

Supporting Information

Aqueous Cross Coupling: Highly efficient Suzuki Reactions of *N*-Heteroaryl Halides and *N*-Heteroarylboronic Acids

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Experimental:

General Experimental:

All chemicals were purchased as reagent grade from commercial suppliers and used without further purification, unless otherwise noted. *n*Butyllithium (2.5 M in hexane) was purchased from Acros. THF was distilled over potassium and benzophenone under an argon-atmosphere, diethylether was distilled over sodium/potassium-alloy and benzophenone under an argon-atmosphere. All experiments were carried out in oven dried glassware under an argon atmosphere, unless otherwise noted. Proton (^1H NMR), carbon (^{13}C NMR), phosphorus (^{31}P NMR) and nitrogen (^{15}N NMR) nuclear magnetic resonance spectra were recorded on Bruker DRX 500 at 500 MHz, 125.75 MHz, 202.46 MHz and 50.69 MHz, respectively at 293 K. The chemical shifts are given in parts per million (ppm) on the delta scale (δ) and are referenced to tetramethylsilane ($\delta = 0$ ppm), ^1H NMR, 65% aq. H_3PO_4 . ($\delta = 0$ ppm), ^{31}P NMR and nitromethane ($\delta = 0$ ppm), ^{15}N NMR. Abbreviations for NMR data: s = singlet; d = doublet; t = triplet; q = quartet; qi = quintet; dd = doublet of doublets; dt = doublet of triplets; dq = doublet of quartets; tt = triplet of triplets; m = multiplet. Mass spectra were recorded on a Finigan MAT 95 magnetic sector spectrometer. Thin layer chromatography (TLC) was performed using Fluka silica gel 60 F 254 (0.2 mm) on aluminum plates. Silica gel columns for chromatography were prepared with *E. Merck* silica gel 60 (0.063-0.20 mesh ASTM). GC experiments were run on a *Clarus* 500 GC with autosampler and FID detector. Column: Varian CP-Sil 8 CB (l = 15 m, $d_i = 0.25$ mm, $d_F = 1.0$ μm), N_2 (flow: 17 cm/sec; split 1:50); Injector-temperature: 270 $^\circ\text{C}$, detector temperature: 350 $^\circ\text{C}$. Temperature program: isotherm 150 $^\circ\text{C}$ for 5 min, heating to 300 $^\circ\text{C}$ with 25 $^\circ\text{C}/\text{min}$, isotherm for 15 min.

Analytical Data of new Coupling Products:

2-p-Tolyl-pyridine

The NMR spectra were identical with the literature.¹

2-p-Tolyl-isonicotinonitrile

¹H NMR (500 MHz, CDCl₃) δ [ppm] 8.75 (dd, ⁵J = 0.5 Hz, ³J = 5.0 Hz, 1 H, CH, ar), 7.84-7.80 (m, 3 H, CH, ar), 7.32 (dd, ⁴J = 1.0 Hz, ³J = 5.0 Hz, 1 H, CH, ar), 7.24 (d, ³J = 8.0 Hz, 2 H, CH, ar), 2.35 (s, 3 H, CH₃); ¹³C{¹H} NMR (125.77 MHz, CDCl₃) δ [ppm] 157.7, 149.5, 139.5, 133.5, 128.8, 125.8, 121.8, 120.7, 120.1, 115.8, 20.3; HRMS calcd. for C₁₃H₁₀N₂: 194.0844, found 194.08414.

2-p-Tolyl-quinoline-3-carbaldehyde

¹H NMR (500 MHz, CD₃CN) δ [ppm] 10.12 (s, 1 H, CHO), 8.85 (s, 1 H, CH, ar), 8.14-8.09 (m, 3 H, CH, ar), 7.91 (ddd, ⁵J = 1.5 Hz, ⁴J = 7.0 Hz, ³J = 8.5 Hz, 1 H, CH, ar), 7.76 (ddd, ⁵J = 1.5 Hz, ⁴J = 7.0 Hz, ³J = 8.5 Hz, 1 H, CH, ar), 7.59 (td, ⁴J = 2.0 Hz, ³J = 8.0 Hz, 2 H, CH, ar), 7.41-7.38 (m, 2 H, CH, ar), 2.45 (s, 3 H, CH₃); ¹³C{¹H} NMR (125.77 MHz, CD₃CN) δ [ppm] 191.1, 159.6, 149.1, 139.2, 137.9, 135.1, 132.3, 130.0, 129.3, 128.8, 128.8, 127.7, 127.1, 126.0, 20.1; HRMS calcd. for C₁₇H₁₃NO: 247.0997, found 247.09700.

4-Methyl-2-p-tolyl-quinoline

The NMR spectra were identical with the literature.²

4-Methyl-2-p-tolyl-pyridine

The NMR spectra were identical with the literature.³

2-p-Tolyl-quinoline

The NMR spectra were identical with the literature.³

¹ Heller, Barbara; Sundermann, Bernd; Buschmann, Helmut; Drexler, Hans-Joachim; You, Jingsong; Holzgrabe, Ulrike; Heller, Eberhard; Oehme, Guenther; *J. Org. Chem.* **2002**, 67, 13, 4414 - 4422.

² Bowman, W. Russell; Fletcher, Anthony J.; Pedersen, Jan M.; Lovell, Peter J.; Elsegood, Mark R. J.; Lopez, Elena Hernandez; McKee, Vickie; Potts, Graeme B. S.; *Tetrahedron*, **2007**, 63, 1, 191 – 203.

³ Gellibert, Françoise; Gouville, Anne-Charlotte de; Woolven, James; Mathews, Neil; Nguyen, Van-Loc; Bertho-Ruault, Cecile; Patikis, Angela; Grygielko, Eugene T.; Laping, Nicholas J.; Huet, Stéphane; *J. Med. Chem.* **2006**, 49, 7, 2210 - 2221.

2-Methoxy-6-p-tolyl-pyridine

^1H NMR (500 MHz, CDCl_3) δ [ppm] 7.93 (d, $^3J = 8.5$ Hz, 2 H, CH, ar), 7.58 (dd, $^3J = 7.5$ Hz, $^3J = 8.0$ Hz, 1 H, CH, ar), 7.29 (dd, $^5J = 0.5$ Hz, $^3J = 7.5$ Hz, 1 H, CH, ar), 7.24 (dd, $^5J = 0.5$ Hz, $^3J = 8.5$ Hz, 2 H, CH, ar), 6.64 (d, $^3J = 8.0$ Hz, 1 H, CH, ar), 4.02 (s, 3 H, OCH_3), 2.39 (s, 3 H, CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CDCl_3) δ [ppm] 164.1, 155.2, 139.5, 139.2, 136.8, 129.7, 127.0, 112.8, 109.2, 53.5, 21.7; HRMS calcd. for $\text{C}_{13}\text{H}_{13}\text{NO}$: 199.0997, found 199.09999.

2-p-Tolyl-pyridin-4-ylamine

^1H NMR (500 MHz, CDCl_3) δ [ppm] 8.25 (d, $^3J = 5.5$ Hz, 1 H, ar), 7.78 (d, $^3J = 8.0$ Hz, 2 H, ar), 7.21 (d, $^3J = 8.0$ Hz, 2 H, ar), 6.85 (s, 1 H, ar), 6.39 (dd, $^3J = 5.5$ Hz, $^4J = 2.5$ Hz, 1 H, ar), 4.35 (s (br), 2 H, NH_2), 2.36 (s, 3 H, CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CDCl_3) δ [ppm] 157.2, 152.6, 159.0, 137.6, 136.0, 128.2, 125.7, 107.2, 105.1, 20.2; HRMS Calcd for $\text{C}_{12}\text{H}_{12}\text{N}_2$: 184.1001, found 184.09808.

4-Methyl-2-m-tolyl-quinoline

^1H NMR (500 MHz, CD_3CN) δ [ppm] 8.06-8.01 (m, 3 H, CH, ar), 7.99-7.96 (m, 1 H, CH, ar), 7.82 (d, $^5J = 0.5$ Hz, 1 H, CH, ar), 7.71 (ddd, $^5J = 1.5$ Hz, $^3J = 6.5$ Hz, $^3J = 8.5$ Hz, 1 H, CH, ar), 7.55 (ddd, $^5J = 1.0$ Hz, $^3J = 6.5$ Hz, $^3J = 8.5$ Hz, 1 H, CH, ar), 7.40 (t, $^3J = 8.0$ Hz, 1 H, CH, ar), 7.30-7.27 (m, 1 H, CH, ar), 2.71 (d, $^5J = 0.5$ Hz, 3 H, CH_3), 2.44 (s, 3 H, CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 156.2, 147.6, 144.9, 139.1, 138.1, 129.7, 129.5, 129.0, 128.3, 127.6, 126.9, 125.7, 124.1, 123.6, 119.0, 20.3, 17.7; HRMS calcd. for $\text{C}_{17}\text{H}_{15}\text{N}$: 233.1205, found 233.12109.

4-Methyl-2-(3-trifluoromethyl-phenyl)-quinoline

^1H NMR (500 MHz, CD_3CN) δ [ppm] 8.54 (s, 1 H, CH, ar), 8.41 (d, $^3J = 7.0$ Hz, 1 H, CH, ar), 8.08-8.02 (m, 2 H, CH, ar), 7.87-7.85 (m, 1 H, CH, ar), 7.78-7.71 (m, 2 H, CH, ar), 7.68 (t, $^3J = 7.5$ Hz, 1 H, CH, ar), 7.60-7.56 (m, 1 H, CH, ar), 2.73-2.72 (m, 3 H, CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 154.2, 147.5, 145.6, 140.0, 130.5, 130.1 (q, $^2J = 31.8$ Hz, CCF_3), 129.6, 129.3, 129.3, 127.1, 126.2, 125.4 (q, $^3J = 4.4$ Hz, CHCCF_3), 123.7, 124.2 (q, $^1J = 271.8$ Hz, CF_3), 123.5 (q, $^3J = 2.9$ Hz, CHCCF_3), 118.7, 17.7; HRMS calcd. for $\text{C}_{17}\text{H}_{12}\text{NF}_3$: 287.0922, found 287.09206.

2-m-Tolyl-quinoline-3-carbaldehyde

^1H NMR (500 MHz, CD_3CN) δ [ppm] 10.10 (s, 1 H, CHO), 8.83 (s, 1 H, CH, ar), 8.12-8.08 (m, 2 H, CH, ar), 7.90 (ddd, $^5J = 1.5$ Hz, $^3J = 7.0$ Hz, $^3J = 9.0$ Hz, 1 H, CH, ar), 7.67 (ddd, $^5J = 1.0$ Hz, $^3J = 7.0$ Hz, $^3J = 8.0$ Hz, 1 H, CH, ar), 7.53-7.50 (m, 1 H, CH, ar), 7.46-7.43 (m, 2 H, CH, ar), 7.40-7.35 (m, 1 H, CH, ar), 2.45 (s, 3 H, CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 191.0, 159.8, 149.0, 138.1, 137.9, 137.8, 132.3, 130.4, 129.5, 129.3, 128.8, 128.0, 127.6, 127.2, 127.1, 126.0, 20.2; HRMS calcd. for $\text{C}_{17}\text{H}_{13}\text{NO}$: 247.0997, found 247.09813.

2-(3-Trifluoromethyl-phenyl)-quinoline-3-carbaldehyde

^1H NMR (500 MHz, CD_3CN) δ [ppm] 10.10 (s, 1 H, CHO), 8.87 (s, 1 H, CH, ar), 8.15-8.10 (m, 2 H, CH, ar), 8.03 (s, 1 H, CH, ar), 7.93 (ddd, $^5J = 1.5$ Hz, $^3J = 7.0$ Hz, $^3J = 8.5$ Hz, 1 H, CH, ar), 7.91-7.84 (m, 2 H, CH, ar), 7.76-7.68 (m, 2 H, CH, ar); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 190.6, 157.7, 148.9, 139.3, 139.2, 133.6, 132.6, 129. (q, $^2J = 32.3$ Hz, CCF_3), 129.2, 128.9, 128.9, 127.6, 127.5, 126.3 (q, $^3J = 3.9$ Hz, CHCCF_3), 126.2, 125.3 (q, $^3J = 3.8$ Hz, CHCCF_3), 124.0 (q, $^1J = 272.4$ Hz, CF_3); HRMS calcd. for $\text{C}_{17}\text{H}_{10}\text{NOF}_3$: 301.0714, found 301.06928.

2-Naphthalen-1-yl-quinoline-3-carbaldehyde

^1H NMR (500 MHz, CD_3CN) δ [ppm] 9.74 (s, 1 H, CHO), 8.96 (s, 1 H, CH, ar), 8.22 (d, $^3J = 8.0$ Hz, 1 H, CH, ar), 8.13 (dd, $^5J = 0.5$ Hz, $^3J = 8.5$ Hz, 1 H, CH, ar), 8.09 (d, $^3J = 8.0$ Hz, 1 H, CH, ar), 8.04 (d, $^3J = 8.0$ Hz, 1 H, CH, ar), 7.96 (ddd, $^5J = 1.0$ Hz, $^3J = 6.5$ Hz, $^3J = 8.5$ Hz, 1 H, CH, ar), 7.75 (ddd, $^5J = 1.5$ Hz, $^3J = 7.0$ Hz, $^3J = 8.5$ Hz, 1 H, CH, ar), 7.67 (dd, $^3J = 7.0$ Hz, $^3J = 8.0$ Hz, 1 H, CH, ar), 7.62-7.52 (m, 3 H, CH, ar), 7.44 (ddd, $^5J = 1.5$ Hz, $^3J = 7.0$ Hz, $^3J = 8.5$ Hz, 1 H, CH, ar); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 190.6, 159.2, 149.3, 137.8, 135.6, 133.2, 132.5, 131.8, 129.5, 128.9, 128.8, 128.8, 128.1, 127.9, 127.5, 126.6, 126.4, 126.0, 125.0, 125.0; HRMS calcd. for $\text{C}_{20}\text{H}_{13}\text{NO}$: 283.0997, found 283.09811.

2-Naphthalen-1-yl-pyridine

The NMR spectra were identical with the literature.⁴

⁴ Song, Chun; Ma, Yudao; Chai, Qiang; Ma, Chanqin; Jiang, Wei; Andrus, Merritt B; *Tetrahedron*, **2005**, 61; 31, 7438-7446.

2-Naphthalen-1-yl-quinoline

The NMR spectra were identical with the literature.⁵

2-Naphthalen-1-yl-pyridin-4-ylamine

¹H NMR (500 MHz, CDCl₃) δ [ppm] 8.20 (d, ³J = 5.5 Hz, 1 H, ar), 8.01 (d, ³J = 8.0 Hz, 1 H, ar), 7.76 (t, ³J = 9.5 Hz, 2 H, ar), 7.43-7.33 (m, 4 H, ar), 6.47 (d, ⁴J = 2.0 Hz, 1 H, ar), 6.27 (dd, ³J = 5.5 Hz, ⁴J = 2.5 Hz, 1 H, ar), 4.37 (s (br), 2 H, NH₂); ¹³C{¹H} NMR (125.77 MHz, CDCl₃) δ [ppm] 158.5, 152.4, 148.5, 138.0, 132.7, 130.2, 127.4, 127.1, 125.8, 125.1, 124.9, 124.7, 124.1, 109.6, 107.1; HRMS Calcd for C₁₅H₁₂N₂: 220.1001, found 220.09869.

4-Methyl-2-naphthalen-1-yl-quinoline

The NMR spectra were identical with the literature.⁶

1-Naphthyl-isonicotinonitrile

¹H NMR (500 MHz, CD₃CN) δ [ppm] 8.75 (dd, ⁵J = 0.5 Hz, ³J = 5.0 Hz, 1 H, CH, ar), 8.75 (dd, ⁴J = 2.5 Hz, ³J = 6.5 Hz, 1 H, CH, ar), 7.82-7.81 (m, 1 H, CH, ar), 7.81-7.79 (m, 2 H, CH, ar), 7.58 (dd, ⁵J = 1.5 Hz, ³J = 5.5 Hz, 1 H, CH, ar), 7.45-7.42 (m, 2 H, CH, ar), 7.38 (ddd, ⁵J = 1.0 Hz, ³J = 7.0 Hz, ³J = 7.5 Hz, 1 H, CH, ar), 7.34 (ddd, ⁵J = 1.0 Hz, ³J = 6.5 Hz, ³J = 8.0 Hz, 1 H, CH, ar); ¹³C{¹H} NMR (125.77 MHz, CD₃CN) δ [ppm] 159.2, 149.6, 135.6, 133.5, 130.3, 129.6, 128.2, 127.8, 127.0, 126.7, 126.1, 125.1, 124.7, 124.0, 121.2, 116.3; HRMS calcd. for C₁₆H₁₀N₂: 230.0844, found 230.08168.

2-Methoxy-6-naphthalen-1-yl-pyridine

The NMR spectra were identical with the literature.⁷

2-Pyridin-3-yl-quinoline-3-carbaldehyde

¹H NMR (500 MHz, CD₃CN) δ [ppm] 10.15 (s, 1 H, CHO), 8.93 (s, 1 H, CH, ar), 8.87 (d, ⁵J = 1.5 Hz, 1 H, CH, ar), 8.73 (dd, ⁵J = 1.5 Hz, ³J = 4.5 Hz, 1 H, CH, ar), 8.19-8.14 (m, 2 H, CH, ar), 8.07-8.04 (m, 1 H, CH, ar), 7.96 (ddd, ⁵J = 1.0 Hz, ³J = 6.5 Hz, ³J = 8.5 Hz, 1 H, CH,

⁵ Zhao, Qiang; Jiang, Chang-Yun; Shi, Mei; Li, Fu-You; Yi, Tao; Cao, Yong; Huang, Chun-Hui; *Organometallics*, **2006**, 25, 15, 3631-3638.

⁶ Thomas, K. R. Justin; Velusamy, Marappan; Lin, Jiann T.; Chien, Chin-Hsiung; Tao, Yu-Tai; Wen, Yuh S.; Hu, Ya-Hui; Chou, Pi-Tai; *Inorg. Chem.* **2005**, 44, 16, 5677-5685.

⁷ Murray, Kenneth John; Porter, Roderick Alan; Prain, Hunter Douglas; Warrington, Brian Herbert; PCT Int. Appl. **1991**, WO 9117987.

ar), 7.73 (ddd, $^5J = 1.0$ Hz, $^3J = 7.0$ Hz, $^3J = 8.0$ Hz, 1 H, CH, ar), 7.54 (ddd, $^5J = 0.5$ Hz, $^3J = 4.5$ Hz, $^3J = 8.0$ Hz, 1 H, CH, ar); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 190.7, 156.5, 150.1, 149.6, 149.0, 139.6, 137.1, 132.7, 129.3, 128.9, 127.7, 127.7, 126.2, 123.9, 122.9; HRMS calcd. for $\text{C}_{15}\text{H}_{10}\text{N}_2\text{O}$: 234.0793, found 234.07699.

[2,3']Bipyridinyl

The NMR spectra were identical with the literature.⁸

2-Pyridin-3-yl-quinoline

The NMR spectra were identical with the literature.⁹

4-Methyl-[2,3']bipyridinyl

The NMR spectra were identical with the literature.¹⁰

4-Methyl-2-pyridin-3-yl-quinoline

The NMR spectra were identical with the literature.¹¹

6-Methoxy-[2,3']bipyridinyl

The NMR spectra were identical with the literature.¹²

[2,3']Bipyridinyl-4-ylamine

^1H NMR (500 MHz, CDCl_3) δ [ppm] 9.01 (d, $^4J = 1.5$ Hz, 1 H, ar), 8.53 (dd, $^3J = 5.0$ Hz, $^4J = 1.5$ Hz, 1 H, ar), 8.22 (d, $^3J = 6.0$ Hz, 1 H, ar), 8.16 (dt, $^3J = 8.0$ Hz, $^4J = 2.0$ Hz, 1 H, ar), 6.29-6.26 (m, 1 H, ar), 6.87 (d, $^4J = 2.0$ Hz, 1 H, ar), 6.44 (dd, $^3J = 6.0$ Hz, $^4J = 2.5$ Hz, 1 H, ar), 4.53 (s, 2 H, NH_2); $^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CDCl_3) δ [ppm] 154.5, 152.8, 149.5,

⁸ Cioffi, Christopher L.; Spencer, William T.; Richards, Justin J.; Herr, R. Jason; *J. Org. Chem.* **2004**, 69, 6, 2210 – 2212.

⁹ a) Barder, Timothy E.; Buchwald, Stephen L.; *Org. Lett.* 2004, 6, 16, 2649-2652. b) Bonnet, Veronique; Mongin, Florence; Trecourt, Francois; Breton, Gilles; Marsais, Francis; Knochel, Paul; Queguiner, Guy, *Synlett*, **2002**, 6, 1008-1010.

¹⁰ Denton, Travis T.; Zhang, Xiaodong; Cashman, John R. *J. med. Chem.* **2005**, 48, 1, 224-239.

¹¹ Vargas M., Leonor Y.; Castelli, Maria V.; Kouznetsov, Vladimir V.; Urbina G., Juan M.; Lopez, Silvia N.; Sortino, Maximiliano; Enriz, Ricardo D.; Ribas, Juan C.; Zacchino, Susana; *Bioorg. Med. Chem.* **2003**, 11, 7, 1531-1550.

Denton, Travis T.; Zhang, Xiaodong; Cashman, John R. *J. med. Chem.* **2005**, 48, 1, 224-239.

¹² Dehmlow, Eckehard V.; Slegers, Arthur; *Liebigs Ann. Chem.* **1992**, 9, 953-9.

148.6, 147.1, 134.4, 133.4, 122.5, 107.9, 105.5; HRMS calcd. for C₁₀H₉N₃: 171.0797, found 171.07820.

4-Methyl-2-phenyl-pyridine (crude)

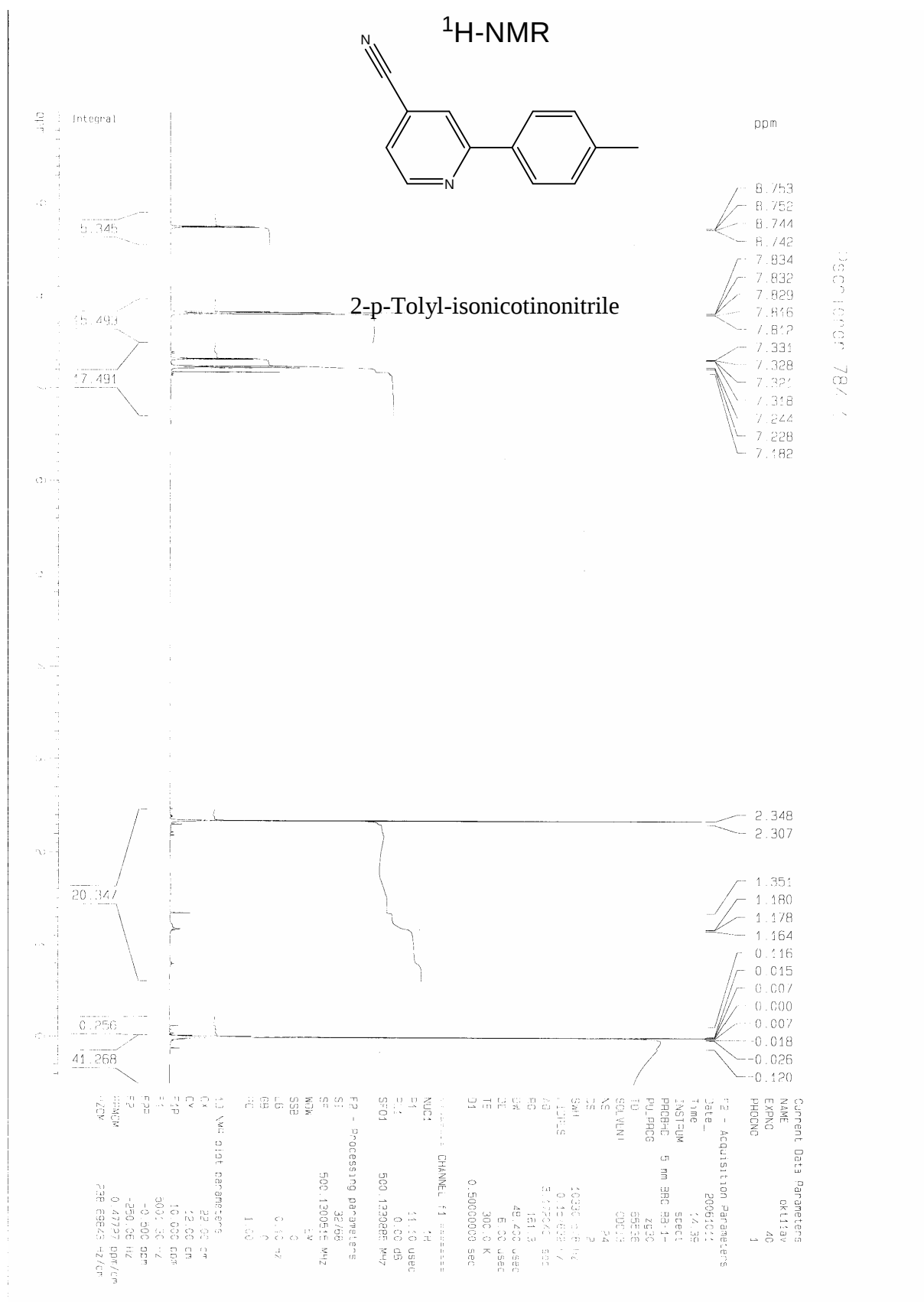
¹H NMR (500 MHz, CDCl₃) δ [ppm] 8.54 (d, ³J = 4.8 Hz, 1 H, CH, ar), 7.98-7.95 (m, 2 H, CH, ar), 7.53 (s, 1 H, CH, ar), 7.48-7.43 (m, 2 H, CH, ar), 7.41-7.37 (m, 1 H, CH, ar), 7.04 (d, ³J = 4.8 Hz, 1 H, CH, ar), 2.40 (s, 3 H, CH₃).

