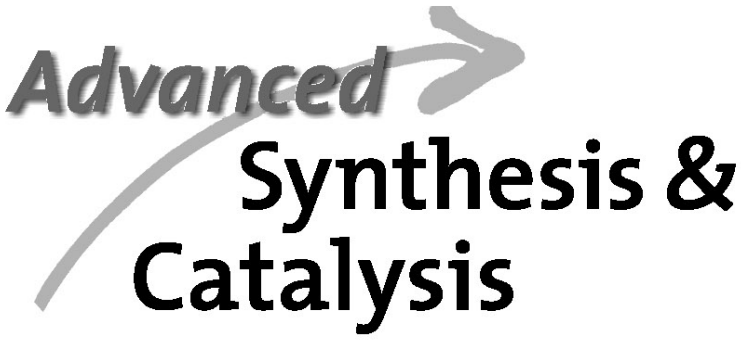

Supporting Information

Domino Reaction of Acyclic α,α-Dialkenoylketene (*S*,*S*)-Acetals and Diamines: Efficient Synthesis of Tetracyclic Thieno[2,3-*b*]thiopyran Fused Imidazo[1,2-*a*]pyridine/pyrido[1,2-*a*]pyrimidines

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Supporting Information

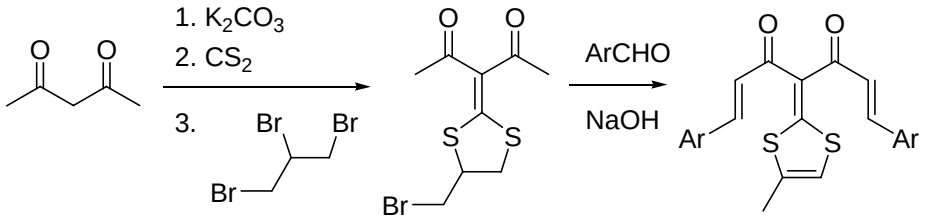
Table of Contents

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 300-400 mesh. ^{1}H (500 Hz) and ^{13}C (125 Hz) NMR spectra were recorded at 25 ºC on a 500 MHz NMR spectrometer, and TMS as internal standard. IR spectra (KBr) were recorded in the range of 400 ~ 4000 cm^{-1}.

II. Synthesis and the analytical data of the substrates 4 and 2a-2g.

Precursors **2a-2g** were synthesized by a two-step reaction starting from pentane-2,4-dione in excellent yields according to the literature: (a) Wang, M.; Xu, X.; Liu, Q.; Xiong, L.; Yang, B.; Gao, L. *Synth. Comm.* **2002**, *32*, 3437–3443. (b) Choi, E. B.; K.Youn, I.; Pak, C. S. *Synthesis* **1991**, 15–18.

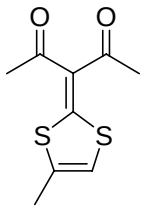


General description for the preparation of **4**: To a solution of pentane-2,4-dione (10.12 mL, 100 mmol) and anhydrous K_2CO_3 (30.1 g, 220 mmol) in DMF (150 mL) was added CS_2 (6.7 mL, 110 mmol) at room temperature. After 30 min, 1,2,3-tribromopropane was added in one portion to the reaction mixture under ice bath and stirred overnight at room temperature. A white solid was obtained after pouring the reaction mixture into ice-water (800 mL). The only product was characterized as 3-(4-bromomethyl-[1,3]dithiolan-2-ylidene)-pentane-2,4-dione **4** with an excellent yield of 91%.

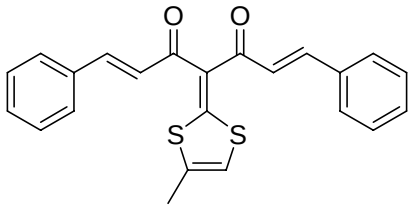
General Procedure for the preparation of **2a-2g**: (with **2a** as an example): To a solution of **4** (295 mg, 1.0 mmol) and benzaldehyde (222.6 mg, 1.0 mmol) in EtOH (10.0 mL) at 0 ºC was added NaOH (200 mg, 5.0 mmol) in one portion. The reaction mixture was stirred at 0 ºC for 10 min, followed by stirring at 25 ºC for 0.5 h. After the starting material **4** was consumed as indicated by TLC, the resulting mixture was then poured

onto ice-water (250 mL) under stirring. The precipitated solid was collected by filtration, washed with water (3 × 30 mL), and dried in *vacuo* to afford the product **2a** as a yellow solid.

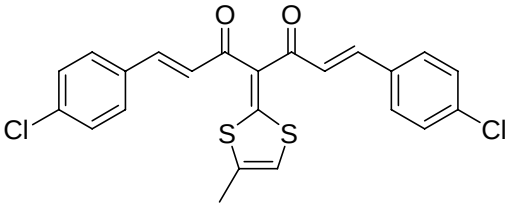
1: White solid. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 2.43 (s, 3H, CH_3), 2.46 (s, 3H, CH_3), 3.46-3.50 (m, 2H), 3.57-3.62 (m, 1H), 3.66-3.69 (m, 1H), 4.02 ppm (m, 1H); IR (KBr, cm^{-1}): ν = 2926, 1619, 1439, 1402, 1269, 1261, 885.



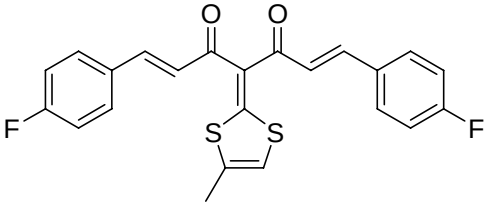
2a: Yellow solid, m.p. 198 ºC. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ 2.49 (s, 3H), 6.96 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 4H), 7.38 (d, *J* = 16.0 Hz, 1H), 7.52 (m, 5H), 7.77 (d, *J* = 16.0 Hz, 2H); IR (KBr, cm^{-1}) IR (KBr, cm^{-1}): ν = 1628, 1572, 1539, 1543, 1370, 1304, 1169. Anal. calcd for $C_{23}H_{18}OS_2$: C, 70.74; H, 4.65; Found: C, 70.78; H, 4.62.



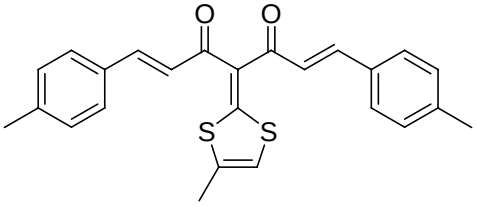
2b: Yellow solid, m.p. 192 ºC. ^{1}H NMR (600 MHz, $CDCl_3$, 293 K, TMS): δ = 2.49 (s, 3H), 6.96 (s, 1H), 7.29 (d, *J* = 8.0 Hz, 4H), 7.29 (d, *J* = 16.0 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 4H), 7.69 (d, *J* = 16.0 Hz, 2H); IR (KBr, cm^{-1}): ν = 1740, 1628, 1560, 1491, 1455, 1370, 1224, 1093.



2c: Yellow solid, m.p. 186 ºC. ^{1}H NMR (600 MHz, $CDCl_3$, 293 K, TMS): δ = 2.48 (s, 3H), 6.94 (s, 1H), 6.98 (m, 4H), 7.23 (d, *J* = 16.0 Hz, 2H), 7.50 (m, 4H), 7.68 (d, *J* = 16.0 Hz, 2H); IR (KBr, cm^{-1}): ν = 3068, 1629, 1576, 1544, 1508, 1451, 1418, 1230.

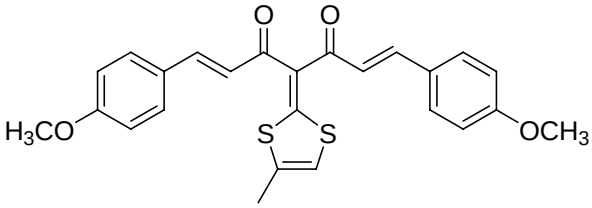


2d: Yellow solid, m.p. 190 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, 293 K, TMS): δ = 2.35 (s, 6H, 2 × Me), 2.46 (s, 3H), 6.90 (s, 1H), 7.12 (d, *J* = 8.0 Hz, 4H), 7.29 (d, *J* = 16.0 Hz, 2H),

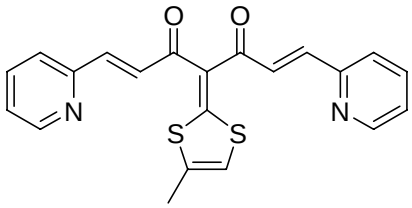


7.43 (d, J = 8.0 Hz, 4H), 7.75 (d, J = 16.0 Hz, 2H); IR (KBr, cm^{-1}): ν = 3070, 1630, 1595, 1517, 1441, 1412,1341, 1224.

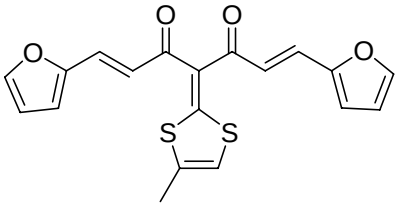
2e: Yellow solid, m.p. 188 ºC. ^{1}H NMR (600 MHz, $CDCl_3$, 293 K, TMS): δ = 2.46 (s, 3H), 3.82 (s, 6H, 2 × OMe), 6.84 (d, J = 8.0 Hz, 4H), 6.89 (s, 1H), 7.22 (d, J = 16.0 Hz, 2H), 7.48-7.49 (d , J = 6.0 Hz, 4H), 7.73 (d, J = 16.0 Hz, 2H); IR (KBr, cm^{-1}): ν = 3058, 2928, 2837, 1624, 1604, 1567, 1511, 1449, 1366, 1255. Anal. calcd for $C_{25}H_{22}O_4S_2$: C, 66.64; H, 4.92; Found: C, 66.81; H, 4.88.



2f: Yellow solid, m.p. 183 ºC. ^{1}H NMR (600 MHz, $CDCl_3$, 293 K, TMS): δ = 2.50 (s, 3H), 6.98 (s, 1H), 7.20 (m, 2H), 7.50 (m, 2H), 7.62 (m, 2H), 7.70 (d, J = 16.0 Hz, 2H), 7.70 (d, J = 16.0 Hz, 2H), 8.52 (m, 2H); IR (KBr, cm^{-1}): ν = 3400, 3024, 1633, 1575, 1538, 1462, 1364, 1293, 1227.



2g: Yellow solid, m.p. 180 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, 293 K, TMS): δ = 2.45 (s, 3H), 6.45 (m, 2H), 6.64 (m, 2H), 6.89 (s, 1H), 7.18 (d, J = 16.0 Hz, 2H), 7.42 (m, 2H), 7.50 (d, J = 16.0 Hz, 2H); IR (KBr, cm^{-1}): ν = 3399, 2170, 1678, 1628, 1549, 1448, 1364, 1289.



III. Synthesis and the analytical data of products 3

3a: white soild. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.72 (s, 1.5 H, Me), 1.73 (s, 1.5 H, Me), 2.33 (broad, NH, 1H), 2.64 (m, 1 H), 2.74 (m, 2 H), 3.07 (m, NCH_2, 2 H), 3.26 (m, NCH_2, 2 H), 3.40 (m, 1 H), 4.53 (m, 1 H), 4.85 (m, 1 H), 7.27 (m, 1 H), 7.36 (m, 7H), 7.58 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 24.5, 24.8, 28.4, 28.6, 43.3, 43.0,

46.8, 46.9, 47.0, 49.6, 55.6, 78.4, 78.5, 127.3, 127.7, 128.1, 128.6, 129.0, 129.3, 132.0, 132.1, 135.4, 135.5, 137.9, 137.9, 139.2, 141.5, 151.9, 152.0, 190.3, 190.4. IR (KBr, cm^{-1}): ν = 3433, 3030, 2927, 1659, 1453, 1401, 762, 698. MS (EI): calcd *m/z* 432.13, found 433.1 $[(M+1)]^+$; Anal. calcd for $C_{25}H_{24}N_2OS_2$: C, 69.41; H, 5.59; N, 6.48; Found: C, 69.67; H, 5.39; N, 6.52.

3b: white solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.70 (s, 1.5 H, Me), 1.72 (s, 1.5 H, Me), 2.32 (broad, NH, 1H), 2.54 (m, 1 H), 2.70 (m, 2 H), 3.02 (m, NCH_2, 2 H), 3.24 (m, NCH_2, 2 H), 3.38 (m, 1 H), 4.47 (m, 1 H), 4.81 (m, 1 H), 7.36 (m, 6H), 7.51 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 24. 5, 24.7, 28.4, 43.3, 43.9, 46.6, 48.7, 54.8, 78.4, 78.5, 128.7, 129.0, 129.5, 131.9, 132.0, 132.9, 134.8, 135.1, 135.2, 136.3, 136.4, 139.4, 140.1, 151.4, 189.9, 190.0. IR (KBr, cm^{-1}): ν = 3294, 2967, 2885, 1648, 1490, 1431, 1401, 1090, 1013, 842. MS (EI): calcd *m/z* 500.06, found 501.1 $[(M+1)]^+$; Anal. calcd for $C_{25}H_{22}Cl_2N_2OS_2$: C, 59.87; H, 4.42; N, 5.59; Found: C, 60.03; H, 4.39; N, 5.65.

3c: light red solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.71 (s, 1.5 H, Me), 1.73 (s, 1.5 H, Me), 2.33 (broad, NH, 1H, disappeared after D_2O was added), 2.58 (m, 1 H), 2.70 (m, 1H), 2.76 (m, 1H), 3.04 (m, NCH_2, 2H), 3.23 (m, NCH_2, 2H), 3.40 (m, 1 H), 4.49 (m, 1 H), 4.85 (m, 1 H), 7.06 (m, 4H), 7.41 (m, 2H), 7.54 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 24.3, 28.1, 42.9, 43. 6, 46.6, 48.5, 54.6, 78.2, 114.9, 115.1, 115.9, 116.0, 128.9, 128.9, 129.1, 129.2, 131.6, 133.4, 134.9, 136.9, 139.0, 151.3, 160.8, 161.6, 162.8, 163.6, 189.9; IR (KBr, cm^{-1}): ν = 3294, 2969, 2886, 1648, 1509, 1456, 1225, 1157, 835. MS (EI): calcd *m/z* 468.11, found 469.1 $[(M+1)]^+$; Anal. calcd for $C_{25}H_{22}F_2N_2OS_2$: C, 64.08; H, 4.73; N, 5.98; Found: C, 64.21; H, 4.71; N, 5.86.

3d: light red solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.71 (s, 1.5H, Me), 1.74 (s, 1.5H, Me), 2.32 (broad, NH, 1H, disappeared after D_2O was added), 2.36 (s, 2 × ArMe, 6 H), 2.61 (m, 1 H), 2.74 (m, 2 H), 3.02 (m, NCH_2, 2 H), 3.26 (m, NCH_2, 2 H), 3.36 (m, 1 H), 4.50 (m, 1 H), 4.82 (m, 1 H), 7.20 (m, 4H), 7.32 (m, 2H), 7.46 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.1, 21.2, 21.2, 24.4, 24.6, 28.2, 28.4, 43.1, 43.7, 46.7, 49.2, 55.1, 55.1, 78.1, 78.3, 127.3, 127.7, 129.0, 129.7, 131.8, 131.9, 134.7, 134.7, 135.3, 135.4, 136.6, 136.6, 138.3, 138.6, 138.9, 151.8, 151.9, 190.3, 190.4; IR (KBr, cm^{-1}): ν = 3440, 2970, 1658, 1453, 815. MS (EI): calcd *m/z* 460.16, found 461.2 $[(M+1)]^+$; Anal. calcd for $C_{27}H_{28}N_2OS_2$: C, 70.40; H, 6.13; N, 6.08; Found: C, 70.66; H, 6.09; N, 6.21.

3e: yellow solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.70 (s, 1.5 H, Me), 1.73

(s, 1.5 H, Me), 2.27 (broad, NH, 1H), 2.61 (m, 1 H), 2.74 (m, 2 H), 3.02 (m, NCH_2, 2 H), 3.26 (m, NCH_2, 2 H), 3.38 (m, 1 H), 3.82 (s, 2 × OMe, 6 H), 4.46 (m, 1 H), 4.80 (m, 1 H), 6.90 (m, 4H), 7.35 (m, 2H), 7.48 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 24.4, 24.7, 28.2, 28.4, 43.0, 43.7, 46.8, 48.8, 48.8, 54.8, 54.8, 55.2, 55.3, 78.0, 78.2, 113.6, 114.3, 128.5, 128.6, 128.8, 129.6, 1229.6, 131.7, 131.8, 133.4, 135.2, 135.3, 138.8, 151.8, 151.9, 185.5, 159.7, 190.3, 190.4; IR (KBr, cm^{-1}): ν = 3298, 2932, 2834, 1659, 1610, 1512, 1456, 1250, 1176, 1034, 830. MS (EI): calcd *m/z* 492.15, found 493.2 $[(M+1)]^+$; Anal. calcd for $C_{27}H_{28}N_2O_3S_2$: C, 65.83; H, 5.73; N, 5.69; Found: C, 66.02; H, 5.70; N, 5.79.

3f: red solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.74 (s, Me), 1.77 (s, Me), 2.37 (broad, NH, 1H), 2.75 (m, 1H), 2.80 (m, 2H), 3.12 (m, 2H), 3.42 (m, 3H), 4.64 (m, 1H), 5.01 (m, 1 H), 7.23 (m, 1H), 7.28 (m, 1H), 7.40 (m, 1H), 7.52 (m, 1H), 7.72 (m, 2H), 8.64 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 24.1, 24.3, 28.1, 28.2, 43.2, 44.0, 45.2, 50.7, 57.9, 58.0, 78.6, 78.7, 122.0, 122.1, 122.5, 122.4, 122.5, 123.2, 131.8, 131.9, 135.3, 136.4, 137.1, 138.5, 138.6, 149.2, 149.6, 150.7, 150.9, 156.9, 160.2, 189.8, 189.9; IR (KBr, cm^{-1}): ν = 3431, 2924, 2854, 1659, 1589, 1456.

3g: red solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.68 (s, 1.5 H, Me), 1.70 (s, 1.5 H, Me), 2.34 (broad, NH, 1H, disappeared after D_2O was added), 2.73 (m, 3 H), 3.12 (m, NCH_2, 2 H), 3.26 (m, 3 H), 4.56 (m, 1 H), 4.88 (m, 1 H), 6.30 (m, 1 H), 6.37 (m, 3H), 7.41 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 23.8, 24.0, 28.0, 28.2, 41.7, 42.9, 43.7, 44.4, 50.6, 77.8, 77.8, 106.6, 108.2, 110.0, 110.6, 131.4, 131.5, 134.3, 138.7, 138.7, 142.1, 142.9, 150.2, 150.6, 150.7, 154.8, 189.7; IR (KBr, cm^{-1}): ν = 3309, 2971, 2359, 1660, 1456, 1011, 738.

