

Supporting Information

Organocatalysis by *p*-sulfonic acid calix[4]arene: a convenient and efficient route to 2,3-dihydroquinazolin-4(1*H*)-ones in water

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EXPERIMENTAL

General: Melting points were determined on a glass disk with an electric hot plate and are uncorrected. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were run in CDCl_3 & $\text{DMSO}-d_6$ solutions (Bruker Avance 400). Chemical shift were recorded as δ values in parts per million (ppm), and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet) and coupling constants J were given in Hz. IR spectra were taken in a Perkin Elmer FTIR-Spectrum 400. Commercially available substrates were freshly distilled before the reaction. Solvents, reagents and chemicals were purchased from Sigma Aldrich and Merck.

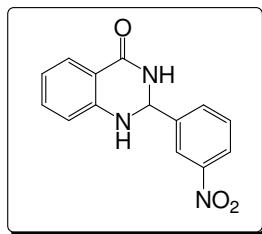
General procedure 2,3-dihydroquinazolin-4(1H)-one:

p-Sulfonic acid calix[4]arene (1 mol%) was added to a solution of 2-aminobenzamide (1 mmol) and aldehyde/ketone (1 mmol) in water (1 mL) and the mixture was stirred at room temperature for a specified period of time. After completion of the reaction, cold distilled water (5 mL) was added to the reaction mixture. Then the product was filtered off and the *p*-sulfonic acid calix[4]arene was recovered by evaporating the water. The recovered *p*-sulfonic acid calix[4]arene was reused for a subsequent fresh batch of the reaction after reactivation. The crude product was recrystallized from hot ethanol to afford the pure product.

Single crystal XRD data of 2-(3-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (**3n**):

Single crystal suitable for X-ray diffraction of (**3n**) was grown from ethanol. The crystals were carefully chosen using a stereo zoom microscope supported by a rotatable polarizing stage. The data was collected at room temperature on Bruker- AXS SMART APEX II, CCD detector.

Crystal data of 3n:



$C_{14}H_{11}N_3O_3$, $M = 269.26$, colorless plate, $0.30 \times 0.25 \times 0.20 \text{ mm}^3$, monoclinic, space group $P21/n$ (No. 14), $a = 10.9782(11)$, $b = 9.8343(8)$, $c = 11.7533(11) \text{ \AA}$, $\alpha = 90$, $\beta = 109.846(10)$, $\gamma = 90^\circ$, $V = 1193.6(2) \text{ \AA}^3$, $Z = 4$, $D_c = 1.498 \text{ g/cm}^3$, $F_{000} = 560$, MoK α radiation, $\lambda = 0.71073 \text{ \AA}$, $T = 100(2) \text{ K}$, $2\theta_{\text{max}} = 60.2^\circ$, 7235 reflections collected, 3141 unique ($R_{\text{int}} = 0.0326$). Final $GooF = 1.002$, $RI = 0.0522$, $wR2 = 0.1342$, R indices based on 3141 reflections with $I > 2\sigma(I)$ (refinement on F^2), 181 parameters, 0 restraints. Lp and absorption corrections applied. Crystallographic data for **3n** have been deposited with the Cambridge Crystallographic Data Center as supplementary publication number CCDC 1026285.

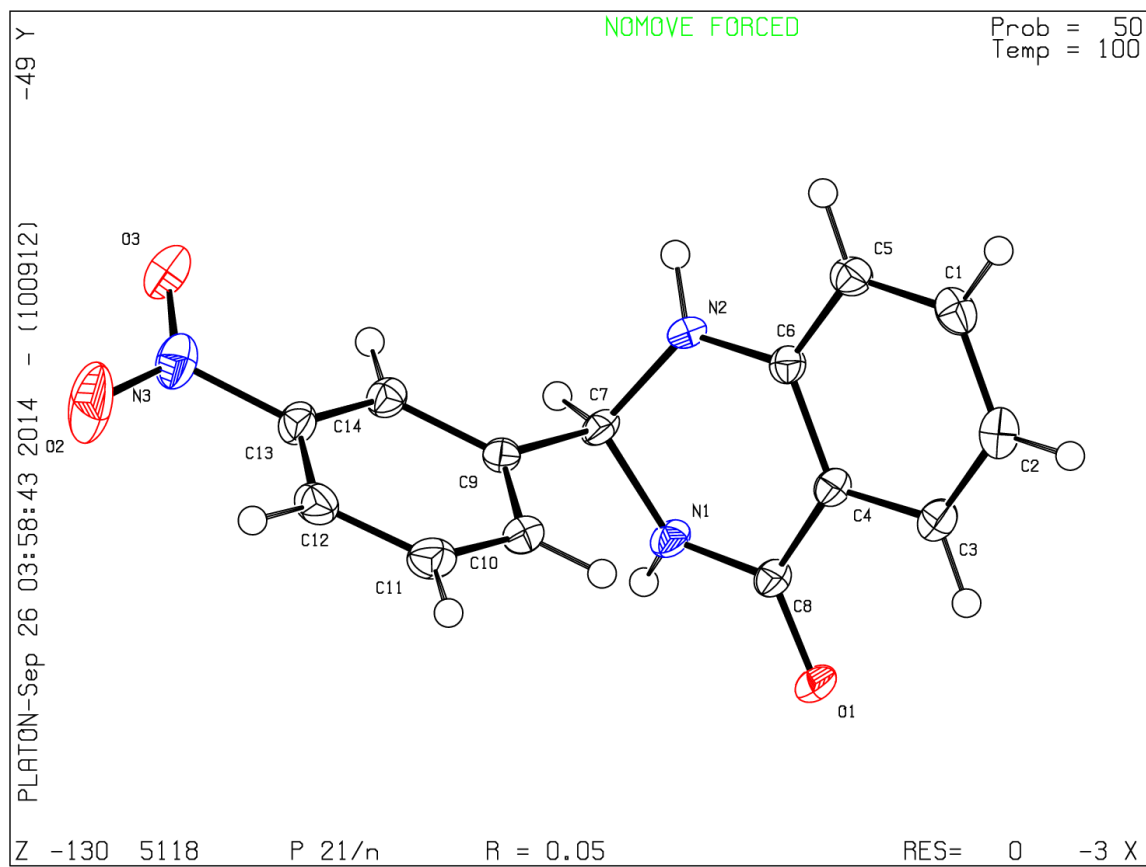


Figure 1: ORTEP view of the compound **3n**.

E-factor Calculations:¹

Table 1 Synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones.: E-factor value for this protocol.^a

Entry	Anthranilamide (mmol)	Aldehyde (mmol)	Product	Isolated yield (%) ^b	Time (min)	E factor (kg waste/kg product) ^c
1	1	4-Methyl benzaldehyde(1)	3a	92	20	0.17
2	1	Benzaldehyde(1)	3b	94	18	0.15

^a All reactions are performed with 1 mol% of *p*-SAC in 1 mL of water at room temperature.

^b Isolated yields.

^c Exclusion of water used for work up procedure, exclusion of the amount of the *p*-SAC used, and exclusion of ethanol used for recrystallization.

Note (Regarding Table 1, SI): When the Authors have not reported the amount of solvent used in the work-up procedure, we have not accounted for solvent and considered that solvent can be recovered. By considering the *p*-SAC catalyst is recyclable and hence, waste is essentially eliminated.

For Entry 1, Table1 (SI)

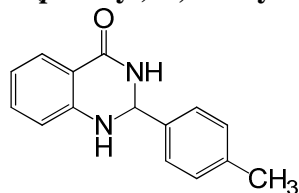
$$\begin{aligned} E &= [0.136 \text{ g (anthranilamide)} + 0.120 \text{ g (4-methyl benzaldehyde)} - 0.219 \text{ g (product} \times \\ &\text{yield)}] / 0.219 \text{ g} \\ &= 0.17 \end{aligned}$$

For Entry 2, Table1 (SI)

$$\begin{aligned} E &= [0.136 \text{ g (anthranilamide)} + 0.106 \text{ g (benzaldehyde)} - 0.210 \text{ g (product} \times \\ &\text{yield)}] / 0.210 \text{ g} \\ &= 0.15 \end{aligned}$$

Characterization data of compounds (3):

2-(*p*-Tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3a):



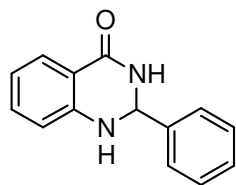
White Solid; Isolated yield: 92%; m.p. 224-225 °C;

IR: 3311, 1657, 1607, 1508, 1484, 1383 cm⁻¹;

¹H NMR (400 MHz, DMSO-*d*₆): δ 8.24 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 2H), 7.27-7.19 (m, 3H), 7.06 (s, 1H), 6.77-6.66 (m, 2H), 5.73 (s, 1H), 2.30 (s, 3H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 164.1, 148.4, 139.1, 138.2, 133.7, 129.3, 127.8, 127.3, 117.5, 115.5, 114.9, 66.9, 21.2.

