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 (^{1}H 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 (δ = 0 ppm), ^{1}H NMR, 65% aq. H_3PO_4. (δ = 0 ppm), ^{31}P NMR and nitromethane (δ = 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 chromatograpy (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 °C, detector temperature: 350 °C. Temperature program: isotherm 150°C for 5 min, heating to 300°C with 25 °C/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

^{1}H NMR (500 MHz, $CDCl_3$) δ [ppm] 8.75 (dd, ^5J = 0.5 Hz, ^3J = 5.0 Hz, 1 H, C*H*, ar), 7.84-7.80 (m, 3 H, C*H*, ar), 7.32 (dd, ^4J = 1.0 Hz, ^3J = 5.0 Hz, 1 H, C*H*, ar), 7.24 (d, ^3J = 8.0 Hz, 2 H, C*H*, ar), 2.35 (s, 3 H, CH_3); $^{13}C\{^1H\}$ NMR (125.77 MHz, $CDCl_3$) 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 $C_{13}H_{10}N_2$: 194.0844, found 194.08414.

2-p-Tolyl-quinoline-3-carbaldehyde

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 10.12 (s, 1 H, C*H*O), 8.85 (s, 1 H, C*H*, ar), 8.14-8.09 (m, 3 H, C*H*, ar), 7.91 (ddd, ^5J = 1.5 Hz, ^4J = 7.0 Hz, ^3J = 8.5 Hz, 1 H, C*H*, ar), 7.76 (ddd, ^5J = 1.5 Hz, ^4J = 7.0 Hz, ^3J = 8.5 Hz, 1 H, C*H*, ar), 7.59 (td, ^4J = 2.0 Hz, ^3J = 8.0 Hz, 2 H, C*H*, ar), 7.41-7.38 (m, 2 H, C*H*, ar), 2.45 (s, 3 H, CH_3); $^{13}C\{^1H\}$ NMR (125.77 MHz, CD_3CN) 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 $C_{17}H_{13}NO$: 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]

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

2-Methoxy-6-p-tolyl-pyridine

^{1}H NMR (500 MHz, $CDCl_3$) δ [ppm] 7.93 (d, ^{3}J = 8.5 Hz, 2 H, C*H*, ar), 7.58 (dd, ^{3}J = 7.5 Hz, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 7.29 (dd, ^{5}J = 0.5 Hz, ^{3}J = 7.5 Hz, 1 H, C*H*, ar), 7.24 (dd, ^{5}J = 0.5 Hz, ^{3}J = 8.5 Hz, 2 H, C*H*, ar), 6.64 (d, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 4.02 (s, 3 H, OCH_3), 2.39 (s, 3 H, CH_3); $^{13}C\{^{1}H\}$ 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 $C_{13}H_{13}NO$: 199.0997, found 199.09999.

2-p-Tolyl-pyridin-4-ylamine

^{1}H NMR (500 MHz, $CDCl_3$) δ [ppm] 8.25 (d, ^{3}J = 5.5 Hz, 1 H, ar), 7.78 (d, ^{3}J = 8.0 Hz, 2 H, ar), 7.21 (d, ^{3}J = 8.0 Hz, 2 H, ar), 6.85 (s, 1 H, ar), 6.39 (dd, ^{3}J = 5.5 Hz, ^{4}J = 2.5 Hz 1 H, ar), 4.35 (s (br), 2 H, NH_2), 2.36 (s, 3 H, CH_3); $^{13}C\{^{1}H\}$ 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 $C_{12}H_{12}N_2$: 184.1001, found 184.09808.

4-Methyl-2-m-tolyl-quinoline

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 8.06-8.01 (m, 3 H, C*H*, ar), 7.99-7.96 (m, 1 H, C*H*, ar), 7.82 (d, ^{5}J = 0.5 Hz, 1 H, C*H*, ar), 7.71 (ddd, ^{5}J = 1.5 Hz, ^{3}J = 6.5 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*, ar), 7.55 (ddd, ^{5}J = 1.0 Hz, ^{3}J = 6.5 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*, ar), 7.40 (t, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 7.30-7.27 (m, 1 H, C*H*, ar), 2.71 (d, ^{5}J = 0.5 Hz, 3 H, CH_3), 2.44 (s, 3 H, CH_3); $^{13}C\{^{1}H\}$ 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 $C_{17}H_{15}N$: 233.1205, found 233.12109.

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

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 8.54 (s, 1 H, C*H*, ar), 8.41 (d, ^{3}J = 7.0 Hz,1 H, C*H*, ar), 8.08-8.02 (m, 2 H, C*H*, ar), 7.87-7.85 (m, 1 H, C*H*, ar), 7.78-7.71 (m, 2 H, C*H*, ar), 7.68 (t, ^{3}J = 7.5 Hz, 1 H, C*H*, ar), 7.60-7.56 (m, 1 H, C*H*, ar), 2.73-2.72 (m, 3 H, CH_3); $^{13}C\{^{1}H\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 154.2, 147.5, 145.6, 140.0, 130.5, 130.1 (q, ^{2}J = 31.8 Hz, *C*CF_3), 129.6, 129.3, 129.3, 127.1, 126.2, 125.4 (q, ^{3}J = 4.4 Hz, *C*HCCF_3), 123.7, 124.2 (q, ^{1}J = 271.8 Hz, *C*F_3), 123.5 (q, ^{3}J = 2.9 Hz, *C*HCCF_3), 118.7, 17.7; HRMS calcd. for $C_{17}H_{12}NF_3$: 287.0922, found 287.09206.

2-m-Tolyl-quinoline-3-carbaldehyde

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 10.10 (s, 1 H, C*H*O), 8.83 (s, 1 H, C*H*, ar), 8.12-8.08 (m, 2 H, C*H*, ar), 7.90 (ddd, ^{5}J = 1.5 Hz, ^{3}J = 7.0 Hz, ^{3}J = 9.0 Hz, 1 H, C*H*, ar), 7.67 (ddd, ^{5}J = 1.0 Hz, ^{3}J = 7.0 Hz, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 7.53-7.50 (m, 1 H, C*H*, ar), 7.46-7.43 (m, 2 H, C*H*, ar), 7.40-7.35 (m, 1 H, C*H*, ar), 2.45 (s, 3 H, CH_3); $^{13}C\{^{1}H\}$ 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 $C_{17}H_{13}NO$: 247.0997, found 247.09813.

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

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 10.10 (s, 1 H, C*H*O), 8.87 (s, 1 H, C*H*, ar), 8.15-8.10 (m, 2 H, C*H*, ar), 8.03 (s, 1 H, C*H*, ar), 7.93 (ddd, ^{5}J = 1.5 Hz, ^{3}J = 7.0 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*, ar), 7.91-7.84 (m, 2 H, C*H*, ar), 7.76-7.68 (m, 2 H, C*H*, ar); $^{13}C\{^{1}H\}$ NMR (125.77 MHz, CD_3CN) δ [ppm] 190.6, 157.7, 148.9, 139.3, 139.2, 133.6, 132.6, 129. (q, ^{2}J = 32.3 Hz, *C*CF_3), 129.2, 128.9, 128.9, 127.6, 127.5, 126.3 (q, ^{3}J = 3.9 Hz, *C*HCCF_3), 126.2, 125.3 (q, ^{3}J = 3.8 Hz, *C*HCCF_3), 124.0 (q, ^{1}J = 272.4 Hz, *C*F_3); HRMS calcd. for $C_{17}H_{10}NOF_3$: 301.0714, found 301.06928.

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

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 9.74 (s, 1 H, C*H*O), 8.96 (s, 1 H, C*H*, ar), 8.22 (d, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 8.13 (dd, ^{5}J = 0.5 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*, ar), 8.09 (d, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 8.04 (d, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 7.96 (ddd, ^{5}J = 1.0 Hz, ^{3}J = 6.5 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*, ar), 7.75 (ddd, ^{5}J = 1.5 Hz, ^{3}J = 7.0 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*, ar), 7.67 (dd, ^{3}J = 7.0 Hz, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 7.62-7.52 (m, 3 H, C*H*, ar), 7.44 (ddd, ^{5}J = 1.5 Hz, ^{3}J = 7.0 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*, ar); $^{13}C\{^{1}H\}$ 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 $C_{20}H_{13}NO$: 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

^{1}H NMR (500 MHz, $CDCl_3$) δ [ppm] 8.20 (d, ^{3}J = 5.5 Hz, 1 H, ar), 8.01 (d, ^{3}J = 8.0 Hz, 1 H, ar), 7.76 (t, ^{3}J = 9.5 Hz, 2 H, ar), 7.43-7.33 (m, 4 H, ar), 6.47 (d, ^{4}J = 2.0 Hz, 1 H, ar), 6.27 (dd, ^{3}J = 5.5 Hz, ^{4}J = 2.5 Hz 1 H, ar), 4.37 (s (br), 2 H, NH_2); ^{13}C{^{1}H} NMR (125.77 MHz, $CDCl_3$) 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 $C_{15}H_{12}N_2$: 220.1001, found 220.09869.

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

The NMR spectra were identical with the literature.[6]

1-Naphthyl-isonicotinonitrile

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 8.75 (dd, ^{5}J = 0.5 Hz, ^{3}J = 5.0 Hz, 1 H, C*H*, ar), 8.75 (dd, ^{4}J = 2.5 Hz, ^{3}J = 6.5 Hz, 1 H, C*H*, ar), 7.82-7.81 (m, 1 H, C*H*, ar), 7.81-7.79 (m, 2 H, C*H*, ar), 7.58 (dd, ^{5}J = 1.5 Hz, ^{3}J = 5.5 Hz, 1 H, C*H*, ar), 7.45-7.42 (m, 2 H, C*H*, ar), 7.38 (ddd, ^{5}J = 1.0 Hz, ^{3}J = 7.0 Hz, ^{3}J = 7.5 Hz, 1 H, C*H*, ar), 7.34 (ddd, ^{5}J = 1.0 Hz, ^{3}J = 6.5 Hz, ^{3}J = 8.0 Hz, 1 H, C*H*, ar); ^{13}C{^{1}H} NMR (125.77 MHz, CD_3CN) 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 $C_{16}H_{10}N_2$: 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

^{1}H NMR (500 MHz, CD_3CN) δ [ppm] 10.15 (s, 1 H, C*H*O), 8.93 (s, 1 H, C*H*, ar), 8.87 (d, ^{5}J = 1.5 Hz, 1 H, C*H*, ar), 8.73 (dd, ^{5}J = 1.5 Hz, ^{3}J = 4.5 Hz, 1 H, C*H*, ar), 8.19-8.14 (m, 2 H, C*H*, ar), 8.07-8.04 (m, 1 H, C*H*, ar), 7.96 (ddd, ^{5}J = 1.0 Hz, ^{3}J = 6.5 Hz, ^{3}J = 8.5 Hz, 1 H, C*H*,

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[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, ^{5}J = 1.0 Hz, ^{3}J = 7.0 Hz, ^{3}J = 8.0 Hz, 1 H, C*H*, ar), 7.54 (ddd, ^{5}J = 0.5 Hz, ^{3}J = 4.5 Hz, ^{3}J = 8.0 Hz, 1 H, C*H*, ar); $^{13}C\{^{1}H\}$ 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 $C_{15}H_{10}N_2O$: 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

^{1}H NMR (500 MHz, $CDCl_3$) δ [ppm] 9.01 (d, ^{4}J = 1.5 Hz, 1 H, ar), 8.53 (dd, ^{3}J = 5.0 Hz, ^{4}J = 1.5 Hz, 1 H, ar), 8.22 (d, ^{3}J = 6.0 Hz, 1 H, ar), 8.16 (dt, ^{3}J = 8.0 Hz, ^{4}J = 2.0 Hz, 1 H, ar), 6.29-6.26 (m, 1 H, ar), 6.87 (d, ^{4}J = 2.0 Hz, 1 H, ar), 6.44 (dd, ^{3}J = 6.0 Hz, ^{4}J = 2.5 Hz, 1 H, ar), 4.53 (s, 2 H, N*H*$_2$); $^{13}C\{^{1}H\}$ NMR (125.77 MHz, $CDCl_3$) δ [ppm] 154.5, 152.8, 149.5,

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[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.; Sleegers, *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 $C_{10}H_9N_3$: 171.0797, found 171.07820.

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

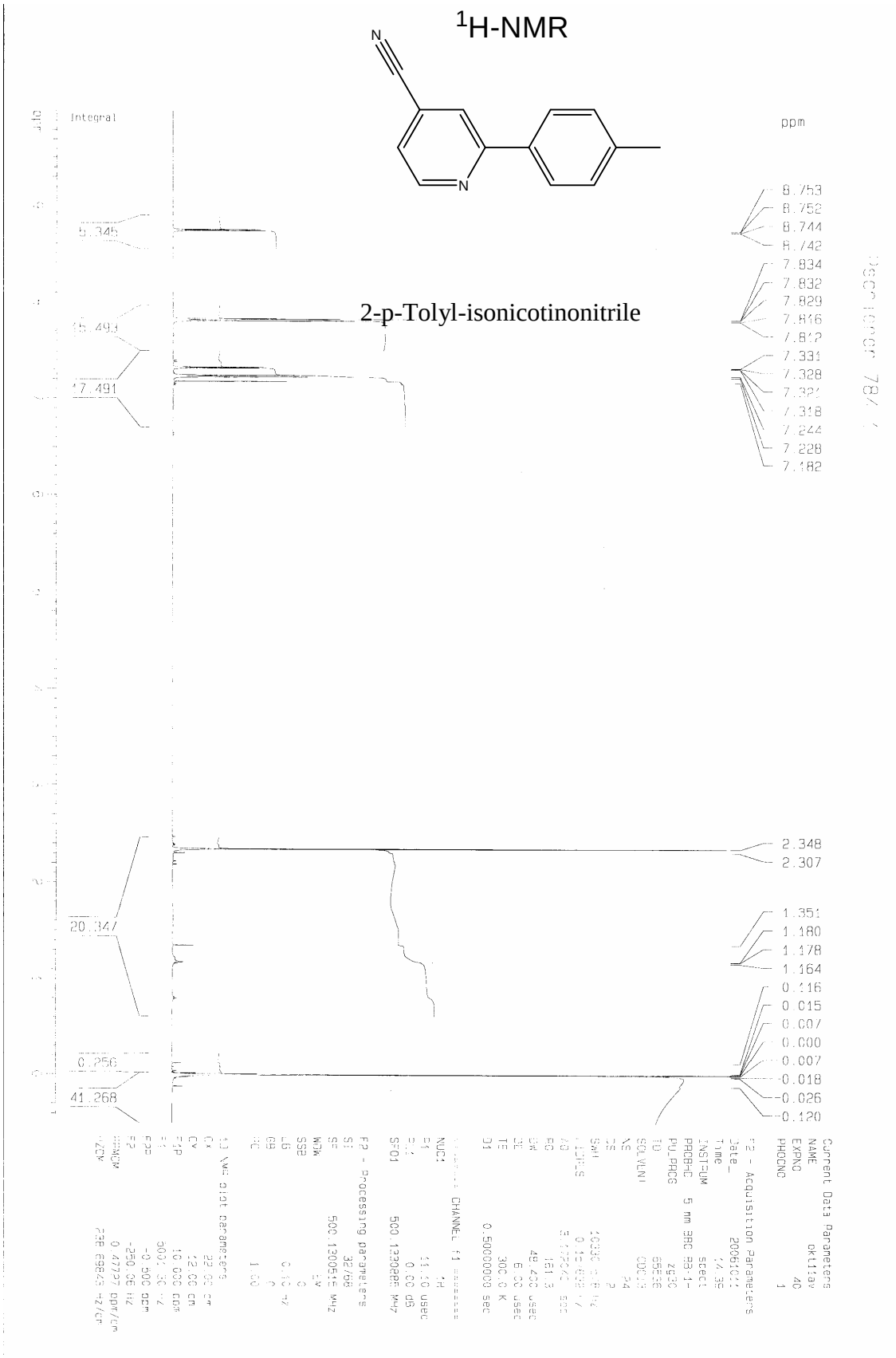
^{1}H NMR (500 MHz, $CDCl_3$) δ [ppm] 8.54 (d, ^3J = 4.8 Hz, 1 H, C*H*, ar), 7.98-7.95 (m, 2 H, C*H*, ar), 7.53 (s, 1 H, C*H*, ar), 7.48-7.43 (m, 2 H, C*H*, ar), 7.41-7.37 (m, 1 H, C*H*, ar), 7.04 (d, ^3J = 4.8 Hz, 1 H, C*H*, ar), 2.40 (s, 3 H, CH_3).