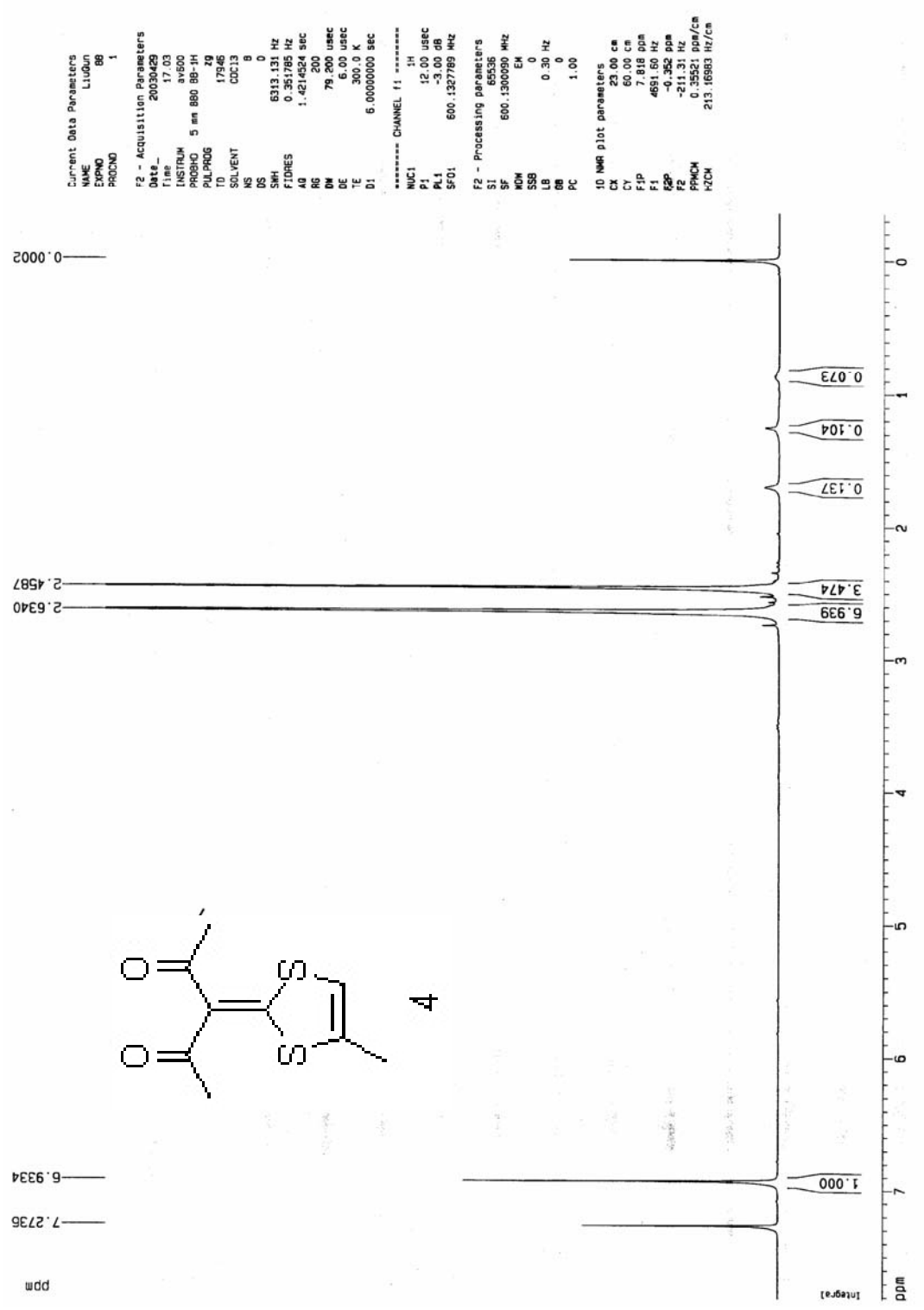
3h: light red solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.48 (m, 1 H), 1.62 (m, 1 H), 1.71 (s, 1.5 H, Me), 1.74 (s, 1.5 H, Me), 1.84 (broad, NH, 1H), 2.36 (m, 1 H), 2.45 (m, 1 H), 2.61 (m, 1 H), 2.86 (m, 1 H), 3.05 (m, 1 H), 3.22 (m, 2 H), 3.36 (m, 1 H), 4.55 (m, 1 H), 4.86 (m, 1 H), 7.28 (m, 1 H), 7.38 (m, 5 H), 7.45 (m, 2H), 7.55 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.5, 40.4, 40.9, 40.9, 46.6, 46.7, 49.4, 49.5, 58.1, 71.2, 71.3, 109.8, 127.0, 127.5, 127.9, 128.0, 128.2, 128.7, 129.0, 132.3, 132.4, 134.8, 134.9, 137.8, 138.9, 141.3, 151.0, 151.1, 190.1, 190.2; IR (KBr, cm^{-1}): ν = 3324, 3029, 2930, 2826, 1656, 1451, 1199, 978, 896; MS (EI): calcd *m/z* 446.15, found 447.2 $[(M+1)]^+$; Anal. calcd for $C_{26}H_{26}N_2OS_2$: C, 69.92; H, 5.87; N, 6.27; Found: C, 70.19; H, 5.75; N, 6.12.

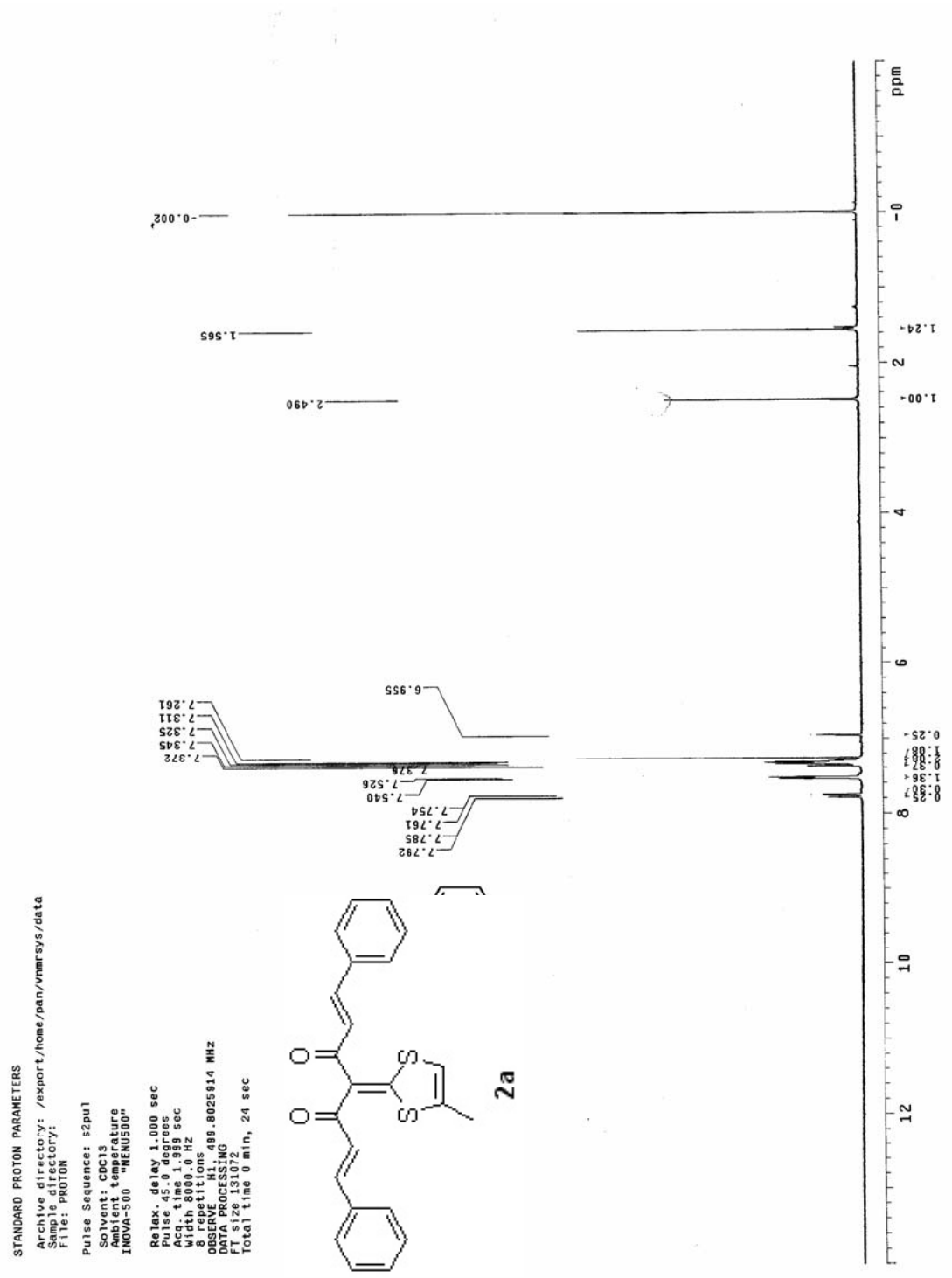
3i: white solid. ^1H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.46 (m, 2 H), 1.69 (s, 1.5

H, Me), 1.72 (s, 1.5 H, Me), 1.82 (broad, NH, 1H), 2.32 (m, 1 H), 2.40 (m, 1 H), 2.60 (m, 1 H), 2.86 (m, 1 H), 3.02 (m, 1 H), 3.20 (m, 2 H), 3.30 (m, 1 H), 4.51 (m, 1 H), 4.82 (m, 1 H), 7.33 (m, 6 H), 7.48 (m, 2 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.7, 40.5, 41.1, 46.6, 46.7, 48.8, 48.9, 57.5, 71.4, 71.5, 128.6, 129.1, 129.4, 132.4, 132.6, 132.9, 134.7, 134.7, 134.8, 136.4, 136.4, 139.2, 140.0, 150.8, 151.0, 190.0, 190.0; IR (KBr, cm^{-1}): ν = 3333, 2927, 1659, 1488, 1454, 823. MS (EI): calcd *m/z* 514.07, found 515.1 $[(M+1)]^+$; Anal. calcd for $C_{26}H_{24}Cl_2N_2OS_2$: C, 60.58; H, 4.69; N, 5.43; Found: C, 60.85; H, 4.64; N, 5.62.

3j: red solid. ^{1}H NMR (500 MHz, $CDCl_3$, 293 K, TMS): δ = 1.45 (m, 2H), 1.74 (m, 3H, Me), 2.33 (broad, NH, 1H), 2.43 (s, 1H), 2.58 (m, 1H), 2.86 (m, 1H), 3.12 (m, 1H), 3.25 (m, 4H), 4.54 (m, 1H), 4.84 (m, 1H), 7.07 (m, 4H), 7.41 (m, 2H), 7.52 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.5, 40.2, 40.9, 46.6, 46.7, 48.5, 48.7, 57.4, 71.3, 115.0, 115.1, 115.9, 116.1 129.2, 129.3, 129.5, 132.2, 132.3, 133.5, 134.6, 136.8, 151.0, 161.7, 163.7, 188.9, 189.9; IR (KBr, cm^{-1}): ν = 3445, 2926, 1660, 1509, 1455, 1226, 835. MS (EI): calcd *m/z* 482.13, found 483.1 $[(M+1)]^+$; Anal. calcd for $C_{26}H_{24}F_2N_2OS_2$: C, 64.71; H, 5.01; N, 5.80; Found: C, 64.93; H, 4.97; N, 5.89.

IV. Copies of ^{1}H and ^{13}C NMR spectra for compounds 4, 2a – 2g and 3a – 3j.

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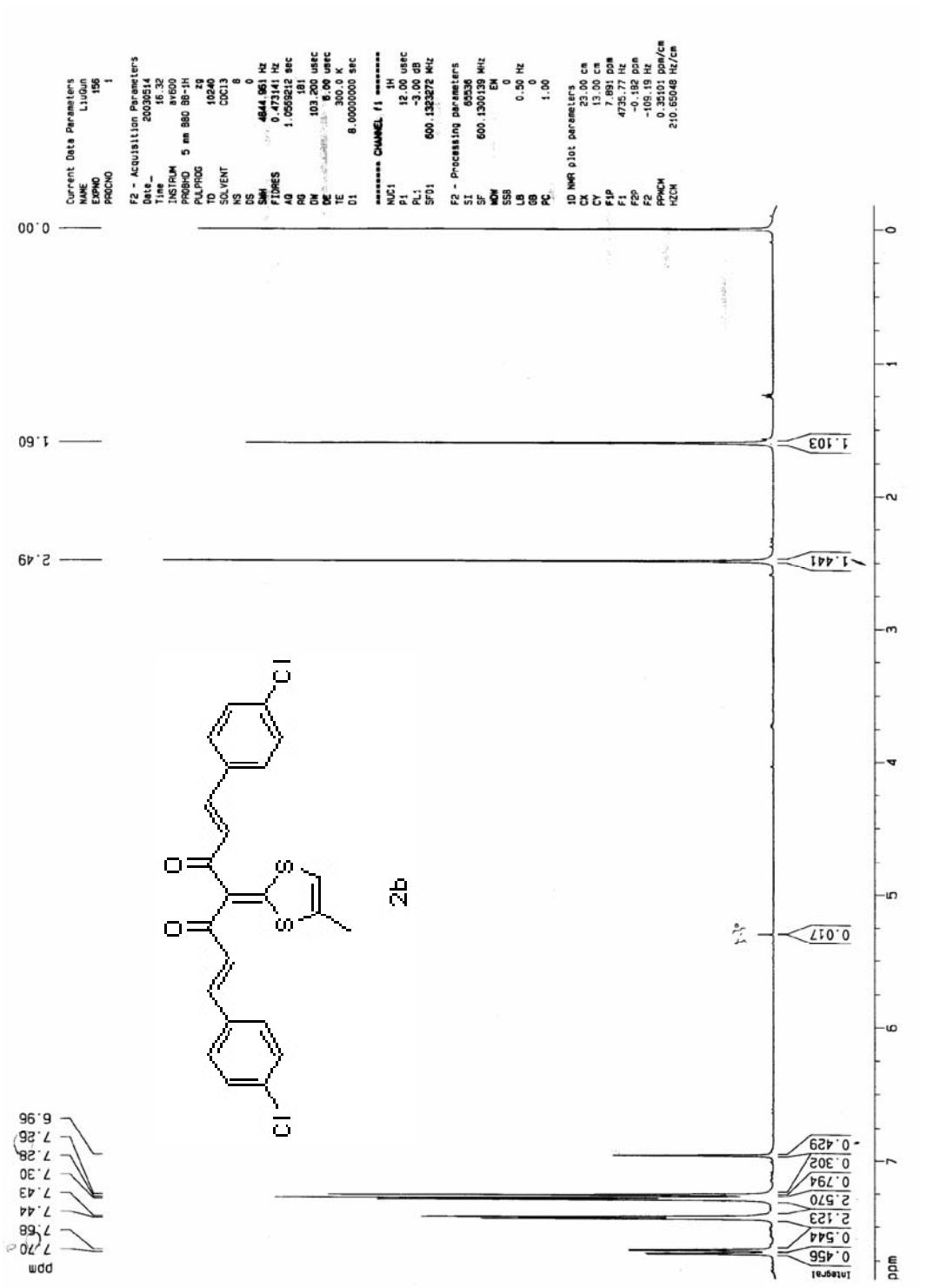
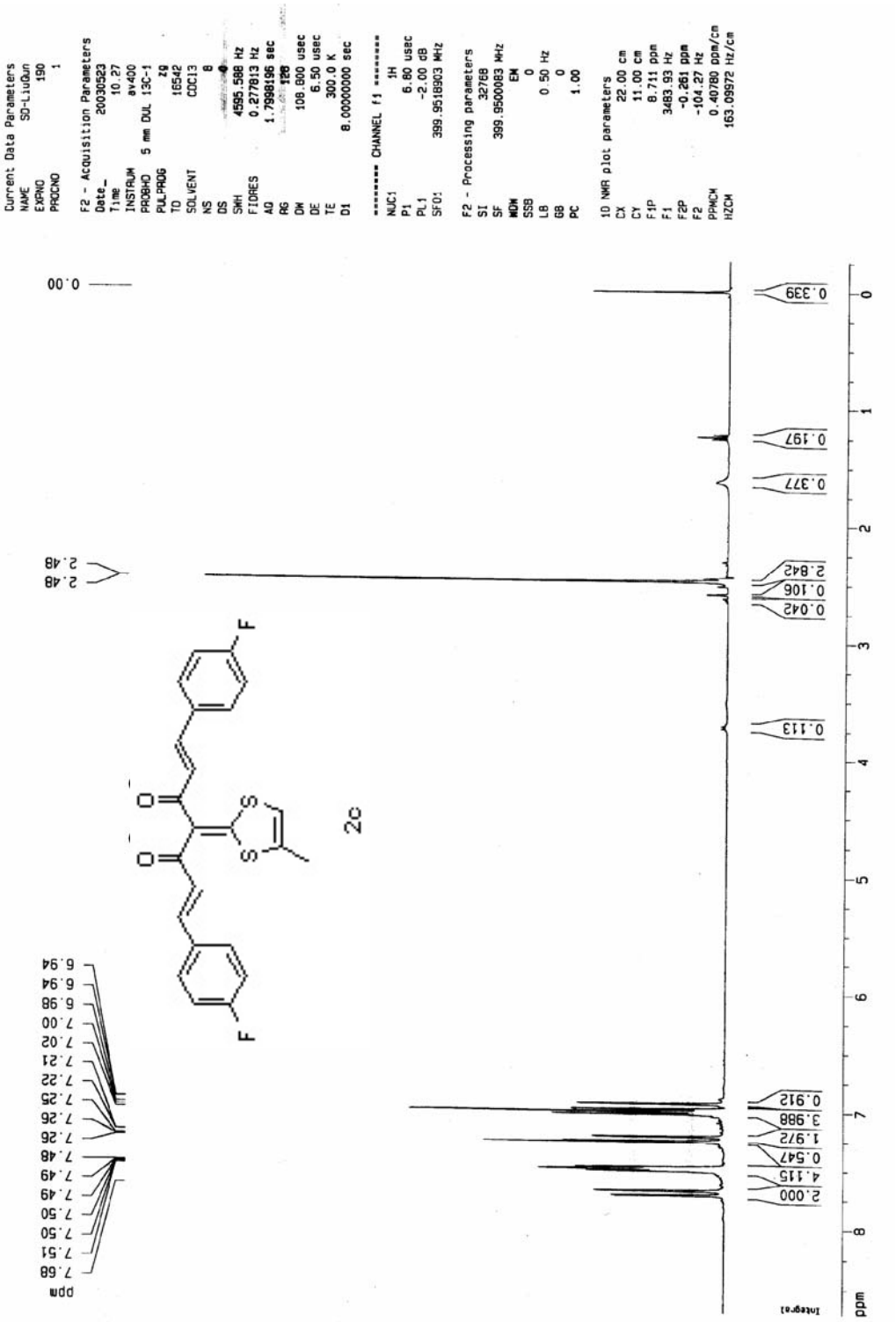
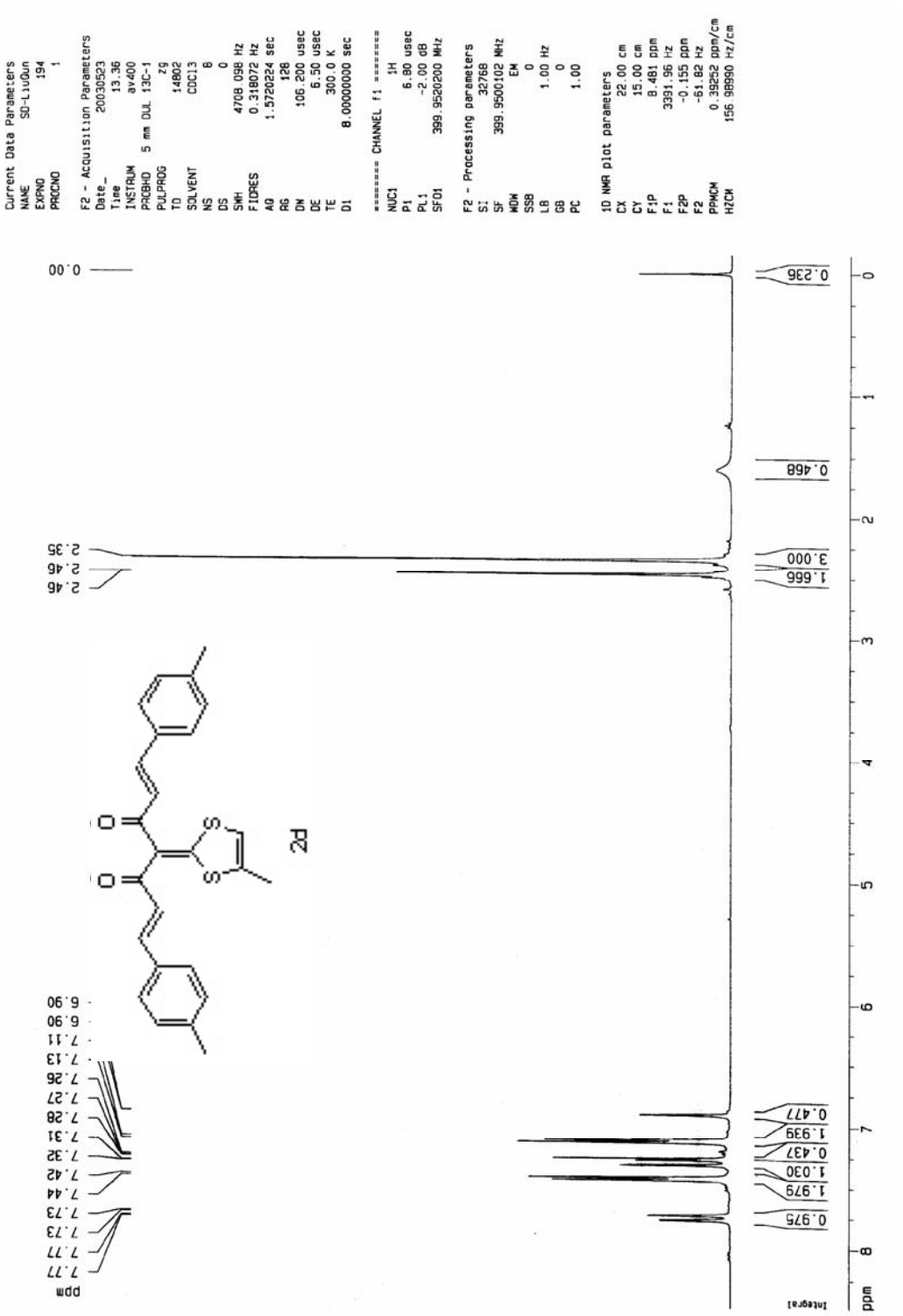
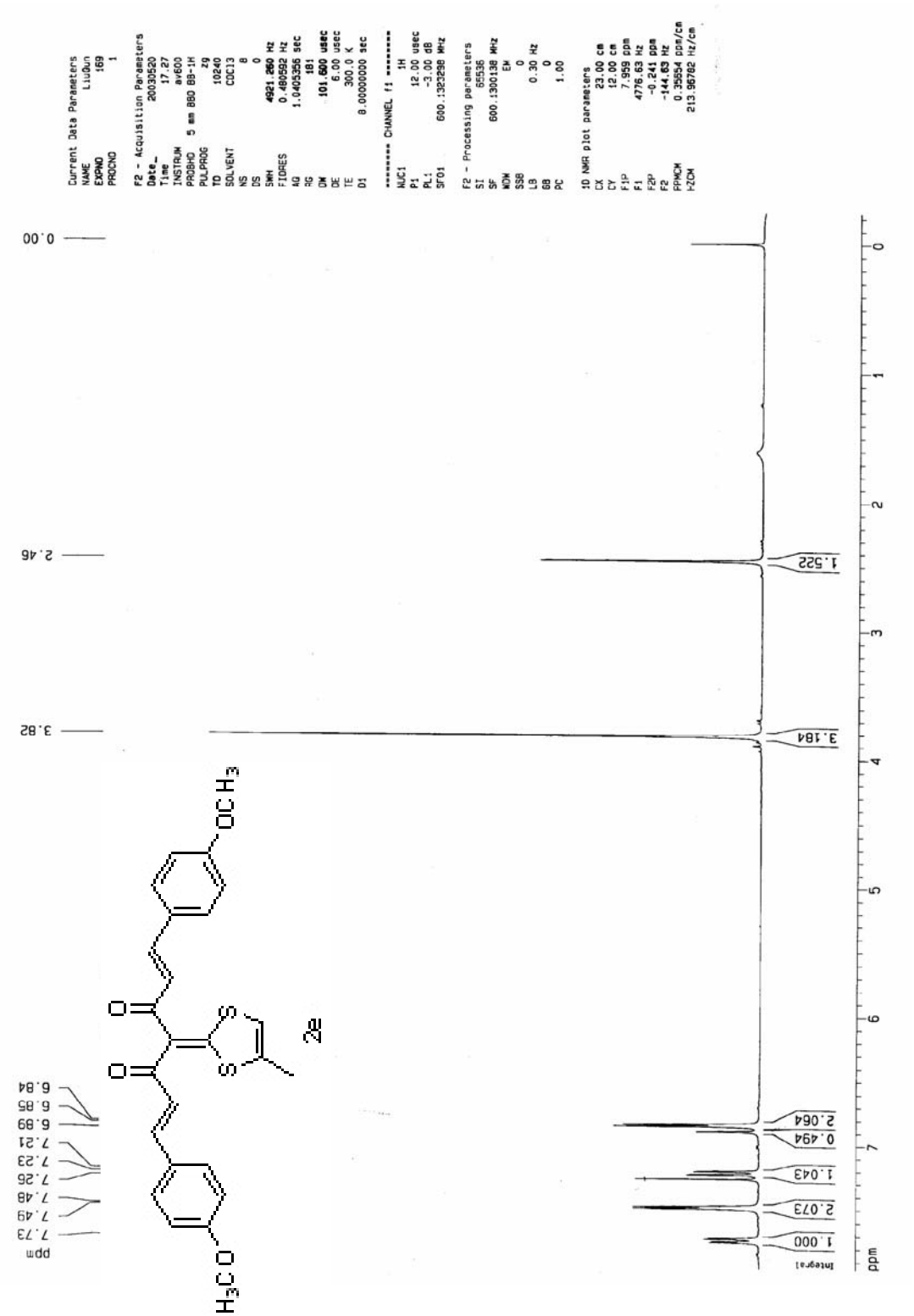
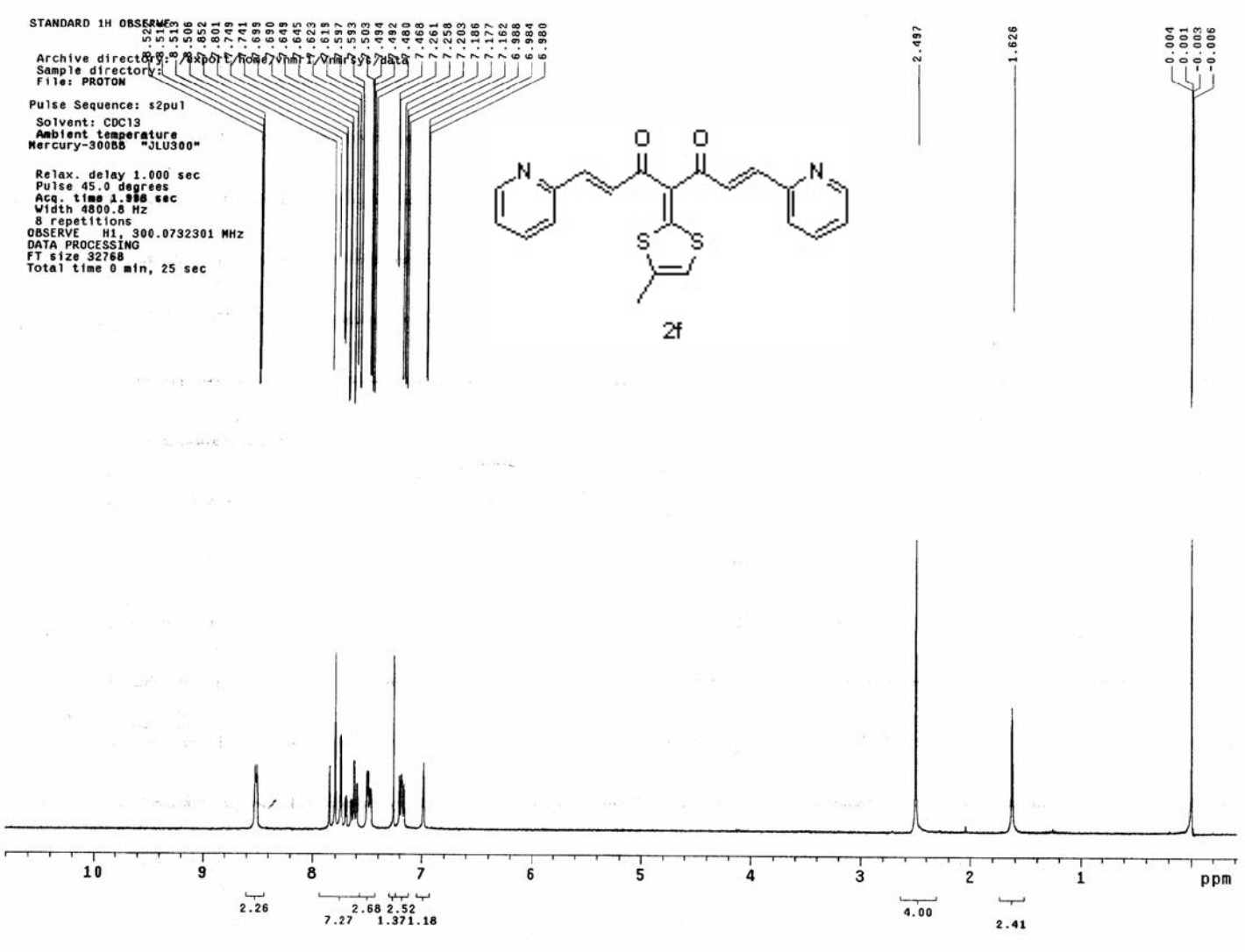
2.490
1.565
-0.002
1.00
1.24
ppm

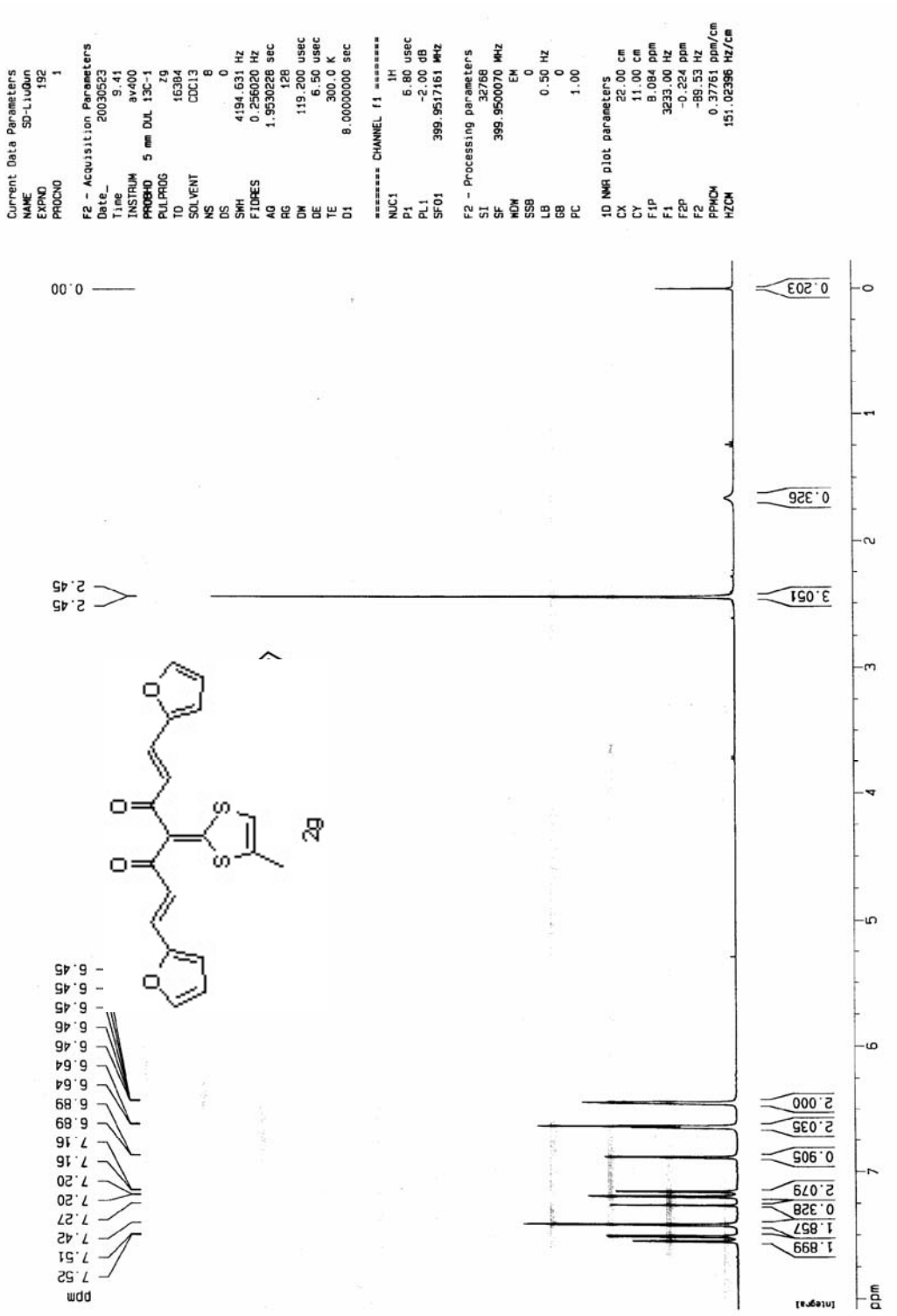

2b
Cl
Cl
O
O
S
S
1.103
1.441
0.017
0.429
0.302
0.794
2.570
2.123
0.544
0.456
Integral
ppm
0.00
1.60
2.49
6.96
7.26
7.28
7.30
7.43
7.44
7.68
7.70

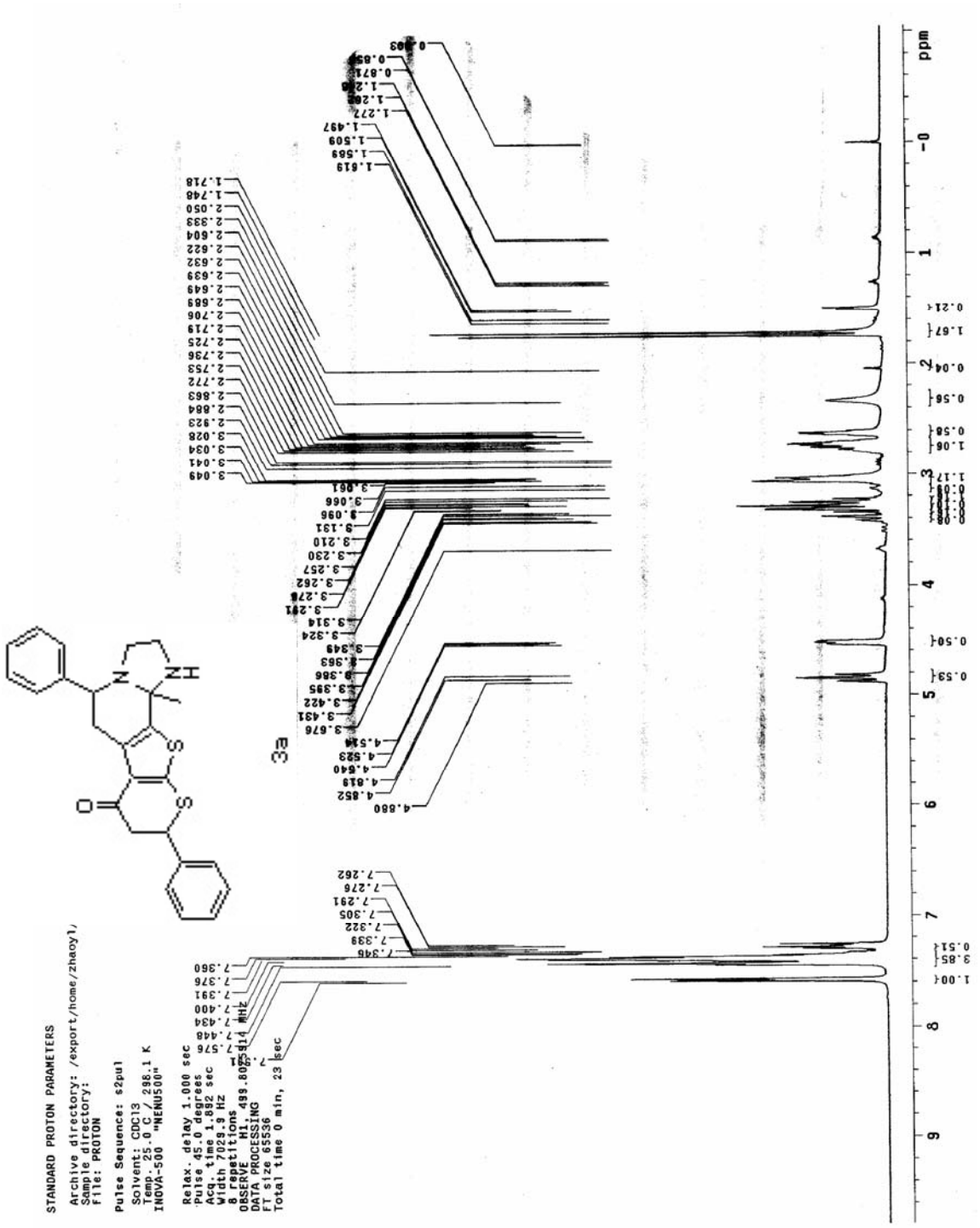

Current Data Parameters
NAME SD-LiuQun
EXPNO 190
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030523
Time 10.27
INSTRUM av400
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16542
SOLVENT CDCl3
NS 8
DS 0
SWH 4595.588 Hz
FIDRES 0.277813 Hz
AQ 1.7998196 sec
RG 128
DW 108.800 usec
DE 6.50 usec
TE 300.0 K
D1 8.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 6.80 usec
PL1 -2.00 dB
SFO1 399.9518903 MHz
F2 - Processing parameters
SI 32768
SF 399.9500083 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 11.00 cm
F1P 8.711 ppm
F1 3483.93 Hz
F2P -0.261 ppm
F2 -104.27 Hz
PPMCM 0.40780 ppm/cm
HZCM 163.09972 Hz/cm
2c
2.48
2.48
0.339
0.197
0.377
2.842
0.106
0.042
0.113
2.000
4.115
0.547
1.972
3.988
0.912
7.68
7.51
7.50
7.50
7.49
7.49
7.48
7.26
7.25
7.22
7.21
7.02
7.00
6.98
6.94
6.94
ppm
Integral
ppm

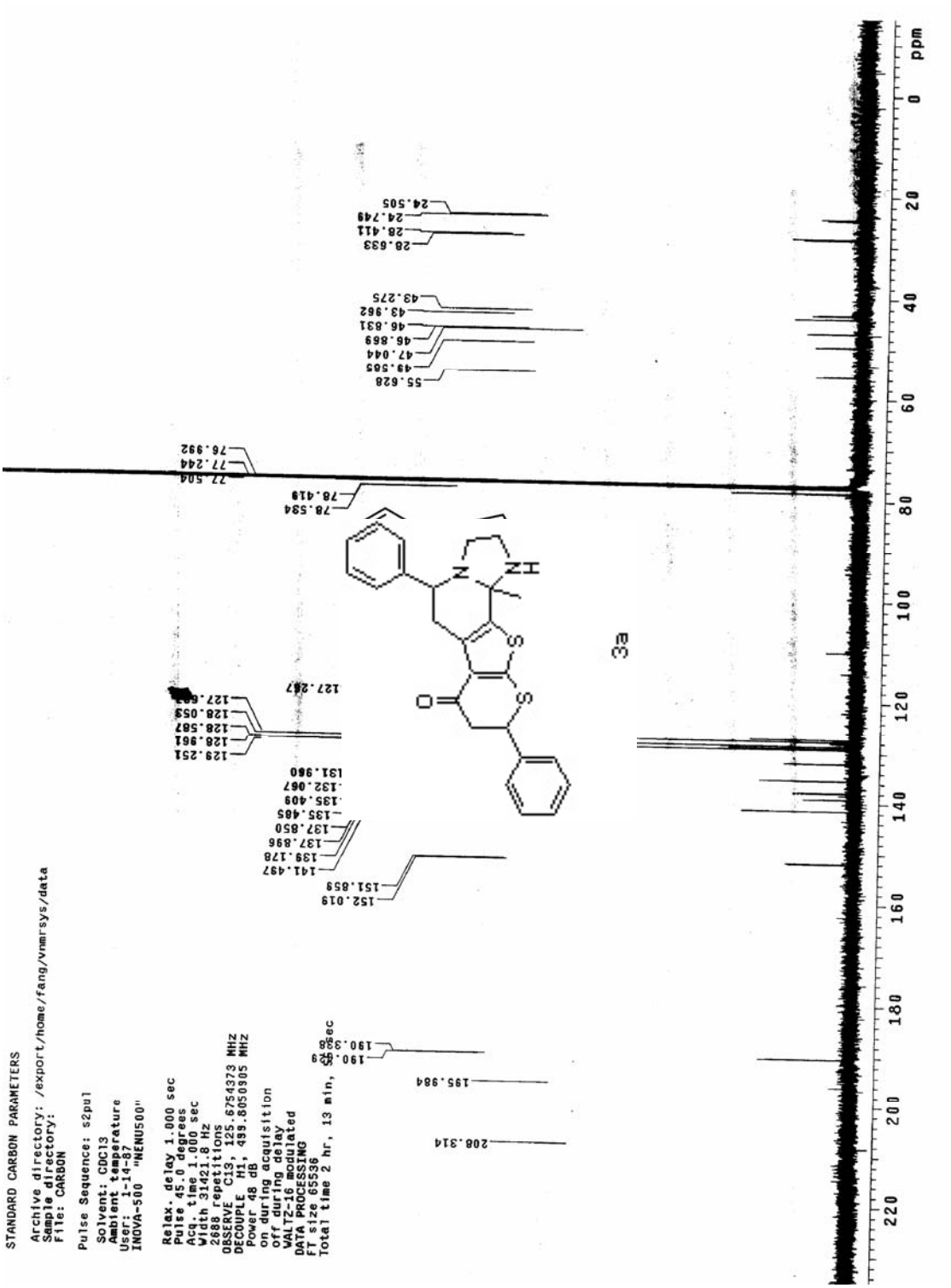

Current Data Parameters
NAME SD-LiuGun
EXPNO 194
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030523
Time 13.36
INSTRUM av400
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 14802
SOLVENT CDCl3
NS 8
DS 0
SWH 4708.098 Hz
FIDRES 0.318072 Hz
AQ 1.5720224 sec
RG 128
DW 106.200 usec
DE 6.50 usec
TE 300.0 K
D1 8.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 6.80 usec
PL1 -2.00 dB
SFO1 399.9520200 MHz
F2 - Processing parameters
SI 32768
SF 399.9500102 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 15.00 cm
F1P 8.481 ppm
F1 3391.96 Hz
F2P -0.155 ppm
F2 -61.82 Hz
PPMCM 0.39252 ppm/cm
HZCM 156.98990 Hz/cm
2d
ppm
Integral

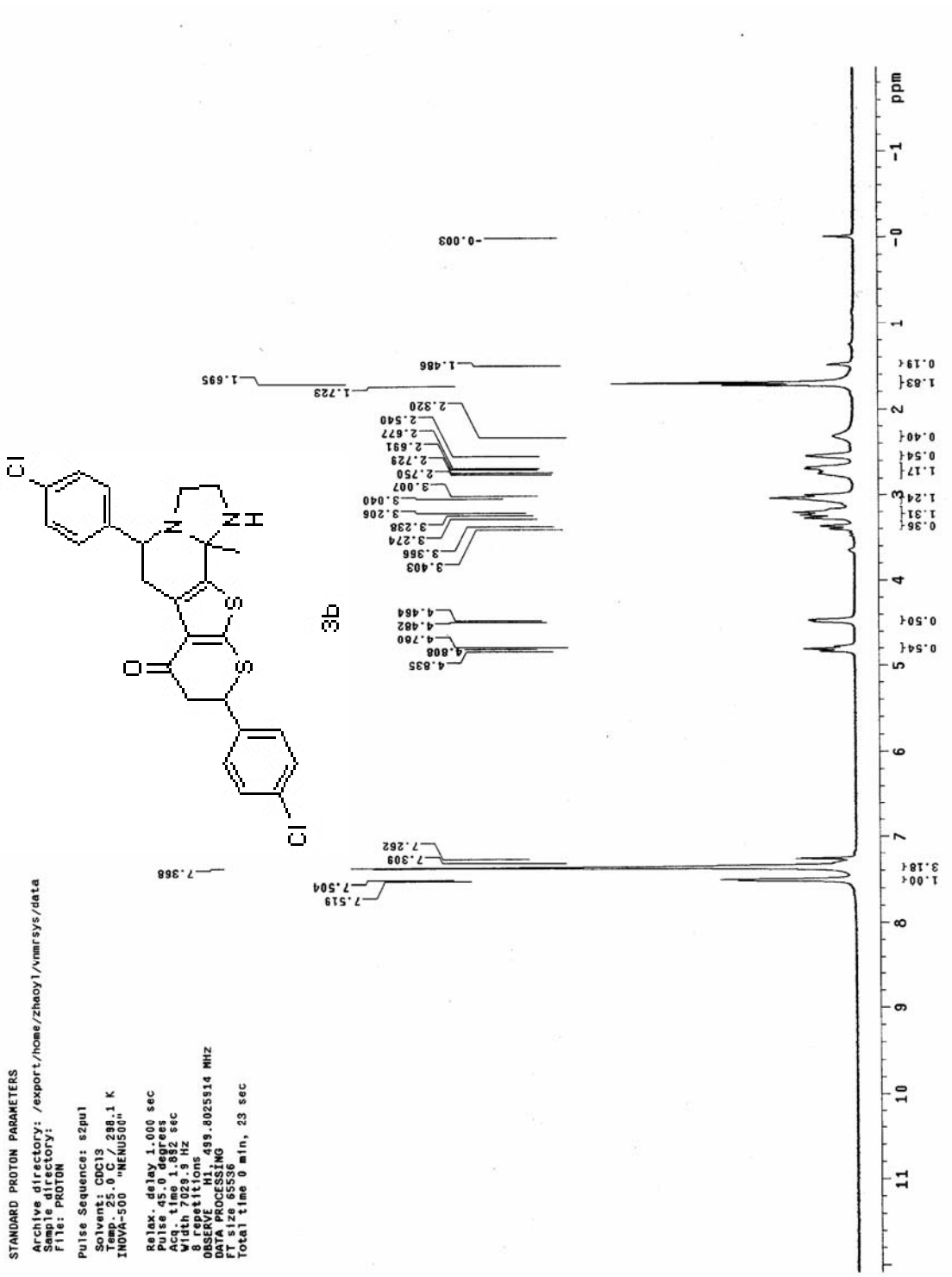

Current Data Parameters
NAME LiuQun
EXPNO 169
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030520
Time 17.27
INSTRUM av600
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 10240
SOLVENT CDCl3
NS 8
DS 0
SWH 4921.260 Hz
FIDRES 0.480592 Hz
AQ 1.0405356 sec
RG 181
DW 101.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -3.00 dB
SFO1 600.1323298 MHz
F2 - Processing parameters
SI 65536
SF 600.1300138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.00 cm
CY 12.00 cm
F1P 7.959 ppm
F1 4776.63 Hz
F2P -0.241 ppm
F2 -144.63 Hz
PPMCM 0.39554 ppm/cm
HZCM 213.96782 Hz/cm
0.00
2.46
3.82
1.522
3.184
2.064
0.494
1.043
2.073
1.000
Integral
ppm
0
1
2
3
4
5
6
7
7.73
7.49
7.48
7.26
7.23
7.21
6.89
6.85
6.84
ppm
2e

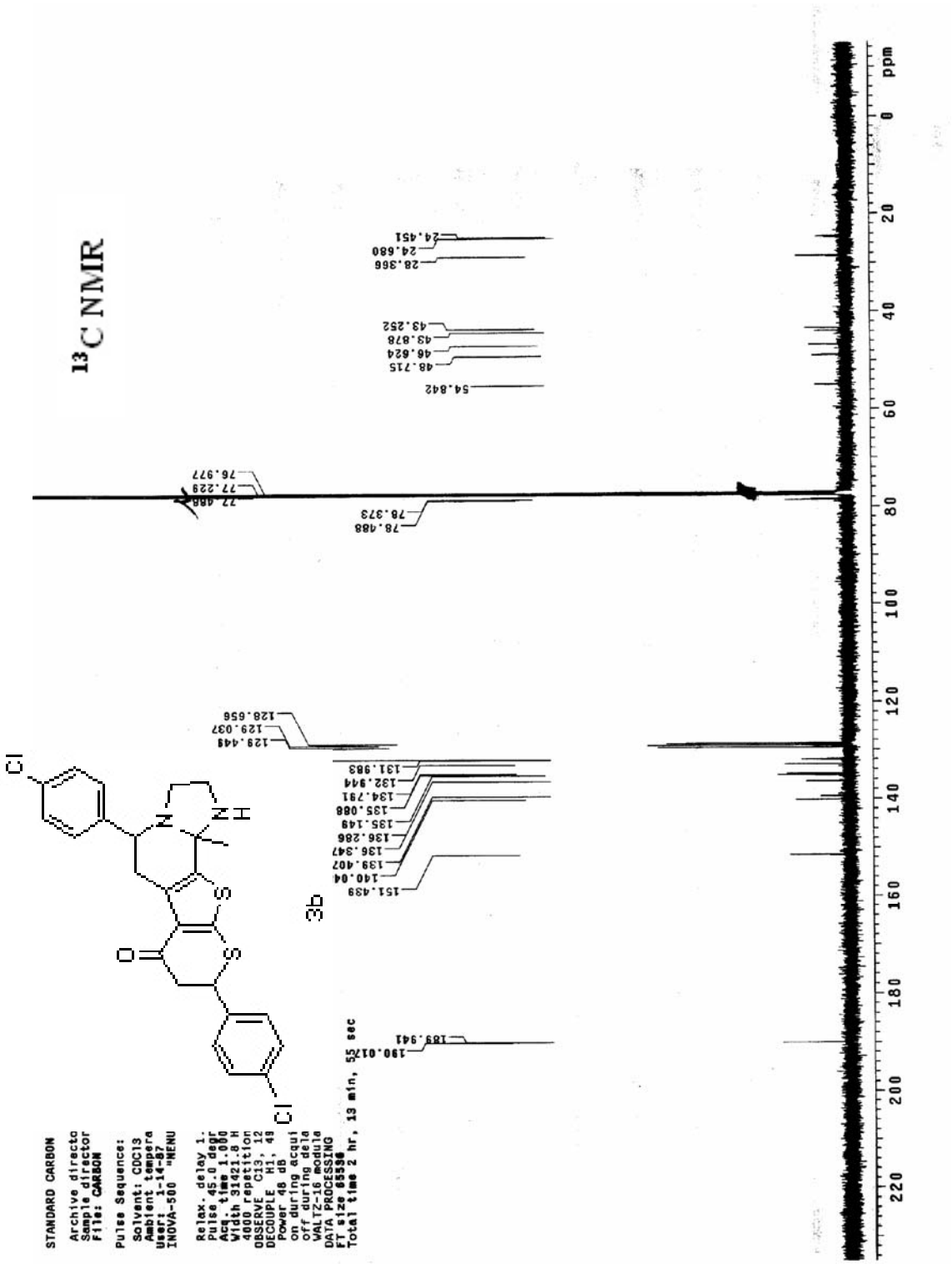

STANDARD 1H OBSERVE
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "JLU300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.998 sec
Width 4800.8 Hz
8 repetitions
OBSERVE H1, 300.0732301 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 25 sec
8.525
8.513
8.506
7.852
7.801
7.749
7.741
7.699
7.690
7.649
7.645
7.623
7.613
7.597
7.593
7.503
7.494
7.492
7.480
7.468
7.261
7.258
7.203
7.186
7.177
7.162
6.988
6.984
6.980
2.497
1.626
0.004
0.001
-0.003
-0.006
O
O
N
N
S
S
2f
10
9
8
7
6
5
4
3
2
1
ppm
2.26
7.27
2.68
2.52
1.37
1.18
4.00
2.41

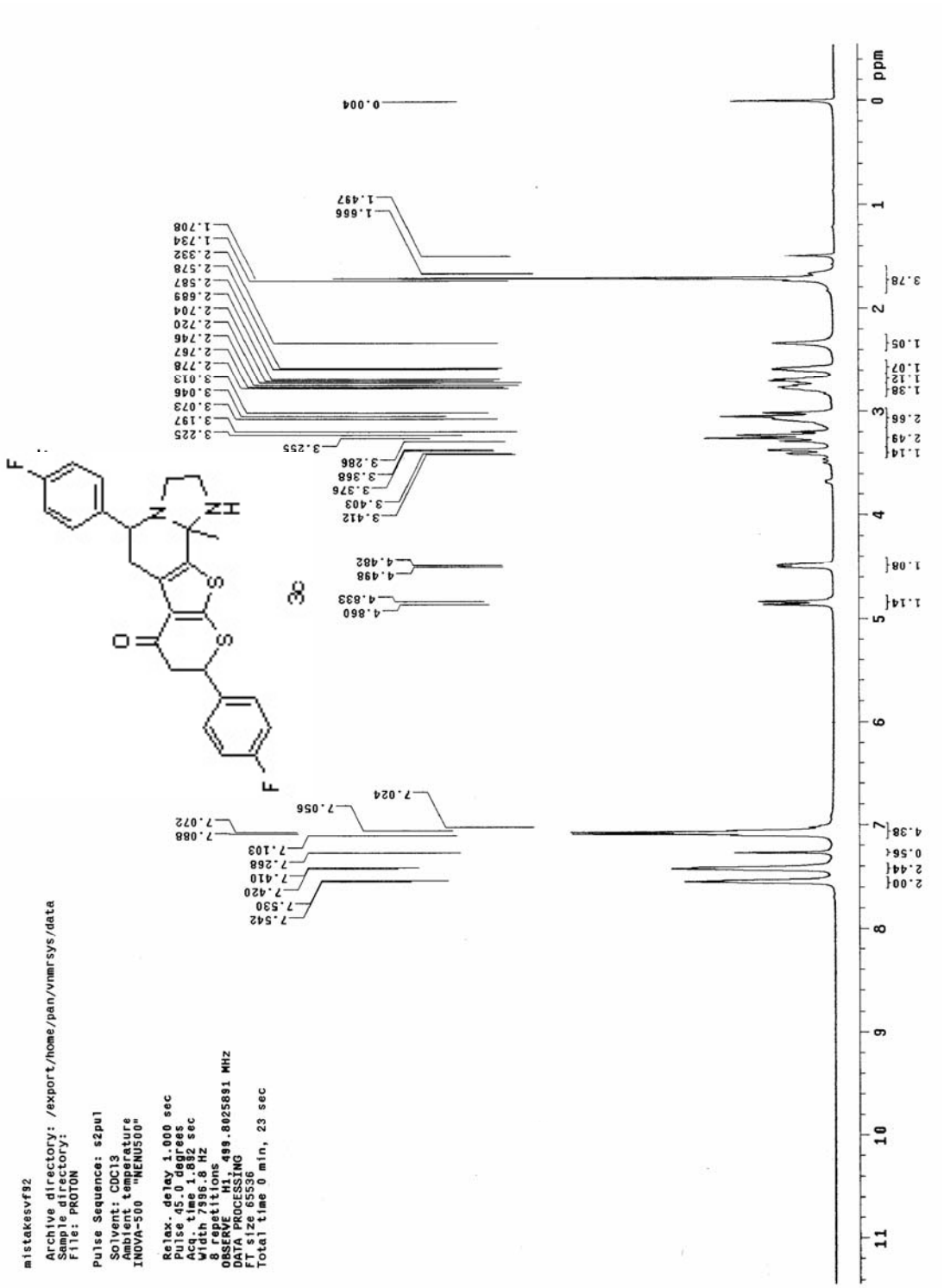

Current Data Parameters
NAME SD-LiuQun
EXPNO 192
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030523
Time 9.41
INSTRUM av400
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 8
DS 0
SWH 4194.631 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 119.200 usec
DE 6.50 usec
TE 300.0 K
D1 8.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 6.80 usec
PL1 -2.00 dB
SFO1 399.9517161 MHz
F2 - Processing parameters
SI 32768
SF 399.9500070 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 11.00 cm
F1P 8.084 ppm
F1 3233.00 Hz
F2P -0.224 ppm
F2 -89.53 Hz
PPMCM 0.37761 ppm/cm
HZCM 151.02396 Hz/cm
0.00
2.45
2g
7.52
7.51
7.42
7.27
7.20
7.20
7.16
7.16
6.89
6.89
6.64
6.64
6.46
6.46
6.45
6.45
6.45
ppm
0.203
0.326
3.051
2.000
2.035
0.905
2.079
0.328
1.857
1.899
[integral]
ppm

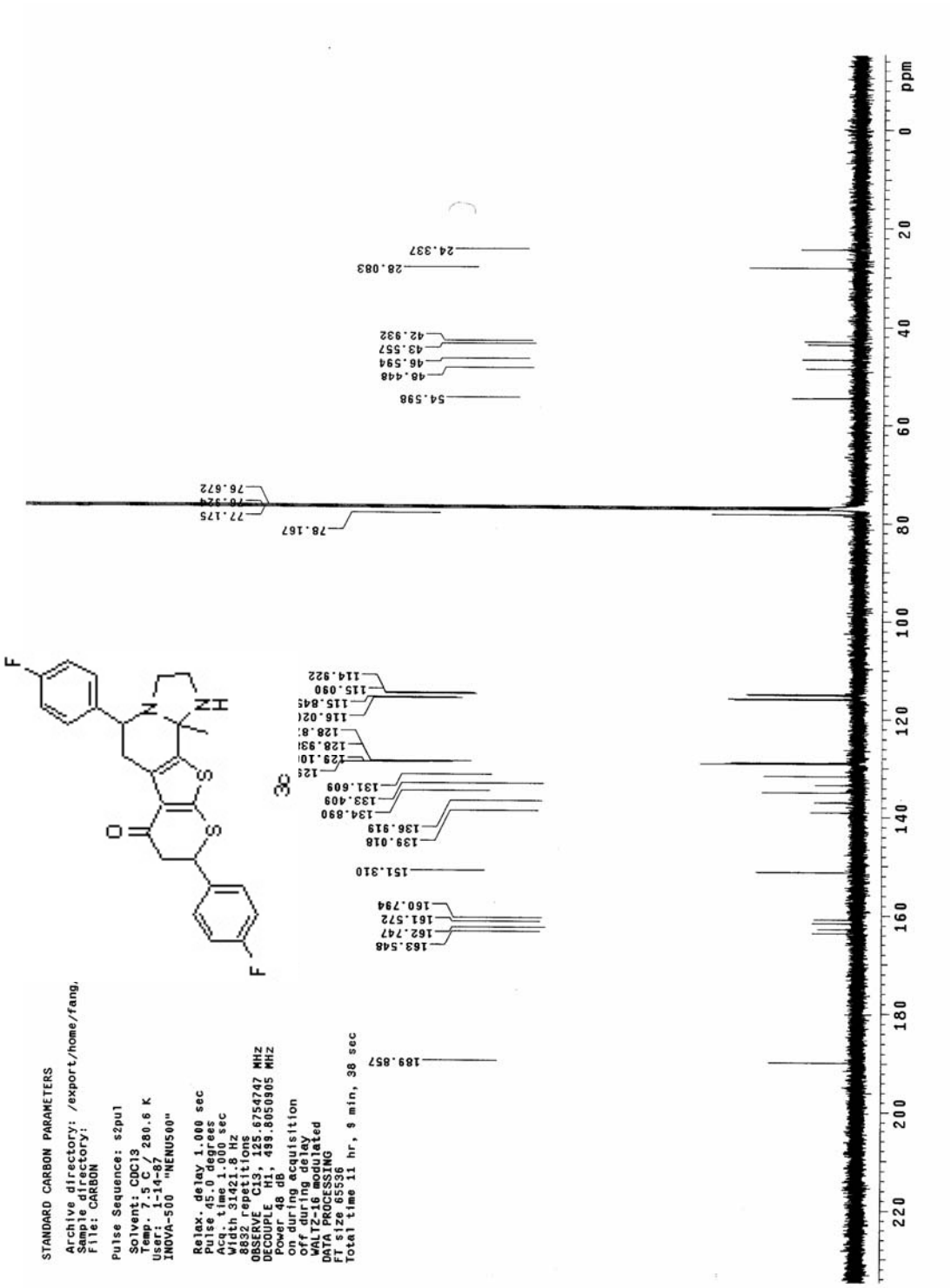

STANDARD PROTON PARAMETERS
Archive directory: /export/home/zhaoyl/
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "NERUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7029.8 Hz
8 repetitions
OBSERVE H1, 499.8025414 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
3a
ppm