2-Phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3b):



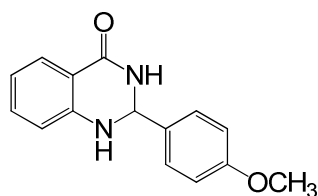
White Solid; Isolated yield: 94%; m.p. 218-220 °C;

IR: 3298, 1651, 1609, 1590, 1505, 1243 cm⁻¹;

¹H NMR (400 MHz, DMSO-*d*₆): δ 8.30 (s, 1H), 7.64 (dd, *J*₁ = 8.0 Hz, *J*₂ = 1.6 Hz, 1H), 7.53-7.50 (m, 2H), 7.42-7.35 (m, 3H), 7.28-7.24 (m, 1H), 7.12 (s, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.71-6.67 (m, 1H), 5.77 (s, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 164.1, 148.3, 142.1, 133.7, 128.9, 128.8 (2C), 127.8, 127.3 (2C), 117.6, 115.4, 114.9, 67.0.

2-(4-Methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3c) :



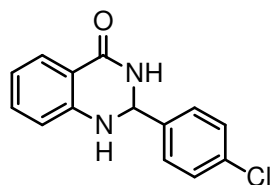
White Solid; Isolated yield: 90%; m.p. 183-184 °C;

IR: 3177, 1654, 1607, 1508, 1435, 1243, 755 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.18 (s, 1H), 7.63-7.60 (m, 1H), 7.44-7.40 (m, 2H), 7.27-7.22 (m, 1H), 7.00-6.93 (m, 3H), 6.75-6.66 (m, 2H), 5.71 (s, 1H), 3.75 (s, 3H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.2, 159.9, 148.5, 133.9, 133.7, 128.7 (2C), 127.8, 117.5, 115.5, 114.9, 114.1 (2C), 66.8, 55.6.

2-(4-Chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3d):



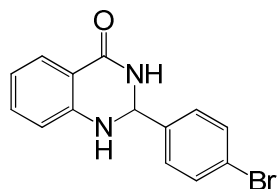
White Solid; Isolated yield: 87%; m.p. 206-208 °C;

IR: 3307, 1666, 1652, 1506, 1482 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.34 (s, 1H), 7.62 (d, $J=7.6$ Hz, 1H), 7.53-7.45 (m, 4H), 7.26 (t, $J=7.6$ Hz, 1H), 7.15 (s, 1H), 6.77-6.67 (m, 2H), 5.78 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.0, 148.1, 141.1, 133.9, 133.4, 129.2, 128.8, 127.8, 117.8, 115.4, 114.9, 66.2.

2-(4-Bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (3e):



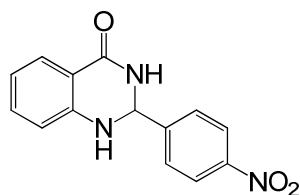
White Solid; Isolated yield: 86%; m.p. 196-198 °C;

IR: 3308, 1666, 1653, 1606, 1481 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.34 (s, 1H), 7.63-7.59 (m, 3H), 7.45 (d, $J = 8.0$ Hz, 2H), 7.28-7.24 (m, 1H), 7.15 (s, 1H), 6.77-6.67 (m, 2H), 5.77 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.0, 148.1, 141.6, 133.9, 131.7(2C), 129.6(2C), 127.8, 122.0, 117.8, 115.4, 114.9, 66.3.

2-(4-Nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (3f):



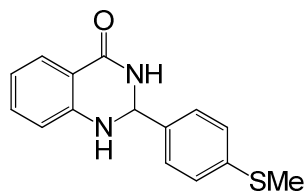
Yellow Solid; Isolated yield: 82%; m.p. 298-300 °C;

IR: 3281, 1644, 1607, 1517, 1387, 1347 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.52 (s, 1H), 8.26 (d, $J = 8.8$ Hz, 2H), 7.75 (d, $J = 8.8$ Hz, 2H), 7.63-7.60 (m, 1H), 7.33-7.25 (m, 2H), 6.79-6.68 (m, 2H), 5.92 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 163.7, 149.7, 147.9, 147.7, 134.0, 128.5(2C), 127.9, 124.0(2C), 117.9, 115.4, 115.0, 65.8.

2-(4-(Methylthio)phenyl)-2,3-dihydroquinazolin-4(1H)-one (3g):



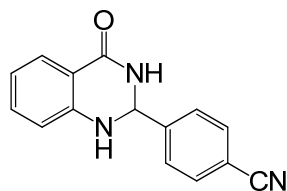
White Solid; Isolated yield: 88%; m.p. 179-180 °C;

IR: 3297, 1664, 1651, 1608, 1485, 1386, 749 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.28 (s, 1H), 7.63 (d, $J = 7.6$ Hz, 1H), 7.44 (d, $J = 8.0$ Hz, 2H), 7.30-7.23 (m, 3H), 7.09 (s, 1H), 6.76 (d, $J = 8.0$ Hz, 1H), 6.69 (t, $J = 7.2$ Hz, 1H), 5.74 (s, 1H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.1, 148.3, 138.9, 138.7, 133.8, 127.9(2C), 127.8, 126.2(2C), 117.6, 115.5, 114.9, 66.6, 15.2.

4-(4-Oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzonitrile (3h):



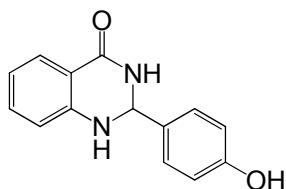
White Solid; Isolated yield: 86%; m.p. 250-251 °C;

IR: 3334, 2227, 1664, 1610, 1504, 1485, 1374, 771 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.48 (s, 1H), 7.88 (d, J = 8.4 Hz, 2H), 7.69 -7.61 (m, 3H), 7.29-7.25 (m, 2H), 6.78 (d, J = 8.0 Hz, 1H), 6.70 (t, J = 7.2 Hz, 1H), 5.87 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 163.8, 147.8(2C), 134.0, 132.9 (2C), 128.2 (2C), 127.9, 119.1, 117.9, 115.4, 115.0, 111.5, 66.0.

2-(4-Hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3i):



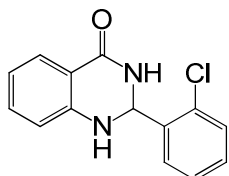
White Solid; Isolated yield: 82%; m.p. 278-280 °C;

IR: 3064, 1672, 1598, 1487, 1284, 764 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 9.54 (s, 1H), 8.15 (s, 1H), 7.65-7.63 (m, 1H), 7.33 (d, J = 8.8 Hz, 2H), 7.27 -7.23 (m, 1H), 6.95 (s, 1H), 6.80-6.75 (m, 3H), 6.71-6.67 (m, 1H), 5.68 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.3, 158.2, 148.6, 133.7, 132.1, 128.8(2C), 127.8, 117.5, 115.4(2C), 114.9, 67.1.

2-(2-Chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3j):



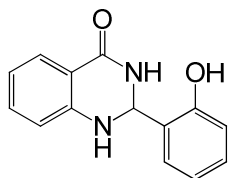
White Solid; Isolated yield: 90%; m.p. 204-205 °C;

IR: 3207, 1665, 1632, 1510, 1487 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.22 (s, 1H), 7.69-7.66 (m, 2H), 7.52-7.49 (m, 1H), 7.42-7.40 (m, 2H), 7.29-7.25 (m, 1H), 7.02 (s, 1H), 6.79-6.71 (m, 2H), 6.16 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.1, 148.1, 138.4, 133.9, 132.3, 130.8, 130.1, 129.2, 127.9 (2C), 118.0, 115.2, 115.0, 64.2.

2-(2-Hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3k):



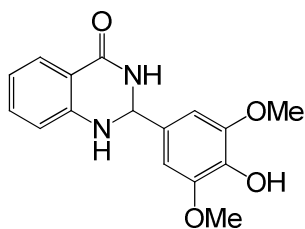
White Solid; Isolated yield: 88%; m.p. 223-224 °C;

IR: 3164, 1654, 1542, 1453, 1384, 762 cm⁻¹;

¹H NMR (400 MHz, DMSO-*d*₆): δ 9.87 (s, 1H), 7.95 (s, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.25 -7.14 (m, 2H), 6.88 (d, *J* = 8.4 Hz, 1H), 6.83-6.76 (m, 3H), 6.68 (t, *J* = 7.6 Hz, 1H), 6.03 (s, 1H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 164.5, 155.0, 148.6, 133.7, 129.7, 128.2, 127.8, 127.6, 119.3, 117.5, 115.8, 115.2, 115.0, 61.7.

