Electronic Supplementary Information

Halonium-initiated electrophilic cascades of 1-alkenoylcyclopropanecarboxamides: efficient access to dihydrofuropyridinones and 3(2*H*)-furanones

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I. General

All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. The products were purified by column chromatography over silica gel. ^{1}H NMR and ^{13}C NMR spectra were recorded at 25 ºC on a Varian 500 MHz and 125 MHz, respectively, and TMS as internal standard. Elemental analyses were measured on an E-2400 analyzer (Perkin-Elmer). Mass spectra were recorded on Agilient 1100 LCMsD mass spectrometer.

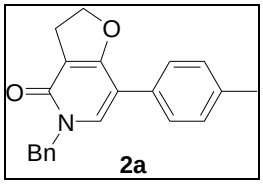
II. Substrates preparation

For the preparation of 1-acetylcyclopropanecarboxamides and 1-alkenoyl-*N*-alkylcyclopropanecarboxamides (**1**), see: a) Z. Zhang, Q. Zhang, S. Sun, T. Xiong, Q. Liu, *Angew. Chem. Int. Ed.* **2007**, *46*, 1726–1729; b) W. Pan, D. W. Dong, K. W. Wang, J. Zhang, W. Rigenhada, D. X. Xiang, Q. Liu, *Org. Lett.* **2007**, *9*, 2421–2423; c) L. Zhao, F. Liang, X. Bi, S. Sun, Q. Liu, *J. Org. Chem.* **2006**, *71*, 1094–1098; d) Y. Li, X. Xu, J. Tan, P. Liao, J. Zhang, Qun Liu, *Org. Lett.* **2010**, *12*, 244–247.

III. Synthesis and analytical data of 2.

General procedure for the preparation of **2** (**2a** as an example): To a solution of 1-alkenoyl-*N*-benzylcyclopropanecarboxamide **1a** (319 mg, 1.0 mmol) in MeCN (2 mL) was added NBS (213 mg, 1.2 mmol) and HCO_2H (0.045 mL, 1.2 mmol). The mixture was stirred at reflux for 8 h. After the starting material **1a** was consumed as indicated by TLC, the reaction mixture was cooled to room temperature and poured into water and then extracted with CH_2Cl_2 (3 × 10 mL). The combined organic phase was washed with water (3 × 10 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by flash chromatography (silica gel, ether : petroleum ether = 3 : 1) to give **2a** (256 mg, 81%) as a white solid.

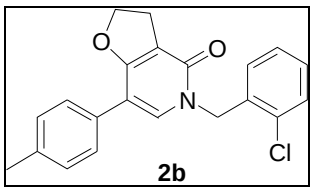
5-Benzyl-7-*p*-tolyl-2,3-dihydrofuro[3,2-*c*]pyridin-4(5*H*)-one (2a)



2a

White solid. m.p. 195-197 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.34 (s, 3H), 3.17-3.20 (t, *J* = 9.5 Hz, 2H), 4.68-4.72 (t, *J* = 9.5 Hz, 2H), 5.18 (s, 2H), 7.16-7.33 (m, 10H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.1, 27.1, 51.3, 73.3, 109.5, 110.7, 127.3, 127.8, 128.0, 128.8, 129.3, 130.0, 136.1, 136.8, 137.3, 160.3, 165.7. MS calcd *m/z* 317.1, found 318.1 $[(M + 1)]^+$. Anal. Calcd for $C_{21}H_{19}NO_2$: C, 79.47; H, 6.03; N, 4.41; Found: C, 79.35; H, 6.02; N, 4.42.

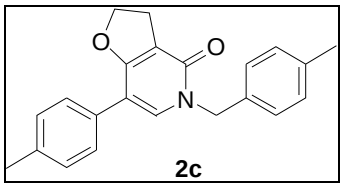
5-(2-Chloro-benzyl)-7-*p*-tolyl-3,5-dihydro-2*H*-furo[3,2-*c*]pyridin-4-one (2b)



2b

White solid. m.p. 217-219 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.35 (s, 3H), 3.19-3.22 (t, *J* = 9.5 Hz, 2H), 4.71-4.75 (t, *J* = 9.5 Hz, 2H), 5.32 (s, 2H), 7.17-7.40 (m, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.1, 27.0, 49.0, 73.4, 109.6, 111.1, 127.3, 127.4, 129.2, 129.3, 129.6, 129.9, 130.3, 133.3, 134.1, 136.5, 137.4, 160.5, 166.2. MS calcd *m/z* 351.1, found 352.1 $[(M + 1)]^+$. Anal. Calcd for $C_{21}H_{18}ClNO_2$: C, 71.69; H, 5.16; N, 3.98; Found: C, 71.83; H, 5.15; N, 3.97.

5-(4-Methyl-benzyl)-7-*p*-tolyl-3,5-dihydro-2*H*-furo[3,2-*c*]pyridin-4-one (2c)

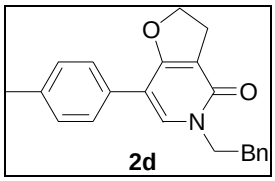


2c

White solid. m.p. 213-215 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.31-2.32 (d, *J* = 3.5 Hz, 3H), 2.34 (s, 3H), 3.17-3.21 (t, *J* = 9.5 Hz, 2H), 4.69-4.73 (t, *J* = 9.5 Hz, 2H), 5.15 (s, 2H), 7.13-7.32 (m, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.0, 27.0, 51.2, 73.4, 109.7, 111.1, 127.4, 128.1, 129.2, 129.5, 129.9, 133.5, 136.1, 137.4, 137.7, 160.5,

166.0. MS calcd *m/z* 331.4, found 332.4 $[(M + 1)]^+$. Anal. Calcd for $C_{22}H_{21}NO_2$: C, 79.73; H, 6.39; N, 4.23; Found: C, 79.80; H, 6.38; N, 4.24.

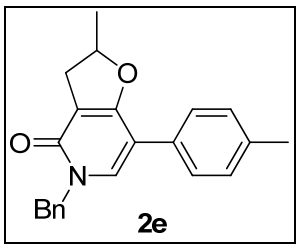
5-Phenethyl-7-phenyl-3,5-dihydro-2*H*-furo[3,2-*c*]pyridin-4-one (2d)



2d

White solid. m.p. 207-209 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.33 (s, 3H), 3.08-3.05 (t, *J* = 6.5 Hz, 2H), 3.19-3.22 (t, *J* = 9.5 Hz, 2H), 4.19-4.22 (t, *J* = 6.5 Hz, 2H), 4.70-4.73 (t, *J* = 9.5 Hz, 2H), 7.08-7.32 (m, 10H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.0, 26.9, 35.5, 51.4, 73.4, 109.6, 110.2, 126.7, 127.3, 128.7, 129.1, 129.1, 129.8, 137.0, 137.2, 38.0, 160.3, 166.2. MS calcd *m/z* 331.1, found 332.1 $[(M + 1)]^+$. Anal. Calcd for $C_{22}H_{21}NO_2$: C, 79.73; H, 6.39; N, 4.23; Found: C, 79.88; H, 6.38; N, 4.22.

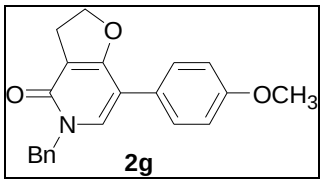
5-Benzyl-2-methyl-7-*p*-tolyl-3,5-dihydro-2*H*-furo[3,2-*c*]pyridin-4-one (2e)



2e

White solid. m.p. 197-199 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.34 (s, 3H), 2.76-2.80 (m, 1H), 3.28-3.33 (m, 1H), 5.08-5.10 (m, 1H), 4.70-4.73 (d, *J* = 1.5 Hz, 2H), 7.16-7.33 (m, 10H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.1, 22.0, 34.2, 51.4, 82.5, 109.3, 111.0, 127.4, 127.9, 128.0, 128.8, 129.2, 130.1, 136.1, 136.8, 137.3, 160.5, 165.1. MS calcd *m/z* 331.1, found 332.1 $[(M + 1)]^+$. Anal. Calcd for $C_{22}H_{21}NO_2$: C, 79.73; H, 6.39; N, 4.23; Found: C, 79.61; H, 6.40; N, 4.24.

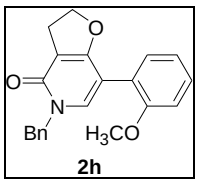
5-Benzyl-7-(4-methoxyphenyl)-2,3-dihydrofuro[3,2-*c*]pyridin-4(5*H*)-one (2g)



2g

White solid. m.p. 199-201 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.17-3.21 (t, *J* = 9.5 Hz, 2H), 3.80 (s, 3H), 4.70-4.73 (t, *J* = 9.5 Hz, 2H), 5.19 (s, 2H), 6.89-6.91 (t, *J* = 6.0 Hz, 2H), 7.27-7.36 (m, 8H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 27.0, 51.1, 55.1, 73.2, 109.3, 110.2, 113.8, 125.2, 127.4, 127.7, 127.8, 128.6, 135.6, 136.8, 158.8, 160.0, 165.5. MS calcd *m/z* 333.1, found 334.1 $[(M + 1)]^{+}$. Anal. Calcd for $C_{21}H_{19}NO_3$: C, 75.66; H, 5.74,; N, 4.20; Found: C, 75.55; H, 5.75; N, 4.21.

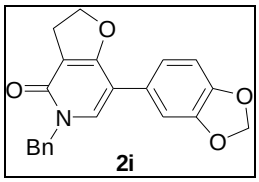
5-Benzyl-7-(2-methoxy-phenyl)-3,5-dihydro-2*H*-furo[3,2-*c*]pyridin-4-one (2h)



2h

White solid. m.p. 191-193ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.17-3.21 (t, *J* = 9.5 Hz, 2H), 3.73 (s, 3H), 4.65-4.70 (m, 2H), 5.17-5.18 (d, *J* = 2.5 Hz, 2H), 6.91-6.98 (m, 2H), 7.25-7.50 (m, 8H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 27.2, 51.3, 55.5, 73.4, 109.1, 111.3, 120.5, 121.6, 127.8, 127.9, 128.2, 128.2, 128.7, 128.8, 129.2, 138.6, 156.6, 160.4, 166.4. MS calcd *m/z* 333.1, found 334.1 $[(M + 1)]^{+}$. Anal. Calcd for $C_{21}H_{19}NO_3$: C, 75.66; H, 5.74,; N, 4.20; Found: C, 75.73; H, 5.73; N, 4.21.

7-(Benzo[*d*][1,3]dioxol-5-yl)-5-benzyl-2,3-dihydrofuro[3,2-*c*]pyridin-4(5*H*)-one (2i)

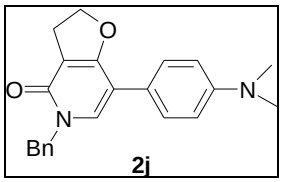


2i

White solid. m.p. 210-212 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.17-3.20 (t, *J* = 9.5 Hz, 2H), 4.69-4.73 (t, *J* = 9.5 Hz, 2H), 5.18 (s, 2H), 5.95 (s, 2H), 6.79-6.93 (m, 3H), 7.27-7.35 (m, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 27.1, 51.2, 73.3, 101.1, 108.4,

109.5, 110.5, 121.0, 126.8, 127.9, 128.0, 128.0, 128.8, 135.9, 136.8, 147.0, 147.7, 160.2, 165.5. MS calcd *m/z* 347.1, found 348.1 $[(M + 1)]^+$. Anal. Calcd for $C_{21}H_{17}NO_4$: C, 72.61; H, 4.93; N, 4.03; Found: C, 72.79; H, 4.94; N, 4.02.

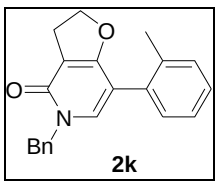
5-Benzyl-7-(4-dimethylamino-phenyl)-3,5-dihydro-2*H*-furo[3,2-*c*]pyridin-4-one (2j)



2j

White solid. m.p. 189-191 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.94 (s, 6H), 3.17-3.21 (t, *J* = 9.5 Hz, 2H), 4.69-4.72 (t, *J* = 9.5 Hz, 2H), 5.19 (s, 2H), 6.71-6.72 (d, *J* =9.0 Hz, 2H), 7.24-7.33 (m, 8H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 27.1, 40.4, 51.2, 73.2, 109.4, 111.1, 112.4, 127.7, 128.0, 128.0, 128.2, 128.7, 128.9, 135.1, 149.9, 160.2, 166.0. MS calcd *m/z* 346.1, found 347.1 $[(M + 1)]^+$. Anal. Calcd for $C_{22}H_{22}N_2O_2$: C, 76.28; H, 6.40,; N, 8.09; Found: C, 76.17; H, 6.41; N, 8.10.

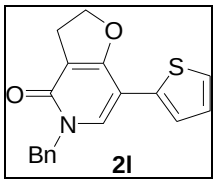
5-Benzyl-7-*o*-tolyl-3,5-dihydro-2*H*-furo[3,2-*c*]pyridin-4-one (2k)



2k

White solid. m.p. 211-213 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.18 (s, 3H), 3.18-3.22 (t, *J* = 9.5 Hz, 2H), 4.64-4.68 (t, *J* = 9.5 Hz, 2H), 5.18 (s, 2H), 7.10-7.34 (m, 10H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 20.0, 27.1, 51.4, 73.4, 109.2, 111.1, 125.8, 128.0, 128.0, 128.4, 128.9, 130.2, 130.2, 132.2, 136.5, 137.2, 137.5, 160.8, 166.6. MS calcd *m/z* 317.1, found 318.1 $[(M + 1)]^+$. Anal. Calcd for $C_{21}H_{19}NO_2$: C, 79.47; H, 6.03; N, 4.41; Found: C, 79.55; H, 6.04; N, 4.42.

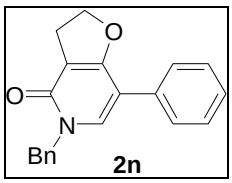
5-Benzyl-7-(thiophen-2-yl)-2,3-dihydrofuro[3,2-*c*]pyridin-4(5*H*)-one (2l)



2l

Yellowish oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.18-3.22 (t, *J* = 9.5Hz, 2H), 4.76-4.79 (d, *J* = 9.5Hz, 2H), 5.18 (s, 2H), 7.00-7.02 (m, 1H), 7.20-7.34 (m, 7H), 7.47 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 27.2, 51.4, 73.6, 105.2, 109.6, 124.0, 124.8, 127.5, 127.6, 127.9, 128.8, 134.6, 135.1, 136.6, 160.0, 164.7. MS calcd *m/z* 309.0, found 310.0 $[(M + 1)]^+$. Anal. Calcd for $C_{18}H_{15}NO_2S$: C, 69.88; H, 4.89; N, 4.53; Found: C, 69.76; H, 4.88; N, 4.54.

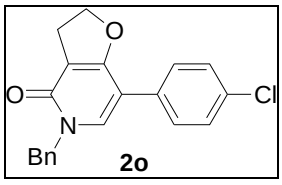
5-Benzyl-7-phenyl-2,3-dihydrofuro[3,2-*c*]pyridin-4(5*H*)-one (2n)



2n

White solid. m.p. 180-182 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.18-3.22 (t, *J* = 9.5 Hz, 2H), 4.71-4.75 (t, *J* = 9.5 Hz, 2H), 5.20 (s, 2H), 7.29-7.44 (m, 11H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 27.1, 51.4, 73,4, 109.7, 111.0, 127.5, 127.9, 128.0, 128.6, 128.8, 128.8, 129.4, 132.9, 136.7, 160.4, 165.8. MS calcd *m/z* 303.1, found 304.1 $[(M + 1)]^+$. Anal. Calcd for $C_{20}H_{17}NO_2$: C, 79.19; H, 5.65; N, 4.62; Found: C, 79.36; H, 5.66; N, 4.61.

5-Benzyl-7-(4-chlorophenyl)-2,3-dihydrofuro[3,2-*c*]pyridin-4(5*H*)-one (2o)



2o

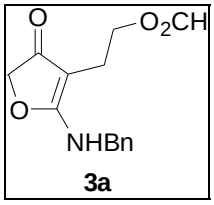
White solid. m.p. 215-217 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.17-3,21 (t, *J* = 9.5 Hz, 2H), 4.71-4.75 (t, *J* = 9.5 Hz, 2H), 5.19 (s, 2H), 7.28-7.41 (m, 10H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.1, 51.4, 73.4, 109.7, 109.7, 127.9, 128.6, 128.7, 128.7, 128.8, 128.8, 130.8, 131.0, 136.3, 160.2, 165.4; MS calcd *m/z* 337.0, found 338.0 [(M

+ 1)]$^+$. Anal. Calcd for $C_{20}H_{16}ClNO_2$: C, 71.11; H, 4.77; N, 4.15; Found: C, 71.21; H, 4.78; N, 4.16.

IV. Synthesis and analytical data of 3.

General procedure for the preparation of **3** (**3b** as an example): To a solution of 1-[3-(4-Nitro-phenyl)-acryloyl]-cyclopropanecarboxylic acid 2-chloro-benzylamide (**1r**) (358 mg, 1.0 mmol) in MeCN (2 mL) was added NBS (213 mg, 1.2 mmol) and HCO_2H (0.045 mL, 1.2 mmol). The mixture was stirred at reflux. After the starting material **1r** was consumed as indicated by TLC, the reaction mixture was cooled to room temperature and poured into water and then extracted with CH_2Cl_2 (3 × 10 mL). The combined organic phase was washed with water (3 × 10 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by flash chromatography (silica gel, ethyl acetate : ether = 2 : 1) to give **3b** (253 mg, 86%) as a white solid.

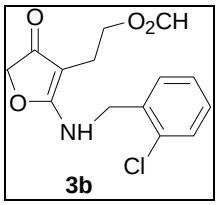
5-Benzylamino-4-(2-methylperoxy-ethyl)-furan-3-one (3a)



3a

White solid. m.p.146-148 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.48-2.51 (t, *J* = 6.5 Hz, 2H), 4.14-4.17 (t, *J* = 6.0 Hz, 2H), 4.53 (s, 2H), 4.56-4.57 (d, *J* = 6.5 Hz, 2H), 6.38 (s, 1H), 7.29-7.39 (m, 5H), 7.90 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 19.6, 45.1, 63.1, 74.4, 88.2, 127.3, 127.8, 128.7, 137.1, 161.1, 178.2, 192.5. MS calcd *m/z* 261.1, found 262.0 [(M + 1)]$^+$. Anal. Calcd for $C_{14}H_{15}NO_4$: C, 64.36; H, 5.79; N, 5.36; Found: C, 64.23; H, 5.80; N, 5.28.

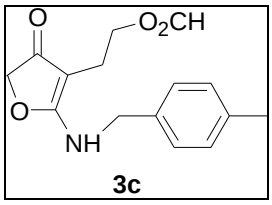
5-(2-Chloro-benzylamino)-4-[1,2]dioxetan-3-ylmethyl-furan-3-one (3b)



3b

White solid. m.p. 152-154 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.48-2.50 (t, *J* = 6.5 Hz, 2H), 4.14-4.17 (t, *J* = 6.5 Hz, 2H), 4.49 (s, 2H), 4.63-4.64(d, *J* = 6.0 Hz, 2H), 6.52 (s, 1H), 7.24-7.29 (m, 2H), 7.34-7.36 (t, *J* = 3.5 Hz, 1H),7.40-7.41 (m, 2H), 7.97 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 19.6, 43.2, 63.8, 74.5, 88.5, 127.2, 129.5, 129.6, 129.7, 133.3, 134.6, 161.0, 178.2, 192.9. MS calcd *m/z* 295.0, found 296.0 $[(M + 1)]^{+}$. Anal. Calcd for $C_{14}H_{14}ClNO_4$: C, 56.86; H, 4.77; N, 4.74; Found: C, 56.78; H, 4.78; N, 4.73.

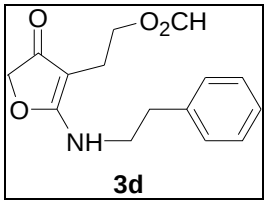
4-[1,2]Dioxetan-3-ylmethyl-5-(4-methyl-benzylamino)-furan-3-one (3c)



3c

White solid. m.p. 165-166 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.31 (s, 3H), 2.44-2.48 (m, 2H), 4.09-4.13 (m, 2H), 4.37-4.38 (d, *J* = 6.0, 2H), 4.46-4.49 (m, 2H), 7.12-7.20 (m, 4H), 7.50 (s, 1H), 7.95 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 19.6, 22.5, 44.8, 62.9, 74.3, 88.0, 127.3, 129.4, 134.3, 137.5, 161,2, 178.1, 192.7. MS calcd *m/z* 275.1, found 275.9 $[(M + 1)]^{+}$. Anal. Calcd for $C_{15}H_{17}NO_4$: C, 65.44; H, 6.22; N, 5.09; Found: C, 65,.53, H, 6,.21; N, 5.10.

4-[1,2]Dioxetan-3-ylmethyl-5-phenethylamino-furan-3-one (3d)

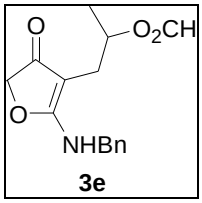


3d

White solid. m.p. 160-162 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.40-2.44 (m, 2H), 2.86-2.93 (m, 2H), 3.60-3.68 (m, 2H), 4.07-4.12 (m, 2H), 4.47 (s, 2H), 6.15 (s, 1H), 7.07-7.09 (d, *J* = 8.5, 2H), 7.31-7.34 (t, *J* = 7.5, 1H), 7.43-7.45 (t, *J* = 8.0, 2H); ^{13}C

NMR ($CDCl_3$, 125 MHz): δ = 19.6, 35.7, 36.1, 42.7, 63.1, 74.3, 88.1, 126.6, 127.6, 128.7, 138.0, 161.1, 178.3, 192.3. MS calcd *m/z* 275.1, found 276.1 $[(M + 1)]^+$. Anal. Calcd for $C_{15}H_{17}NO_4$: C, 65.44; H, 6.22; N, 5.09; Found: C, 65.31; H, 6.21; N, 5.08.

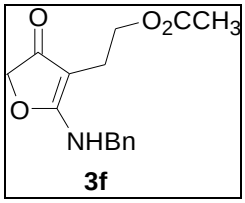
5-Benzylamino-4-(2-methylperoxy-propyl)-furan-3-one (3e)



3e

White solid. m.p. 149-151 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 1.26 (s, 3H), 2.29-2.33 (m, 1H), 2.45-2.49 (m, 1H), 4.43-4.50 (m, 2H), 4.53-4.55 (t, *J* = 5.5 Hz, 2H), 4.85-4.89 (m, 1H), 7.16-7.47 (m, 6H), 7.88 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 19.1, 26.4, 44.8, 71.1, 74.2, 87.9, 127.5, 128.5, 128.8, 137.1, 161.0, 178.0, 192.2. MS calcd *m/z* 275.1, found 276.1 $[(M + 1)]^+$. Anal. Calcd for $C_{15}H_{17}NO_4$: C, 65.44; H, 6.22; N, 5.09; Found: C,65.37; H, 6.23; N, 5.10.