The ¹H-NMR spectrum was identical with the literature.¹³

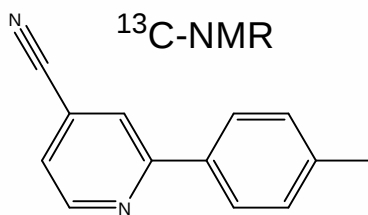
¹³

McLoughlin, Padraig T.F.; Clyne, Mairead A.; Aldabbagh, Fawaz; *Tetrahedron*; **2004**; 60; 37; 8065 – 8072.

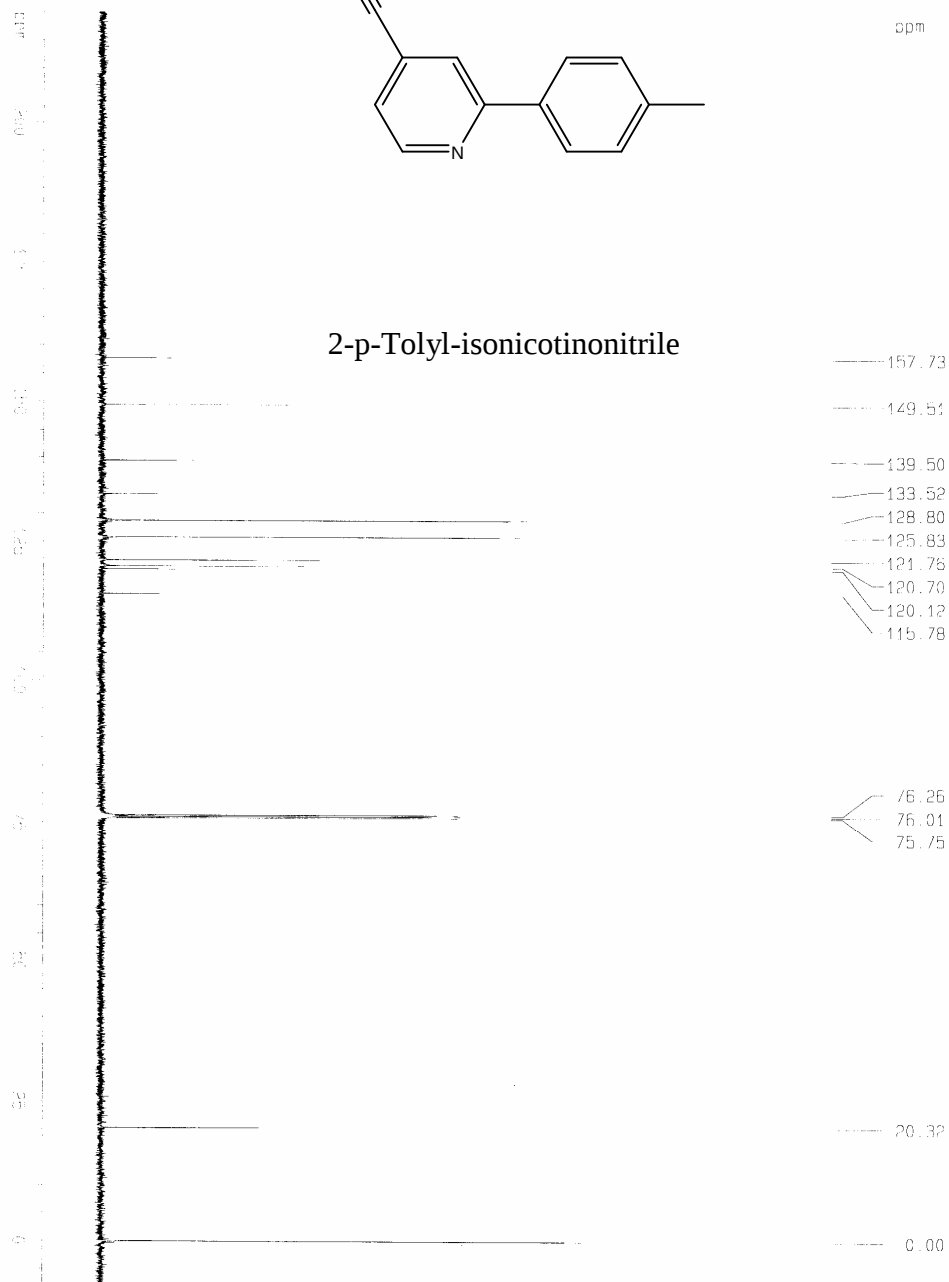
NMR-Spectra



PSCHREIER 784-1



2-p-Tolyl-isonicotinonitrile



Current Data Parameters

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EXPNO	41			
PROCNO	1			

F2 - Acquisition Parameters

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d12	0.0000000 sec

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

Parameter	Value
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P1	7.40 usec
PL1	4.00 dB
SFO1	125.770343 MHz

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

Parameter	Value
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F2 Processing parameters

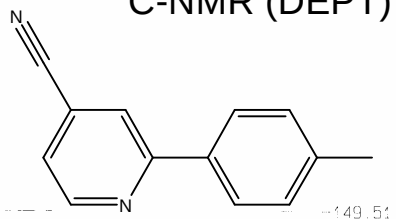
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10 NMR list parameters

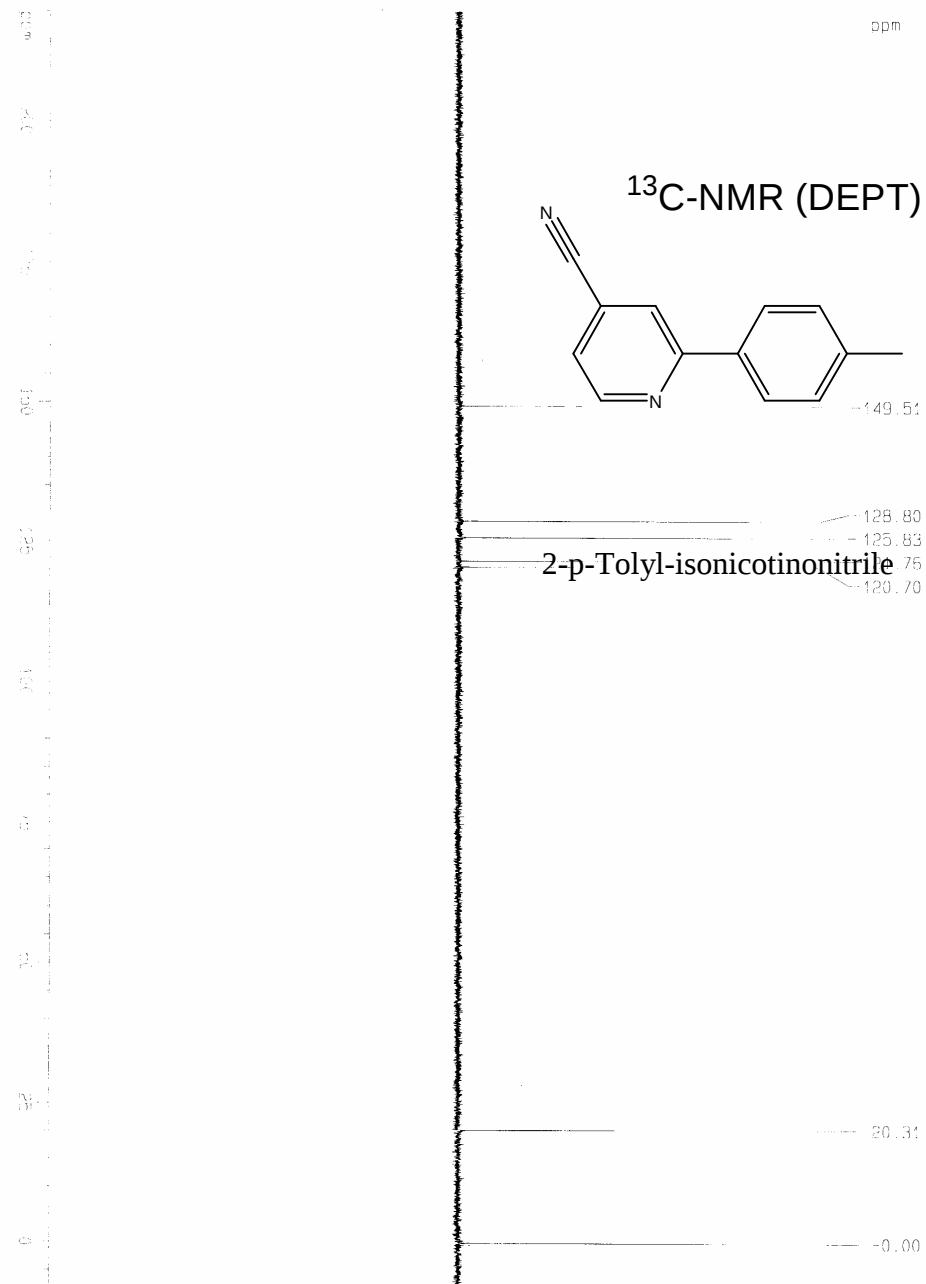
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PSCH1692P 784 1

¹³C-NMR (DEPT)



2-p-Tolyl-isonicotinonitrile



Current Data Parameters
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F2 - Acquisition Parameters

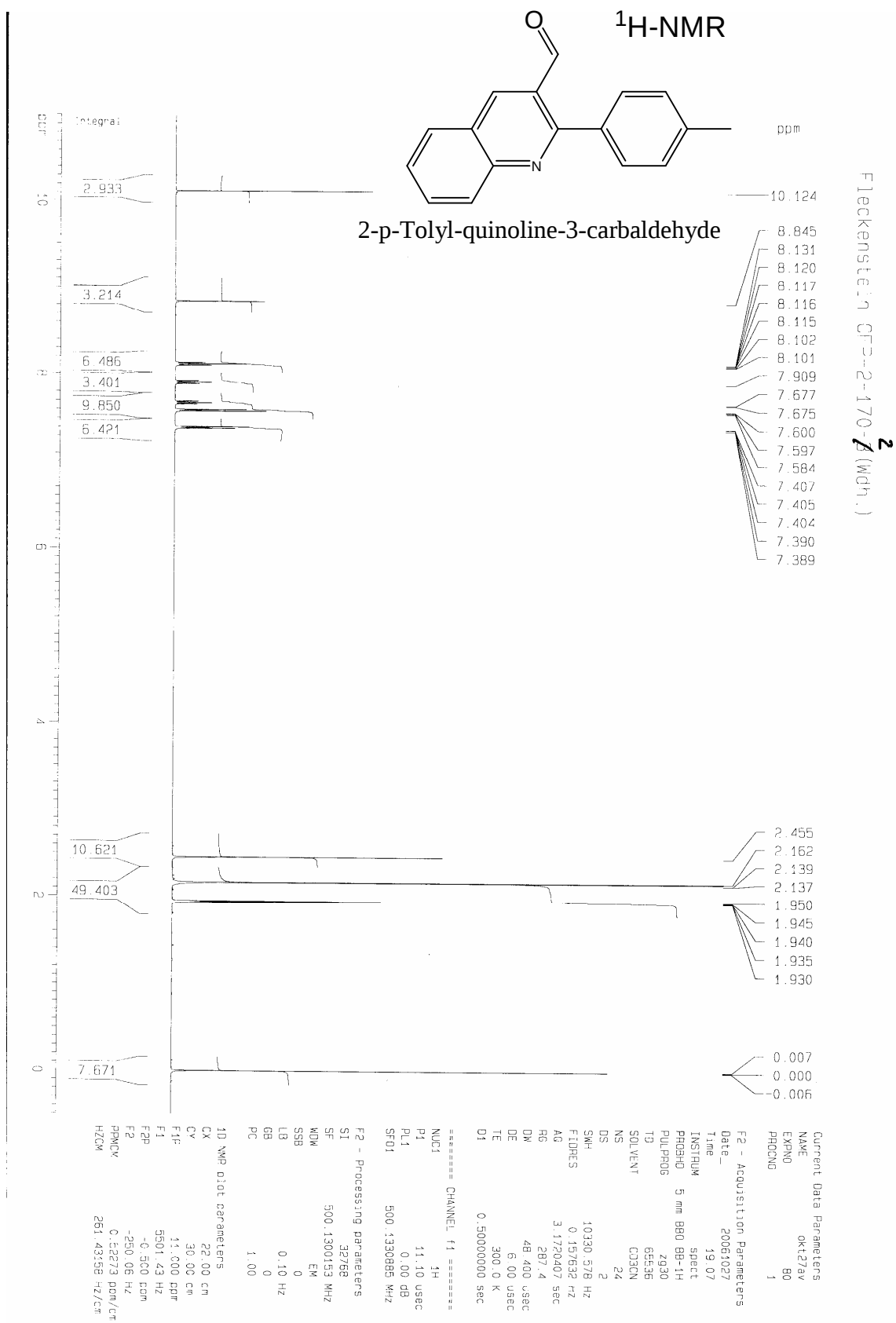
Date_ 20051011
Time 14.15
INSTRUM spect
PROBHD 5 mm BBO BB-7H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 325
DS 4
SWH 31953.884 MHz
FIDRES 0.972659 Hz
AQ 0.674621 sec
RG 656
GB 16.860 MHz
PC 19.00 MHz
TE 300.2 K
CNS 2 1.40000000 sec
D1 2.00000000 sec
d2 0.00344878 sec
d12 0.00020000 sec
DELTA 0.00009422 sec

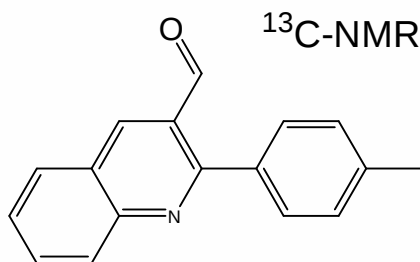
===== CHANNEL f1 =====
NUC1 13C
P1 1.00 usec
PL1 14.00 dB
PL2 14.00 dB
PL3 14.00 dB
SF01 125.761343 MHz

===== CHANNEL f2 =====
COPPRG2 x617116
NUC2 1H
P3 11.00 usec
PL3 14.00 dB
PL4 14.00 dB
PL5 14.00 dB
PL6 14.00 dB
PL7 14.00 dB
PL8 14.00 dB
PL9 14.00 dB
PL10 14.00 dB
PL11 14.00 dB
PL12 14.00 dB
SF02 500.136059 MHz

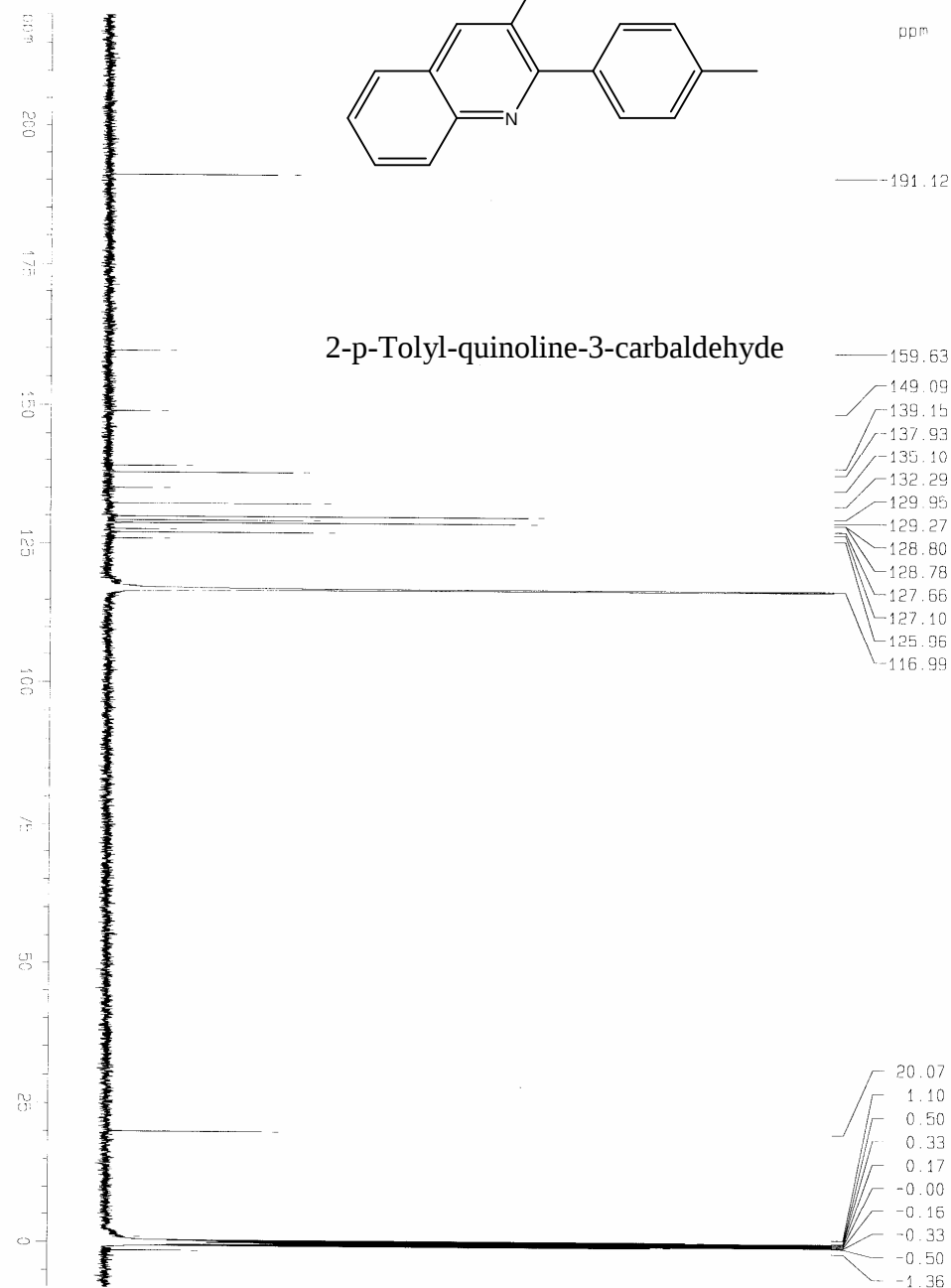
F2 - PULPROG zgpg30
SI 32768
SF 125.761343 MHz
WDW EM
SSB 0
Z 2.00 Hz
GB 0
PC 1.00

13 NMR 5.00 usec
CX 72.00 usec
CY 9.00 usec
F10 270.000 MHz
F11 77.000 MHz
F12 77.000 MHz
F2 125.761343 MHz
PRCK 16.000 MHz
FREQ 125.761343 MHz





2-p-Tolyl-quinoline-3-carbaldehyde



Current Data Parameters
 NAME ok127av
 EXPNO 81
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 2006/02/7
 Time 20.11
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 3000
 DS 4
 SWH 37593.984 Hz
 FIDRES 0.573639 Hz
 AQ 0.8716921 sec
 RG 8152
 DM 13.300 usec
 DE 5.00 usec
 TE 300.0 K
 D1 0.4000001 sec
 d11 0.0300000 sec
 d12 0.0002000 sec

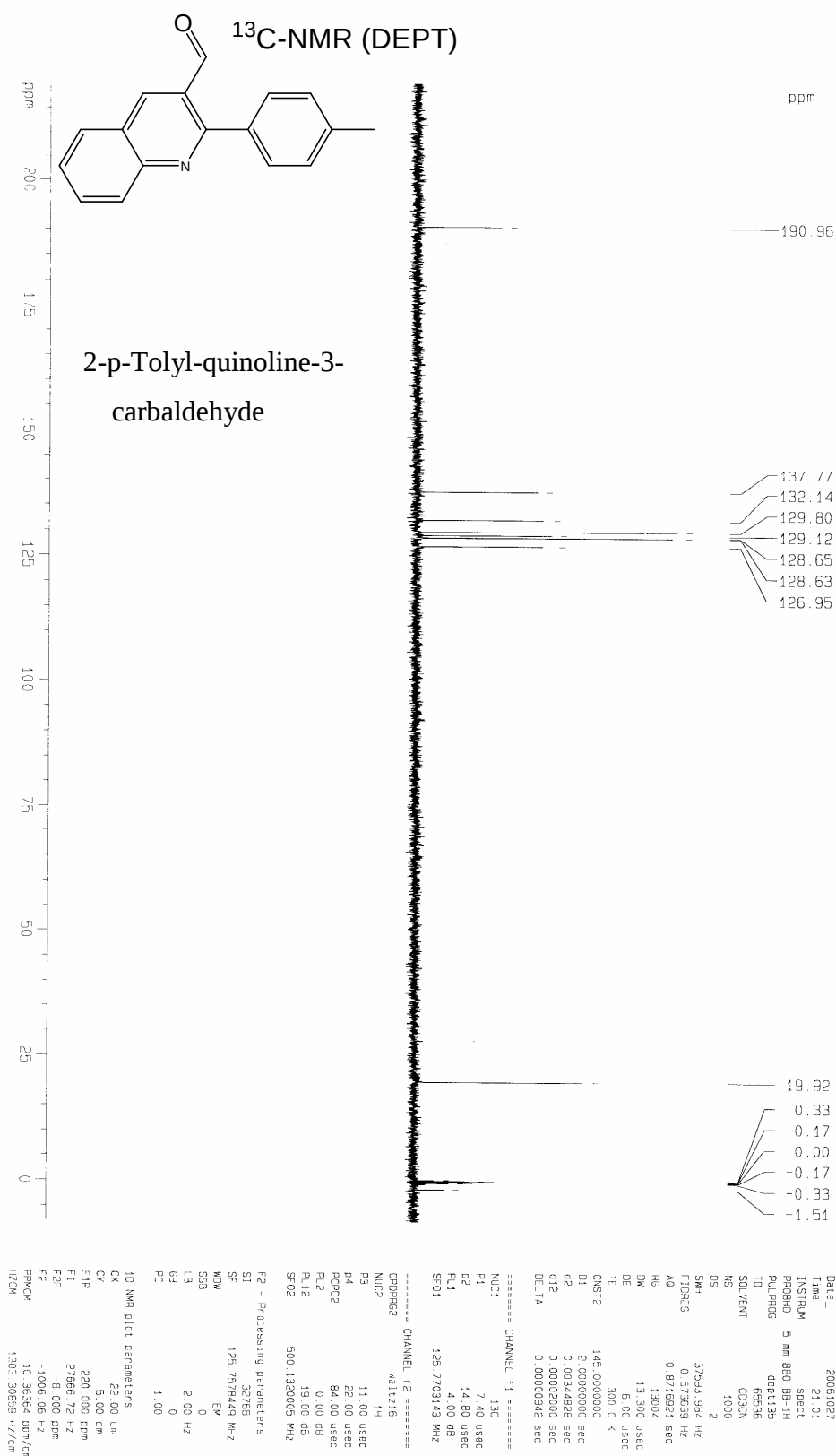
===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 4.00 dB
 SF01 125.7703143 MHz