2-(4-Hydroxy-3,5-dimethoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3l):



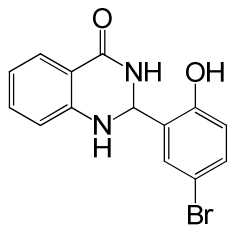
White Solid; Isolated yield: 84%; m.p. 223-224 °C;

IR: 3334, 1660, 1610, 1463, 1329, 762 cm⁻¹;

¹H NMR (400 MHz, DMSO-*d*₆): δ 8.45 (s, 1H), 8.10 (s, 1H), 7.64-7.61 (m, 1H), 7.28-7.24 (m, 1H), 6.96 (s, 1H), 6.80-6.67 (m, 4H), 5.67 (s, 1H), 3.76 (s, 6H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 164.3, 148.7, 148.2(2C), 136.4, 133.7, 131.3, 127.8, 117.6, 115.5, 114.9, 105.2 (2C), 67.6, 56.4 (2C).

2-(5-Bromo-2-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3m):



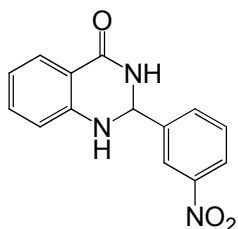
White Solid; Isolated yield: 85%; m.p. 262-264 °C;

IR: 3198, 1638, 1613, 1486, 1247, 751 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 10.25 (s, 1H), 8.03 (s, 1H), 7.64 (d, $J = 7.6$ Hz, 1H), 7.42 (d, $J = 2.4$ Hz, 1H), 7.35 -7.32 (m, 1H), 7.27-7.23 (m, 1H), 6.86-6.78 (m, 3H), 6.70 (t, $J = 7.6$ Hz, 1H), 5.98 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 164.3, 154.5, 148.3, 133.8, 132.3, 130.2(2C), 127.8, 118.1, 117.7, 115.1, 115.0, 110.3, 61.4.

2-(3-Nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (3n):



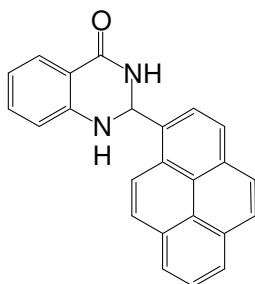
Yellow Solid; Isolated yield: 88%; m.p. 196-198 $^{\circ}\text{C}$;

IR: 3288, 1652, 1612, 1487, 1342 cm^{-1} ;

^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.54 (s, 1H), 8.38 (s, 1H), 8.22-8.20 (m, 1H), 7.96 (d, $J = 7.6$ Hz, 1H), 7.70 (t, $J = 8.0$ Hz, 1H), 7.63(d, $J = 7.6$ Hz, 1H), 7.35 (s, 1H), 7.30-7.26 (m, 1H), 6.80 (d, $J = 8.0$ Hz, 1H) 6.71 (t, $J = 7.6$ Hz, 1H), 5.96 (s, 1H).

^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 163.8, 148.2, 147.8, 144.8, 134.1, 133.8, 130.5, 127.9, 123.7, 122.0, 118.0, 115.4, 115.1, 65.7.

2-(Pyren-1-yl)-2,3-dihydroquinazolin-4(1H)-one (3o):



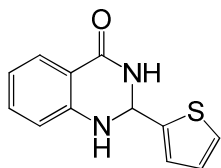
Yellow Solid; Isolated yield: 82%; m.p. 196-198 $^{\circ}\text{C}$;

IR: 3402, 1662, 1612, 1484, 1390, 833 cm^{-1} ;

^1H NMR (400 MHz, DMSO- d_6): δ 8.83 (d, J = 9.6 Hz, 1H), 8.44 (s, 1H), 8.36-8.34 (m, 4H), 8.29 (d, J = 9.2 Hz, 1H), 8.24 (d, J = 2.8 Hz, 2H), 8.12 (t, J = 7.6 Hz, 1H), 7.81-7.78 (m, 1H), 7.33-7.30 (m, 1H), 7.25 (s, 1H), 6.90 (s, 1H), 6.85-6.78 (m, 2H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 164.6, 149.1, 133.8, 133.5, 131.7, 131.2, 130.6, 128.9, 128.3, 128.1, 128.0, 127.8, 126.9, 126.6, 126.0, 125.9, 125.2, 124.7, 124.4, 124.1, 117.9, 115.7, 115.1, 66.0.

2-(Thiophen-2-yl)-2,3-dihydroquinazolin-4(1H)-one(3p):



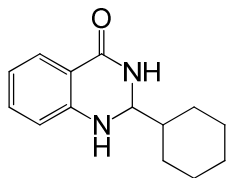
White Solid; Isolated yield: 86%; m.p. 223-224 °C;

IR: 3287, 1650, 1607, 1515, 1487, 763 cm^{-1} ;

^1H NMR (400 MHz, DMSO- d_6): δ 8.46 (s, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 4.8 Hz, 1H), 7.29-7.25 (m, 2H), 7.14 (d, J = 2.8 Hz, 1H), 6.99 (t, J = 3.6 Hz, 1H), 6.79 -6.70 (m, 2H), 6.03 (s, 1H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 163.6, 147.7, 146.9, 133.8, 127.8, 126.9, 126.4, 126.2, 118.0, 115.6, 115.2, 63.0.

2-Cyclohexyl-2,3-dihydroquinazolin-4(1H)-one(3q):



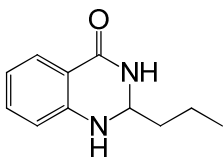
White Solid; Isolated yield: 82%; m.p. 223-224 °C;

IR: 3173, 2924, 1644, 1609, 1505, 1070, 751 cm^{-1} ;

^1H NMR (400 MHz, DMSO- d_6): δ 7.87 (s, 1H), 7.56 (d, J = 7.6 Hz, 1H), 7.20 (t, J = 8.0 Hz, 1H), 6.74 (d, J = 8.0 Hz, 1H), 6.63 -6.55 (m, 2H), 4.45 (s, 1H), 1.72-1.56 (m, 6H), 1.16-1.12 (m, 5H).

^{13}C NMR (100 MHz, DMSO- d_6): δ 164.2, 148.8, 133.5, 127.7, 126.9, 116.9, 115.2, 114.5, 69.0, 43.3, 27.5, 27.1, 26.4, 26.0.

2-Propyl-2,3-dihydroquinazolin-4(1H)-one(3r):



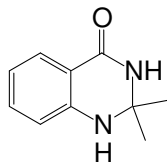
White Solid; Isolated yield: 68%; m.p. 149-150 °C;

IR: 2911, 1642, 1607, 1515, 1483, 748 cm⁻¹;

¹H NMR (400 MHz, CDCl₃): δ 7.91-7.9 (m, 1H), 7.34-7.29 (m, 1H), 6.87 (t, *J* = 7.2 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 2H), 4.91 (t, *J* = 5.6 Hz, 1H), 1.82 -1.77 (m, 2H), 1.55-1.48 (m, 2H), 1.02 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 165.6, 147.5, 133.8, 128.5, 119.3, 116.0, 114.7, 65.1, 37.6, 17.4, 13.8.