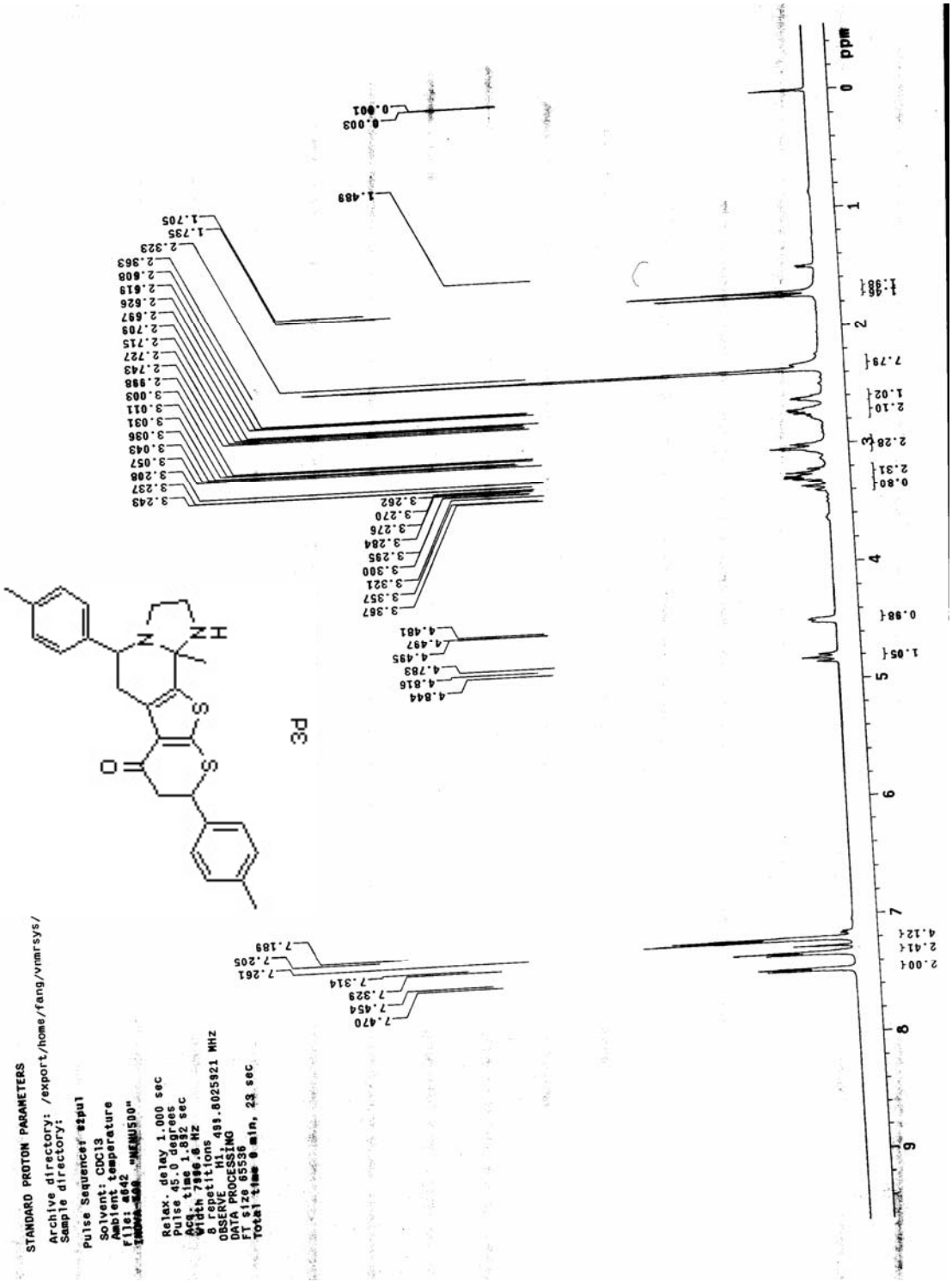

STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 31421.8 Hz
2688 repetitions
OBSERVE C13, 125.6754373 MHz
DECOUPLE H1, 499.8050905 MHz
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
FT size 65536
Total time 2 hr, 13 min, 25 sec
208.314
195.984
190.358
190.329
152.019
151.859
141.497
139.178
137.896
137.850
135.485
135.409
132.067
131.980
129.251
128.961
128.587
128.053
127.247
78.584
78.419
77.504
77.244
76.992
55.628
49.585
47.044
46.869
46.831
43.962
43.275
28.693
28.411
24.749
24.505
3a
ppm

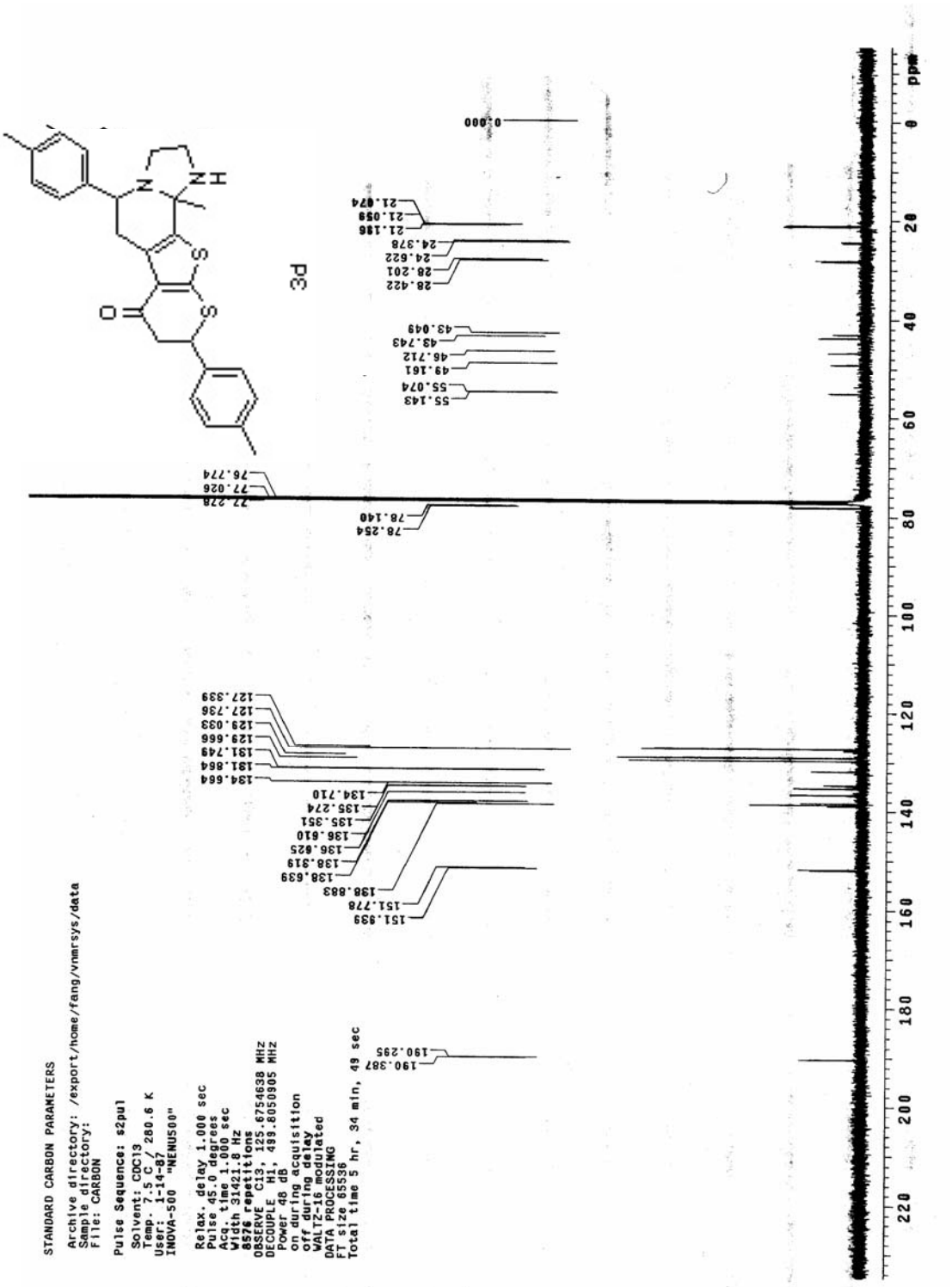

STANDARD PROTON PARAMETERS
Archive directory: /export/home/zhaoyl/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7028.9 Hz
8 repetitions
OBSERVE H1, 499.8025914 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
3b
Cl
Cl
O
S
S
N
H
7.368
7.519
7.504
7.309
7.262
4.835
4.808
4.760
4.482
4.464
3.403
3.366
3.274
3.238
3.206
3.040
3.007
2.750
2.729
2.691
2.677
2.540
2.320
1.723
1.695
1.486
0.003
ppm

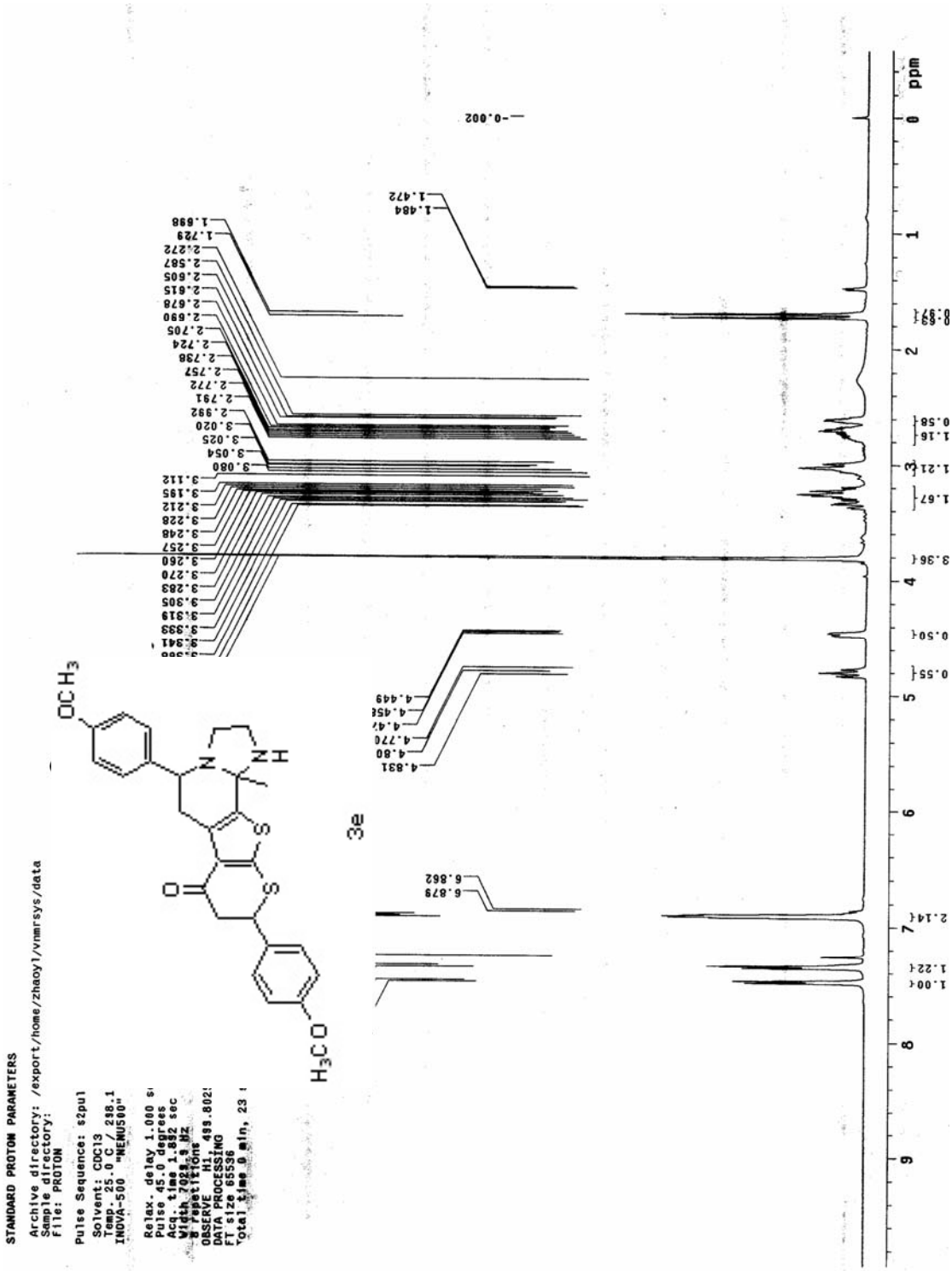

^{13}C NMR
3b
Cl
Cl
O
S
S
N
H
STANDARD CARBON
Archive directo
Sample director
File: CARBON
Pulse Sequence:
Solvent: CDCl3
Ambient temperatu
User: lc-ms7
INOVA-500 "MENU
Relax. delay 1.
Pulse 45.0 degr
Acq. time 1.080
Width 31421.8 H
4000 repetition
OBSERVE C13, 12
DECOUPLE H1, 49
Power 48 dB
on during acqui
off during dela
WALTZ-16 modula
DATA PROCESSING
FT size 65536
Total time 2 hr, 13 min, 55 sec
189.941
190.012
151.439
140.040
139.407
136.347
136.286
135.149
135.088
134.791
132.944
131.983
129.448
129.037
128.656
78.488
78.373
77.488
77.228
76.977
54.842
48.715
46.624
43.878
43.252
28.366
24.680
24.451
ppm

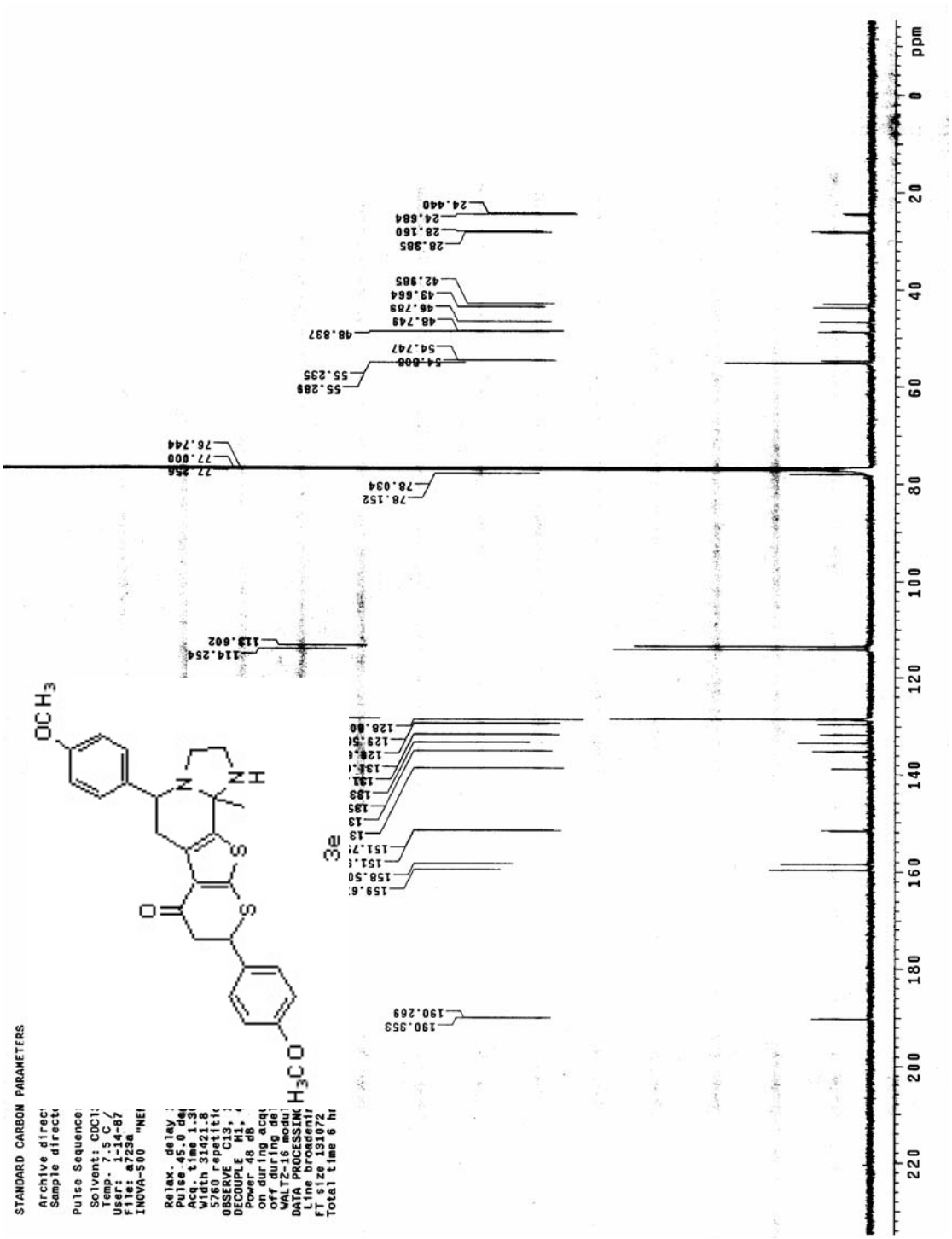

mistakesvf92
Archive directory: /export/home/pan/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025891 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
30
F
N
NH
S
S
O
F
0.004
1.497
1.666
1.708
1.734
2.332
2.578
2.587
2.689
2.704
2.720
2.746
2.767
2.778
3.013
3.046
3.073
3.197
3.225
3.255
3.286
3.368
3.376
3.403
3.412
4.482
4.498
4.833
4.860
7.024
7.056
7.072
7.088
7.103
7.268
7.410
7.420
7.530
7.542
3.78
1.05
1.07
1.12
1.38
2.66
2.49
1.14
1.08
1.14
4.38
0.56
2.44
2.00
ppm

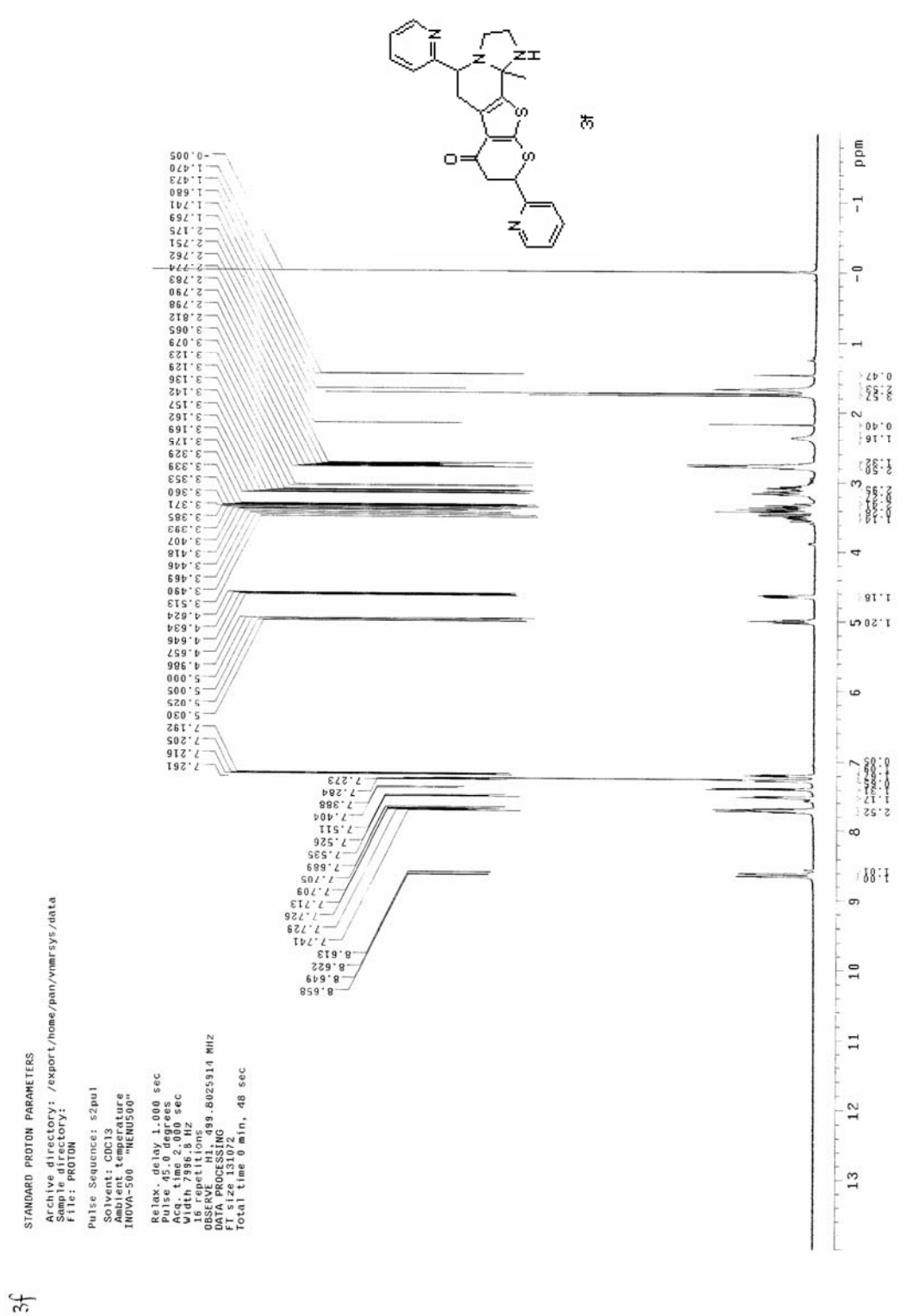

STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 7.5 C / 280.6 K
User: 1-14-07
INOVA-500 "NEMUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 31421.8 Hz
8832 repetitions
OBSERVE C13, 125.8754747 MHz
DECOUPLE H1, 499.8050905 MHz
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
FT size 65536
Total time 11 hr, 9 min, 36 sec
189.857
163.548
162.747
161.572
160.794
151.310
139.018
136.919
134.890
133.409
131.609
129.107
128.938
128.8
116.020
115.845
115.090
114.922
78.167
77.175
76.924
76.672
54.598
48.448
46.594
43.557
42.932
28.083
24.337
ppm
F
O
S
S
N
NH
F