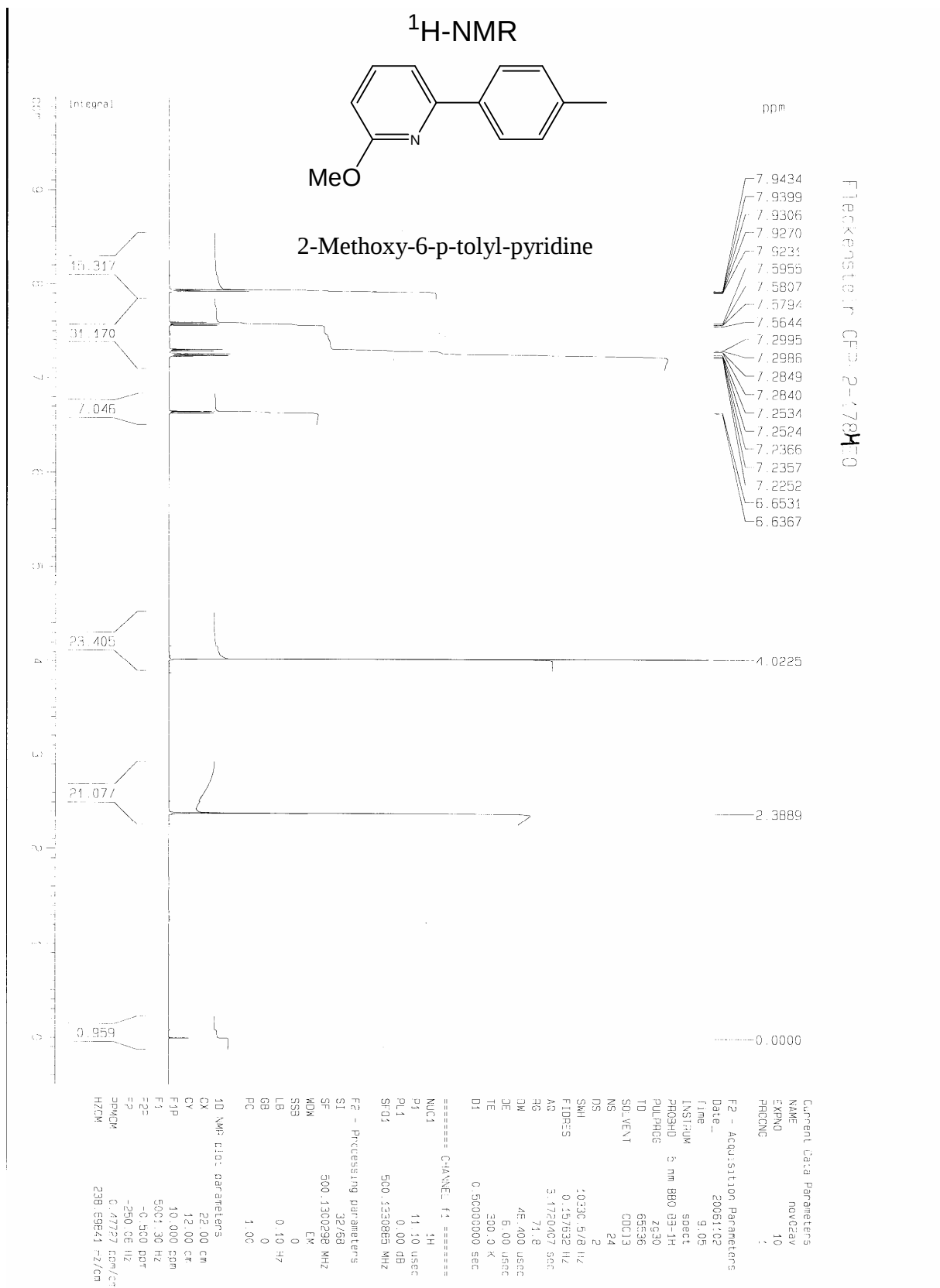
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 84.00 usec
 PL2 0.00 dB
 PL12 19.00 dB
 PL13 19.00 dB
 SF02 500.132005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7578259 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

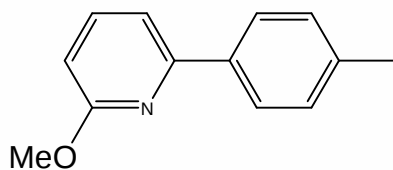
1D NMR file parameters
 CX 22.00 cm
 CY 80.00 cm
 F1P 220.000 ppm
 F1 27656.72 Hz
 F2P -6.000 ppm
 F2 -1006.06 Hz
 PPM0V 10.36564 ppm/cm
 V1CM 1303.30947 Hz/cm

Fleckenstein CFP-2-170-3 (Wdh.)

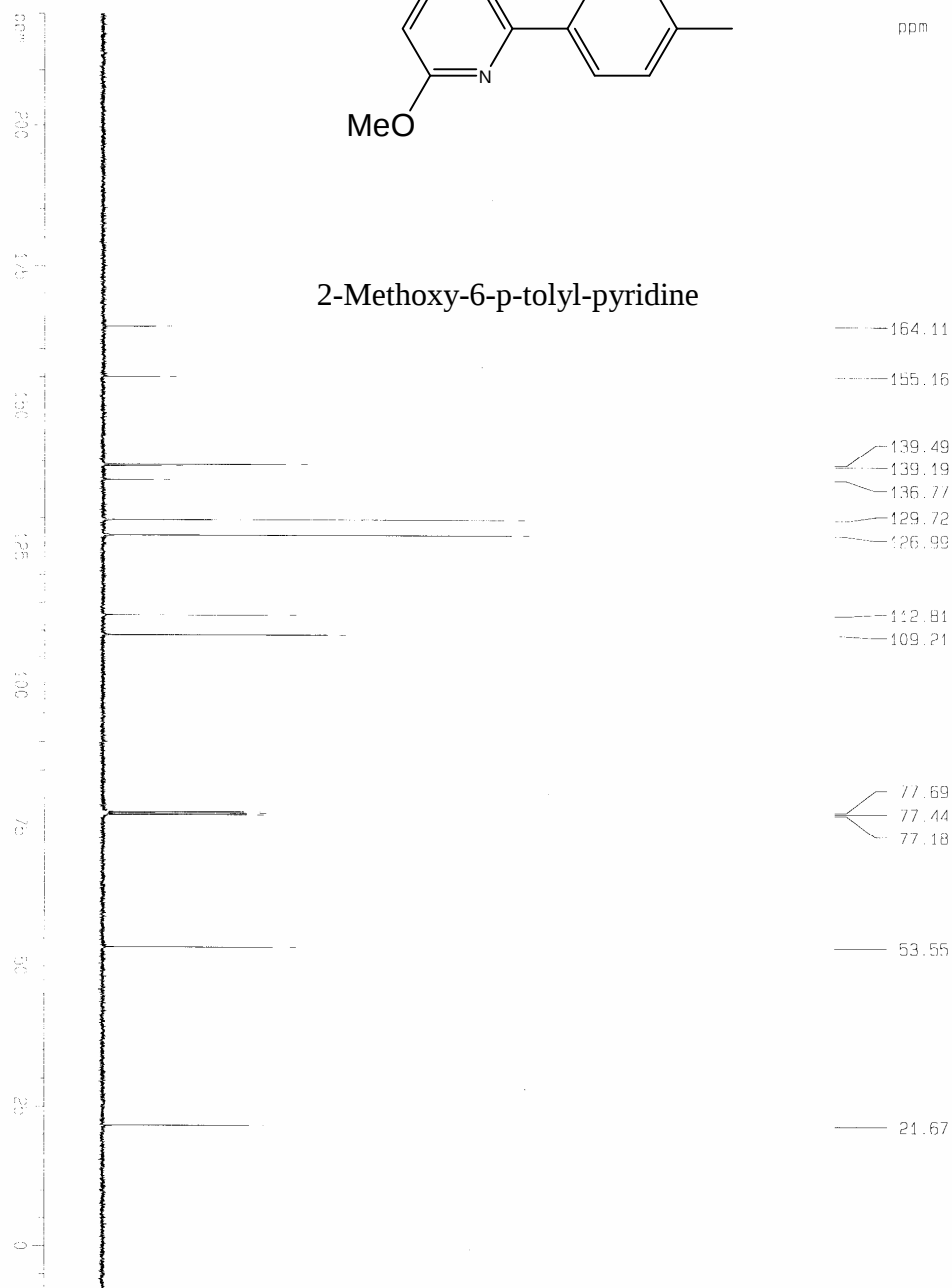




¹³C-NMR



2-Methoxy-6-p-tolyl-pyridine



Hockenstein CFP-2-1/8H2O

Current Data Parameters
NAME nov2aw
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061102
Time 5.09
INSTRUM spect
PROBHD 5 mm BBO-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 152
DS 4
SWH 37453.984 Hz
FIDRES 0.174339 Hz
AQ 0.6716921 sec
RG 652
FSC2
DE 13.300 usec
TE 6.00 usec
T1 3.00 sec
T1 0.0300000 sec
d11 0.0300000 sec
d12 0.0000000 sec

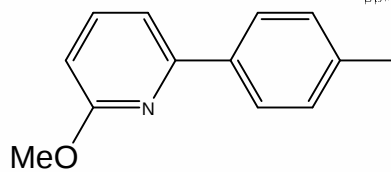
===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 4.00 dB
SFO1 125.770343 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 19.00 usec
PL2 0.00 dB
SFO2 500.132000 MHz

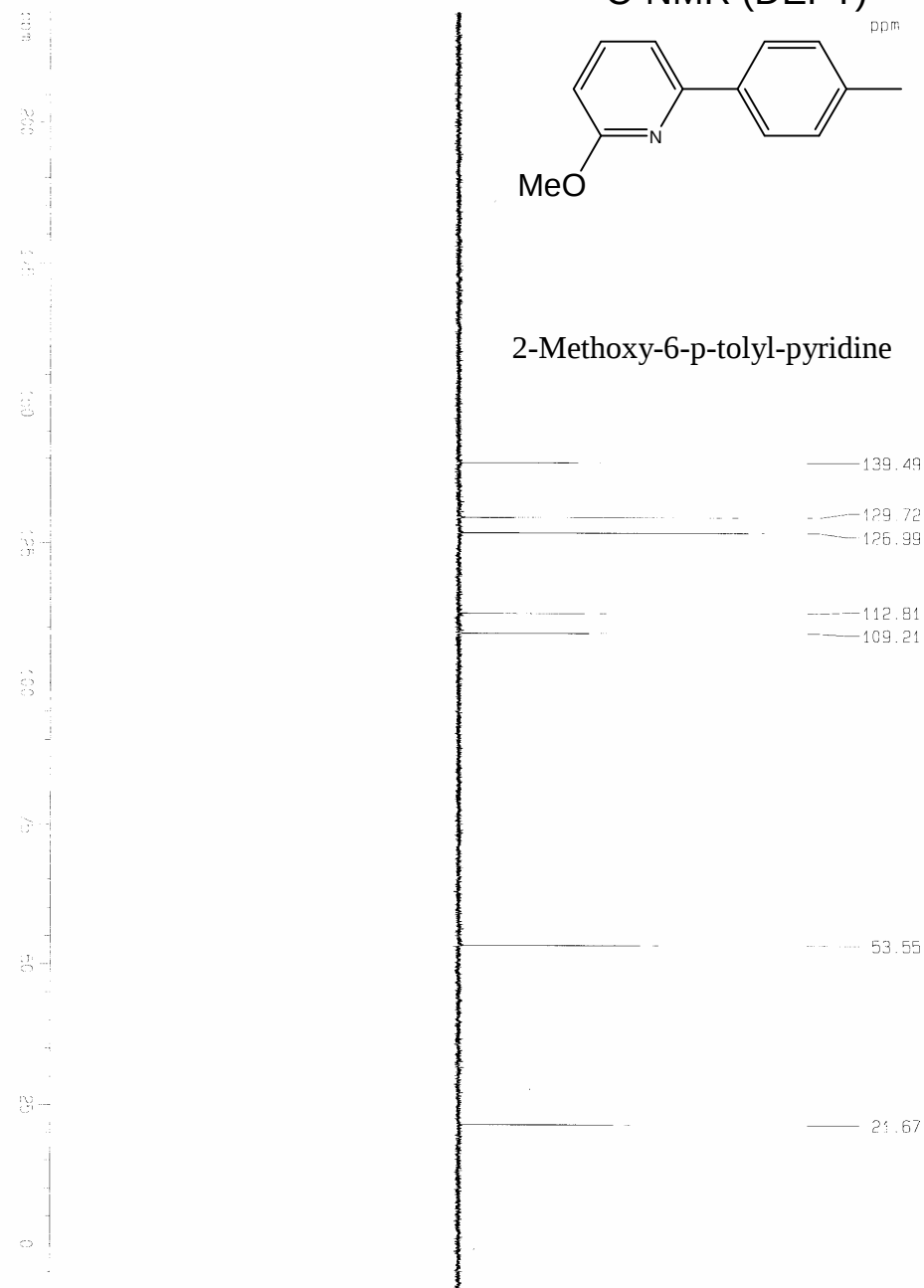
F2 - Processing parameters
SI 32768
SF 125.757350 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR file parameters
CX 22.00 cm
CY 7.00 cm
F1F 220.000 cm
Z1 21666.70 Hz
Z2 -21666.70 Hz
F2-NMR 10.000000 Hz
F2-NUC 13C
F2-PC 1.000000

¹³C-NMR (DEPT)



2-Methoxy-6-p-tolyl-pyridine



Current Data Parameters
NAME nov02av
EXPNO 12
PROCNO 1

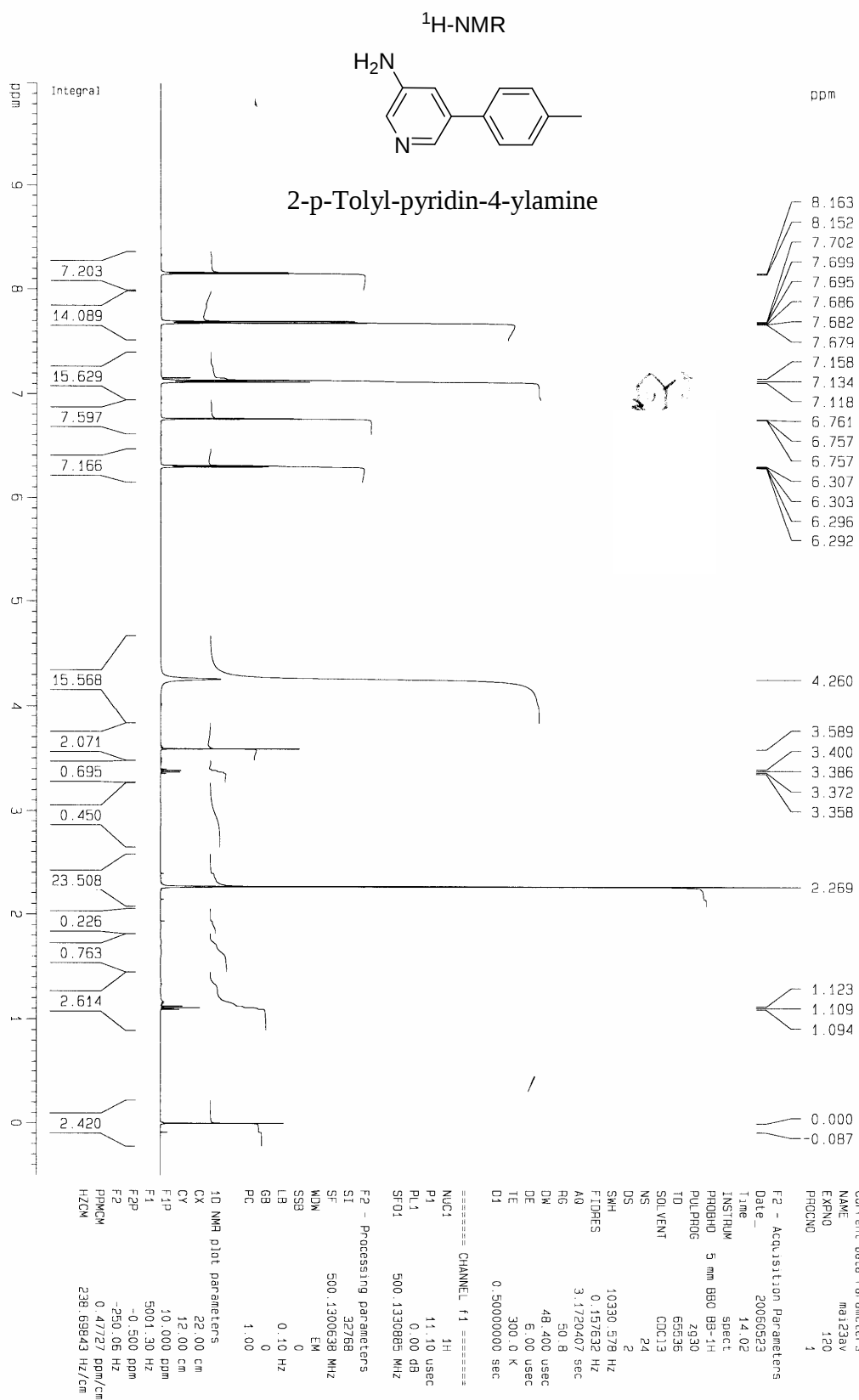
F2 - Acquisition Parameters
Date_ 20061102
Time 9.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
SOLVENT DMSO
NS 40
DS 2
SWH 3759.980 MHz
FIDRES 0.57855 Hz
AQ 0.876961 sec
RG 1024
TM 13.500 sec
JR 6.00 usec
TL 300.0 K
CNS12 140.3000000 sec
D1 2.0000000 sec
d2 0.0034678 sec
d12 0.0000200 sec
DELTA 0.0000942 sec

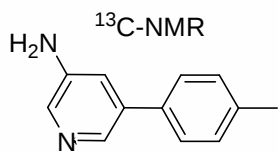
===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 14.80 dB
SFO1 125.7703143 MHz

===== CHANNEL f2 =====
COPRG2 waltz16
NUC2 1H
P2 11.00 usec
PL2 22.00 dB
PL12 0.00 dB
PL12 15.00 dB
SFO2 500.1320005 MHz

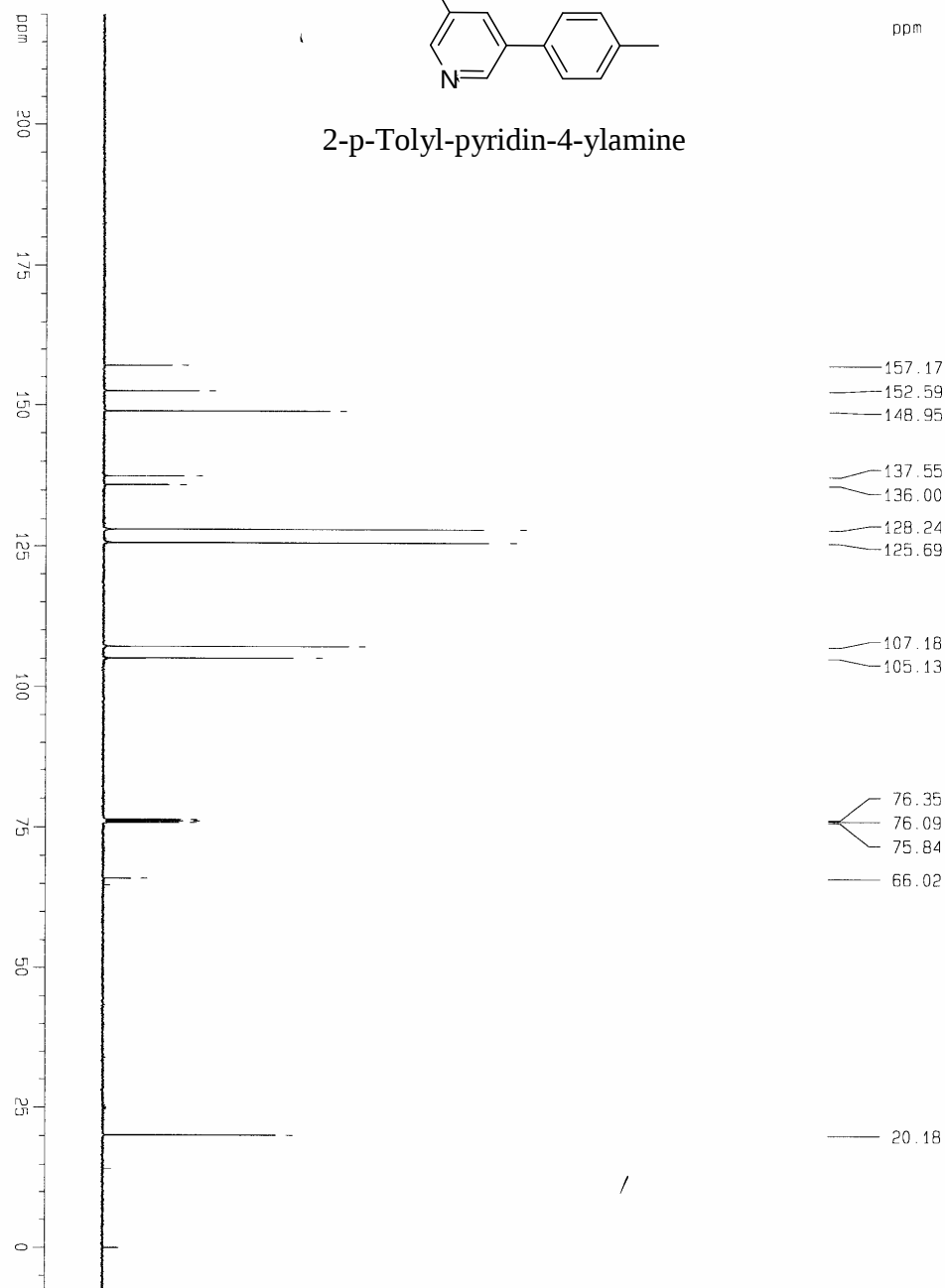
F2 - Processing parameters
SI 32768
SF 125.7577590 MHz
WDW EM
SSB 0
GB 2.00 usec
PC 1.00

10 MHz 110t detectors
CX 22.00 usec
CY 5.00 usec
F1P 720.000 MHz
F2P 720.000 MHz
F2 1206.00 MHz
P2 10.00000000 sec
P2 10.00000000 sec
P2 10.00000000 sec





2-p-Tolyl-pyridin-4-ylamine



Current Data Parameters
NAME ma.23av
EXPNO 121
PROCNO 1

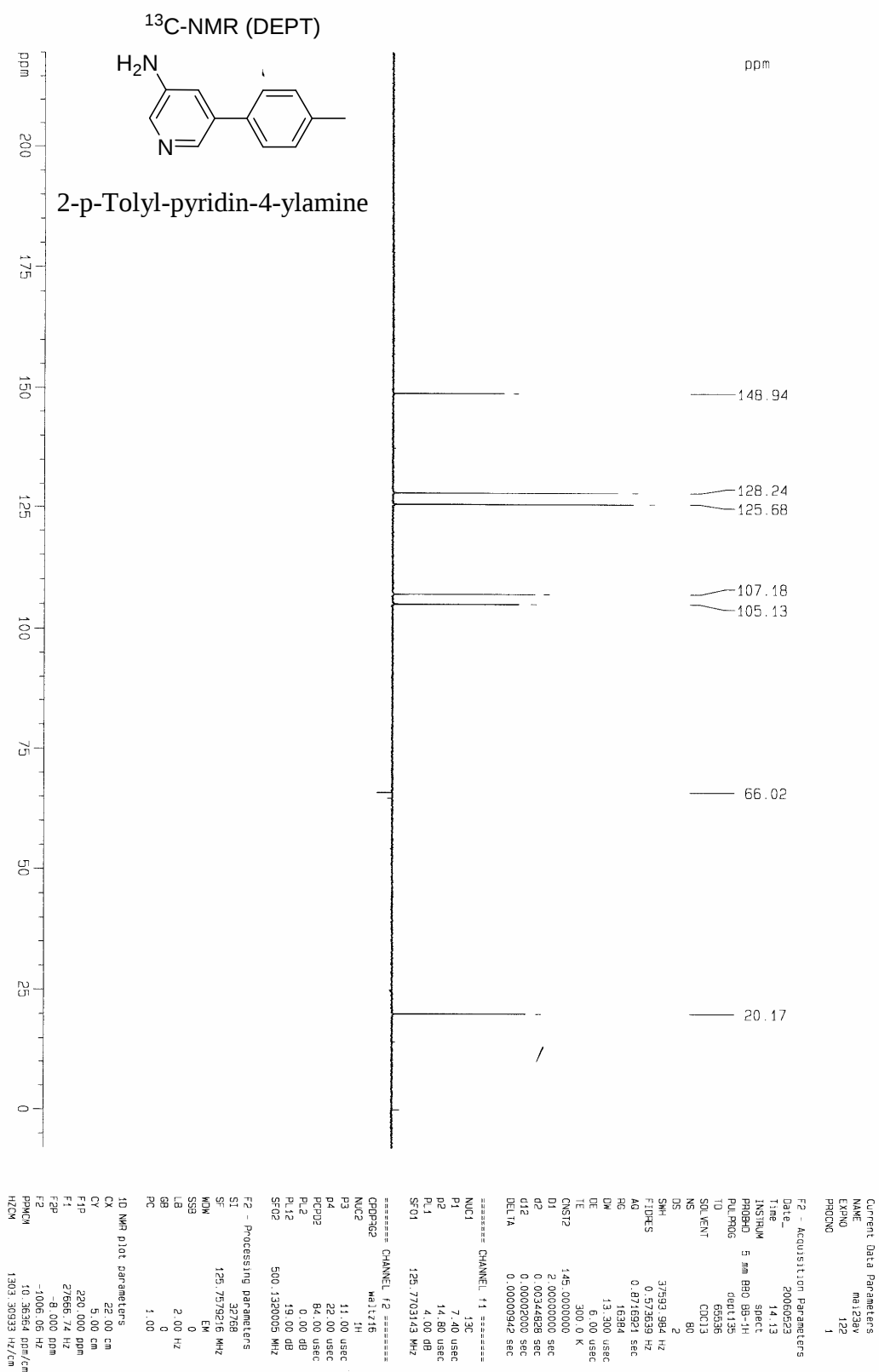
F2 - Acquisition Parameters
Date_ 20060523
Time 14.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 37693.984 Hz
FIDRES 0.57639 Hz
AQ 0.876921 sec
RG 5160.6
DM 13.300 usec
DE 6.00 usec
TE 300.0 K
D1 0.4000001 sec
d11 0.0300000 sec
d12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 ¹³C
P1 7.40 usec
PL1 4.00 dB
SFO1 125.770343 MHz