2,2-Dimethyl-2,3-dihydroquinazolin-4(1H)-one(3s):



White Solid; Isolated yield: 64%; m.p. 185-186 °C;

IR: 3211, 1645, 1598, 1510, 1487 cm⁻¹;

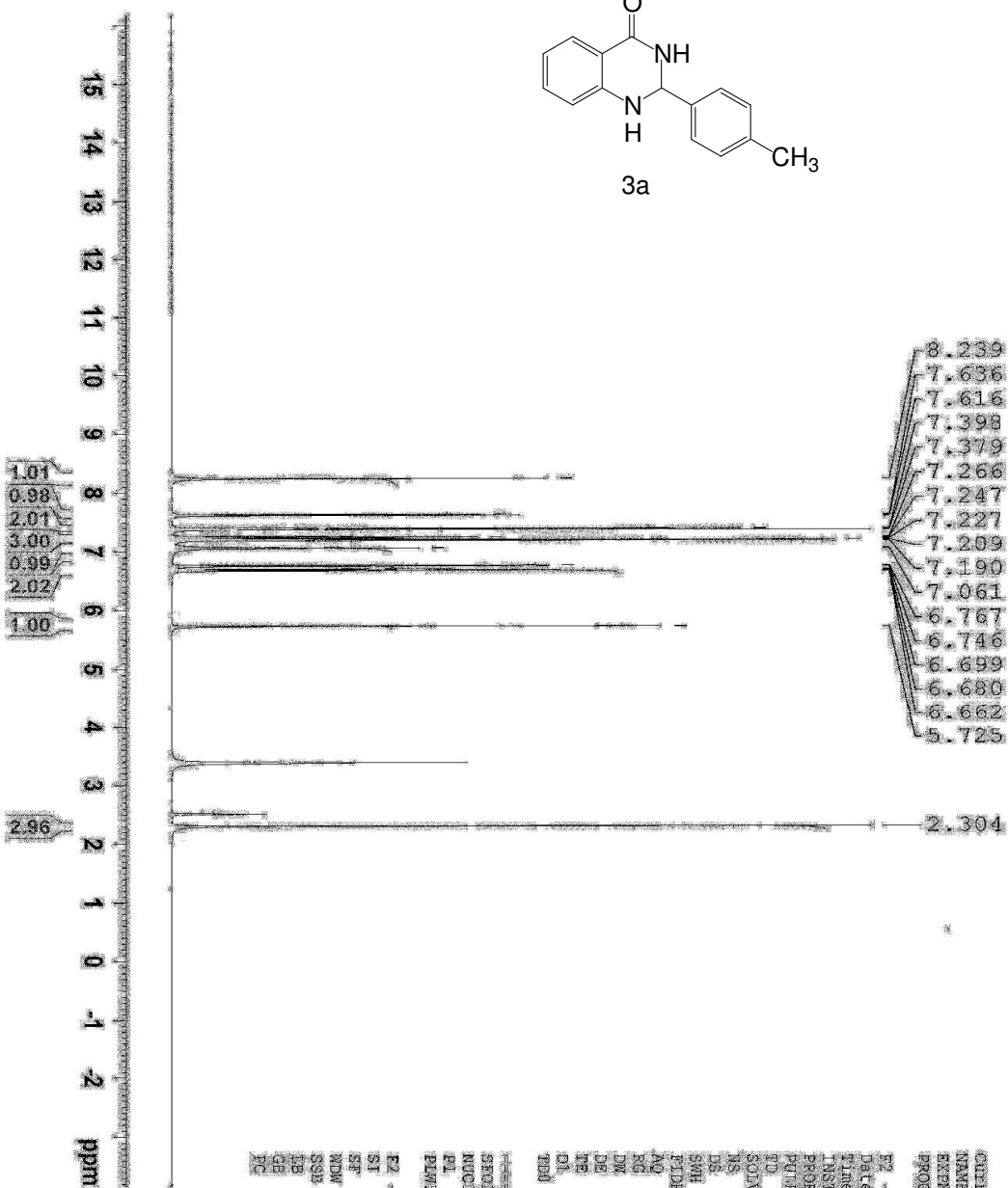
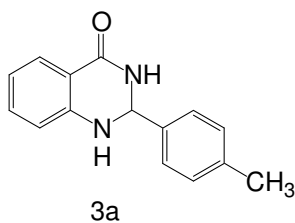
¹H NMR (400 MHz, DMSO-*d*₆): δ 7.94 (s, 1H), 7.59(d, *J* = 7.6 Hz, 1H), 7.24 -7.20 (m, 1H), 6.64-6.63 (m, 3H), 1.39 (s, 6H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 163.5, 147.5, 133.7, 127.6, 116.9, 114.7, 114.3, 67.3, 29.5(2C).

Reference:

1. A. Kamal, V. Srinivasulu, B. N. Seshadri, N. Markandeya, A. Alarifi and N. Shankaraiah, *Green Chem.* 2012, **14**, 2513.

¹H NMR

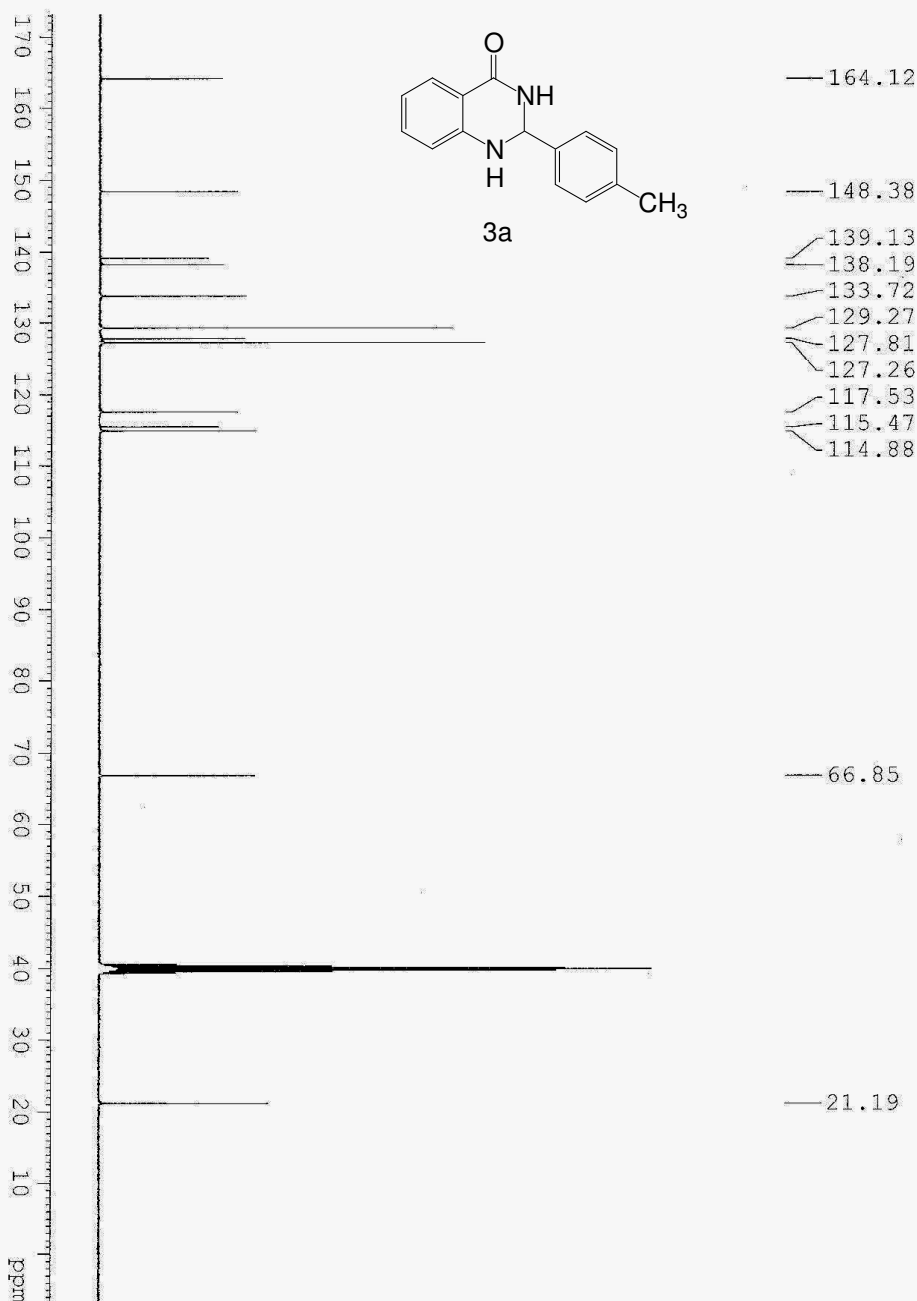
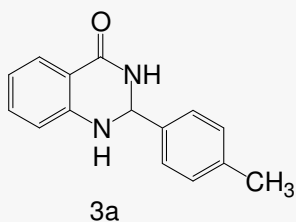


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NAME Sep03-2014 p-ns
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 801.820 Hz
FIDRES 0.132266 Hz
AQ 4.0894986 sec
RG 69.03
DE 62.400 usec
TE 298.2 K
D1 1.0000000 sec
TD1 1

===== CHANNEL f1 =====
NUC1 400.1324710 MHz
P1 15.50 usec
PL1 12.00000000 dB
===== CHANNEL f2 =====
SI 5536
SF 400.1300000 MHz
WDW EM
SSB 0
GB 0
PC 1.00