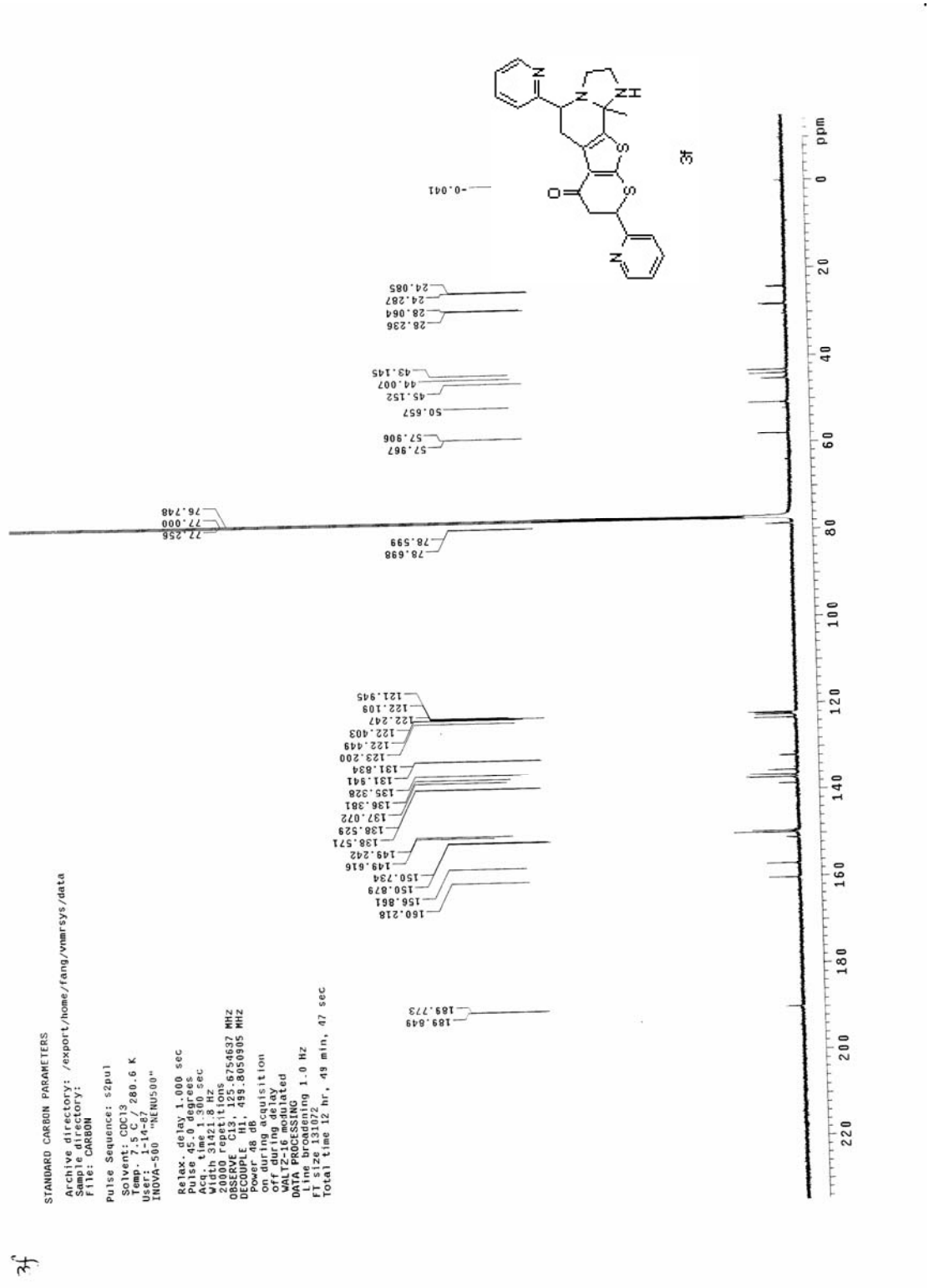

STANDARD PROTON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/
Sample directory:
Pulse Sequence: stpul
Solvent: CDCl3
Ambient temperature
File: a842
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 7186.8 Hz
8 repetitions
OBSERVE H1, 499.8025921 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
3d
ppm

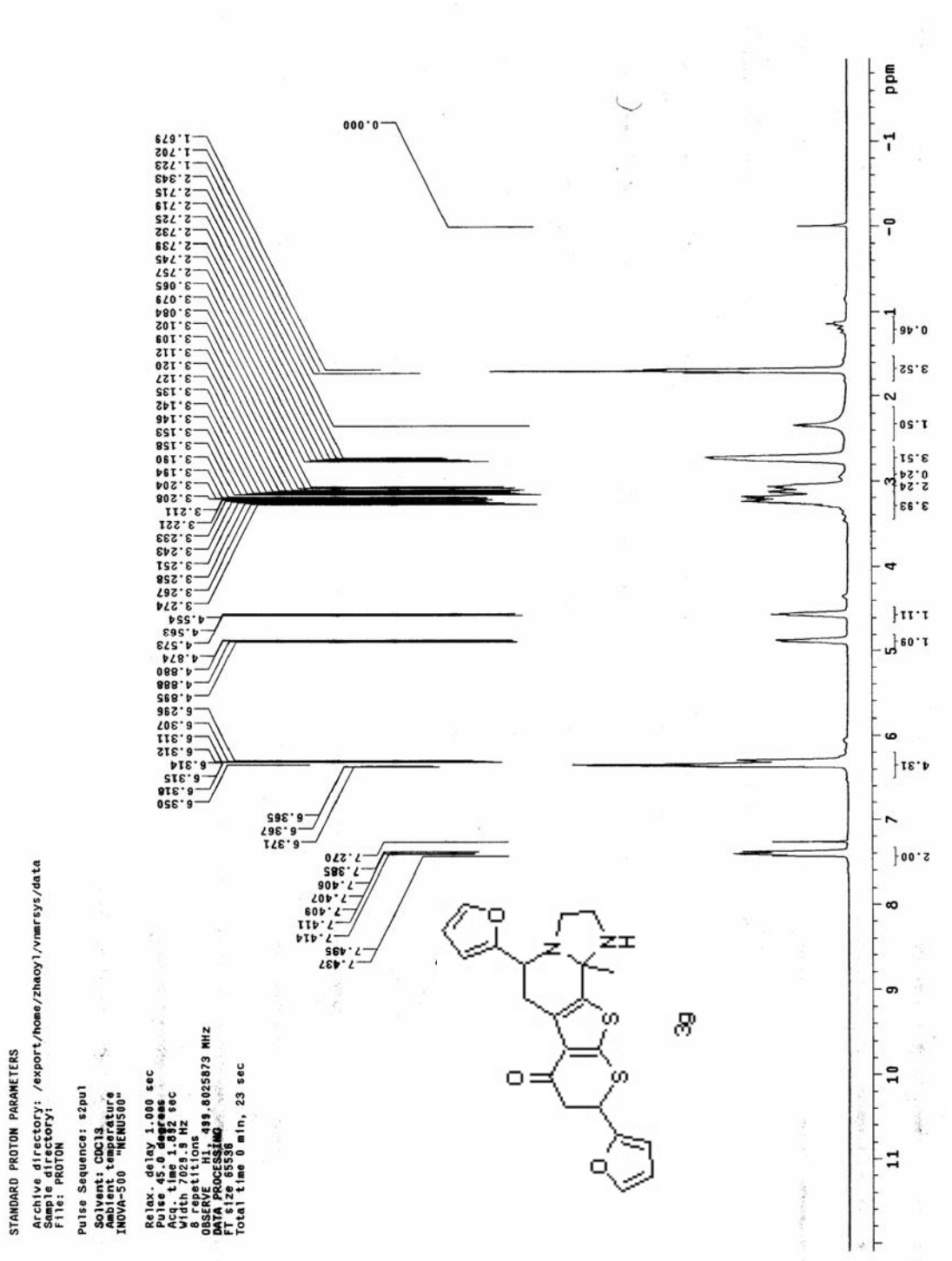

STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 7.5 C / 280.6 K
User: 1-14-07
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 31421.1 Hz
8576 repetitions
OBSERVE C13, 125.6754638 MHz
DECOUPLE H1, 499.8050905 MHz
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
FT size 65536
Total time 5 hr, 34 min, 49 sec
3d
O
S
S
N
H
190.387
190.295
151.939
151.778
138.883
138.639
138.319
136.825
136.610
135.351
135.274
134.710
134.664
131.864
131.749
129.666
129.033
127.796
127.339
77.228
77.026
76.774
78.254
78.140
55.143
55.074
49.161
46.712
43.743
43.049
28.422
28.201
24.622
24.378
21.186
21.059
21.074
0.000
ppm

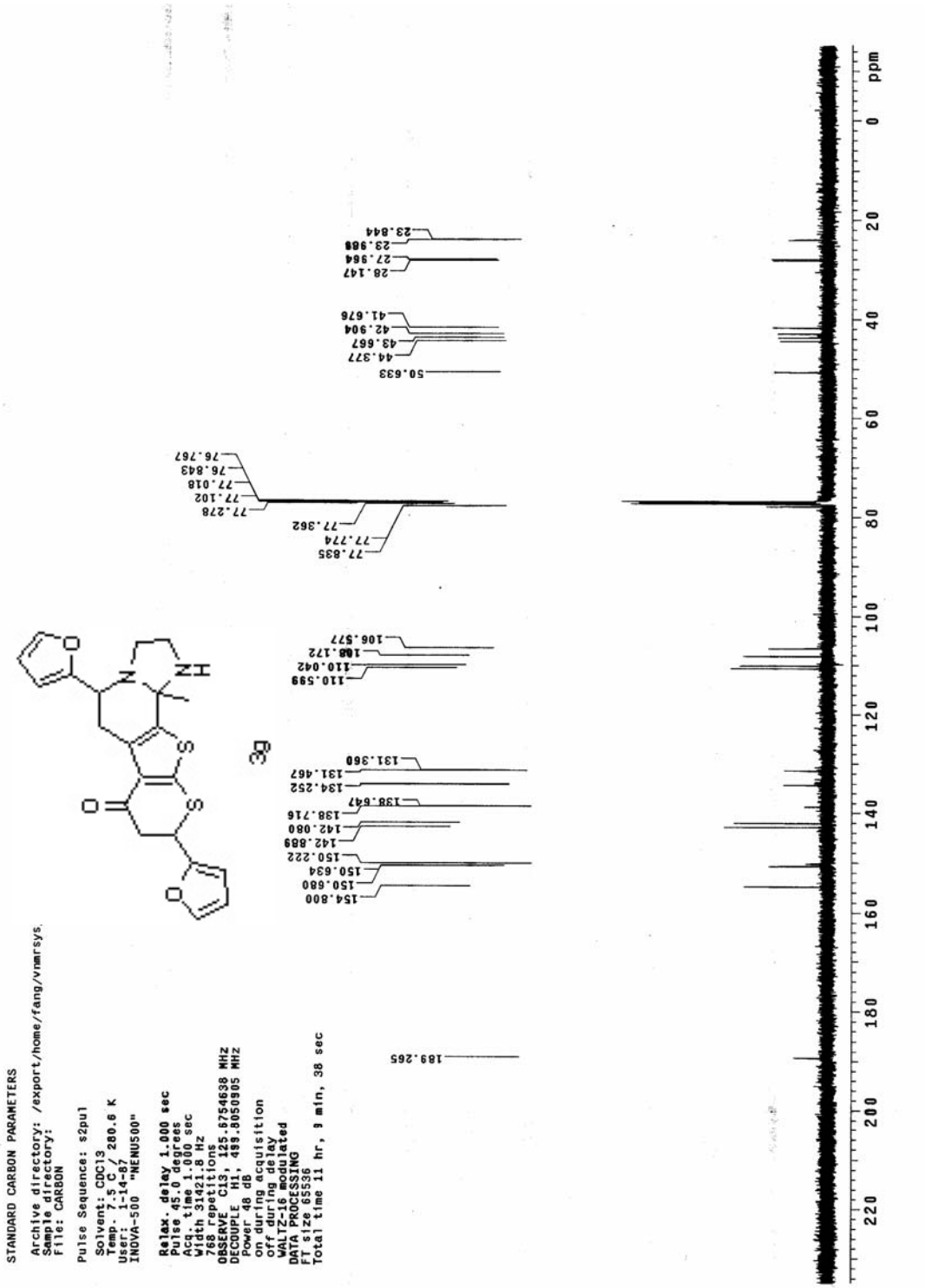

STANDARD PROTON PARAMETERS
Archive directory: /export/home/zhaoy1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1
INOVA-500 "NEMU500"
Relax. delay 1.000 s
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 7028.9 Hz
8 repetitions
OBSERVE H1, 499.802
DATA PROCESSING
FT size 65536
Total time 0 min, 23
OCH3
H3CO
3e
ppm

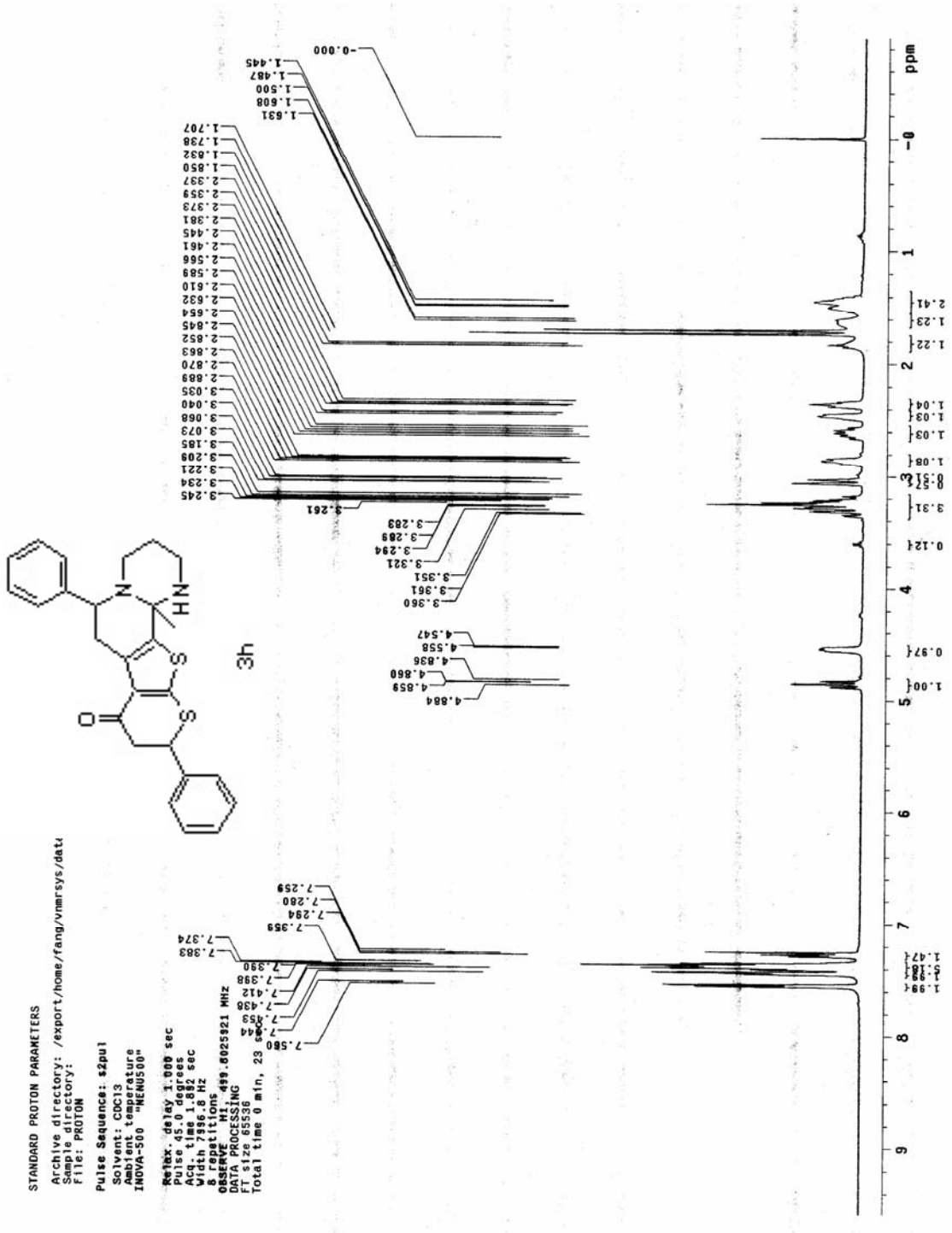

STANDARD CARBON PARAMETERS
Archive direc
Sample directo
Pulse Sequence
Solvent: CDCl3
Temp. 7.5 C /
User: 1-14-87
File: a723a
INOVA-500 "NEI
Relax. delay
Pulse 45.0 deg
Acq. time 1.8
Width 31421.8
5760 repetitio
OBSERVE C13,
DECOUPLE H1,
Power 48 dB
on during acqu
off during de
WALTZ-16 modu
DATA PROCESSING
Line broadening
FT size 131072
Total time 6 ho
OCH3
H3CO
3e
190.353
190.269
159.6
158.50
151.7
128.80
114.254
113.602
78.152
78.034
77.356
77.000
76.744
55.289
55.235
54.808
54.747
48.837
48.749
48.789
43.664
42.985
28.385
28.160
24.684
24.440
ppm

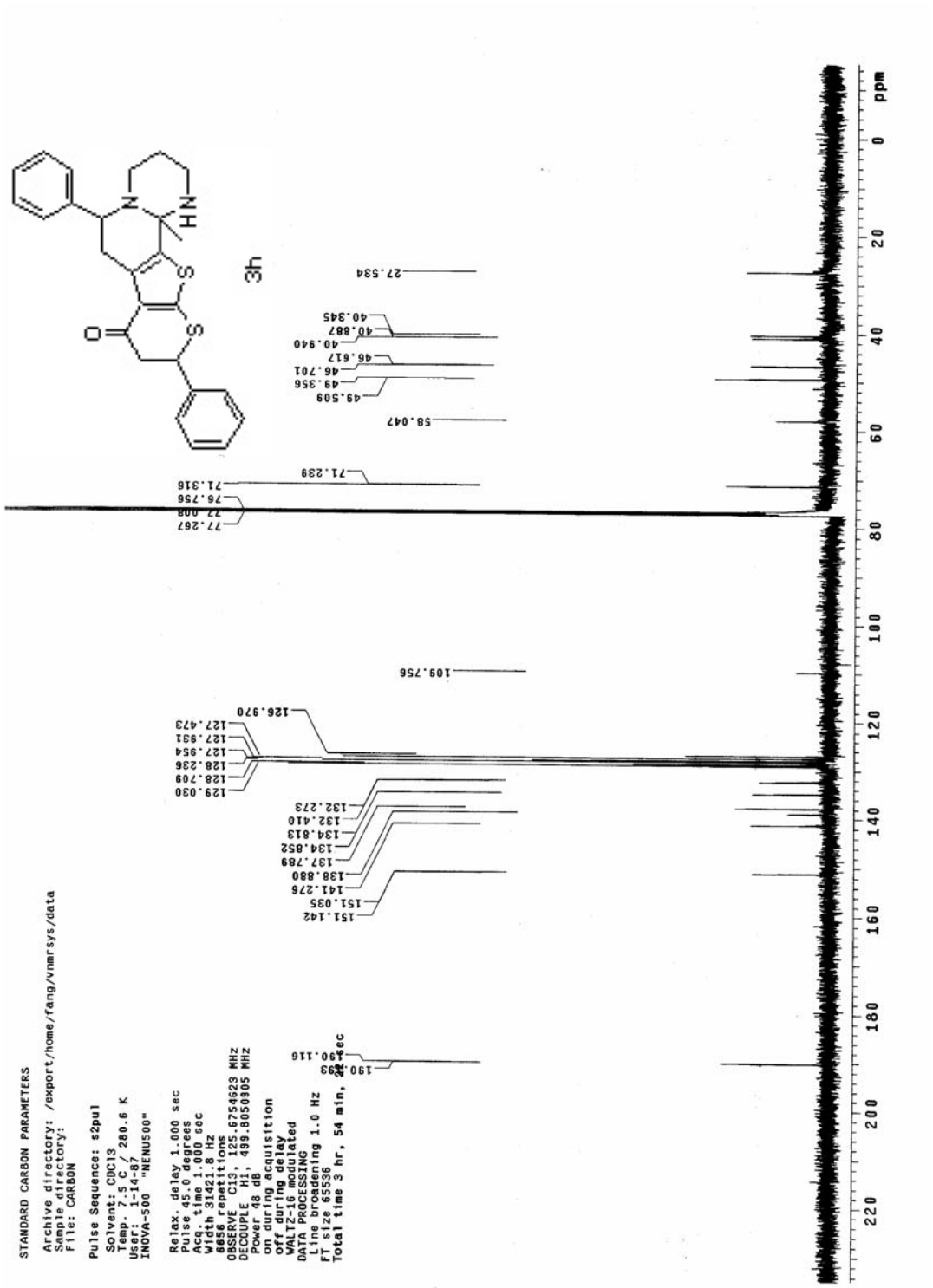

3f
STANDARD PROTON PARAMETERS
Archive directory: /export/home/pan/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 7996.8 Hz
16 repetitions
OBSERVE H1, 499.8025914 MHz
DATA PROCESSING
FT size 131072
Total time 0 min, 48 sec
3f
ppm