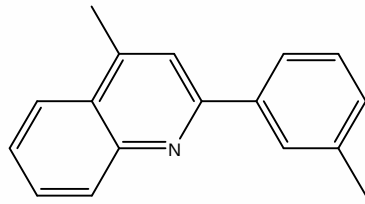
===== CHANNEL f2 =====
CFOPRG2 waltz16
NUC2 ¹H
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 500.132005 MHz

F2 - Processing parameters
SI 32768
SF 125.7575205 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

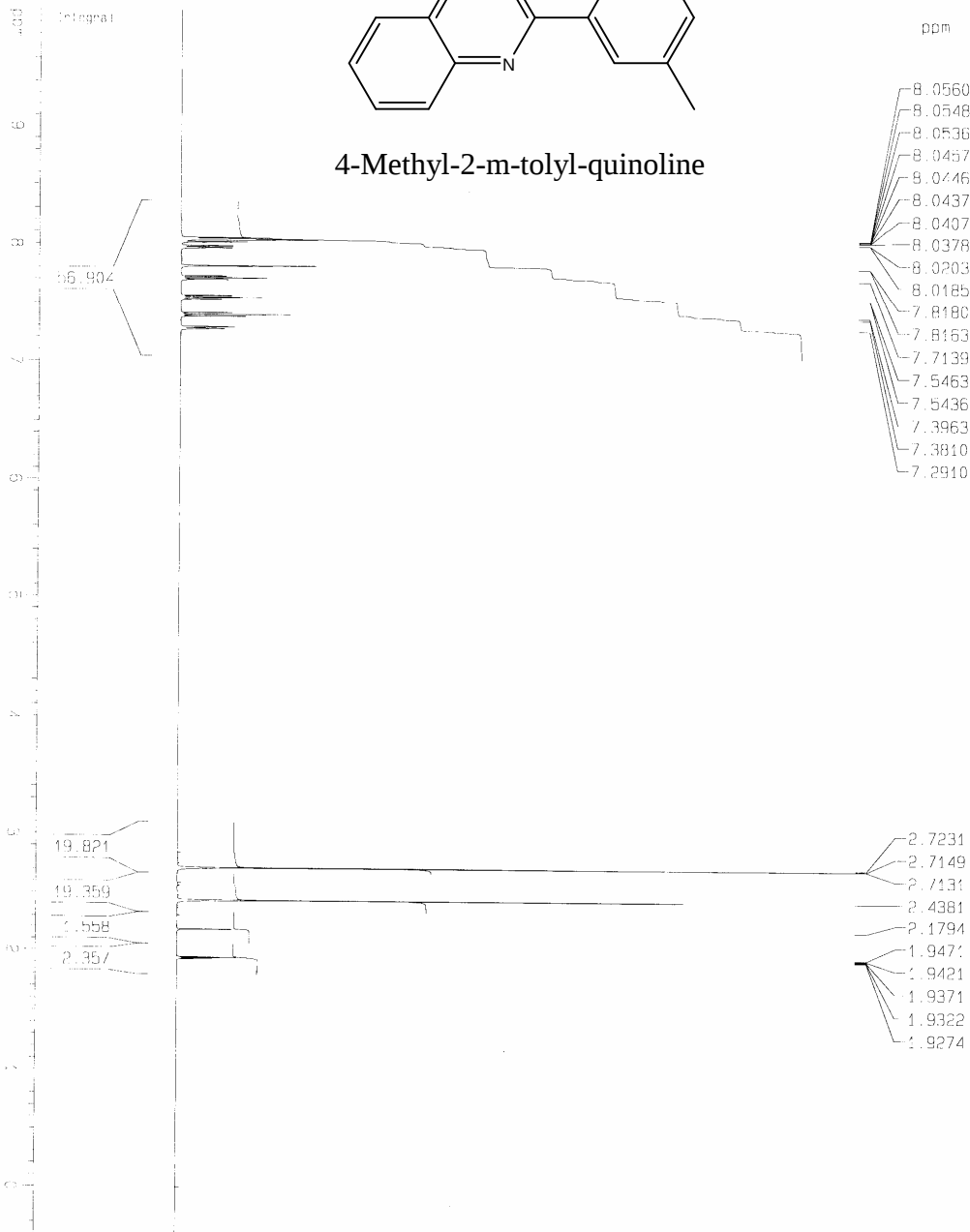
1D NMR plot parameters
CX 22.00 cm
CY 7.00 cm
F1P 220.000 ppm
F1 2766.74 Hz
F2P -8.000 ppm
F2 -106.06 Hz
FREQ 10.36564 ppm/cm
HZCM 1303.30933 Hz/cm



¹H-NMR



4-Methyl-2-m-tolyl-quinoline



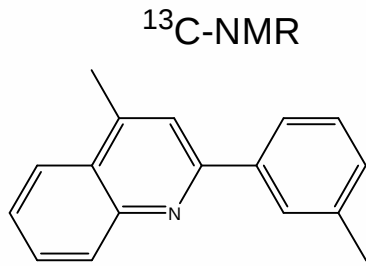
Current Data Parameters
NAME: nvoBay
EXPNO: 20
PROCNO: 1

F2 - Acquisition Parameters
Date_: 2006108
Time: 8:57
INSTRUM: spect
PROBHD: 5 mm BBO GB-1H
PULPROG: zg30
TD: 65536
SOLVENT: CDCl3
NS: 24
DS: 2
SWH: 10330.678 Hz
FIDRES: 0.157537 Hz
AQ: 3.1720407 sec
RG: 71.8
DW: 48.400 usec
DE: 6.00 usec
TE: 300.0 K
D1: 0.50000000 sec

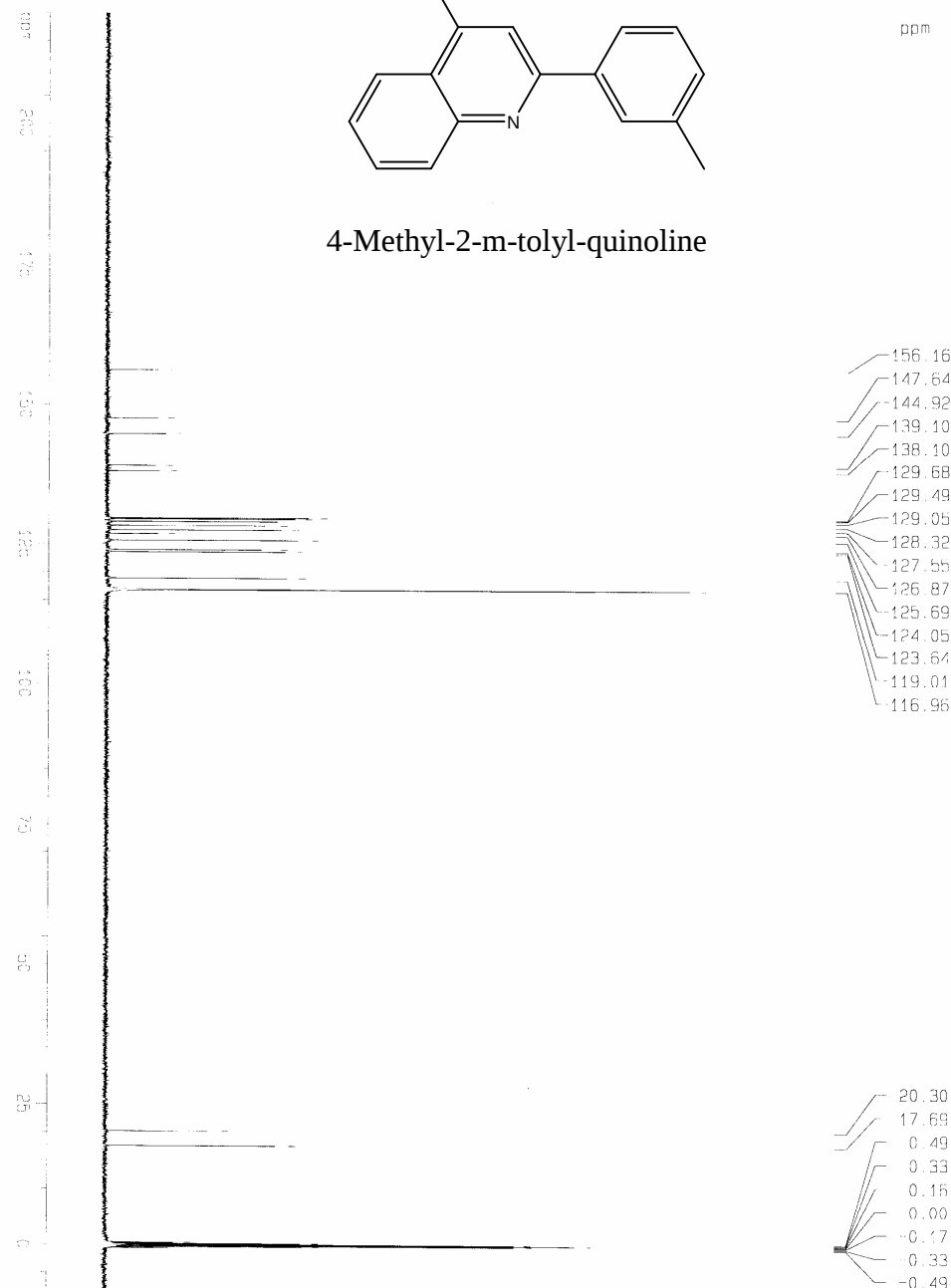
***** CHANNEL f1 *****
NUC1: 1H
P1: 11.10 usec
PL1: 0.00 dB
SFO1: 500.1360993 MHz

F2 - Processing parameters
SI: 32768
SF: 500.1360993 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

F3 - NMR D101 parameters
CX: 22.00 usec
CY: 12.00 usec
FAP: 10.000 usec
F1: 500.1360993 MHz
F2: -0.500 usec
F3: -250.00 usec
PCYC: 0.4127 usec/cycle
HZCW: 238.69659 Hz/cm



4-Methyl-2-m-tolyl-quinoline



Current Data Parameters
NAME nov08av
F2PNO 21
F2COND 1

F2 - Acquisition Parameters
Date_ 20061108
Time 9.02
INSTRUM spect
PROBHD E TM 5BD BB-1H
PULPROG zgpg30
TD 65536
SOLVENT C3CN
NS 216
DS 4
SWH 37593.984 Hz
F2-HES 0.517639 Hz
AQ 0.8176524 sec
RG 11565.2
DM 13.300 usec
DS 6.00 usec
TE 300.0 K
D1 0.4000001 sec
D11 0.0300000 sec
d12 0.0002000 sec

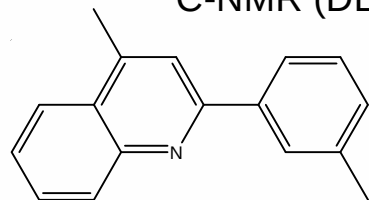
===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 4.00 dB
SF01 125.770343 MHz

===== CHANNEL f2 =====
COPPRG2 waltz16
NUC2 1H
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SF02 500.1320005 MHz

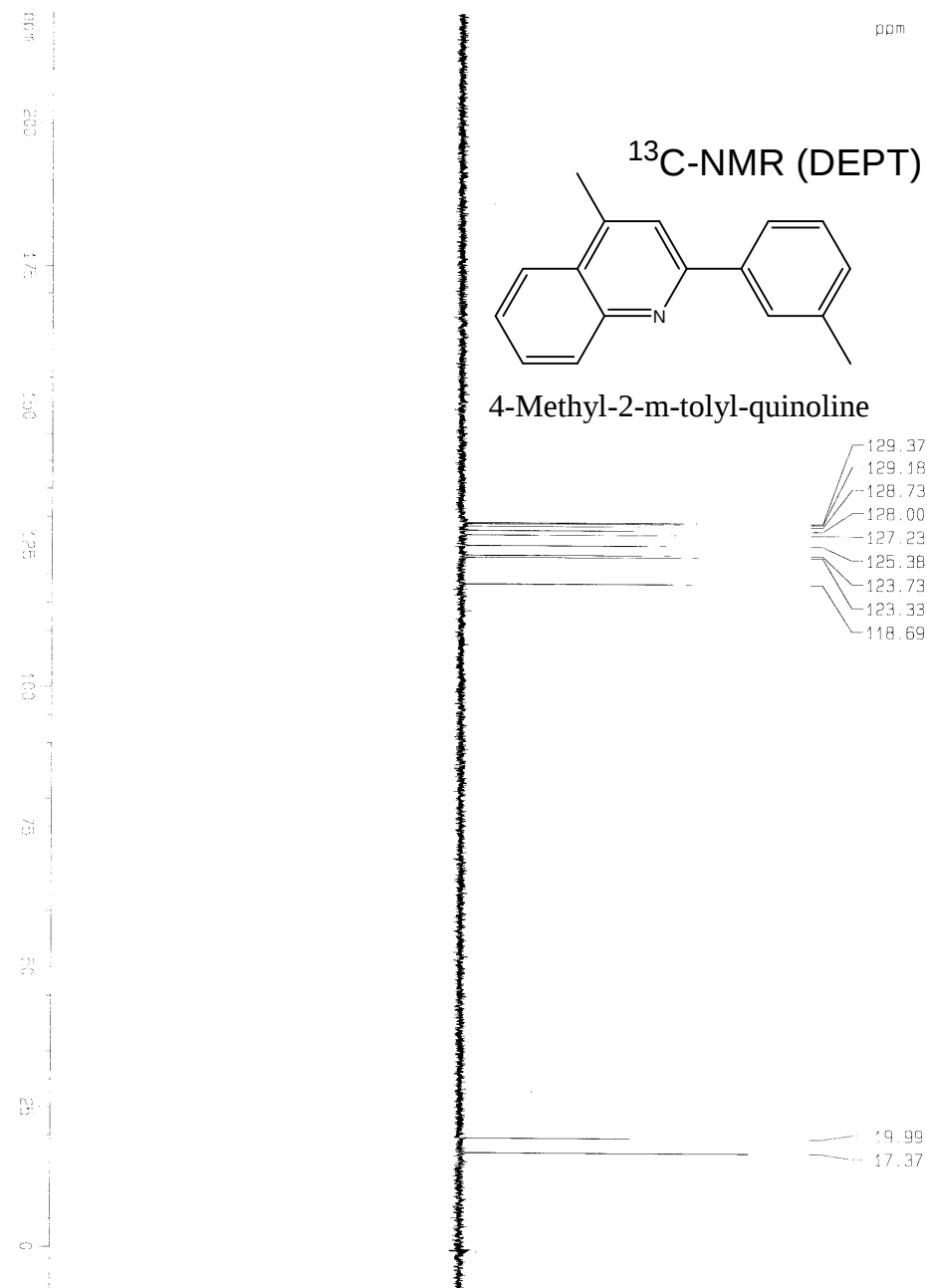
F2 - Processing parameters
SI 32768
SF 125.757289 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 10.00 cm
F1D 220.000.000
Z1 7.05872 Hz
F2D 7.05872 Hz
Z2 7.05872 Hz
SOLVENT 125.770343 MHz
PC 1.00

¹³C-NMR (DEPT)



4-Methyl-2-m-tolyl-quinoline



Current Data Parameters
NAME novobay
EXPNO 22
PROCNO 1

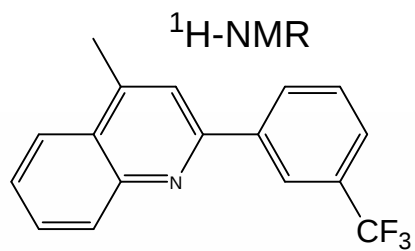
F2 - Acquisition Parameters
Date_ 20061108
Time 9.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 65
DS 2
SWH 37563.884 Hz
FIDRES 0.573639 Hz
AQ 0.8716921 sec
RG 13004
DE 13.400 usec
TE 300.0 K
CNS12 145.0000000
D1 2.00000000 sec
d2 0.00344628 sec
d12 0.00002000 sec
DELTA 0.00009342 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 14.80 usec
PC1 4.00 dB
SFO1 125.770343 MHz

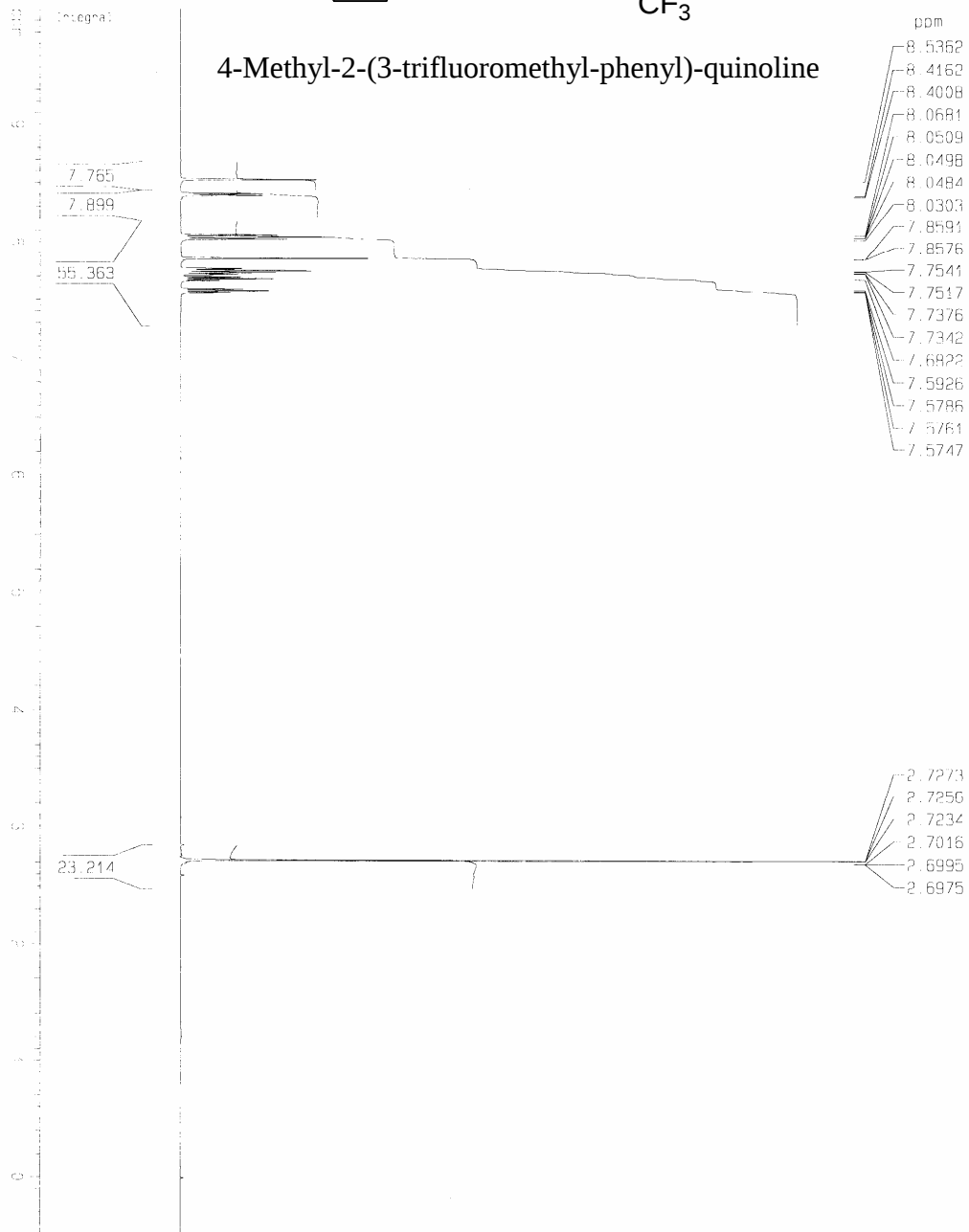
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 11.00 usec
PL2 22.00 usec
PC2 0.00 dB
SFO2 500.132005 MHz

F2 - Processing parameters
SI 32768
SF 125.757665 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

F2 NMR file parameters
CX 22.00 cm
CY 5.00 cm
F1c 270.000 MHz
F1 2766.731 Hz
F2 -8.000 Hz
F2C 276.6731 MHz
F2Cv 10.3654 cm/cm
F2Cv 153.3084 Hz/cm