5-Benzylamino-4-(2-ethylperoxy-ethyl)-furan-3-one (3f)



3f

Yellowish oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 1.86 (s, 3H), 2.44-2.46 (t, *J* =6.5 Hz, 2H), 4.01-4.04 (t, *J* =6.0 Hz, 2H), 4.52 (s, 2H), 4.55-4.57 (d, *J* = 6.0 Hz, 2H), 6.72 (s, 1H), 7.27-7.38 (m, 5H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 19.5, 20.7, 45.1, 63.8, 74.5, 88.7, 127.2, 127.9, 128.8, 136.9, 171.3, 178.2, 192.3. MS calcd *m/z* 275.1, found 275.7 $[(M + 1)]^+$. Anal. Calcd for $C_{15}H_{17}NO_4$: C, 65.44; H, 6.22; N, 5.09; Found: C, 65.57; H, 6.23; N, 5.08.

V. X-ray crystallographic information of **2a**, **2i** and **3b.**

Table S1. Crystallographic Data for Compounds 2a, **2i** and **3b**

	Compound 2a	**Compound 2i**	**Compound 3b**
Formula	$C_{21}H_{19}NO_2$	$C_{21}H_{17}NO_4$	$C_{14}H_{14}ClNO_4$
M_r	317.37	347.36	295.71
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	Pna2(1)	P 21/c	Cc
Temperature	293(2)	293(2)	293(2)
***a* (Å)**	11.2914(17)	19.023(5)	4.670(3)
***b* (Å)**	8.1975(13)	8.279(5)	24.712(3)
***c* (Å)**	18.139(3)	11.214(5)	12.388(3)
α **(deg)**	90.00	90.00	90.00
β **(deg)**	90.00	103.913(5)	91.024(3)
γ **(deg)**	90.00	90.00	90.00
***V* (Å^3)**	1679.0(4)	1714.3(14)	1429.4(10)
Z	4	4	4
$D_{calc.}$ **(g cm^{-3})**	1.256	1.346	1.374
μ **/ mm^{-1}**	0.081	0.094	0.279
***F* (000)**	672	728	616
Crystal size, mm^3	0.37 × 0.32 × 0.27	0.22 × 0.15 ×0.13	0.37 × 0.33 × 0.24
Index ranges	$-13 \le h \le 13$ $-9 \le k \le 9$ $-15 \le l \le 21$	$-15 \le h \le 24$ $-11 \le k \le 7$ $-15 \le l \le 14$	$-5 \le h \le 5$ $-28 \le k \le 27$ $-14 \le l \le 11$
Reflections collected	7918	7634	3555
Independent reflections	2341 [R(int) = 0.0546]	3980 [R(int) = 0.0441]	1957 [R(int) = 0.0384]
Goodness-of-fit on F^2	1.043	0.982	1.003
Final R_1, wR_2	R_1 = 0.0447, wR_2 = 0.1177	R_1 = 0.0606, wR_2 = 0.1239	R_1 = 0.0435, wR_2 = 0.1049
***R* indices (all data)**	R_1 = 0.0761, wR_2 = 0.1462	R_1 = 0.1663, wR_2 = 0.1644	R_1 = 0.0645, wR_2 = 0.1191

Summary of Data CCDC 826841

Authors: Fushun Liang, Ying Wei, Shaoxia Lin, Juan Zhang, Zaihai Niu, Qiang Fu

Journal: Chem.Commun. (0182)

Formula: C21 H19 N1 O2

Unit cell parameters: a 11.2914(17) b 8.1975(13) c 18.139(3)

alpha 90.00 beta 90.00 gamma 90.00

space group Pna21

Summary of Data CCDC 829460

Authors: Fushun Liang, Ying Wei, Shaoxia Lin, Juan Zhang, Zaihai Niu, Qiang Fu

Journal: Chem.Commun. (0182)

Formula: C21 H17 N1 O4

Unit cell parameters: a 19.023(5) b 8.279(5) c 11.214(5) beta 103.913(5)

space group P21/c

Summary of Data CCDC 839385

Authors: Fushun Liang, Ying Wei, Shaoxia Lin, Juan Zhang, Zaihai Niu, Qiang Fu

Journal: Chem.Commun. (0182)

Formula: C14 H14 Cl1 N1 O4

Unit cell parameters: a 4.670 b 24.712 c 12.388 beta 91.02

space group Cc

VI. ORTEP drawings for compounds **2a**, **2i** and **3b**

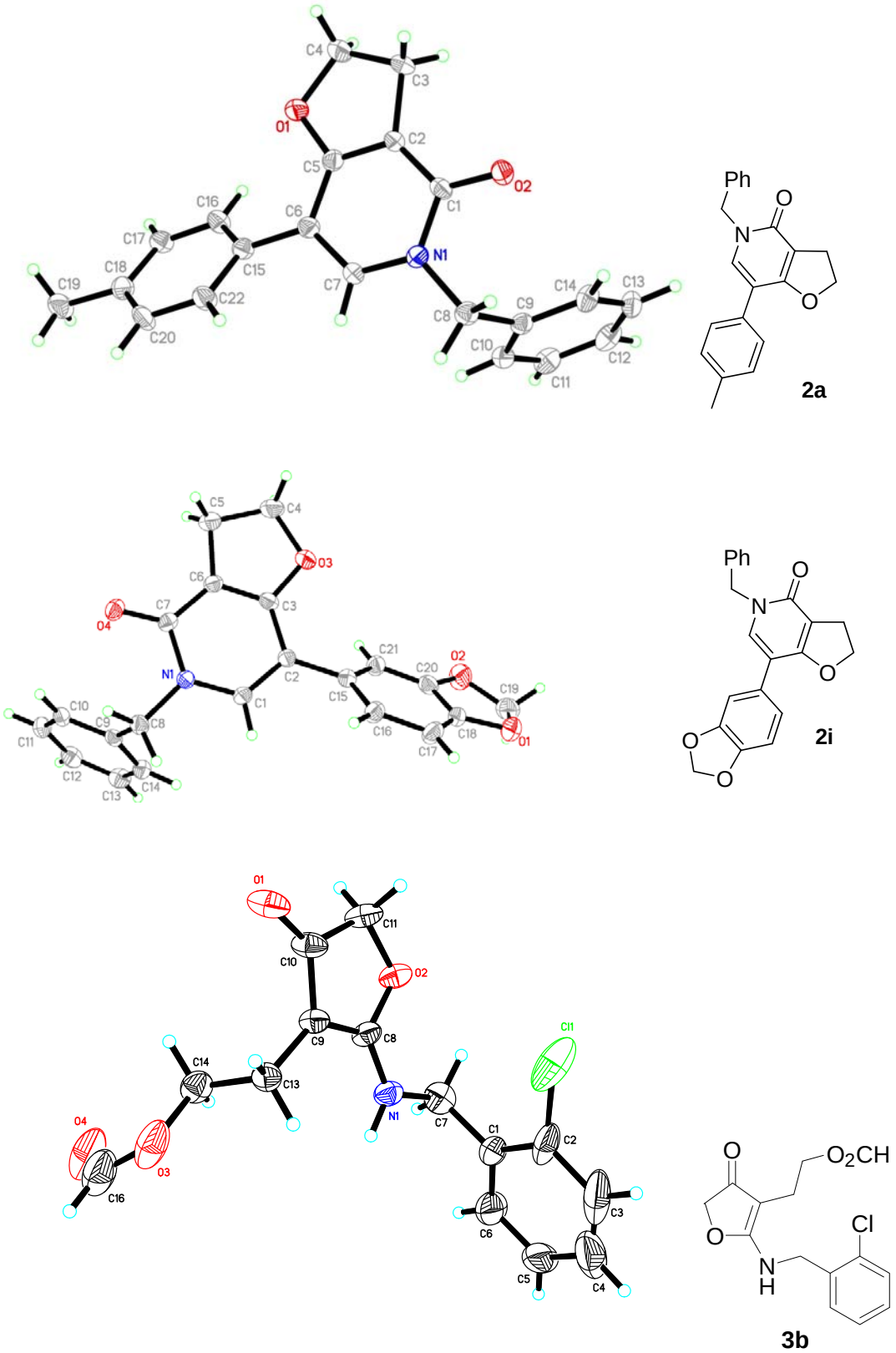
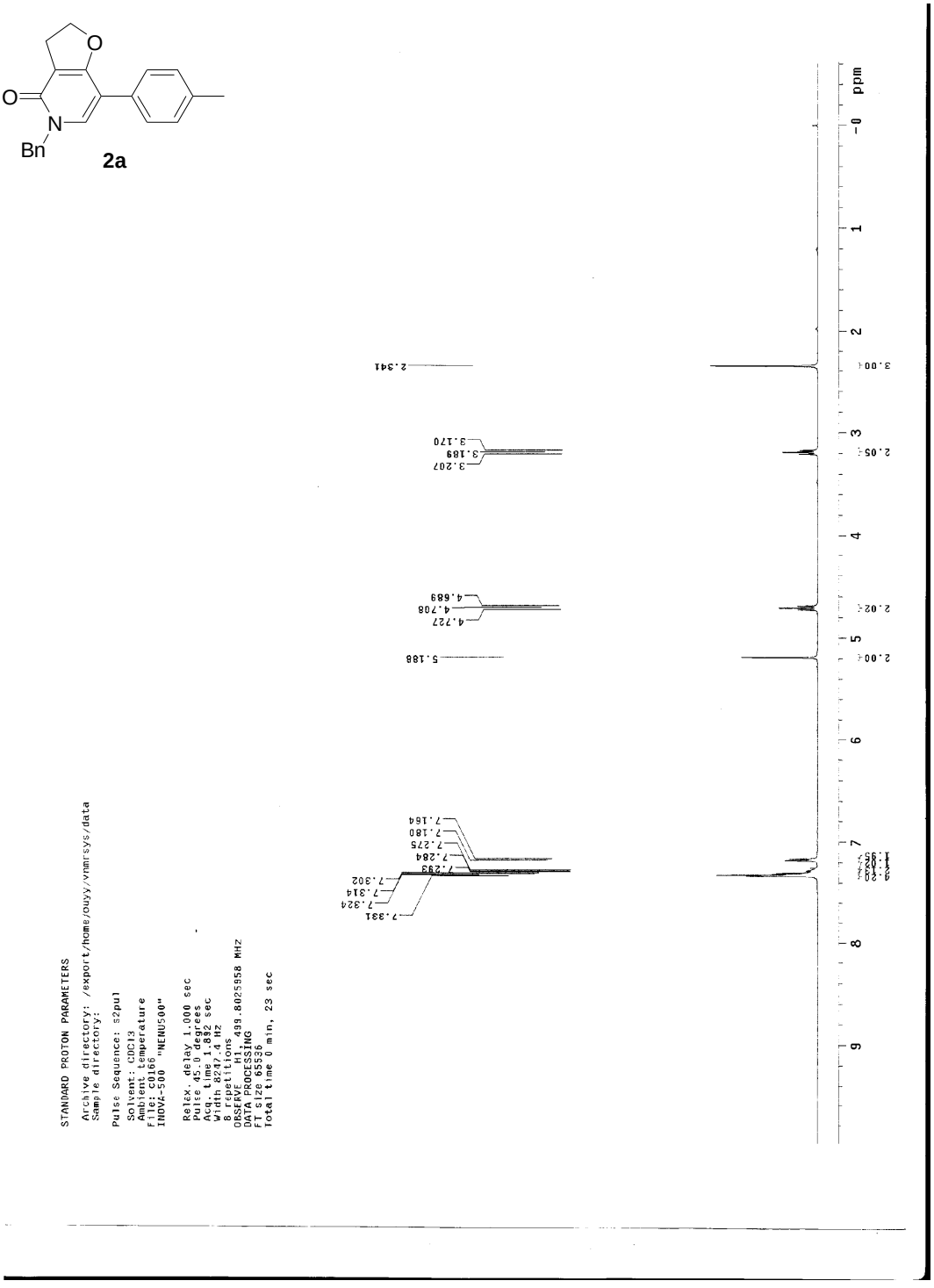
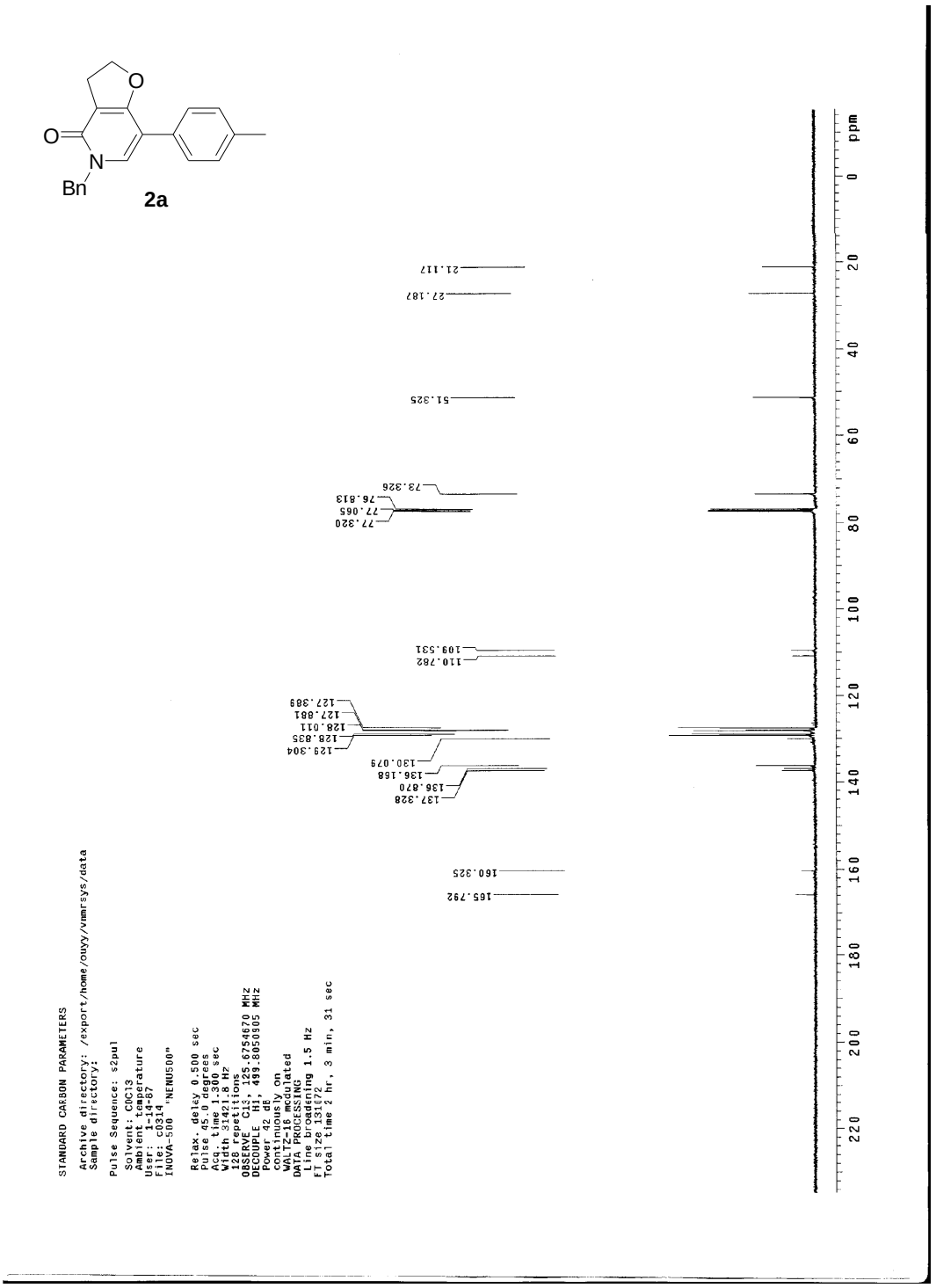


FIGURE S1. ORTEP Drawings of **2a**, **2i** and **3b.**

VII. Copies of ^{1}H and ^{13}C NMR spectra for compounds 2 and 3.

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O
N
Bn
2a
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27.187
51.325
73.326
76.813
77.065
77.320
109.531
110.782
127.369
127.681
128.011
128.835
129.304
130.079
136.168
136.870
137.328
160.325
165.792
ppm
0
20
40
60
80
100
120
140
160
180
200
220
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Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c014
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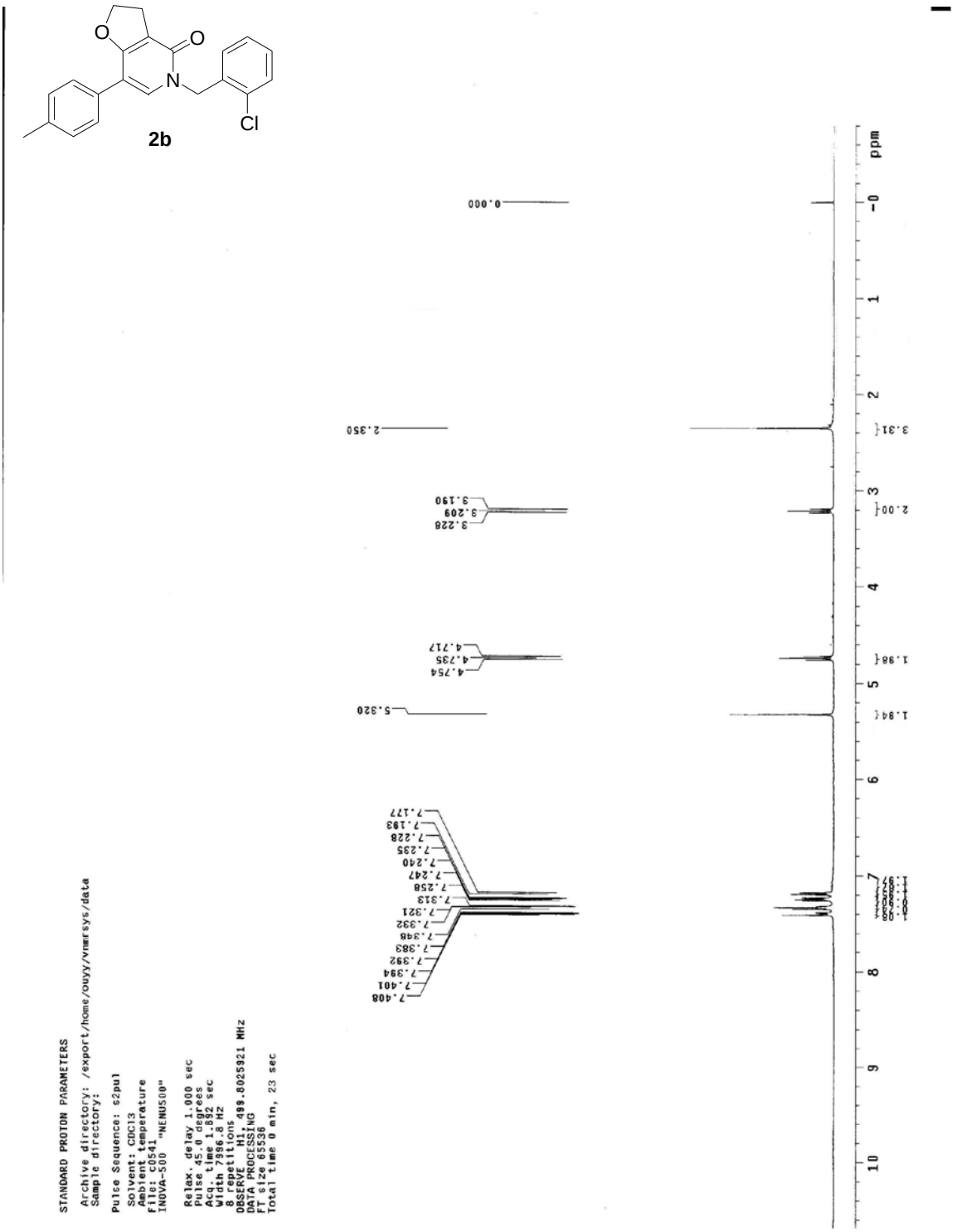
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6756670 MHz
DECOUPLE H1, 499.8050005 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 32772
Total time 2 hr, 3 min, 31 sec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N
Cl
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3.228
4.717
4.735
4.754
5.320
7.177
7.193
7.228
7.235
7.240
7.247
7.258
7.313
7.321
7.332
7.348
7.383
7.392
7.394
7.401
7.408
3.31
2.00
1.98
1.94
ppm
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Pulse 45.0 degrees
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Width 7896.8 HZ
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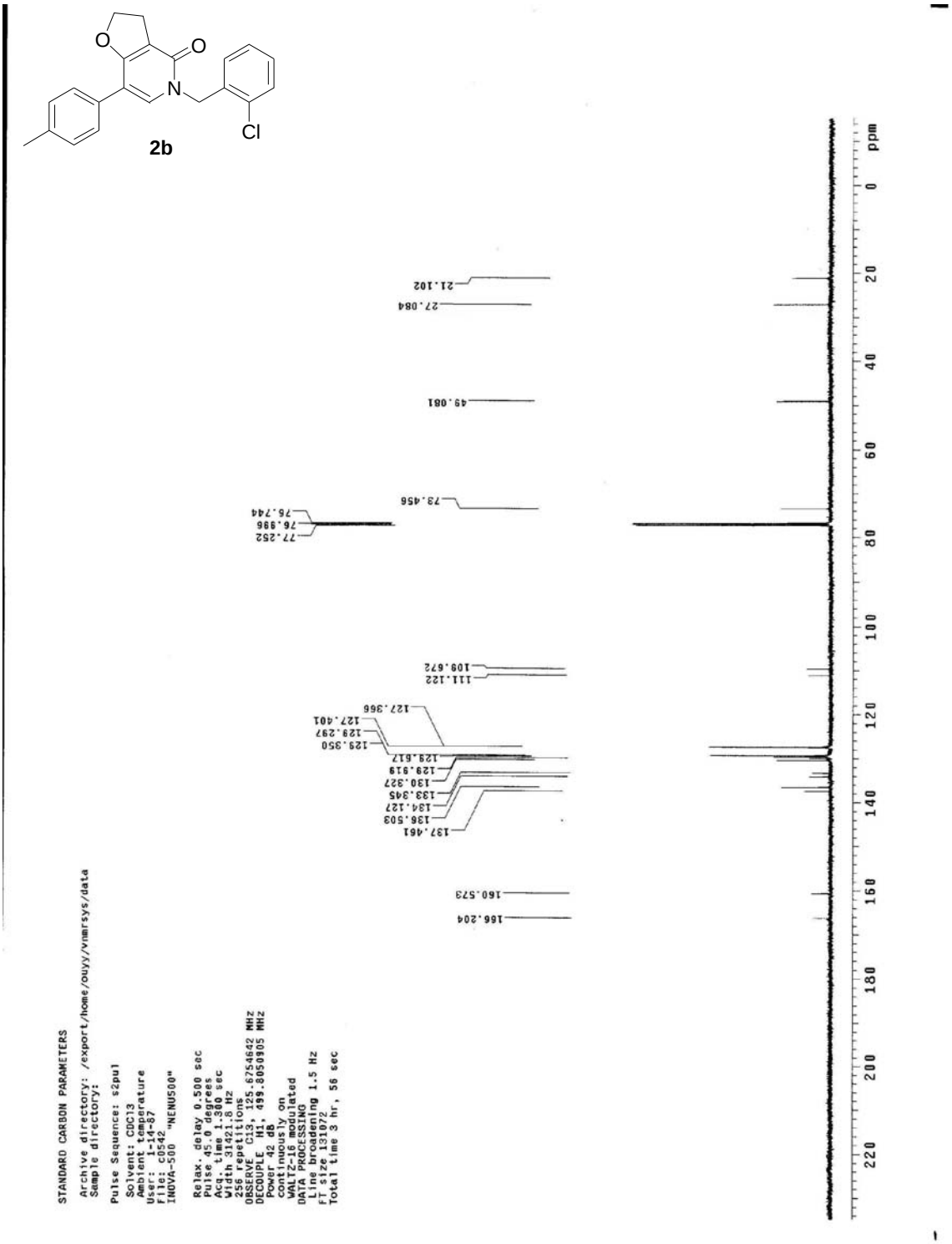
Total time 0 min, 23 sec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Cl
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77.252
109.672
111.122
127.366
127.401
129.297
129.350
129.817
129.819
130.327
133.345
134.127
136.503
137.461
160.573
166.204
ppm
0
20
40
60
80
100
120
140
160
180
200
220
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Sample directory:
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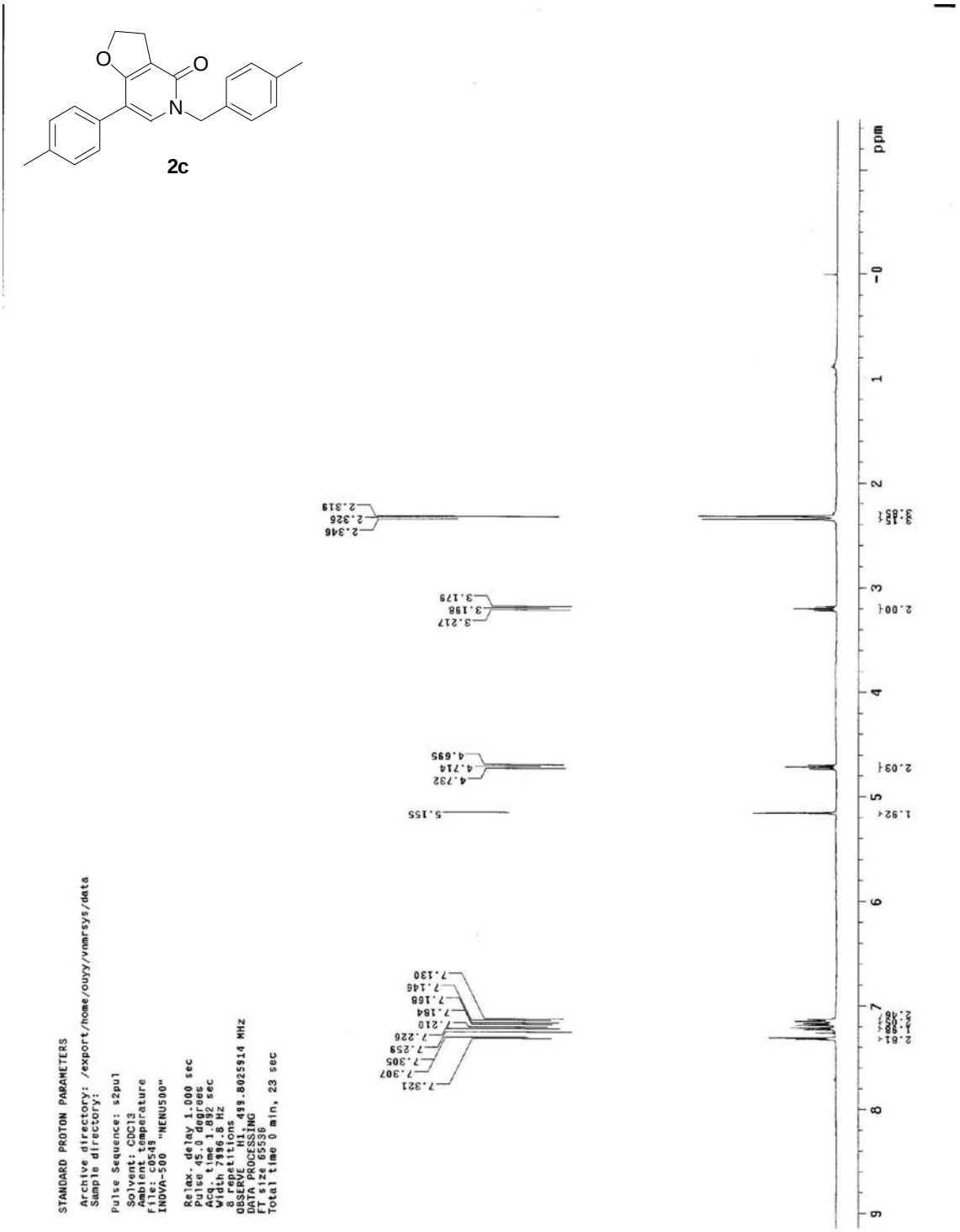
Solvent: CDCl3
Ambient temperature
User: l-14-87
File: c0542
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec


O
O
N
2c
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2.326
2.319
3.217
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3.179
4.732
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4.695
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7.321
7.307
7.305
7.259
7.226
7.210
7.184
7.168
7.146
7.130
ppm
STANDARD PROTON PARAMETERS
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Ambient temperature
File: c0549.fid
"MENU500"
INOVA-500
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Pulse 45.0 degrees
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8 repetitions
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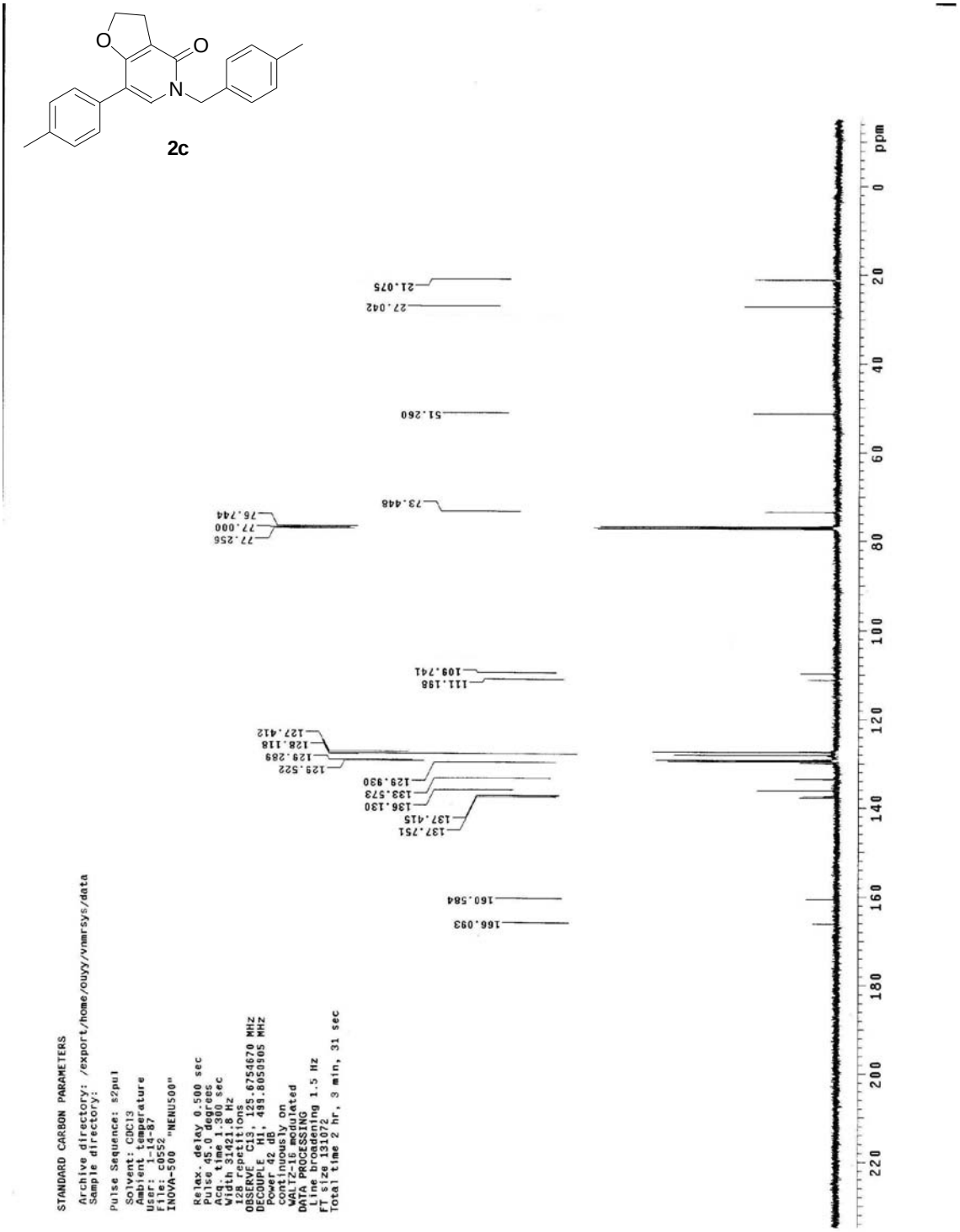
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec


2c
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73.448
76.744
77.000
77.256
109.741
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127.412
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129.289
129.522
129.930
133.573
136.130
137.415
137.751
160.584
166.093
ppm
0
20
40
60
80
100
120
140
160
180
200
220
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Ambient temperature
User: l-14-87
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Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
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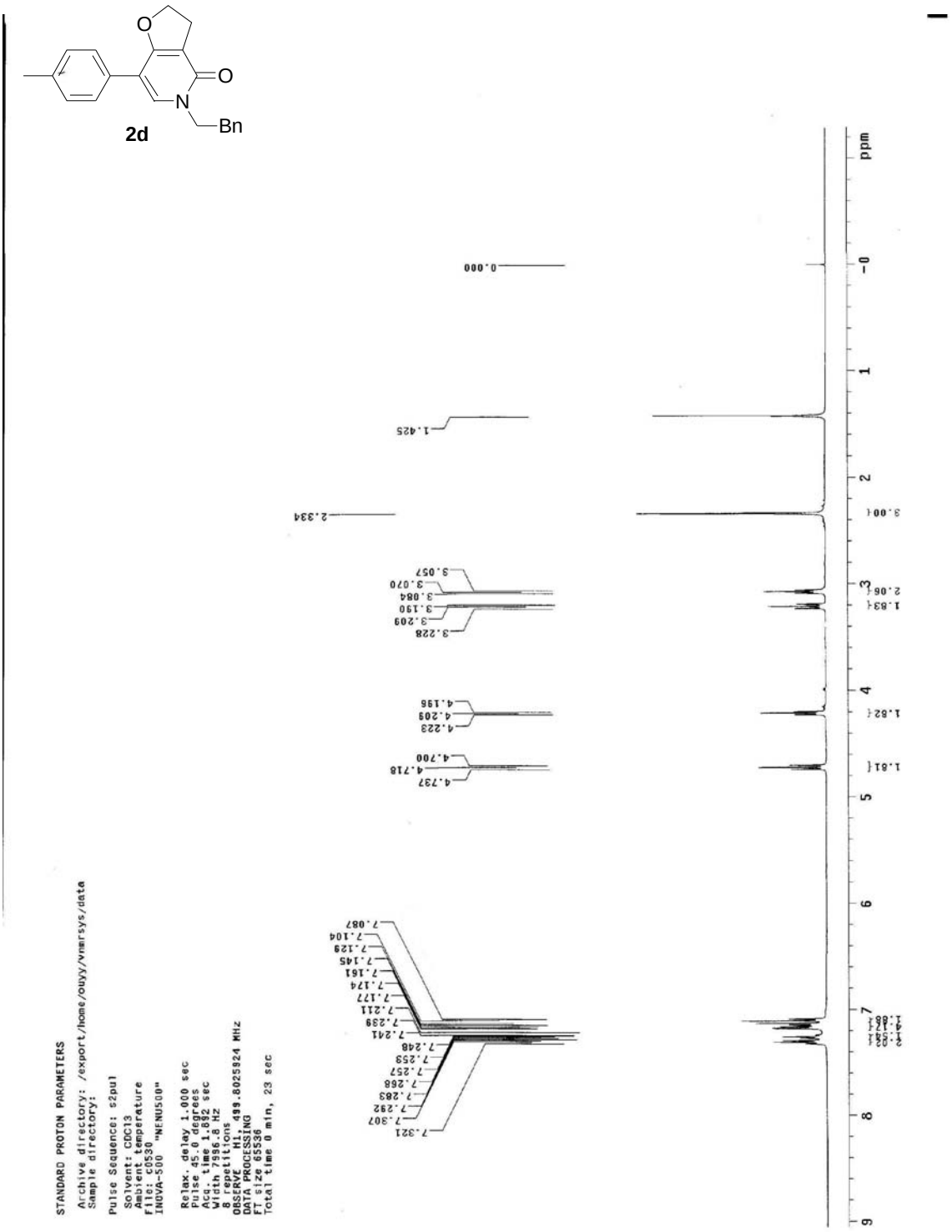
DECOUPLE H1, 499.8059505 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec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O
N
Bn
2d
ppm
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2.334
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3.070
3.084
3.190
3.209
3.228
4.196
4.209
4.223
4.700
4.718
4.737
7.087
7.104
7.129
7.145
7.161
7.174
7.177
7.211
7.239
7.241
7.248
7.259
7.257
7.268
7.283
7.292
7.307
7.321
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Sample directory:
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Solvent: CDCl3
Ambient temperature
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INOVA-500 "NENU500"
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Pulse 45.0 degrees
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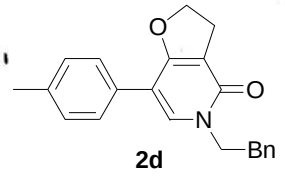
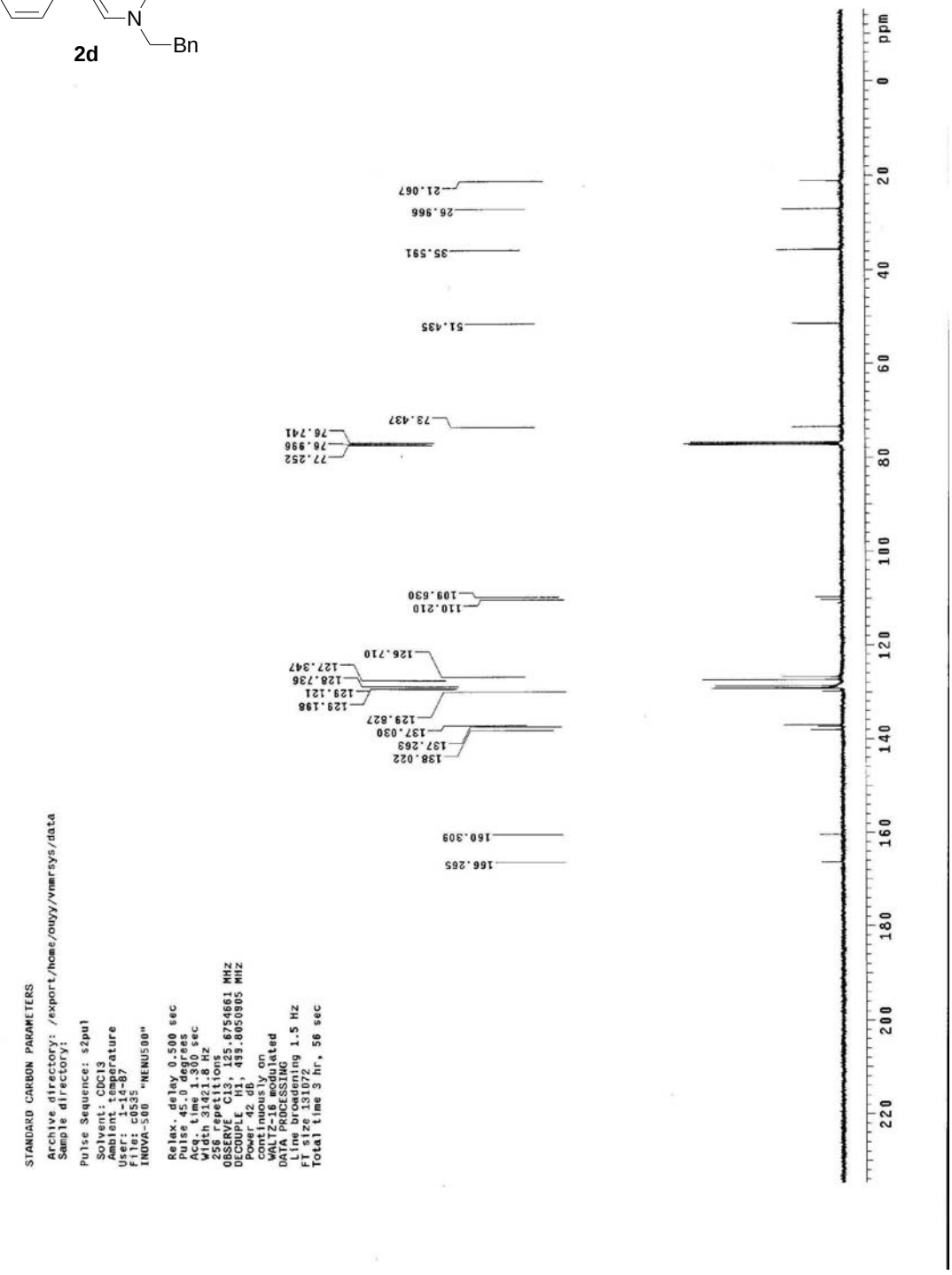
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec



2d



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Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c0535
INOVA-500 "NENUS00"
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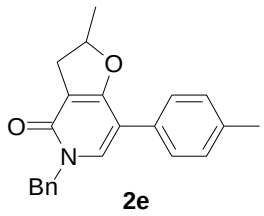
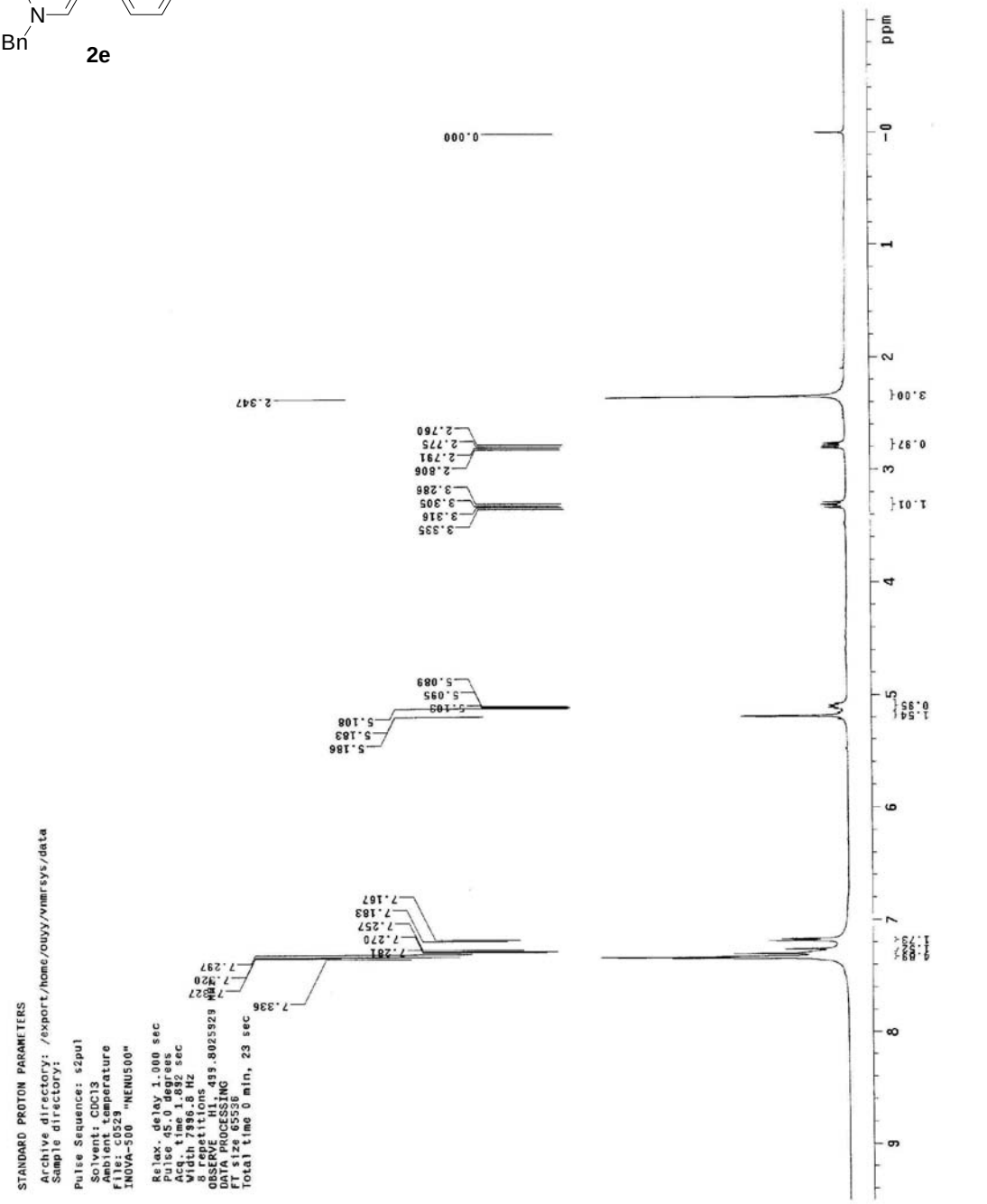
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.6050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec


O
O
N
Bn

2e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Sample directory:
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Solvent: CDCl3
Ambient temperature
File: c0529
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
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Width 7996.8 Hz
8 repetitions
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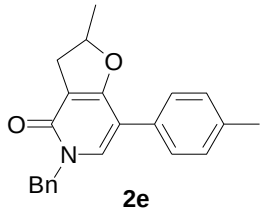
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm


O
O
N
Bn

2e

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77.015
77.271
82.570
109.314
111.053
127.420
127.916
128.072
128.850
129.297
130.159
136.164
136.812
137.312
160.500
165.174
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c0540
INOVA-500 "NENUS00"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754687 MHz
DECOUPLE H1, 499.8050905 MHz
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WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
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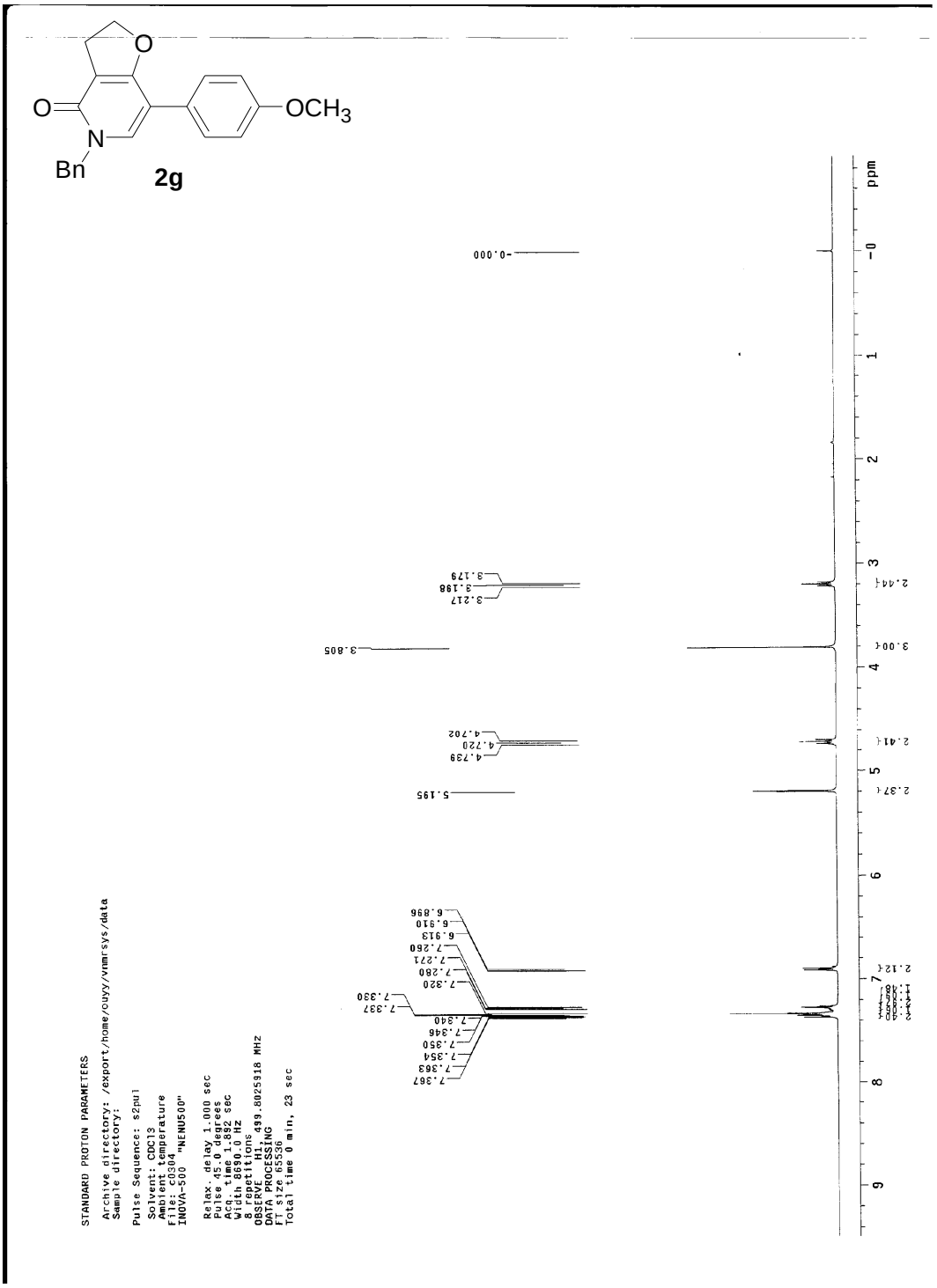
Total time 2 hr, 3 min, 31 sec


O
O
N
Bn
OCH3
2g
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Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
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Solvent: CDCl3
Ambient temperature
Fill-CDCl3-04 "NENU500"
INOVA-500
Relax. delay 1.000 sec
Pulse 45.0 degrees
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8 repetitions
OBSERVE H1 499.8025918 MHz
DATA PROCESSING
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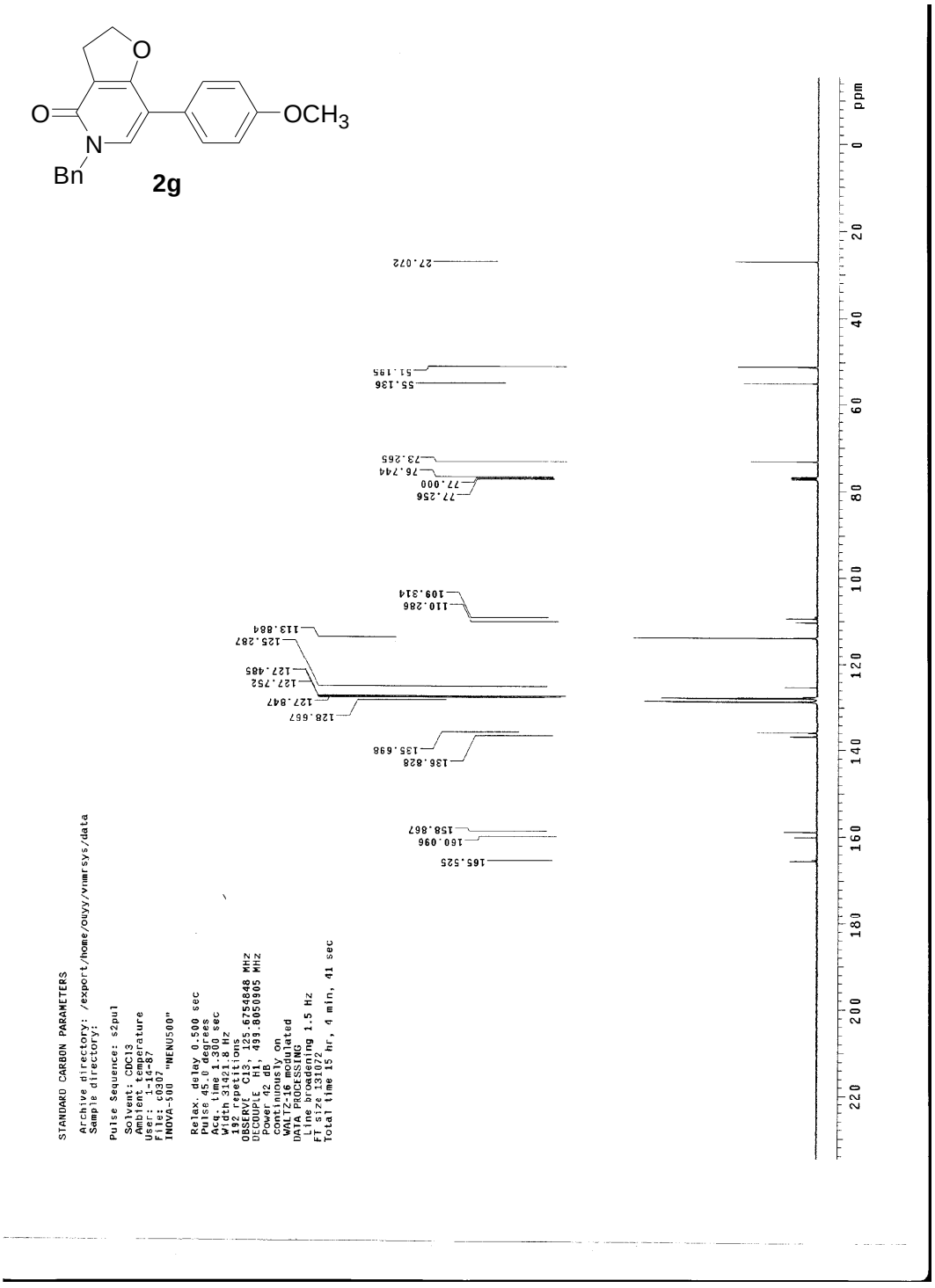
Total time 0 min, 23 sec
ppm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N
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113.884
125.287
127.485
127.752
127.847
128.667
135.698
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165.525
ppm
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20
40
60
80
100
120
140
160
180
200
220
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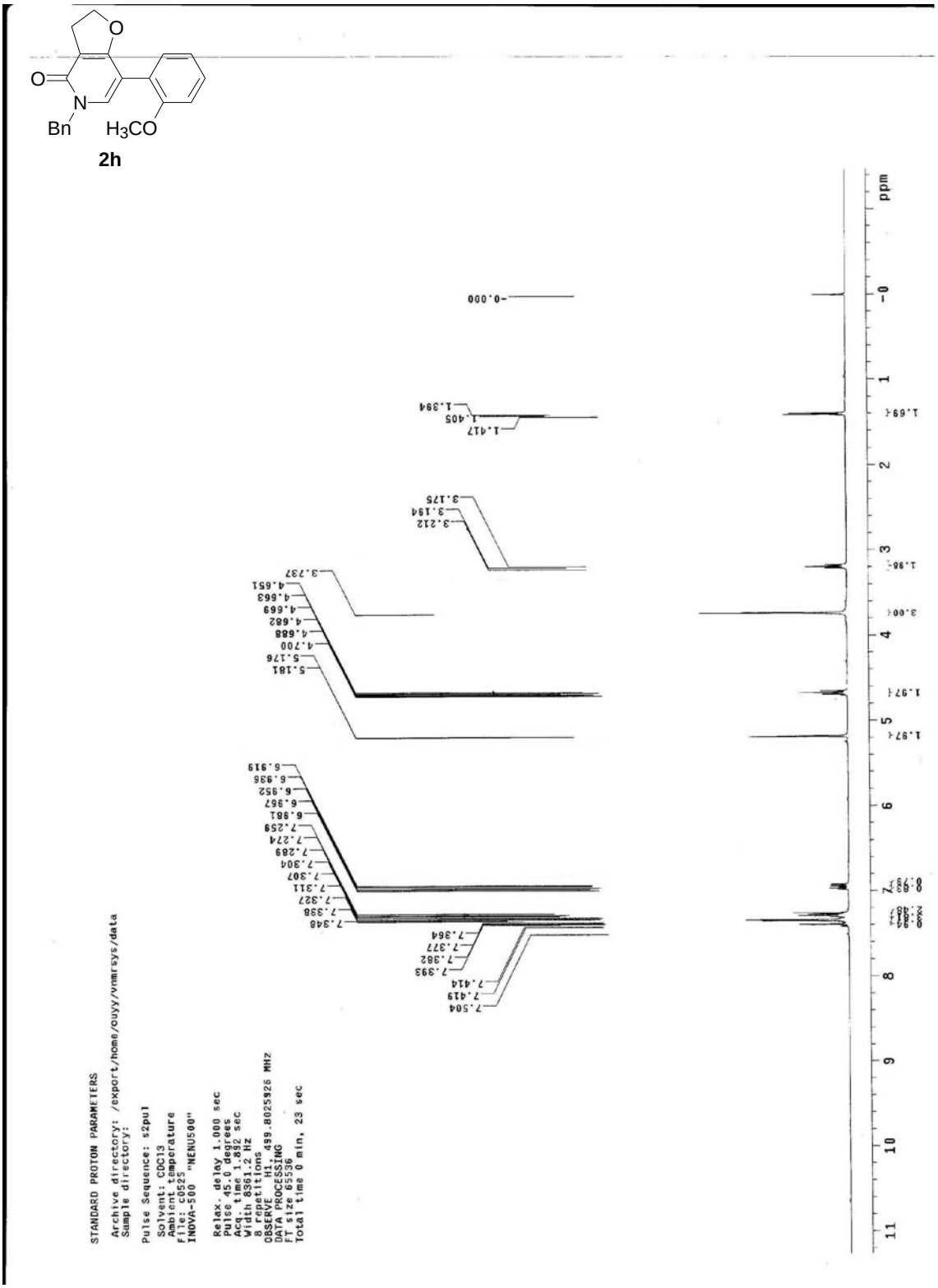
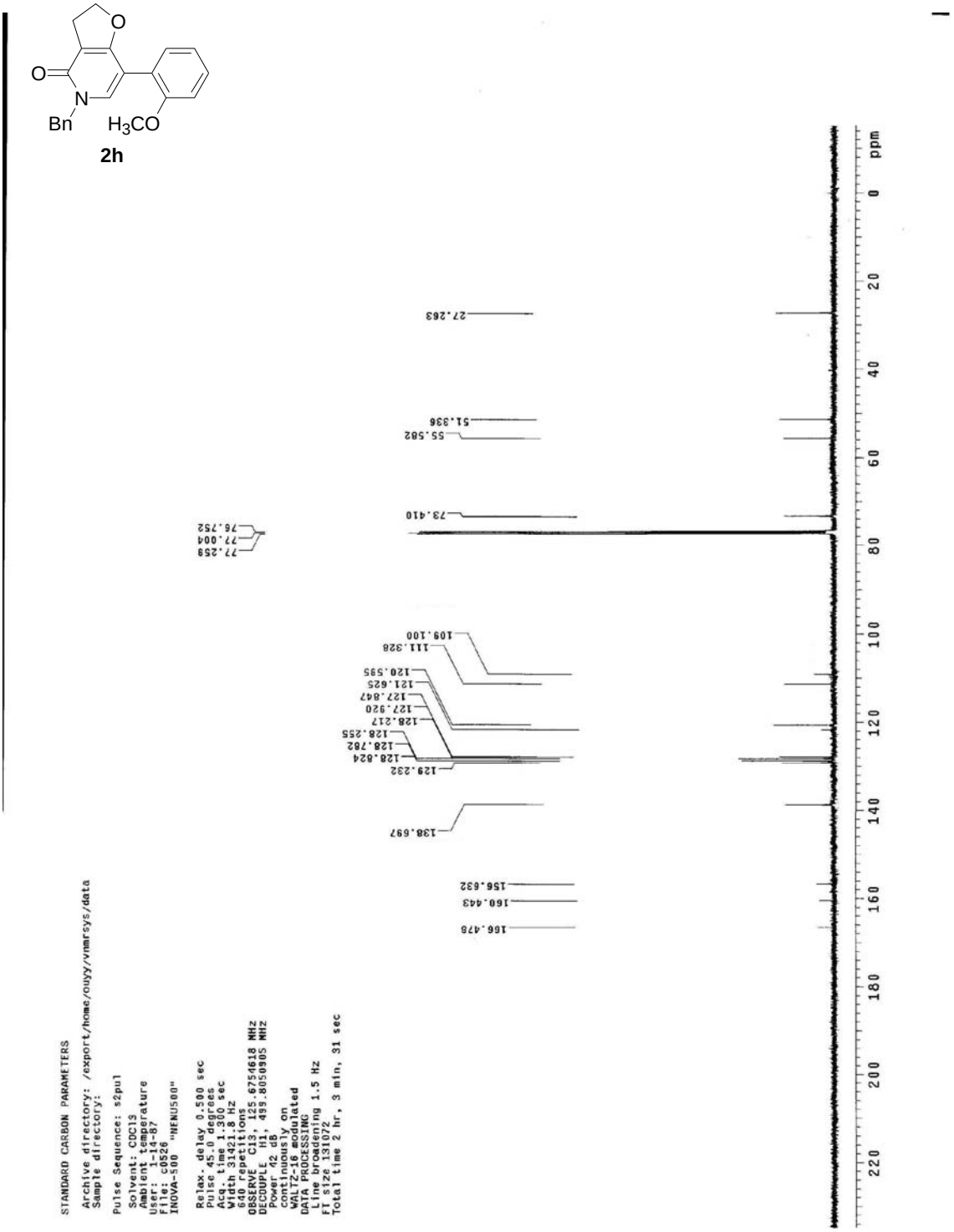
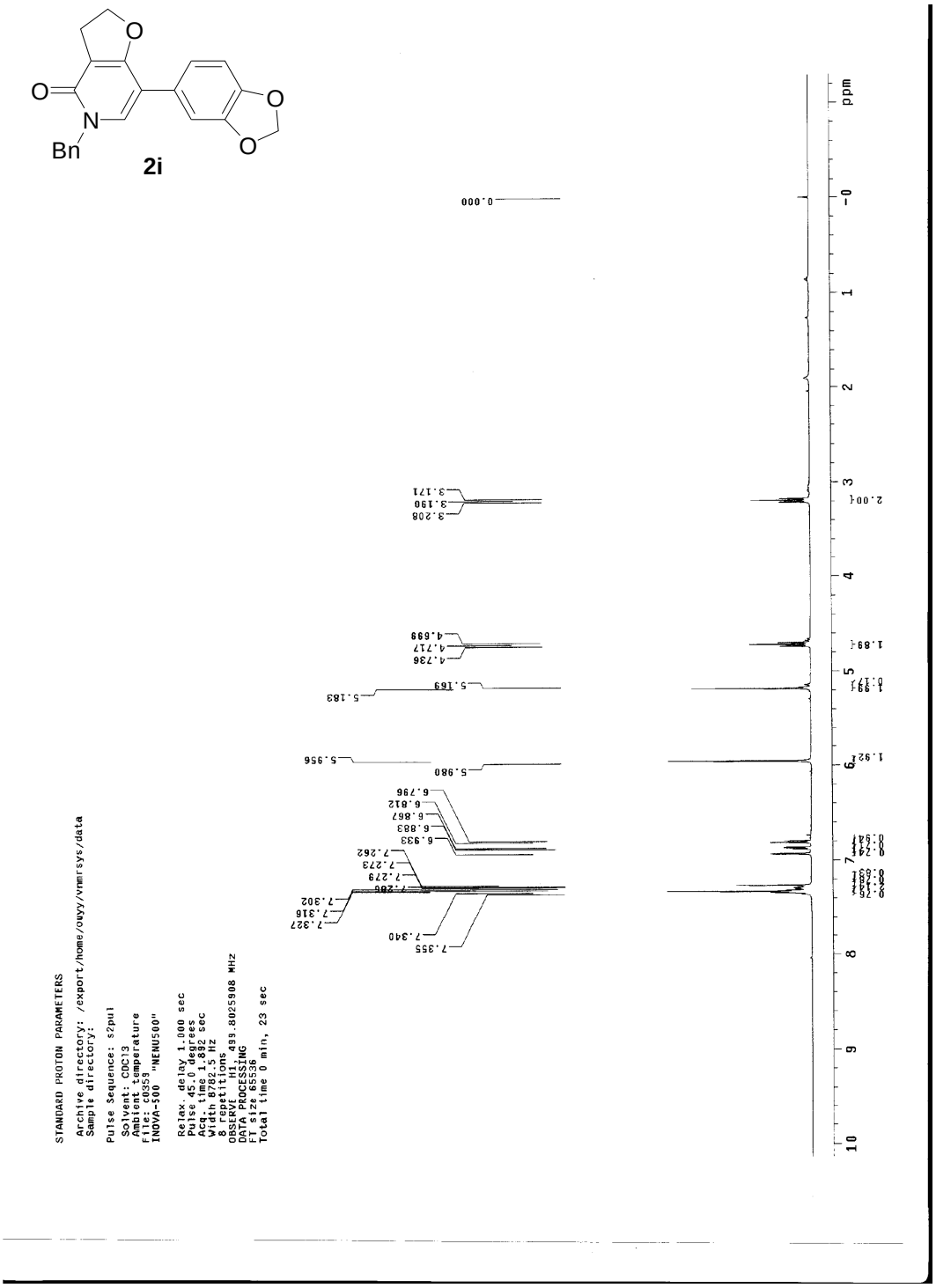
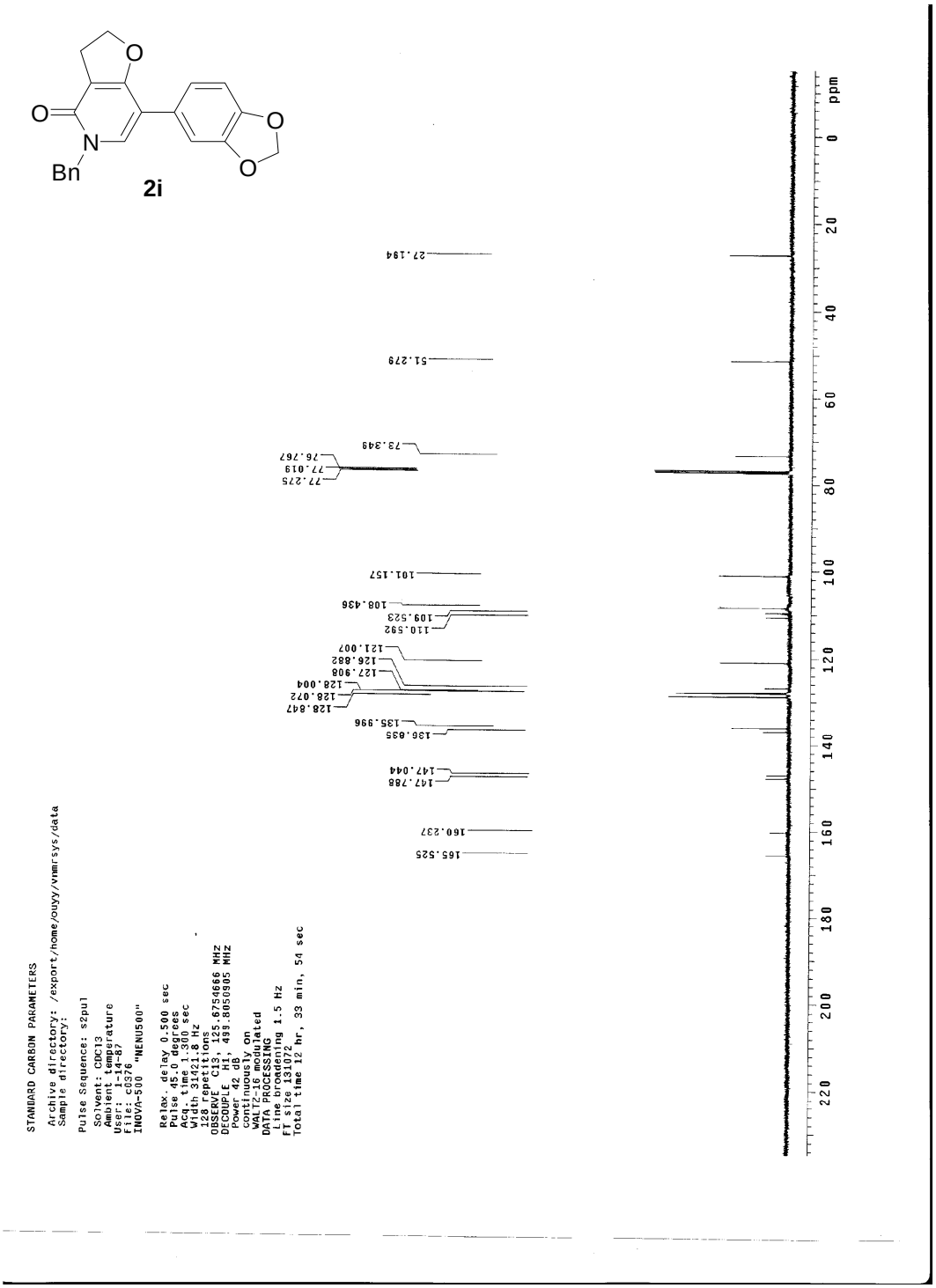
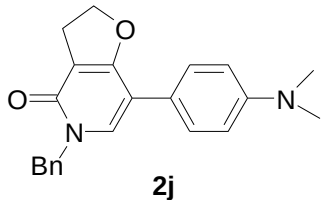
Solvent: CDCl3
Ambient temperature
User: ouyy
File: c07
INOVA-500 "WENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754848 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 15 hr, 4 min, 41 sec


O
O
N
Bn
H3CO
2h
ppm
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c0525
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 8361.2 Hz
8 repetitions
OBSERVE H1, 499.8025926 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec


O
O
N
Bn
H3CO
2h
27.263
51.336
55.502
73.410
76.752
77.004
77.259
109.100
111.328
120.595
121.625
127.847
127.920
128.217
128.255
128.782
128.824
129.232
138.697
156.632
160.443
166.478
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: ouyy-87
File: cd526
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
640 repetitions
OBSERVE C13, 125.6754618 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec

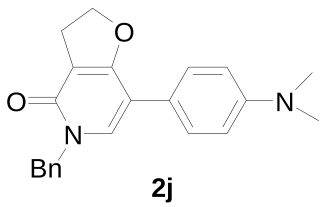

O
O
N
Bn
O
O
2i
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
FILE /dsk
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8782.5 Hz
8 repetitions
OBSERVE H1, 499.8025908 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
0.000
3.171
3.190
3.208
4.699
4.717
4.736
5.169
5.183
5.956
5.980
6.796
6.812
6.867
6.883
6.933
7.262
7.273
7.279
7.286
7.302
7.316
7.327
7.340
7.355
ppm


O
O
N
Bn
O
O
2i
27.194
51.279
73.349
76.767
77.019
77.275
101.157
108.436
109.523
110.592
121.007
126.882
127.908
128.004
128.072
128.847
135.996
136.035
147.044
147.788
160.237
165.525
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c0376 "NENU500"
INOVA-500
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 12 hr, 33 min, 54 sec

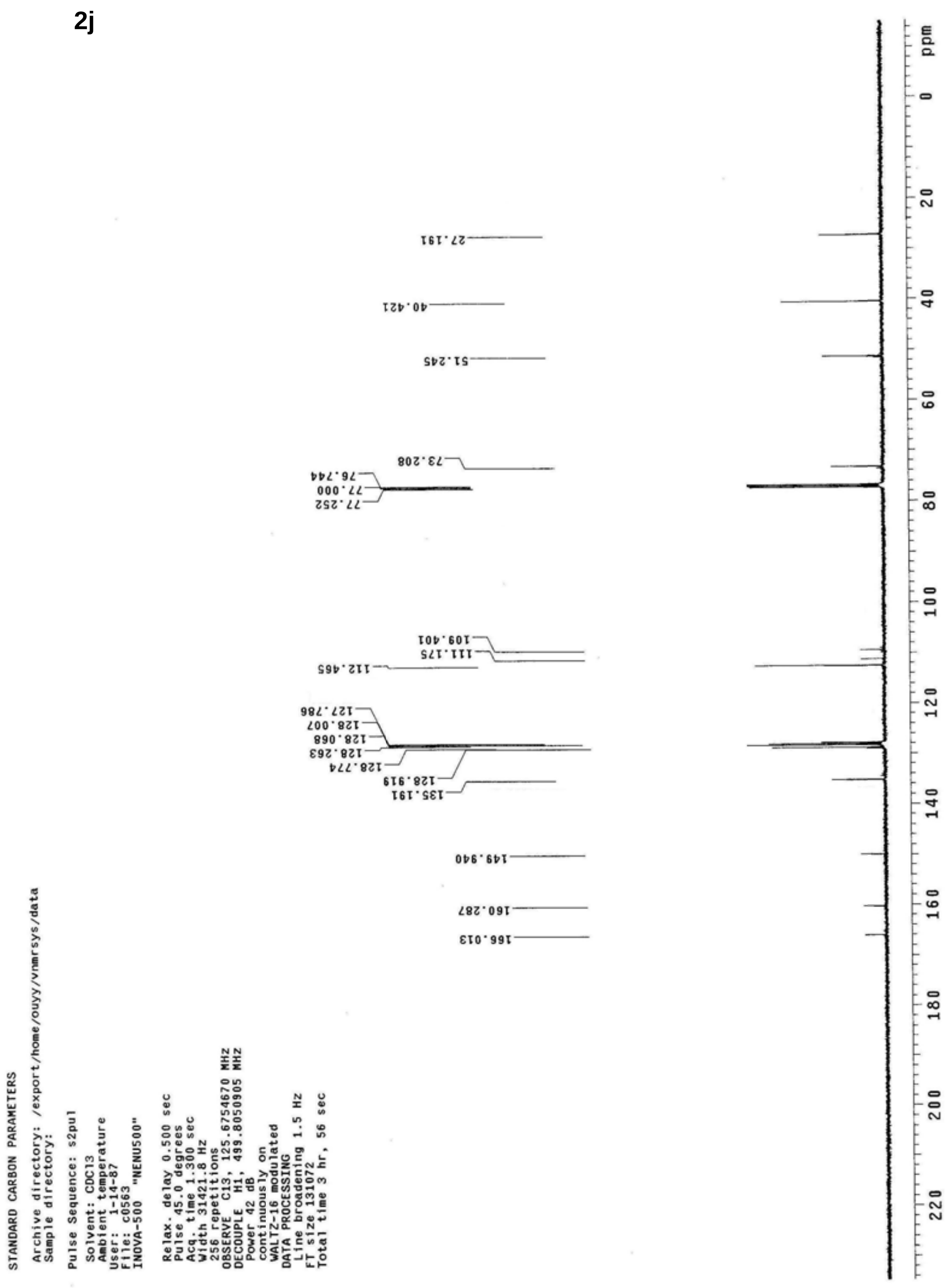

O
O
N
Bn
N

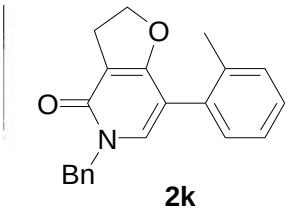
2j

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c0557
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 7896.8 Hz
8 repetitions
OBSERVE H1, 499.8025919 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
0.000
2.947
3.174
3.193
3.212
4.692
4.711
4.729
5.180
6.711
6.729
7.245
7.259
7.295
7.300
7.310
7.313
7.321
7.329
7.351
ppm

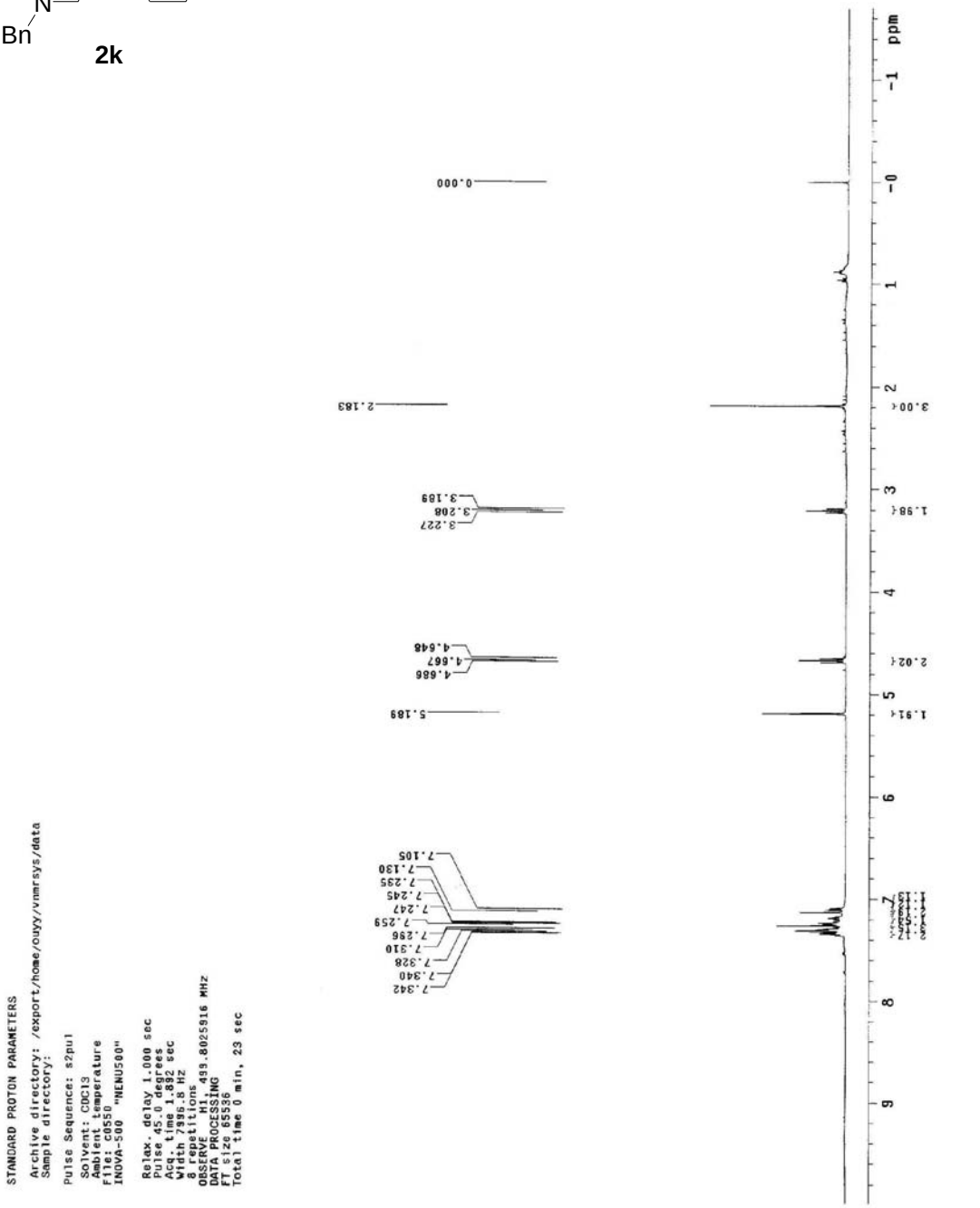

O
O
N
N
Bn

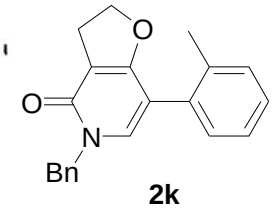
2j


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c0563
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
27.191
40.421
51.245
73.208
76.744
77.000
77.252
109.401
111.175
112.465
127.786
128.007
128.068
128.263
128.774
128.919
135.191
149.940
160.287
166.013
ppm
0
20
40
60
80
100
120
140
160
180
200
220

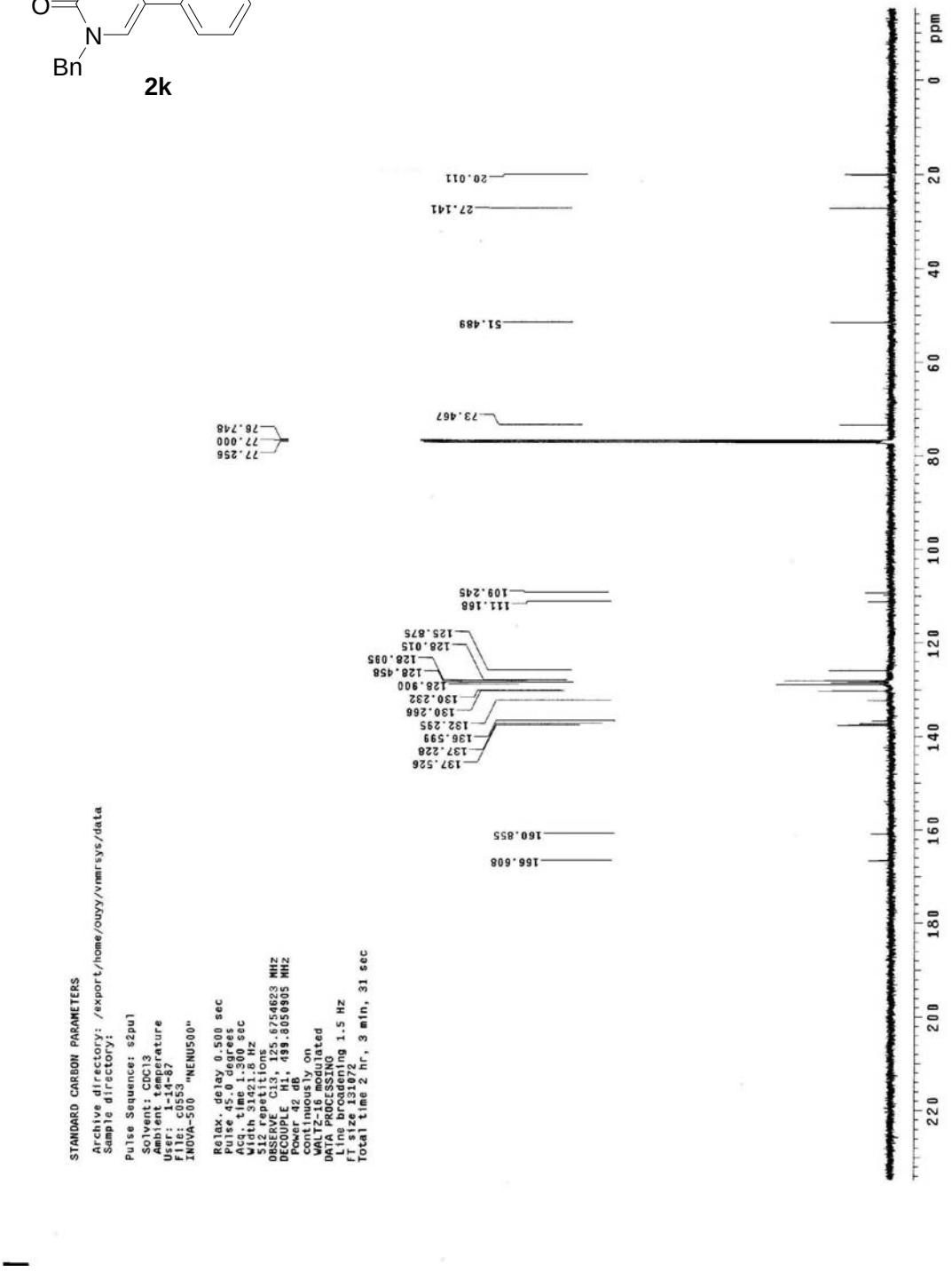

O
O
N
Bn

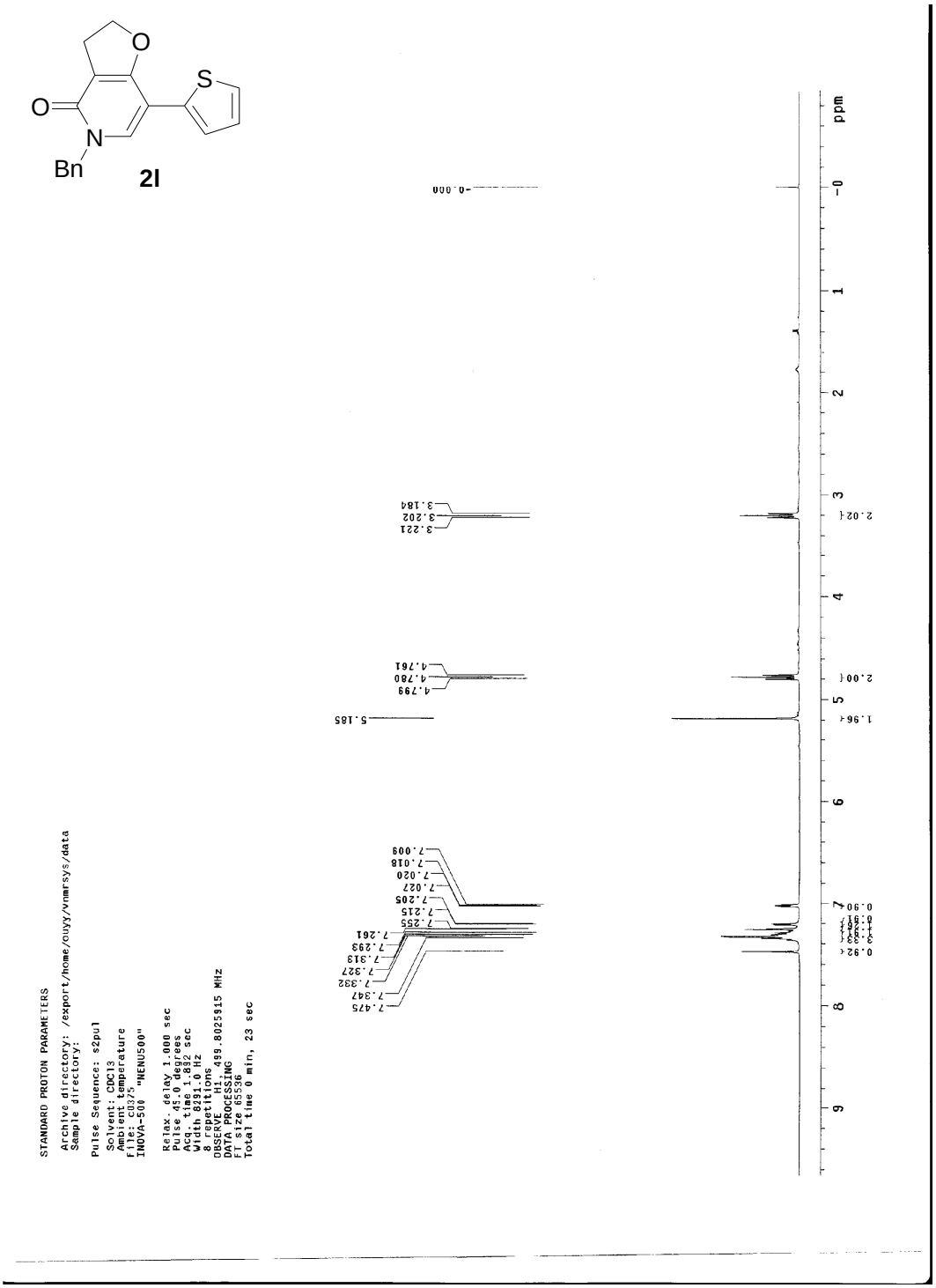
2k

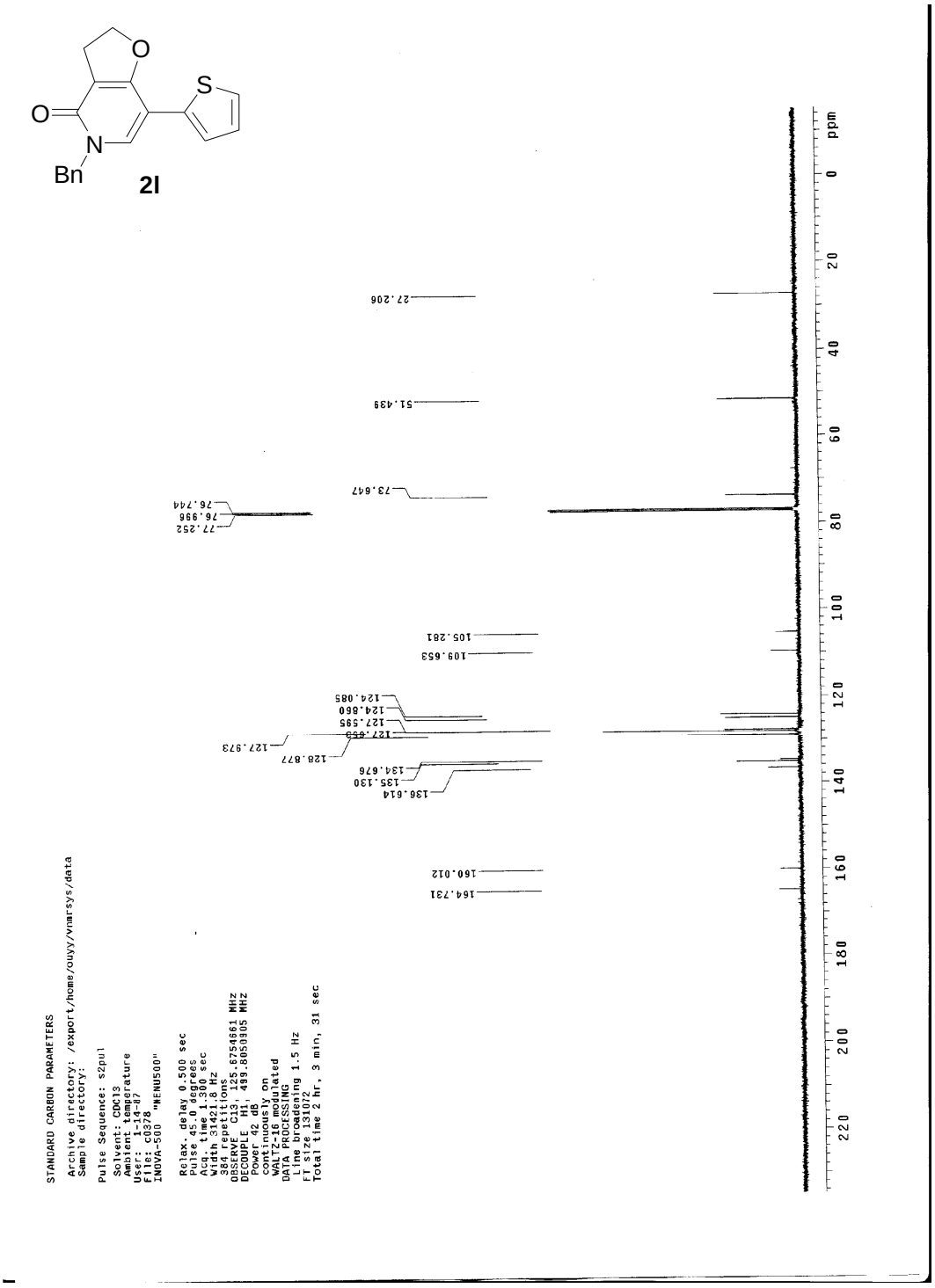

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c0550
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025916 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
0.000
2.183
3.189
3.208
3.227
4.648
4.667
4.686
5.189
7.105
7.130
7.235
7.245
7.247
7.259
7.286
7.310
7.328
7.340
7.342
ppm

