

Electronic Supplementary Material (ESI) for ChemComm
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Electronic Supplementary Information

DABCO-catalyzed ring opening of activated cyclopropanes and recyclization leading to γ -lactams with an all-carbon quaternary center

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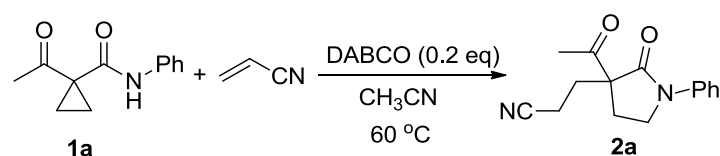
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I. General information:

All reagents were purchased from commercial sources and used without further 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 °C on a Varian 500 MHz and 125 MHz, respectively, with TMS as the internal standard. Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and are uncorrected. High resolution mass spectra were recorded on Bruck microtof. All reactions were monitored by TLC with Taizhou GF254 silica gel coated plates. Flash column chromatography was carried out using 200-300 mesh silica gel at increased pressure.

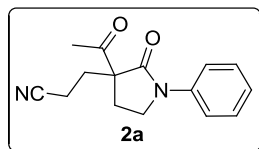
II. General procedure for the construction of γ -lactams (2a as an example):



To a solution of **1a** (203 mg, 1.0 mmol) and DABCO (44 mg, 0.2 mmol) in CH₃CN (2.0 mL) was added acrylonitrile (0.08 mL, 1.1 mmol) in a 25 mL flask. The reaction mixture was stirred at 60 °C for 6 h, cooled down to room temperature, poured into brine and extracted with EtOAc. The combined organic phase was washed with water (3 × 10 mL), dried over anhydrous MgSO₄, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography (petroleum ether/diethyl ether) to afford the desired product **2a** (238 mg, 93%).

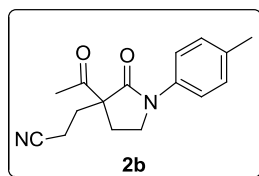
III. Characterization of the products

3-(3-acetyl-2-oxo-1-phenylpyrrolidin-3-yl)propanenitrile (2a)



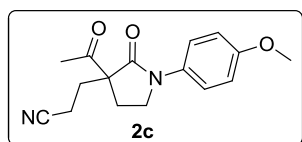
Colorless crystals. m.p. 86-88 °C. ^1H NMR (500 MHz, CDCl_3): δ = 2.00-2.06 (m, 1H), 2.34 (s, 3H), 2.35-2.46 (m, 4H), 2.77-2.82 (m, 1H), 3.81-3.89 (m, 2H), 7.20-7.23 (t, J = 7.5 Hz, 1H), 7.39-7.42 (t, J = 7.5 Hz, 2H), 7.60-7.61 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 13.0, 26.1, 26.1, 29.6, 29.8, 45.8, 62.7, 118.8, 120.0, 125.4, 129.0, 138.5, 170.4, 203.5. HRMS (ESI-TOF): Calc for $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_2$ [$\text{M}+\text{H}$]: 257.1290; found: 257.1290.

3-(3-acetyl-2-oxo-1-(*p*-tolyl)pyrrolidin-3-yl)propanenitrile (2b)



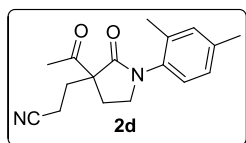
White solid. m.p. 91-93 °C. ^1H NMR (500 MHz, CDCl_3): δ = 1.98-2.04 (m, 1H), 2.14 (s, 3H), 2.30-2.46 (m, 10H), 2.74-2.79 (m, 1H), 3.77-3.87 (m, 2H), 7.18-7.20 (d, J = 8.5 Hz, 2H), 7.46-7.47 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 13.0, 20.9, 26.1, 26.2, 29.8, 30.9, 46.0, 62.6, 118.9, 120.0, 129.5, 135.3, 136.0, 170.2, 203.7. HRMS (ESI-TOF): Calc for $\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_2$ [$\text{M}+\text{H}$]: 271.1447; found: 271.1453.

3-(3-acetyl-1-(4-methoxyphenyl)-2-oxopyrrolidin-3-yl)propanenitrile (2c)



Colorless crystals. ^1H NMR (500 MHz, CDCl_3): δ = 2.00-2.04 (m, 1H), 2.33 (s, 3H), 2.34-2.39 (m, 2H), 2.42-2.46 (m, 4H), 2.74-2.79 (m, 1H), 3.77-3.84 (m, 5H), 6.91-6.93 (m, 2H), 7.48-7.50 (m, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 13.0, 26.1, 26.2, 29.8, 46.2, 55.4, 62.4, 114.1, 118.9, 121.8, 131.6, 157.1, 170.0, 203.8. HRMS (ESI-TOF): Calc for $\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_3$ [$\text{M}+\text{H}$]: 287.1396; found: 287.1391.

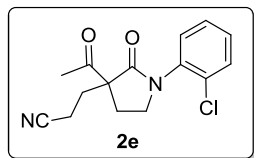
3-(3-acetyl-1-(2,4-dimethylphenyl)-2-oxopyrrolidin-3-yl)propanenitrile (2d)



White solid. m.p. 74-76 °C. ^1H NMR (500 MHz, CDCl_3): δ = 2.05-2.11 (m, 1H), 2.14 (s, 3H), 2.32 (s, 3H), 2.33-2.45 (m, 5H), 2.46-2.50 (m, 2H), 2.74-2.79 (m, 1H), 3.60-3.65 (m, 1H), 3.68-3.73 (m, 1H), 6.98-6.99 (d, J = 8.0 Hz, 1H), 7.04-7.05 (d, J = 8.5 Hz, 1H), 7.09 (s, 1H). ^{13}C NMR (125

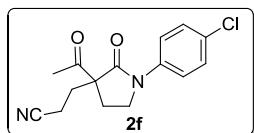
MHz, CDCl₃): δ = 12.9, 17.6, 20.9, 26.1, 27.1, 29.6, 47.7, 61.3, 118.9, 126.0, 127.6, 131.8, 133.7, 134.7, 138.2, 170.4, 204.0. HRMS (ESI-TOF): Calc for C₁₇H₂₀N₂O₂ [M+H]: 285.1603; found: 285.1607.

3-(3-acetyl-1-(2-chlorophenyl)-2-oxopyrrolidin-3-yl)propanenitrile (2e)



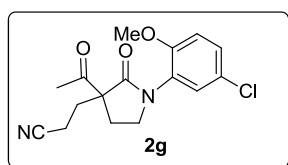
White solid. m.p. 77-79 °C. ¹H NMR (500 MHz, CDCl₃): δ = 2.09-2.14 (m, 1H), 2.33-2.42 (m, 5H), 2.45-2.50 (m, 2H), 2.78-2.83 (m, 1H), 3.68-3.72 (m, 1H), 3.75-3.80 (m, 1H), 7.25-7.27 (m, 1H), 7.30-7.35 (m, 2H), 7.47-7.49 (m, 1H). ¹³C NMR (125 MHz, CDCl₃): δ = 12.9, 26.2, 27.3, 29.5, 47.0, 61.0, 119.0, 128.0, 129.1, 129.8, 130.5, 132.0, 135.1, 171.2, 203.7. HRMS (ESI-TOF): Calc for C₁₅H₁₅ClN₂O₂ [M+H]: 291.0900; found: 291.0984.

3-(3-acetyl-1-(4-chlorophenyl)-2-oxopyrrolidin-3-yl)propanenitrile (2f)



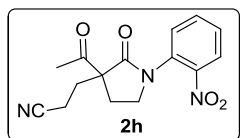
White solid. m.p. 119-121 °C. ¹H NMR (500 MHz, CDCl₃): δ = 2.00-2.06 (m, 1H), 2.33 (s, 3H), 2.34-2.45 (m, 4H), 2.79-2.83 (m, 1H), 3.77-3.85 (m, 2H), 7.35-7.37 (d, *J* = 8.5 Hz, 2H), 7.56-7.58 (t, *J* = 9.5 Hz, 2H). ¹³C NMR (125 MHz, CDCl₃): δ = 13.0, 25.9, 26.1, 29.8, 45.8, 62.7, 118.7, 121.0, 129.0, 130.6, 137.1, 170.4, 203.3. HRMS (ESI-TOF): Calc for C₁₅H₁₅ClN₂O₂ [M+H]: 291.0900; found: 291.0905.

3-(3-acetyl-1-(5-chloro-2-methoxyphenyl)-2-oxopyrrolidin-3-yl)propanenitrile (2g)



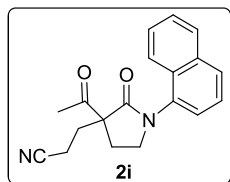
White solid. m.p. 55-57 °C. ¹H NMR (500 MHz, CDCl₃): δ = 2.05-2.11 (m, 1H), 2.26-2.38 (m, 5H), 2.43-2.56 (m, 2H), 2.70-2.75 (m, 1H), 3.66-3.74 (m, 2H), 3.82 (s, 3H), 6.90-6.92 (d, *J* = 8.5 Hz, 1H), 7.22-7.22 (d, *J* = 2.5 Hz, 2H), 7.27-7.30 (m, 1H). ¹³C NMR (125 MHz, CDCl₃): δ = 12.8, 26.1, 27.4, 29.4, 46.9, 55.9, 60.8, 113.0, 119.1, 125.4, 127.0, 128.4, 129.1, 153.3, 171.6, 203.9. HRMS (ESI-TOF): Calc for C₁₆H₁₇ClN₂O₃ [M+H]: 321.1006; found: 321.1010.

3-(3-acetyl-1-(2-nitrophenyl)-2-oxopyrrolidin-3-yl)propanenitrile (2h)



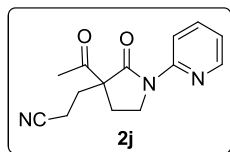
Colorless oil. ^1H NMR (500 MHz, CDCl_3): δ = 2.15-2.19 (m, 1H), 2.31-2.45 (m, 7H), 2.86-2.91 (m, 1H), 3.82-3.86 (m, 1H), 3.89-3.94 (m, 1H), 7.35-7.36 (m, 1H), 7.47-7.51 (m, 1H), 7.67-7.71 (m, 1H), 8.00-8.02 (m, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ = 12.8, 26.1, 27.0, 29.2, 30.9, 47.2, 61.4, 118.8, 125.6, 127.0, 128.3, 131.1, 134.0, 145.3, 171.0, 203.0. HRMS (ESI-TOF): Calc for $\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}_4$ [M+H]: 302.1141; found: 302.1147.

3-(3-acetyl-1-(naphthalen-1-yl)-2-oxopyrrolidin-3-yl)propanenitrile (2i)



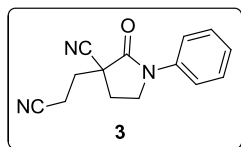
Colorless oil. ^1H NMR (500 MHz, CDCl_3): δ = 2.19-2.25 (m, 1H), 2.41-2.60 (m, 7H), 2.87-2.92 (m, 1H), 3.75-3.78 (m, 1H), 3.79-3.91 (m, 1H), 7.33-7.35 (d, J = 7.0 Hz, 1H), 7.49-7.60 (m, 4H), 7.86-7.92 (m, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 13.1, 26.3, 27.4, 29.8, 48.8, 61.7, 118.9, 121.8, 124.7, 125.6, 126.6, 127.1, 128.7, 129.0, 129.3, 134.3, 134.5, 171.5, 204.2. HRMS (ESI-TOF): Calc for $\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_2$ [M+H]: 307.1447; found: 307.1446.

3-(3-acetyl-2-oxo-1-(pyridin-2-yl)pyrrolidin-3-yl)propanenitrile (2j)



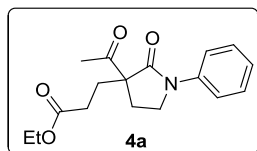
White solid. m.p. 83-85 °C. ^1H NMR (500 MHz, CDCl_3): δ = 1.97-2.02 (m, 1H), 2.32 (s, 3H), 2.33-2.39 (m, 2H), 2.43-2.47 (m, 2H), 2.69-2.74 (m, 1H), 3.99-4.05 (m, 1H), 4.15-4.19 (m, 1H), 7.09-7.12 (m, 1H), 7.72-7.75 (m, 1H), 8.35-8.39 (m, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 12.9, 25.8, 26.1, 29.6, 44.3, 63.3, 114.6, 118.8, 120.2, 137.7, 147.6, 150.9, 171.3, 203.2. HRMS (ESI-TOF): Calc for $\text{C}_{14}\text{H}_{15}\text{N}_3\text{O}_2$ [M+H]: 257.1164; found: 257.1171.

3-(2-cyanoethyl)-2-oxo-1-phenylpyrrolidine-3-carbonitrile (3)



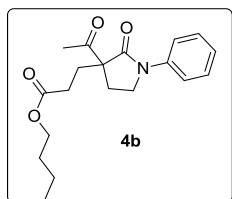
Colorless oil. ^1H NMR (500 MHz, CDCl_3): δ = 2.10-2.27 (m, 1H), 2.28-2.32 (m, 1H), 2.37-2.43 (m, 1H), 2.61-2.73 (m, 2H), 2.81-2.88 (m, 1H), 3.84-3.89 (m, 1H), 3.95-4.00 (m, 1H), 7.22-7.25 (t, J = 7.0 Hz, 1H), 7.38-7.42 (t, J = 7.0 Hz, 2H), 7.55-7.57 (d, J = 7.0 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 13.3, 29.8, 30.6, 44.8, 45.3, 117.5, 118.1, 120.2, 125.9, 129.0, 137.7, 166.0. HRMS (ESI-TOF): Calc for $\text{C}_{14}\text{H}_{13}\text{N}_3\text{O}$ [M+H]: 239.1059; found: 239.1055.

ethyl 3-(3-acetyl-2-oxo-1-phenylpyrrolidin-3-yl)propanoate (4a)



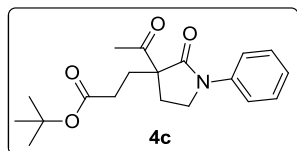
White solid. m.p. 56-58 °C. ^1H NMR (500 MHz, CDCl_3): δ = 1.24-1.27 (t, J = 7.5 Hz, 3H), 1.86-1.92 (m, 1H), 2.22-2.33 (m, 3H), 2.35 (s, 3H), 2.45-2.50 (m, 1H), 2.79-2.83 (m, 1H), 3.71-3.75 (m, 1H), 3.79-3.84 (m, 1H), 4.12-4.16 (m, 2H), 7.16-7.19 (t, J = 7.5 Hz, 1H), 7.36-7.40 (t, J = 8.5 Hz, 2H), 7.59-7.61 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 14.1, 25.6, 26.1, 29.7, 45.9, 60.7, 63.4, 119.9, 125.1, 128.9, 138.9, 171.0, 172.4, 204.6. HRMS (ESI-TOF): Calc for $\text{C}_{17}\text{H}_{21}\text{NO}_4$ [M+H]: 303.1471; found: 303.1477.

butyl 3-(3-acetyl-2-oxo-1-phenylpyrrolidin-3-yl)propanoate (4b)



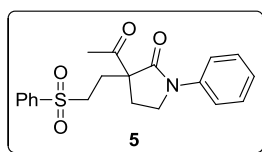
White solid. m.p. 36-38 °C. ^1H NMR (500 MHz, CDCl_3): δ = 0.92-0.94 (t, J = 7.5 Hz, 3H), 1.33-1.41 (m, 2H), 1.57-1.63 (m, 2H), 1.86-1.92 (m, 1H), 2.21-2.36 (m, 6H), 2.43-2.48 (m, 1H), 2.76-2.81 (m, 1H), 3.70-3.83 (m, 2H), 4.06-4.09 (t, J = 6.5 Hz, 2H), 7.15-7.18 (t, J = 7.5 Hz, 1H), 7.35-7.38 (t, J = 8.0 Hz, 2H), 7.60-7.61 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 13.5, 18.8, 25.3, 25.8, 29.4, 30.3, 45.6, 63.1, 64.4, 119.6, 124.8, 128.6, 138.8, 170.8, 172.2, 204.3. HRMS (ESI-TOF): Calc for $\text{C}_{19}\text{H}_{25}\text{NO}_4$ [M+H]: 332.1862; found: 332.1867.

tert-butyl 3-(3-acetyl-2-oxo-1-phenylpyrrolidin-3-yl)propanoate (4c)



White solid. m.p. 74-76 °C. ^1H NMR (500 MHz, CDCl_3): δ = 1.44 (s, 9H), 1.86-1.92 (m, 1H), 2.16-2.62 (m, 3H), 2.34 (s, 3H), 2.39-2.46 (m, 1H), 2.77-2.81 (m, 1H), 2.70-3.83 (m, 2H), 7.15-7.18 (t, J = 7.5 Hz, 1H), 7.35-7.39 (t, J = 7.5 Hz, 2H), 7.59-7.61 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 25.4, 26.0, 27.9, 29.7, 30.7, 45.8, 63.3, 80.7, 119.8, 124.9, 128.8, 138.9, 171.0, 171.5, 204.6. HRMS (ESI-TOF): Calc for $\text{C}_{19}\text{H}_{25}\text{NO}_4$ [M+H]: 332.1862; found: 332.1867.

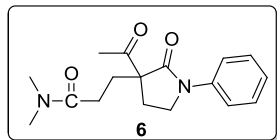
3-acetyl-1-phenyl-3-(2-(phenylsulfonyl)ethyl)pyrrolidin-2-one (5)



White solid. m.p. 121-123 °C. ^1H NMR (500 MHz, CDCl_3): δ = 1.86-1.88 (m, 1H), 2.19 (s, 3H), 2.26-2.30 (t, J = 8.0 Hz, 1H), 2.36-2.40 (m, 1H), 2.63-2.66 (m, 1H), 3.10-3.13 (m, 2H), 3.74-3.80 (m, 2H), 7.14-7.17 (t, J = 7.0 Hz, 1H), 7.33-7.36 (t, J = 8.0 Hz, 2H), 7.53-7.57 (t, J = 8.5 Hz, 4H).

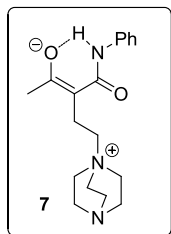
7.63-7.66 (t, J = 8.0 Hz, 1H), 7.88-7.90 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 25.8, 26.1, 26.9, 45.6, 51.5, 61.9, 119.8, 125.2, 127.8, 128.8, 129.3, 133.8, 138.3, 138.4, 170.3, 203.7. HRMS (ESI-TOF): Calc for $\text{C}_{20}\text{H}_{21}\text{NO}_4\text{S}$ [$\text{M}+\text{H}$]: 372.1270; found: 372.1267.

3-(3-acetyl-2-oxo-1-phenylpyrrolidin-3-yl)-*N,N*-dimethylpropanamide (6)



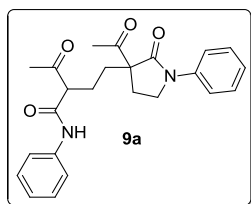
White solid. m.p. 61-63 °C. ^1H NMR (500 MHz, CDCl_3): δ = 1.93-1.98 (m, 1H), 2.22-2.45 (m, 7H), 2.73-2.78 (m, 1H), 2.94 (s, 3H), 3.00 (s, 3H), 3.75-3.82 (m, 2H), 7.16-7.19 (d, J = 7.0 Hz, 1H), 7.36-7.39 (t, J = 7.5 Hz, 2H), 7.60-7.61 (t, J = 7.5 Hz, 2H). ^{13}C NMR (125 MHz, CDCl_3): δ = 25.9, 26.2, 28.4, 29.5, 35.5, 37.2, 45.9, 63.4, 119.9, 125.0, 128.9, 139.0, 171.4, 171.5, 205.2. HRMS (ESI-TOF): Calc for $\text{C}_{17}\text{H}_{22}\text{N}_2\text{O}_3$ [$\text{M}+\text{H}$]: 303.1709; found: 303.1712.

1,3-zwitterion (7)



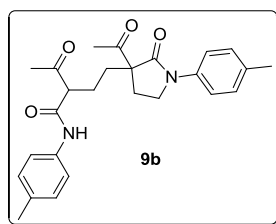
White solid. m.p. 173-175 °C. ^1H NMR (500 MHz, D_2O): δ = 1.75-1.76 (d, J = 7.5 Hz, 3H), 2.32-2.35 (t, J = 8.0 Hz, 2H), 2.72-2.75 (t, J = 8.5 Hz, 2H), 2.79-2.80 (d, J = 6.5 Hz, 6H), 3.01-3.02 (d, J = 6.5 Hz, 6H), 6.83-6.86 (t, J = 7.0 Hz, 1H), 7.11-7.14 (t, J = 8.0 Hz, 2H), 7.25-7.26 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, D_2O): δ = 20.4, 24.1, 44.2, 51.8, 63.7, 93.2, 119.9, 123.1, 129.5, 139.6, 170.0, 181.4. HRMS (ESI-TOF): Calc for $\text{C}_{18}\text{H}_{25}\text{N}_3\text{O}_2$ [$\text{M}+\text{H}$]: 316.2025; found: 316.2021.

2-acetyl-4-(3-acetyl-2-oxo-1-phenylpyrrolidin-3-yl)-*N*-phenylbutanamide (9a)



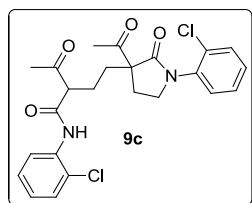
Colorless oil. ^1H NMR (500 MHz, CDCl_3): δ = 1.88-2.00 (m, 4H), 2.14-2.19 (m, 1H), 2.29 (s, 3H), 2.32-2.33 (d, J = 4.0 Hz, 3H), 2.79-2.82 (m, 1H), 3.46-3.54 (m, 1H), 3.73-3.85 (m, 2H), 7.11-7.20 (m, 2H), 7.30-7.39 (m, 4H), 7.52-7.58 (m, 4H), 8.30-8.35 (d, J = 25.0 Hz, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ = 24.5, 24.6, 25.4, 25.6, 26.0, 28.8, 29.2, 32.0, 32.3, 46.2, 46.3, 61.5, 61.6, 63.9, 63.9, 120.0, 120.0, 120.2, 120.0, 124.7, 125.3, 125.3, 128.9, 137.4, 137.4, 138.7, 166.3, 166.3, 171.3, 171.4, 204.6, 204.6, 205.5, 205.6. HRMS (ESI-TOF): Calc for $\text{C}_{24}\text{H}_{26}\text{N}_2\text{O}_4$ [$\text{M}+\text{H}$]: 407.1971; found: 407.1976.

2-acetyl-4-(3-acetyl-2-oxo-1-(*p*-tolyl)pyrrolidin-3-yl)-*N*-(*p*-tolyl)butanamide (9b)



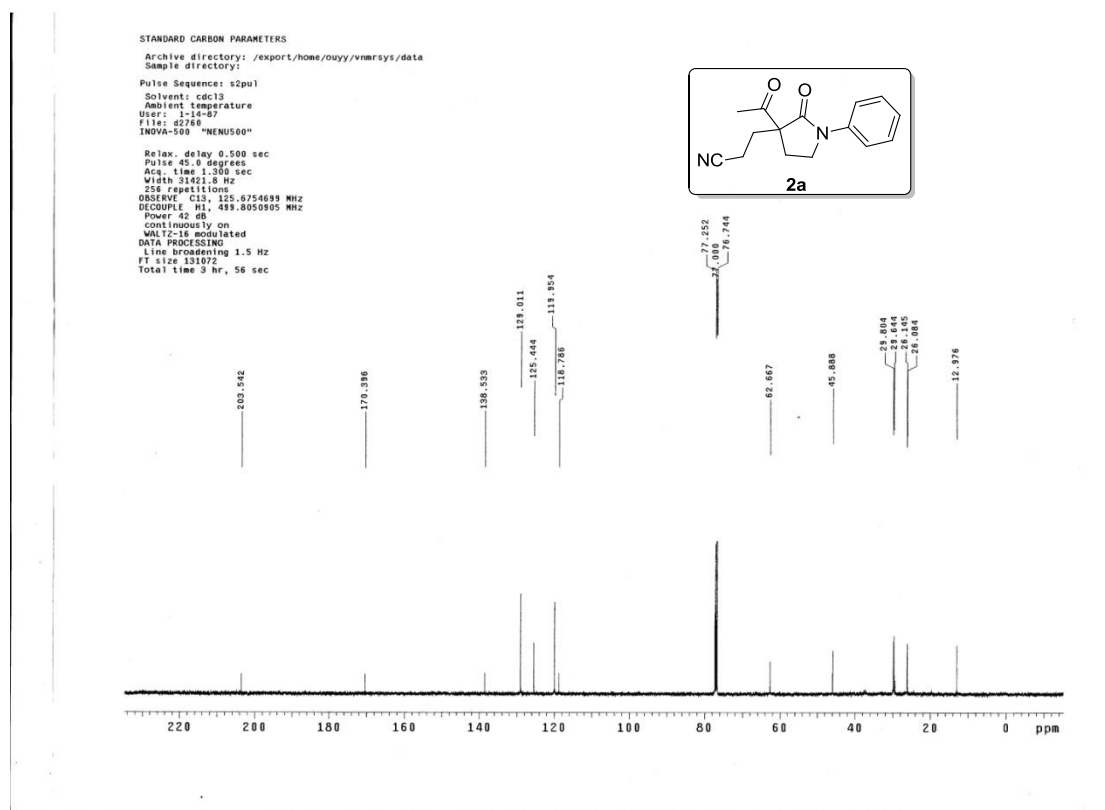
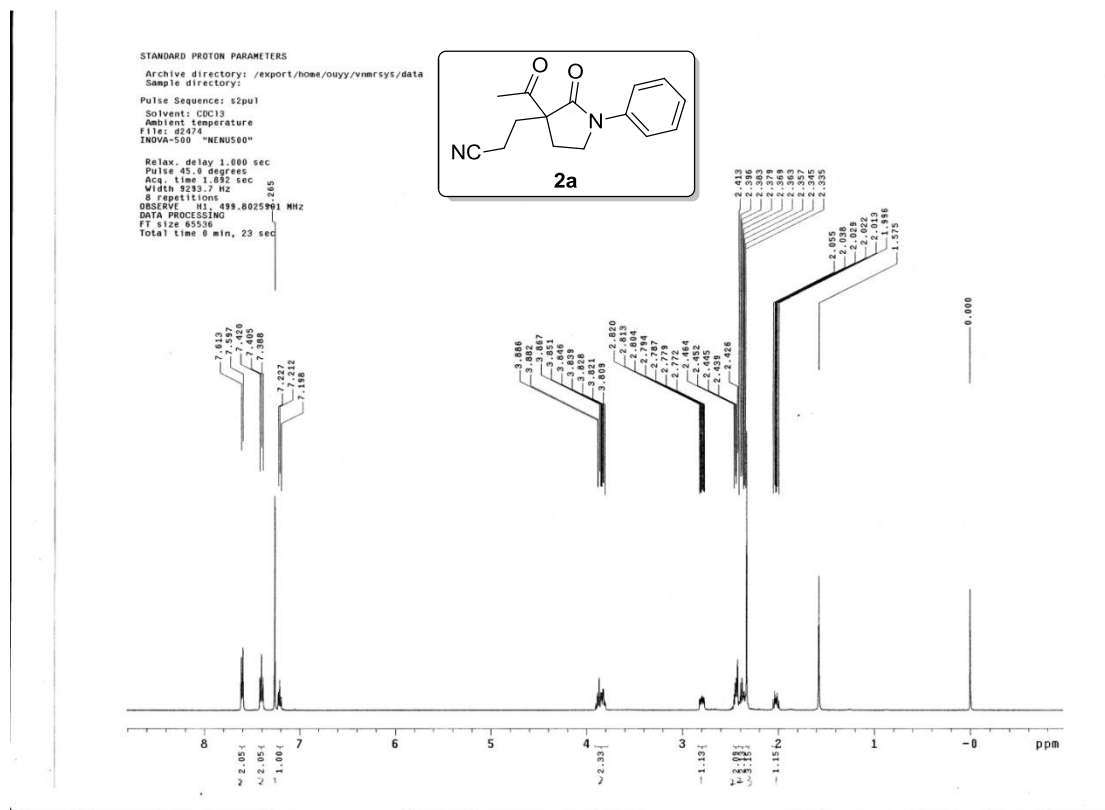
Colorless oil. ^1H NMR (500 MHz, CDCl_3): δ = 1.85-2.00 (m, 4H), 2.13-2.17 (m, 1H), 2.25-2.38(m, 12H), 2.76-2.83 (m, 1H), 3.43-3.51 (m, 1H), 3.68-3.83 (m, 2H), 7.07-7.17 (m, 4H), 7.38-7.44 (m, 4H), 8.21-8.26 (d, J = 27.5 Hz, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ = 20.8, 24.5, 24.7, 25.4, 25.7, 26.0, 26.0, 28.8, 29.2, 32.0, 32.3, 46.3, 46.4, 61.5, 61.6, 63.8, 63.8, 120.0, 120.0, 120.3, 120.3, 129.4, 129.4, 129.4, 134.3, 134.3, 134.8, 134.9, 135.1, 135.2, 136.2, 166.1, 166.2, 171.1, 171.2, 204.7, 204.8, 205.6, 205.7. HRMS (ESI-TOF): Calc for $\text{C}_{26}\text{H}_{30}\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$: 435.2284; found: 435.2288.

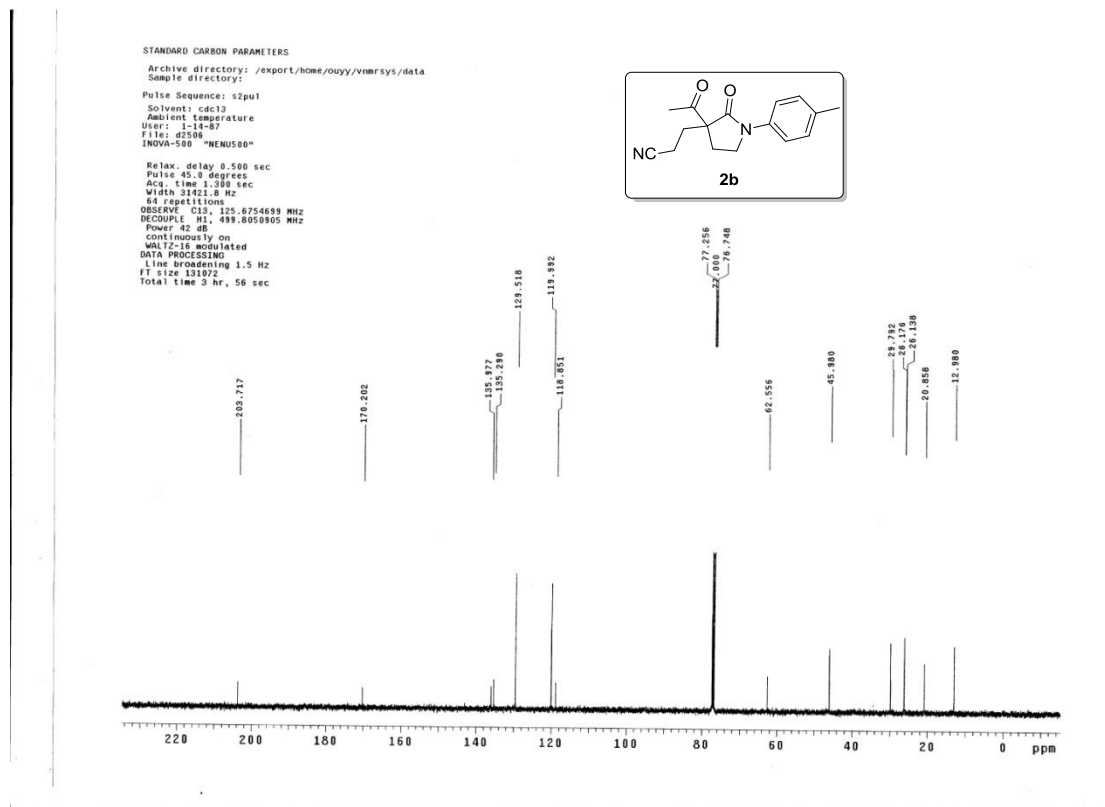
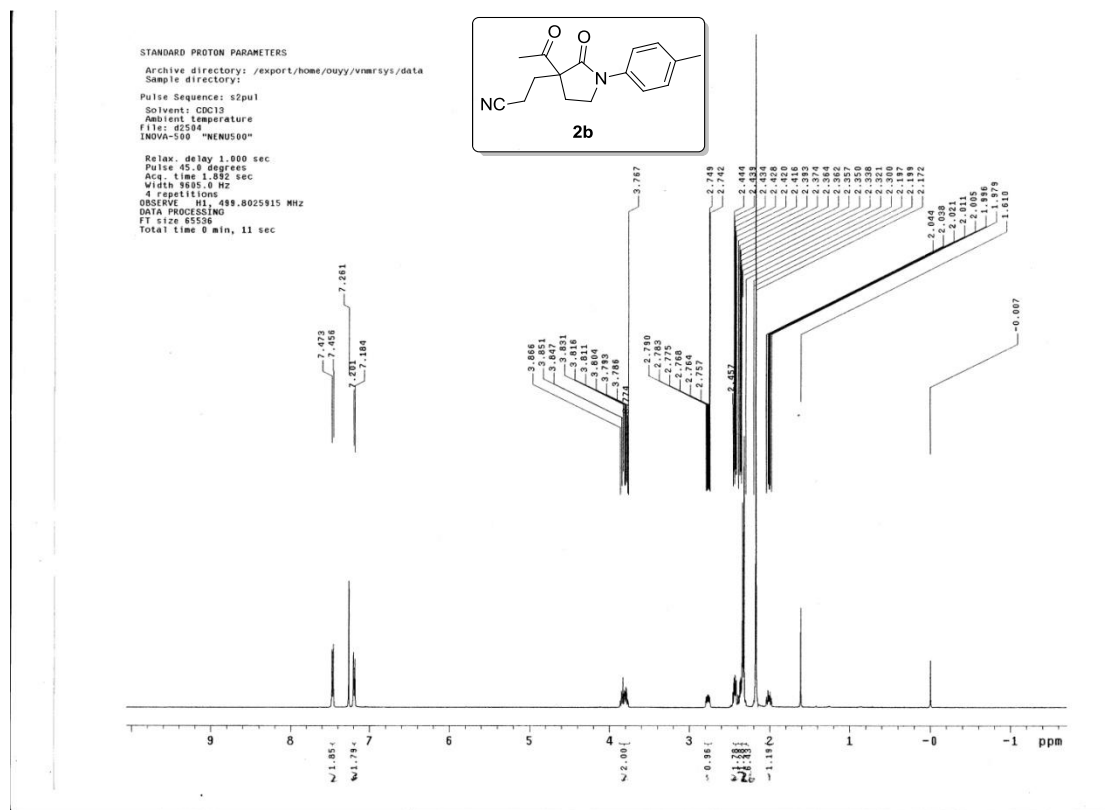
2-acetyl-4-(3-acetyl-1-(2-chlorophenyl)-2-oxopyrrolidin-3-yl)-*N*-(2-chlorophenyl)butanamide (9c)



Colorless oil. ^1H NMR (500 MHz, CDCl_3): δ = 1.94-2.18 (m, 5H), 2.33-2.40 (m, 6H), 2.85-2.88 (m, 1H), 3.56-3.74 (m, 3H), 7.07-7.10 (t, J = 7.0 Hz, 1H), 7.22-7.47 (m, 6H), 8.23-8.25 (m, 1H), 8.54-8.63 (d, J = 41.5 Hz, 1H). ^{13}C NMR (125 MHz, CDCl_3): δ = 25.2, 25.4, 26.0, 26.0, 26.5, 26.8, 29.3, 29.4, 29.8, 31.8, 31.9, 47.2, 47.3, 61.2, 61.6, 62.3, 62.4, 122.3, 122.3, 123.8, 123.9, 125.4, 127.5, 127.5, 127.9, 129.1, 129.1, 129.5, 129.5, 130.4, 132.0, 132.0, 134.0, 135.5, 135.6, 166.2, 166.2, 171.8, 171.8, 204.5, 204.6, 205.7, 206.0. HRMS (ESI-TOF): Calc for $\text{C}_{24}\text{H}_{24}\text{Cl}_2\text{N}_2\text{O}_4$ $[\text{M}+\text{H}]^+$: 475.1191; found: 475.1187.

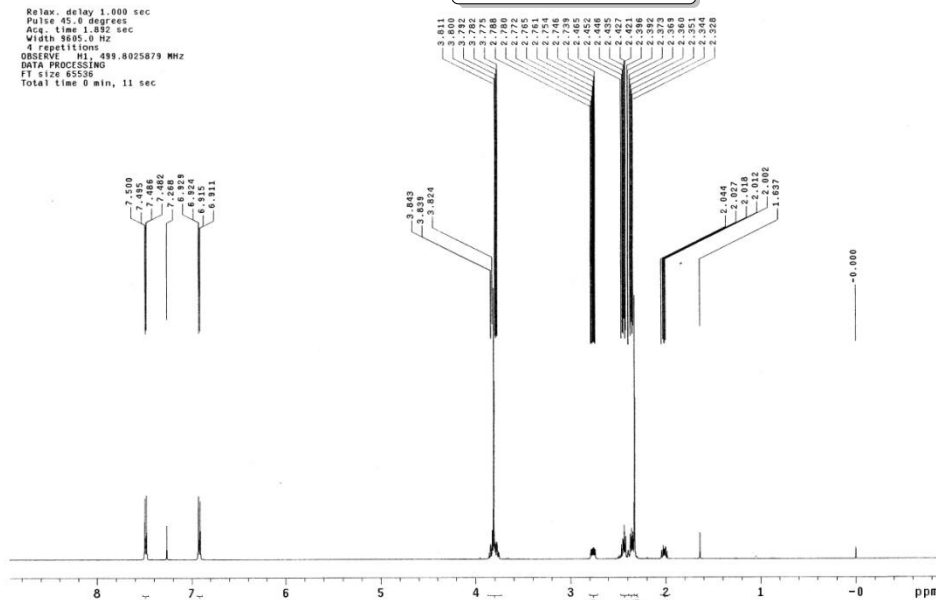
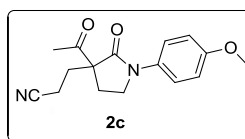
IV. ^1H and ^{13}C NMR spectra of compounds 2-7.





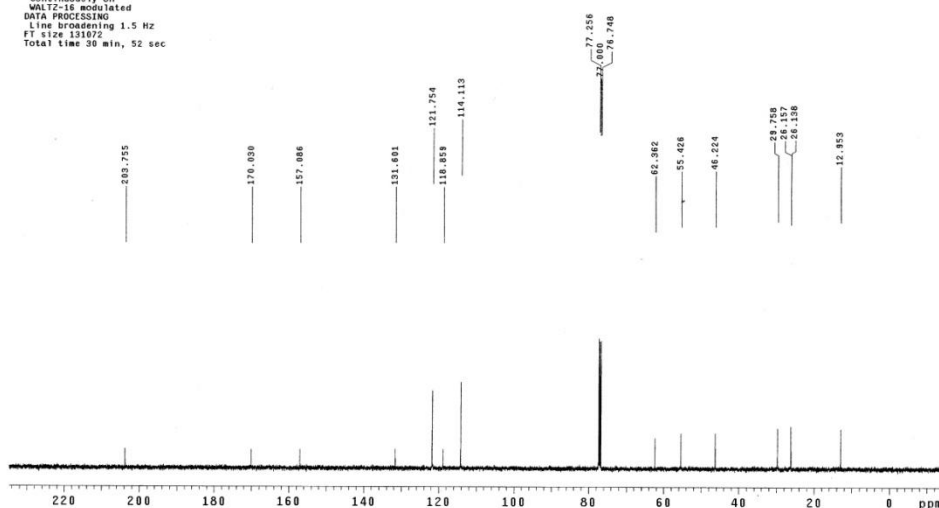
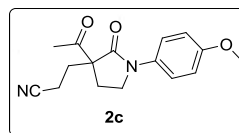
STANDARD PROTON PARAMETERS

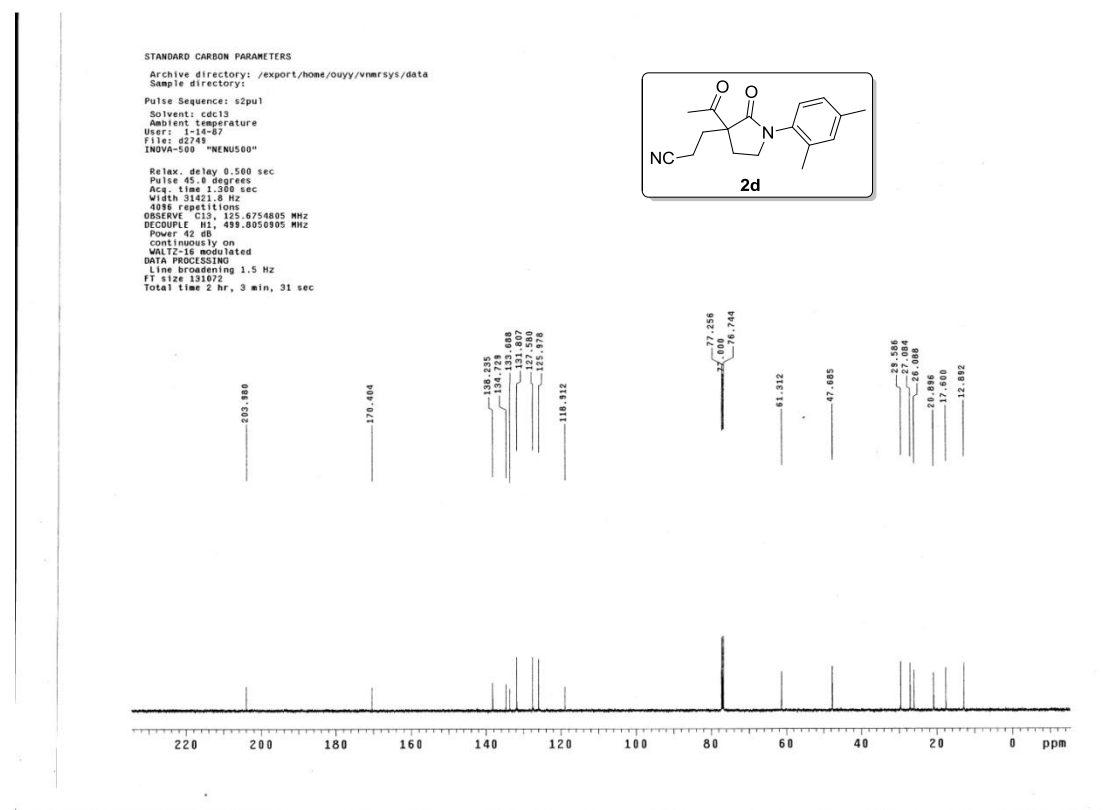
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
File: d2514
INOVA-500 "MNU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8605.0 Hz
4 repetitions
OBSERVE H1 499.8025879 MHz
DATA PROCESSING
F1 size 85538
Total time 0 min, 11 sec