4-Methyl-2-(3-trifluoromethyl-phenyl)-quinoline



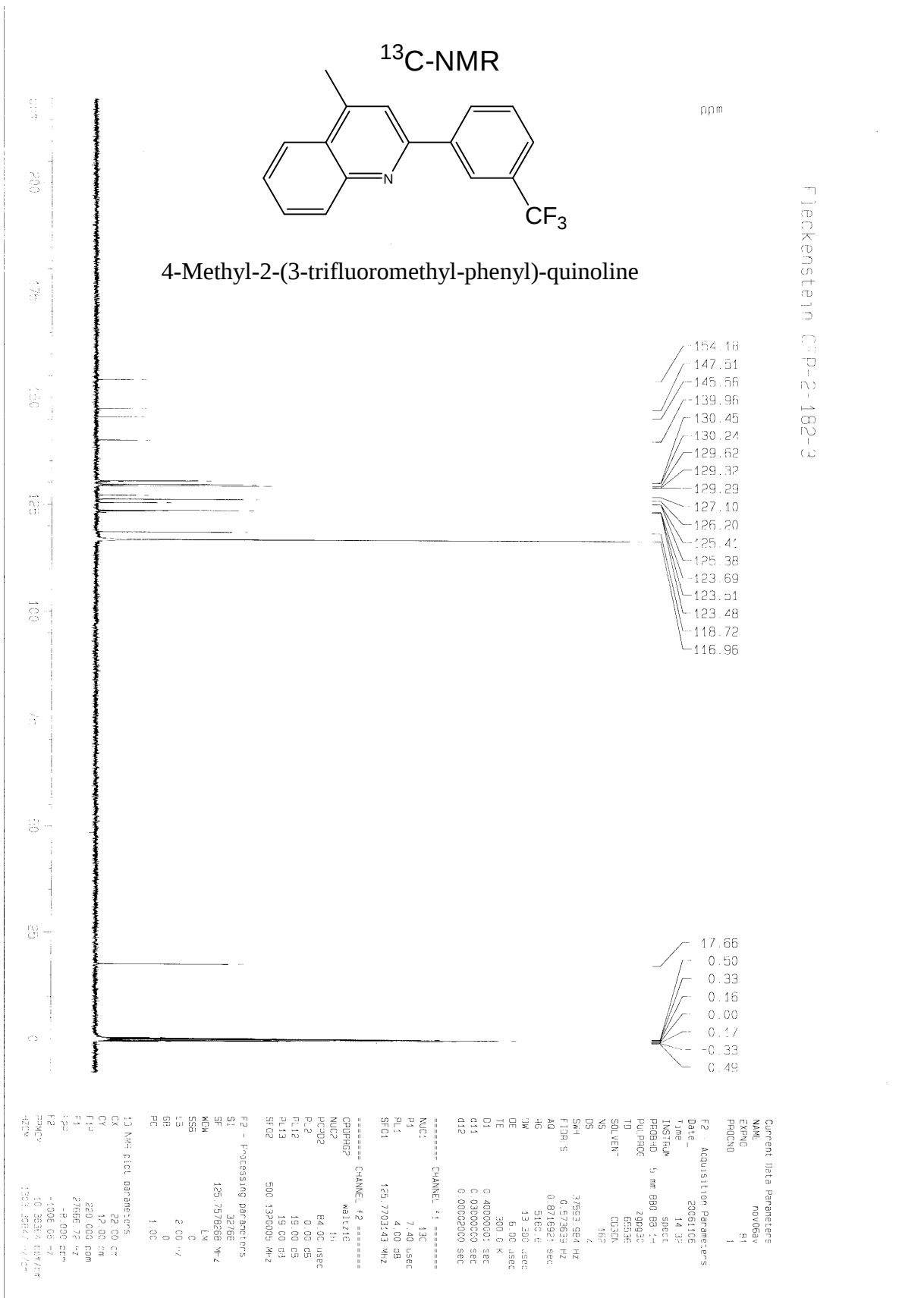
Flockenstein CTP-2-182-3

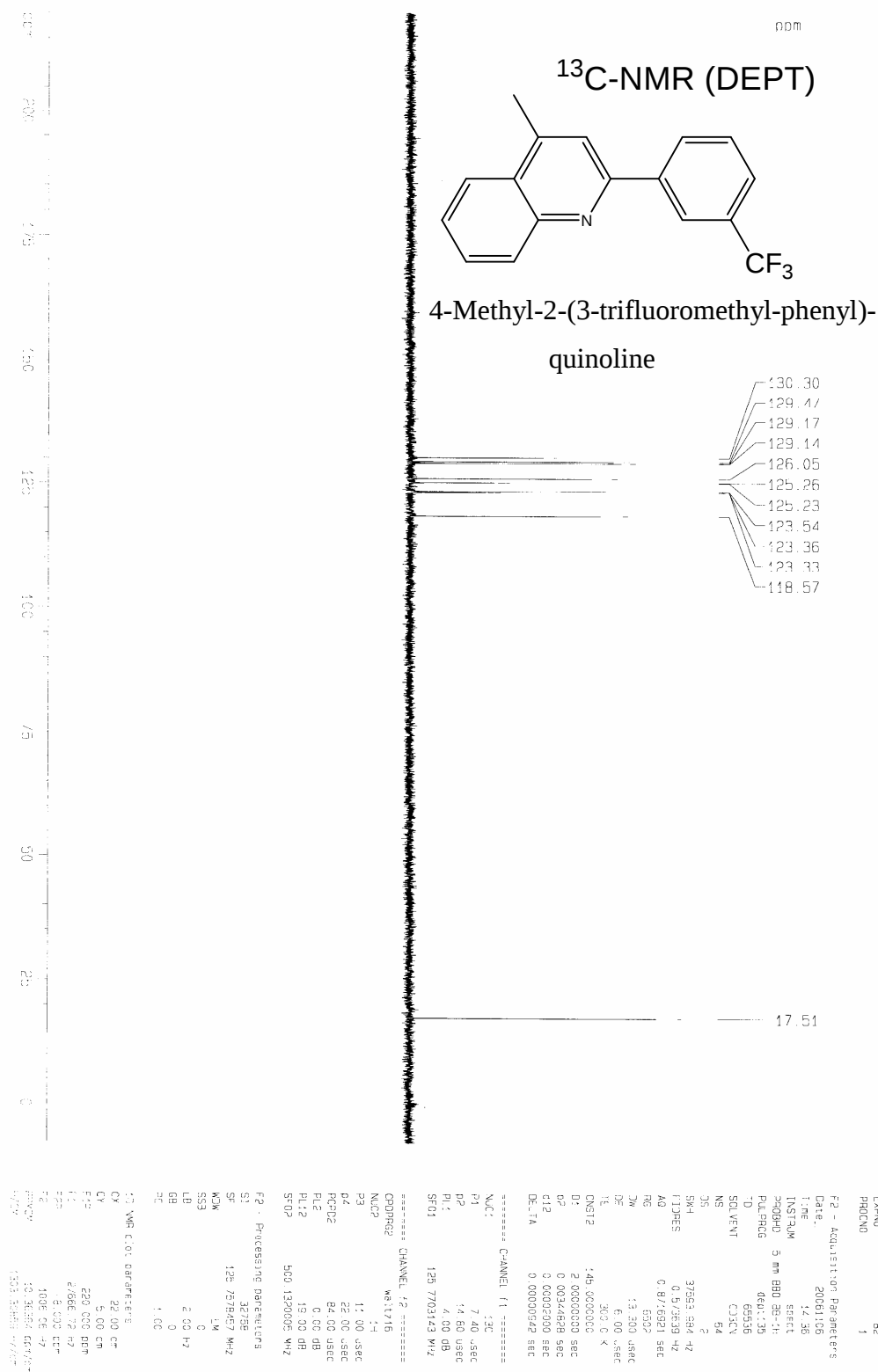
Current Data Parameters
 NAME novocav
 EXAMID B0
 FIDENC 1

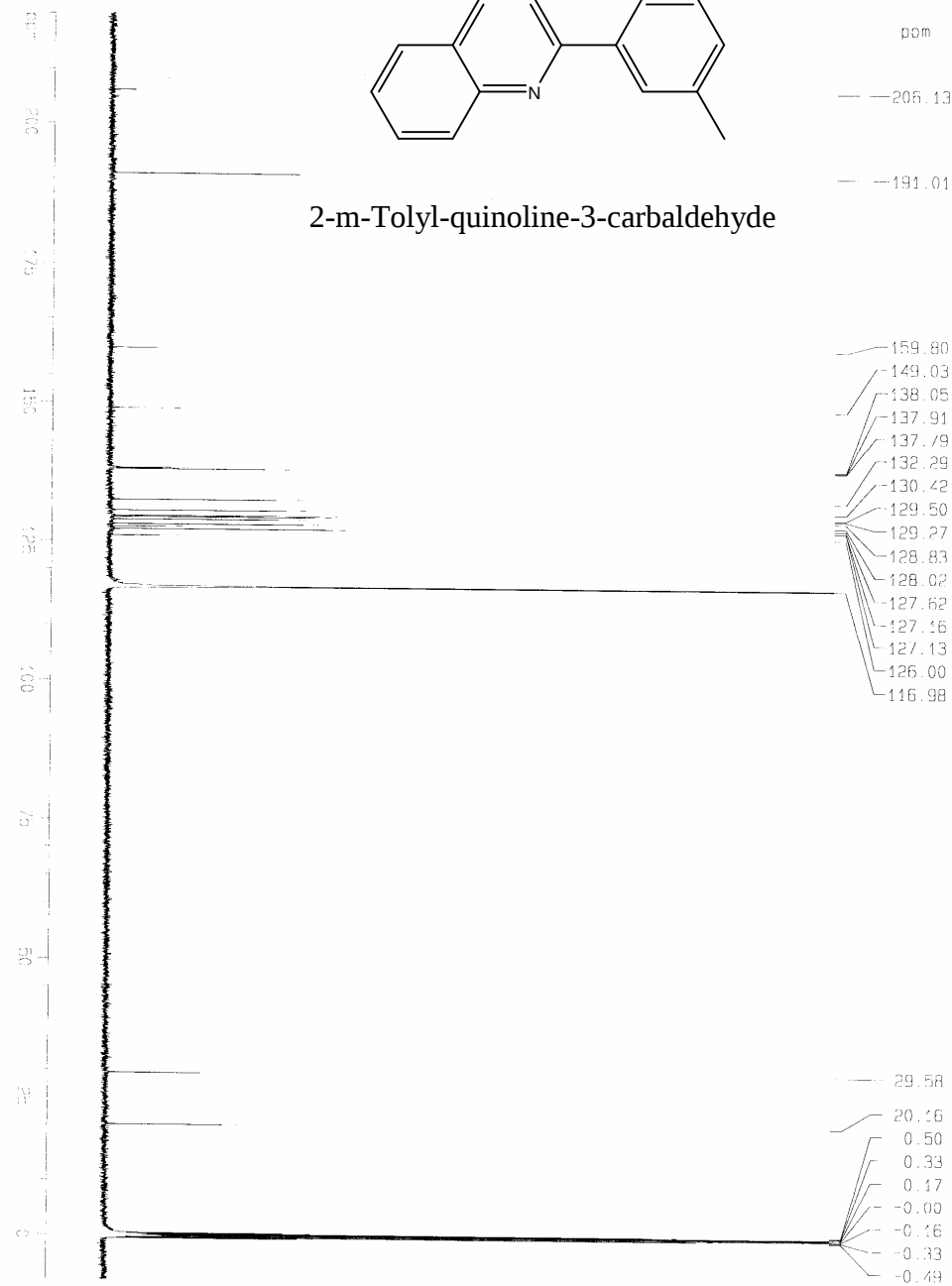
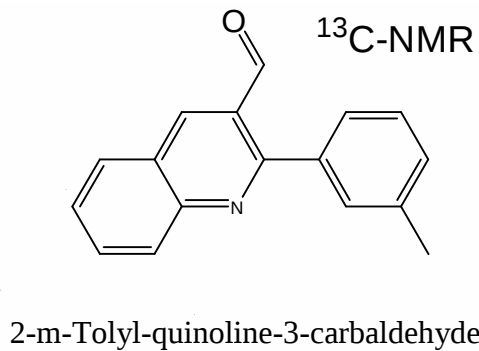
F2 - Acquisition Parameters
 Date_ 20061106
 Time 14.29
 INSTRUM spect
 PROBHD 5 mm BBO BB-3H
 PULPROG zgpg30
 TC 65536
 SOLVENT CD3CN
 NS 2
 DS 2
 SWH 10330.878 Hz
 FIDRES 0.187832 Hz
 AQ 3.1270202 sec
 RG 343.7
 DN 46.400 usec
 DE 6.00 usec
 TE 300.0 K
 TF 0.50000000 sec

F2 - Processing parameters
 SI 32768
 SF 500.1300178 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 EC 1.00

1D NMR 01ct parameters
 CX 22.00 cm
 CY 12.00 cm
 FZ 10.000000 cm
 F1 500.130172
 F2 -0.500000
 F3 -250.00 Hz
 FREQC 0.4772700 MHz
 FZCW 238.69535 Hz/cm







Current Data Parameters

NAME	VALUE
EXCND	142
PROGND	1

F2 - Acquisition Parameters

NAME	VALUE
Date	2006-10-9
Time	20:58
INSTRUM	spec
PROBHD	5 mm BBO 56-71
PULPROG	zgpg30
TD	65536
COLN	CD3CN
SOLVENT	1000
NS	4
DS	4
SWH	37483.984 Hz
FIDRES	0.57359 Hz
AQ	0.876921 sec
RG	5192
DE	13.500 usec
TE	300.0 K
D1	0.0300000 sec
d11	0.0300000 sec
d12	0.0002000 sec

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

NAME	VALUE
NUC1	¹³ C
P1	7.40 usec
PL1	4.00 dB
SECT1	125.7703143 MHz

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

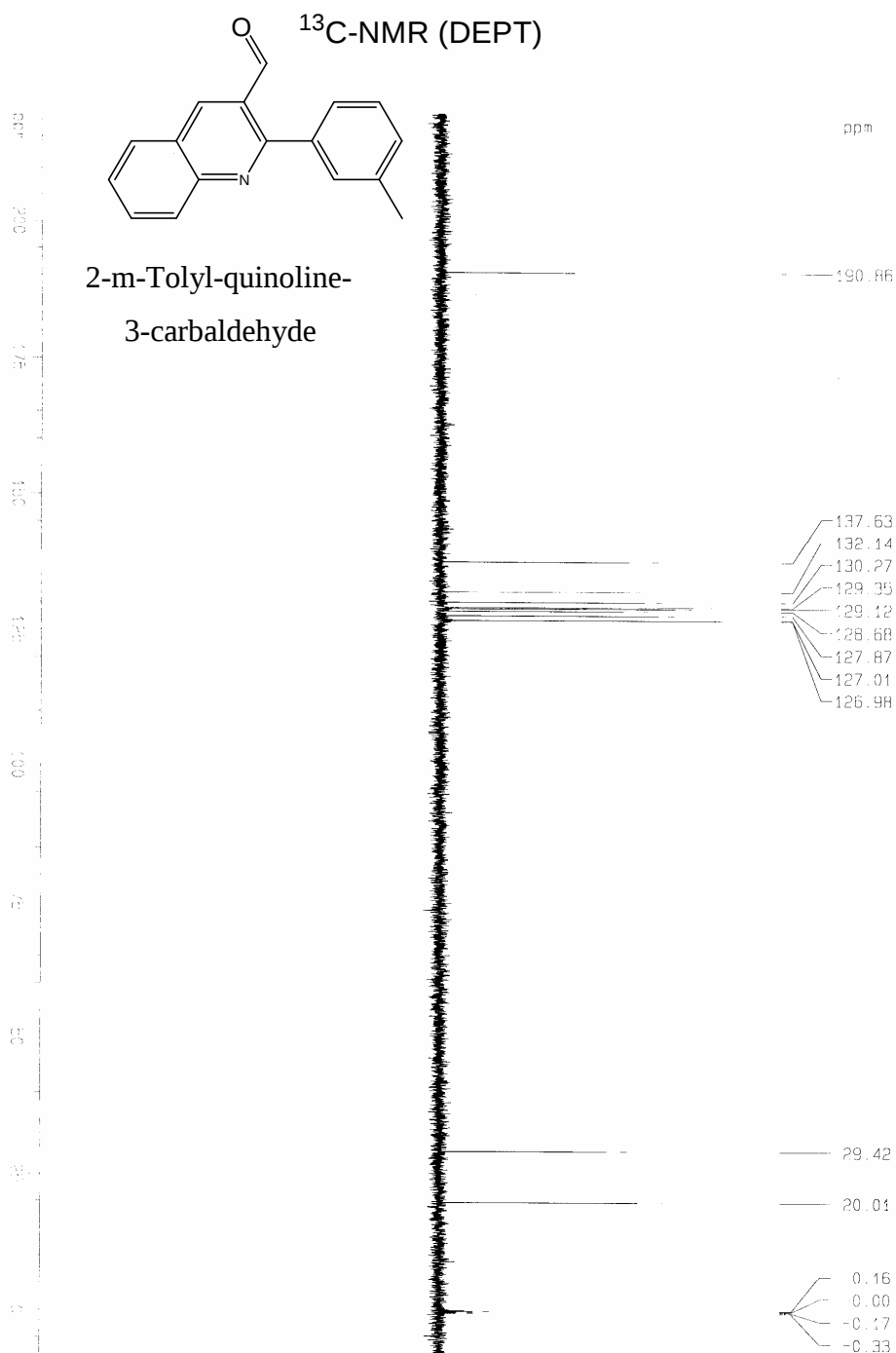
NAME	VALUE
CHRG2	4811.716
NUC2	¹³ C
PCPG2	86.00 usec
PL2	0.00 dB
PL12	19.00 dB
PL13	19.00 dB
SECT2	500.1320005 MHz

F2 - Processing Parameters

NAME	VALUE
SI	32768
SF	120.7578262 MHz
WIM	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00

1D VSR 0.100 usec

NAME	VALUE
QX	32.00 CF
QY	50.00 CF
FL1	220.000 CF
FL2	270.000 CF
FL3	270.000 CF
FL4	270.000 CF
FL5	270.000 CF
FL6	270.000 CF
FL7	270.000 CF
FL8	270.000 CF
FL9	270.000 CF
FL10	270.000 CF
FL11	270.000 CF
FL12	270.000 CF
FL13	270.000 CF
FL14	270.000 CF
FL15	270.000 CF
FL16	270.000 CF
FL17	270.000 CF
FL18	270.000 CF
FL19	270.000 CF
FL20	270.000 CF
FL21	270.000 CF
FL22	270.000 CF
FL23	270.000 CF
FL24	270.000 CF
FL25	270.000 CF
FL26	270.000 CF
FL27	270.000 CF
FL28	270.000 CF
FL29	270.000 CF
FL30	270.000 CF
FL31	270.000 CF
FL32	270.000 CF
FL33	270.000 CF
FL34	270.000 CF
FL35	270.000 CF
FL36	270.000 CF
FL37	270.000 CF
FL38	270.000 CF
FL39	270.000 CF
FL40	270.000 CF
FL41	270.000 CF
FL42	270.000 CF
FL43	270.000 CF
FL44	270.000 CF
FL45	270.000 CF
FL46	270.000 CF
FL47	270.000 CF
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FL50	270.000 CF
FL51	270.000 CF
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FL53	270.000 CF
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FL55	270.000 CF
FL56	270.000 CF
FL57	270.000 CF
FL58	270.000 CF
FL59	270.000 CF
FL60	270.000 CF
FL61	270.000 CF
FL62	270.000 CF
FL63	270.000 CF
FL64	270.000 CF
FL65	270.000 CF
FL66	270.000 CF
FL67	270.000 CF
FL68	270.000 CF
FL69	270.000 CF
FL70	270.000 CF
FL71	270.000 CF
FL72	270.000 CF
FL73	270.000 CF
FL74	270.000 CF
FL75	270.000 CF
FL76	270.000 CF
FL77	270.000 CF
FL78	270.000 CF
FL79	270.000 CF
FL80	270.000 CF
FL81	270.000 CF
FL82	270.000 CF
FL83	270.000 CF
FL84	270.000 CF
FL85	270.000 CF
FL86	270.000 CF
FL87	270.000 CF
FL88	270.000 CF
FL89	270.000 CF
FL90	270.000 CF
FL91	270.000 CF
FL92	270.000 CF
FL93	270.000 CF
FL94	270.000 CF
FL95	270.000 CF
FL96	270.000 CF
FL97	270.000 CF
FL98	270.000 CF
FL99	270.000 CF
FL100	270.000 CF



Current Data Parameters

NAME	VALUE
EXPNO	142
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20061109	21:11

INSTRUM spect

PROBHD 5 mm BBO BB-1H

PULPROG zgpg30

TD 65536

SD VPR1

NS 200

DS 2

SWH 37953.884 Hz

FIDRES 0.073635 Hz

AQ 0.671621 sec

RG 6502

DM 13.500 usec

DE 6.00 usec

TE 300.0 K

CN12 1425.000000

SI 2.00000000 sec

CP 0.00344228 sec

CI2 0.00000000 sec

DELTA 0.00000042 sec

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

NUC1	13C
P1	7.40 usec
P2	14.80 usec
PL1	4.00 dB
SFO1	125.7703143 MHz

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

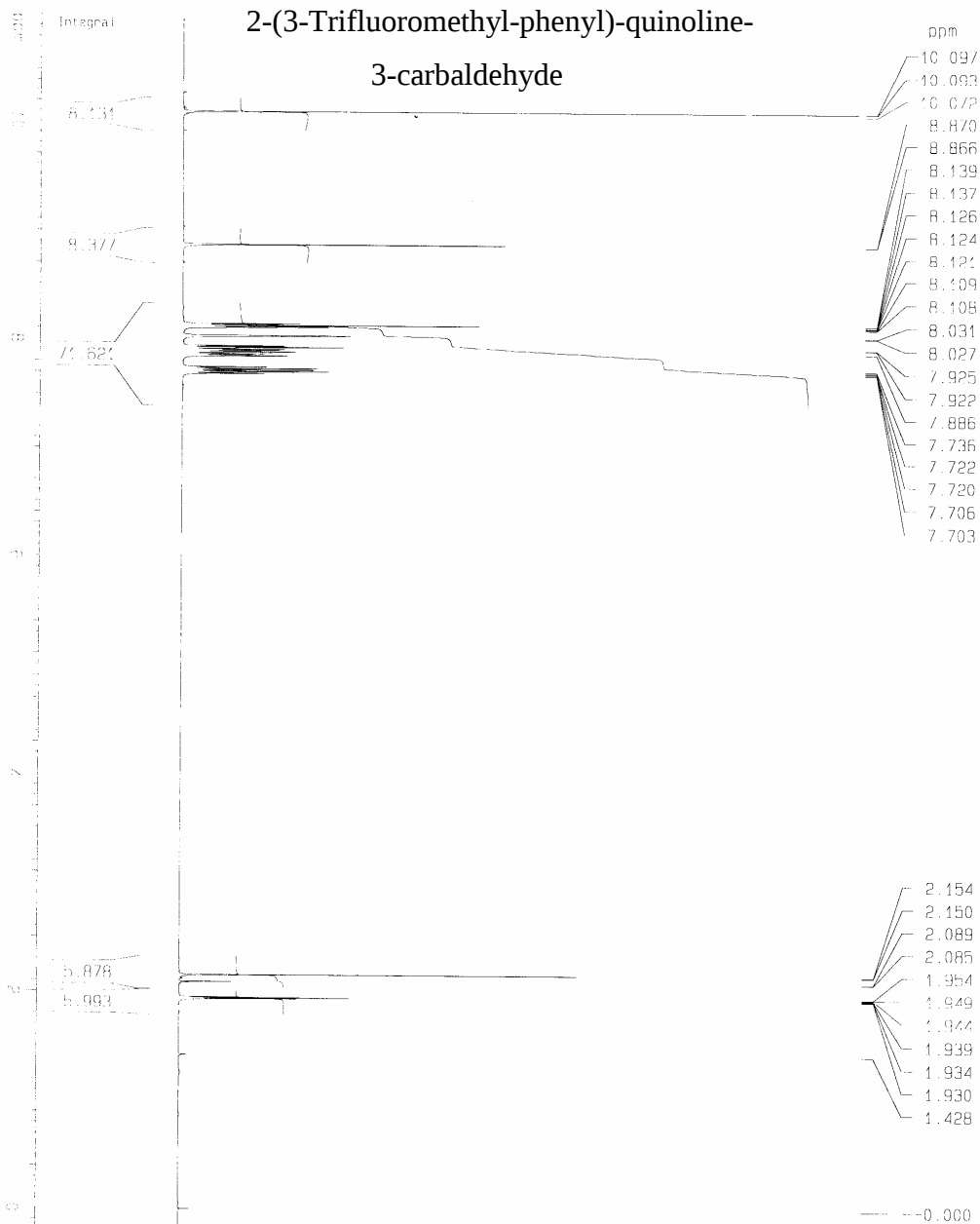
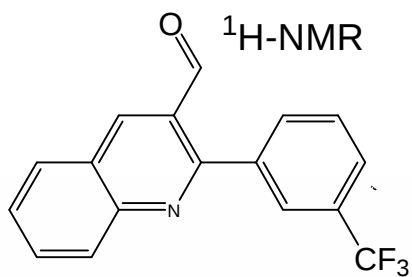
CPDPRG2	WALTZ16
NUC2	1H
P3	11.00 usec
P4	22.00 usec
PCPD2	84.00 usec
PL2	0.00 dB
PL12	19.00 dB
SFO2	500.132005 MHz

F2 - Processing Parameters

SI	12789
SF	125.757649 MHz
WDW	EM
SSB	0
GB	2.00 Hz
PC	1.00

1D NMR data parameters

CX	22.00 cm
CV	5.00 cm
FLP	220.000 cm
F1	21666.72 Hz
F2	5.000 cm
PRGCM	10.0000 cm
WDW	1001.0000 Hz



