yl)ethanone (1h)[10]



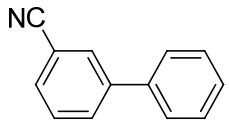
Hexane, R_f=0.5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (s, 3H), 7.41-7.49 (m, 3H), 7.62-7.68 (m, 4H), 8.03 (d, *J*=8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.3, 126.9, 127.0, 128.0, 128.6, 128.7, 135.6, 139.5, 145.4, 197.3; MS (EI): *m/z* (relative intensity) 196.1 (M^+, 47), 181.1 (100), 152.1 (54), 76.1 (8).

1-(2-methoxy-[1,1'-biphenyl]-4-yl)ethanone (1i)[11]



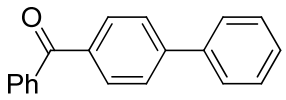
EA:Hexane = 1:9, R_f=0.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.66 (s, 3H), 3.89 (s, 3H), 7.41-7.49 (m, 4H), 7.59-7.65 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.4, 55.4, 109.8, 121.5, 127.4, 127.9, 129.2, 130.6, 135.4, 137.1, 137.2, 156.5, 197.3; MS (EI): *m/z* (relative intensity) 226.1 (M^+, 67), 211.1 (100), 183.1 (10), 168.1 (27).

[1,1'-biphenyl]-3-carbonitrile (1j)[12]



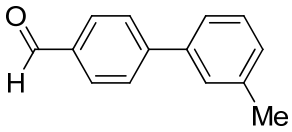
EA:Hexane = 1:9, R_f=0.15; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.51 (m, 3H), 7.54-7.57 (m, 3H), 7.61-7.63 (m, 1H), 7.79-7.82 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 112.6, 118.5, 126.7, 128.1, 128.8, 129.3, 130.3, 130.4, 131.1, 138.4, 142.0; MS (EI): *m/z* (relative intensity) 179.1 (M^+, 100), 151.0 (13), 76.0 (8), 63.1 (5); HRMS: calcd. for $C_{24}H_{29}NO$: 347.2244, found 347.2253.

[1,1'-biphenyl]-4-yl(phenyl)methanone (1k)[13]



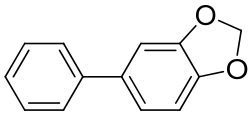
Hexane, R_f=0.55; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.46 (m, 1H), 7.53 (q, *J*=7.2 Hz, 6H), 7.61-7.65 (m, 1H), 7.69-7.75 (m, 4H), 7.89-7.96 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 126.7, 127.1, 128.0, 128.1, 128.8, 129.8, 130.5, 132.2, 136.0, 137.5, 139.7, 144.9, 196.0; MS (EI):*m/z* (relative intensity) 258.1 (M^+, 76), 181.1 (100), 152.1 (46), 105.1 (20).

3'-methyl-[1,1'-biphenyl]-4-carbaldehyde (1l)[14]



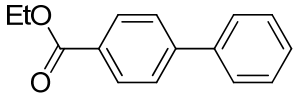
EA:Hexane = 1:9, R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.48 (s, 3H), 7.26-7.28 (m, 1H), 7.38-7.48 (m, 3H), 7.75-7.77(m, 2H), 7.95-7.97 (m, *2*H), 10.06 (s, 1H); ^{13}C NMR (100 Hz, $CDCl_3$) δ 21.3, 124.3, 127.4, 127.9, 128.7, 129.1, 130.0, 134.9, 138.4, 139.4, 147.1, 191.7; MS (EI): *m/z* (relative intensity) 196.1 (M^+, 100), 165.1 (36), 152.1 (47), 115.1 (7).

5-phenylbenzo[*d*][1,3]dioxole (1m)[15]



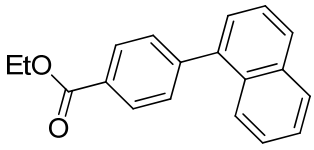
EA:Hexane = 1:4, R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.06 (s, 2H), 6.99 (t, *J*=6.8 Hz, 1H), 7.15-7.21 (m, 2H), 7.39-7.45 (m, 1H), 7.49-7.54 (m, 2H), 7.61-7.65 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 101.0, 107.6, 108.5, 120.5, 126.8, 128.7, 135.5, 140.9, 147.0, 148.1; MS (EI): *m/z* (relative intensity) 198.1 (M^+, 100), 139.1 (48), 98.8 (10), 63.1 (5).

Ethyl [1,1'-biphenyl]-4-carboxylate (1n)[13]



Hexane, R_f=0.55; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.46 (t, *J*=6.8 Hz, 3H), 4.45 (q, *J*=7.2 Hz, 2H), 7.42-7.50 (m, 3H), 7.63-7.69 (m, 4H), 8.18 (d, *J*=8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.1, 60.7, 126.7, 127.0, 127.8, 128.6, 129.0, 129.8, 139.7, 145.2, 166.1; MS (EI): *m/z* (relative intensity) 210 (M^+, 65), 195 (100), 180 (30), 152 (25).

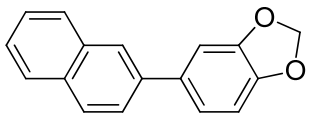
Ethyl 4-(naphthalen-1-yl)benzoate (1o)[16]



DCM:Hexane = 1:20, R_f=0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.52 (t, *J*=6.8 Hz, 3H), 4.54 (q, *J*=6.8 Hz, 2H), 7.47-7.50 (m, 2H), 7.56-7.58 (m, 2H), 7.64 (d, *J*=6.8 Hz, 2H), 7.93-7.98 (m, 3H); 8.30 (d, *J*=7.2 Hz, 2H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 60.7, 125.1, 125.4, 125.7, 126.1,

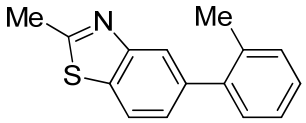
126.7, 128.0, 128.2, 129.2, 129.3, 129.8, 131.0, 133.6, 138.9, 145.2, 166.2; MS (EI): *m/z* (relative intensity) 276.1 (M^+, 100), 248.1 (13), 231.1 (51), 202.1 (70).

5-(naphthalen-2-yl)benzo[*d*][1,3]dioxole (1p)[17]



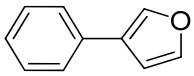
EA:Hexane = 3:7, R_f=0.5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.09 (s, 2H), 7.04 (d, *J*=8.0 Hz, 1H), 7.29-7.32 (m, 1H), 7.35 (s, 1H), 7.59-7.62 (m, 2H), 7.79 (d, *J*=8.8 Hz, 1H), 7.97-7.99 (m, 3H), 8.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 101.1, 107.7, ,108.5, 120.8, 125.1, 125.3, 125.6, 126.2, 127.5, 128.0, 128.3, 132.3, 133.6, 135.3, 138.1, 147.1, 148.1 MS (EI): *m/z* (relative intensity) 248.1 (M^+, 100), 189.1 (46), 123.7 (12), 94.5 (7).

2-methyl-5-*o*-tolylbenzo[*d*]thiazole (2a)[18]



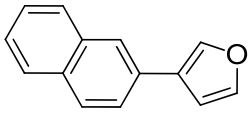
EA:Hexane = 1:20, R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.36 (s, 3H), 2.84 (s, 3H), 7.31-7.35 (m, 5H), 7.82 (d, *J*=8.0 Hz, 1H), 8.03 (s, 1H), 7.93-7.98 (m, 4H);^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 20.2, 120.5, 122.5, 125.8, 125.5, 127.1, 129.6, 130.1, 133.9, 135.0, 139.7, 141.0, 153.2, 167.0; MS (EI): *m/z* (relative intensity) 239.1 (M^+, 100), 197.0 (21), 165.1 (50), 1552.1 (12).

3-phenylfuran (2b)[19]



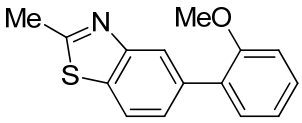
EA:Hexane = 1:4, R_f=0.7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.80 (s, 1H), 7.36-7.38 (m, 1H), 7.50-7.49 (m, 2H), 7.56-7.60 (m, 3H), 7.82-7.83 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.8, 125.8, 126.4, 126.9, 128.7, 132.4, 138.4, 143.6; MS (EI): *m/z* (relative intensity) 144.1 (M^+, 96), 115.1 (100), 89.1 (15), 63.1 (13).

3-(naphthalen-2-yl)furan (2c)



EA:Hexane = 1:4, R_f=0.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (s, 1H), 7.57-7.64 (m, 3H), 7.72 (d, *J*=8.4 Hz, 1H), 7.93-7.96 (m, 4H), 8.04 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.8, 123.9, 124.4, 125.6, 126.3, 126.4, 127.6, 127.8, 128.4, 129.7, 132.5, 133.7, 138.8, 143.7; MS (EI): *m/z* (relative intensity) 194.1 (M^+, 100), 165.1 (76), 139.1 (10), 115.1 (6). $C_{26}H_{21}N_2PH^+$: 194.0732, found 194.0738

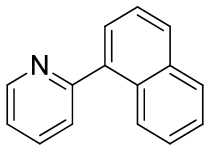
5-(2-methoxyphenyl)-2-methylbenzo[*d*]thiazole (2d)[20]



EA:Hexane = 1:20, R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.85 (s, 3H), 3.82 (s, 3H), 7.02 (d, *J*=8.0 Hz, 1H), 7.09 (t, *J*=7.6 Hz, 1H), 7.35-7.39 (m, 1H), 7.43-7.45 (m, 1H), 7.57-7.59 (m, 1H), 7.84 (d, *J*=8.0 Hz, 1H), 8.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.8, 55.1, 111.0, 120.4,

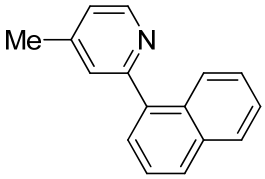
120.6, 123.0, 126.2, 128.5, 129.8, 130.7, 133.9, 136.3, 153.2, 156.2, 166.7; MS (EI): *m/z* (relative intensity) 255.1 (M^+, 100), 240.0 (26), 199.0 (31), 171.0 (12).

2-(naphthalen-1-yl)pyridine (2e)[21]



EA:Hexane = 1:20, R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.31 (m, 1H), 7.52-7.61 (m, 4H), 7.65-7.67 (m, 1H), 7.75-7.79 (m, 1H), 7.95(d, *J*=8.0 Hz, 2H), 8.19 (d, *J*=6.8 Hz, 1H), 8.84-8.85 (m, 1H),; ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.7, 124.8, 125.0, 125.4, 125.6, 126.2, 127.2, 128.1, 128.6, 130.9, 133.7, 136.1, 138.3, 149.2, 59.0; MS (EI): *m/z* (relative intensity) 205.1 (M^+, 38), 176.1 (10), 102.1 (8), 88.1 (4).

4-methyl-2-(naphthalen-1-yl)pyridine (2f)[22]

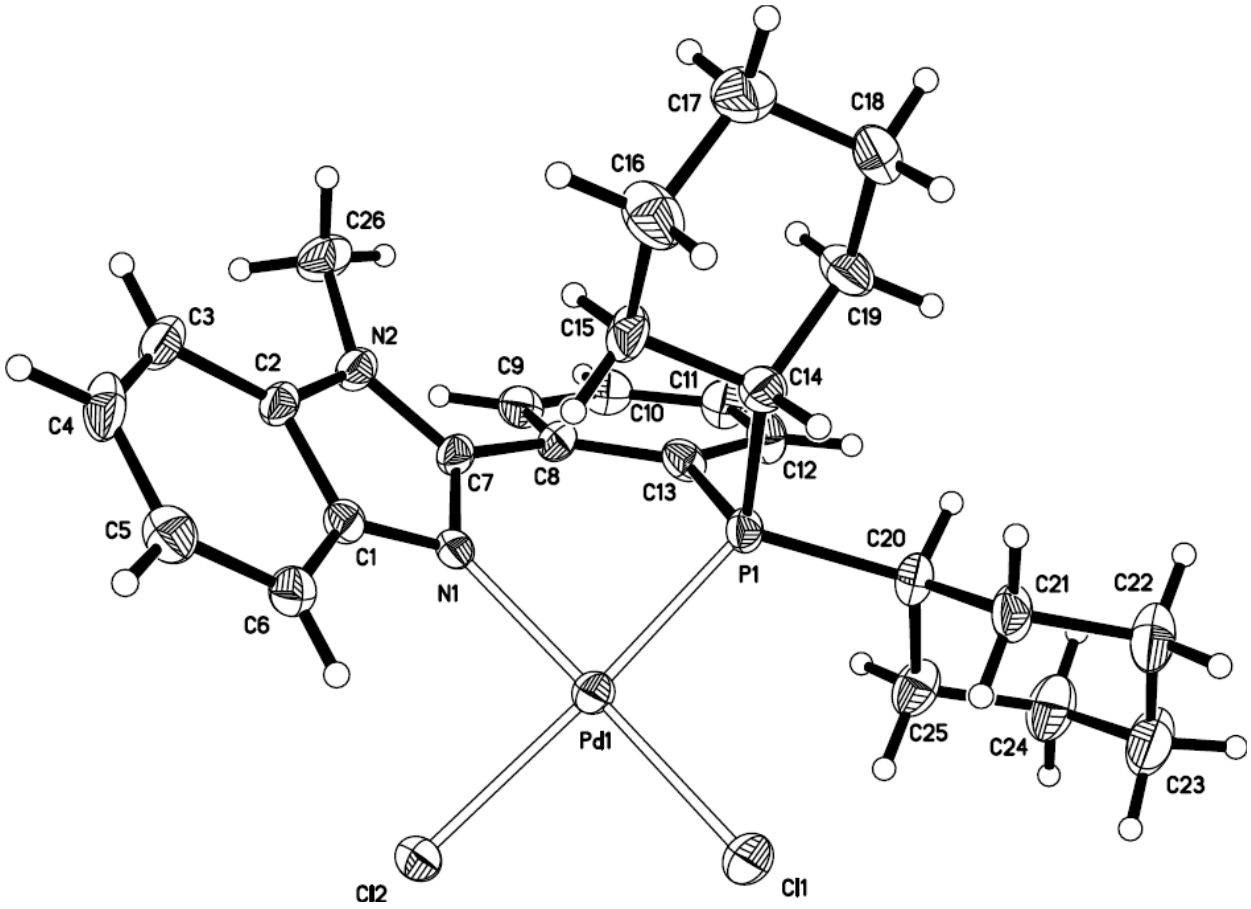


EA:Hexane = 1:20, R_f=0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H,), 7.12 (s, 1H), 7.41 (s, 1H), 7.51-7.65 (m, 4H), 7.93 (d, *J*=6.8 Hz, 2H), 8.17-8.20 (m, 1H), 8.69 (d, *J*=4.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 122.7, 125.0, 125.4, 125.5, 125.6, 126.1, 127.0, 128.0, 128.4, 131.0, 133.6, 138.4, 147.1, 148.9, 159.8; MS (EI): *m/z* (relative intensity) 219.1 (M^+, 41), 204.1 (11), 189.1 (5), 108.7 (7).

6. X-ray crystal data of complex Pd-L2

Table 1. Crystal data and structure refinement for BCSOCM43 (31 Mar 2011).

Identification code	socm43	
Empirical formula	$PdCl_2(C_{26}H_{33}N_2P)\ .CH_2Cl_2$	
Formula weight	666.74	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.2097(6) Å	α= 99.428(6)°.
	b = 10.1097(6) Å	β= 97.595(6)°.
	c = 18.0481(16) Å	γ = 113.505(4)°.
Volume	1483.49(19) $Å^3$	
Z	2	
Density (calculated)	1.493 Mg/m^3	
Absorption coefficient	1.059 mm^{-1}	
F(000)	680	
Crystal size	0.50 x 0.40 x 0.18 mm^3	
Theta range for data collection	2.29 to 27.87°.	
Index ranges	-12<=h<=12, -13<=k<=13, -23<=l<=23	
Reflections collected	26578	
Independent reflections	6987 [R(int) = 0.4427]	
Completeness to theta = 27.87°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8323 and 0.6196	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6987 / 4 / 335	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0716, wR2 = 0.1649	
R indices (all data)	R1 = 0.2766, wR2 = 0.2023	
Largest diff. peak and hole	1.156 and -0.928 $e.Å^{-3}$	



ORTEP representation of complex Pd-**L2** (30% probability ellipsoids). Hydrogen atoms have been omitted for clarity. Selected bond distances (Å) and angles (deg): Pd(1)-N(1), 2.011(2); Pd(1)-P(1), 2.2493(8); Pd(1)-Cl(1), 2.2969(9); Pd(1)-Cl(2), 2.3744(8); P(1)-C(20), 1.837(3); P(1)-C(14), 1.846(4); P(1)-C(13), 1.854(3); N(1)-C(1), 1.393(3); N(1)-C(7), 1.336(4); N(1)-Pd(1)-P(1), 86.05(7); N(1)-Pd(1)-Cl(1), 170.26(7); P(1)-Pd(1)-Cl(1), 96.35(3); N(1)-Pd(1)-Cl(2), 88.90(7).

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for socm43. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	3051(1)	4581(1)	1733(1)	32(1)
Cl(1)	5470(1)	4711(1)	2347(1)	55(1)
Cl(2)	2934(1)	2789(1)	669(1)	39(1)
P(1)	3106(1)	6536(1)	2558(1)	31(1)
N(1)	758(2)	4175(2)	1276(1)	31(1)
N(2)	-1514(2)	4408(2)	939(1)	35(1)
C(1)	-536(2)	2786(2)	1162(1)	32(1)
C(2)	-1993(3)	2912(2)	944(1)	33(1)
C(3)	-3512(3)	1723(2)	809(2)	46(1)
C(4)	-3518(3)	392(2)	891(2)	51(1)
C(5)	-2051(3)	257(2)	1096(2)	46(1)
C(6)	-566(3)	1429(2)	1241(1)	38(1)
C(7)	115(2)	5110(2)	1144(1)	31(1)
C(8)	1072(2)	6735(2)	1293(1)	32(1)
C(9)	635(2)	7481(2)	775(1)	41(1)
C(10)	1477(3)	9019(2)	910(1)	45(1)
C(11)	2675(3)	9794(2)	1552(2)	47(1)
C(12)	3105(3)	9039(2)	2067(1)	45(1)
C(13)	2334(3)	7501(2)	1932(1)	35(1)
C(14)	1820(3)	6082(2)	3267(1)	38(1)
C(15)	157(3)	4788(2)	2968(2)	45(1)
C(16)	-727(4)	4410(3)	3613(2)	62(1)
C(17)	-876(3)	5760(3)	4053(2)	60(1)
C(18)	762(3)	7058(3)	4347(2)	58(1)
C(19)	1656(3)	7439(2)	3709(2)	52(1)
C(20)	5076(3)	7983(2)	3123(1)	40(1)
C(21)	5793(3)	7607(2)	3833(1)	46(1)
C(22)	7332(4)	8959(3)	4290(2)	65(1)
C(23)	8574(4)	9528(3)	3818(2)	73(1)
C(24)	7872(4)	9866(3)	3108(2)	64(1)
C(25)	6343(3)	8514(2)	2629(1)	49(1)

C(26)	-2697(2)	5018(2)	741(2)	51(1)
C(27)	3677(5)	12408(5)	3633(3)	104(3)
Cl(3)	3009(2)	13463(2)	4233(1)	155(1)
C(27')	4530(7)	13278(8)	3910(6)	102(4)
Cl(3')	2405(4)	12363(4)	3585(3)	208(2)
Cl(4)	5091(1)	11933(1)	4110(1)	114(1)

Table 3. Bond lengths [Å] and angles [°] for socm43.

Pd(1)-N(1)	2.0113(17)
Pd(1)-P(1)	2.2493(6)
Pd(1)-Cl(1)	2.2969(7)
Pd(1)-Cl(2)	2.3744(6)
P(1)-C(20)	1.8371(19)
P(1)-C(14)	1.846(3)
P(1)-C(13)	1.854(2)
N(1)-C(7)	1.336(3)
N(1)-C(1)	1.392(2)
N(2)-C(7)	1.345(3)
N(2)-C(2)	1.397(3)
N(2)-C(26)	1.483(3)
C(1)-C(6)	1.393(3)
C(1)-C(2)	1.408(3)
C(2)-C(3)	1.391(3)
C(3)-C(4)	1.376(4)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.418(4)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.361(3)
C(5)-H(5A)	0.9300
C(6)-H(6A)	0.9300
C(7)-C(8)	1.479(2)
C(8)-C(13)	1.385(3)
C(8)-C(9)	1.406(3)
C(9)-C(10)	1.393(2)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.360(3)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.407(4)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.390(2)
C(12)-H(12A)	0.9300
C(14)-C(15)	1.517(3)

C(14)-C(19)	1.544(3)
C(14)-H(14A)	0.9800
C(15)-C(16)	1.521(4)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.528(4)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.503(3)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.514(4)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-C(21)	1.536(4)
C(20)-C(25)	1.541(4)
C(20)-H(20A)	0.9800
C(21)-C(22)	1.528(3)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(23)	1.503(5)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.509(5)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(24)-C(25)	1.534(3)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600

C(27)-Cl(4)	1.733(5)
C(27)-Cl(3)	1.735(5)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27')-Cl(4)	1.707(9)
C(27')-Cl(3')	1.762(6)
C(27')-H(27C)	0.9700
C(27')-H(27D)	0.9700

N(1)-Pd(1)-P(1)	86.05(5)
N(1)-Pd(1)-Cl(1)	170.26(5)
P(1)-Pd(1)-Cl(1)	96.35(2)
N(1)-Pd(1)-Cl(2)	88.90(5)
P(1)-Pd(1)-Cl(2)	168.21(2)
Cl(1)-Pd(1)-Cl(2)	90.41(2)
C(20)-P(1)-C(14)	104.89(10)
C(20)-P(1)-C(13)	104.10(9)
C(14)-P(1)-C(13)	108.17(11)
C(20)-P(1)-Pd(1)	118.79(9)
C(14)-P(1)-Pd(1)	115.72(6)
C(13)-P(1)-Pd(1)	104.21(7)
C(7)-N(1)-C(1)	106.59(17)
C(7)-N(1)-Pd(1)	130.31(11)
C(1)-N(1)-Pd(1)	122.26(14)
C(7)-N(2)-C(2)	108.34(18)
C(7)-N(2)-C(26)	129.19(16)
C(2)-N(2)-C(26)	122.46(16)
N(1)-C(1)-C(6)	130.9(2)
N(1)-C(1)-C(2)	108.61(17)
C(6)-C(1)-C(2)	120.48(17)
C(3)-C(2)-N(2)	132.2(2)
C(3)-C(2)-C(1)	122.7(2)
N(2)-C(2)-C(1)	105.02(16)
C(4)-C(3)-C(2)	116.0(3)
C(4)-C(3)-H(3A)	122.0
C(2)-C(3)-H(3A)	122.0

C(3)-C(4)-C(5)	121.3(2)
C(3)-C(4)-H(4A)	119.3
C(5)-C(4)-H(4A)	119.3
C(6)-C(5)-C(4)	122.6(2)
C(6)-C(5)-H(5A)	118.7
C(4)-C(5)-H(5A)	118.7
C(5)-C(6)-C(1)	116.9(2)
C(5)-C(6)-H(6A)	121.5
C(1)-C(6)-H(6A)	121.5
N(1)-C(7)-N(2)	111.43(15)
N(1)-C(7)-C(8)	123.66(17)
N(2)-C(7)-C(8)	124.6(2)
C(13)-C(8)-C(9)	121.13(15)
C(13)-C(8)-C(7)	120.93(19)
C(9)-C(8)-C(7)	117.92(16)
C(10)-C(9)-C(8)	119.53(17)
C(10)-C(9)-H(9A)	120.2
C(8)-C(9)-H(9A)	120.2
C(11)-C(10)-C(9)	120.1(2)
C(11)-C(10)-H(10A)	120.0
C(9)-C(10)-H(10A)	120.0
C(10)-C(11)-C(12)	120.01(18)
C(10)-C(11)-H(11A)	120.0
C(12)-C(11)-H(11A)	120.0
C(13)-C(12)-C(11)	121.27(19)
C(13)-C(12)-H(12A)	119.4
C(11)-C(12)-H(12A)	119.4
C(8)-C(13)-C(12)	117.9(2)
C(8)-C(13)-P(1)	122.20(13)
C(12)-C(13)-P(1)	119.78(16)
C(15)-C(14)-C(19)	109.7(2)
C(15)-C(14)-P(1)	116.15(17)
C(19)-C(14)-P(1)	113.01(15)
C(15)-C(14)-H(14A)	105.7
C(19)-C(14)-H(14A)	105.7
P(1)-C(14)-H(14A)	105.7

C(14)-C(15)-C(16)	111.7(2)
C(14)-C(15)-H(15A)	109.3
C(16)-C(15)-H(15A)	109.3
C(14)-C(15)-H(15B)	109.3
C(16)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	107.9
C(15)-C(16)-C(17)	111.0(2)
C(15)-C(16)-H(16A)	109.4
C(17)-C(16)-H(16A)	109.4
C(15)-C(16)-H(16B)	109.4
C(17)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
C(18)-C(17)-C(16)	110.9(3)
C(18)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17A)	109.5
C(18)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	108.1
C(17)-C(18)-C(19)	112.2(2)
C(17)-C(18)-H(18A)	109.2
C(19)-C(18)-H(18A)	109.2
C(17)-C(18)-H(18B)	109.2
C(19)-C(18)-H(18B)	109.2
H(18A)-C(18)-H(18B)	107.9
C(18)-C(19)-C(14)	111.2(2)
C(18)-C(19)-H(19A)	109.4
C(14)-C(19)-H(19A)	109.4
C(18)-C(19)-H(19B)	109.4
C(14)-C(19)-H(19B)	109.4
H(19A)-C(19)-H(19B)	108.0
C(21)-C(20)-C(25)	110.5(2)
C(21)-C(20)-P(1)	115.09(14)
C(25)-C(20)-P(1)	113.02(16)
C(21)-C(20)-H(20A)	105.8
C(25)-C(20)-H(20A)	105.8
P(1)-C(20)-H(20A)	105.8

C(22)-C(21)-C(20)	109.4(2)
C(22)-C(21)-H(21A)	109.8
C(20)-C(21)-H(21A)	109.8
C(22)-C(21)-H(21B)	109.8
C(20)-C(21)-H(21B)	109.8
H(21A)-C(21)-H(21B)	108.2
C(23)-C(22)-C(21)	113.2(3)
C(23)-C(22)-H(22A)	108.9
C(21)-C(22)-H(22A)	108.9
C(23)-C(22)-H(22B)	108.9
C(21)-C(22)-H(22B)	108.9
H(22A)-C(22)-H(22B)	107.7
C(22)-C(23)-C(24)	111.5(3)
C(22)-C(23)-H(23A)	109.3
C(24)-C(23)-H(23A)	109.3
C(22)-C(23)-H(23B)	109.3
C(24)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	108.0
C(23)-C(24)-C(25)	111.3(2)
C(23)-C(24)-H(24A)	109.4
C(25)-C(24)-H(24A)	109.4
C(23)-C(24)-H(24B)	109.4
C(25)-C(24)-H(24B)	109.4
H(24A)-C(24)-H(24B)	108.0
C(24)-C(25)-C(20)	110.4(2)
C(24)-C(25)-H(25A)	109.6
C(20)-C(25)-H(25A)	109.6
C(24)-C(25)-H(25B)	109.6
C(20)-C(25)-H(25B)	109.6
H(25A)-C(25)-H(25B)	108.1
N(2)-C(26)-H(26A)	109.5
N(2)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
N(2)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Cl(4)-C(27)-Cl(3)	114.2(3)
Cl(4)-C(27)-H(27A)	108.7
Cl(3)-C(27)-H(27A)	108.7
Cl(4)-C(27)-H(27B)	108.7
Cl(3)-C(27)-H(27B)	108.7
H(27A)-C(27)-H(27B)	107.6
Cl(4)-C(27')-Cl(3')	105.0(4)
Cl(4)-C(27')-H(27C)	110.7
Cl(3')-C(27')-H(27C)	110.7
Cl(4)-C(27')-H(27D)	110.7
Cl(3')-C(27')-H(27D)	110.7
H(27C)-C(27')-H(27D)	108.8
C(27')-Cl(4)-C(27)	30.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for socm43. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	32(1)	37(1)	29(1)	7(1)	4(1)	18(1)
Cl(1)	51(1)	75(1)	43(1)	1(1)	-7(1)	40(1)
Cl(2)	41(1)	37(1)	38(1)	4(1)	7(1)	20(1)
P(1)	32(1)	34(1)	25(1)	4(1)	0(1)	13(1)
N(1)	33(1)	35(1)	25(1)	-1(1)	3(1)	18(1)
N(2)	27(1)	42(1)	33(1)	8(1)	3(1)	14(1)
C(1)	33(1)	35(1)	24(1)	4(1)	7(1)	13(1)
C(2)	24(1)	45(1)	24(1)	5(1)	4(1)	10(1)
C(3)	26(1)	56(1)	43(1)	7(1)	1(1)	9(1)
C(4)	42(2)	41(1)	40(1)	4(1)	6(1)	-8(1)
C(5)	51(1)	43(1)	43(1)	8(1)	13(1)	18(1)
C(6)	36(1)	35(1)	40(1)	6(1)	8(1)	13(1)
C(7)	26(1)	40(1)	24(1)	5(1)	3(1)	13(1)
C(8)	27(1)	36(1)	32(1)	9(1)	3(1)	14(1)
C(9)	47(1)	54(1)	29(1)	10(1)	6(1)	31(1)
C(10)	55(1)	45(1)	49(1)	23(1)	15(1)	29(1)
C(11)	51(1)	39(1)	52(1)	13(1)	7(1)	21(1)
C(12)	50(1)	43(1)	35(1)	5(1)	-2(1)	17(1)
C(13)	47(1)	39(1)	26(1)	8(1)	10(1)	24(1)
C(14)	38(1)	44(1)	34(1)	9(1)	9(1)	19(1)
C(15)	27(1)	42(1)	45(1)	4(1)	6(1)	-5(1)
C(16)	77(2)	54(1)	47(2)	9(1)	26(2)	16(1)
C(17)	54(2)	64(1)	62(2)	14(1)	27(1)	20(1)
C(18)	58(2)	58(1)	43(2)	-8(1)	8(1)	18(1)
C(19)	63(1)	53(1)	39(1)	3(1)	21(1)	25(1)
C(20)	33(1)	37(1)	37(1)	4(1)	-4(1)	9(1)
C(21)	46(1)	56(1)	27(1)	5(1)	-3(1)	17(1)
C(22)	55(2)	70(1)	47(2)	4(1)	-10(2)	15(1)
C(23)	46(2)	94(2)	57(2)	9(1)	-7(2)	16(1)
C(24)	43(2)	55(1)	69(2)	15(1)	1(2)	-1(1)
C(25)	36(1)	57(1)	46(1)	22(1)	6(1)	9(1)

C(26)	40(1)	69(1)	56(1)	20(1)	5(1)	34(1)
C(27)	127(4)	162(4)	58(5)	23(3)	28(4)	97(3)
Cl(3)	227(1)	173(1)	195(2)	123(1)	129(1)	161(1)
C(27')	52(6)	94(5)	106(6)	41(4)	-5(5)	-22(4)
Cl(3')	121(2)	295(3)	267(4)	157(2)	72(3)	105(2)
Cl(4)	134(1)	135(1)	96(1)	26(1)	35(1)	79(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for socm43.

	x	y	z	U(eq)
H(3A)	-4467	1822	673	55
H(4A)	-4503	-437	809	61
H(5A)	-2105	-668	1133	56
H(6A)	385	1328	1386	46
H(9A)	-209	6953	346	49
H(10A)	1218	9515	561	54
H(11A)	3211	10824	1651	57
H(12A)	3921	9580	2507	54
H(14A)	2399	5783	3653	46
H(15A)	275	3926	2713	54
H(15B)	-484	5036	2592	54
H(16A)	-140	4071	3965	75
H(16B)	-1801	3609	3399	75
H(17A)	-1570	6027	3716	72
H(17B)	-1373	5512	4483	72
H(18A)	1408	6827	4730	70
H(18B)	627	7915	4595	70
H(19A)	2726	8242	3928	62
H(19B)	1072	7777	3355	62
H(20A)	4878	8843	3320	48
H(21A)	5006	7328	4154	55
H(21B)	6046	6775	3673	55
H(22A)	7043	9748	4495	78
H(22B)	7808	8698	4722	78
H(23A)	8970	8791	3666	88
H(23B)	9486	10423	4128	88
H(24A)	8676	10156	2797	77
H(24B)	7604	10692	3259	77
H(25A)	6627	7716	2436	59
H(25B)	5886	8775	2192	59

H(26A)	-2125	6058	766	77
H(26B)	-3397	4881	1099	77
H(26C)	-3333	4509	229	77
H(27A)	2748	11505	3344	124
H(27B)	4152	12959	3267	124
H(27C)	5041	13701	3515	122
H(27D)	4833	14065	4368	122

Table 6. Torsion angles [°] for socm43.

N(1)-Pd(1)-P(1)-C(20)	-164.79(11)
Cl(1)-Pd(1)-P(1)-C(20)	24.69(9)
Cl(2)-Pd(1)-P(1)-C(20)	-99.92(13)
N(1)-Pd(1)-P(1)-C(14)	69.05(10)
Cl(1)-Pd(1)-P(1)-C(14)	-101.48(9)
Cl(2)-Pd(1)-P(1)-C(14)	133.91(12)
N(1)-Pd(1)-P(1)-C(13)	-49.57(9)
Cl(1)-Pd(1)-P(1)-C(13)	139.90(7)
Cl(2)-Pd(1)-P(1)-C(13)	15.29(13)
P(1)-Pd(1)-N(1)-C(7)	39.6(2)
Cl(1)-Pd(1)-N(1)-C(7)	144.3(2)
Cl(2)-Pd(1)-N(1)-C(7)	-129.7(2)
P(1)-Pd(1)-N(1)-C(1)	-128.44(17)
Cl(1)-Pd(1)-N(1)-C(1)	-23.8(4)
Cl(2)-Pd(1)-N(1)-C(1)	62.22(17)
C(7)-N(1)-C(1)-C(6)	-178.1(2)
Pd(1)-N(1)-C(1)-C(6)	-7.6(3)
C(7)-N(1)-C(1)-C(2)	0.8(2)
Pd(1)-N(1)-C(1)-C(2)	171.36(15)
C(7)-N(2)-C(2)-C(3)	177.2(3)
C(26)-N(2)-C(2)-C(3)	-2.3(4)
C(7)-N(2)-C(2)-C(1)	-0.2(2)
C(26)-N(2)-C(2)-C(1)	-179.7(2)
N(1)-C(1)-C(2)-C(3)	-178.1(2)
C(6)-C(1)-C(2)-C(3)	1.0(4)
N(1)-C(1)-C(2)-N(2)	-0.4(2)
C(6)-C(1)-C(2)-N(2)	178.7(2)
N(2)-C(2)-C(3)-C(4)	-177.9(3)
C(1)-C(2)-C(3)-C(4)	-0.9(4)
C(2)-C(3)-C(4)-C(5)	-0.3(4)
C(3)-C(4)-C(5)-C(6)	1.6(4)
C(4)-C(5)-C(6)-C(1)	-1.5(4)
N(1)-C(1)-C(6)-C(5)	179.1(2)
C(2)-C(1)-C(6)-C(5)	0.2(4)

C(1)-N(1)-C(7)-N(2)	-1.0(3)
Pd(1)-N(1)-C(7)-N(2)	-170.47(15)
C(1)-N(1)-C(7)-C(8)	172.4(2)
Pd(1)-N(1)-C(7)-C(8)	2.9(3)
C(2)-N(2)-C(7)-N(1)	0.8(3)
C(26)-N(2)-C(7)-N(1)	-179.8(2)
C(2)-N(2)-C(7)-C(8)	-172.6(2)
C(26)-N(2)-C(7)-C(8)	6.8(4)
N(1)-C(7)-C(8)-C(13)	-38.3(3)
N(2)-C(7)-C(8)-C(13)	134.2(2)
N(1)-C(7)-C(8)-C(9)	143.1(2)
N(2)-C(7)-C(8)-C(9)	-44.3(3)
C(13)-C(8)-C(9)-C(10)	-0.5(4)
C(7)-C(8)-C(9)-C(10)	178.0(2)
C(8)-C(9)-C(10)-C(11)	-2.2(4)
C(9)-C(10)-C(11)-C(12)	2.2(4)
C(10)-C(11)-C(12)-C(13)	0.5(4)
C(9)-C(8)-C(13)-C(12)	3.1(4)
C(7)-C(8)-C(13)-C(12)	-175.4(2)
C(9)-C(8)-C(13)-P(1)	-172.31(19)
C(7)-C(8)-C(13)-P(1)	9.2(3)
C(11)-C(12)-C(13)-C(8)	-3.1(4)
C(11)-C(12)-C(13)-P(1)	172.4(2)
C(20)-P(1)-C(13)-C(8)	164.2(2)
C(14)-P(1)-C(13)-C(8)	-84.6(2)
Pd(1)-P(1)-C(13)-C(8)	39.0(2)
C(20)-P(1)-C(13)-C(12)	-11.1(2)
C(14)-P(1)-C(13)-C(12)	100.1(2)
Pd(1)-P(1)-C(13)-C(12)	-136.3(2)
C(20)-P(1)-C(14)-C(15)	-173.81(19)
C(13)-P(1)-C(14)-C(15)	75.5(2)
Pd(1)-P(1)-C(14)-C(15)	-40.9(2)
C(20)-P(1)-C(14)-C(19)	58.06(19)
C(13)-P(1)-C(14)-C(19)	-52.58(17)
Pd(1)-P(1)-C(14)-C(19)	-169.00(14)
C(19)-C(14)-C(15)-C(16)	-56.2(3)

P(1)-C(14)-C(15)-C(16)	174.1(2)
C(14)-C(15)-C(16)-C(17)	56.6(3)
C(15)-C(16)-C(17)-C(18)	-55.1(3)
C(16)-C(17)-C(18)-C(19)	55.3(4)
C(17)-C(18)-C(19)-C(14)	-55.8(3)
C(15)-C(14)-C(19)-C(18)	55.4(3)
P(1)-C(14)-C(19)-C(18)	-173.25(18)
C(14)-P(1)-C(20)-C(21)	51.4(2)
C(13)-P(1)-C(20)-C(21)	164.94(19)
Pd(1)-P(1)-C(20)-C(21)	-79.8(2)
C(14)-P(1)-C(20)-C(25)	179.61(18)
C(13)-P(1)-C(20)-C(25)	-66.8(2)
Pd(1)-P(1)-C(20)-C(25)	48.4(2)
C(25)-C(20)-C(21)-C(22)	56.3(3)
P(1)-C(20)-C(21)-C(22)	-174.2(2)
C(20)-C(21)-C(22)-C(23)	-55.6(4)
C(21)-C(22)-C(23)-C(24)	55.1(4)
C(22)-C(23)-C(24)-C(25)	-54.6(4)
C(23)-C(24)-C(25)-C(20)	56.3(4)
C(21)-C(20)-C(25)-C(24)	-57.5(3)
P(1)-C(20)-C(25)-C(24)	171.9(2)
Cl(3')-C(27')-Cl(4)-C(27)	20.6(4)
Cl(3)-C(27)-Cl(4)-C(27')	-57.1(7)

Symmetry transformations used to generate equivalent atoms:

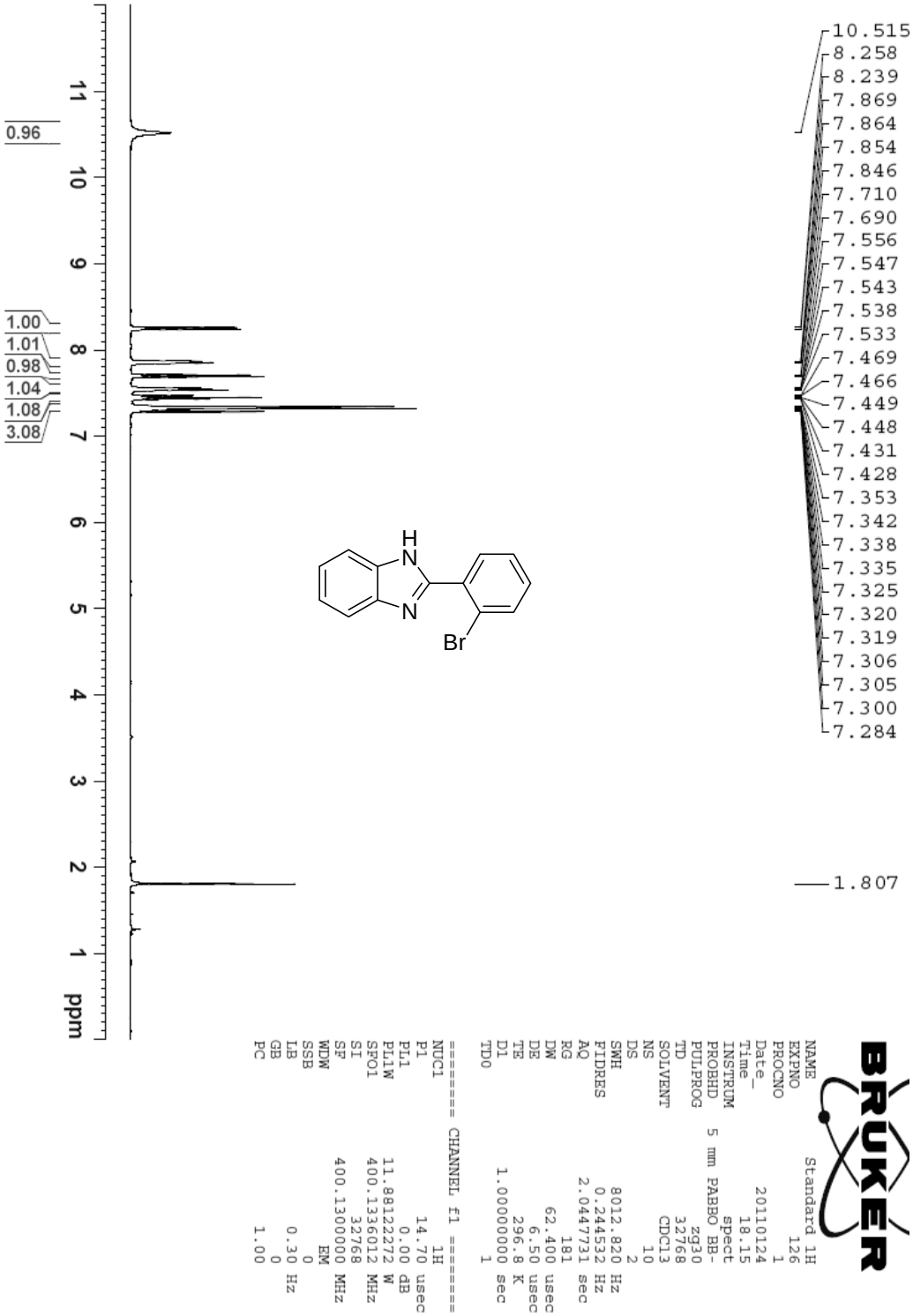
Table 7. Hydrogen bonds for socm43 [Å and °].