The ^{1}H-NMR spectrum was identical with the literature.[13]

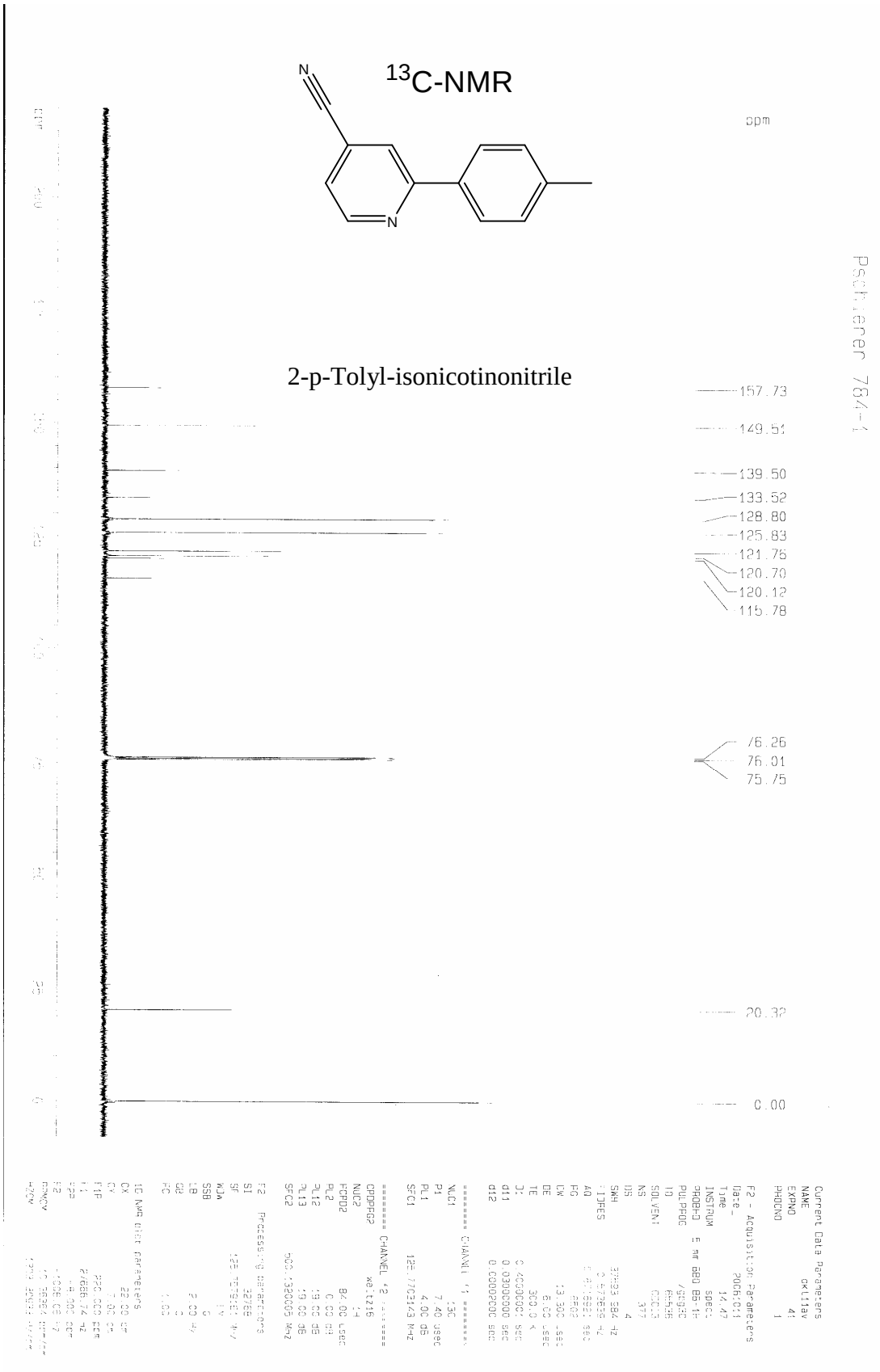
[13] McLoughlin, Padraig T.F.; Clyne, Mairead A.; Aldabbagh, Fawaz; *Tetrahedron*; **2004**; *60*; 37; 8065 – 8072.

NMR-Spectra

^{1}H-NMR



2-p-Tolyl-isonicotinonitrile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120.12
115.78
76.26
76.01
75.75
20.32
0.00

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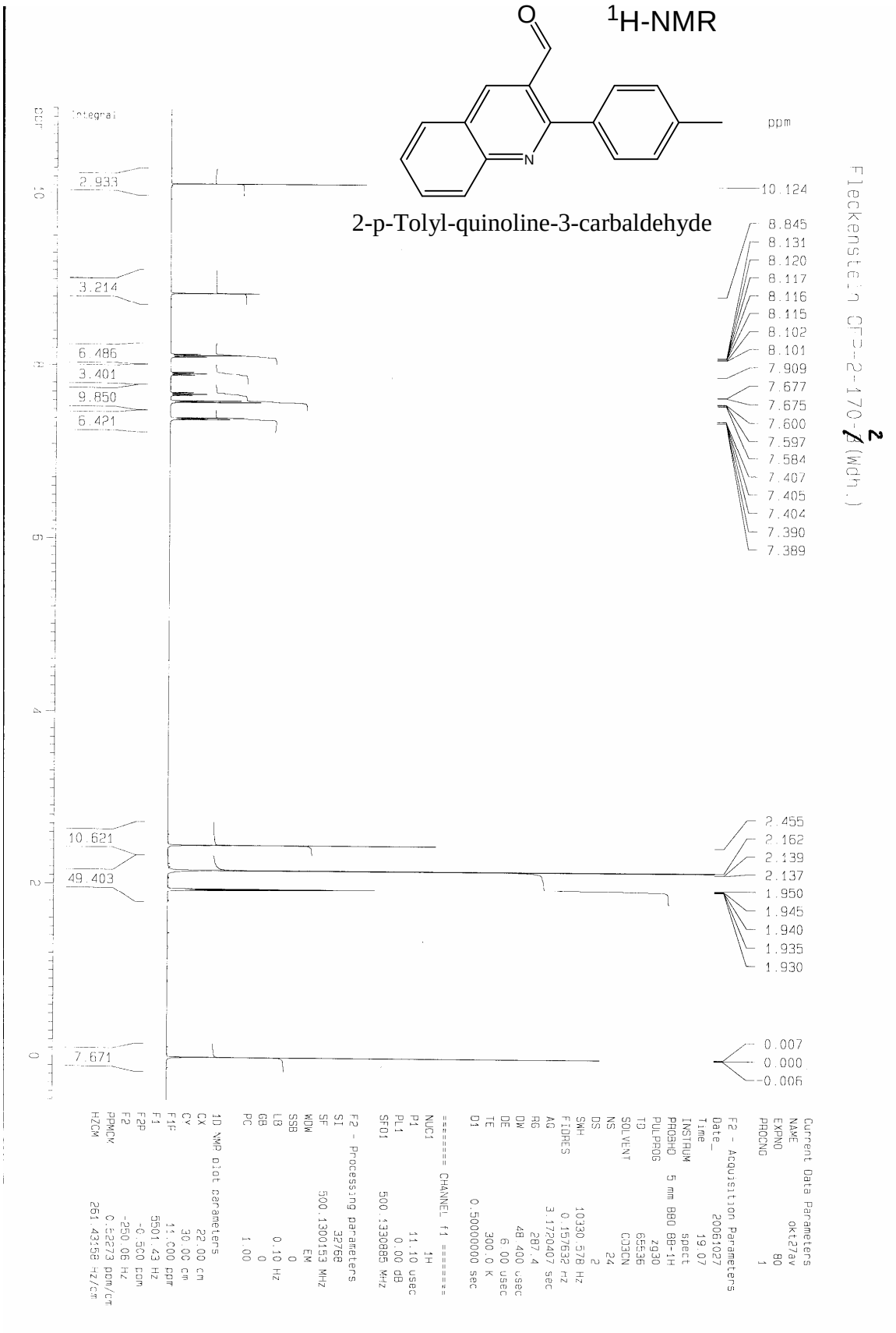
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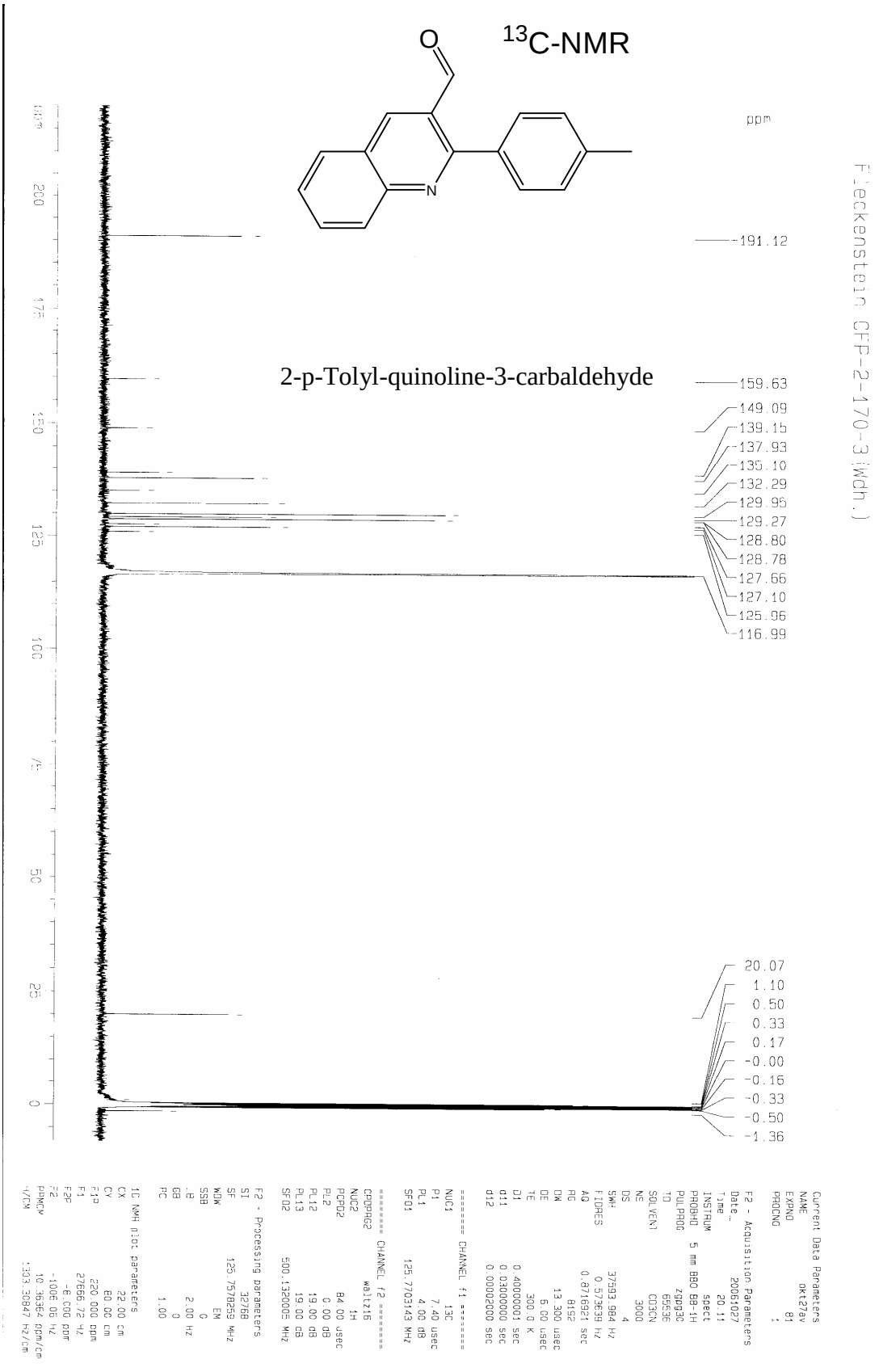
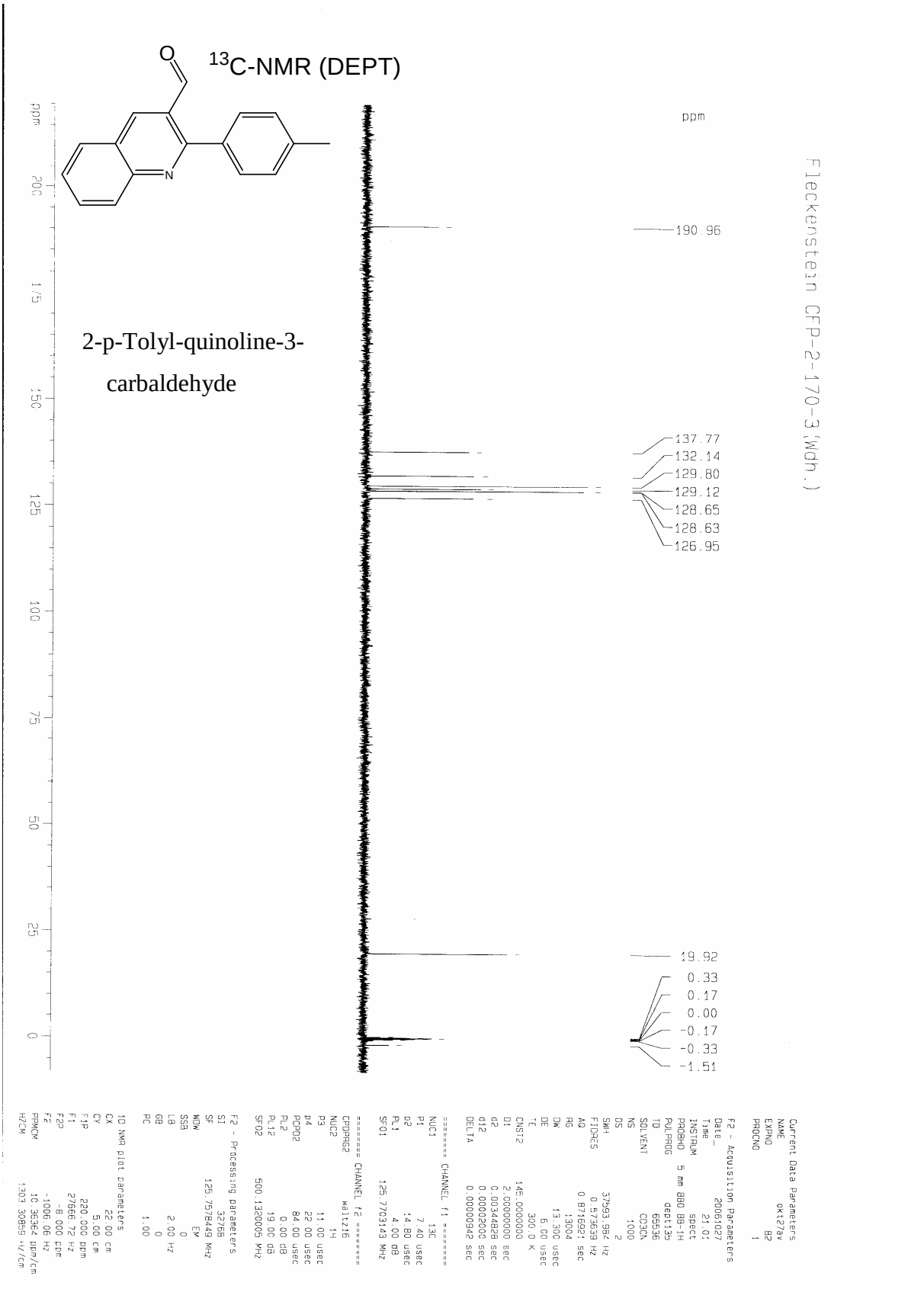
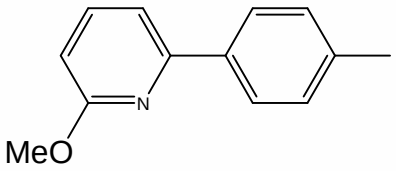
HZCM 261.43758 Hz/cm


^{13}C-NMR
O
N
ppm
191.12
159.63
149.09
139.15
137.93
135.10
132.29
129.96
129.27
128.80
128.78
127.66
127.10
125.96
116.99
20.07
1.10
0.50
0.33
0.17
-0.00
-0.16
-0.33
-0.50
-1.36
200
175
150
125
100
75
50
25
0
Fleckenstein CFP-2-170-3.iwdh.)
2-p-Tolyl-quinoline-3-carbaldehyde

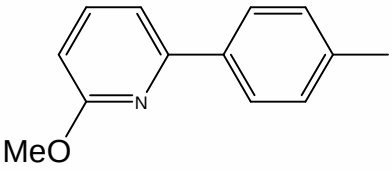

13C-NMR (DEPT)
2-p-Tolyl-quinoline-3-carbaldehyde
ppm
190.96
137.77
132.14
129.80
129.12
128.65
128.63
126.95
19.92
0.33
0.17
0.00
-0.17
-0.33
-1.51
Fleckenstein CFP-2-170-3 (wdh.)