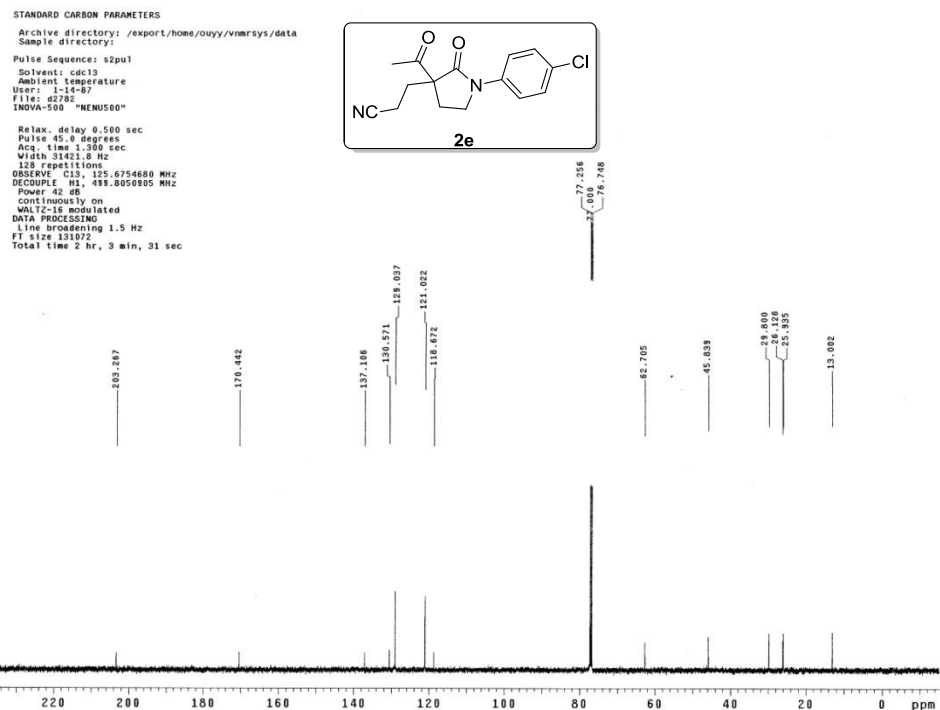
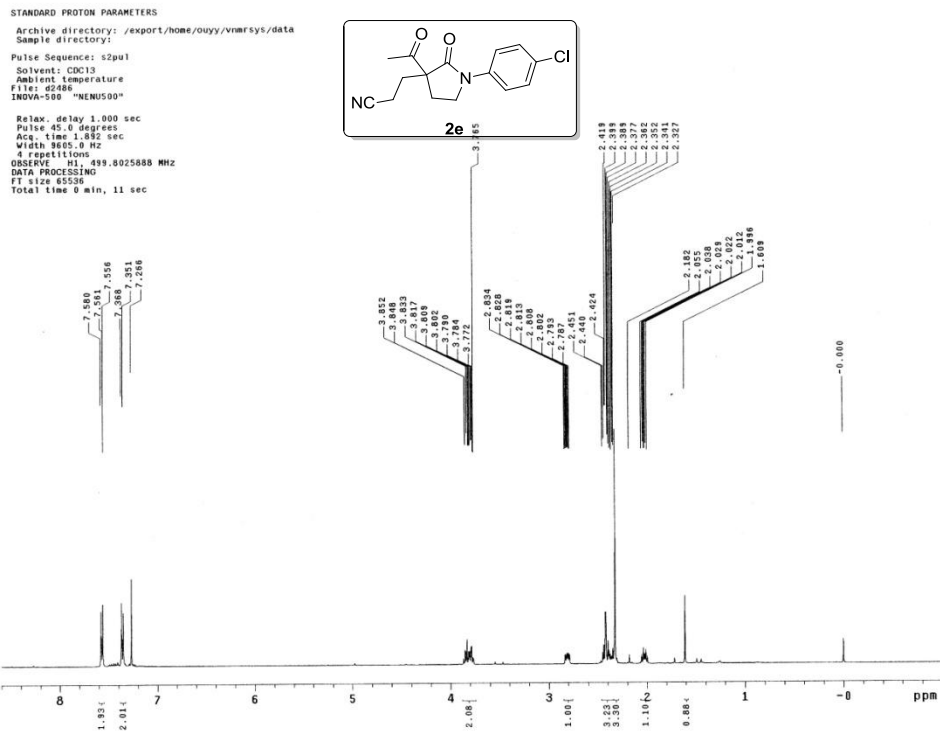


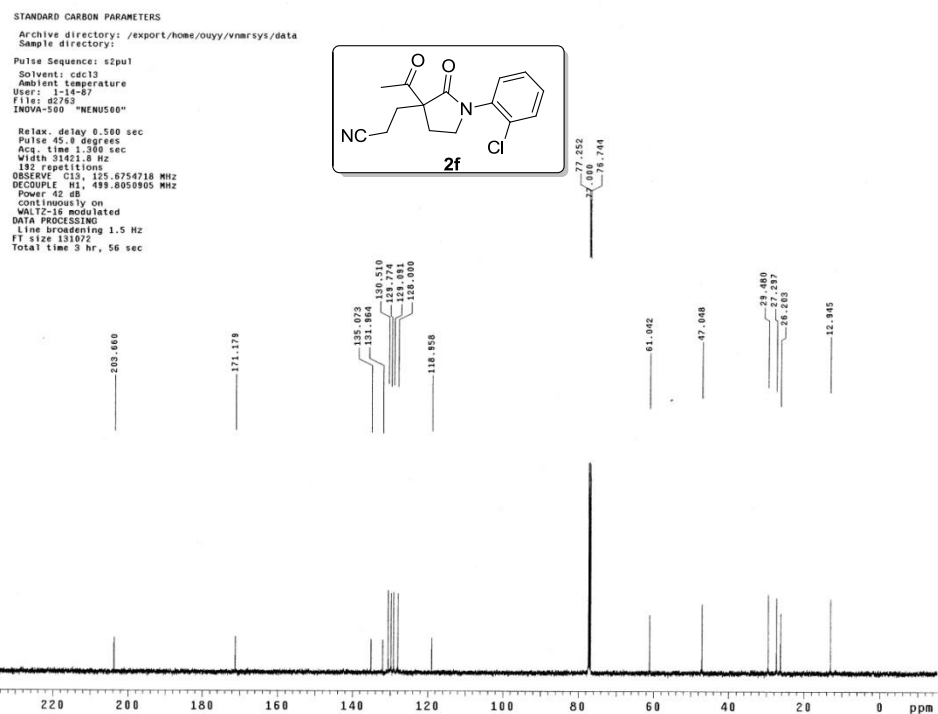
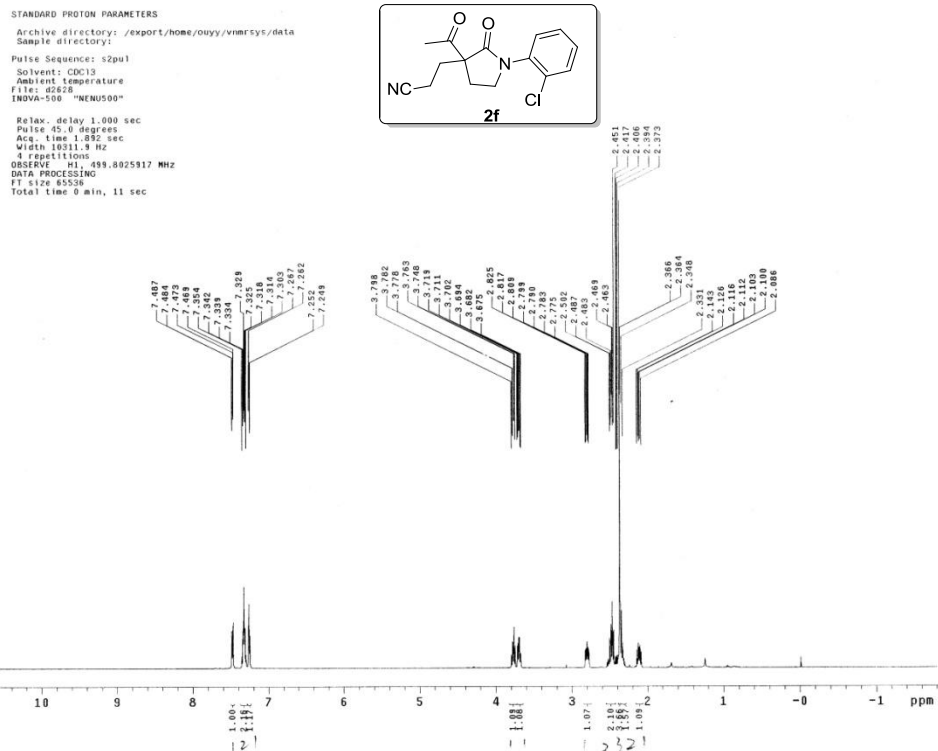
STANDARD CARBON PARAMETERS

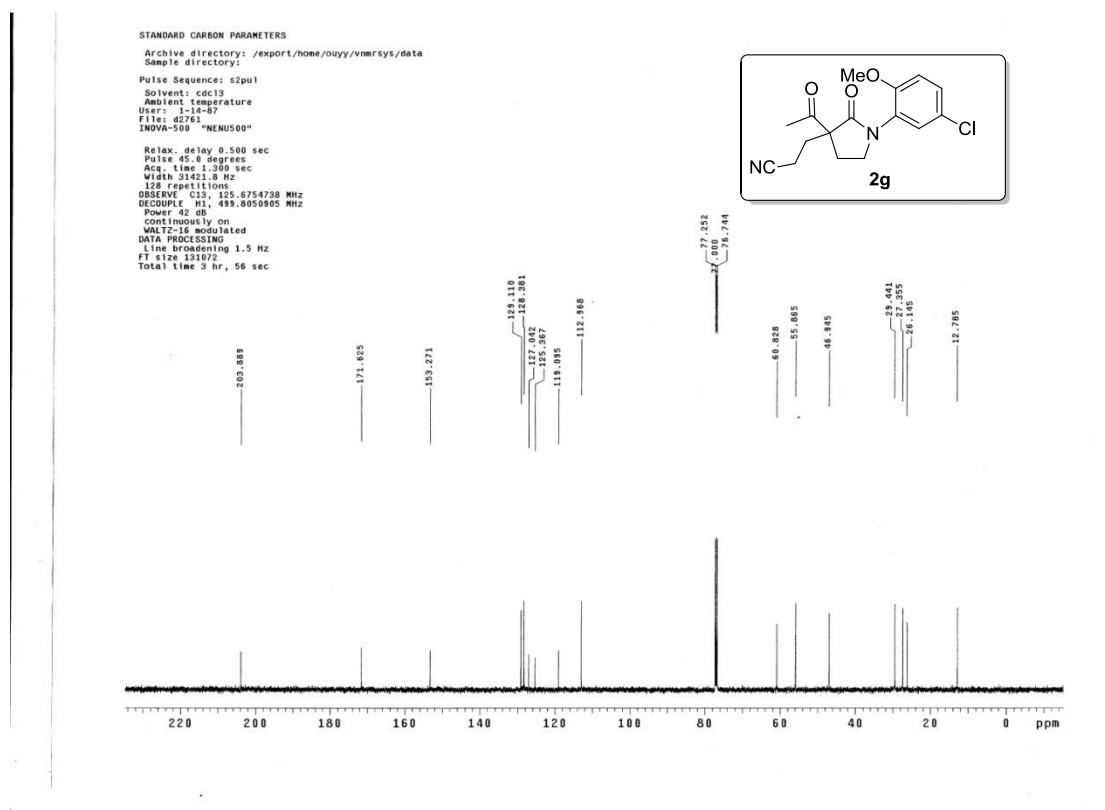
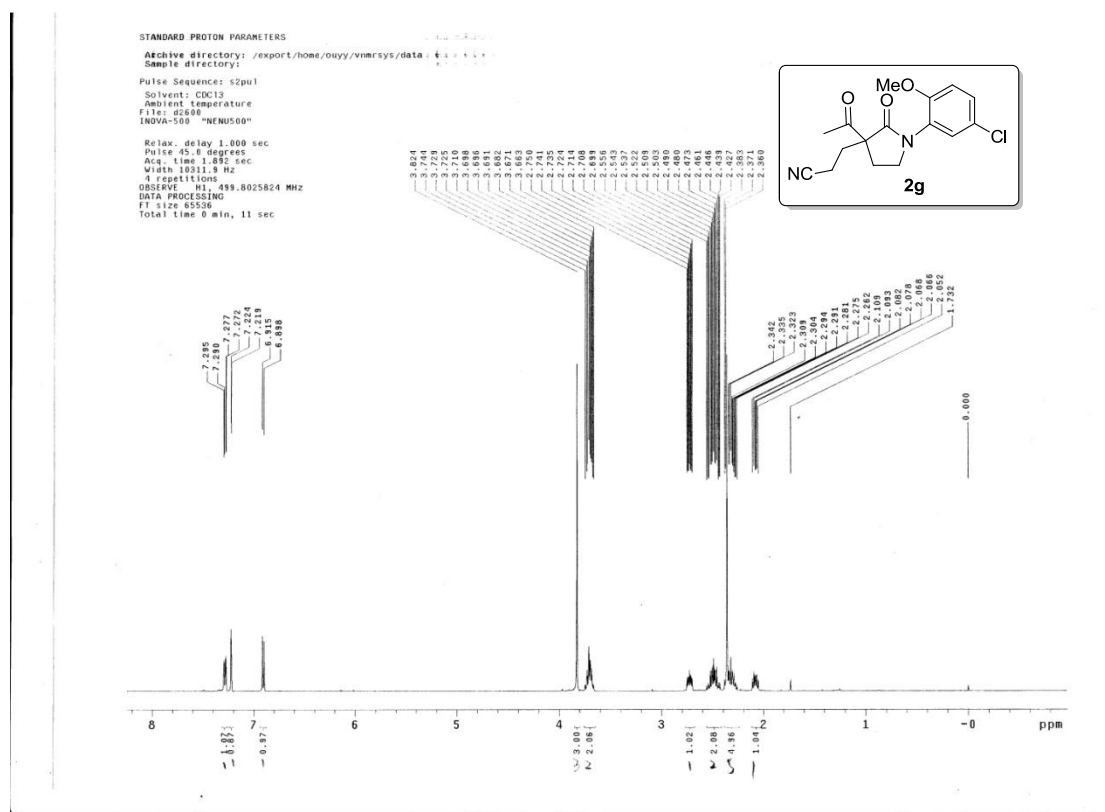
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pu1
Solvent: cdcl3
Ambient temperature
User: i-14-07
File: d2514
INOVA-500 "MNU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.388 sec
Width 21621.0 Hz
64 repetitions
OBSERVE C13 125.6754718 MHz
DECOUPLE H1 499.8058905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
F1 size 151072
Total time 30 min, 52 sec