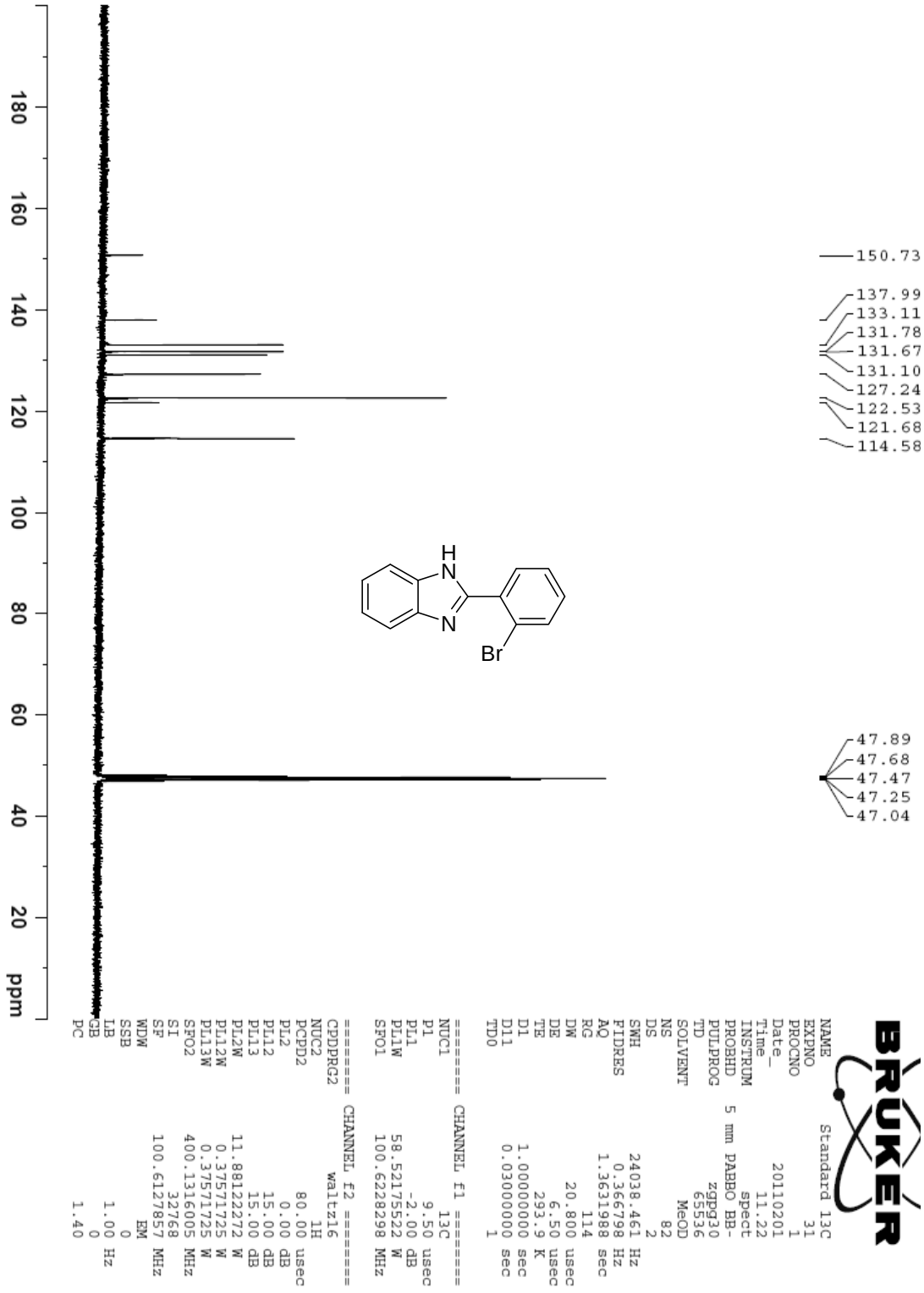
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(27)-H(27B)...Cl(1)#1	0.97	2.67	3.640(5)	174.5

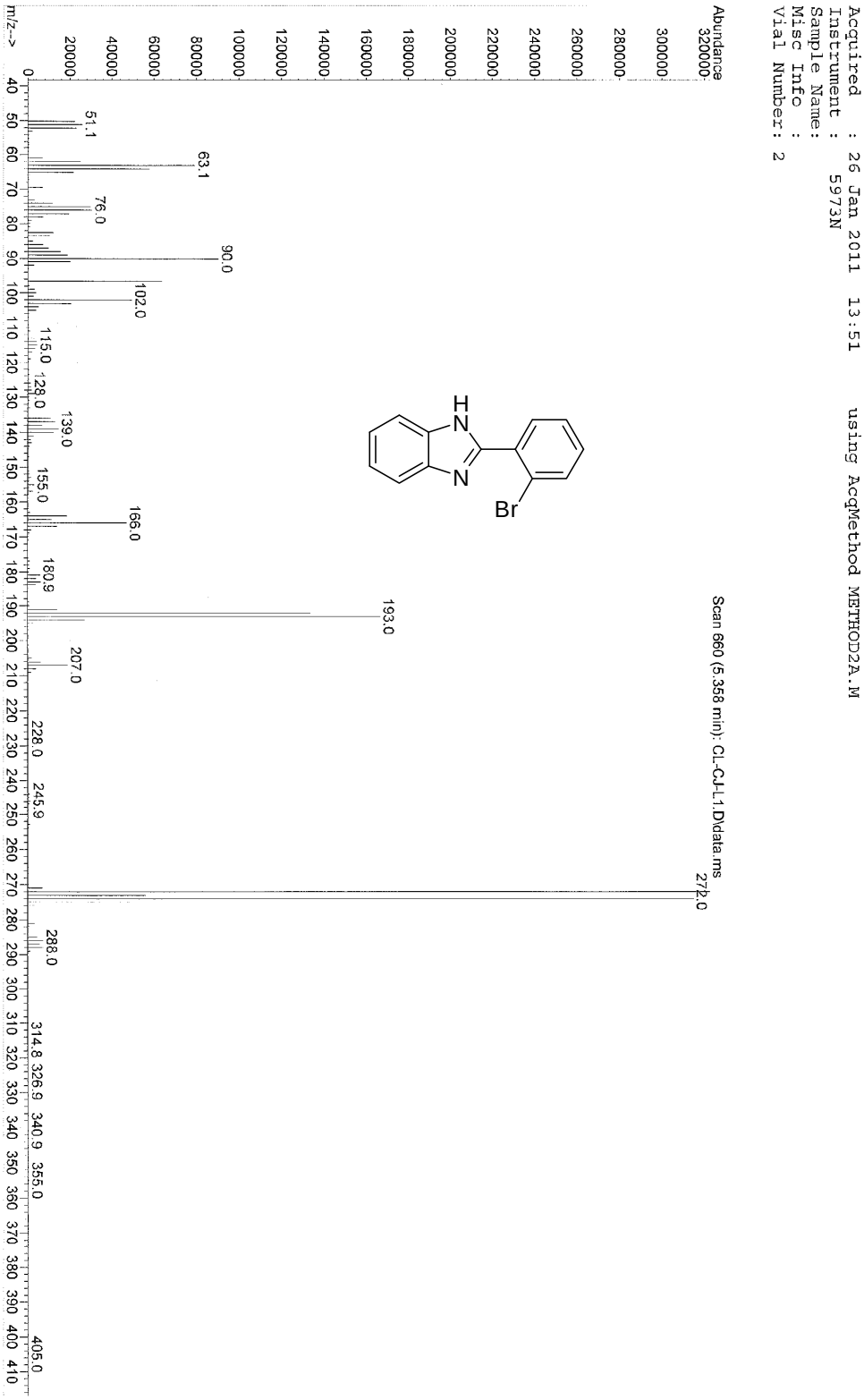
Symmetry transformations used to generate equivalent atoms:

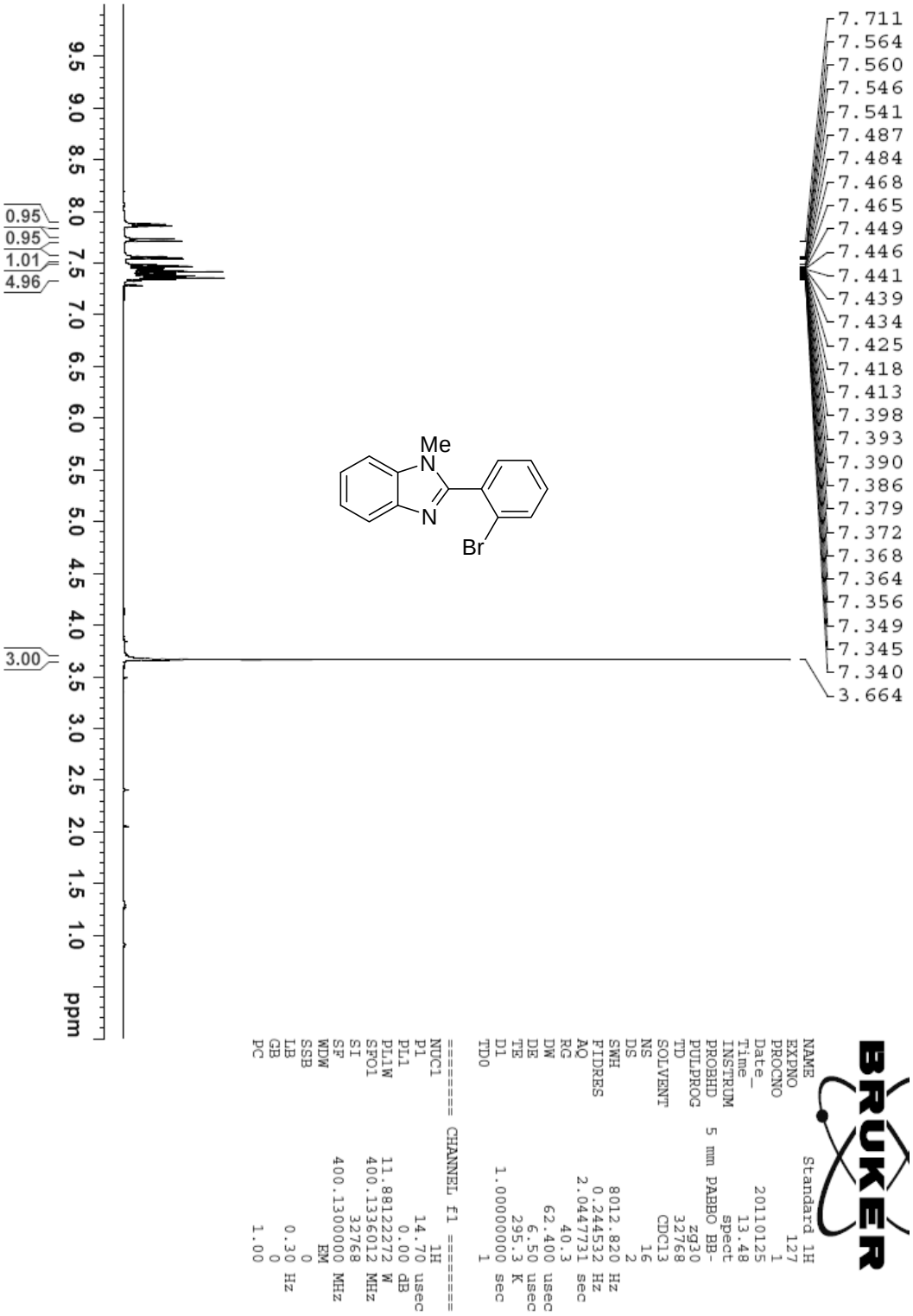
#1 x,y+1,z

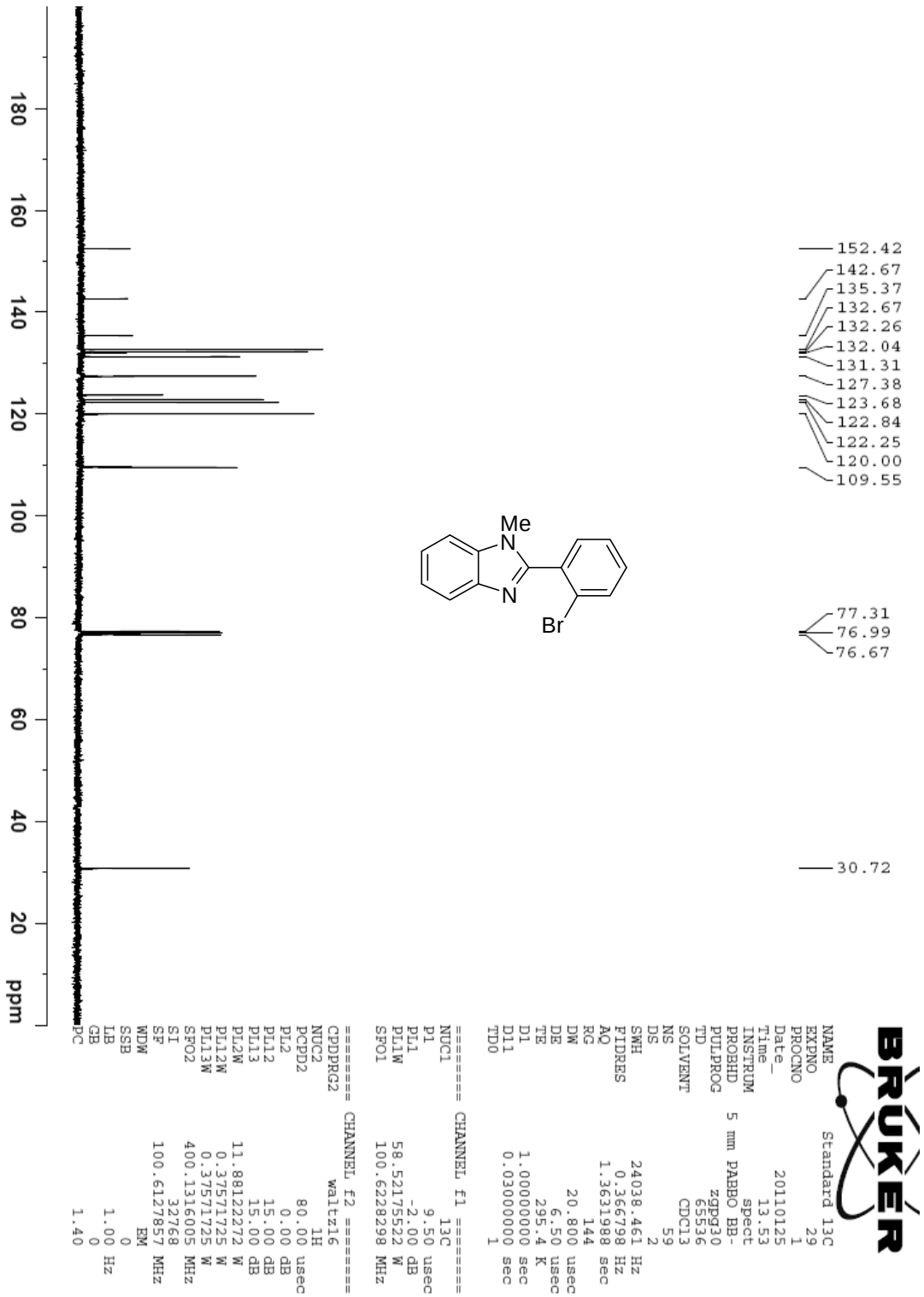
7. ^{1}H, ^{13}C, ^{31}P NMR, MS and HRMS spectra

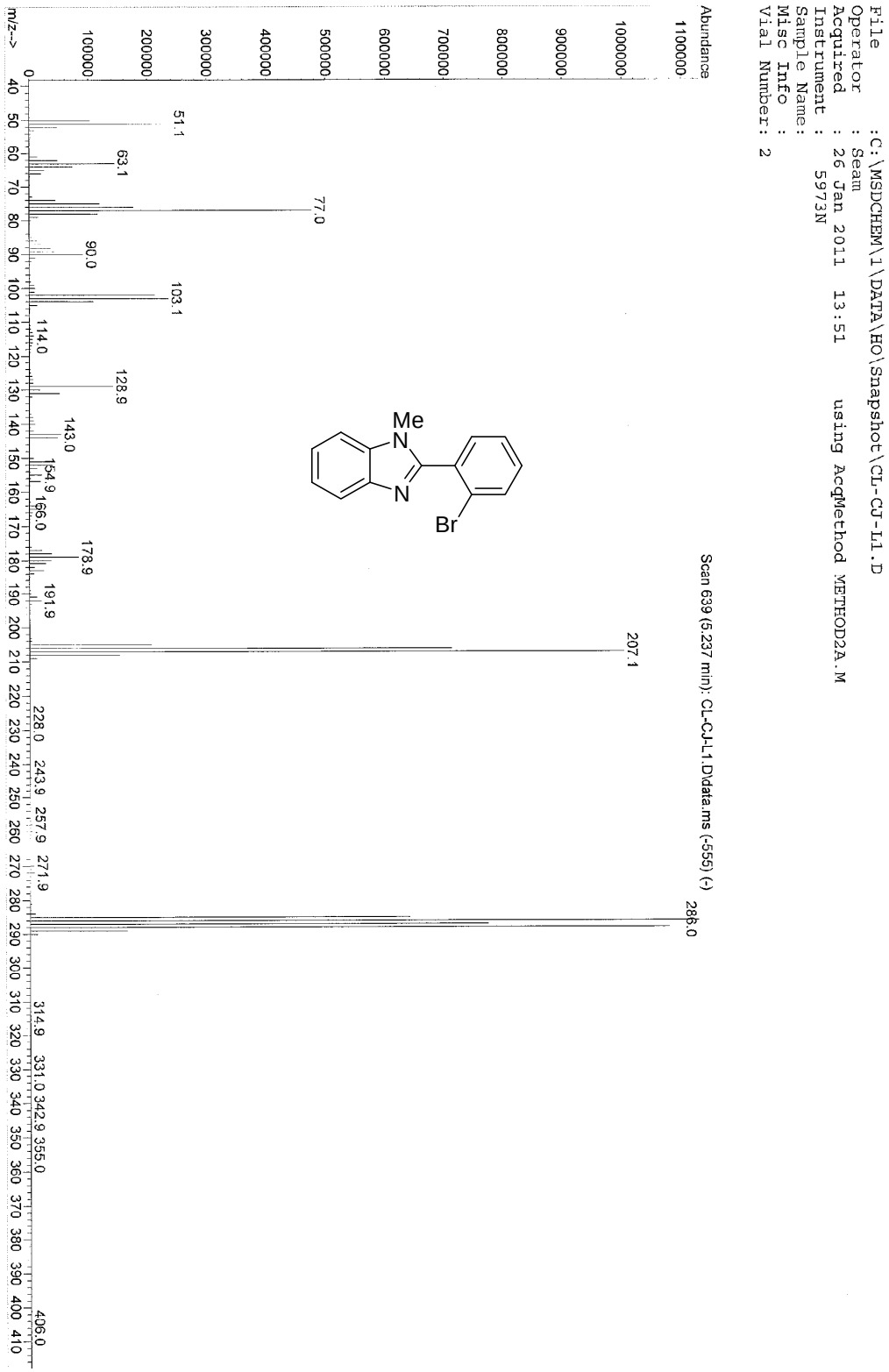


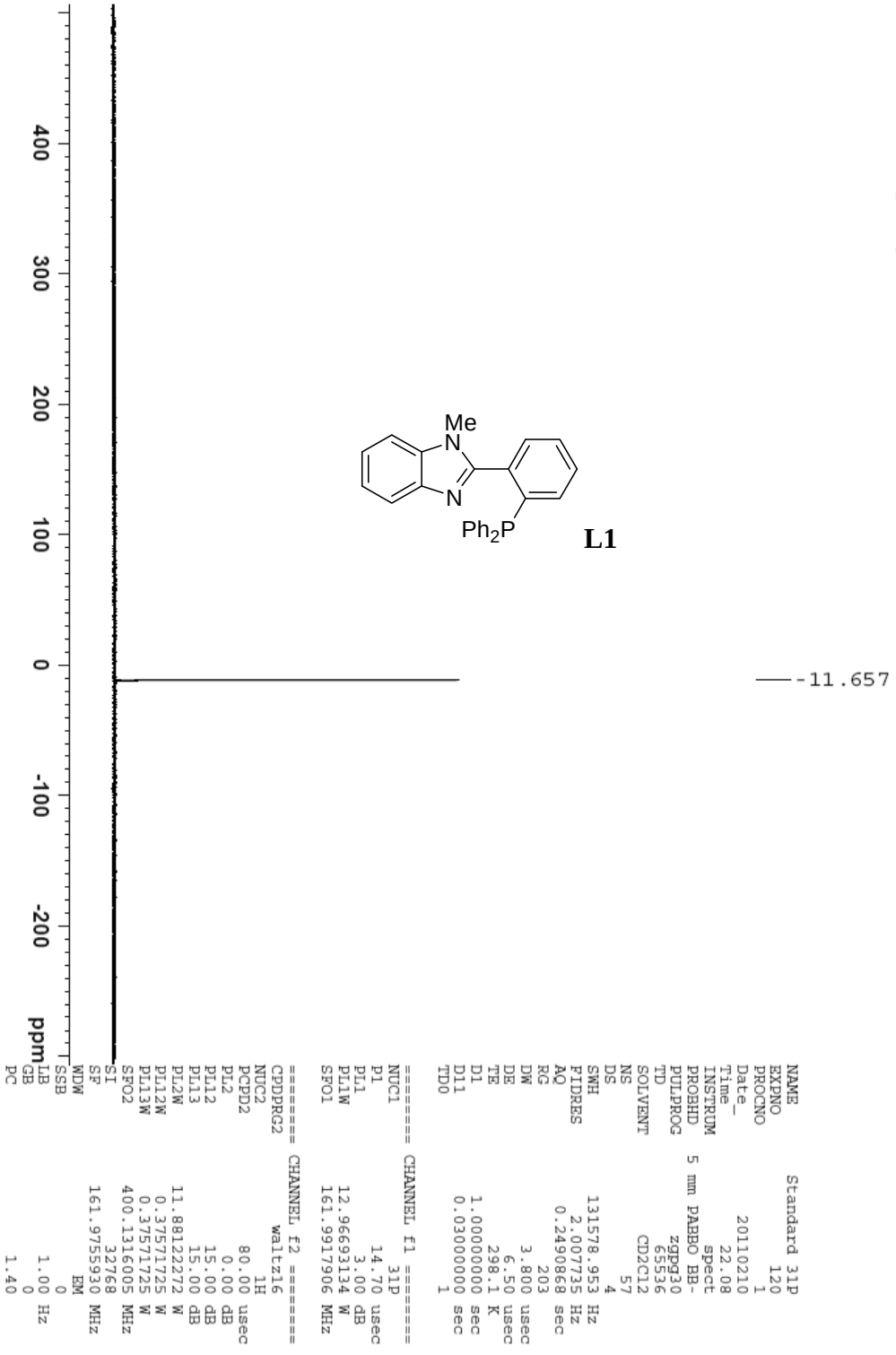

150.73
137.99
133.11
131.78
131.67
131.10
127.24
122.53
121.68
114.58
47.89
47.68
47.47
47.25
47.04
H
N
N
Br
180
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME Standard 13C
EXPNO 31
PROCNO 1
Date_ 20110201
Time_ 11.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 82
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127857 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


File :C:\MSDCHEM\1\DATA\HO\Snapshot\CL-CJ-L1.D
Operator : Seam
Acquired : 26 Jan 2011 13:51 using AcqMethod METHOD2A.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 2
Abundance
m/z-->
Scan 660 (5.358 min): CL-CJ-L1.D\data.ms
H
N
N
Br
51.1
63.1
76.0
90.0
102.0
115.0
128.0
139.0
155.0
166.0
180.9
193.0
207.0
228.0
245.9
272.0
288.0
314.8
326.9
340.9
355.0
405.0


7.711
7.564
7.560
7.546
7.541
7.487
7.484
7.468
7.465
7.449
7.446
7.441
7.439
7.434
7.425
7.418
7.413
7.398
7.393
7.390
7.386
7.379
7.372
7.368
7.364
7.356
7.349
7.345
7.340
3.664
Me
N
N
Br
0.95
0.95
1.01
4.96
3.00
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
NAME Standard 1H
EXPNO 127
PROCNO 1
Date_ 20110125
Time_ 13.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


152.42
142.67
135.37
132.67
132.26
132.04
131.31
127.38
123.68
122.84
122.25
120.00
109.55
77.31
76.99
76.67
30.72
Me
N
N
Br
180
160
140
120
100
80
60
40
20
ppm
NAME Standard 13C
EXPNO 29
PROCNO 1
Date_ 20110125
Time_ 13.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 59
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127857 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
1.40
PC

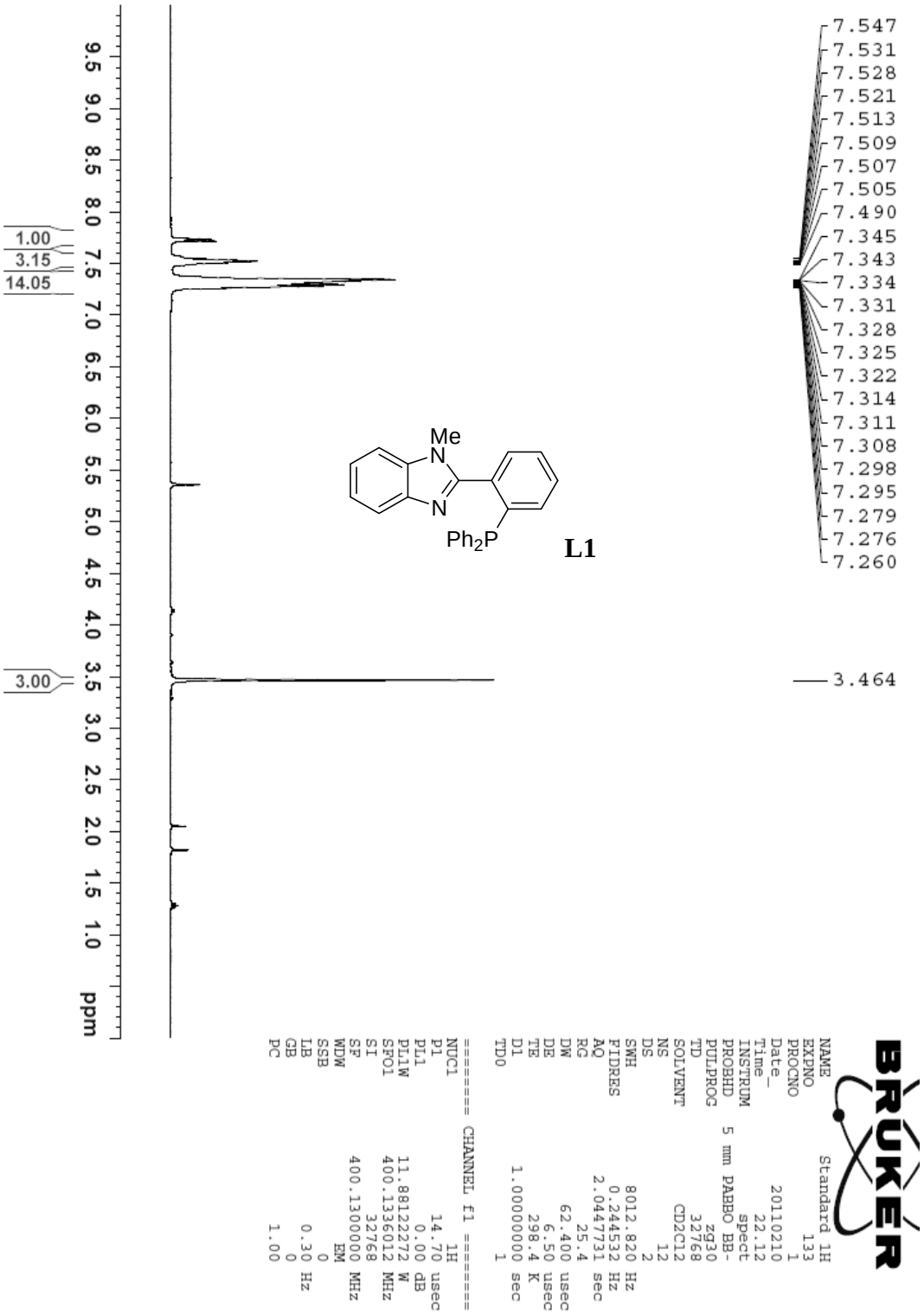

File :C:\MSDCHEM\1\DATA\HO\Snapshot\CL-CJ-L1.D
Operator : Seam
Acquired : 26 Jan 2011 13:51 using AcqMethod METHOD2A.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 2
Abundance
Scan 639 (5.237 min): CL-CJ-L1.D\data.ms (-556) (-)
m/z-->




```
NAME                                    Standard 31p
EXPNO                                   120
PROCNO                                  1
Date_                                   20110210
Time_                                   22.08
INSTRUM                                 spect
PROBHD                 5 mm PABBO BB-
PULPROG                                 zgpg30
TD                                      65536
SOLVENT                                 CD2Cl2
NS                                      57
DS                                      4
SWH                                     131578.953 Hz
FIDRES                                  2.007735 Hz
AQ                                      0.2490868 sec
RG                                      203
DW                                      3.800 usec
DE                                      6.50 usec
TE                                      298.1 K
D1                                      1.00000000 sec
D11                                     0.03000000 sec
TD0                                     1

======== CHANNEL f1 ========
NUC1                                    31P
P1                                      14.70 usec
PL1                                     3.00 dB
PL1W                                    12.96693134 W
SFO1                                    161.9917906 MHz

======== CHANNEL f2 ========
CPDPRG2                                 waltz16
NUC2                                    1H
PCPD2                                   80.00 usec
PL2                                     0.00 dB
PL12                                    15.00 dB
PL13                                    15.00 dB
PL2W                                    11.88122272 W
PL12W                                   0.37571725 W
PL13W                                   0.37571725 W
SFO2                                    400.1316005 MHz
SI                                      32768
SF                                      161.9755930 MHz
WDW                                     EM
SSB                                     0
LB                                      1.00 Hz
GB                                      0
PC                                      1.40
```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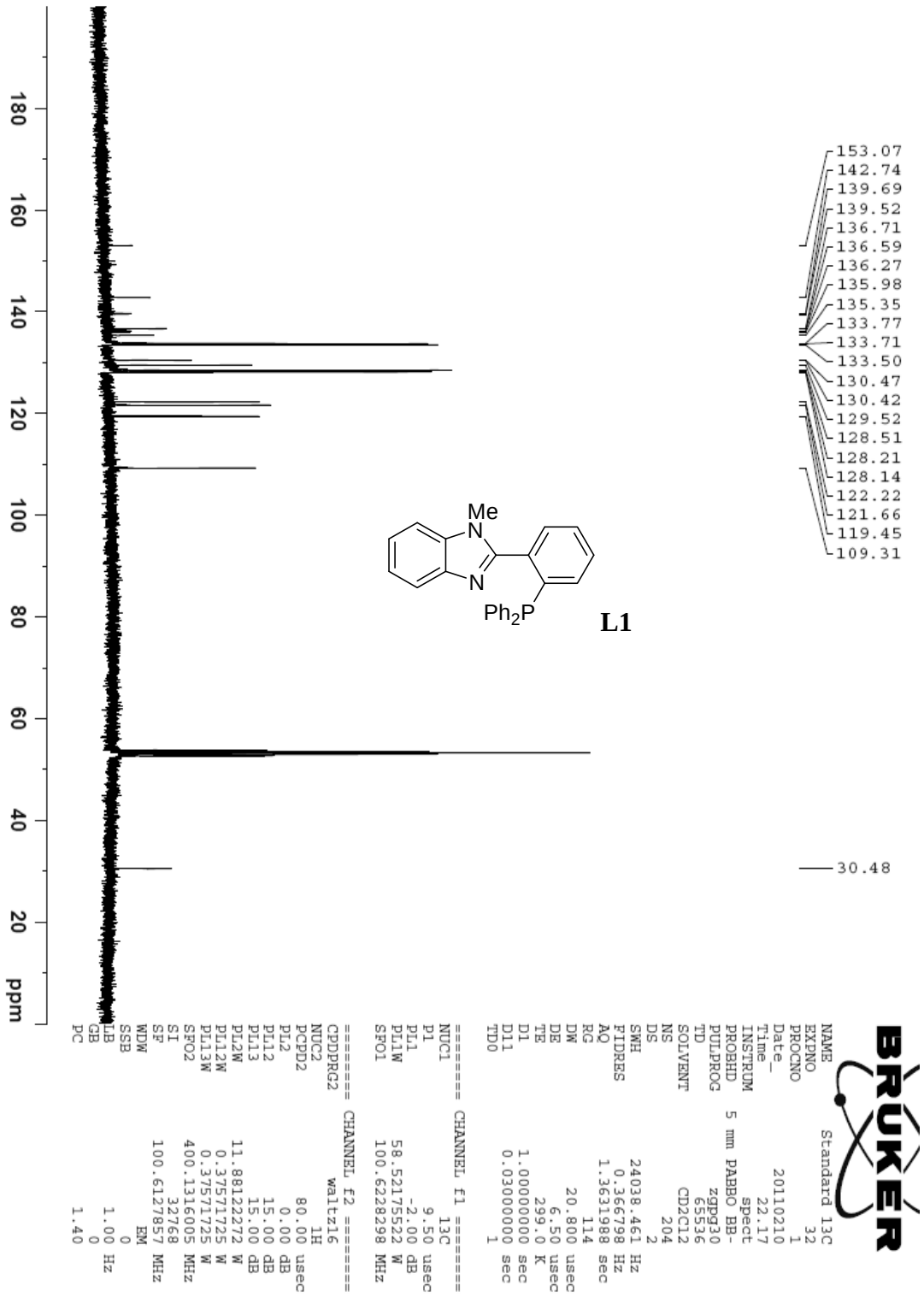
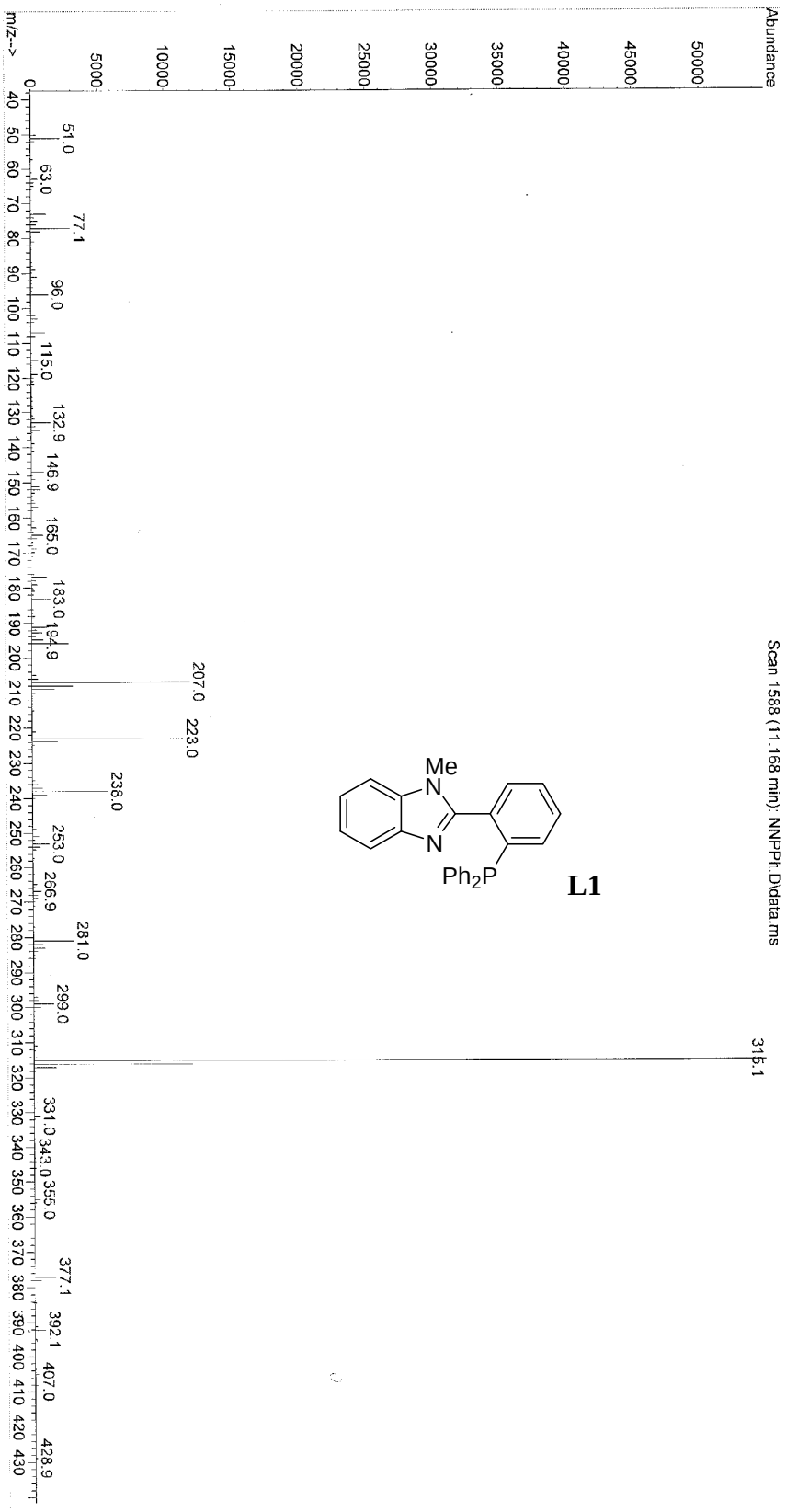
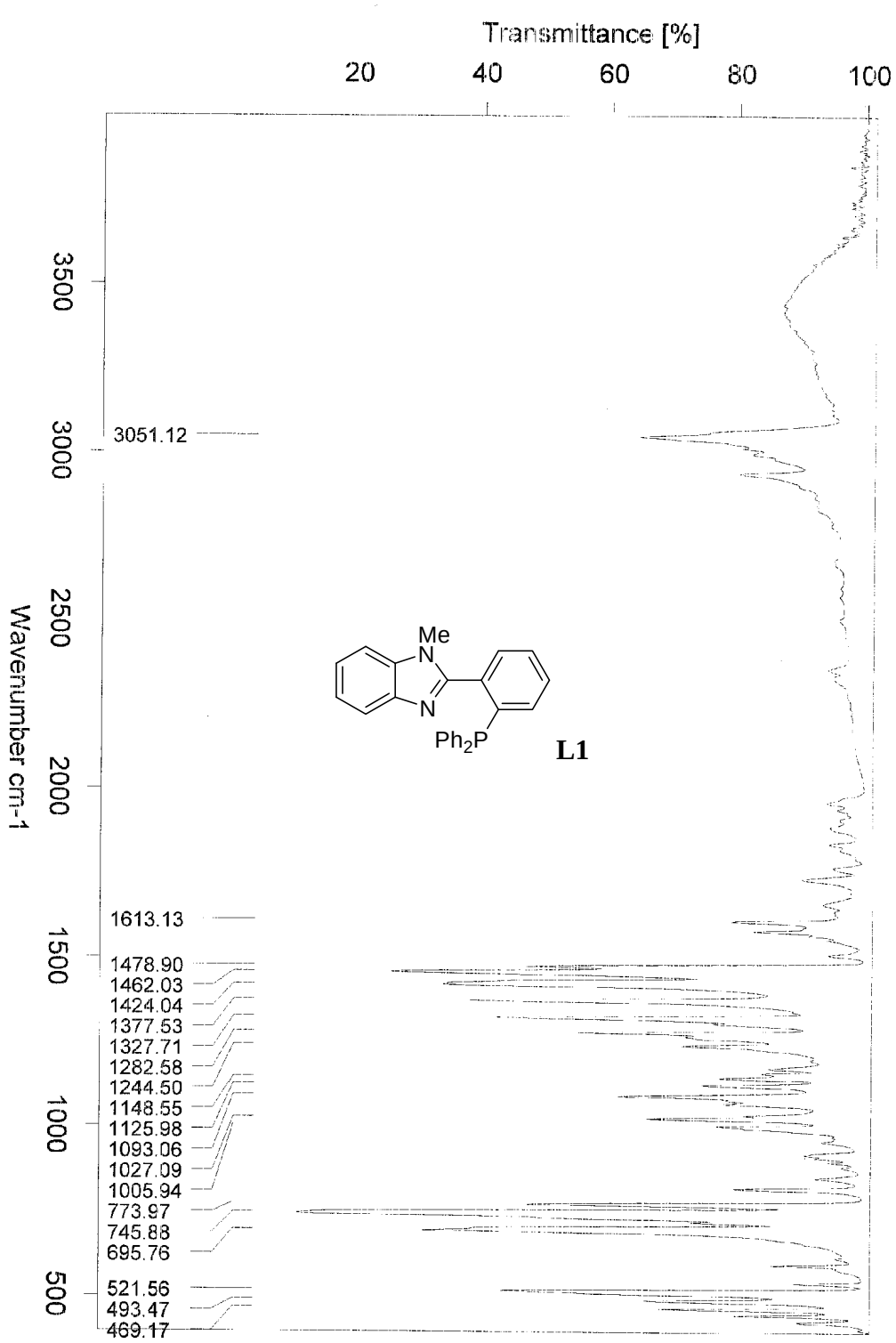
7.531
7.528
7.521
7.513
7.509
7.507
7.505
7.490
7.345
7.343
7.334
7.331
7.328
7.325
7.322
7.314
7.311
7.308
7.298
7.295
7.279
7.276
7.260
3.464
1.00
3.15
14.05
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
Me
N
N
Ph2P
L1
BRUKER
NAME Standard 1H
EXPNO 133
PROCNO 1
Date_ 20110210
Time_ 22.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CD2Cl2
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 25.4
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


153.07
142.74
139.69
139.52
136.71
136.59
136.27
135.98
135.35
133.77
133.71
133.50
130.47
130.42
129.52
128.51
128.21
128.14
122.22
121.66
119.45
109.31
30.48
Me
N
N
Ph2P
L1
180
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME Standard 13C
EXPNO 32
PROCNO 1
Date_ 20110210
Time_ 22.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 204
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127857 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
CB 1.40
PC


File :C:\msdchem\1\DATA\DIC\NNPPh.D
Operator : Seam
Acquired : 10 Feb 2011 16:27 using AcqMethod METHOD2F.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 2
Abundance
m/z-->
Scan 1588 (11.168 min): NNPPr.D\data.ms
Me
N
N
Ph2P
L1

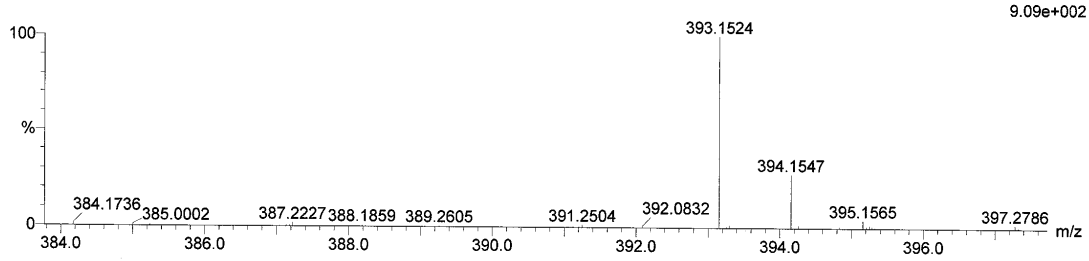

Transmittance [%]
20
40
60
80
100
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3051.12
1613.13
1478.90
1462.03
1424.04
1377.53
1327.71
1282.58
1244.50
1148.55
1125.98
1093.06
1027.09
1005.94
773.97
745.88
695.76
521.56
493.47
469.17
Me
N
N
Ph2P

L1

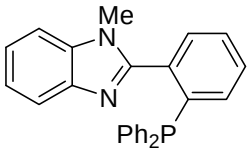
mental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

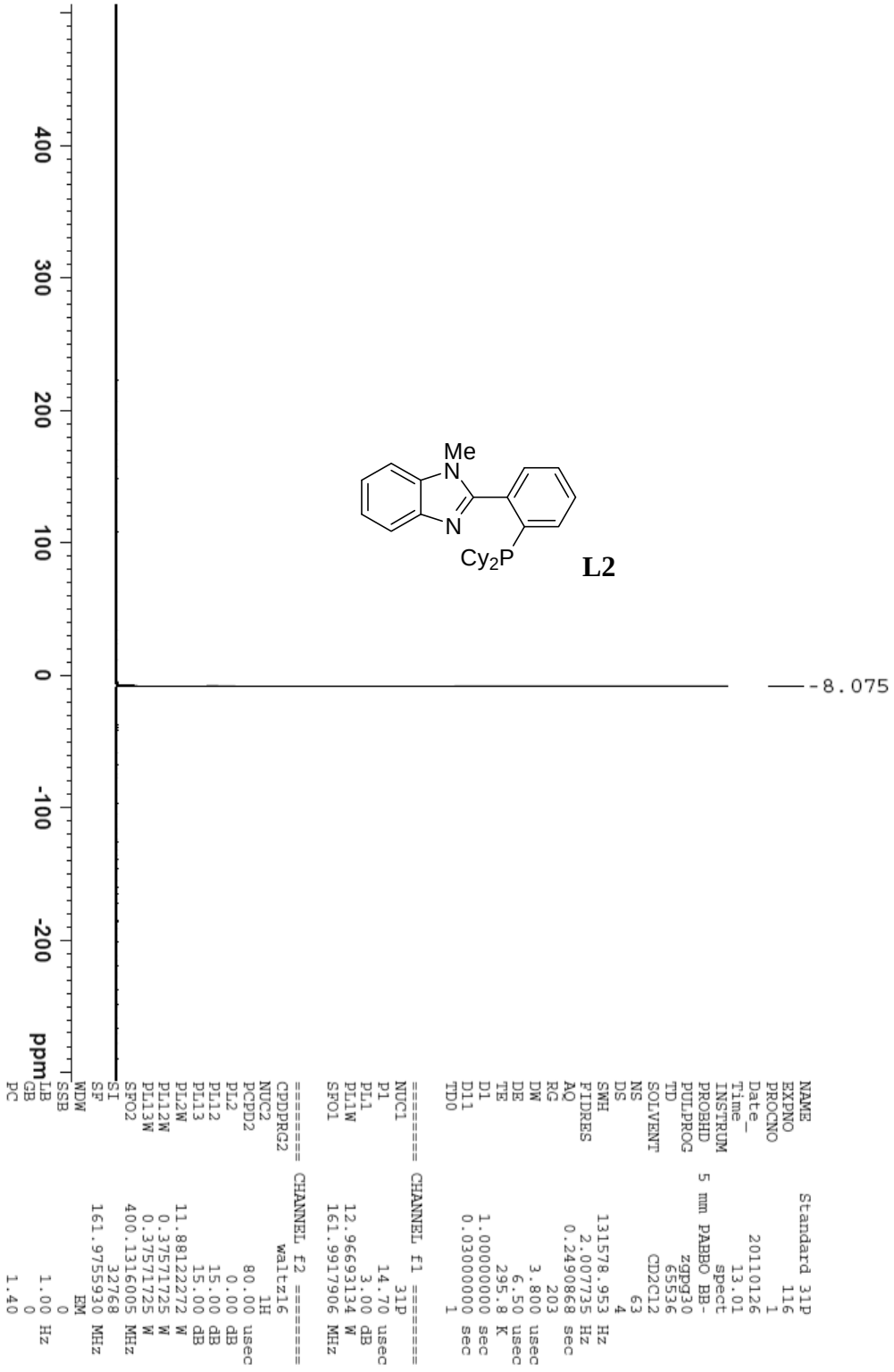
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-26 H: 0-26 N: 0-3 Na: 0-1 P: 0-1
Kin-Dept-16022011-HS S10 51 (0.967) Cn (Cen,4, 80.00, Ar); Sm (SG, 2x3.00); Sb (5,40.00); Cm (40:58)
TOF MS ES+



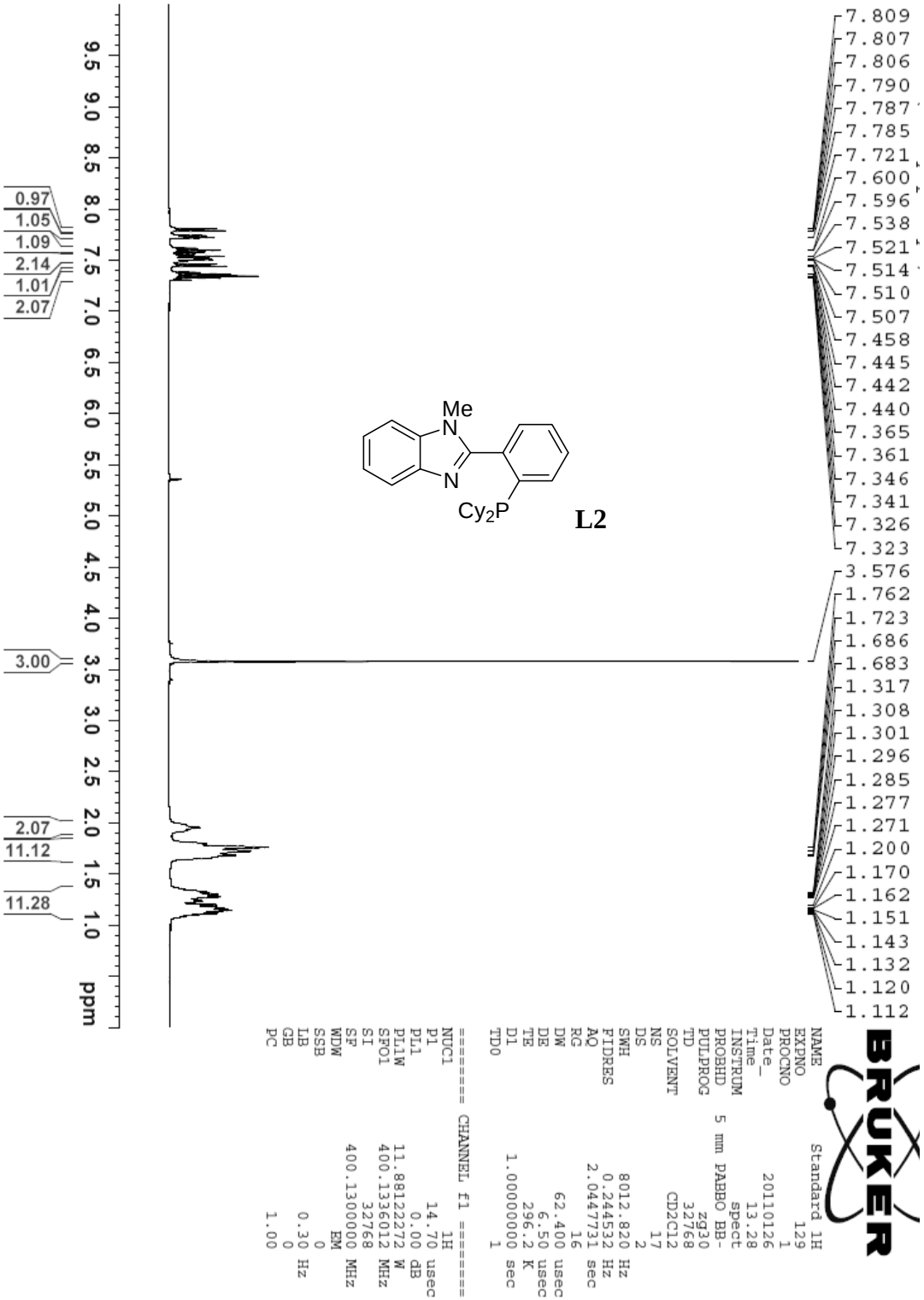
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
393.1524	393.1521	0.3	0.8	17.5	1.0	C26 H22 N2 P



L1


Me
N
N
Cy2P
-8.075
400
300
200
100
0
-100
-200
ppm
NAME Standard 31p
EXPNO 116
PROCNO 1
Date_ 20110126
Time_ 13.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 63
DS 4
SWH 131578.953 Hz
FIDRES 2.007735 Hz
AQ 0.2490868 sec
RG 203
DW 3.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
========== CHANNEL f1 ==========
NUC1 31p
P1 14.70 usec
PL1 3.00 dB
PL1W 12.96693134 W
SFO1 161.9917906 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 161.9755930 MHz
EM
0
1.00 Hz
0
1.40
SSB
LB
GB
PC
WDW

L2


Me
N
N
Cy2P
L2
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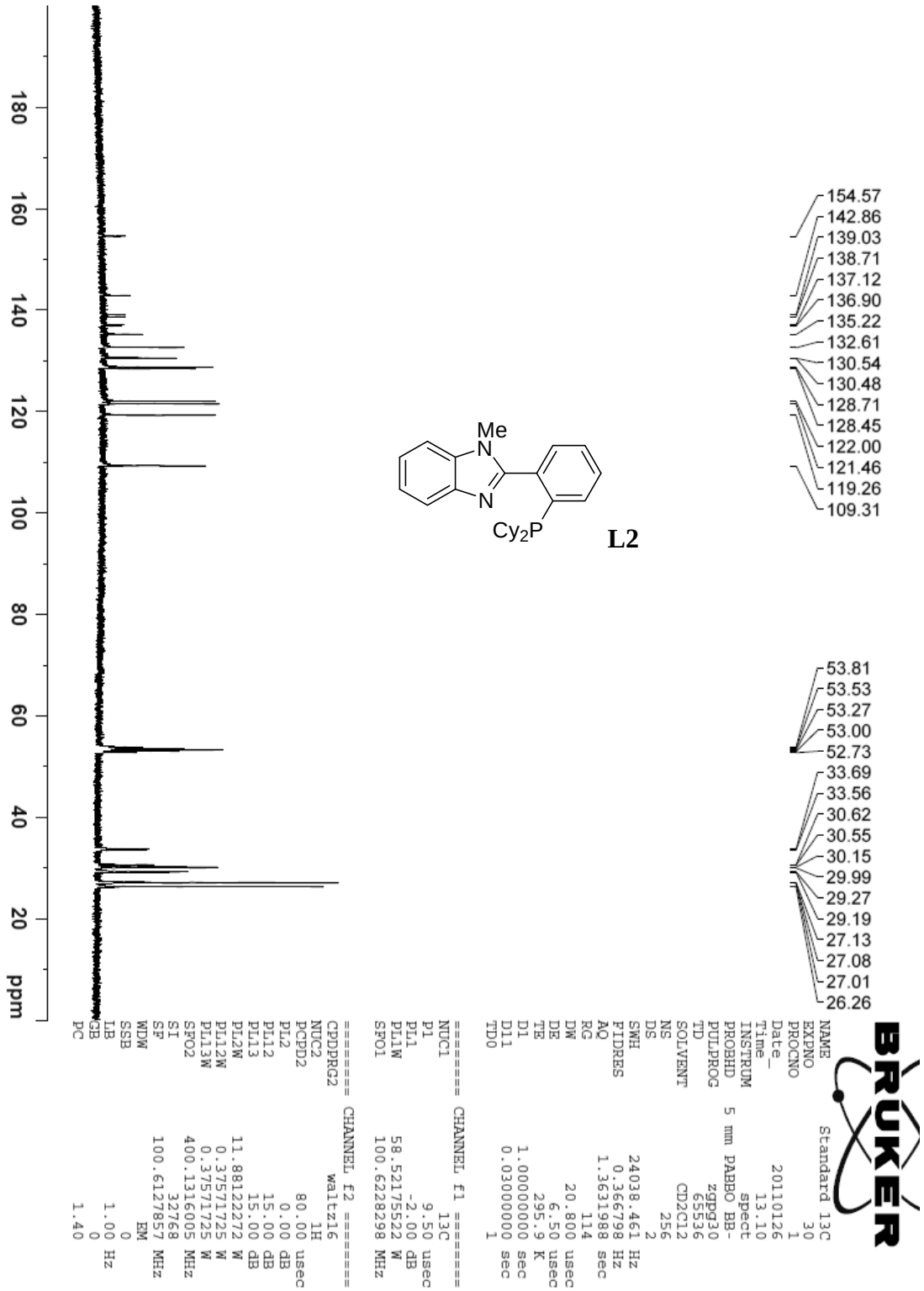
7.807
7.806
7.790
7.787
7.785
7.721
7.600
7.596
7.538
7.521
7.514
7.510
7.507
7.458
7.445
7.442
7.440
7.365
7.361
7.346
7.341
7.326
7.323
3.576
1.762
1.723
1.686
1.683
1.317
1.308
1.301
1.296
1.285
1.277
1.271
1.200
1.170
1.162
1.151
1.143
1.132
1.120
1.112
0.97
1.05
1.09
2.14
1.01
2.07
3.00
2.07
11.12
11.28
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
NAME Standard 1H
EXPNO 129
PROCNO 1
Date_ 20110126
Time_ 13.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CD2Cl2
NS 17
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 16
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER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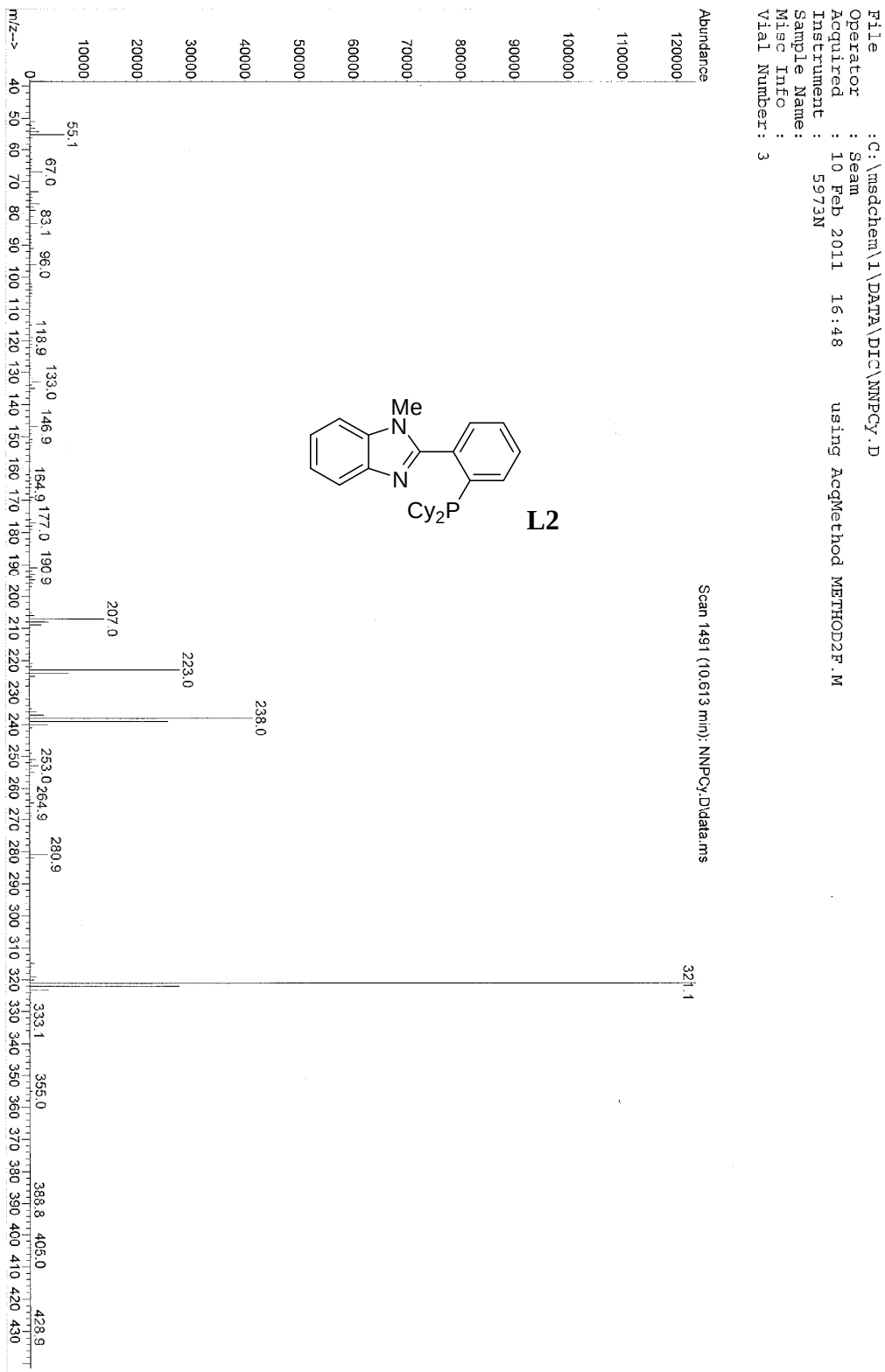
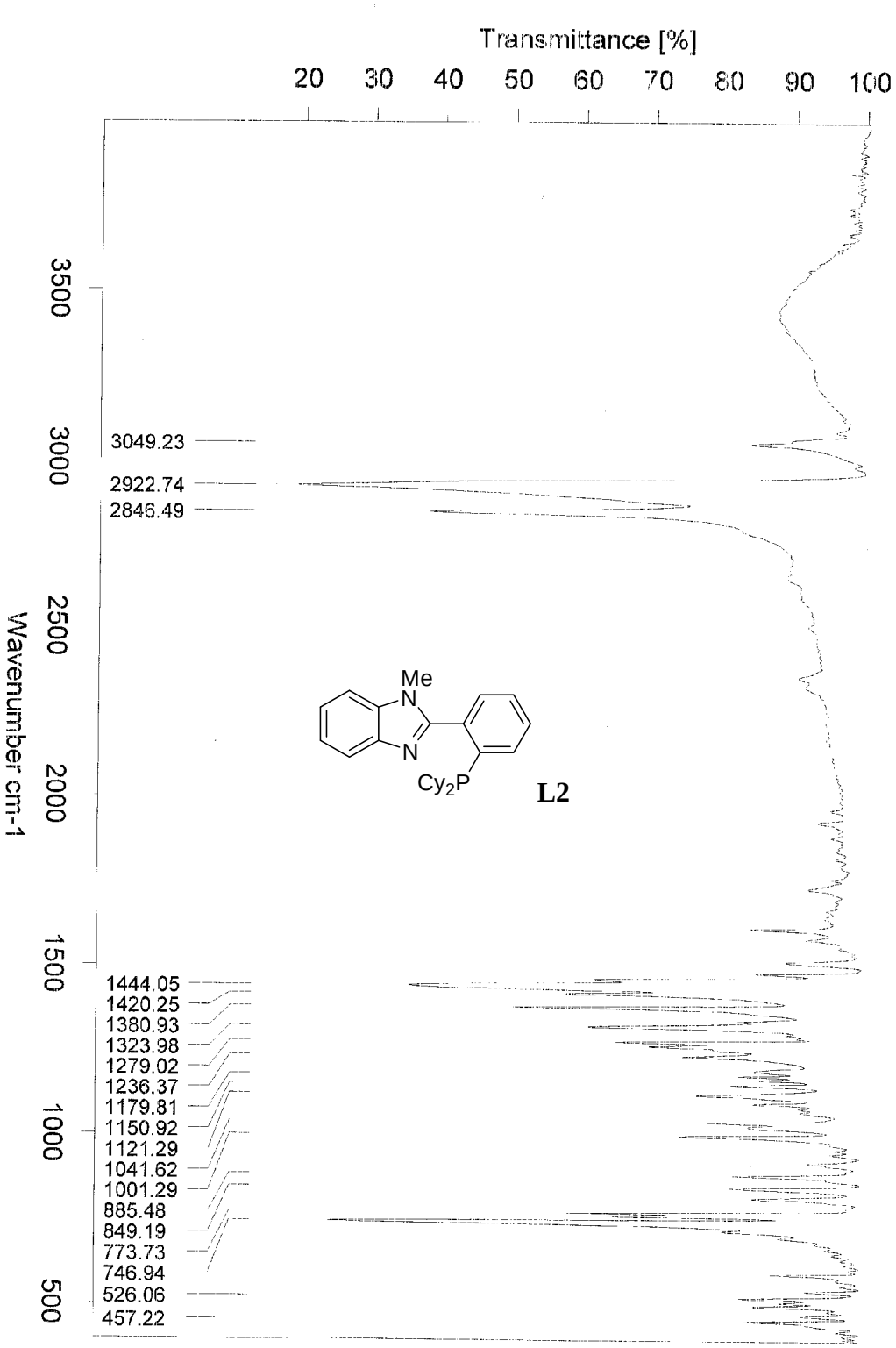
142.86
139.03
138.71
137.12
136.90
135.22
132.61
130.54
130.48
128.71
128.45
122.00
121.46
119.26
109.31
Me
N
N
Cy2P
L2
53.81
53.53
53.27
53.00
52.73
33.69
33.56
30.62
30.55
30.15
29.99
29.27
29.19
27.13
27.08
27.01
26.26
180
160
140
120
100
80
60
40
20
ppm
BRUKER
NAME Standard 13C
EXPNO 30
PROCNO 1
Date_ 20110126
Time_ 13.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 256
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127857 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


File :C:\msdchem\1\DATA\DIC\NNPCy.D
Operator : Seam
Acquired : 10 Feb 2011 16:48 using AcqMethod METHOD2F.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
Scan 1491 (10.613 min): NNPCy.D\data.ms
m/z-->
Me
N
N
Cy2P
L2


Transmittance [%]
20
30
40
50
60
70
80
90
100
Wavenumber cm-1
3500
3000
2500
2000
1500
1000
500
3049.23
2922.74
2846.49
1444.05
1420.25
1380.93
1323.98
1279.02
1236.37
1179.81
1150.92
1121.29
1041.62
1001.29
885.48
849.19
773.73
746.94
526.06
457.22
Me
N
N
Cy2P

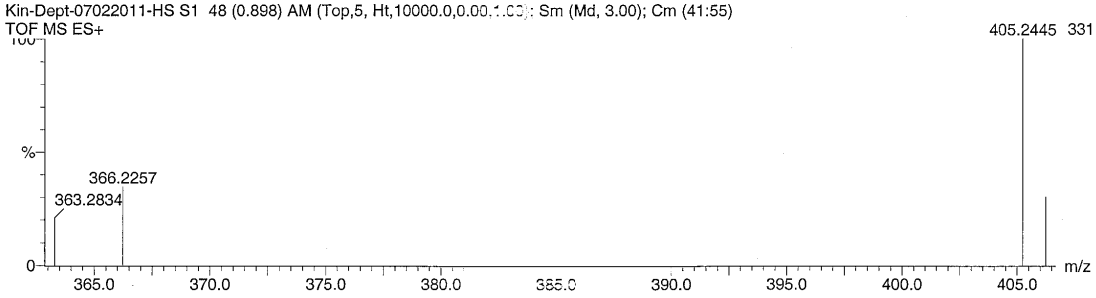
L2

ental Composition Report **Page 1**

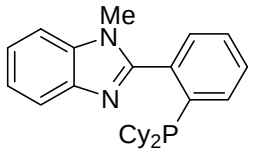
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-34 N: 0-4 Na: 0-1 P: 0-2

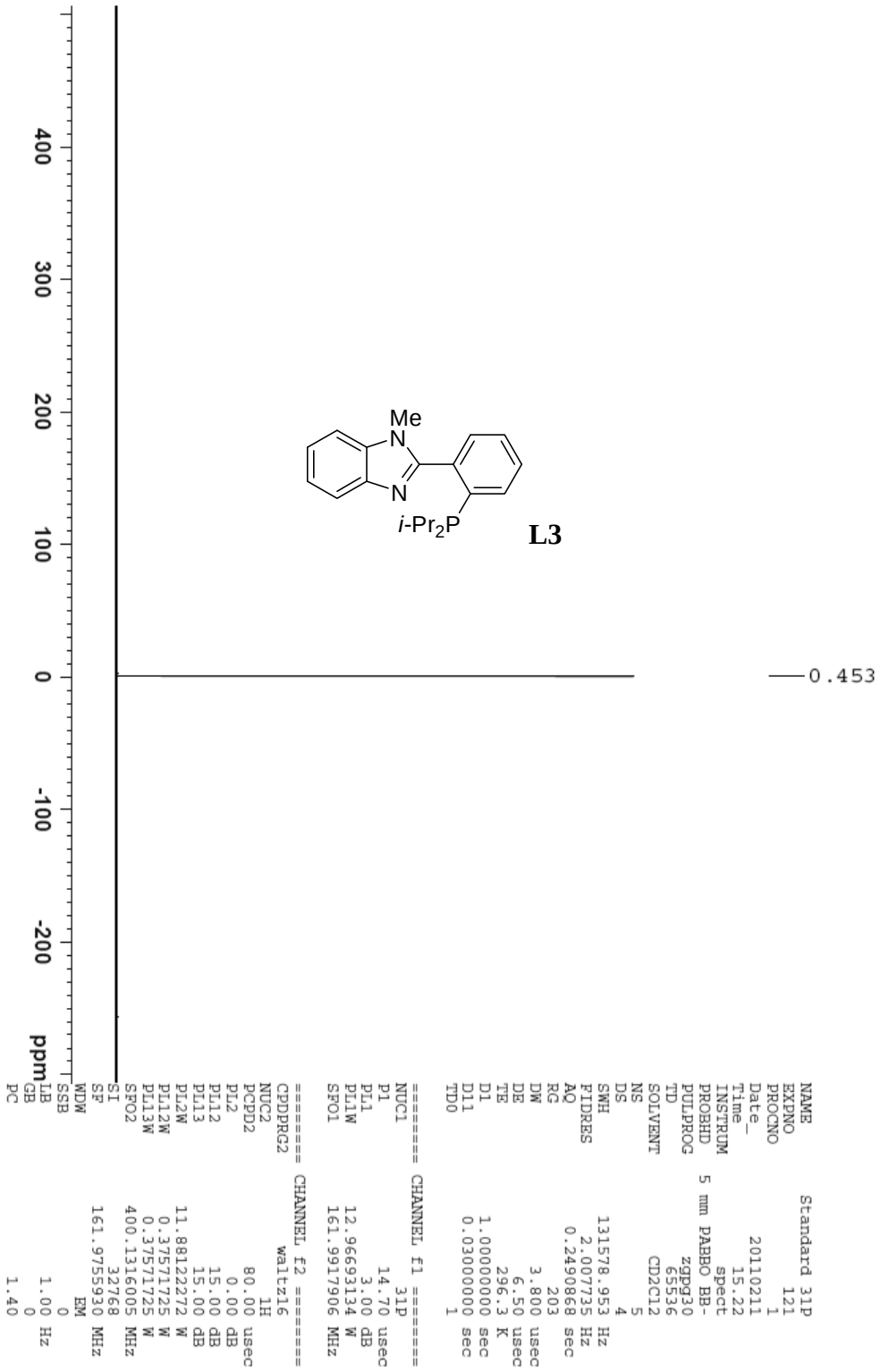
Kin-Dept-07022011-HS S1 48 (0.898) AM (Top,5, Ht,10000.0,0.00 : Sm (Md, 3.00); Cm (41:55)



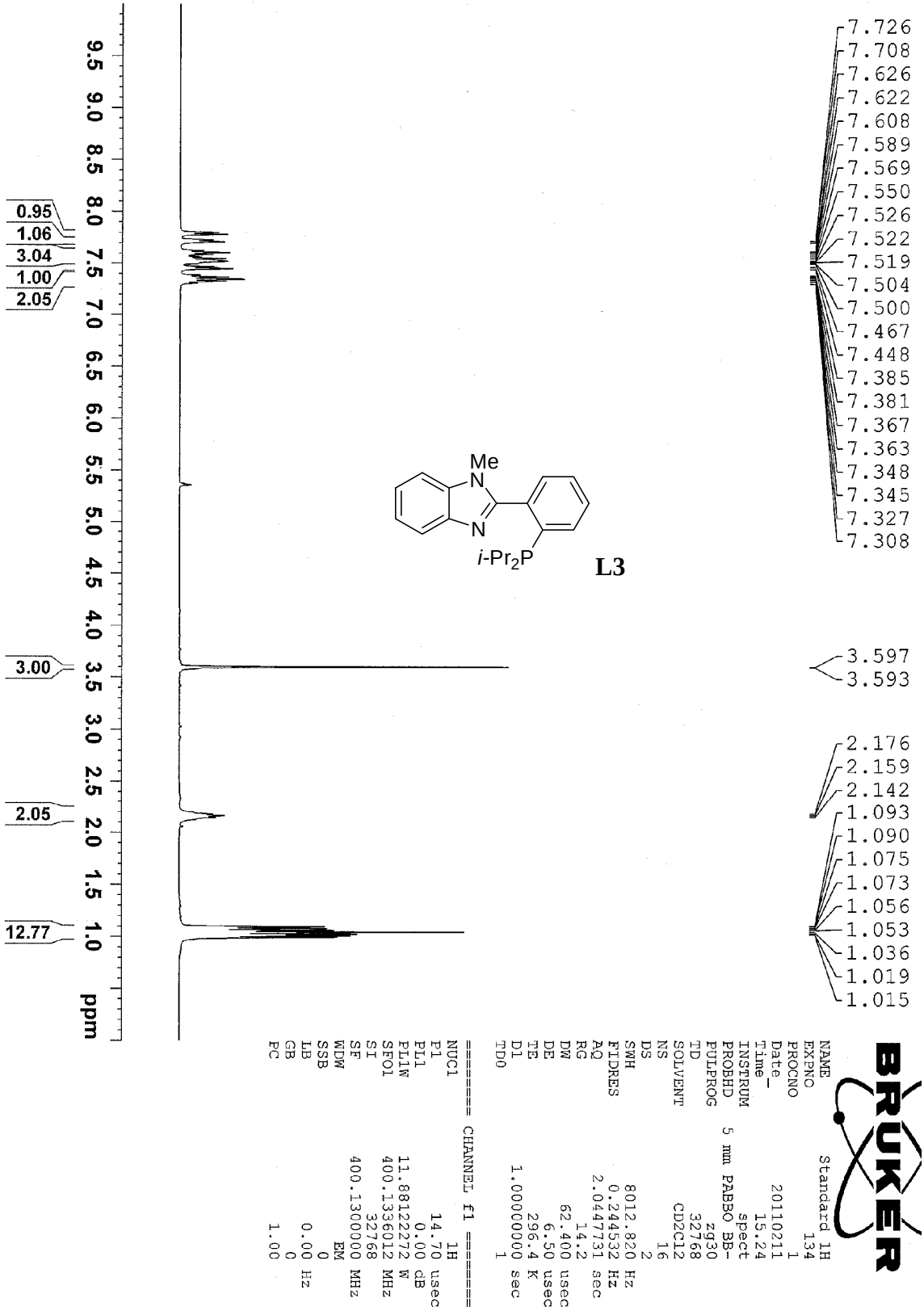
Minimum:				-100.0		
Maximum:		5.0	20.0	1000.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
405.2445	405.2460	-1.5	-3.7	11.5	2773074.0	C26 H34 N2 P

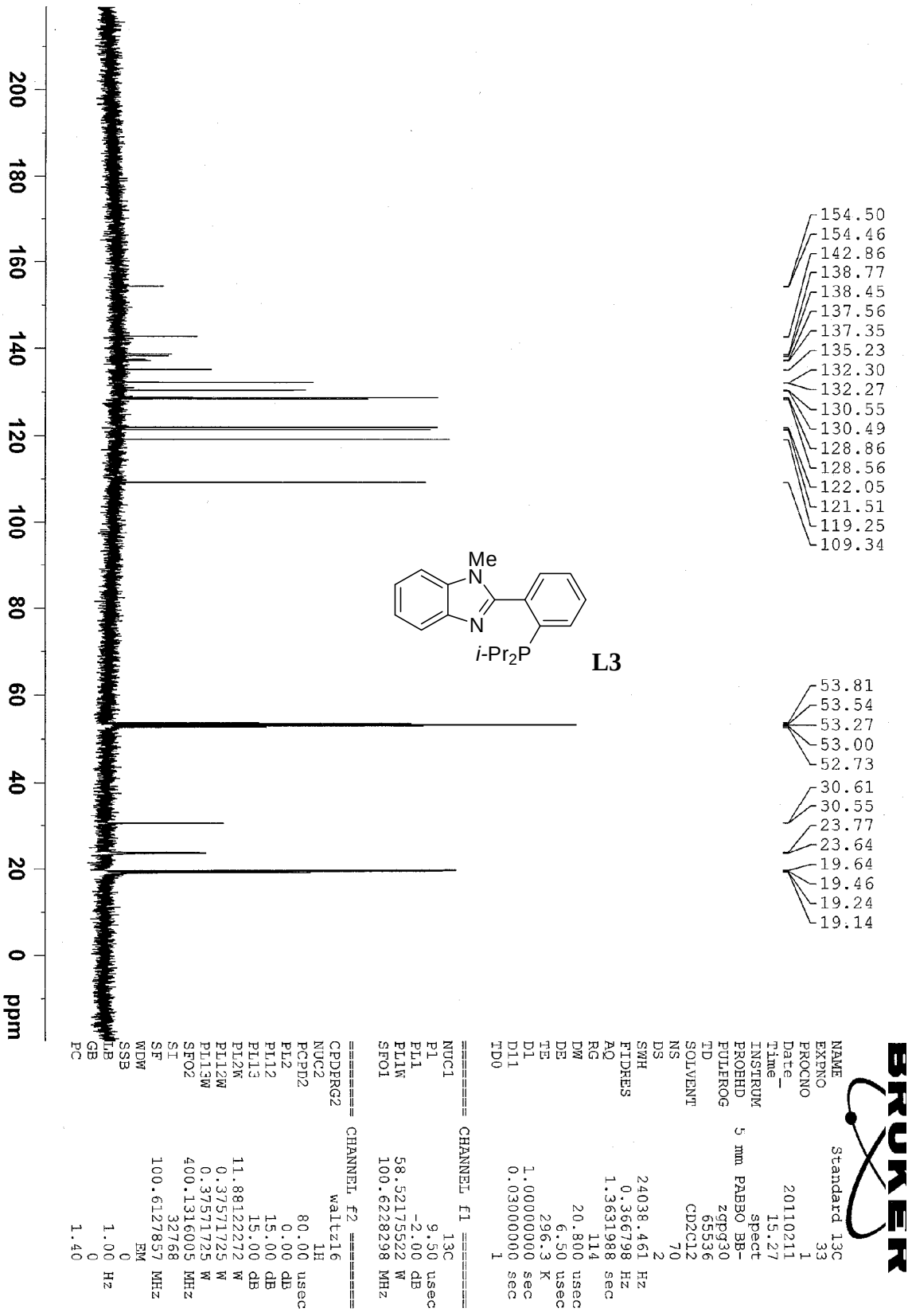


L2

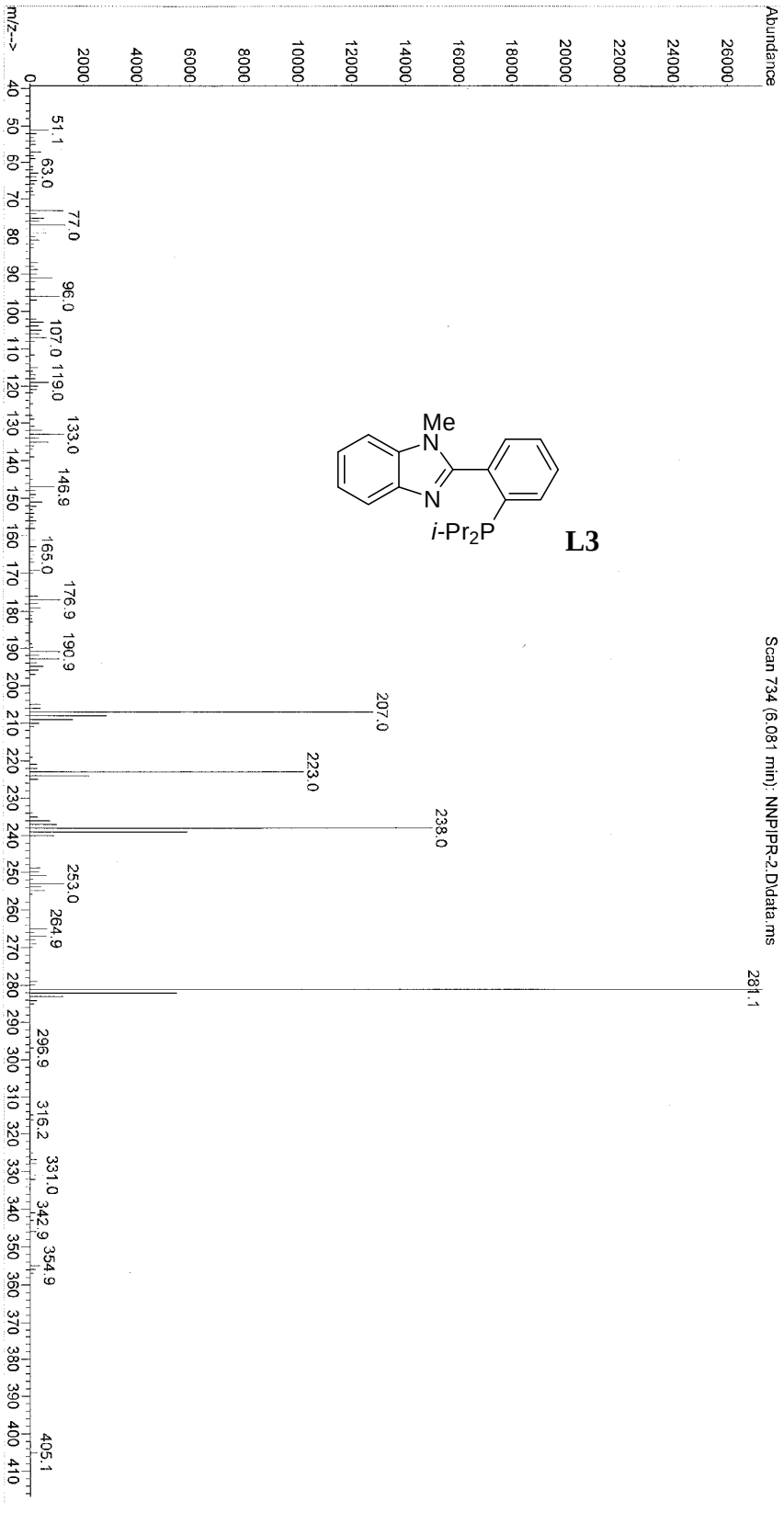



```
NAME                                   Standard 31p
EXPNO                                          121
PROCNO                                           1
Date_                                     20110211
Time_                                        15.22
INSTRUM                                      spect
PROBHD                 5 mm PABBO BB-
PULPROG                                   zgpg30
TD                                         65536
SOLVENT                                   CD2Cl2
NS                                             5
DS                                             4
SWH                                    131578.953 Hz
FIDRES                                   2.007735 Hz
AQ                                       0.2490868 sec
RG                                           203
DW                                       3.800 usec
DE                                       6.50 usec
TE                                       296.3 K
D1                                       1.00000000 sec
D11                                      0.03000000 sec
TD0                                            1

======== CHANNEL f1 ========
NUC1                                         31p
P1                                        14.70 usec
PL1                                        3.00 dB
PL1W                                   12.96693134 W
SFO1                                   161.9917906 MHz

======== CHANNEL f2 ========
CPDPRG2                                   waltz16
NUC2                                         1H
PCPD2                                     80.00 usec
PL2                                        0.00 dB
PL12                                      15.00 dB
PL13                                      15.00 dB
PL2W                                   11.88122272 W
PL12W                                   0.37571725 W
PL13W                                   0.37571725 W
SFO2                                   400.1316005 MHz
SI                                         32768
SF                                     161.9755930 MHz
WDW                                            EM
SSB                                            0
LB                                         1.00 Hz
GB                                             0
PC                                         1.40
```

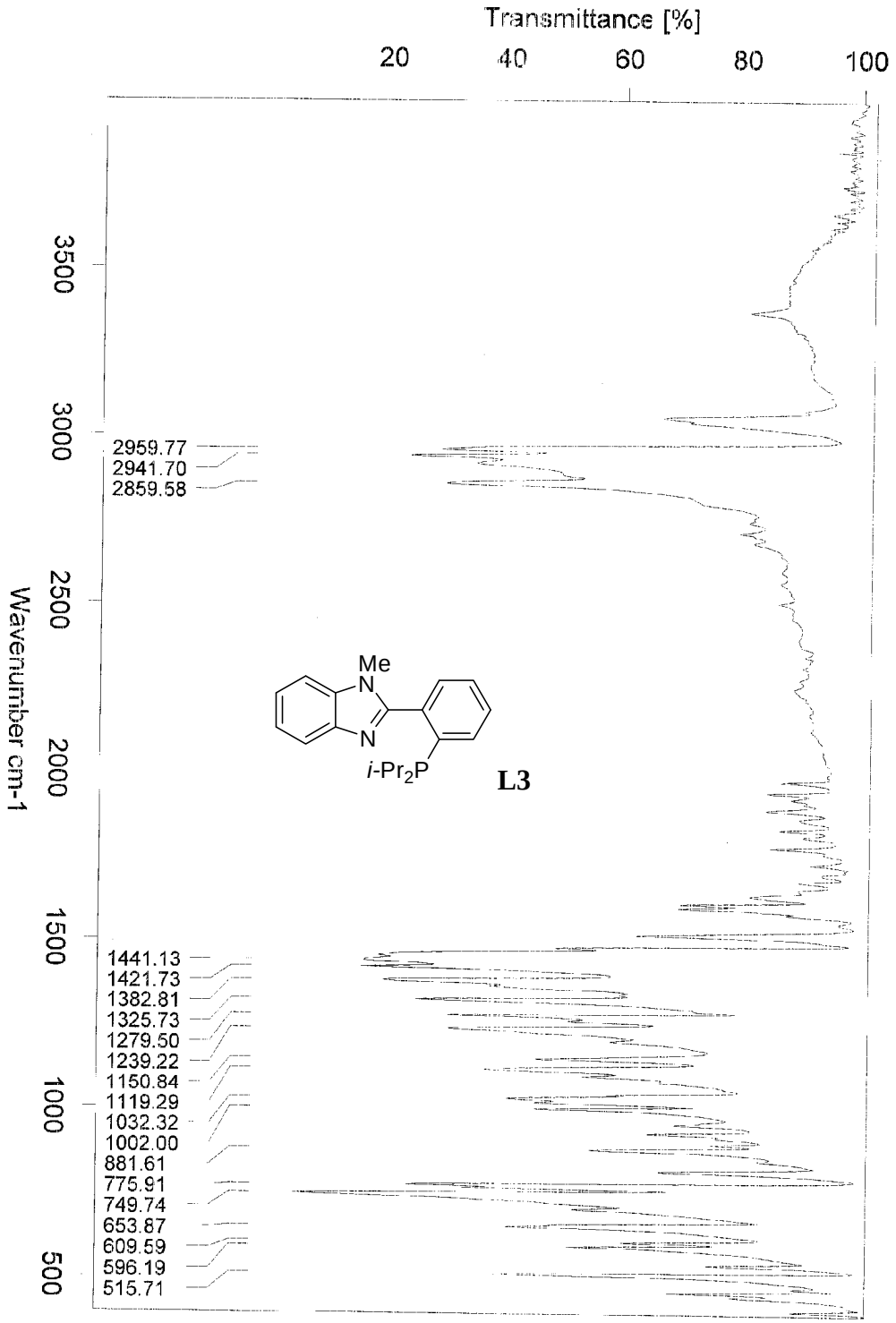

7.726
7.708
7.626
7.622
7.608
7.589
7.569
7.550
7.526
7.522
7.519
7.504
7.500
7.467
7.448
7.385
7.381
7.367
7.363
7.348
7.345
7.327
7.308
3.597
3.593
2.176
2.159
2.142
1.093
1.090
1.075
1.073
1.056
1.053
1.036
1.019
1.015
0.95
1.06
3.04
1.00
2.05
3.00
2.05
12.77
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
Me
N
N
i-Pr2P
L3
NAME Standard 1H
EXPNO 134
PROCNO 1
Date_ 20110211
Time_ 15.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CD2Cl2
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 14.2
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00


154.50
154.46
142.86
138.77
138.45
137.56
137.35
135.23
132.30
132.27
130.55
130.49
128.86
128.56
122.05
121.51
119.25
109.34
Me
N
N
i-Pr2P
L3
53.81
53.54
53.27
53.00
52.73
30.61
30.55
23.77
23.64
19.64
19.46
19.24
19.14
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
NAME Standard 13C
EXPNO 33
PROCNO 1
Date_ 20110211
Time_ 15.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 70
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127857 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

File :C:\MSDCHEM\1\DATA\CMSO\Snapshot\NNPIPR-2.D
Operator : Seam
Acquired : 10 Feb 2011 17:31 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 4



L3



L3

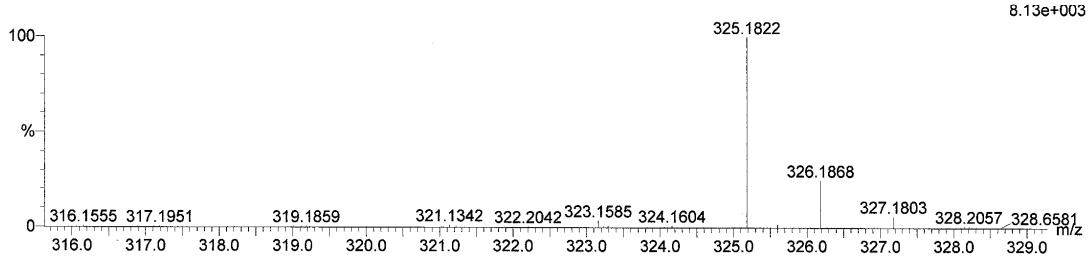
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

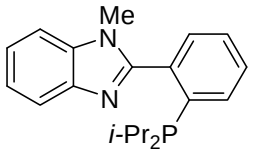
Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-26 H: 0-26 N: 0-3 Na: 0-1 P: 0-1

Kin-Dept-16022011-HS_2 S9 59 (1.117) Cn (Cen,4, 80.00, Ar); Sm (SG, 2x3.00); Sb (5,40.00); Cm (58:65)
TOF MS ES+

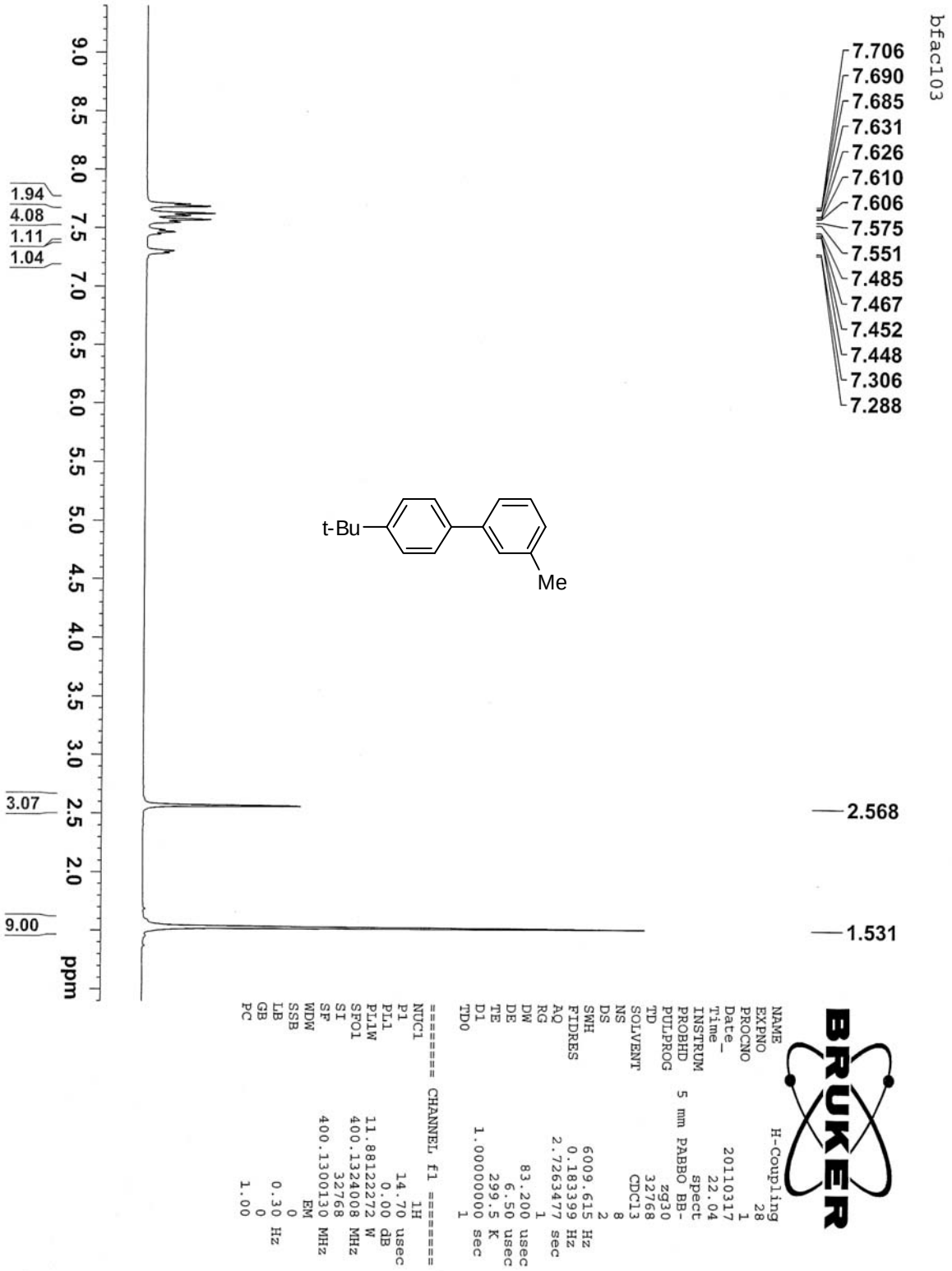
8.13e+003

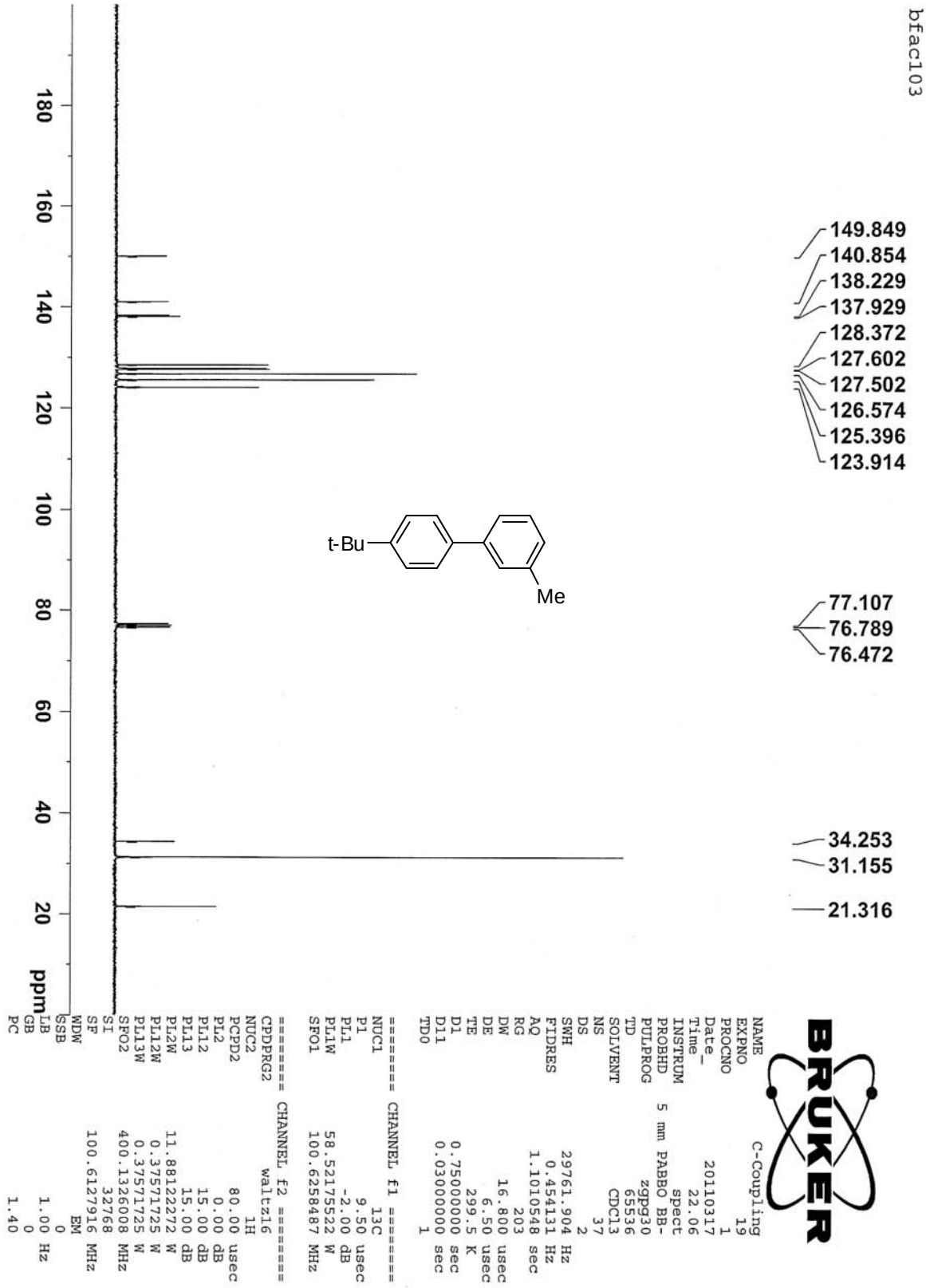


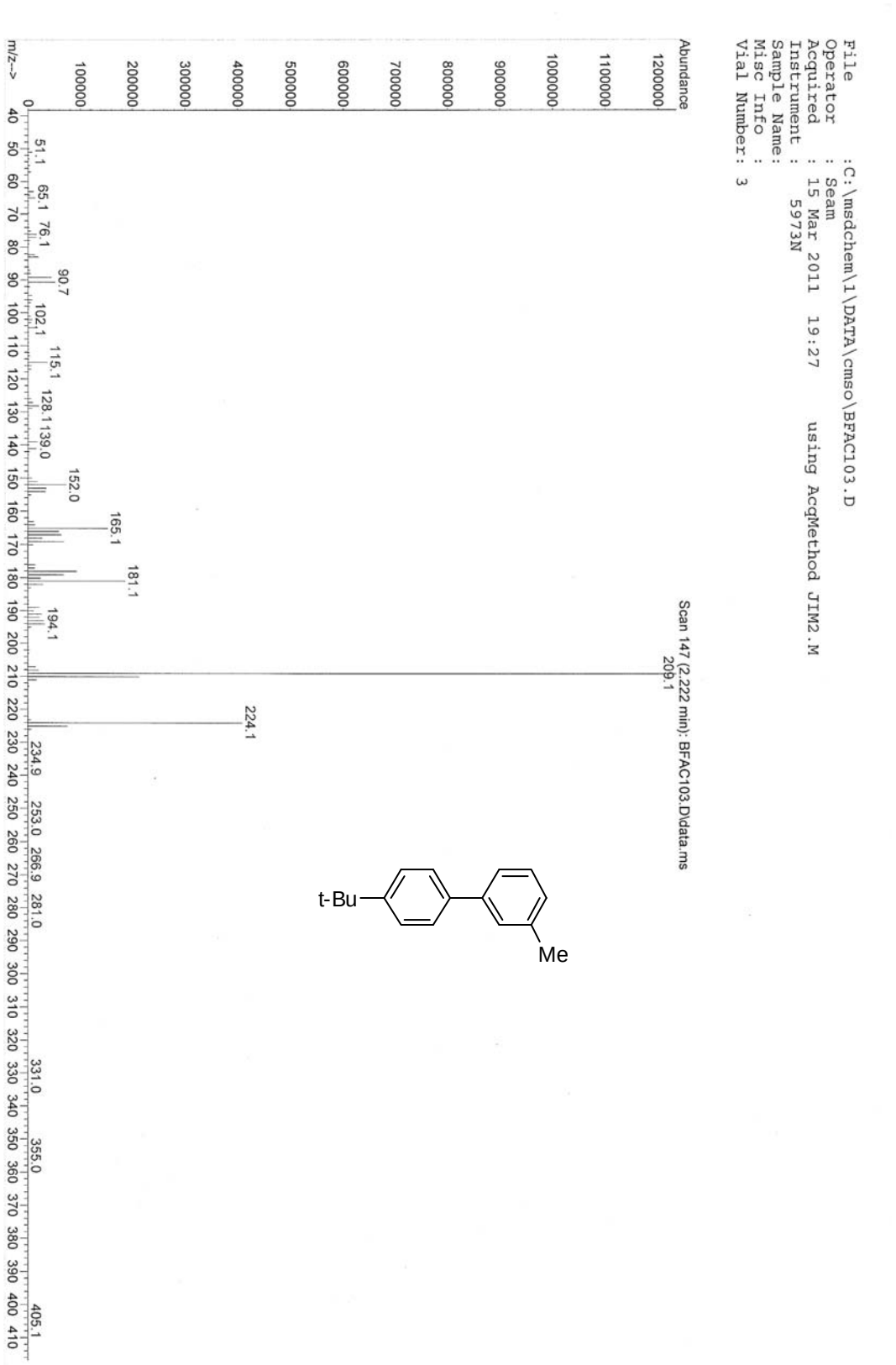
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
325.1822	325.1834	-1.2	-3.7	9.5	76.6	C20 H26 N2 P