^{1}H-NMR

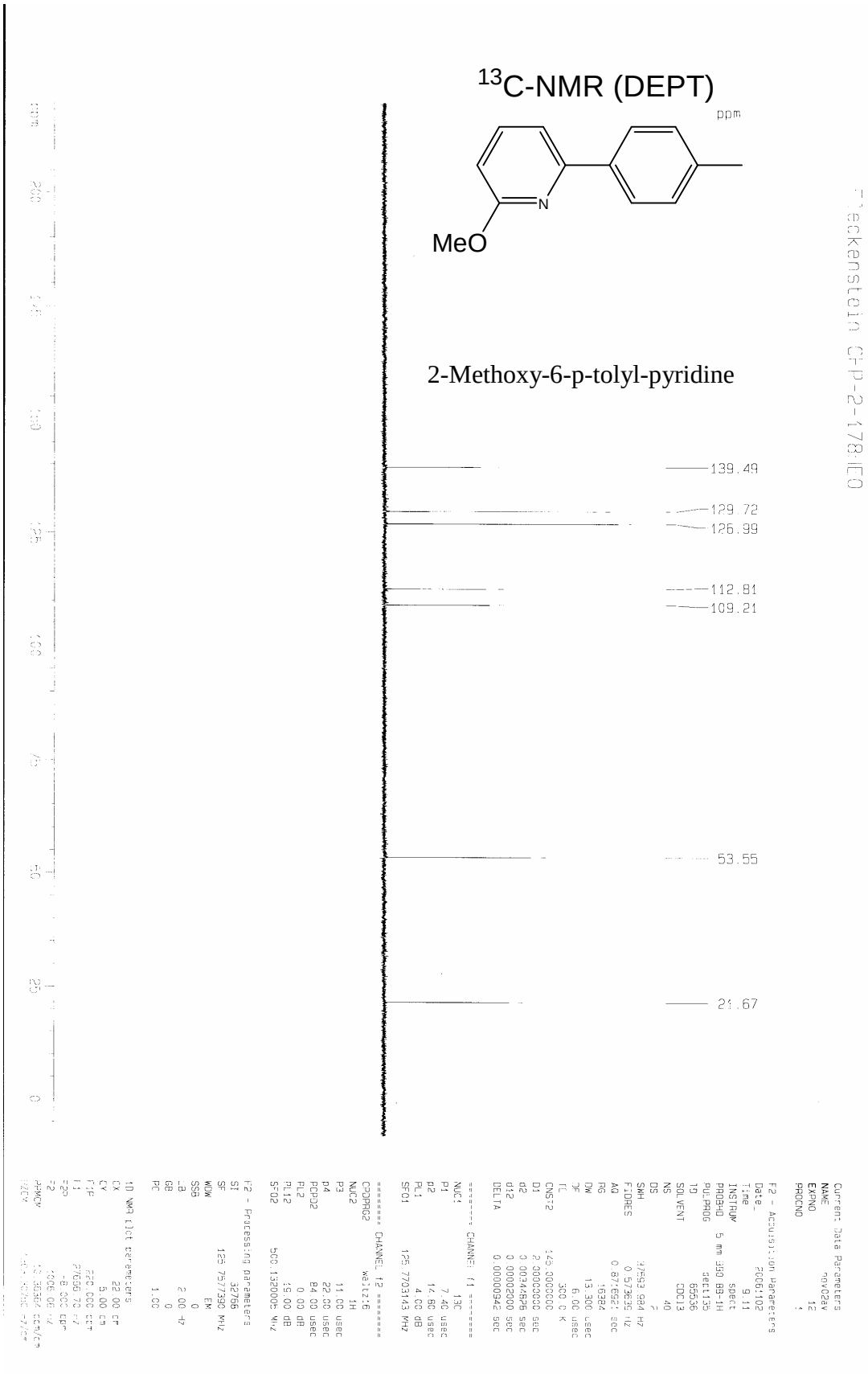


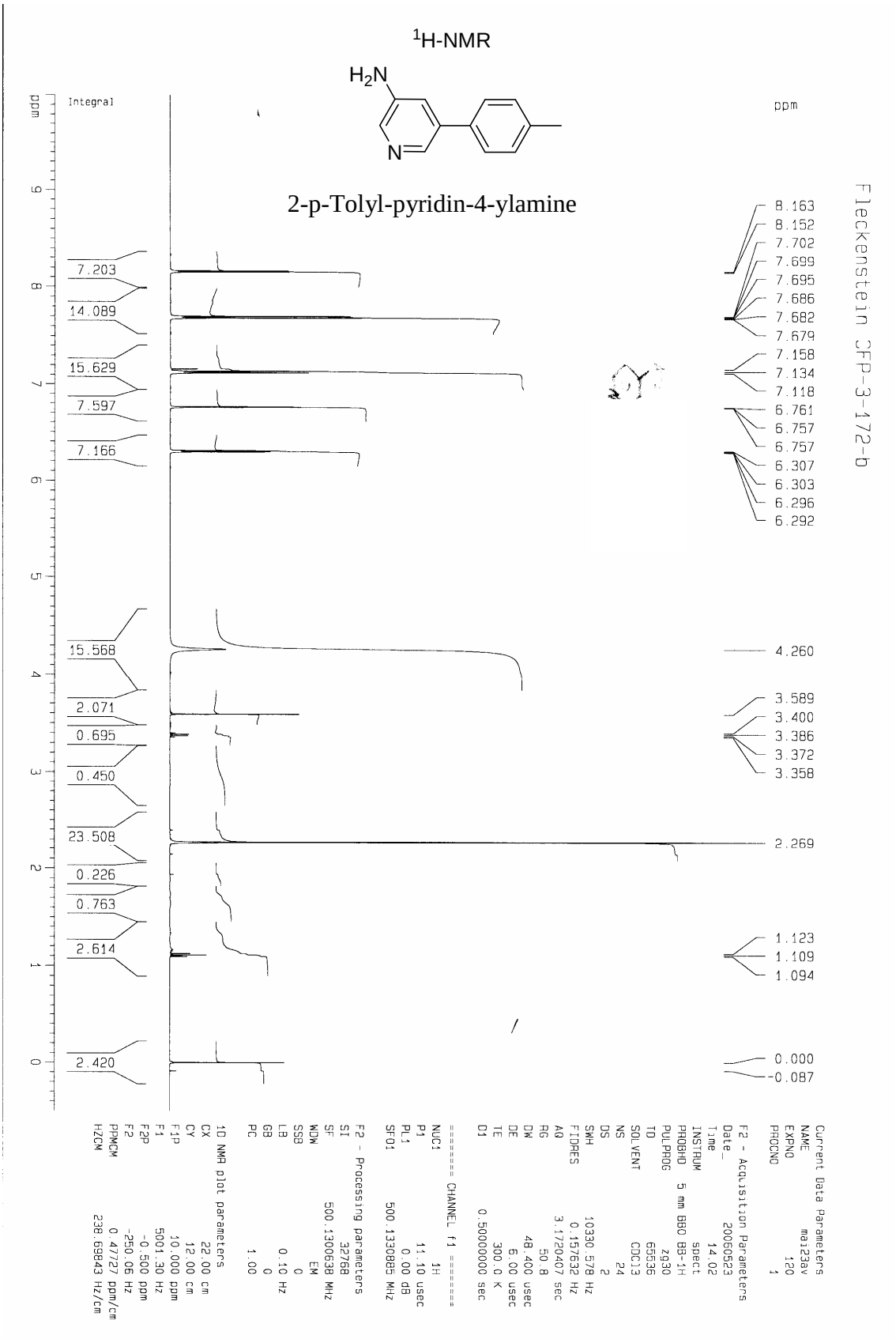
2-Methoxy-6-p-tolyl-pyridine

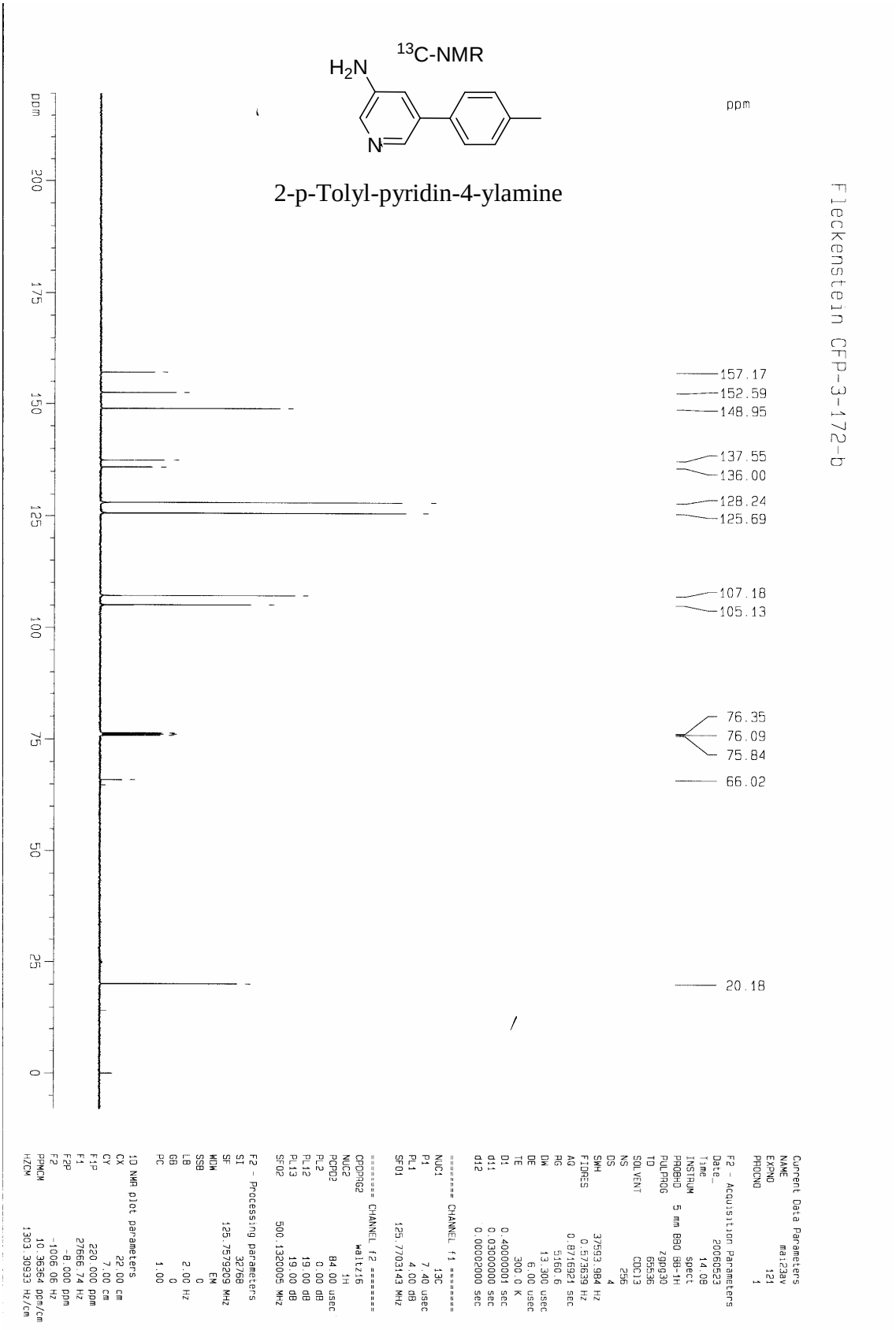
^{13}C-NMR

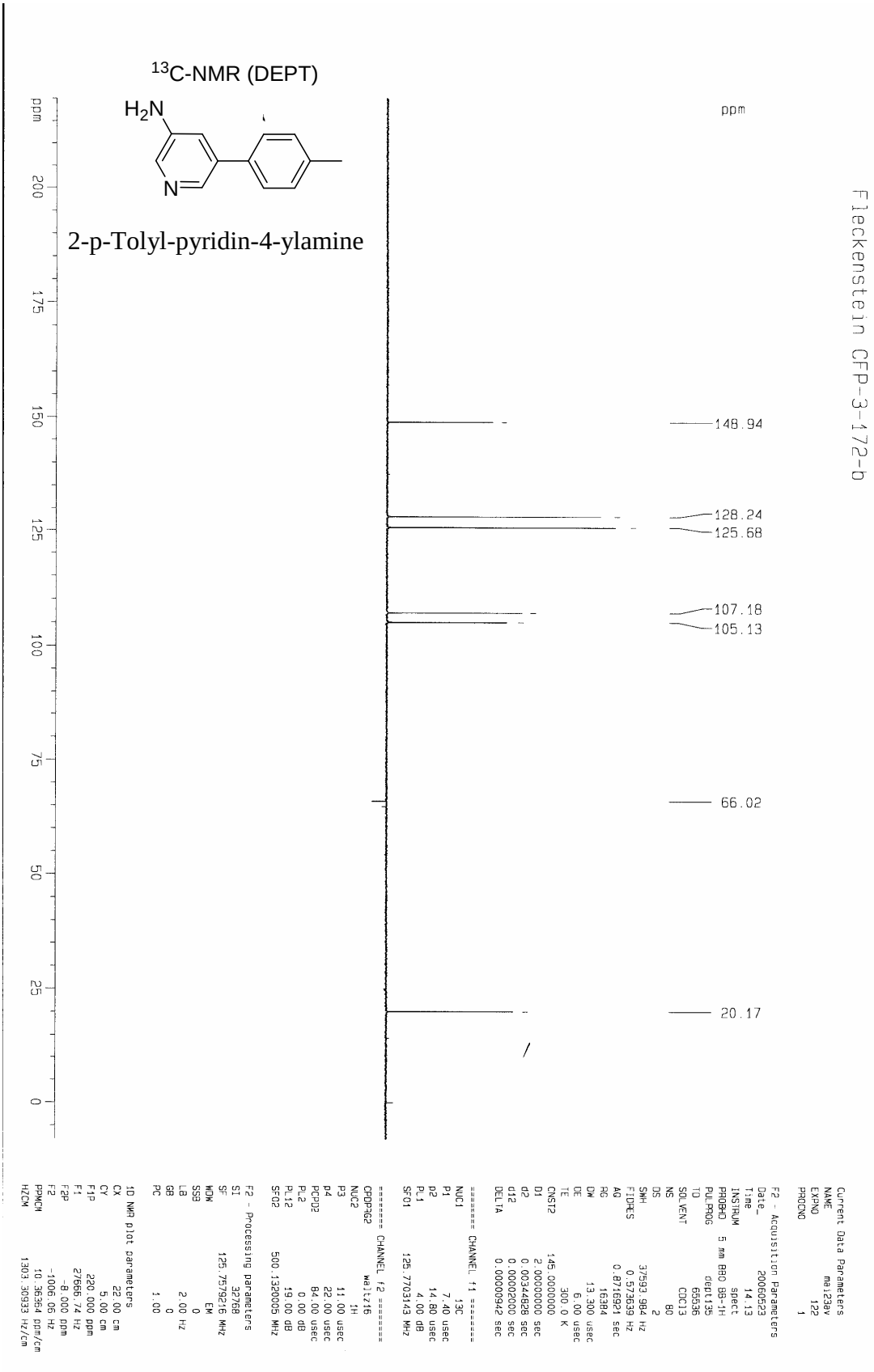


2-Methoxy-6-p-tolyl-pyridine

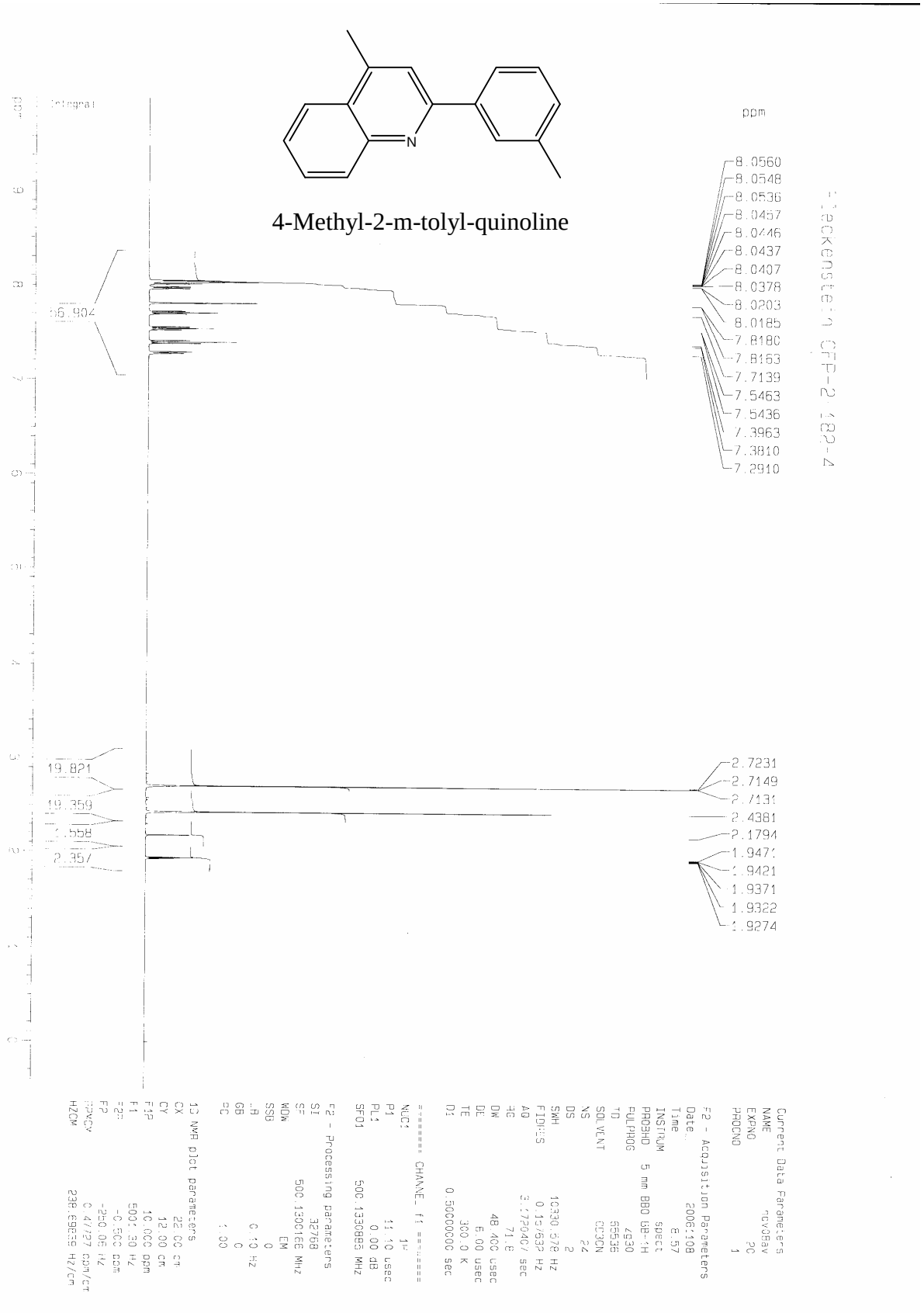

13C-NMR (DEPT)
ppm
N
MeO
2-Methoxy-6-p-tolyl-pyridine
139.49
129.72
126.99
112.81
109.21
53.55
21.67
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
CNST2
D1
d2
d12
DELTA
======== CHANNEL f1 ========
NUC1
P1
p2
PL1
SFO1
======== CHANNEL f2 ========
CPDPRG2
NUC2
P3
p4
PCPD2
PL2
PL12
SFO2
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D WNMR plot parameters
CX
CY
F1P
F2P
PPMCM