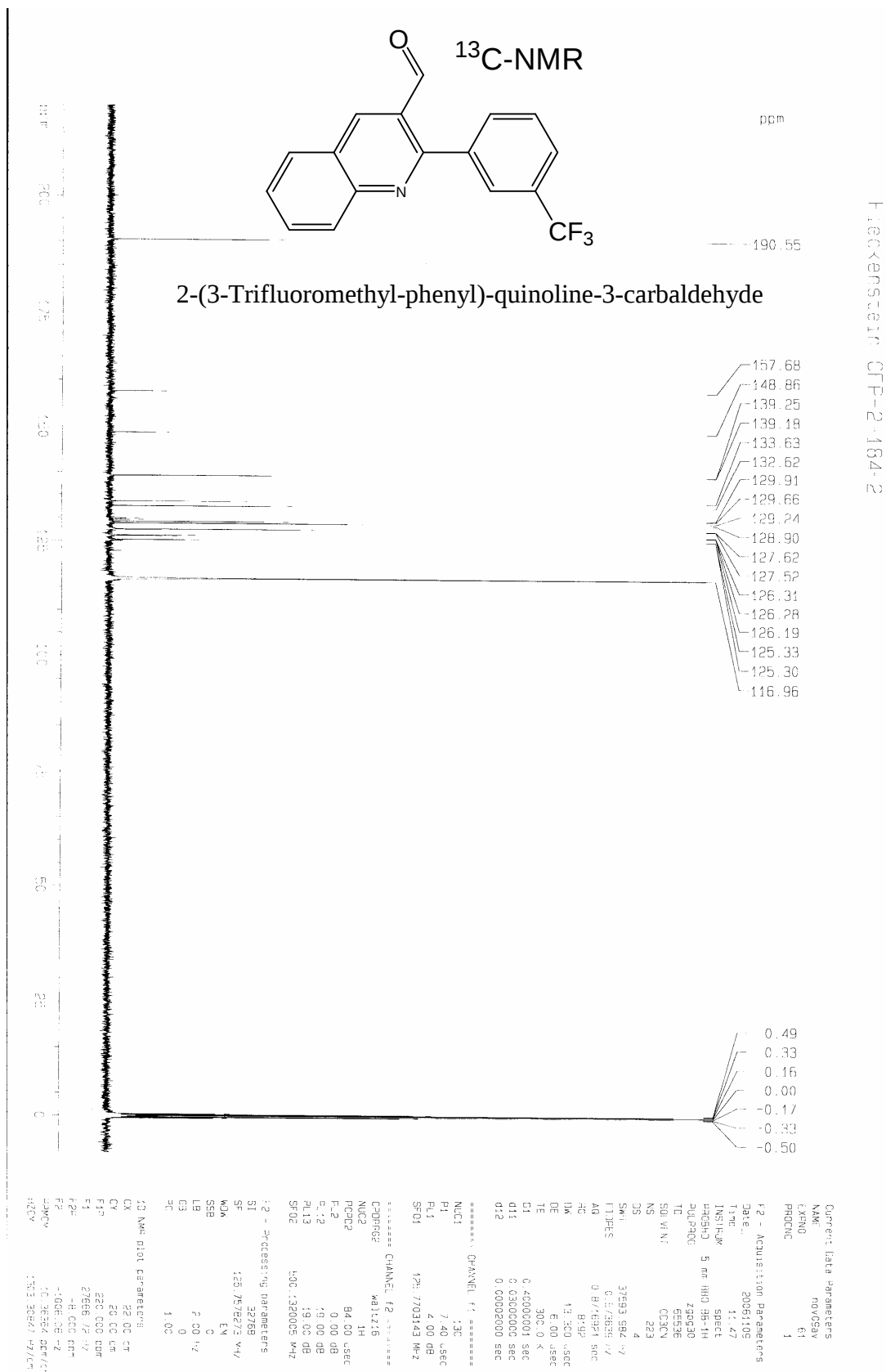
Current Data Parameters
 NAME nov09av
 EXPNO 50
 PROCNO 1

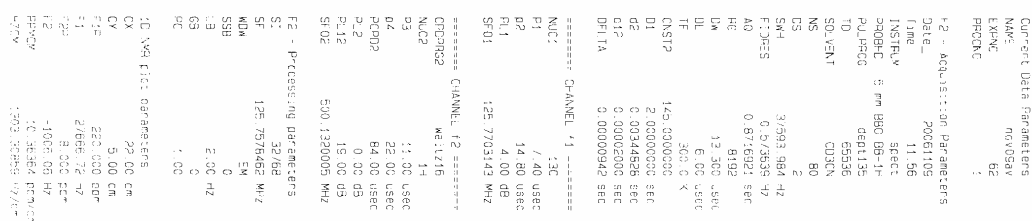
F2 - Acquisition Parameters
 Date_ 20061109
 Time 11:28
 INSTRUM spect
 PROBD 5 mm 300 3H
 PULPROG zgpg30
 TO 65536
 SOLVENT CUCN
 NS 24
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.15432 Hz
 AC 3.776727 sec
 QC 181
 JM 48.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.5000000 sec

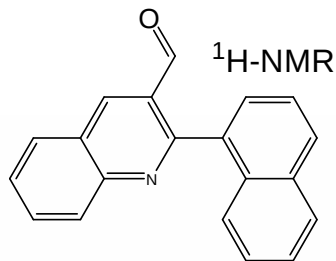
===== CHANNEL f1 =====
 NUC1 13C
 P1 11.10 usec
 PL1 0.00 dB
 SF01 500.130053 MHz
 SFO1 500.130053 MHz

F2 - Processing parameters
 SI 32768
 SF 500.130053 MHz
 WDM EV
 SSB 0
 FB 0.10 Hz
 GB 0
 PC 1.00

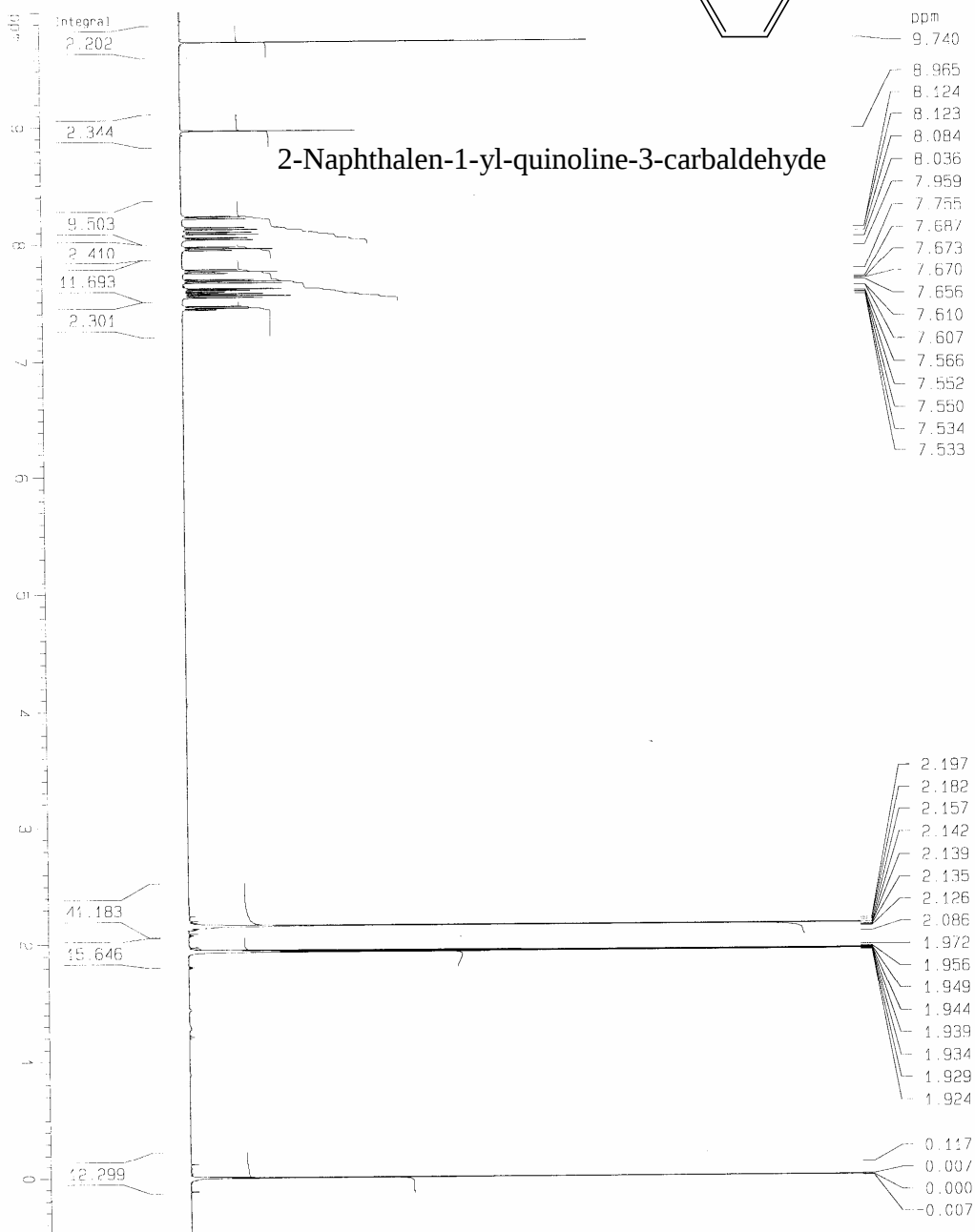
F2 - NMR plot parameters
 CX 22.00 cm
 CY 12.00 cm
 ZF 11.000 cm
 F1 500.130053 MHz
 F2 0.5000000 MHz
 F3 0.5000000 MHz
 F4 0.5000000 MHz
 F5 0.5000000 MHz
 F6 0.5000000 MHz
 F7 0.5000000 MHz
 F8 0.5000000 MHz
 F9 0.5000000 MHz
 F10 0.5000000 MHz
 F11 0.5000000 MHz
 F12 0.5000000 MHz
 F13 0.5000000 MHz
 F14 0.5000000 MHz
 F15 0.5000000 MHz
 F16 0.5000000 MHz
 F17 0.5000000 MHz
 F18 0.5000000 MHz
 F19 0.5000000 MHz
 F20 0.5000000 MHz
 F21 0.5000000 MHz
 F22 0.5000000 MHz
 F23 0.5000000 MHz
 F24 0.5000000 MHz
 F25 0.5000000 MHz
 F26 0.5000000 MHz
 F27 0.5000000 MHz
 F28 0.5000000 MHz
 F29 0.5000000 MHz
 F30 0.5000000 MHz
 F31 0.5000000 MHz
 F32 0.5000000 MHz
 F33 0.5000000 MHz
 F34 0.5000000 MHz
 F35 0.5000000 MHz
 F36 0.5000000 MHz
 F37 0.5000000 MHz
 F38 0.5000000 MHz
 F39 0.5000000 MHz
 F40 0.5000000 MHz
 F41 0.5000000 MHz
 F42 0.5000000 MHz
 F43 0.5000000 MHz
 F44 0.5000000 MHz
 F45 0.5000000 MHz
 F46 0.5000000 MHz
 F47 0.5000000 MHz
 F48 0.5000000 MHz
 F49 0.5000000 MHz
 F50 0.5000000 MHz
 F51 0.5000000 MHz
 F52 0.5000000 MHz
 F53 0.5000000 MHz
 F54 0.5000000 MHz
 F55 0.5000000 MHz
 F56 0.5000000 MHz
 F57 0.5000000 MHz
 F58 0.5000000 MHz
 F59 0.5000000 MHz
 F60 0.5000000 MHz
 F61 0.5000000 MHz
 F62 0.5000000 MHz
 F63 0.5000000 MHz
 F64 0.5000000 MHz
 F65 0.5000000 MHz
 F66 0.5000000 MHz
 F67 0.5000000 MHz
 F68 0.5000000 MHz
 F69 0.5000000 MHz
 F70 0.5000000 MHz
 F71 0.5000000 MHz
 F72 0.5000000 MHz
 F73 0.5000000 MHz
 F74 0.5000000 MHz
 F75 0.5000000 MHz
 F76 0.5000000 MHz
 F77 0.5000000 MHz
 F78 0.5000000 MHz
 F79 0.5000000 MHz
 F80 0.5000000 MHz
 F81 0.5000000 MHz
 F82 0.5000000 MHz
 F83 0.5000000 MHz
 F84 0.5000000 MHz
 F85 0.5000000 MHz
 F86 0.5000000 MHz
 F87 0.5000000 MHz
 F88 0.5000000 MHz
 F89 0.5000000 MHz
 F90 0.5000000 MHz
 F91 0.5000000 MHz
 F92 0.5000000 MHz
 F93 0.5000000 MHz
 F94 0.5000000 MHz
 F95 0.5000000 MHz
 F96 0.5000000 MHz
 F97 0.5000000 MHz
 F98 0.5000000 MHz
 F99 0.5000000 MHz
 F100 0.5000000 MHz







2-Naphthalen-1-yl-quinoline-3-carbaldehyde



Fieckenstein CFP-2-170-3A

3

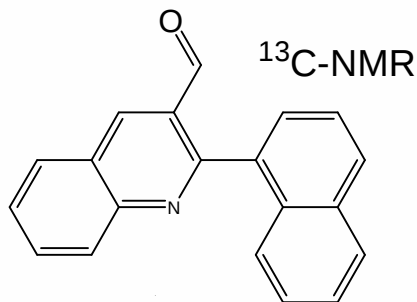
Current Data Parameters
 NAME: dk130av
 EXPNO: 30
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20061030
 Time: 10.14
 INSTRUM: spect
 PROBHD: 5 mm 380 GB-1H
 PULPROG: zg30
 TD: 65536
 SOLVENT: CD3CN
 NS: 32
 DS: 2
 SWH: 10330.578 Hz
 FIDRES: 0.157632 Hz
 AQ: 3.1720407 sec
 RG: 362
 DW: 48.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 0.50000000 sec

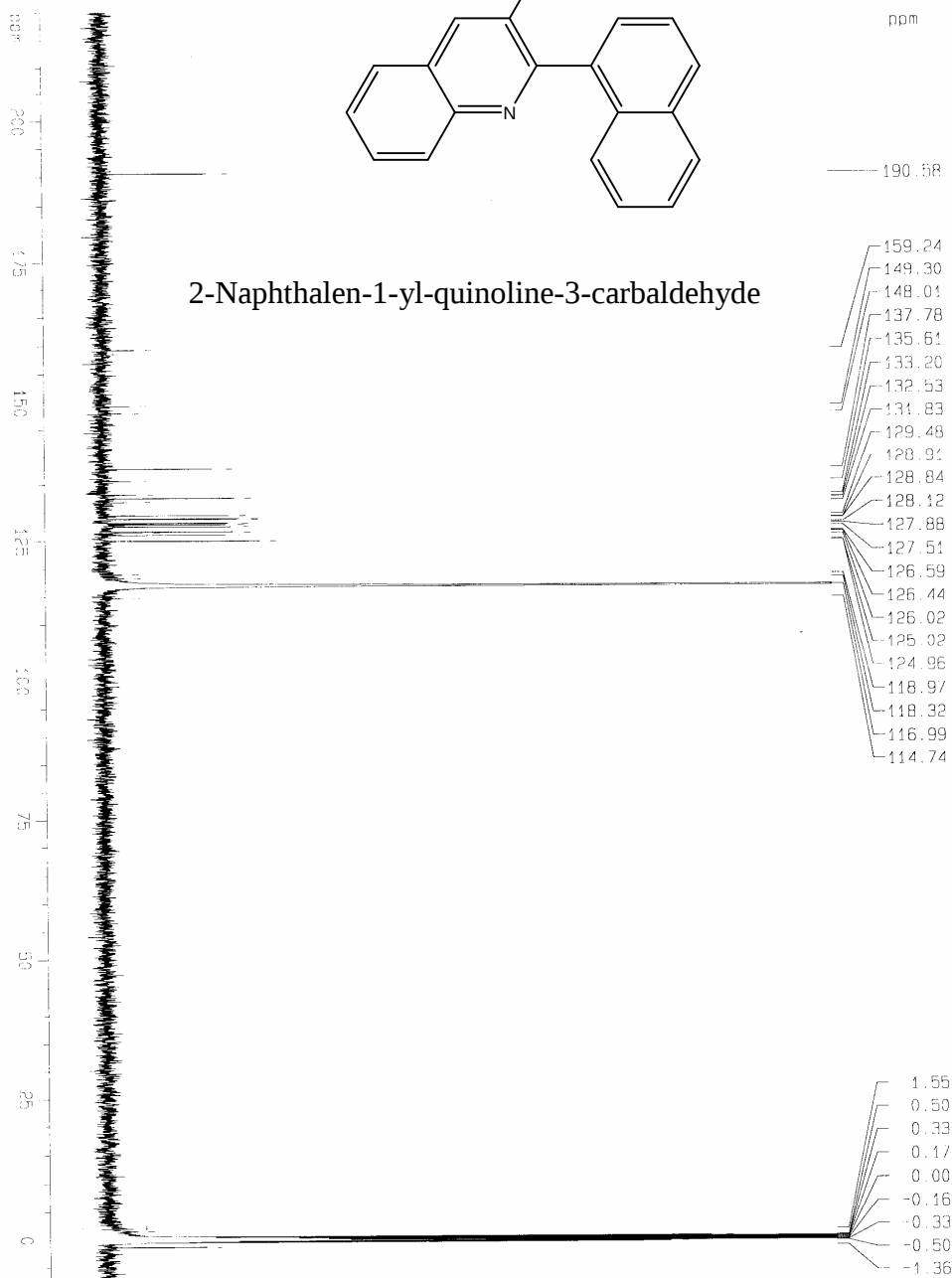
===== CHANNEL f1 =====
 NUC1: 1H
 P1: 11.10 usec
 PL1: 0.00 dB
 SF01: 500.1330885 MHz

F2 - Processing parameters
 SI: 32768
 SF: 500.1300156 MHz
 WDK: EM
 SSB: 0
 LB: 0.10 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.00 cm
 CY: 150.00 cm
 FAP: 10.000 ppm
 F1: 5001.30 Hz
 F2: -0.500 ppm
 F3: -250.06 Hz
 PPMCH: 0.4727 ppm/cm
 HZCM: 238.59839 Hz/cm



2-Naphthalen-1-yl-quinoline-3-carbaldehyde



Current Data Parameters

NAME	OK130A
EXPNO	31
F2PROC	1

F2 - Acquisition Parameters

Date_	20061030
Time	10.16
INSTRUM	spect
PROBHD	5 mm BBO BB-4H
PULPROG	zgpg30
TD	65536
SOLVENT	CD3CN
NS	1000
DS	4
SWH	37593.984 Hz
FIDRES	0.574639 Hz
AQ	0.8716921 sec
RG	3165.6
DM	13.300 usec
DE	6.00 usec
TE	300.0 K
D1	0.4000001 sec
d12	0.0300000 sec
d12	0.00002000 sec

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

NUC1	¹³ C
P1	7.40 usec
PL1	4.00 dB
SFO1	125.770343 MHz

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

CPDPRG2	waltz16
NUC2	^{1H}
PCPD2	64.00 usec
PL2	0.00 dB
PL12	19.00 dB
PL13	19.00 dB
SFO2	500.1320005 MHz

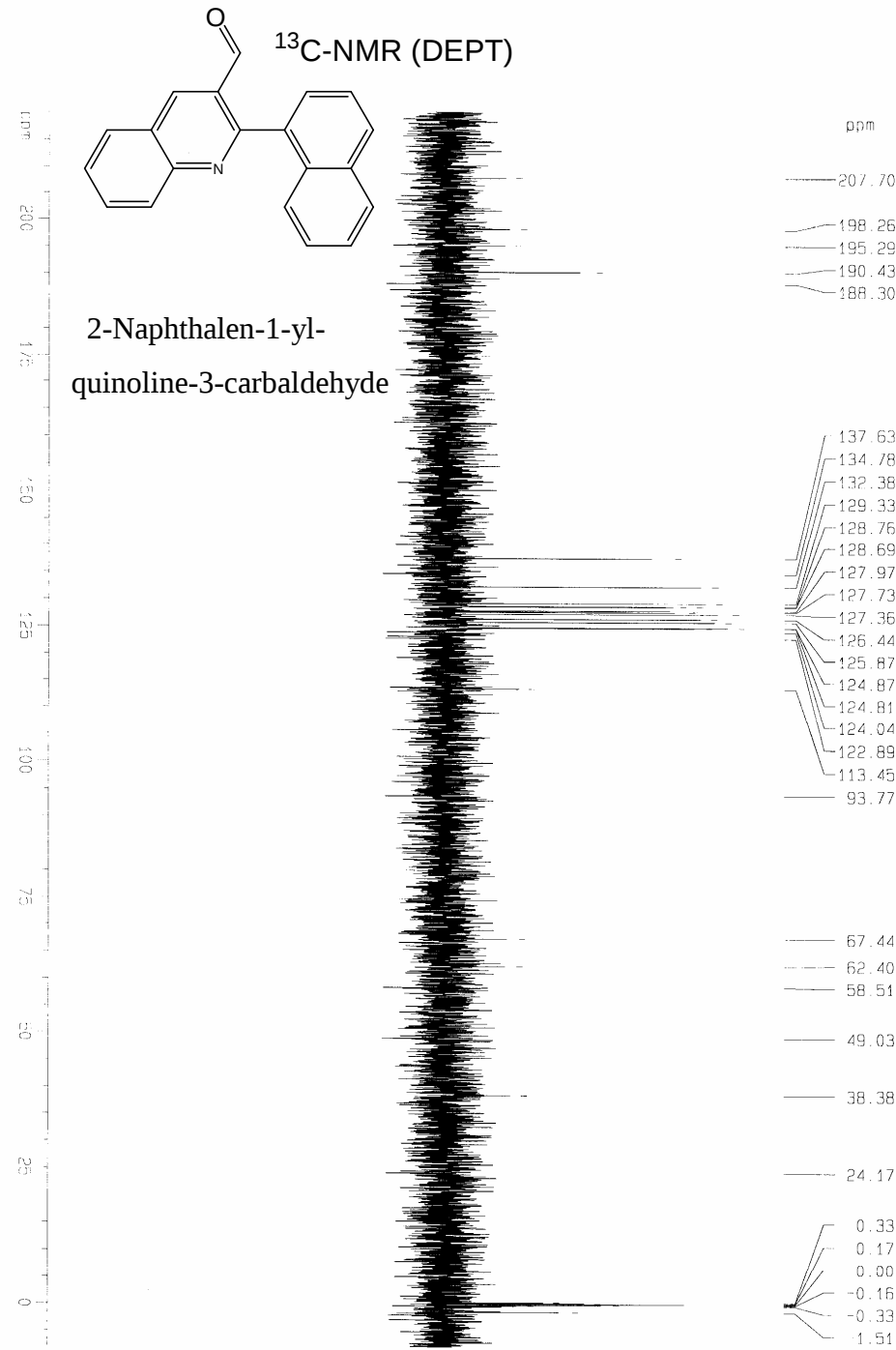
F2 - Processing parameters

SI	32768
SE	125.7678259 MHz
KIC4	EW
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

1D NMR PLOT parameters

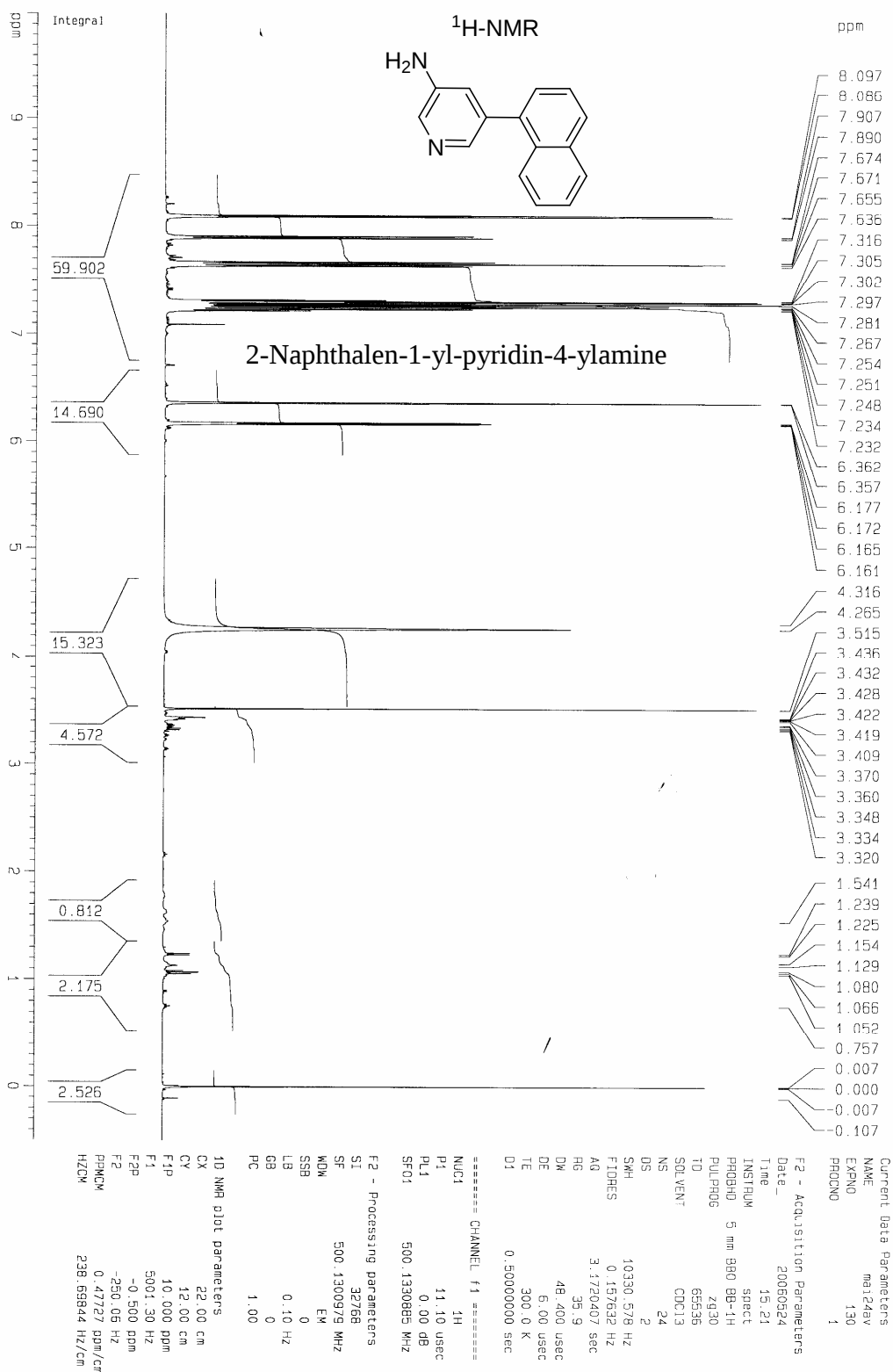
CX	22.00 C°
CY	100.00 C°
F1P	220.000 CPM
F2P	27566.72 Hz
F2P	-8.000 CPM
PHCXY	10.36364 100%/C°
HZCXY	1303.30847 Hz/C°