¹³C -p-me-cho



Current Data Parameters
 NAME Sep08-2014Matiur--p-Me
 EXPG 10
 PROCNO 1

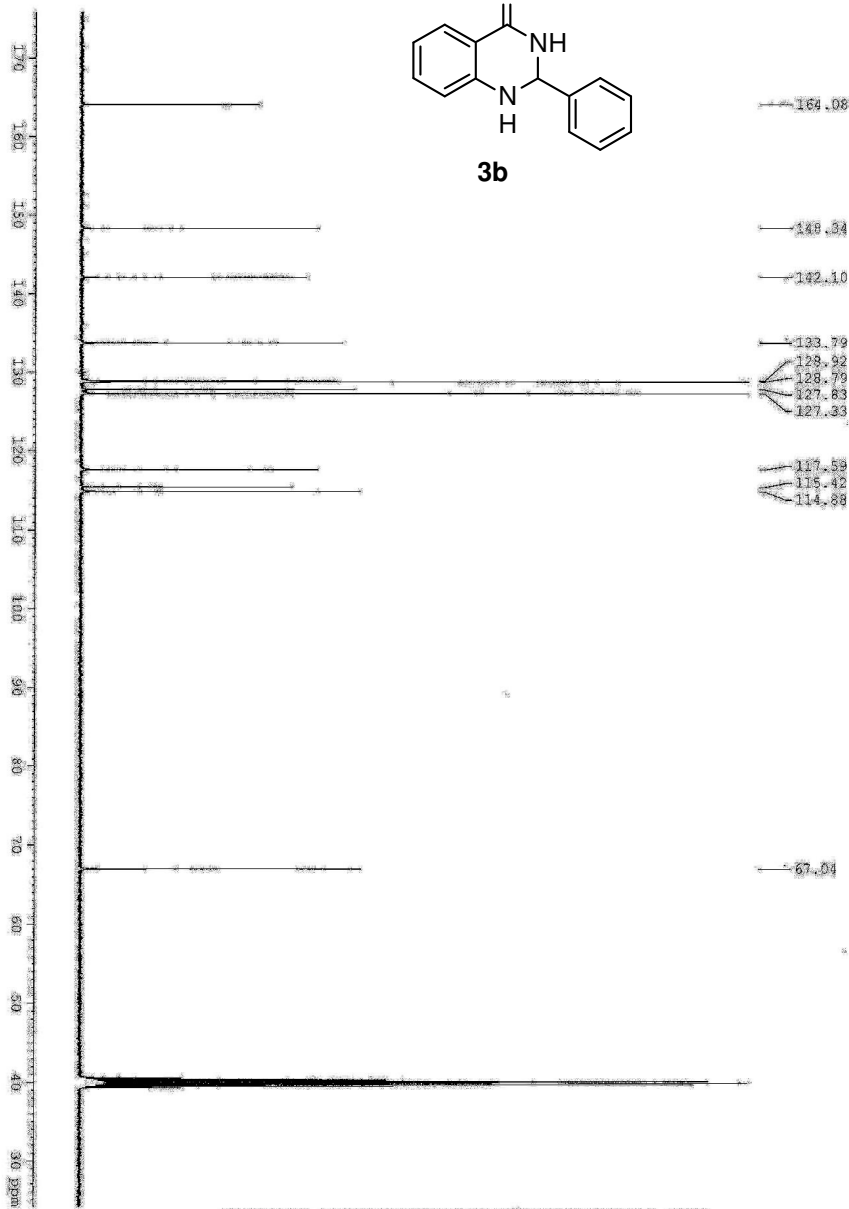
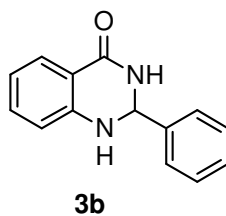
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 Time 13.15
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 PROBRD 5 mm EBBB0 SB/
 PULPROG zgpg30
 DO 65336
 SFO 400.133000
 SOLVENT 1024
 NS 4
 DS 4
 SMH 24038.461 Hz
 EIRMS 0.366798 Hz
 AQ 1.361988 sec
 RG 128
 SS 70.300 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999999 sec
 INPR 13
 NUC1 13C
 PL 10.00 usec
 PLW1 52.00000000 W
 SFO1 100.628293 MHz
 CPOPRG2 1H
 FID2 12.00000000 W
 PLW2 0.35563001 W
 PLW3 0.28830001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127650 MHz
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 EC 1.40


$$\text{1H-CHO}$$


NAME	DATE	TIME	LOCATION	REMARKS
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6. NAME	7. DATE	8. TIME	9. LOCATION	10. REMARKS
11. NAME	12. DATE	13. TIME	14. LOCATION	15. REMARKS
16. NAME	17. DATE	18. TIME	19. LOCATION	20. REMARKS
21. NAME	22. DATE	23. TIME	24. LOCATION	25. REMARKS
26. NAME	27. DATE	28. TIME	29. LOCATION	30. REMARKS
31. NAME	32. DATE	33. TIME	34. LOCATION	35. REMARKS
36. NAME	37. DATE	38. TIME	39. LOCATION	40. REMARKS
41. NAME	42. DATE	43. TIME	44. LOCATION	45. REMARKS
46. NAME	47. DATE	48. TIME	49. LOCATION	50. REMARKS
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56. NAME	57. DATE	58. TIME	59. LOCATION	60. REMARKS
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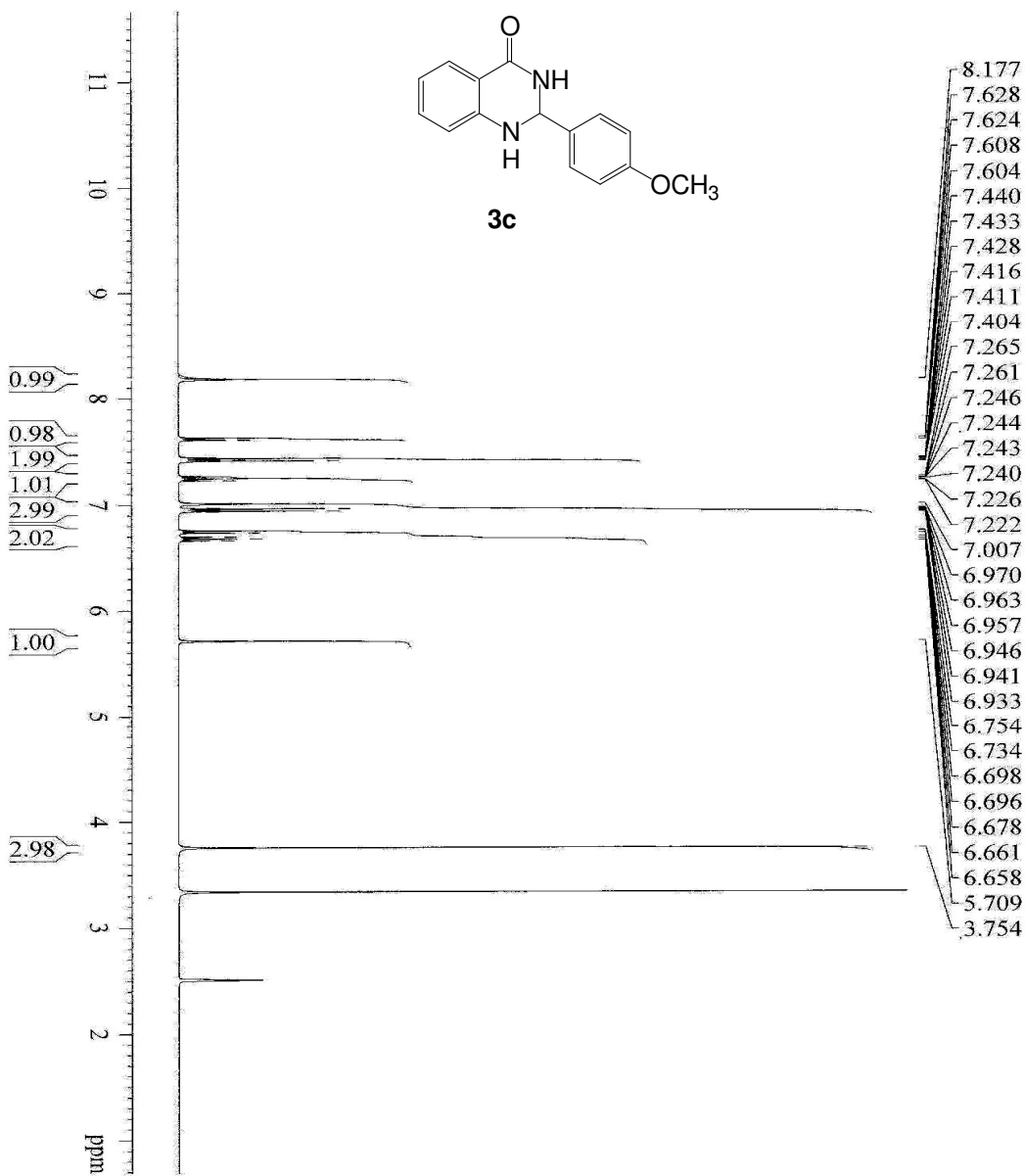
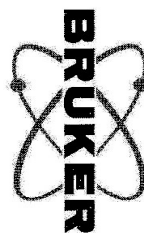
13C -CHO