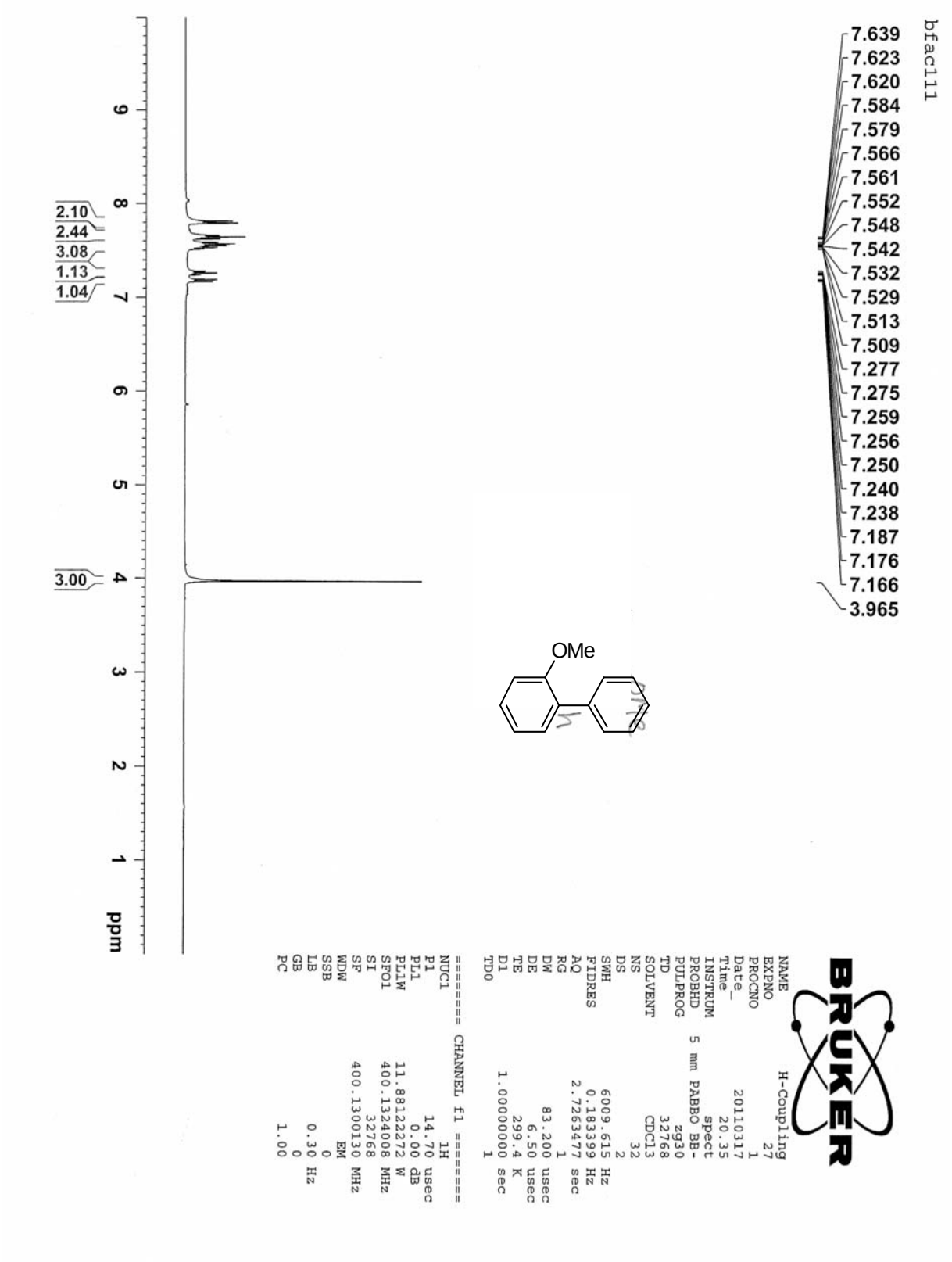


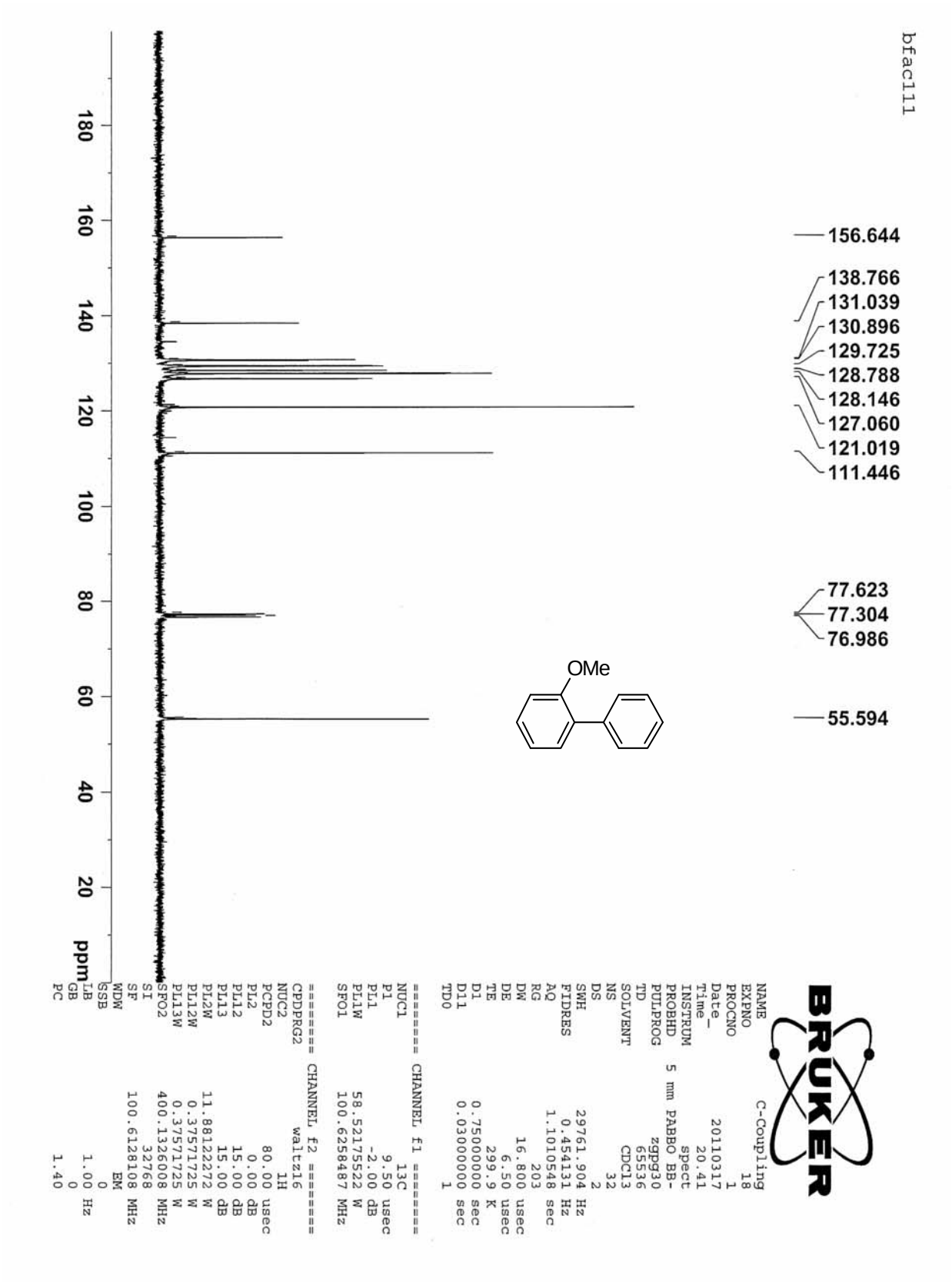
L3

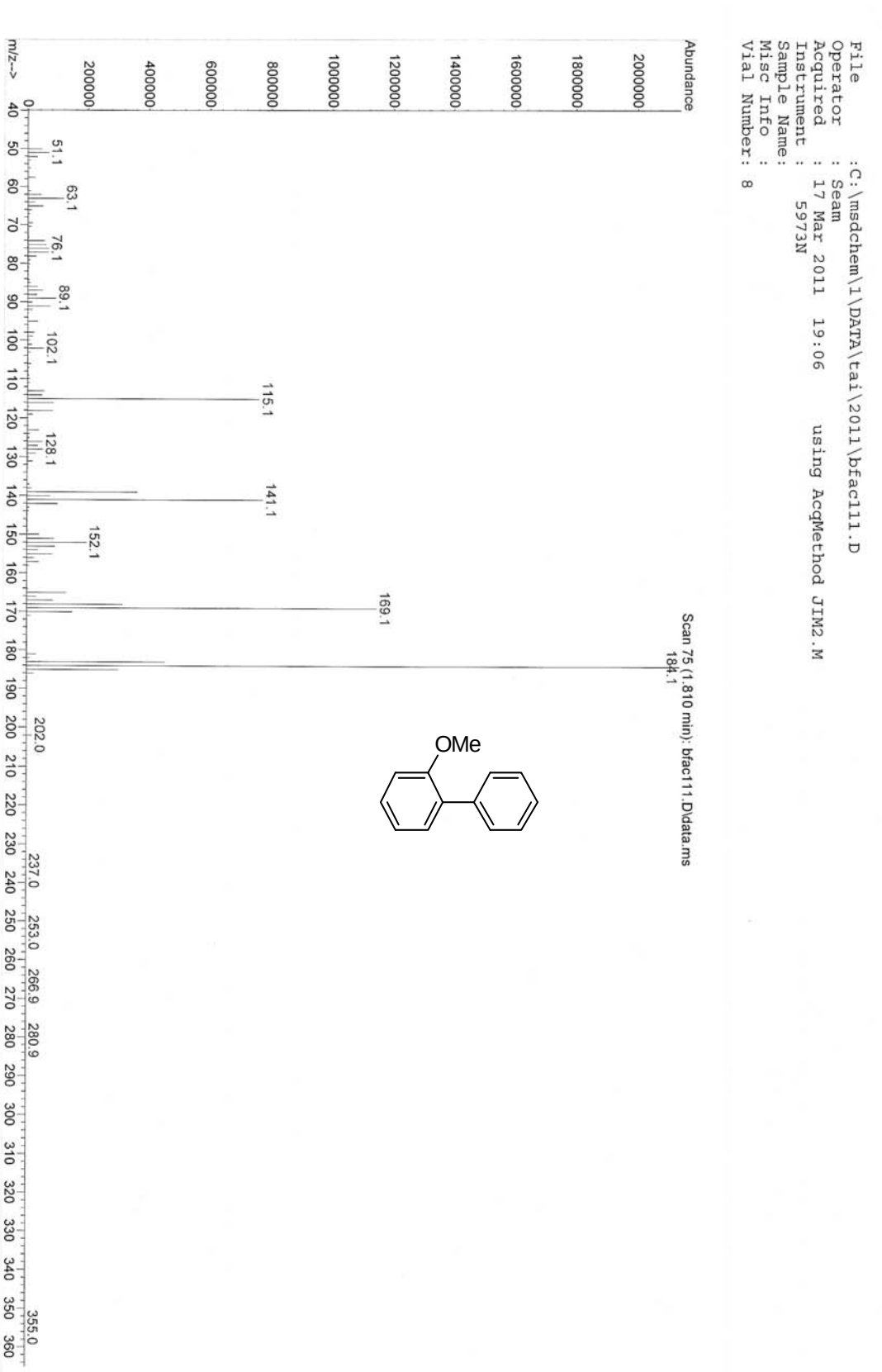

bfac103
7.706
7.690
7.685
7.631
7.626
7.610
7.606
7.575
7.551
7.485
7.467
7.452
7.448
7.306
7.288
t-Bu
Me
2.568
1.531
1.94
4.08
1.11
1.04
3.07
9.00
ppm
NAME H-Coupling
EXPNO 28
PROCNO 1
Date_ 20110317
Time_ 22.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 1
DW 83.200 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PLIW 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

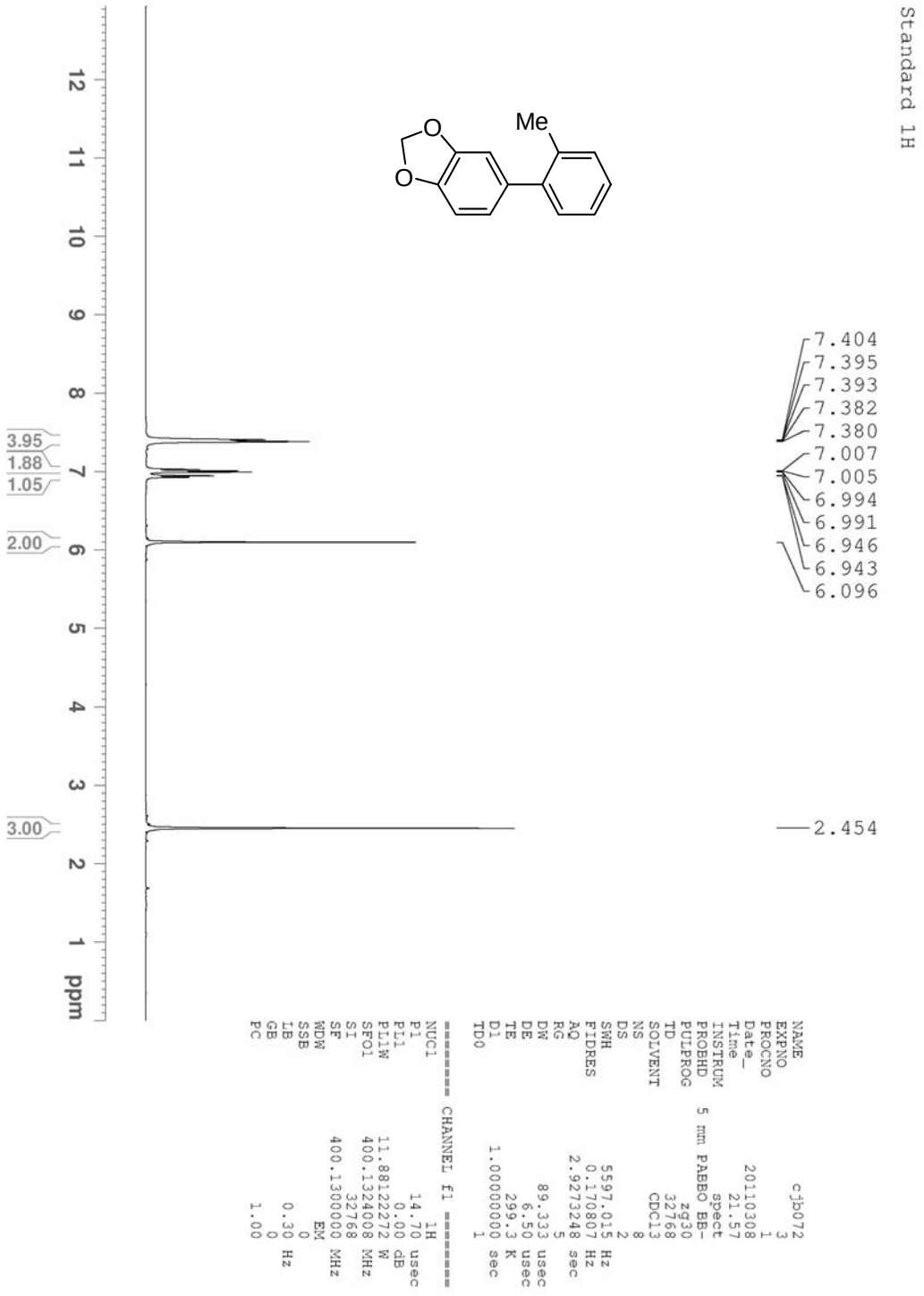

bfac103
149.849
140.854
138.229
137.929
128.372
127.602
127.502
126.574
125.396
123.914
77.107
76.789
76.472
34.253
31.155
21.316
t-Bu
Me
ppm
180
160
140
120
100
80
60
40
20
BRUKER
NAME C-Coupling
EXPNO 19
PROCNO 1
Date_ 20110317
Time_ 22.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 37
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.5 K
D1 0.75000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6258487 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1326008 MHz
SI 32768
SF 100.6127916 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

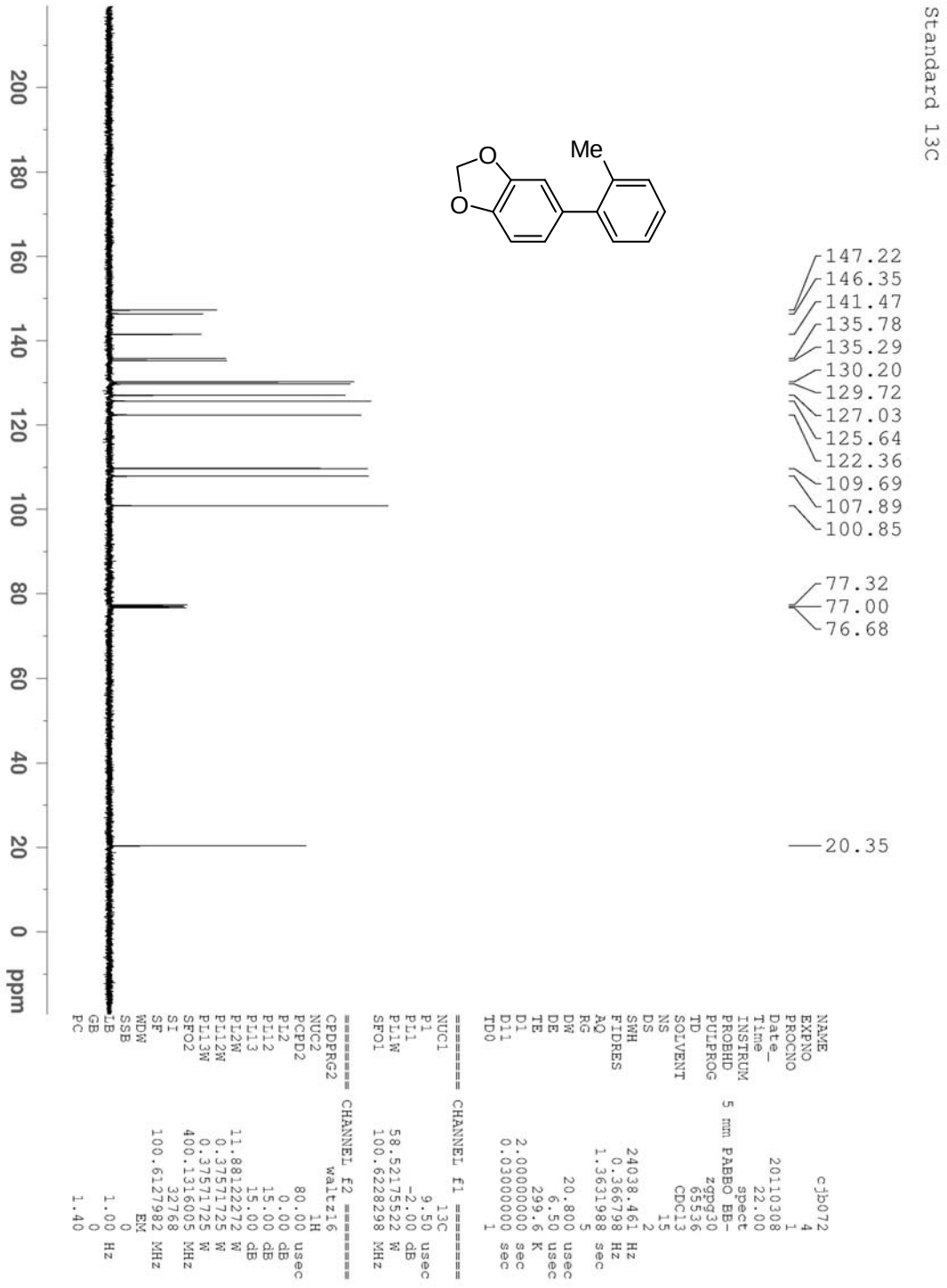

File :C:\msdchem\1\DATA\cmso\BFAC103.D
Operator : Seam
Acquired : 15 Mar 2011 19:27 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
Scan 147 (2.222 min): BFAC103.D\data.ms
209.1
224.1
181.1
165.1
152.0
194.1
90.7
115.1
102.1
128.1
139.0
76.1
65.1
51.1
234.9
253.0
266.9
281.0
331.0
355.0
405.1
m/z-->
t-Bu
Me

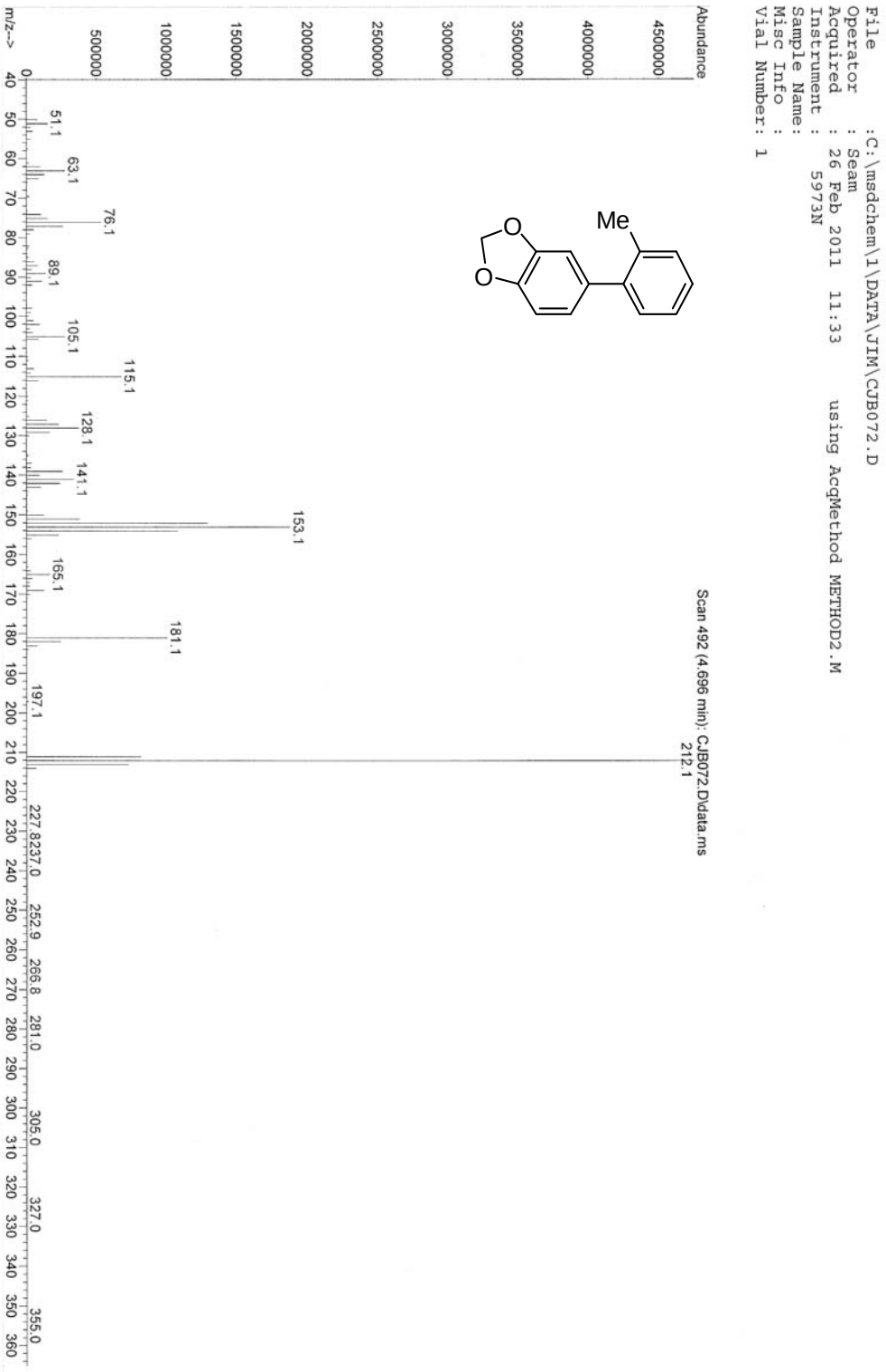

bfac111
7.639
7.623
7.620
7.584
7.579
7.566
7.561
7.552
7.548
7.542
7.532
7.529
7.513
7.509
7.277
7.275
7.259
7.256
7.250
7.240
7.238
7.187
7.176
7.166
3.965
OMe
2.10
2.44
3.08
1.13
1.04
3.00
9
8
7
6
5
4
3
2
1
ppm
BRUKER
NAME H-Coupling
EXPNO 27
PROCNO 1
Date_ 20110317
Time_ 20.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 1
DW 83.200 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

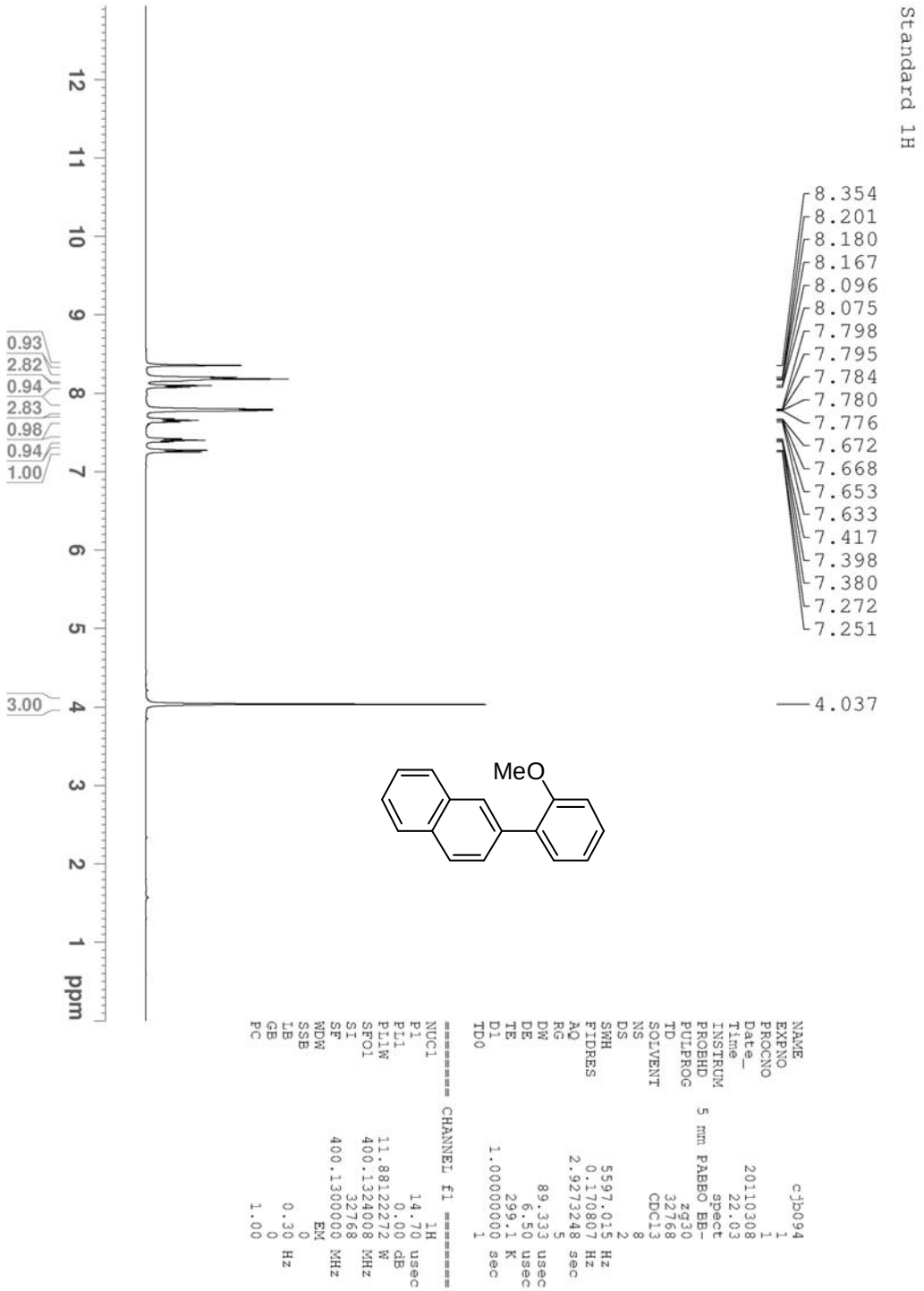

bfac111
156.644
138.766
131.039
130.896
129.725
128.788
128.146
127.060
121.019
111.446
77.623
77.304
76.986
55.594
OMe
BRUKER
NAME C-Coupling
EXPNO 18
PROCNO 1
Date_ 20110317
Time_ 20.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.9 K
D1 0.75000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6258487 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1326008 MHz
SI 32768
SF 100.6128108 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 160 140 120 100 80 60 40 20 ppm

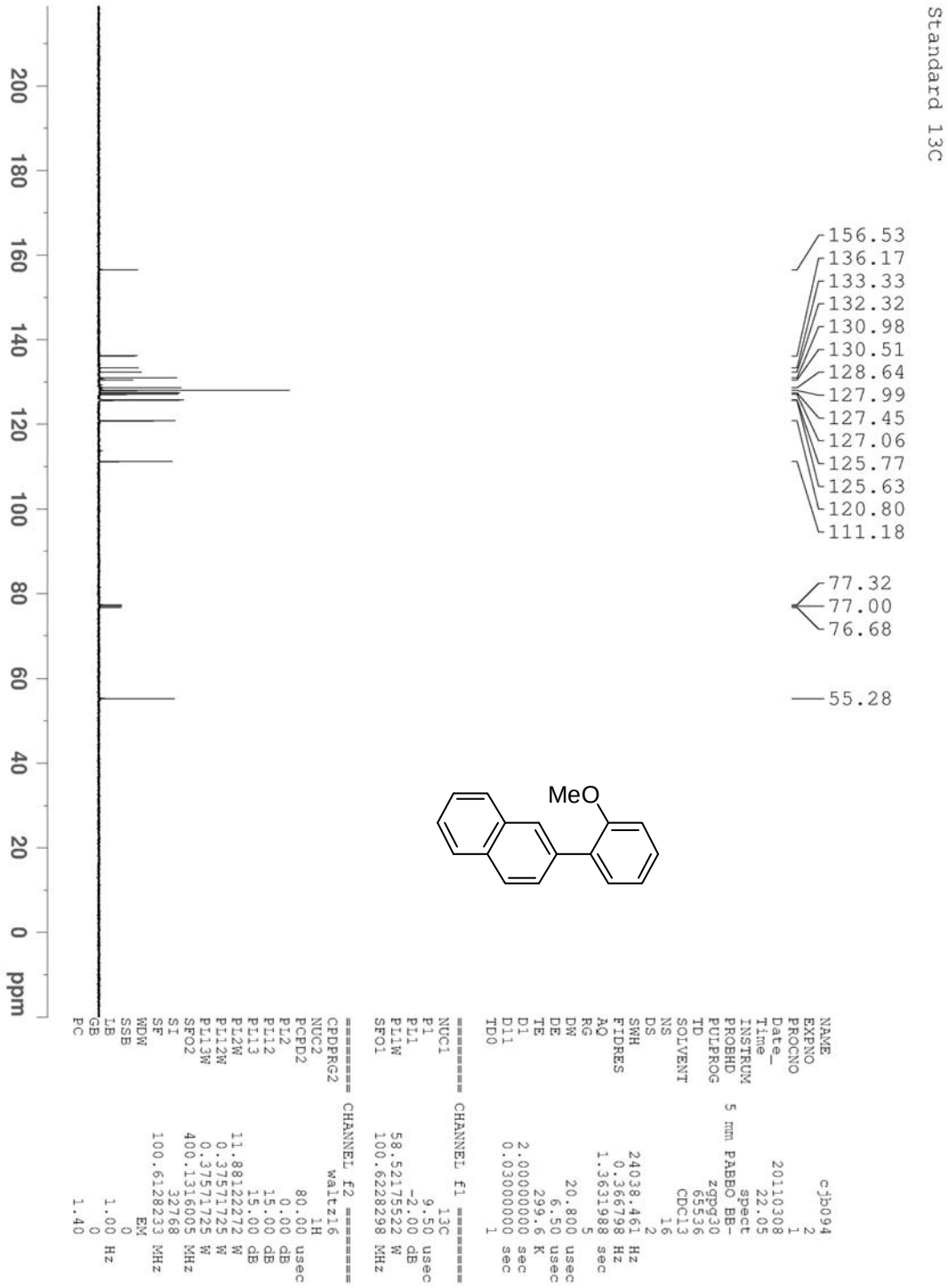

File :C:\msdchem\1\DATA\tai\2011\bfac111.D
Operator : Seam
Acquired : 17 Mar 2011 19:06 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 8
Abundance
m/z-->
Scan 75 (1.810 min): bfac111.D\data.ms
184.1
115.1
141.1
169.1
OMe

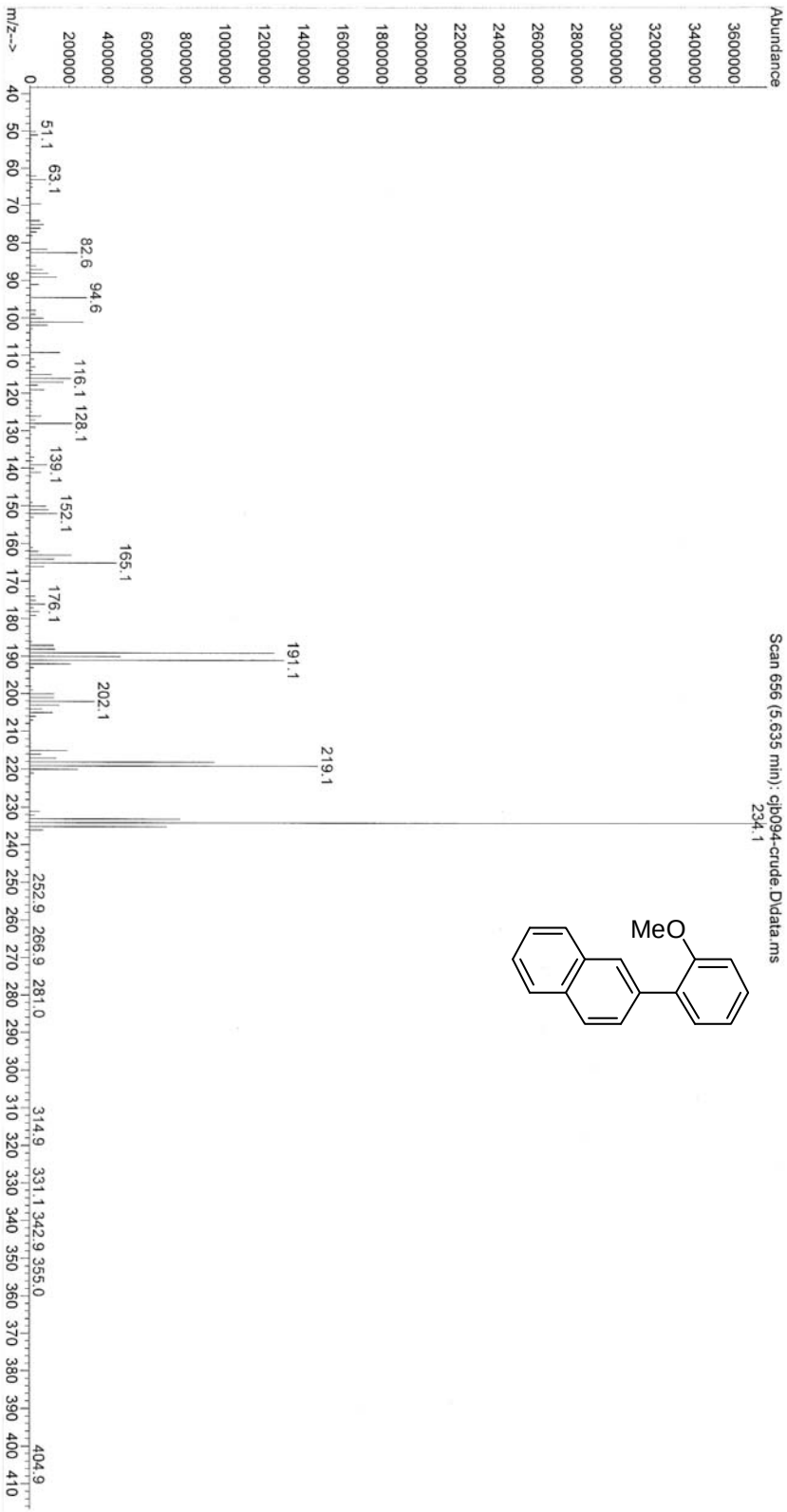

Standard 1H
Me
O
O
7.404
7.395
7.393
7.382
7.380
7.007
7.005
6.994
6.991
6.946
6.943
6.096
2.454
3.95
1.88
1.05
2.00
3.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
NAME cjb072
EXPNO 3
PROCNO 1
Date_ 20110308
Time_ 21.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.927248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

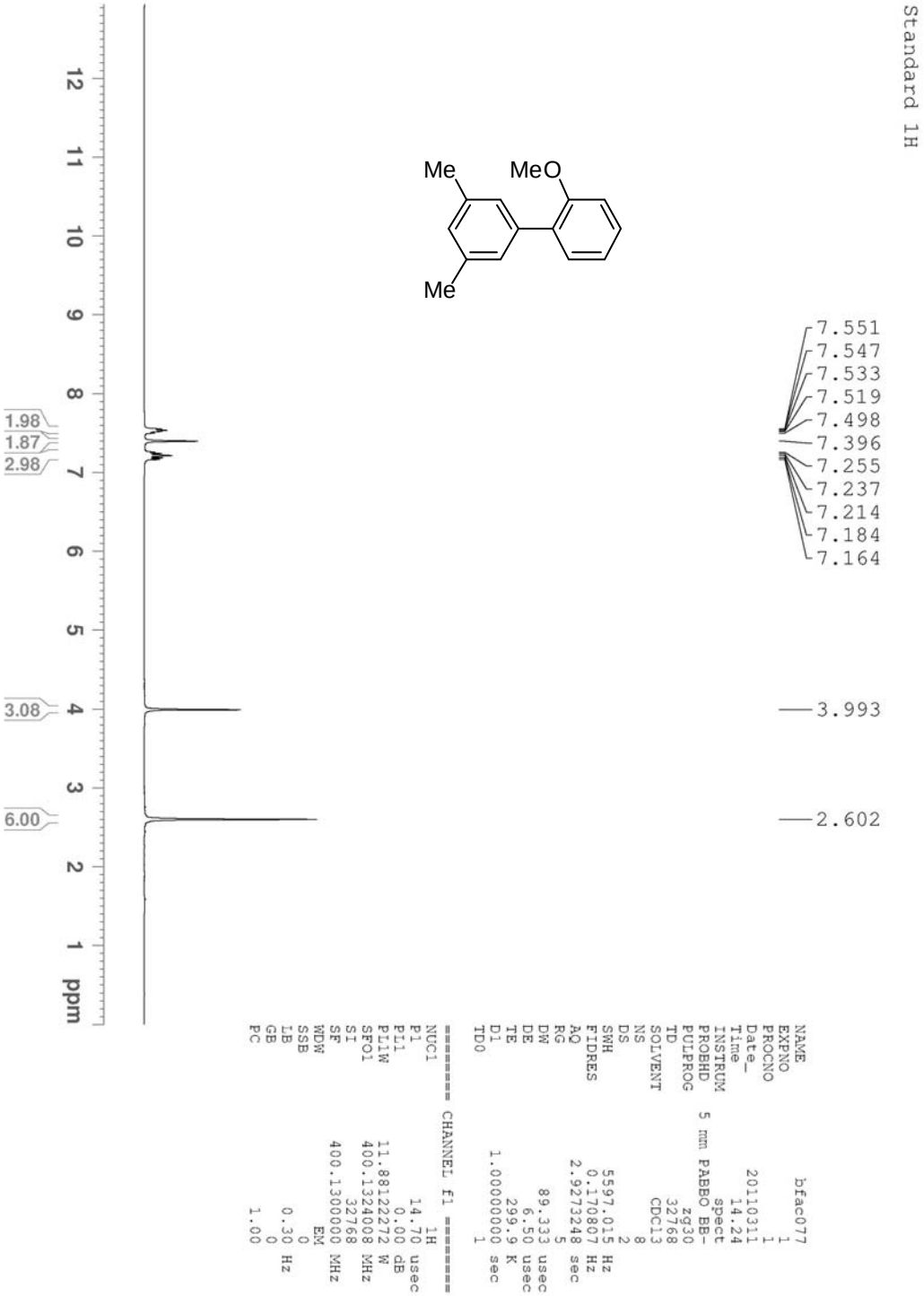

Standard 13C
Me
O
O
147.22
146.35
141.47
135.78
135.29
130.20
129.72
127.03
125.64
122.36
109.69
107.89
100.85
77.32
77.00
76.68
20.35
200
180
160
140
120
100
80
60
40
20
0
ppm

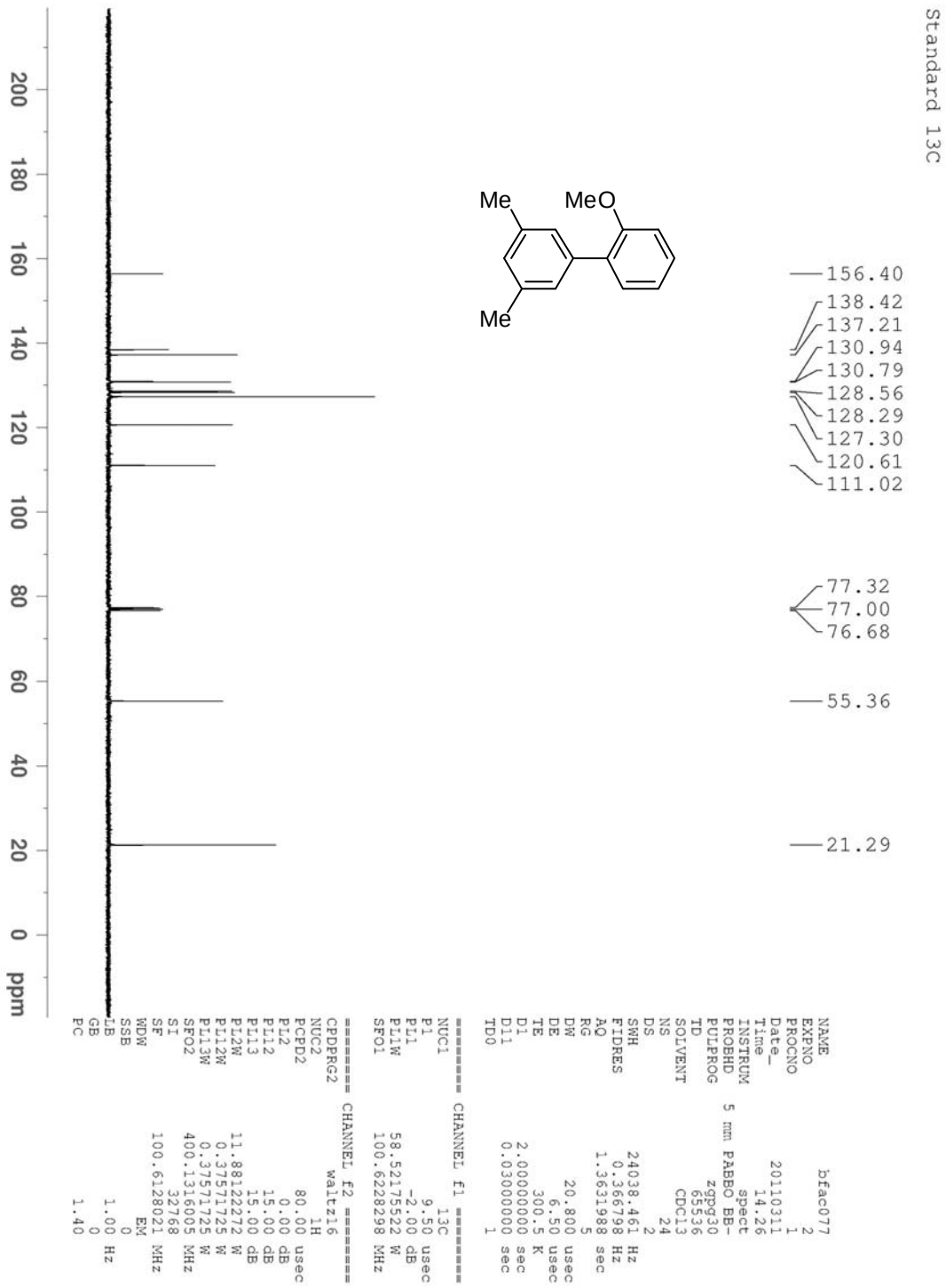

File :C:\msdchem\1\DATA\JIM\CJB072.D
Operator : Seam
Acquired : 26 Feb 2011 11:33 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1
Abundance
m/z-->
Scan 492 (4.696 min): CJB072.D\data.ms
212.1
153.1
115.1
76.1
63.1
51.1
89.1
105.1
128.1
141.1
165.1
181.1
197.1
227.8
237.0
252.9
266.8
281.0
305.0
327.0
355.0
O
O
Me


Standard 1H
8.354
8.201
8.180
8.167
8.096
8.075
7.798
7.795
7.784
7.780
7.776
7.672
7.668
7.653
7.633
7.417
7.398
7.380
7.272
7.251
4.037
0.93
2.82
0.94
2.83
0.98
0.94
1.00
3.00
MeO
12 11 10 9 8 7 6 5 4 3 2 1 ppm
NAME cjb094
EXPNO 1
PROCNO 1
Date_ 20110308
Time_ 22.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.927248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

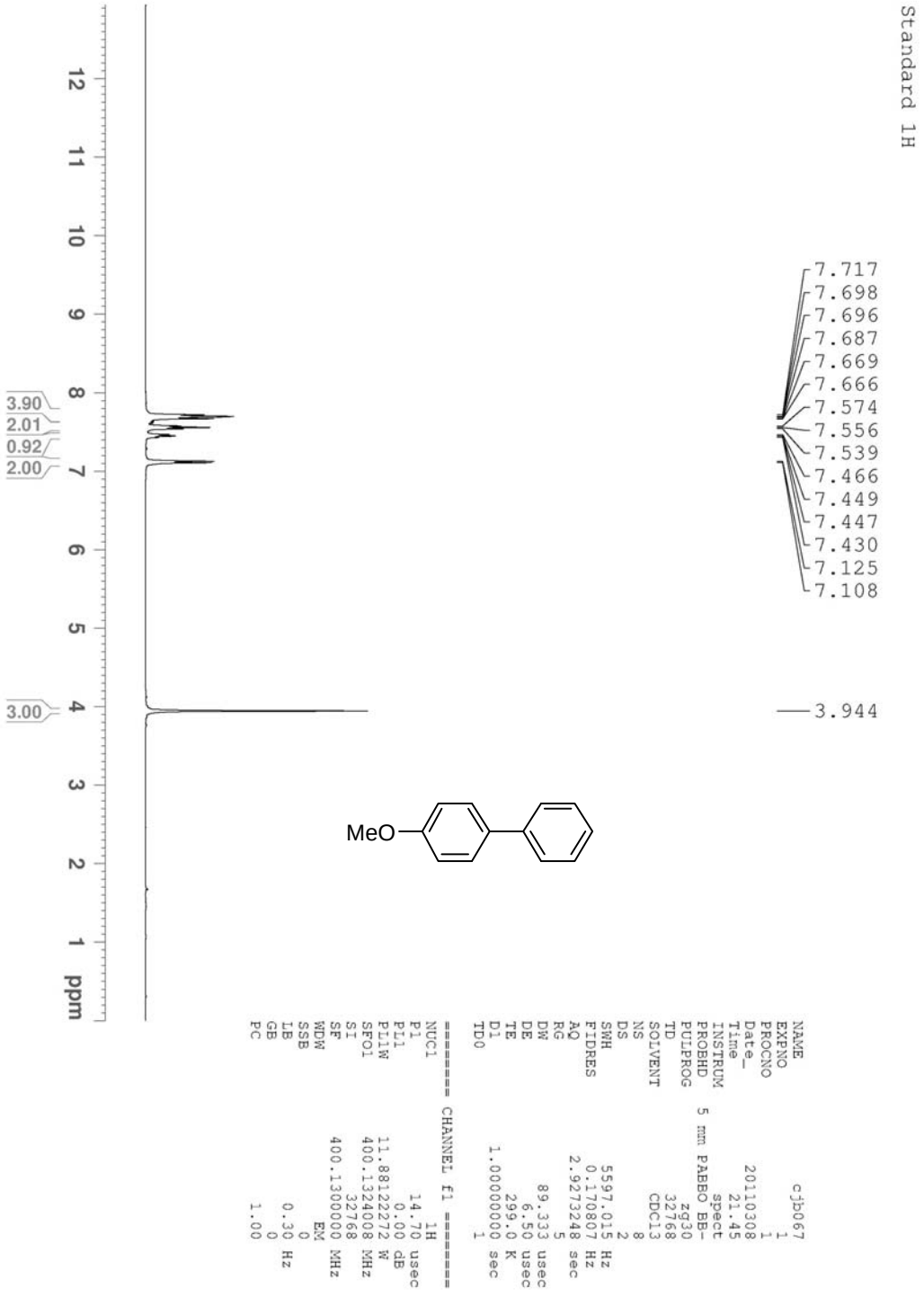

Standard 13C
156.53
136.17
133.33
132.32
130.98
130.51
128.64
127.99
127.45
127.06
125.77
125.63
120.80
111.18
77.32
77.00
76.68
55.28
MeO
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME cjb094
EXPNO 2
PROCNO 1
Date_ 20110308
Time 22.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128233 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

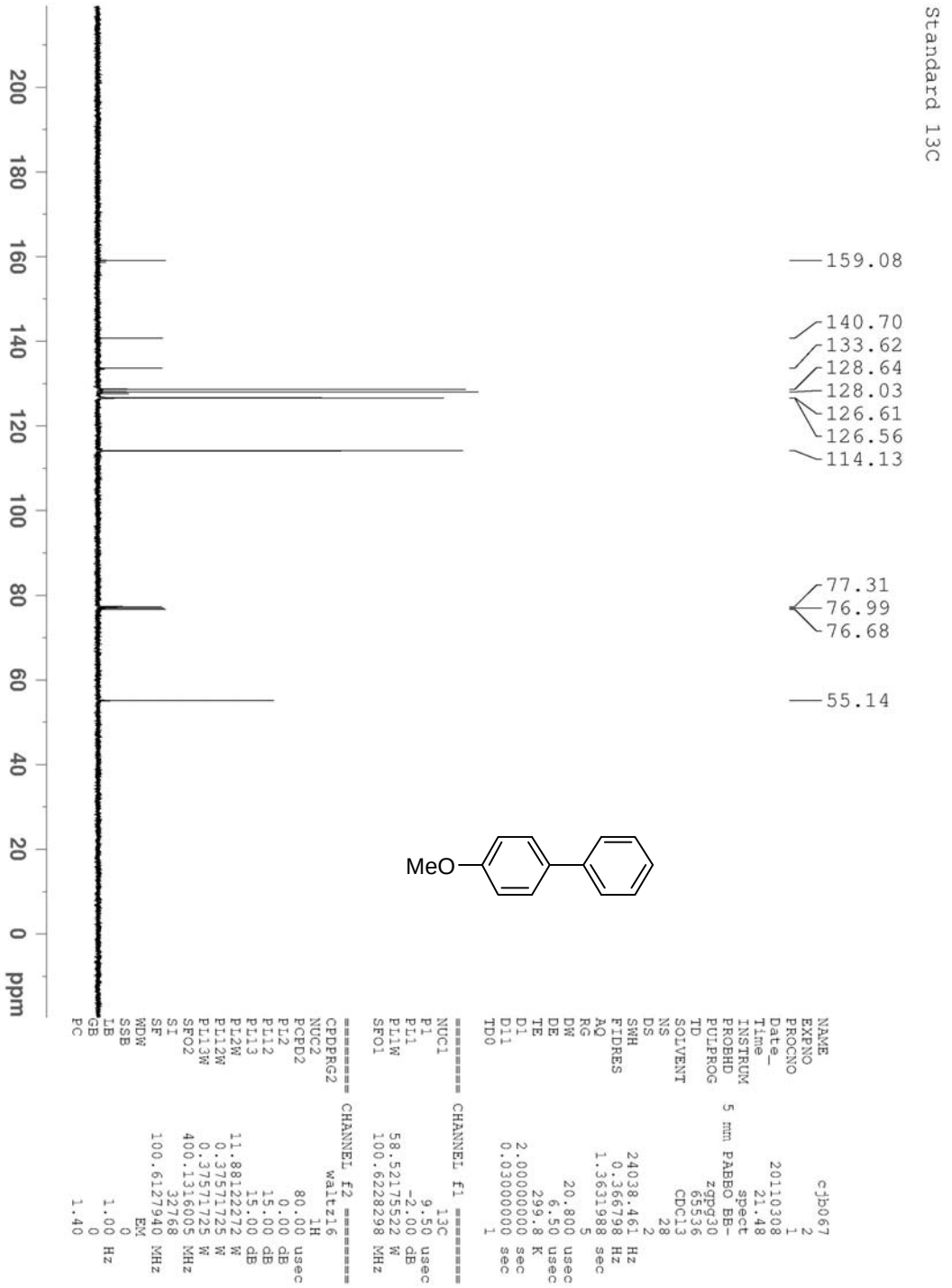

File :C:\msdchem\1\DATA\JIM\cjb094-crude.D
Operator : Seam
Acquired : 5 Mar 2011 23:40 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
Scan 656 (5.635 min): cjb094-crude.D\data.ms
234.1
191.1
219.1
202.1
165.1
94.6
82.6
MeO
m/z-->

