

Supporting Information

Suzuki-Miyaura Coupling of Aryl Tosylates Catalyzed by an Array of Indolyl Phosphine-Palladium Catalysts

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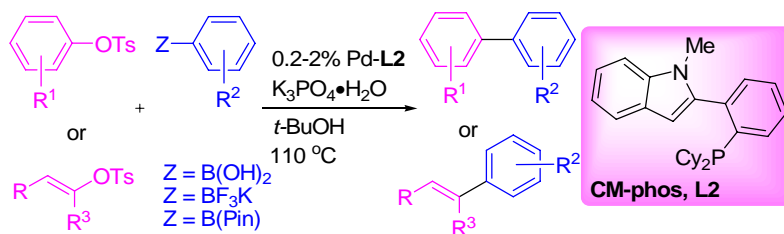


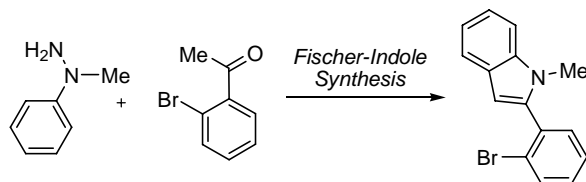
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1. General considerations.

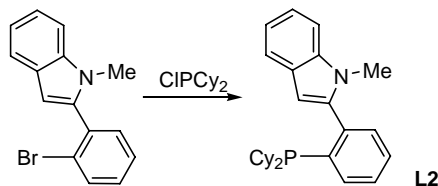
Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All Suzuki-Miyaura reactions were performed in resealable screw cap schlenk flask (approx. 20 mL volume) in the presence of Teflon coated magnetic stirrer bar (3 mm \times 8 mm). Toluene and tetrahydrofuran (THF) were distilled from sodium and sodium benzophenone ketyl under nitrogen, respectively.¹ *tert*-Butanol was distilled from sodium under nitrogen.¹ Chlorodiphenylphosphine (Tech grade) was distilled under vacuum prior to use. Most commercially available arylboronic acids were used as received. Some arylboronic acids may require further recrystallization depending on the received conditions. 1-Naphthylboronic acid and 2,4-di-*tert*-butyl-6-methoxyphenylboronic acid were synthesized according to literature methods (see section 4). New bottle of *n*-butyllithium was used (*Note*: since the concentration of *n*-BuLi from old bottle may vary, we recommend to perform a titration prior to use). K₃PO₄•H₂O was purchased directly from commercial supplier and used without grinding. Thin layer chromatography was performed on precoated silica gel 60 F₂₅₄ plates. Silica gel (70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected instrument. ¹H NMR spectra were recorded on a 400 MHz spectrometer. Spectra were referenced internally to the residual proton resonance in CDCl₃ (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. ¹³C NMR spectra were referenced to CDCl₃ (δ 77.0 ppm, the middle peak). ³¹P NMR spectra were referenced to 85% H₃PO₄ externally. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a ESIMS mass spectrometer. GC-MS analysis was conducted on a GCD system using a column with dimension of 30 m \times 0.25 mm. The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from GC-FID system. All yields reported refer to isolated yield of compounds estimated to be greater than 95% purity as determined by capillary gas chromatography (GC) or ¹H NMR. Compounds described in the literature were characterized by comparison of their ¹H, and/or ¹³C 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. **L4-L8** were prepared according to our previous publication (*Org. Lett.* **2007**, 9, 2795).

2. Preparation of indolyl phosphine ligands L1-L3 and L9



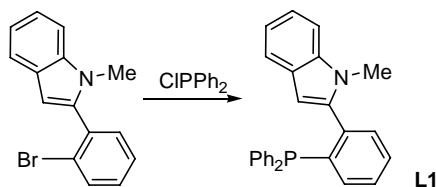
General procedure for Fischer-indole synthesis: 2'-Bromoacetophenone (1.31 mL, 10 mmol) was mixed with *N*-methylphenylhydrazine (1.3 mL, 11 mmol) in phosphoric acid (5 mL) and stirred at room temperature for 30 min. PPA (25-30 g) was added to the mixture and an exothermic reaction ensued whereupon the mixture was heated slowly to 120 °C and kept at this temperature for 1 h. The mixture was poured into ice water and then extracted with Et₂O (3 × ~150 mL). The organic phases were combined, dried over Na₂SO₄ and concentrated under reduced pressure. The crude product was filtered through a short silica pad (3 × ~10 cm) and washed with hexane then EA/Hexane (1:9). The solution was evaporated to yield a light yellow solid. Small amount of cold hexane was used to further wash the product. The product was then dried under vacuum to afford *N*-methyl-2-(2'-bromophenyl)indole (2.35 g, 75%) as a light yellow solid. Melting point. 85.5-87.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 3.61 (s, 3H), 6.56 (s, 1H), 7.20-7.45 (m, 6H), 7.70-7.75 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 30.5, 102.0, 109.4, 119.7, 120.6, 121.6, 125.0, 127.1, 127.5 130.0, 132.6 132.7, 134.1, 137.1, 139.5; IR (cm⁻¹) 3049.43, 2933.63, 1536.35, 1457.76, 1431.08, 1382.94, 1337.55, 1309.58, 1164.78, 1061.55, 1023.56, 791.60, 749.44, 662.83, 578.63, 536.74, 454.92; MS (EI): *m/z* (relative intensity) 285 (M⁺, 100), 204 (75), 190 (10), 178 (20); HRMS: calcd. for C₁₅H₁₂BrNH⁺: 286.0231, found 286.0280.

N-Methyl-2-(2'- Dicyclohexylphosphinophenyl)indole (L2)



General procedure for ligand synthesis: *N*-methyl-2-(2'-bromophenyl)indole (2.2 g, 7.7 mmol) was dissolved in freshly distilled THF (25 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 °C in dry ice/acetone bath. Titrated *n*-BuLi (8.47 mmol) was added dropwise by syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (1.87 mL, 8.47 mmol) in THF (5 mL) was added. The reaction was allowed to warm to room temperature and stirred overnight. Solvent was removed under reduced pressure. After the solvent was removed under vacuum, the product was successively washed with cold MeOH/EtOH mixture. The product was then dried under vacuum. White solid of *N*-methyl-2-(2'-dicyclohexylphosphinophenyl)indole (**L2**) (2.75g, 88%) were obtained. Melting point. 171.9-174.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 1.20-1.80 (m, 22H), 3.53 (s, 3H), 6.44 (s, 1H), 7.15(t, *J*=7.4 Hz, 1H), 7.24-7.27 (m, 1H), 7.36-7.50 (m, 4H), 7.66 (d, *J*=7.7 Hz, 2H); ¹³C NMR (100MHz, CDCl₃) δ 25.5, 26.2, 27.1, 28.9, 29.3, 29.5, 30.1, 30.7, 103.2, 109.3, 119.3, 120.2 121.0, 127.6, 127.8, 128.0, 128.2, 128.4, 131.8, 131.9, 132.7, 136.6 (unresolved complex C-P splittings were observed); ³¹P NMR (162 MHz, C₆D₆) δ -9.87; IR (cm⁻¹) 2422.67, 3050.84, 2924.05, 2846.58, 1445.74, 1384.98, 1338.55, 1309.68, 1264.17, 1123.17, 1001.01, 886.58, 848.87, 769.86, 746.53, 523.77; MS (EI): *m/z* (relative intensity) 403(M⁺, 25), 348 (5), 321 (30), 238 (100), 222 (30), 207 (20); HRMS: calcd. for C₂₇H₃₄NP: 403.2423, found 403.2414.

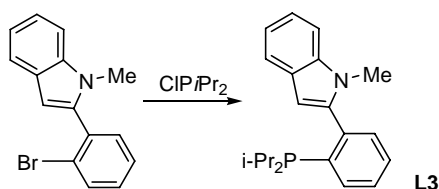
***N*-Methyl-2-(2'-Diphenylphosphinophenyl)indole (L1)**



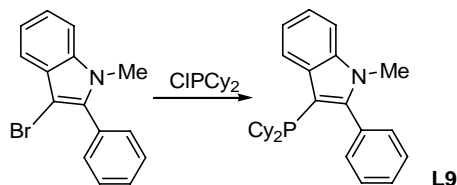
General procedures for the synthesis of ligand **L2** were followed. *N*-Methyl-2-(2'-bromophenyl)indole (1.89 g, 6.6 mmol), *n*-BuLi (6.9 mmol), chlorodiphenylphosphine (1.25 mL, 7.0 mmol) were used to afford *N*-methyl-2-(2'-diphenylphosphinophenyl)indole (**L1**) (1.65 g, 64%) as a white crystal. Melting point. 122.0-125.5 °C; ¹H NMR (400 MHz, C₆D₆) δ 3.18 (s, 3H), 6.55 (s, 1H), 7.08-7.66 (m, 18H); ¹³C NMR (100 MHz, CD₂Cl₂) δ 30.5, 103.7, 103.8, 109.5, 119.5, 120.4, 121.5, 127.6, 128.5 (overlapped), 128.6, 128.7, 128.8, 131.6 (overlapped), 133.7,

133.8, 133.9, 137.2, 137.4, 137.5, 139.6 (overlapped) (unresolved complex C-P splittings were observed); ^{31}P NMR (162 MHz, C_6D_6) δ -12.02; IR (cm^{-1}) 3446.06, 3048.19, 2931.48, 1582.52, 1461.53, 1429.92, 1377.43, 1359.35, 1336.25, 1308.54, 1235.94, 1176.72, 1123.94, 1093.80, 1025.26, 999.97, 924.13, 943.98, 769.18, 745.33, 695.27, 539.41, 495.26; MS (EI): m/z (relative intensity) 391 (M^+ , 100), 376 (50), 314 (30), 298 (27), 281 (5), 261 (5), 236 (50), 222 (40), 204 (25); HRMS: calcd. for $\text{C}_{27}\text{H}_{22}\text{NPH}^+$: 392.1568, found 392.1579.

***N*-Methyl-2-(2'-Diisopropylphosphinophenyl)indole (**L3**)**



General procedures for the synthesis of ligand **L2** were followed. *N*-Methyl-2-(2'-bromophenyl)indole (1.66 g, 5.8 mmol), *n*-BuLi (6.38 mmol), chlorodiisopropylphosphine (1.03 mL, 6.4 mmol) were used to afford *N*-methyl-2-(2'-diisopropylphosphinophenyl)indole (**L3**) (1.41 g, 75%) as white crystal. Melting point. 146.1-147.8 °C; ^1H NMR (400 MHz, CD_2Cl_2) δ 1.06-1.15 (m, 12H), 1.80-2.80 (m, 2H), 3.61 (s, 3H), 6.52 (s, 1H), 7.23-7.77 (m, 8H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 20.0, 20.2, 23.3, 25.7 (overlapped), 30.8 (overlapped), 103.3 (overlapped), 109.4, 119.4, 120.1, 121.1, 127.8, 128.2, 128.4, 131.7, 131.8, 132.5, 132.6, 136.7, 137.9, 138.1, 140.6, 140.9, 141.5, 141.5 (overlapped) (unresolved complex C-P splitting was observed); ^{31}P NMR (162 MHz, CD_2Cl_2) δ -1.29; IR (cm^{-1}) 3445.89, 3050.50, 2941.77, 2860.55, 1542.40, 1454.90, 1420.35, 1380.67, 1336.26, 1309.58, 1237.42, 1119.75, 1005.64, 880.09, 778.80, 747.64, 676.90, 653.14, 606.16, 583.14, 531.39, 459.25; MS (EI): m/z (relative intensity) 323 (M^+ , 20), 280 (100), 236 (40), 222 (30), 204 (5); HRMS: calcd. for $\text{C}_{21}\text{H}_{26}\text{NP}$: 323.1797, found 323.1803.

Independent synthesis of ligand **L9** for a **L2/L9** ligand comparison study.***N*-Methyl-2-phenyl-3-(dicyclohexylphosphino)indole (**L9**).**

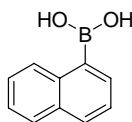
The synthesis of *N*-methyl-2-phenyl-3-bromoindole followed to the literature method.^[2] *N*-Methyl-2-phenyl-3-bromoindole (0.855 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 °C in dry ice/acetone bath. Titrated *n*-BuLi (3.3 mmol) was added dropwise by syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.66 mL, 3.3 mmol) in THF (5 mL) was added. The reaction was allowed to warm to room temperature and stirred overnight. Solvent was removed under reduced pressure. After the solvent was removed under vacuum, the product was successively washed with cold MeOH/EtOH mixture. The product was then dried under vacuum. White solid of *N*-methyl-2-phenyl-3-(dicyclohexylphosphino)indole (**L9**) (0.85 g, 71%) were obtained. Melting point. 122.0-123.2 °C; ¹H NMR (400 MHz, C₆D₆) δ 1.19-2.55 (m, 22H), 3.08 (s, 3H), 7.19-7.39 (m, 6H), 7.51 (d, *J*=7.3 Hz, 2H), 8.16-8.18 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 26.8, 27.3, 27.5 (overlapped), 27.6, 30.7 (overlapped), 31.0, 31.1, 32.5, 32.8, 34.8, 34.9, 105.1, 105.3, 110.3, 120.5, 122.1 (Overlapped), 127.8, 127.9, 131.3 (overlapped), 132.1 (overlapped), 133.3 (overlapped), 138.8 (overlapped), 149.8, 150.2 (unresolved complex C-P splittings were observed); ³¹P NMR (162 MHz, C₆D₆) δ -18.36; IR (cm⁻¹) 3049.36, 2921.78, 2845.98, 1465.12, 1443.10, 1372.54, 1336.47, 1264.83, 1106.31, 1021.29, 887.02, 849.63, 795.91, 737.94, 698.91, 619.86, 550.50; MS (EI): *m/z* (relative intensity) 403(M⁺, 25), 348 (5), 321 (30), 238 (100), 222 (25), 207 (10); HRMS: calcd. for C₂₇H₃₄NPH⁺: 404.2507, found 404.2511.

3. Preparation of aryl tosylates

4-*tert*-Butylphenyl tosylate^[3], 3,5-dimethylphenyl tosylate^[4], 4-benzoylphenyl tosylate^[5], 2-acetylphenyl tosylate^[6], 2-cyanophenyl tosylate^[7], 5-formyl-2-methoxyphenyl tosylate^[6], 3-acetylphenyl tosylate^[8], 4-(methoxycarbonyl)phenyl tosylate^[5], 4-methoxyphenyl tosylate^[9], 6-(tosyloxy)quinoline^[10] and 8-(tosyloxy)quinoline^[11] were prepared from their corresponding phenols with TsCl in the presence of triethylamine in CH₂Cl₂ according to the literature method.^[9] 1,2-Dihydro-3-naphthyl tosylate was prepared according to the literature method.^[12]

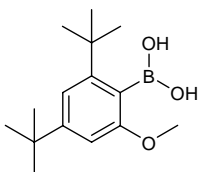
4. Procedures for preparation arylboronic acid substrates

1-Naphthylboronic acid¹³



Anhydrous THF (20 mL) was added to 1-bromonaphthalene (5.56 mL, 40 mmol) under nitrogen at room temperature. *n*-Butyllithium (44 mmol) was added dropwise to the solution at -78 °C and stirred for 30 min. The reaction mixture was transferred to a solution of B(*Oi*-Pr)₃ (18.6 mL, 80 mmol) in THF (10 mL) at -78 °C *via* cannular under nitrogen. The solution was warm to room temperature and stirred overnight. Diluted HCl (10%, 20 mL) was added to the mixture and stirred for 30 min. The organic layer was separated and the aqueous phase was extracted by diethyl ether (50 mL × 3). The combined organic extracts were washed with brine and dried over MgSO₄. The solvent was removed and the residue was crystallized under ether/hexane to give colorless crystals (5.0 g, 72%). The product was used without further characterization.

2,4-Di-*tert*-butyl-6-methoxyphenylboronic acid¹⁴

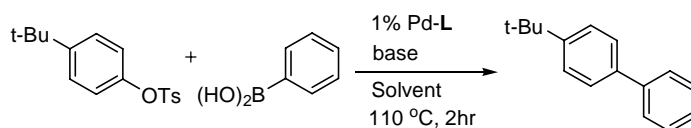


n-Butyllithium (1.6 M in hexane, 25 mL, 40 mmol) was added to a solution of 2-bromo-3,5-di-*tert*-butylanisole (12 g, 40 mmol) in THF (20 mL) at -78 °C under nitrogen. The mixture was stirred for 1 h and then transferred to a solution of distilled B(OMe)₃ (9.1 mL, 80 mmol) in THF (10 mL) at -78 °C under nitrogen. It was allowed to warm to room temperature and water was added. The organic layer was separated, and the aqueous phase was extracted with ether (3 × ~100 mL). The combined organic phases were washed with brine. After removing of solvent, the residue was redissolved in ethanol (60 mL). A solution of NaOH (2 M) was added and the mixture was stirred for 2 h. Solvent was rotary-evaporated, and the remaining aqueous layer was extracted with ether (3 × ~100 mL). The ethereal layer was then washed with brine and dried over

MgSO₄. The solvent was removed, and the residue was recrystallized from ether/hexane to give 2,4-di-*tert*-butyl-6-methoxyphenylboronic acid as colorless crystals (7.8 g, 74%). The product was used without further characterization.

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

General procedure for screening: Pd(OAc)₂ (2.3 mg, 0.010 mmol) and ligand (Pd:L = 1:4) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. The tube was evacuated and flushed with nitrogen for three times. Precomplexation was applied by adding freshly distilled dichloromethane and Et₃N into the tube. The palladium complex stock solution was stirred and warmed using hair drier for about 1 to 2 minutes until the solvent started boiling. The solvent was then evaporated under high vacuum. 4-*tert*-Butylphenyl tosylate (1.0 mmol), phenylboronic acid (2.0 mmol) and base (3.0 mmol) were loaded into the tube, and the system was further evacuated and flushed with nitrogen for three times. The solvent (3.0 mL) was added with stirring at room temperature for several minutes. The tube was then placed into a preheated oil bath (110 °C) and stirred for the time as indicated. 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.



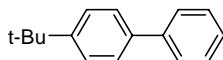
entry	Ligand	base	Solvent	GC yield (%)
1	L1	K ₃ PO ₄	<i>t</i> -BuOH	<1
2	L2	K ₃ PO ₄	<i>t</i> -BuOH	93
3	L3	K ₃ PO ₄	<i>t</i> -BuOH	86
4	L2	K ₃ PO ₄	DMF	99
5	L2	Cs ₂ CO ₃	<i>t</i> -BuOH	85
6	L2	KO <i>t</i> -Bu	<i>t</i> -BuOH	14
7	L2	K ₃ PO ₄	Dioxane	45
8	L2	K ₃ PO ₄	THF	46

6. General procedures for Suzuki-Miyaura couplings of aryl tosylates

General procedure for Suzuki-Miyaura coupling of aryl tosylates: Pd(OAc)₂ (2.3 mg, 0.010 mmol) and ligand (Pd:L = 1:4) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. The tube was evacuated and flushed with nitrogen for several times. Precomplexation was applied by adding freshly distilled dichloromethane and Et₃N into the tube. The solution was stirred and warmed using hair drier for about 1 to 2 minutes until the solvent started boiling. The solvent was then evaporated under high vacuum. Aryl tosylate (1.0 mmol), aryl boronic acid (2.0 mmol) and K₃PO₄•H₂O (3.0 mmol) were loaded into the tube, and the system was further evacuated and flushed with nitrogen for several times. The solvent *tert*-butanol (3.0 mL) was then added. The tube was stirred at room temperature for several minutes and then placed into a preheated oil bath (110 °C) for the time period as indicated in Table 2. 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.

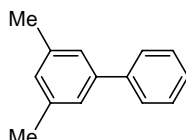
7. Characterization data for coupling products

4-*tert*-Butylbiphenyl (Table 2, entry 1 and 2).^[15]



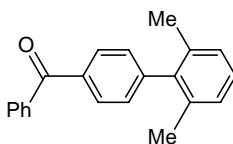
Hexane, $R_f=0.55$; ^1H NMR (400 MHz, CDCl_3) δ 1.72 (s, 9H), 7.64 (t, $J=7.4$ Hz, 1H), 7.72-7.82 (m, 4H), 7.89-7.96 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 31.3, 34.4, 125.6, 126.7, 126.9, 128.6, 138.2, 140.9, 150.0; MS (EI): m/z (relative intensity) 210 (M^+ , 35), 195 (100), 178 (20), 167 (30).

3,5-Dimethylbiphenyl (Table 2, entry 3).^[16]



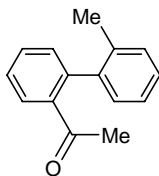
Hexane, $R_f=0.55$; ^1H NMR (400 MHz, CDCl_3) δ 2.76 (s, 6H), 7.37(s, 1H), 7.63(s, 2H), 7.67-7.71 (m, 1H), 7.77-7.80 (m, 2H), 7.95-7.99 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.2, 125.0, 126.9, 127.0, 128.5, 128.8, 138.0, 141.1, 141.3, MS (EI): m/z (relative intensity) 182 (M^+ , 100), 167 (70), 152 (25).

4-(2,6-Dimethylphenyl)benzophenone (Table 2, entry 4).



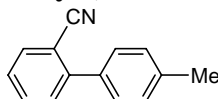
EA:Hexane = 1:20, $R_f=0.4$; white solid, m.p. = 76.5-78.9 °C; ^1H NMR (400 MHz, CDCl_3) δ 2.13 (s, 6H), 7.17-7.32 (m, 5H), 7.51-7.63 (m, 3H), 7.92-7.97 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.5, 127.1, 127.2, 127.9, 128.7, 129.6, 130.0, 131.9, 135.1, 135.5, 137.3, 140.3, 145.4, 195.8; MS (EI): m/z (relative intensity) 286 (M^+ , 80), 209 (100), 181 (25), 165 (50), 105 (45). HRMS: calcd. for $\text{C}_{21}\text{H}_{18}\text{O}$: 287.1436, found 287.1442.

2-Acetyl-2'-methylbiphenyl (Table 2, entry 5).^[17]



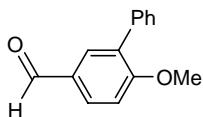
DCM:Hexane = 2:8, R_f =0.2; ^1H NMR (400 MHz, CDCl_3) δ 1.98 (s, 3H), 2.14 (s, 3H), 7.13 (d, J =7.4 Hz, 1H), 7.21-7.30 (m, 4H), 7.40-7.52 (m, 2H), 7.69-7.71(m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 19.9, 29.5, 125.6, 127.2, 127.8, 128.0, 129.3, 130.0, 130.4, 130.7, 135.3, 139.9, 140.3, 140.5, 202.7; MS (EI): m/z (relative intensity) 210 (M^+ , 10), 195 (100), 177 (15), 165 (45), 152 (30).

2-Cyano-4'-methylbiphenyl (Table 2, entry 6).^[18]



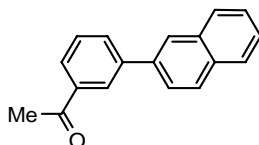
DCM:Hexane = 2:8, R_f =0.35; ^1H NMR (400 MHz, CDCl_3) δ 2.43 (s, 3H), 7.32 (d, J =7.9 Hz, 2H), 7.40 (dt, J =1.1, 7.6 Hz, 1H), 7.49-7.51 (m, 3H), 7.61 (dt, J = 1.2, 7.7 Hz, 1H), 7.74 (dd, J =0.8, 7.7 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.8, 110.6, 118.5, 126.9, 128.2, 129.0, 129.6, 132.4, 133.3, 134.9, 138.2, 145.0; MS (EI): m/z (relative intensity) 193 (M^+ , 100), 177 (10), 165 (35)

3-Phenyl-4-methoxybenzaldehyde (Table 2, entry 7).^[19]



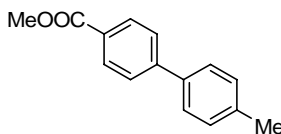
EA:Hexane = 1:9, R_f =0.4; ^1H NMR (400 MHz, CDCl_3) δ 3.82 (s, 3H), 7.04 (d, J =8.3 Hz, 1H), 7.37-7.84 (m, 7H), 9.89 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 55.3, 110.7, 127.1, 127.7, 129.0, 129.4, 130.8, 131.0, 131.6, 136.7, 161.0, 190.3; MS (EI): m/z (relative intensity) 212 (M^+ , 100), 197(3), 183(5), 168(25).

3-(2-Naphthyl)acetophenone (Table 2, entry 8).



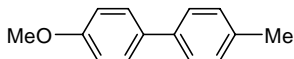
EA:Hexane = 1:9, R_f =0.35; White solid, m.p. = 69.5-71.8 °C; ^1H NMR (400 MHz, CDCl_3) δ 2.60 (s, 3H), 7.45-7.50 (m, 3H), 7.68 (dd, J =1.6, 8.5 Hz, 1H), 7.78-7.89 (m, 5H), 8.00 (bs, 1H), 8.30 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 26.2, 124.7, 125.5, 125.8, 126.0, 126.5, 126.8, 127.2, 127.8, 128.2, 128.6, 131.3, 132.4, 133.2, 136.8, 137.2, 140.9, 197.5; MS (EI): m/z (relative intensity) 246 (M^+ , 100), 231 (90), 202 (95). HRMS: calcd. for $\text{C}_{18}\text{H}_{14}\text{O}$: 247.1123, found 247.1106.

Methyl 4-(4'-tolyl)benzoate (Table 2, entry 9).^[20]



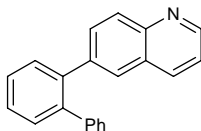
EA:Hexane = 1:9, R_f =0.5; ^1H NMR (400 MHz, CDCl_3) δ 2.42 (s, 3H), 3.95 (s, 3H), 7.27 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 8.3 Hz), 8.12 (d, J = 8.3 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 21.0, 51.8, 126.5, 126.9, 128.4, 129.4, 129.9, 136.8, 137.9, 145.3, 166.8; MS (EI): m/z (relative intensity) 226 (M^+ , 85), 195 (100), 165 (40), 152 (50), 139 (10).

4-(4'-Tolyl)anisole (Table 2, entry 10).^[21]



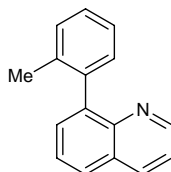
Hexane, R_f =0.1; ^1H NMR (400 MHz, CDCl_3) δ 2.53 (s, 3H), 3.94 (s, 3H), 7.10 (d, J =8.7 Hz, 2H), 7.37 (d, J =7.9 Hz, 2H), 7.61 (d, J =8.0 Hz, 2H), 7.66 (d, J =8.7 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.9, 55.0, 114.0, 126.4, 127.8, 129.3, 133.5, 136.1, 137.8, 158.8; MS (EI): m/z (relative intensity) 198 (M^+ , 100), 183 (60), 165 (10), 155 (35).

5-(2-Biphenyl)quinoline (Table 3, entry 1).



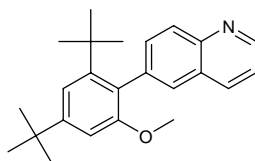
EA:Hexane = 1:9, R_f =0.15; light yellow viscous liquid; ^1H NMR (400 MHz, CDCl_3) δ 7.18 (bs, 5H), 7.25-7.54 (m, 6H), 7.69 (s, 1H), 7.94-7.98 (m, 2H), 8.85 (d, J = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 120.8, 126.4, 127.4, 127.7, 127.8, 127.9, 128.3, 129.6, 130.4, 130.5, 131.7, 135.6, 139.2, 139.7, 140.4, 140.8, 146.8, 149.9; MS (EI): m/z (relative intensity) 281 (M^+ , 100), 266 (30), 252 (20); HRMS: calcd. for $\text{C}_{21}\text{H}_{15}\text{N}$: 281.1199, found 281.1203.

7-(2'-Tolyl)quinoline (Table 3, entry 2).^[23]

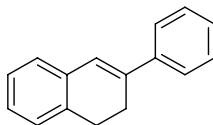


EA:Hexane = 1:9, R_f =0.25; ^1H NMR (400 MHz, CDCl_3) δ 2.28 (s, 3H), 7.42-7.53 (m, 5H), 7.67-7.76 (m, 2H), 7.92-8.25 (m, 2H), 9.07-9.09 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.1, 120.4, 125.0, 125.7, 127.1, 127.2, 127.9, 129.3, 129.8, 129.9, 135.6, 136.4, 139.5, 141.0, 146.1, 149.8; MS (EI): m/z (relative intensity) 218 (M^+ , 85), 204 (100), 188 (5), 176 (3).

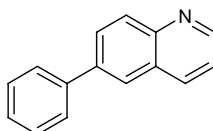
6-(2,4-Di-*tert*-butyl-6-methoxyphenyl)quinoline (Table 3, entry 3).



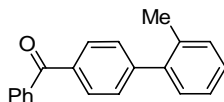
EA:Hexane = 1:9, R_f =0.15; white solid, m.p. = 136.4-138.1 °C. ^1H NMR (400 MHz, CDCl_3) δ 1.19 (s, 9H), 1.42 (s, 9H), 3.56 (s, 3H), 6.92 (s, 1H); 7.24-7.31 (m, 4H), 8.02 (d, J =7.9 Hz, 1H), 8.14 (d, J =8.5 Hz, 1H), 8.87 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 31.1, 32.5, 34.8, 36.6, 55.5, 105.7, 116.0, 120.5, 127.0, 127.2, 127.5, 129.2, 133.9, 135.5, 138.3, 147.0, 148.4, 149.6, 150.6, 157.3; MS (EI): m/z (relative intensity) 347 (M^+ , 100), 332 (75), 317 (5), 302 (3), 290 (5), 276(75), 261(30); HRMS: calcd. for $\text{C}_{24}\text{H}_{29}\text{NO}$: 347.2244, found 347.2253.

1,2-Dihydro-3-phenylnaphthalene (Table 3, entry 4).^[24]

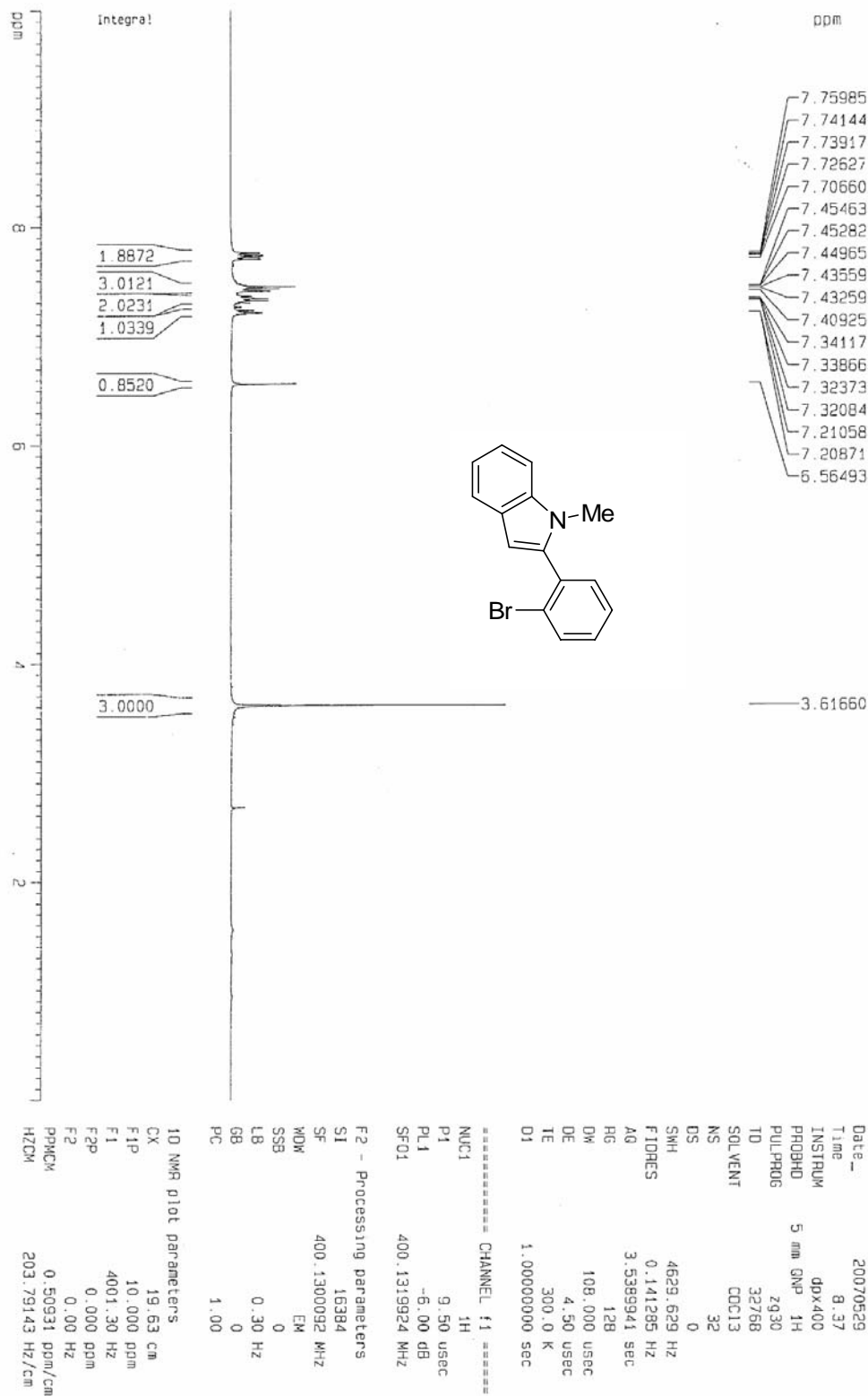
Hexane, $R_f=0.4$; ^1H NMR (400 MHz, CDCl_3) δ 3.00-3.04 (m, 2H), 3.21-3.25 (m, 2H), 7.19 (s, 1H), 7.44-7.69 (m, 7H), 7.84-7.85 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 26.1, 27.9, 124.2, 124.9, 126.4, 126.5, 126.8, 127.0, 127.1, 128.2, 134.5, 138.3, 140.8; MS (EI): m/z (relative intensity) 206 (M^+ , 100), 191 (20), 178 (5), 165 (5), 128 (30), 91(55);

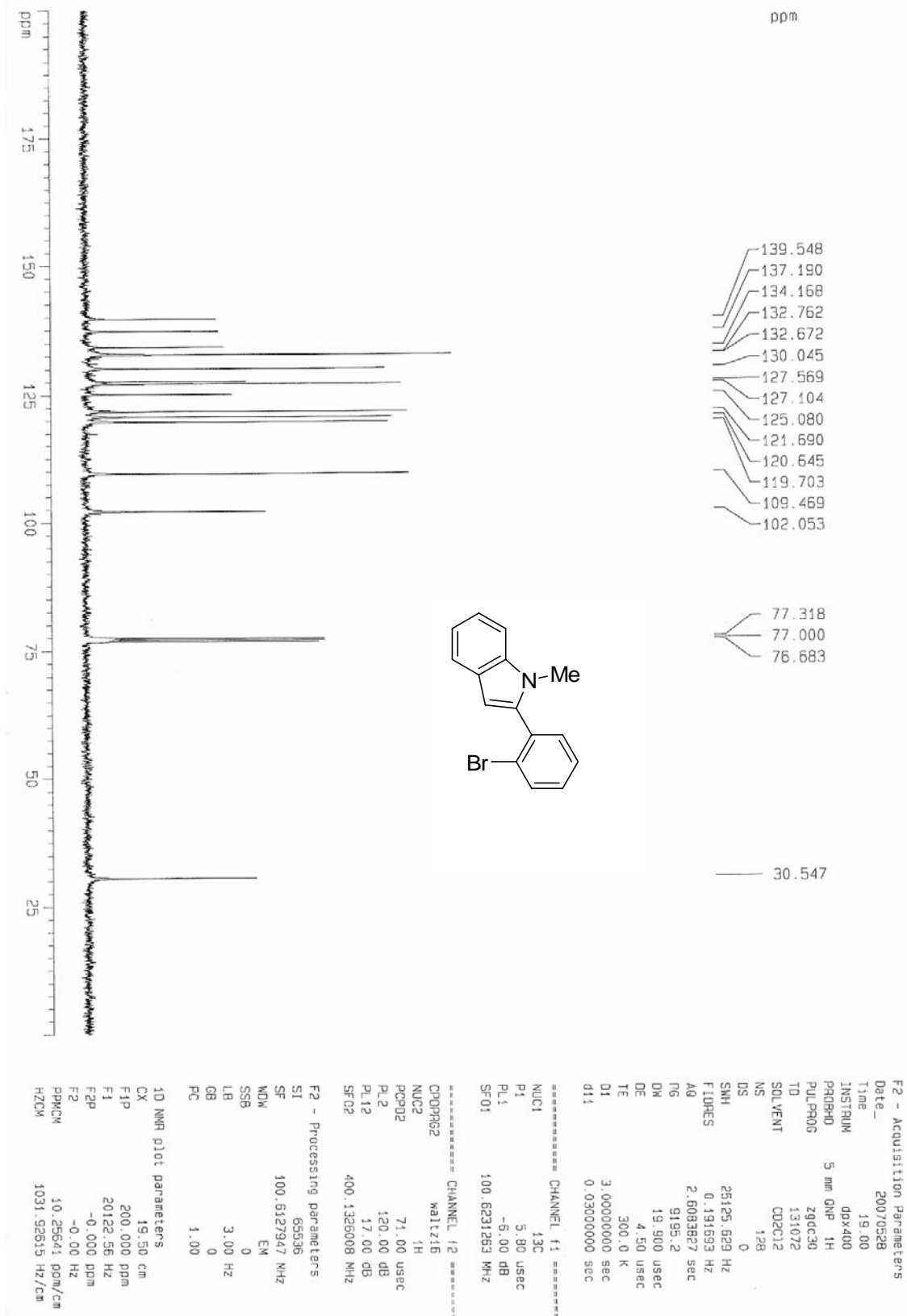
6-Phenylquinoline (Table 3, entry 5).^[20]

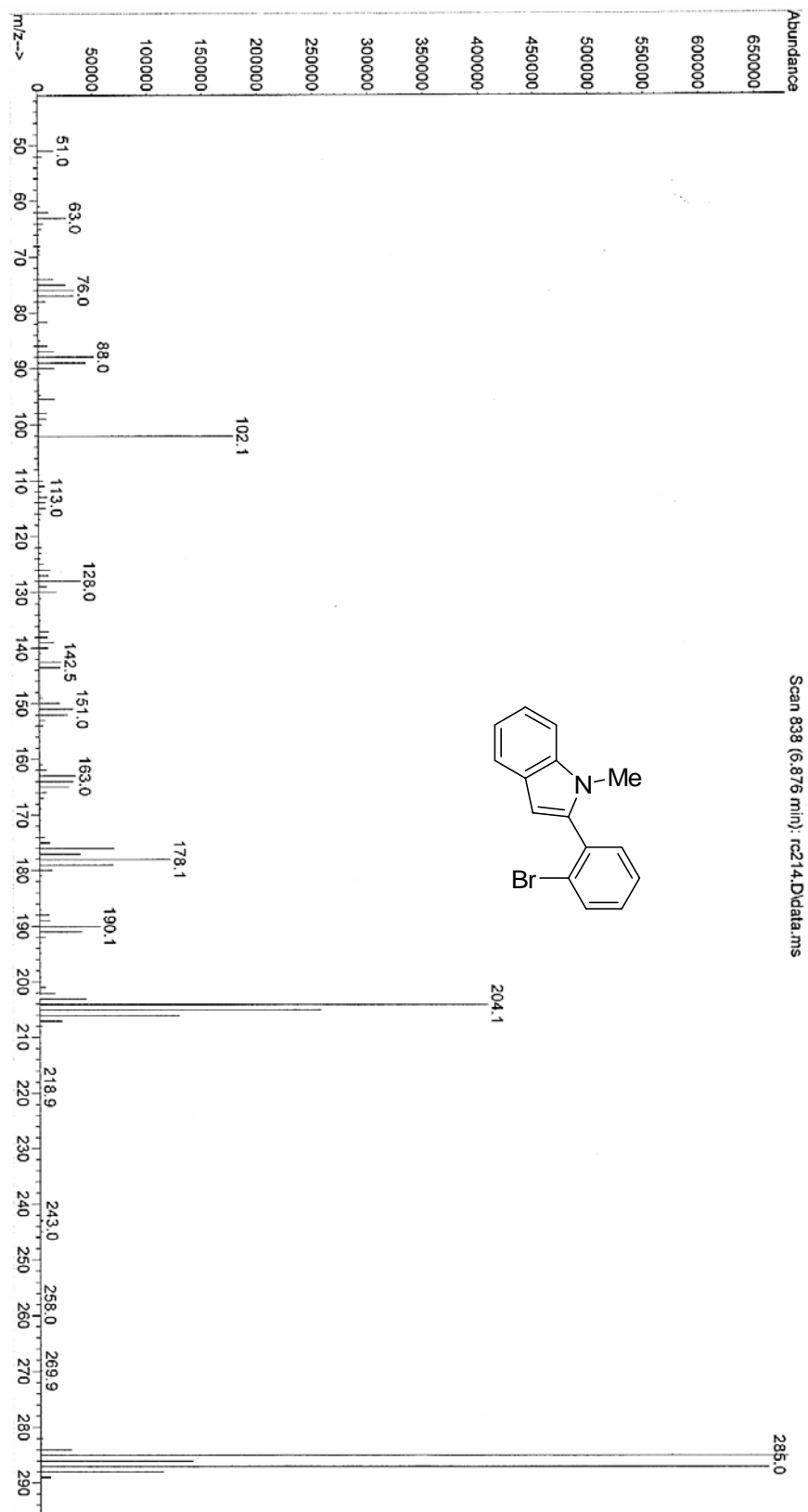
EA:Hexane = 2:8, $R_f=0.25$; ^1H NMR (400 MHz, CDCl_3) δ 7.21-7.33 (m, 2H), 7.37-7.71 (m, 2H), 7.58-7.60 (m, 2H), 7.82-7.87 (m, 2H), 7.96-8.15 (m, 2H), 8.83 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 121.0, 125.0, 127.0, 127.3, 128.0, 128.5, 128.7, 129.4, 135.7, 138.7, 139.7, 147.2, 149.9; MS (EI): m/z (relative intensity) 205 (M^+ , 100), 176 (10).

4-(2'-Tolyl)benzophenone (Scheme 1).^[22]

EA:Hexane = 1:20, $R_f=0.4$; ^1H NMR (400 MHz, CDCl_3) δ 2.36 (s, 3H), 7.30-7.33 (m, 4H), 7.46-7.61 (m, 5H), 7.90-7.93 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 20.2, 125.7, 127.6, 128.0, 128.9, 129.3, 129.7, 130.3, 132.0, 135.6, 137.4, 140.4, 146.0, 195.9; MS (EI): m/z (relative intensity) 272 (M^+ , 70), 195 (100), 164 (40), 152 (40), 105 (40).