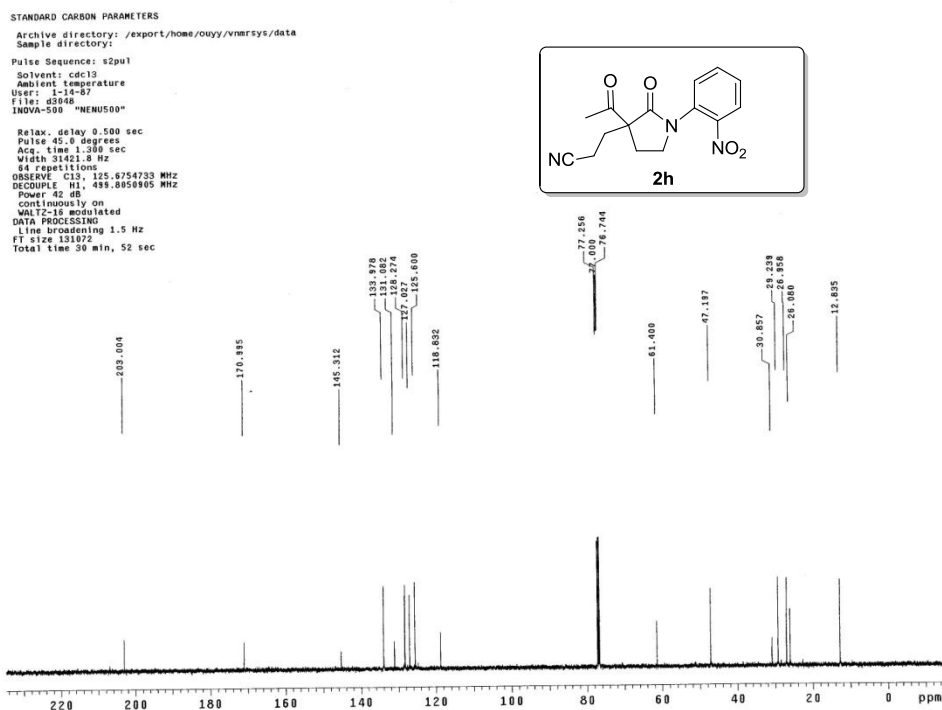
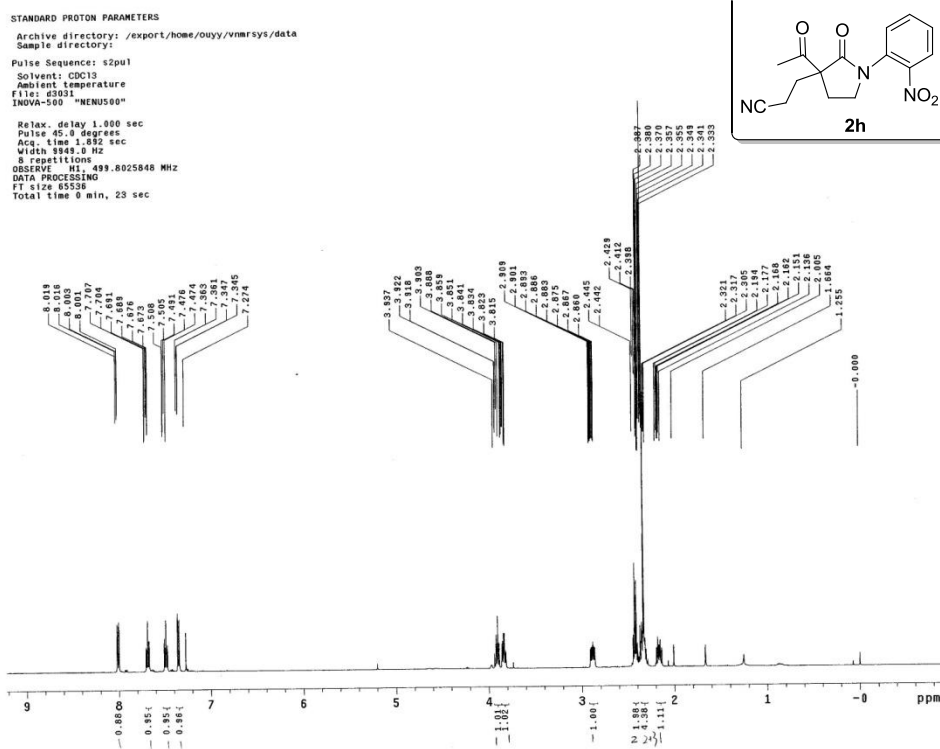


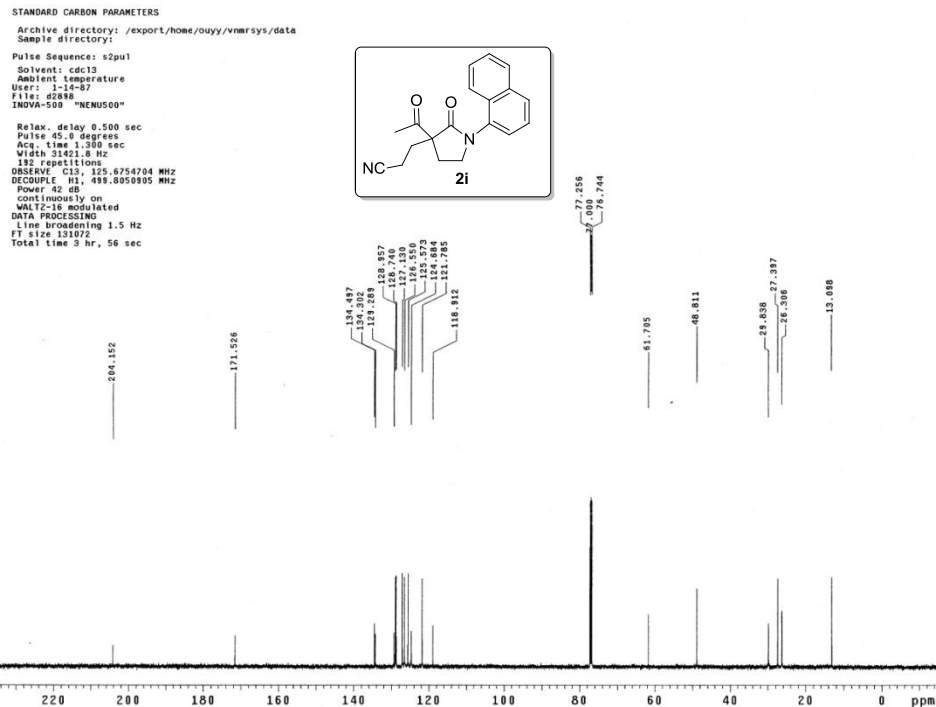
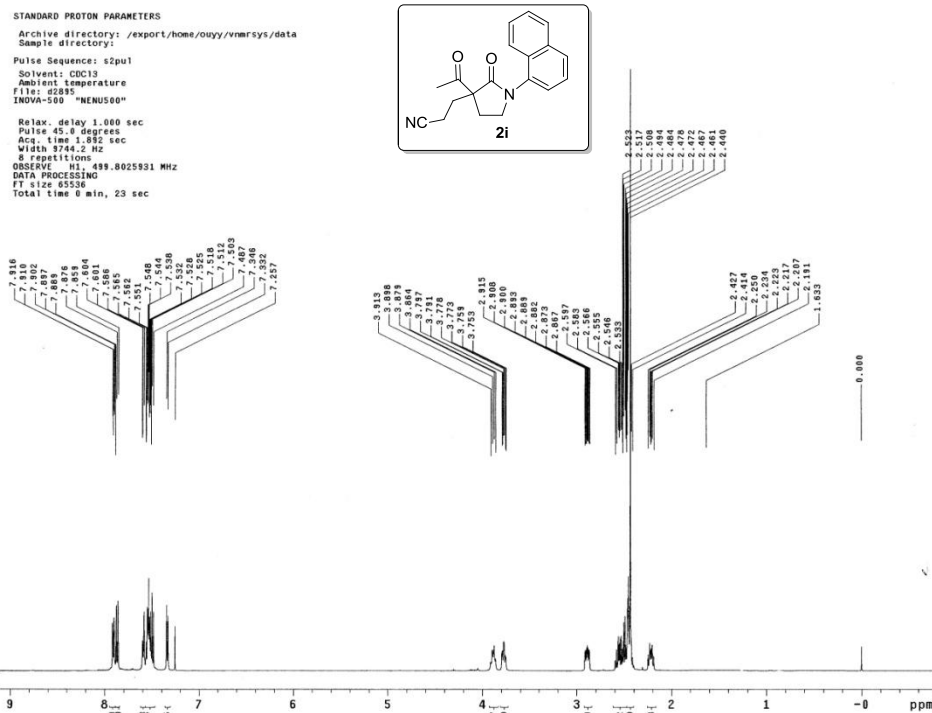












STANDARD PROTON PARAMETERS

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

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

File: d3184

INDVA-500 "MENU500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 8848.0 Hz