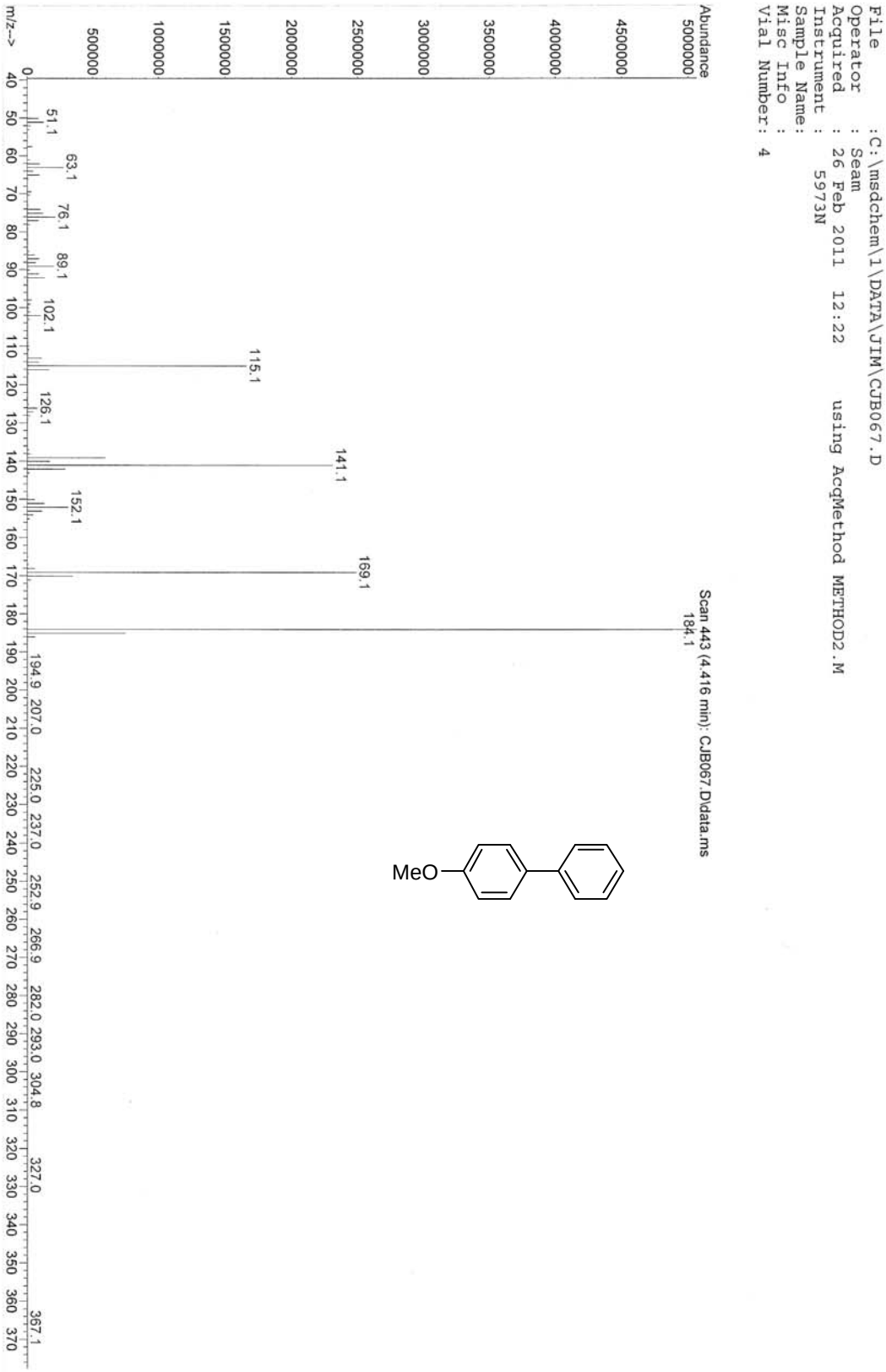

Standard 1H
Me
MeO
Me
7.551
7.547
7.533
7.519
7.498
7.396
7.255
7.237
7.214
7.184
7.164
3.993
2.602
1.98
1.87
2.98
3.08
6.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
NAME bfac077
EXPNO 1
PROCNO 1
Date_ 20110311
Time 14.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.927248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PLIW 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

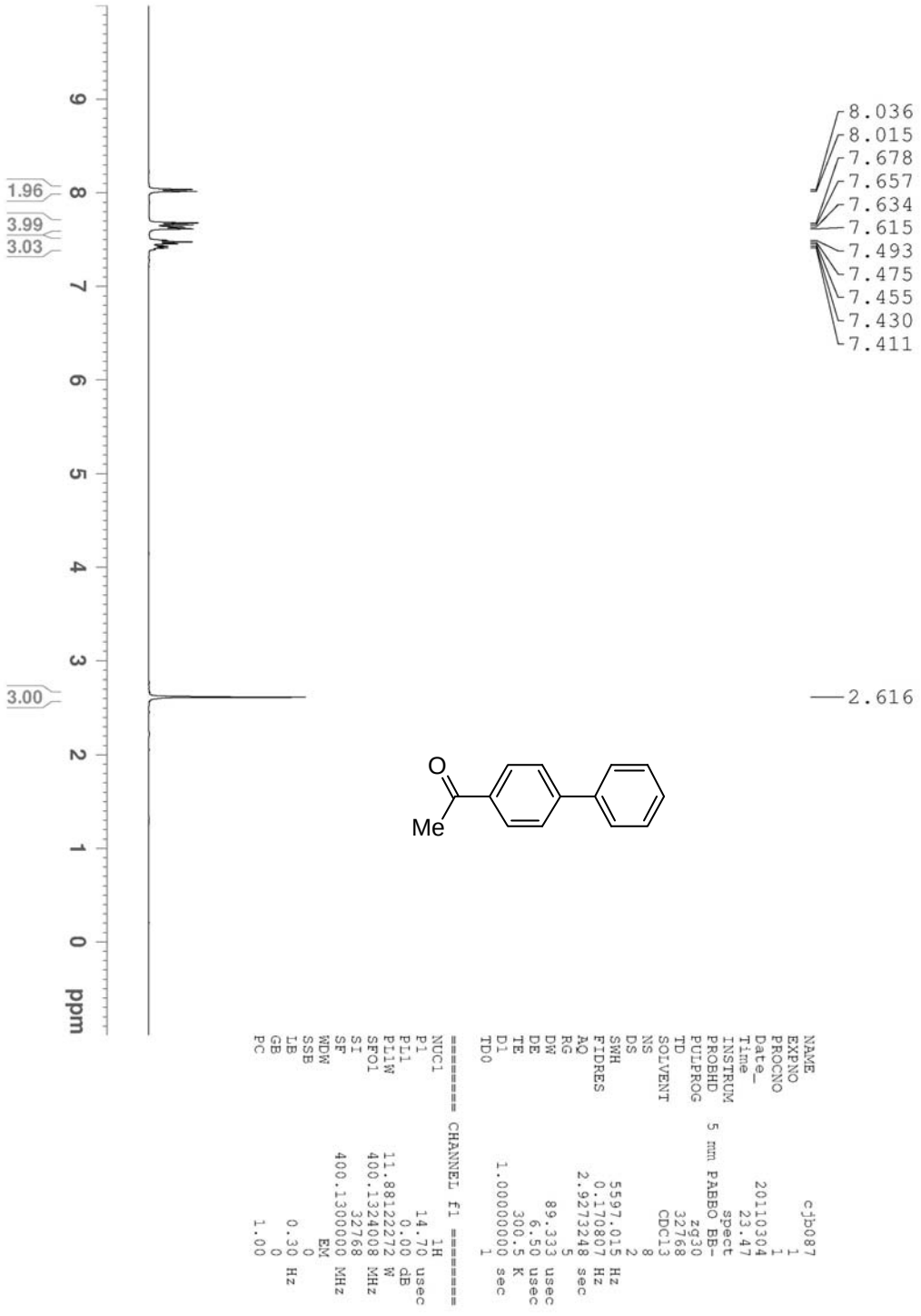

Standard 13C
Me
MeO
Me
156.40
138.42
137.21
130.94
130.79
128.56
128.29
127.30
120.61
111.02
77.32
77.00
76.68
55.36
21.29
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME bfac077
EXPNO 2
PROCNO 1
Date_ 20110311
Time 14.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128021 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

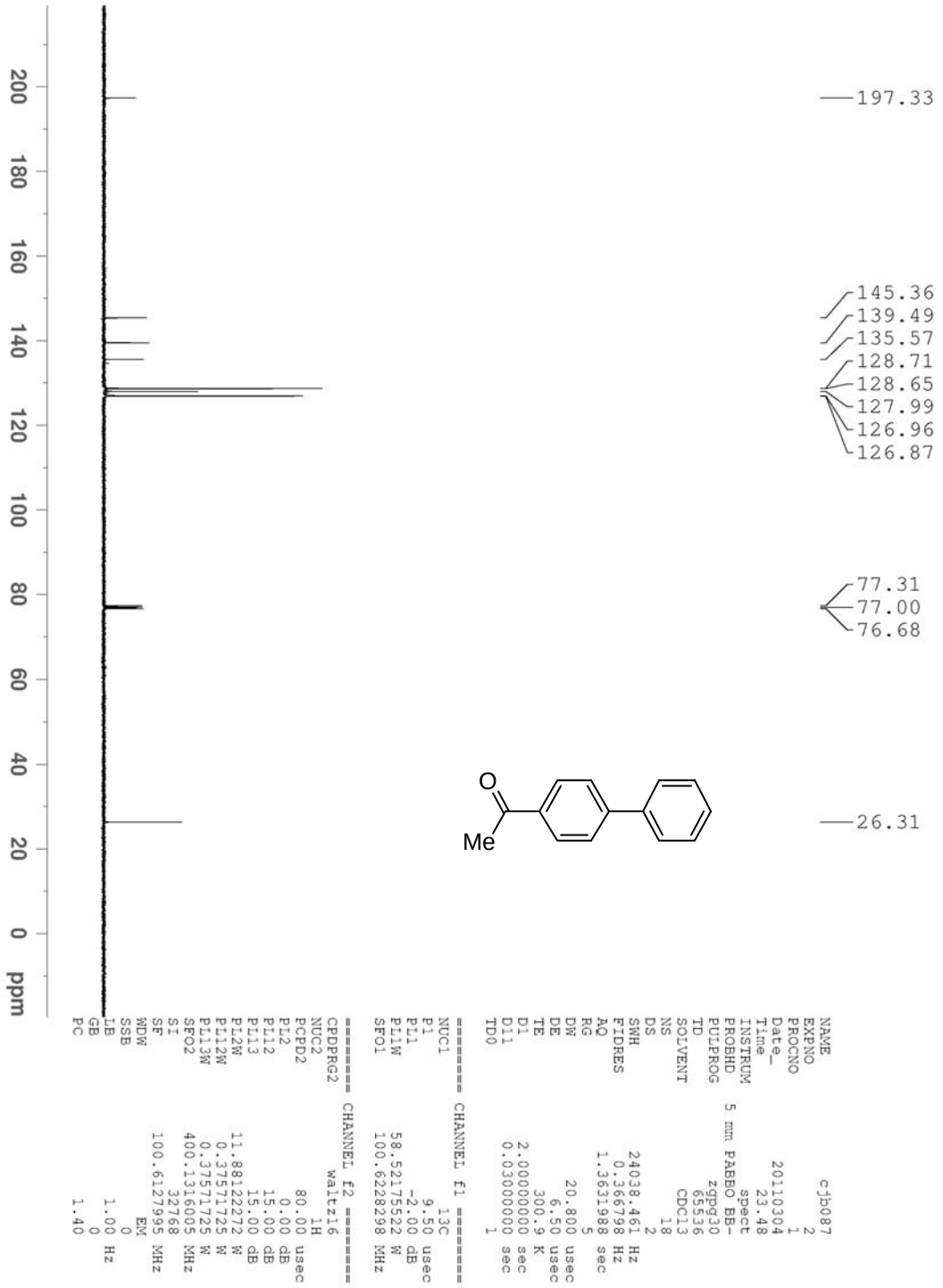

File :C:\msdchem\1\DATA\cmso\bfac77.D
Operator : Seam
Acquired : 10 Mar 2011 15:58 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 6
Me
MeO
Me
Abundance
m/z-->
Scan 110 (2.010 min): bfac77.D\data.ms
212.1
182.1
197.1
152.1
165.1
119.1
91.1
77.1
63.1
51.1
129.1
141.1
105.1
227.9
237.0
251.2
262.0
277.1
331.1
355.0


Standard 1H
7.717
7.698
7.696
7.687
7.669
7.666
7.574
7.556
7.539
7.466
7.449
7.447
7.430
7.125
7.108
3.944
3.90
2.01
0.92
2.00
3.00
MeO
12 11 10 9 8 7 6 5 4 3 2 1 ppm
NAME cjb067
EXPNO 1
PROCNO 1
Date_ 20110308
Time 21.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

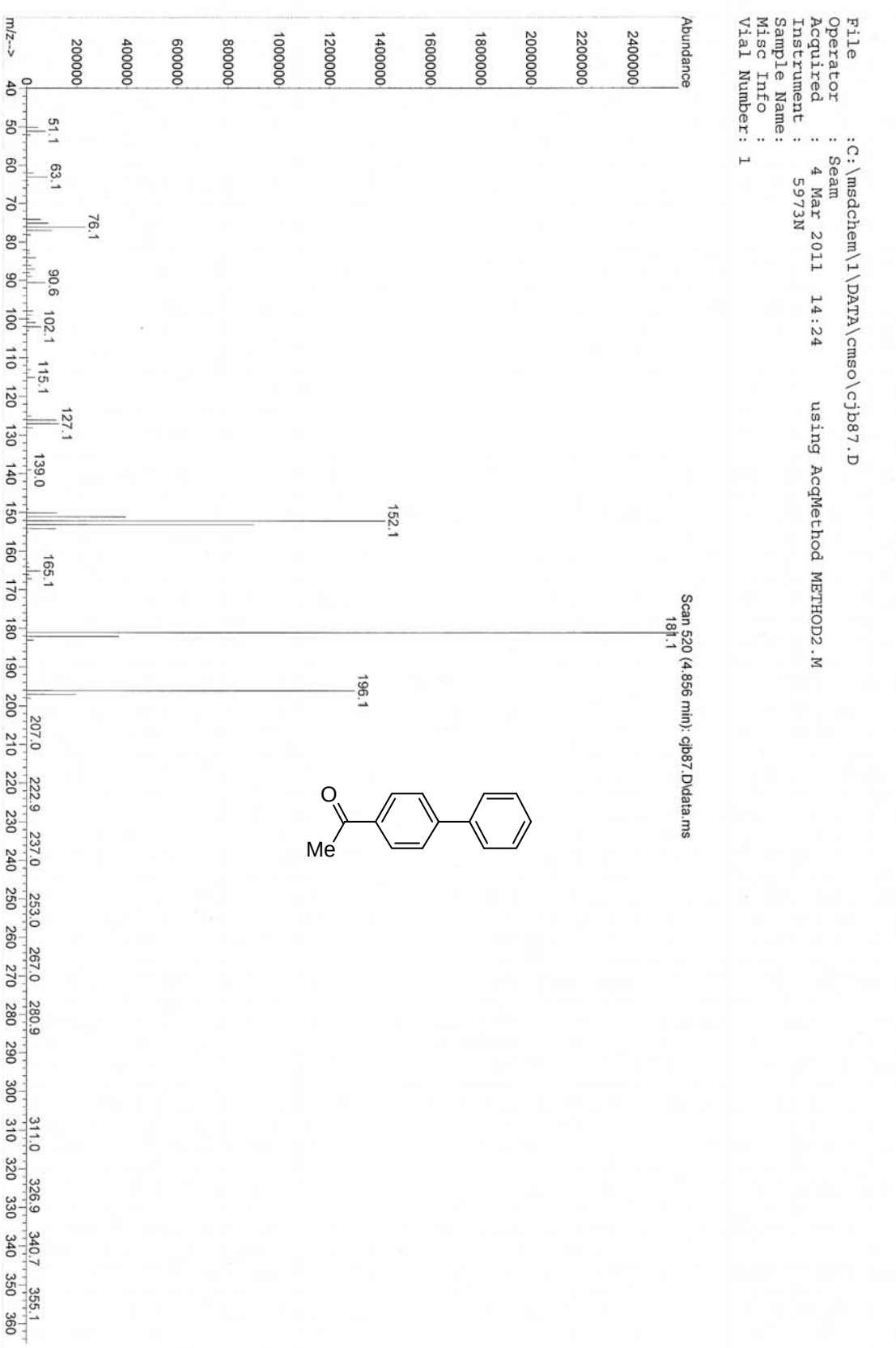

Standard 13C
159.08
140.70
133.62
128.64
128.03
126.61
126.56
114.13
77.31
76.99
76.68
55.14
MeO
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME cjb067
EXPNO 2
PROCNO 1
Date_ 20110308
Time 21.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 28
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127940 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

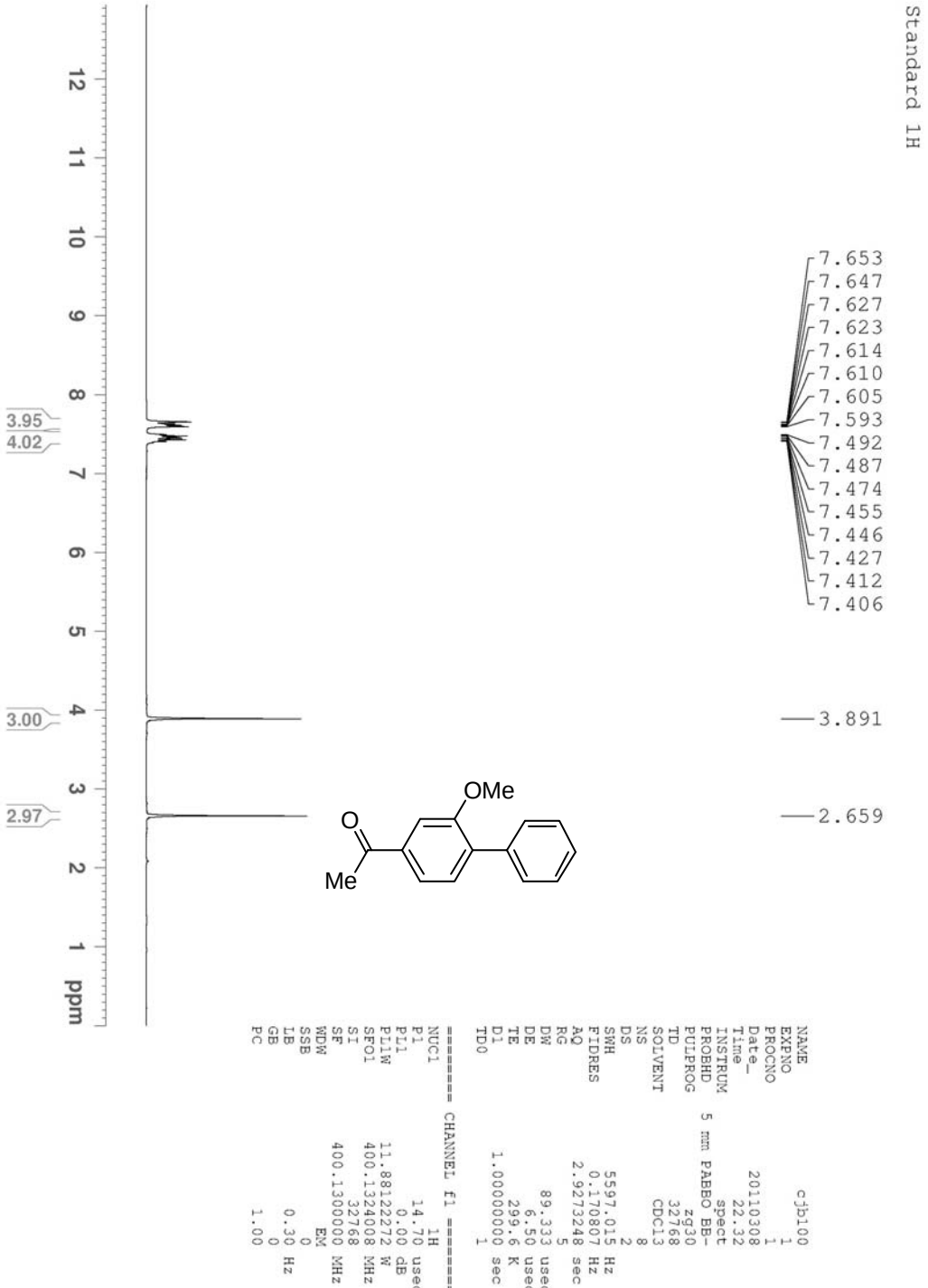

File :C:\msdchem\1\DATA\JIM\CJB067.D
Operator : Seam
Acquired : 26 Feb 2011 12:22 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 4
Abundance
Scan 443 (4.416 min): CJB067.D\data.ms
184.1
141.1
169.1
115.1
51.1
63.1
76.1
89.1
102.1
126.1
152.1
194.9
207.0
225.0
237.0
252.9
266.9
282.0
293.0
304.8
327.0
367.1
m/z-->
MeO

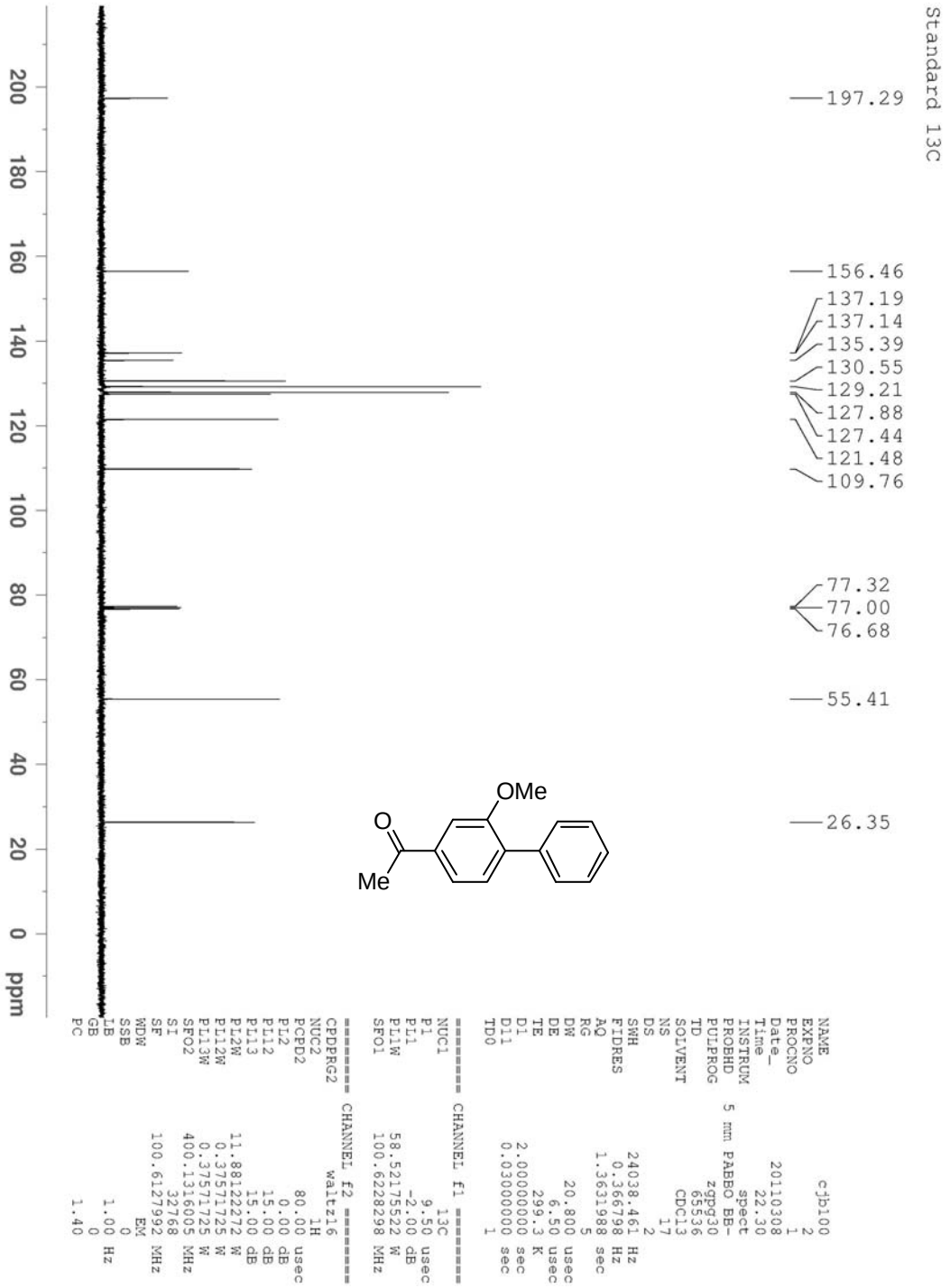

8.036
8.015
7.678
7.657
7.634
7.615
7.493
7.475
7.455
7.430
7.411
2.616
1.96
3.99
3.03
3.00
O
Me
ppm
NAME cjb087
EXPNO 1
PROCNO 1
Date_ 20110304
Time_ 23.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 300.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

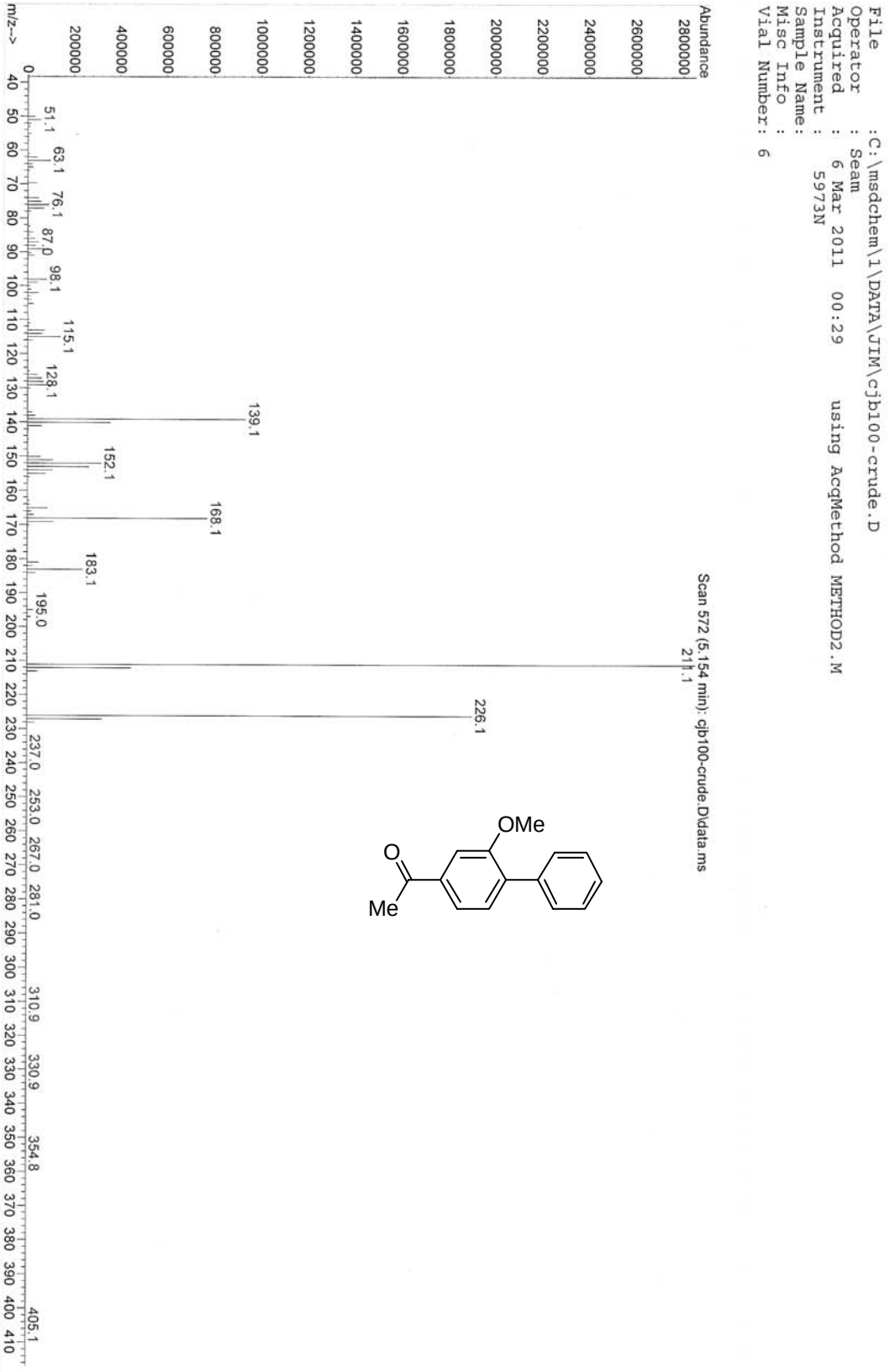


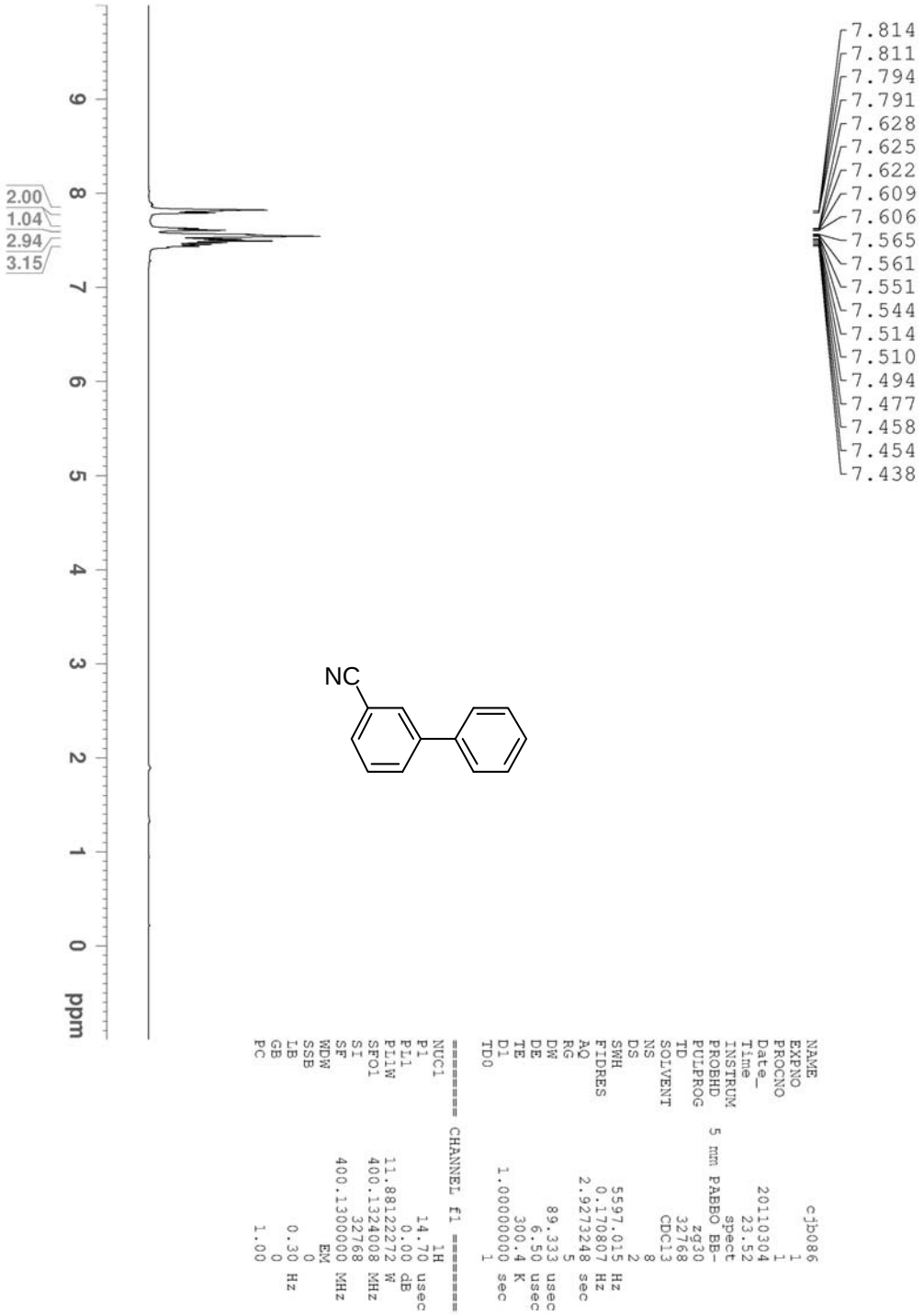

```
NAME                                    cjb087
EXPNO                                        2
PROCNO                                       1
Date_                             20110304
Time_                                 23.48
INSTRUM                                spect
PROBHD     5 mm PABBO BB-
PULPROG                             zgpg30
TD                                   65536
SOLVENT                              CDCl3
NS                                      18
DS                                       2
SWH                              24038.461 Hz
FIDRES                            0.366798 Hz
AQ                                1.3631988 sec
RG                                       5
DW                                  20.800 usec
DE                                   6.50 usec
TE                                 300.9 K
D1                                2.00000000 sec
D11                               0.03000000 sec
TD0                                      1

======== CHANNEL f1 ========
NUC1                                   13C
P1                                    9.50 usec
PL1                                  -2.00 dB
PL1W                            58.52175522 W
SFO1                           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                            waltz16
NUC2                                   1H
PCPD2                                80.00 usec
PL2                                   0.00 dB
PL12                                 15.00 dB
PL13                                 15.00 dB
PL2W                            11.88122272 W
PL12W                            0.37571725 W
PL13W                            0.37571725 W
SFO2                           400.1316005 MHz
SI                                   32768
SF                             100.6127995 MHz
WDW                                     EM
SSB                                      0
LB                                    1.00 Hz
GB                                       0
PC                                    1.40
```

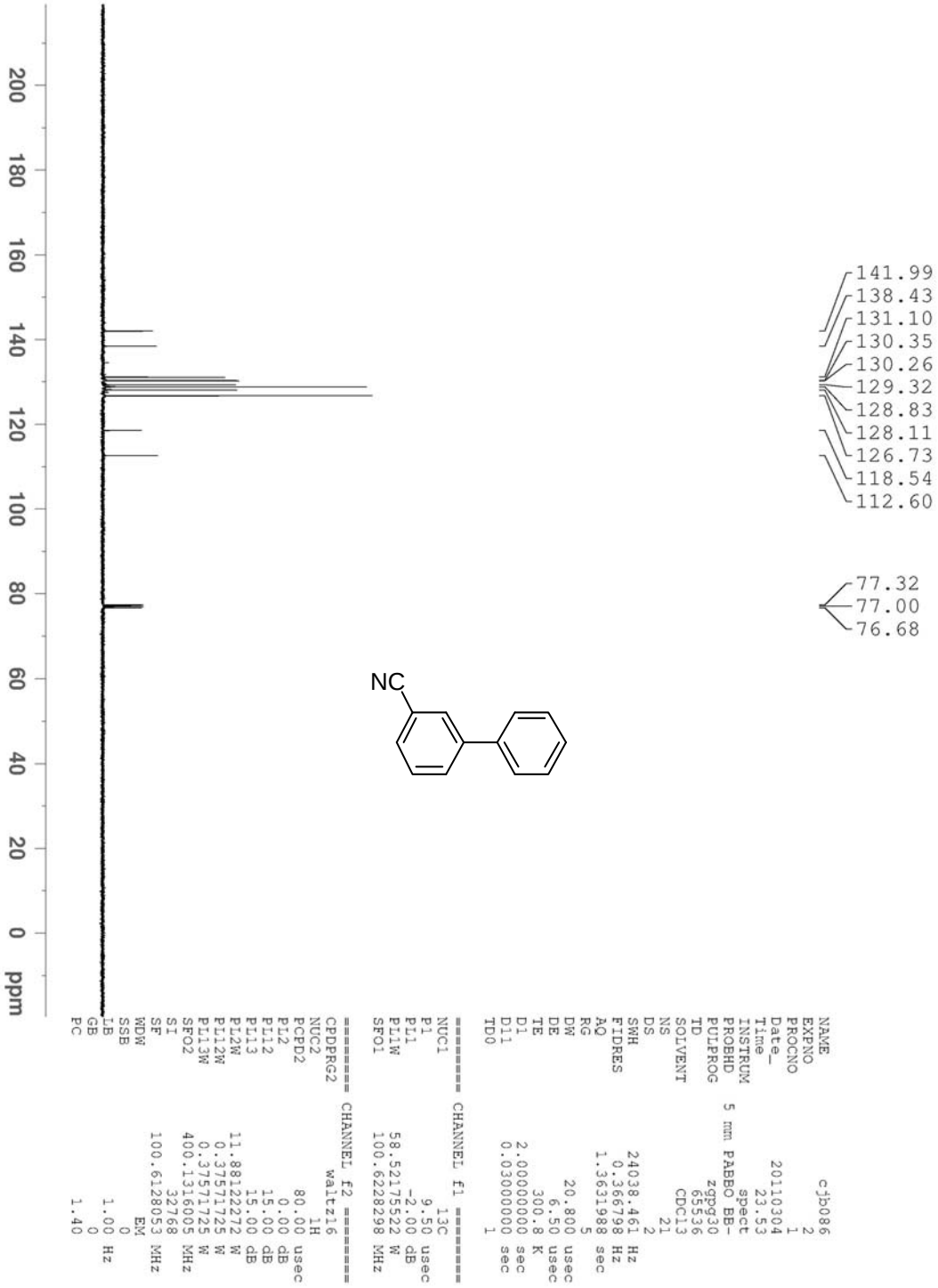

File :C:\msdchem\1\DATA\cmso\cjb87.D
Operator : Seam
Acquired : 4 Mar 2011 14:24 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1
Abundance
Scan 520 (4.856 min): cjb87.D\data.ms
181.1
152.1
196.1
76.1
165.1
127.1
O
Me
m/z-->

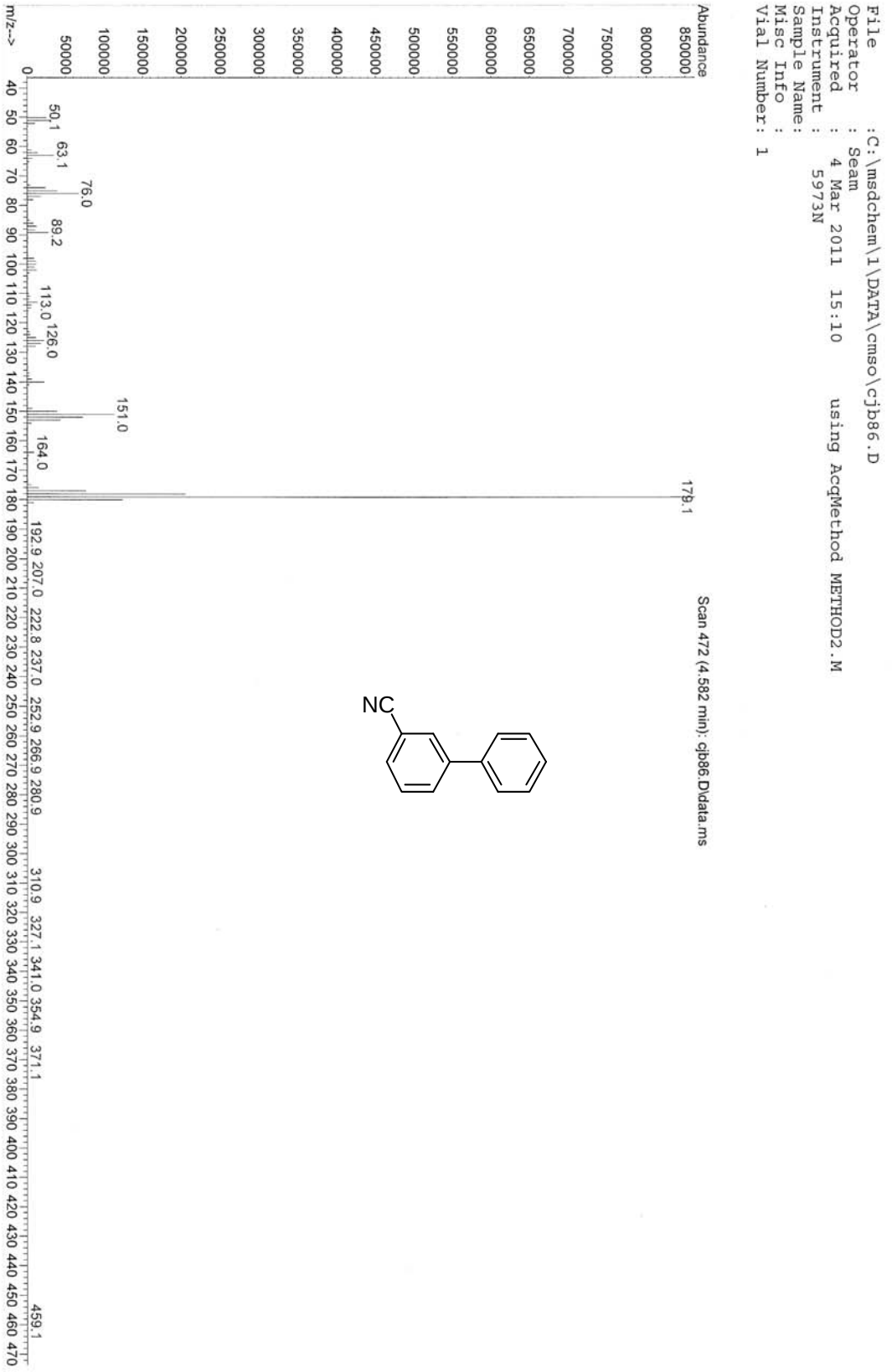

Standard 1H
7.653
7.647
7.627
7.623
7.614
7.610
7.605
7.593
7.492
7.487
7.474
7.455
7.446
7.427
7.412
7.406
3.891
2.659
3.95
4.02
3.00
2.97
OMe
O
Me
12
11
10
9
8
7
6
5
4
3
2
1
ppm
NAME cjb100
EXPNO 1
PROCNO 1
Date_ 20110308
Time 22.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

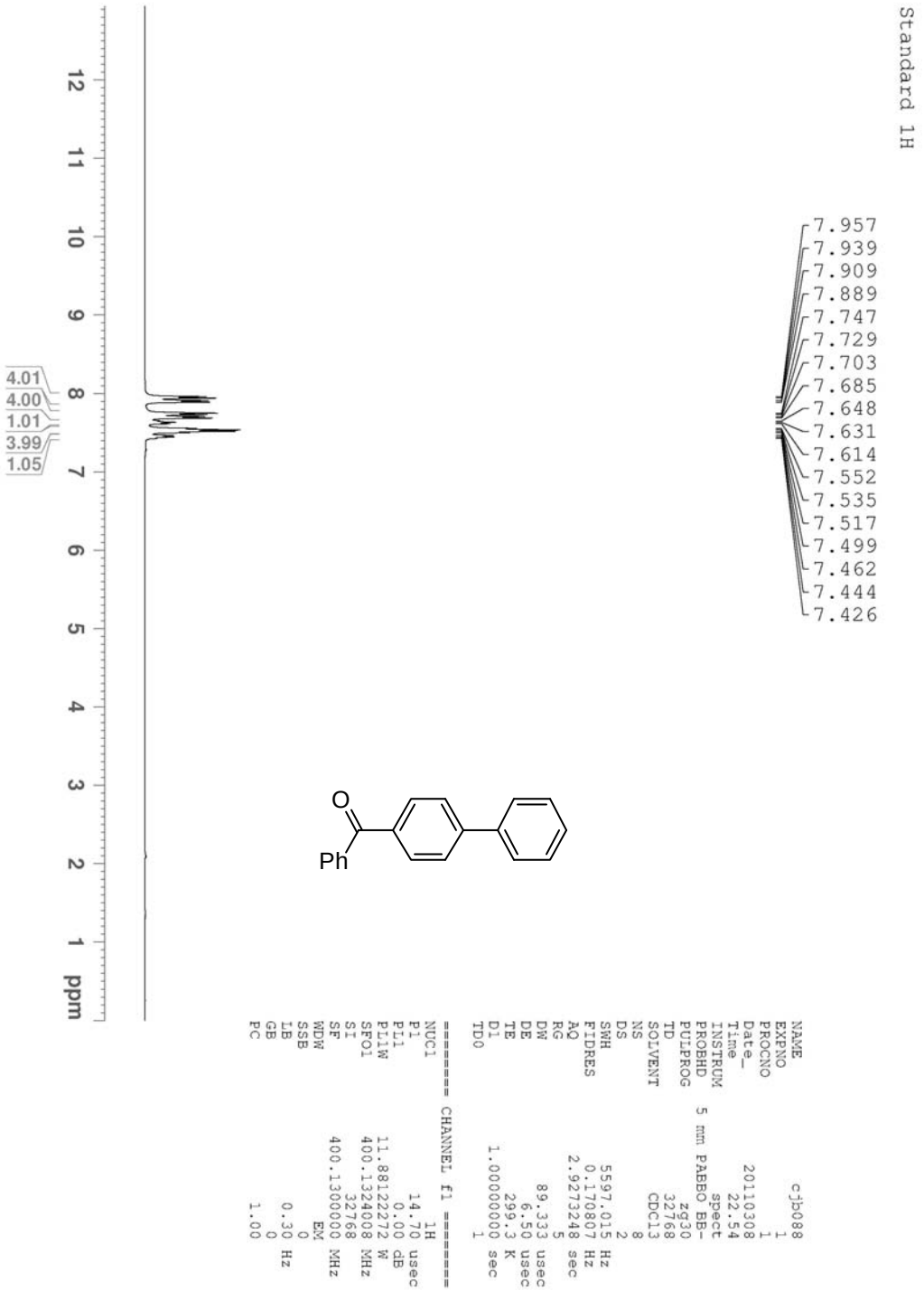

Standard 13C
197.29
156.46
137.19
137.14
135.39
130.55
129.21
127.88
127.44
121.48
109.76
77.32
77.00
76.68
55.41
26.35
OMe
O
Me
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME cjb100
EXPNO 2
PROCNO 1
Date_ 20110308
Time 22.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 17
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127992 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