1H-NMR
H2N
N
2-p-Tolyl-pyridin-4-ylamine
Fleckenstein CFP-3-172-b
ppm
Integral
8.163
8.152
7.702
7.699
7.695
7.686
7.682
7.679
7.158
7.134
7.118
6.761
6.757
6.757
6.307
6.303
6.296
6.292
4.260
3.589
3.400
3.386
3.372
3.358
2.269
1.123
1.109
1.094
0.000
-0.087
7.203
14.089
15.629
7.597
7.166
15.568
2.071
0.695
0.450
23.508
0.226
0.763
2.614
2.420
Current Data Parameters
NAME mai23av
EXPNO 120
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060523
Time 14.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 50.8
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 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300638 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 12.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.06 Hz
PPMCM 0.47727 ppm/cm
HZCM 238.69843 Hz/cm

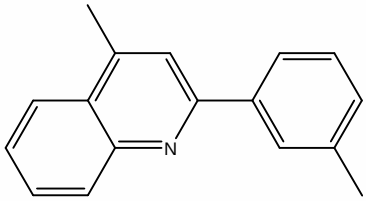

13C-NMR
H2N
N
2-p-Tolyl-pyridin-4-ylamine
Fleckenstein CFP-3-172-b
ppm
157.17
152.59
148.95
137.55
136.00
128.24
125.69
107.18
105.13
76.35
76.09
75.84
66.02
20.18
Current Data Parameters
NAME mai23av
EXPNO 121
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060523
Time 14.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8716321 sec
RG 5160.6
DW 13.300 usec
DE 6.00 usec
TE 300.0 K
D1 0.40000001 sec
D11 0.03000000 sec
D12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
PL1 4.00 dB
SF01 125.7703143 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7579209 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 27666.74 Hz
F2P -8.000 ppm
F2 -1006.06 Hz
PPMCM 10.36364 ppm/cm
HZCM 1303.30933 Hz/cm


^{13}C-NMR (DEPT)
H_2N
N
2-p-Tolyl-pyridin-4-ylamine
ppm
148.94
128.24
125.68
107.18
105.13
66.02
20.17
Fleckenstein CFP-3-172-b

^{1}H-NMR


N
4-Methyl-2-m-tolyl-quinoline
ppm
8.0560
8.0548
8.0536
8.0457
8.0446
8.0437
8.0407
8.0378
8.0203
8.0185
7.8180
7.8163
7.7139
7.5463
7.5436
7.3963
7.3810
7.2910
2.7231
2.7149
2.4381
2.1794
1.9421
1.9371
1.9322
1.9274
19.821
19.350
2.558
2.357
Integral
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM

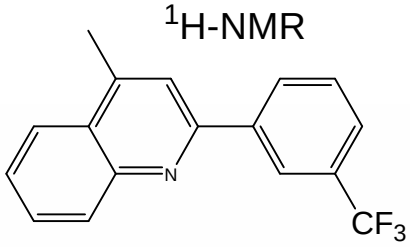
^{13}C-NMR



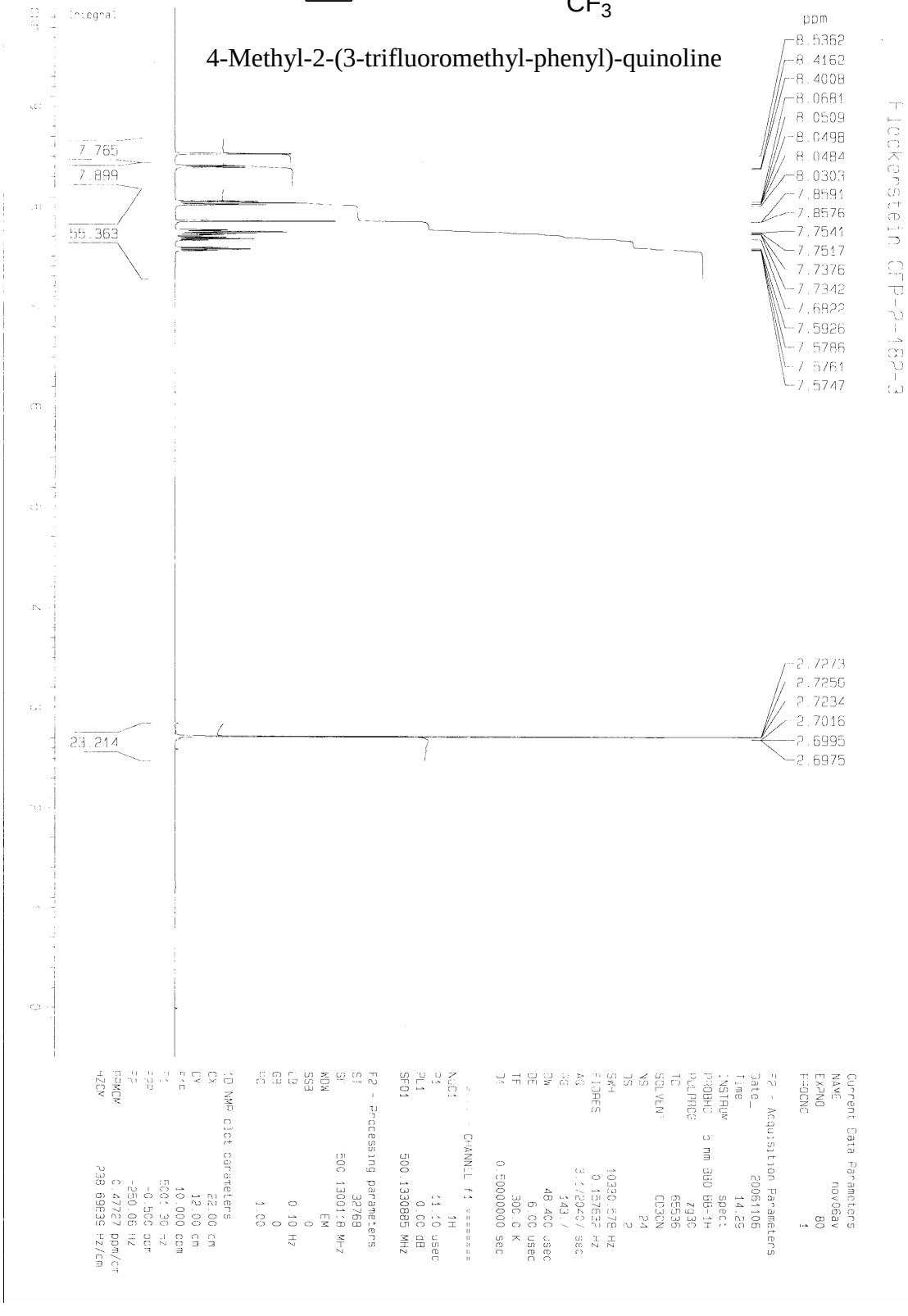
4-Methyl-2-m-tolyl-quinoline

Fleckenstein CFP-2-102.4
^{13}C-NMR (DEPT)
4-Methyl-2-m-tolyl-quinoline
ppm
129.37
129.18
128.73
128.00
127.23
125.38
123.73
123.33
118.69
19.99
17.37
200
175
150
125
100
75
50
25
0