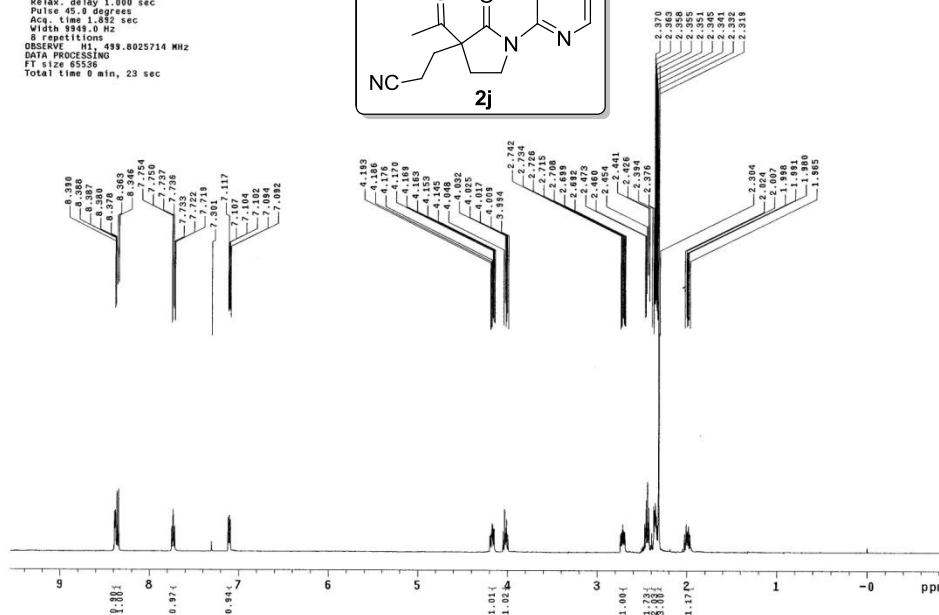
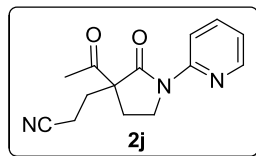
8 repetitions

OBSERVE H1 499.8025714 MHz

DATA PROCESSING

FT size 65536

Total time 8 min, 23 sec



STANDARD CARBON PARAMETERS

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

Sample directory:

Pulse Sequence: s2pu1

Solvent: cdc13

Ambient temperature

User: 1-14-07

File: d3184

INDVA-500 "MENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 52421.8 Hz

64 repetitions

OBSERVE C13 125.6754771 MHz

DECOUPLE H1 499.8050905 MHz

Power 42 dB

CONTINUOUSLY ON

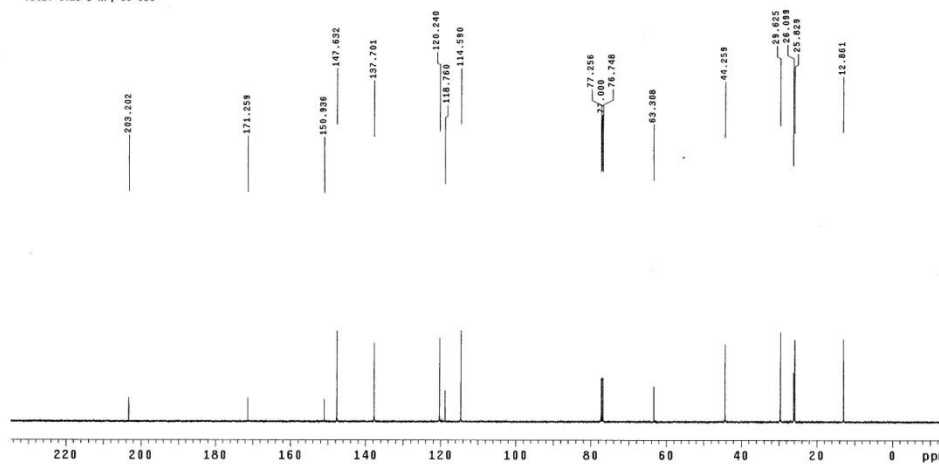
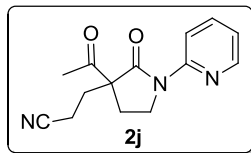
WALTZ-16 modulated

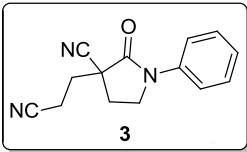
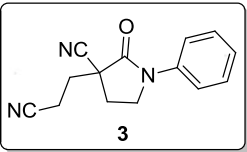
DATA PROCESSING

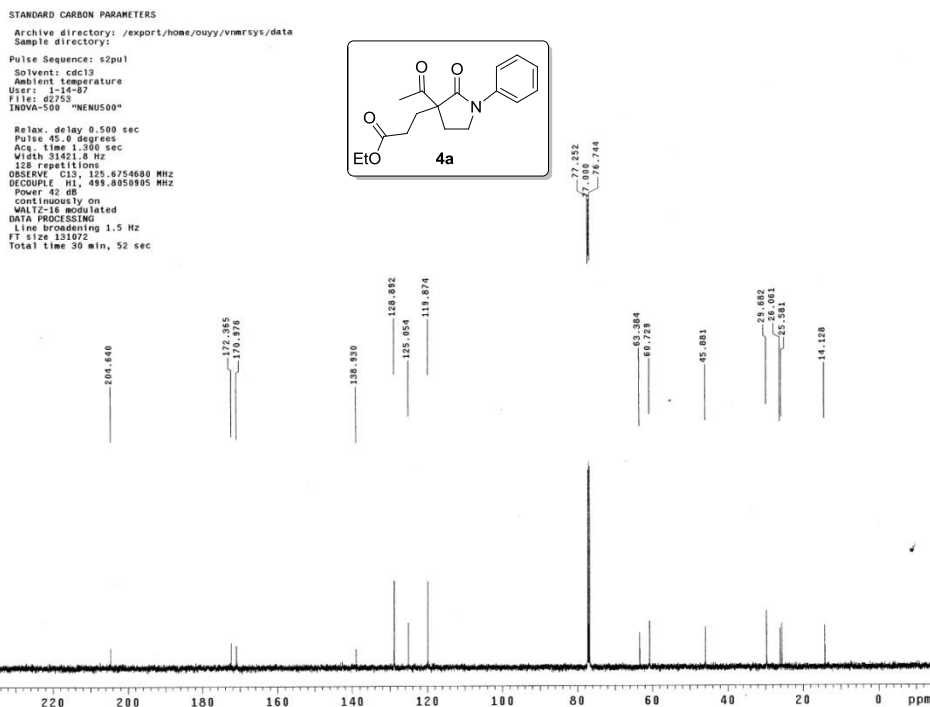
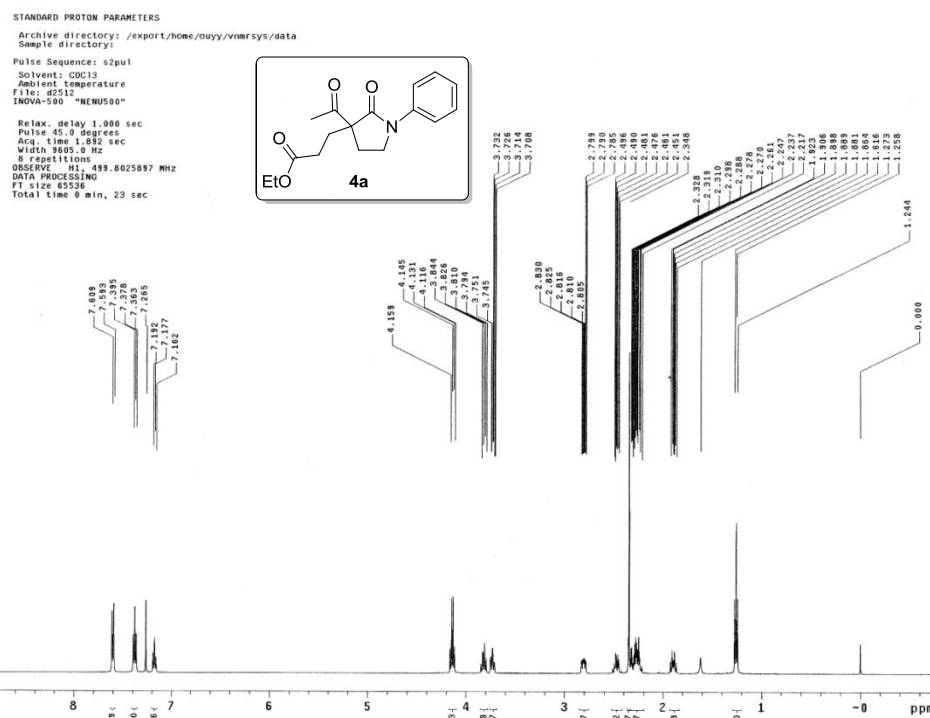
Line broadening 1.5 Hz

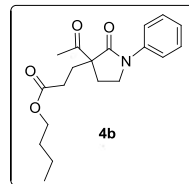
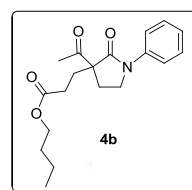
FT size 131072

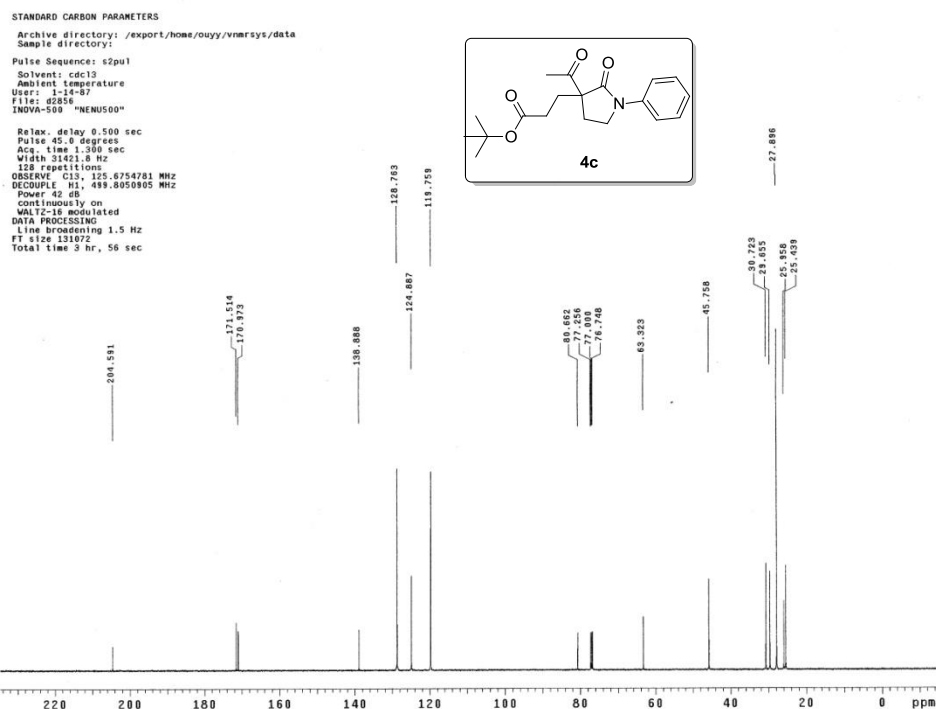
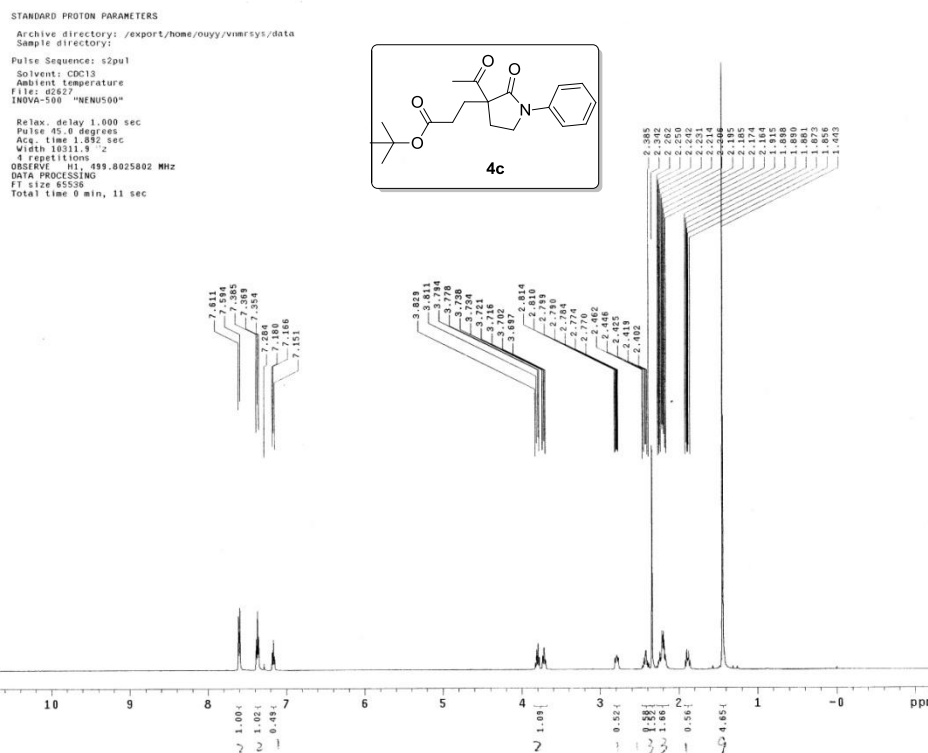
Total time 3 hr, 56 sec