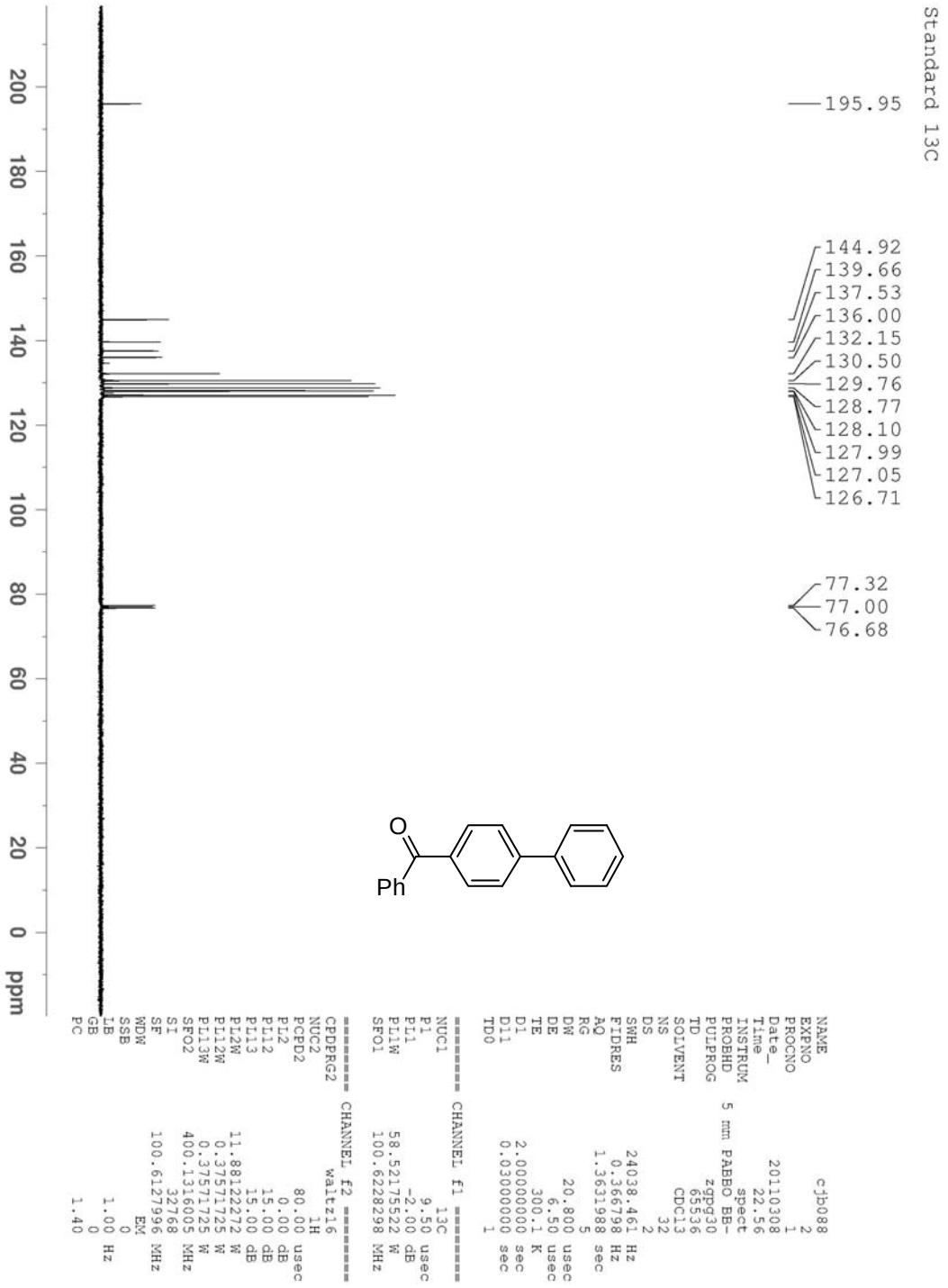

File :C:\msdchem\1\DATA\JIM\cjb100-crude.D
Operator : Seam
Acquired : 6 Mar 2011 00:29 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 6
Abundance
m/z-->
Scan 572 (5.154 min): cjb100-crude.D\data.ms
211.1
226.1
139.1
168.1
152.1
183.1
195.0
115.1
128.1
98.1
87.0
76.1
63.1
51.1
OMe
O
Me

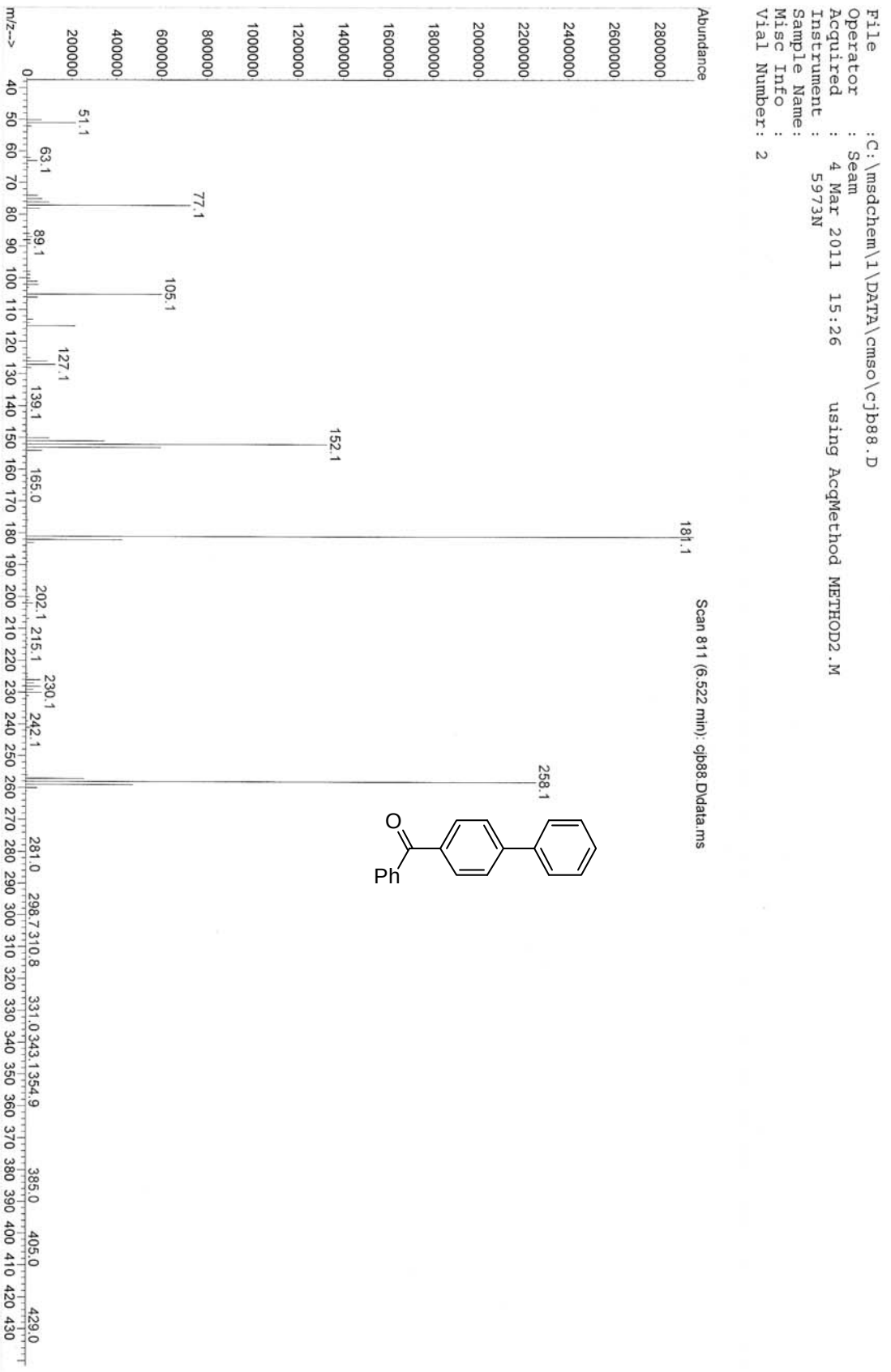

7.814
7.811
7.794
7.791
7.628
7.625
7.622
7.609
7.606
7.565
7.561
7.551
7.544
7.514
7.510
7.494
7.477
7.458
7.454
7.438
2.00
1.04
2.94
3.15
9
8
7
6
5
4
3
2
1
0
ppm
NC
NAME cjb086
EXPNO 1
PROCNO 1
Date_ 20110304
Time 23.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 300.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

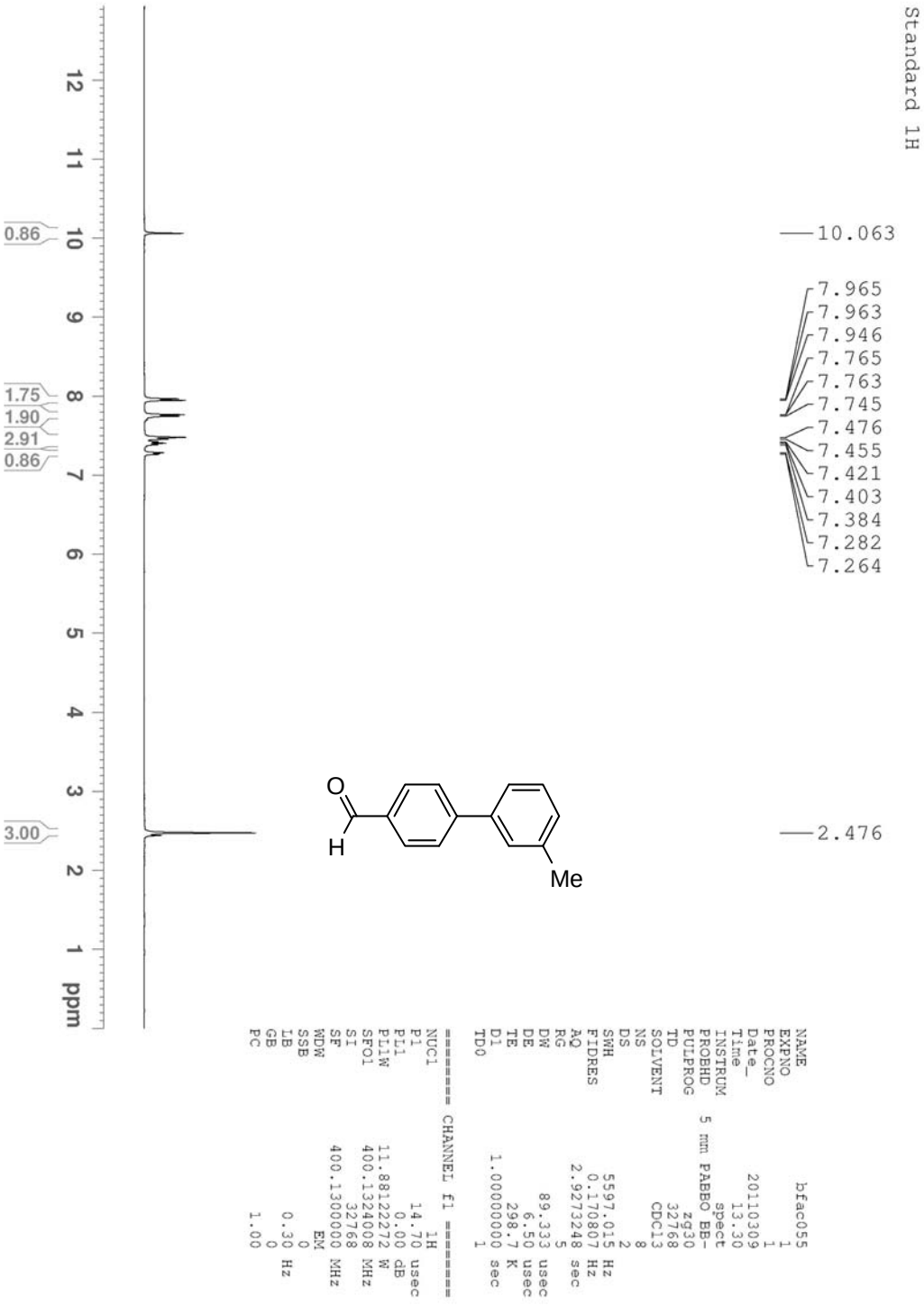

141.99
138.43
131.10
130.35
130.26
129.32
128.83
128.11
126.73
118.54
112.60
77.32
77.00
76.68
NC
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME cjb086
EXPNO 2
PROCNO 1
Date_ 20110304
Time 23.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 300.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

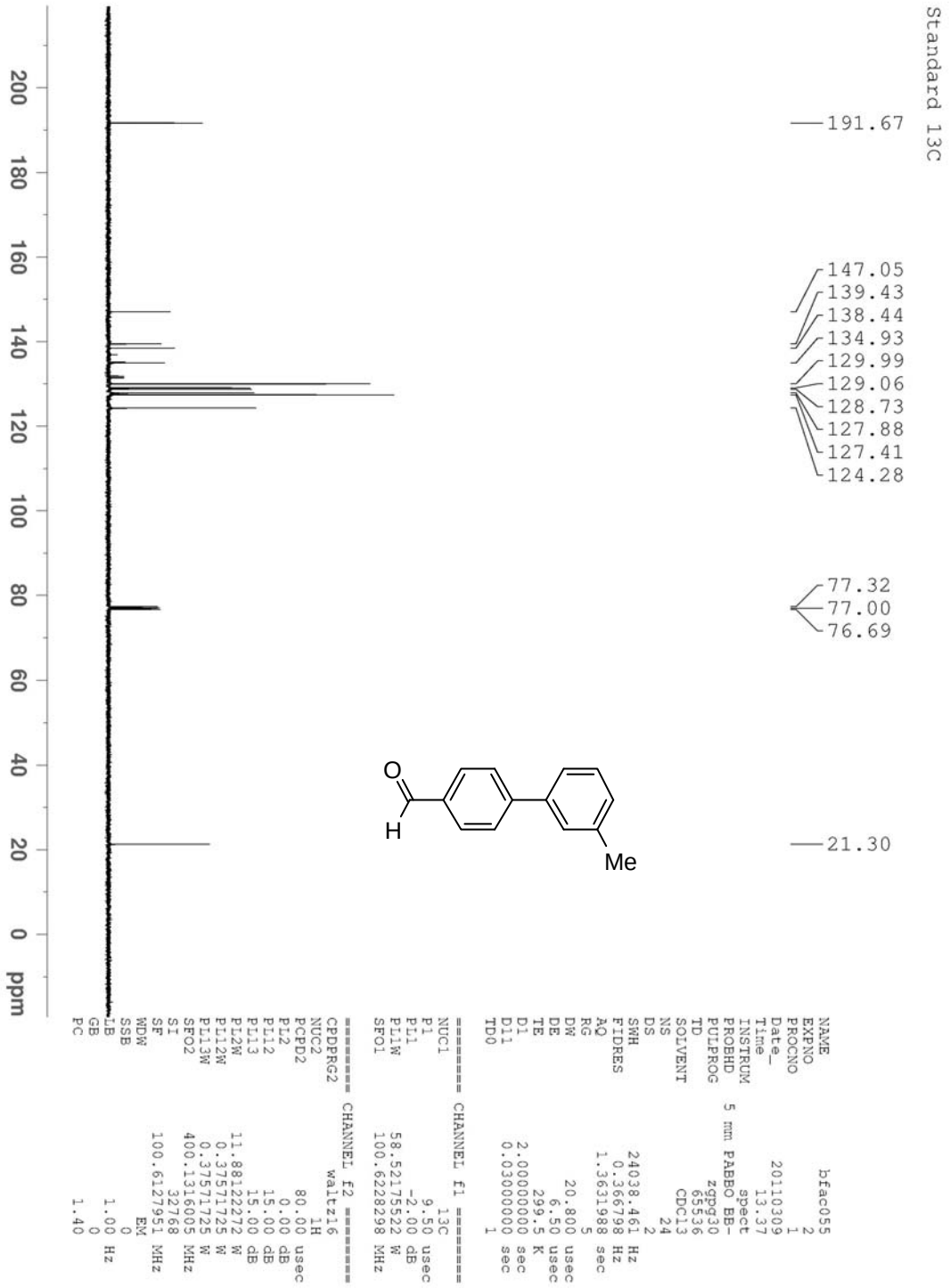

File :C:\msdchem\1\DATA\cmso\cjb86.D
Operator : Seam
Acquired : 4 Mar 2011 15:10 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1
Abundance
m/z-->
Scan 472 (4.582 min): cjb86.D\data.ms
NC

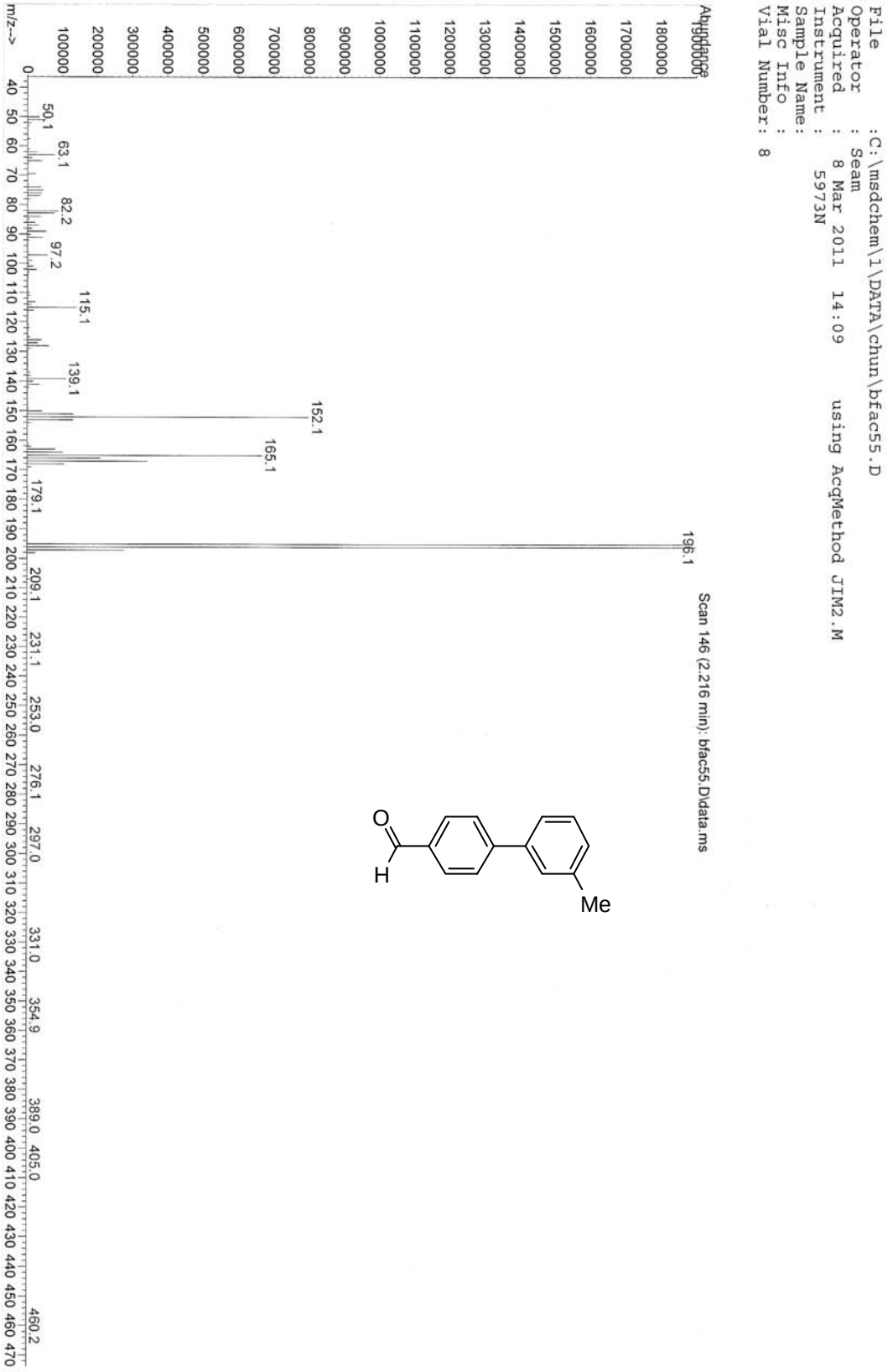

Standard 1H
7.957
7.939
7.909
7.889
7.747
7.729
7.703
7.685
7.648
7.631
7.614
7.552
7.535
7.517
7.499
7.462
7.444
7.426
4.01
4.00
1.01
3.99
1.05
12 11 10 9 8 7 6 5 4 3 2 1 ppm
O
Ph
NAME cjb088
EXPNO 1
PROCNO 1
Date_ 20110308
Time 22.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

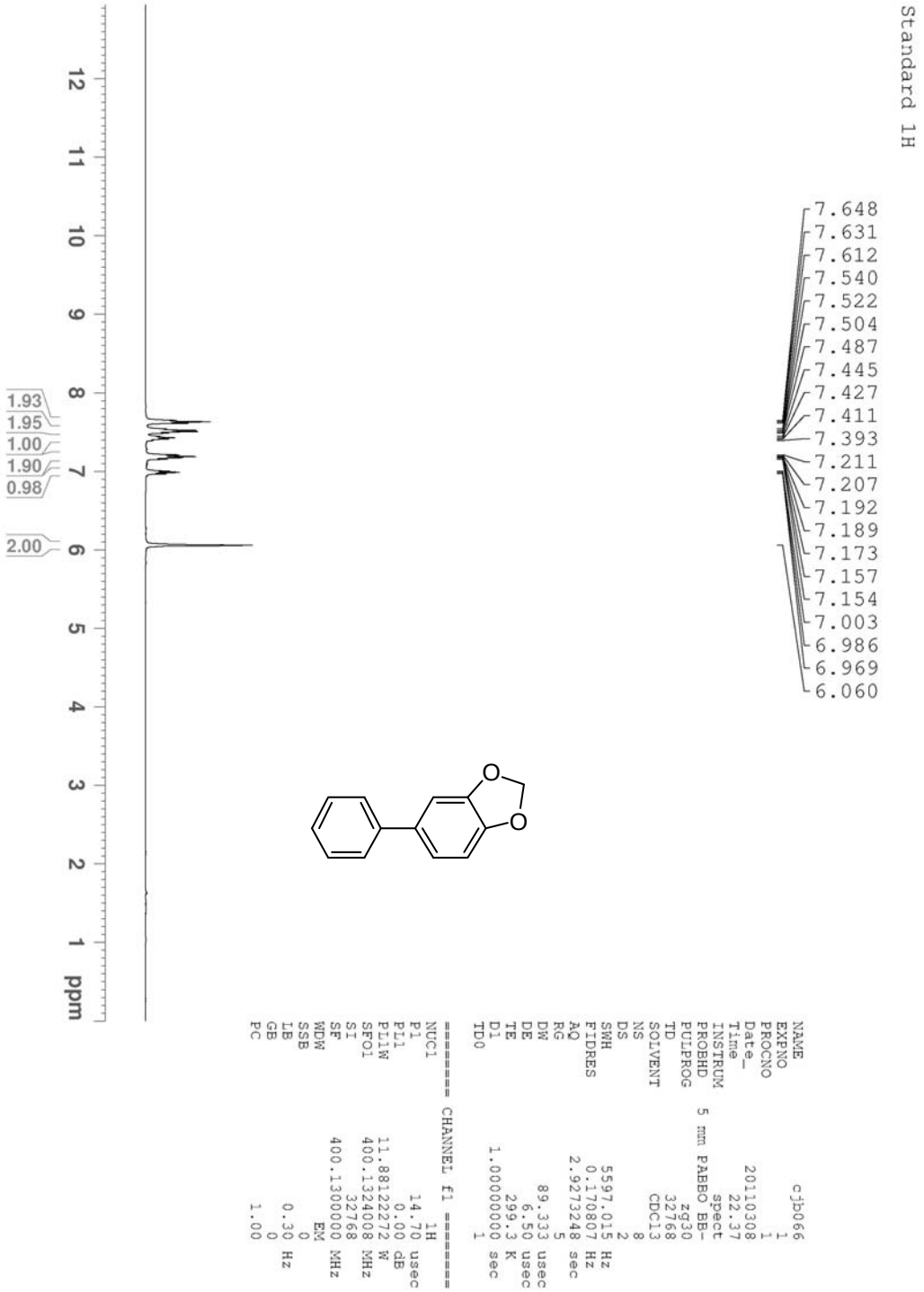

Standard 13C
195.95
144.92
139.66
137.53
136.00
132.15
130.50
129.76
128.77
128.10
127.99
127.05
126.71
77.32
77.00
76.68
O
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME cjb088
EXPNO 2
PROCNO 1
Date_ 20110308
Time 22.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127996 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

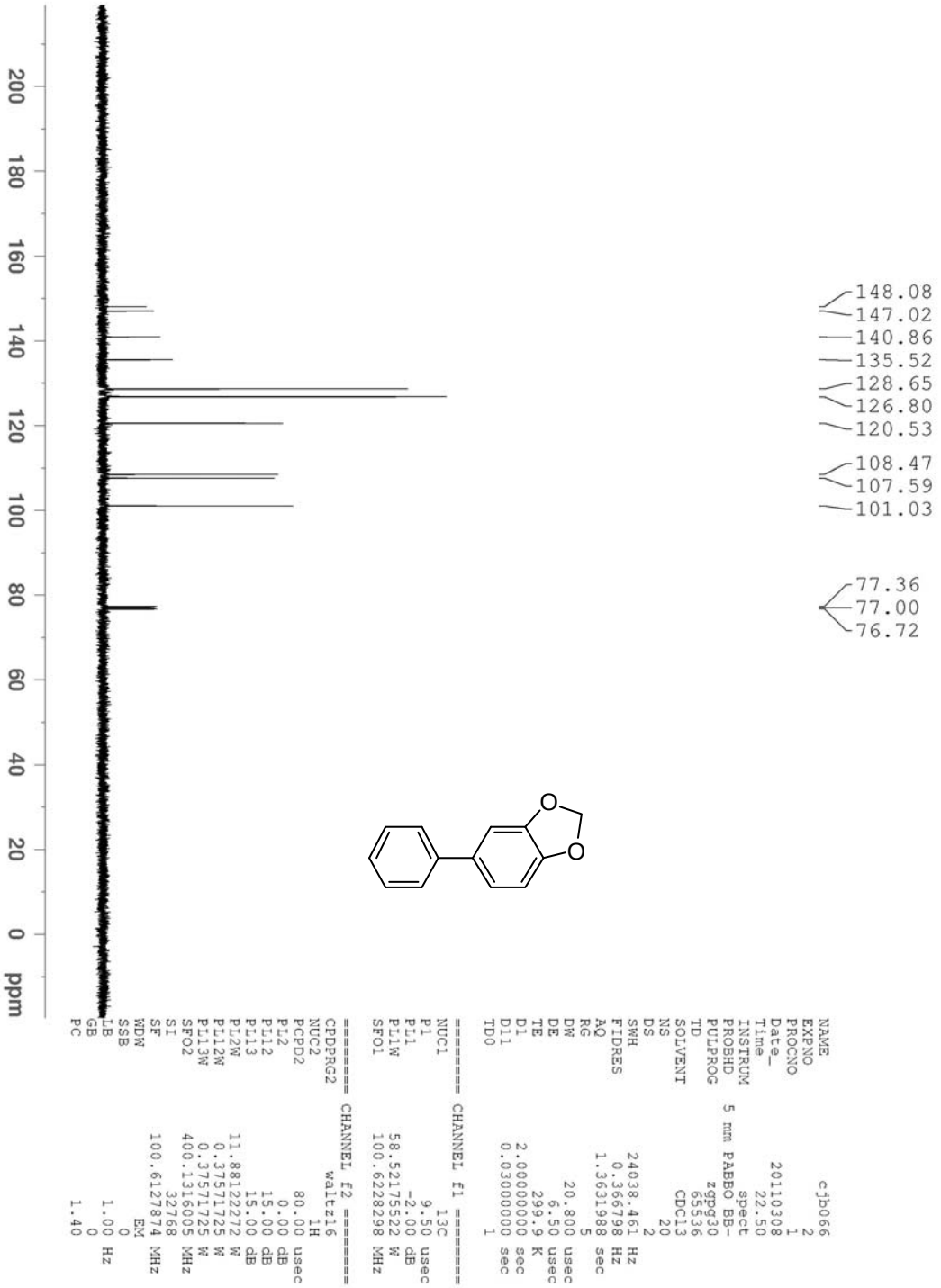

File :C:\msdchem\1\DATA\cmso\cjb88.D
Operator : Seam
Acquired : 4 Mar 2011 15:26 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 2
Abundance
m/z-->
Scan 811 (6.522 min): cjb88.D\data.ms
181.1
258.1
152.1
77.1
105.1
51.1
63.1
89.1
127.1
139.1
165.0
202.1
215.1
230.1
242.1
O
Ph



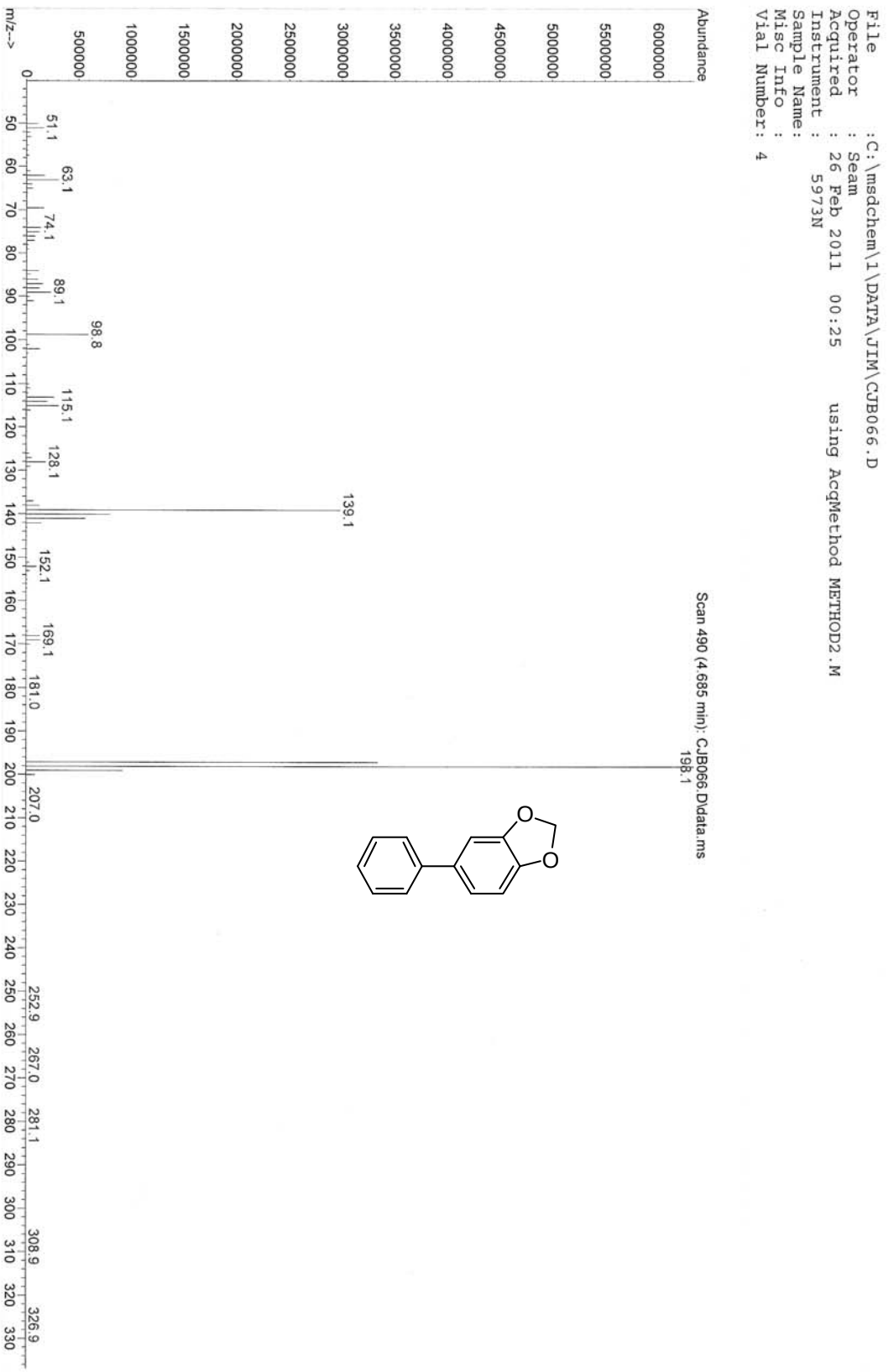


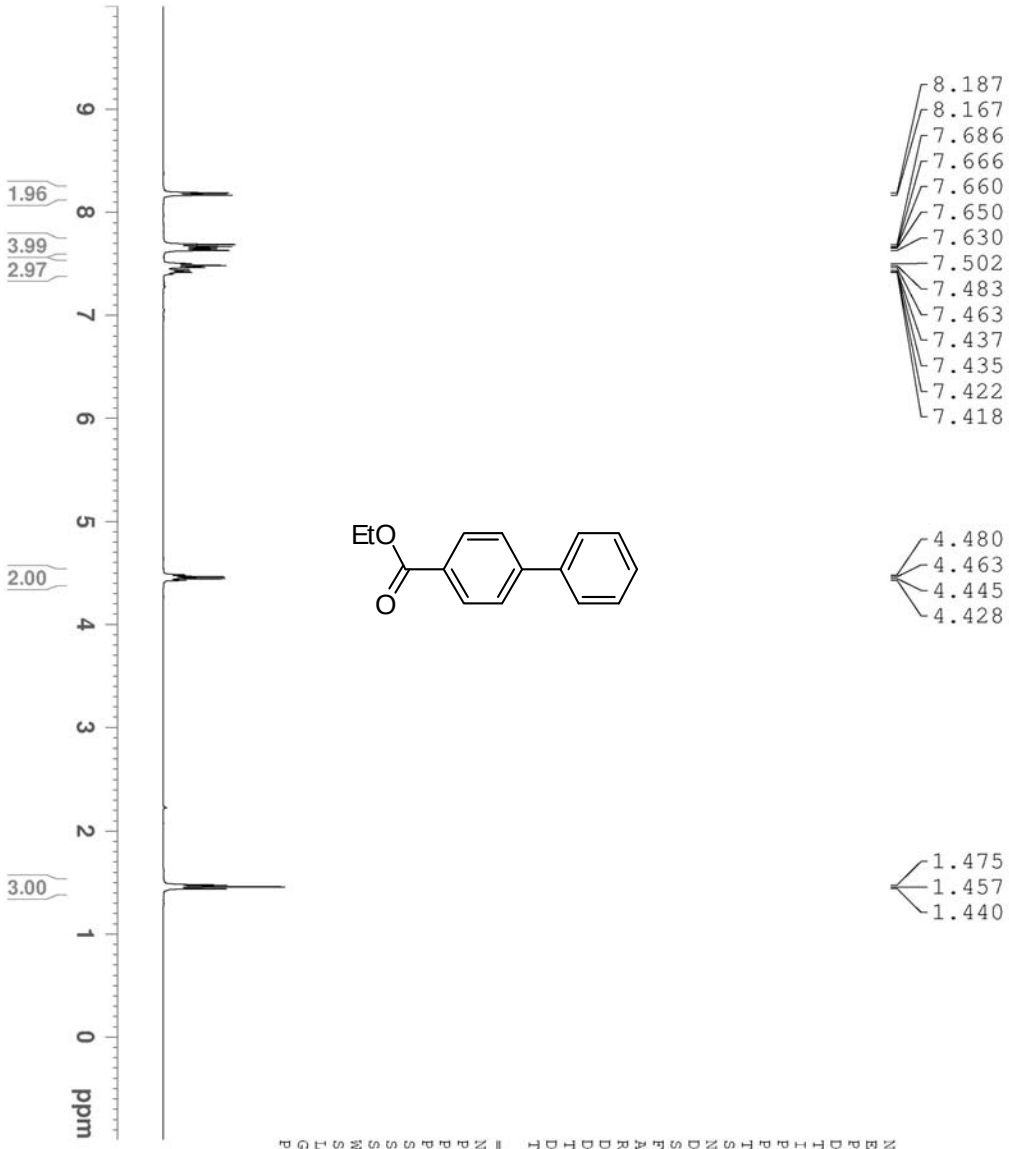

File :C:\msdchem\1\DATA\chun\bfac55.D
Operator : Seam
Acquired : 8 Mar 2011 14:09 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 8
Abundance
m/z-->
Scan 146 (2.216 min): bfac55.D\data.ms
196.1
152.1
165.1
139.1
115.1
82.2
97.2
63.1
50.1
179.1
O
H
Me