Fleckenstein CPD-2-170-3A

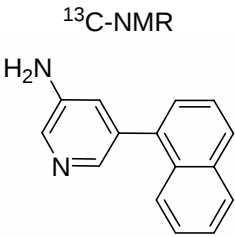


Current Data Parameters
NAME OKL30ay
EXPNO 32
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061020
Time 10:46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SFO 125.760443 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
F2 - Processing parameters
SI 32768
SF 125.760443 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
F2 - NMR plot parameters
CX 22.00 cm
CY 5.00 cm
F1 220.000 MHz
F2 756.672 MHz
F2 - 1006.05 MHz
DPRCM 10.36364 cm/cm
HZCM 1303.30855 V/cm

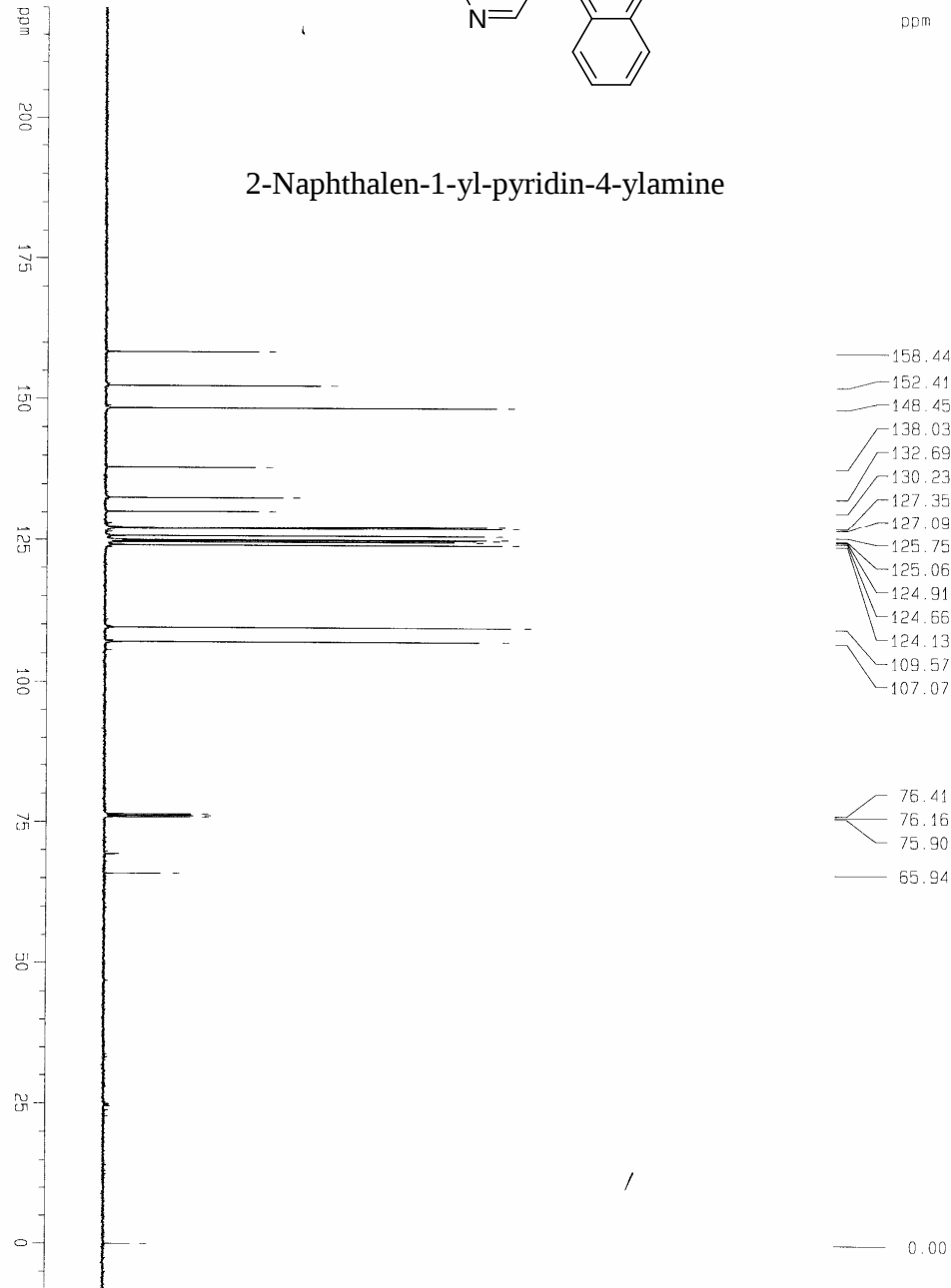
Fleckenstein CFP-3-172-C



Fleckenstein CFP-3-172-C



2-Naphthalen-1-yl-pyridin-4-ylamine



Current Data Parameters
NAME: m324v
EXPNO: 131
PROCNO: 1

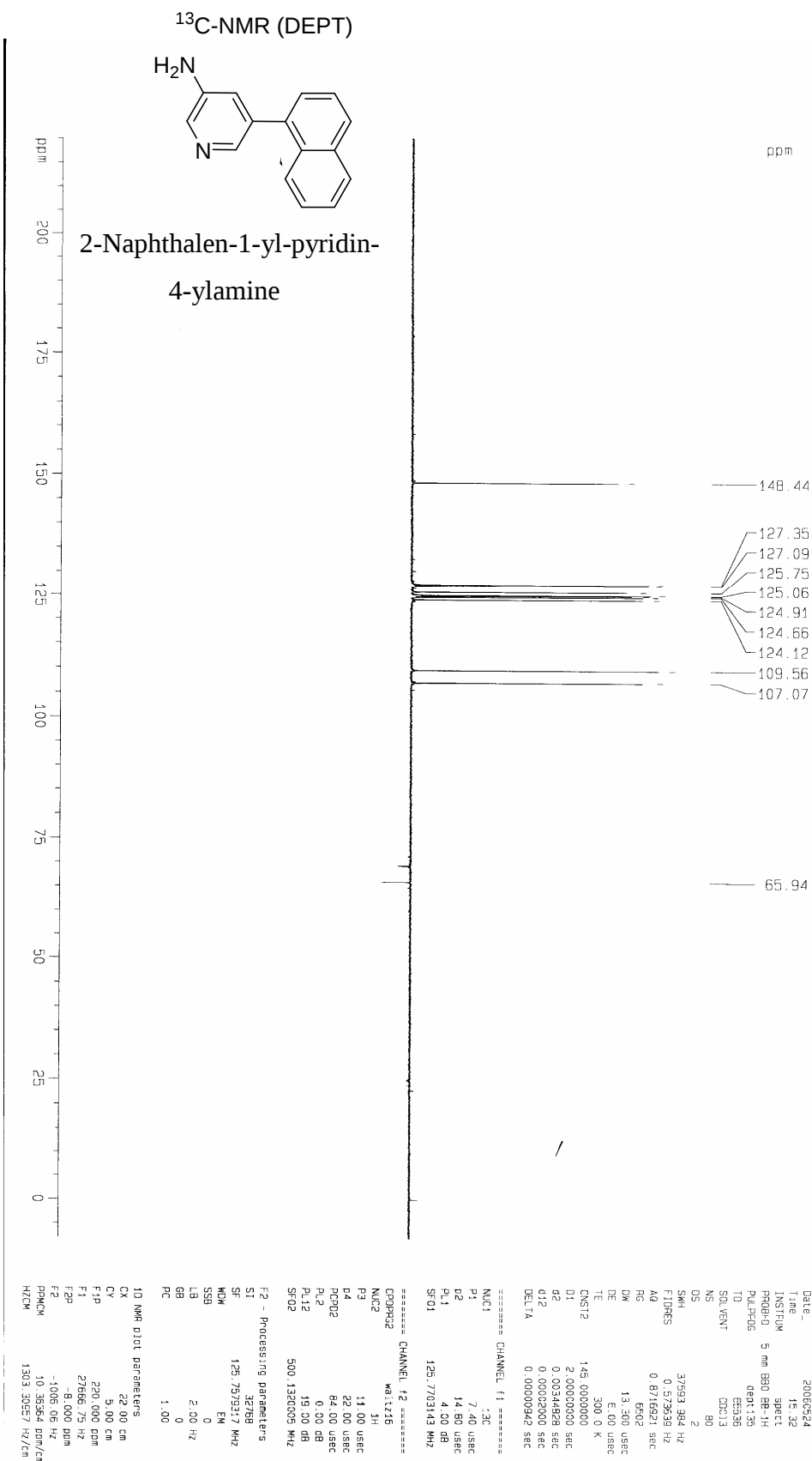
F2 - Acquisition Parameters
Date_: 20060524
Time: 15.27
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 256
DS: 4
SWH: 37593.984 Hz
FIDRES: 0.57639 Hz
AQ: 0.8716921 sec
RG: 13004
DM: 13.300 usec
DE: 6.00 usec
TE: 300.0 K
D1: 0.4000001 sec
d11: 0.0300000 sec
d12: 0.0002000 sec

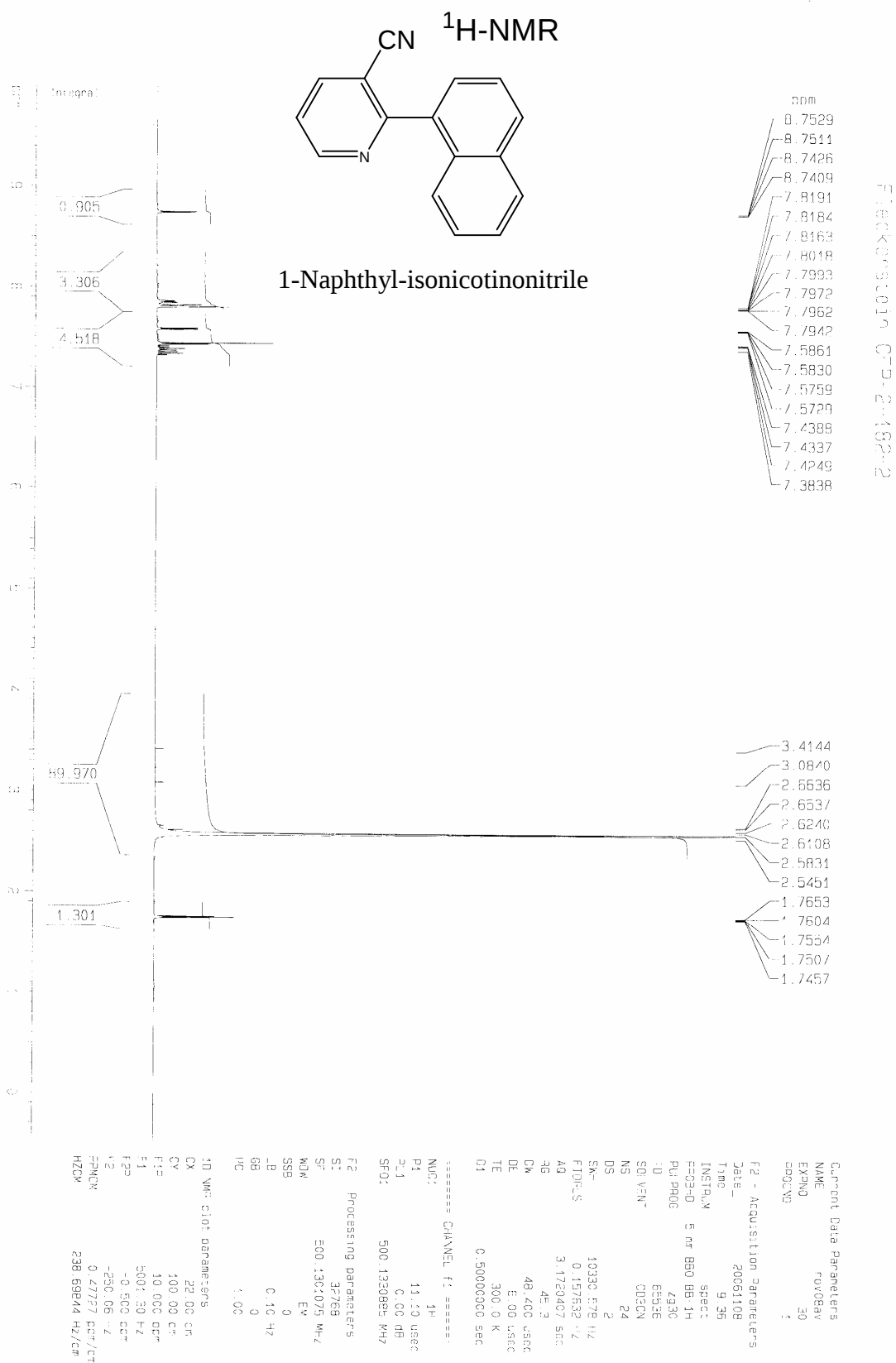
===== CHANNEL f1 =====
NUC1: ¹³C
P1: 7.40 usec
PL1: 4.00 dB
SFO1: 125.7703143 MHz

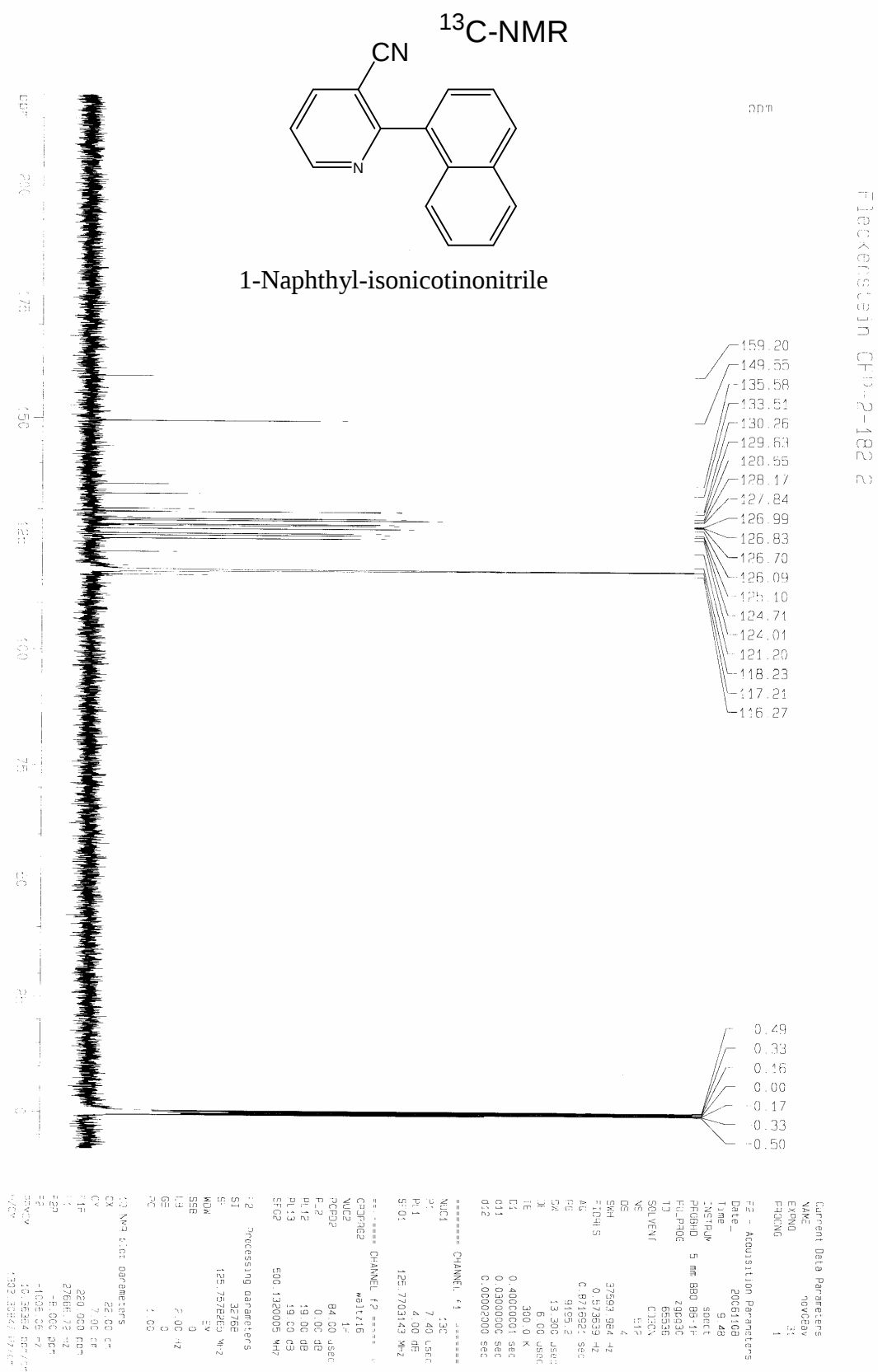
===== CHANNEL f2 =====
CPRPG2: waltz16
NUC2: ¹H
PCPD2: 64.00 usec
PL2: 0.00 dB
PL12: 19.00 dB
PL13: 19.00 dB
SFO2: 500.1320005 MHz

F2 - Processing parameters
SI: 32768
SF: 125.770314 MHz
WDW: EM
SSB: 0
LB: 2.00 Hz
GB: 0
PC: 1.00

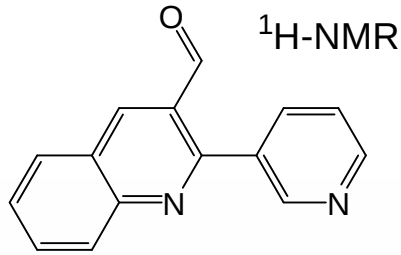
1D NMR plot parameters
CX: 22.00 cm
CY: 7.00 cm
F1P: 220.000 ppm
F1: 27866.75 Hz
F2P: -6.000 ppm
F2: -1006.06 Hz
PPHMC: 10.36364 ppm/cm
HZCM: 1303.30957 Hz/cm











Fleckenstein CPD-2-170-1

Current Data Parameters

NAME	VALUE
EXPNO	20
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20051030	9.12

INSTRUM spect

PROBHD 5 mm BBO BB-1H

PULPROG zg30

TD 65536

SOLVENT CD3CN

NS 32

DS 2

SWH 10330.578 Hz

FIDRES 0.137632 Hz

AQ 3.1720407 sec

RG 362

DM 48.400 usec

DE 6.00 usec

TE 300.0 K

C1 0.50000000 sec

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

NUC1 1H

P1 11.50 usec

PL1 0.00 dB

SFO1 500.130086 MHz

F2 - Processing parameters

SI	SI
32768	500.130086 MHz

WDW EM

SSB 0

LB 0.10 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX	CY
22.00 CT	50.00 CM

F3 11.000 ppm

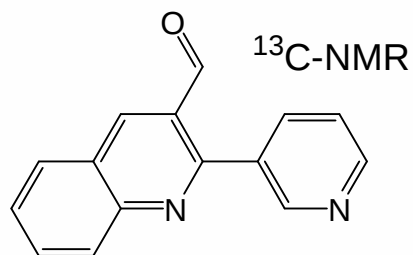
F4 5501.43 Hz

F2 0.500 ppm

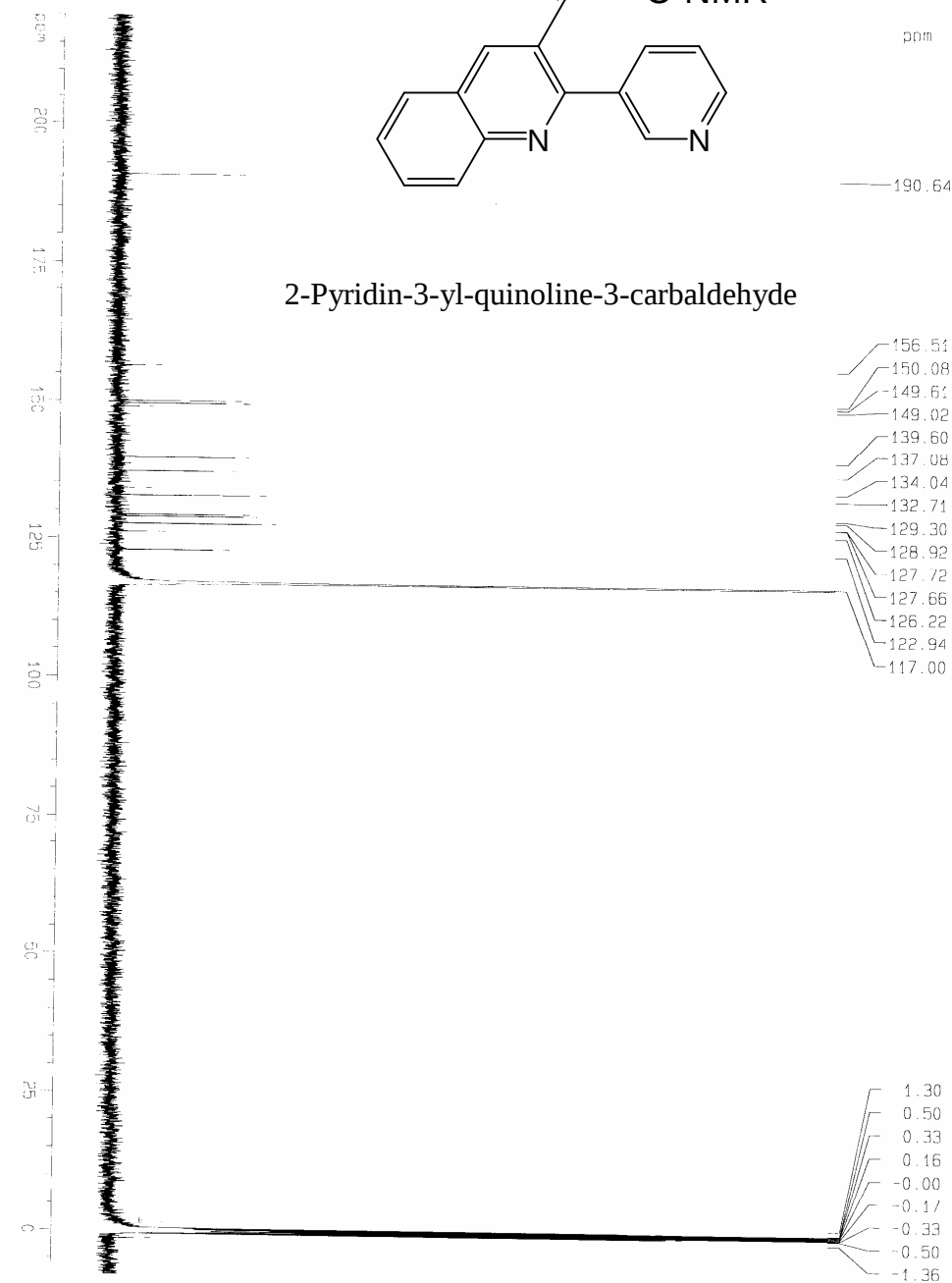
F2 250.06 Hz

PPMCM 0.52272 ppm/cm

HZCM 261.43158 Hz/cm



2-Pyridin-3-yl-quinoline-3-carbaldehyde



Current Data Parameters
NAME OK1308Y
EXPNO 21
PROCNO 1

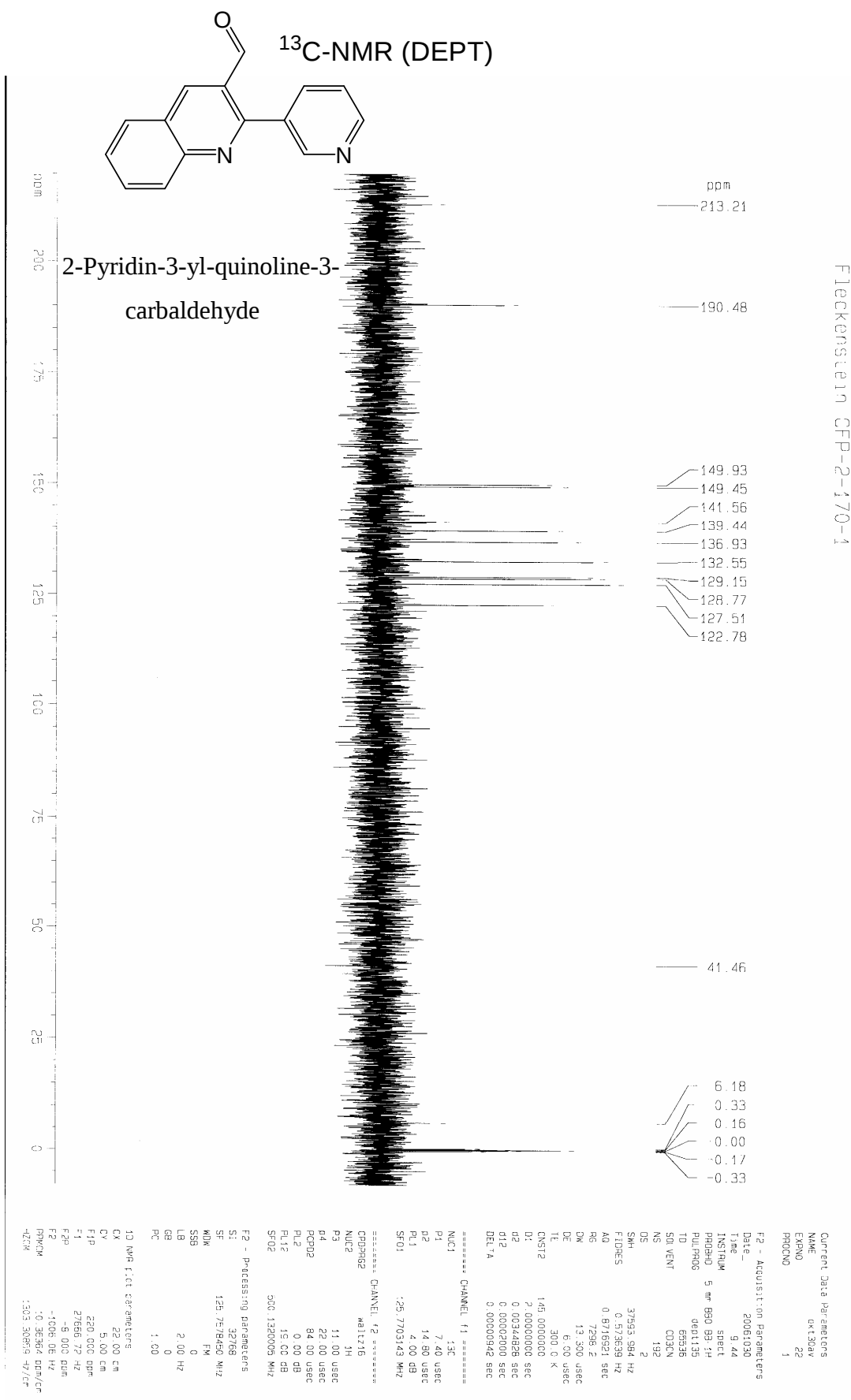
F2 - Acquisition Parameters
Date_ 20061030
Time 9:34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CLICH
NS 1000
DS 4
SWH 37593.584 Hz
FIDRES 0.573639 Hz
AQ 0.8716921 sec
RG 4096
DM 13.300 usec
DE 6.00 usec
TE 300.0 K
D1 0.40000001 sec
d11 0.03000000 sec
d12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 4.00 dB
SFO1 125.7703143 MHz