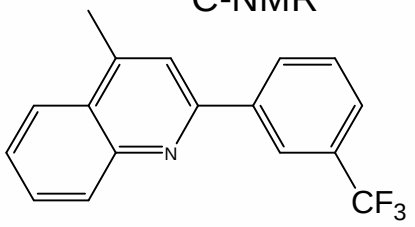
^{1}H-NMR



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

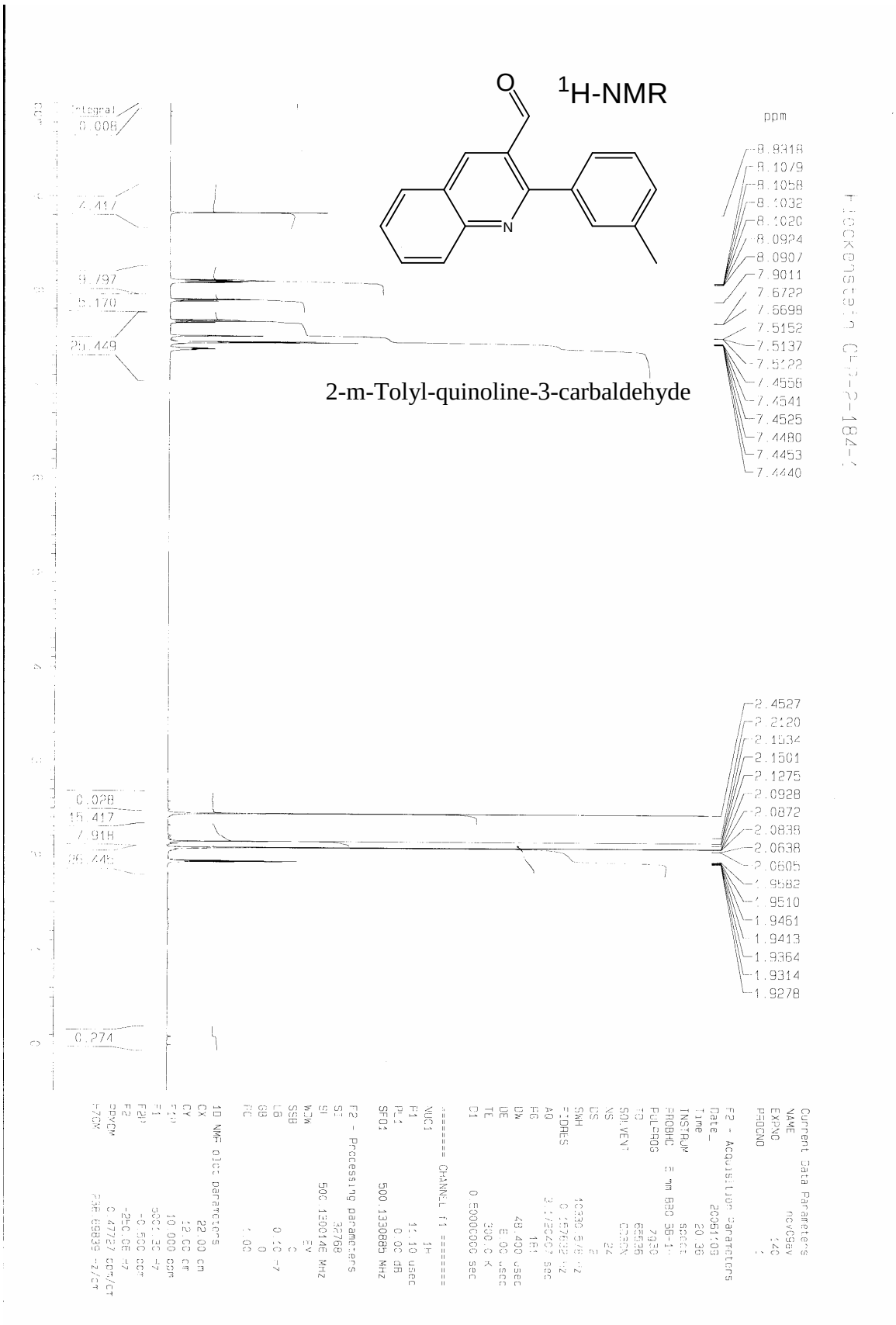


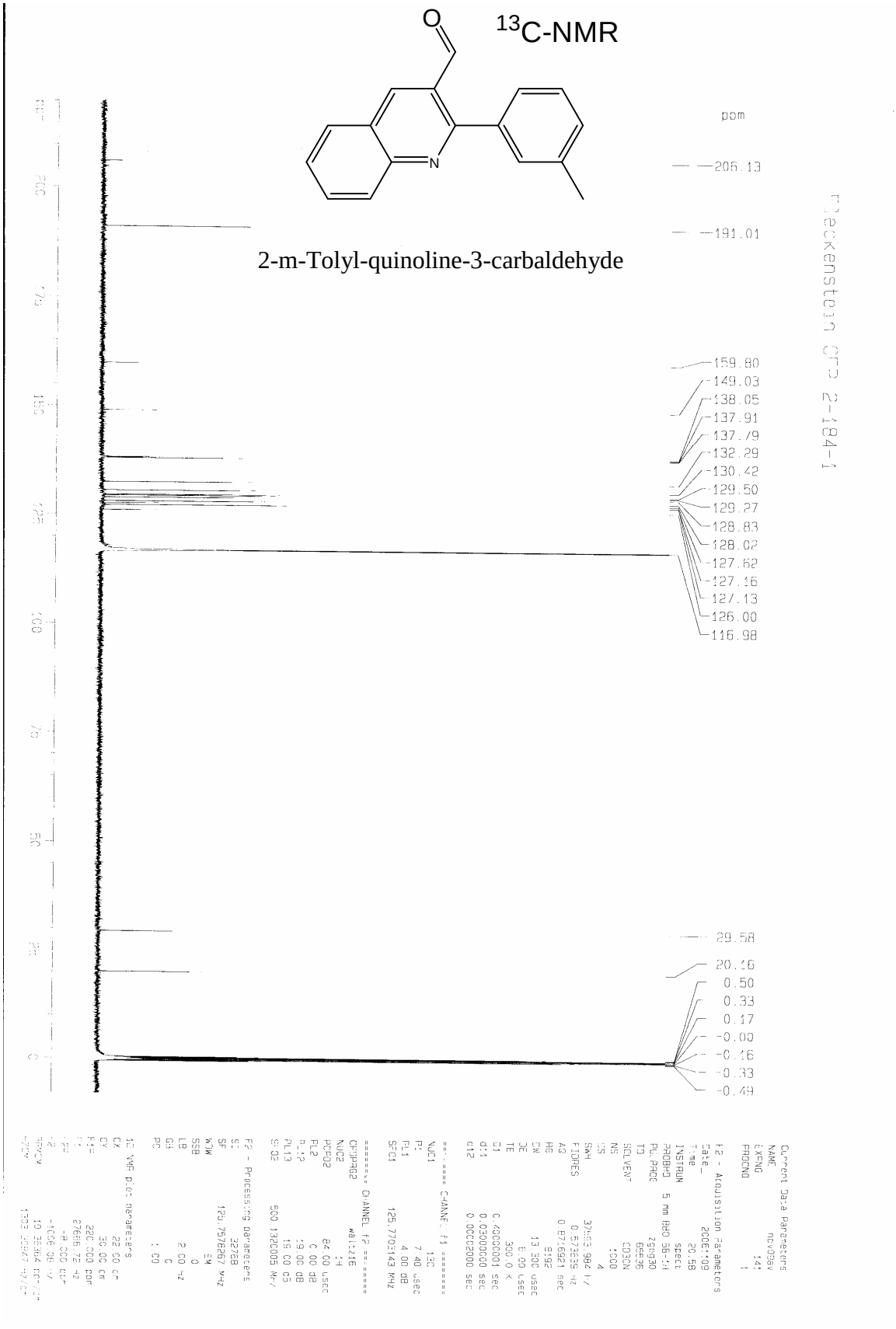
^{13}C-NMR



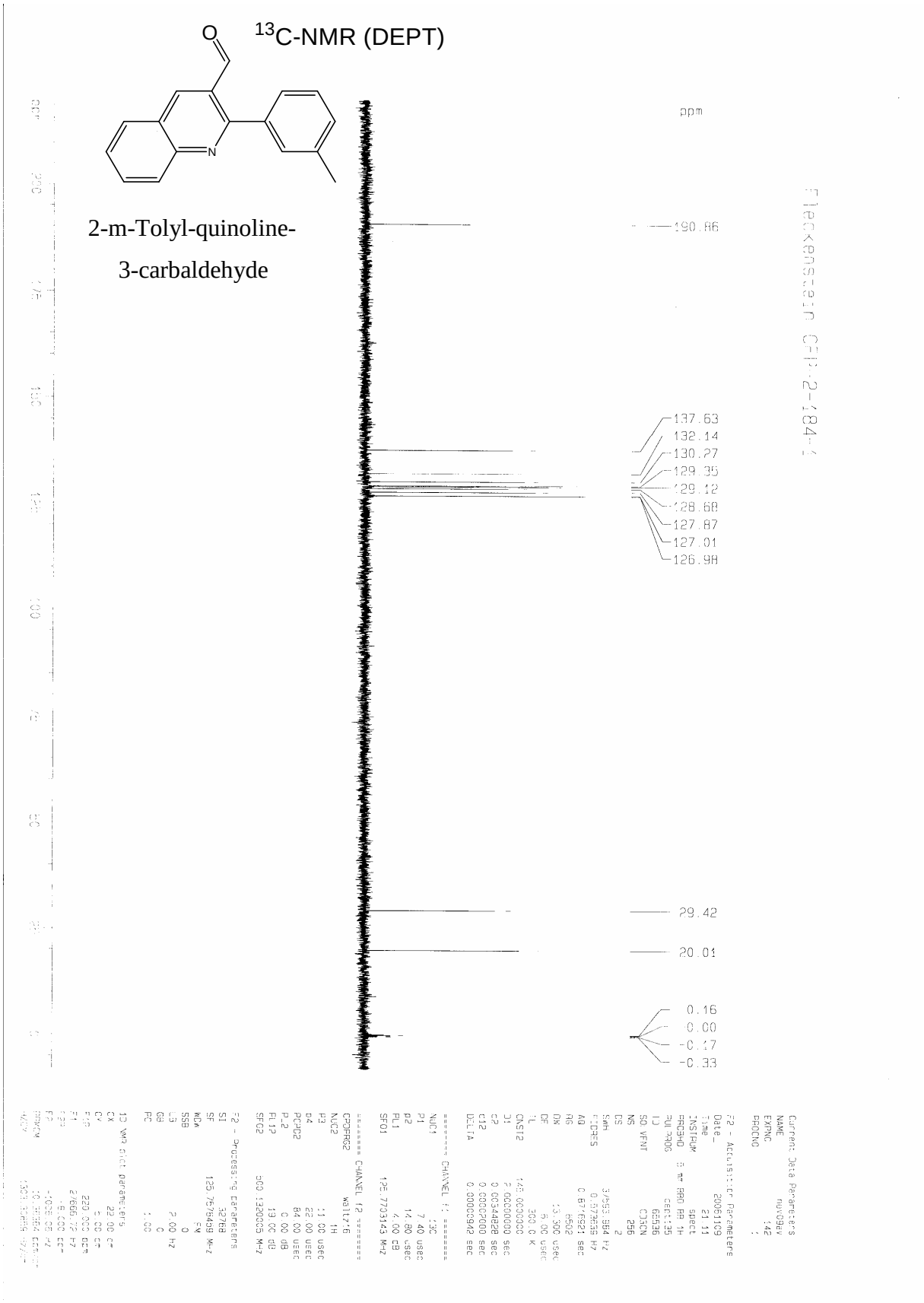
4-Methyl-2-(3-trifluoromethyl-phenyl)-quinoline

^{13}C-NMR (DEPT)
4-Methyl-2-(3-trifluoromethyl-phenyl)-quinoline
ppm
130.30
129.47
129.17
129.14
126.05
125.26
125.23
123.54
123.36
123.33
118.57
17.51

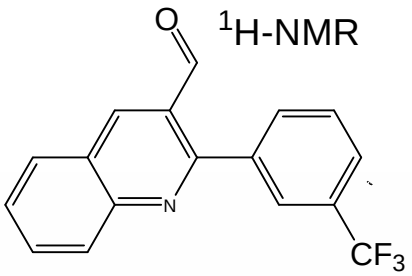

1H-NMR
2-m-Tolyl-quinoline-3-carbaldehyde
ppm



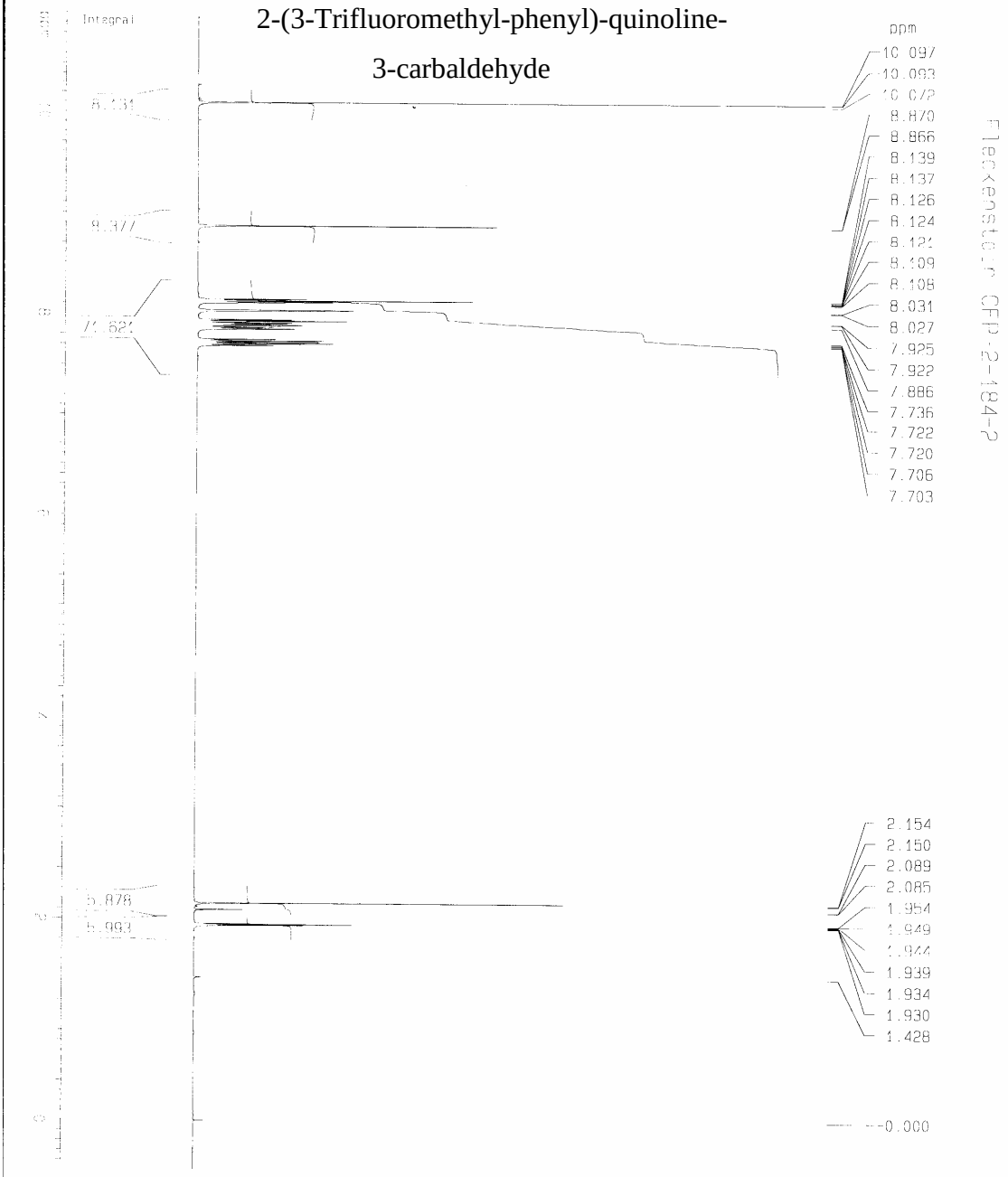
2-m-Tolyl-quinoline-3-carbaldehyde

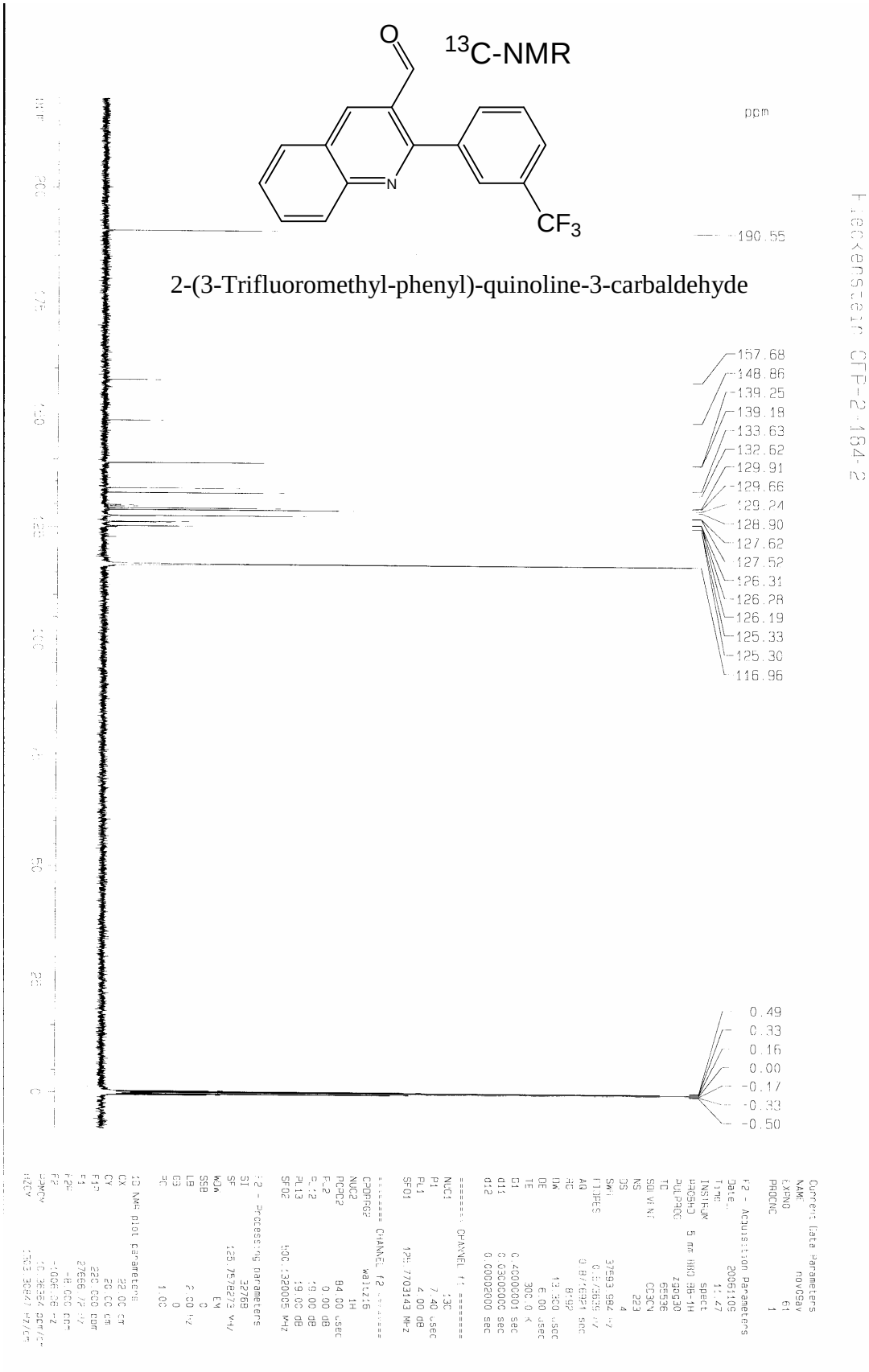

O
N
13C-NMR (DEPT)
2-m-Tolyl-quinoline-
3-carbaldehyde
ppm
190.86
137.63
132.14
130.27
129.35
129.12
128.68
127.87
127.01
126.98
29.42
20.01
0.16
0.00
-0.17
-0.33

^{1}H-NMR

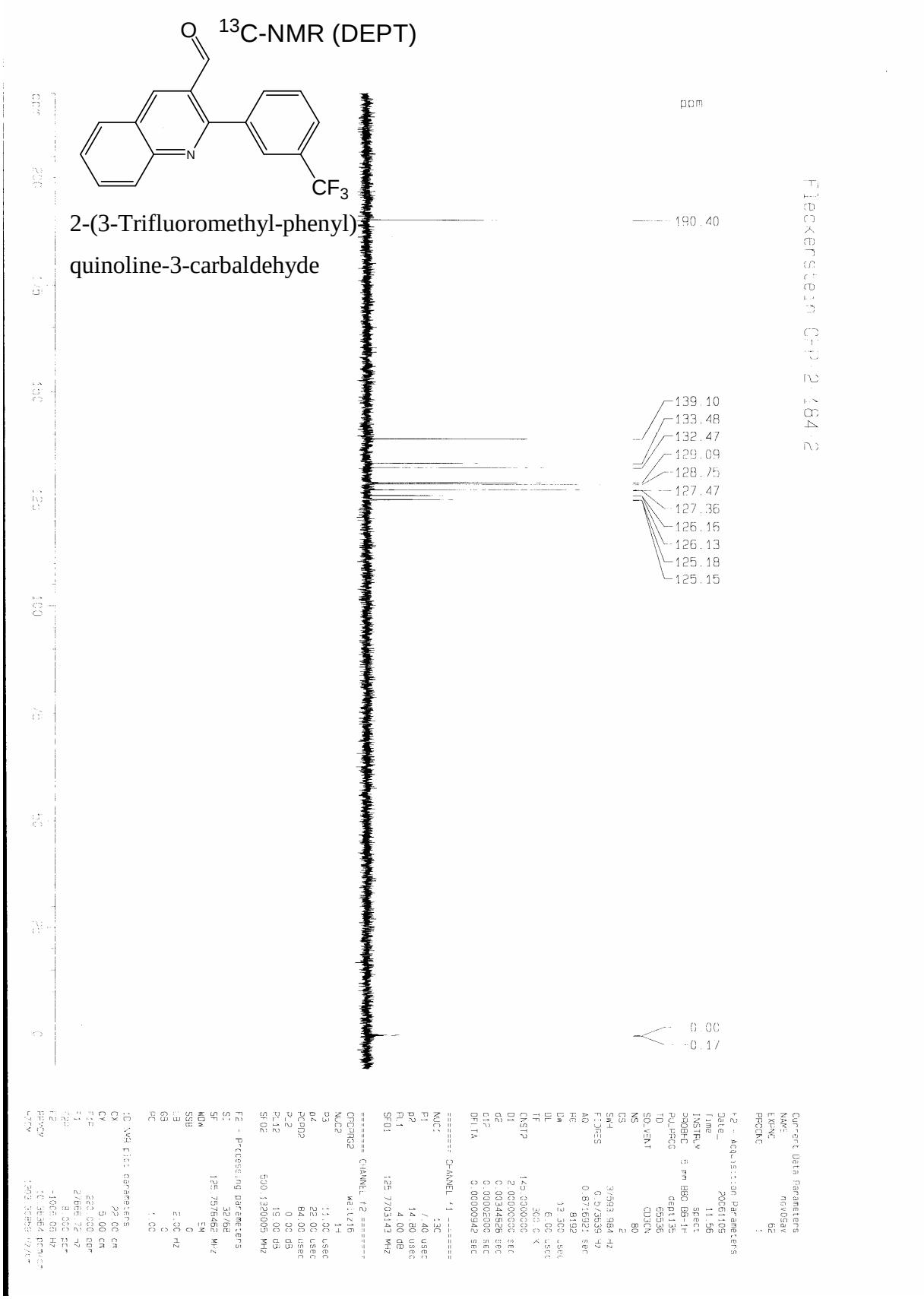


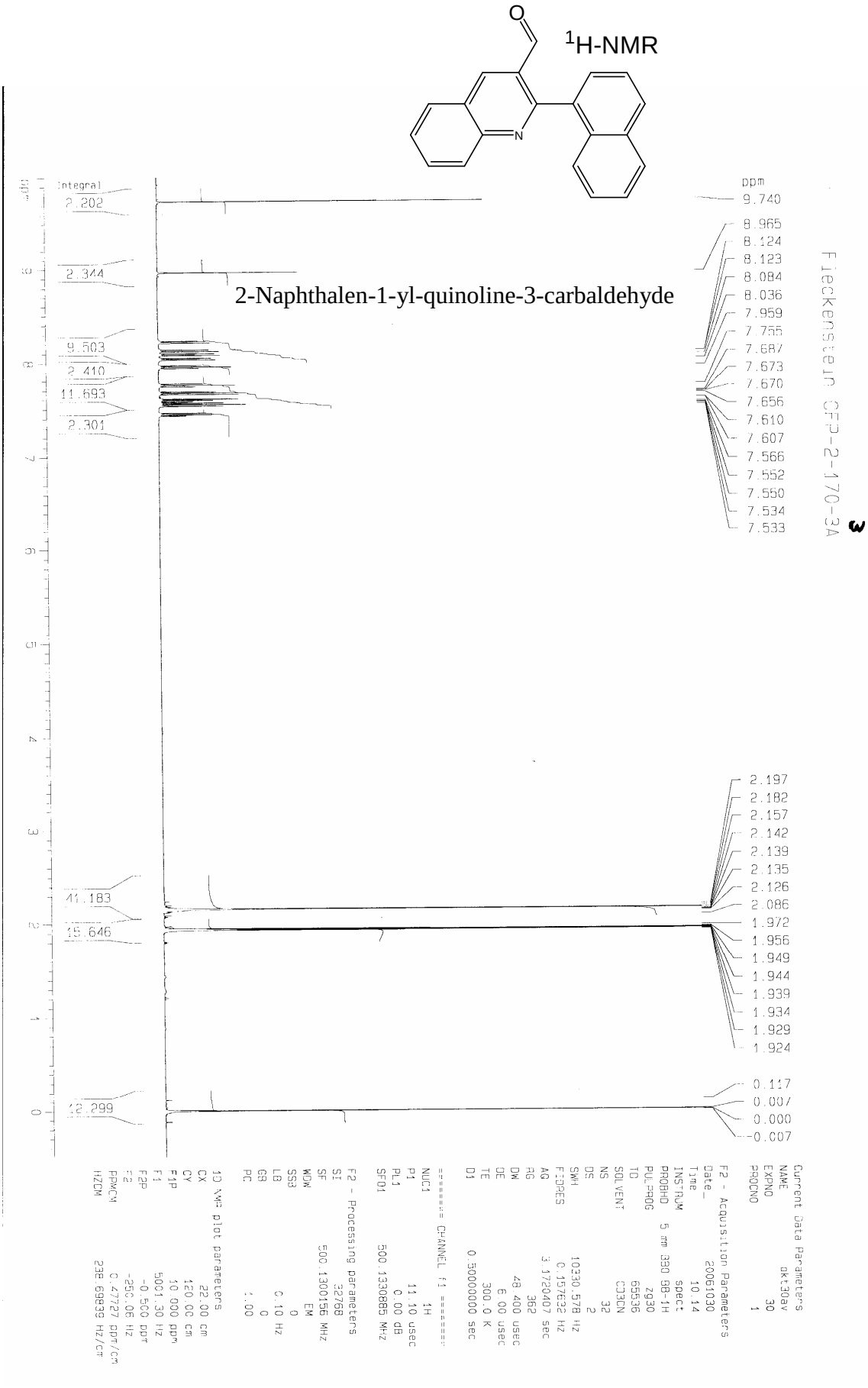
2-(3-Trifluoromethyl-phenyl)-quinoline-3-carbaldehyde