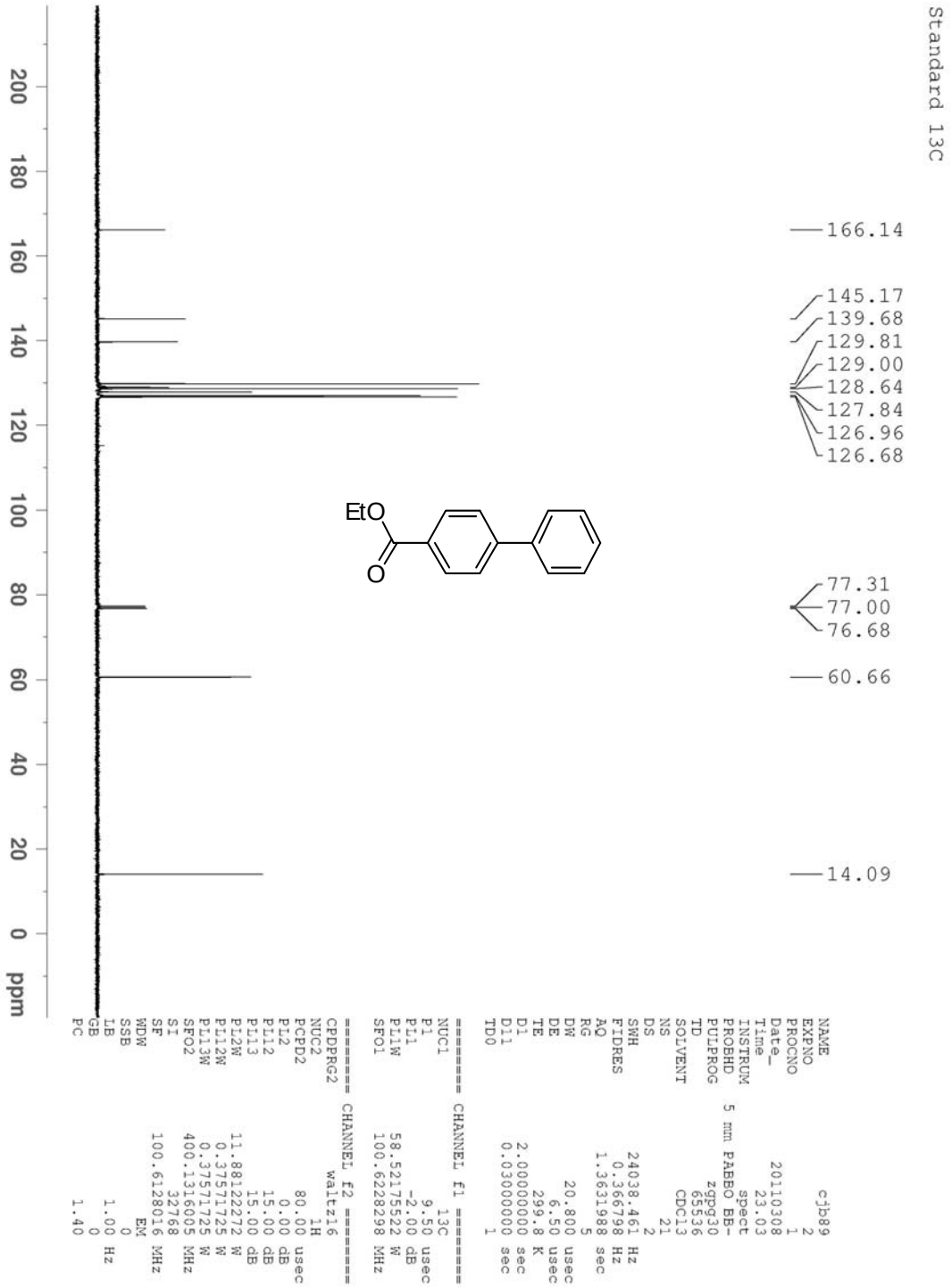


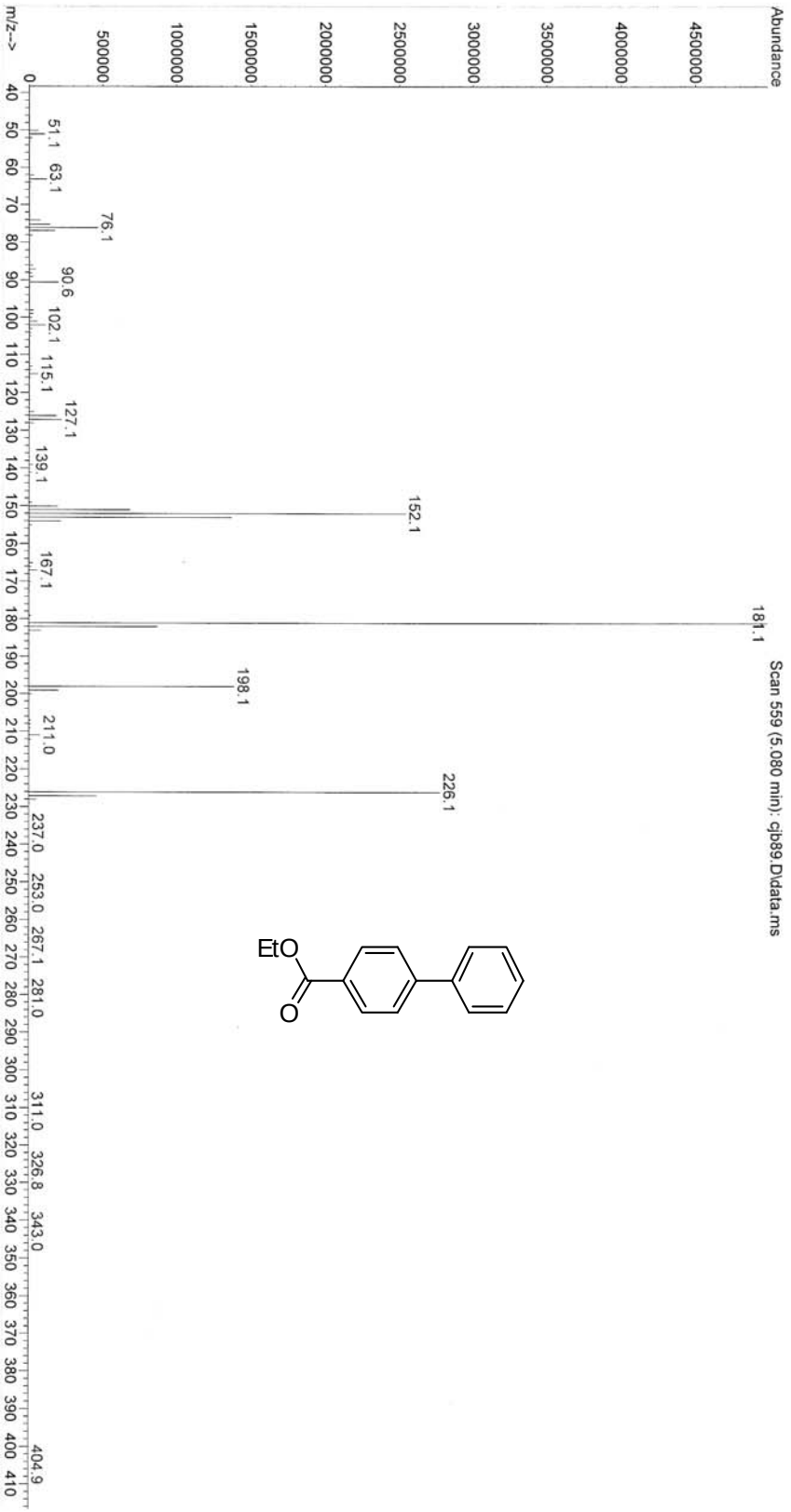


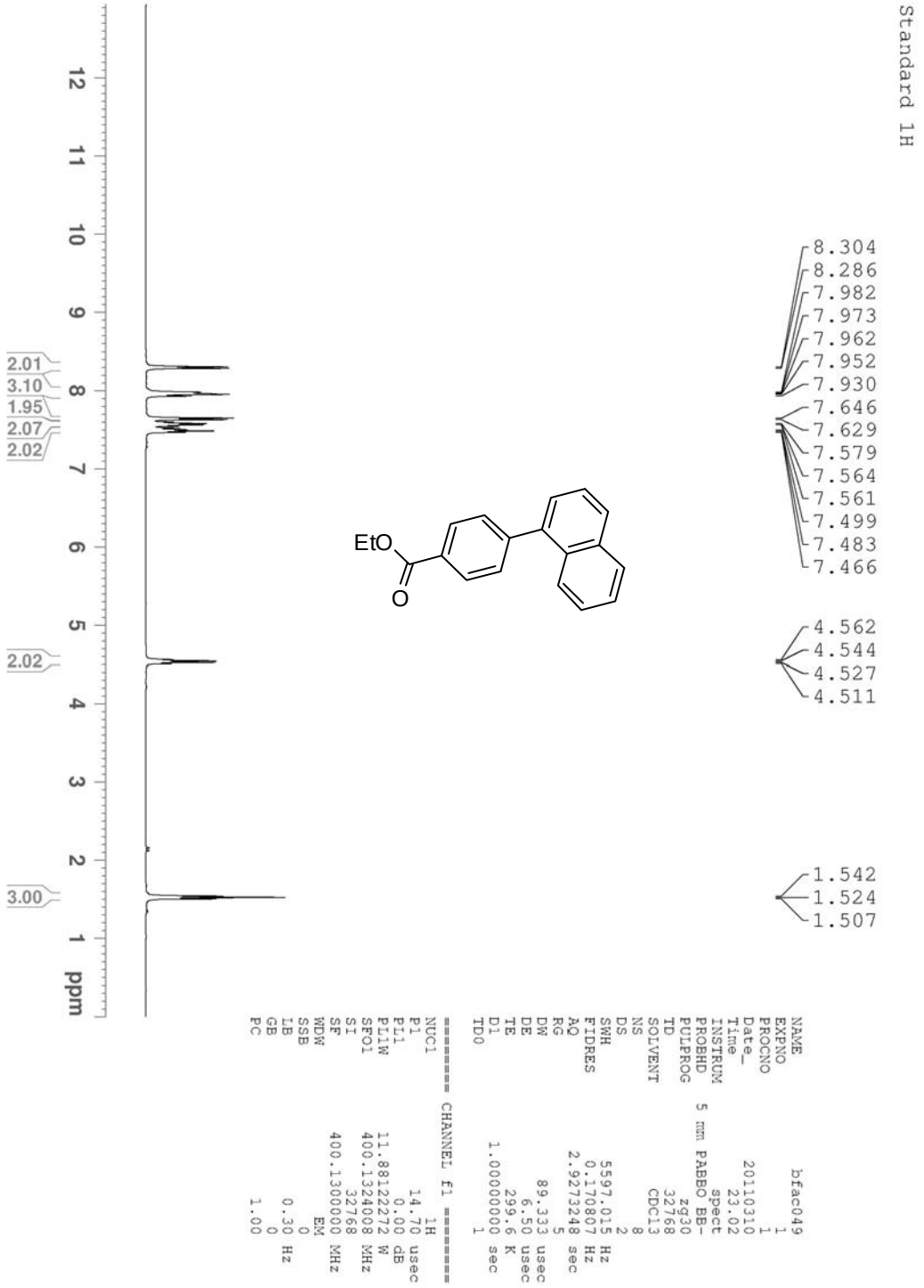

```
NAME                    cjb066
EXPNO                        2
PROCNO                       1
Date_                 20110308
Time                     22.50
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          20
DS                           2
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                           5
DW                      20.800 usec
DE                       6.50 usec
TE                       299.9 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                          1

========== CHANNEL f1 ==========
NUC1                        13C
P1                         9.50 usec
PL1                       -2.00 dB
PL1W                58.52175522 W
SFO1                100.6228298 MHz

========== CHANNEL f2 ==========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.00 dB
PL13                    15.00 dB
PL2W                11.88122272 W
PL12W                0.37571725 W
PL13W                0.37571725 W
SFO2                400.1316005 MHz
SI                       32768
SF                  100.6127874 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

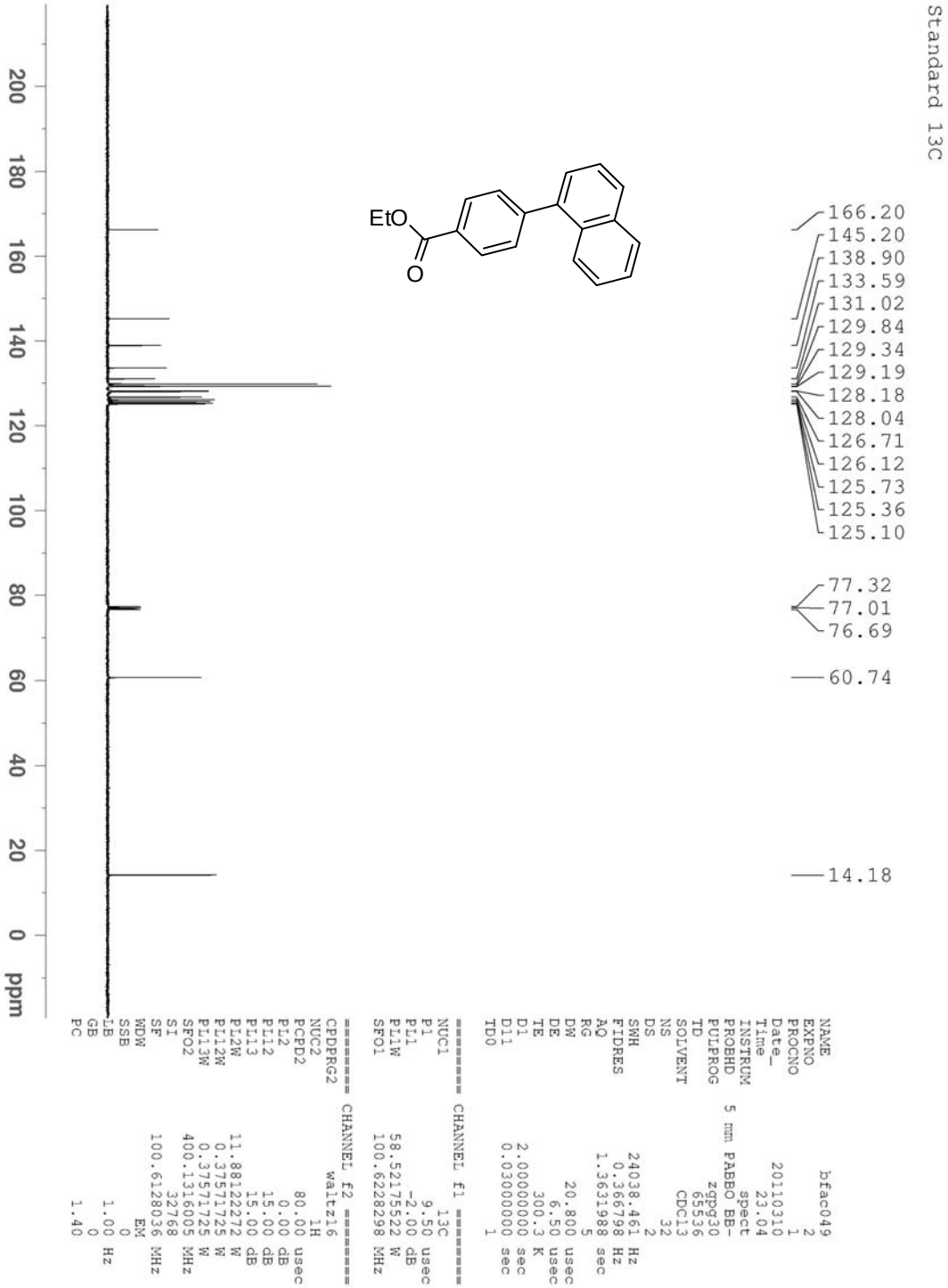

File :C:\msdchem\1\DATA\JIM\CJB066.D
Operator : Seam
Acquired : 26 Feb 2011 00:25 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 4
Abundance
m/z-->
Scan 490 (4.685 min): CJB066.D\data.ms
198.1
139.1
98.8
51.1
63.1
74.1
89.1
115.1
128.1
152.1
169.1
181.0
207.0
252.9
267.0
281.1
308.9
326.9
O
O

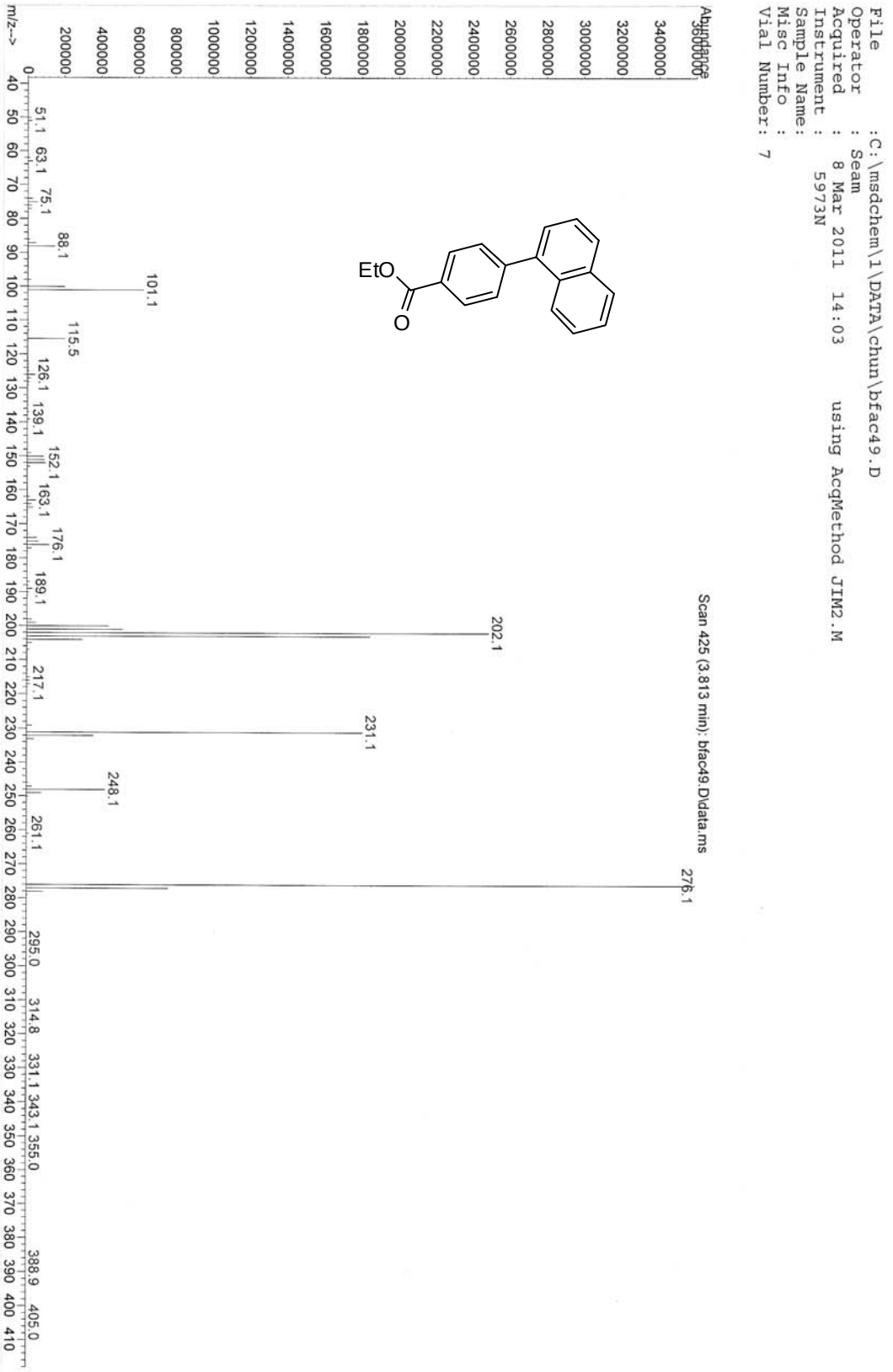

8.187
8.167
7.686
7.666
7.660
7.650
7.630
7.502
7.483
7.463
7.437
7.435
7.422
7.418
4.480
4.463
4.445
4.428
1.475
1.457
1.440
EtO
O
1.96
3.99
2.97
2.00
3.00
ppm
NAME cjb89
EXPNO 1
PROCNO 1
Date_ 20110308
Time_ 23.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

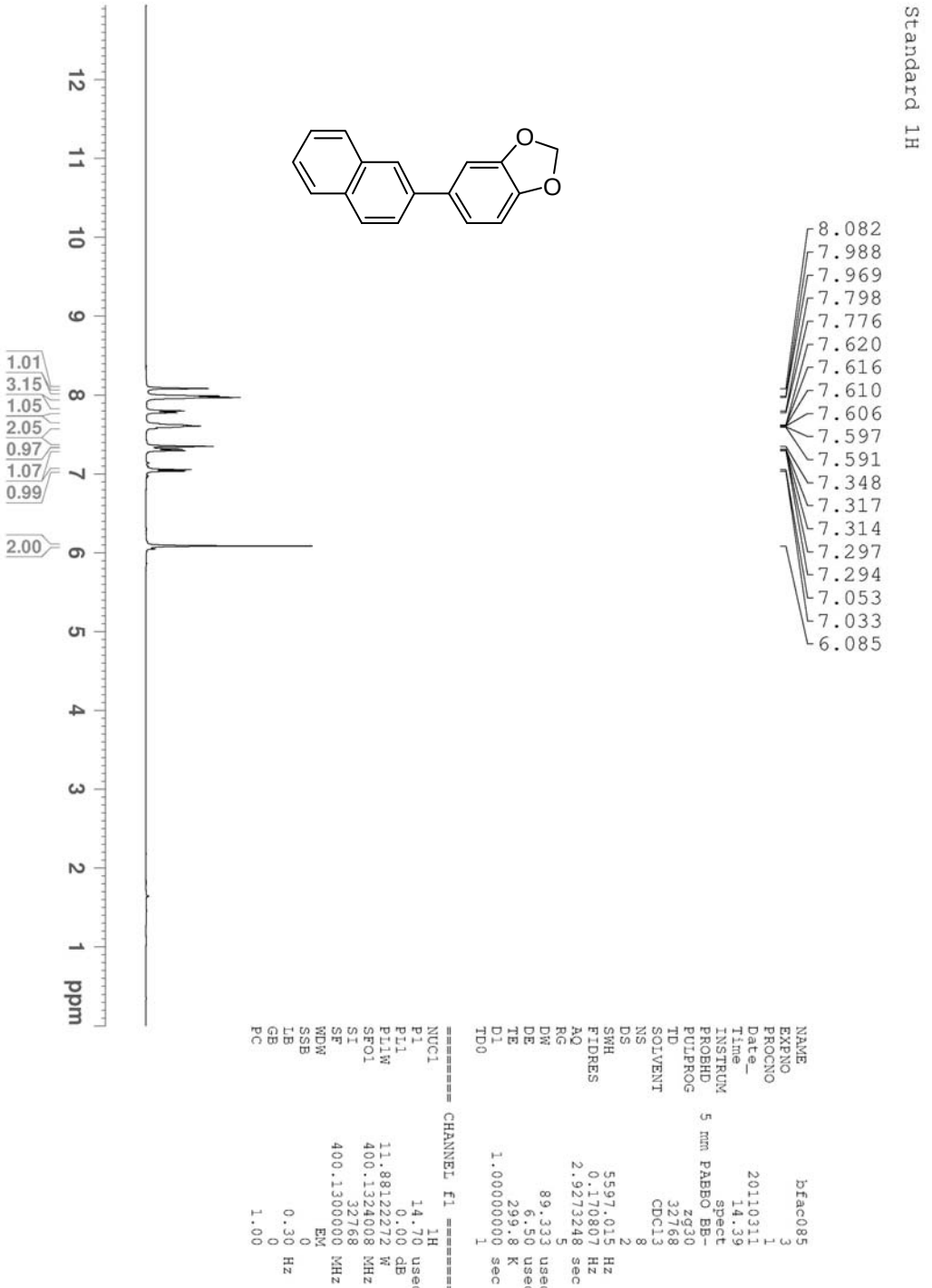

Standard 13C
166.14
145.17
139.68
129.81
129.00
128.64
127.84
126.96
126.68
77.31
77.00
76.68
60.66
14.09
EtO
O
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME cjb89
EXPNO 2
PROCNO 1
Date_ 20110308
Time_ 23.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128016 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

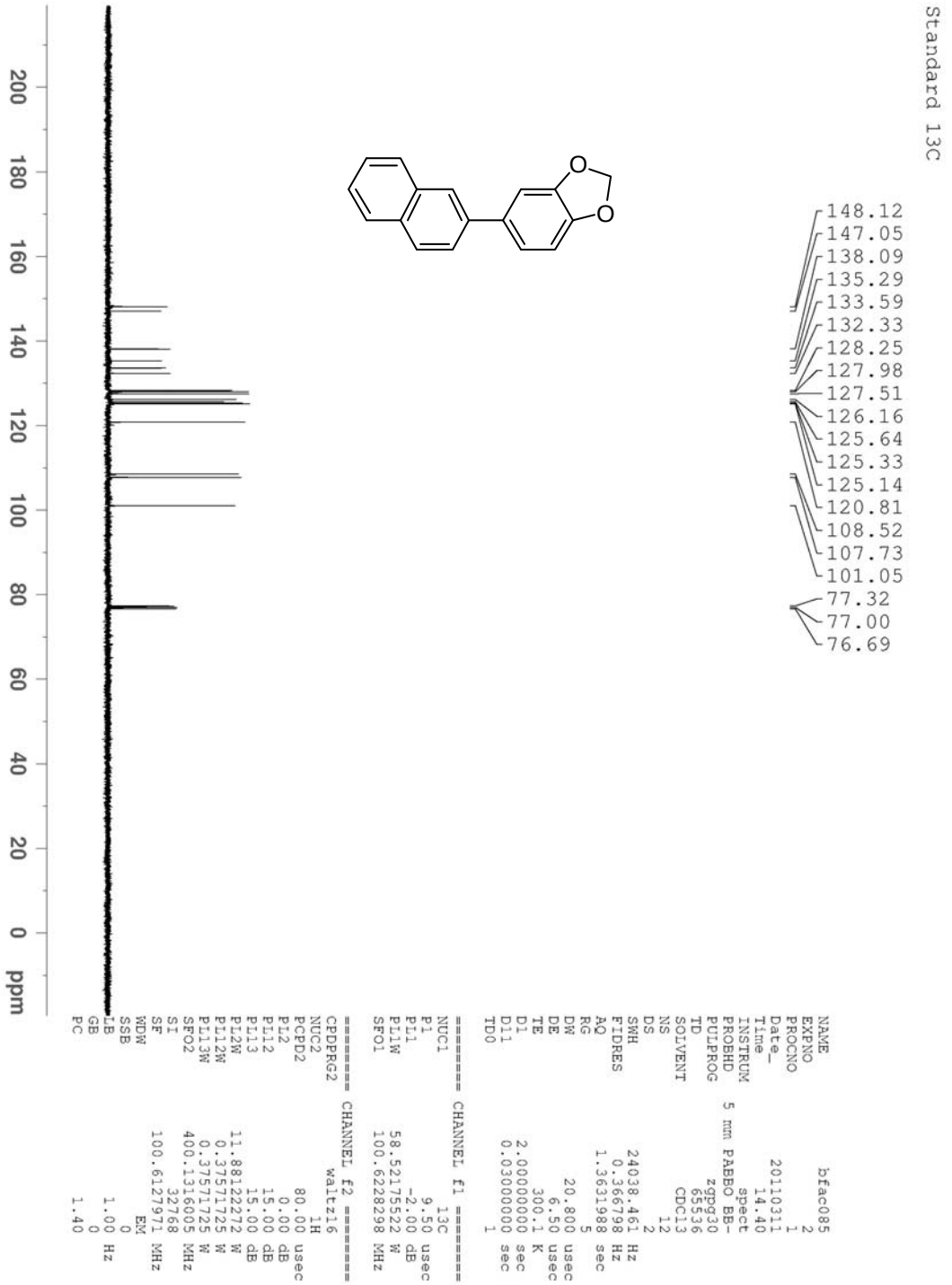

File :C:\msdchem\1\DATA\cmso\cjb89.D
Operator : Seam
Acquired : 4 Mar 2011 15:41 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
Scan 559 (5.080 min): cjb89.D\data.ms
181.1
152.1
76.1
226.1
198.1
EtO
O

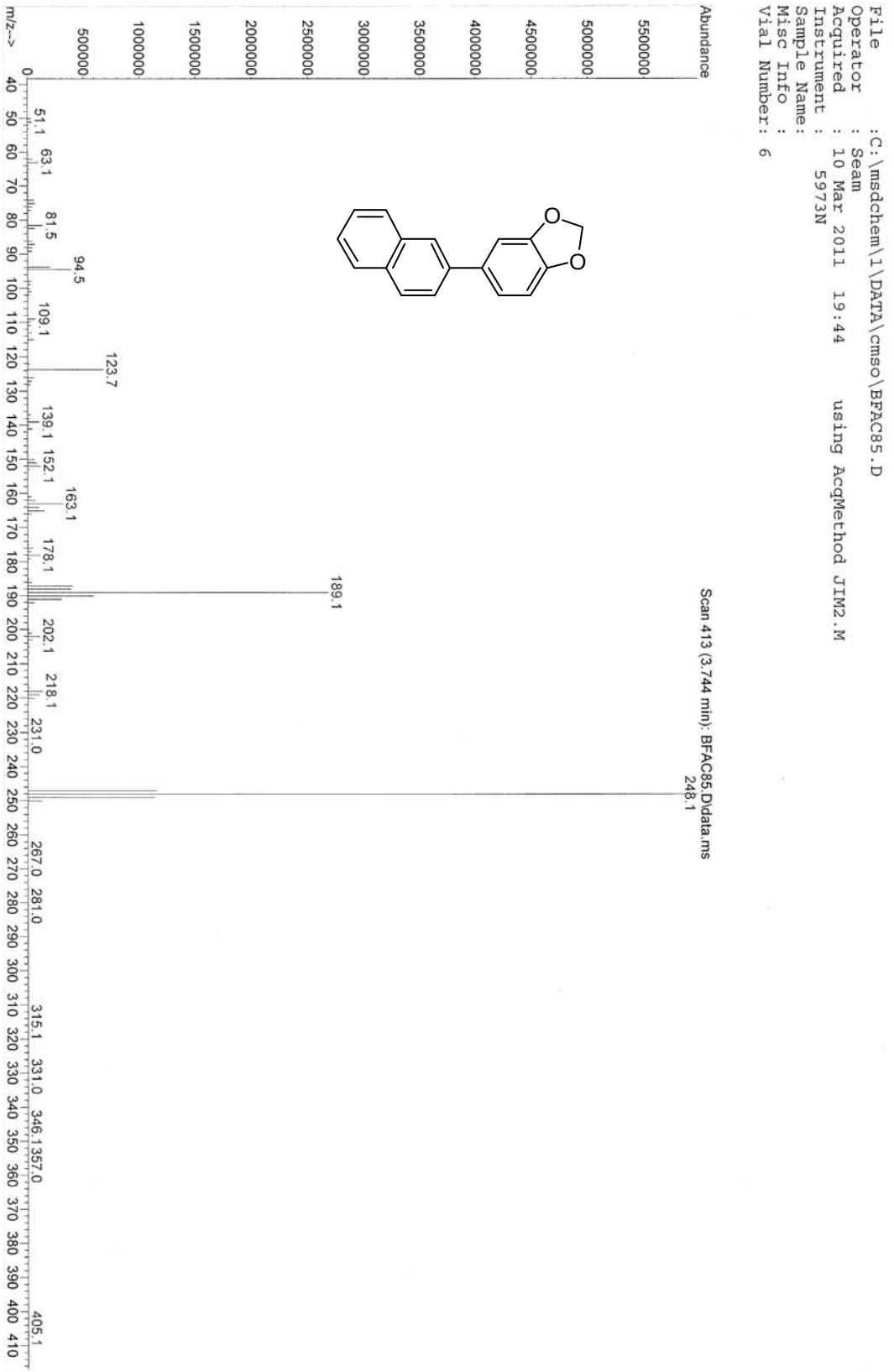

Standard 1H
8.304
8.286
7.982
7.973
7.962
7.952
7.930
7.646
7.629
7.579
7.564
7.561
7.499
7.483
7.466
4.562
4.544
4.527
4.511
1.542
1.524
1.507
EtO
O
2.01
3.10
1.95
2.07
2.02
2.02
3.00
12 11 10 9 8 7 6 5 4 3 2 1 ppm
NAME bfac049
EXPNO 1
PROCNO 1
Date_ 20110310
Time 23.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.927248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

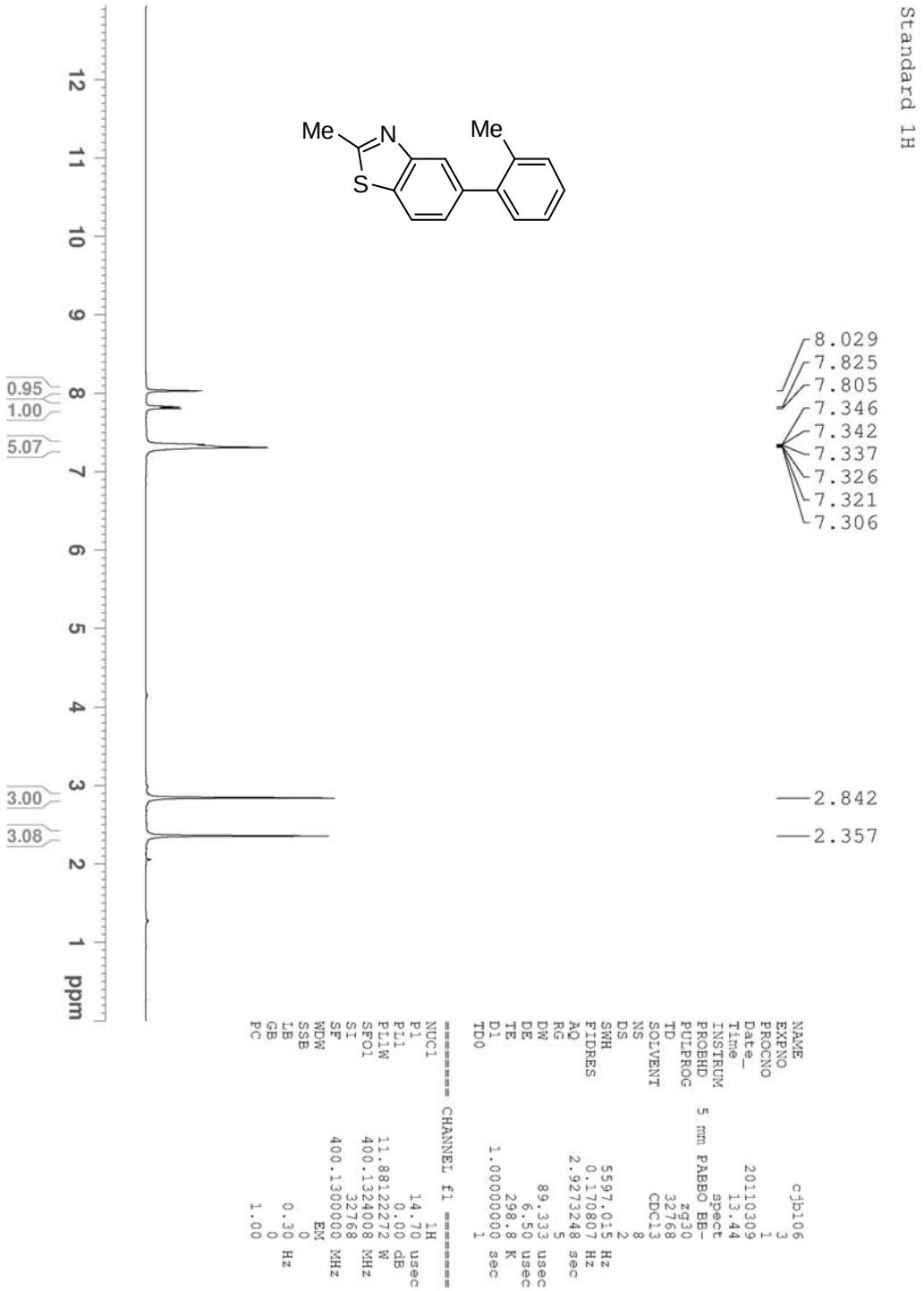


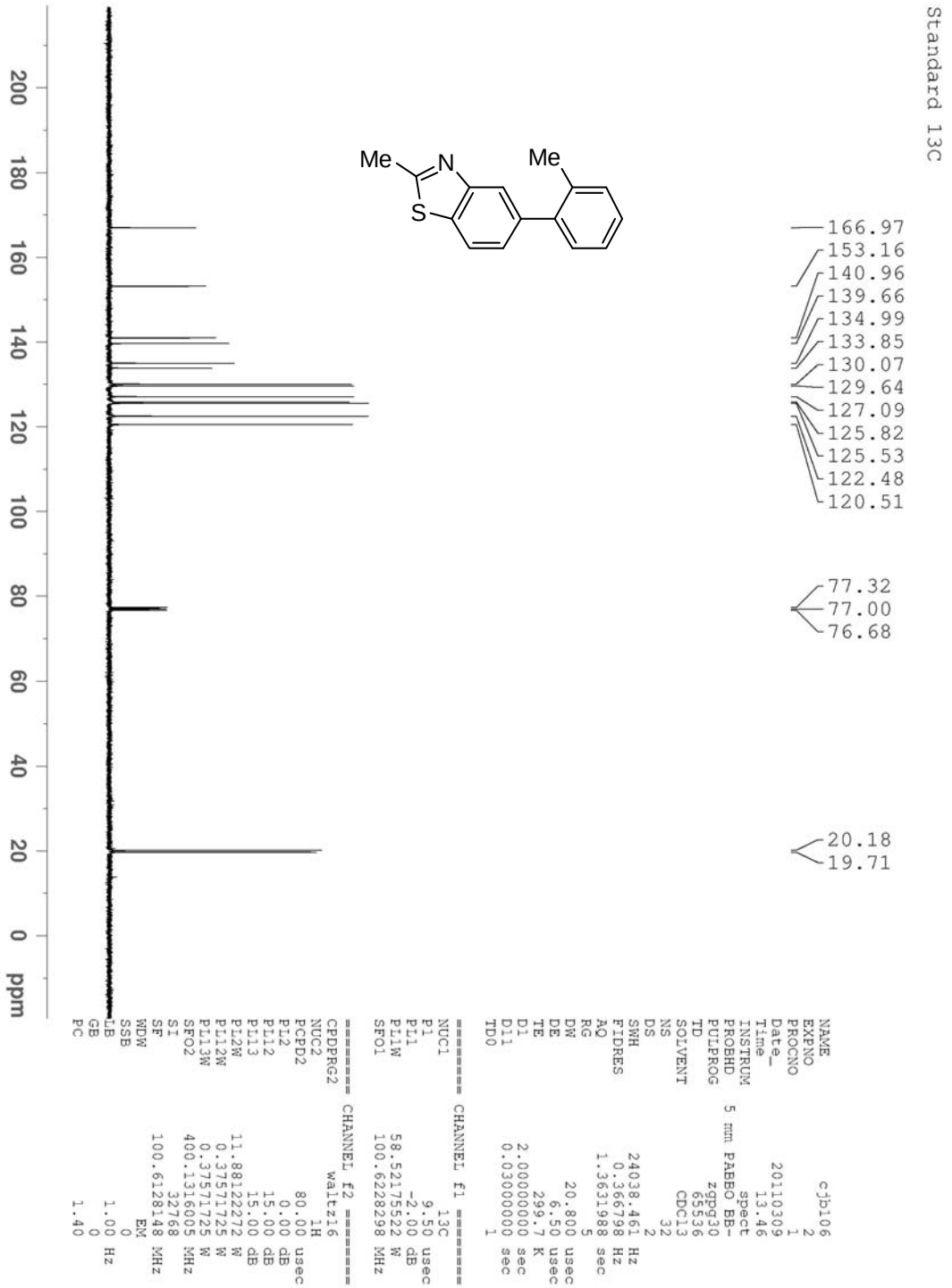

File :C:\msdchem\1\DATA\chun\bfac49.D
Operator : Seam
Acquired : 8 Mar 2011 14:03 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 7
Abundance
m/z-->
Scan 425 (3.813 min): bfac49.D\data.ms
EtO
O
276.1
202.1
231.1
248.1
261.1
101.1
88.1
115.5
51.1
63.1
75.1
126.1
139.1
152.1
163.1
176.1
189.1
217.1
295.0
314.8
331.1
343.1
355.0
388.9
405.0

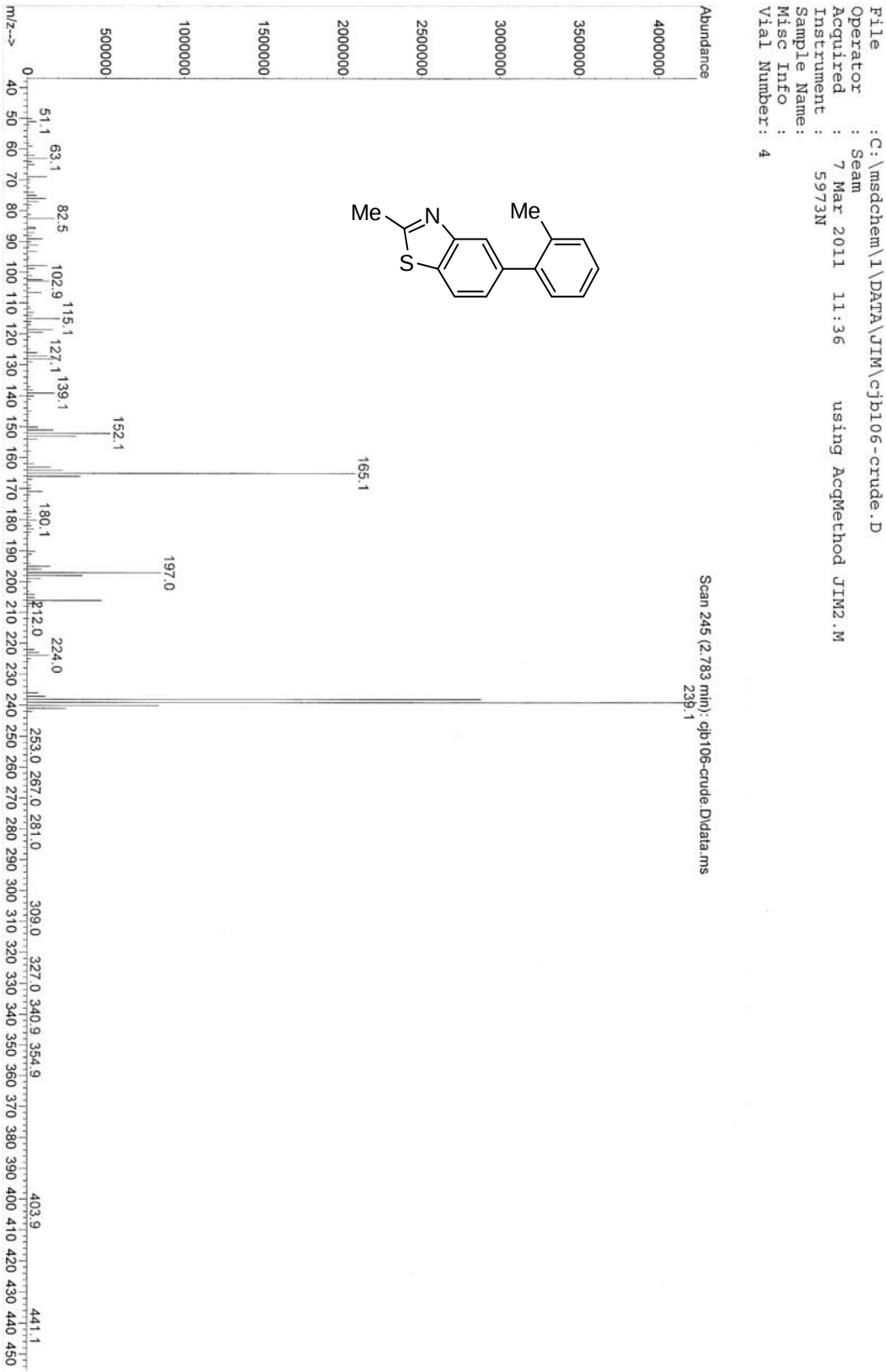

Standard 1H
8.082
7.988
7.969
7.798
7.776
7.620
7.616
7.610
7.606
7.597
7.591
7.348
7.317
7.314
7.297
7.294
7.053
7.033
6.085
1.01
3.15
1.05
2.05
0.97
1.07
0.99
2.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
O
O
NAME bfac085
EXPNO 3
PROCNO 1
Date_ 20110311
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

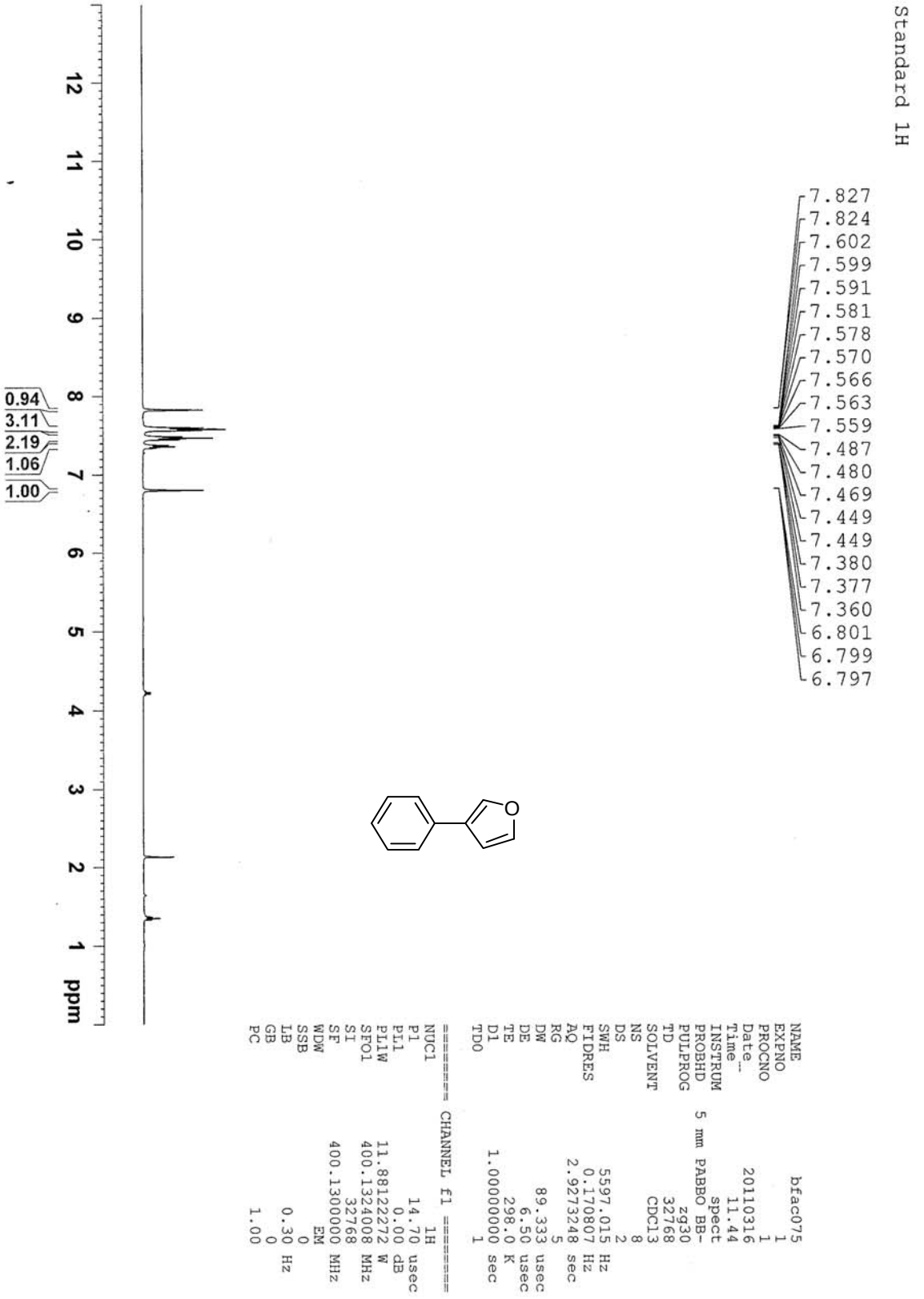

Standard 13C
148.12
147.05
138.09
135.29
133.59
132.33
128.25
127.98
127.51
126.16
125.64
125.33
125.14
120.81
108.52
107.73
101.05
77.32
77.00
76.69
O
O
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME bfac085
EXPNO 2
PROCNO 1
Date_ 20110311
Time 14.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127971 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

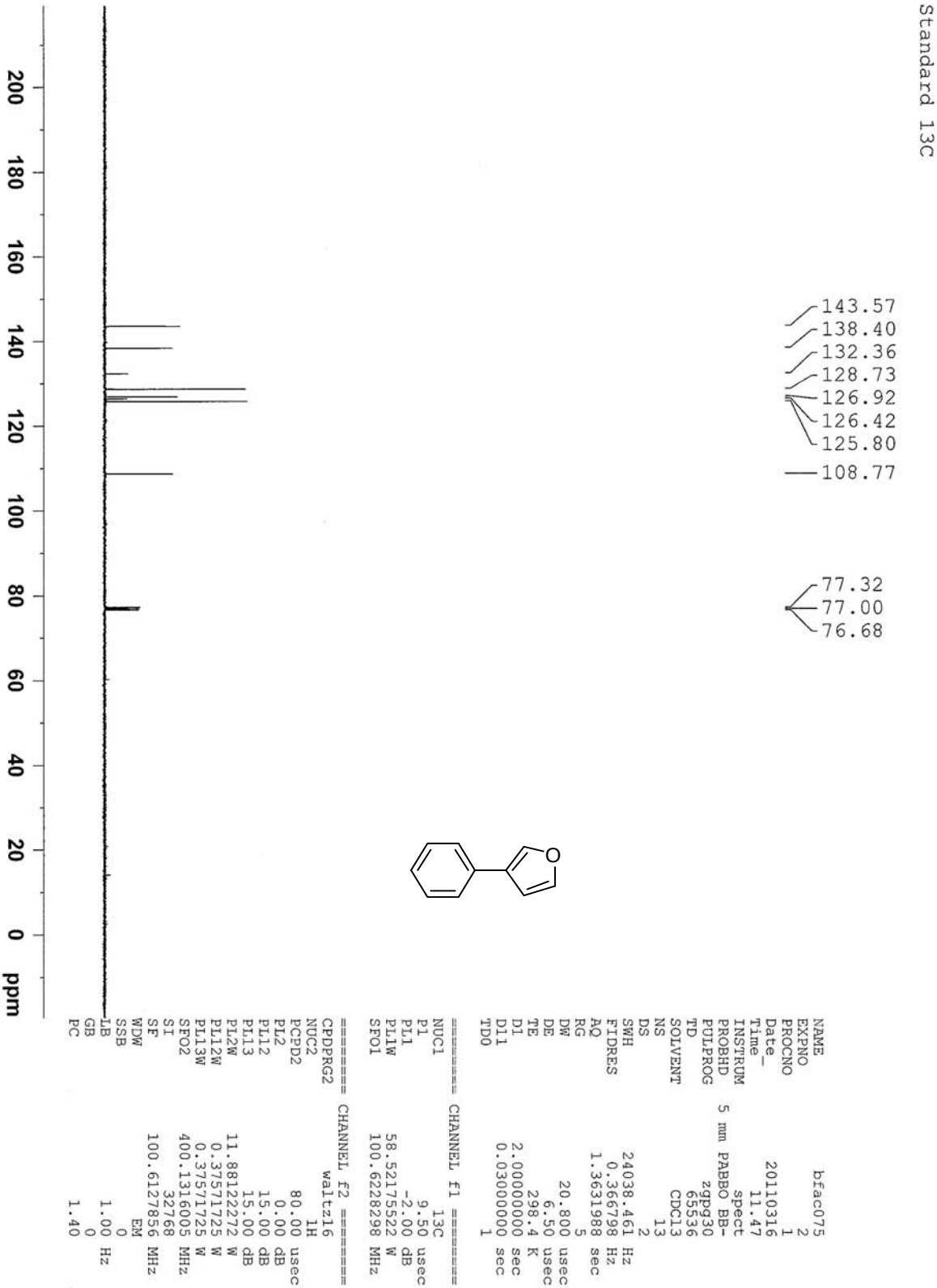

File :C:\msdchem\1\DATA\cmso\BFAC85.D
Operator : Seam
Acquired : 10 Mar 2011 19:44 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 6
Abundance
Scan 413 (3.744 min): BFAC85.D\data.ms
248.1
189.1
123.7
94.5
m/z-->


Standard 1H
Me
N
S
Me
8.029
7.825
7.805
7.346
7.342
7.337
7.326
7.321
7.306
2.842
2.357
0.95
1.00
5.07
3.00
3.08
12
11
10
9
8
7
6
5
4
3
2
1
ppm
NAME cjb106
EXPNO 3
PROCNO 1
Date_ 20110309
Time_ 13.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.927248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

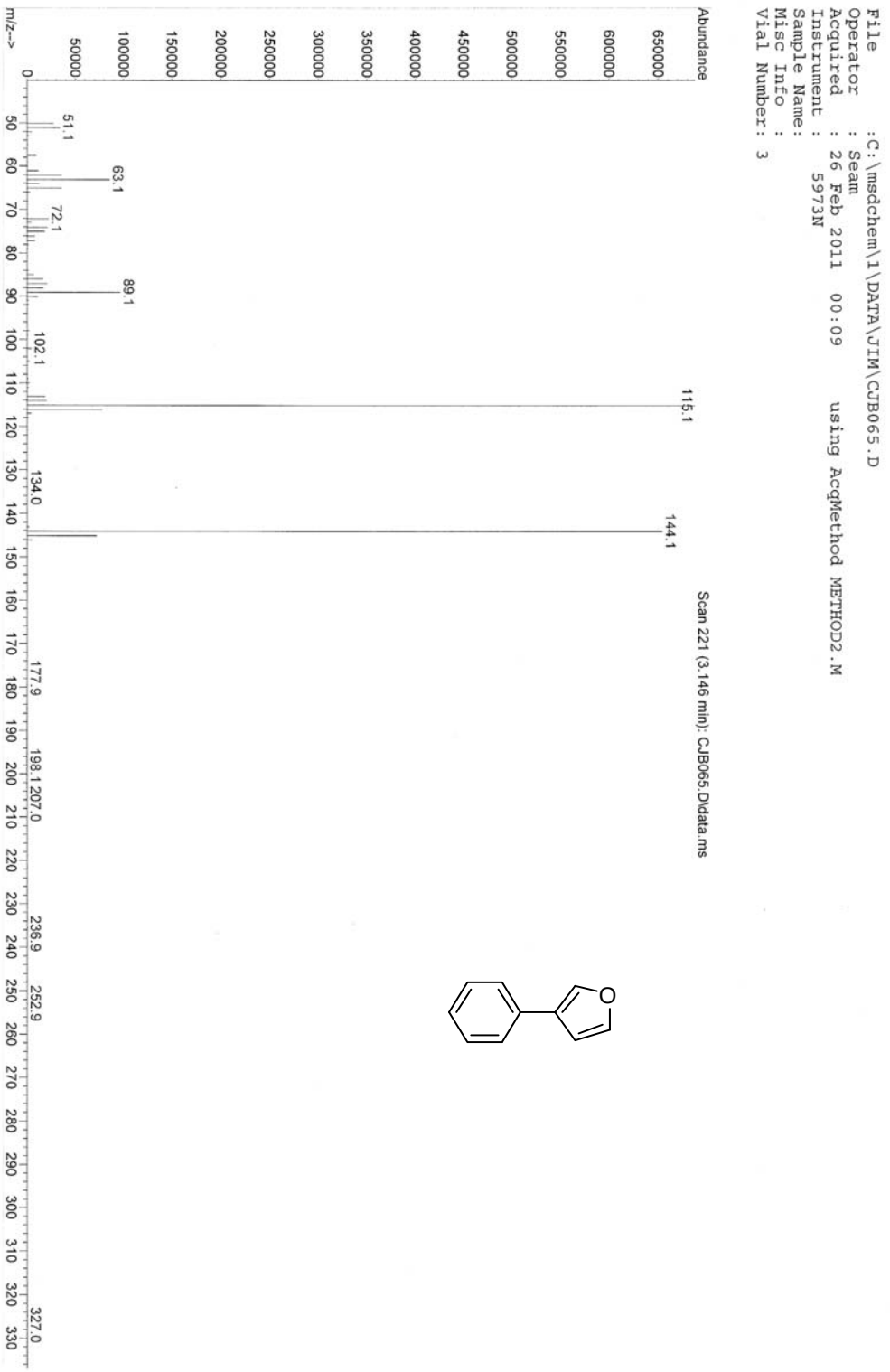

Standard 13C
Me
N
Me
S
166.97
153.16
140.96
139.66
134.99
133.85
130.07
129.64
127.09
125.82
125.53
122.48
120.51
77.32
77.00
76.68
20.18
19.71
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME cjb106
EXPNO 2
PROCNO 1
Date_ 20110309
Time_ 13.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128148 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

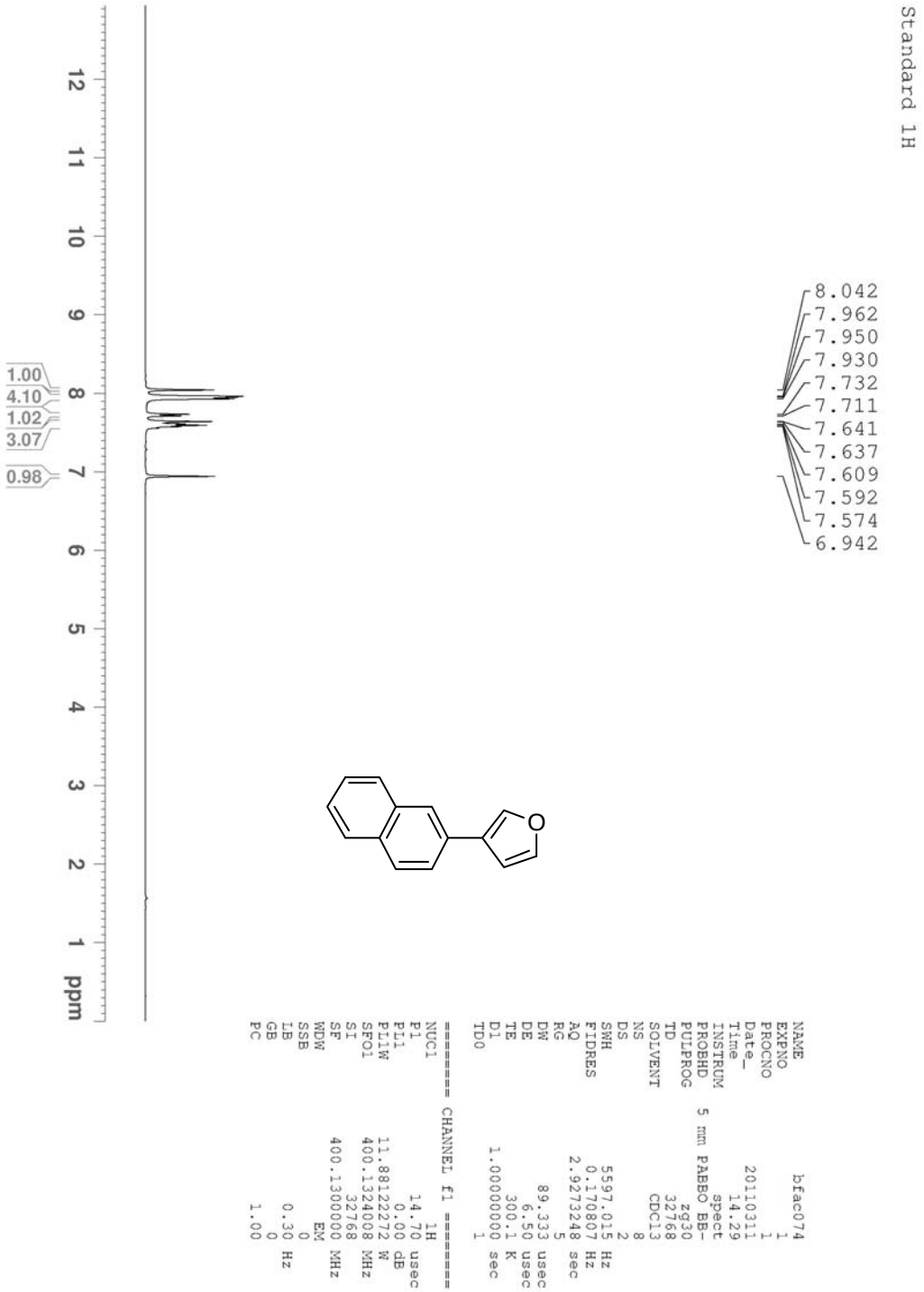

File :C:\msdchem\1\DATA\JIM\cjb106-crude.D
Operator : Seam
Acquired : 7 Mar 2011 11:36 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 4
Abundance
m/z-->
Scan 245 (2.783 min): cjb106-crude.D\data.ms
Me
N
S
Me
239.1
165.1
152.1
197.0
180.1
212.0
224.0
51.1
63.1
82.5
102.9
115.1
127.1
139.1
253.0
267.0
281.0
309.0
327.0
340.9
354.9
403.9
441.1

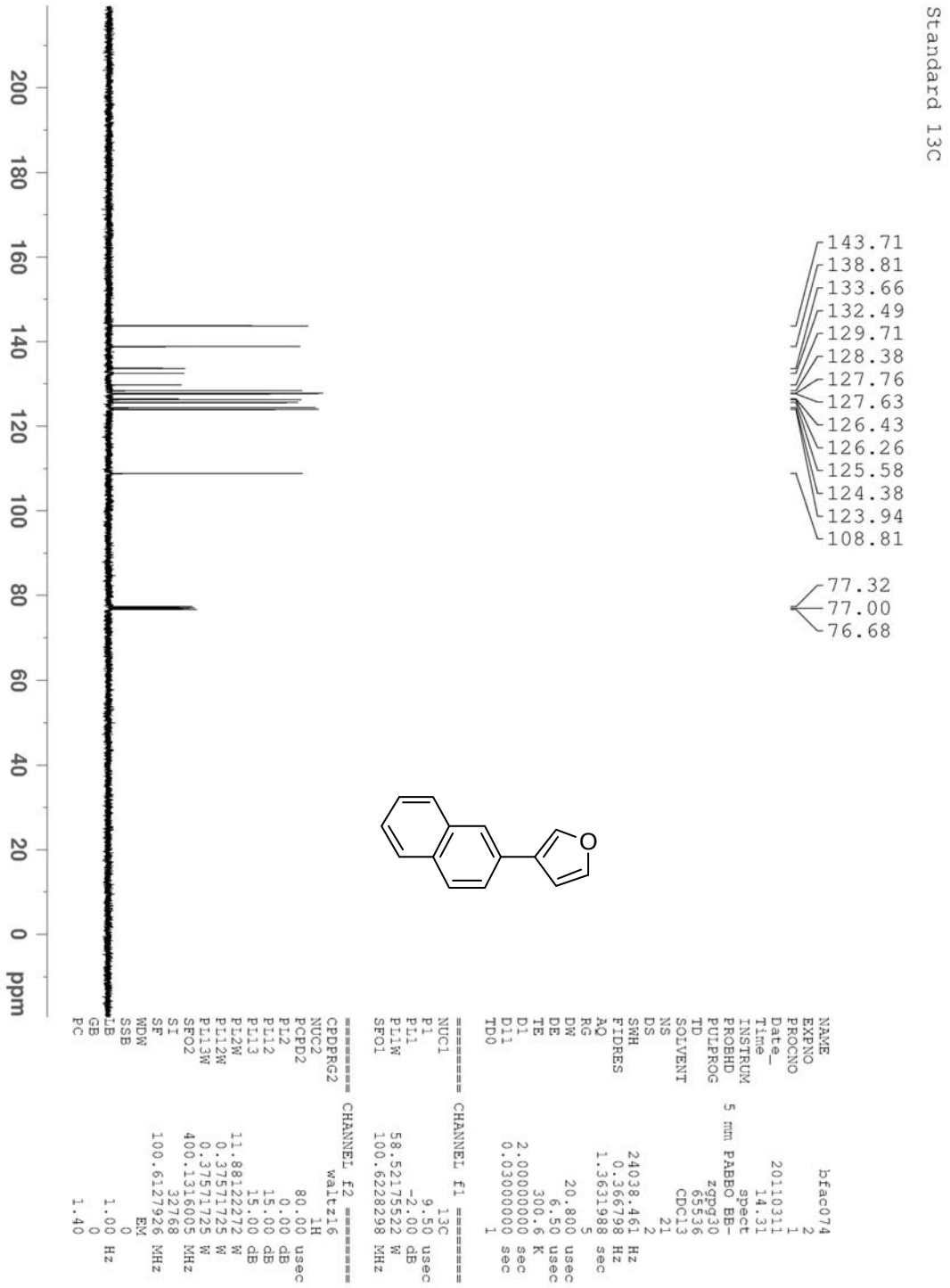

Standard 1H
7.827
7.824
7.602
7.599
7.591
7.581
7.578
7.570
7.566
7.563
7.559
7.487
7.480
7.469
7.449
7.449
7.380
7.377
7.360
6.801
6.799
6.797
0.94
3.11
2.19
1.06
1.00
12 11 10 9 8 7 6 5 4 3 2 1 ppm
O
NAME bfac075
EXPNO 1
PROCNO 1
Date_ 20110316
Time_ 11.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



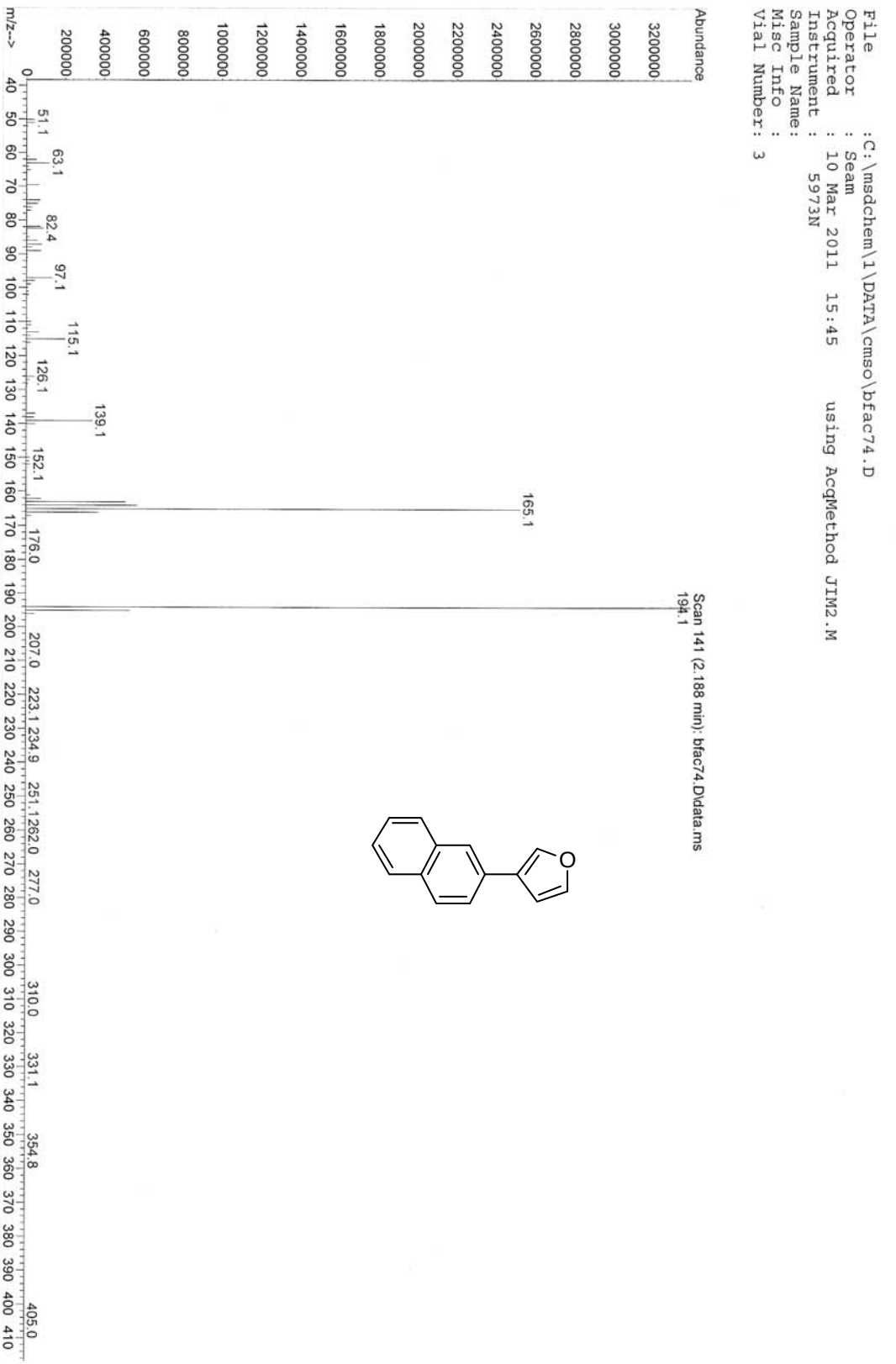