8. ^1H , ^{13}C , ^{31}P NMR, MS, HRMS and IR spectra



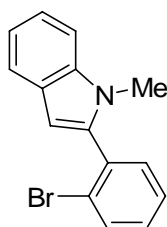


Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 60.0

Selected filters: None



Monoisotopic Mass, Even Electron Ions

7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

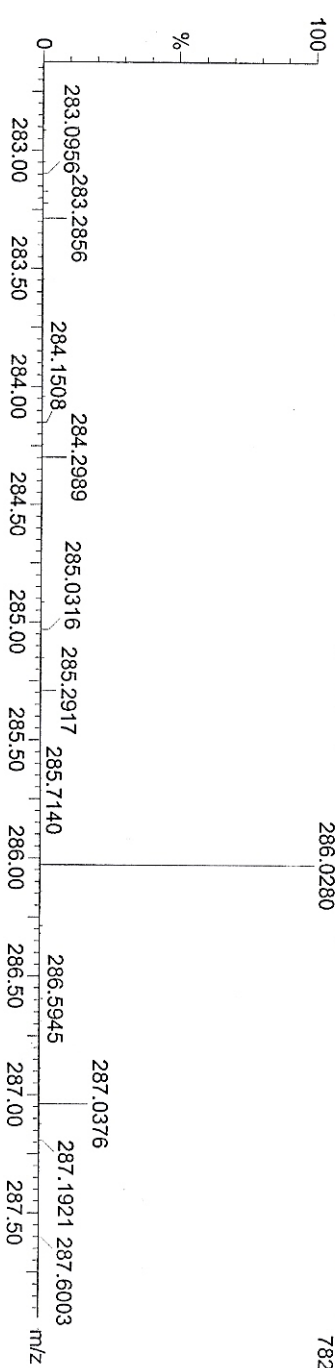
Elements Used:

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So Chau Ming, N-methyl 2(2Bromophenyl)indole

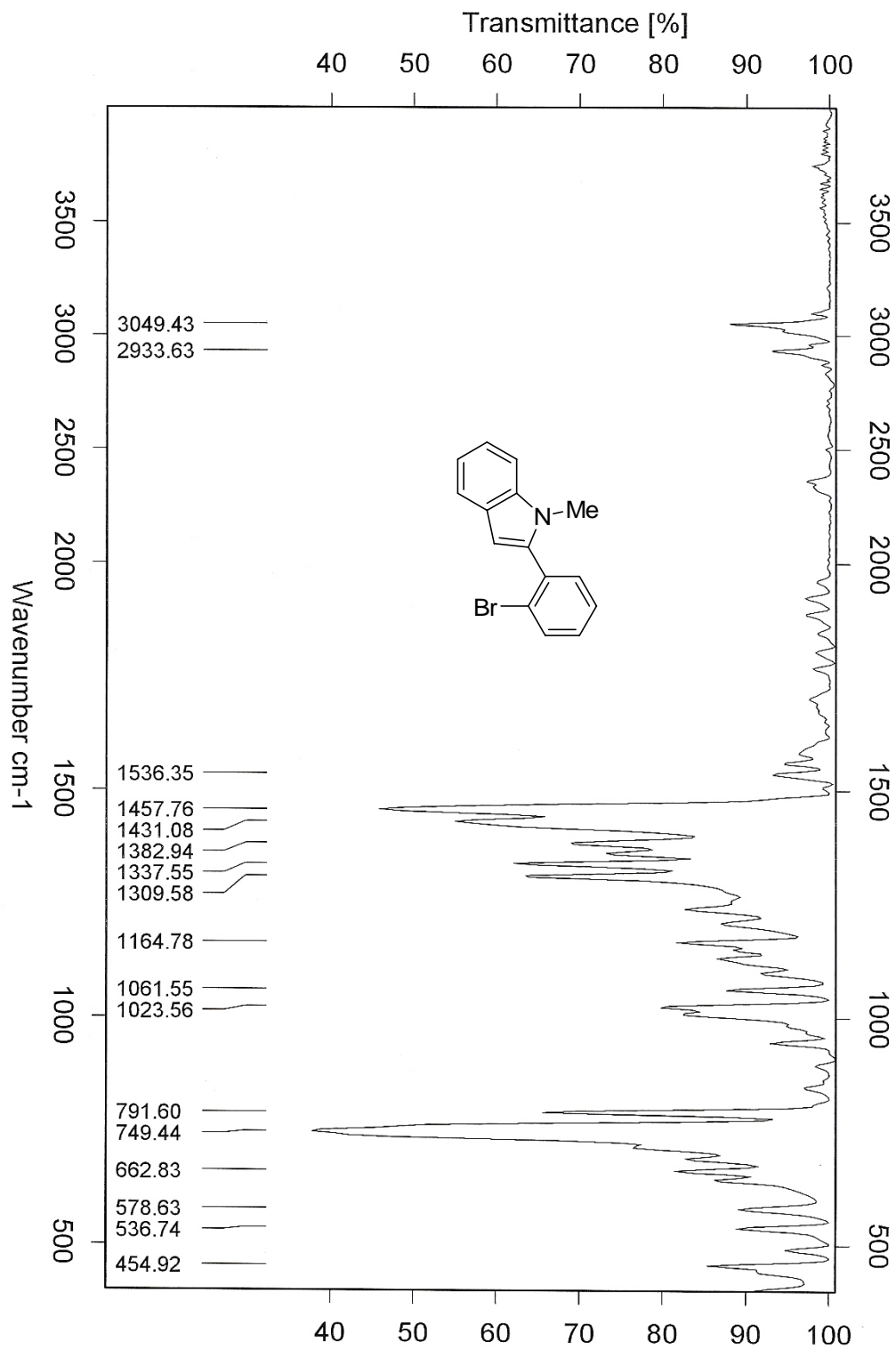
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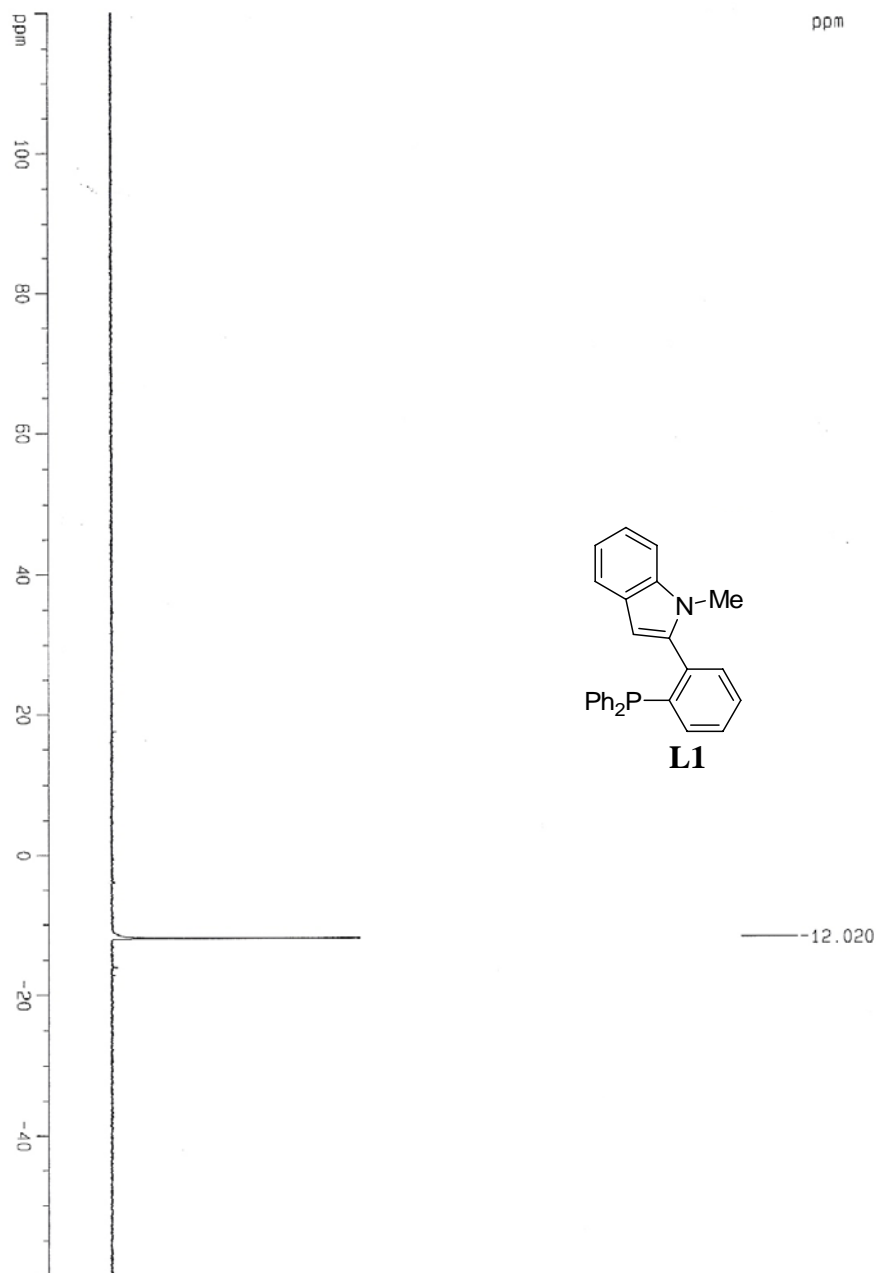
286.0280

15-Jun-2007
TOF MS ES+
782

Minimum: -1.5
Maximum: 60.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Current Data Parameters
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 PROCNO 1

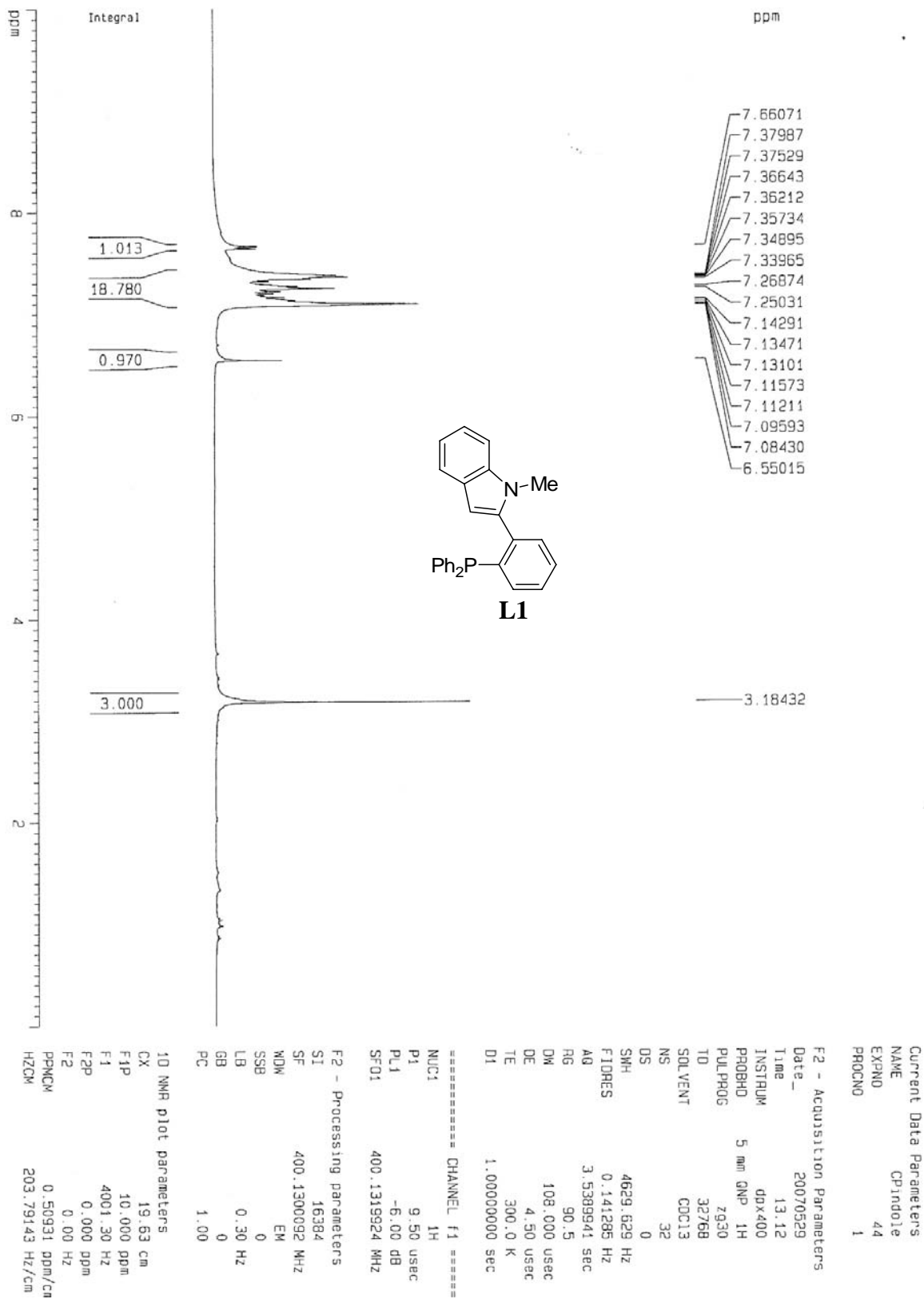
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 32
 DS 0
 SM 49651.801 Hz
 FIDRES 0.742520 Hz
 AQ 0.6734324 sec
 RG 13004
 DM 10.275 uSBC
 DE 4.50 uSBC
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec

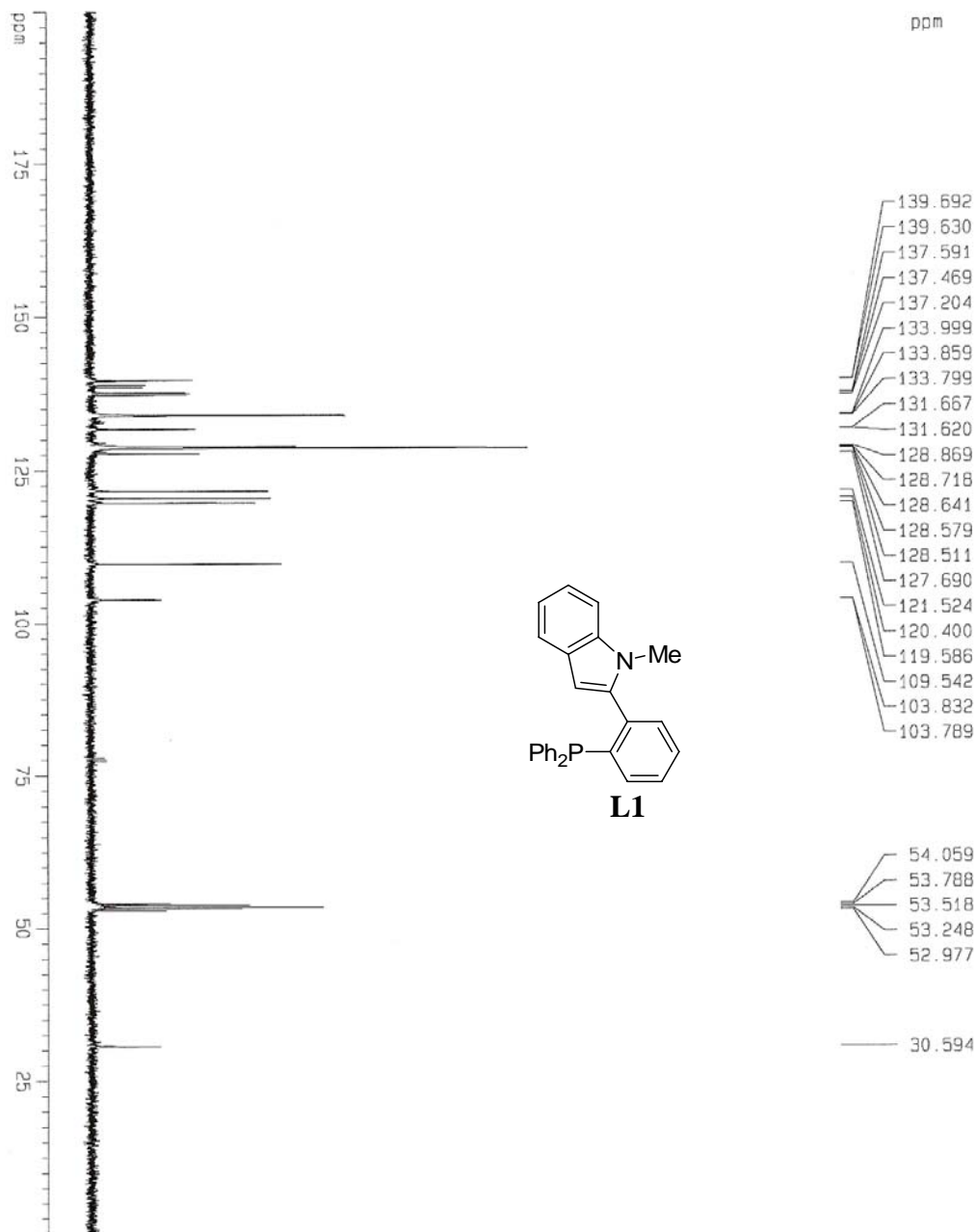
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 NUC2 1H
 PCPD2 71.00 uSBC
 PL2 120.00 dB
 PL12 17.00 dB
 SFO2 400.1324008 MHz

F2 - Processing parameters
 SI 32768
 SF 161.9755831 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1P 120.000 ppm
 F1 19437.07 Hz
 F2P -60.000 ppm
 F2 -9718.54 Hz
 PPMCK 9.00000 ppm/cf
 HZCK 1457.78027 Hz/cm





Current Data Parameters

NAME	CCPindole
EXPNO	25
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
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INSTRUM dpx400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 131072
SOLVENT CDCl₃
NS 96
DS 0
SWH 25125.629 Hz
FIDRES 0.191693 Hz
AQ 2.6083827 sec
RG 9195.2
DW 19.900 usec
DE 4.50 usec
TE 300.0 K
D1 3.00000000 sec
d11 0.03000000 sec

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NUC1	13C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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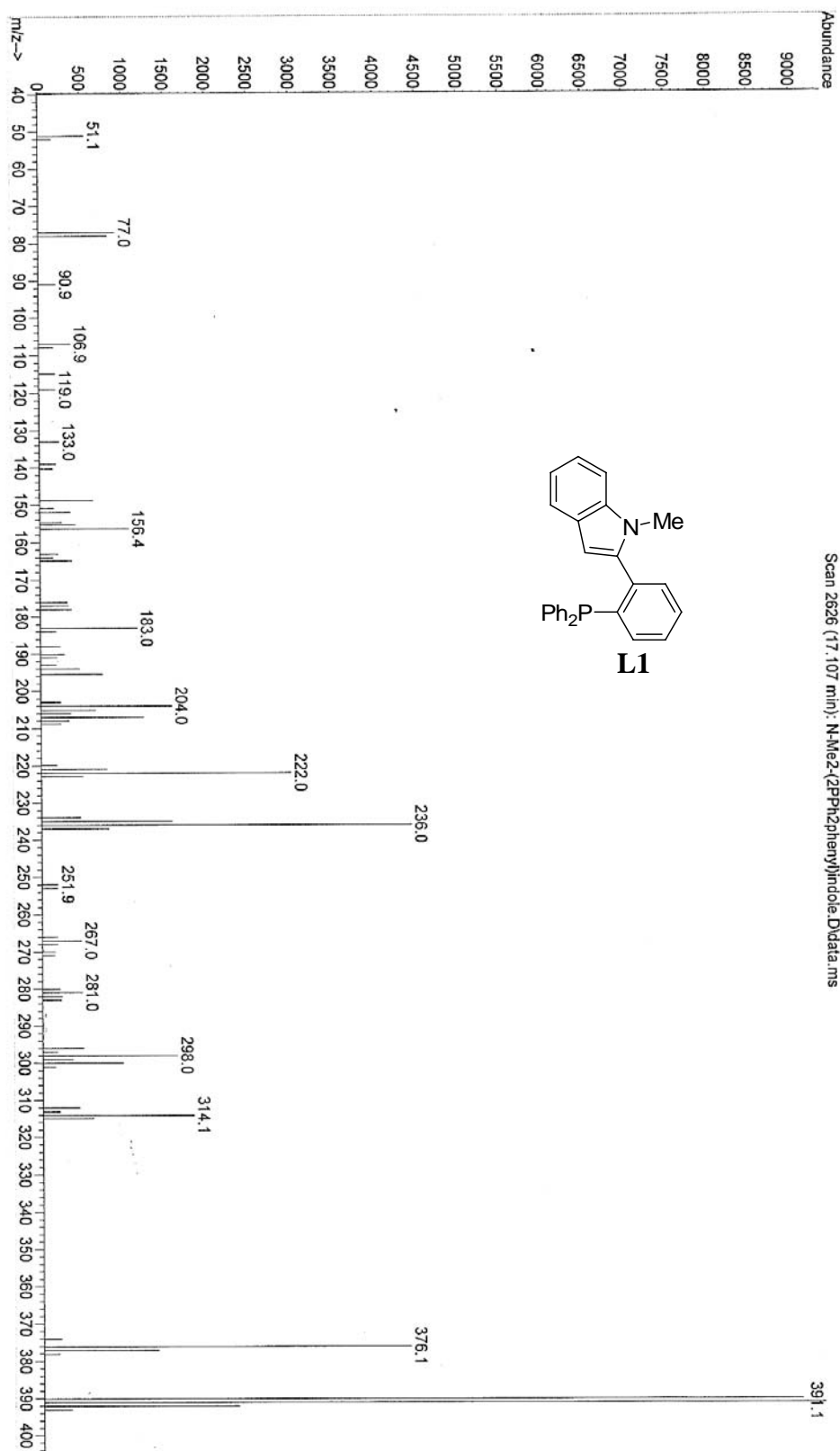
CPDPRG2	waltz16
NUC2	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SI	65536
SF	100.6127679 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.50 cm
F1P	200.000 ppm
F1	20122.55 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCK	10.25641 ppm/cm
HZCK	1031.92590 Hz/cm



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 60.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

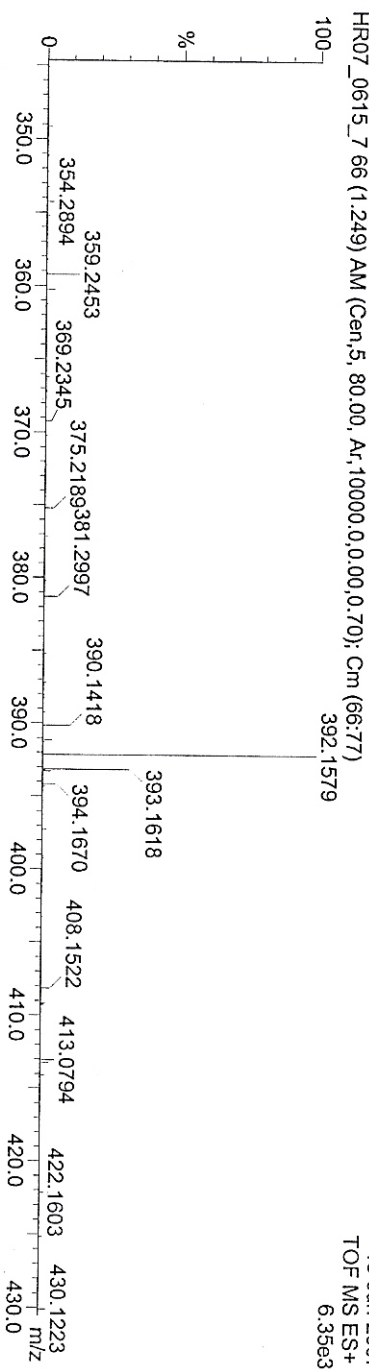
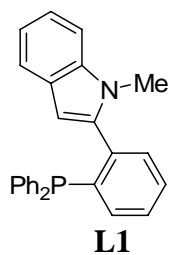
9 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

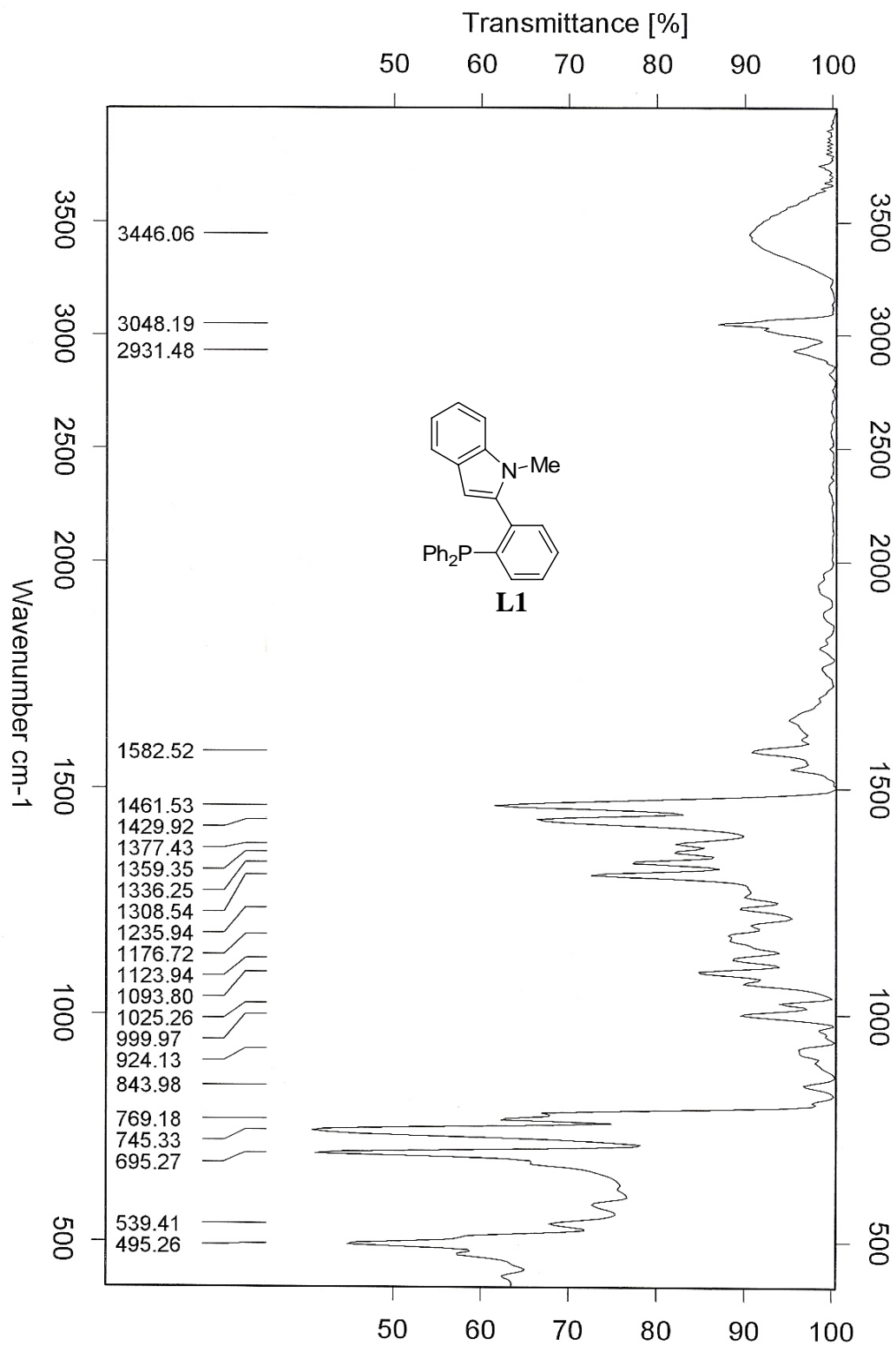
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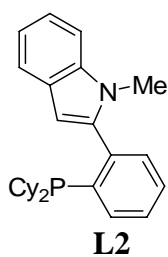
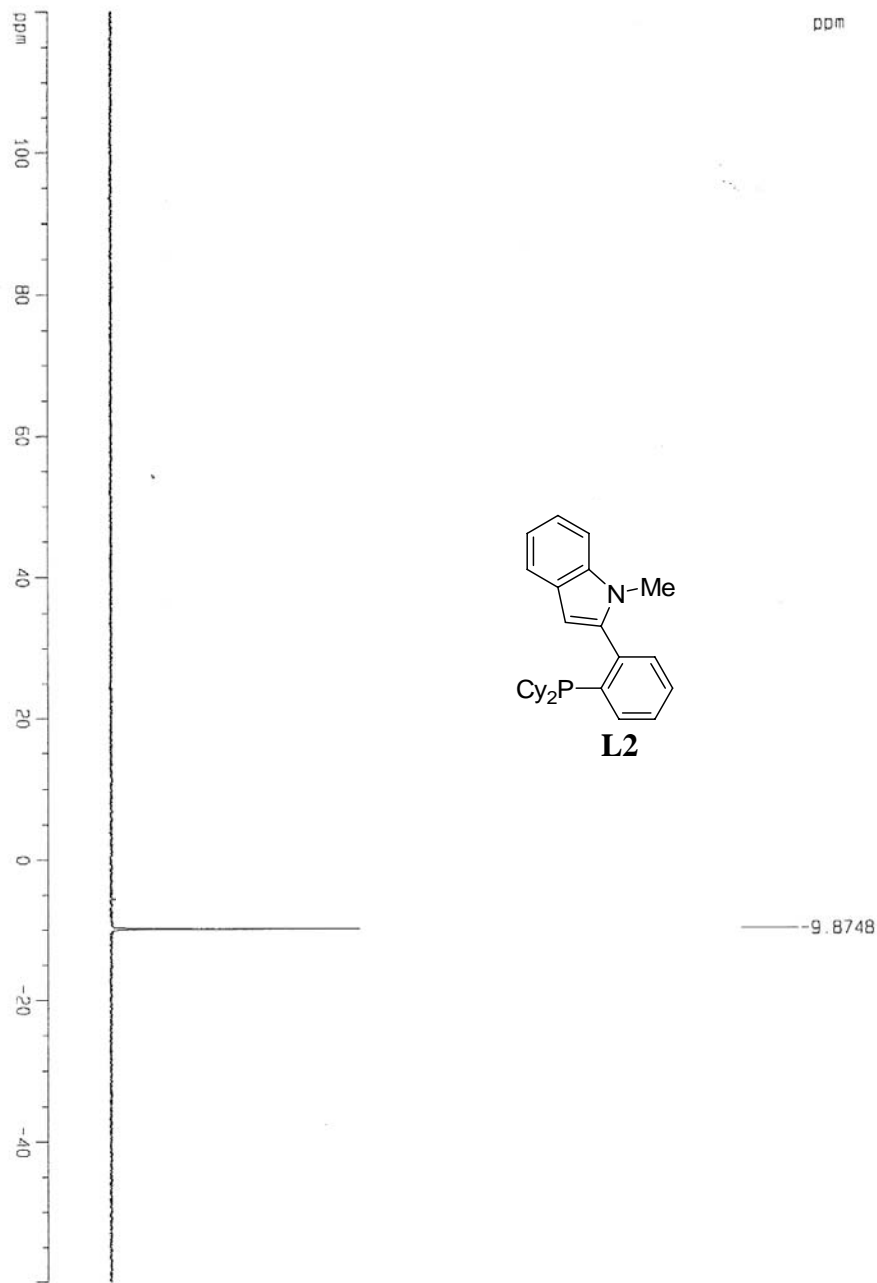
So Chau Ming, 2-(N-methylindolyl)phenyl/Ph₂phosphine

HR07_0615_7 66 (1.249) AM (Cen,5, 80.00, Ar,10000.0,0.00,0.70); Cm (66.77)

15-Jun-2007
TOF MS ES+
6.35e3

Minimum:							
Maximum:							
		5.0	100.0	-1.5			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
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Current Data Parameters
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 EXPNO 31
 PROCNO 1

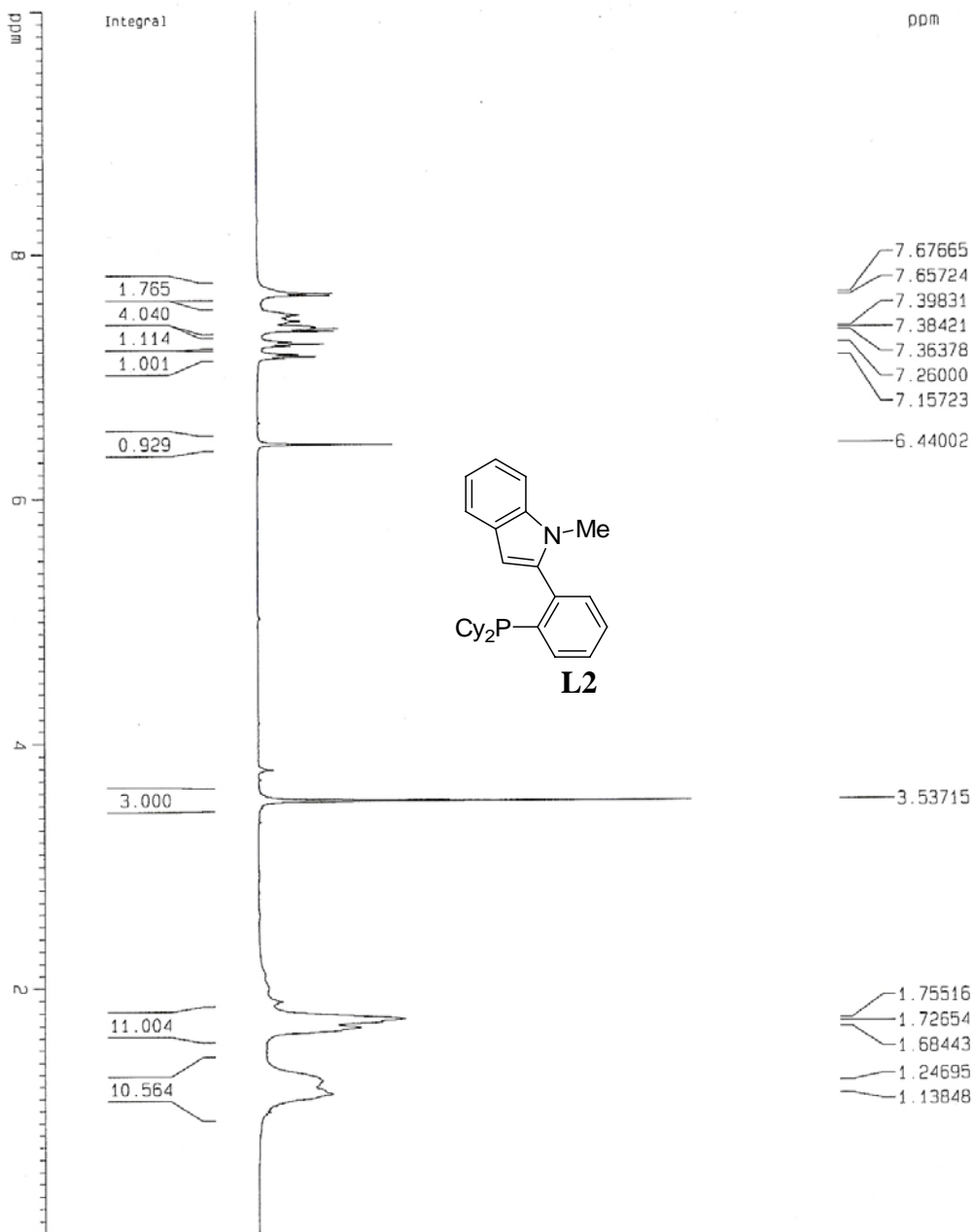
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 TO 655.36
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 48661.801 Hz
 FIDRES 0.742520 Hz
 AQ 0.6734324 sec
 RG 13004
 DW 10.275 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 31P
 P1 7.20 usec
 PL1 -5.00 dB
 SF01 161.985115 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 71.00 usec
 PL2 120.00 dB
 PL12 17.00 dB
 SF02 400.1324008 MHz

F2 - Processing parameters
 S1 32768
 SF 161.9755831 MHz
 KW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 FIP 120.000 ppm
 F1 19437.07 Hz
 F2P -160.000 ppm
 F2 -9718.54 Hz
 PPMCH 9.00000 ppm/cm
 HZCN 1457.78027 Hz/cm



Current Data Parameters
NAME CPIndo1e
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070516
Time 20.10
INSTRUM dpx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4629.629 Hz
FIDRES 0.141285 Hz
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RG 35.9
DW 108.000 usec
DE 4.50 usec
TE 300.0 K
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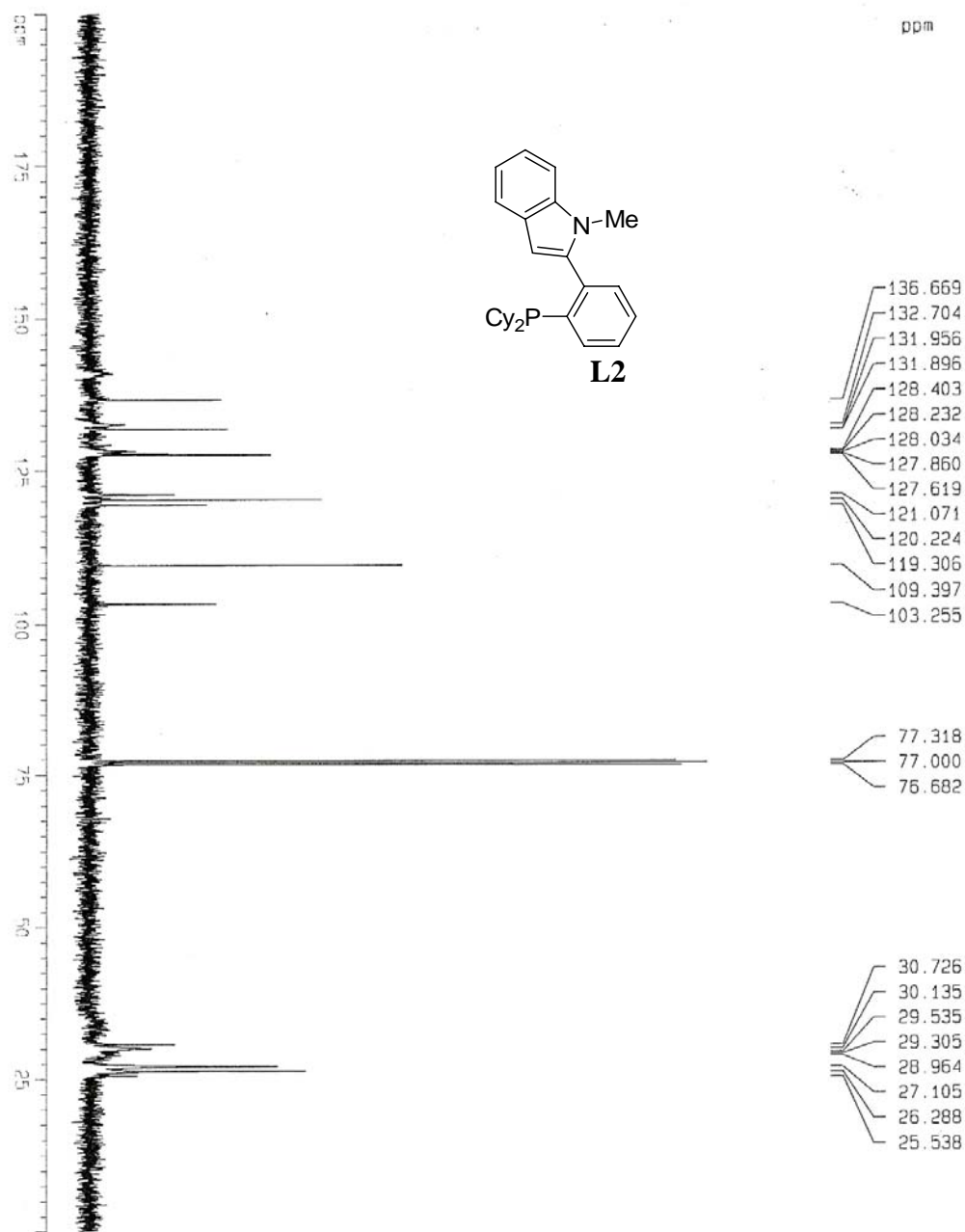
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F2 - Processing parameters

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SF 400.130092 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 19.63 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.50931 ppm/cm
HZCM 203.79143 Hz/cm



Current Data Parameters

NAME	CCPIndole
EXPNO	21
PROCNO	1

F2 - Acquisition Parameters

Date_	20070515
Time	20.14
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PROBHD	5 mm GNP 1H
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl ₃
NS	128
DS	0
SWH	25125.629 Hz
FIDRES	0.191693 Hz
AQ	2.6083827 sec
RG	9195.2
DW	19.900 usec
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TE	300.0 K
D1	3.00000000 sec
d11	0.03000000 sec

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

NUC1	¹³ C
P1	5.80 usec
PL1	-6.00 dB
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===== CHANNEL f2 =====