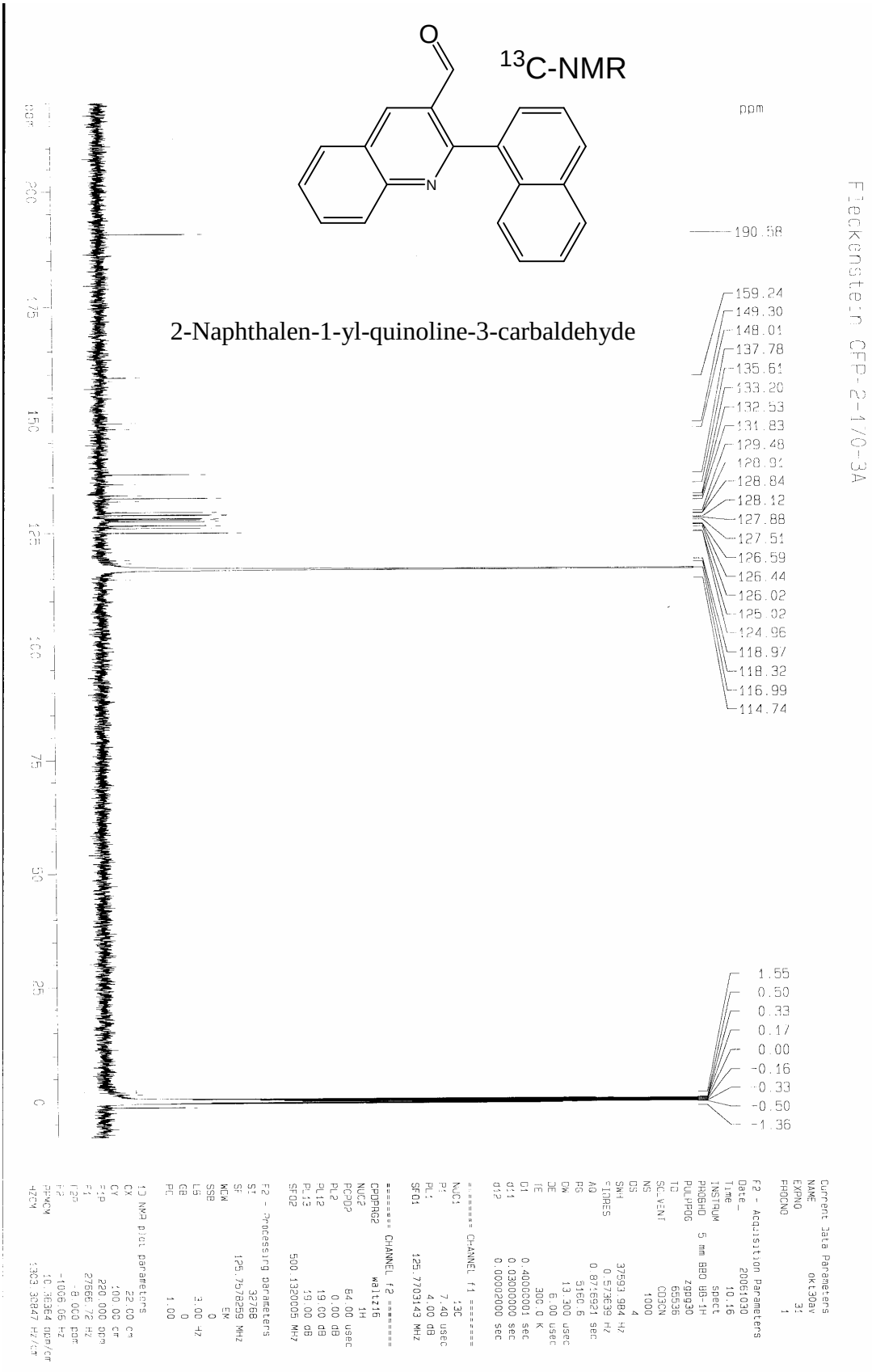


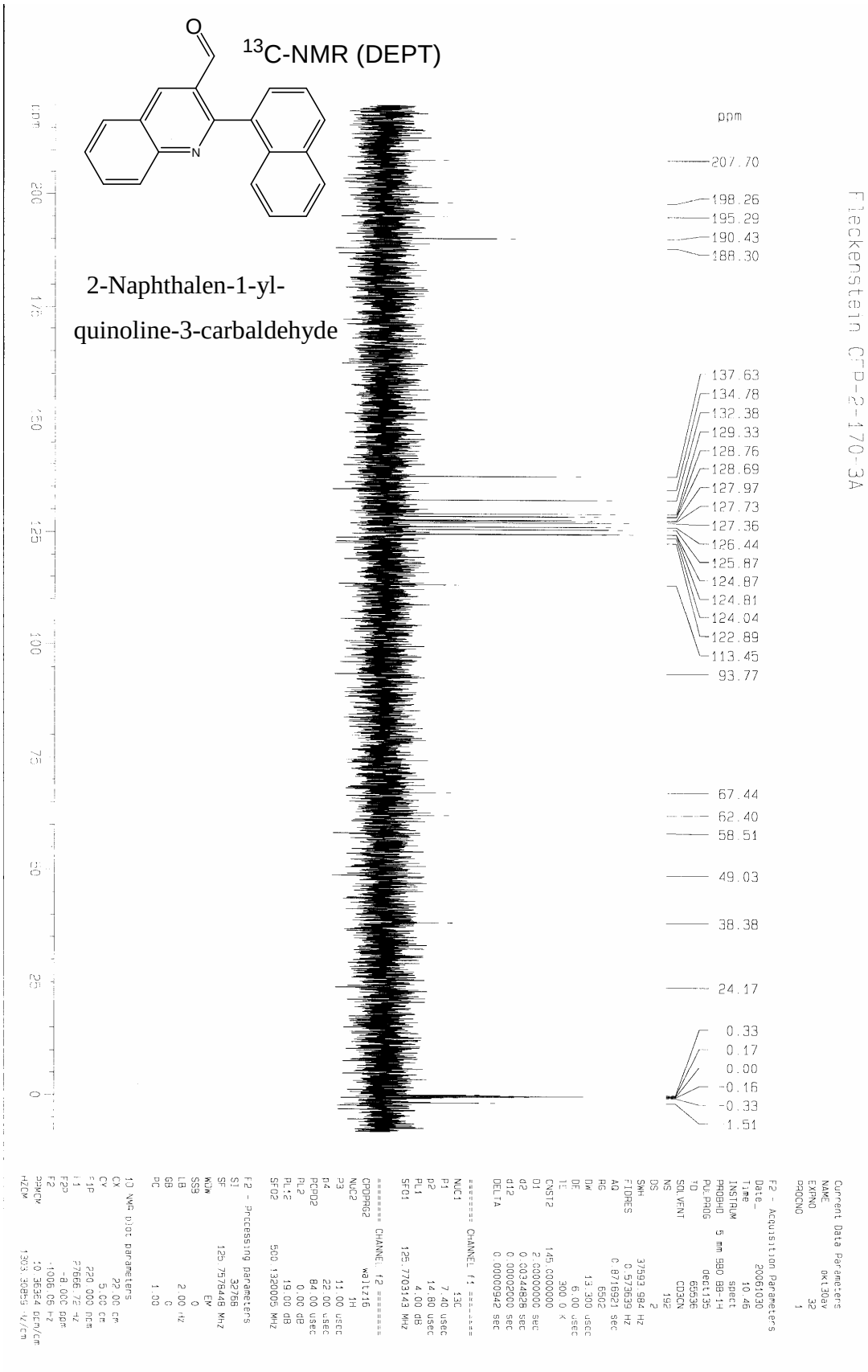


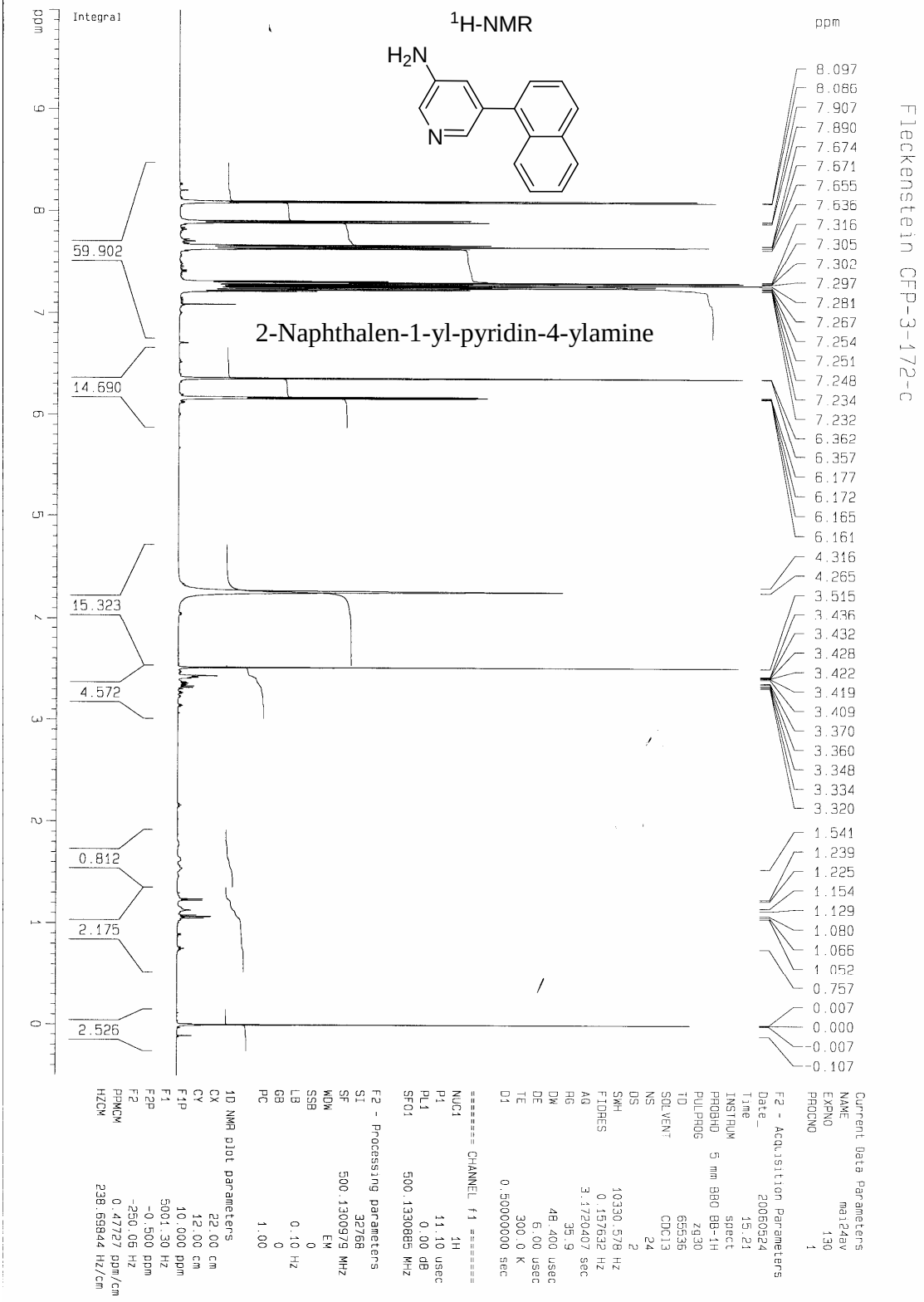
2-(3-Trifluoromethyl-phenyl)-quinoline-3-carbaldehyde


13C-NMR (DEPT)
2-(3-Trifluoromethyl-phenyl)-quinoline-3-carbaldehyde
O
N
CF3
ppm
190.40
139.10
133.48
132.47
129.09
128.75
127.47
127.36
126.16
126.13
125.18
125.15
0.00
-0.17

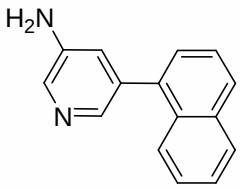

1H-NMR
2-Naphthalen-1-yl-quinoline-3-carbaldehyde
Fleckenstein CFP-2-170-3A
Integral
2.202
2.344
9.503
2.410
11.693
2.301
41.183
15.646
12.299
ppm
9.740
8.965
8.124
8.123
8.084
8.036
7.959
7.755
7.687
7.673
7.670
7.656
7.610
7.607
7.566
7.552
7.550
7.534
7.533
2.197
2.182
2.157
2.142
2.139
2.135
2.126
2.086
1.972
1.956
1.949
1.944
1.939
1.934
1.929
1.924
0.117
0.007
0.000
-0.007
Current Data Parameters
NAME okt30av
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061030
Time 10.14
INSTRUM spect
PROBHD 5 mm 330 BB-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
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300156 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 120.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.06 Hz
PPMCM 0.47727 ppm/cm
HZCM 238.69939 Hz/cm


13C-NMR
2-Naphthalen-1-yl-quinoline-3-carbaldehyde
Fleckenstein CFP-2-1/0-3A
ppm
190.58
159.24
149.30
148.01
137.78
135.61
133.20
132.53
131.83
129.48
128.91
128.84
128.12
127.88
127.51
126.59
126.44
126.02
125.02
124.96
118.97
118.32
116.99
114.74
1.55
0.50
0.33
0.17
0.00
-0.16
-0.33
-0.50
-1.36
Current Data Parameters
NAME
EXPNO
PROCNO
f2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
D11
D12
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
======== CHANNEL f2 ========
CPDPRG2
NUC2
PCPD2
PL2
PL12
PL13
SFO2
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM

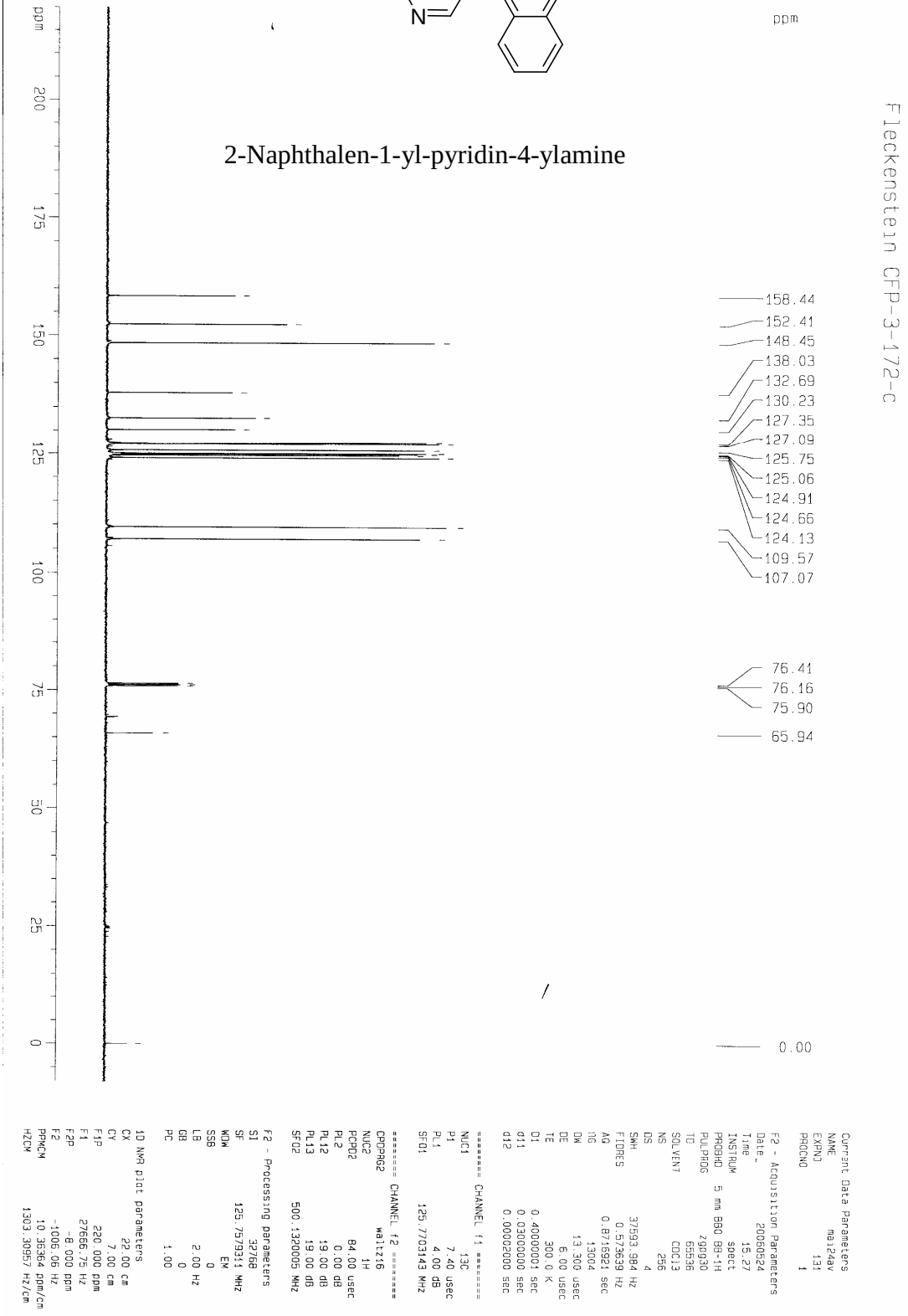

13C-NMR (DEPT)
2-Naphthalen-1-yl-
quinoline-3-carbaldehyde
Fleckenstein CTP-2-170-3A
ppm
207.70
198.26
195.29
190.43
188.30
137.63
134.78
132.38
129.33
128.76
128.69
127.97
127.73
127.36
126.44
125.87
124.87
124.81
124.04
122.89
113.45
93.77
67.44
62.40
58.51
49.03
38.38
24.17
0.33
0.17
0.00
-0.16
-0.33
-1.51


^{1}H-NMR
H_2N
N
2-Naphthalen-1-yl-pyridin-4-ylamine
Fleckenstein CFP-3-172-c
Integral
ppm
59.902
14.690
15.323
4.572
0.812
2.175
2.526
8.097
8.086
7.907
7.890
7.674
7.671
7.655
7.636
7.316
7.305
7.302
7.297
7.281
7.267
7.254
7.251
7.248
7.234
7.232
6.362
6.357
6.177
6.172
6.165
6.161
4.316
4.265
3.515
3.436
3.432
3.428
3.422
3.419
3.409
3.370
3.360
3.348
3.334
3.320
1.541
1.239
1.225
1.154
1.129
1.080
1.066
1.052
0.757
0.007
0.000
-0.007
-0.107
Current Data Parameters
NAME ma124av
EXPNO 130
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060524
Time 15.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 35.9
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 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300979 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 12.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.05 Hz
PPMCM 0.47727 ppm/cm
HZCM 238.65844 Hz/cm

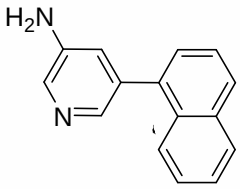
^{13}C-NMR



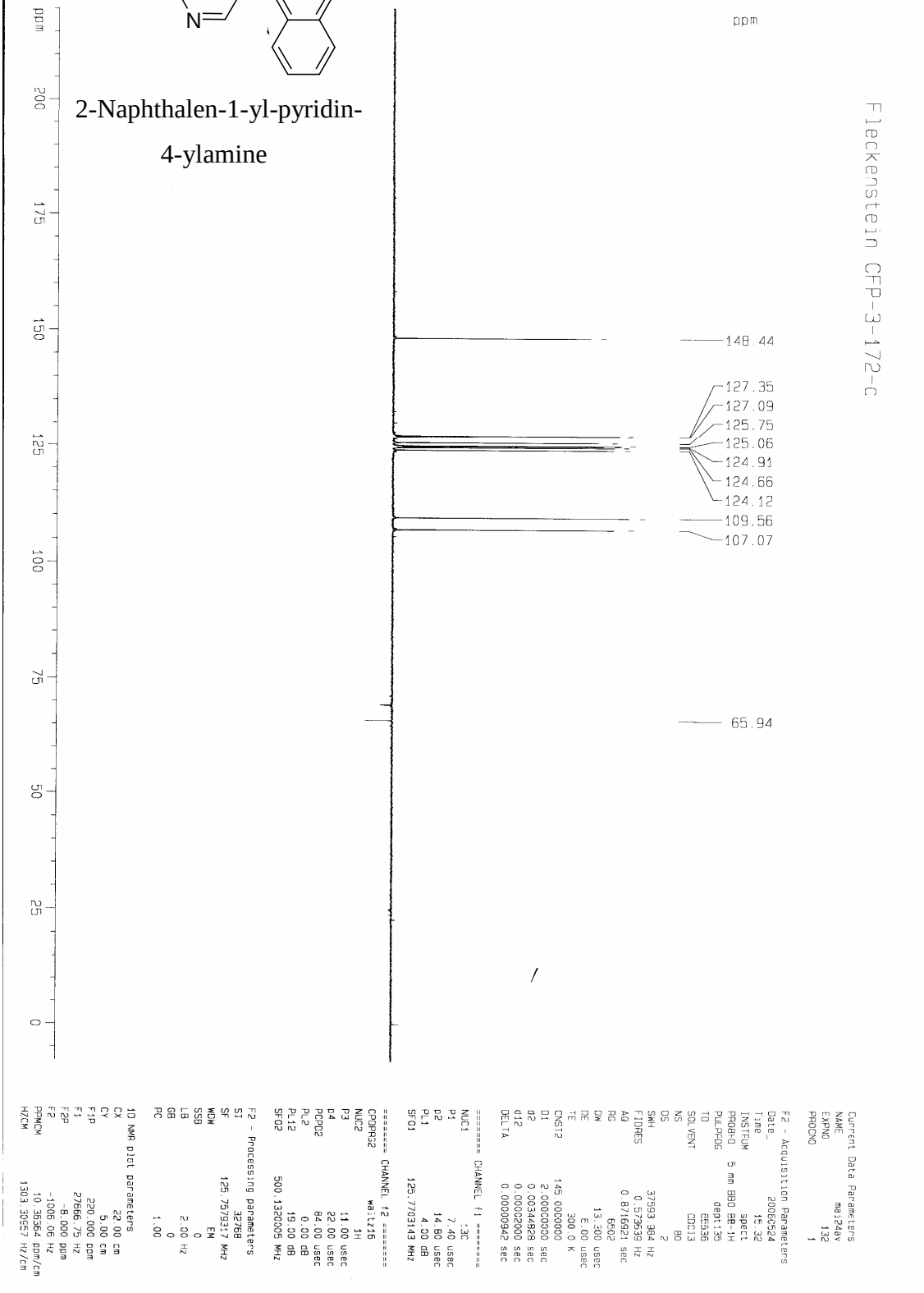
2-Naphthalen-1-yl-pyridin-4-ylamine



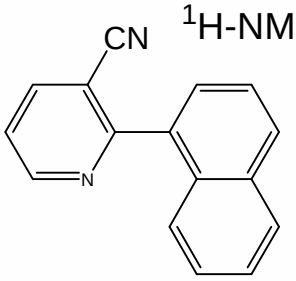
^{13}C-NMR (DEPT)



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

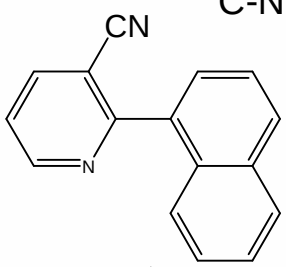


^{1}H-NMR



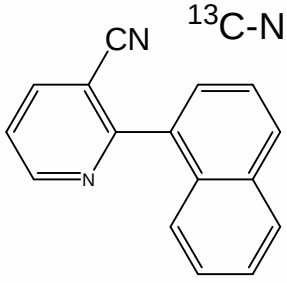
1-Naphthyl-isonicotinonitrile

^{13}C-NMR

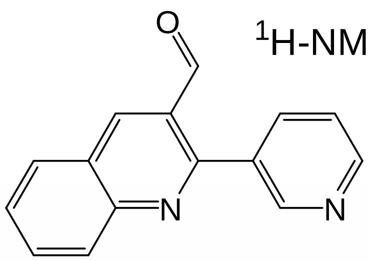


1-Naphthyl-isonicotinonitrile

^{13}C-NMR (DEPT)