```
NAME                                    bfac075
EXPNO                                         2
PROCNO                                        1
Date_                               20110316
Time                                    11.47
INSTRUM                                  spect
PROBHD                  5 mm PABBO BB-
PULPROG                              zgpg30
TD                                    65536
SOLVENT                               CDCl3
NS                                       13
DS                                        2
SWH                                 24038.461 Hz
FIDRES                                0.366798 Hz
AQ                                    1.3631988 sec
RG                                        5
DW                                   20.800 usec
DE                                    6.50 usec
TE                                   298.4 K
D1                                    2.00000000 sec
D11                                   0.03000000 sec
TD0                                       1

======== CHANNEL f1 ========
NUC1                                    13C
P1                                    9.50 usec
PL1                                  -2.00 dB
PL1W                                58.52175522 W
SFO1                               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                             waltz16
NUC2                                    1H
PCPD2                                80.00 usec
PL2                                   0.00 dB
PL12                                 15.00 dB
PL13                                 15.00 dB
PL2W                                11.88122272 W
PL12W                                0.37571725 W
PL13W                                0.37571725 W
SFO2                               400.1316005 MHz
SI                                       32768
SF                                 100.6127856 MHz
WDW                                         EM
SSB                                          0
LB                                    1.00 Hz
GB                                           0
PC                                    1.40
```


File :C:\msdchem\1\DATA\JIM\CJB065.D
Operator : Seam
Acquired : 26 Feb 2011 00:09 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
m/z-->
Scan 221 (3.146 min): CJB065.D\data.ms
115.1
144.1
89.1
63.1
51.1
72.1
102.1
134.0
177.9
198.1
207.0
236.9
252.9
327.0
O


Standard 1H
8.042
7.962
7.950
7.930
7.732
7.711
7.641
7.637
7.609
7.592
7.574
6.942
1.00
4.10
1.02
3.07
0.98
12
11
10
9
8
7
6
5
4
3
2
1
ppm
O
NAME bfac074
EXPNO 1
PROCNO 1
Date_ 20110311
Time 14.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PLIW 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
NAME                                    bfac074
EXPNO                                         2
PROCNO                                        1
Date_                                  20110311
Time_                                     14.31
INSTRUM                                   spect
PROBHD     5 mm PABBO BB-
PULPROG                               zgpg30
TD                                         65536
SOLVENT                                  CDCl3
NS                                            21
DS                                             2
SWH                                    24038.461 Hz
FIDRES                                     0.366798 Hz
AQ                                         1.3631988 sec
RG                                             5
DW                                        20.800 usec
DE                                         6.50 usec
TE                                       300.6 K
D1                                         2.00000000 sec
D11                                        0.03000000 sec
TD0                                            1

======== CHANNEL f1 ========
NUC1                                         13C
P1                                         9.50 usec
PL1                                       -2.00 dB
PL1W                                   58.52175522 W
SFO1                                  100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                                  waltz16
NUC2                                         1H
PCPD2                                     80.00 usec
PL2                                        0.00 dB
PL12                                      15.00 dB
PL13                                      15.00 dB
PL2W                                   11.88122272 W
PL12W                                   0.37571725 W
PL13W                                   0.37571725 W
SFO2                                  400.1316005 MHz
SI                                         32768
SF                                    100.6127926 MHz
WDW                                           EM
SSB                                            0
LB                                         1.00 Hz
GB                                             0
PC                                         1.40
```

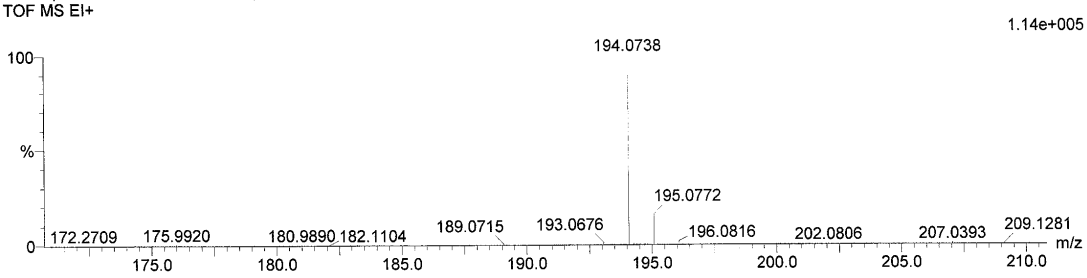

File :C:\msdchem\1\DATA\cmso\bfac74.D
Operator : Seam
Acquired : 10 Mar 2011 15:45 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 3
Abundance
Scan 141 (2.188 min): bfac74.D\data.ms
194.1
165.1
139.1
115.1
97.1
82.4
63.1
51.1
176.0
152.1
126.1
207.0
223.1
234.9
251.1
262.0
277.0
310.0
331.1
354.8
405.0
m/z-->

ental Composition Report

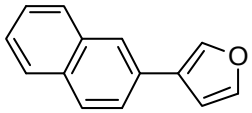
Page 1

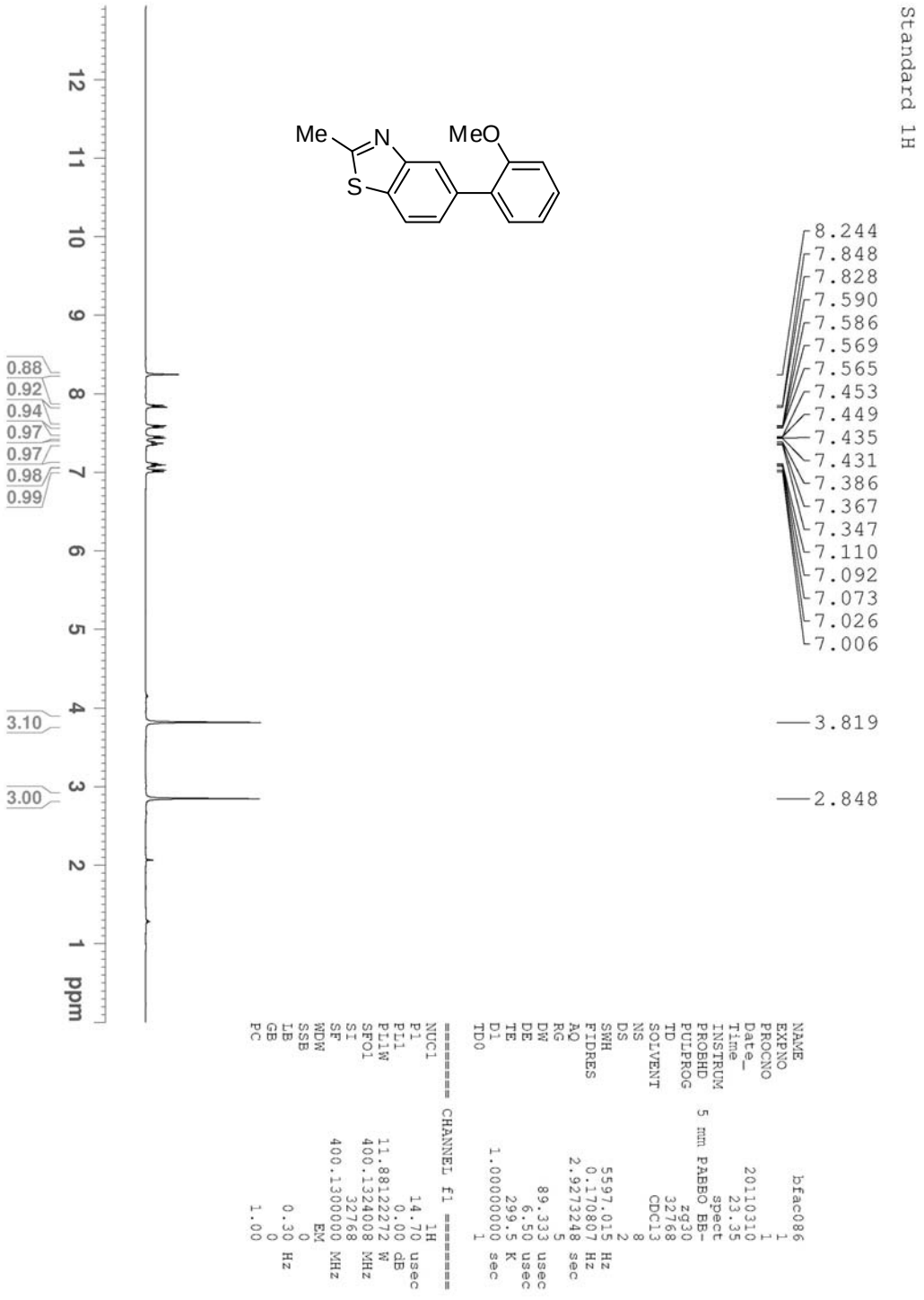
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

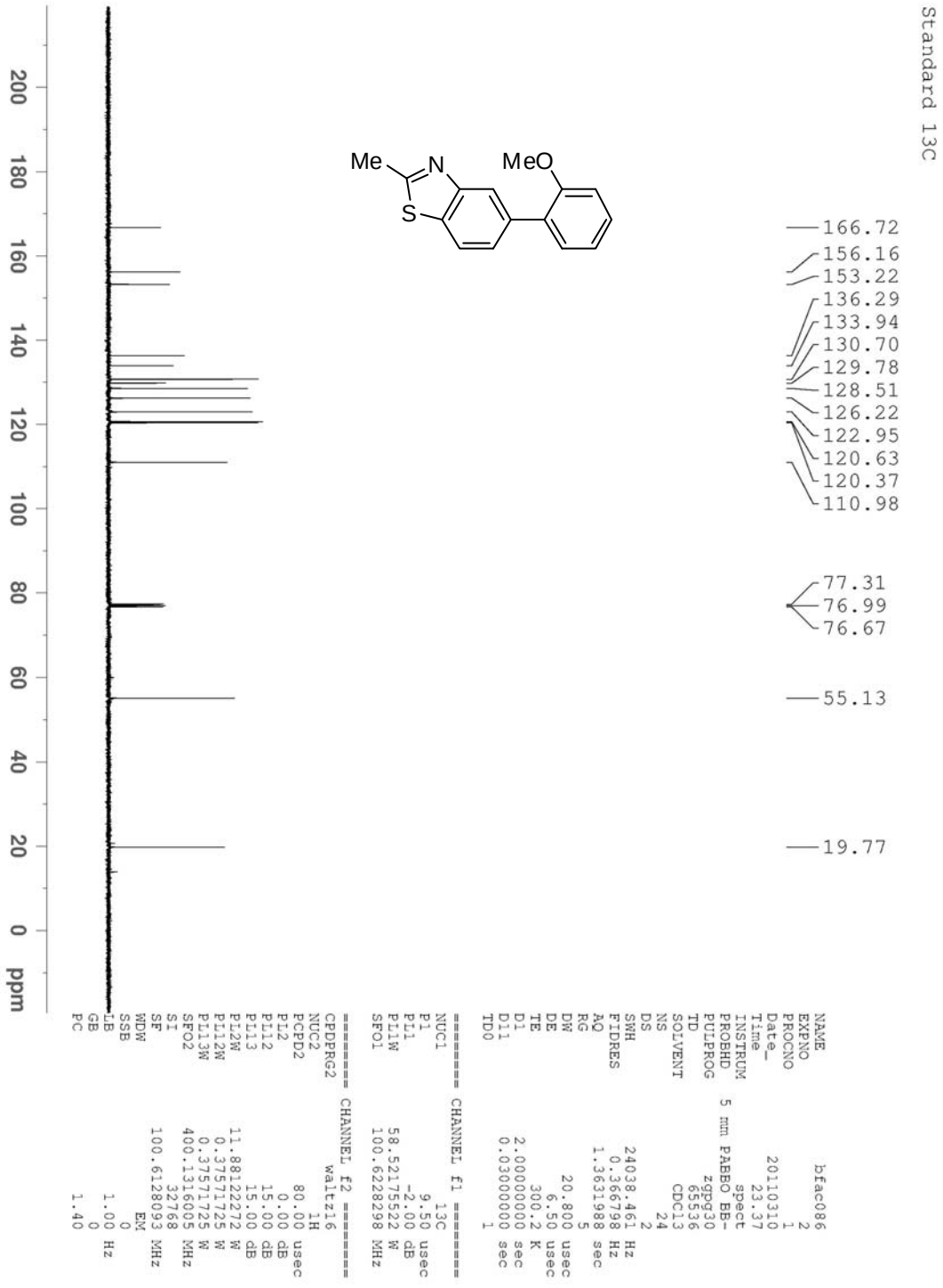
Monoisotopic Mass, Odd and Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-14 H: 0-11 O: 0-1 Na: 0-1 39K: 0-1
Kin-Dept-2903011 chan kin ho 40 (0.667) Cm (39:48)
TOF MS EI+

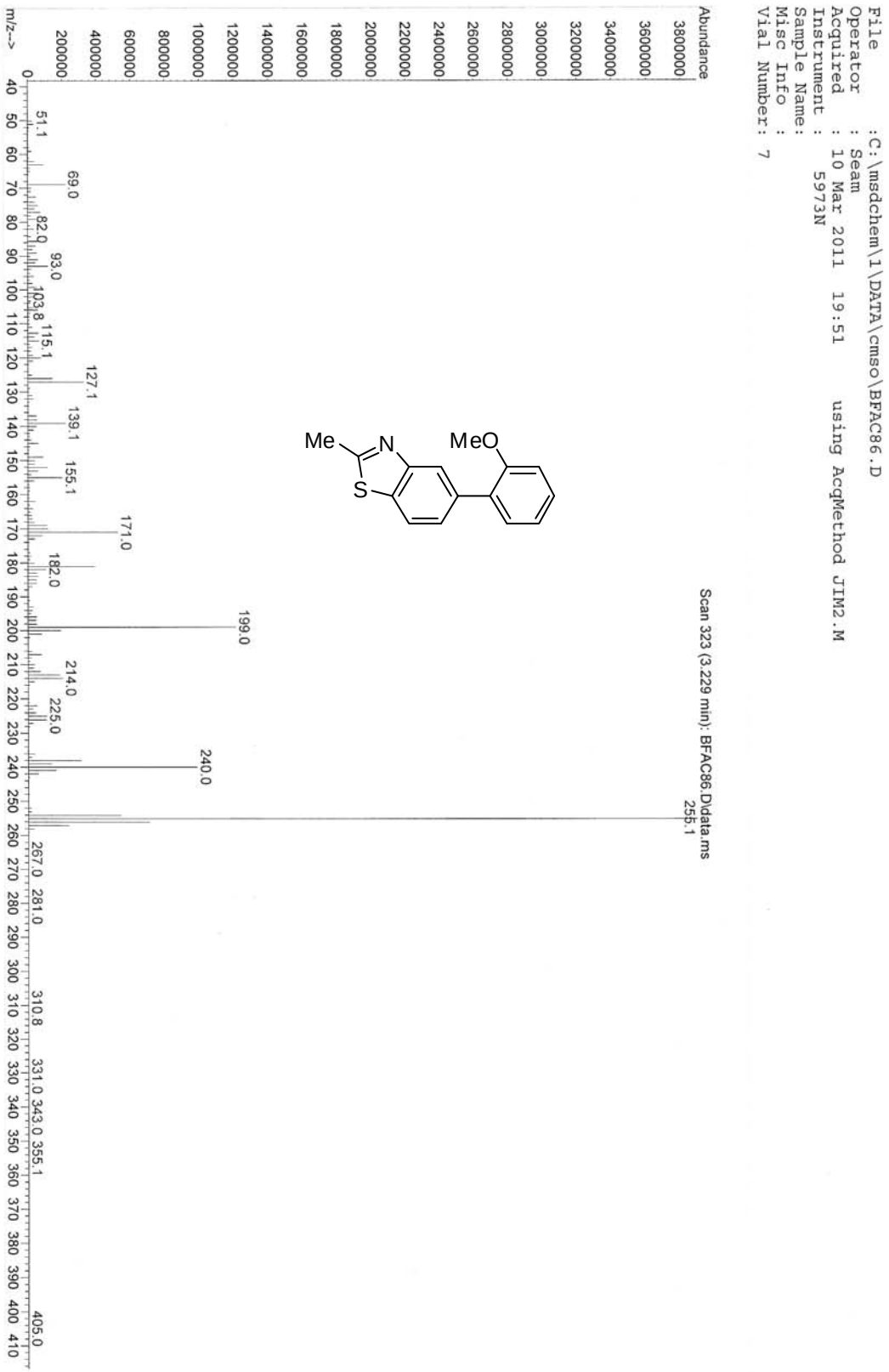


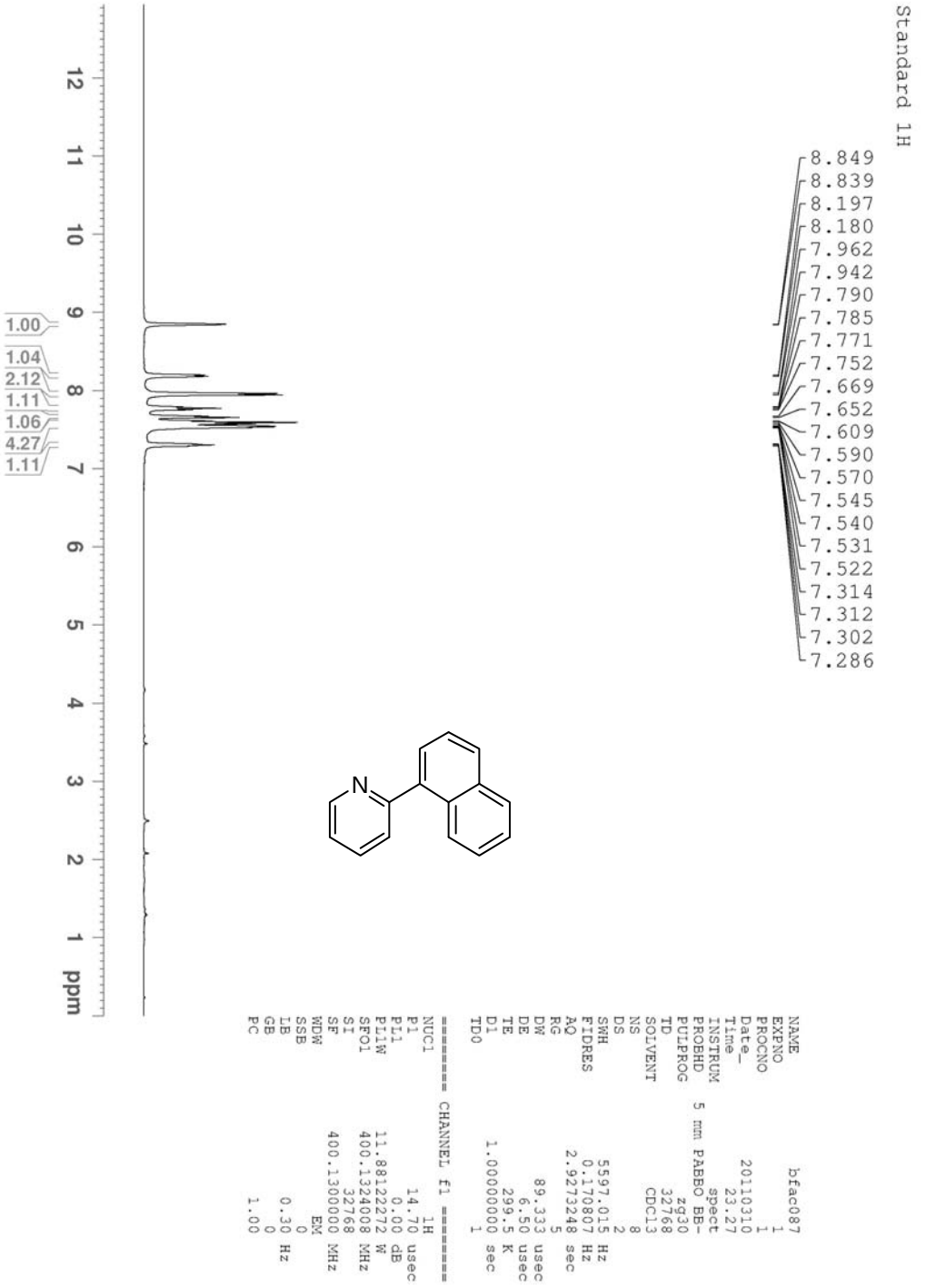
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
194.0738	194.0732	0.6	3.1	10.0	24.1	C14 H10 O

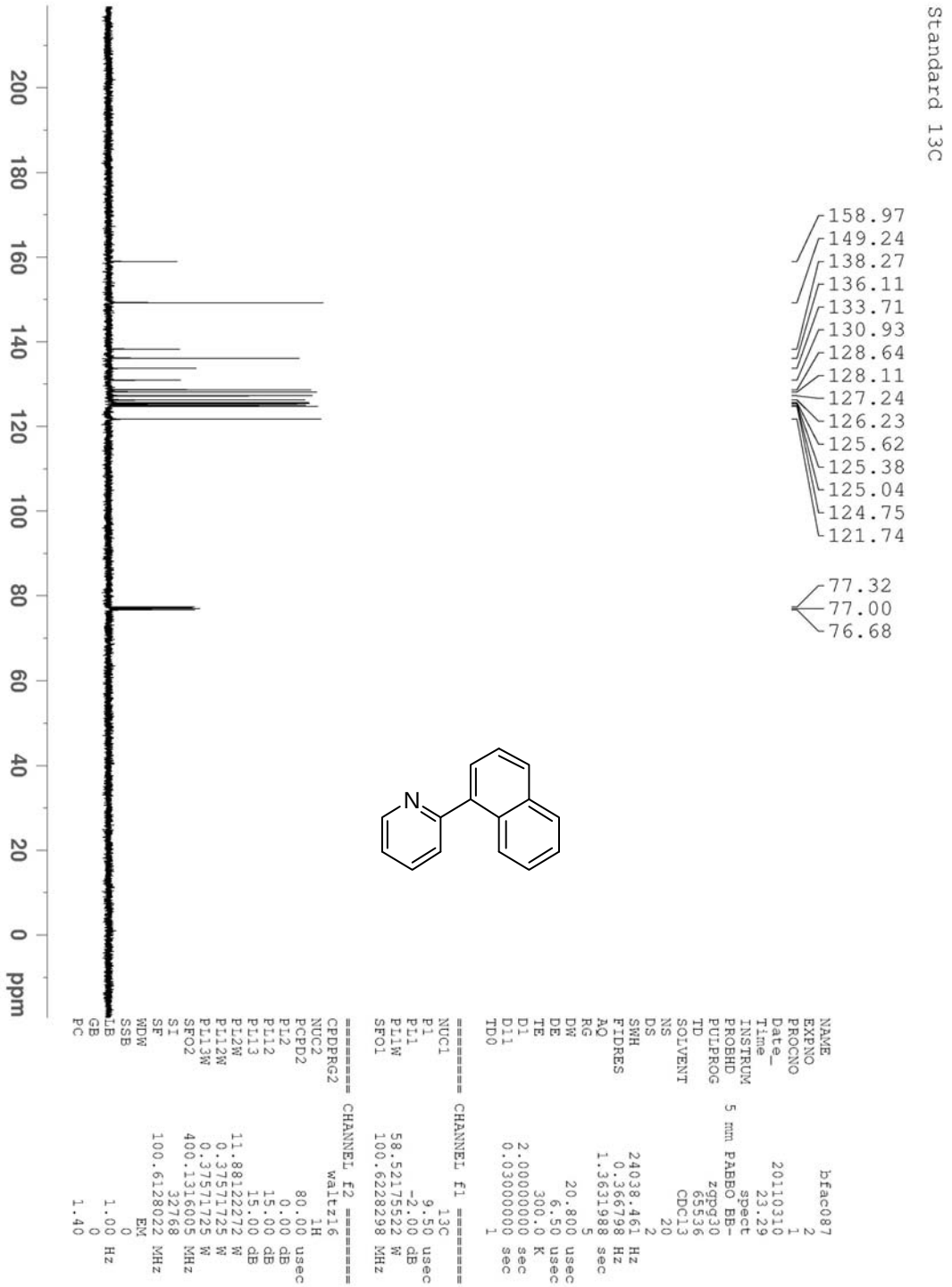


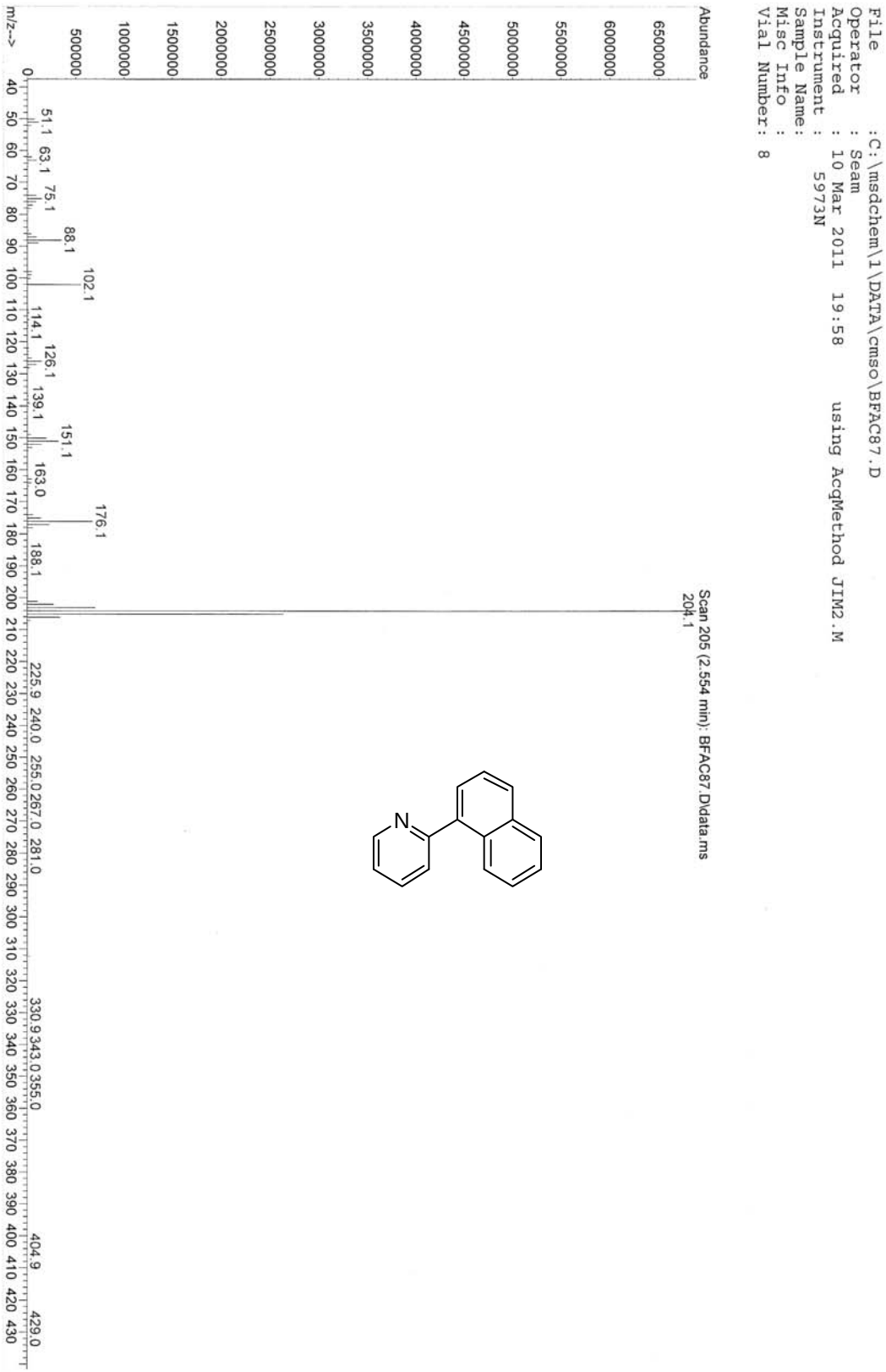

Standard 1H
Me
N
MeO
S
8.244
7.848
7.828
7.590
7.586
7.569
7.565
7.453
7.449
7.435
7.431
7.386
7.367
7.347
7.110
7.092
7.073
7.026
7.006
3.819
2.848
0.88
0.92
0.94
0.97
0.97
0.98
0.99
3.10
3.00
12 11 10 9 8 7 6 5 4 3 2 1 ppm
NAME bfac086
EXPNO 1
PROCNO 1
Date_ 20110310
Time_ 23.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

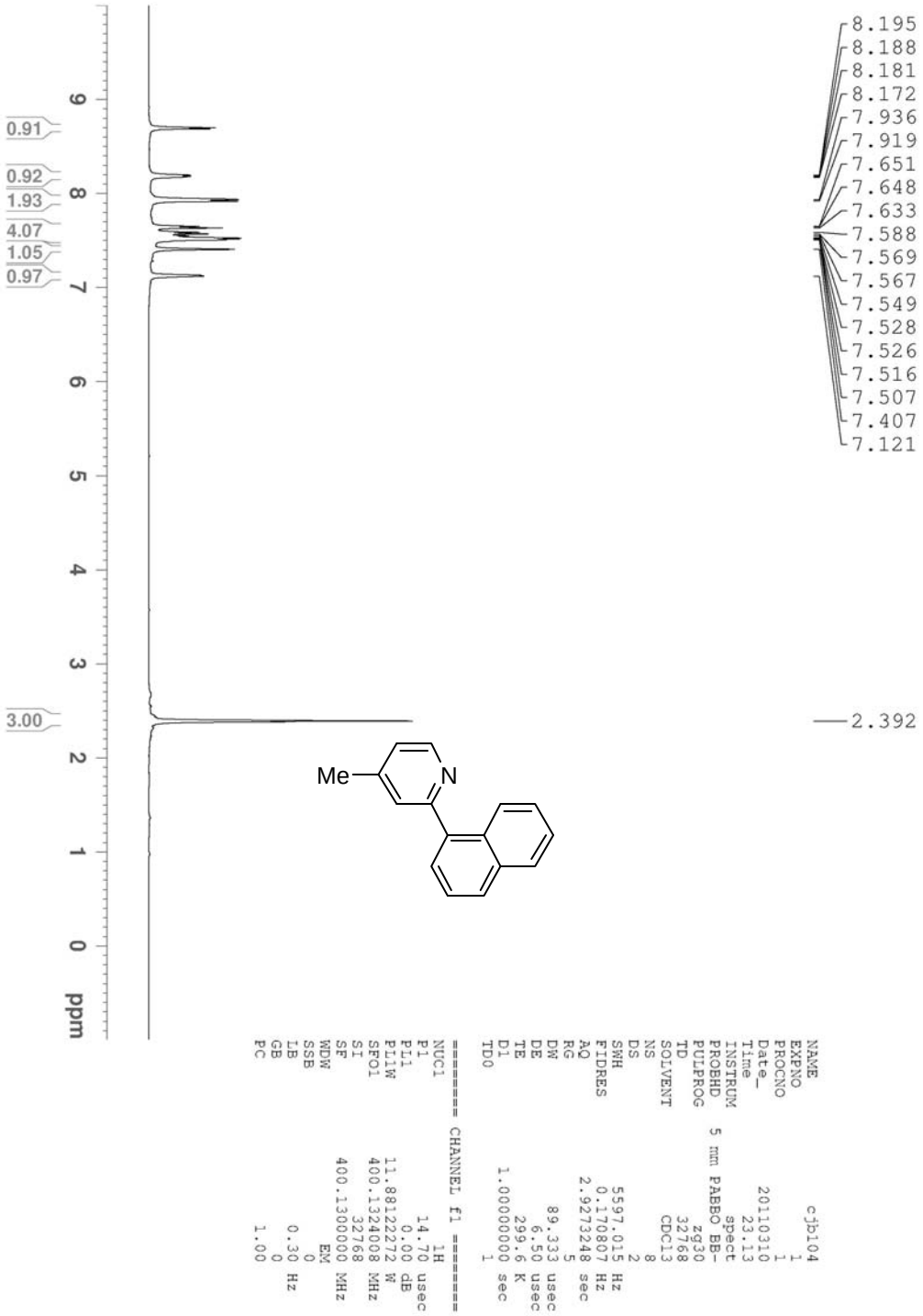

Standard 13C
Me
N
MeO
S
166.72
156.16
153.22
136.29
133.94
130.70
129.78
128.51
126.22
122.95
120.63
120.37
110.98
77.31
76.99
76.67
55.13
19.77
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME bfac086
EXPNO 2
PROCNO 1
Date_ 20110310
Time_ 23.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 24
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128093 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

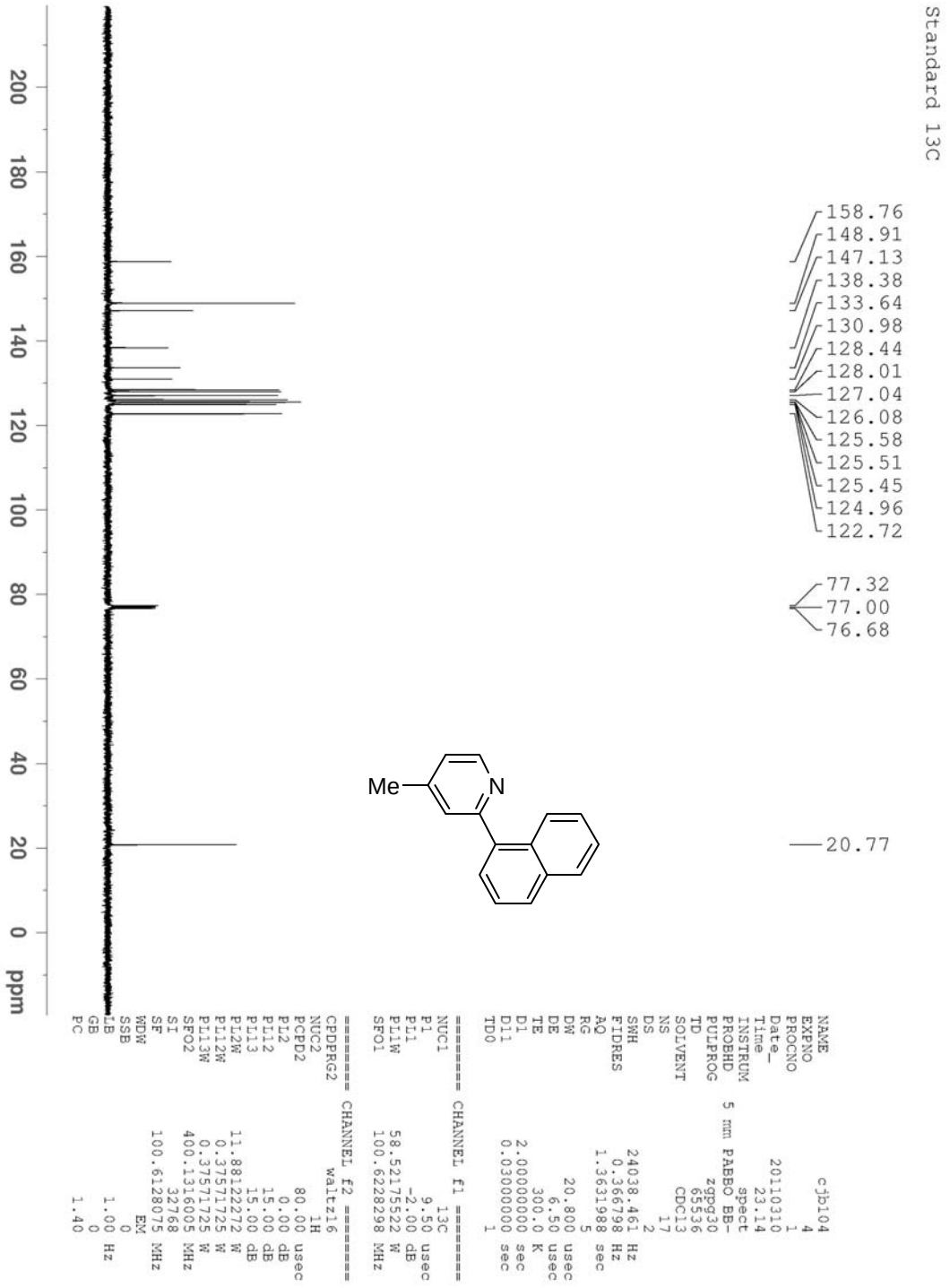

File :C:\msdchem\1\DATA\cmso\BFAC86.D
Operator : Seam
Acquired : 10 Mar 2011 19:51 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 7
Abundance
Scan 323 (3.229 min): BFAC86.D\data.ms
255.1
199.0
240.0
171.0
127.1
69.0
51.1
82.0
93.0
103.8
115.1
139.1
155.1
182.0
214.0
225.0
267.0
281.0
310.8
331.0
343.0
355.1
405.0
m/z-->
Me
N
MeO
S

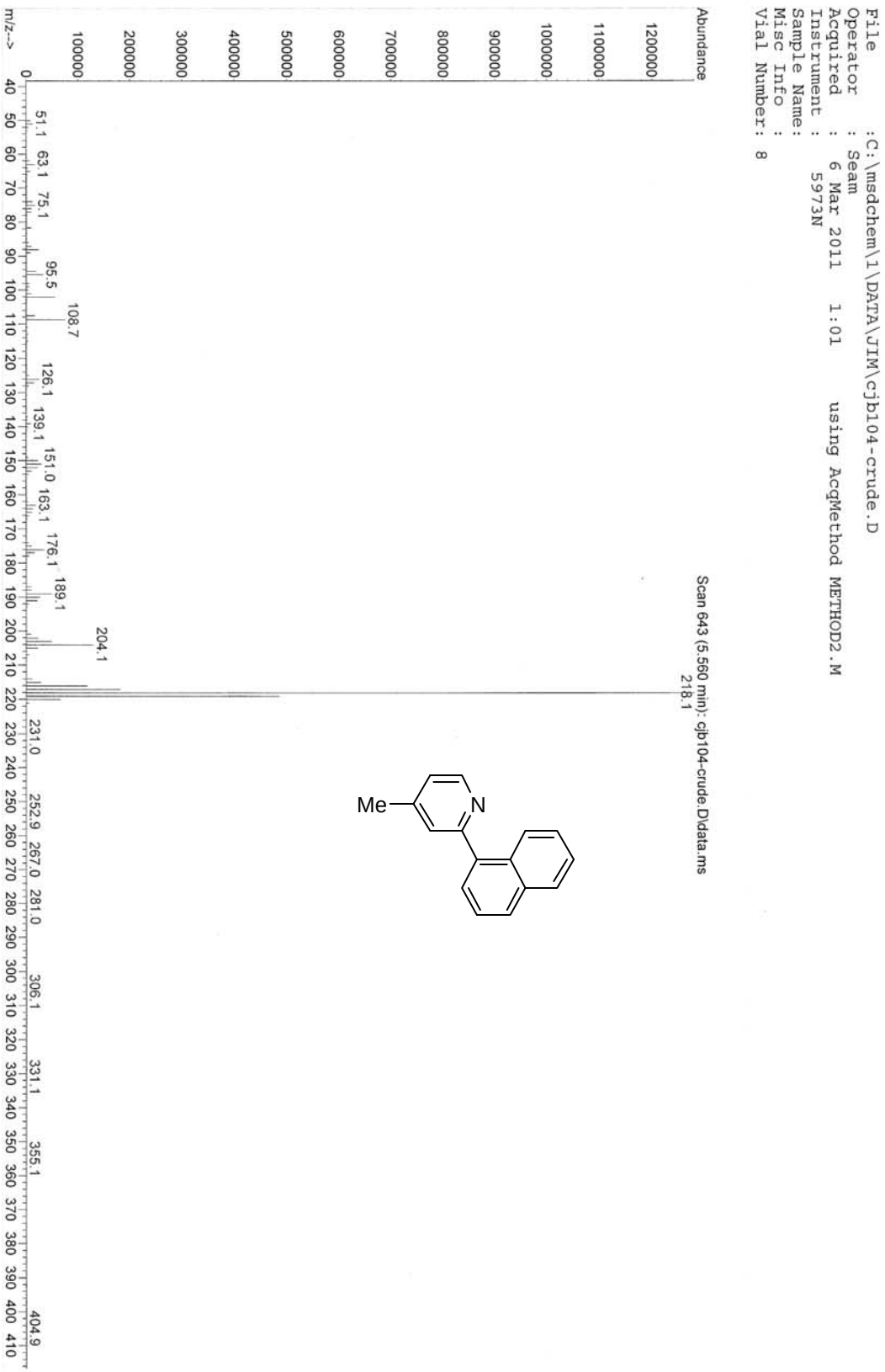

Standard 1H
8.849
8.839
8.197
8.180
7.962
7.942
7.790
7.785
7.771
7.752
7.669
7.652
7.609
7.590
7.570
7.545
7.540
7.531
7.522
7.314
7.312
7.302
7.286
1.00
1.04
2.12
1.11
1.06
4.27
1.11
12 11 10 9 8 7 6 5 4 3 2 1 ppm
N
NAME bfac087
EXPNO 1
PROCNO 1
Date_ 20110310
Time 23.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


Standard 13C
158.97
149.24
138.27
136.11
133.71
130.93
128.64
128.11
127.24
126.23
125.62
125.38
125.04
124.75
121.74
77.32
77.00
76.68
N
200
180
160
140
120
100
80
60
40
20
0
ppm
NAME bfac087
EXPNO 2
PROCNO 1
Date_ 20110310
Time_ 23.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 20
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 5
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128022 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


File :C:\msdchem\1\DATA\cmso\BFAC87.D
Operator : Seam
Acquired : 10 Mar 2011 19:58 using AcqMethod JIM2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 8
Abundance
Scan 205 (2.554 min): BFAC87.D\data.ms
204.1
m/z-->


8.195
8.188
8.181
8.172
7.936
7.919
7.651
7.648
7.633
7.588
7.569
7.567
7.549
7.528
7.526
7.516
7.507
7.407
7.121
2.392
0.91
0.92
1.93
4.07
1.05
0.97
3.00
ppm
Me
N
NAME cjb104
EXPNO 1
PROCNO 1
Date_ 20110310
Time 23.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 5597.015 Hz
FIDRES 0.170807 Hz
AQ 2.9273248 sec
RG 5
DW 89.333 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




File :C:\msdchem\1\DATA\JIM\cjb104-crude.D
Operator : Seam
Acquired : 6 Mar 2011 1:01 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 8
Abundance
Scan 643 (5.560 min): cjb104-crude.D\data.ms
218.1
204.1
108.7
95.5
51.1
63.1
75.1
126.1
139.1
151.0
163.1
176.1
189.1
231.0
252.9
267.0
281.0
306.1
331.1
355.1
404.9
m/z-->
Me
N

10. References.

1. Armarego, W. L. F.; Perrin, D. D., In *Purification of Laboratory Chemicals*, 4th, Ed. Butterworth-Heinemann: Oxford UK: 1996.
2. Reddy, K. R.; Krishna, G. G., Palladium-imidazole derivatives as highly active catalysts for Heck reactions. *Tetrahedron Lett* **2005,** *46* (4), 661-663.
3. Letsinger, R. L.; MacLean, D. B., Organoboron Compounds. XVI. Coöperative Functional Group Effects in Reactions of Boronoarylbenzimidazoles. *Journal of the American Chemical Society* **1963,** *85* (15), 2230-2236.
4. Andrus, M. B.; Song, C., *Org. Lett.* **2001,** *3*, 3761-3764.
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