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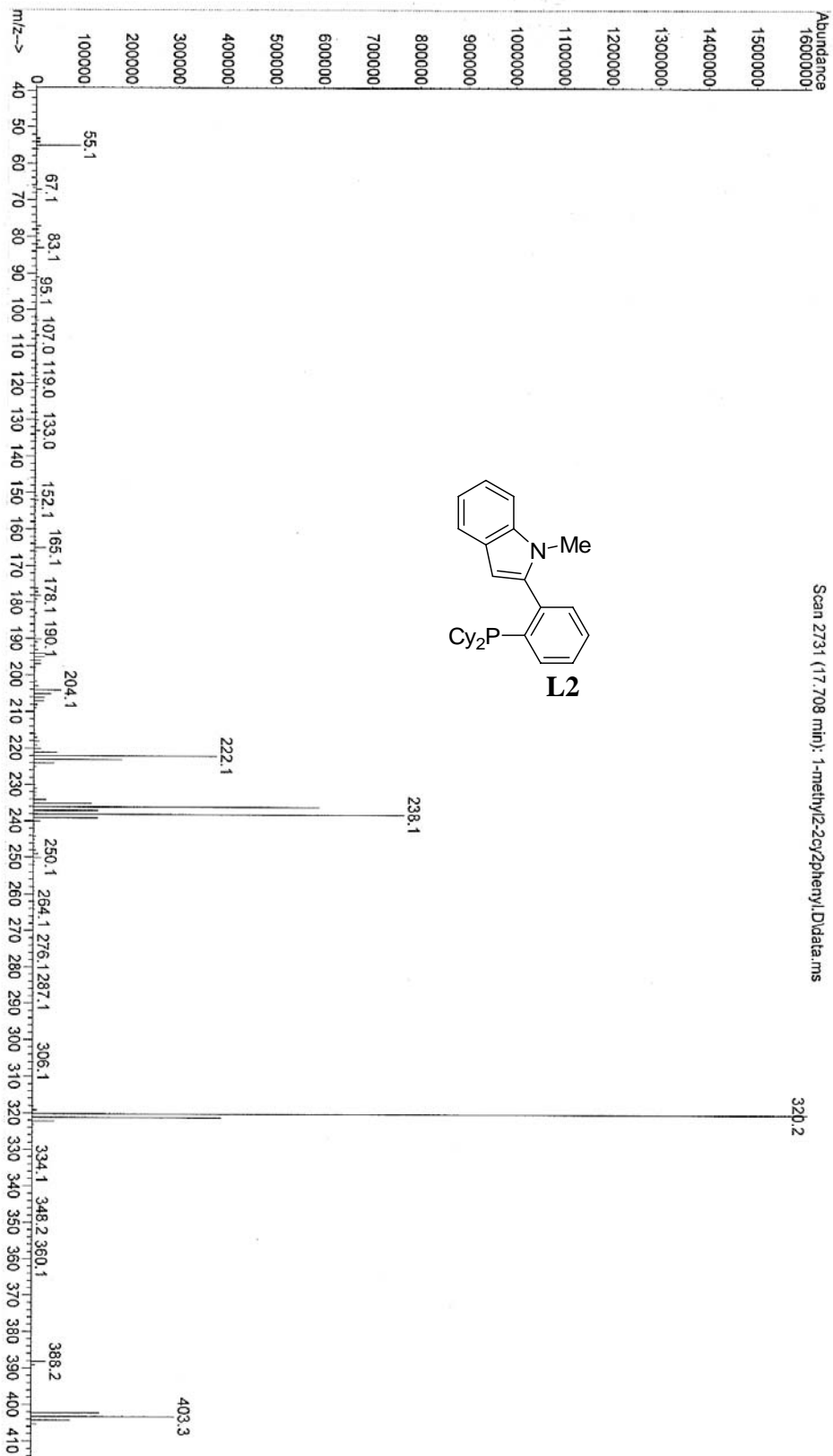
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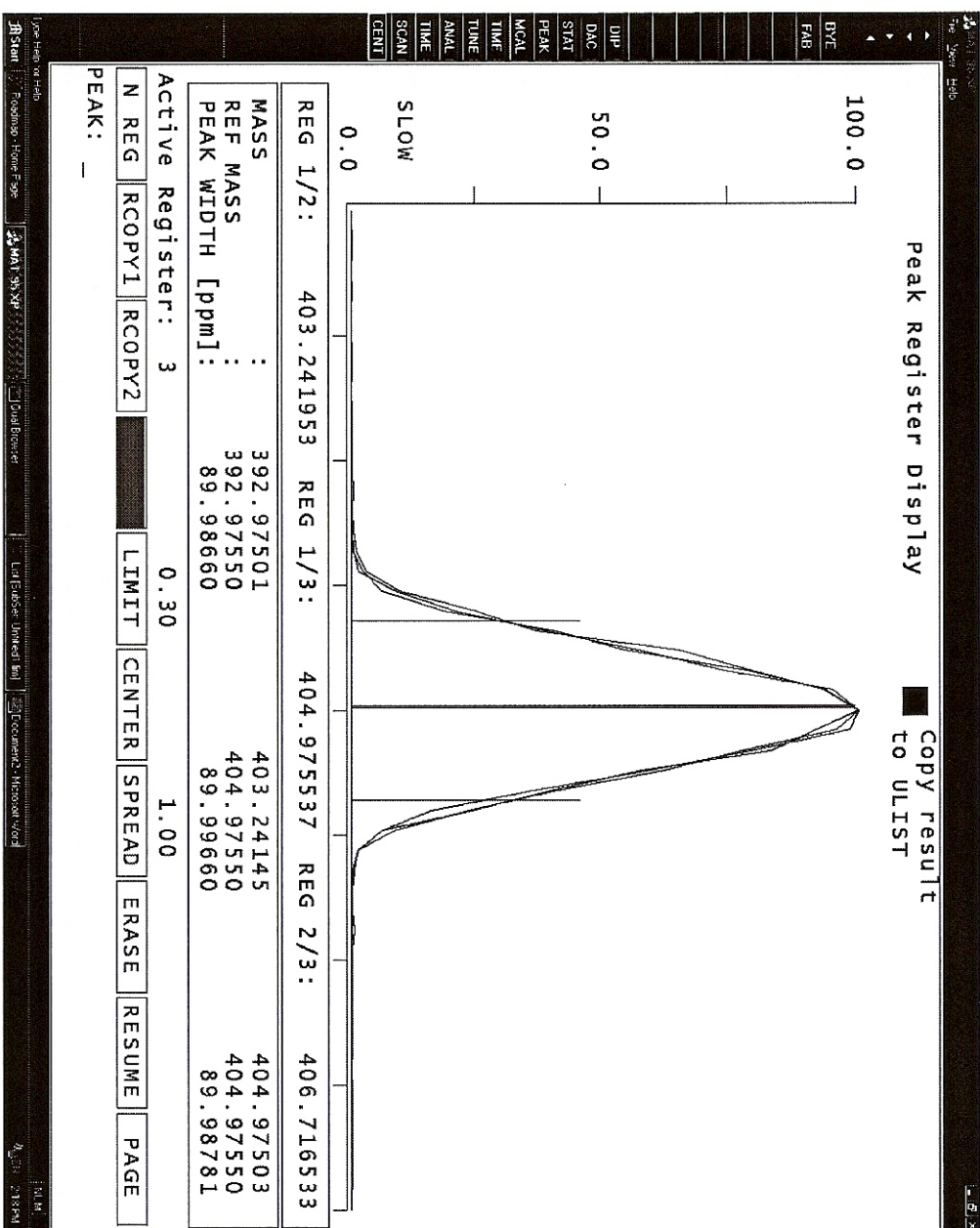
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SSB	0
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1D NMR plot parameters

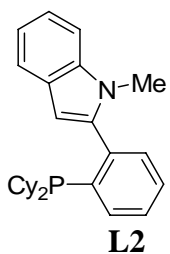
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HZCM	1031.92803 Hz/cm

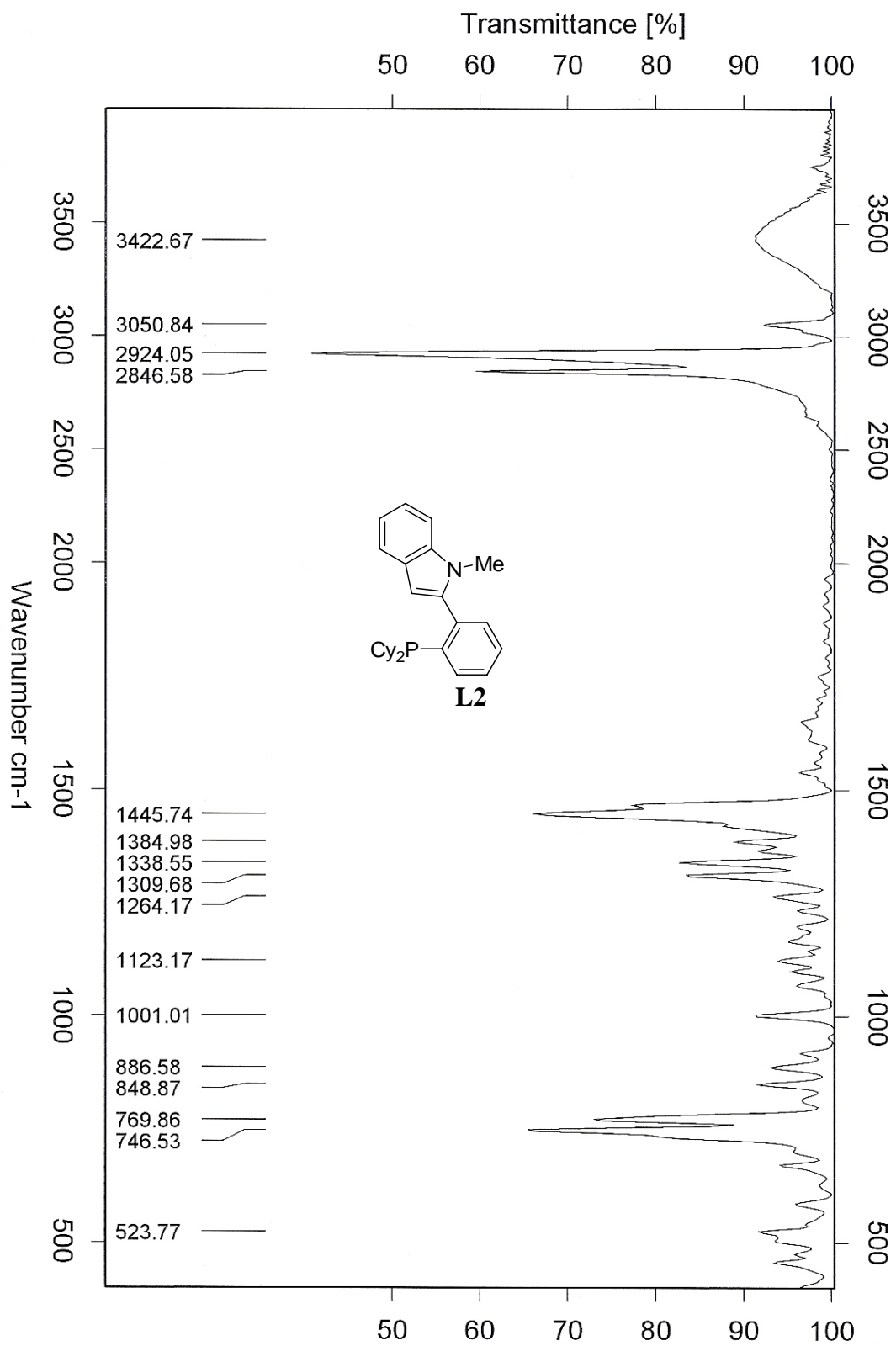
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Instrument : 5973N
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Sample Name :
Misc Info :

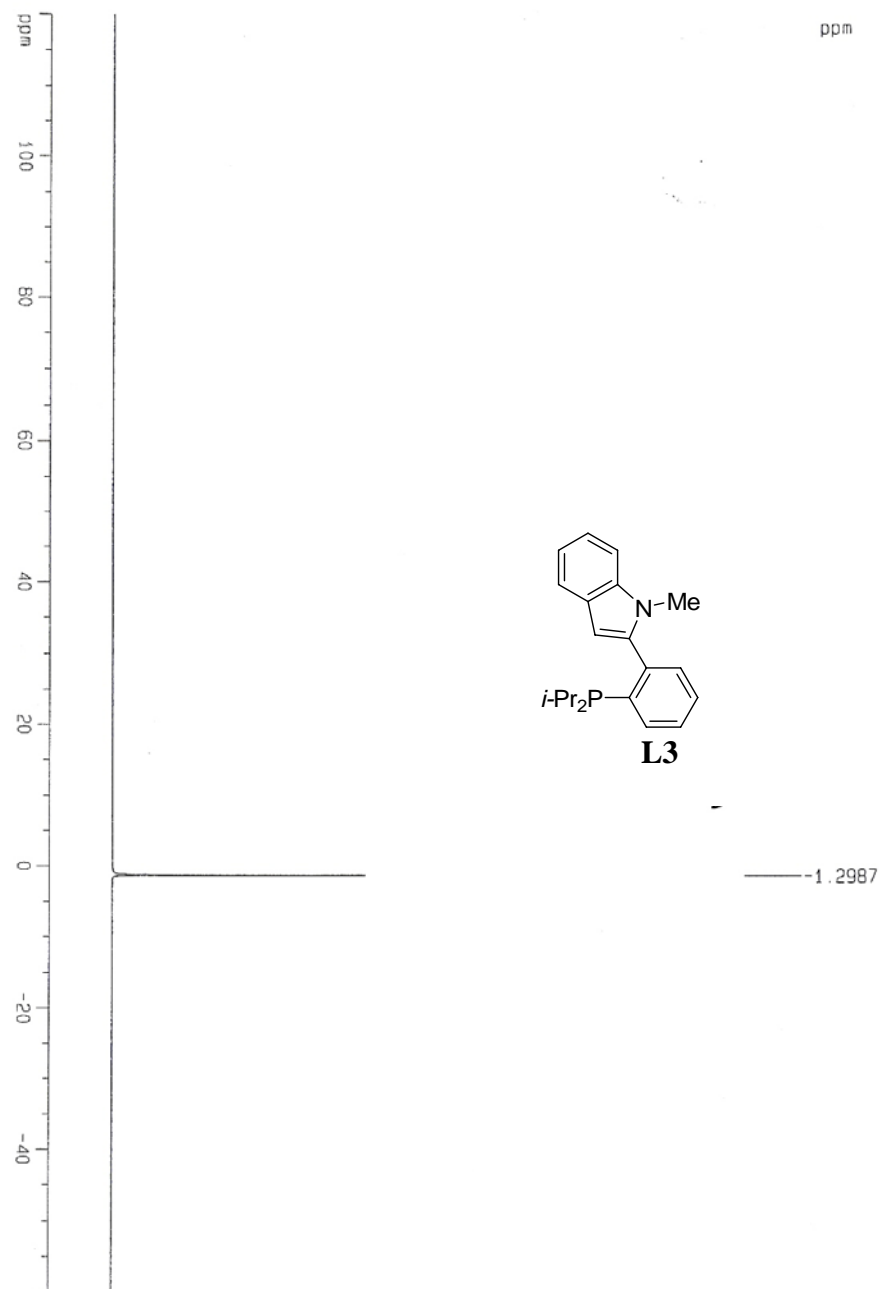




Molecular formula:
C₂₇H₃₄N₁P₁
[M]⁺ (theoretical)
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Current Data Parameters
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 PROCNO 1

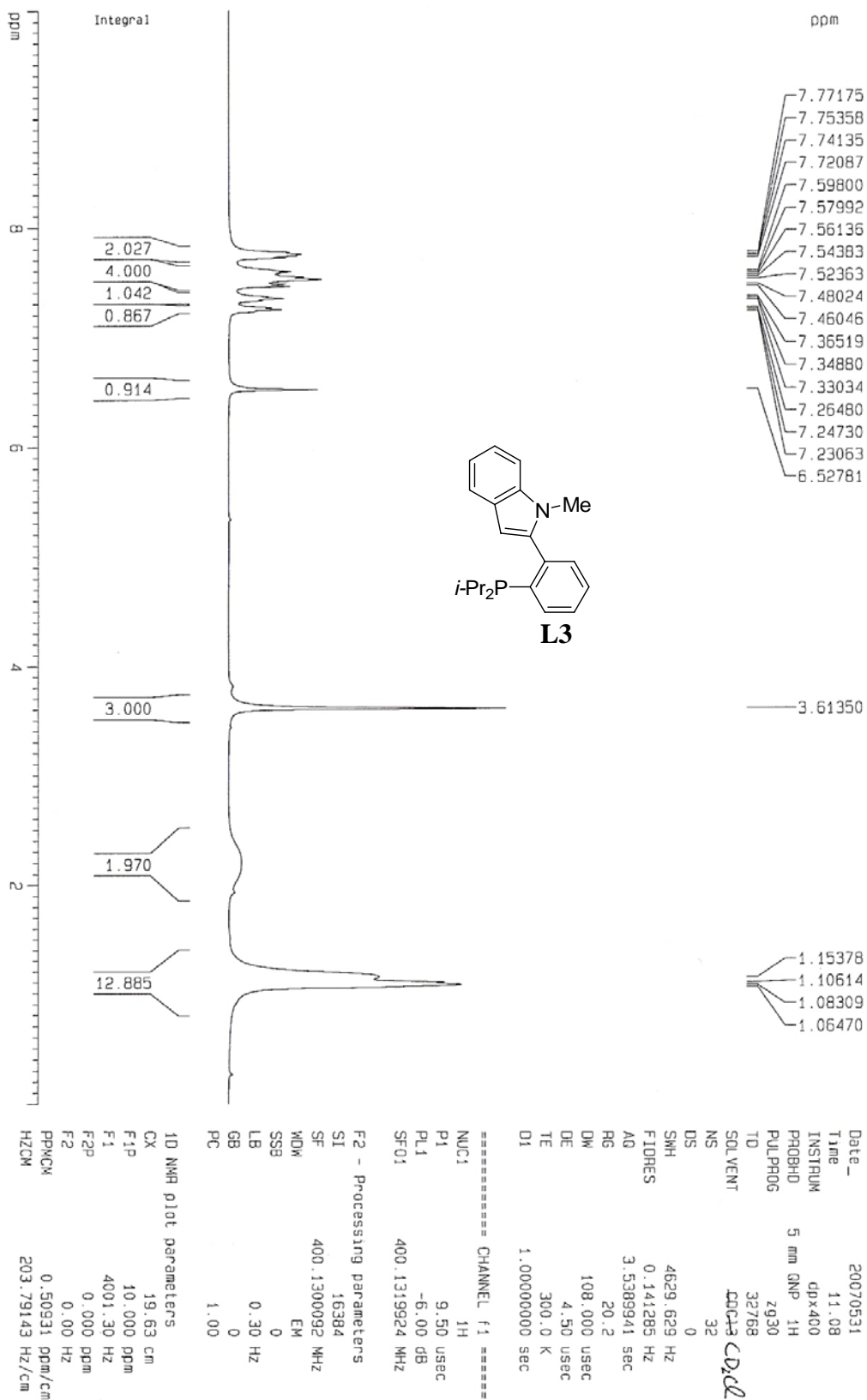
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 TO 65536
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 NS 32
 DS 0
 SWH 48661.801 Hz
 FIDRES 0.742520 Hz
 AQ 0.6734324 sec
 RG 6502
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 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec

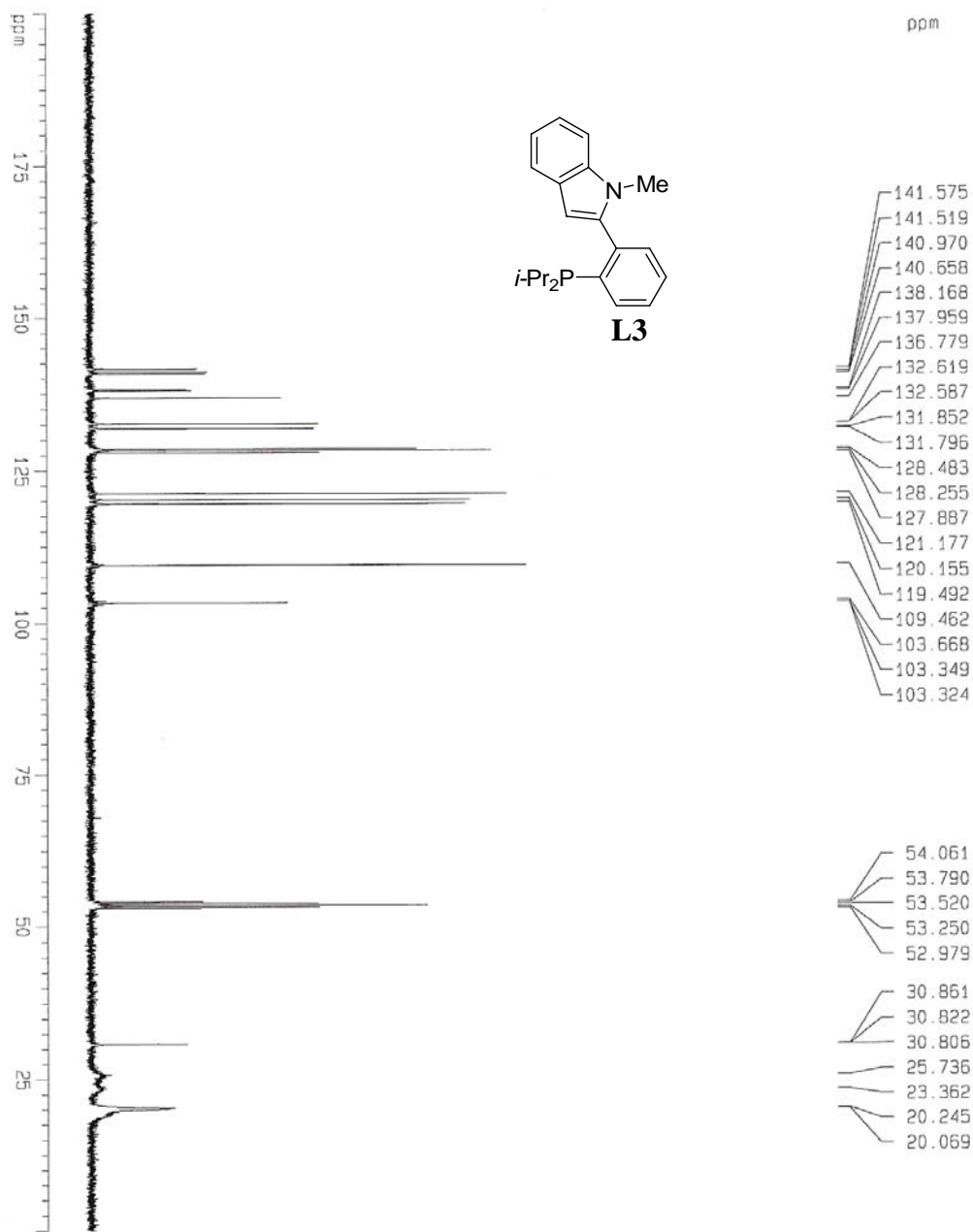
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 SF01 161.9651115 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 71.00 usec
 PL2 120.00 dB
 PL12 17.00 dB
 SF02 400.1324008 MHz

F2 - Processing parameters
 SI 32768
 SF 161.9755831 MHz
 KOK EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 20.00 cm
 F1P 120.000 ppm
 F1 19437.07 Hz
 F2P -60.000 ppm
 F2 -9718.54 Hz
 PPMCM 9.00000 ppm/cm
 HZCM 1457.78027 Hz/cm





Current Data Parameters

NAME	CCP1nd01e
EXPNO	26
PROCNO	1

F2 - Acquisition Parameters

Date_	20070531
Time	11.20
INSTRUM	ddx400
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl ₃
NS	128
DS	0
SWH	25125.629 Hz
FIDRES	0.191693 Hz
AQ	2.6083827 sec
RG	9195.2
DE	19.900 usec
TE	4.50 usec
D1	3.00000000 sec
d11	0.03000000 sec

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

NUC1	¹³ C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	h81t216
NUC2	¹ H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

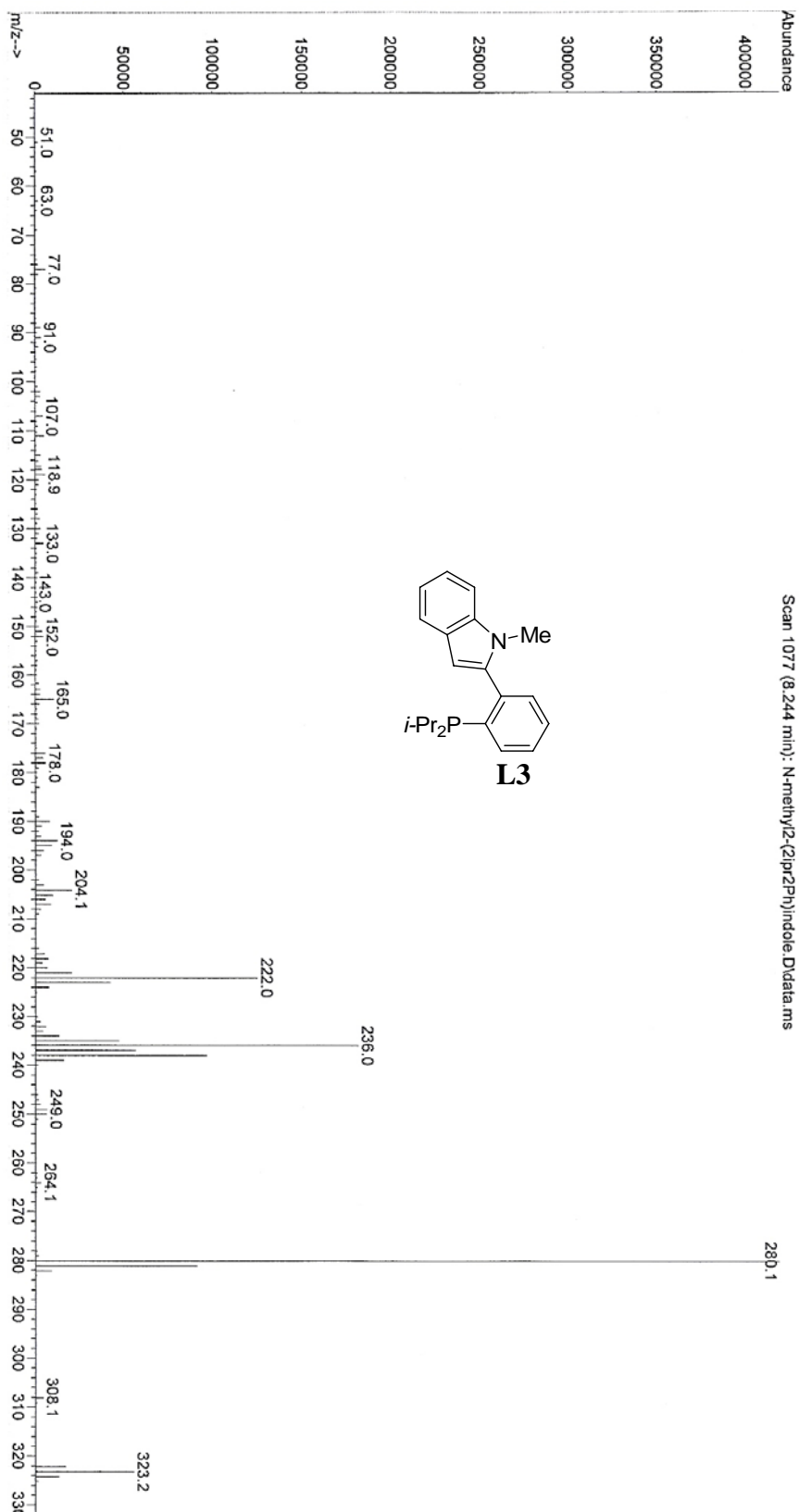
F2 - Processing parameters

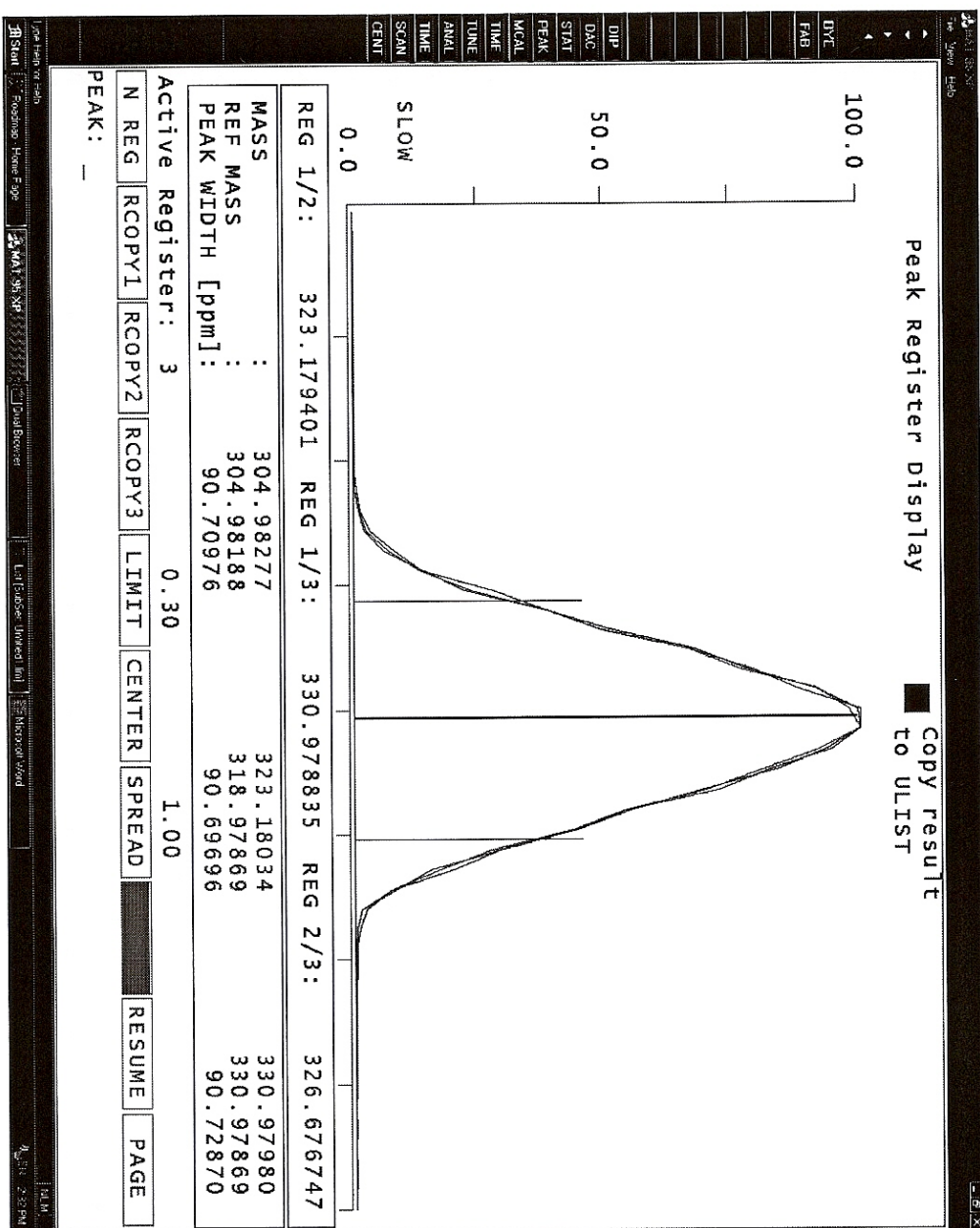
SI	65536
SF	100.6127679 MHz
KDM	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

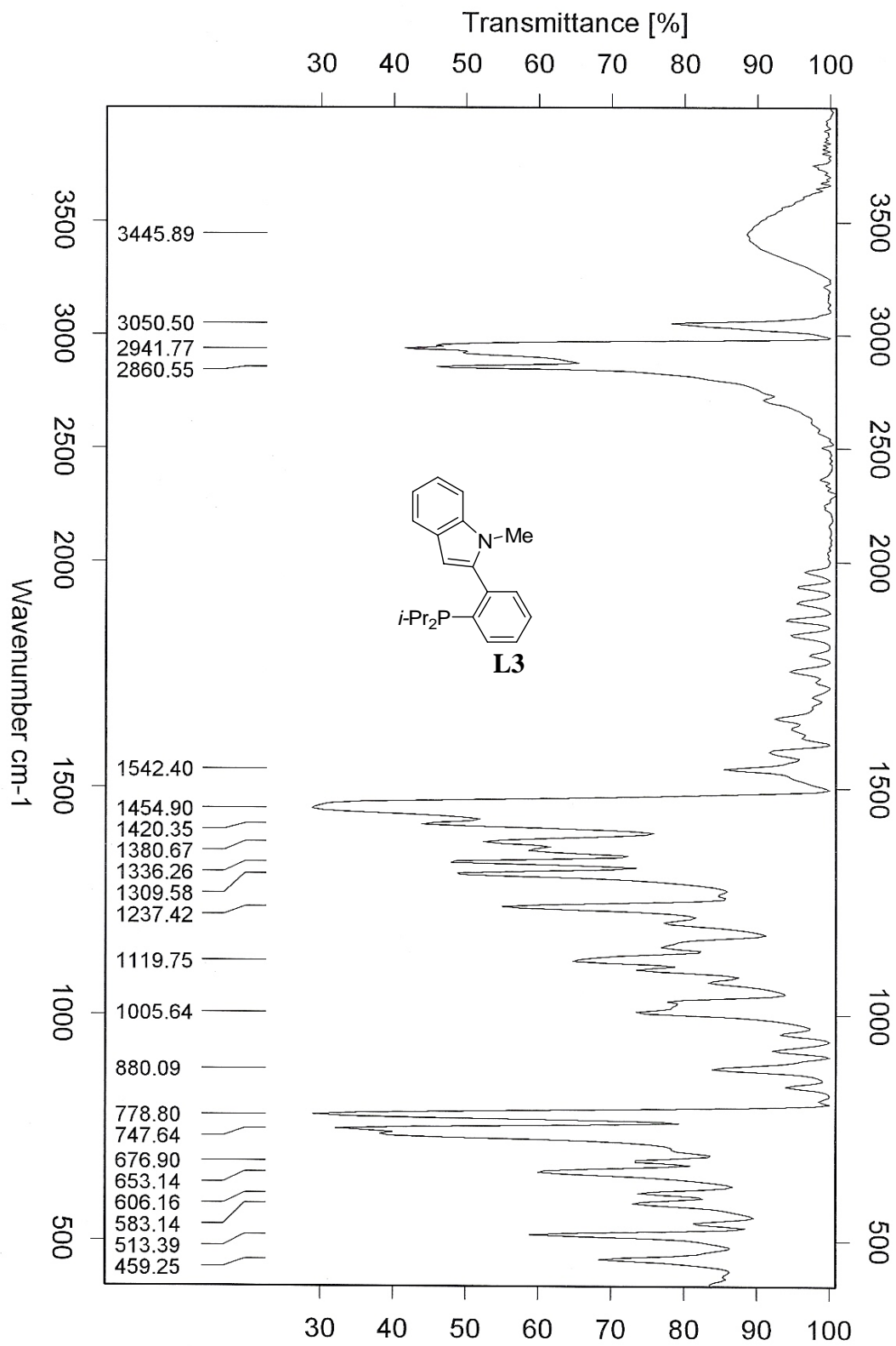
1D NMR plot parameters

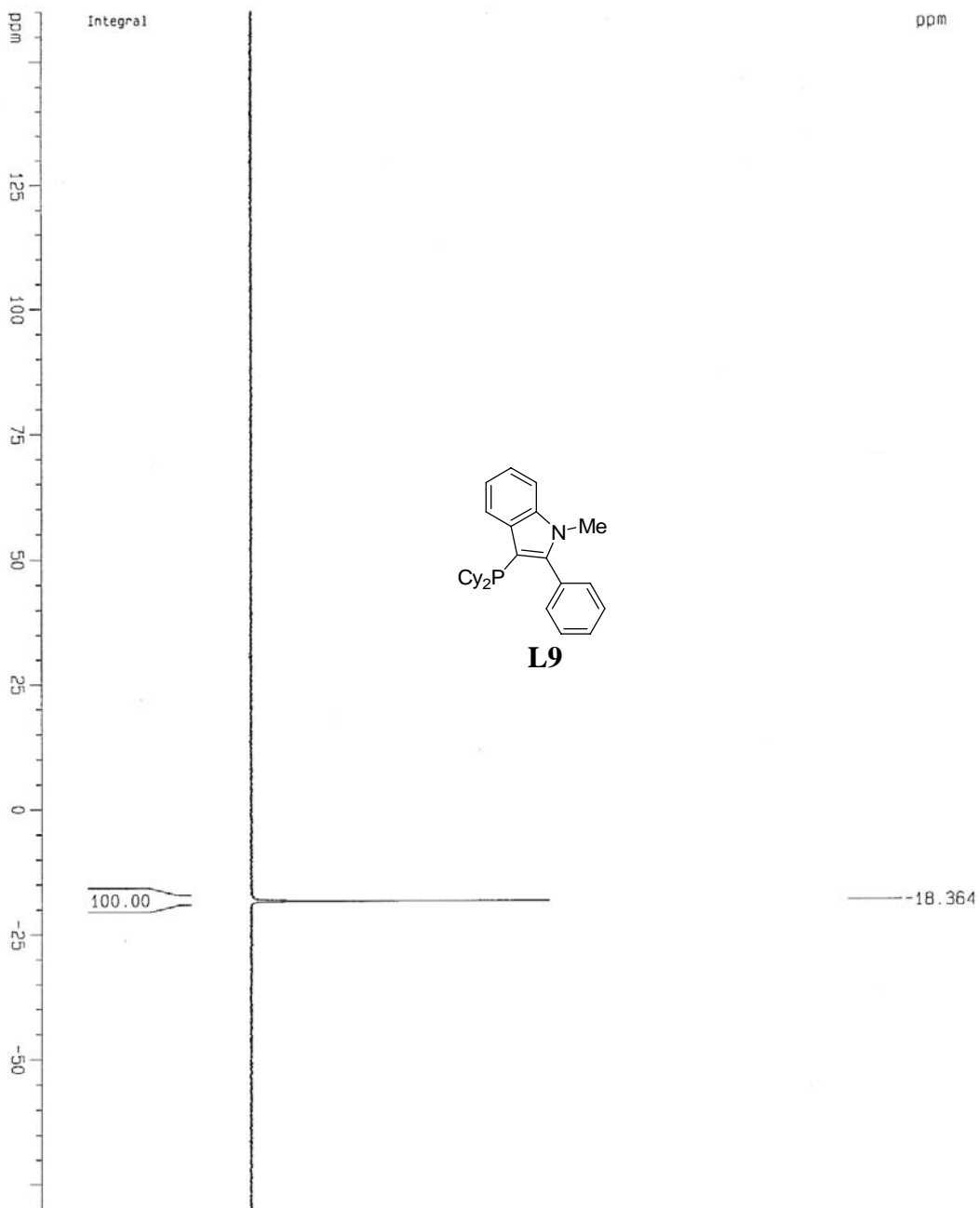
CX	19.50 cm
F1P	200.000 ppm
F1	20122.55 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCK	10.25641 ppm/cm
HZCK	1031.92590 Hz/cm

File : C:\msdchem\1\DATA\cmsc\C-Pphos\N-methyl2-(2ipr2Ph) indole.D
Operator :
Acquired : 30 May 2007 20:57 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 8



Accurate Mass Measurement:





Current Data Parameters

NAME	Pincode
EXPNO	100
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070102	20.54

INSTRUM 60x400
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 128
DS 0
SWH 40661.801 Hz
FIDRES 0.742920 Hz
AQ 0.6734324 sec
RG 13004
DM 10.275 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec

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

NUC1	31P
P1	7.20 usec
PL1	-6.00 dB
SFO1	161.905115 MHz

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

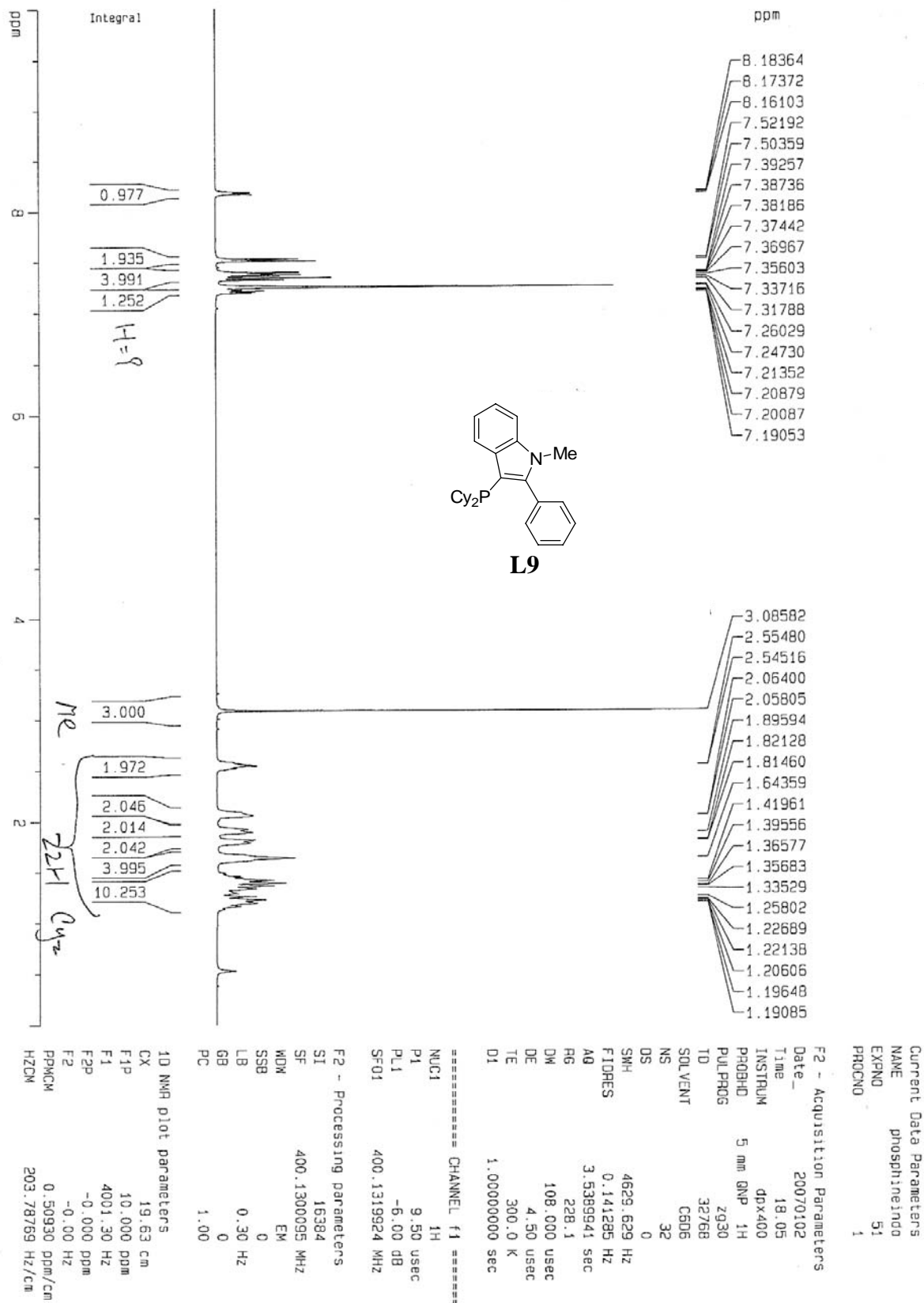
CPDPRG2	waltz16
NUC2	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1319010 MHz