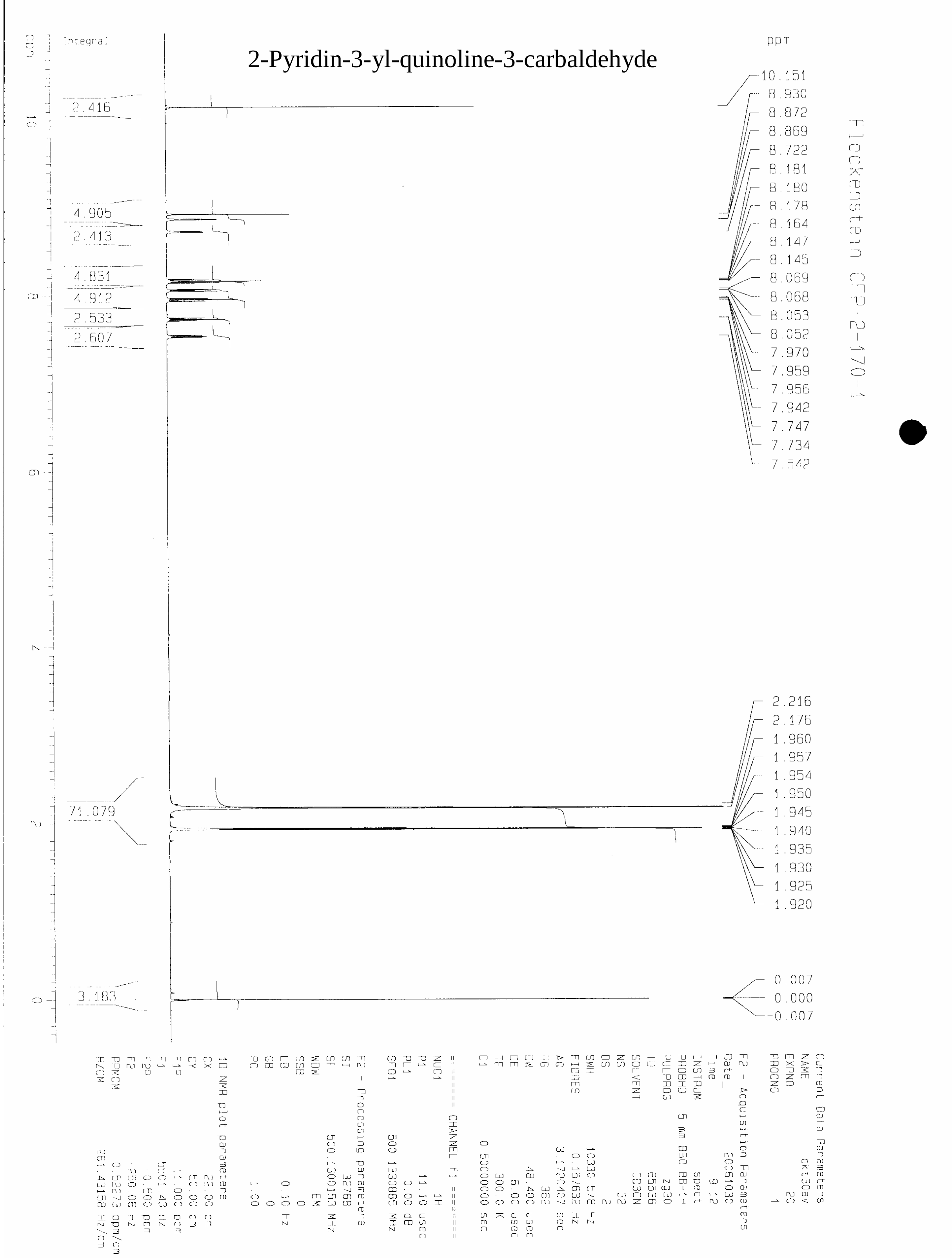


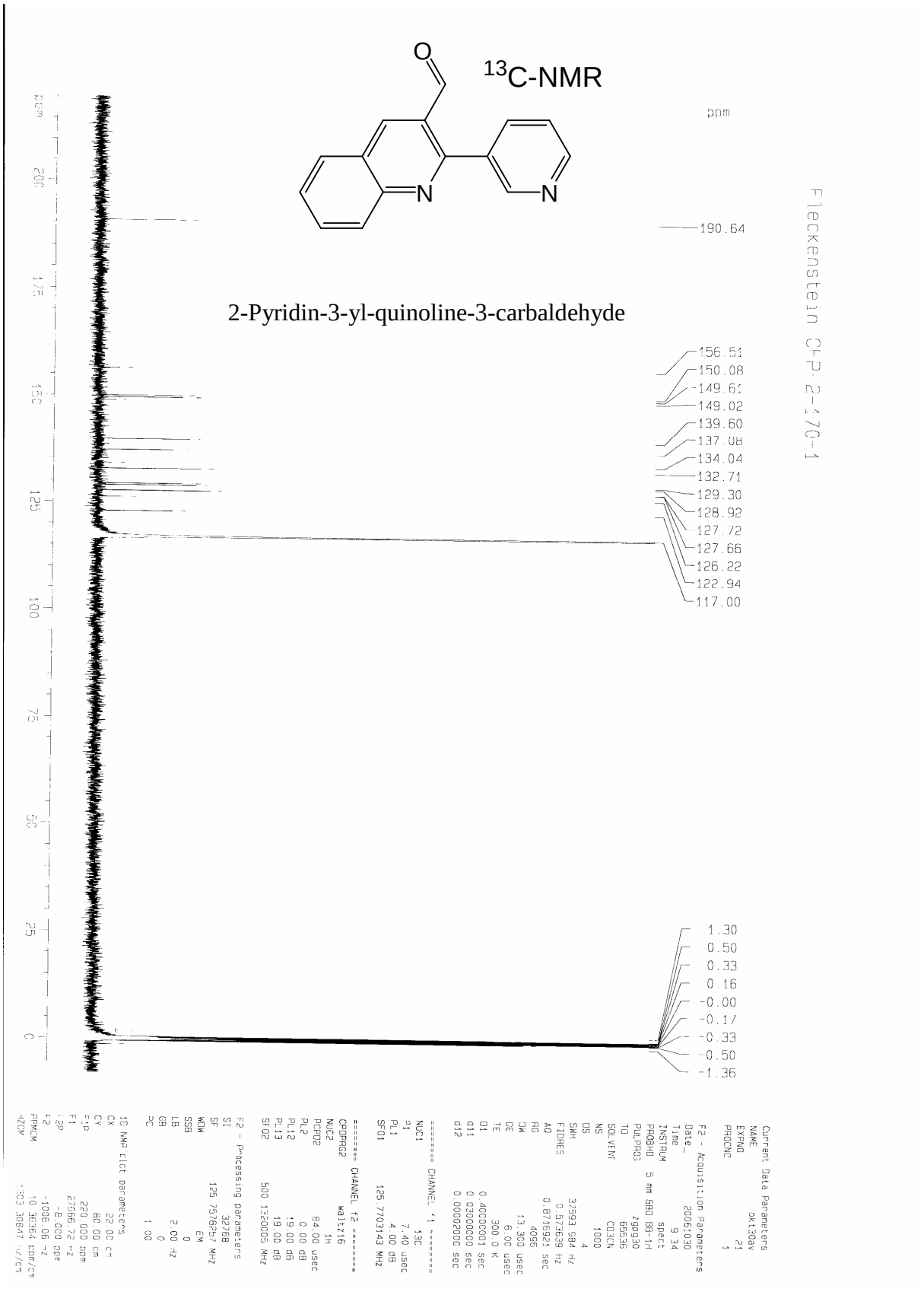
1-Naphthyl-isonicotinonitrile



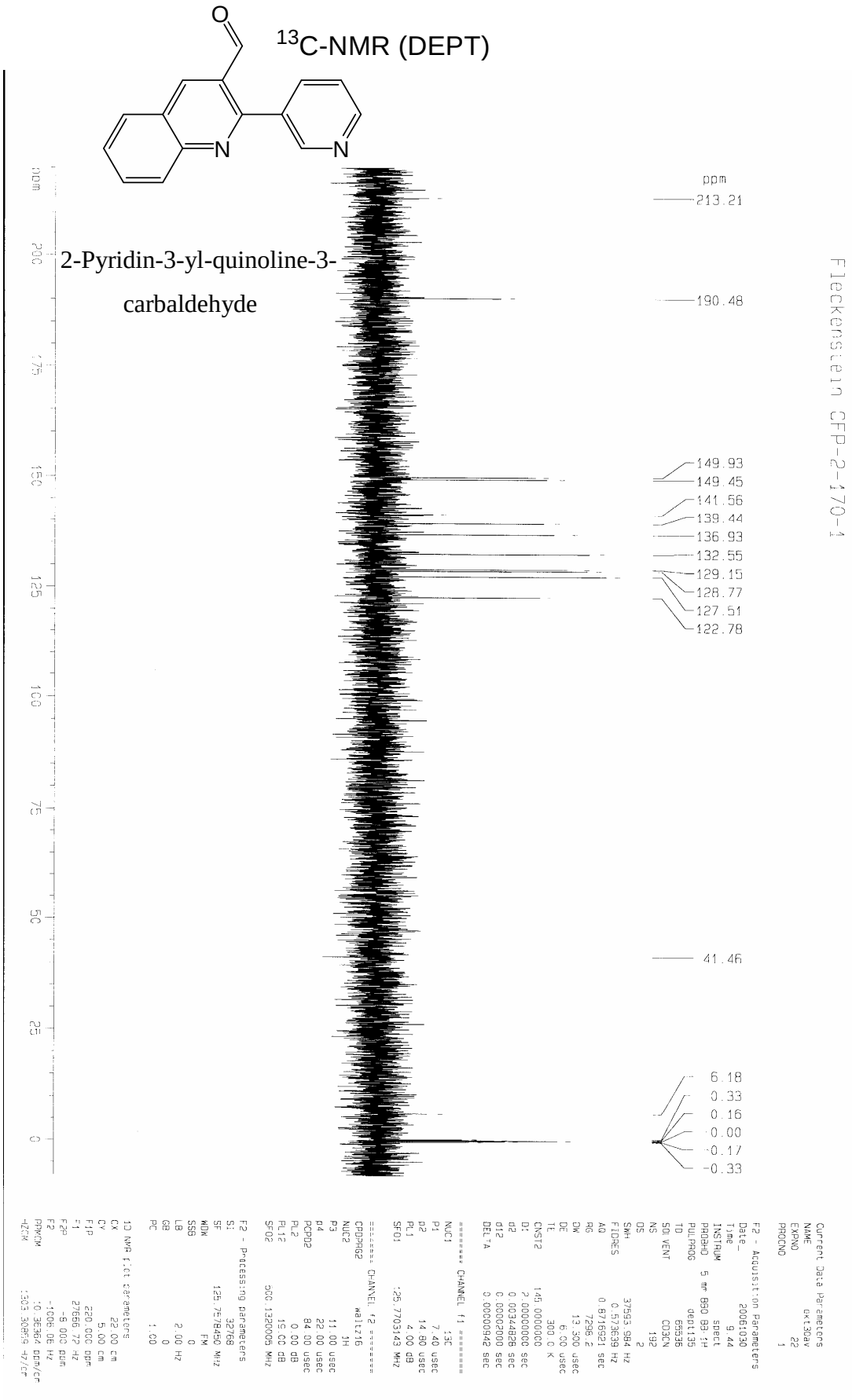
^{1}H-NMR

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

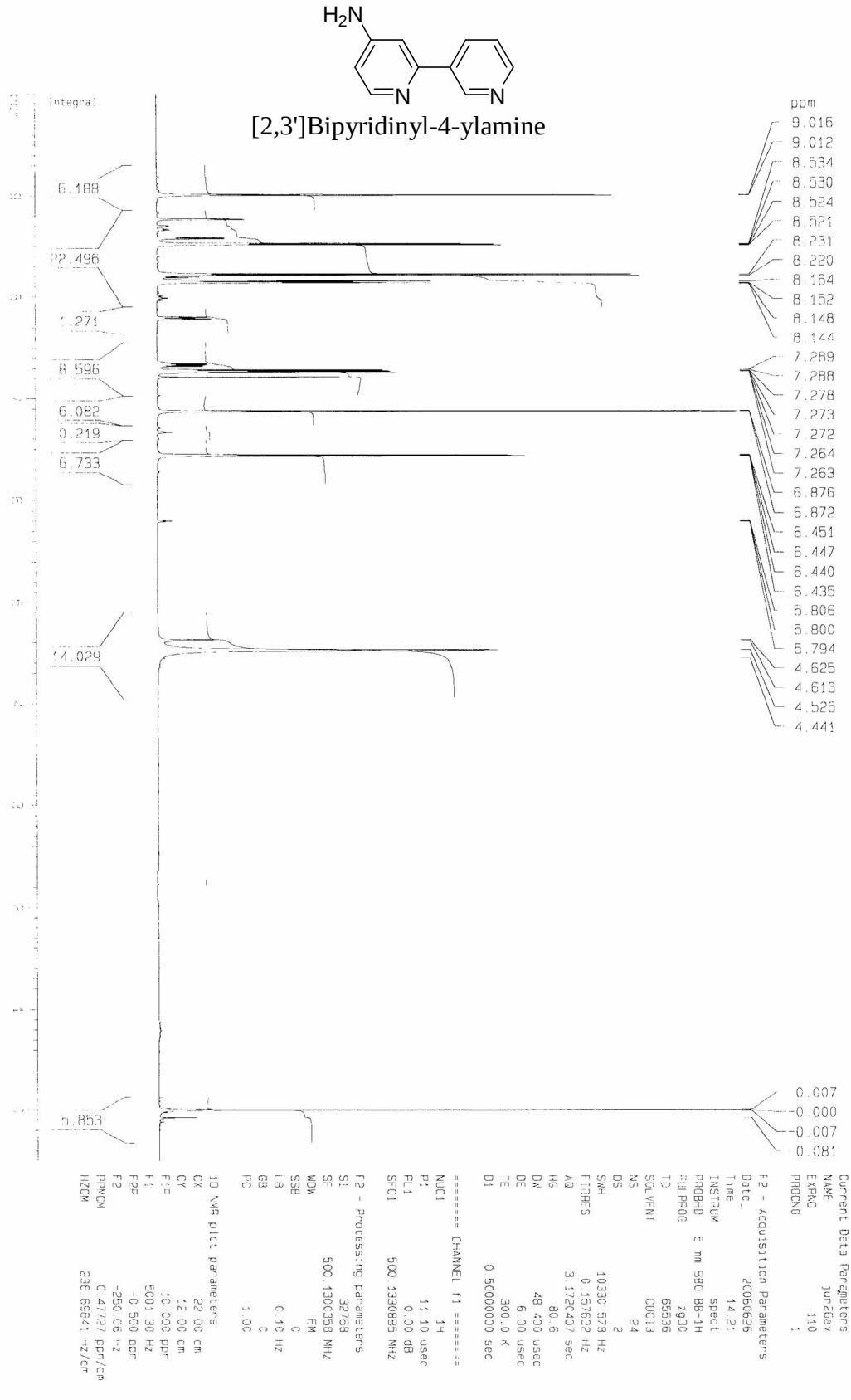




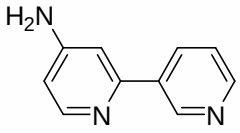
2-Pyridin-3-yl-quinoline-3-carbaldehyde


O
N
N
13C-NMR (DEPT)
2-Pyridin-3-yl-quinoline-3-carbaldehyde
ppm
213.21
190.48
149.93
149.45
141.56
139.44
136.93
132.55
129.15
128.77
127.51
122.78
41.46
6.18
0.33
0.16
0.00
-0.17
-0.33
Fleckenstein CFP-2-170-1

^{1}H-NMR

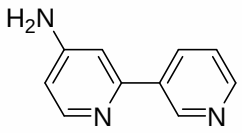

H2N
N
N
[2,3']Bipyridinyl-4-ylamine
Integral
6.188
22.496
1.271
8.596
6.082
0.219
6.733
14.029
5.853
ppm
9.016
9.012
8.534
8.530
8.524
8.521
8.231
8.220
8.164
8.152
8.148
8.144
7.289
7.288
7.278
7.273
7.272
7.264
7.263
6.876
6.872
6.451
6.447
6.440
6.435
5.806
5.800
5.794
4.625
4.613
4.526
4.441
0.007
0.000
-0.007
0.081
Flockenstein CFP-3-188-a
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F2P
PPMCM
HZCM

^{13}C-NMR



[2,3']Bipyridinyl-4-ylamine

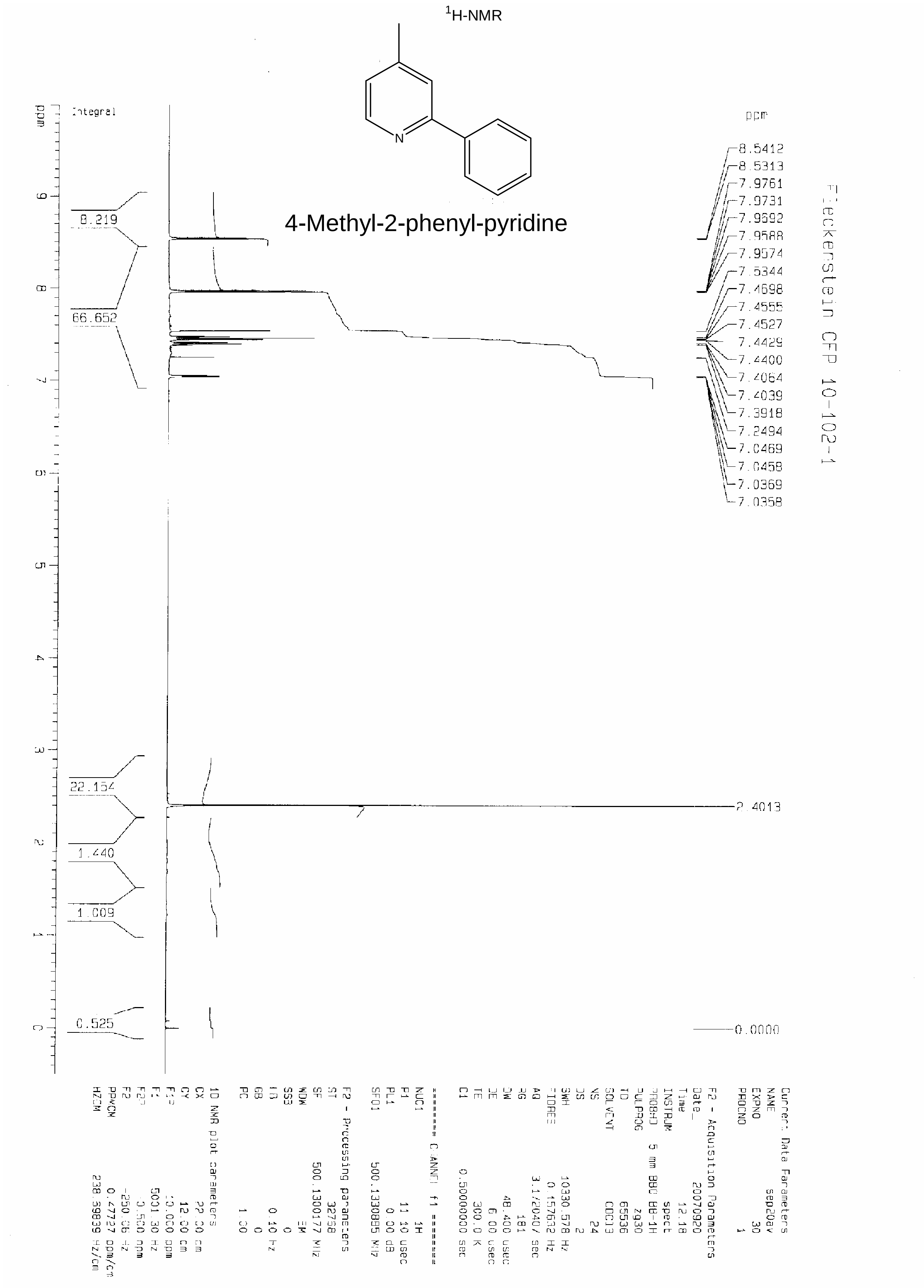
^{13}C-NMR (DEPT)



[2,3']Bipyridinyl-4-ylamine

^{1}H-NMR

4-Methyl-2-phenyl-pyridine



Software Version	: 6.3.1.0504	Date	: 19.09.2007 09:40:12
Operator	: tcprocess	Sample Name	:
Sample Number	: 001	Study	: Picolin-Kupplung
AutoSampler	: BUILT-IN	Rack/Vial	: 0/21
Instrument Name	: pancho	Channel	: A
Instrument Serial #	: None	A/D mV Range	: 1000
Delay Time	: 0,00 min	End Time	: 26,00 min
Sampling Rate	: 12,5000 pts/s		
Sample Volume	: 1,000000 ul		
Sample Amount	: 1,0000	Area Reject	: 0,000000
Data Acquisition Time	: 19.09.2007 08:24:02	Dilution Factor	: 1,00
		Cycle	: 1

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

DEFAULT REPORT

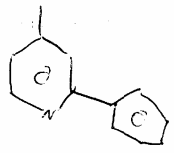
Peak #	Time [min]	Area [µV·s]	Height [µV]	Area [%]	Norm. Area [%]	BL	Area/Height [s]	
1	2,255	60687,79	31396,54	0,43	0,43	BB	1,9329	
2	2,350	49127,50	31758,62	0,35	0,35	BV	1,5469	
3	2,391	7087860,05	987876,66	50,18	50,18	VB	7,1748	
4	2,741	1448367,25	584270,78	10,25	10,25	BB	2,4789	
5	9,408	37679,85	21285,94	0,27	0,27	BB	1,7702	
6	10,717	5442084,75	985256,27	38,53	38,53	BB	5,5235	← Produkt
		14125807,20	2,64e+06	100,00	100,00			

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

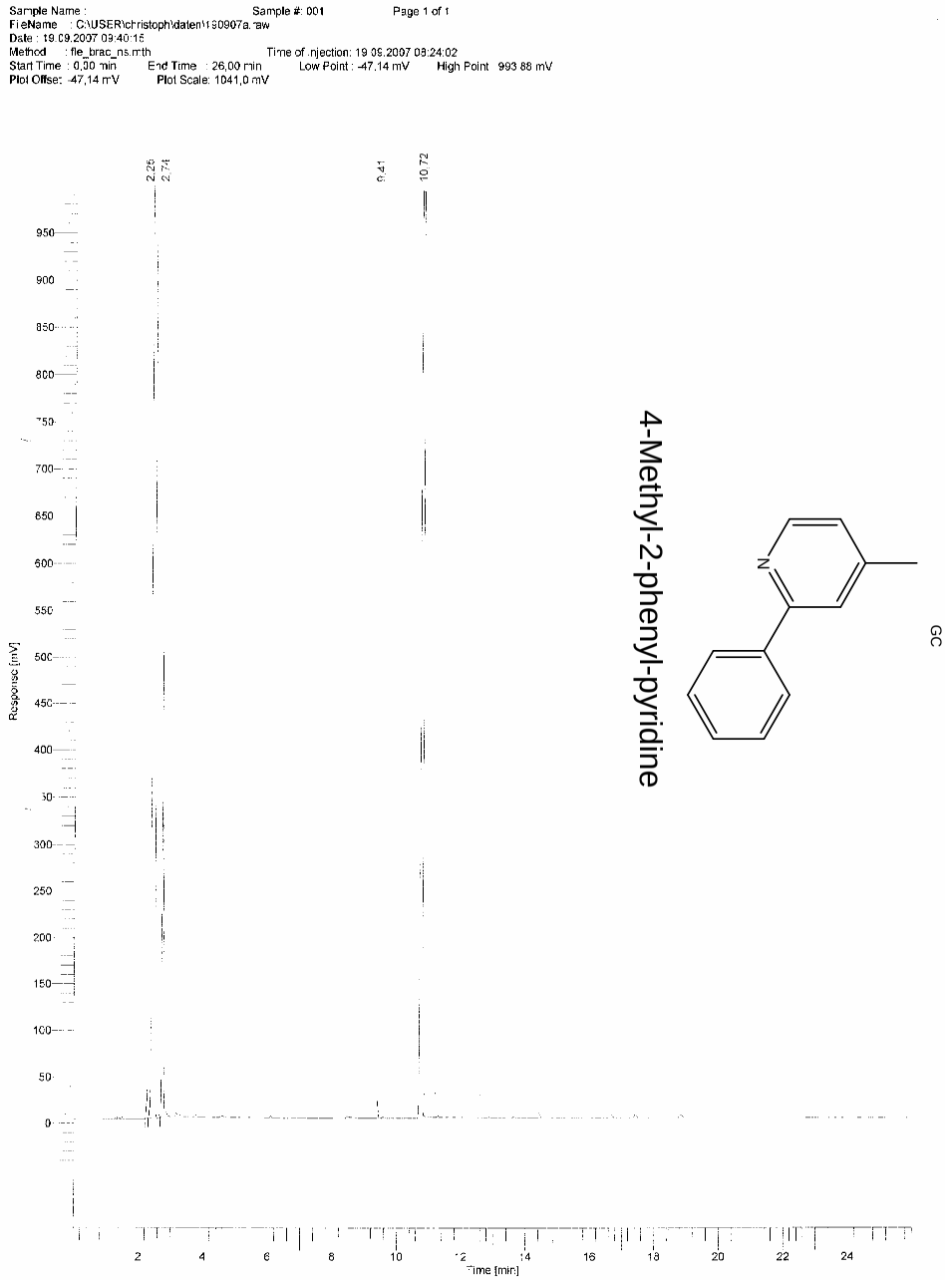
Missing Component Report
Component Expected Retention (Calibration File)

All components were found

CFP-10-101-1



Chromatogram



4-Methyl-2-phenyl-pyridine

GC