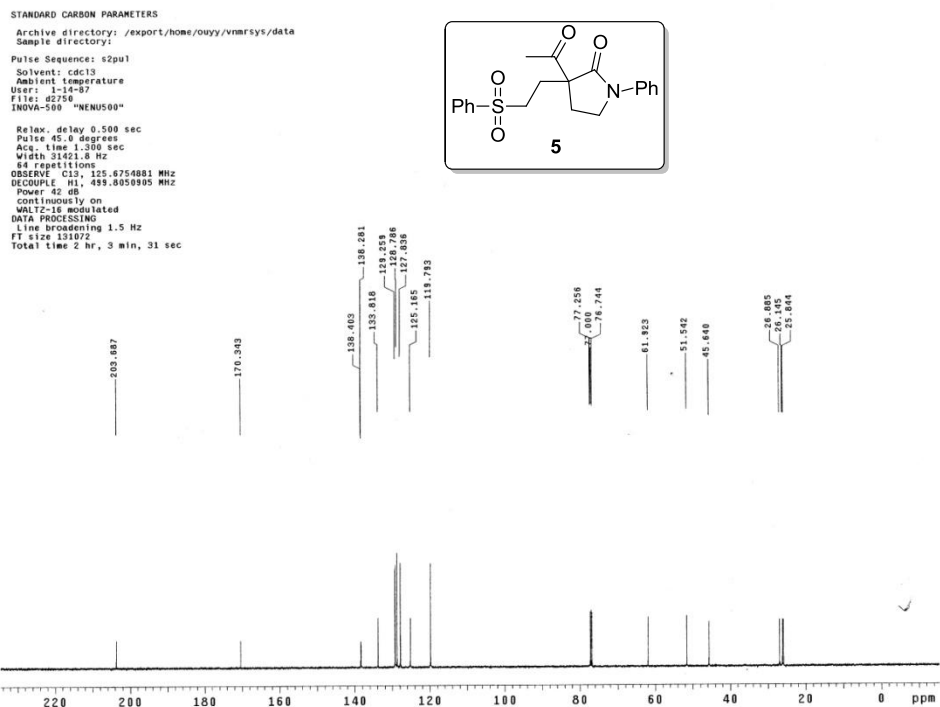
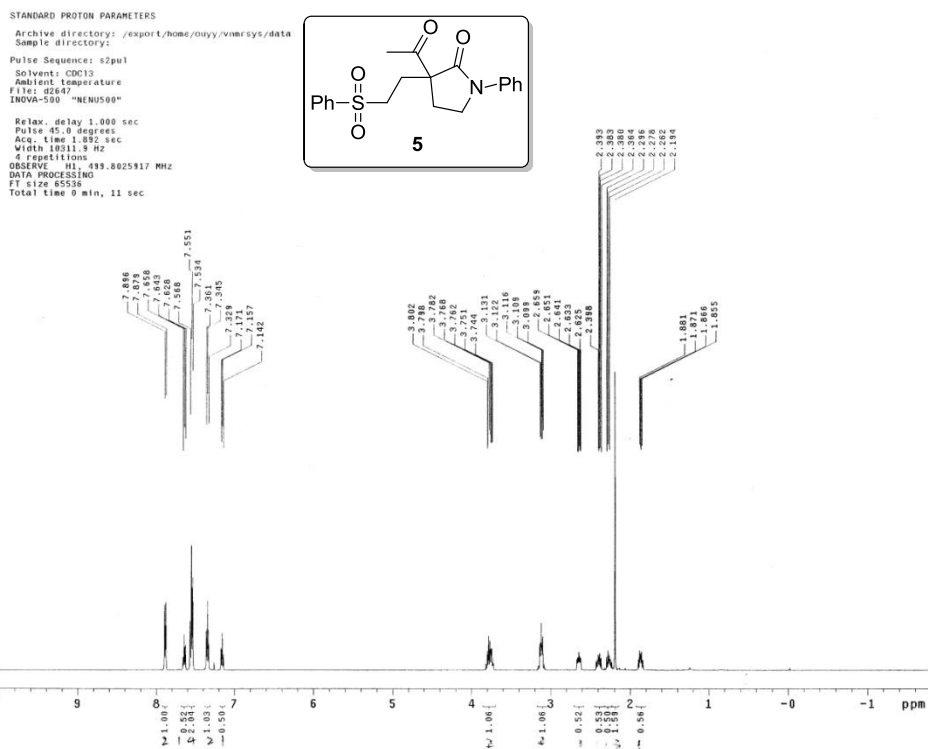


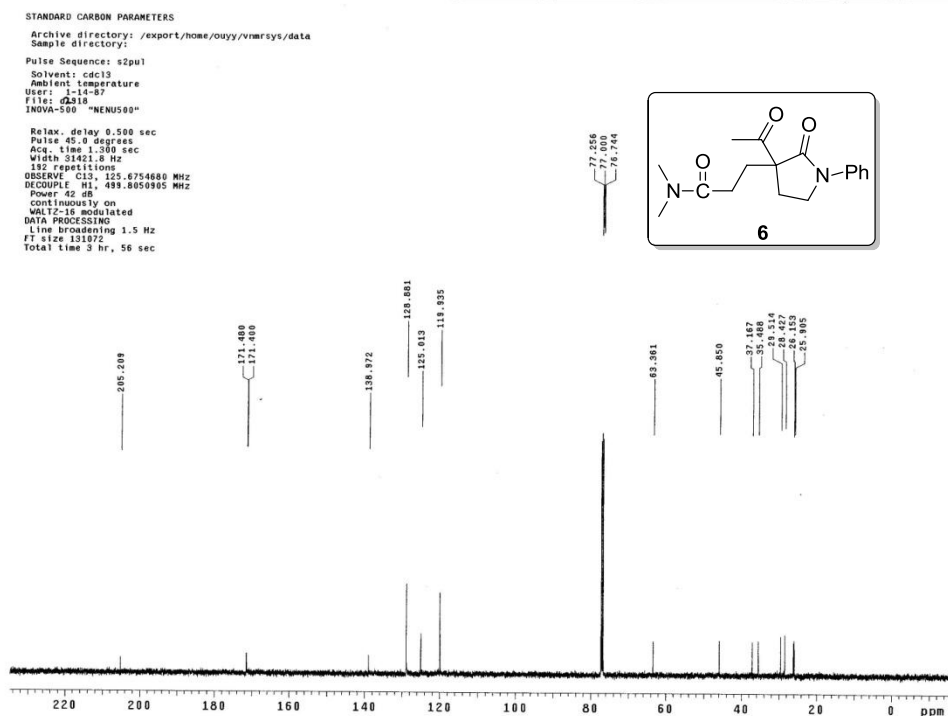
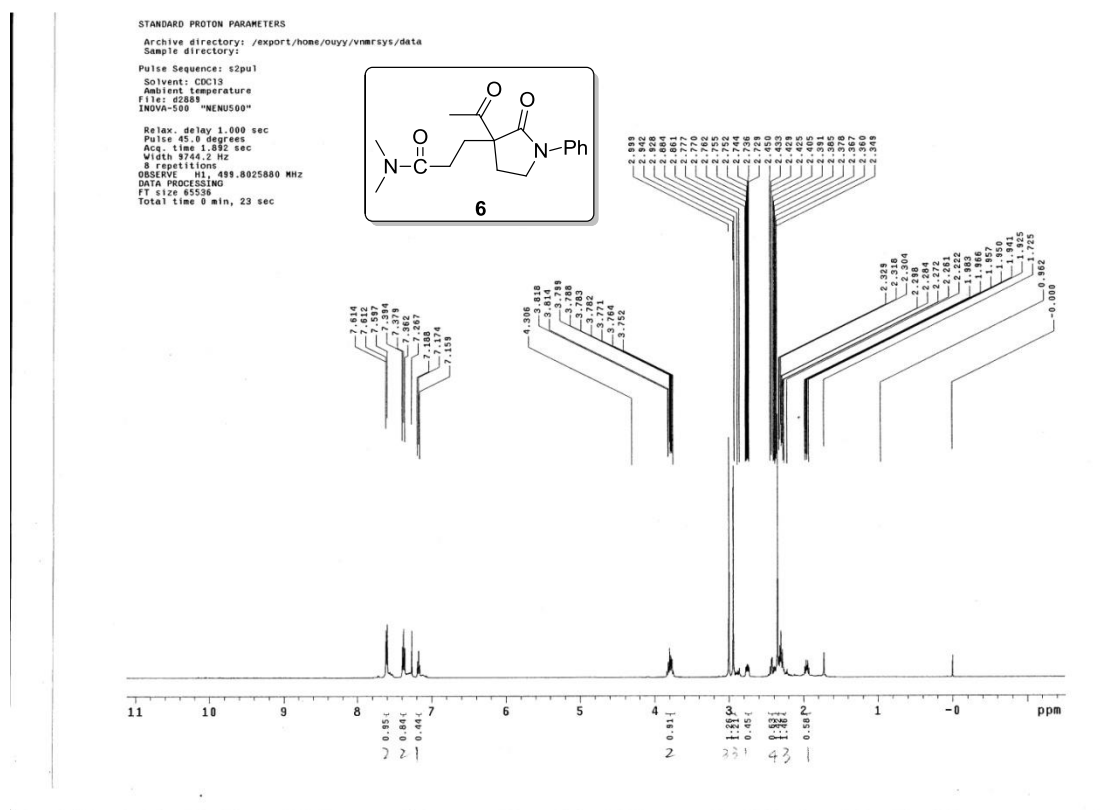


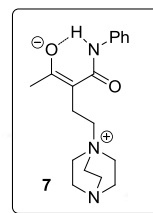












```
C13      16PPR 1402      2014.04.14
Archive directory: /export/home/lp/vmrsys/data
Sample directory:
Pulse sequence: szpul
Solvent: D2O
Ambient temperature:
User: 1-14-87
File: sz082
INDV=500 "MENU500"

Relax. delay 0.500 sec
Pulse 45.00 degrees
Acq. time 1.360 sec
Width 31601.0 Hz
250 repetitions
DESRULE C13, 125.675945 MHz
ACQUACQPL H1, 499.8063750 MHz
Power 42.00
Continuous lyz
MW 472.16 modulated
LINE PROCESSING
Line broadening 2.0 Hz
F1 size 131072
Total time 15 hr, 4 min, 41 sec
```