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 P53: 1.00
 P54: 1.00
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 P80: 1.00
 P81: 1.00
 P82: 1.00
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 P84: 1.00
 P85: 1.00
 P86: 1.00
 P87: 1.00
 P88: 1.00
 P89: 1.00
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 P91: 1.00
 P92: 1.00
 P93: 1.00
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 P99: 1.00
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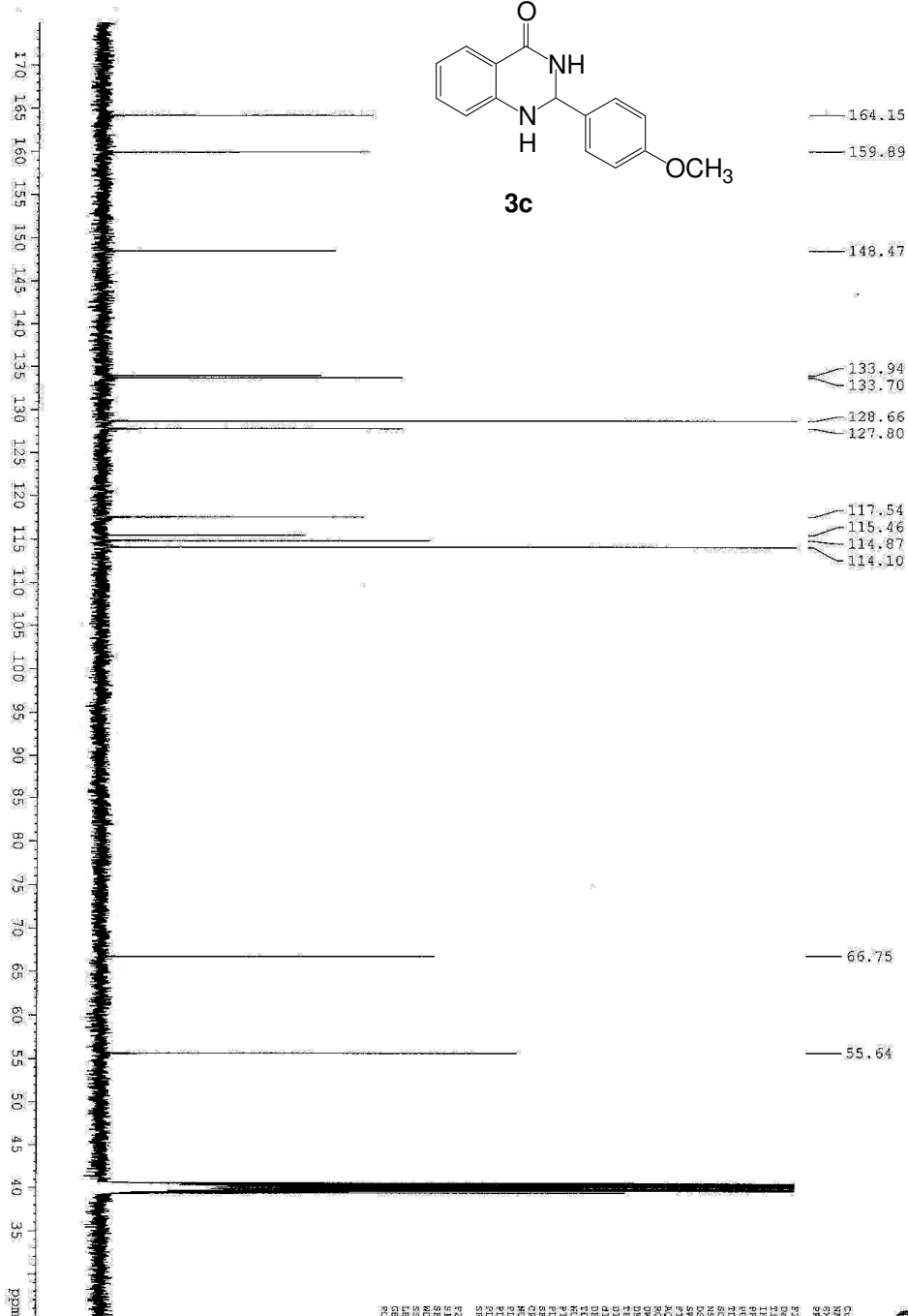
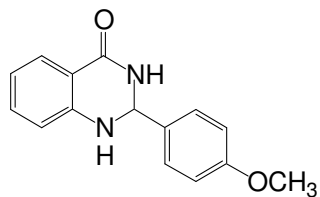


1H-p_OME



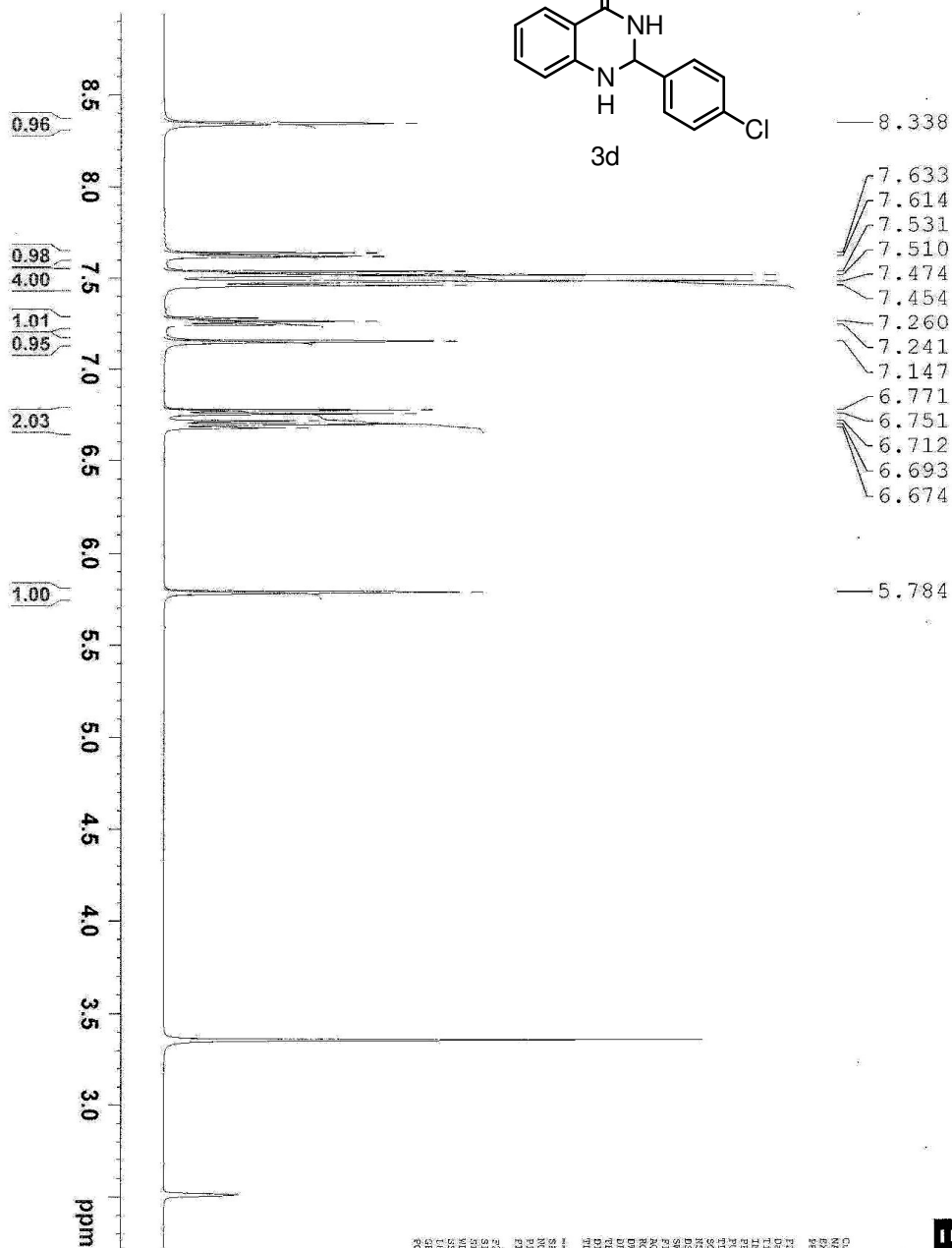
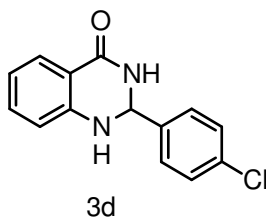
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NAME Sep01-2014, 101416-0008
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140909
Time 15.16
INSTRUM spect
PROBHD 5 mm BBO-400
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 12
DS 2
SWH 812.820 Hz
FIDRES 0.114260 Hz
AQ 0.09456 sec
RG 153.9
RW 62.400 usec
BS 5.50 usec
TZ 298.1 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
SFO1 400.134710 MHz
NUC1 1H
P1 15.50 usec
PL1 12.0000000 W
PL11
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C -p-OMe



Current Data Parameters
NAME Sep08-2014_Met14F-p-OMe
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 2011.11.19
Time 11:59
INSTRUM spect
PROBHD 5 mm BBO-1H-13C
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 800
DS 4
SWH 2403.464 Hz
FIDRES 0.3444 Hz
AQ 1.321088 sec
RG 128.31 usec
DE 13.951 Hz
TE 300.2 K
D1 5.00 sec
d11 0.041 sec
DELTA 1.8999999 sec
NUC1 13C
F1 101.60 usec
P1 12.00 usec
SFO 100.626183 MHz
CPOBPG2
NUC2 1H
P2 12.00 usec
F2 400.1460000 MHz
PL2 0.35562001 W
SFO2 400.1460000 MHz
F2 - Processing parameters
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SF 100.626183 MHz
SF2 400.1460000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.70

¹H-p-Cl-CHO

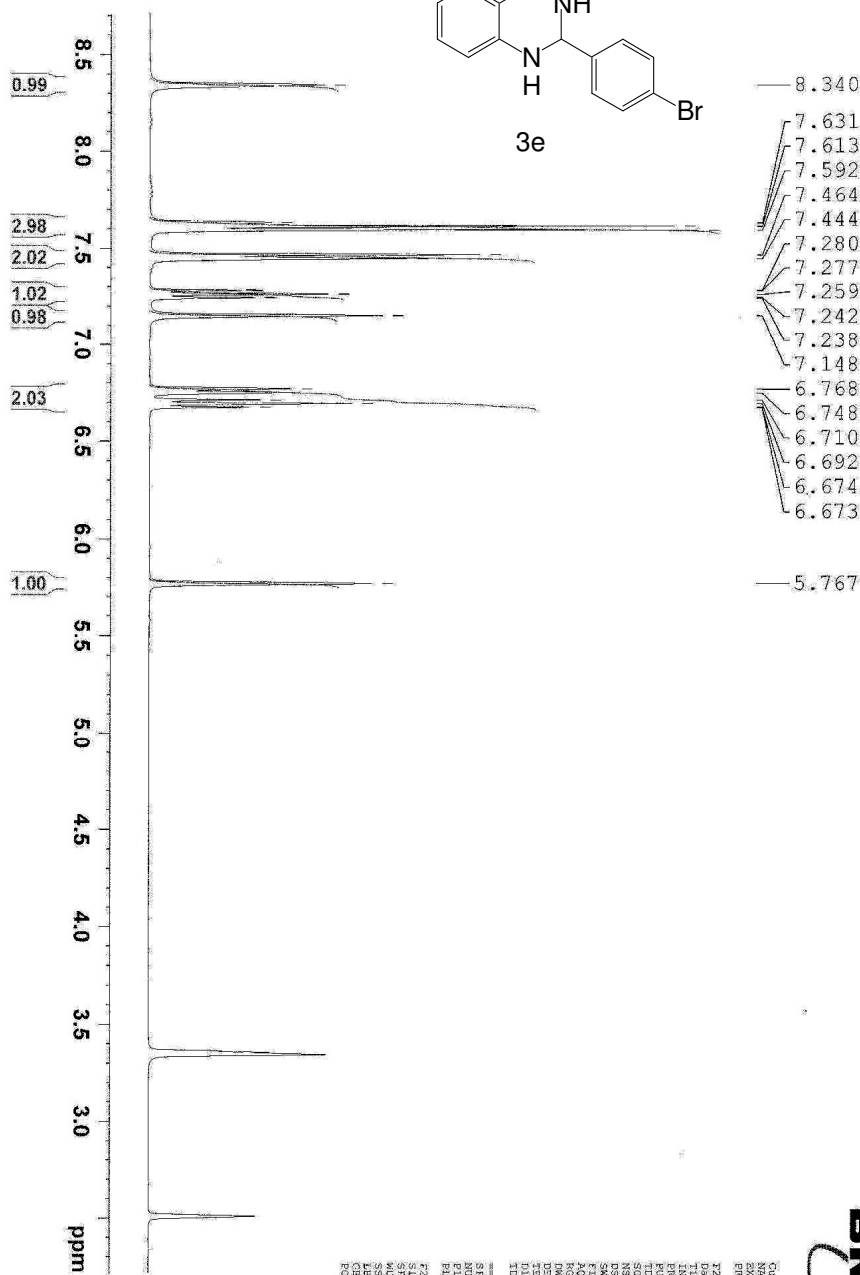
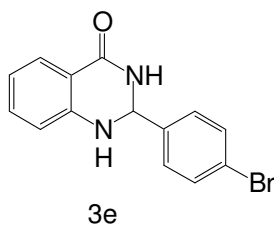


Current Data Parameters
 NAME Sep23-2013_Na1m-p-Cl-CHO
 EXNO 10
 PROCNO 1
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 Date_ 20130923
 Time_ 12:50:41
 INSTRUM spect
 PULPROG zgpg30
 FIDRES 5 mm BMRB B1/7
 TD 65536
 AQ 4.232
 SOLVENT DMSO
 NS 63
 DS 4
 SWH 8032.860 Hz
 F1RES 0.122266 Hz
 F2 400.146398 MHz
 ACQ 4.0000000 sec
 DE 2.0000000 sec
 TE 300.2 K
 D1 1.0000000 sec
 TDO 1
 ----- CHANNEL f1 -----
 SFO1 400.146398 MHz
 NUQ1 1H
 P1 12.0000000 sec
 PL1 0 dB
 FWH 12.00000000 Hz
 SFO2 Processing parameters
 SI 32768
 SF 400.146060 MHz
 EQ 1
 VM 0
 UG 0.30 Hz
 GB 0
 PC 1.00