3f
STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 7.5 C / 280.6 K
User: 1-14-87
INOVA-500 "NERUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
2000 repetitions
OBSERVE C13, 125.6754637 MHz
DECOUPLE H1, 499.8050905 MHz
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 12 hr, 49 min, 47 sec
189.773
189.649
160.218
156.861
150.879
150.734
149.616
149.242
138.571
138.529
137.072
136.381
135.328
131.941
131.834
123.200
122.449
122.403
122.247
122.109
121.945
78.698
78.599
77.258
77.000
76.748
57.987
57.906
50.657
45.152
44.007
43.145
28.236
28.064
24.287
24.085
-0.041
ppm

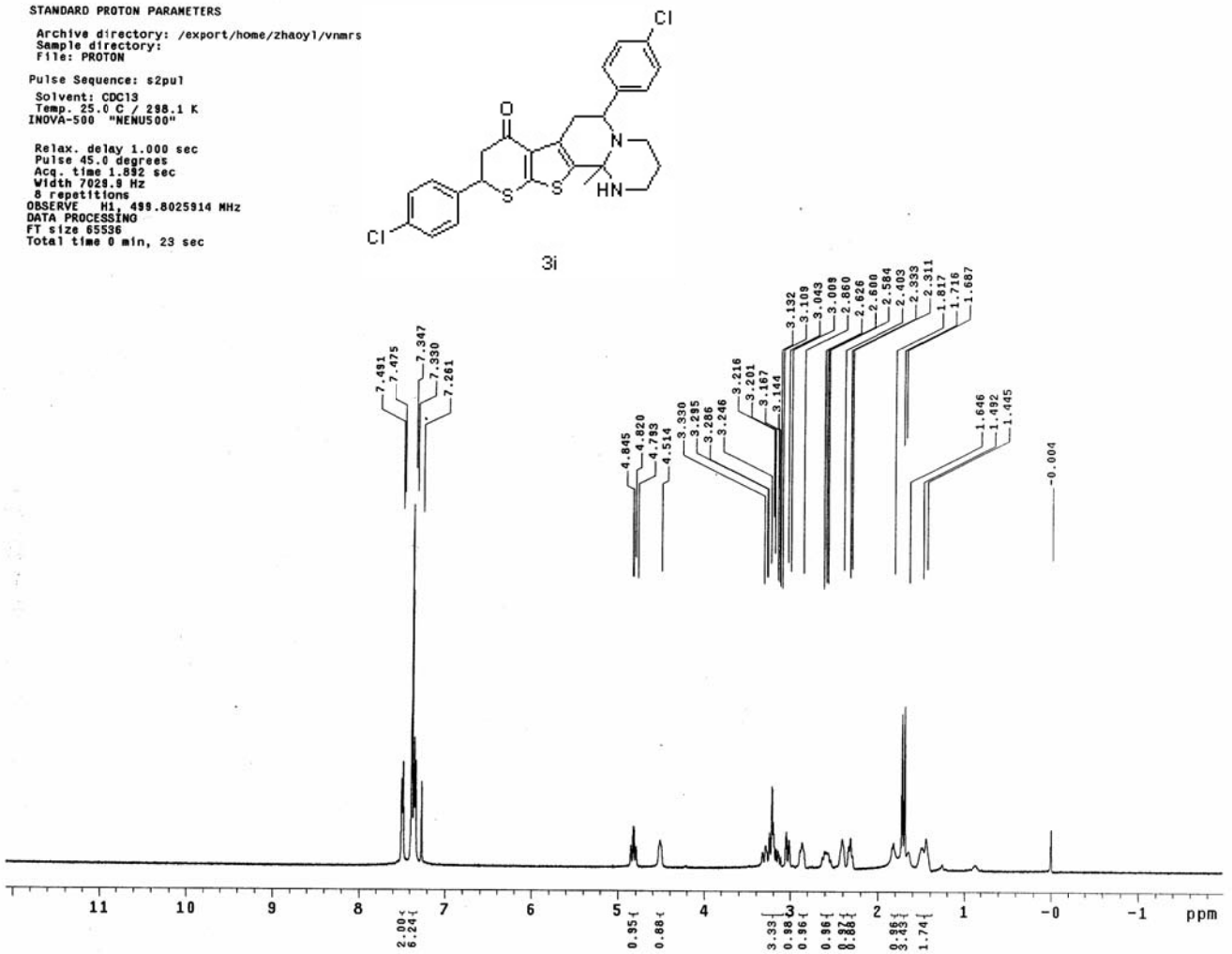

STANDARD PROTON PARAMETERS
Archive directory: /export/home/zhaoyl/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7029.9 Hz
8 repetitions
OBSERVE H1, 499.8025873 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
3g
ppm

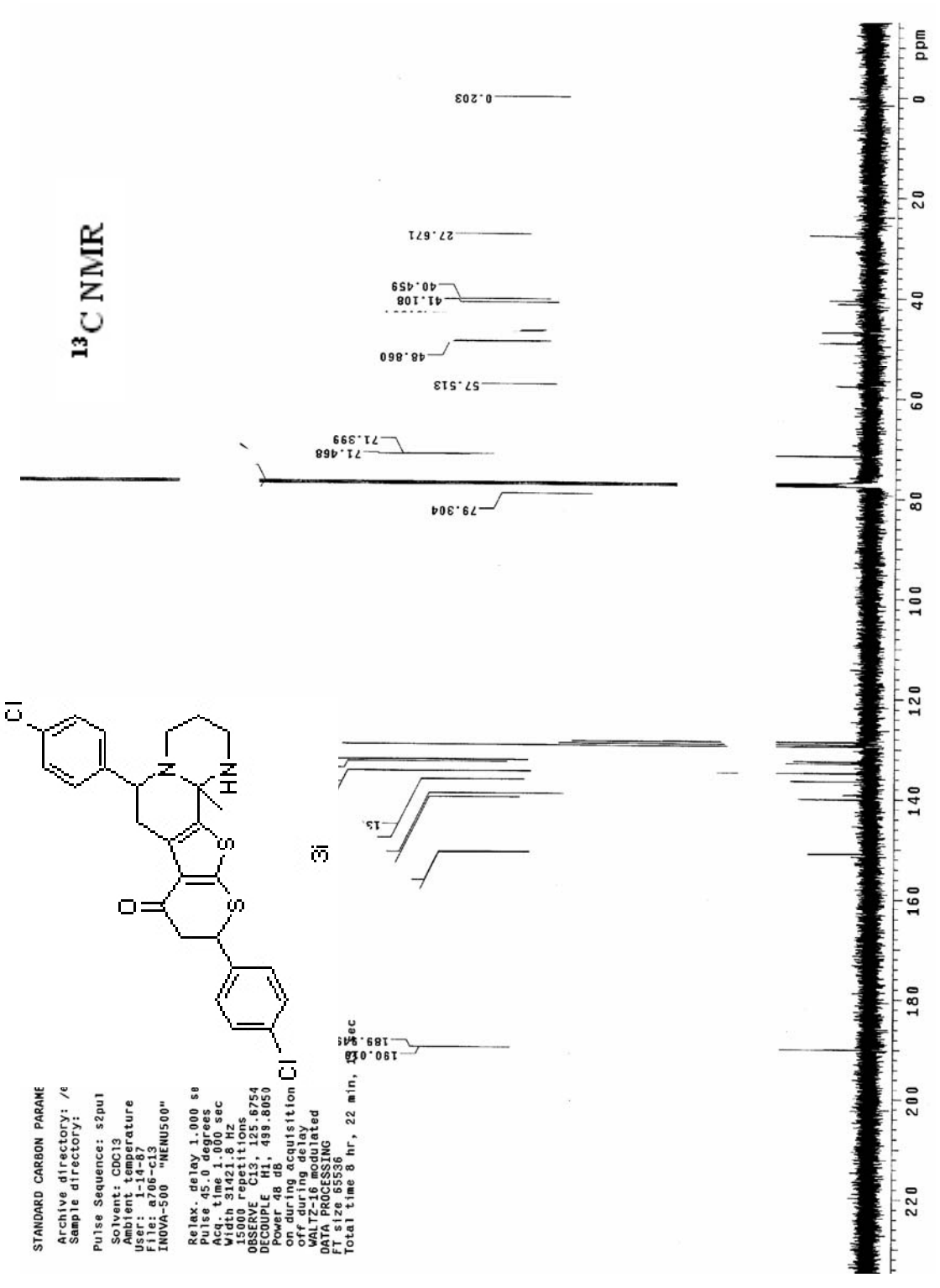

STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang/vnmrsys
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 7.5 C / 280.6 K
User: 1-14-87
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 31421.8 Hz
768 repetitions
OBSERVE C13, 125.6754638 MHz
DECOUPLE H1, 499.8050905 MHz
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
FT size 65536
Total time 11 hr, 1 min, 38 sec
8g
189.265
154.800
150.680
150.634
150.222
142.889
142.080
138.716
138.647
134.252
131.467
131.360
110.599
110.042
108.172
106.577
77.835
77.774
77.362
77.278
77.102
77.018
76.643
76.767
50.633
44.377
43.667
42.904
41.676
28.147
27.964
23.968
23.844
ppm

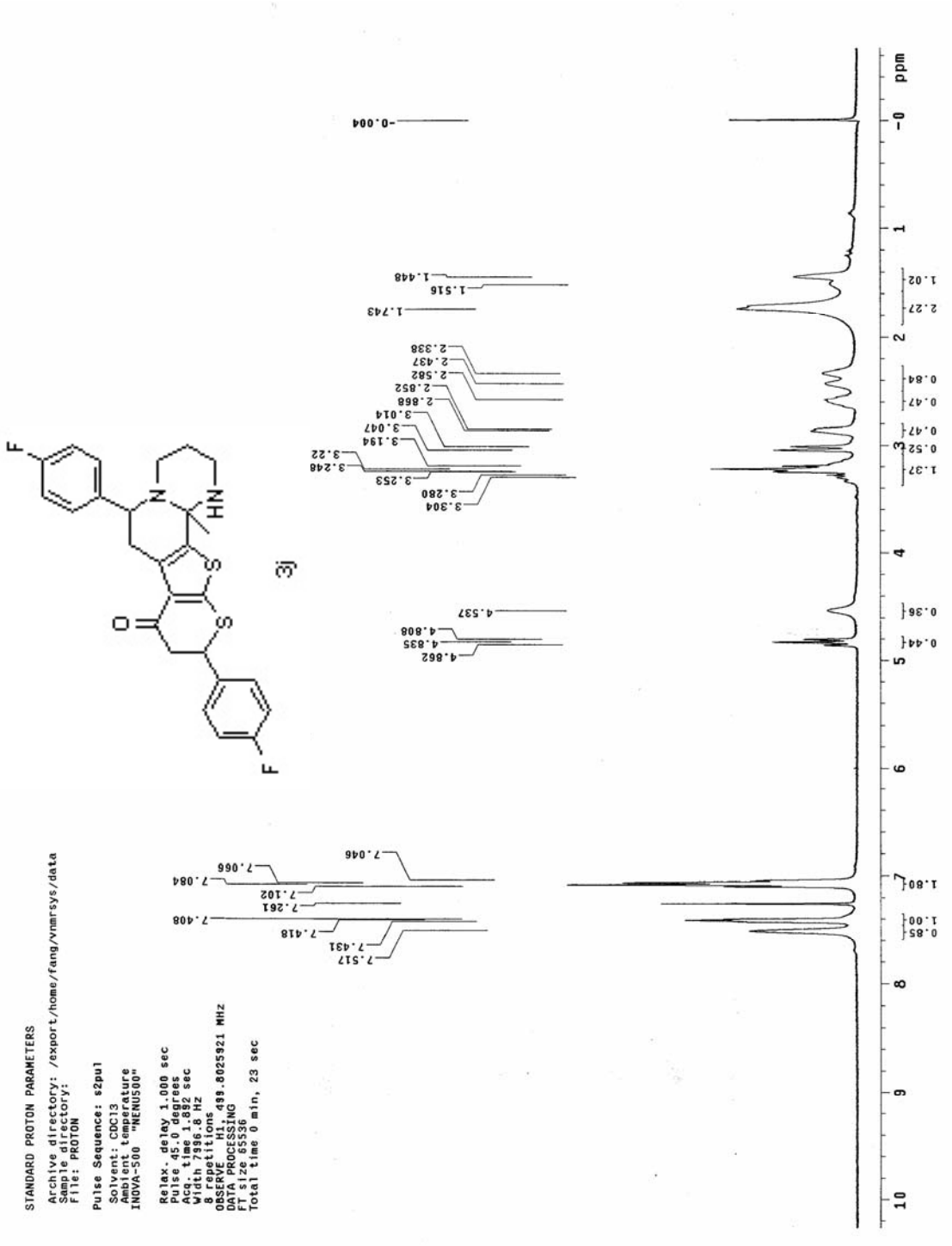

STANDARD PROTON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.6025921 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
3h
ppm

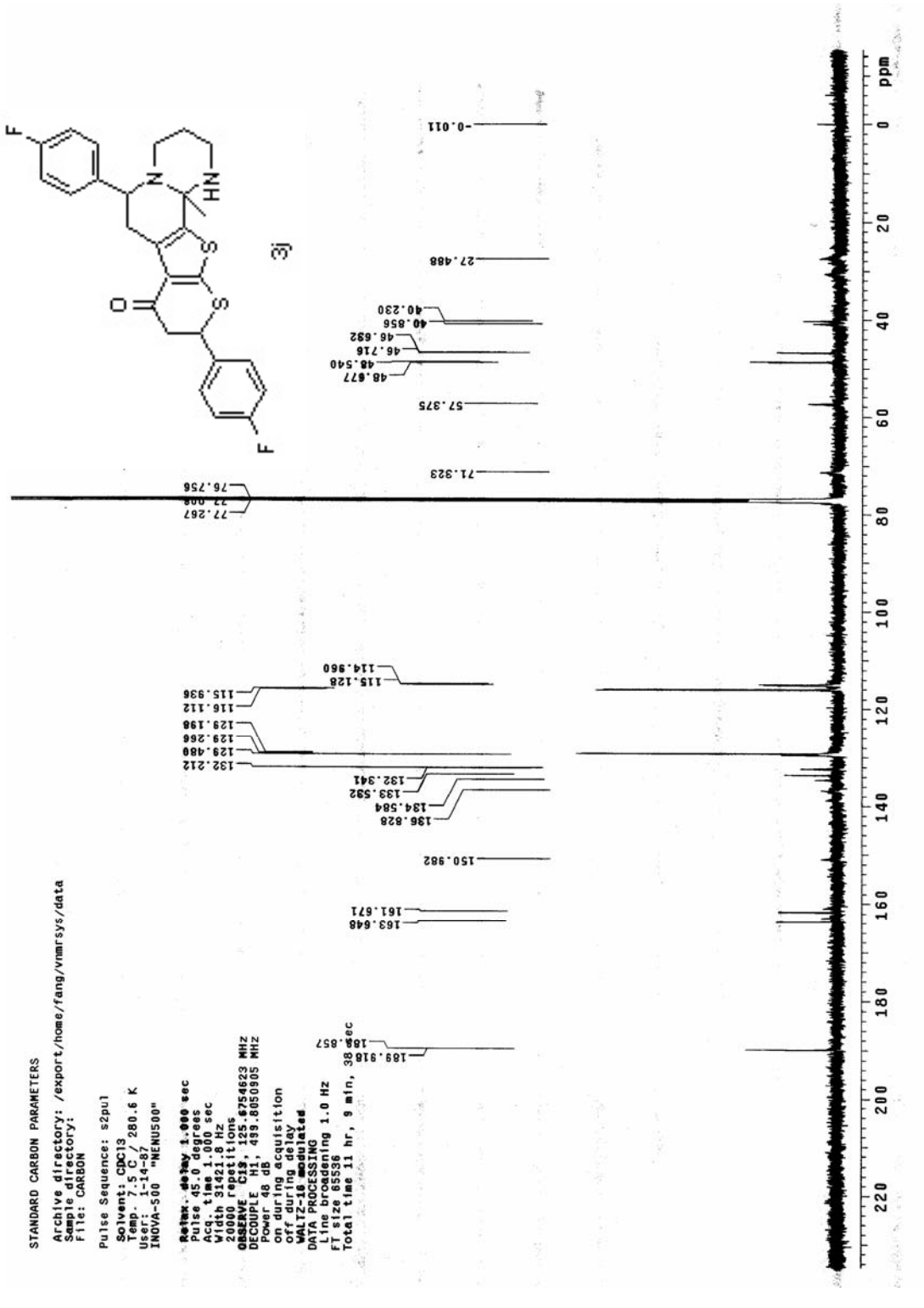

3h
27.534
40.345
40.887
40.940
46.617
46.701
49.356
49.509
58.047
71.239
71.316
76.756
77.008
77.267
109.756
126.970
127.473
127.931
127.954
128.236
128.709
129.030
132.273
132.410
134.613
134.852
137.789
138.880
141.276
151.035
151.142
190.116
190.393
STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 7.5 C / 280.6 K
User: 1-14+87
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 31421.8 Hz
65536 repetitions
OBSERVE C13, 125.6754623 MHz
DECOUPLE H1, 499.8050905 MHz
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 3 hr, 54 min, 24 sec
220
200
180
160
140
120
100
80
60
40
20
0
ppm

3i

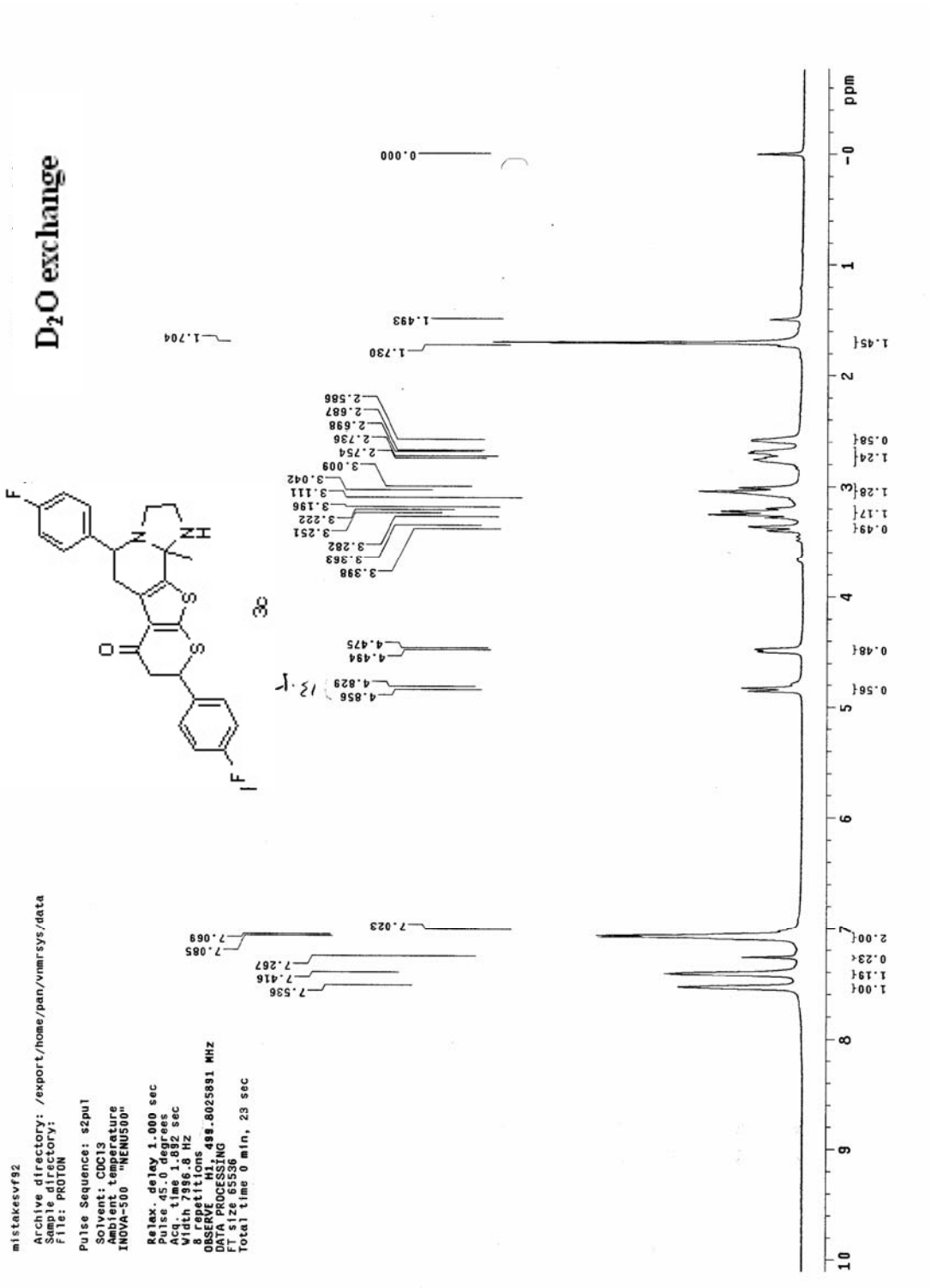

STANDARD PROTON PARAMETERS
Archive directory: /export/home/zhaoyl/vnmrs
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7028.8 Hz
8 repetitions
OBSERVE H1, 499.8025914 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
Cl
O
N
S
S
HN
Cl
7.491
7.475
7.347
7.330
7.261
4.845
4.820
4.793
4.514
3.330
3.295
3.286
3.246
3.216
3.201
3.167
3.144
3.132
3.109
3.043
3.009
2.860
2.626
2.600
2.584
2.403
2.333
2.311
1.817
1.716
1.687
1.646
1.492
1.445
-0.004
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
2.00
6.24
0.95
0.88
3.33
0.88
0.96
0.96
0.87
0.88
0.86
3.43
1.74

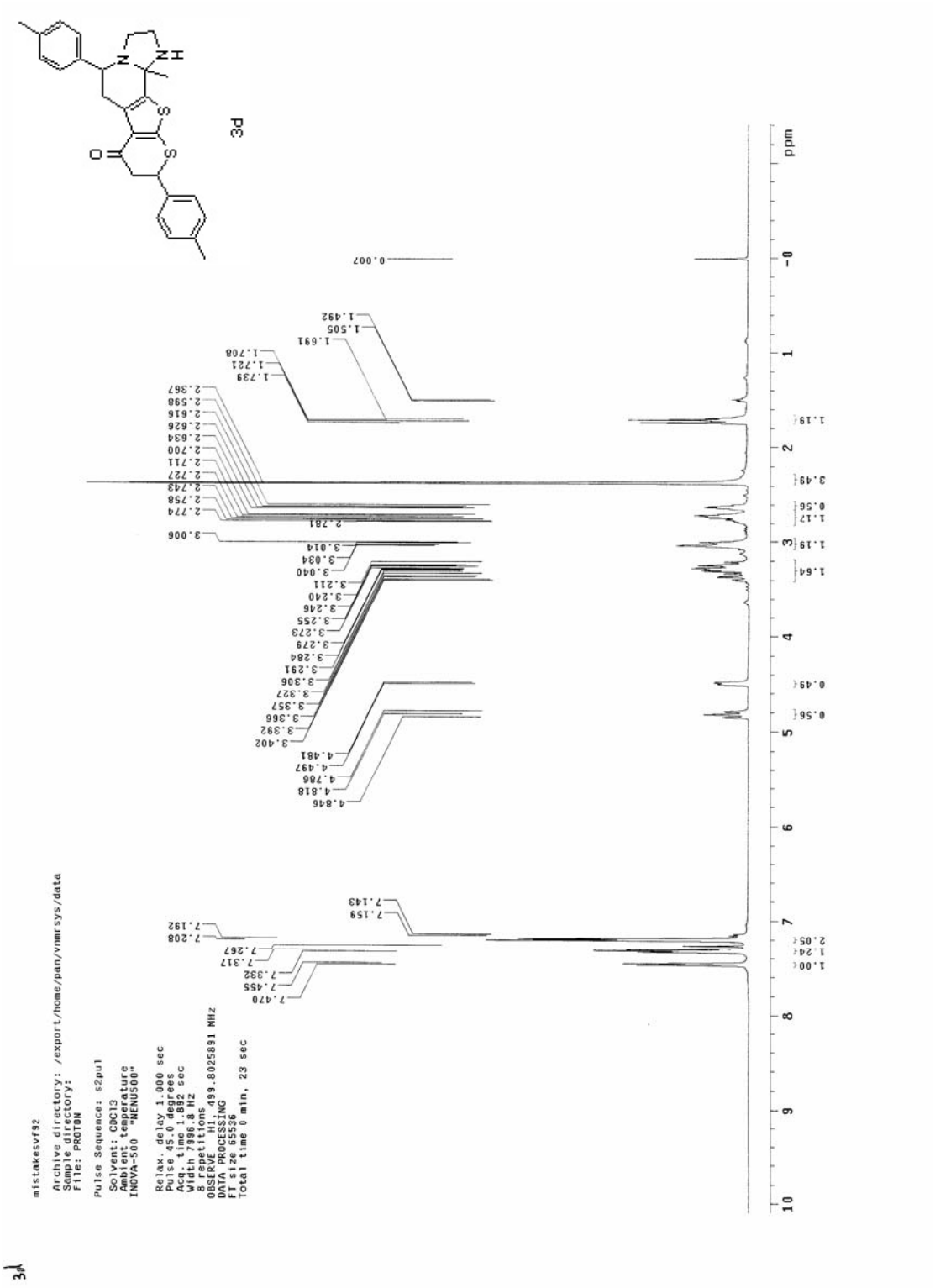

^{13}C NMR
3i
STANDARD CARBON PARAME
Archive directory: /e
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: a706-c13
INOVA-500 "NENU500"
Relax. delay 1.000 se
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 31421.8 Hz
15000 repetitions
OBSERVE C13, 125.6754
DECOUPLE H1, 499.8050
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
FT size 65536
Total time 8 hr, 22 min,
189.340
180.010
79.304
71.468
71.399
57.513
48.860
41.108
40.459
27.671
0.203
ppm

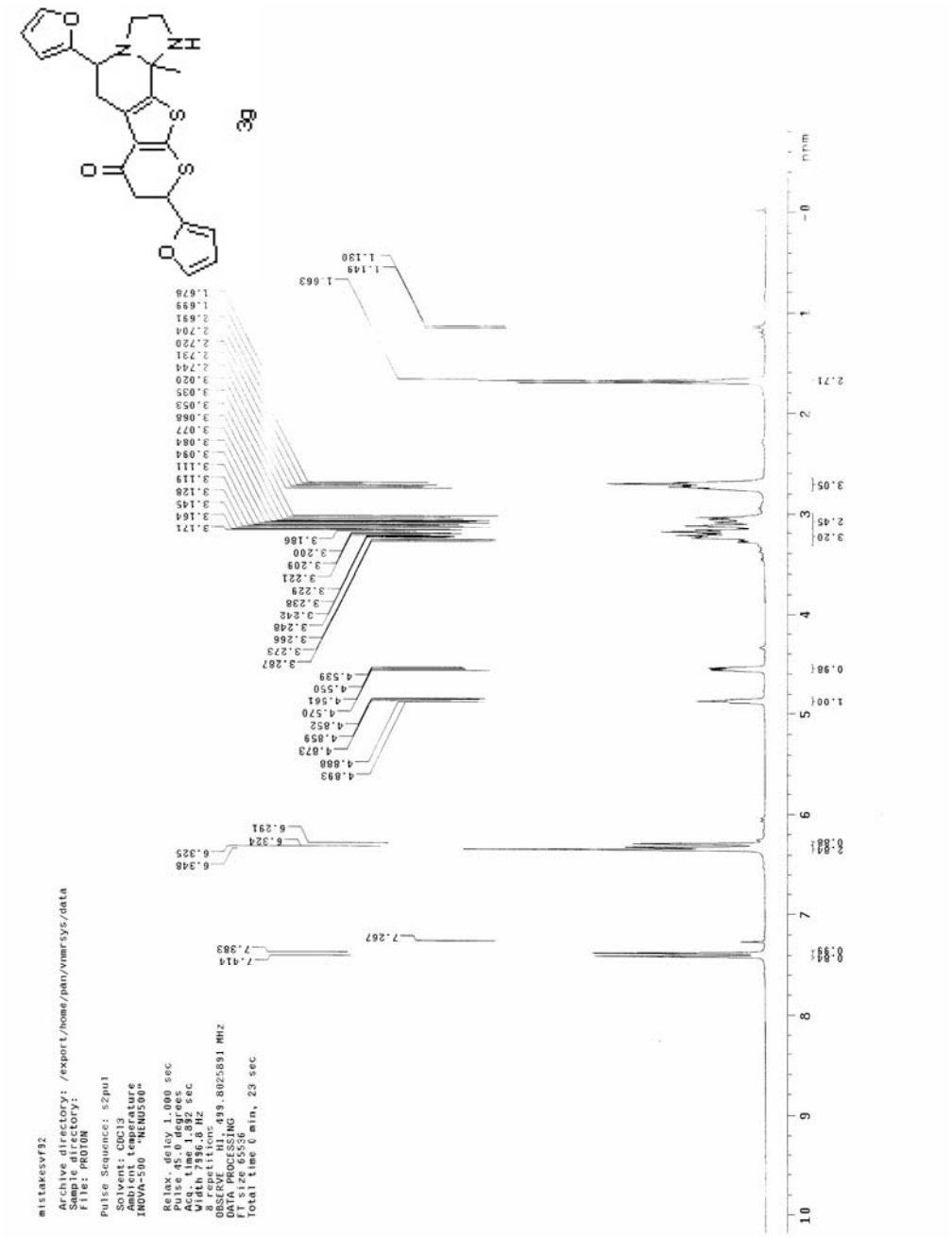

STANDARD PROTON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025921 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
3j
F
O
S
S
N
NH
F
7.517
7.431
7.418
7.408
7.261
7.102
7.084
7.066
7.046
4.862
4.835
4.808
4.537
3.304
3.280
3.253
3.246
3.220
3.194
3.047
3.014
2.868
2.852
2.582
2.437
2.338
1.743
1.516
1.448
-0.004
ppm
10
9
8
7
6
5
4
3
2
1
0
0.85
1.00
1.80
0.36
0.44
1.37
0.52
0.47
0.47
0.84
0.47
2.27
1.02


STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 7.5 C / 280.6 K
User: 1-14-87
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.800 sec
Width 31421.8 Hz
20000 repetitions
OBSERVE C13, 125.6754623 MHz
DECOUPLE H1, 499.8050905 MHz
Power 48 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 11 hr, 9 min, 38 sec
3j
F
N
HN
S
O
S
F
189.916
188.857
163.648
161.671
150.982
136.828
134.584
133.582
132.341
132.212
129.480
129.266
129.196
116.112
115.936
115.128
114.960
77.267
77.008
76.756
71.323
57.375
48.677
48.540
46.716
46.682
40.856
40.230
27.488
-0.011
ppm
0
20
40
60
80
100
120
140
160
180
200
220

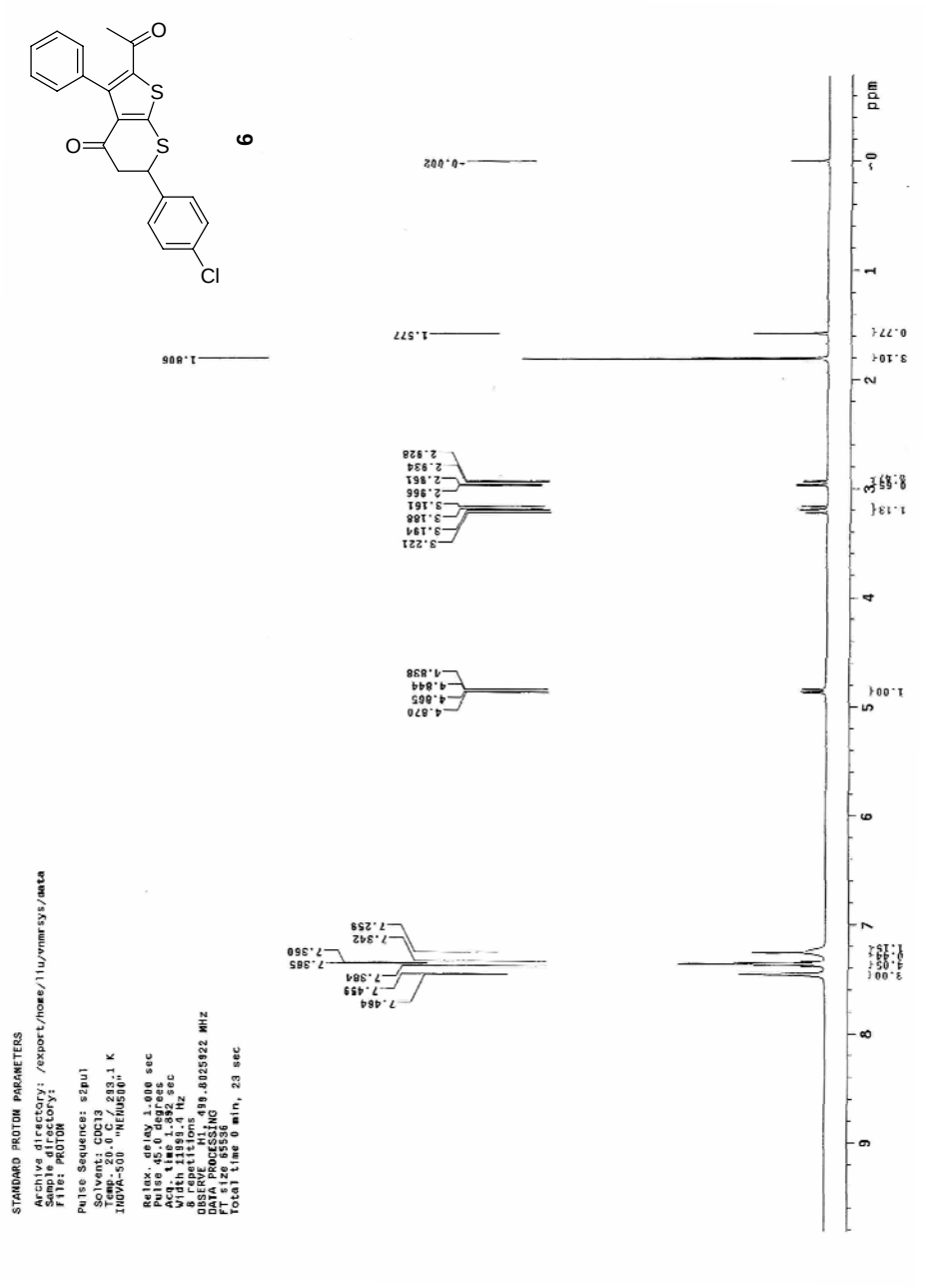
V. Copies of ^{1}H NMR spectra for compounds 3c, 3d and 3g by D_2O exchange.

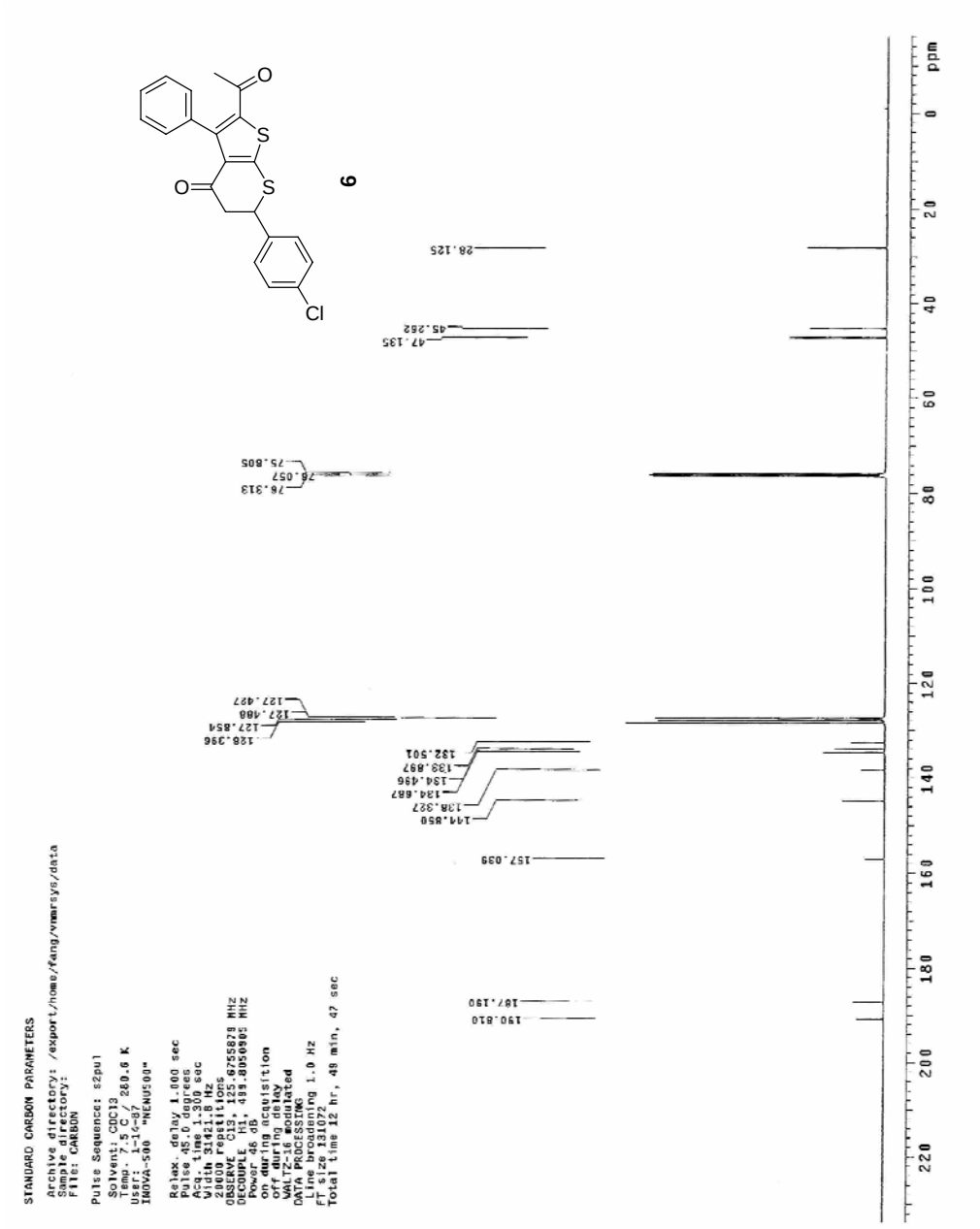



3d
mistakesvf92
Archive directory: /export/home/pan/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7936.8 Hz
8 repetitions
OBSERVE H1, 499.8025891 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm


3g
mistakesvf92
Archive directory: /export/home/pan/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7196.8 Hz
8 repetitions
OBSERVE H1, 499.8025891 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1.130
1.149
1.663
1.676
1.699
1.691
2.704
2.720
2.731
2.744
3.020
3.035
3.053
3.068
3.077
3.084
3.094
3.111
3.119
3.128
3.145
3.164
3.171
3.186
3.200
3.209
3.221
3.229
3.236
3.242
3.248
3.266
3.273
3.287
4.539
4.550
4.561
4.570
4.652
4.659
4.673
4.886
4.893
6.291
6.324
6.325
6.348
7.267
7.383
7.414
2.71
3.05
2.45
3.20
0.98
1.00
0.88
0.99
ppm

VI. Copies of ^{1}H NMR spectra for compound 6




STANDARD CARBON PARAMETERS
Archive directory: /export/home/fang/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 7.5 C / 280.6 K
User: 11-16-07
INOVA-500 "NCNU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
20000 repetitions
OBSERVE C13, 125.6755878 MHz
DECOUPLE H1, 499.8050905 MHz
Power 46 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 12 hr, 48 min, 47 sec
O
S
O
S
Cl
6
28.125
45.262
47.135
75.805
76.057
76.313
127.397
127.460
127.854
128.396
132.501
133.897
134.496
134.687
138.827
144.850
157.039
187.190
190.810
220
200
180
160
140
120
100
80
60
40
20
0
ppm