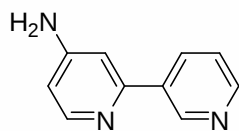
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 1H
PL2 0.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 500.132005 MHz

F2 - Processing parameters
SI 32768
SF 125.7576257 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
SC 1.00

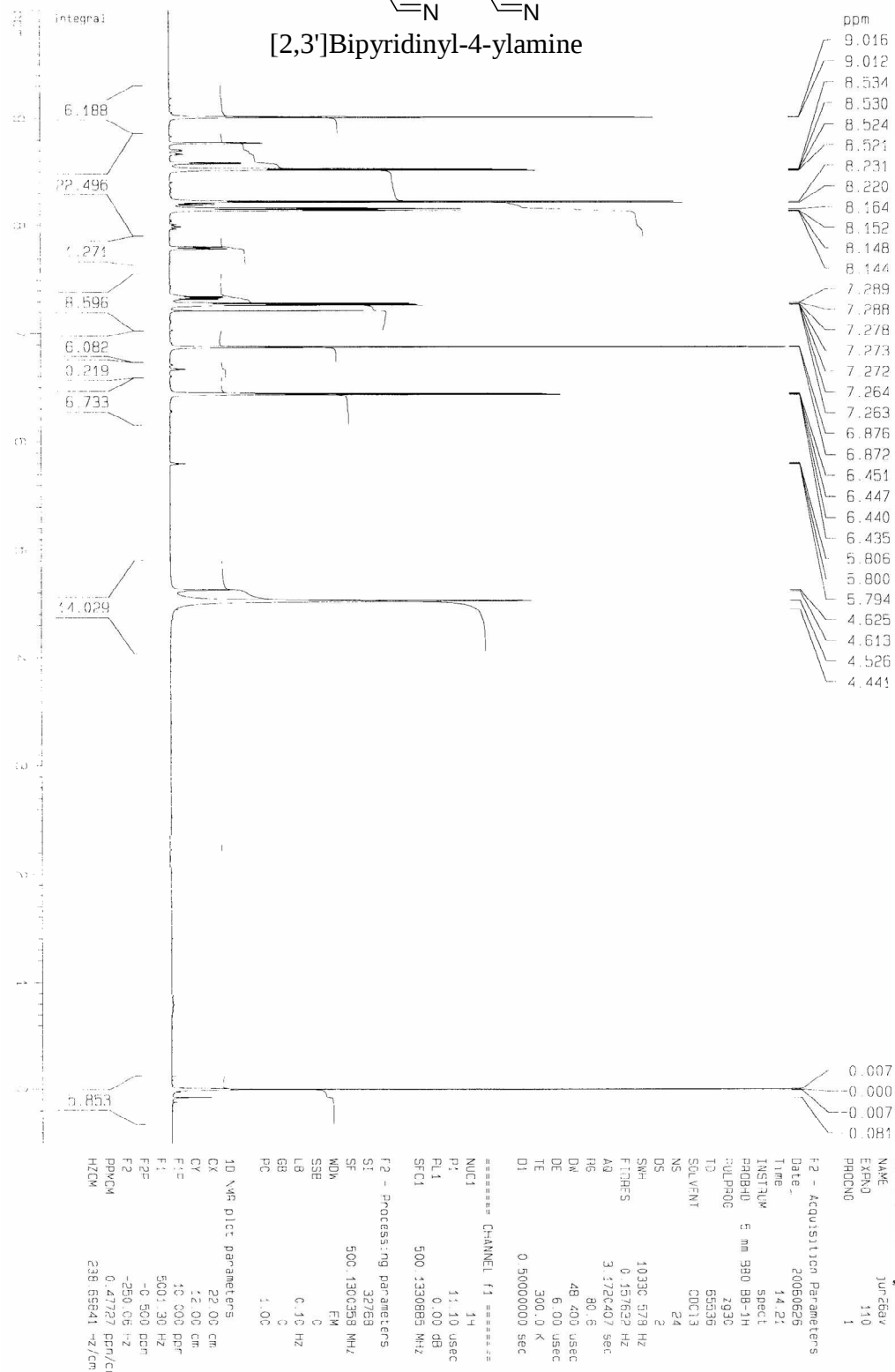
1D NMR elct parameters
CX 22.00 cm
CY 60.00 cm
FAP 220.000 mm
F1 27565.72 Hz
F2 -20.000 dB
F2 -1036.06 Hz
FPMCM 10.36364 dB/cy
FZCV 1303.30847 Hz/cy



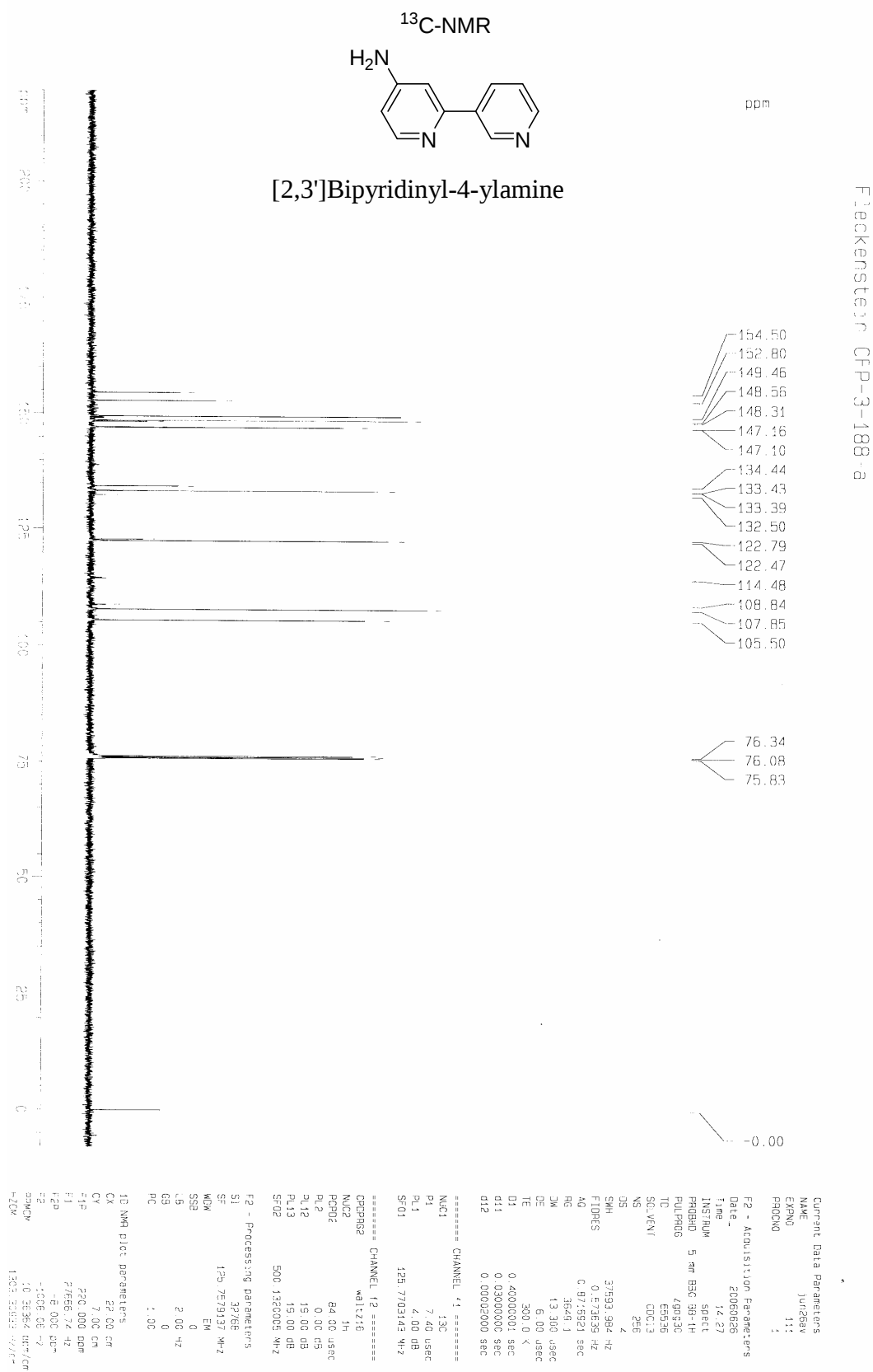
¹H-NMR

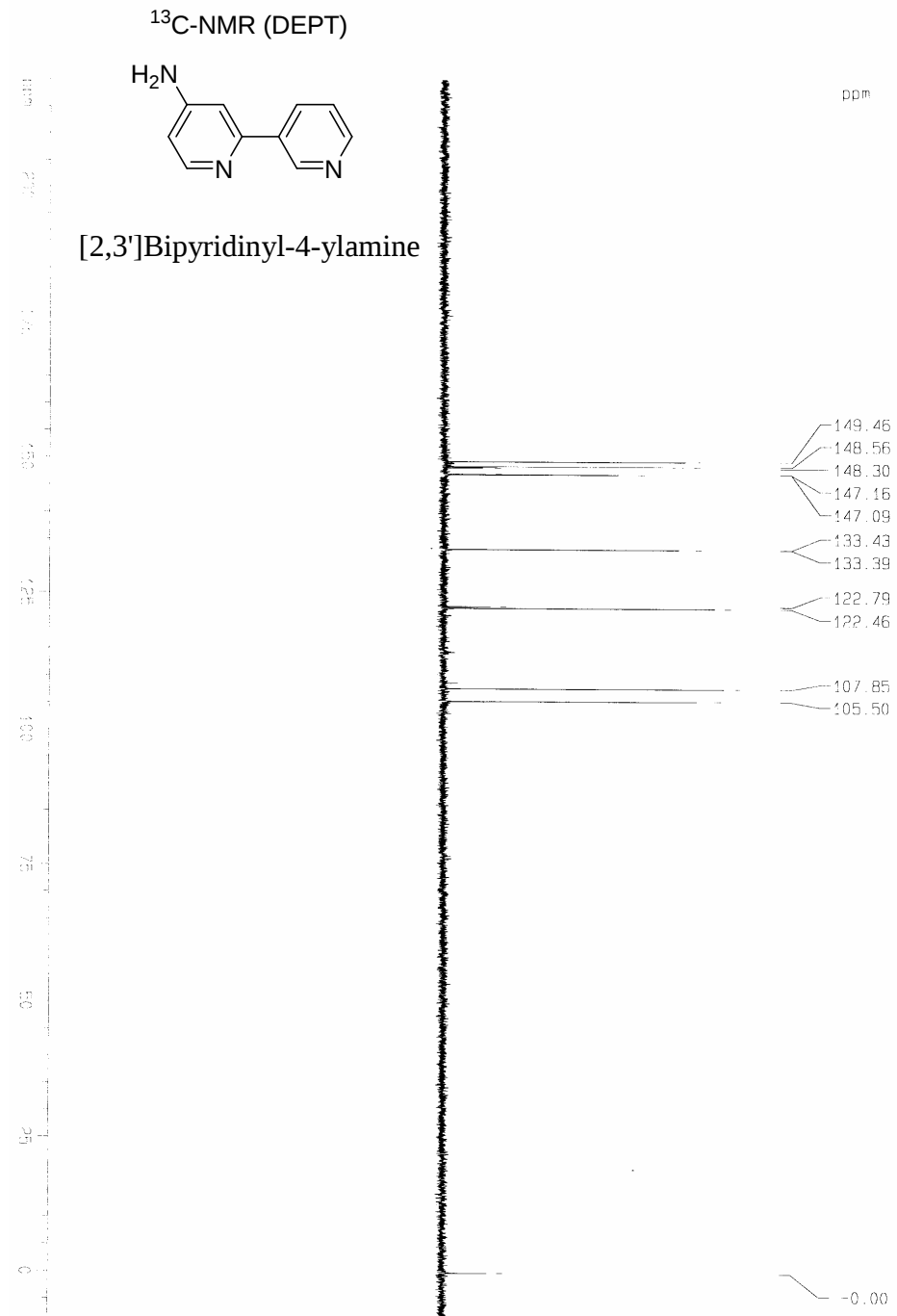


[2,3']Bipyridinyl-4-ylamine



Flockenstein CFP-3-188-a





Current Data Parameters

NAME: 10726ay

EXPNO: 112

PROCNO: 1

F2 - Acquisition Parameters

Date_: 20060826

Time: 14:31

INSTRUM: spect

PROBHD: 5 mm BBO BB-1H

PULPROG: zgpg30

TD: 65536

SOLVENT: DMS-d6

NS: 80

DS: 2

SWH: 37553.984 Hz

FIDRES: 0.173639 Hz

AQ: 0.871692 sec

RG: 659.7

DM: 13.300 usec

DE: 5.00 usec

TE: 300.2 K

CONTR: 145.000000

DI: 2.00000000 sec

DE: 0.00344828 sec

DE2: 0.00022000 sec

DELTA: 0.0000942 sec

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

NUC1: ¹³C

P1: 7.40 usec

P2: 14.80 usec

PL1: 4.00 dB

PL2: 120.7703143 MHz

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

CPDPRG2: waltz16

NUC2: ¹H

P3: 11.00 usec

P4: 22.00 usec

PL3: 84.00 usec

PL4: 0.00 dB

PL5: 19.00 dB

SFO2: 500.136005 MHz

F2 - Processing parameters

SI: 32768

SF: 125.759139 MHz

WDW: EM

SSB: 0

LB: 2.00 Hz

GB: 0

PC: 1.00

1D NMR plot parameters

CX: 22.00 cm

CY: 5.00 cm

F10: 220.000 MHz

F1: 276.6672 Hz

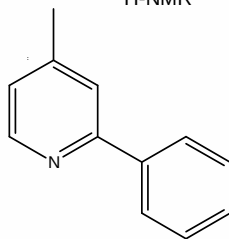
F20: 5.000 MHz

F2: 10.38564 MHz

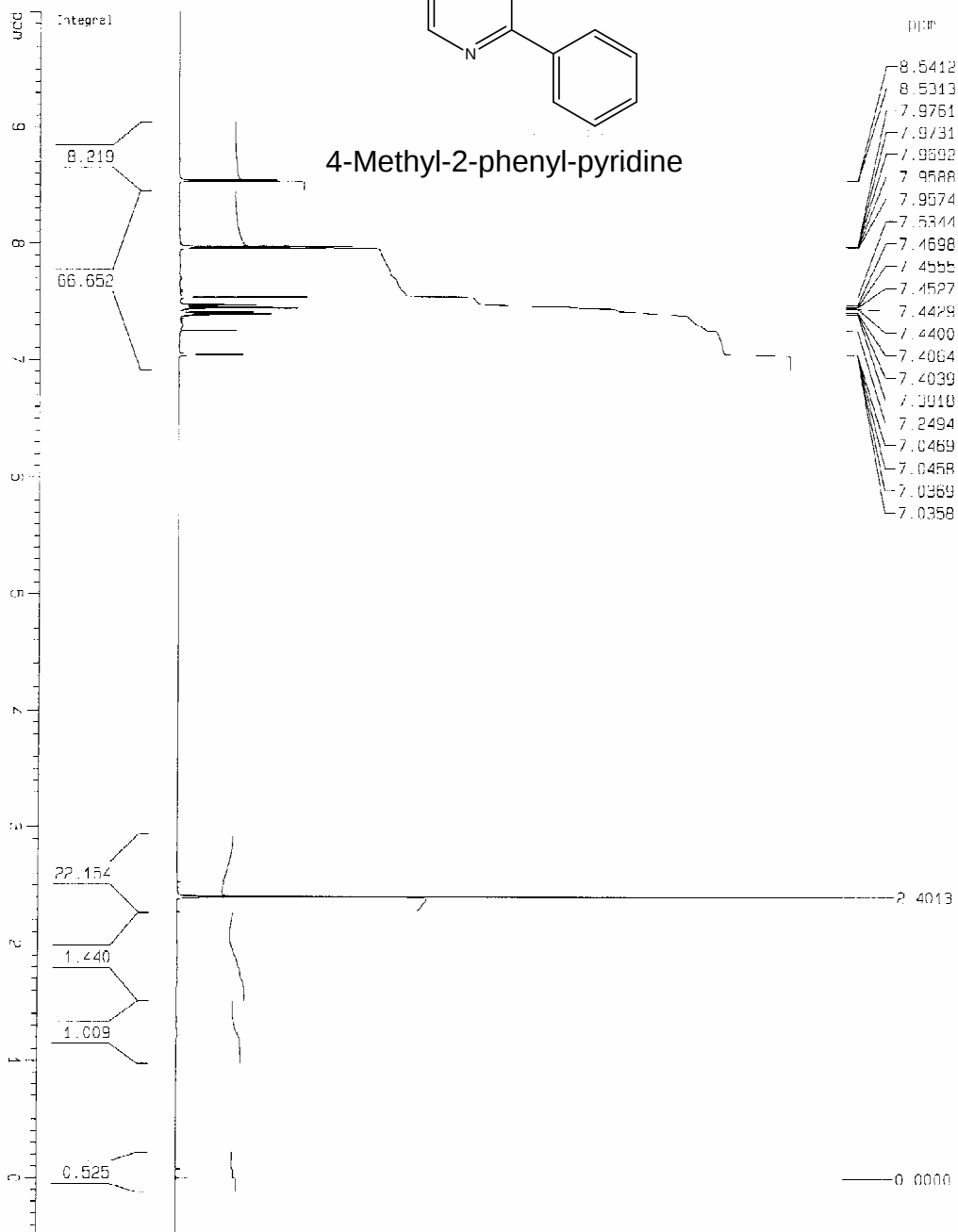
NUC1: ¹³C

NUC2: ¹H

¹H-NMR



4-Methyl-2-phenyl-pyridine



Current Data Parameters
NAME sedday
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070920
Time 22.23
INSTRUM spect
PROBHD 5 mm BBO BB-2H
PULPROG zgpg30
TD 2635
FIDRES 0.0000
SOLVENT CDCl3
NS 24
DS 2
SWH 10330.578 Hz
FIDRES 0.157332 Hz
AQ 3.170407 sec
RG 181
GB 48.400 sec
TE 6.00 sec
DE 300.0 K
C1 0.5000000 sec
===== C1 ANTI f1 =====
NUC1 1H
P1 11.10 sec
PL1 0.00 dB
SFO1 500.1330895 MHz
F2 - Processing parameters
SI 32768
SF 500.1330895 MHz
WDW EM
SSP 0
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 14.00 cm
F2 10.000 cm
F1 2001.30 Hz
F2 10.500 cm
F2 -250.06 Hz
PROCN 0.47227 cm/cm
HZCW 218.56899 Hz/cm

Software Version	: 6.3.1.0504	Date	: 19.09.2007 09:40:12
Operator	: tprocess	Sample Name	: Picolin-Kupplung
Sample Number	: 001	Study	: 0/21
AutoSampler	: BUILT-IN	Rack/Vial	: A
Instrument Name	: pancho	Channel	: 1000
Instrument Serial #	: None	A/D mV Range	: 26.00 min
Delay Time	: 0.00 min	End Time	: 0.00 min
Sampling Rate	: 12.5000 pts/s	Area Reject	: 0.000000
Sample Volume	: 1.000000 ul	Dilution Factor	: 1.00
Sample Amount	: 1.0000	Cycle	: 1
Data Acquisition Time	: 19.09.2007 08:24:02		

Raw Data File : C:\USER\christoph\daten\190907a.raw
Inst Method : c:\user\christoph\methoden\file_brac_ns.mth from C:\USER\christoph\daten\190907a.raw
Proc Method : c:\user\christoph\methoden\file_brac_ns.mth from
Callb Method : c:\user\christoph\methoden\file_brac_ns.mth from
Report Format File: c:\user\christoph\methoden\default.rpt
Sequence File : C:\USER\markus\methoden\Acetylene-Reinheit.seq

DEFAULT REPORT

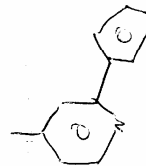
Peak #	Time [min]	Area [µV·s]	Height [µV]	Area [%]	Norm. Area [%]	BL	Area/Height [s]
1	2.255	60687.79	31396.54	0.43	0.43	BB	1.9329
2	2.350	49127.50	31758.62	0.35	0.35	BV	1.5469
3	2.391	7087860.05	987876.66	50.18	50.18	VB	7.1748
4	2.741	1448367.25	584270.78	10.25	10.25	BB	2.4789
5	9.408	37679.85	21285.94	0.27	0.27	BB	1.7702
6	10.717	5442084.75	985256.27	38.53	38.53	BB	5.5235
		14125807.20	2.64e+06	100.00	100.00		

Warning -- Signal level out-of-range in peak

Missing Component Report
Component Expected Retention (Calibration File)

All components were found

C.F.P. - AC - 1001 - 1



Chromatogram

Sample Name : C:\USER\christoph\daten\190907a.raw
File Name : C:\USER\christoph\daten\190907a.raw
Date : 19.09.2007 09:40:12
Start Time : 0.00 min
End Time : 26.00 min
Low Point : -47.14 mV
High Point : 993.88 mV
Plot Scale : 1941.0 mV