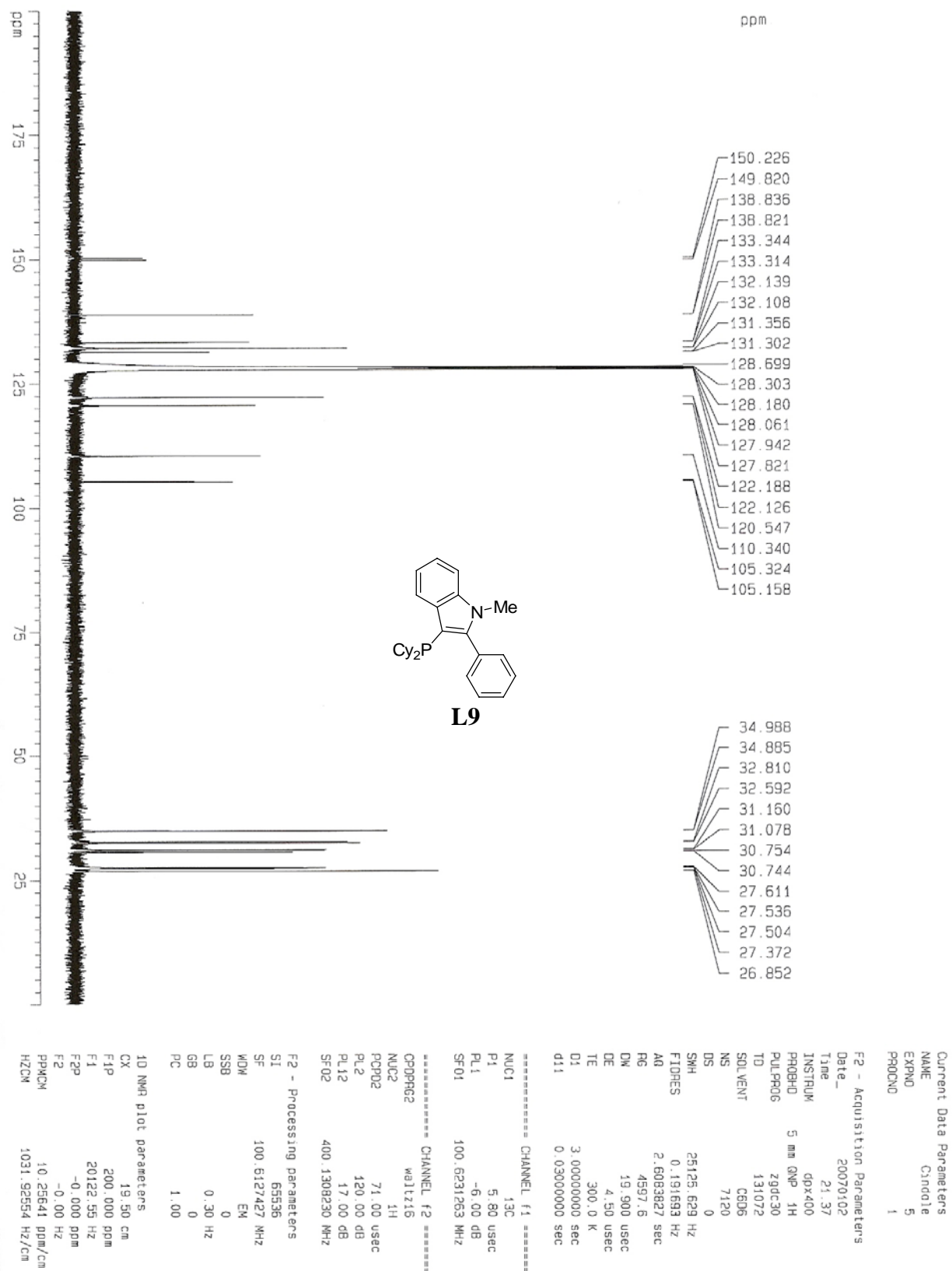
F2 - Processing parameters

SF	32768
SF	161.9755831 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

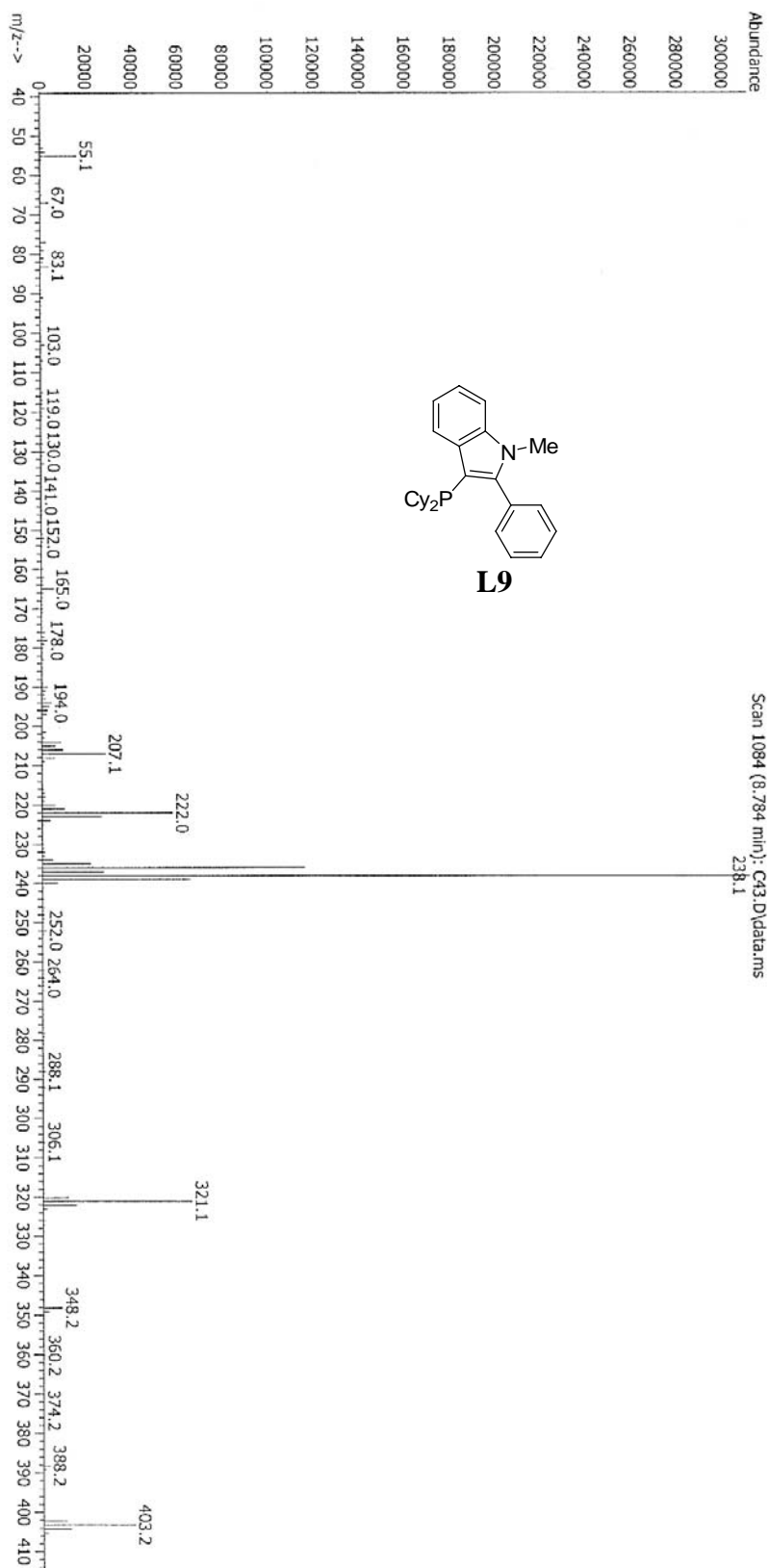
10 NMR plot parameters

CX	20.00 cm
F1P	150.000 ppm
F1	25815.09 Hz
F2P	-80.000 ppm
F2	-12598.05 Hz
PPMCH	12.00000 ppm/ci
HZCM	1943.70591 Hz/cm





File :D:\msdchem\1\DATA\cms0\catalysis\C43.D
Operator :
Acquired : 20 Dec 2006 16:56 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 2



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 60.0

Selected filters: None

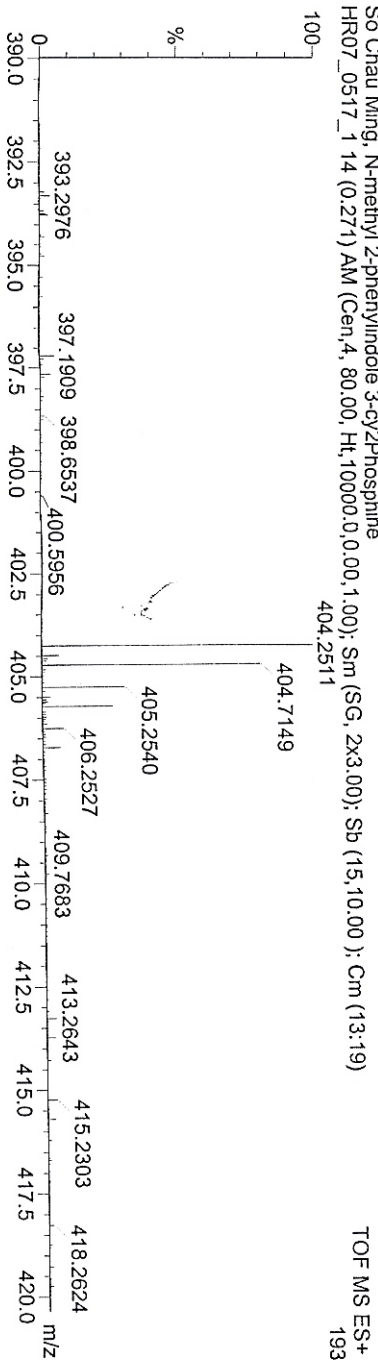
Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-28 H: 0-1000 N: 0-1 O: 0-1 P: 0-1

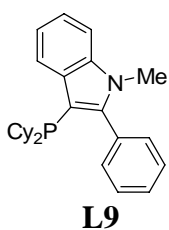
So Chau Ming, N-methyl 2-phenylindole 3-cy2Phosphine
HR07_0517_1 14 (0.271) AM (Cen, 4, 80.00, Ht, 10000.0, 0.00, 1.00); Sm (SG, 2x3.00); Sb (15, 10.00); Cm (13, 19)

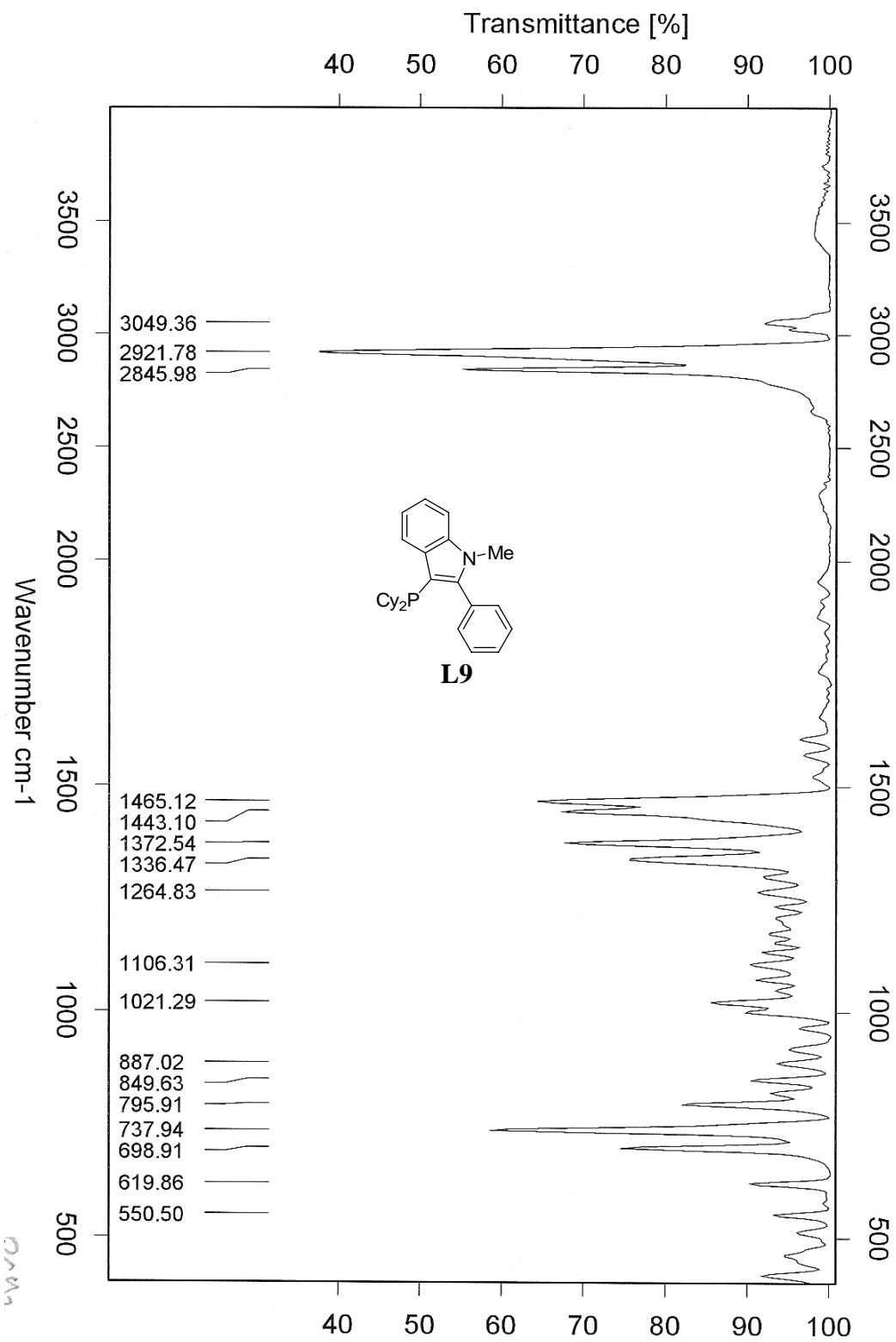


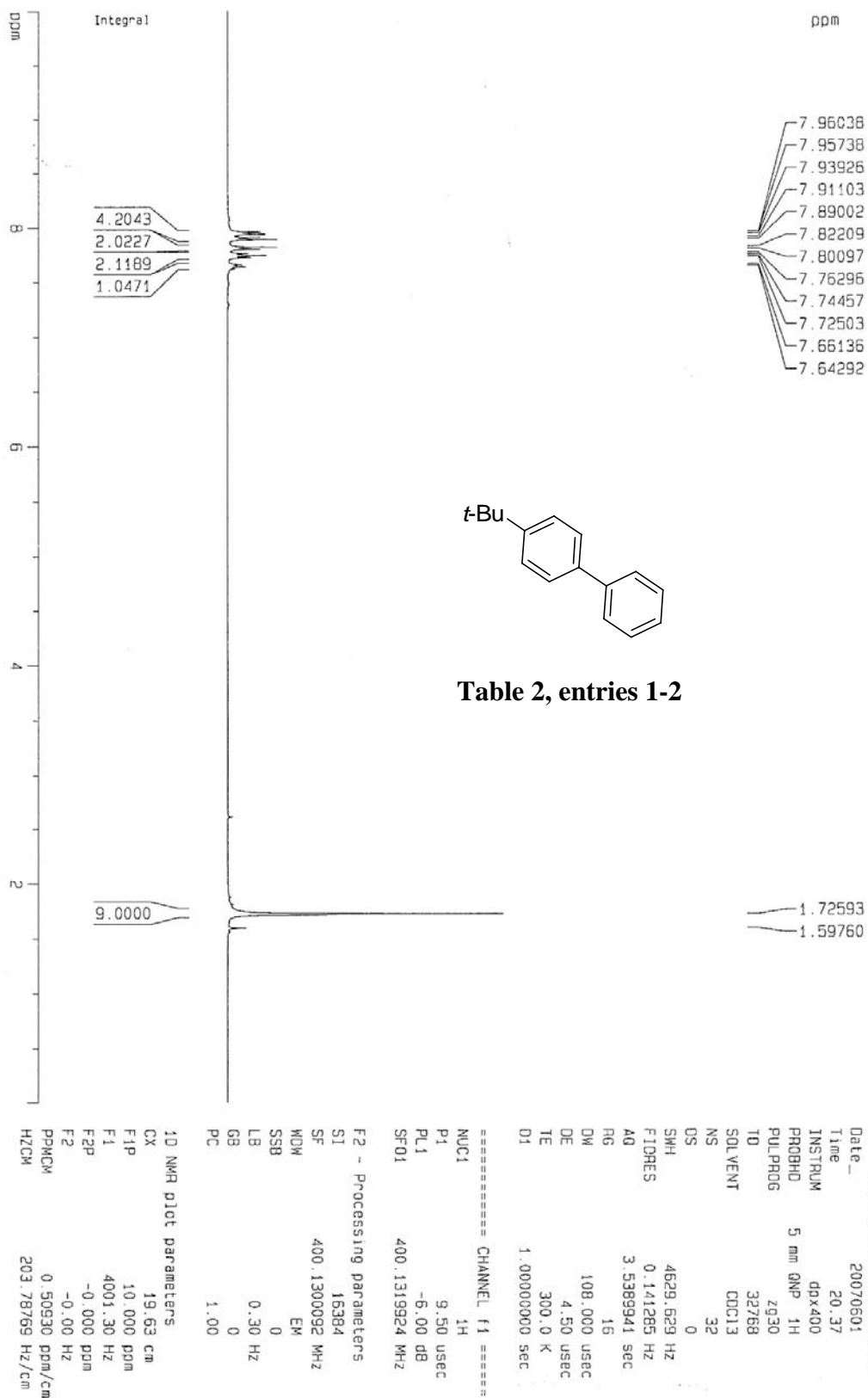
Minimum:
Maximum:

5.0 5.0 -1.5 60.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
404.2511	404.2507	0.4	1.0	11.5	1.1	C27 H35 N P







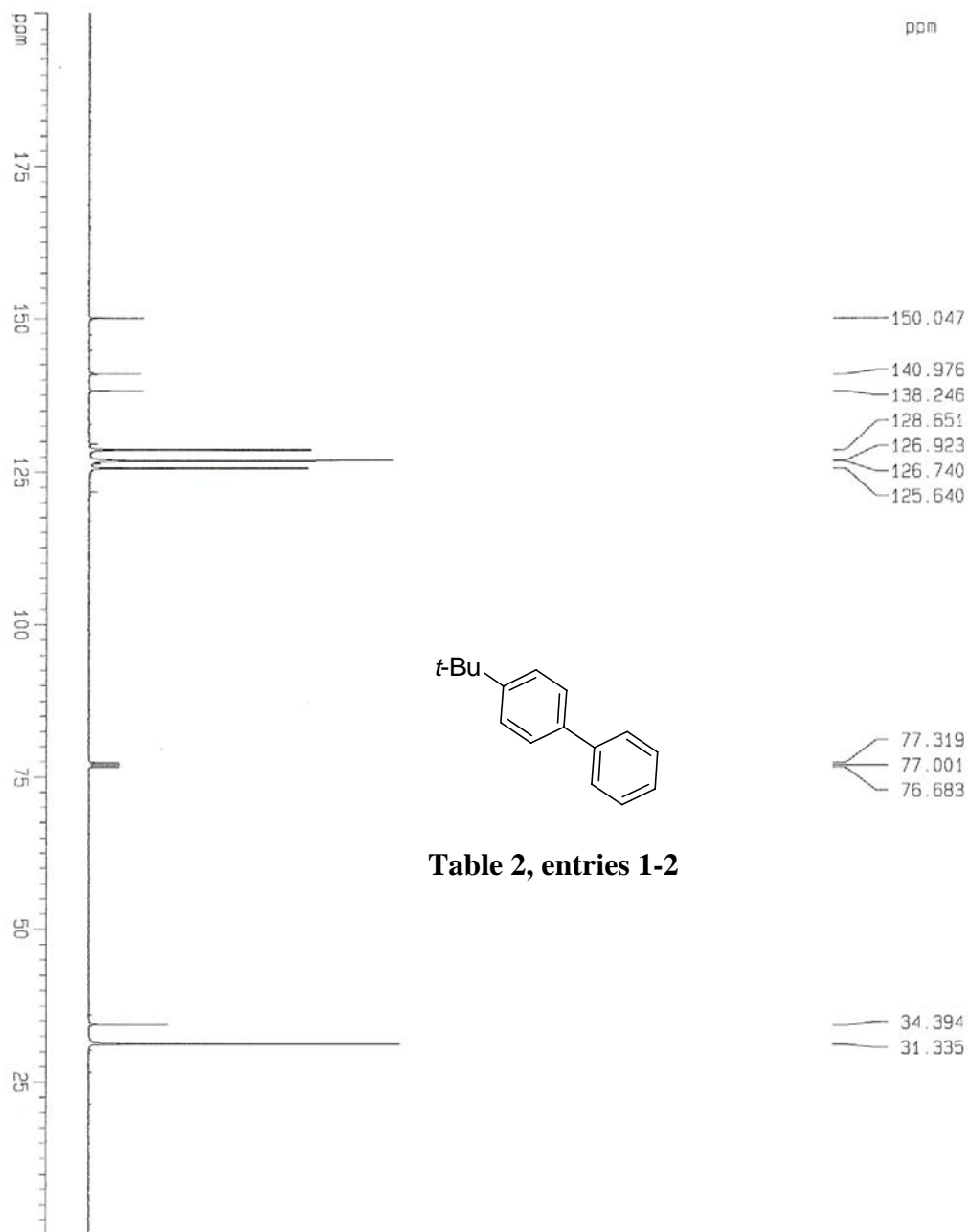


Table 2, entries 1-2

Current Data Parameters

NAME	Coupling	
EXPNO	30	
PROCNO	1	

F2 - Acquisition Parameters

Date_	20070601
Time	20.41
INSTRUM	gpx400
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl3
NS	64
DS	0
SWH	25125.629 Hz
FIDRES	0.191693 Hz
AQ	2.5003827 sec
RG	8192
DM	19.900 usec
DE	4.50 usec
TE	300.0 K
D1	3.00000000 sec
d11	0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SI	65536
SF	100.6128150 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.50 cm
F1P	200.000 ppm
F1	20122.56 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPKCM	10.25641 ppm/cm
HZCM	1031.92638 Hz/cm

File : C:\msdchem\1\DATA\cmso\CT\c289-2.D
Operator :
Acquired : 1 Jun 2007 19:37 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1

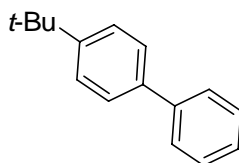
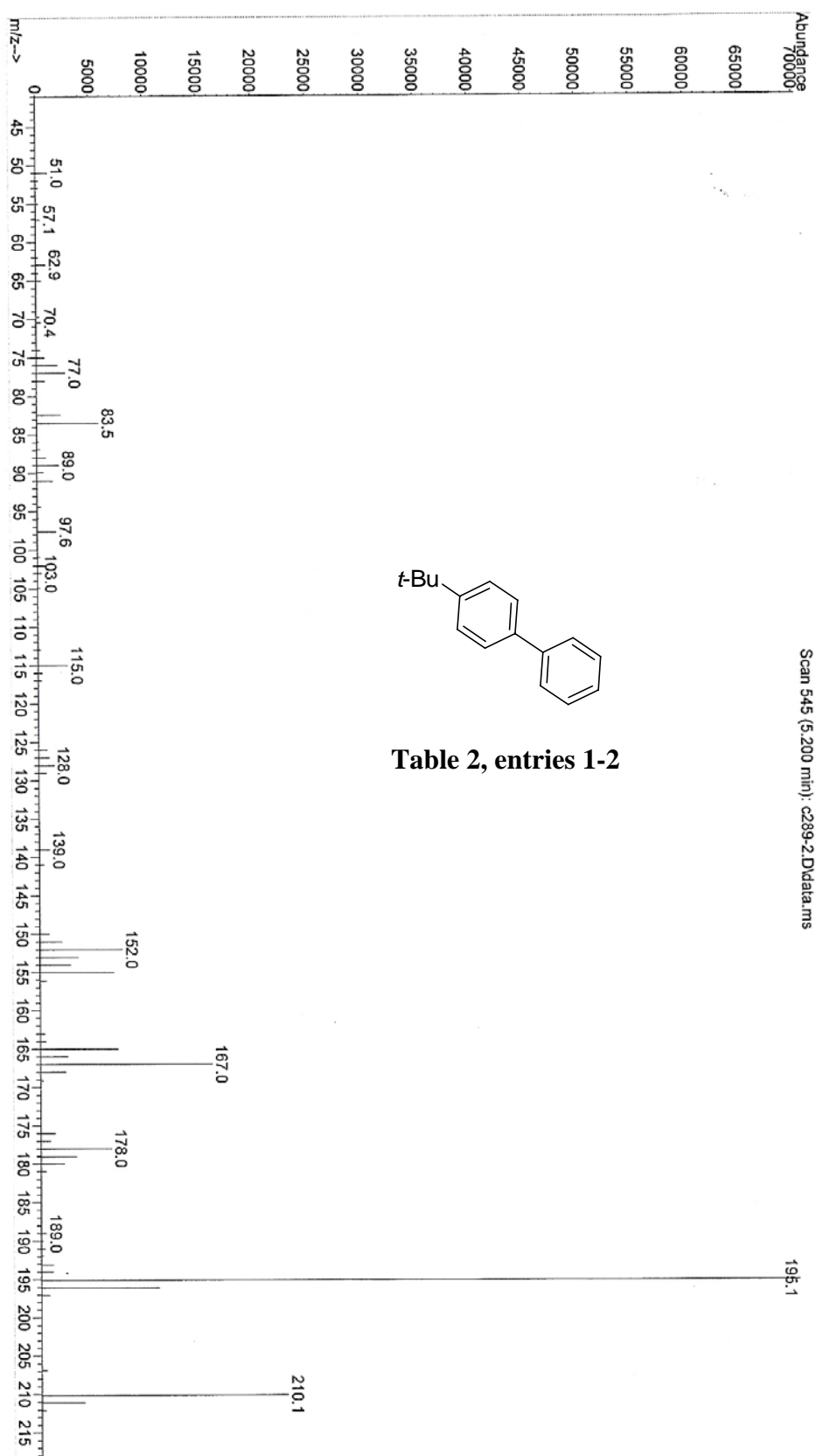
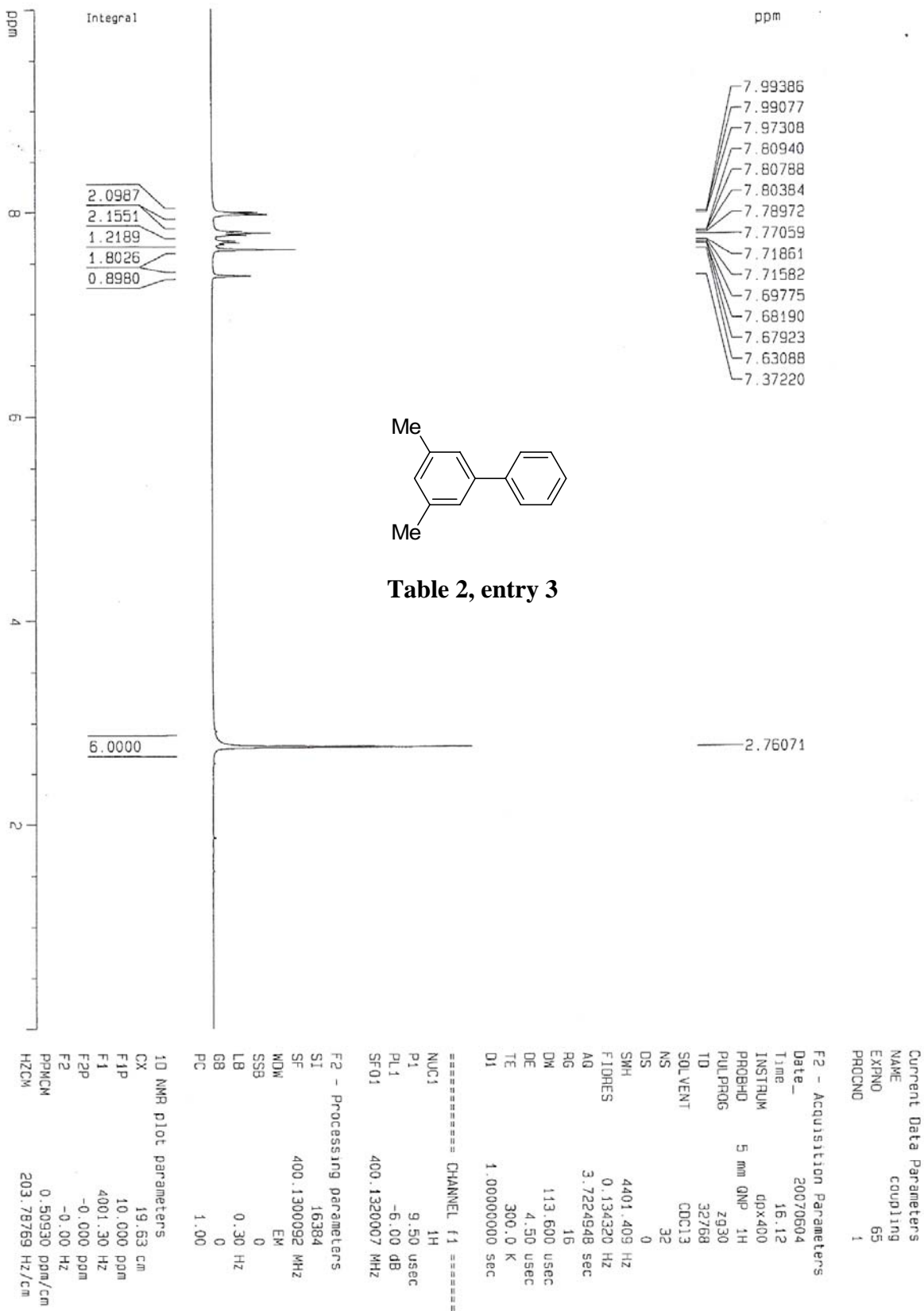


Table 2, entries 1-2





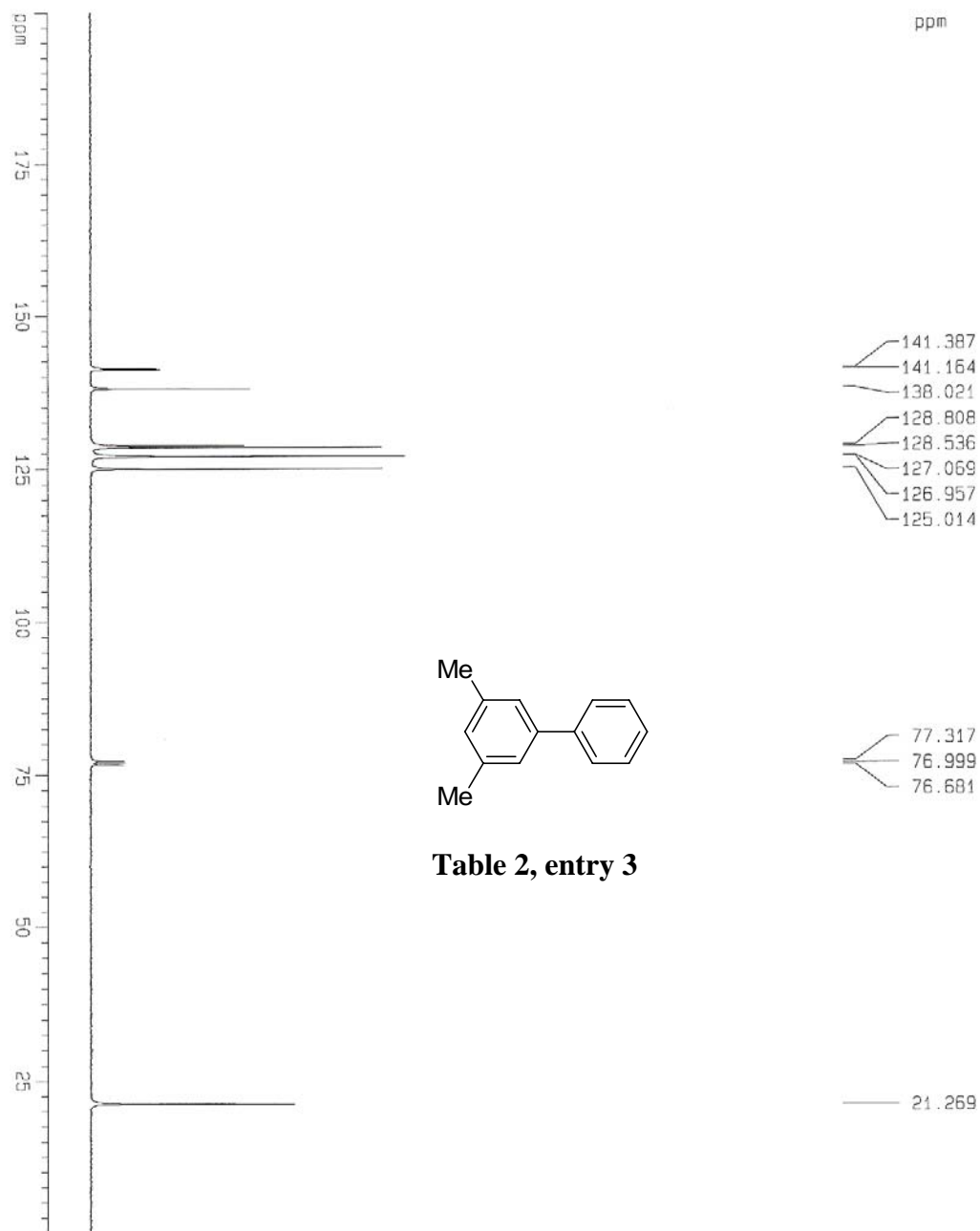


Table 2, entry 3

```

Current Data Parameters
NAME          Coupling
EXPNO         31
PROCNO        1

F2 - Acquisition Parameters
Date_         20070604
Time          15.15
INSTRUM       dpx400
PROBHD        5 mm QNP 1H
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            64
DS            0
SWH           25125.629 Hz
FIDRES        0.191693 Hz
AQ            2.6093827 sec
RG            8192
DE            19.900 usec
TE            300.0 K
D1            3.00000000 sec
d11           0.03000000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            5.80 usec
PL1           -6.00 dB
SFO1         100.6231263 MHz

===== CHANNEL f2 =====
CPOPRG2       waltz16
NUC2          1H
PCPD2         71.00 usec
PL2           120.00 dB
PL12         17.00 dB
SFO2         400.1326008 MHz

F2 - Processing parameters
SI            65536
SF            100.6128242 MHz
WDW           EM
SSB           0
LB            4.00 Hz
GB            0
PC            1.00

1D NMR plot parameters
CX            19.50 cm
F1P           200.000 ppm
F1            201.2256 Hz
F2P           -0.000 ppm
F2            -0.00 Hz
PPMCK         10.25641 ppm/c
HZCK          1031.92539 Hz/cm
  
```

File : C:\msdchem\1\DATA\cms0\CT\c307.D
Operator :
Acquired : 4 Jun 2007 12:28 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 3

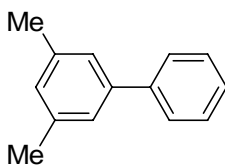
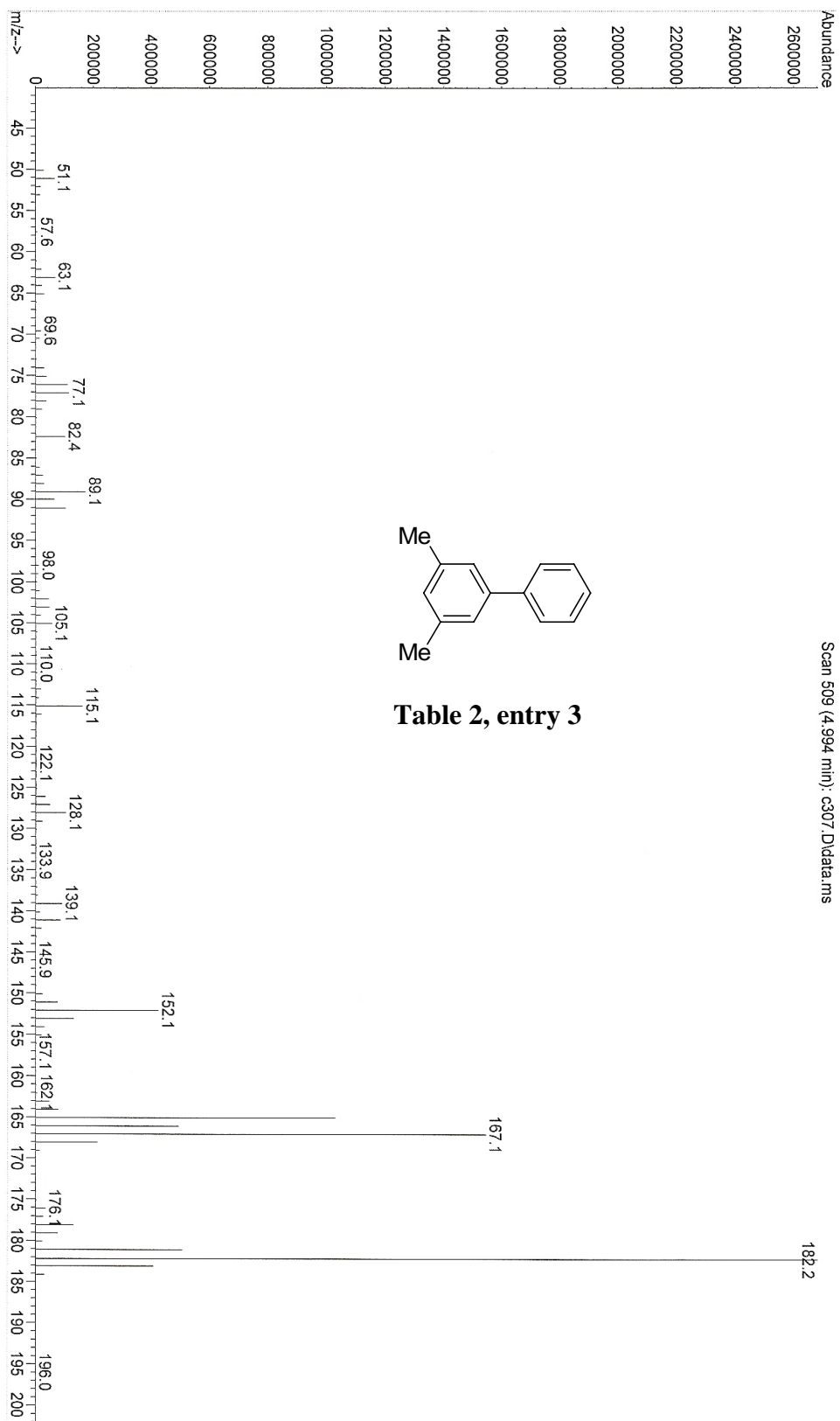


Table 2, entry 3



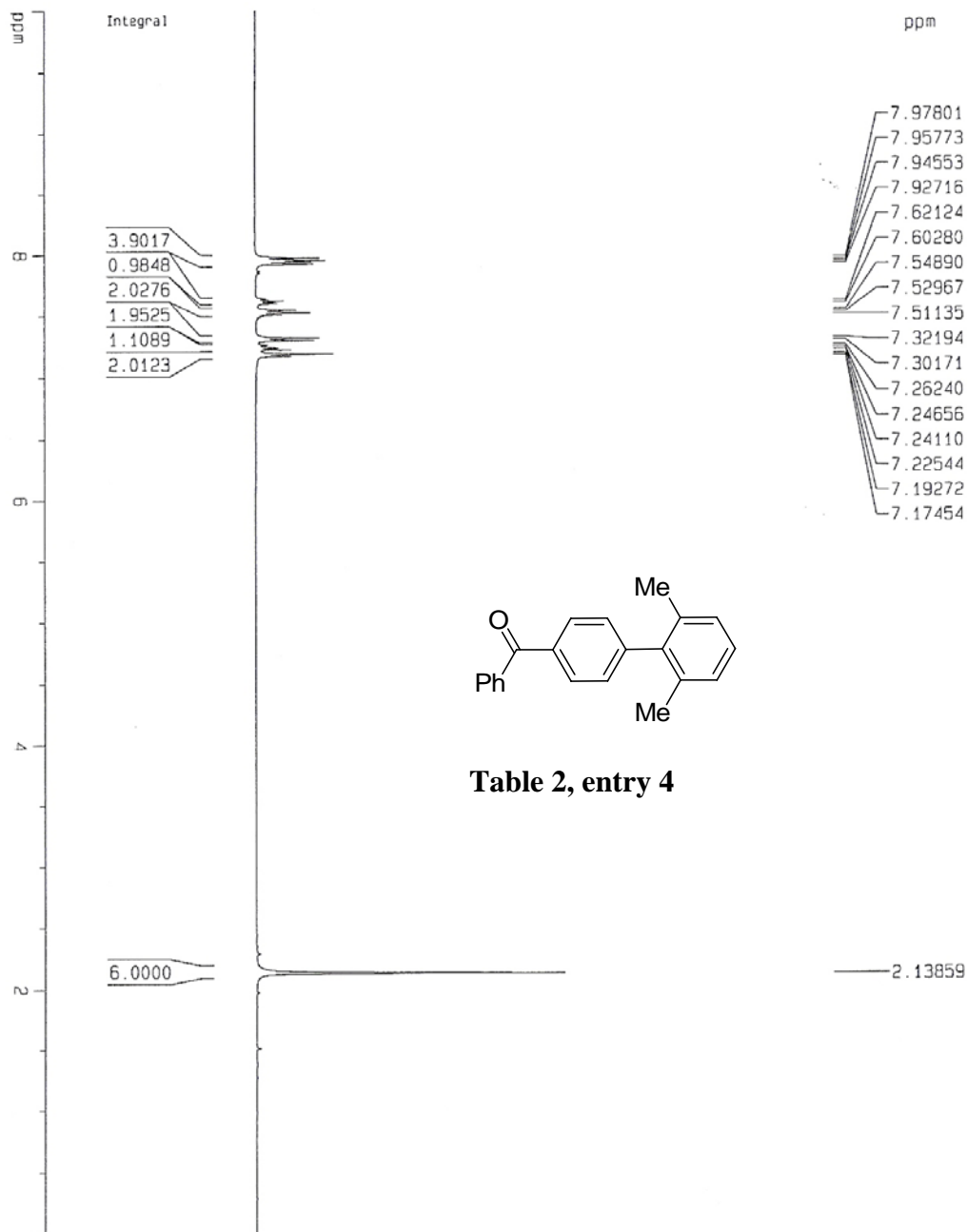


Table 2, entry 4

Current Data Parameters

NAME	COUPLING
EXPNO	75
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070620	17.06
INSTRUM	dx400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	4401.409 Hz
FIDRES	0.134320 Hz
AQ	3.7224948 sec
RG	18
DM	113.600 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	16384
SF	400.130088 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.63 cm
F1P	10.000 ppm
F1	4001.30 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCK	0.50930 ppm/c
HZCM	203.78769 Hz/cm

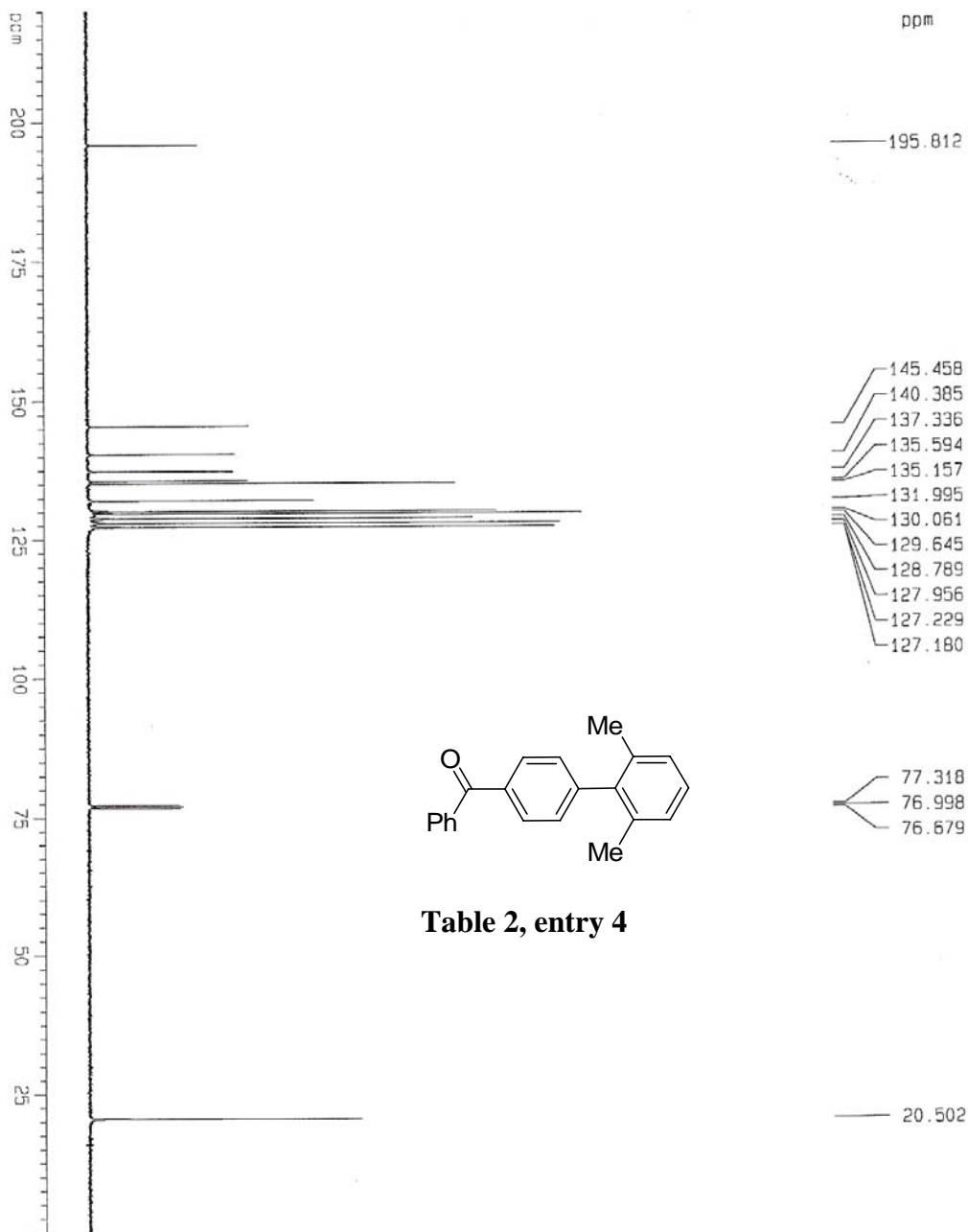


Table 2, entry 4

```

Current Data Parameters
NAME                      Coupling
EXPNO                     40
PROCNO                    1

F2 - Acquisition Parameters
Date_                     20070620
Time                      17.08
INSTRUM                  dp400
PROBHD                   5 mm QNP 1H
PULPROG                  zgpg30
TD                        131072
SOLVENT                  CDCl3
NS                        64
DS                        0
SWH                      25125.629 Hz
FIDRES                   0.191693 Hz
AQ                        2.6083827 sec
RG                        9192
DM                        19.900 usec
DE                        4.50 usec
TE                        300.0 K
D1                        3.00000000 sec
d11                       0.03000000 sec

===== CHANNEL f1 =====
NUC1                      13C
P1                         5.80 usec
PL1                       -6.00 dB
SFO1                      100.6231263 MHz

===== CHANNEL f2 =====
CPDPRG2                  waltz16
NUC2                      1H
PCPD2                     71.00 usec
PL2                       120.00 dB
PL12                      17.00 dB
SFO2                      400.1326008 MHz

F2 - Processing parameters
SI                        65536
SF                        100.6128177 MHz
WDW                        EM
SSB                        0
LB                        1.50 Hz
GB                        0
PC                        1.00

1D NMR plot parameters
CX                        19.50 cm
F1P                       220.000 ppm
F1                         22134.82 Hz
F2P                       -0.000 ppm
F2                        -0.00 Hz
PPMCM                     11.28205 ppm/cm
HZCM                     1135.11902 Hz/cm

```

File : C:\msdchem\1\DATA\cms0\CT\c348.D
Operator :
Acquired : 20 Jun 2007 13:17 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1

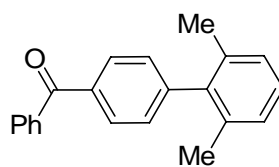
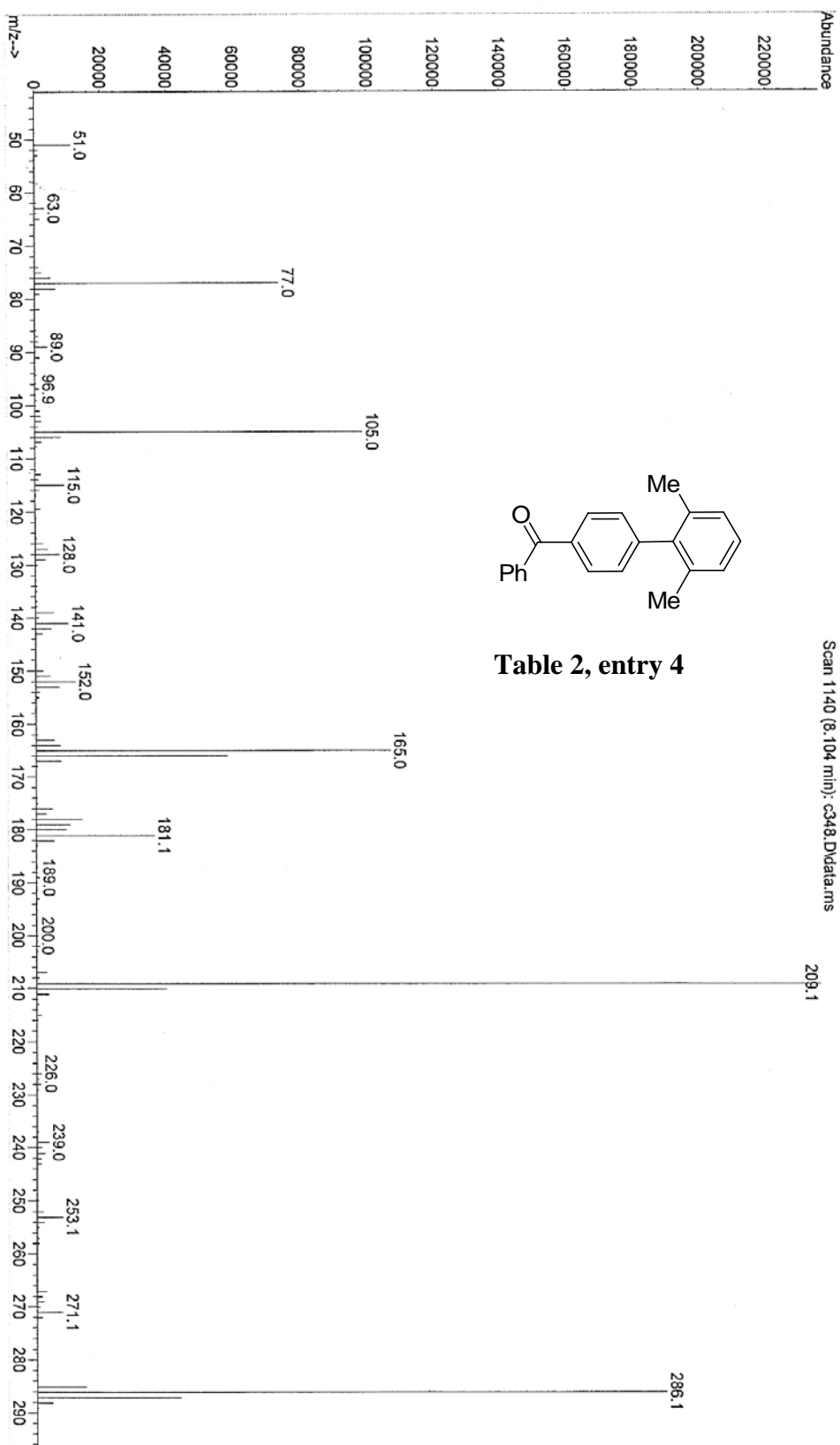


Table 2, entry 4



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-21 H: 0-1000 O: 0-1

So chau Ming, 4-(2',6'-dimethylphenyl)benzophenone

HR07_0724_4 47 (0.891) AM (Gen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (31.57)

287.1442

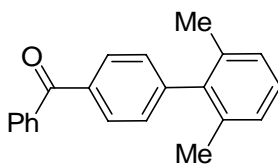
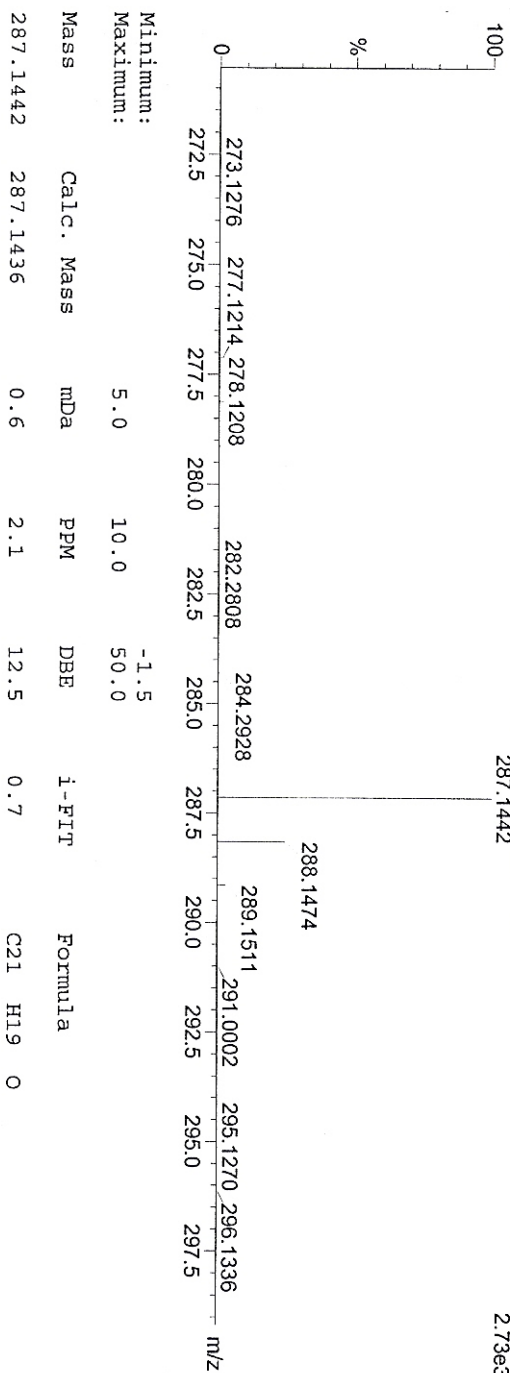
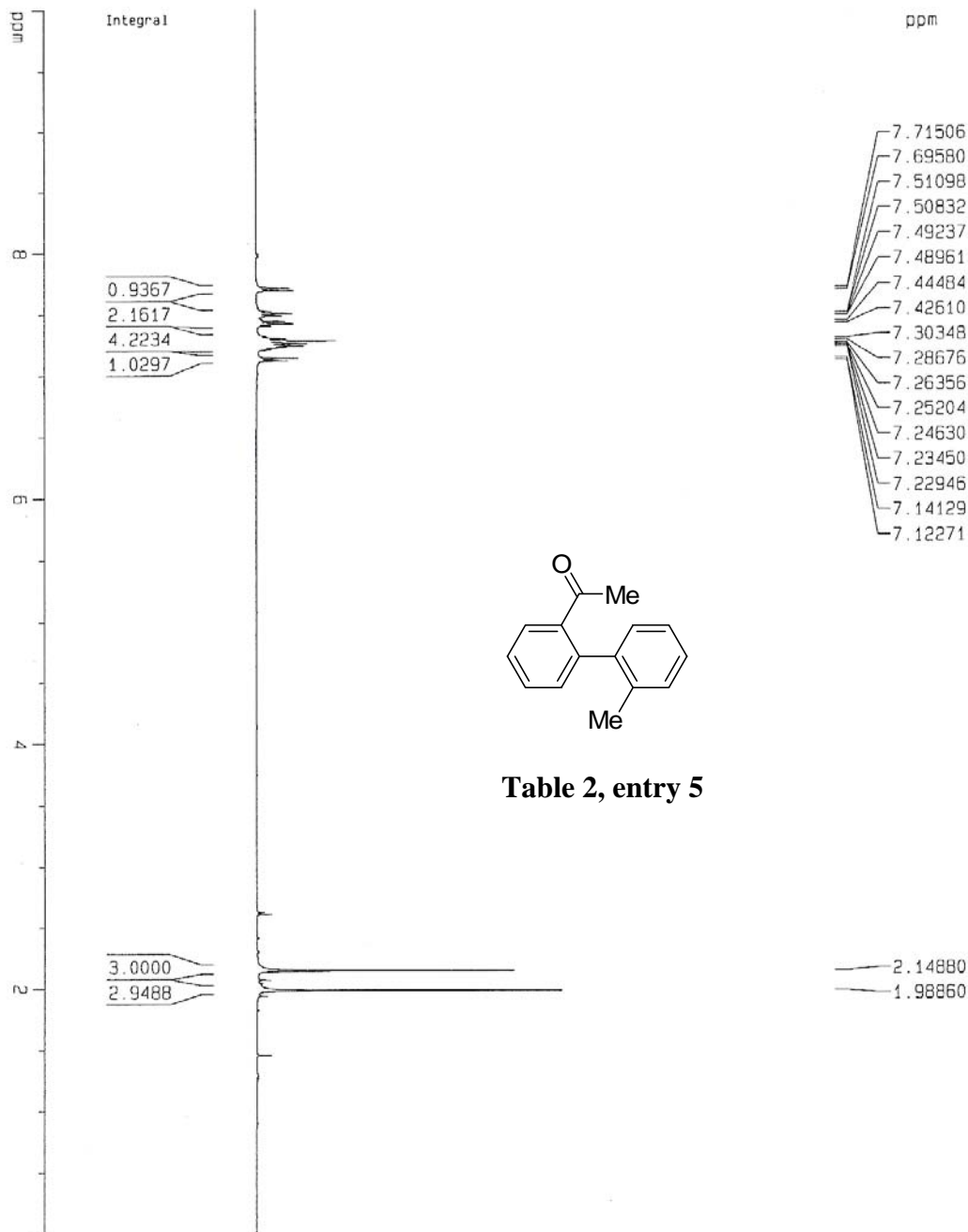
TOF MS ES+
2.73e3

Table 2, entry 4



Minimum: 5.0
Maximum: 10.0
-1.5
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
287.1442	287.1436	0.6	2.1	12.5	0.7	C21 H19 O



Current Data Parameters

NAME	coupling
EXPNO	72
PROCNO	1

F2 - Acquisition Parameters

Date_	20070615
Time	18.13
INSTRUM	cpd400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	4401.409 Hz
FIDRES	0.134320 Hz
RG	3.7224548 sec
DW	35.9
DE	113.600 usec
TE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.132007 MHz

F2 - Processing parameters

SI	16384
SF	400.130088 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.63 cm
F1P	10.000 ppm
F1	4001.30 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	0.50930 ppm/c
HZCM	203.78769 Hz/cm

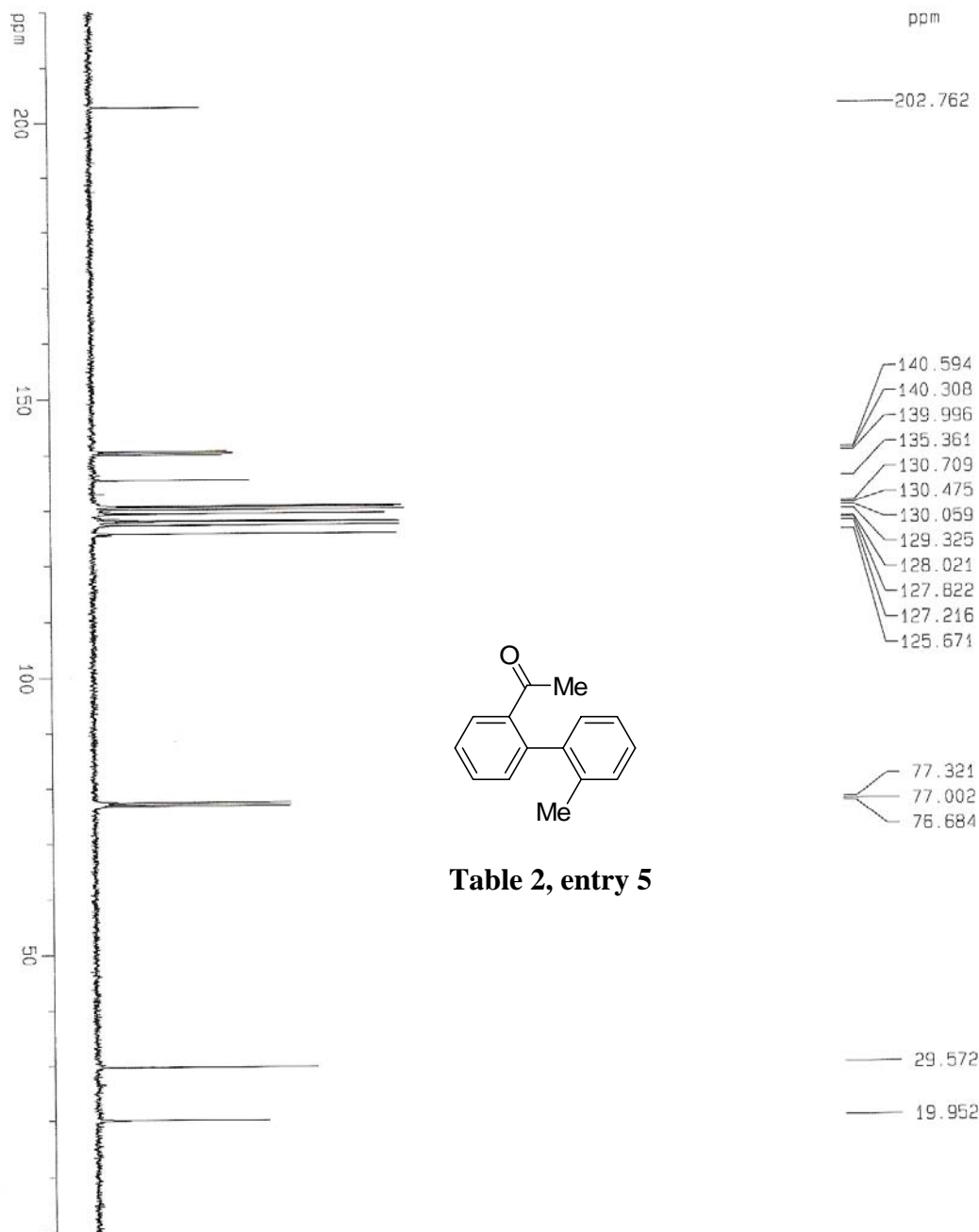


Table 2, entry 5

Current Data Parameters

NAME	Coupling
EXPNO	38
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070615	18.15
INSTRUM	ddx400
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl3
NS	64
DS	0
SWH	25125.629 Hz
FIDRES	0.191693 Hz
AQ	2.6093827 sec
RG	8192
DW	19.500 usec
DE	4.50 usec
TE	300.0 K
D1	3.00000000 sec
d11	0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	zgpg30
NUC2 <td>1H</td>	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SI	65536
SF	100.6127909 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.50 cm
F1P	220.000 ppm
F1	22134.81 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCK	11.28205 ppm
HZCM	1136.11877 Hz

File : C:\msdchem\1\DATA\cms0\CT\c301-3.D
Operator :
Acquired : 7 Jun 2007 15:13 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 2

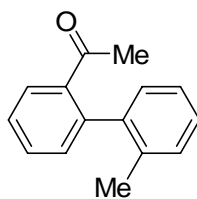
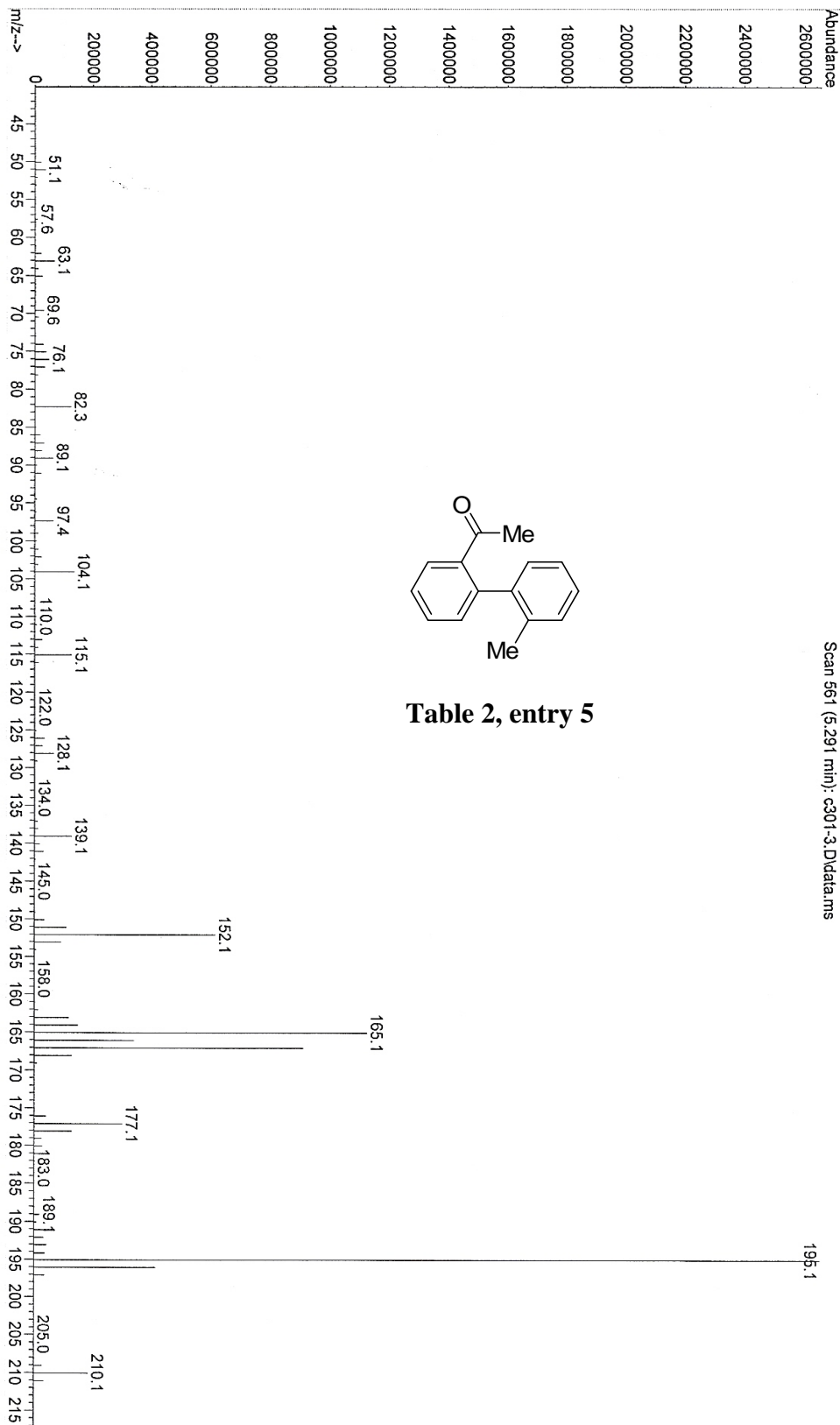


Table 2, entry 5



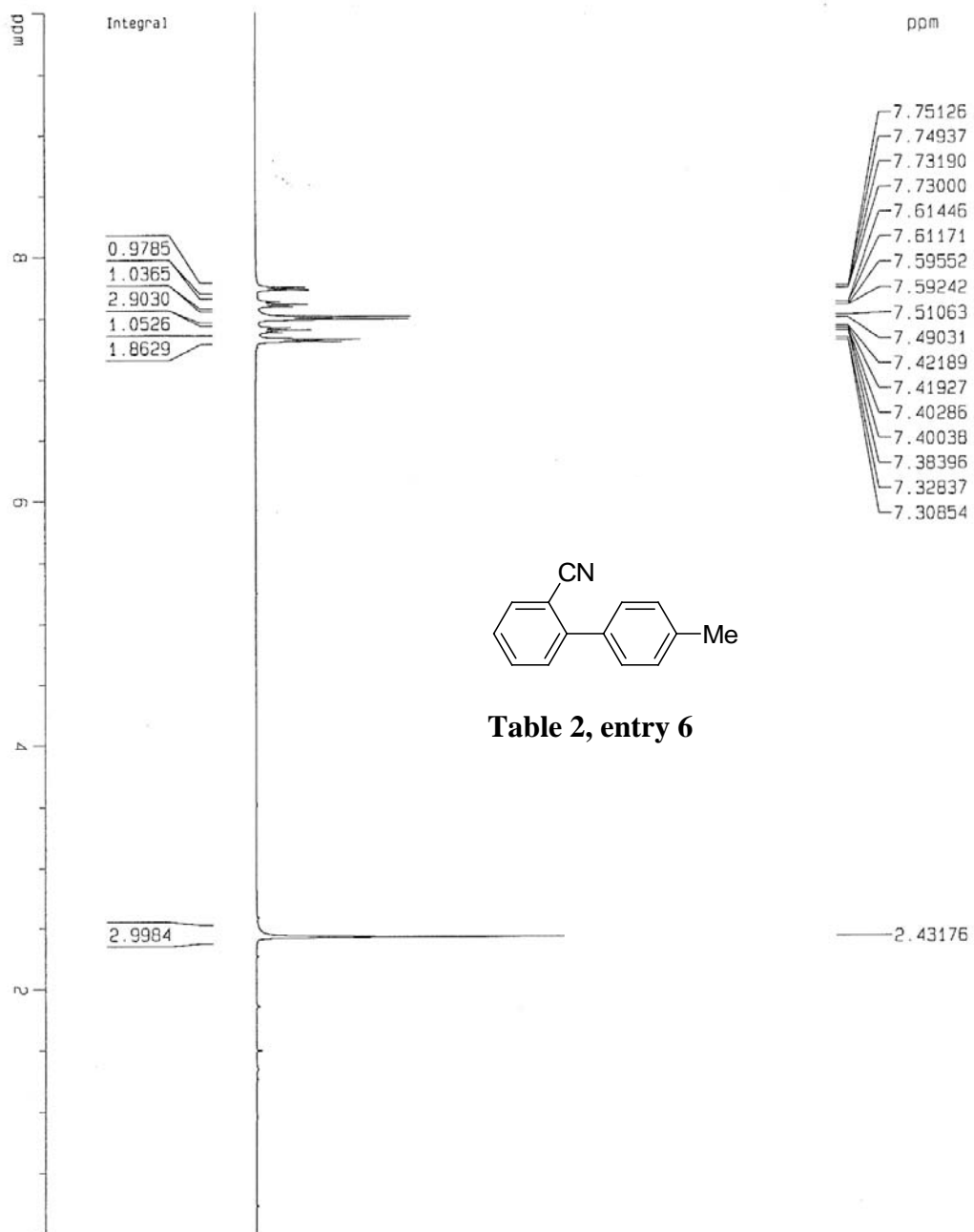


Table 2, entry 6

Current Data Parameters

NAME	coupling
EXPNO	67
PROCNO	1

F2 - Acquisition Parameters

Date_	20070606
Time	13.16
INSTRUM	dp400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	4401.409 Hz
FIDRES	0.134320 Hz
AQ	3.7224948 sec
RG	28.5
DK	113.600 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.1320007 MHz

F2 - Processing Parameters

SI	16384
SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.63 cm
F1P	10.000 ppm
F1	4001.30 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	0.50930 ppm/c
HZCM	203.78769 Hz/cm

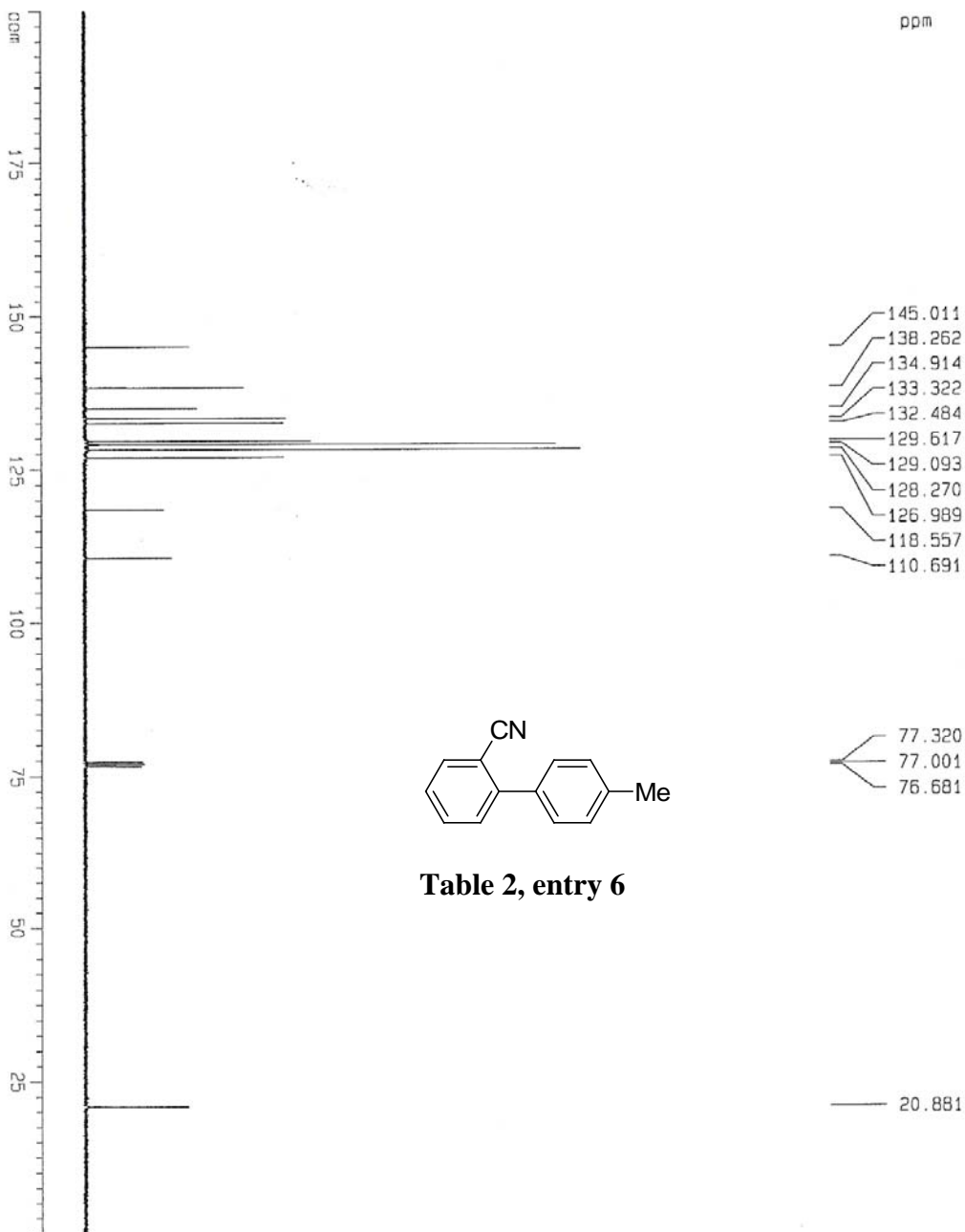


Table 2, entry 6

Current Data Parameters

NAME	Coupling
EXPNO	33
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070605	13.21

INSTRUM 5 mm QNP 1H
PROBHD zgpg30
PULPROG zgpg30
TO 131072
SOLVENT CDCl3
NS 32
DS 0
SWH 25125.629 Hz
FIDRES 0.191693 Hz
AQ 2.6083827 sec
RG 8192
DM 19.900 usec
DE 4.50 usec
TE 300.0 K
D1 3.00000000 sec
d11 0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	waltz16
NUC2 <td>1H</td>	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SI	65536
SF	100.6128139 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.50 cm
F1P	200.000 ppm
F1	20122.56 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	10.25641 ppm/c
HZCM	1031.92639 Hz/cm

File : C:\msdchem\1\DATA\cms0\CT\c316.D
Operator :
Acquired : 5 Jun 2007 12:22 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 2

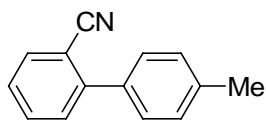
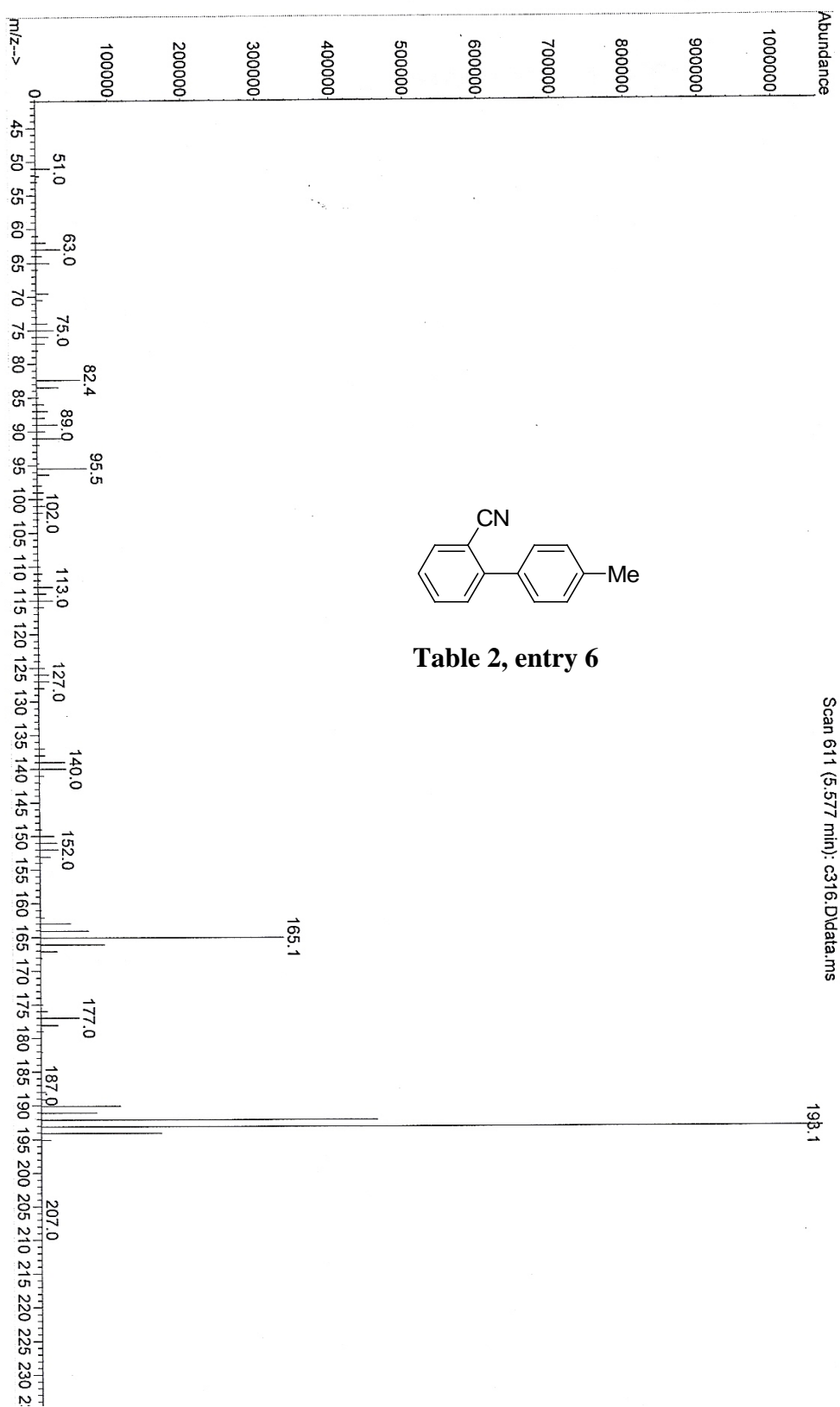


Table 2, entry 6



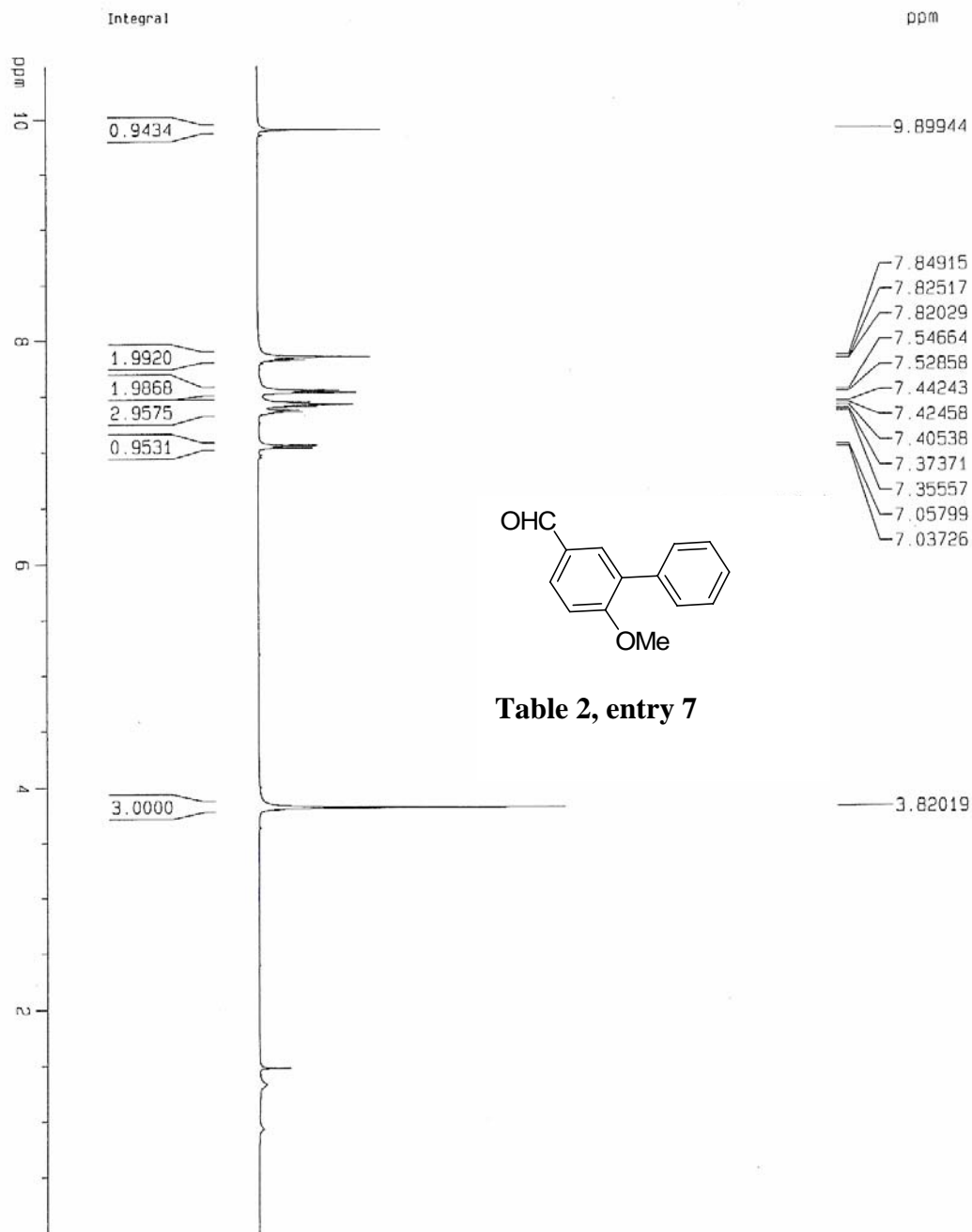


Table 2, entry 7

Current Data Parameters

NAME	coupling
EXPNO	71
PROCNO	1

F2 - Acquisition Parameters

Date_	20070610
Time	17.05
INSTRUM	gdx400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	4401.409 Hz
FIDRES	0.134320 Hz
AQ	3.7224948 sec
RG	16
DM	113.600 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	16384
SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.63 cm
F1P	11.000 ppm
F1	4401.43 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	0.56023 ppm/c
HZCM	224.16646 Hz/cm

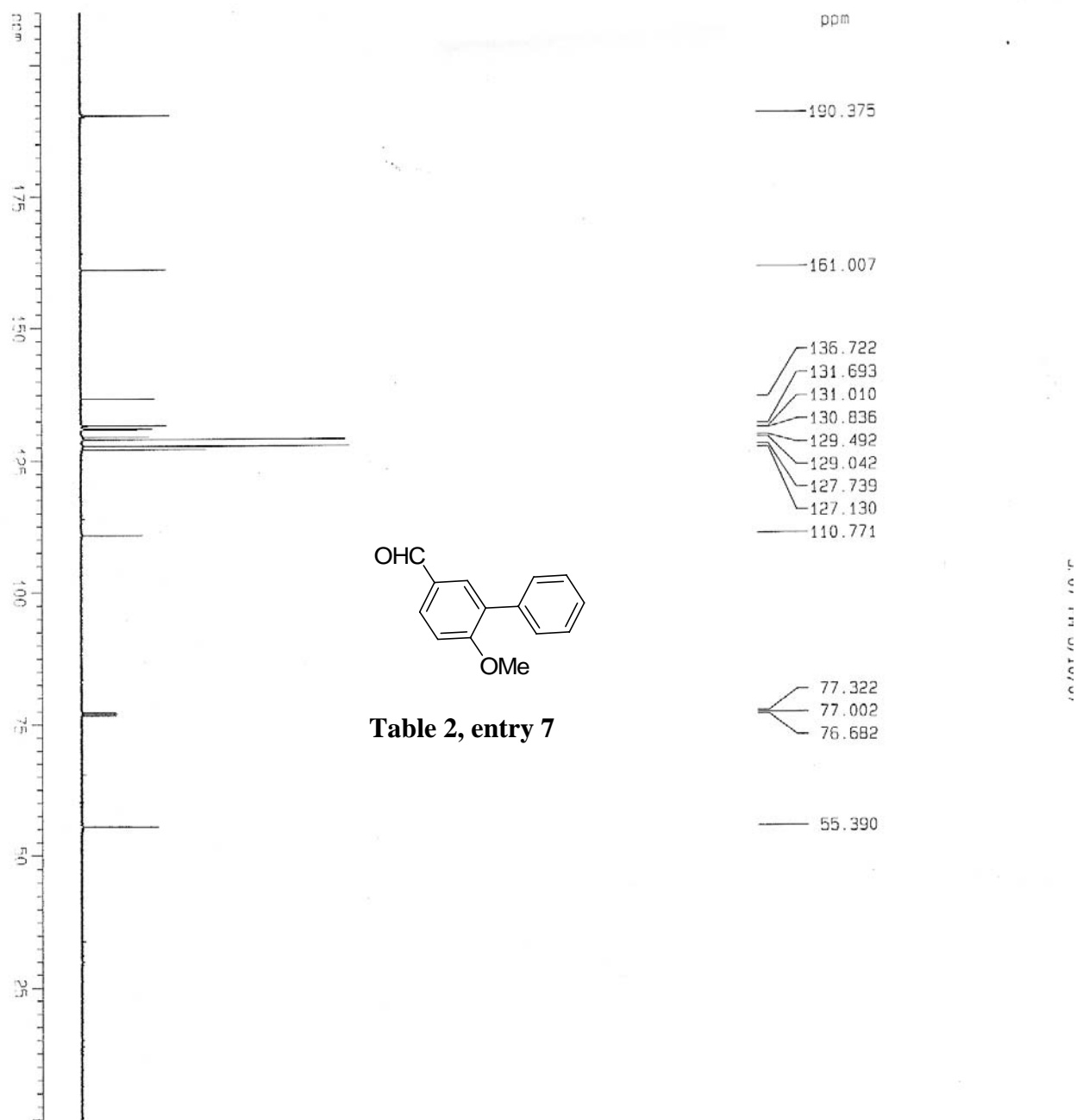


Table 2, entry 7

```

Current Data Parameters
NAME                      Coupling
EXPNO                     35
PROCNO                    1

F2 - Acquisition Parameters
Date_                    20070610
Time                     17.07
INSTRUM                  gpc400
PROBHD                   5 mm QNP 1H
PULPROG                  zgpg30
TD                       131072
SOLVENT                  CDCl3
NS                        45
DS                        0
SWH                      25125.629 Hz
FIDRES                   0.191693 Hz
AQ                        2.6083827 sec
RG                        8192
DE                       19.500 usec
TE                       300.0 K
D1                       3.00000000 sec
d11                      0.03000000 sec

===== CHANNEL f1 =====
NUC1                      13C
P1                        5.80 usec
PL1                      -6.00 dB
SF01                     100.6231253 MHz

===== CHANNEL f2 =====
CPDPRG2                  waltz16
NUC2                      1H
PCPD2                    71.00 usec
PL2                      120.00 dB
PL12                     17.00 dB
SF02                     400.1326008 MHz

F2 - Processing parameters
SI                        65536
SF                      100.6128189 MHz
WDW                      EM
SSB                      0
LB                       0.50 Hz
GB                      0
PC                       1.00

1D NMR plot parameters
CX                      19.50 cm
F1P                     210.000 ppm
F1                      21128.69 Hz
F2P                     0.000 ppm
F2                      0.00 Hz
PPWCH                  10.76923 ppm/
HZCH                   1083.52236 Hz/c

```

File : C:\msdchem\1\DATA\cms0\CT\c322-1.D
Operator :
Acquired : 8 Jun 2007 14:14 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1

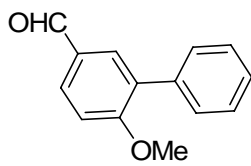
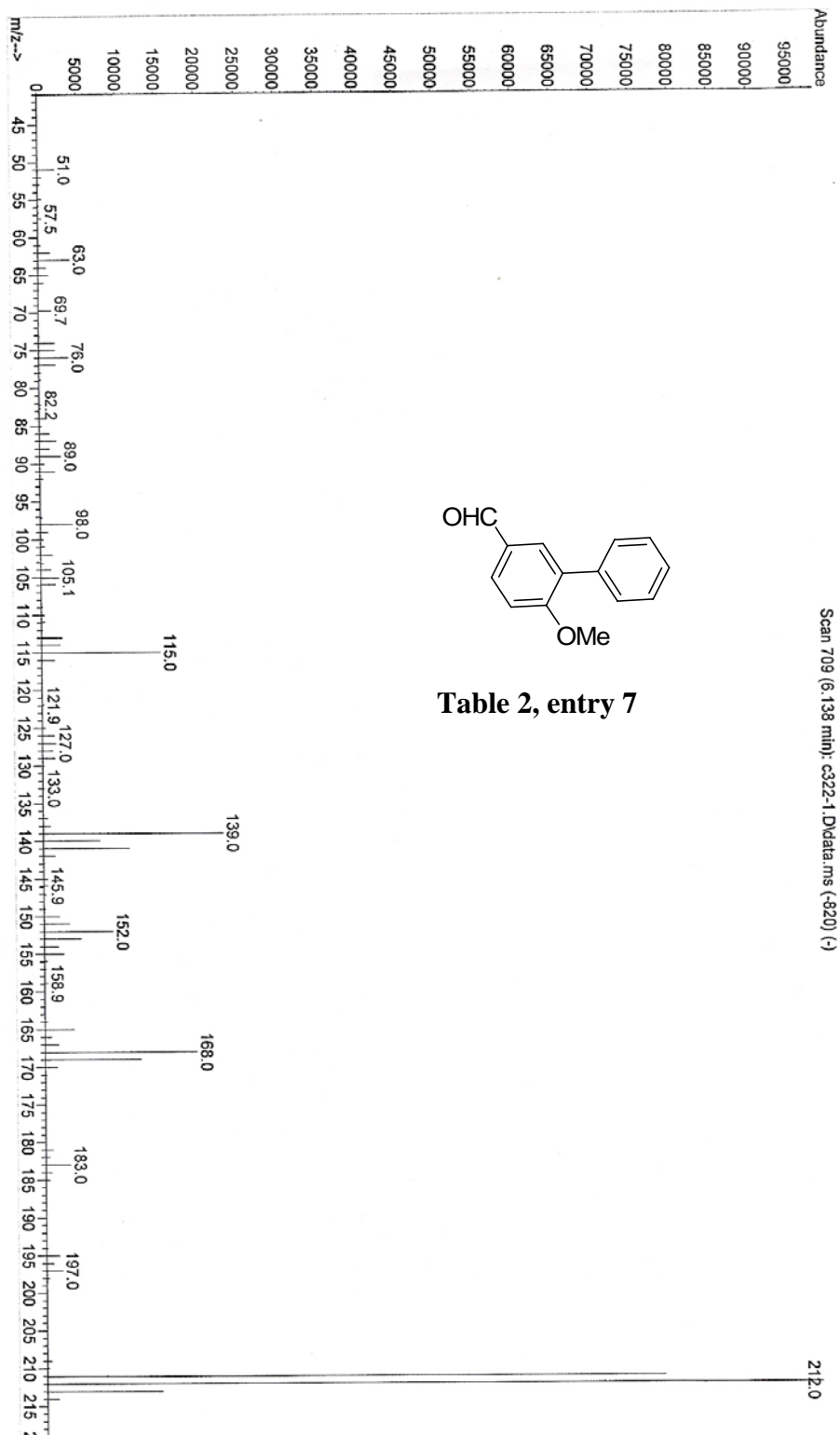
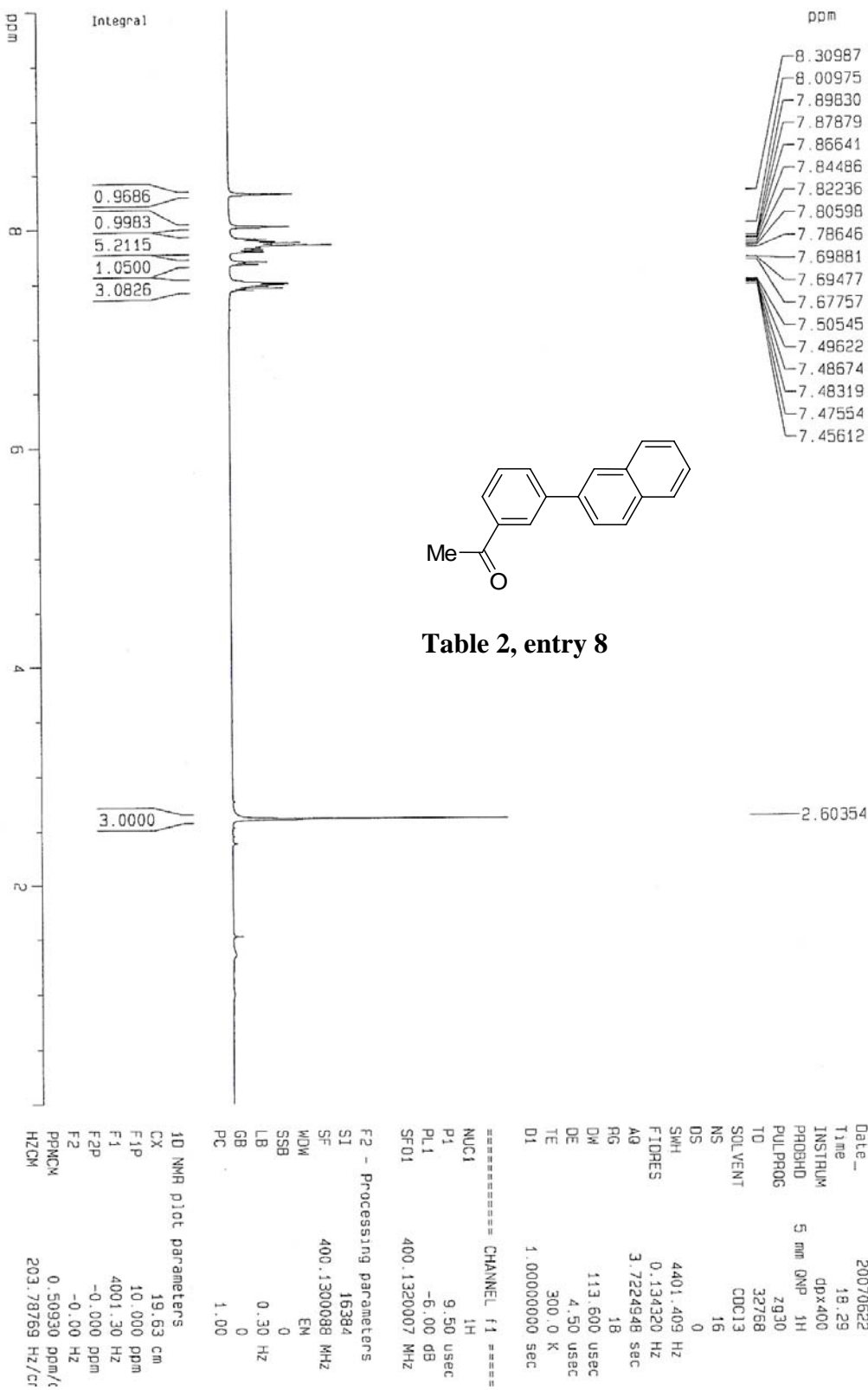


Table 2, entry 7





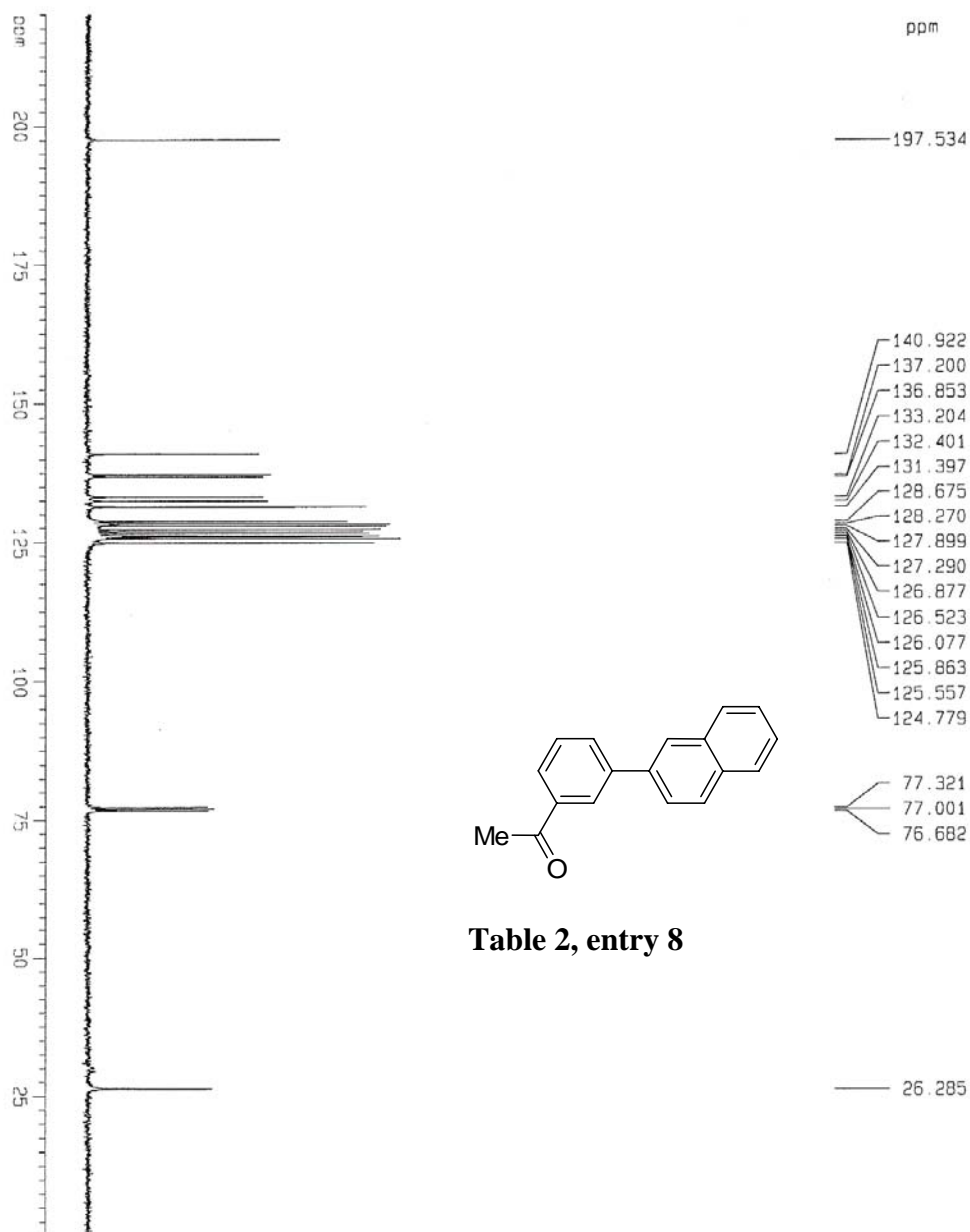


Table 2, entry 8

Current Data Parameters

NAME	Coupling
EXPNO	43
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070622	18:31

INSTRUM: dx400
PROBHD: 5 mm QNP 1H
PULPROG: zgpg30
TD: 131072
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 25125.629 Hz
FIDRES: 0.191693 Hz
AQ: 2.6083627 sec
RG: 8192
DM: 19.900 usec
DE: 4.50 usec
TE: 300.0 K
D1: 3.00000000 sec
d11: 0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-5.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	waltz16
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SI	65536
SF	100.6128181 MHz
MDM	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.50 cm
F1P	220.000 ppm
F1	22134.82 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCK	11.28205 ppm/C
HZCK	1135.11902 Hz/C

File : C:\msdchem\1\DATA\cms0\CT\c353.D
Operator :
Acquired : 22 Jun 2007 14:35 using AcqMethod METHOD02.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 1

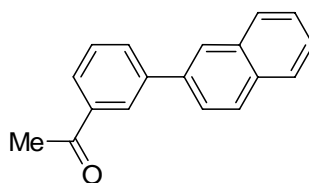
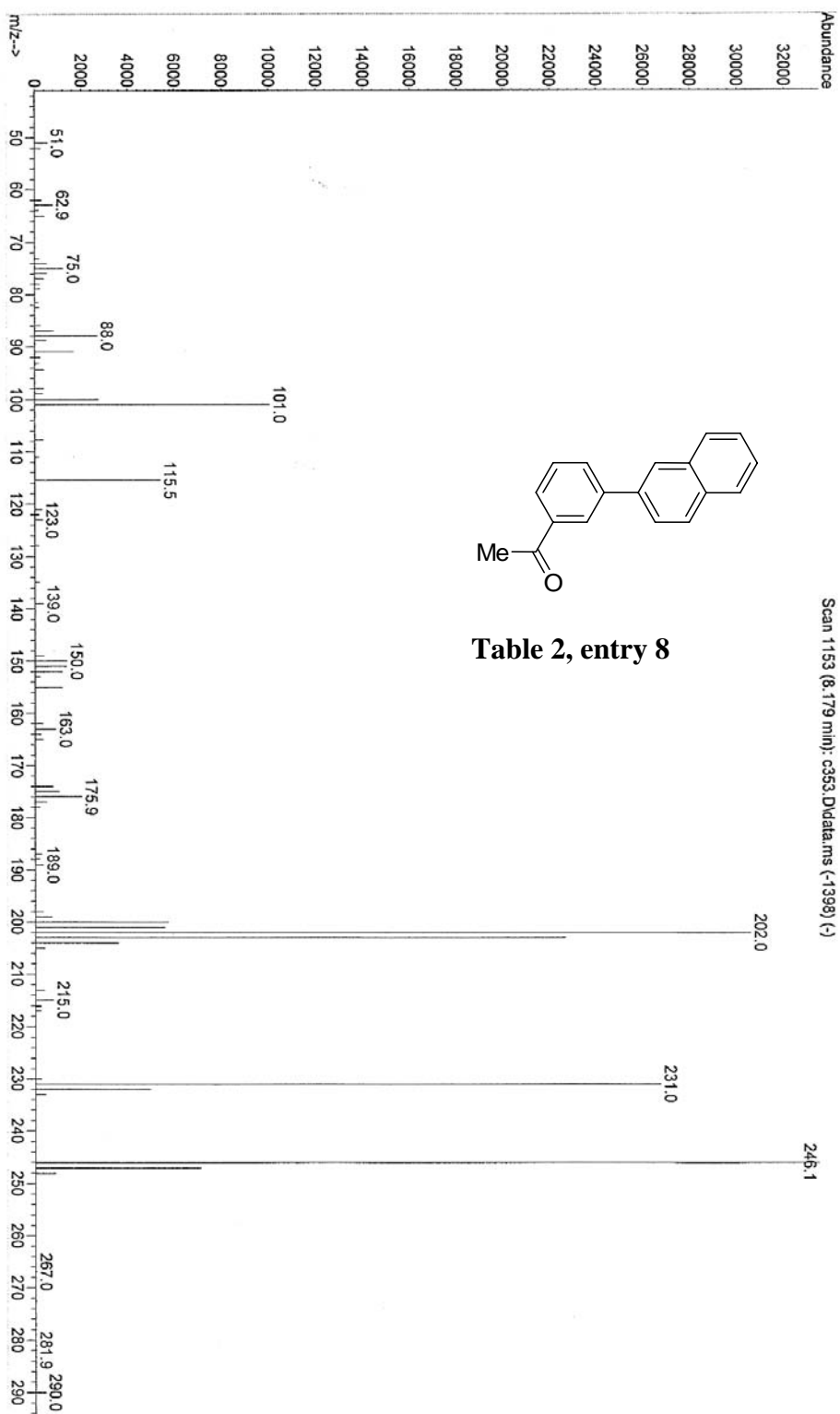


Table 2, entry 8



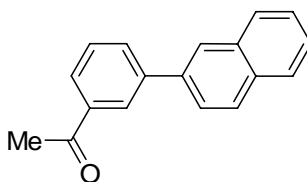


Table 2, entry 8

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

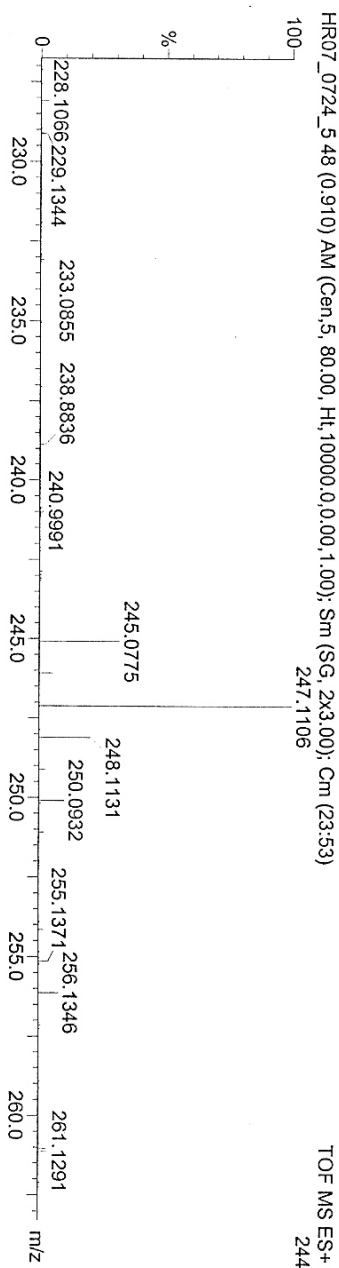
8 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

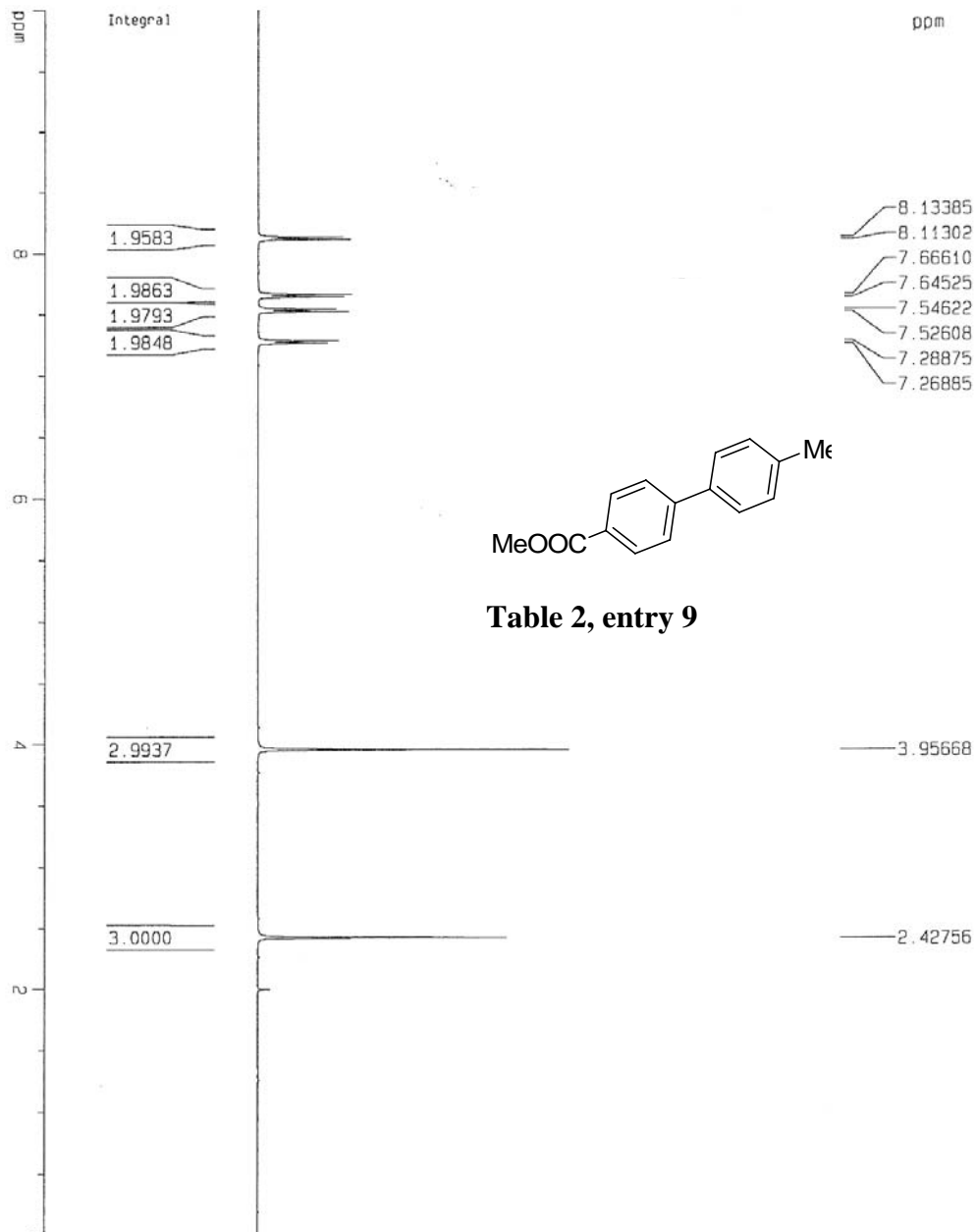
C: 0-21 H: 0-1000 O: 0-1

So Chau Ming, 3-naphthylacetophenone

HR07_0724_5.48 (0.910) AM (Cen,5, 80.00, Ht,10000.0,0.00,1.00); Sm (SG, 2x3.00); Cm (23.53)



Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
247.1106	247.1123	-1.7	-6.9	11.5	0.1	C18 H15 O



Current Data Parameters

NAME	coupling
EXPNO	81
PROCNO	1

F2 - Acquisition Parameters

Date_	20070627
Time	21.21
INSTRUM	gpc400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	4401.409 Hz
FIDRES	0.134320 Hz
AQ	3.7224948 sec
RG	40.3
DW	113.600 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	¹ H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.132006 MHz

F2 - Processing parameters

SI	16384
SF	400.130077 MHz
WDW	EM
SSB	0
LB	0.70 Hz
GB	0
PC	1.00

1D NMR plot parameters

CK	19.63 cm
F1P	10.000 ppm
F1	4001.30 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	0.50930 ppm/°C
HZCM	203.78769 Hz/°C

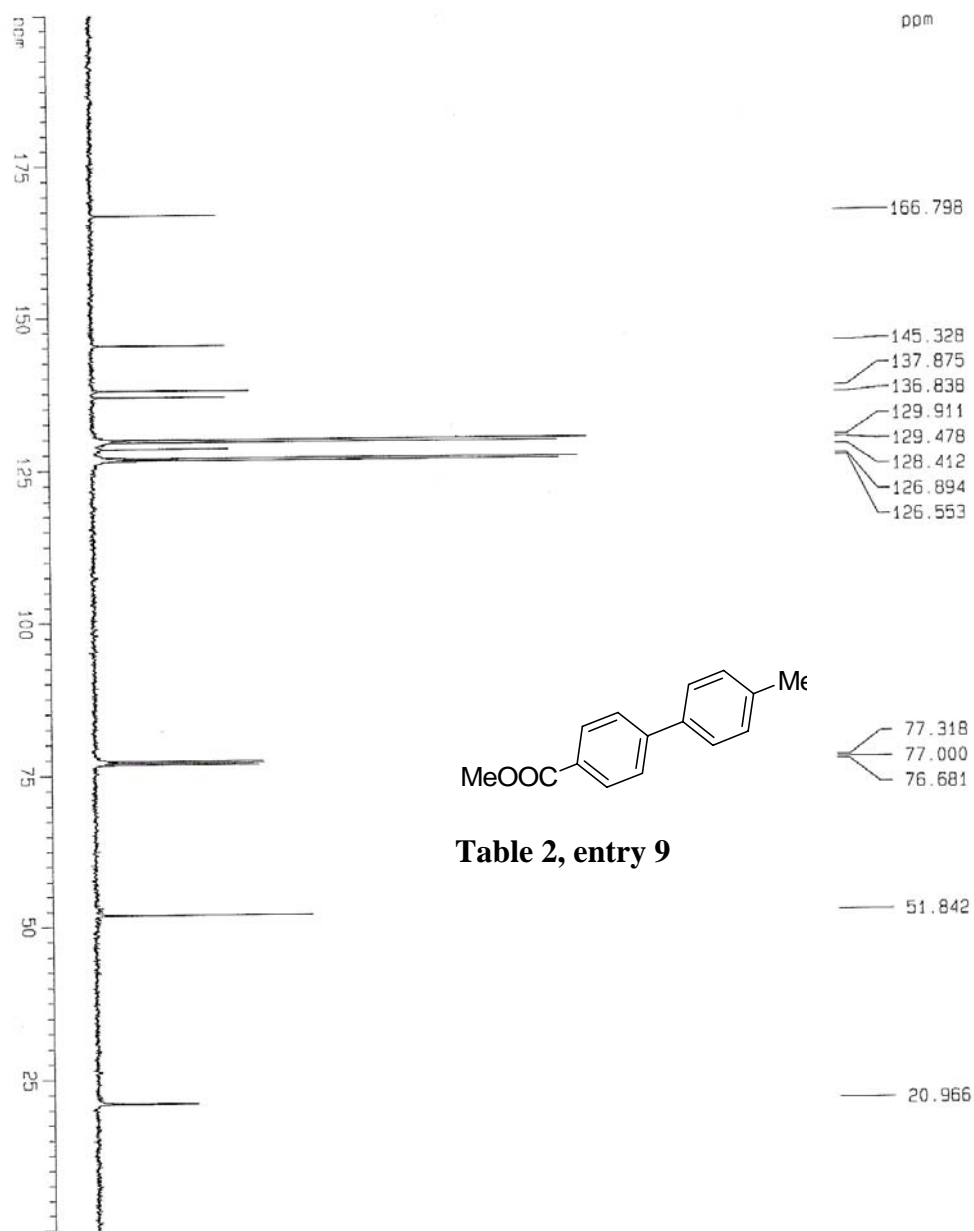


Table 2, entry 9

Current Data Parameters

NAME	COUPLING
EXPNO	46
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070627	21.24

INSTRUM 5 mm QNP 1H
PROBHD zgpg30
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 64
DS 0
SWH 25125.629 Hz
FIDRES 0.191693 Hz
AQ 2.5083827 sec
RG 8192
DM 19.900 usec
DE 4.50 usec
TE 300.0 K
D1 3.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.80 usec
PL1 -6.00 dB
SF01 100.621263 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 71.00 usec
PL2 120.00 dB
PL12 17.00 dB
SF02 400.132608 MHz

F2 - Processing parameters

SF	SI
100.6127917 MHz	65536

WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX	F1P	F1	F2P	F2	PPMCM	HZCM
19.50 cm	200.000 ppm	20122.56 Hz	-0.000 ppm	-0.00 Hz	10.25641 ppm/Hz	1031.92615 Hz/C

File : C:\msdchem\1\DATA\cms0\CT\c364.D
Operator :
Acquired : 26 Jun 2007 16:17 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1

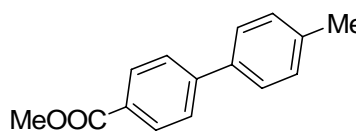
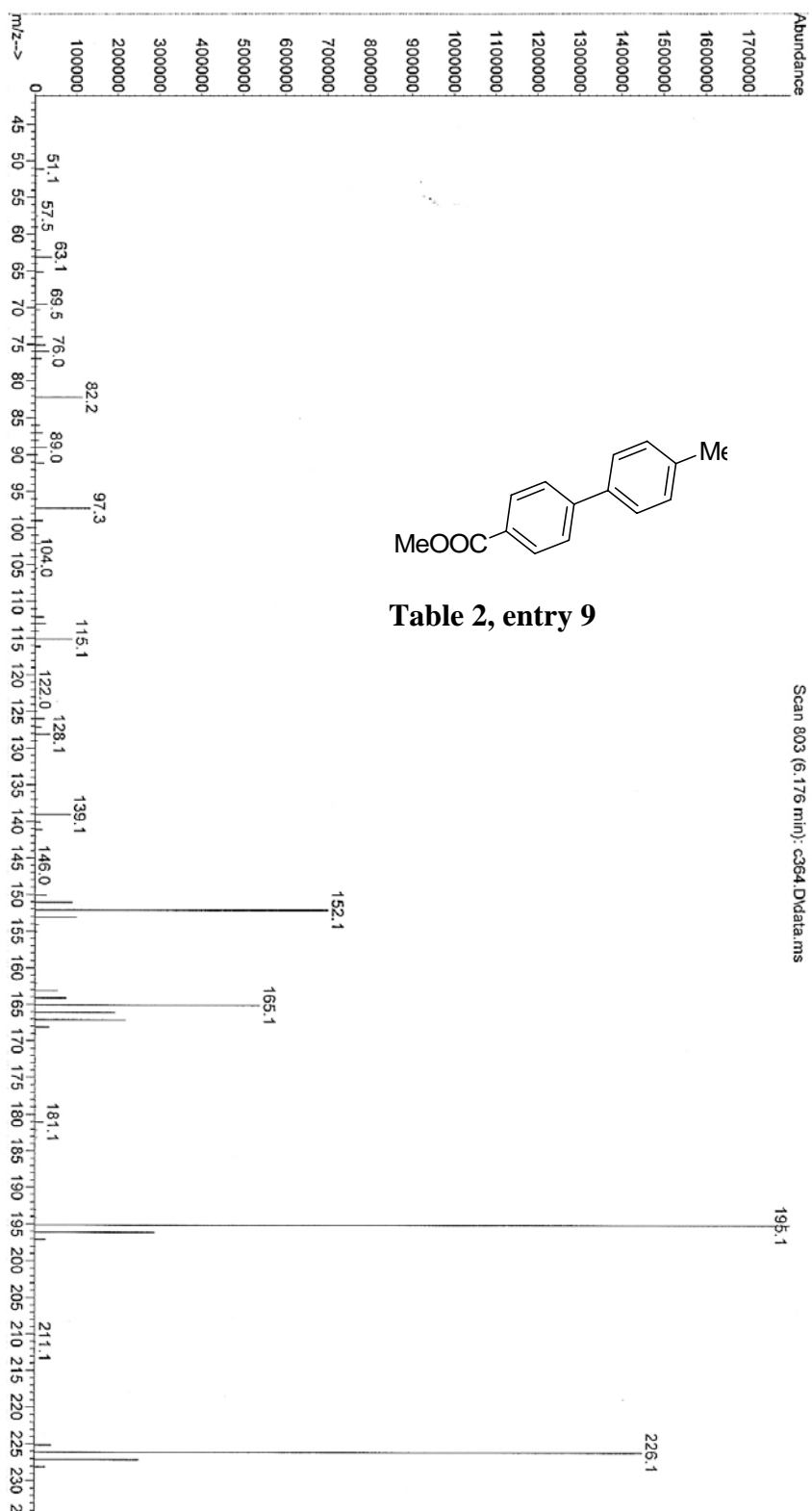
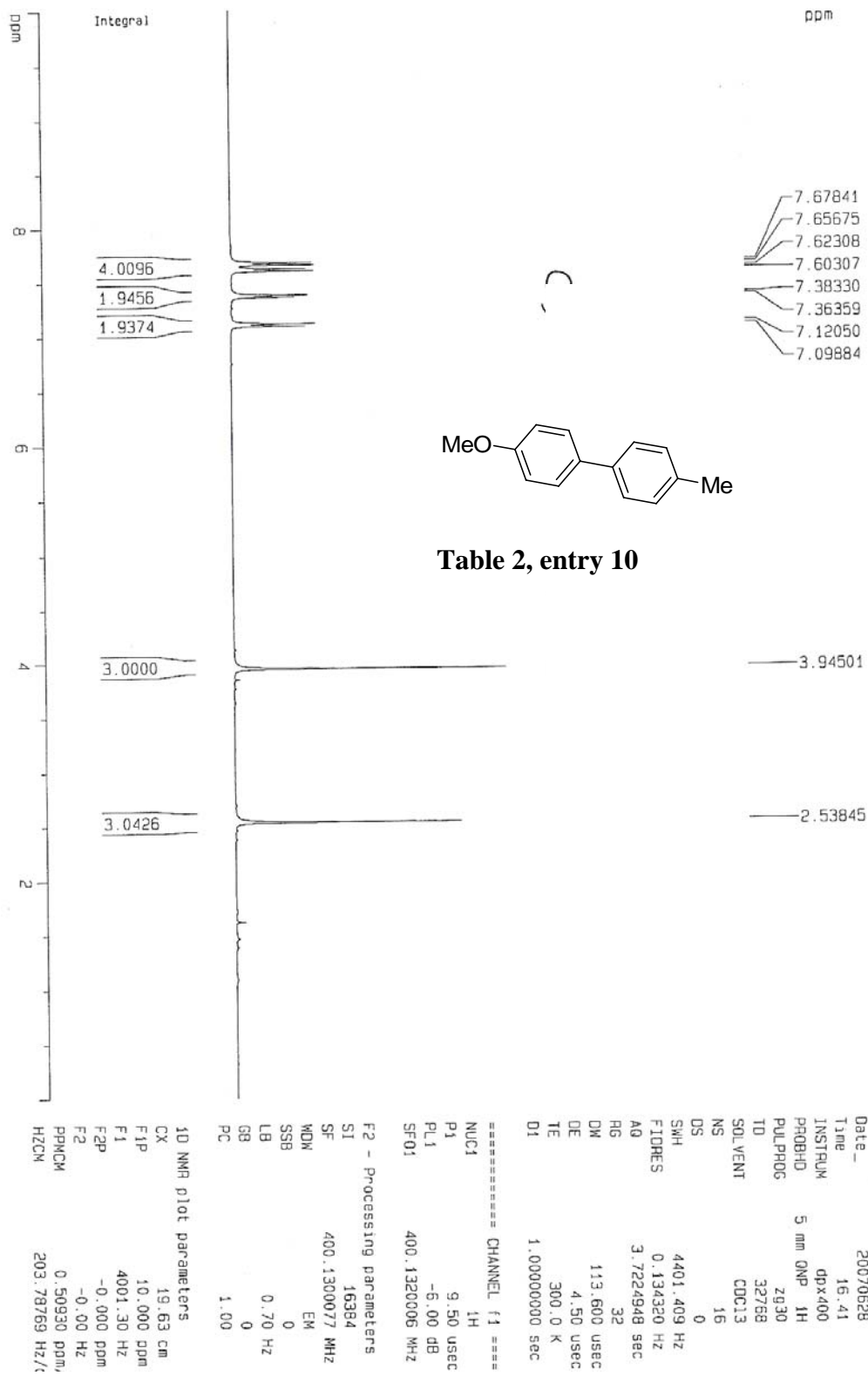


Table 2, entry 9





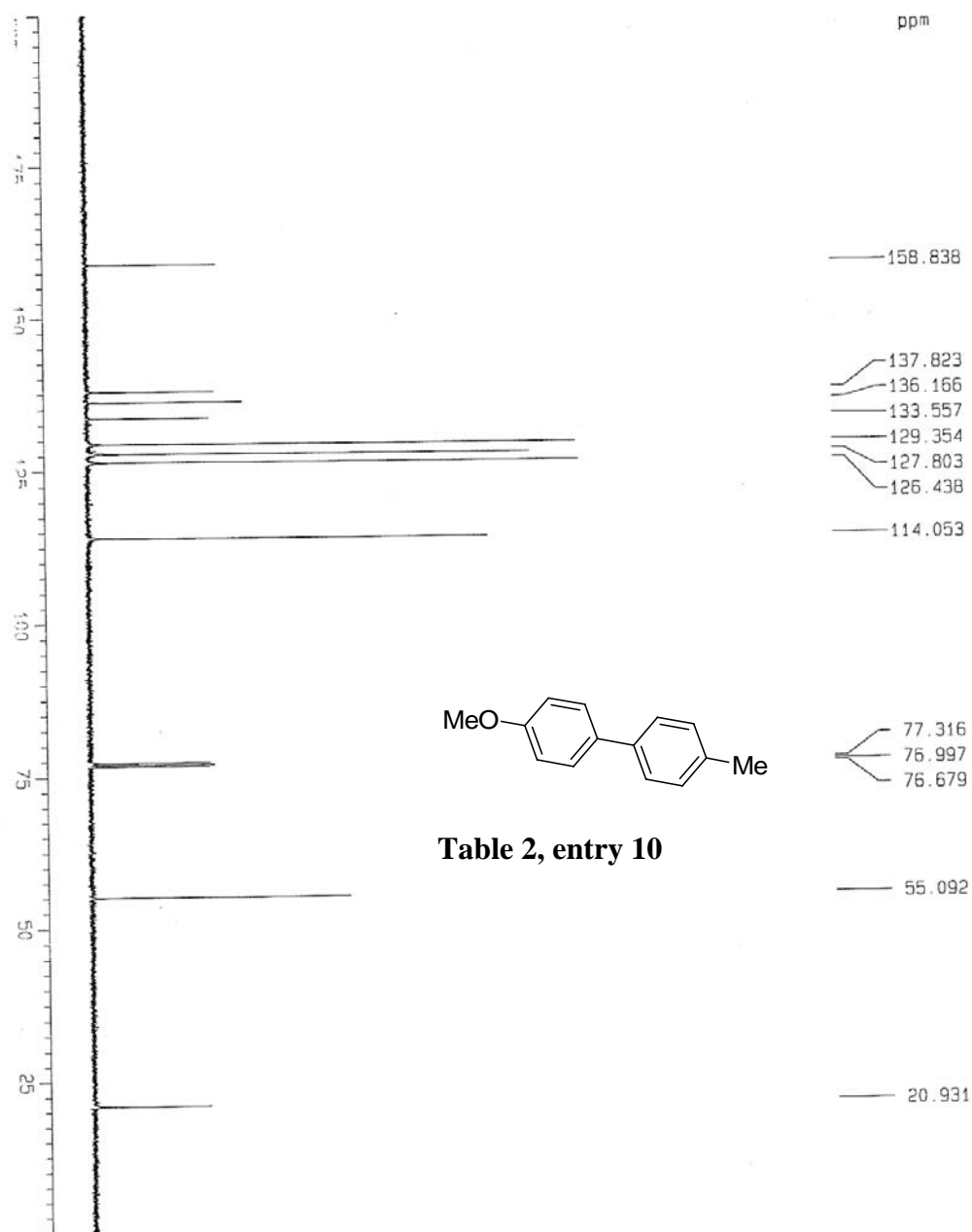


Table 2, entry 10

Current Data Parameters

NAME	COUPLING
EXPNO	48
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070529	16.37
INSTRUM	gpc400
PROBHD	5 mm QNP 1H
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl3
NS	33
DS	0
SWH	25125.629 Hz
FIDRES	0.191693 Hz
AQ	2.6083827 sec
RG	8192
DW	19.900 usec
DE	4.50 usec
TE	300.0 K
D1	3.00000000 sec
d11	0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SI	65536
SF	100.6127986 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.50 cm
F1P	200.000 ppm
F1	20122.56 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	10.25641 ppm/
HZCM	1031.92615 Hz/c

File : C:\msdchem\1\DATA\cms0\CT\c368.D
Operator : Fbm
Acquired : 27 Jun 2007 15:44 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 1

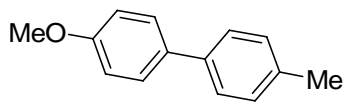
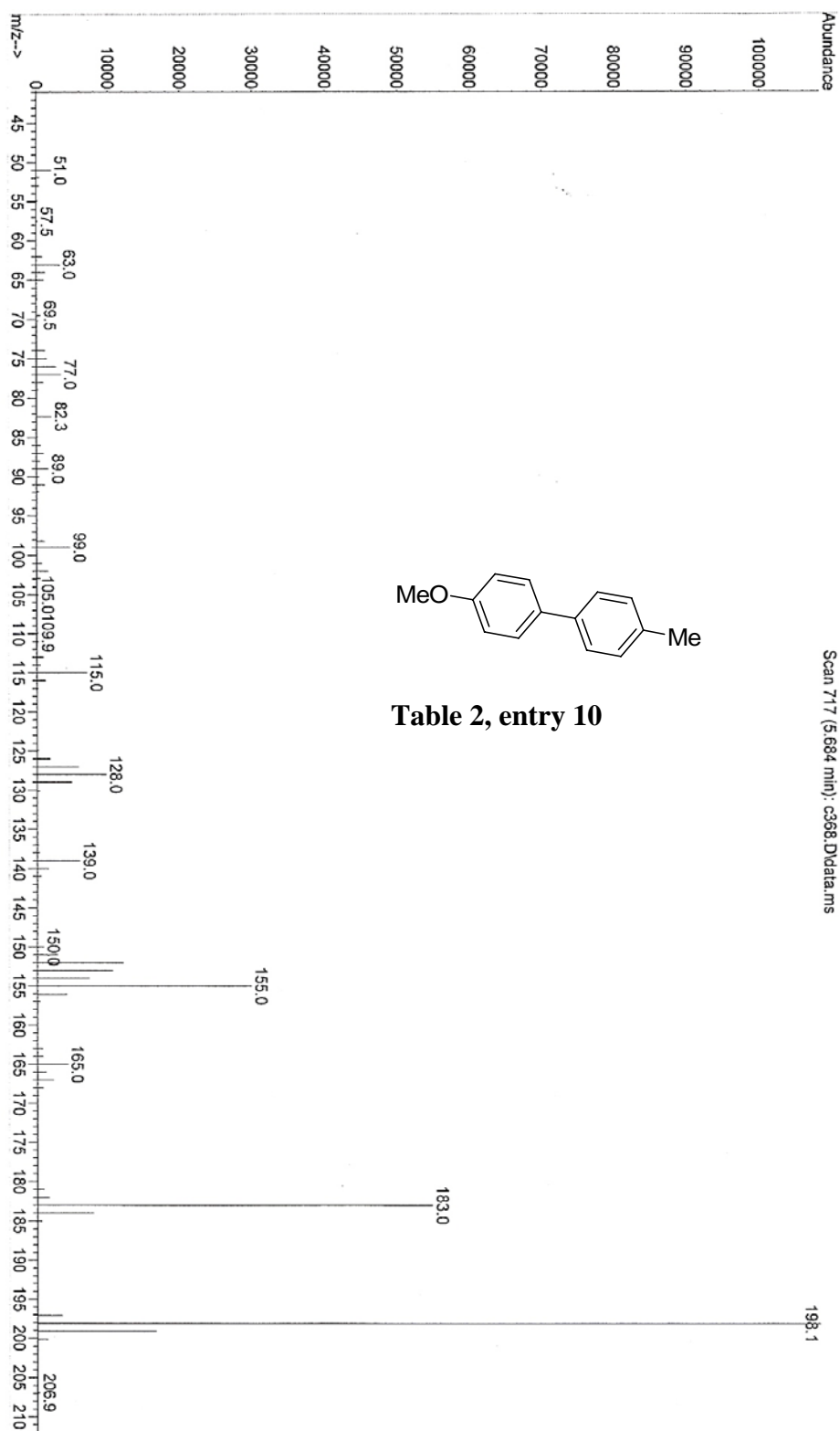
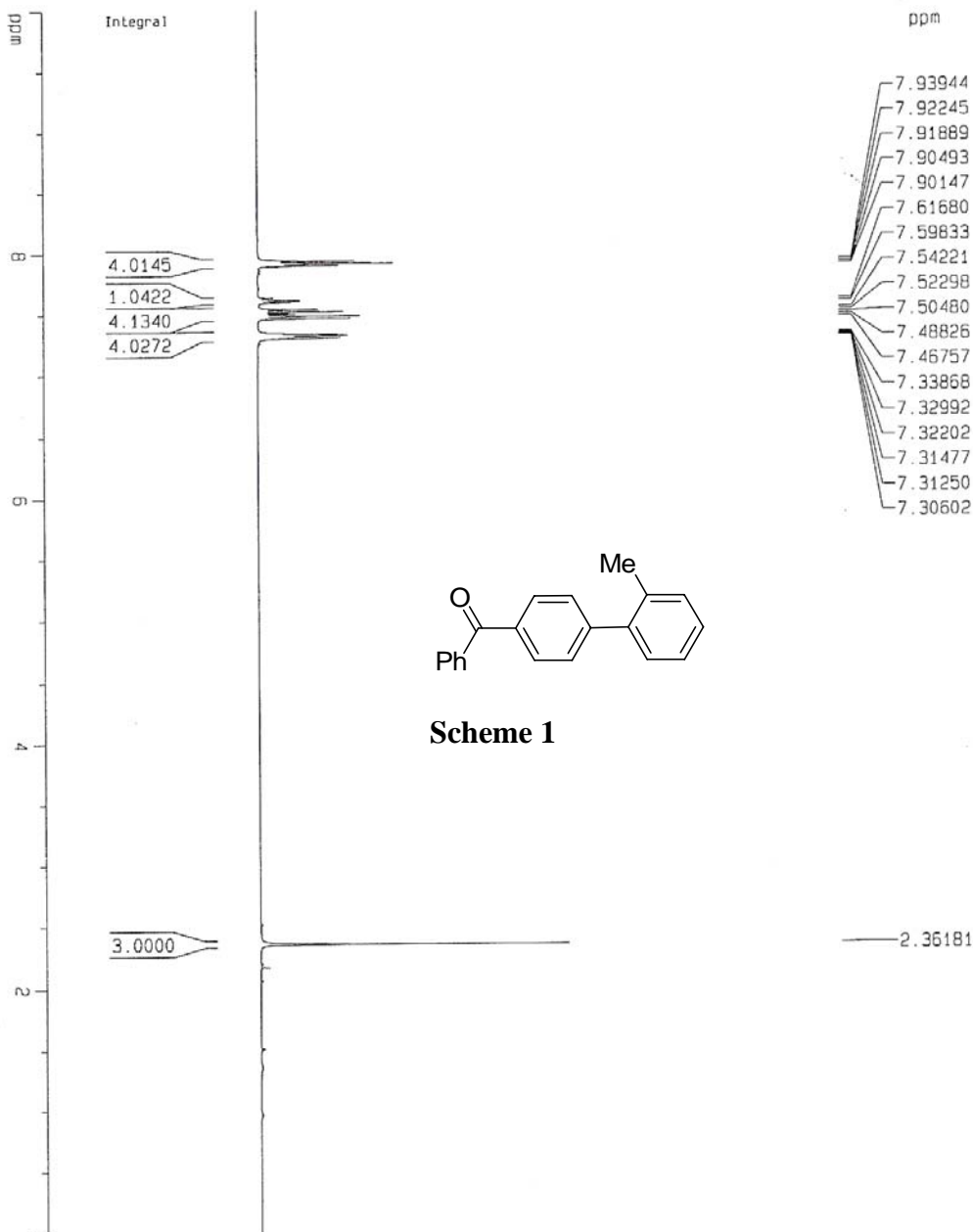


Table 2, entry 10





Current Data Parameters

NAME	COUPLING
EXPNO	79
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070625	18.14

INSTRUM dpx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 16
DS 0
SWH 4401.409 Hz
FIDRES 0.134320 Hz
AQ 3.7224948 sec
RG 18
DM 113.600 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

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

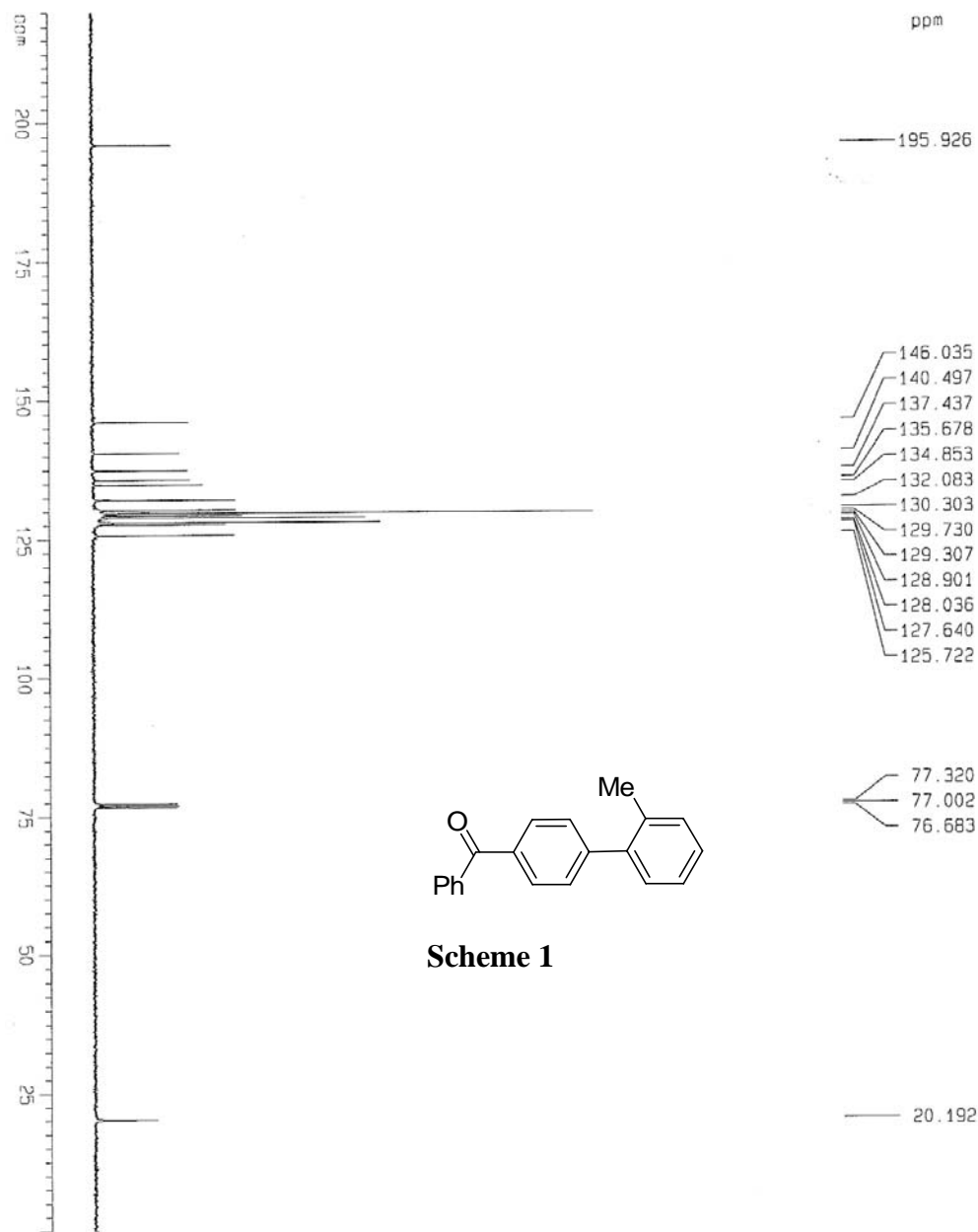
NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	16384
SF	400.1300077 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

10 NMR plot parameters

CX	19.63 cm
F1P	10.000 ppm
F1	4001.30 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	0.50930 ppm/
HZCM	203.78769 Hz/c



Scheme 1

Current Data Parameters

NAME	Coupling
EXPNO	44
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070625	18.16

INSTRUM: dpk400
PROBHD: 5 mm QNP 1H
PULPROG: zgpg30
TD: 131072
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 25125.629 Hz
FIDRES: 0.191693 Hz
AQ: 2.6093827 sec
RG: 8192
DM: 19.900 usec
DE: 4.50 usec
TE: 300.0 K
D1: 3.00000000 sec
d11: 0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

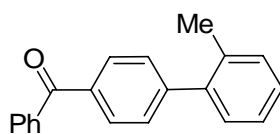
F2 - Processing parameters

SI	65536
SF	100.6128078 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

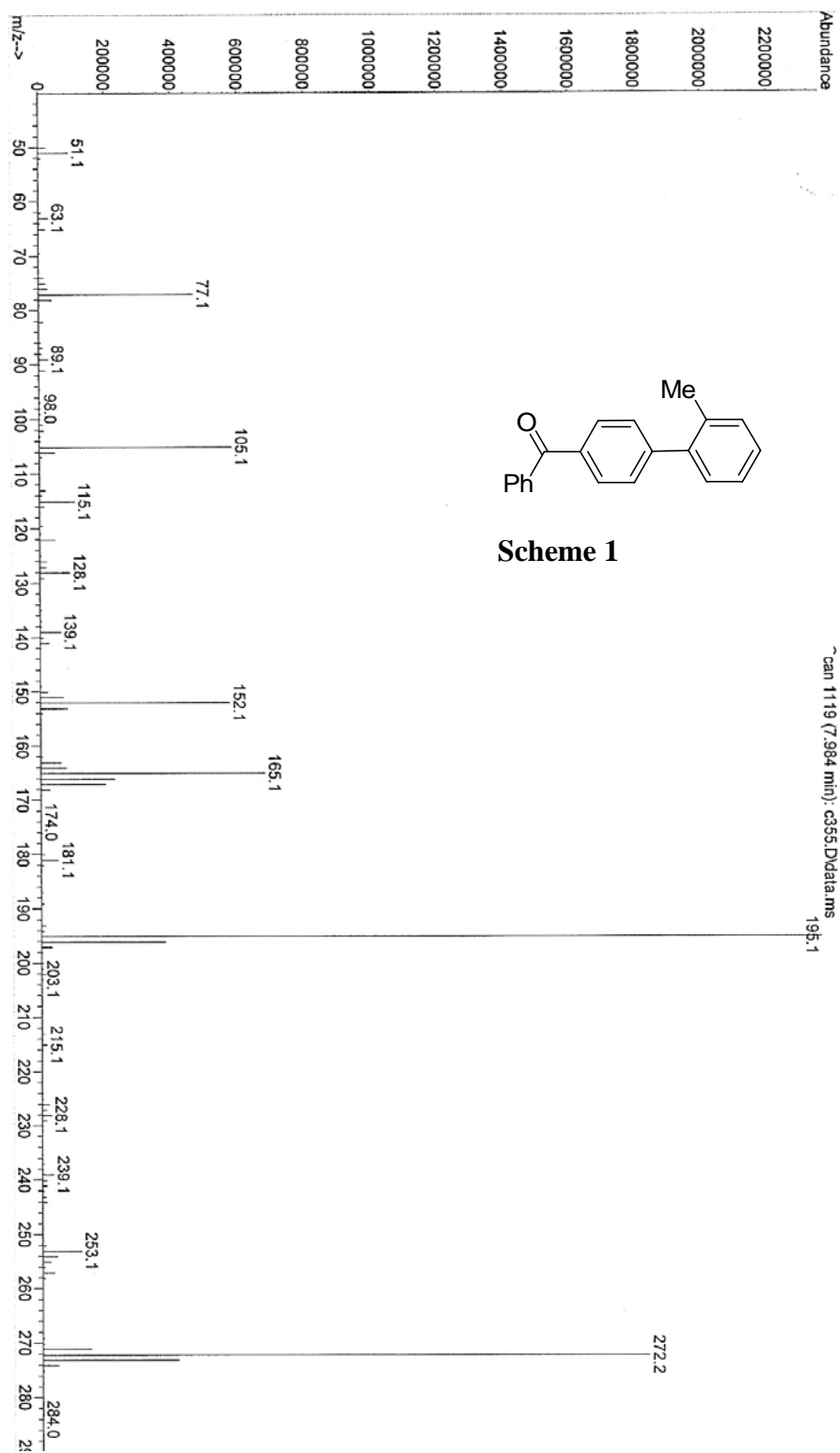
1D NMR plot parameters

CX	19.50 cm
F1P	220.000 ppm
F1	22134.82 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	11.28205 ppm/
HZCM	1135.11890 Hz/C

File : C:\msdchem\1\DATA\cmso\CT\c355.D
Operator :
Acquired : 22 Jun 2007 14:56 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 2



Scheme 1



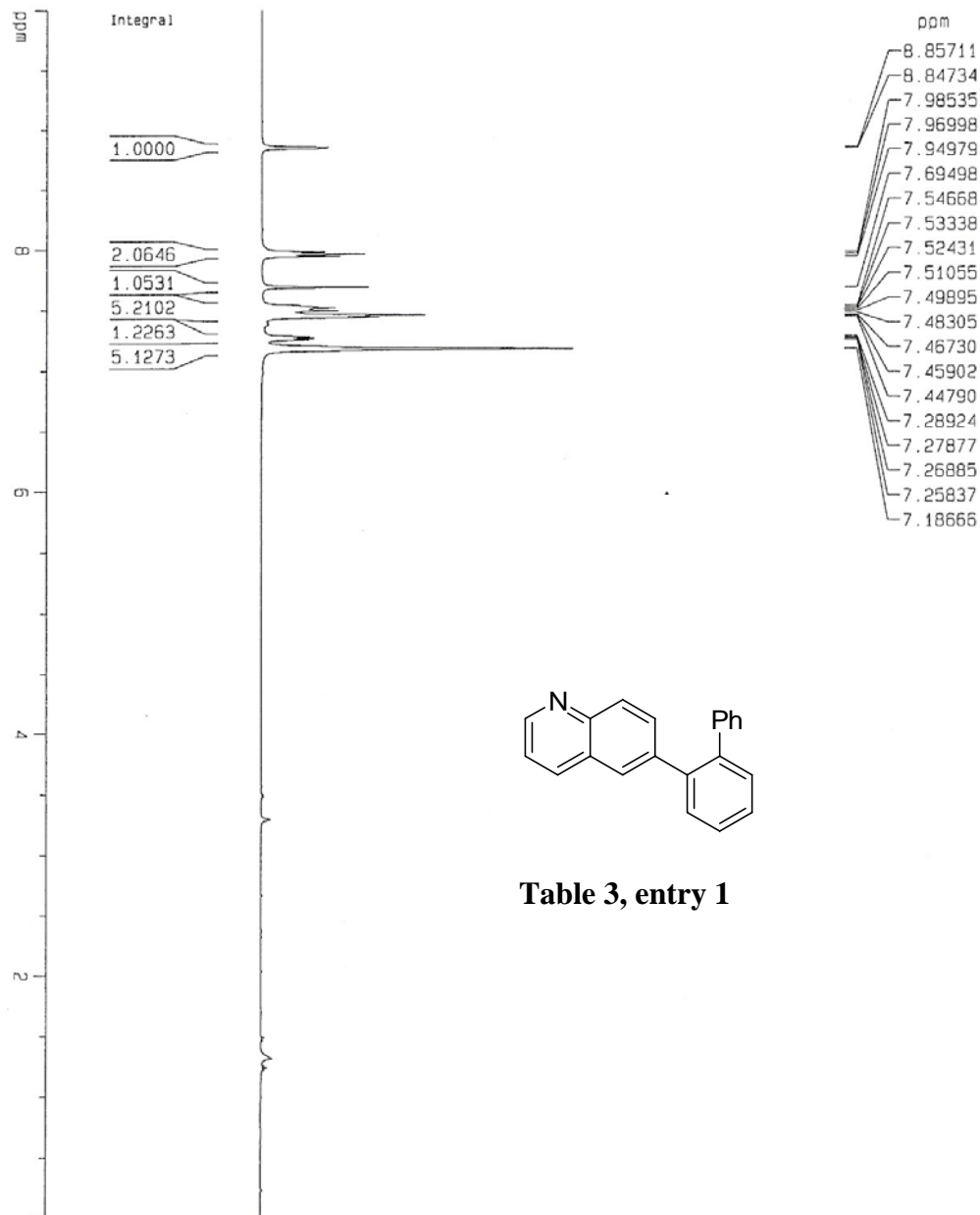


Table 3, entry 1

Current Data Parameters

NAME	coupling
EXPNO	70
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070608	21.01
INSTRUM	dp400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SMH	4401.409 Hz
FIDRES	0.134320 Hz
AQ	3.7224948 sec
RG	32
DM	113.600 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SI	16384
SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.63 cm
F1P <td>10.000 ppm</td>	10.000 ppm
F1 <td>4001.30 Hz</td>	4001.30 Hz
F2P <td>-0.000 ppm</td>	-0.000 ppm
F2 <td>-0.00 Hz</td>	-0.00 Hz
PPMCM <td>0.50930 ppm/c</td>	0.50930 ppm/c
HZCM <td>203.78769 Hz/cm</td>	203.78769 Hz/cm

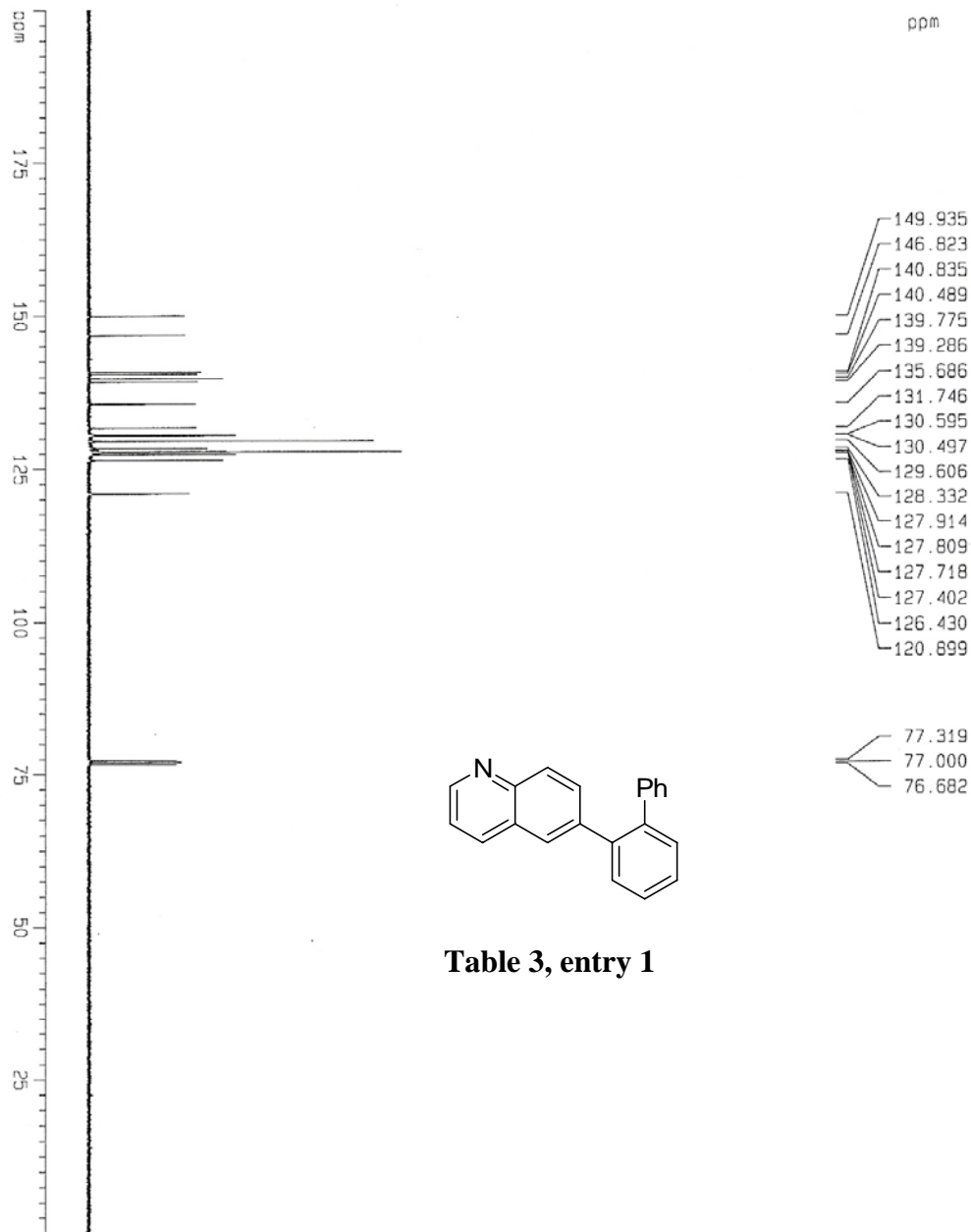


Table 3, entry 1

Current Data Parameters

NAME	COUPLING
EXPNO	35
PROCNO	1

F2 - Acquisition Parameters

Date_	20070608
Time	21.04
INSTRUM	gpc400
PROBHD	5 mm GNP 1H
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl3
NS	64
DS	0
SWH	25125.629 Hz
FIDRES	0.191693 Hz
AQ	2.6083827 sec
RG	8192
DW	19.900 usec
DE	4.50 usec
TE	300.0 K
D1	3.00000000 sec
d11	0.03000000 sec

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

NUC1	¹³ C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	waltz16
NUC2	¹ H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SI	65536
SF	100.6128059 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.50 cm
F1P	200.000 ppm
F1	20122.56 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCK	10.25641 ppm/cm
HZCM	1031.92627 Hz/cm

File : C:\msdchem\1\DATA\cmso\CT\c324.D
Operator :
Acquired : 8 Jun 2007 14:31 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 3

Scan 1109 (8.427 min): c324.D\data.ms

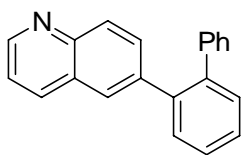
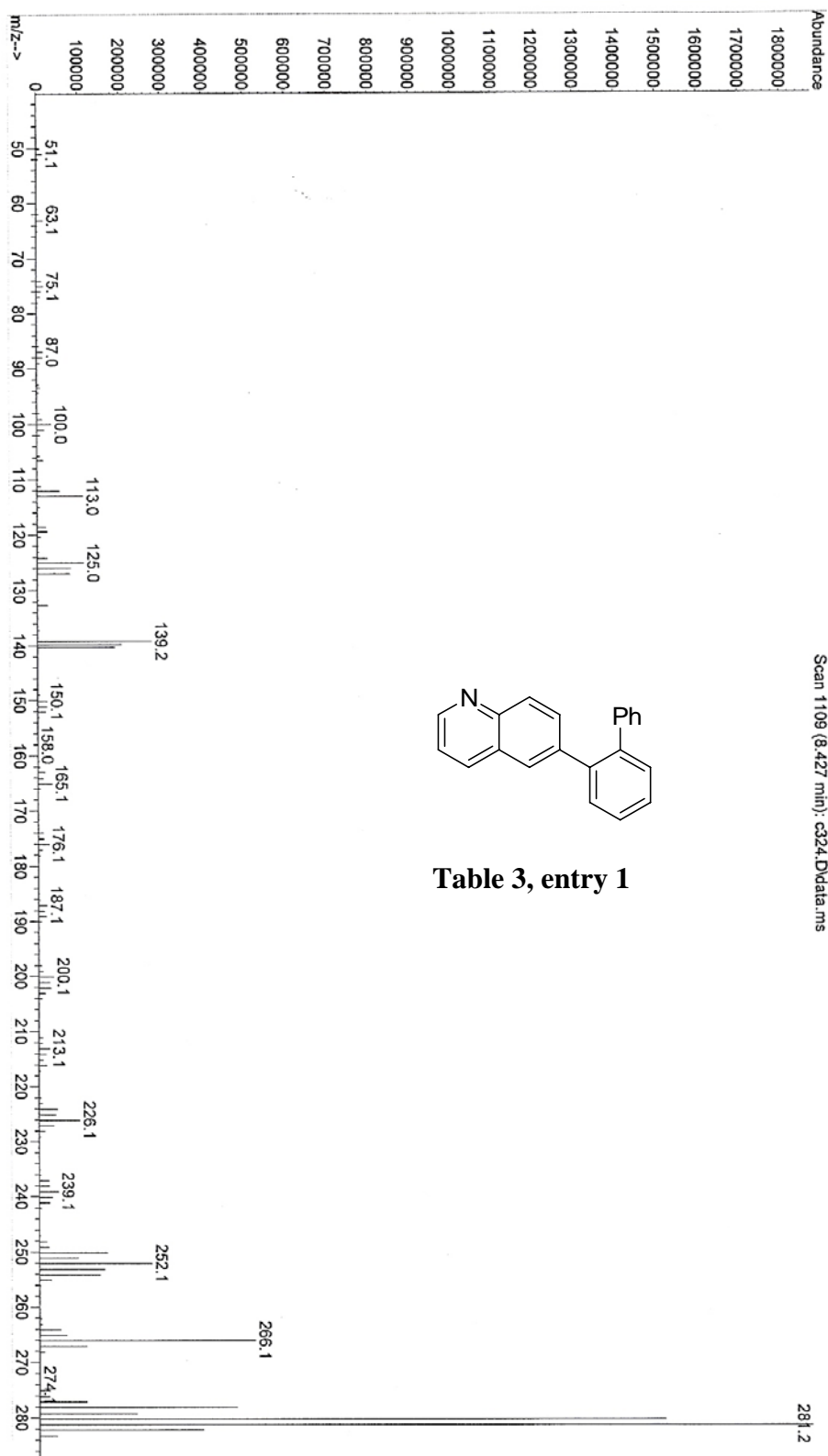
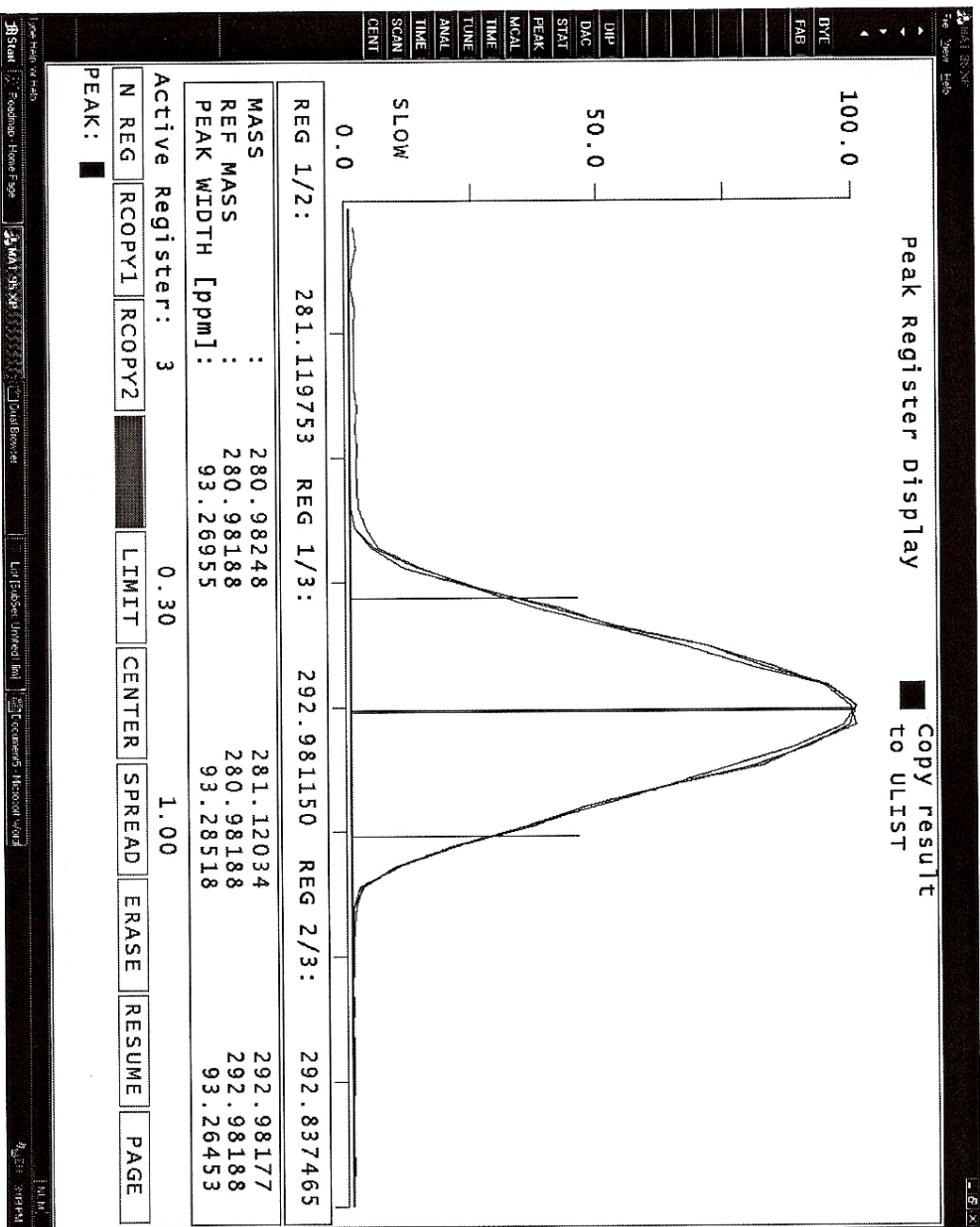


Table 3, entry 1



Accurate Mass Measurement:

Molecular formula:
 $C_{21}H_{15}N_1$
 $[M]^+$ (theoretical)
 = 281.1199

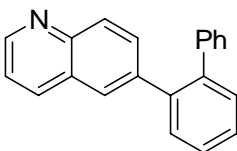


Table 3, entry 1

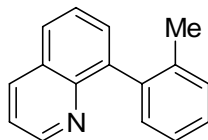
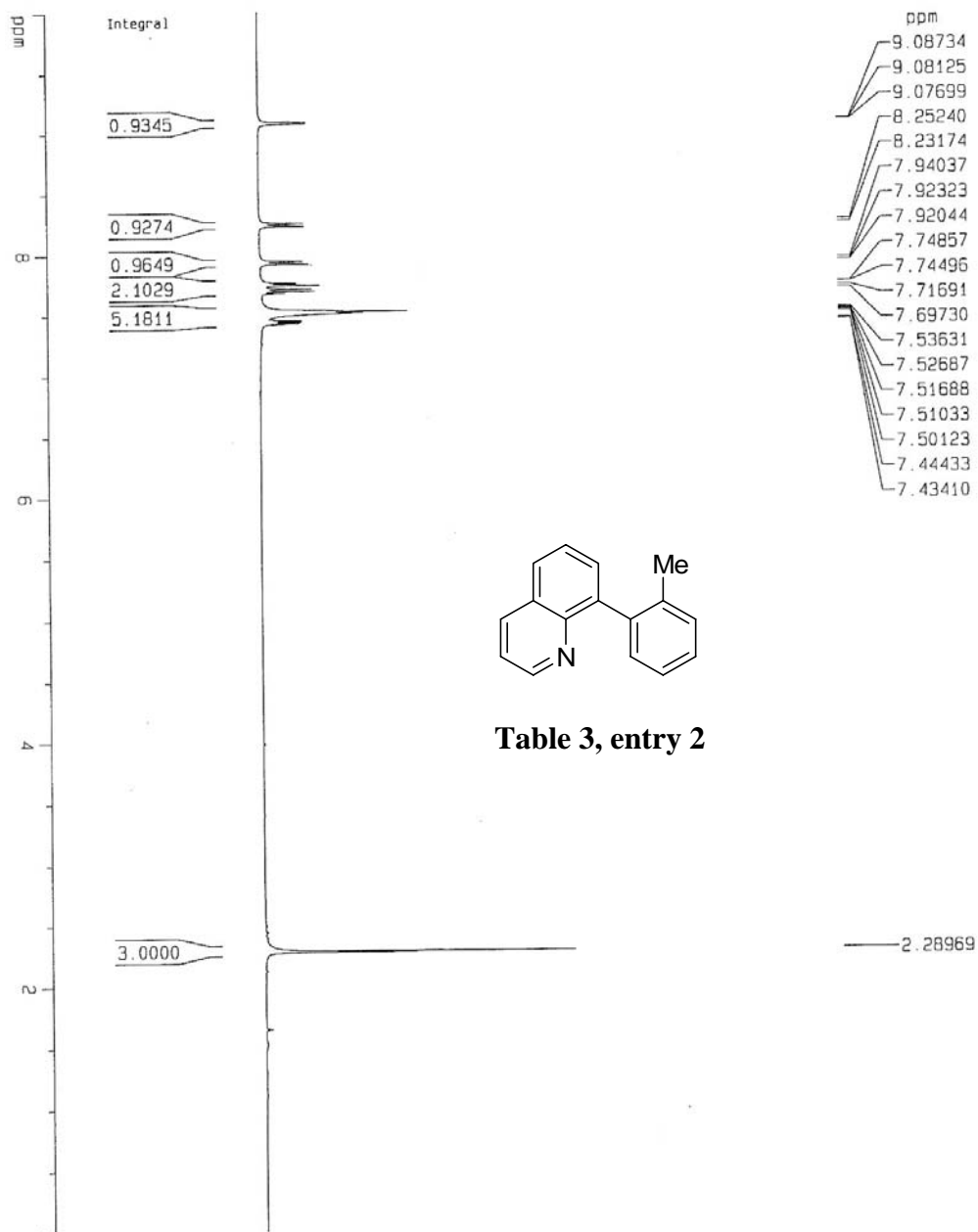


Table 3, entry 2

Current Data Parameters

NAME	COUPLING
EXPNO	76
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070621	20.16
INSTRUM	cp400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	4401.409 Hz
FIDRES	0.134320 Hz
AQ	3.7224948 sec
RG	18
DW	113.600 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	1H
P1	9.50 usec
PL1	-5.00 dB
SFO1	400.1320007 MHz

F2 - Processing parameters

SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	19.63 cm
F1P	10.000 ppm
F1	4001.30 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPKCM	0.50930 ppm/c
HZCM	203.78769 Hz/cm

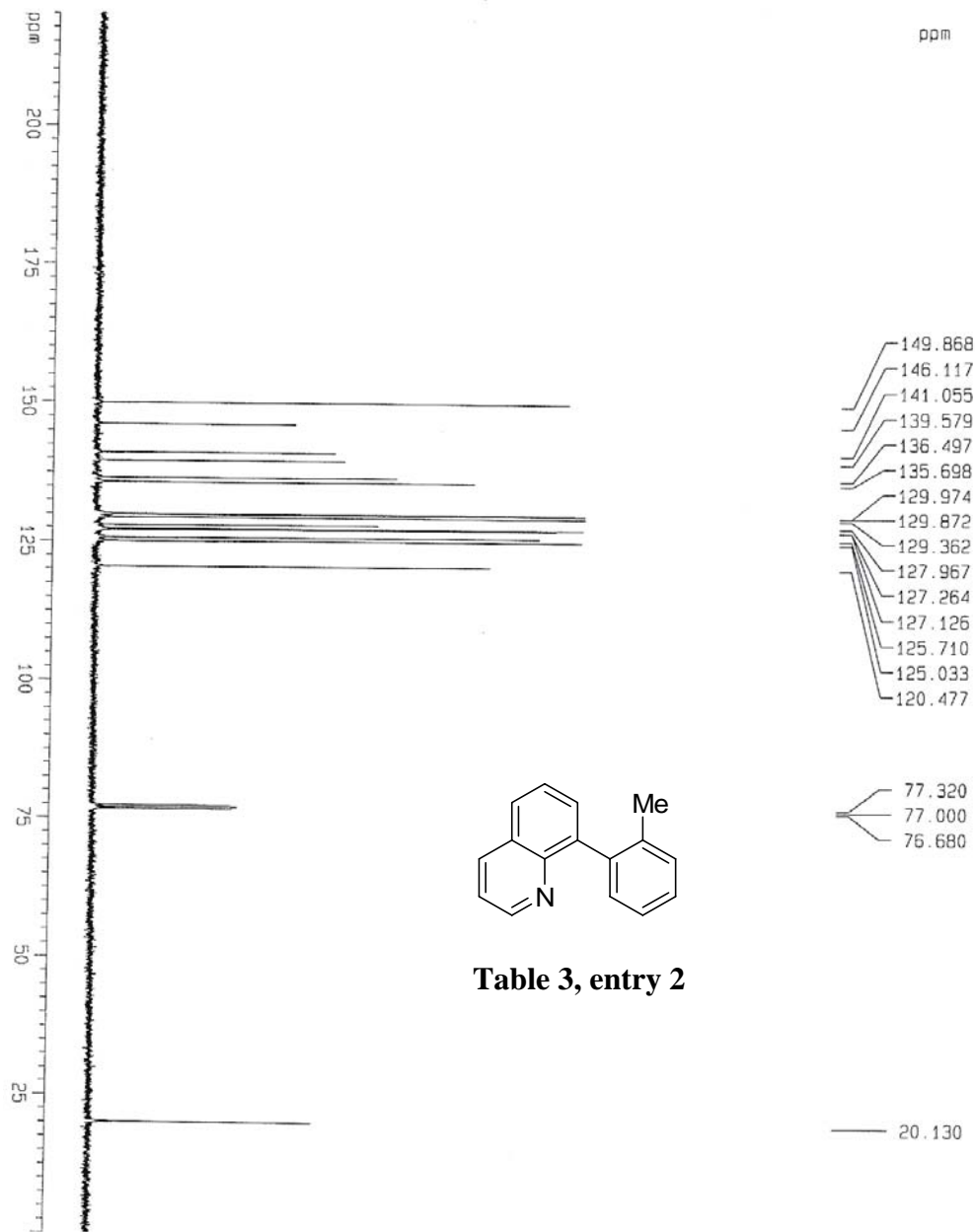


Table 3, entry 2

Current Data Parameters

NAME	EXPNO	PROCNO	COUPLING
NAME	41	1	

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SMH	FIDRES	AQ	RG	DM	DE	TE	D1
20070621	20.19	dp400	5 mm QNP 1H	zgpg30	131072	CDCl3	32	0	25125.629 Hz	0.191693 Hz	2.6083927 sec	8192	19.900 usec	4.50 usec	300.0 K	0.03000000 sec

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

NUC1	P1	PL1	SFO1
13C	5.80 usec	-6.00 dB	100.6231263 MHz

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

CPDPRG2	NUC2	P2	PL2	SFO2
zgpg30	1H	71.00 usec	120.00 dB	400.1326008 MHz

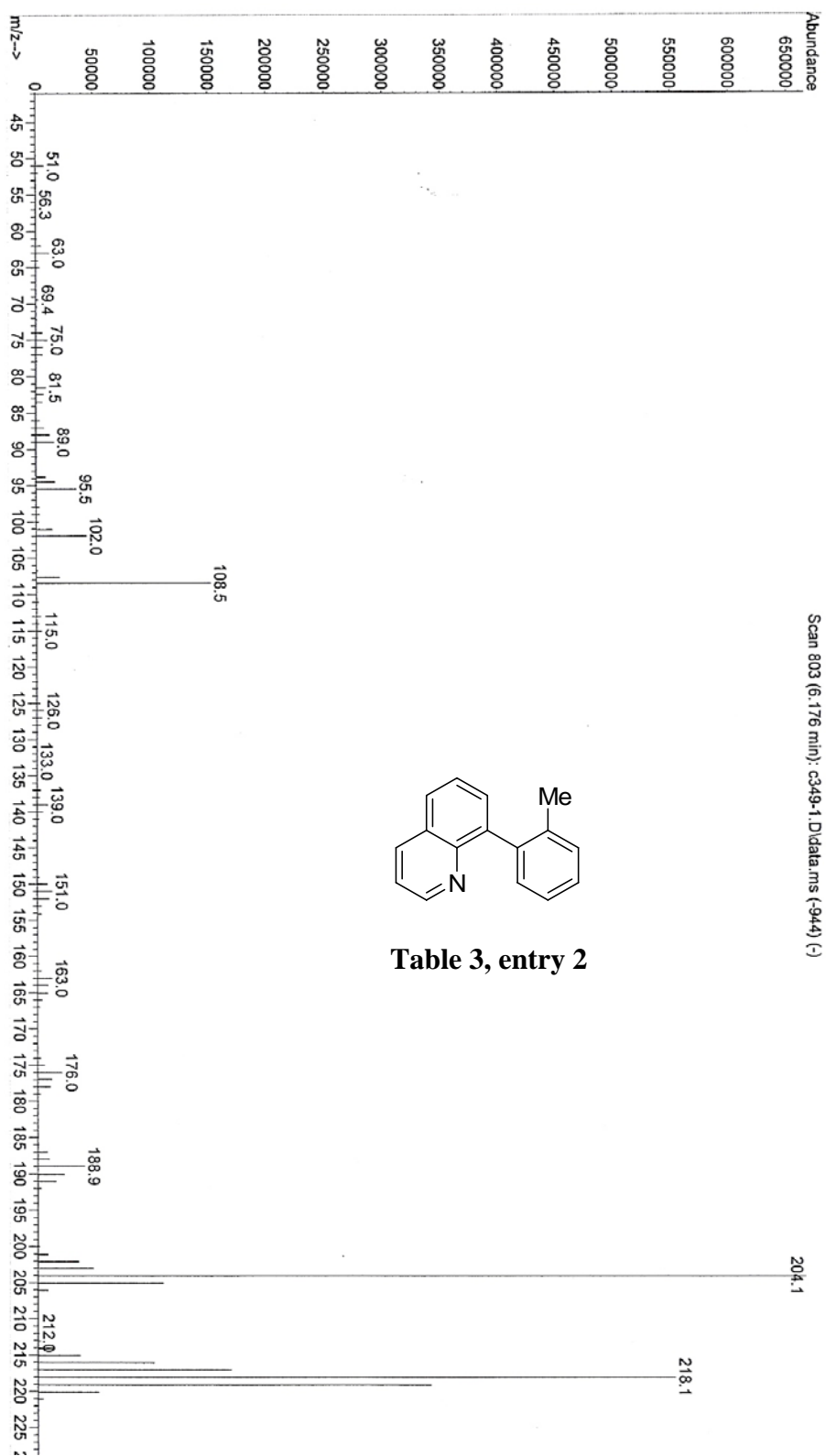
F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
65536	100.6126380 MHz	EM	0	1.50 Hz	0	1.00

10 NMR plot parameters

CX	F1P	F2P	PPMCK
19.50 cm	220.000 ppm	-0.000 ppm	11.28205 ppm/cm
	22134.82 Hz	-0.00 Hz	1135.11926 Hz/cm

File : C:\msdchem\1\DATA\cmso\CT\c349-1.D
Operator :
Acquired : 21 Jun 2007 14:46 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 1



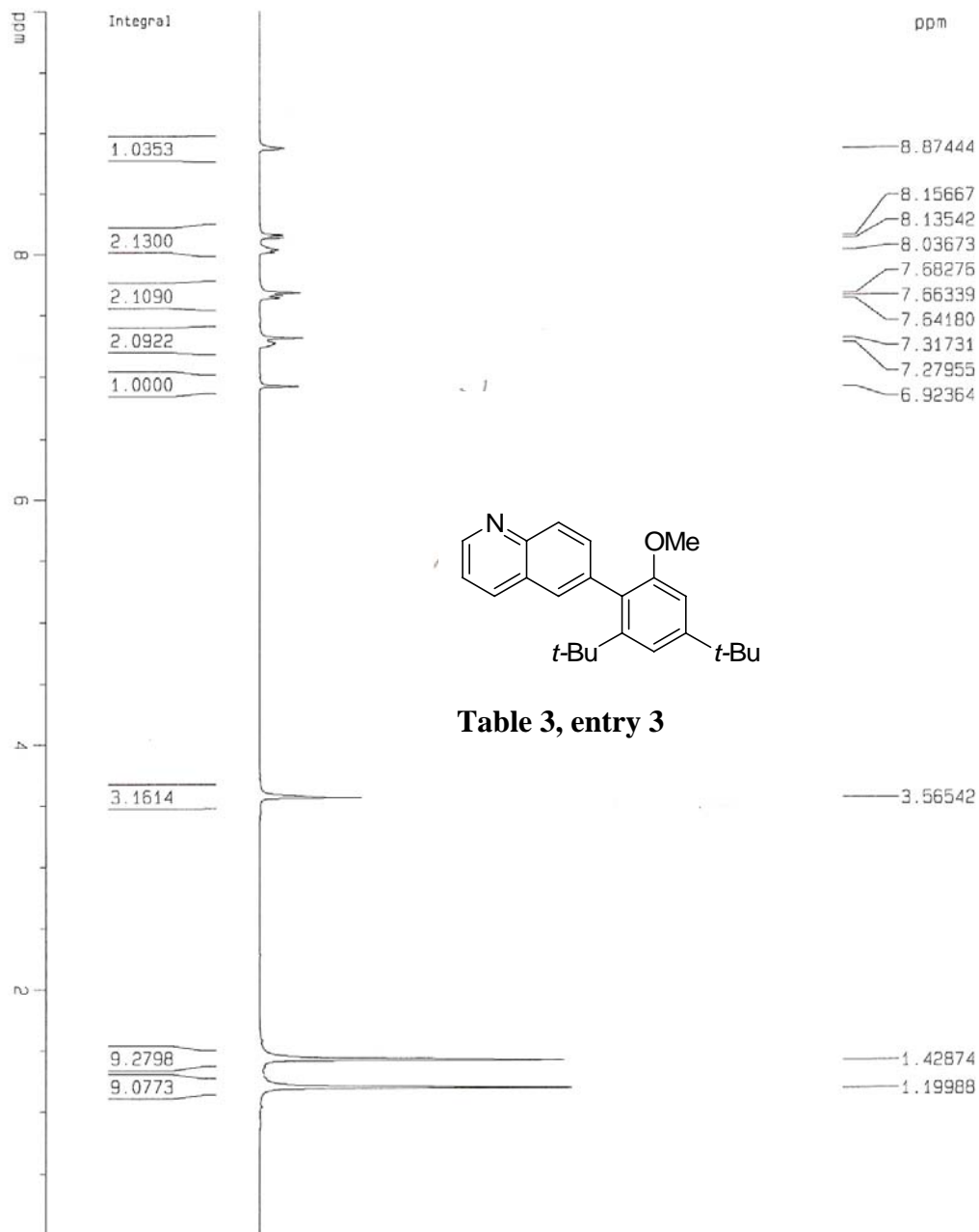


Table 3, entry 3

Current Data Parameters

NAME	COUPLING
EXPNO	80
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070625	21.39
INSTRUM	cp400
PROBHD	5 mm QNP 1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SMH	4401.409 Hz
FIDRES	0.134320 Hz
AQ	3.7224948 sec
RG	18
DM	113.600 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec

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

NUC1	P1	PL1	SFO1
¹ H	9.50 usec	-6.00 dB	400.132006 MHz

F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
16384	400.1300077 MHz	EM	0	0.70 Hz	0	1.00

1D NMR plot parameters

CX	F1P	F1	F2P	F2	PPMCM	HZCM
19.63 cm	10.000 ppm	4001.30 Hz	-0.000 ppm	-0.00 Hz	0.50930 ppm/Hz	203.78769 Hz/Hz

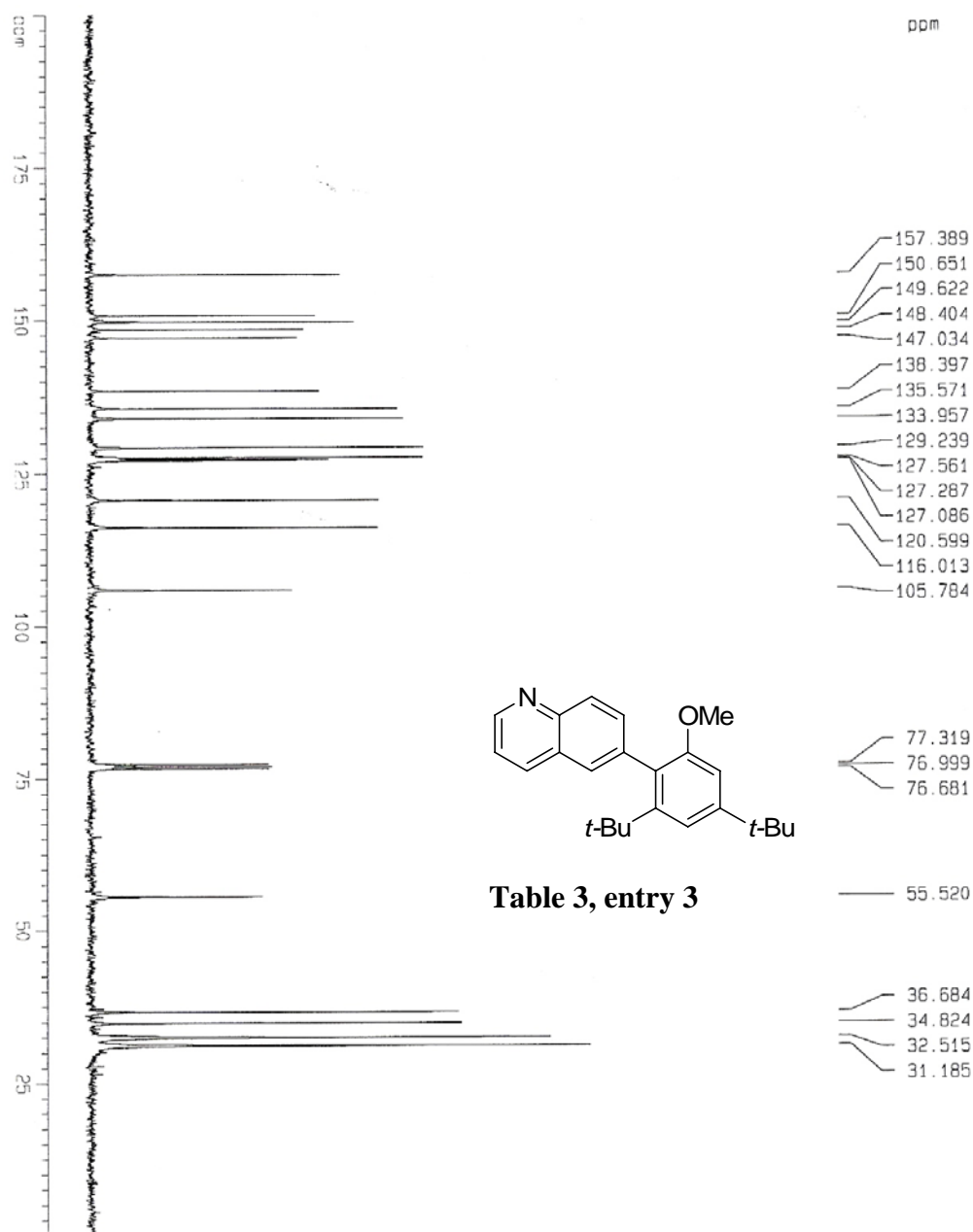


Table 3, entry 3

Current Data Parameters

NAME	Coupling
EXPNO	45
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070625	21.41

INSTRUM: dpx400
PROBHD: 5 mm QNP 1H
PULPROG: zgpg30
TO: 131072
SOLVENT: CDCl3
NS: 64
DS: 0
SWH: 25125.629 Hz
FIDRES: 0.191693 Hz
AQ: 2.6093827 sec
RG: 8192
DM: 19.900 usec
DE: 4.50 usec
TE: 300.0 K
D1: 3.00000000 sec
d11: 0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-6.00 dB
SFO1	100.6231263 MHz

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

CHPROG2	waltz16
NUC2 <td>1H</td>	1H
PCPD2 <td>71.00 usec</td>	71.00 usec
PL2 <td>120.00 dB</td>	120.00 dB
PL12 <td>17.00 dB</td>	17.00 dB
SFO2 <td>400.1326068 MHz</td>	400.1326068 MHz

F2 - Processing parameters

SI	65536
SF <td>100.6128082 MHz</td>	100.6128082 MHz
WDW <td>EM</td>	EM
SSB <td>0</td>	0
LB <td>4.00 Hz</td>	4.00 Hz
GB <td>0</td>	0
PC <td>1.00</td>	1.00

10 NMR plot parameters

CX	19.50 cm
F1P <td>200.000 ppm</td>	200.000 ppm
F1 <td>20122.56 Hz</td>	20122.56 Hz
F2P <td>-0.000 ppm</td>	-0.000 ppm
F2 <td>-0.00 Hz</td>	-0.00 Hz
PPMCK <td>10.2564 ppm/</td>	10.2564 ppm/
HZCM <td>1031.92627 Hz/c</td>	1031.92627 Hz/c

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Operator :
Acquired : 25 Jun 2007 14:58 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 2

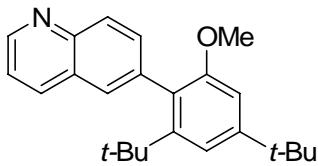
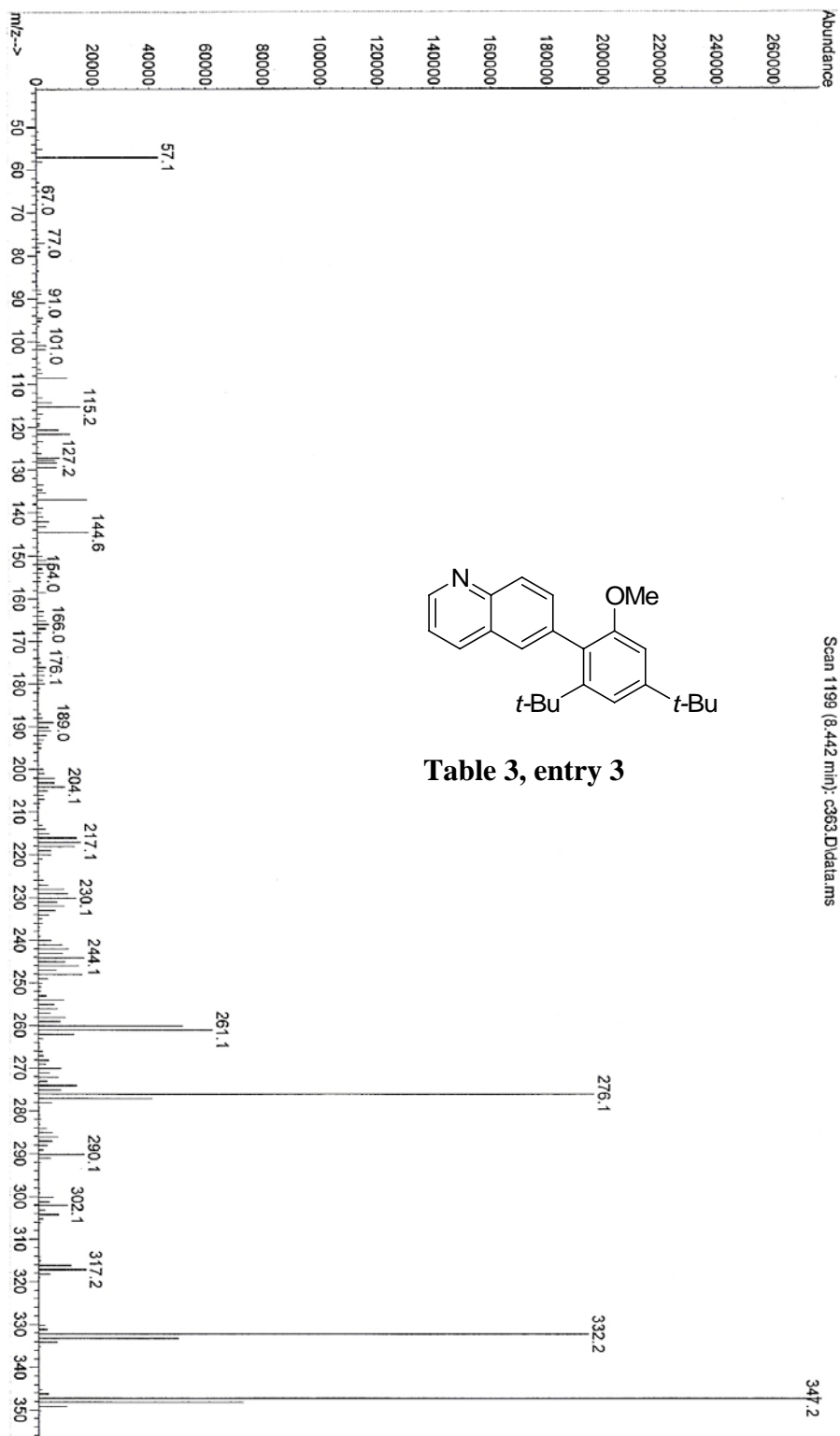
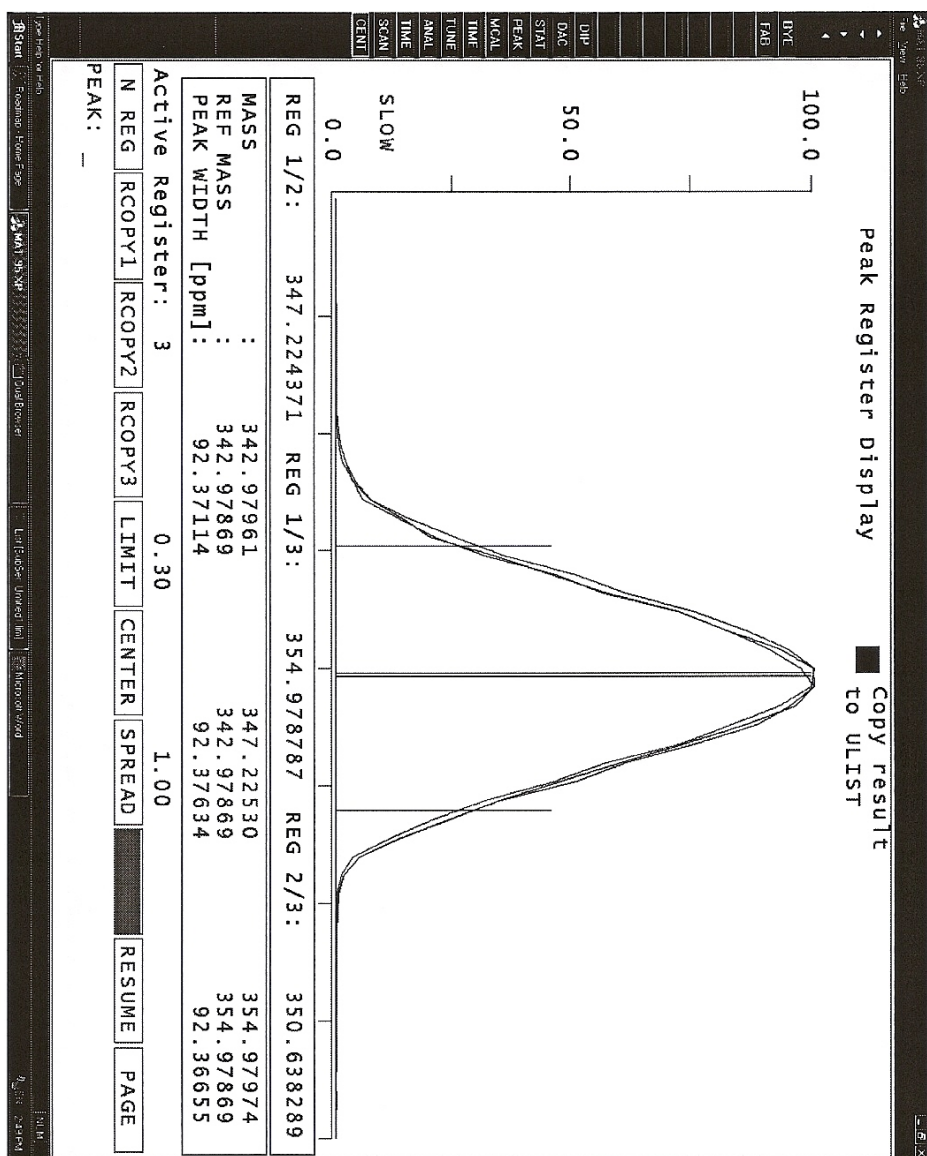


Table 3, entry 3



Accurate Mass Measurement:

Molecular formula:
 $C_{24}H_{29}N_1O_1$
 $[M]^+$ (theoretical)
 = 347.2244

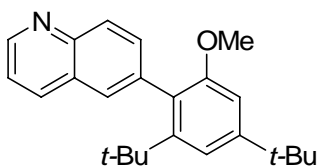
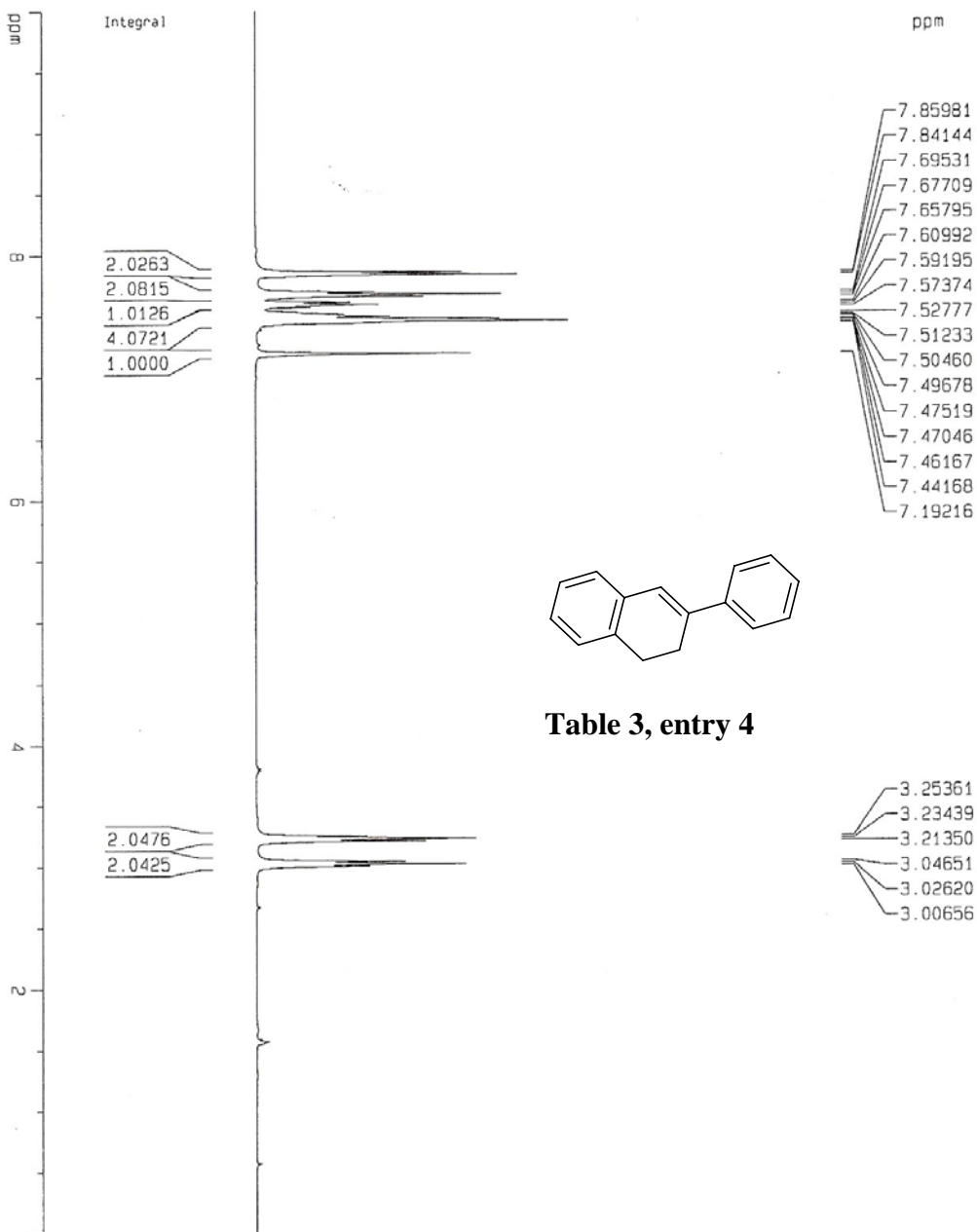


Table 3, entry 3



Current Data Parameters

NAME	COUPLING
EXPNO	82
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070627	21.32

INSTRUM dx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 4401.409 Hz
FIDRES 0.134320 Hz
AQ 3.7224948 sec
RG 18
RW 113.600 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

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

NUC1	1H
P1	9.50 usec
PL1	-6.00 dB
SFO1	400.1320006 MHz

F2 - Processing parameters

SI	16384
SF	400.1300077 MHz
WDW	EM
SSB	0
LB	0.70 Hz
GB	0
PC	1.00

10 NMR plot parameters

CX	19.63 cm
F1P <td>10.000 ppm</td>	10.000 ppm
F1 <td>4001.30 Hz</td>	4001.30 Hz
F2P <td>-0.000 ppm</td>	-0.000 ppm
F2 <td>-0.00 Hz</td>	-0.00 Hz
PPMCM <td>0.50930 ppm/</td>	0.50930 ppm/
HZCM <td>203.78769 Hz/c</td>	203.78769 Hz/c

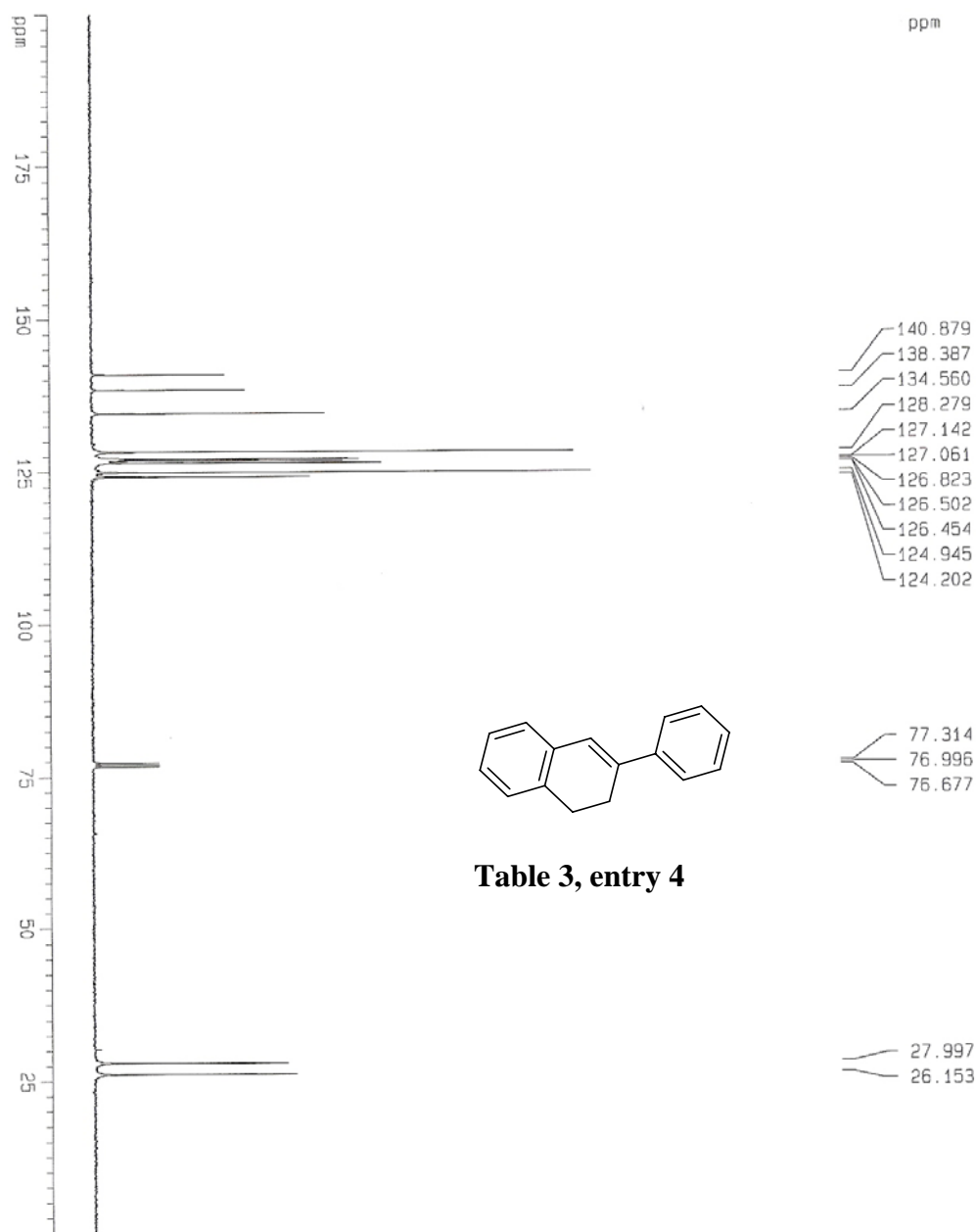


Table 3, entry 4

```

Current Data Parameters
NAME          Coupling
EXPNO         47
PROCNO        1

F2 - Acquisition Parameters
Date_         20070627
Time          21.34
INSTRUM       spect
PROBHD        5 mm QNP 1H
PULPROG       zgpg30
TD            131072
SOLVENT       CDCl3
NS            64
DS            0
SMH           25125.629 Hz
FIDRES        0.191693 Hz
AQ            2.6083827 sec
RG            4096
DM            19.900 usec
DE            4.50 usec
TE            300.0 K
D1            3.0000000 sec
d11           0.0300000 sec

===== CHANNEL f1 =====
NUC1          13C
P1            5.80 usec
PL1           -6.00 dB
SF01          100.6231263 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         71.00 usec
PL2           120.00 dB
PL12          17.00 dB
SF02          400.1325008 MHz

F2 - Processing parameters
SI            65536
SF            100.6128258 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.00

1D NMR plot parameters
CX            19.50 cm
F1P           200.000 DPM
F1            20122.56 Hz
F2P           -0.000 DPM
F2            -0.00 Hz
PPMCK         10.25641 ppm/cm
HZCM          1031.92639 Hz/cm

```

File : C:\msdchem\1\DATA\cms0\CT\c370.D
Operator : flm
Acquired : 27 Jun 2007 14:02 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name:
Misc Info :
Vial Number: 2

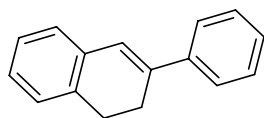
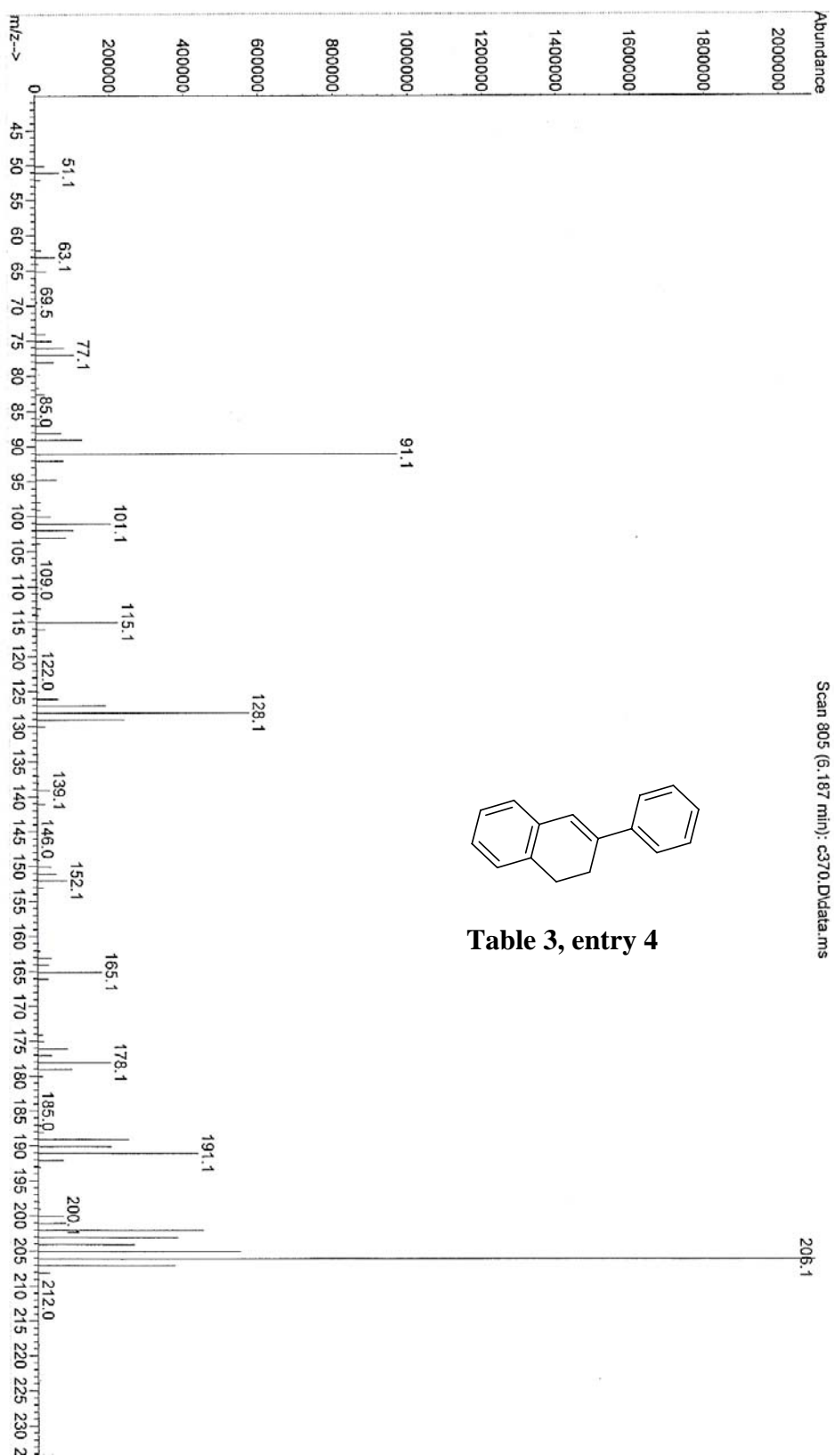
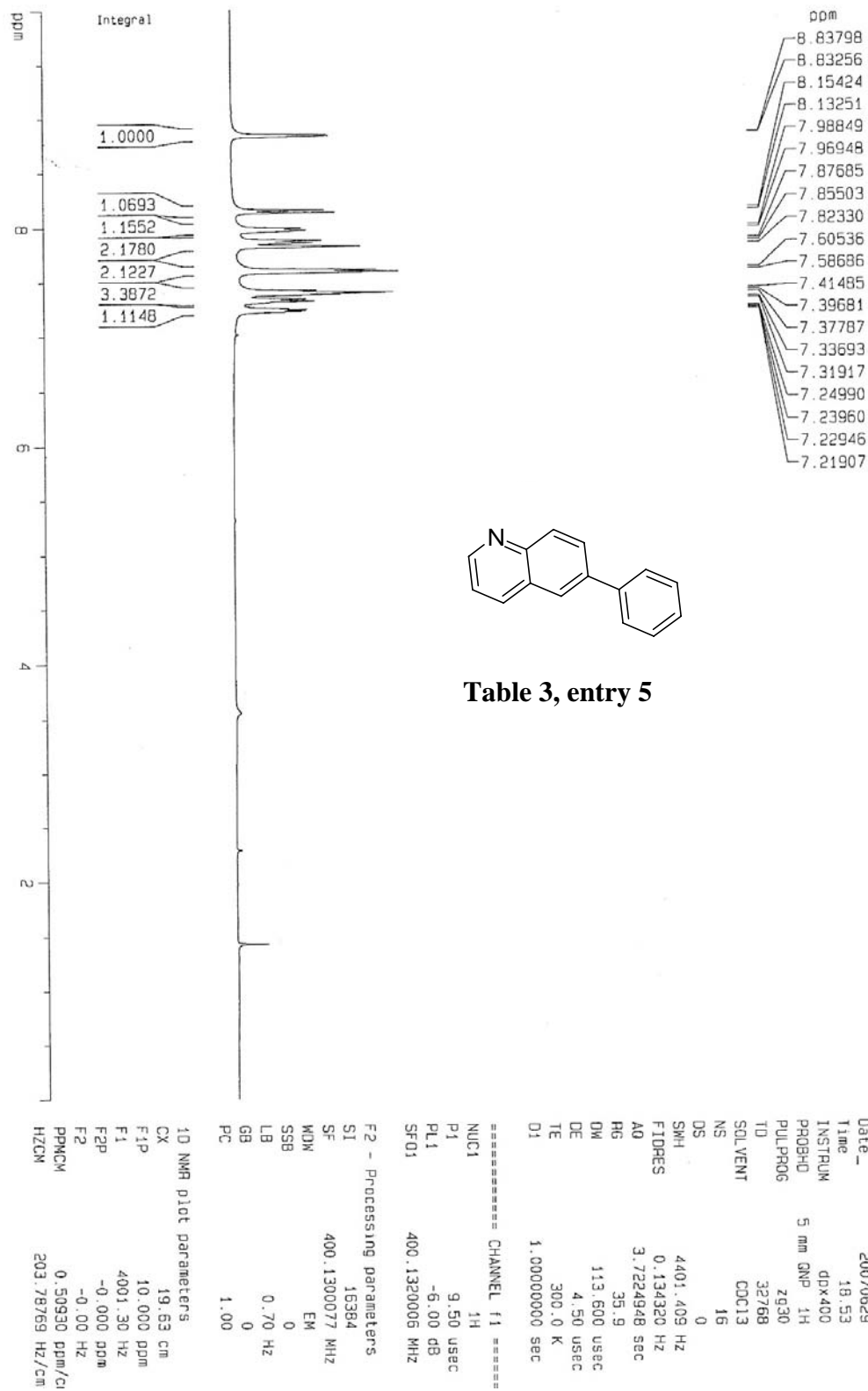


Table 3, entry 4





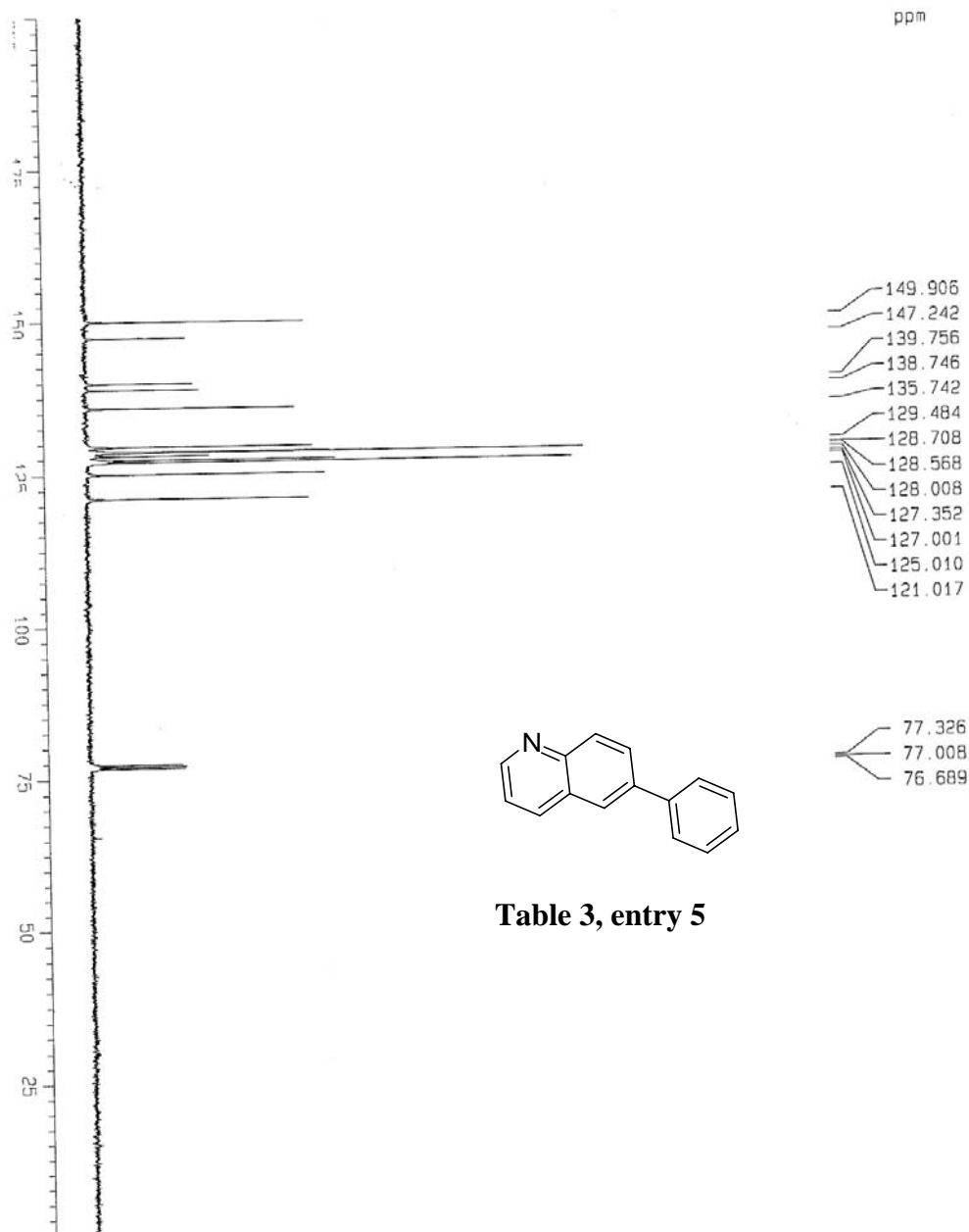


Table 3, entry 5

Current Data Parameters

NAME	Coupling
EXPNO	51
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070629	18.55

INSTRUM: gpc400
PROBHD: 5 mm QNP 1H
PULPROG: zgpg30
TD: 131072
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 25125.629 Hz
FIDRES: 0.191693 Hz
AQ: 2.6083827 sec
RG: 8192
DM: 19.900 usec
DE: 4.50 usec
TE: 300.0 K
D1: 3.00000000 sec
d11: 0.03000000 sec

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

NUC1	13C
P1	5.80 usec
PL1	-5.00 dB
SFO1	100.6231263 MHz

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

CPDPRG2	WALTZ16
NUC2	1H
PCPD2	71.00 usec
PL2	120.00 dB
PL12	17.00 dB
SFO2	400.1326008 MHz

F2 - Processing parameters

SF	65536
MOM	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

10 NMR plot parameters

CX	19.50 cm
F1P	200.000 ppm
F1	20122.56 Hz
F2P	-0.000 ppm
F2	-0.00 Hz
PPMCM	10.25641 ppm
HZCM	1031.92627 Hz

File : C:\msdchem\1\DATA\cms0\CT\c360-78hr.D
Operator : Fbm
Acquired : 26 Jun 2007 18:29 using AcqMethod METHOD2.M
Instrument : 5973N
Sample Name :
Misc Info :
Vial Number: 1

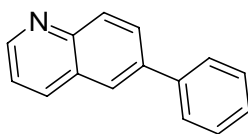
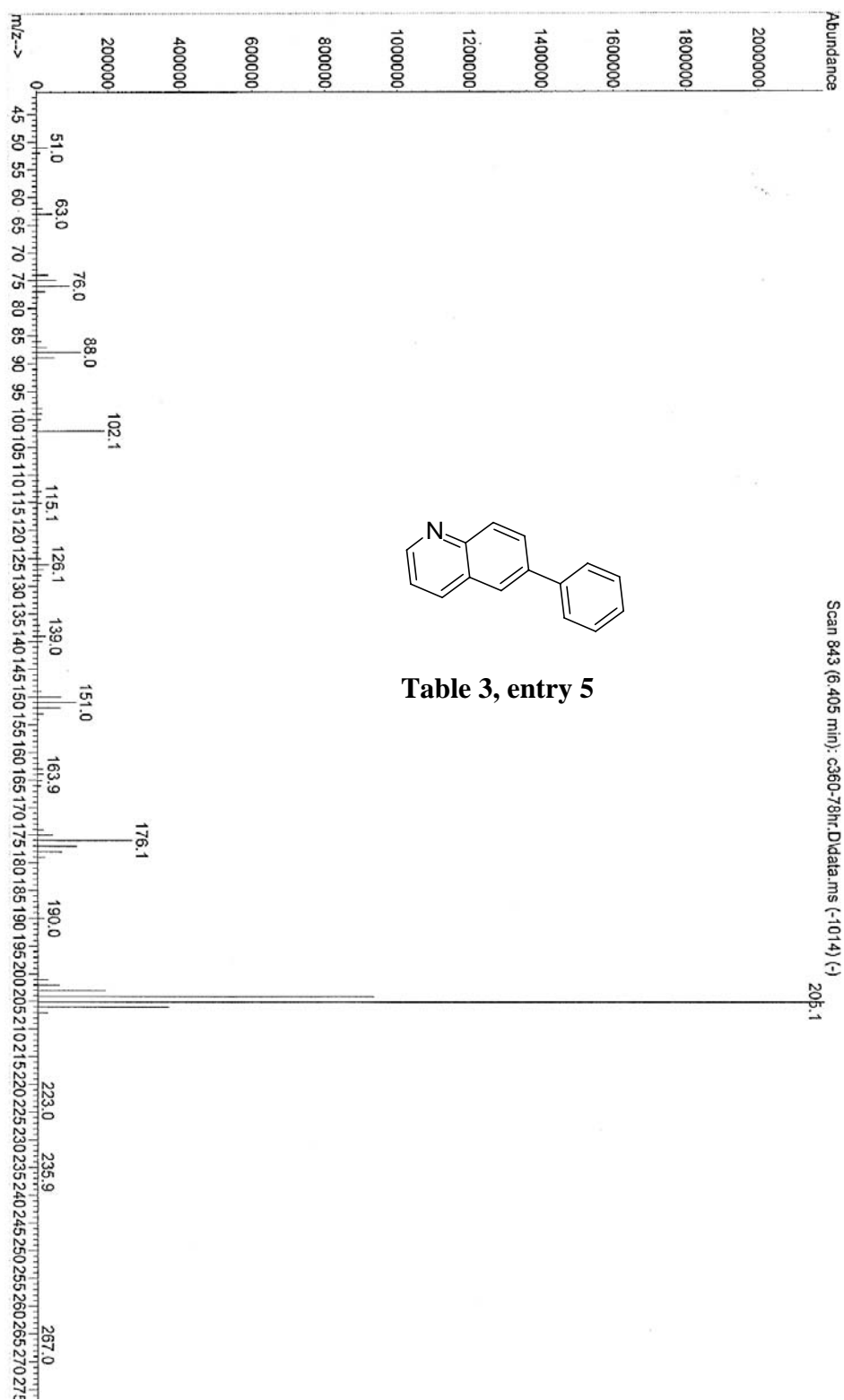


Table 3, entry 5



9. References.

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