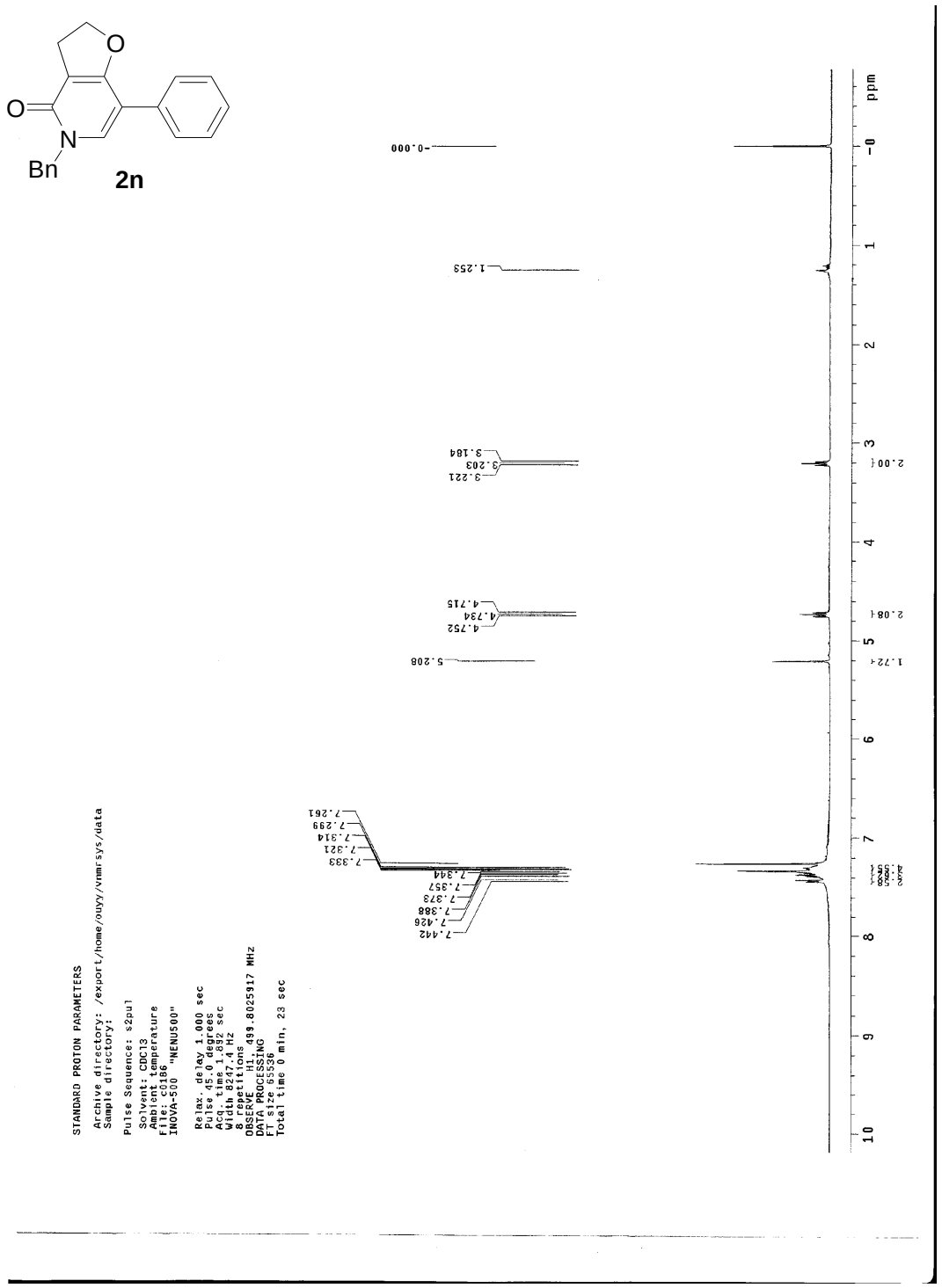

O
O
N
Bn

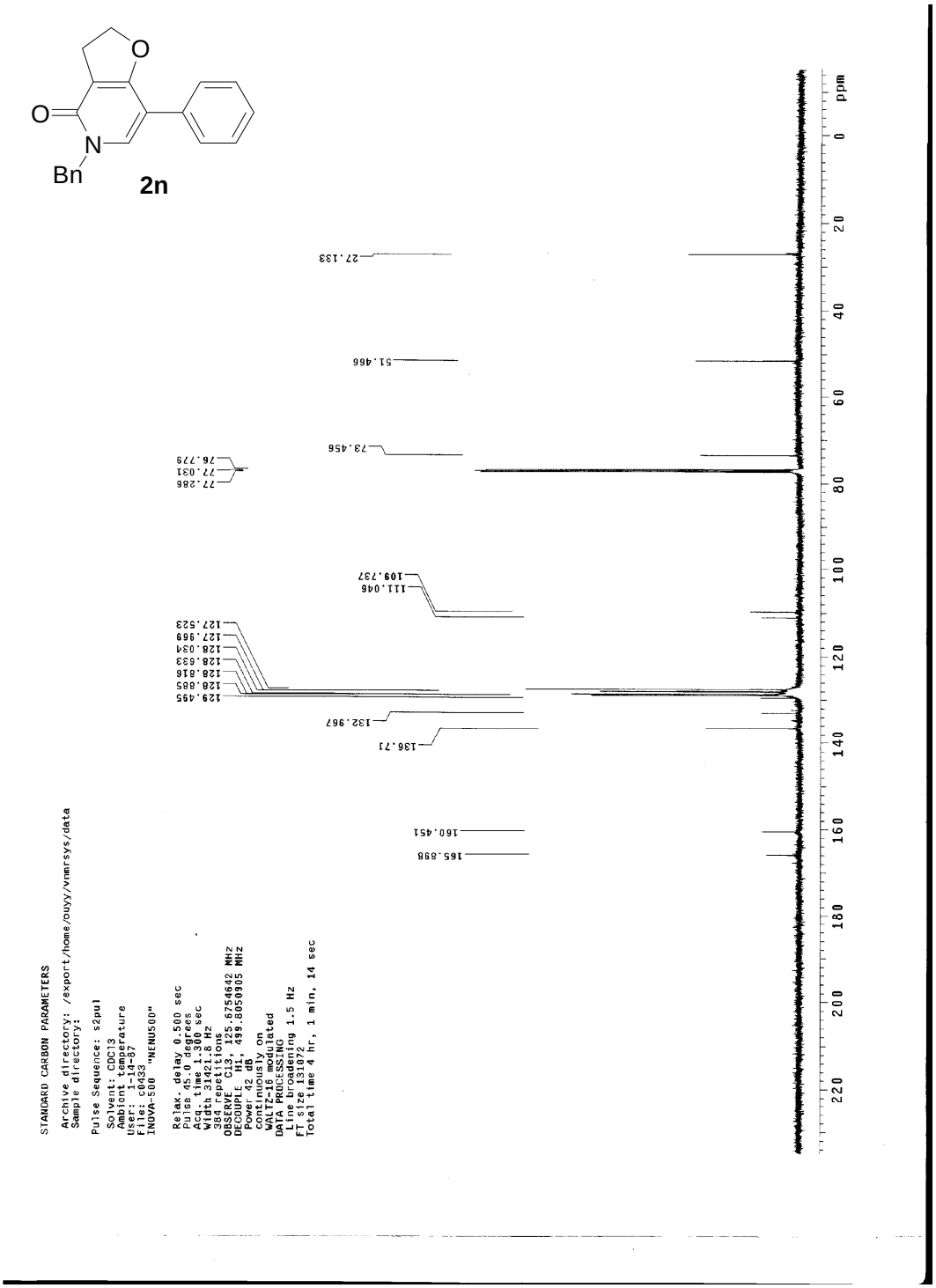
2k

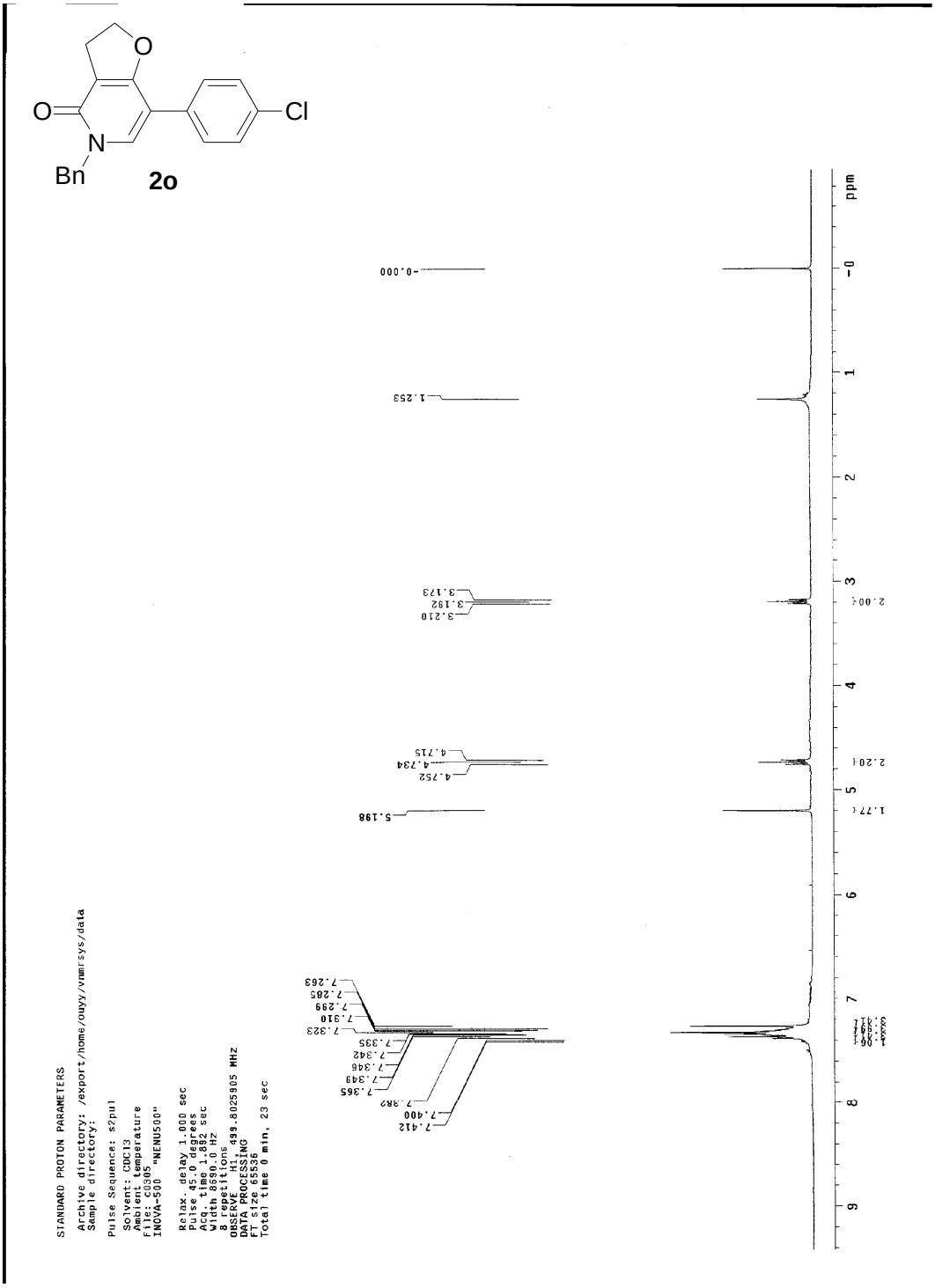

20.011
27.141
51.489
73.467
77.256
77.000
78.748
109.245
111.188
125.875
128.015
128.095
128.458
128.900
130.232
130.266
132.295
136.599
137.228
137.526
160.855
166.608
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c0553
INOVA-500 "NENUS00"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
512 repetitions
OBSERVE C13, 125.6754823 MHz
DECOUPLE H1, 499.6059605 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec

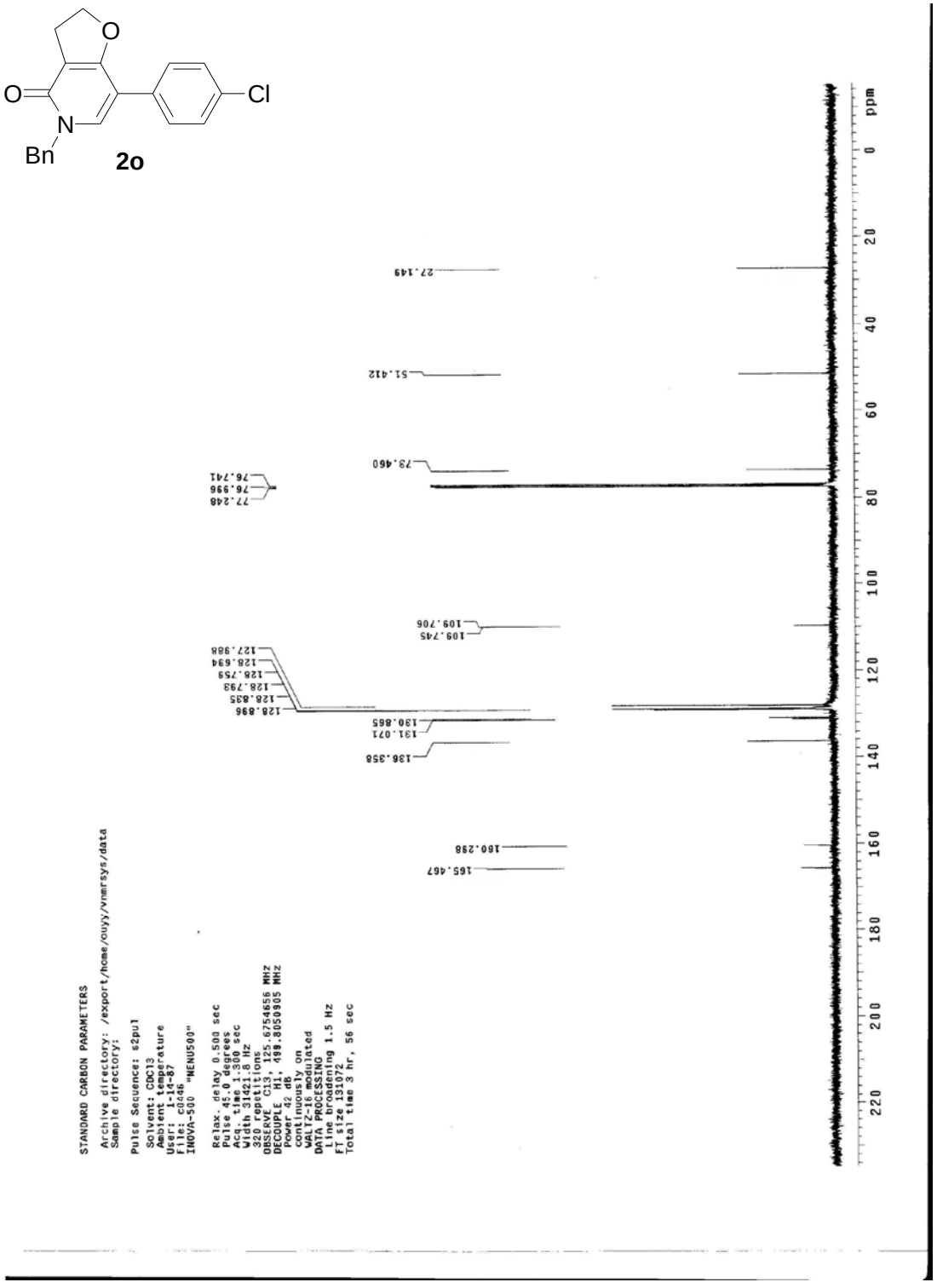

O
S
O
N
Bn
2l
STANDARD PROTON PARAMETERS
Archive directory: /export/home/cuyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: CD375
INOVA-500 "WENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8191.0 Hz
8 repetitions
OBSERVE H1, 499.8025915 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
0.000
3.184
3.202
3.221
4.761
4.780
4.799
5.185
7.009
7.018
7.020
7.027
7.205
7.215
7.255
7.261
7.293
7.313
7.327
7.332
7.347
7.475
ppm
2.02
2.00
1.96
0.92

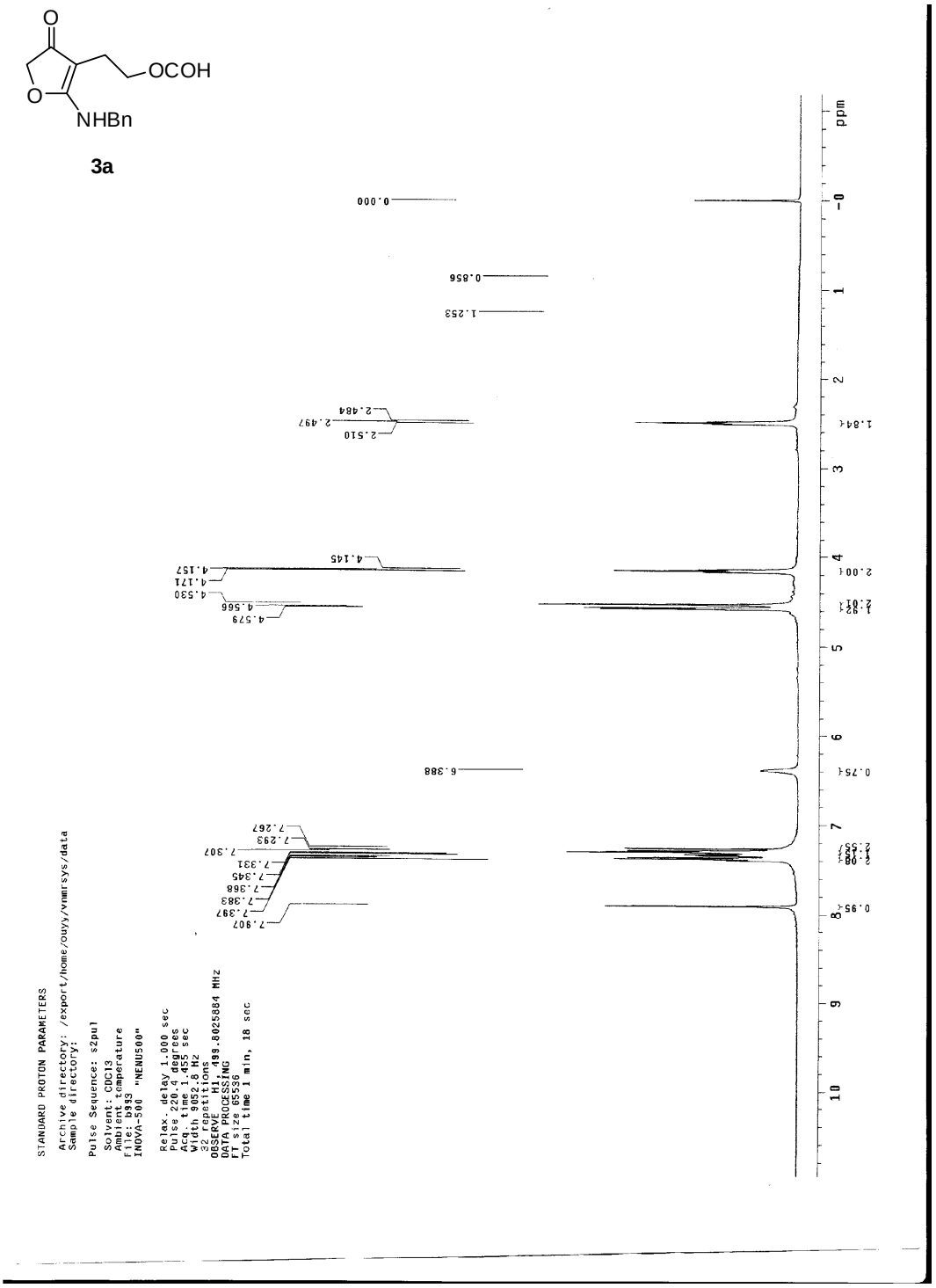

O
S
O
N
Bn
2l
27.206
51.439
73.647
76.744
76.998
77.252
105.281
109.653
124.085
124.660
127.595
127.659
127.973
128.877
134.676
135.130
136.614
160.012
164.731
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: c8378
INOVA-500 "WENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
384 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8053805 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec

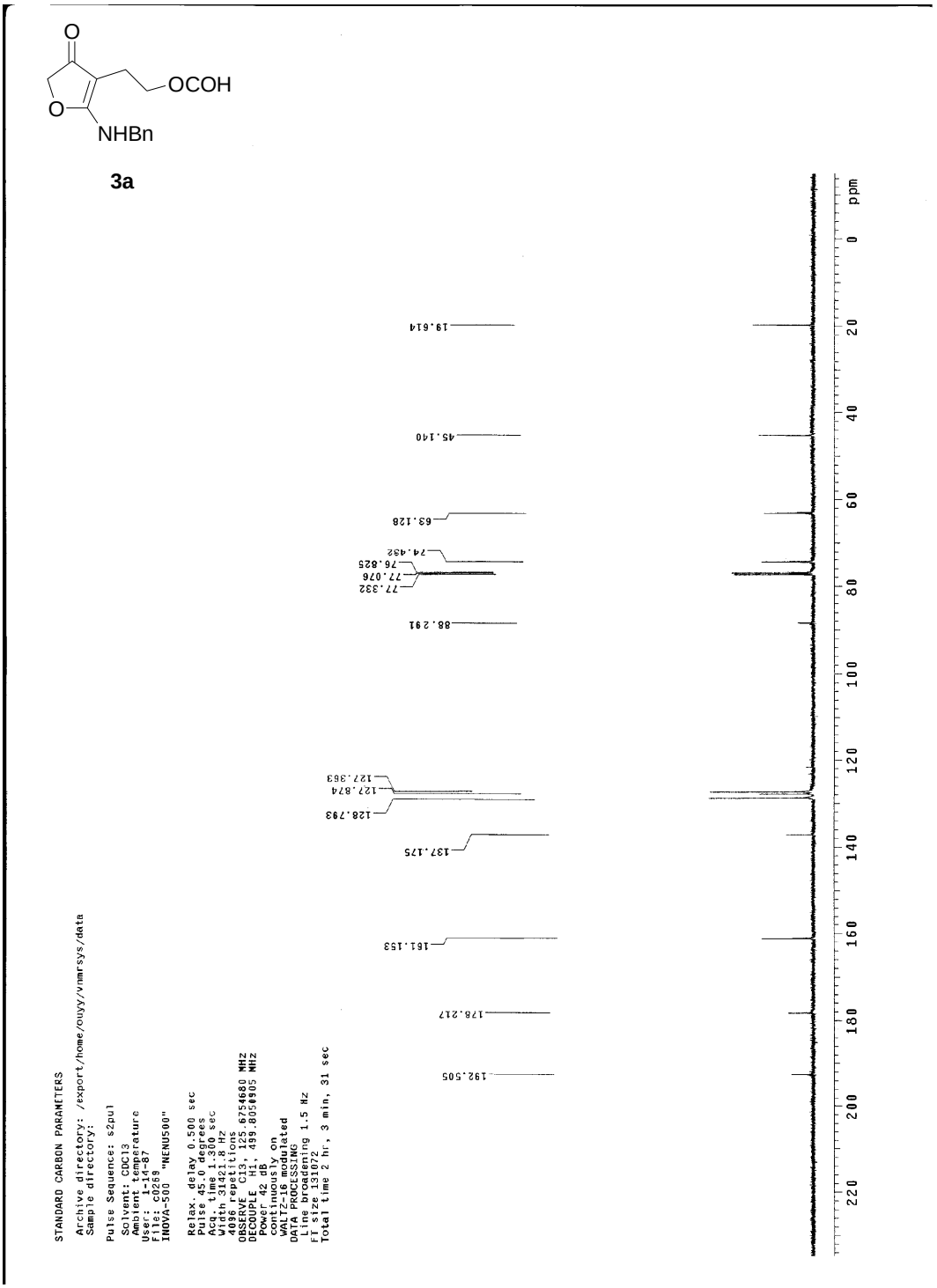

O
O
N
Bn
2n
0.000
1.253
3.184
3.203
3.221
4.715
4.734
4.752
5.208
7.261
7.299
7.314
7.321
7.333
7.344
7.357
7.373
7.388
7.426
7.442
ppm
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c08 "NENU500"
INOVA-500
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8247.4 Hz
8 repetitions
OBSERVE H1 499.8025917 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec

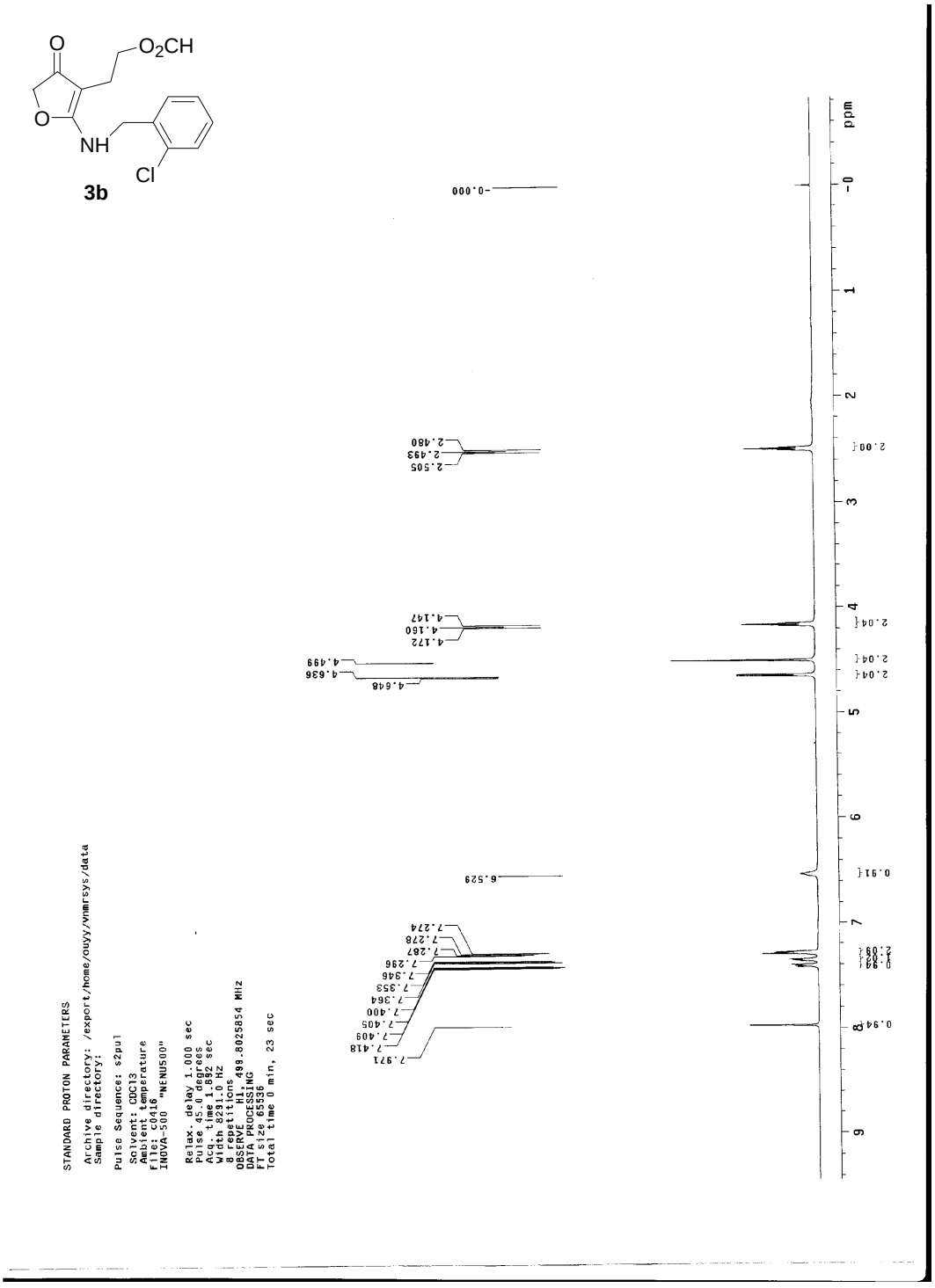

O
O
N
Bn
2n
27.133
51.466
73.456
76.779
77.031
77.286
109.737
111.046
127.523
127.969
128.034
128.633
128.816
128.885
129.495
132.967
136.71
160.451
165.898
0
20
40
60
80
100
120
140
160
180
200
220
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: c0433
INOVA-500 "WENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31446.8 Hz
384 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 4 hr, 1 min, 14 sec

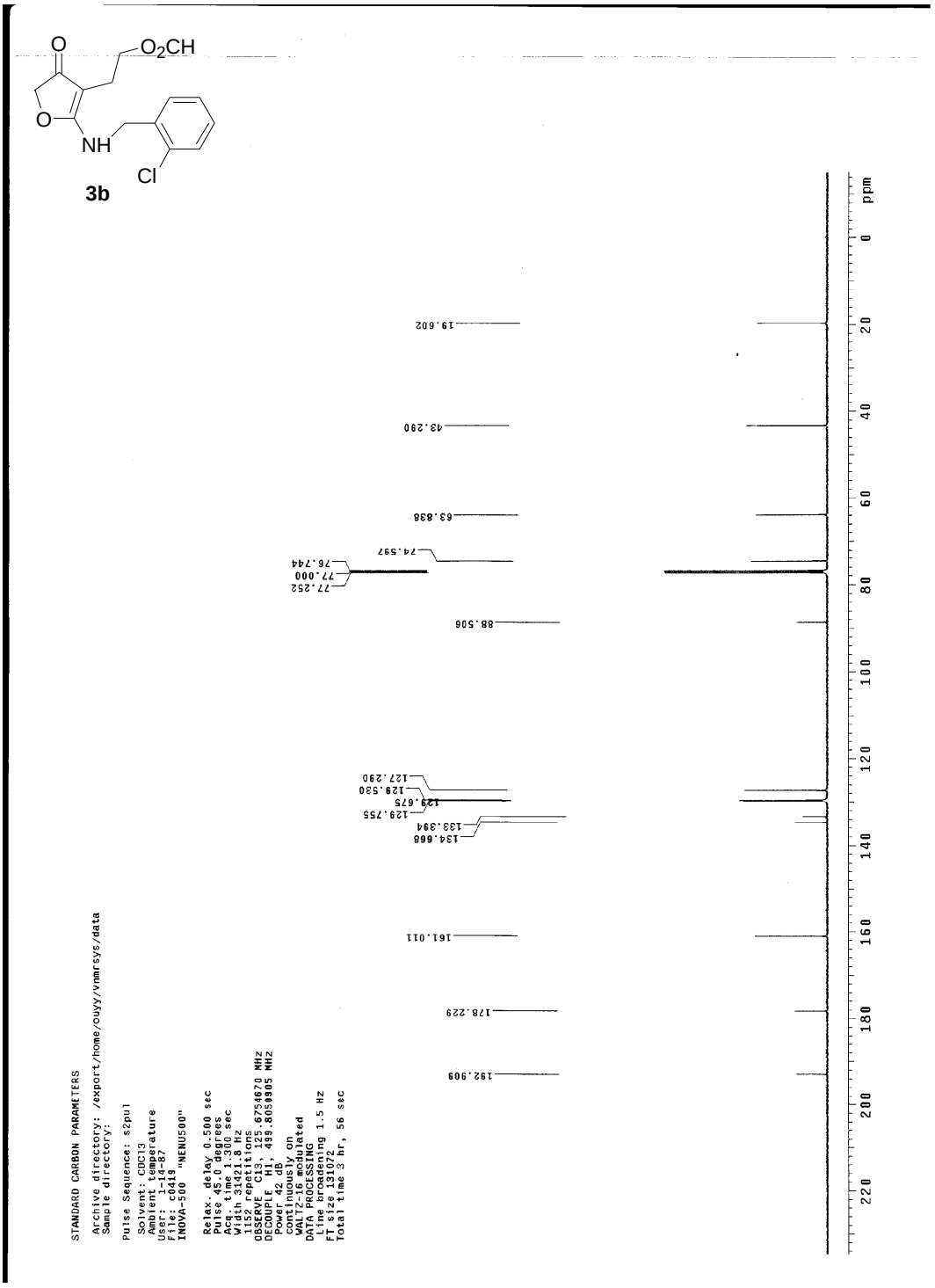

O
O
N
Bn
Cl
2o
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: C:\05 "NENU500"
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8680.0 Hz
8 repetitions
OBSERVE H1, 499.8025905 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
0.000
1.253
3.173
3.192
3.210
4.715
4.734
4.752
5.198
7.263
7.285
7.299
7.310
7.323
7.335
7.342
7.348
7.349
7.365
7.382
7.400
7.412
ppm

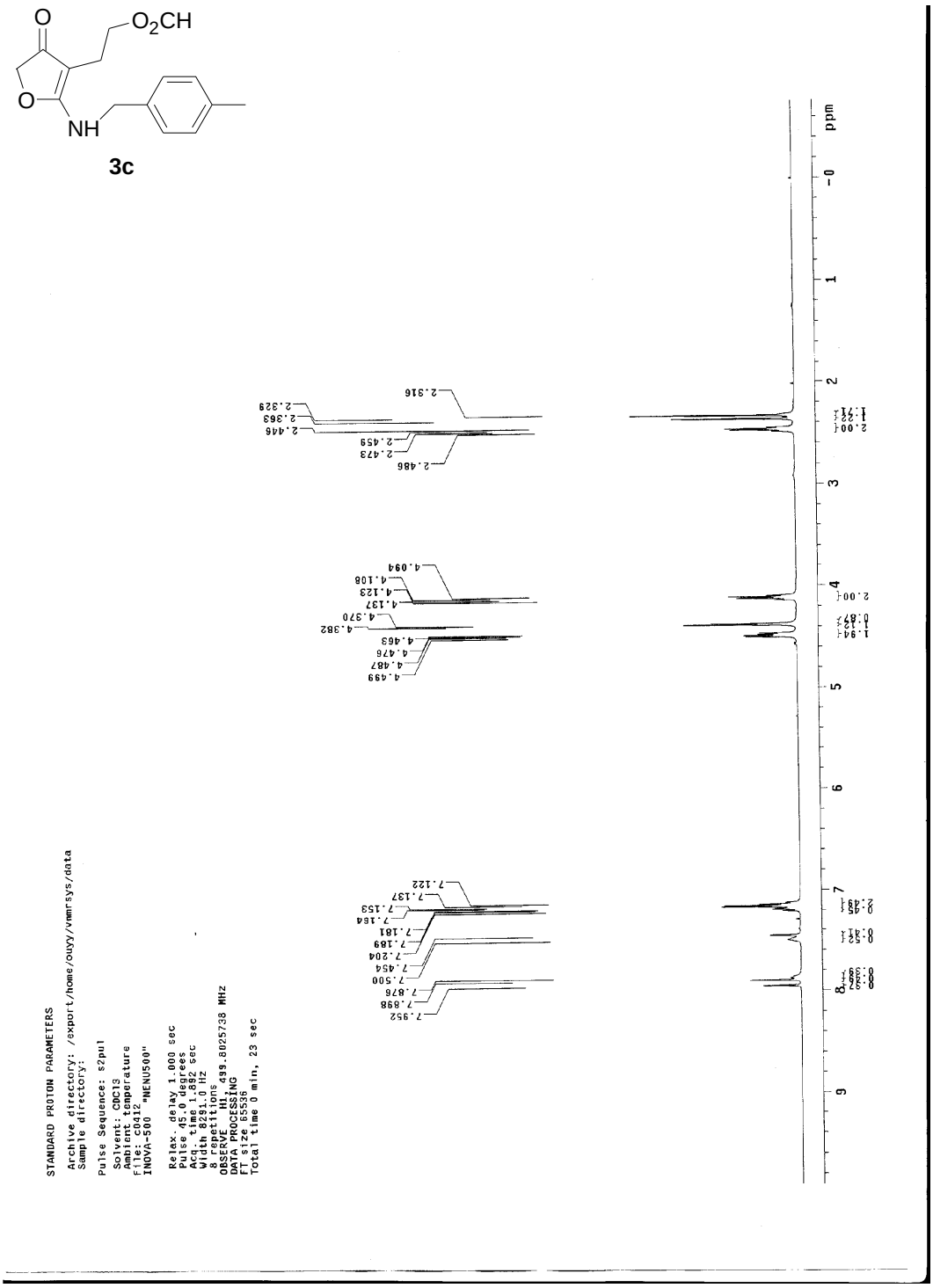

O
O
N
Bn
Cl
2o
27.149
51.412
73.460
76.741
76.996
77.248
109.706
109.745
127.988
126.694
126.759
126.793
126.835
126.896
130.865
131.071
136.358
160.286
165.467
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-id-87
File: cole
INOVA-500 "WENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
320 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8059905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec

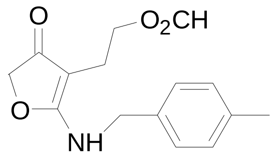

O
OCOH
O
NHBn
3a
0.000
0.856
1.253
2.484
2.497
2.510
4.145
4.157
4.171
4.530
4.566
4.579
6.388
7.267
7.293
7.307
7.331
7.345
7.368
7.383
7.397
7.907
ppm
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: b993
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 220.4 degrees
Acq. time 1.455 sec
Width 8012.8 Hz
32 repetitions
OBSERVE H1, 499.8025884 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 18 sec


O
OCOH
O
NHBn
3a
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c0269
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.800 sec
Width 31212.8 Hz
4096 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8059905 MHz
Power 42 dB
continuously ON
WALTZ16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
19.614
45.140
63.128
74.482
76.825
77.076
77.332
88.291
127.363
127.874
128.793
137.175
161.153
178.217
192.505
ppm
0
20
40
60
80
100
120
140
160
180
200
220

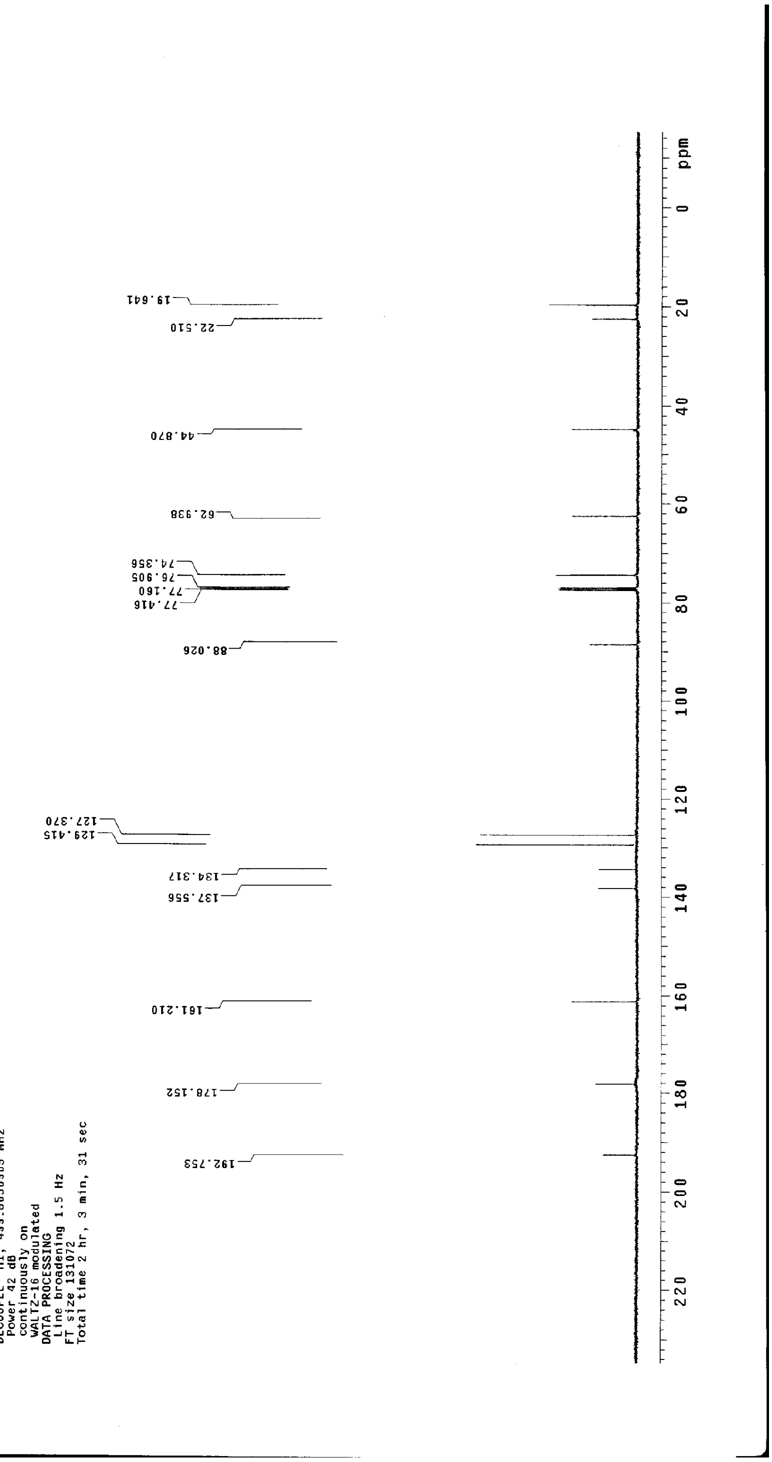

O
O2CH
O
NH
Cl
3b
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c0416 "NENU500"
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.842 sec
Width 8011.0 HZ
8 repetitions
OBSERVE H1, 499.8025854 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
0.000
2.480
2.493
2.505
4.147
4.160
4.172
4.488
4.636
4.648
6.529
7.274
7.278
7.287
7.296
7.346
7.353
7.364
7.400
7.405
7.409
7.418
7.971
ppm

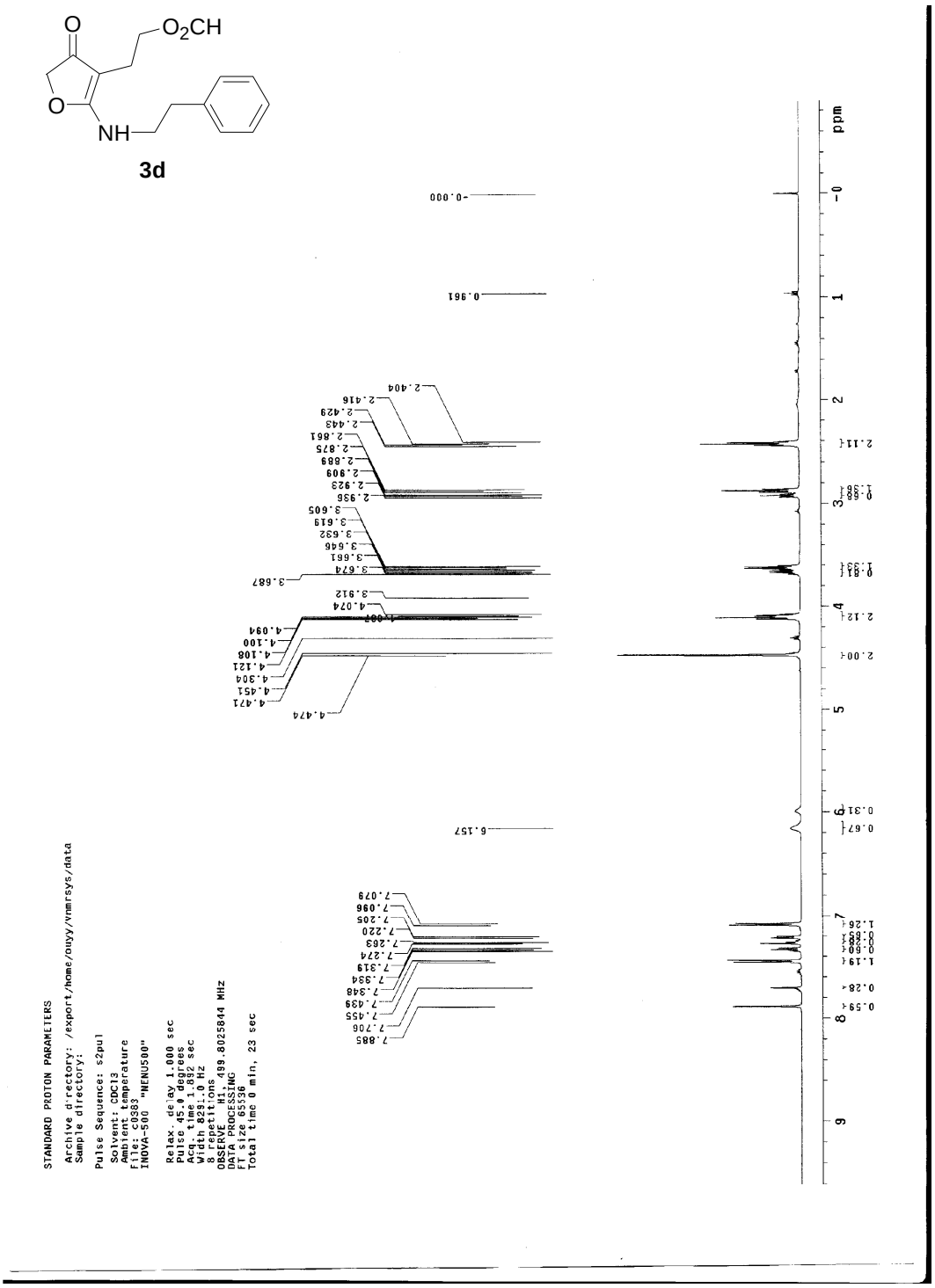

O
O2CH
O
NH
Cl
3b
19.602
43.290
63.838
74.597
76.744
77.000
77.252
88.506
127.290
129.580
129.673
129.755
133.394
134.668
161.011
178.229
192.909
0
20
40
60
80
100
120
140
160
180
200
220
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: tq-87
File: c013
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
1500 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8059905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec

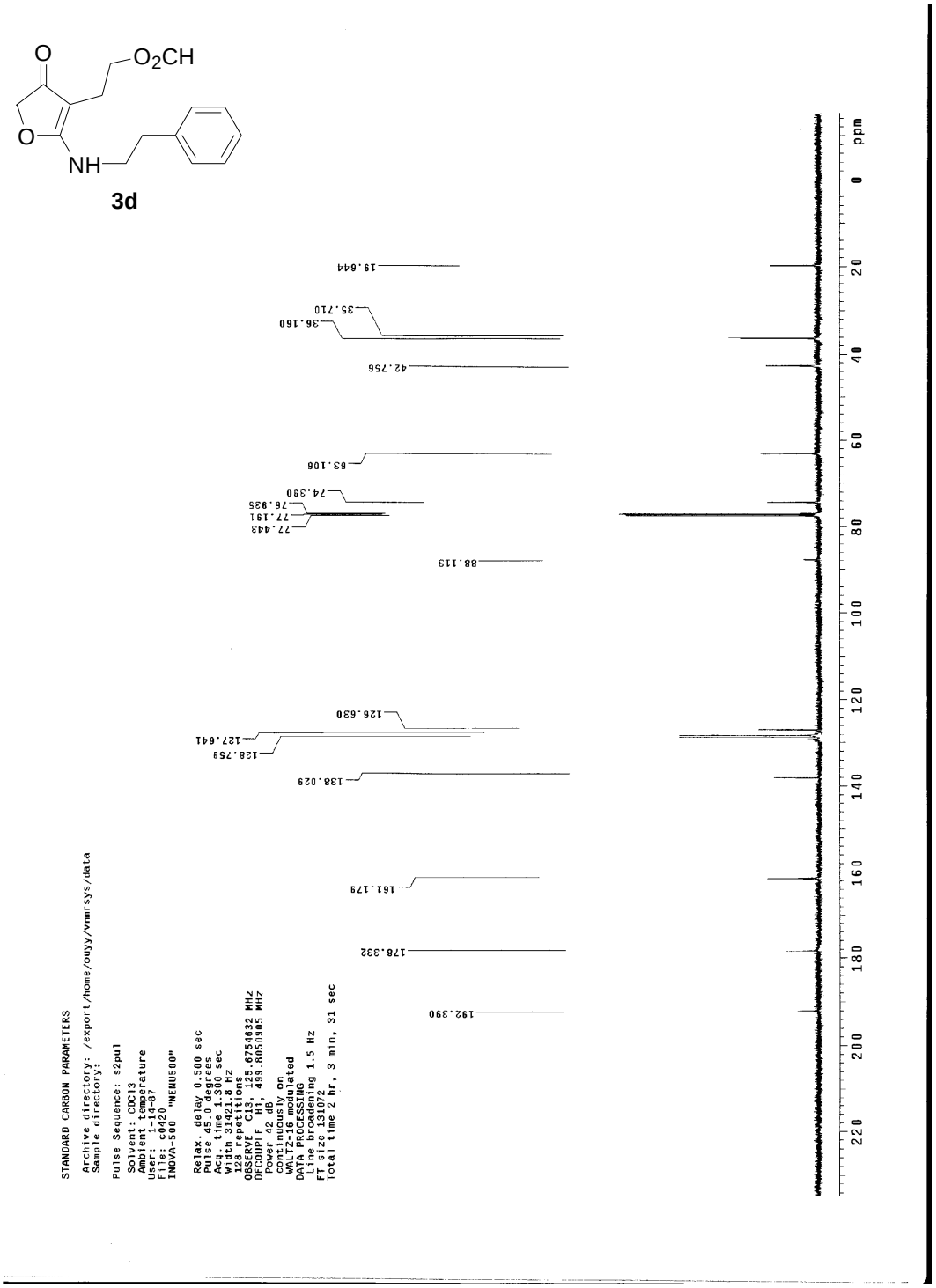

O
O2CH
O
NH
3c
2.316
2.329
2.383
2.446
2.459
2.473
2.486
4.094
4.108
4.123
4.137
4.370
4.382
4.463
4.476
4.487
4.499
7.122
7.137
7.153
7.164
7.181
7.189
7.204
7.454
7.500
7.876
7.898
7.952
ppm
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: cd12 "NENU50"
INOVA-500 "NENU50"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8291.0 Hz
8 repetitions
OBSERVE H1, 499.8025738 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec

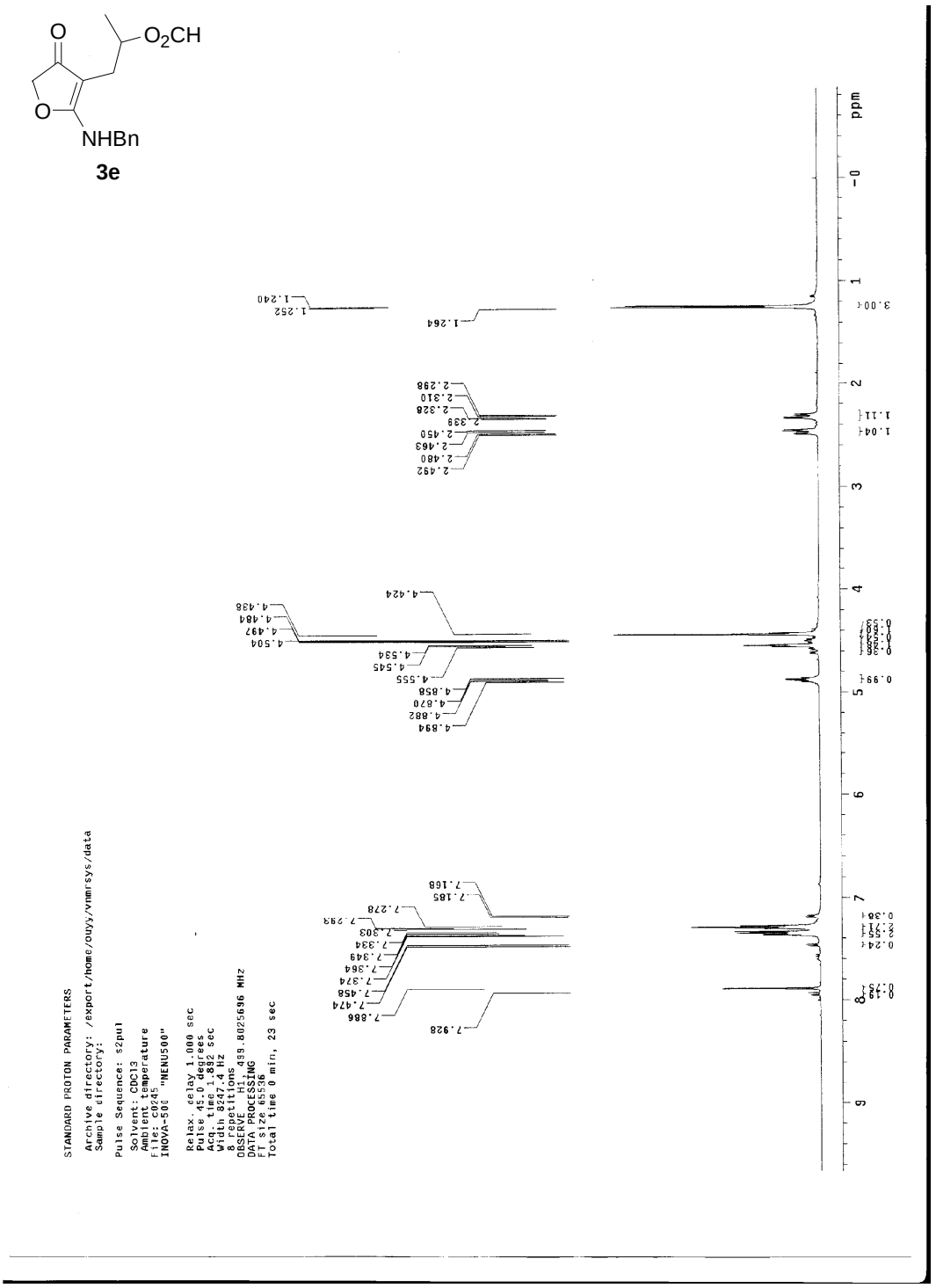

O
O2CH
O
NH

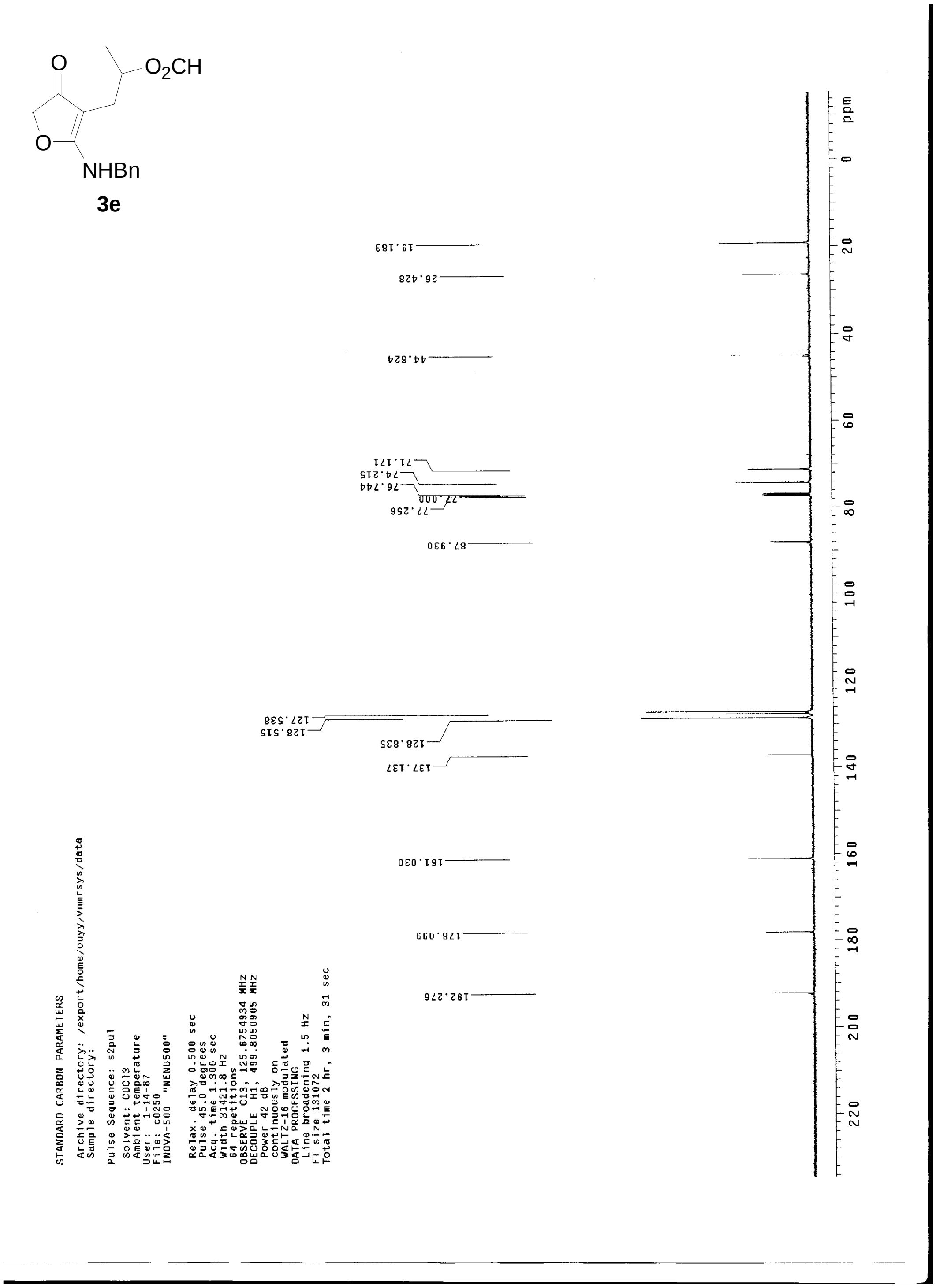
3c

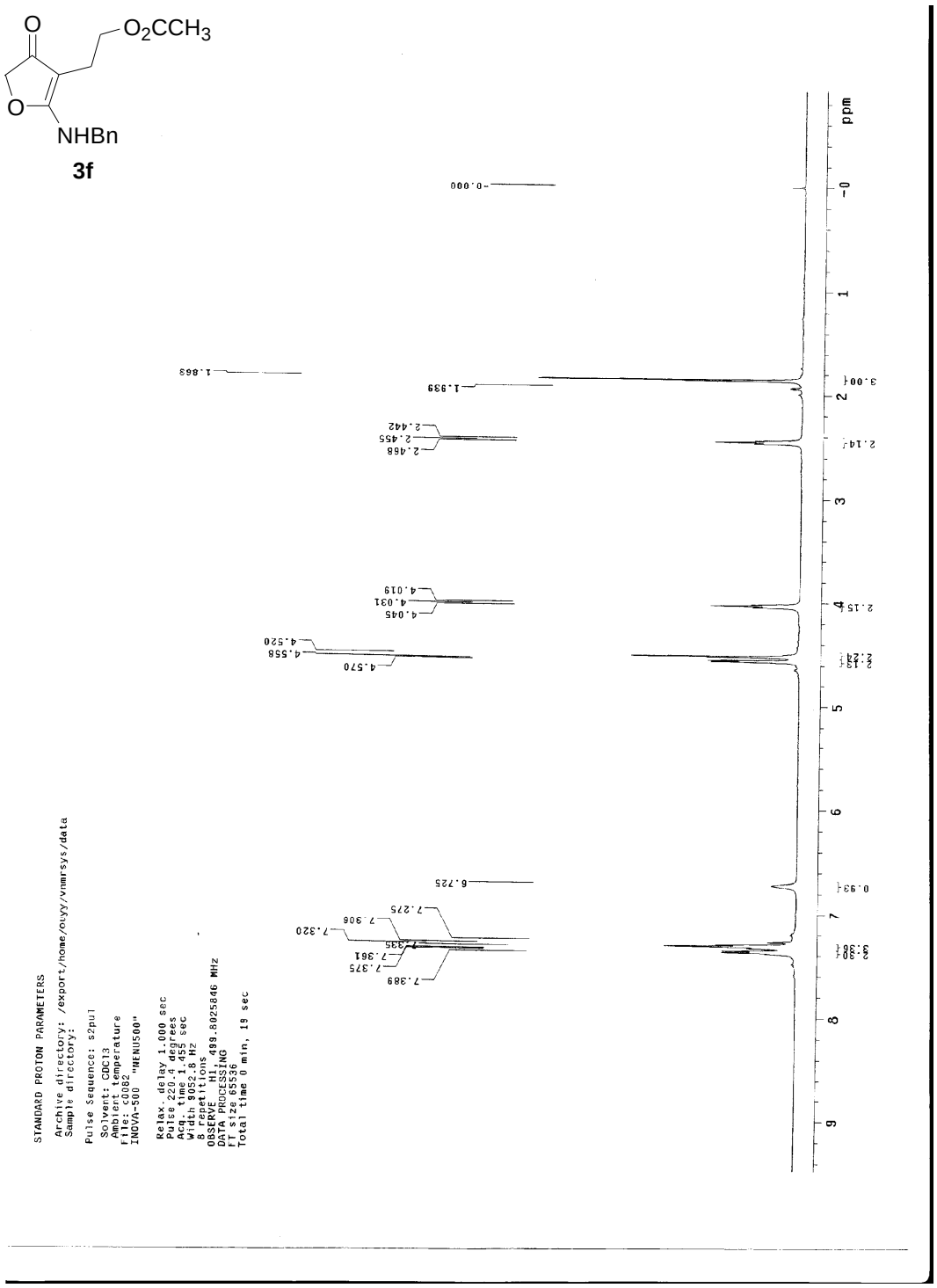

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: c0415
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754646 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
19.641
22.510
44.870
62.938
74.356
76.905
77.160
77.416
88.026
127.370
129.415
134.317
137.556
161.210
178.152
192.753
ppm
0
20
40
60
80
100
120
140
160
180
200
220

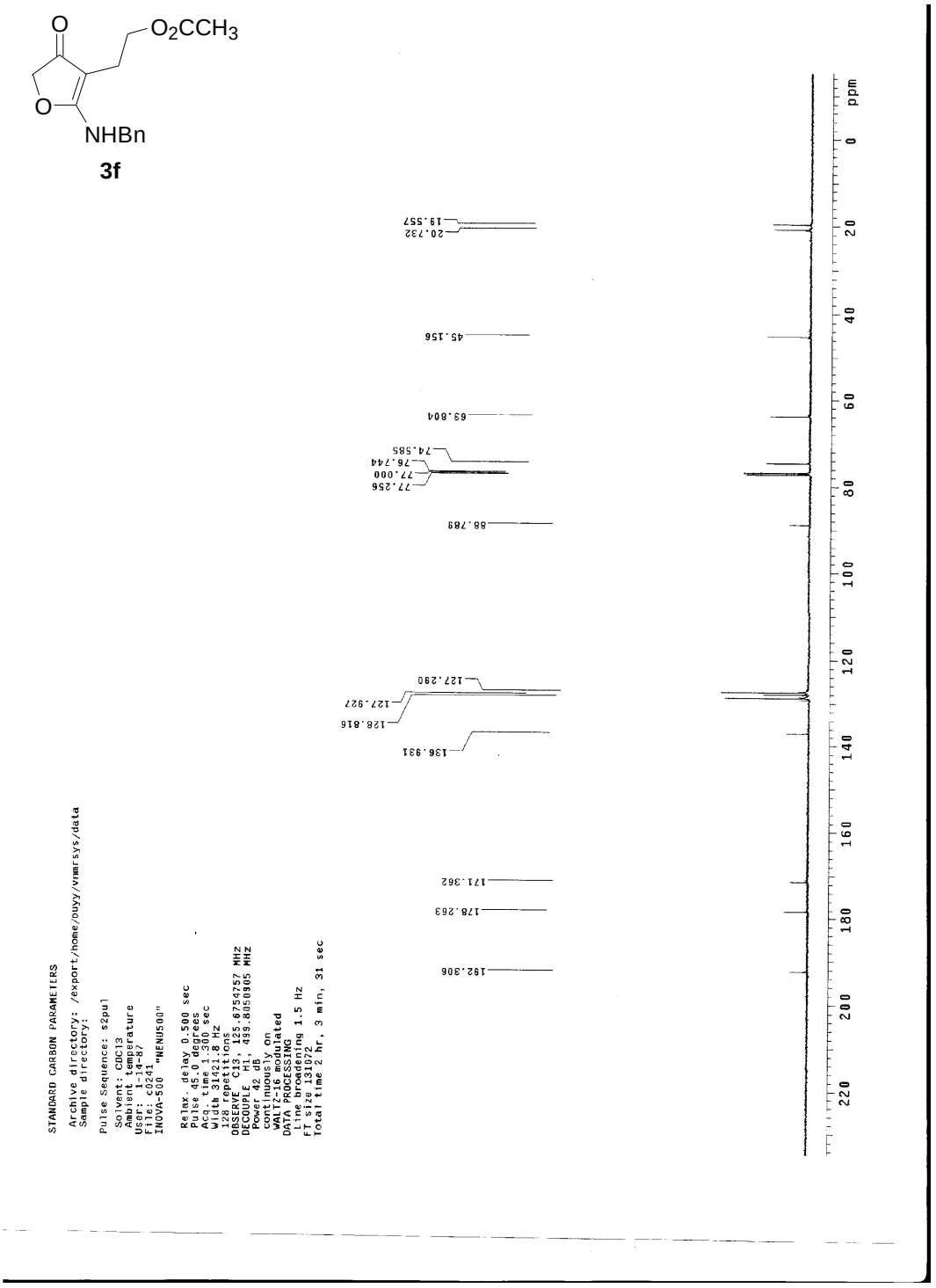

O
O2CH
O
NH
3d
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: C0383
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 8231.0 Hz
8 repetitions
OBSERVE H1, 499.8025844 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

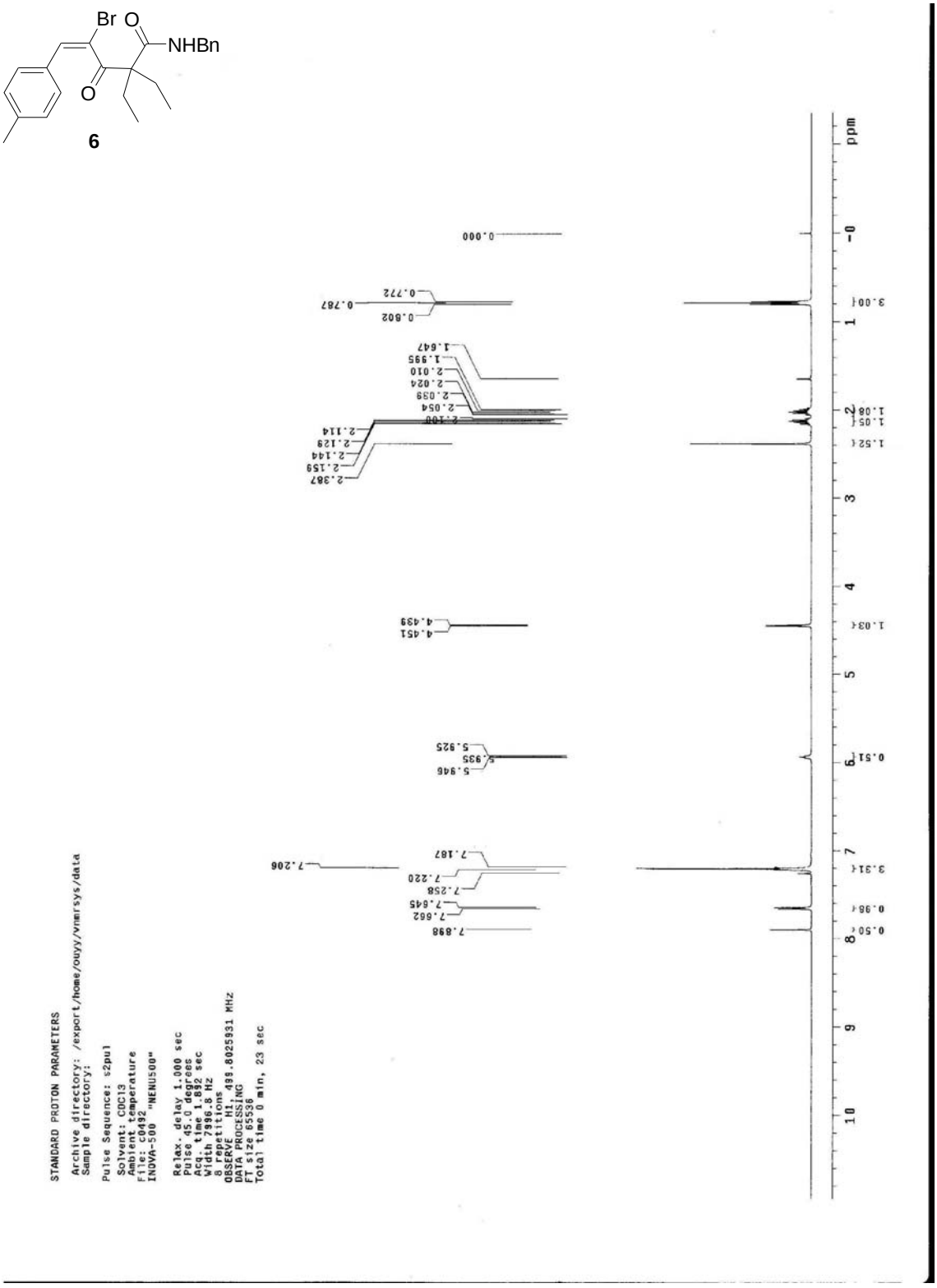

O
O2CH
O
NH
3d
19.644
35.710
36.160
42.756
63.106
74.390
76.935
77.181
77.443
88.113
126.630
127.641
128.759
138.029
161.179
178.332
192.390
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: liq-87
File: c020
INOVA-500 "MENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754632 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec


O
O2CH
O
NHBn
3e
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c0245
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8247.4 Hz
8 repetitions
OBSERVE H1, 499.8025696 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm




O
O2CCH3
O
NHBn
3f
ppm
0.000
1.868
1.889
2.442
2.455
2.468
4.019
4.031
4.045
4.520
4.558
4.570
6.725
7.275
7.308
7.320
7.335
7.361
7.375
7.389
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c082.fid
INOVA-500 "WENU500"
Relax. delay 1.000 sec
Pulse 220.4 degrees
Acq. time 1.455 sec
Width 9052.8 Hz
8 repetitions
OBSERVE H1, 499.8025846 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 19 sec


O
O2CCH3
O
NHBn
3f
19.557
20.732
45.156
63.804
74.585
76.744
77.000
77.256
88.789
127.290
127.927
128.816
136.931
171.362
178.263
182.306
ppm
0
20
40
60
80
100
120
140
160
180
200
220
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c0241 "MENUS60"
INOVA-500
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.380 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754757 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec


Br
O
NHBn
O
6
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c0492
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 7998.8 Hz
8 repetitions
OBSERVE H1, 499.8025931 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm