

Supporting Information

Multicomponent reactions of chalcones, malononitrile in DMF leading to γ -ketoamides

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General methods

Analytical data for compounds 3

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

General methods

All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. The products were purified by column chromatography over silica gel. ^1H NMR and ^{13}C NMR spectra were recorded at 25 $^\circ\text{C}$ on a Varian 500 MHz and 125 MHz, respectively, and TMS as internal standard. High resolution mass spectra (HRMS) were recorded on Bruck microTof by using ESI method. Data for ^1H NMR are reported as follows: chemical shift (ppm), and multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration; Data for ^{13}C NMR are reported as ppm. Melting points were measured on an X₄-type micro-melting point apparatus and were uncorrected.

Analytical data for compounds 3

***N,N*-dimethyl-4-oxo-2,4-diphenylbutanamide (3a).** Pale yellow oil. ^1H NMR (500 MHz, CDCl_3): δ = 2.96 (s, 3H), 3.03 (d, J = 3.5 Hz, 3H), 3.07 (d, J = 3.0 Hz, 1H), 4.10-4.16 (m, 1H), 4.53-4.56 (m, 1H), 7.27-7.29 (m, 1H), 7.32-7.35 (m, 4H), 7.43 (t, J = 7.5 Hz, 2H), 7.53 (t, J = 7.5 Hz, 1H), 7.97 (d, J = 7.5 Hz, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ = 36.0, 37.2, 44.2, 44.4, 127.2, 127.8, 128.2, 128.5, 129.0, 133.1, 136.5, 139.3, 172.2, 198.7; HRMS (ESI-TOF): calcd for $\text{C}_{18}\text{H}_{19}\text{NO}_2$ 282.1494 ($\text{M}+\text{H}^+$), found 282.1487.

***N,N*-dimethyl-4-oxo-2-phenyl-4-(*p*-tolyl)butanamide (3b).** White solid. m.p. 112-114 $^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ = 2.37 (s, 3H), 2.95 (s, 3H), 3.01-3.02 (m, 3H), 3.05 (d, J = 3.5 Hz, 1H), 4.07-4.13 (m, 1H), 4.52-4.55 (m, 1H), 7.21 (d, J = 8.0 Hz, 2H), 7.24 (t, J = 3.0 Hz, 1H), 7.31-7.36 (m, 4H), 7.87 (d, J = 8.0 Hz, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ = 21.5, 35.9, 37.0, 44.0, 44.2, 127.0, 127.7, 128.1, 128.8, 129.0, 134.0, 139.3, 143.7, 172.1, 198.2; HRMS (ESI-TOF): calcd for $\text{C}_{19}\text{H}_{21}\text{NO}_2$ 296.1651 ($\text{M}+\text{H}^+$), found 296.1646.

4-(4-methoxyphenyl)-*N,N*-dimethyl-4-oxo-2-phenylbutanamide (3c). White solid. m.p. 93-95 $^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ = 2.95 (s, 3H), 2.99 (d, J = 3.5 Hz, 1H), 3.03 (s, 3H), 3.83 (s, 3H), 4.05-4.11 (m, 1H), 4.52-4.55 (m, 1H), 6.89 (d, J = 8.5 Hz, 2H), 7.27 (s, 1H), 7.32-7.37 (m, 4H), 7.95 (d, J = 8.5 Hz, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ = 35.9, 37.1, 44.0, 44.1, 55.3, 113.5, 127.0, 127.8, 128.9, 129.6, 130.3, 139.4, 163.4, 172.2, 197.1; HRMS (ESI-TOF): calcd for $\text{C}_{19}\text{H}_{21}\text{NO}_3$ 312.1600 ($\text{M}+\text{H}^+$), found 312.1609.

4-(4-chlorophenyl)-*N,N*-dimethyl-4-oxo-2-phenylbutanamide (3d). White solid. m.p. 91-93 $^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ = 2.95 (s, 3H), 2.98 (t, J = 15 Hz, 1H), 3.01 (s, 3H), 4.06-4.11 (m, 1H), 4.51-4.54 (m, 1H), 7.28 (t, J = 4.0 Hz, 1H), 7.34 (d, J = 4.5 Hz, 4H), 7.40 (d, J = 1.5 Hz, 2H), 7.91 (d, J = 8.5 Hz, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ = 36.0, 37.1, 44.3, 44.4, 127.2, 127.7, 128.7, 129.0, 129.6, 134.9, 139.1, 139.4, 172.0, 197.5; HRMS (ESI-TOF): calcd for $\text{C}_{18}\text{H}_{18}\text{ClNO}_2$ 316.1104 ($\text{M}+\text{H}^+$), found 316.1113.

***N,N*-dimethyl-4-(naphthalen-2-yl)-4-oxo-2-phenylbutanamide (3e).** Pale yellow solid. m.p. 115-117 $^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ = 2.97 (s, 3H), 3.04 (s, 3H), 3.17-3.21 (m, 1H), 4.24-4.30 (m, 1H), 4.59-4.62 (m, 1H), 7.25-7.29 (m, 1H), 7.34-7.41 (m, 4H), 7.49-7.53 (m, 1H), 7.55-7.58 (m, 1H), 7.83-7.85 (m, 2H), 7.90 (d, J = 7.5 Hz, 1H), 8.01-8.03 (m, 1H), 8.51 (s, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ = 36.0, 37.2, 44.2, 44.5, 123.8, 126.6, 127.1, 127.6, 127.8, 128.2, 128.3, 129.0, 129.5, 130.0, 132.4, 133.9, 135.5, 139.3, 172.2, 198.6; HRMS (ESI-TOF): calcd for $\text{C}_{19}\text{H}_{21}\text{NO}_3$ 312.1600 ($\text{M}+\text{H}^+$), found 312.1609.

4-(furan-2-yl)-*N,N*-dimethyl-4-oxo-2-phenylbutanamide (3f). White solid. m.p. 93-95 $^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ = 2.91-2.95 (m, 1H), 2.96 (s, 3H), 2.99 (s, 3H), 3.90-3.96 (m, 1H), 4.51-4.54 (m, 1H), 6.49-6.50 (m, 1H), 7.19 (d, J = 3.5 Hz, 1H), 7.26 (d, J = 8.5 Hz, 1H), 7.33 (d, J = 4.5 Hz, 4H), 7.55 (d, J = 1.5 Hz, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ = 35.9, 37.1, 43.8, 43.9, 112.1, 117.4, 127.1, 127.8, 128.9, 139.1, 146.3, 152.3, 171.9, 187.5; HRMS (ESI-TOF): calcd for $\text{C}_{16}\text{H}_{17}\text{NO}_3$ 272.1287 ($\text{M}+\text{H}^+$), found 272.1279.

***N,N*-dimethyl-4-oxo-2-phenyl-4-(thiophen-2-yl)butanamide (3g).** Pale yellow solid. m.p. 100-102 $^\circ\text{C}$. ^1H NMR (500 MHz, CDCl_3): δ = 2.95 (s, 3H), 3.00 (s, 3H), 3.01-3.05 (m, 1H), 4.00-4.05 (m, 1H), 4.52-4.55 (m, 1H), 7.07-7.09 (m, 1H),

7.26-7.28 (m, 1H), 7.32-7.36 (m, 4H), 7.59-7.60 (m, 1H), 7.74 (t, J = 2.0 Hz, 1H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 35.9, 37.1, 44.0, 44.8, 127.1, 127.8, 128.0, 128.9, 132.1, 133.5, 139.0, 143.7, 171.9, 191.4; HRMS (ESI-TOF): calcd for C₁₆H₁₇NO₂S 288.1058 (M+H⁺), found 288.1051.

2-(4-methoxyphenyl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3i). White solid. m.p. 79-81 °C. ^1H NMR (500 MHz, CDCl₃): δ = 2.95 (s, 3H), 3.01-3.05 (m, 4H), 3.78 (s, 3H), 4.06-4.12 (m, 1H), 4.08-4.51 (m, 1H), 6.87 (d, J = 8.5 Hz, 2H), 7.27 (d, J = 8.5 Hz, 2H), 7.41 (t, J = 7.5 Hz, 2H), 7.51 (d, J = 7.5 Hz, 1H), 7.96 (t, J = 3.5 Hz, 2H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 35.8, 37.0, 43.1, 43.4, 55.1, 114.2, 128.0, 128.3, 128.7, 131.1, 132.9, 136.5, 158.5, 172.4, 198.7; HRMS (ESI-TOF): calcd for C₁₉H₂₁NO₃ 312.1600 (M+H⁺), found 312.1607.

2-(2-methoxyphenyl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3j). White solid. m.p. 109-111 °C. ^1H NMR (500 MHz, CDCl₃): δ = 2.93-2.96 (m, 6H), 2.98 (d, J = 3.0 Hz, 1H), 3.84 (s, 3H), 3.96-4.02 (m, 1H), 4.97-5.00 (m, 1H), 6.89-6.96 (m, 2H), 7.24-7.30 (m, 2H), 7.41 (t, J = 7.5 Hz, 2H), 7.51 (d, J = 7.5 Hz, 1H), 7.98 (d, J = 7.5 Hz, 2H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 35.8, 36.6, 36.8, 42.7, 55.3, 110.3, 121.0, 127.3, 128.1, 128.2, 128.3, 132.8, 136.7, 155.8, 172.8, 199.0; HRMS (ESI-TOF): calcd for C₁₉H₂₁NO₃ 312.1600 (M+H⁺), found 312.1612.

2-(4-(dimethylamino)phenyl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3k). White solid. m.p. 149-151 °C. ^1H NMR (500 MHz, CDCl₃): δ = 2.94 (d, J = 4.0 Hz, 8H), 2.99 (d, J = 3.5 Hz, 1H), 3.03 (d, J = 3.5 Hz, 4H), 4.07-4.12 (m, 1H), 4.43-4.46 (m, 1H), 6.70 (d, J = 8.5 Hz, 2H), 7.21 (d, J = 8.5 Hz, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.51 (d, J = 7.5 Hz, 1H), 7.97 (d, J = 7.5 Hz, 2H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 30.9, 35.9, 37.2, 40.5, 43.2, 44.6, 112.9, 126.8, 128.1, 128.4, 128.5, 132.9, 136.7, 149.6, 172.8, 199.1; HRMS (ESI-TOF): calcd for C₂₀H₂₄N₂O₂ 325.1916 (M+H⁺), found 325.1907.

2-(benzo[d][1,3]dioxol-5-yl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3l). Pale yellow solid. m.p. 82-84 °C. ^1H NMR (500 MHz, CDCl₃): δ = 2.95 (s, 3H), 3.01 (d, J = 4.0 Hz, 1H), 3.05 (s, 3H), 4.04-4.10 (m, 1H), 4.44-4.47 (m, 1H), 5.95 (d, J = 1.5 Hz, 2H), 6.75-6.81 (m, 2H), 6.87 (s, 1H), 7.41-7.48 (m, 2H), 7.53 (t, J = 7.5 Hz, 1H), 7.97 (d, J = 7.0 Hz, 2H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 29.7, 36.1, 37.2, 43.7, 44.5, 101.1, 108.1, 108.6, 121.0, 128.1, 128.5, 132.9, 133.1, 136.5, 146.6, 148.1, 172.3, 198.8; HRMS (ESI-TOF): calcd for C₁₉H₁₉NO₄ 326.1392 (M+H⁺), found 326.1386.

2-(4-fluorophenyl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3m). Pale yellow oil. ^1H NMR (500 MHz, CDCl₃): δ = 2.96 (s, 3H), 3.05 (d, J = 14.5 Hz, 3H), 3.07 (d, J = 3.5 Hz, 1H), 4.06-4.12 (m, 1H), 4.53-4.56 (m, 1H), 7.02 (t, J = 9.0 Hz, 2H), 7.32-7.35 (m, 2H), 7.43 (t, J = 7.5 Hz, 2H), 7.54 (t, J = 7.5 Hz, 1H), 7.97 (d, J = 8.0 Hz, 2H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 36.0, 37.1, 43.2, 44.4, 115.7, 115.9, 128.1, 128.5, 129.3, 129.4, 133.1, 134.9, 135.0, 136.4, 160.9, 162.8, 172.1, 198.5; HRMS (ESI-TOF): calcd for C₁₈H₁₈FNO₂ 300.1392 (M+H⁺), found 300.1400.

2-(4-chlorophenyl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3n). Pale yellow oil. ^1H NMR (500 MHz, CDCl₃): δ = 2.96 (s, 3H), 3.03 (s, 3H), 3.07 (d, J = 4.0 Hz, 1H), 4.06-4.11 (m, 1H), 4.52-4.55 (m, 1H), 7.31 (s, 4H), 7.43 (t, J = 7.5 Hz, 2H), 7.54 (t, J = 7.5 Hz, 1H), 7.96 (t, J = 4.0 Hz, 2H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 36.0, 37.2, 43.4, 44.3, 128.1, 128.5, 129.1, 129.2, 133.0, 133.2, 136.4, 137.7, 171.8, 198.4; HRMS (ESI-TOF): calcd for C₁₈H₁₈CINO₂ 316.1104 (M+H⁺), found 316.1112.

2-(2-chlorophenyl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3o). Pale yellow oil. ^1H NMR (500 MHz, CDCl₃): δ = 2.95 (s, 3H), 2.97 (d, J = 5.0 Hz, 3H), 3.00 (d, J = 2.5 Hz, 1H), 3.98-4.03 (m, 1H), 4.99-5.01 (m, 1H), 7.22-7.25 (m, 2H), 7.40-7.44 (m, 4H), 7.52 (d, J = 7.5 Hz, 1H), 7.99 (t, J = 4.0 Hz, 2H); ^{13}C NMR (CDCl₃, 125 MHz): δ = 35.9, 36.8, 40.7, 42.4, 127.5, 128.1, 128.4, 128.5, 128.7, 129.7, 132.9, 133.0, 136.4, 136.8, 171.7, 198.1; HRMS (ESI-TOF): calcd for C₁₈H₁₈CINO₂ 316.1104 (M+H⁺), found 316.1109.

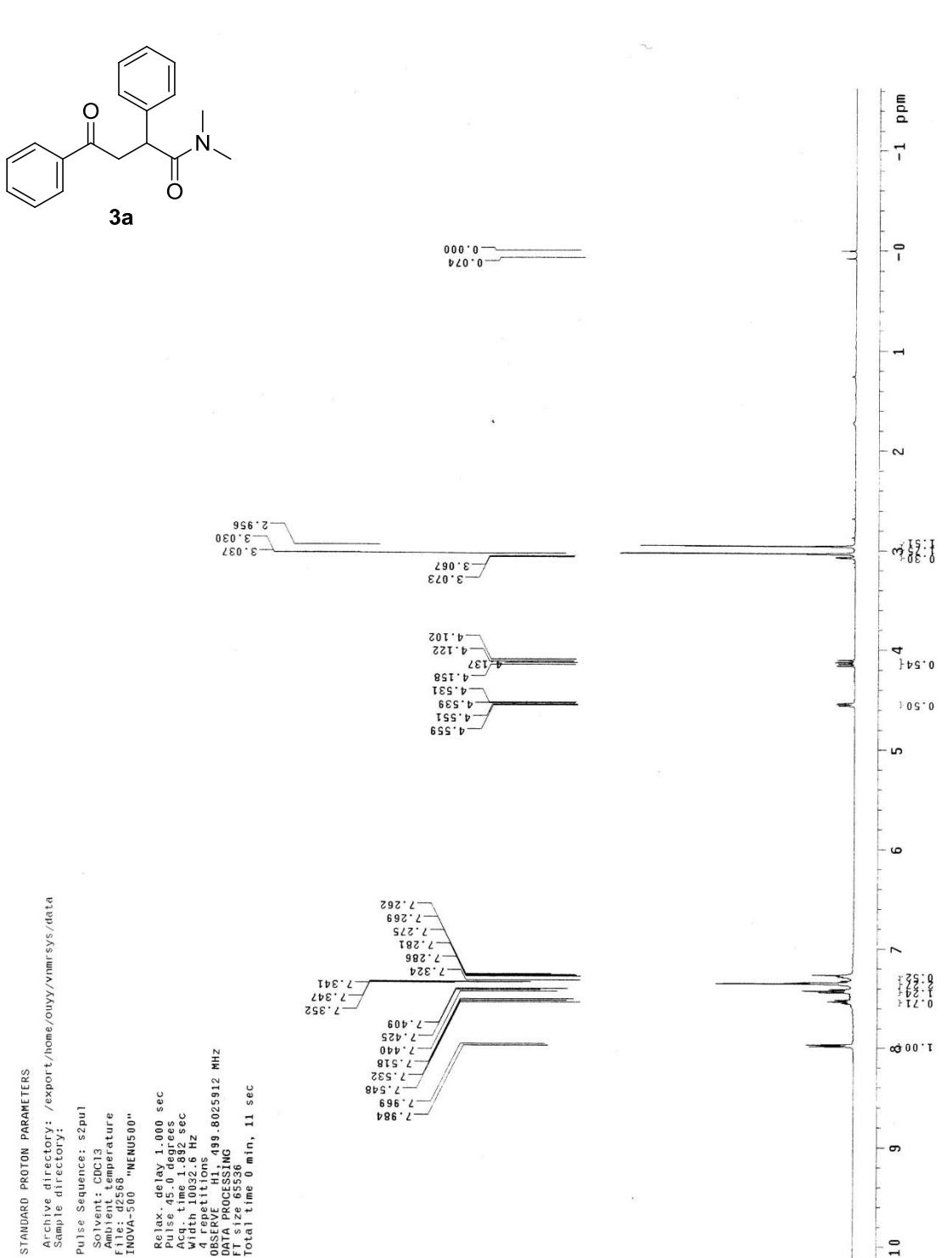
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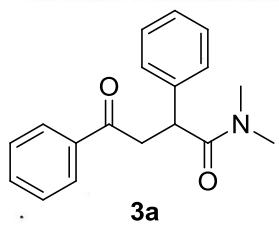
N,N-dimethyl-2-(3-nitrophenyl)-4-oxo-4-phenylbutanamide (3q). Pale yellow solid. m.p. 125-127 °C. ¹H NMR (500 MHz, CDCl₃): δ = 2.98 (s, 3H), 3.10 (s, 3H), 3.13-3.18 (m, 1H), 4.12-4.17 (m, 1H), 4.69-4.71 (m, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.52-7.56 (m, 2H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 7.5 Hz, 2H), 8.14-8.16 (m, 1H), 8.26 (s, 1H); ¹³C NMR (CDCl₃, 125 MHz): δ = 36.2, 37.3, 43.4, 44.2, 122.4, 123.0, 128.1, 128.6, 130.0, 133.4, 134.1, 136.2, 141.4, 148.6, 171.2, 197.8; HRMS (ESI-TOF): calcd for C₁₈H₁₈N₂O₄ 327.1345 (M+H⁺), found 327.1339.

N,N-dimethyl-2-(naphthalen-1-yl)-4-oxo-4-phenylbutanamide (3r). White solid. m.p. 129-131 °C. ¹H NMR (500 MHz, CDCl₃): δ = 2.79 (s, 3H), 3.01 (s, 3H), 3.04 (d, *J* = 3.5 Hz, 1H), 4.20-4.26 (m, 1H), 5.33-5.36 (m, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.41-7.46 (m, 2H), 7.48-7.51 (t, *J* = 6.0 Hz, 2H), 7.52-7.55 (m, 1H), 7.78-7.80 (m, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.98 (d, *J* = 7.0 Hz, 2H), 8.13 (d, *J* = 8.5 Hz, 1H); ¹³C NMR (CDCl₃, 125 MHz): δ = 35.9, 37.0, 40.1, 43.1, 122.1, 124.8, 125.7, 125.8, 126.7, 127.8, 128.1, 128.3, 129.2, 130.3, 133.0, 134.0, 135.2, 136.4, 172.4, 198.8; HRMS (ESI-TOF): calcd for C₂₂H₂₁NO₂ 332.1651 (M+H⁺), found 332.1646.

2-(furan-2-yl)-N,N-dimethyl-4-oxo-4-phenylbutanamide (3s). Pale yellow solid. m.p. 96-98 °C. ¹H NMR (500 MHz, CDCl₃): δ = 2.99 (s, 3H), 3.18 (s, 3H), 3.22-3.27 (m, 1H), 4.11-4.16 (m, 1H), 4.70-4.73 (m, 1H), 6.18 (d, *J* = 3.0 Hz, 1H), 6.33 (t, *J* = 3.0 Hz, 1H), 7.35 (d, *J* = 0.5 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 2H); ¹³C NMR (CDCl₃, 125 MHz): δ = 36.1, 37.4, 37.5, 40.9, 106.4, 110.5, 128.1, 128.5, 133.2, 136.3, 141.9, 152.3, 170.2, 198.2; HRMS (ESI-TOF): calcd for C₁₆H₁₇NO₃ 272.1287 (M+H⁺), found 272.1276.

N,N-dimethyl-4-oxo-4-phenyl-2-(thiophen-2-yl)butanamide (3t). Pale yellow solid. m.p. 108-110 °C. ¹H NMR (500 MHz, CDCl₃): δ = 2.98 (s, 3H), 3.16 (s, 3H), 3.19-3.23 (m, 1H), 4.14-4.20 (m, 1H), 4.84-4.87 (m, 1H), 6.95-6.98 (m, 2H), 7.20 (d, *J* = 5.0 Hz, 1H), 7.42-7.48 (m, 2H), 7.53-7.57 (m, 1H), 7.97 (d, *J* = 8.5 Hz, 2H); ¹³C NMR (CDCl₃, 125 MHz): δ = 36.1, 37.4, 38.7, 44.9, 124.6, 125.1, 126.9, 128.1, 128.5, 133.2, 136.3, 141.5, 171.6, 198.2; HRMS (ESI-TOF): calcd for C₁₆H₁₇NO₂S 288.1058 (M+H⁺), found 288.1051.





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Ambient temperature

User: 1-14-87

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Pulse: 45.0 deg sec

Acq. time: 0.10 sec

With 31421.3 Hz

6000 repetitions

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continuous on

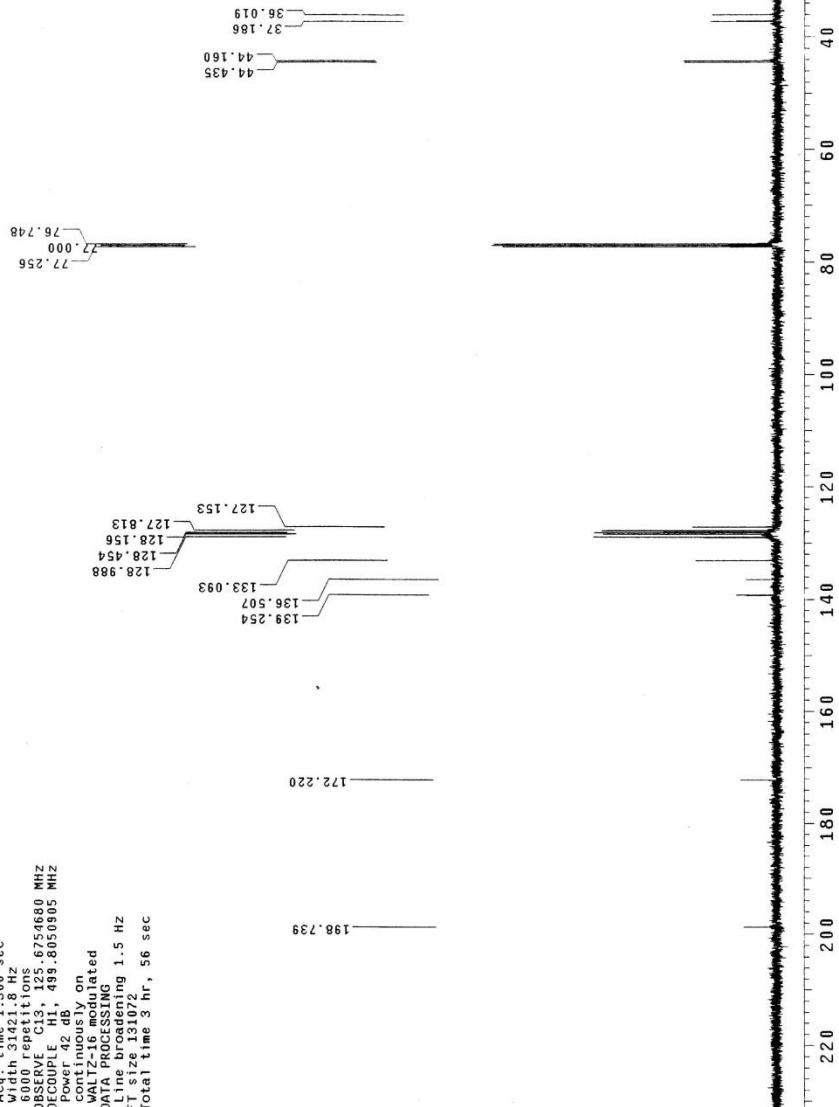
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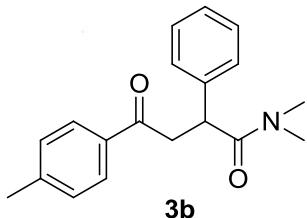
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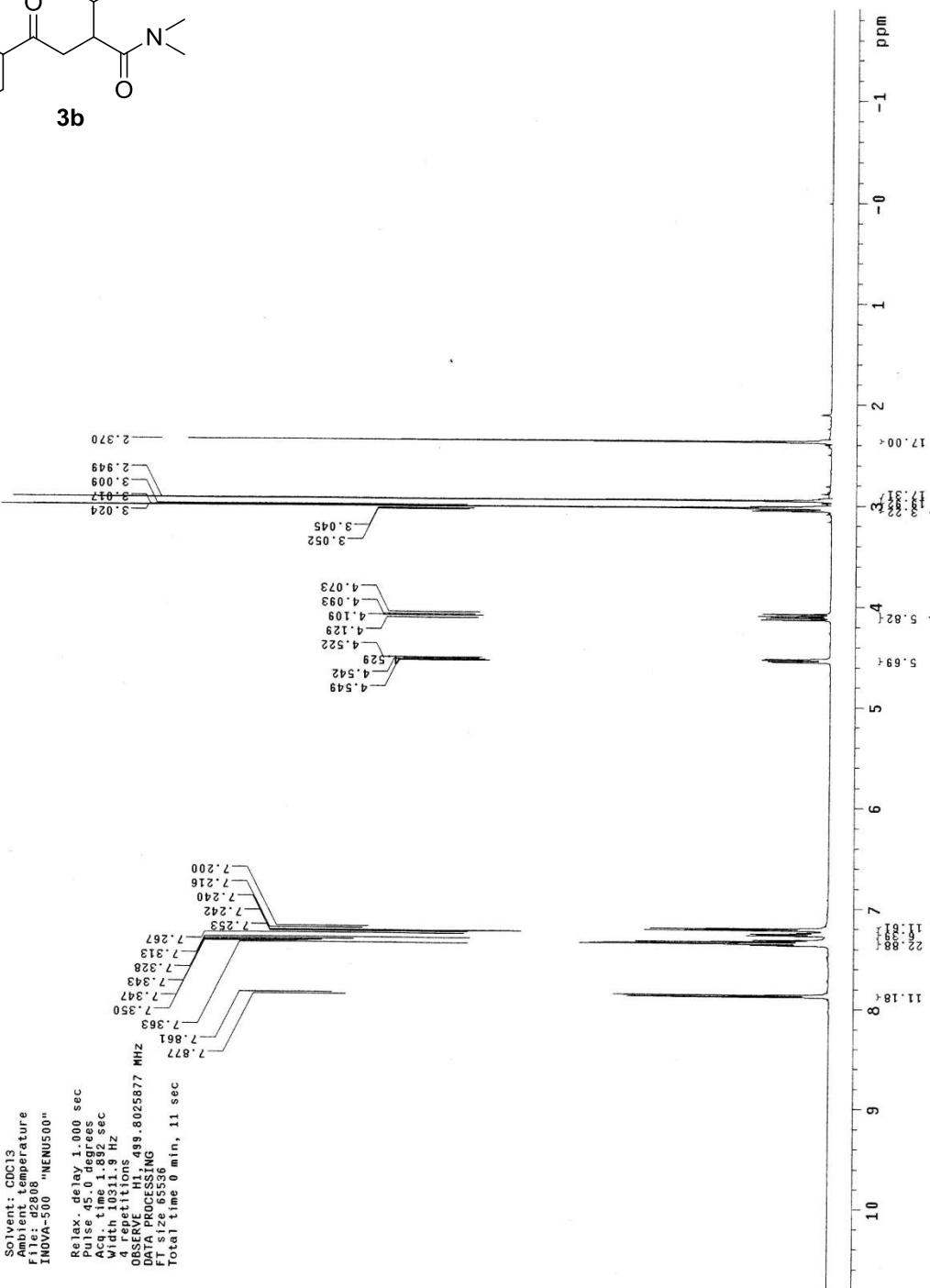
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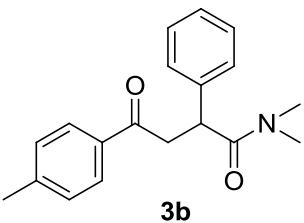
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DATA PROCESSING
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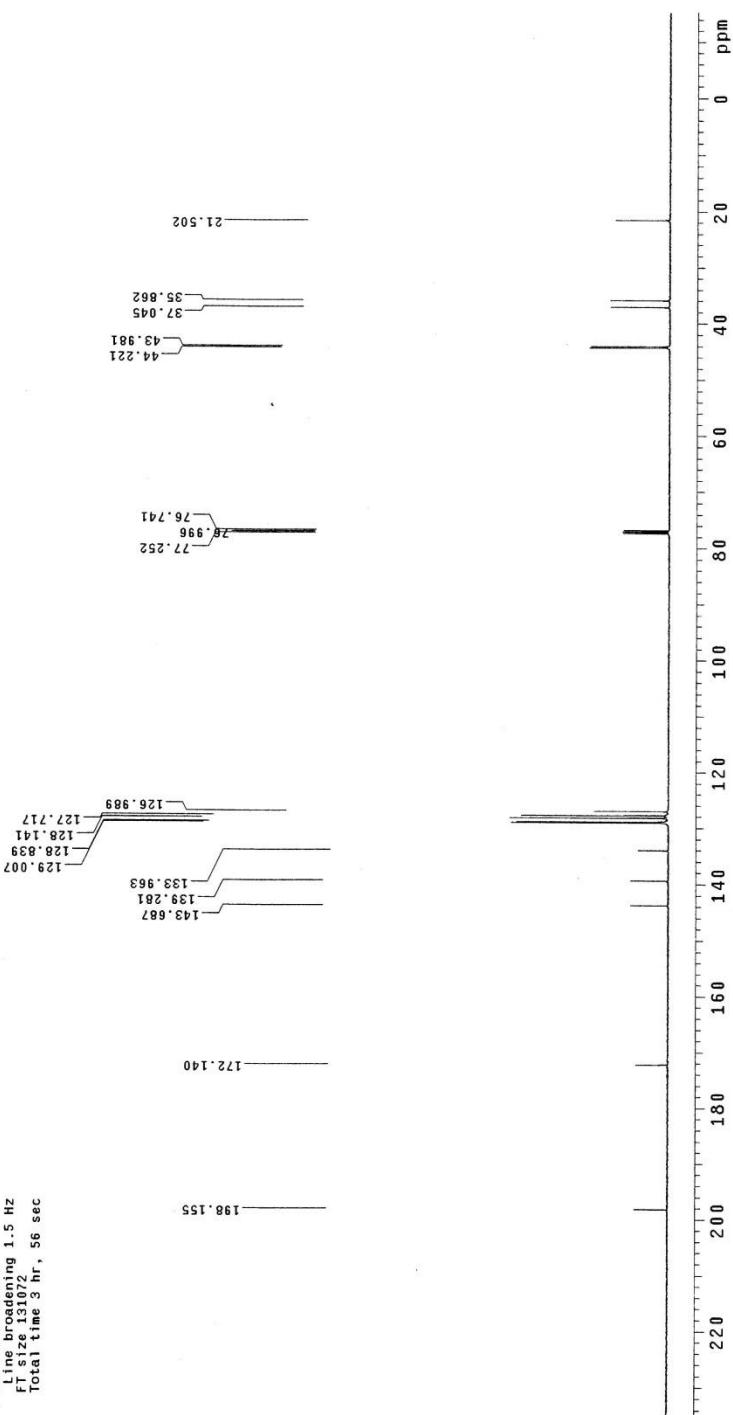
STANDARD CARBON PARAMETERS

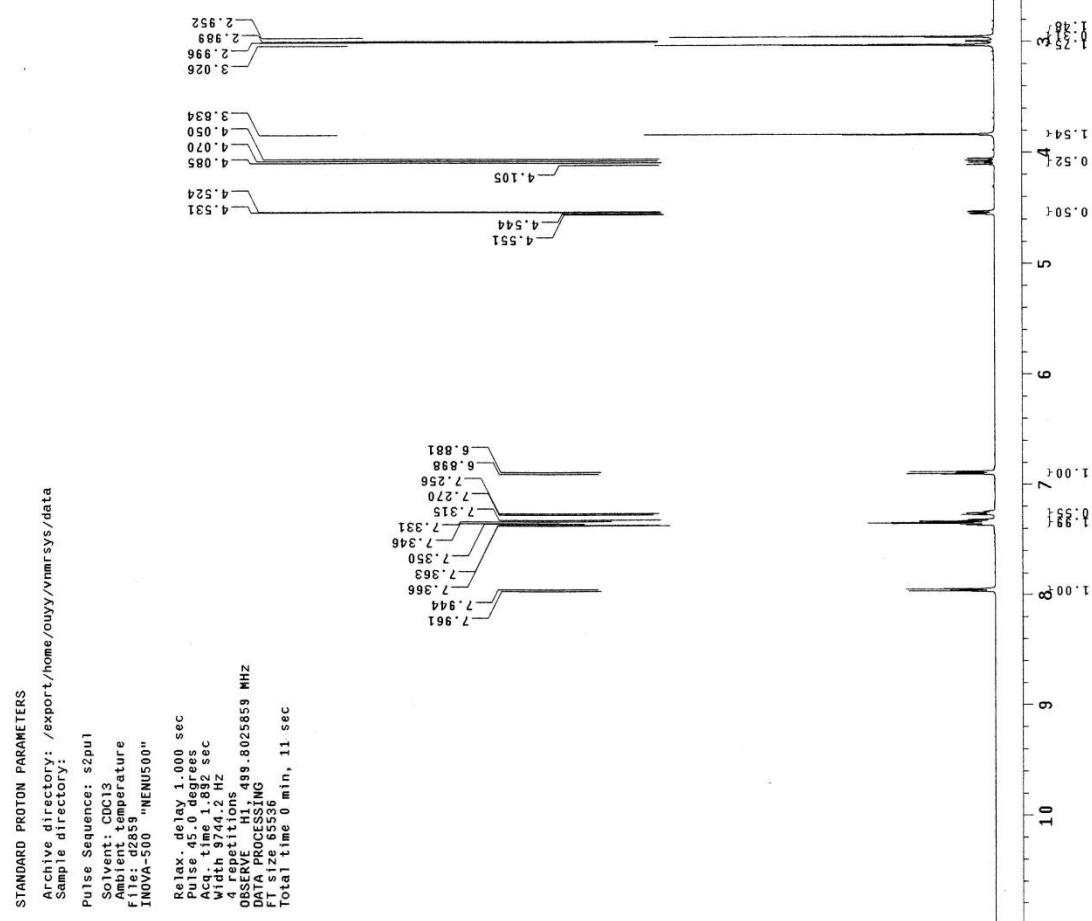
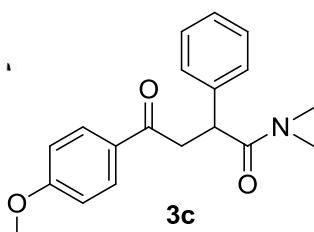
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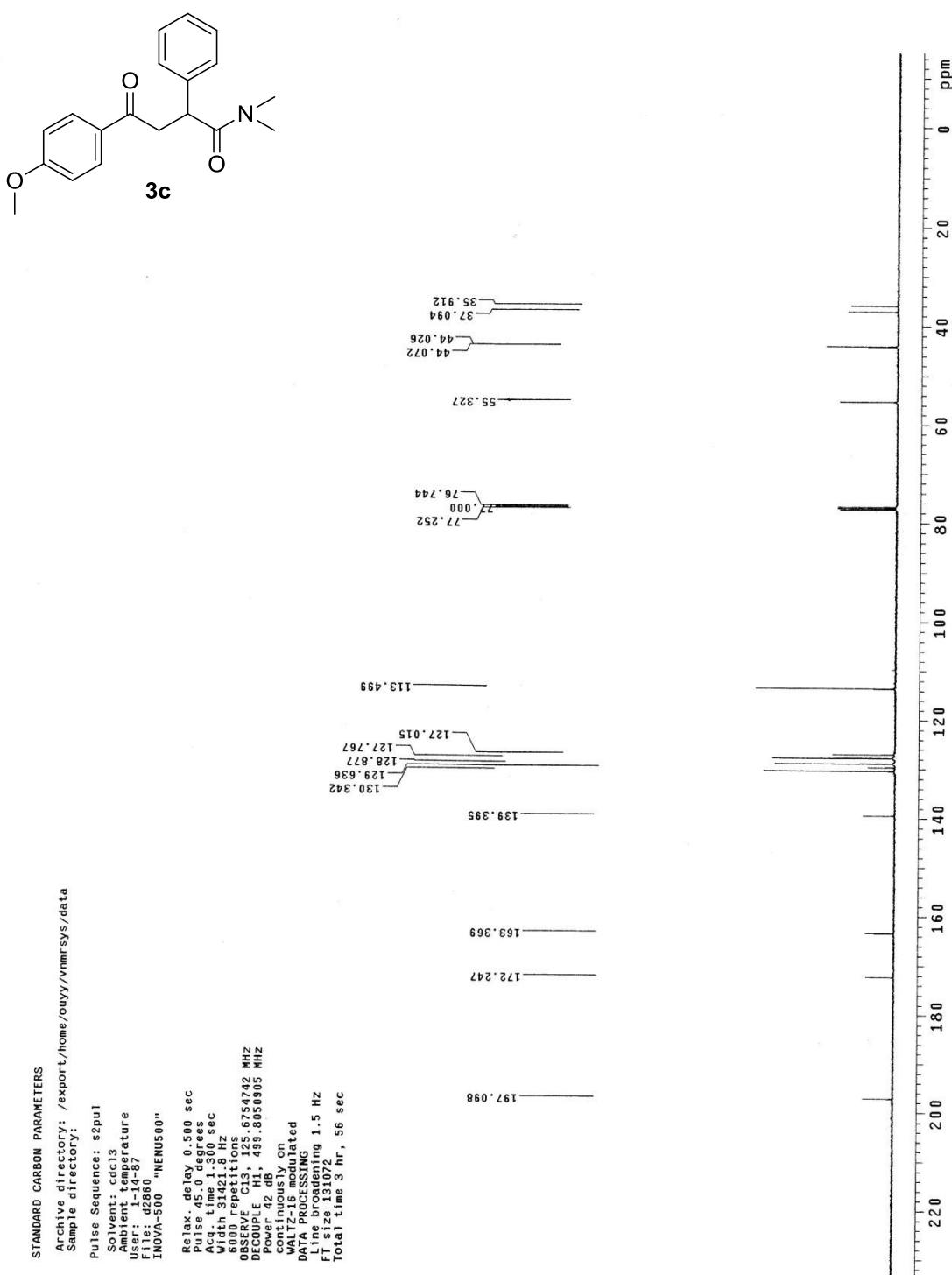
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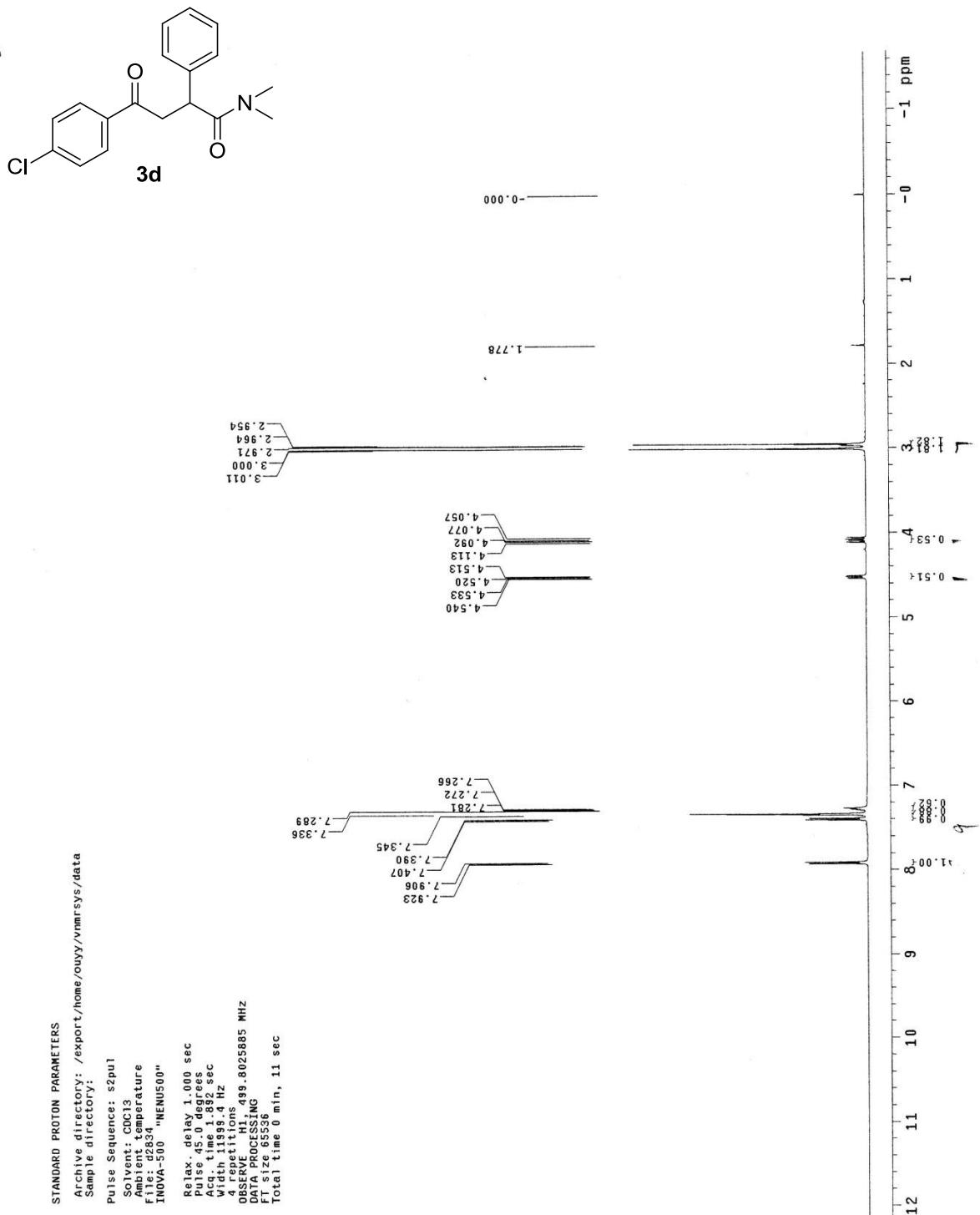
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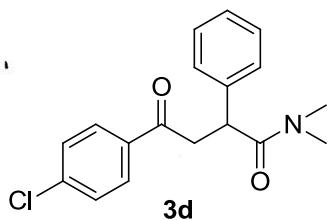




STANDARD PROTON PARAMETERS







STANDARD CARBON PARAMETERS

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Sample directory:

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Solvent: cdcl₃

Ambient temperature

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File: 02839

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Relax, delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

64 repetitions

OBSERVE C13, 125.6754680 MHz

DECOUPLE H1, 499.8050905 MHz

Power 42 dB

Pont 2000

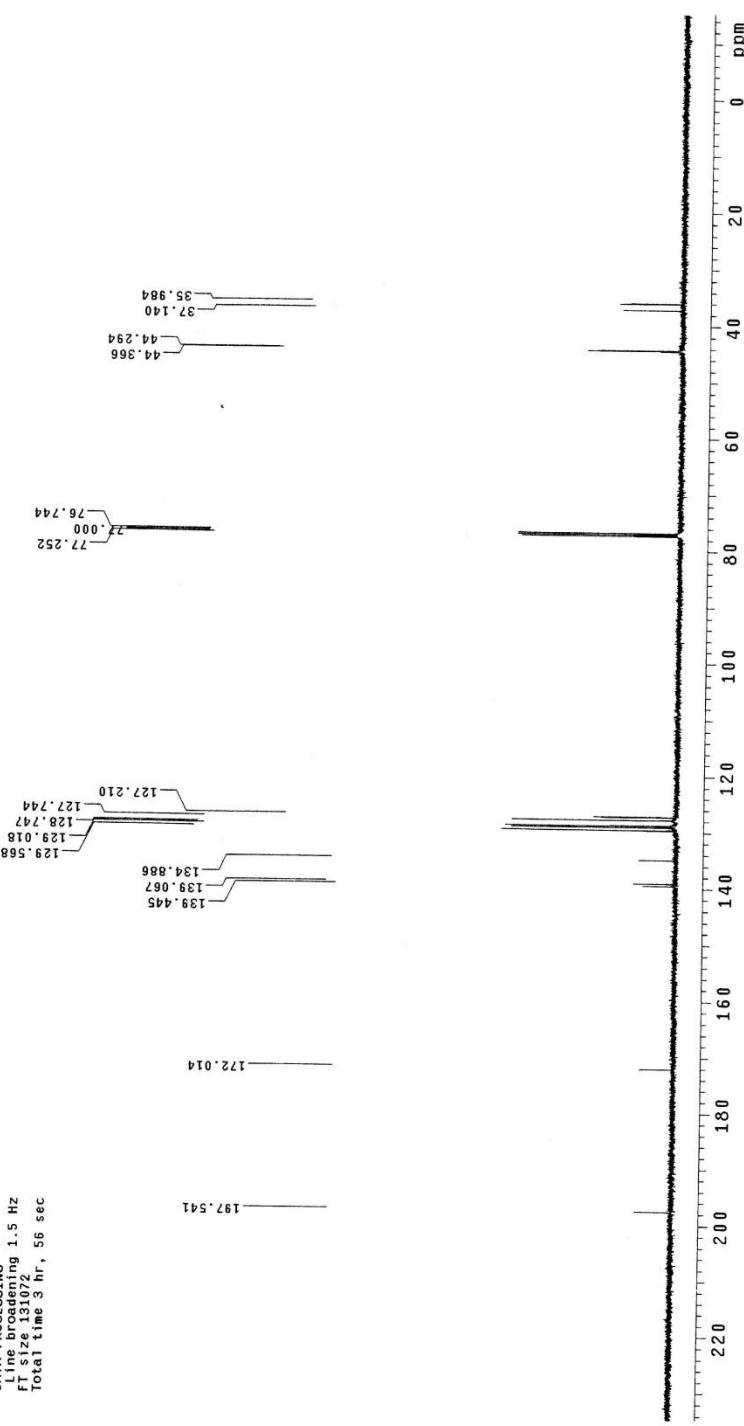
Water suppression on

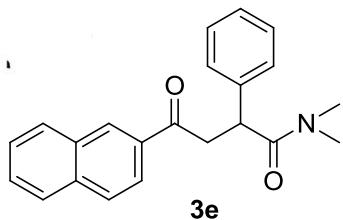
DATA PROCESSING

Line broadening 1.5 Hz

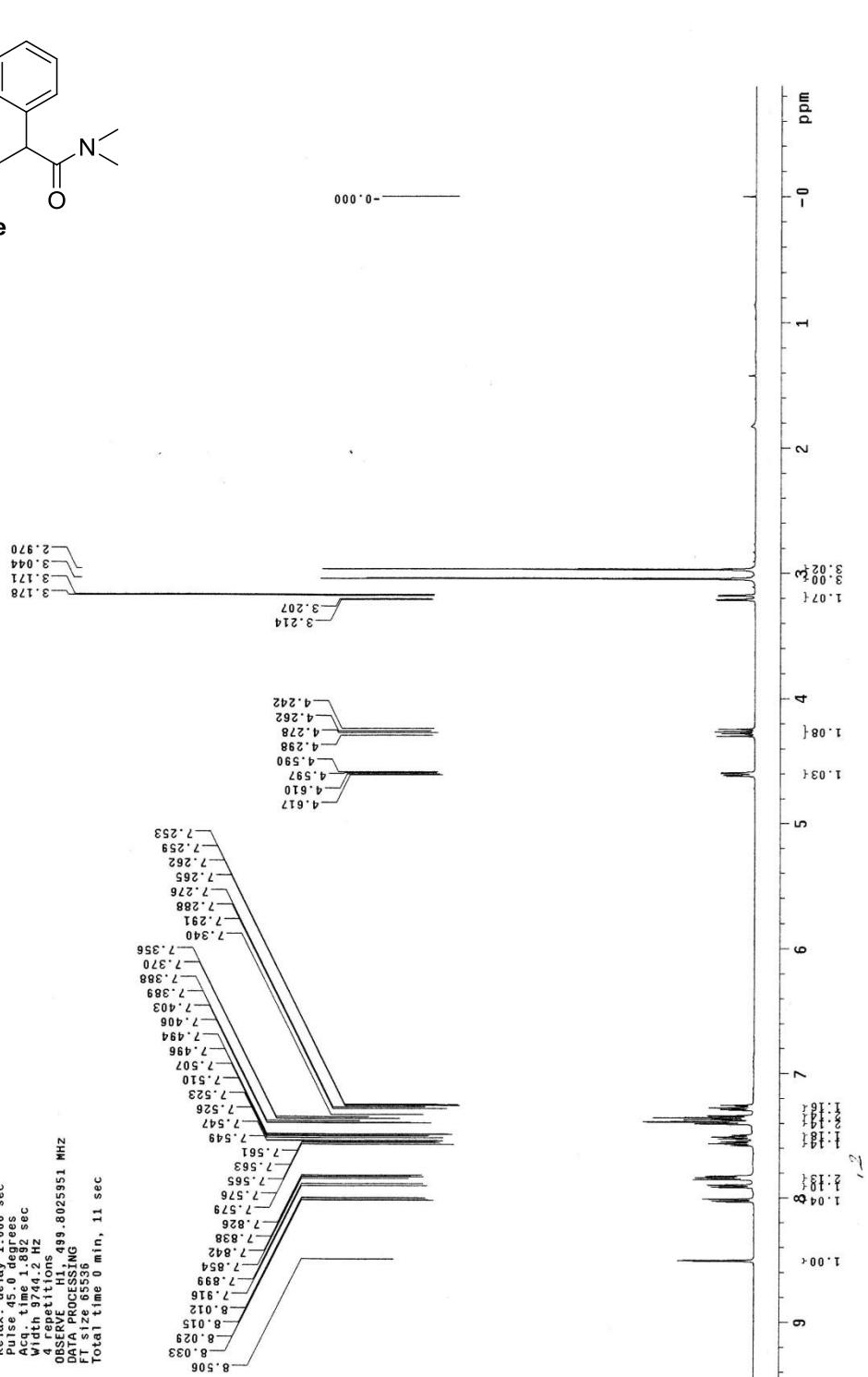
FT size 3372

Total time 9 hr, 56 sec

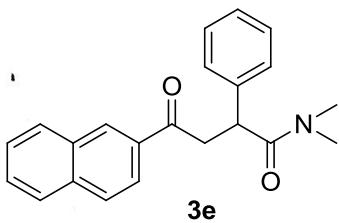




3e



STANDARD PROTON PARAMETERS



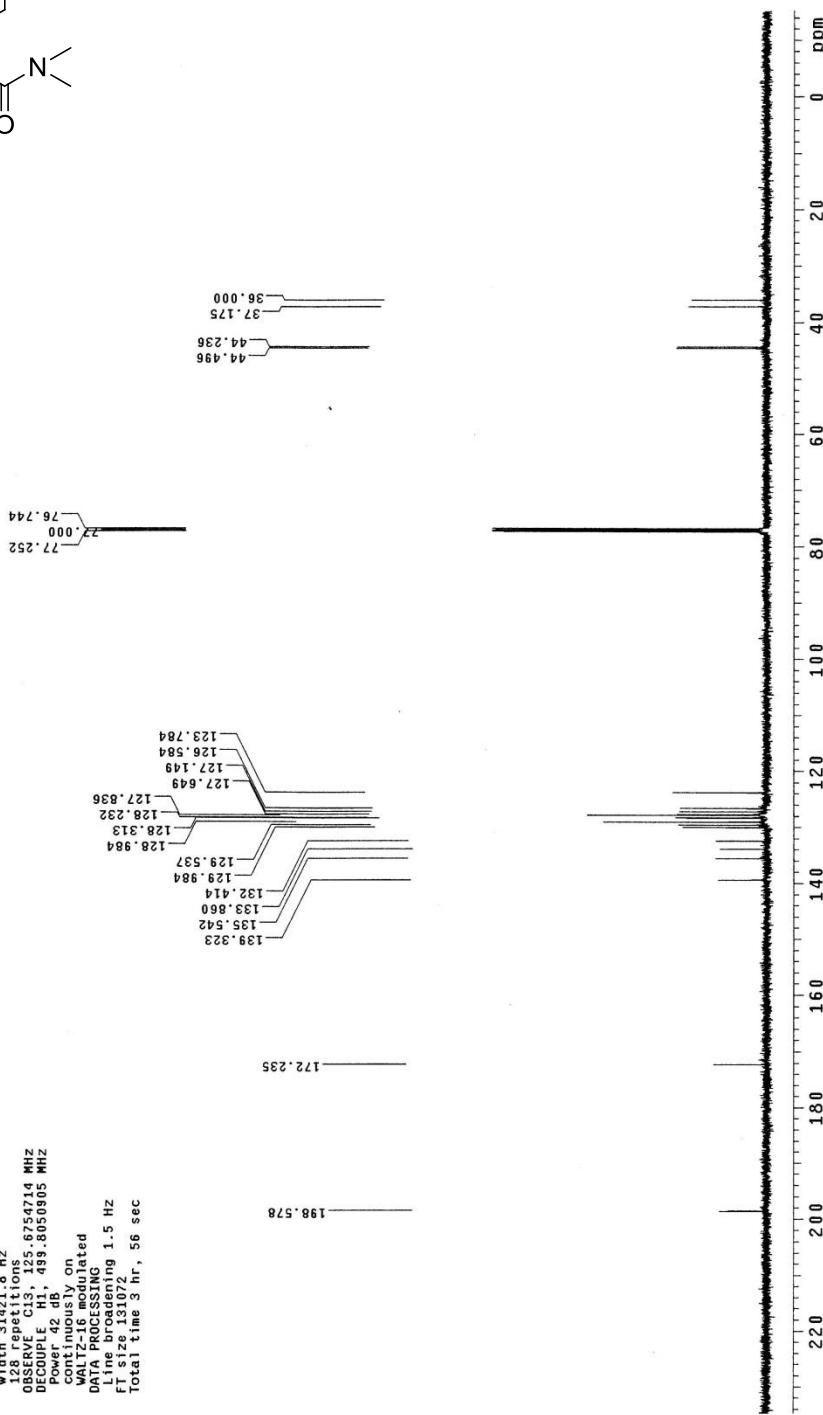
STANDARD CARBON PARAMETERS

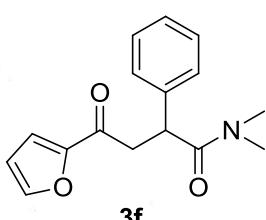
```

Archive directory: /export/home/ouyy/vnmrfsys/data
Sample directory:
Pulse Sequence: s2pu1
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2333
INOVA-500 "NENU500"

Relax, delay 0.500 sec
Pulse 45.0 degrees
Acc. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 135.675414 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
Fit size 13072
Total time 3 hr, 56 sec

```



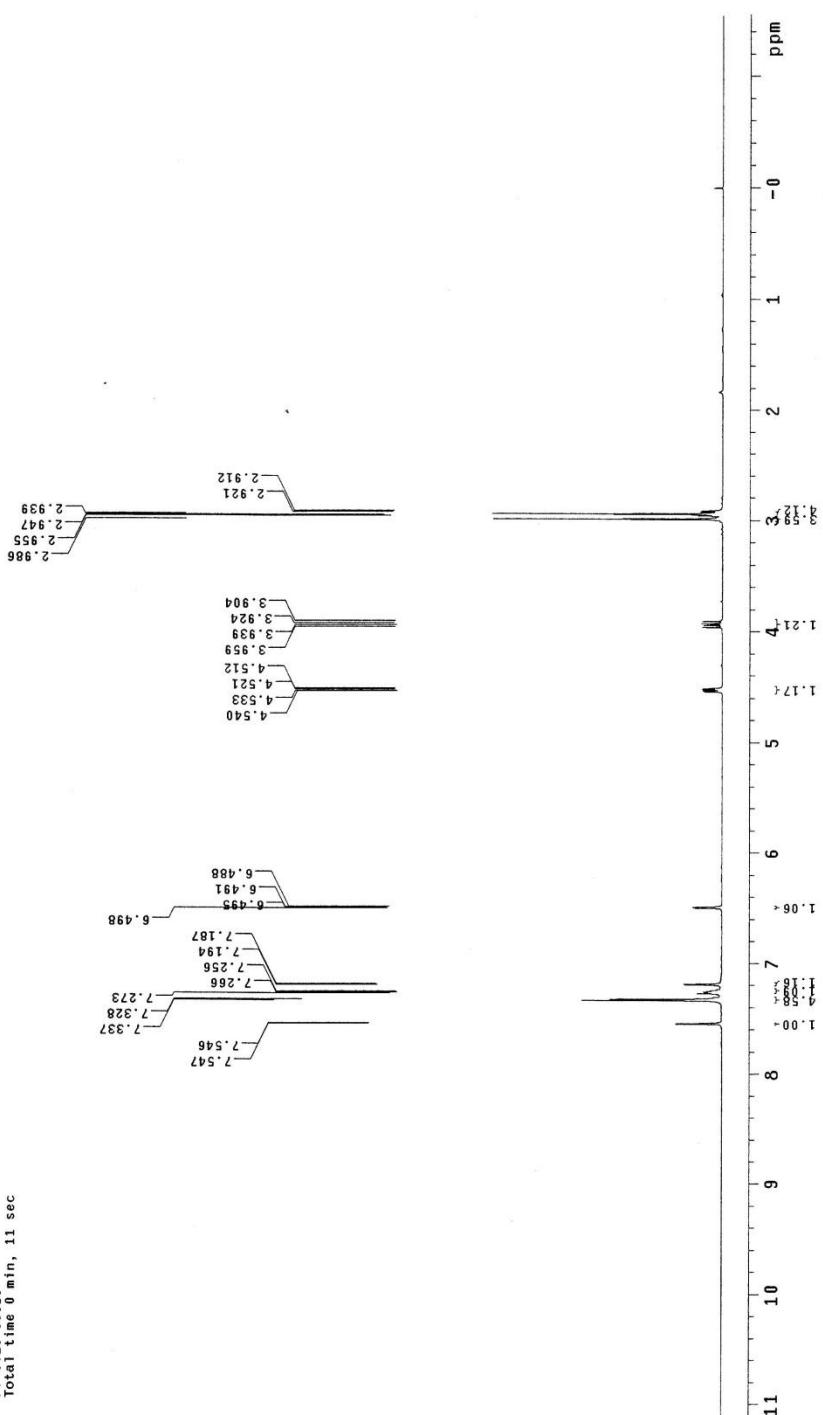


STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pu1

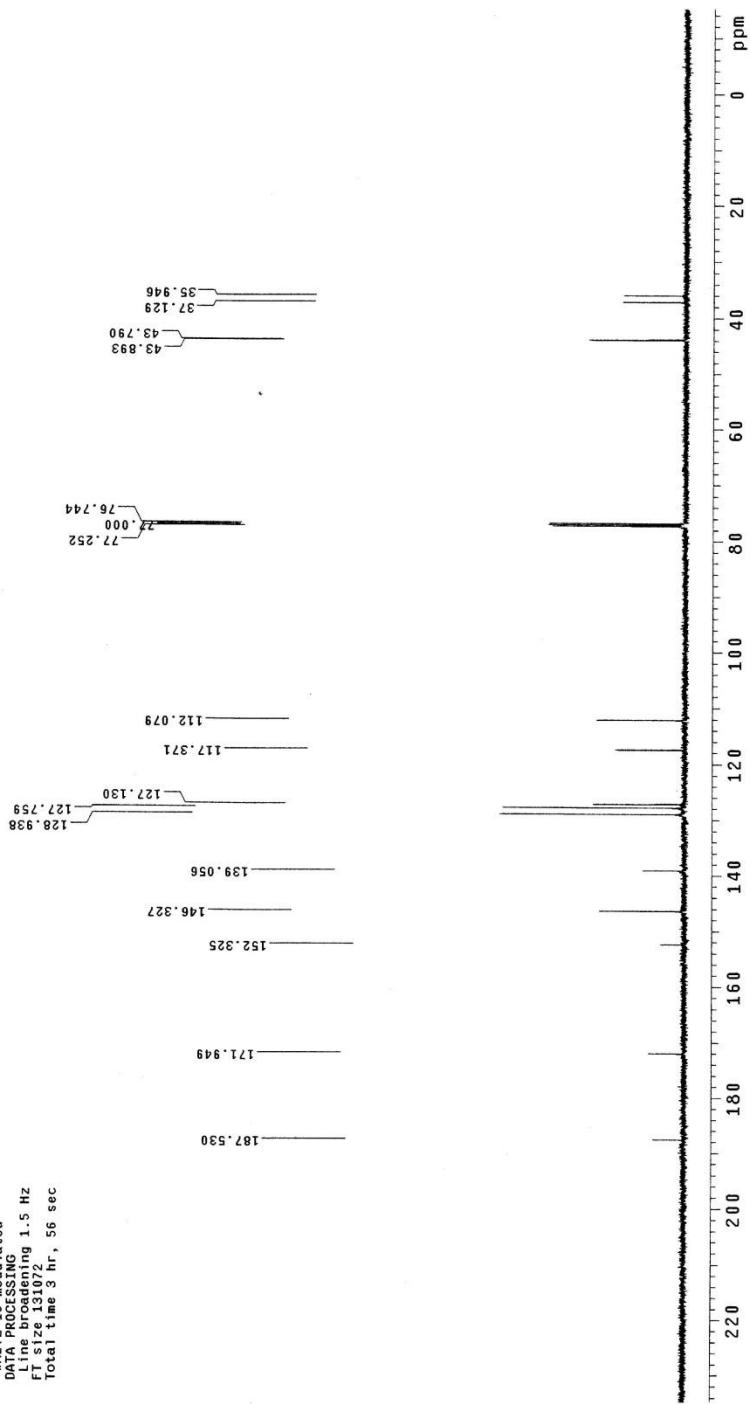
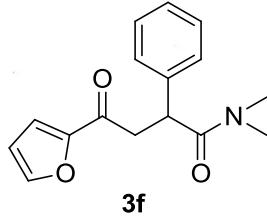
Solvent: CDCl₃
 Ambient temperature
 F11c: d25B
 INOVA-500 "NEN/500"

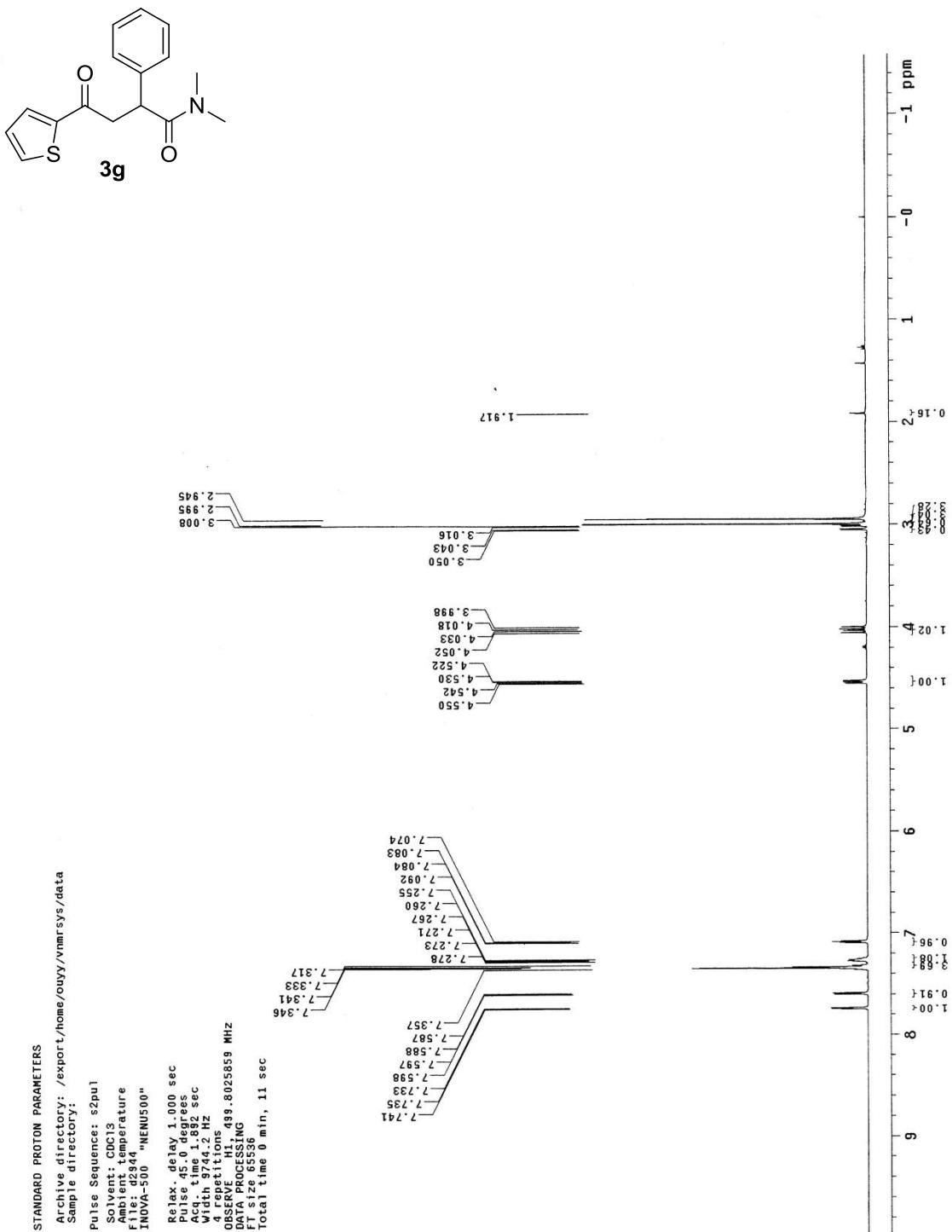
Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acc. time 1.892 sec
 Width 9.744.2 Hz
 4 repetitions
 OBSERVE: H1, 499.8025850 MHz
 DATA PROCESSING
 FT size 65536
 Total z-time 0 min, 11 sec

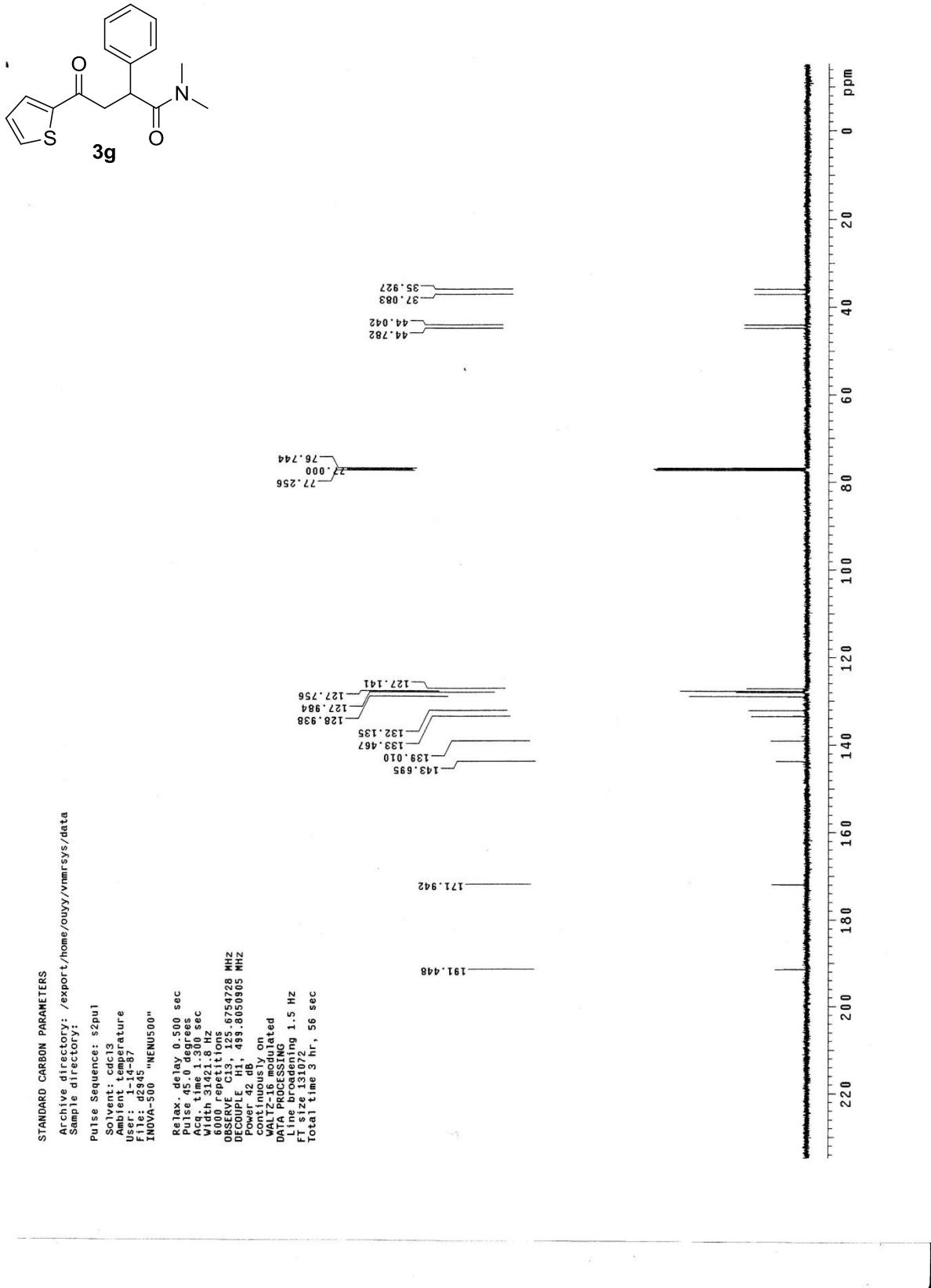


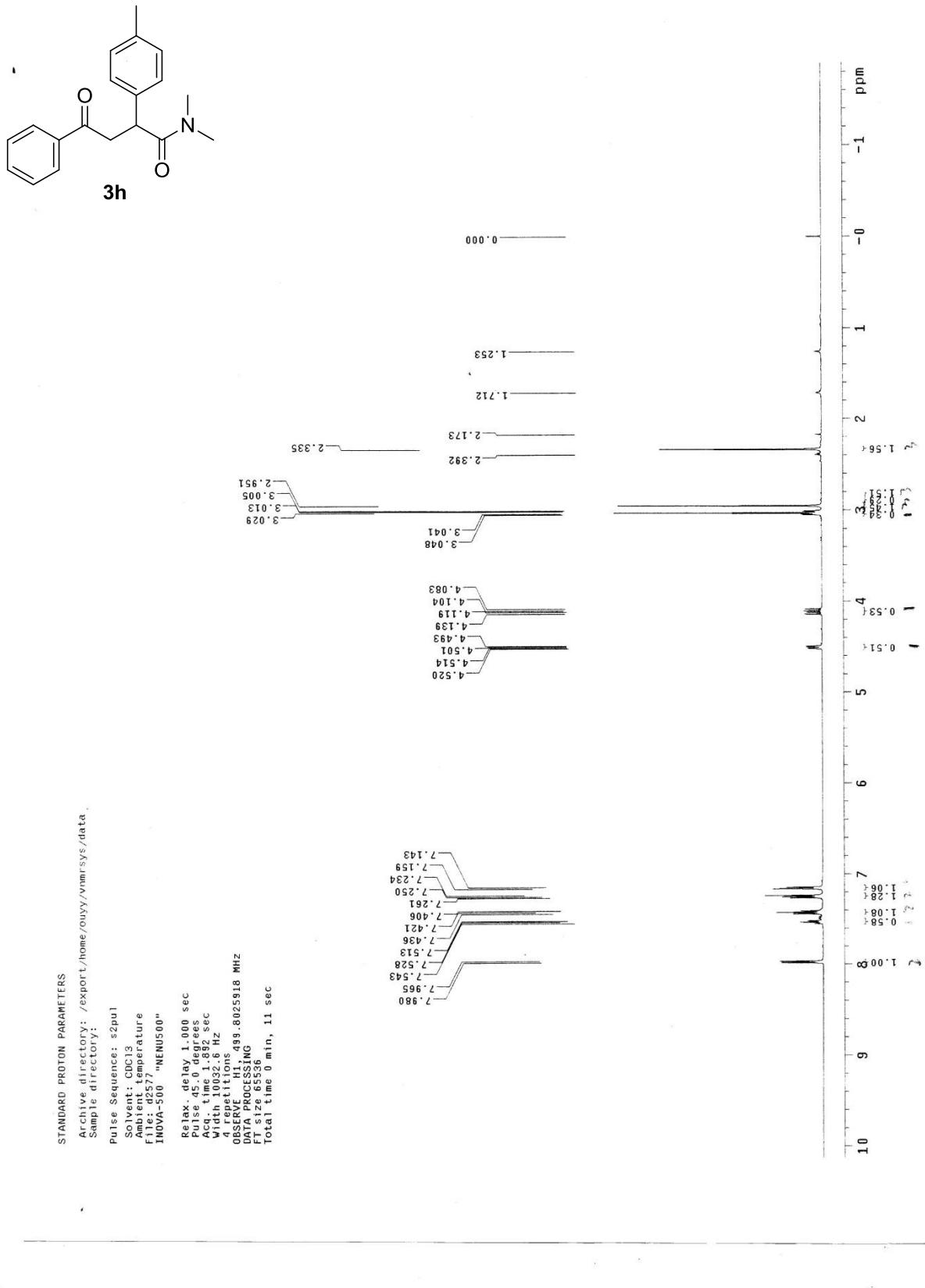
STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

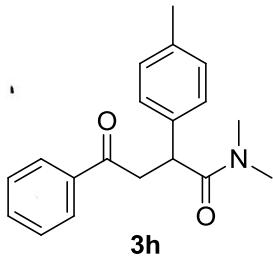
Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
User: 1-14-87
File: d2867
INOVA-500 "INENU500"
Relax: delay 0.500 sec
Pulse 45.0 degrees
Acc. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.675464 MHz
DECOUPLE H1, 499.805095 MHz
Power 42 dB
continuous on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
Fit size 13102
Total time 3 hr, 56 sec











STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data

Sample directory:

Pulse Sequence: s2pu1

Solvent: cdcl₃

Ambient temperature

User: 1-14-87

File: d2582

INOVA-500 "NEMUS00"

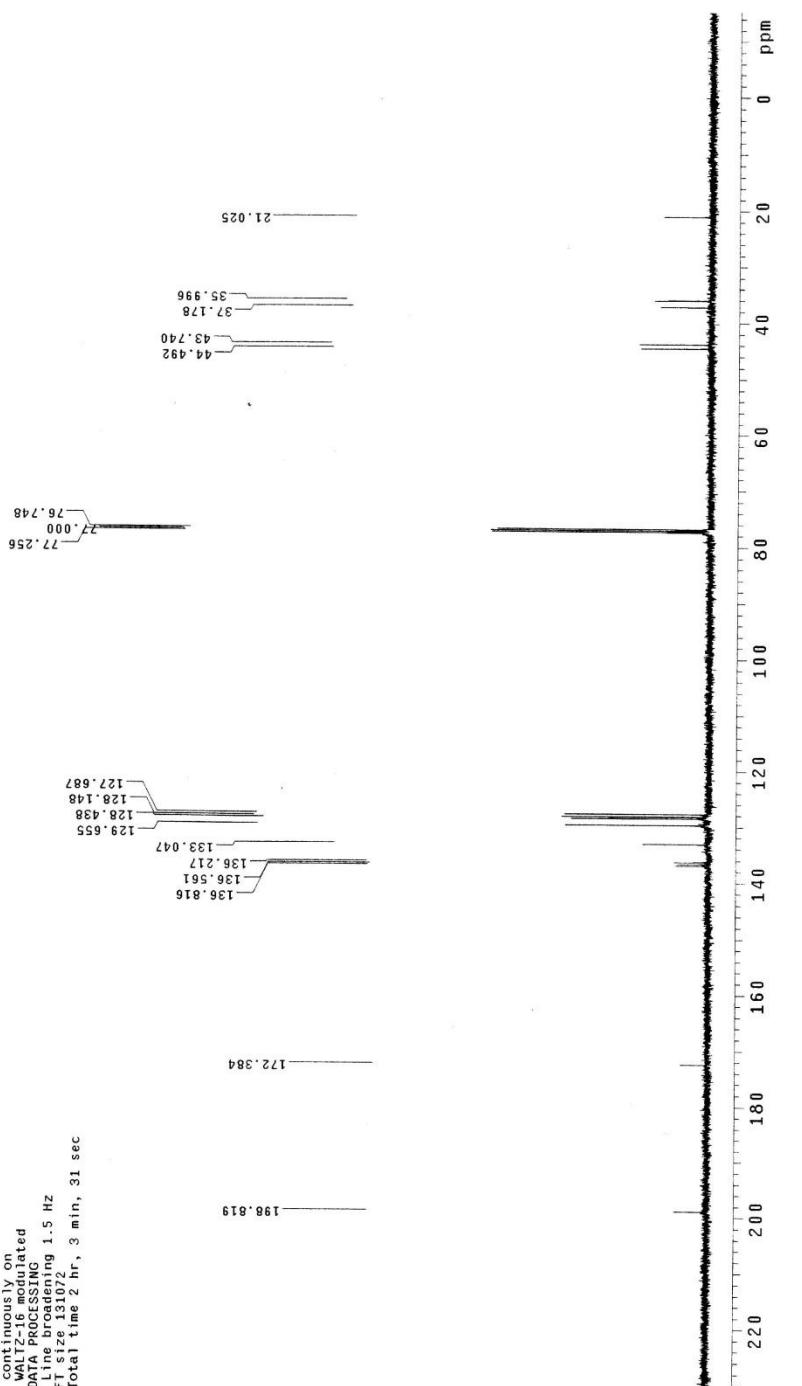
Relax 1 delay 0.500 sec
pulse 45.0 degrees
Ave 1
With 3121.30 sec
64 repetitions
OBSERVE C13, 125.675625 MHz
DECOUPLE H1, 498.805095 MHz
Power 42 dB
continuous on
WALTZ-16 modulated

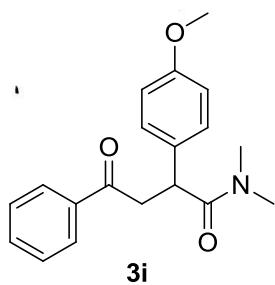
DATA PROCESSING

Line broadening 1.5 Hz

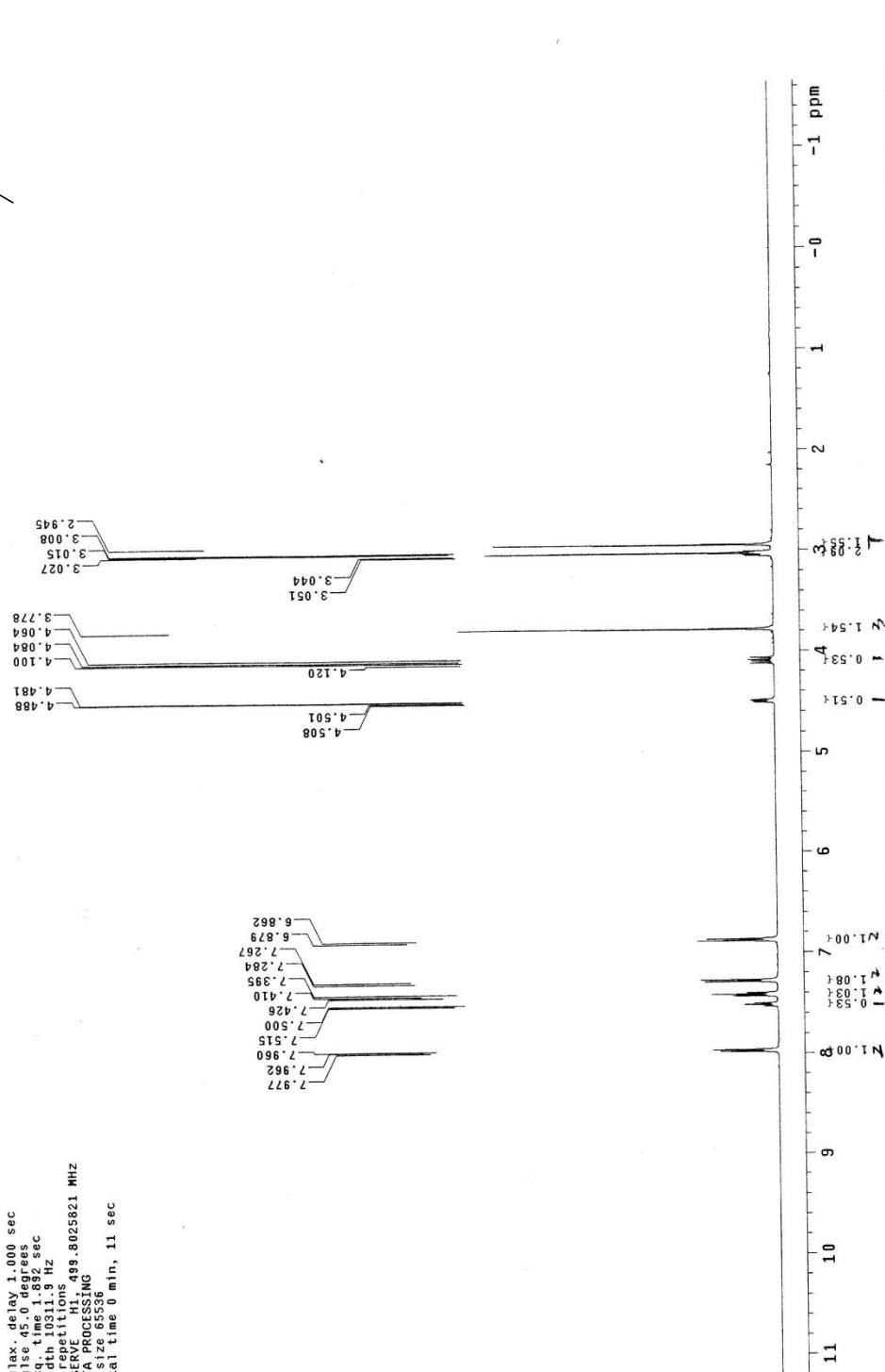
FT size 131072

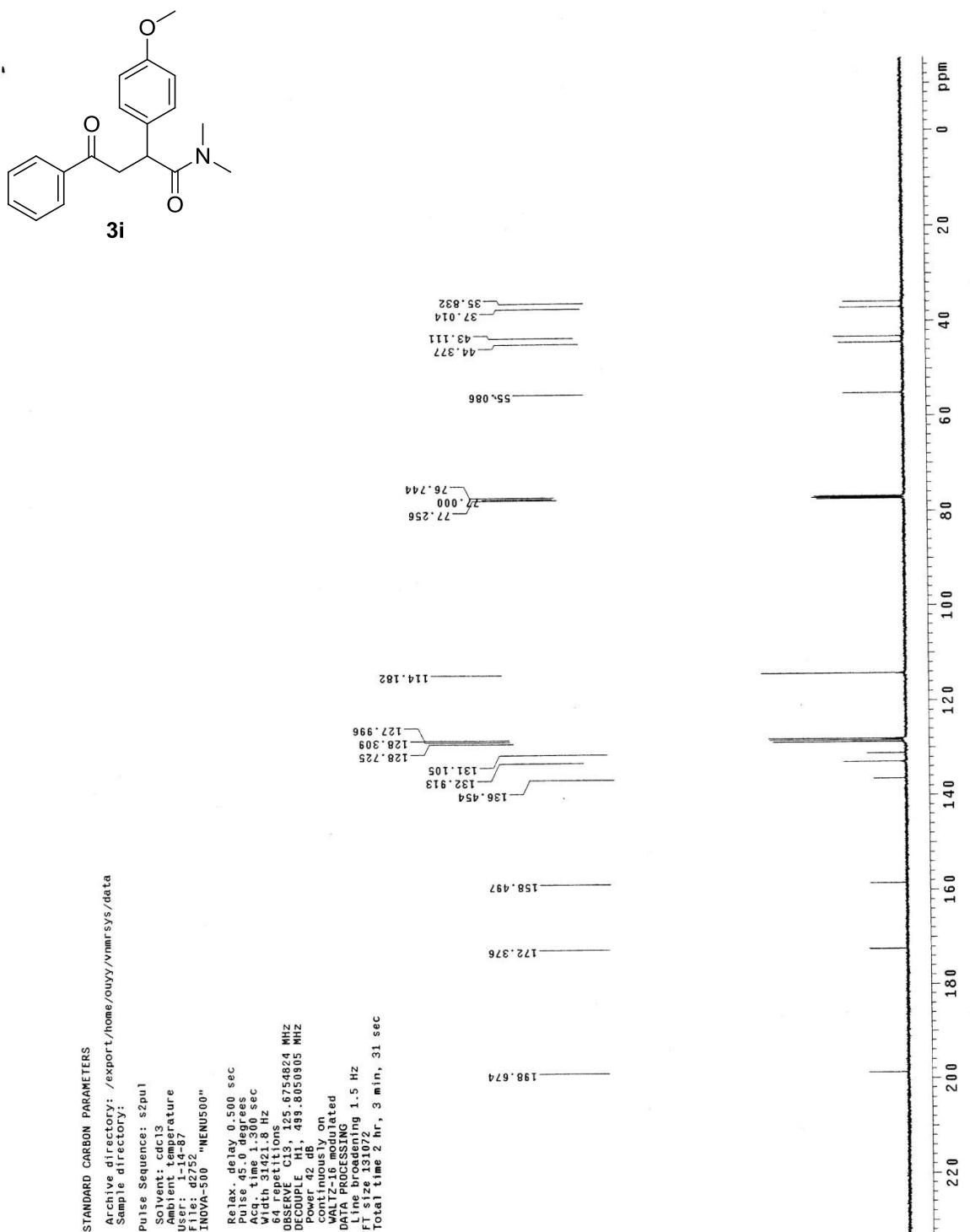
Total time 2 hr, 3 min, 31 sec

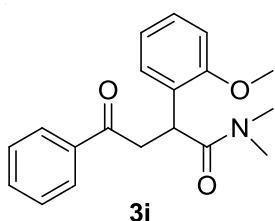




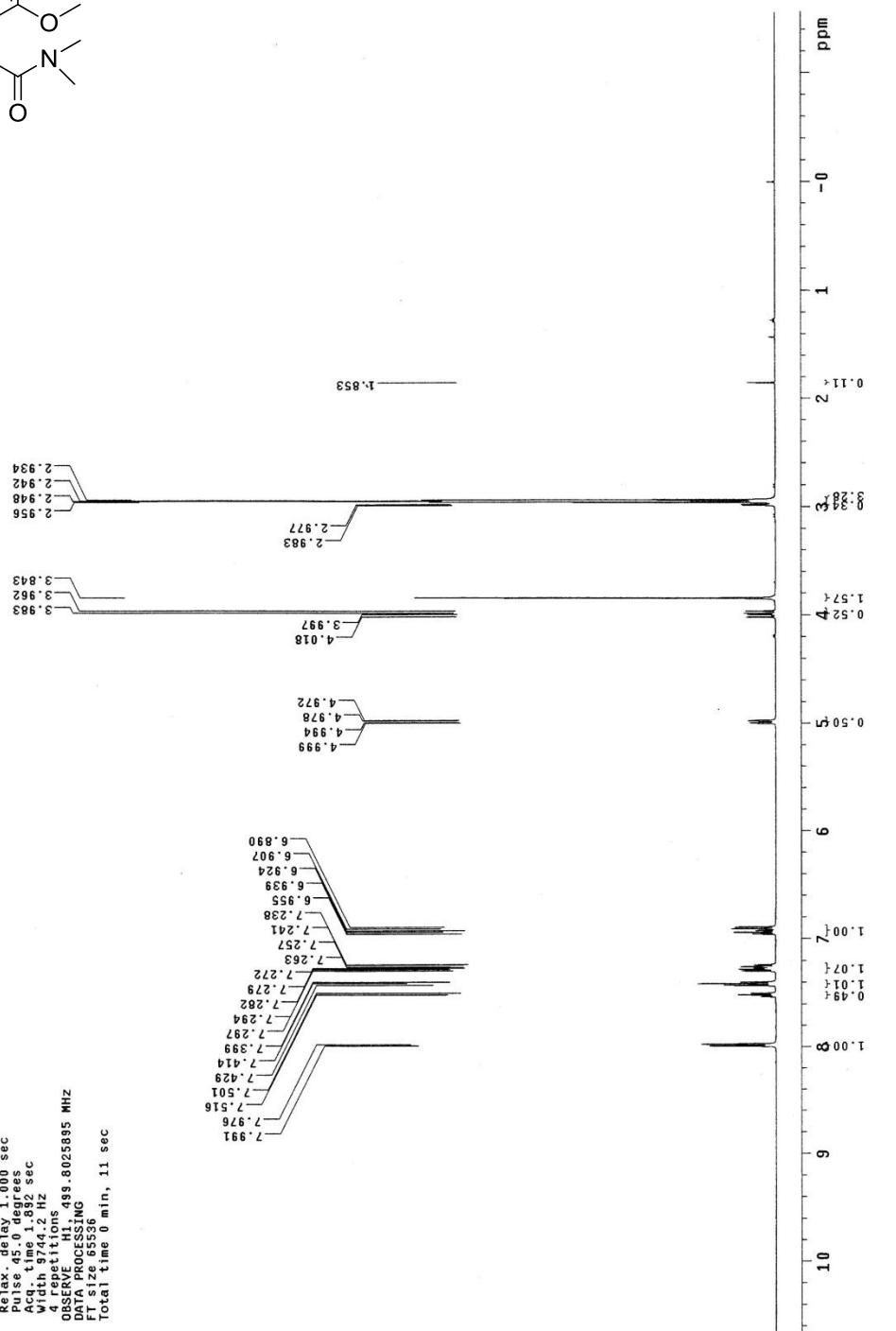
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouuyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: ODC13
Ambient temperature
File: d2751, "MENU500"
INOVA-500
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.892 sec
Width 10311.9 Hz
4 repetitions
OBSERVE H1, 499.8025821 MHz
DATA PROCESSING
FT size 65536
Total time 50 min, 11 sec







3j



STANDARD PROTON PARAMETERS

```

Archive directory: /export/home/ouy/vnmr/syndata
Sample directory: /export/home/ouy/vnmr/syndata

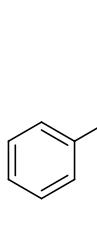
Pulse Sequence: s2pu1
Sovent: CDC13
Ambient temperature
F1[1]: d2442
INNOVA: "NMRNU500"

Relax, delay 1.000 sec
Pulse 45, 0 degrees
Acq. time 1.92 sec
FID time 4.12 Hz
Acq. time 4.12 sec
Data processing time 499.8025835 MHz
Data processing time 65535.65536
Total acquisition time 0 min, 11 sec

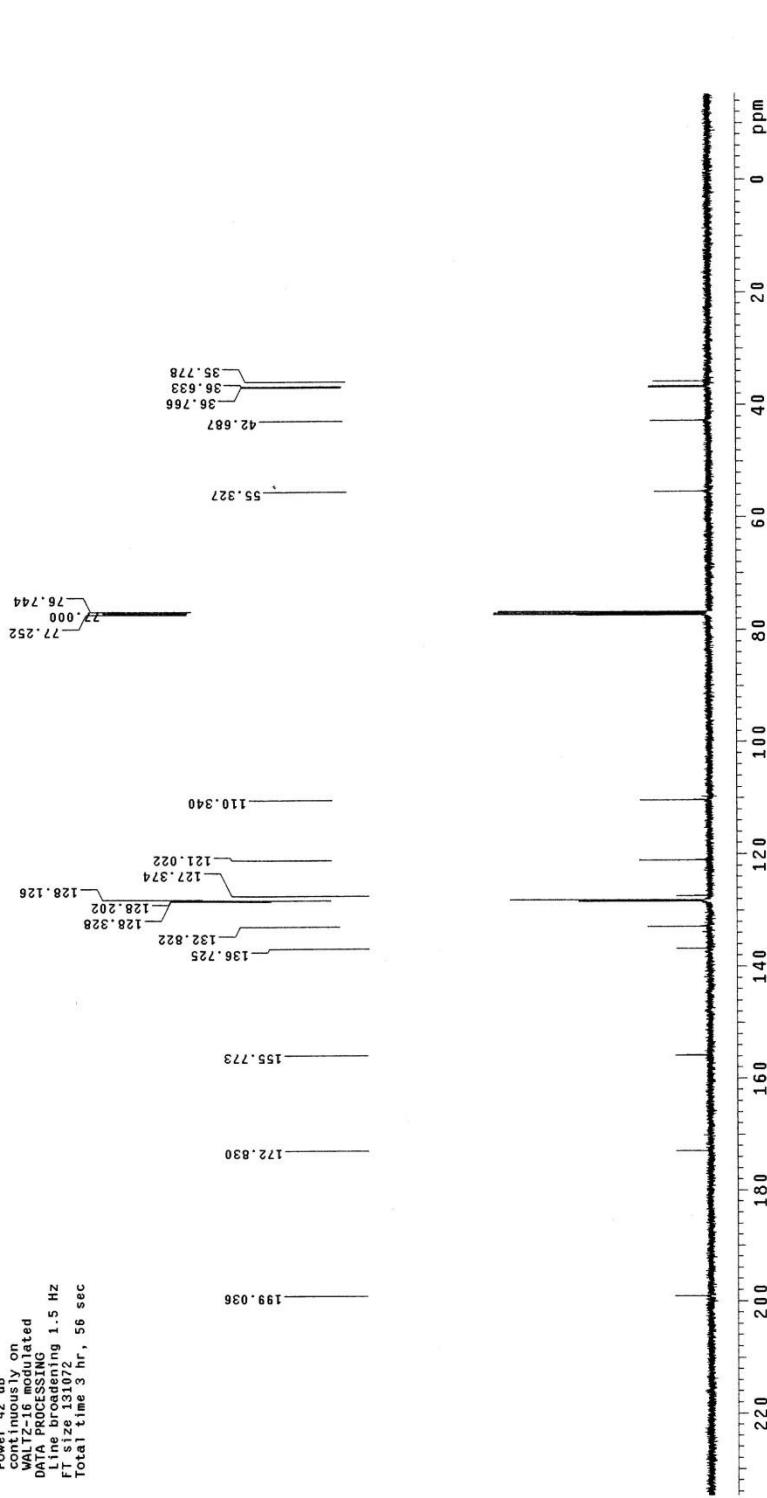
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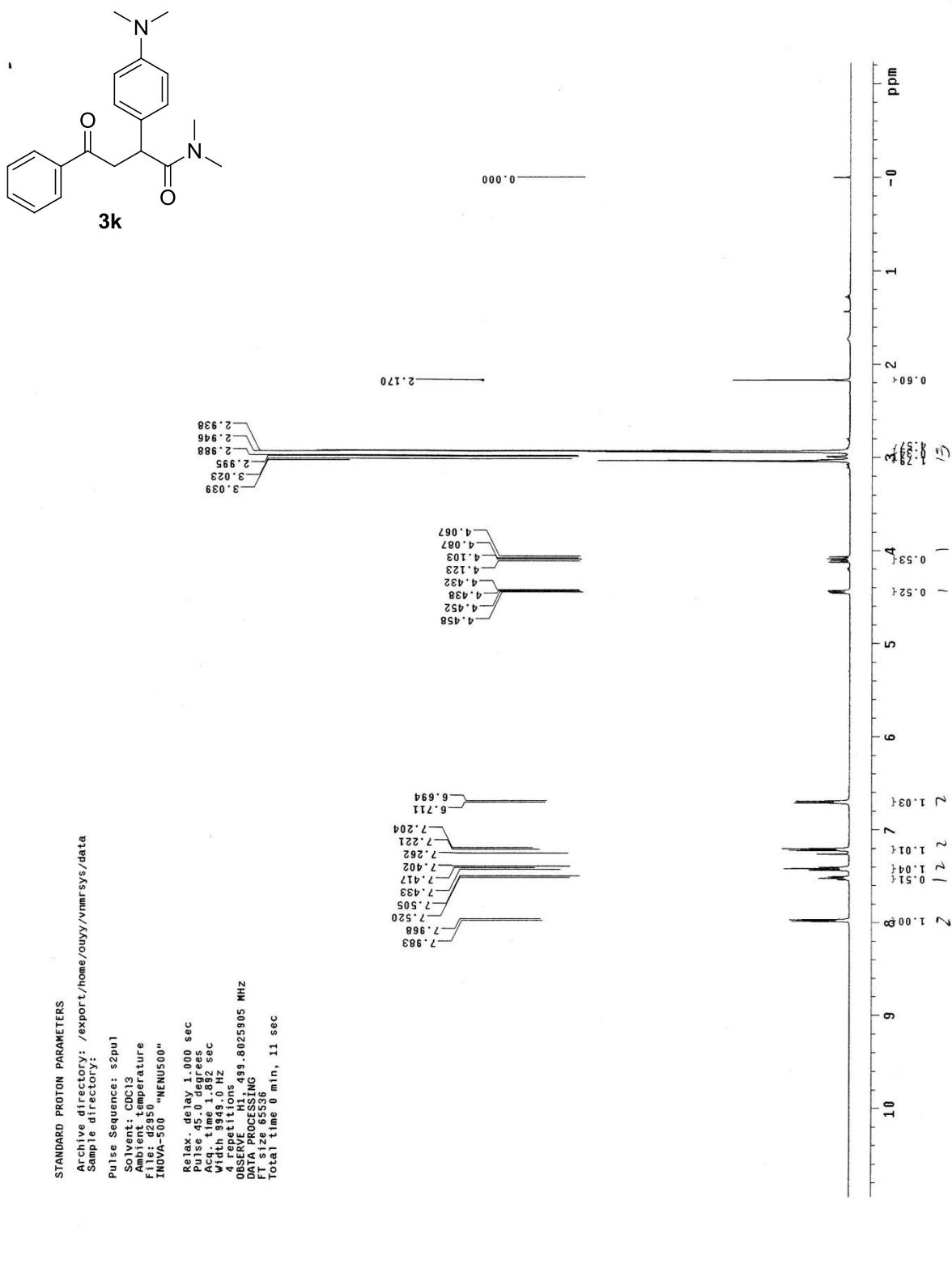
STANDARD CARBON PARAMETERS

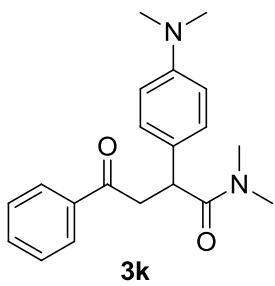
Archive directory: /export/home/ouyu/vnmrsys/data
Sample directory:
Pulse Sequence: s2pu1
Solvent: ccl3
Ambient Temperature
User: 1-14-87
File: d943 "INNOVA-500"
Relax, delay 0.500 sec
Pulse, 45.0 degrees
Acq. time 1.310 sec
Width 31121.8 Hz
64 repetitions
OBSERVE C13, 125.675404 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
contuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec



3j

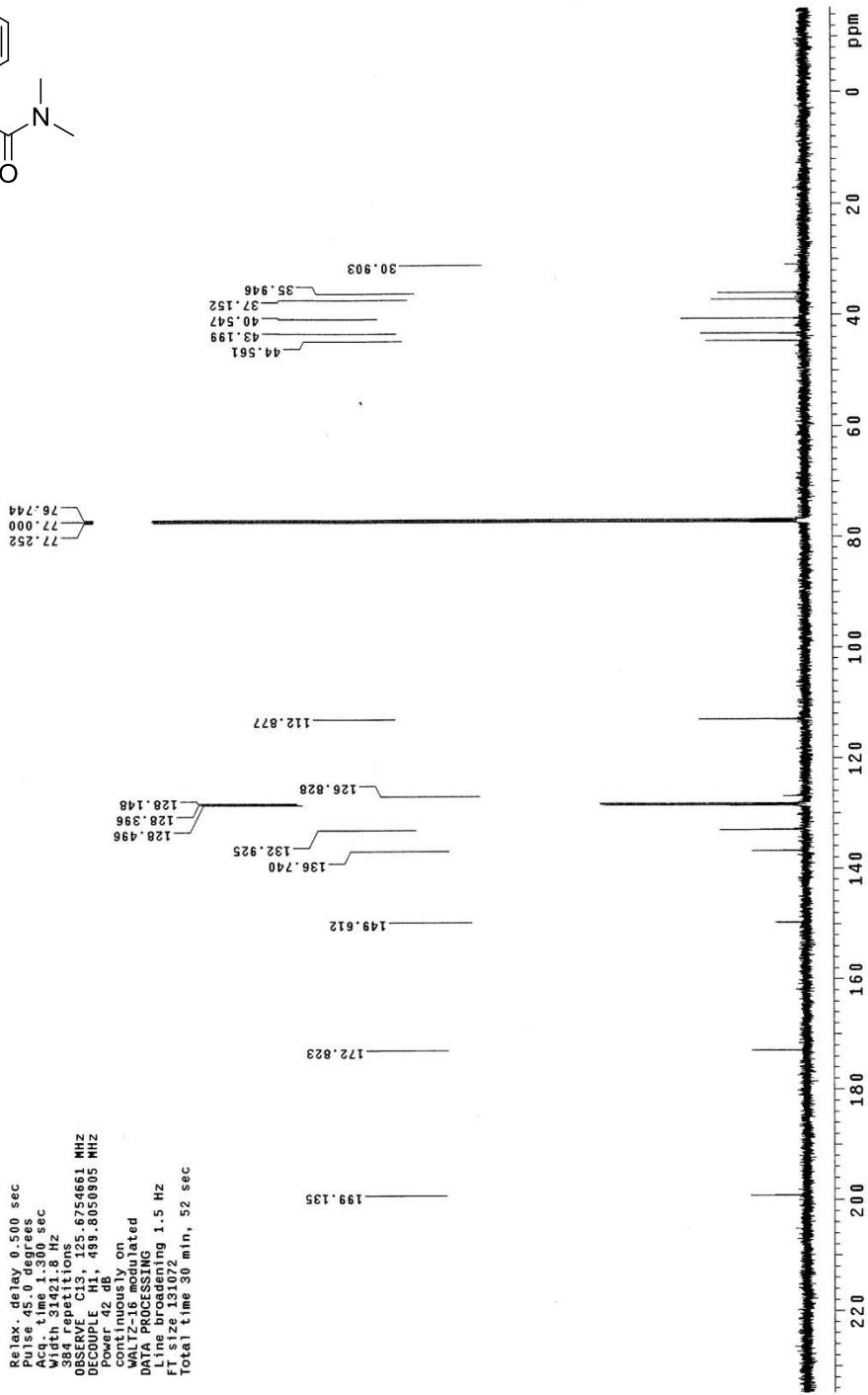


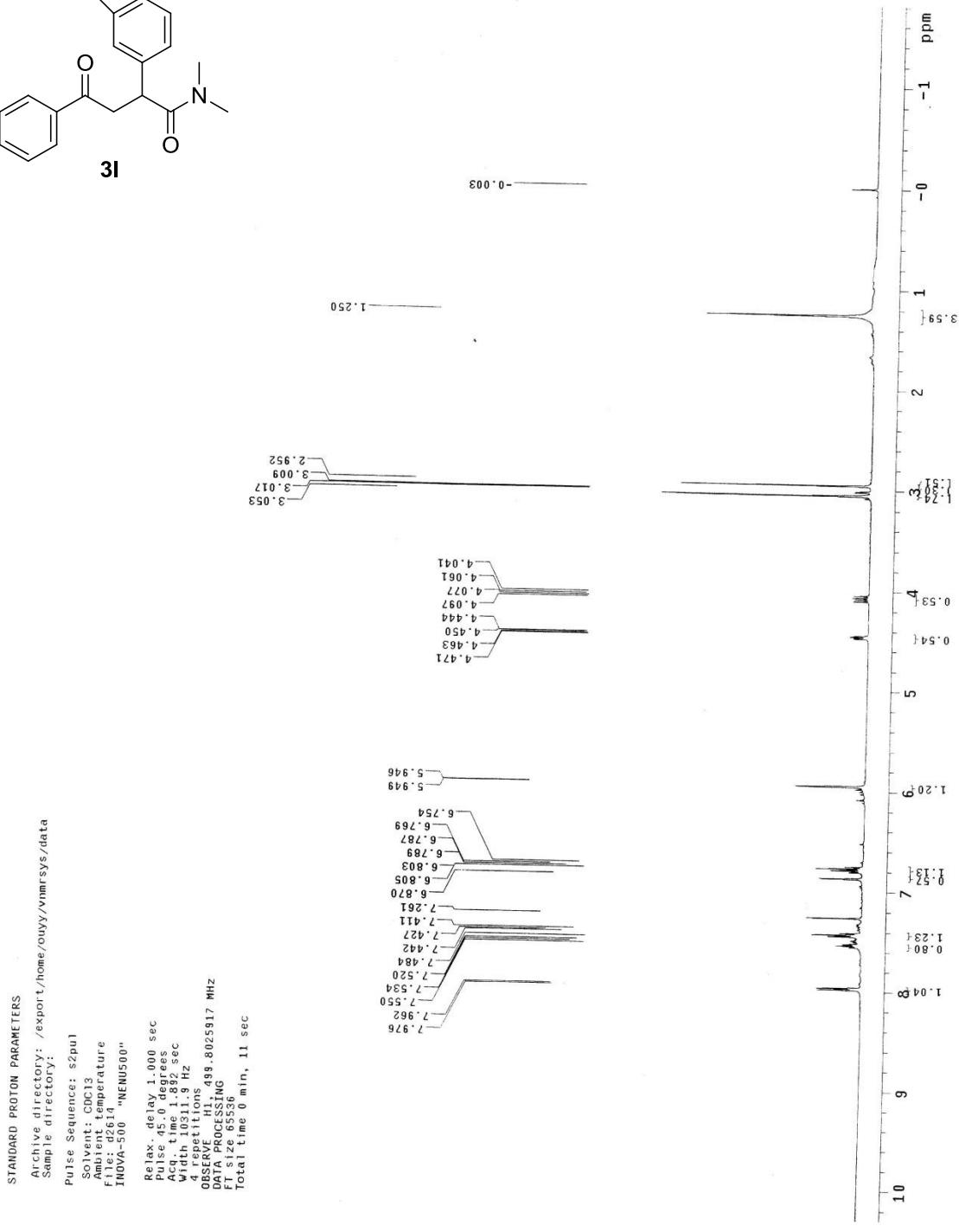
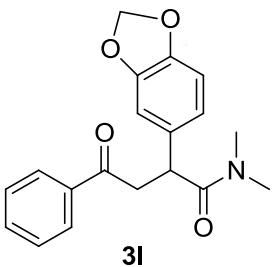


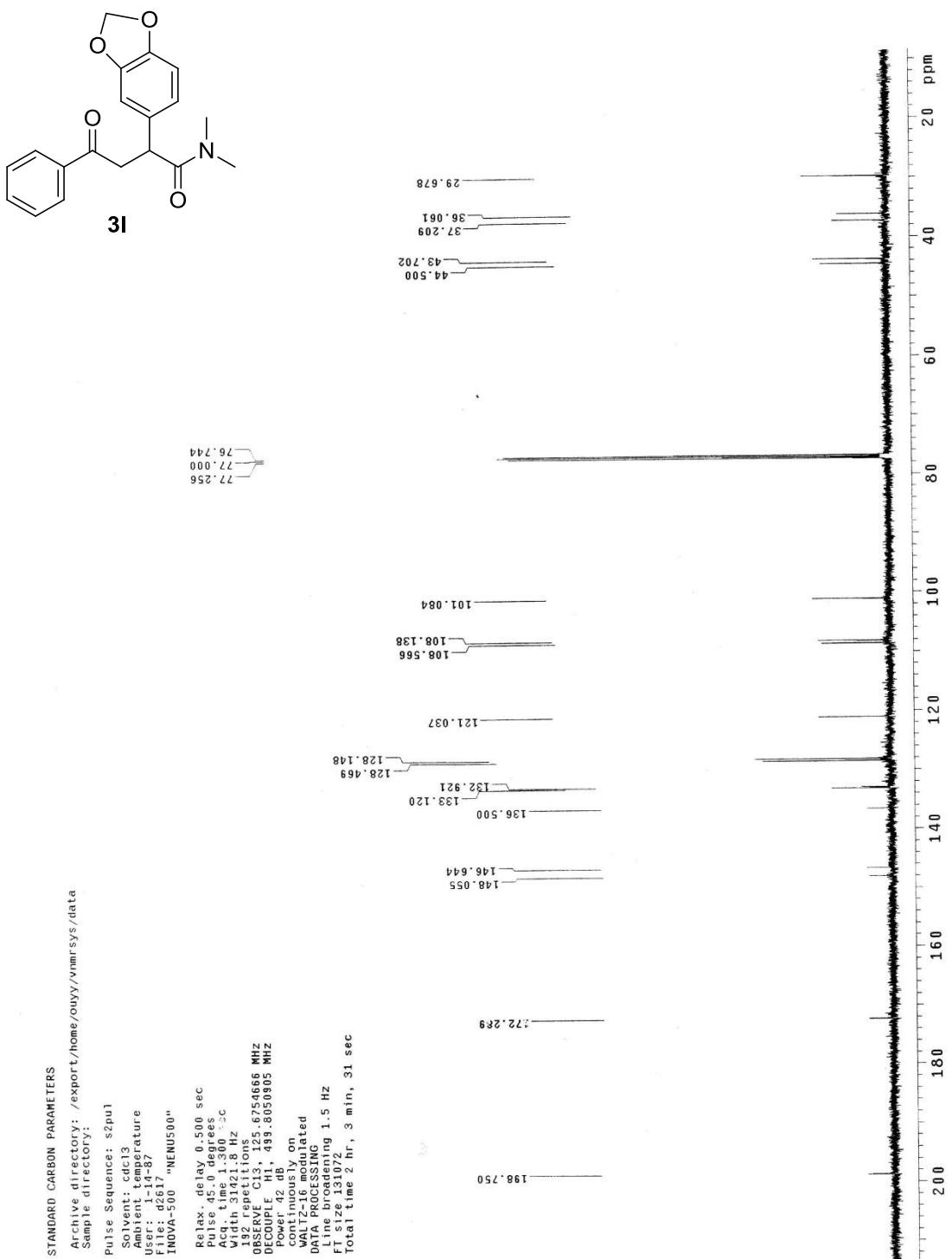


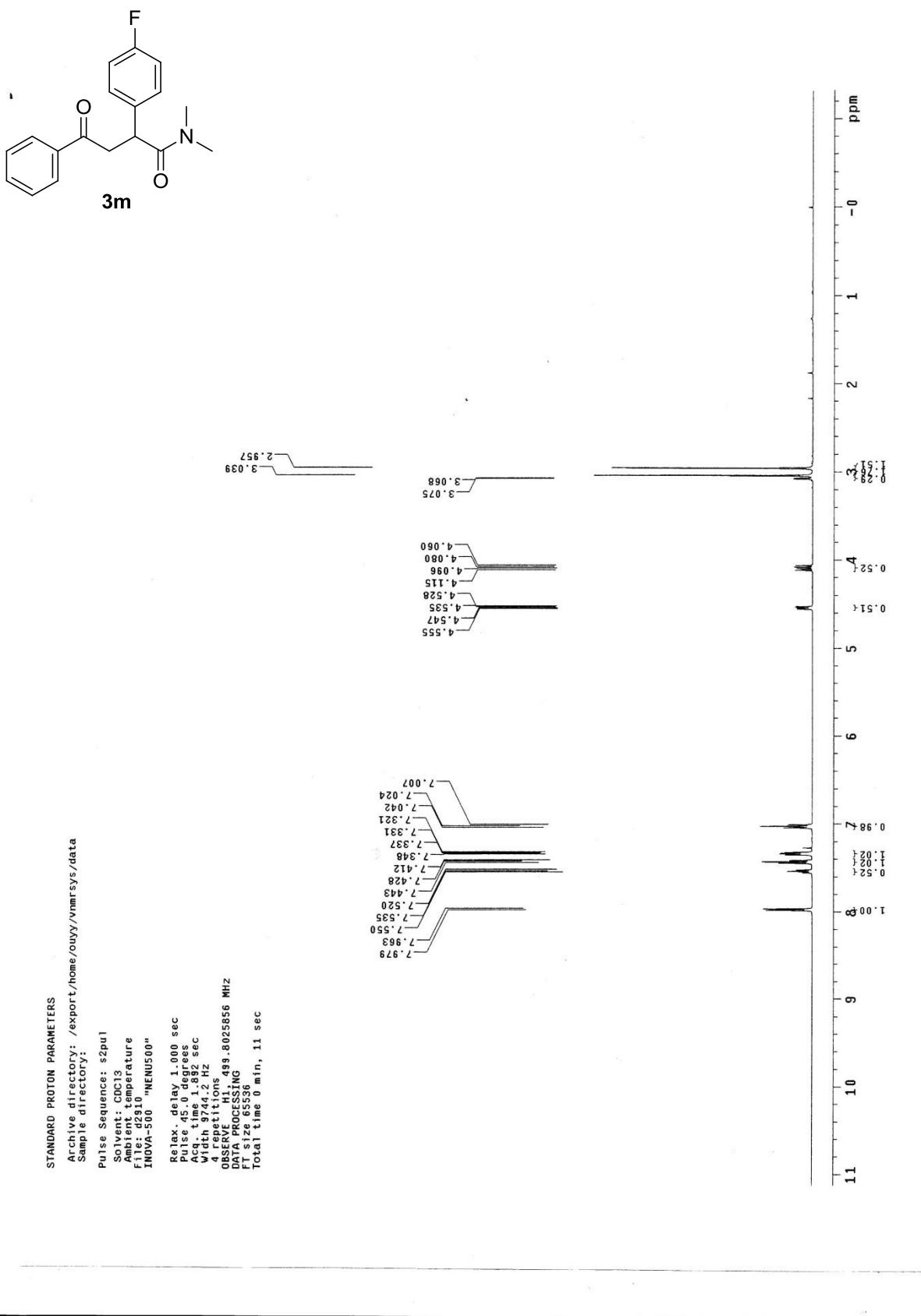
STANDARD CARBON PARAMETERS

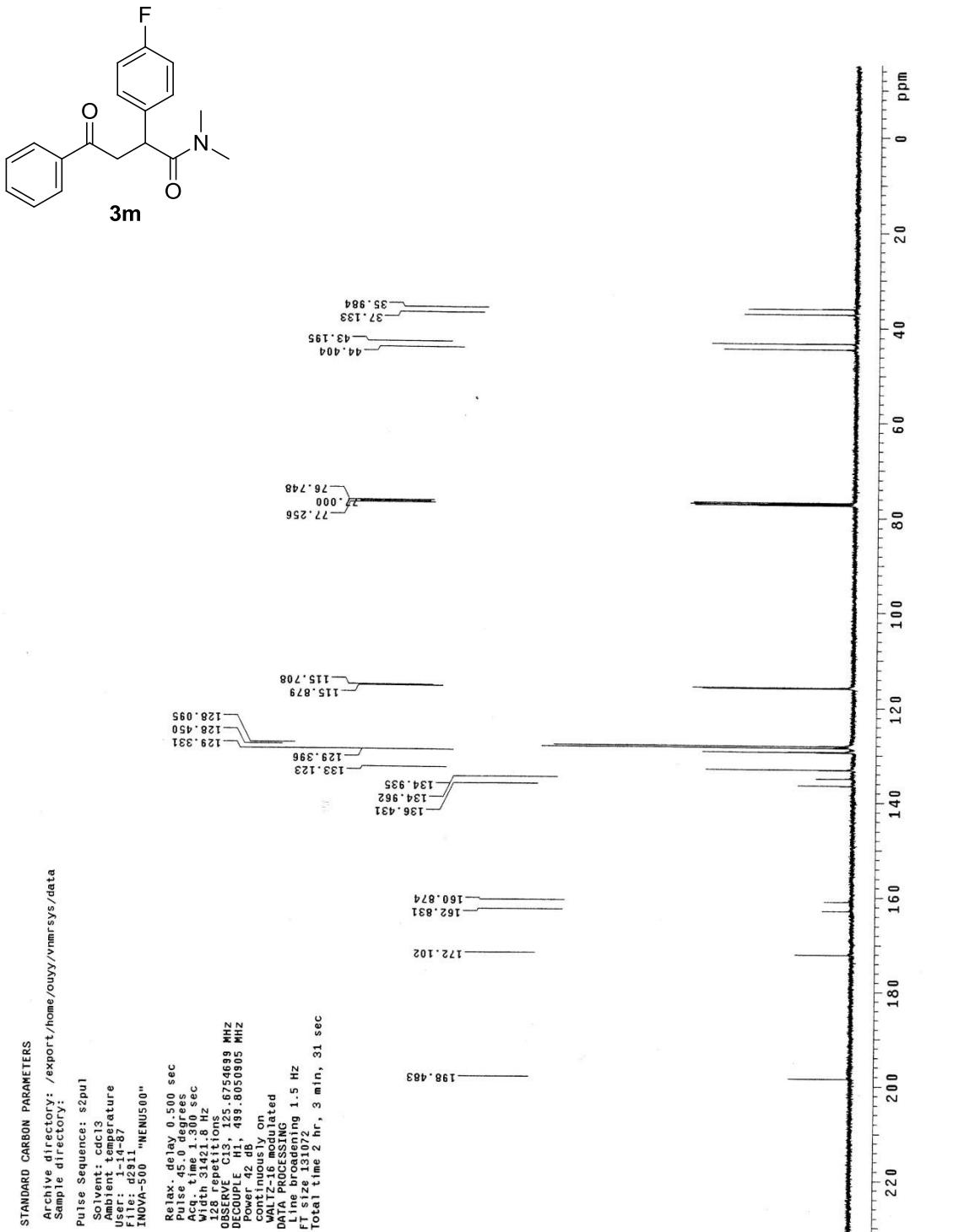
Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: cdcl₃
 Ambient temperature
 User: 1-14-87
 File: d251
 INOVA-500 "NENU500"
 Relax delay 0.500 sec
 P1s 45.0 0.00 0.68
 ACh tine 1.30 0 sec
 With 314.21.8 Hz
 384.496 repitions
 OBSERVE C13 125.675461 MHz
 DECOUPLE H1 498.805095 MHz
 Power 42 dB
 continuous on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 30 min, 52 sec

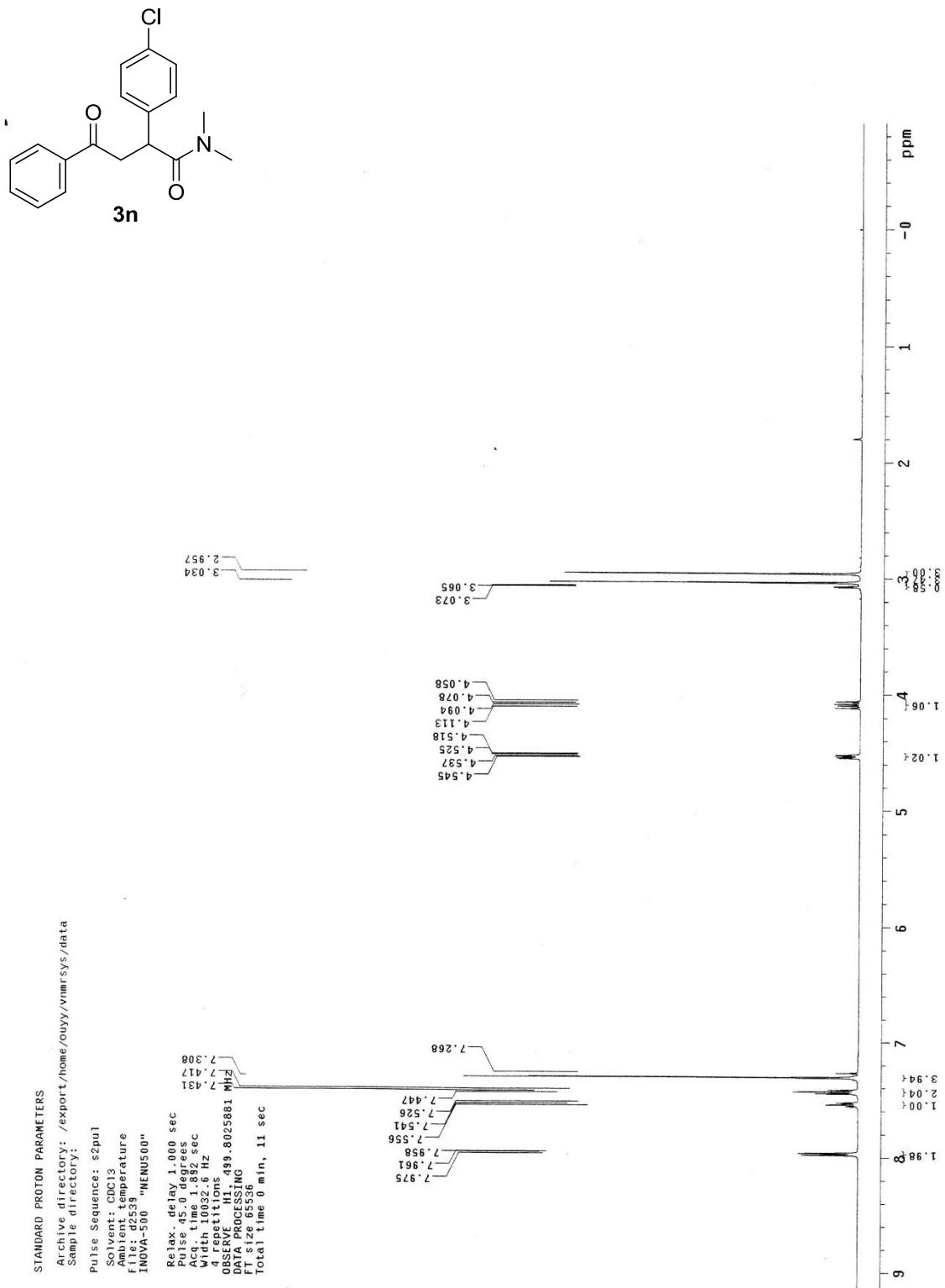


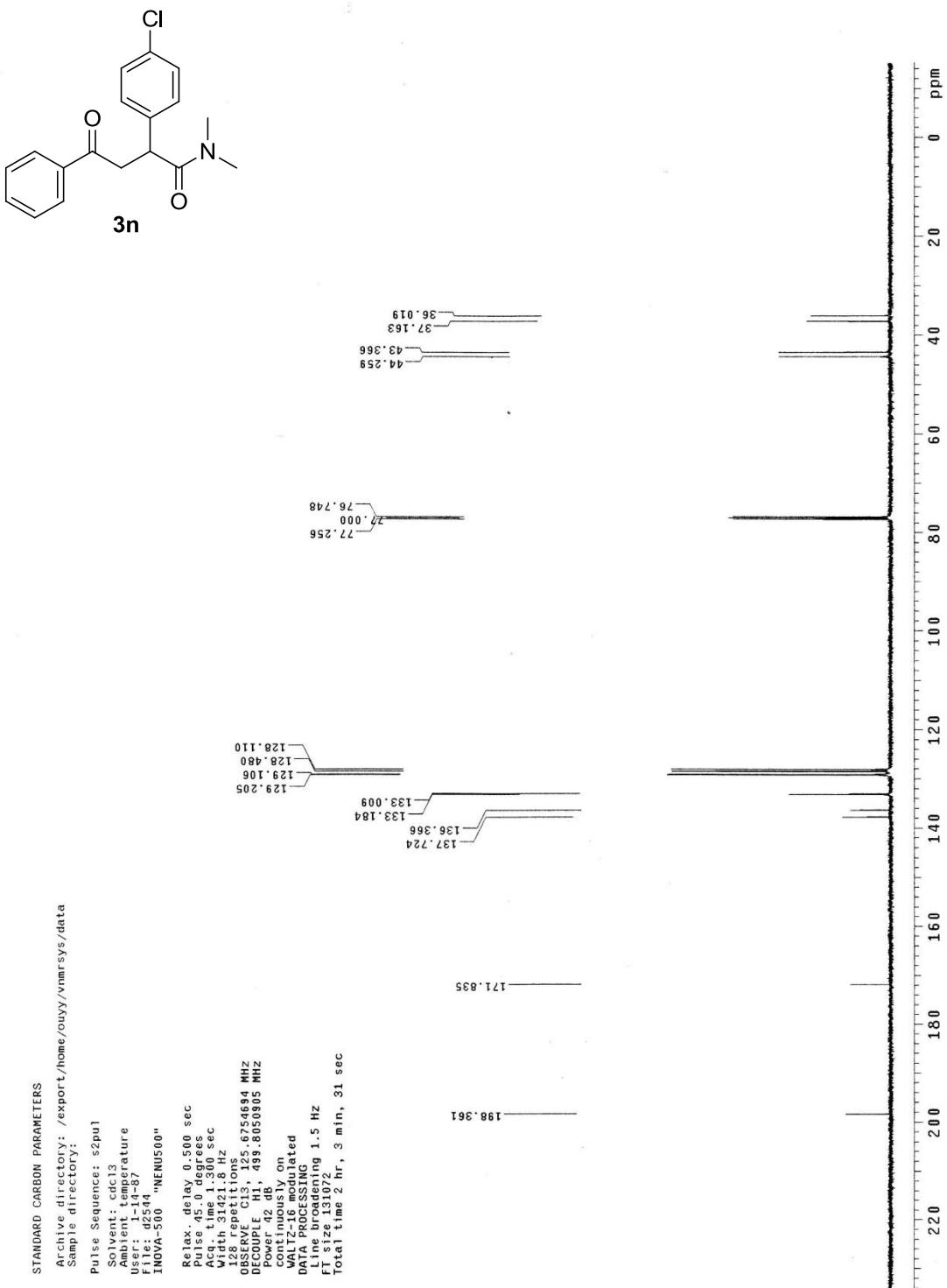


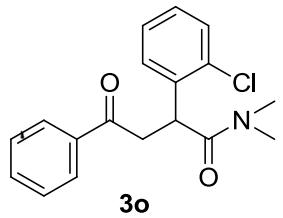






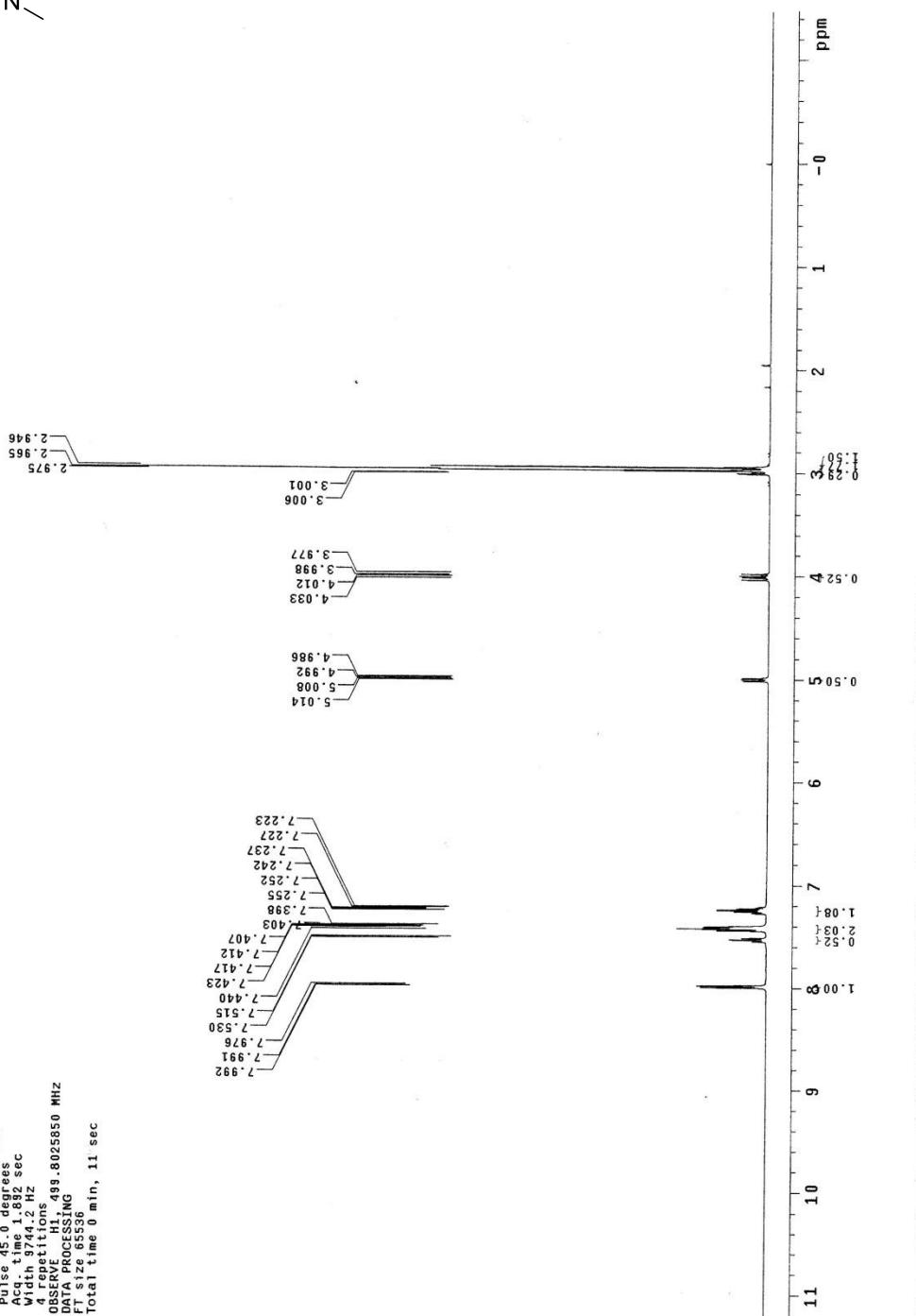






STANDARD PROTON PARAMETERS

Archive directory: /export/t/home/ouyy/vnmrSys/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: CDCl₃
 Ambient temperature
 F11: d212
 INOVA-500
 "NENU500"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 9.944.2 Hz
 4 Repetitions
 OBSERVE F11, 499.8025850 MHz
 DATA PROCESSING
 FIT size 65536
 Total time 0 min, 11 sec



STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyyv/nmrsys/data

Sample directory:

Pulse Sequence: s2pu1

Solvent: cdc13

Ambient temperature

User: 1-14-87

File: 12913

INOVA-500 "NENUS00"

Relax-delay 0.500 sec

pulse 45.0 degrees

Acq. time 1.310 sec

With 3121.8 Hz

4096 points

OBSERVE C13, 125

DECOUPLE H1, 498.8050935 MHz

Power 42 dB

continuous on

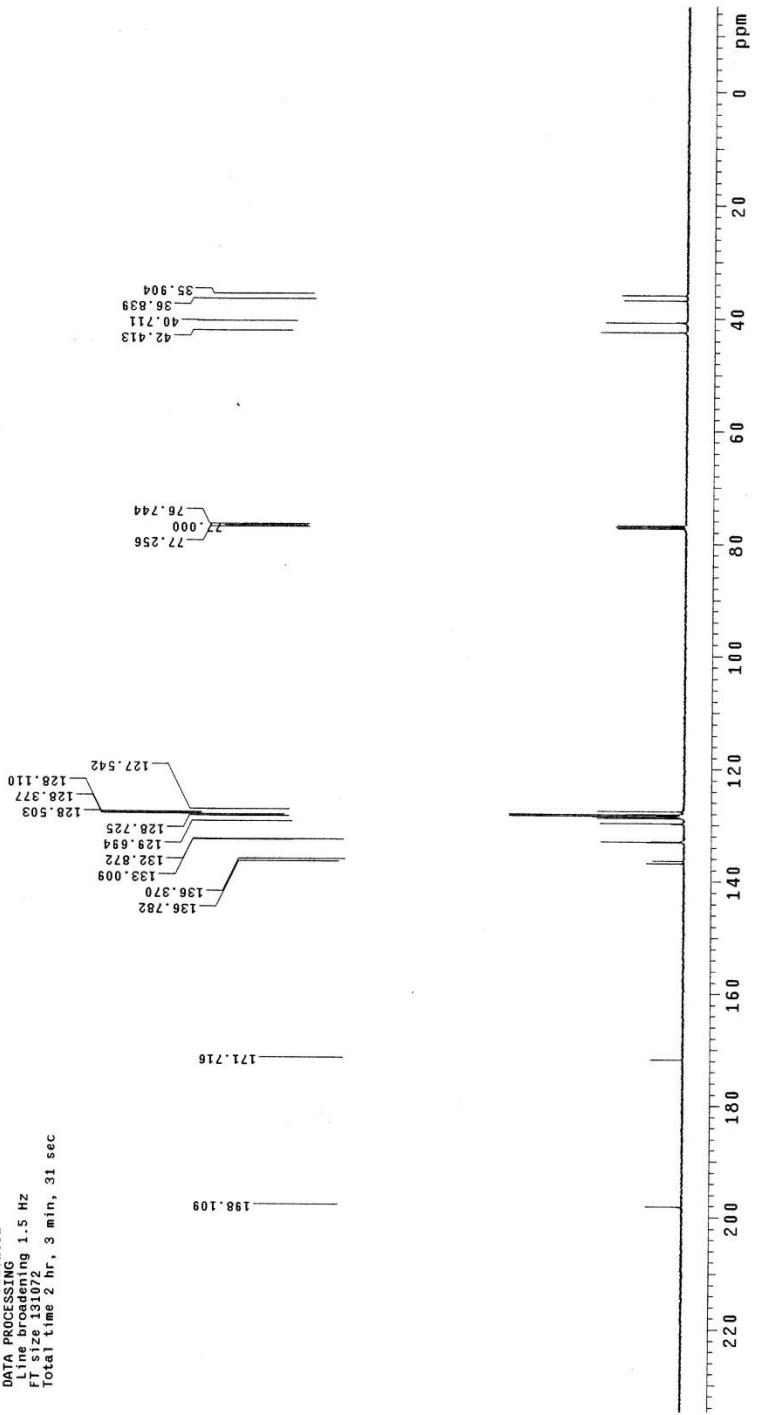
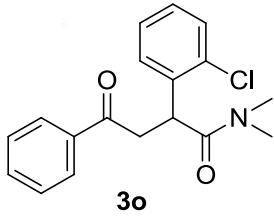
WALTZ-16 modulated

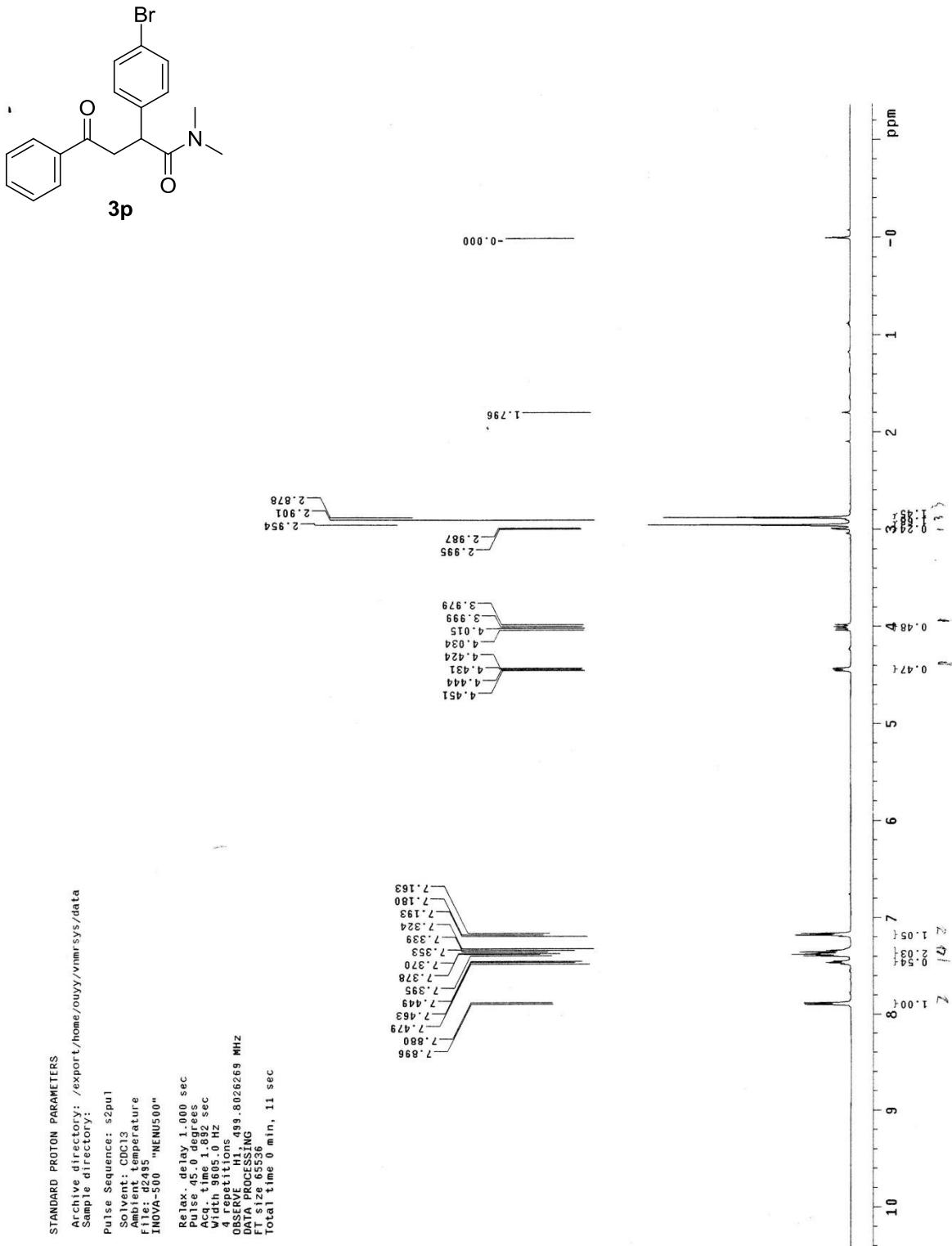
DATA PROCESSING

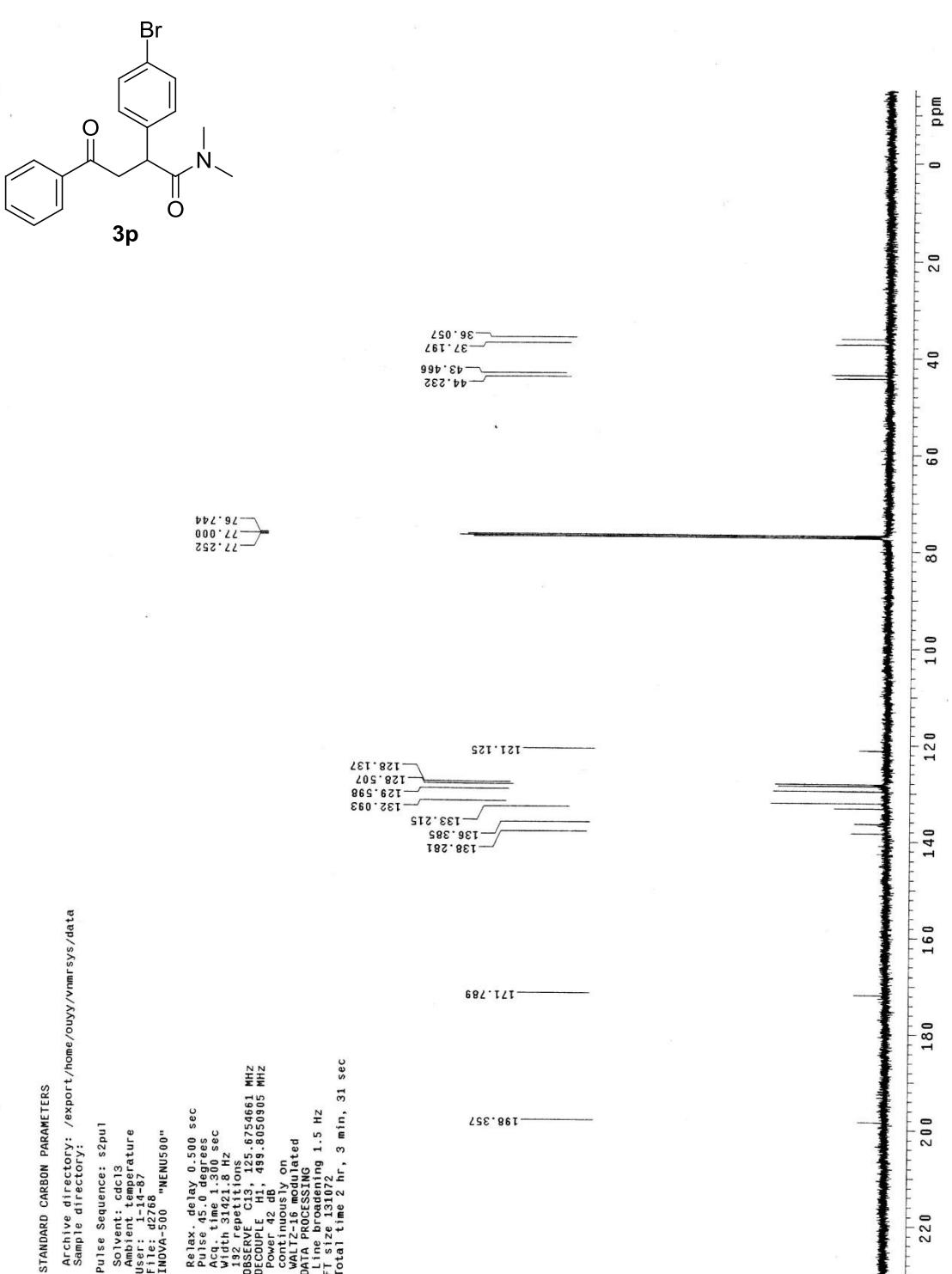
Line broadening 1.5 Hz

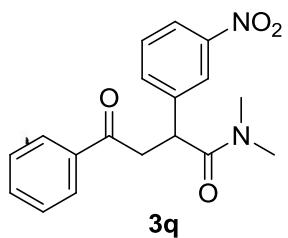
FT size 131072

Total time 2 hr, 3 min, 31 sec

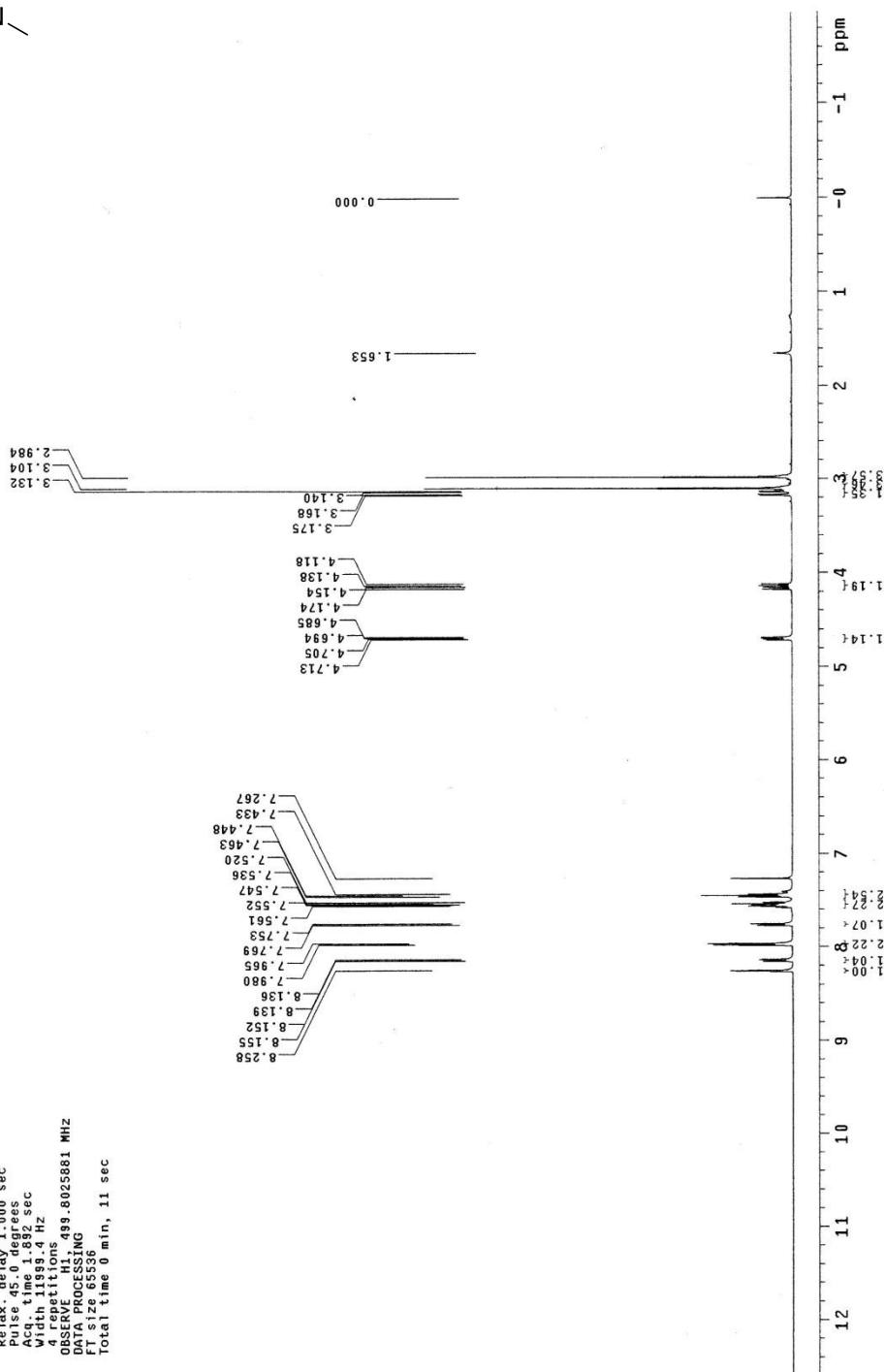


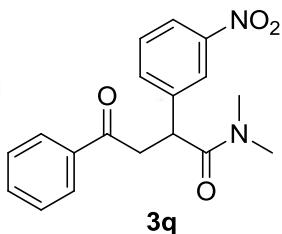






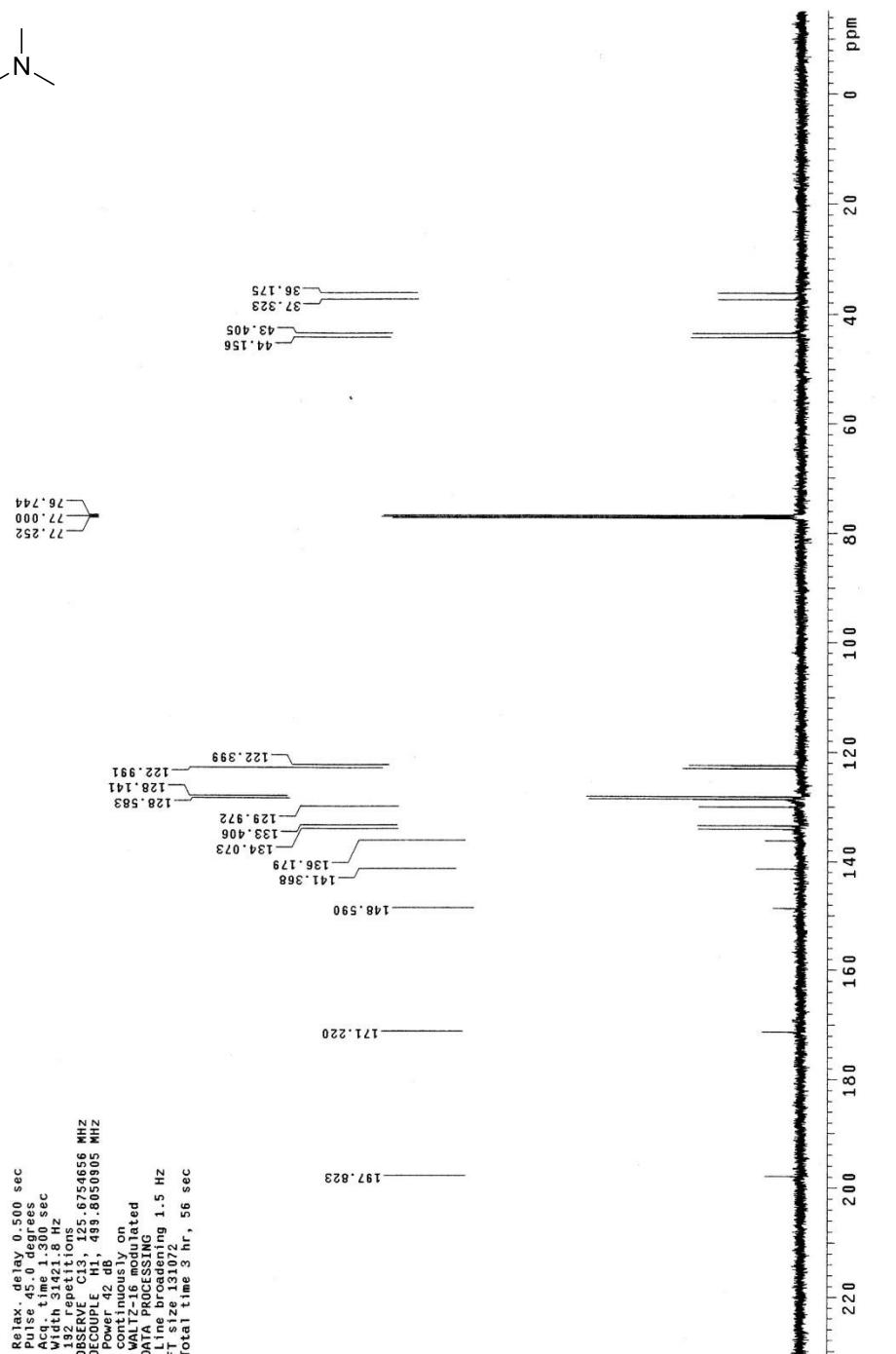
STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouvy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pu1
Solvent: CDCl₃
Ambient temperature
File: d2332
INOVA-500 "INENUS00"
Relax delay 1.000 sec
Pulse 45°, 1.000 sec
Apt 1.189 sec
Width 1199.4 Hz
4 repetitions
OBSERVE 11.499.8025881 MHz
DATA PROCESSING
FT size 65336
Total time 0 min, 11 sec

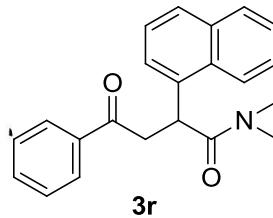




STANDARD CARBON PARAMETERS

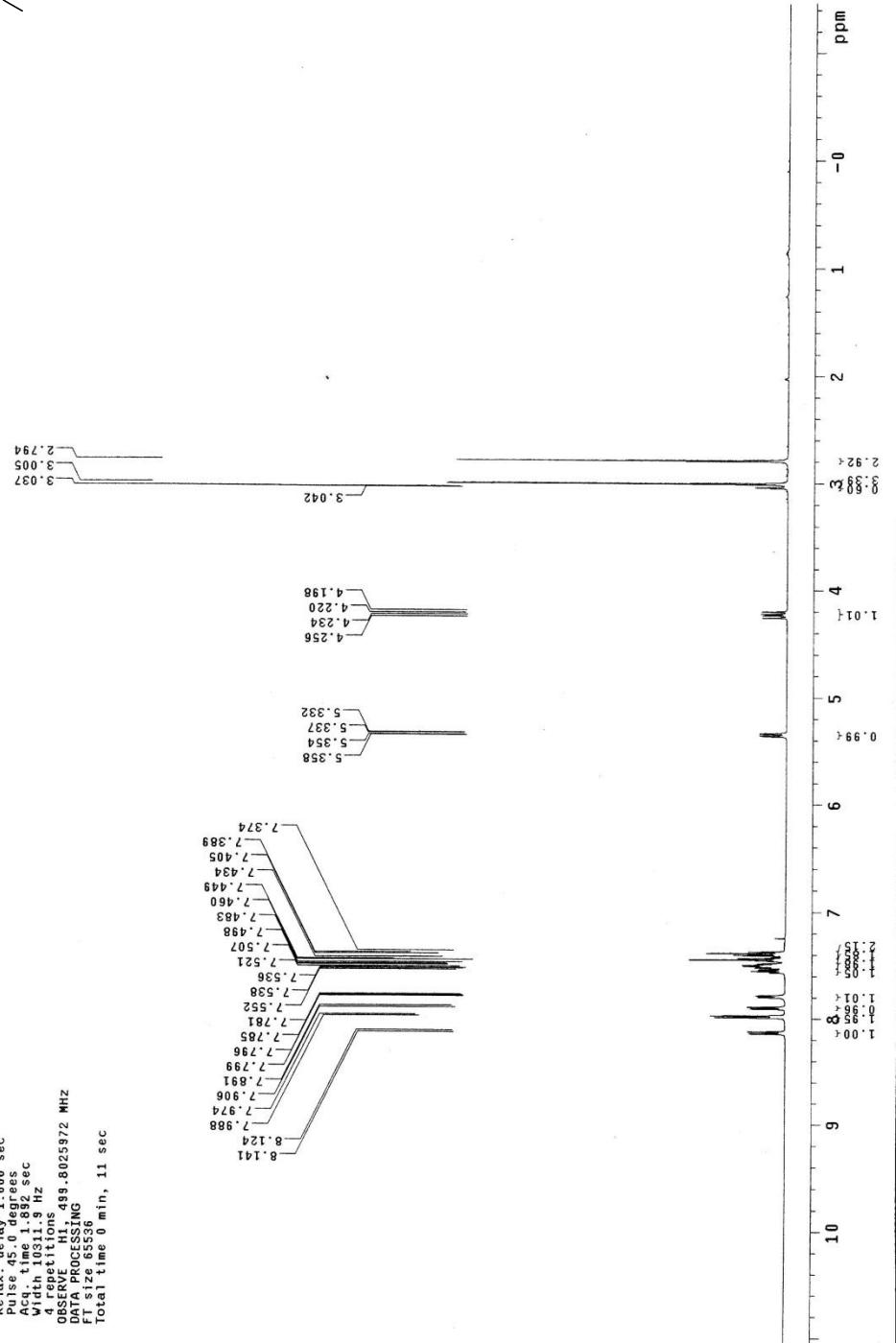
Archive directory: /export/v/home/ouyy/vnmrfsys/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: cdcl3
 Ambient temperature
 User: 1-14-87
 File: d2833
 INOVA-500 "NEMUS00"

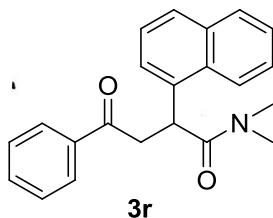




STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pu1
Solvent: CDCl₃
Ambient temperature
File: d2778 .INNOVA-500
INOVA-500

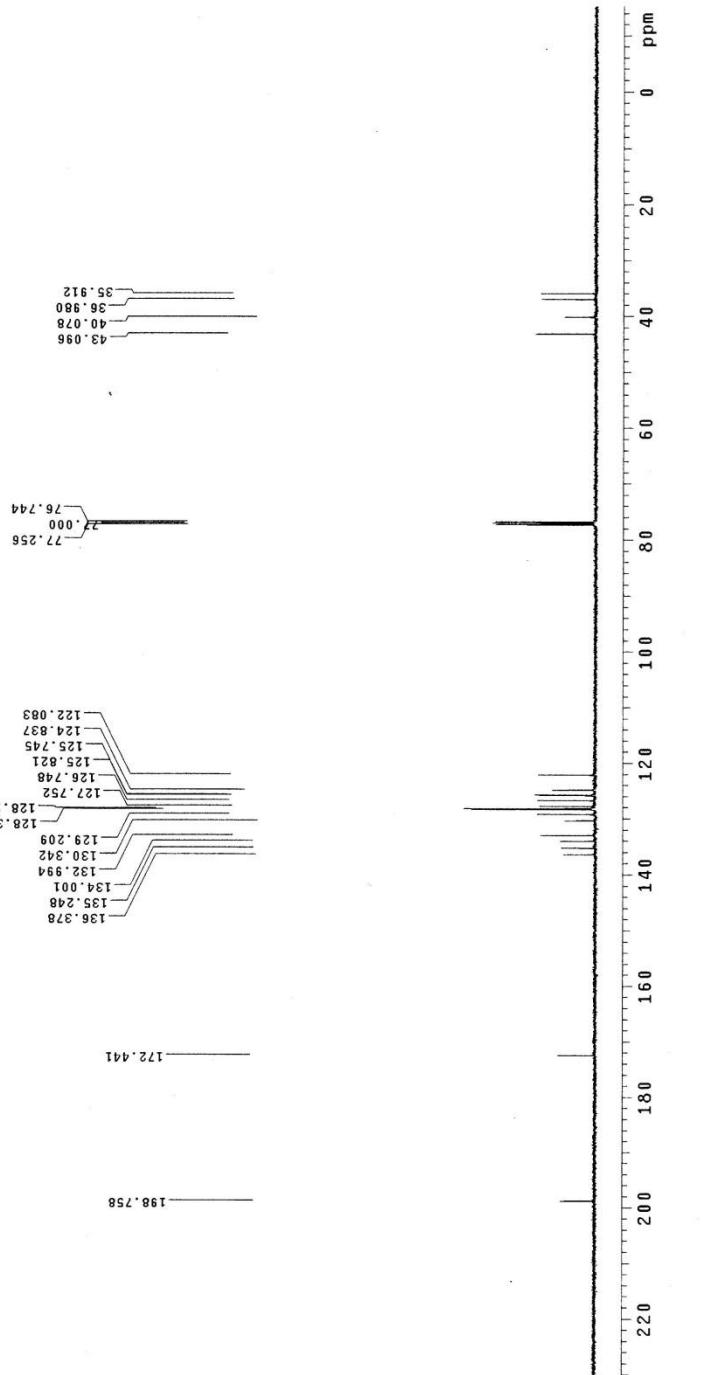
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10311.9 Hz
4 repetitions
OBSERVE H1, 499.8025972 MHz
DATA PROCESSING
Fit size 65536
Total time 0 min, 11 sec

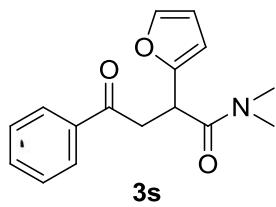




STANDARD CARBON PARAMETERS
 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: cdcl3
 Ambient temperature
 User: 1-14-87
 File: d2779
 INOVA-500 "NENNU500"

 Relax. delay 5.00 sec
 Pulse 45.0 degrees
 Acq. 4.00 sec
 Wdt 31421.8 Hz
 64 repetitions
 OBSERVE C13, 125.674810 MHz
 DECOUPL F1 H1, 459.805095 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

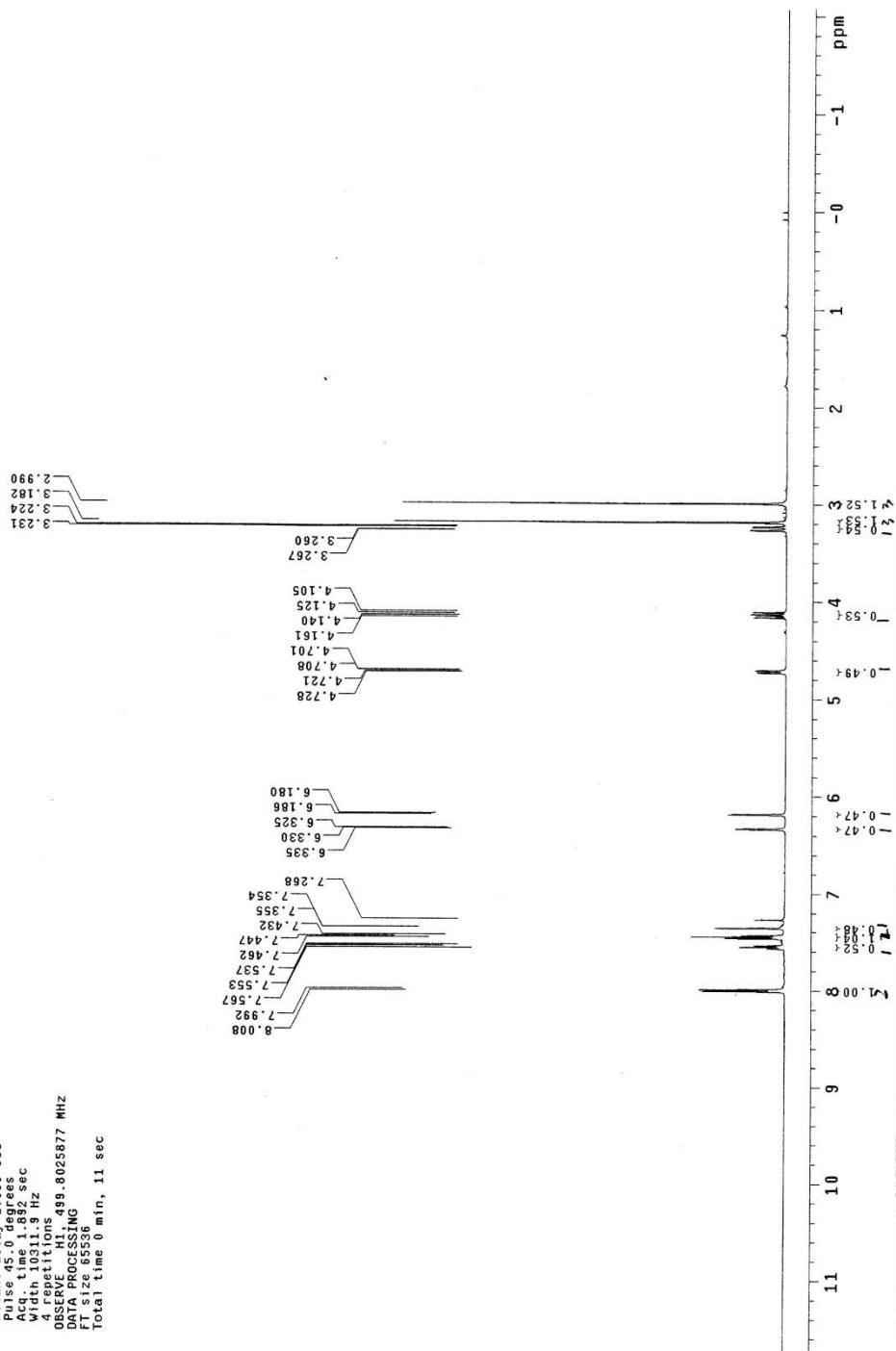


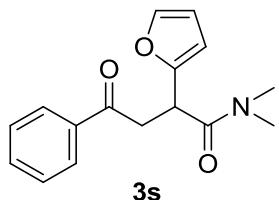


```

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouuy/vnmr/svs/data
Sample directory: s2pu1
Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
FILE: d2780 "NEMUS09"
INOVA-500

```





STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

Solvent: cdcl₃

Ambient temperature

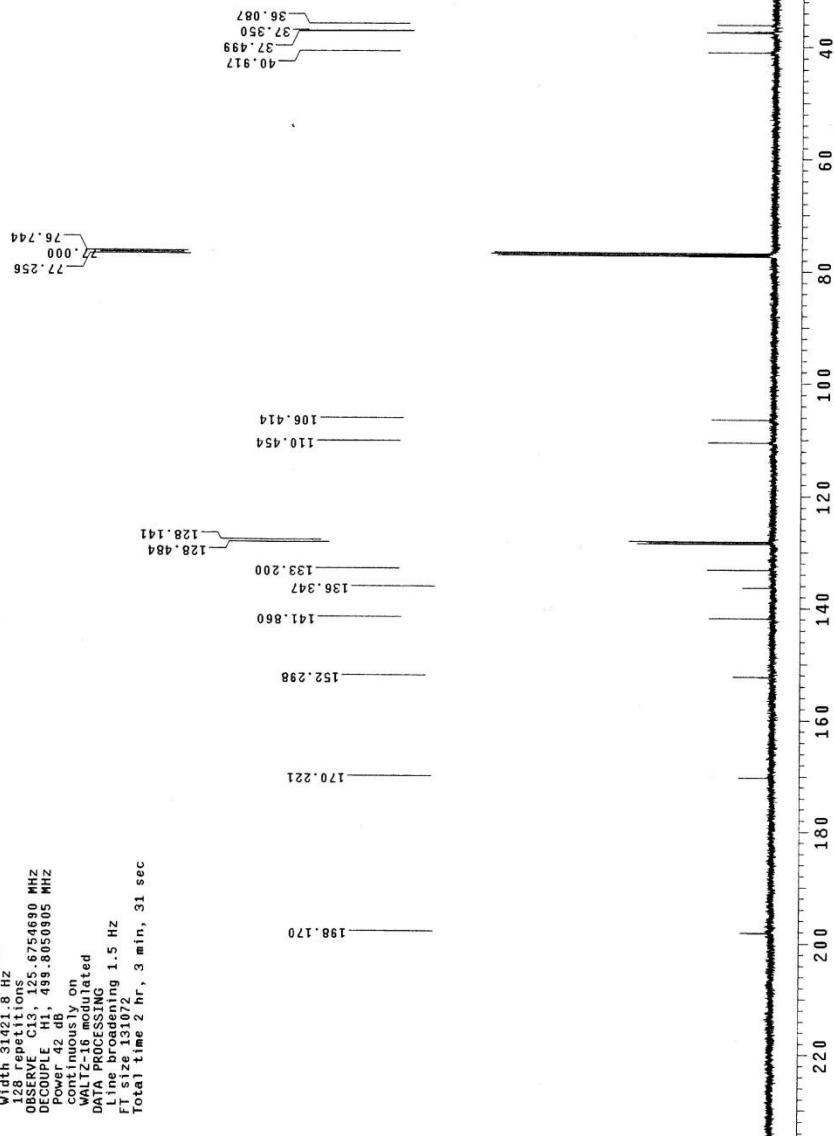
User: 1-14-87

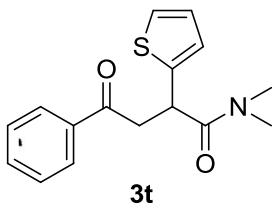
File: d281

INDIA-500

"NENUS00"

Relax. delay 0.500 sec
Pulse 95.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131024
Total time 2 hr, 3 min, 31 sec





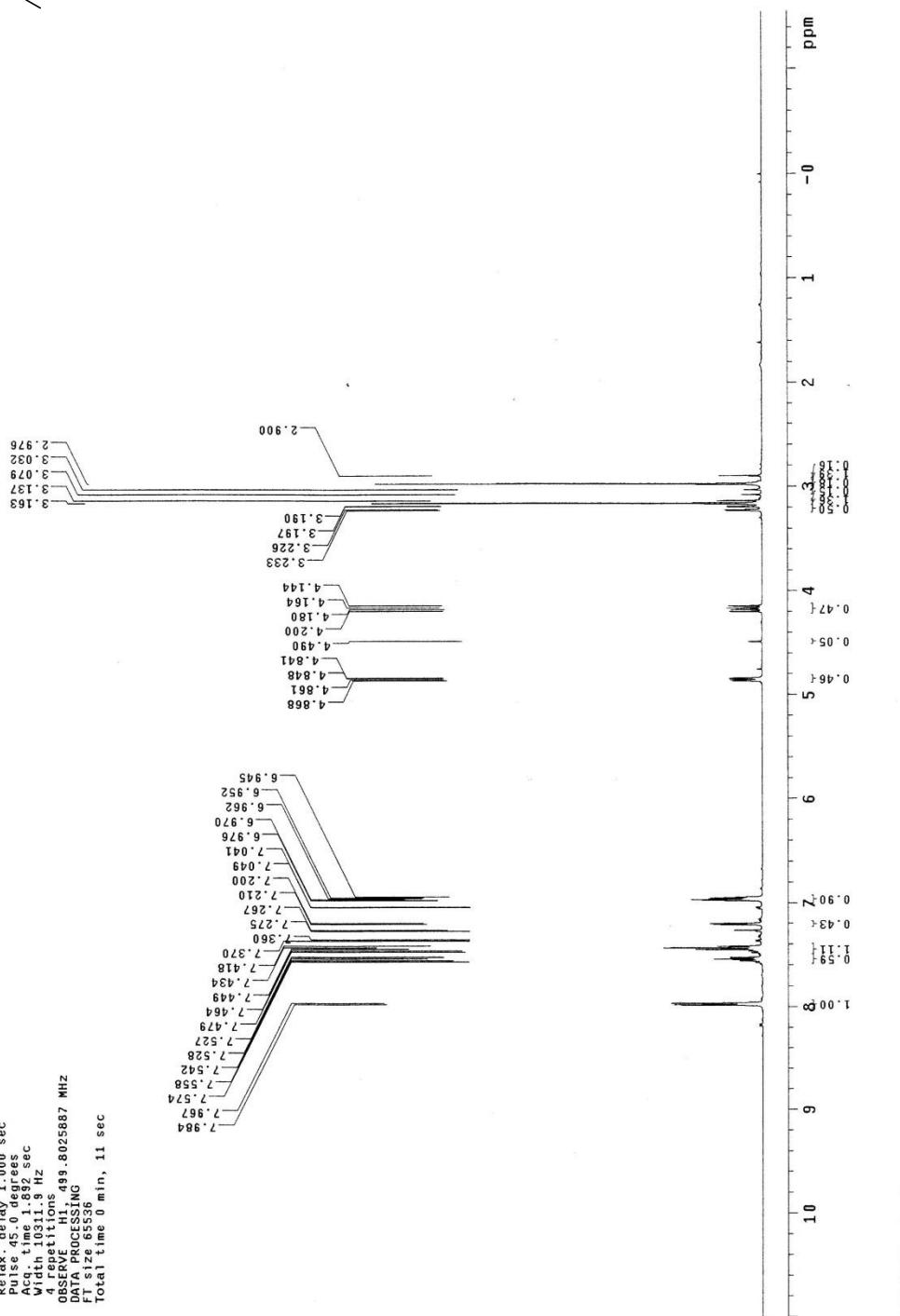
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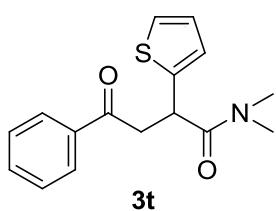
STANDARD PROTON PARAMETERS
Archive directory: /export/
Sample directory: /s2pu

Pulse Sequence: s2pu1
Solvint: C6C13
Ambient temperature
FI 1.0: d2766
INNOVA-500 "NENNU500"

Relax delay 1,000 sec
Pulse 45.0 deg66
Acq time 1.892 sec
With 1031.9 Hz
4 reactions
OBSERVE H1 439.8025887 MHz
DATA PROCESSING
Total time 0 min, 11 sec

```





STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2p1
Solvent: cdcl₃
Ambient temperature
User: 1-16-87
File: d276?
INNOVA-500 "HENNU500"
Relax, delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 3141.8 Hz
4096 repetitions
OBSERVE C13, 125.6754714 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
FT size 131072
Line broadening 1.5 Hz
Total time 2 hr, 3 min, 31 sec