21

1H-4-Br-CHO



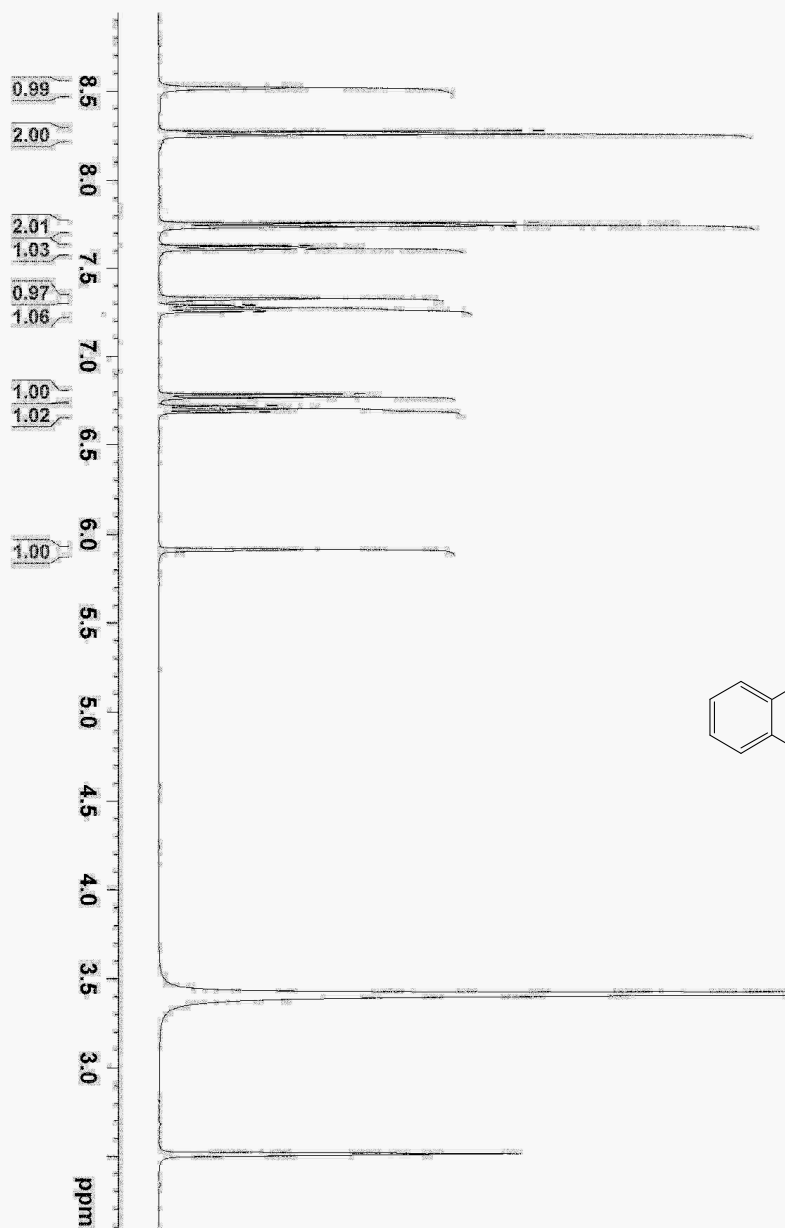
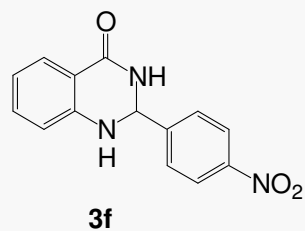
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NAME: 3e
EXPNO: 1
PROCNO: 1
Date_ Acquired: 20100414
Time: 13:20
INSTRUM: spect
PROBHD: 5 mm PABBO
PULPROG: zgpg30
TD: 65536
SOLVENT: DMS
NS: 128
DS: 2
SWH: 8012.800 Hz
AQ: 4.0122664 sec
RG: 123.93 umsec
DE: 6.50 umsec
TE: 298.1 K
TDO: 1.000000 sec
TDC: 1

===== CHANNEL f1 =====
NUC1: 13C
P1: 15.50 umsec
PL1: 0.00000000 K
B1: 400.1500000 MHz
SFO: 400.1500000 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.00

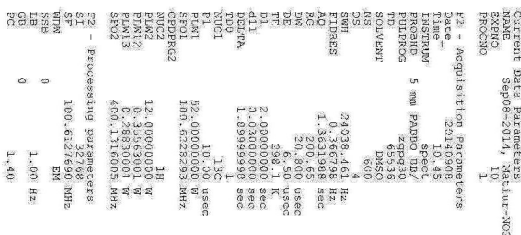
PC
L. 46

1H-4-NO2

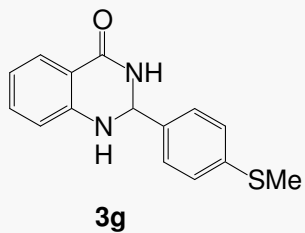
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6.761
6.717
6.698
6.680
5.912



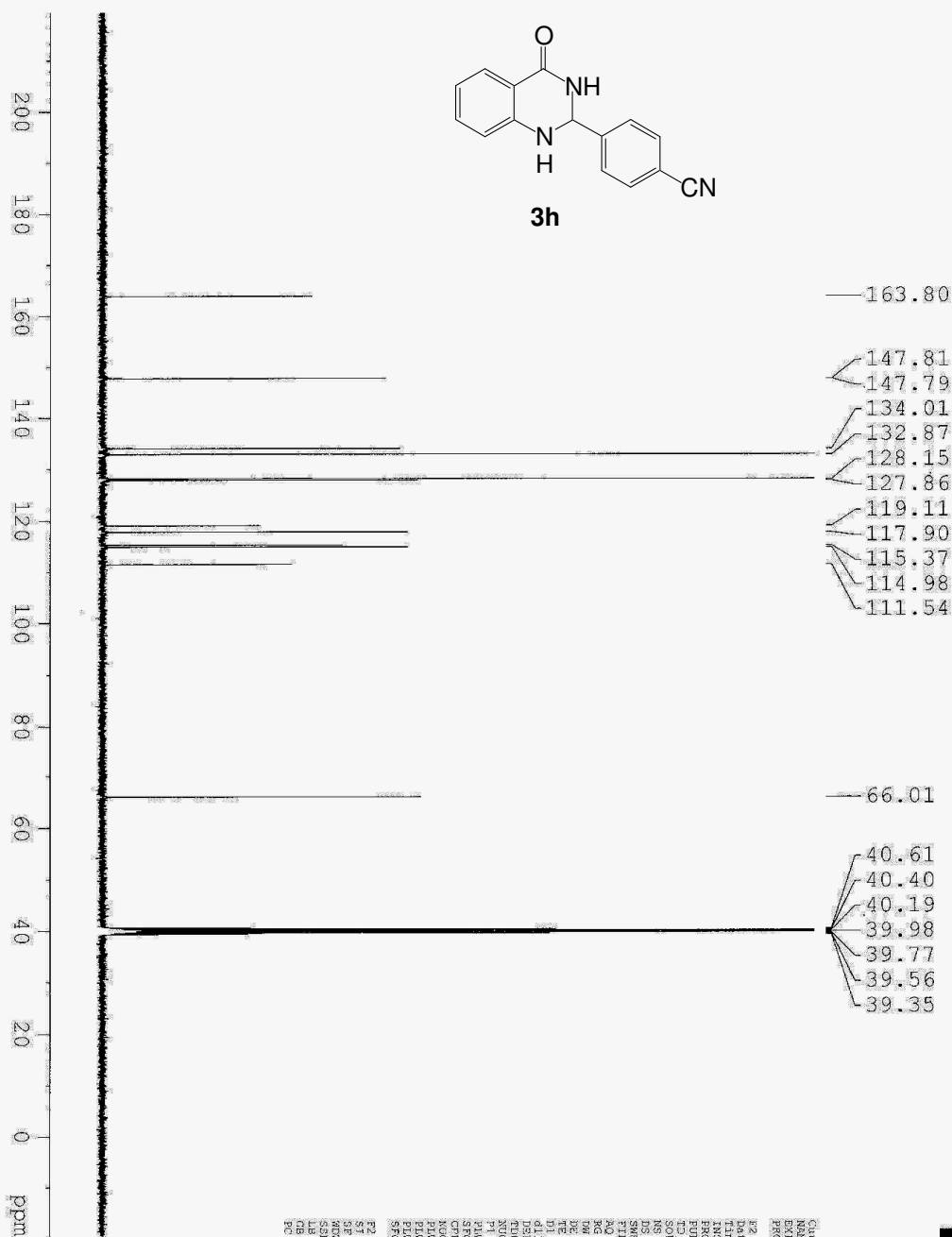
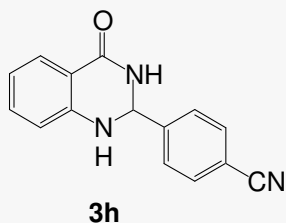
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NAME 10011-2011_10
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110117
Time 10:37
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PROBHD 5 mm PABO BB/4
PULPROG zgpg30
F2 - Processing Parameters
SI 32
SF 400.1360000 MHz
WDW EM
SSB 0
LB 0.30 MHz
GB 0
PC 1.00
SFO1 400.1324710 MHz
NUC1 13C
P1 15.50 uSec
PL1 0.00000000 W
PL2
PL3
F2 - Processing Parameters
SI 32
SF 400.1360000 MHz
WDW EM
SSB 0
LB 0.30 MHz
GB 0
PC 1.00
SFO1 400.1324710 MHz
NUC1 13C
P1 15.50 uSec
PL1 0.00000000 W
PL2
PL3
F2 - Acquisition Parameters
Date_ 20110117
Time 10:37
INSTRUM spect
PROBHD 5 mm PABO BB/4
PULPROG zgpg30
F2 - Processing Parameters
SI 32
SF 400.1360000 MHz
WDW EM
SSB 0
LB 0.30 MHz
GB 0
PC 1.00
SFO1 400.1324710 MHz
NUC1 13C
P1 15.50 uSec
PL1 0.00000000 W
PL2
PL3



BRUKER

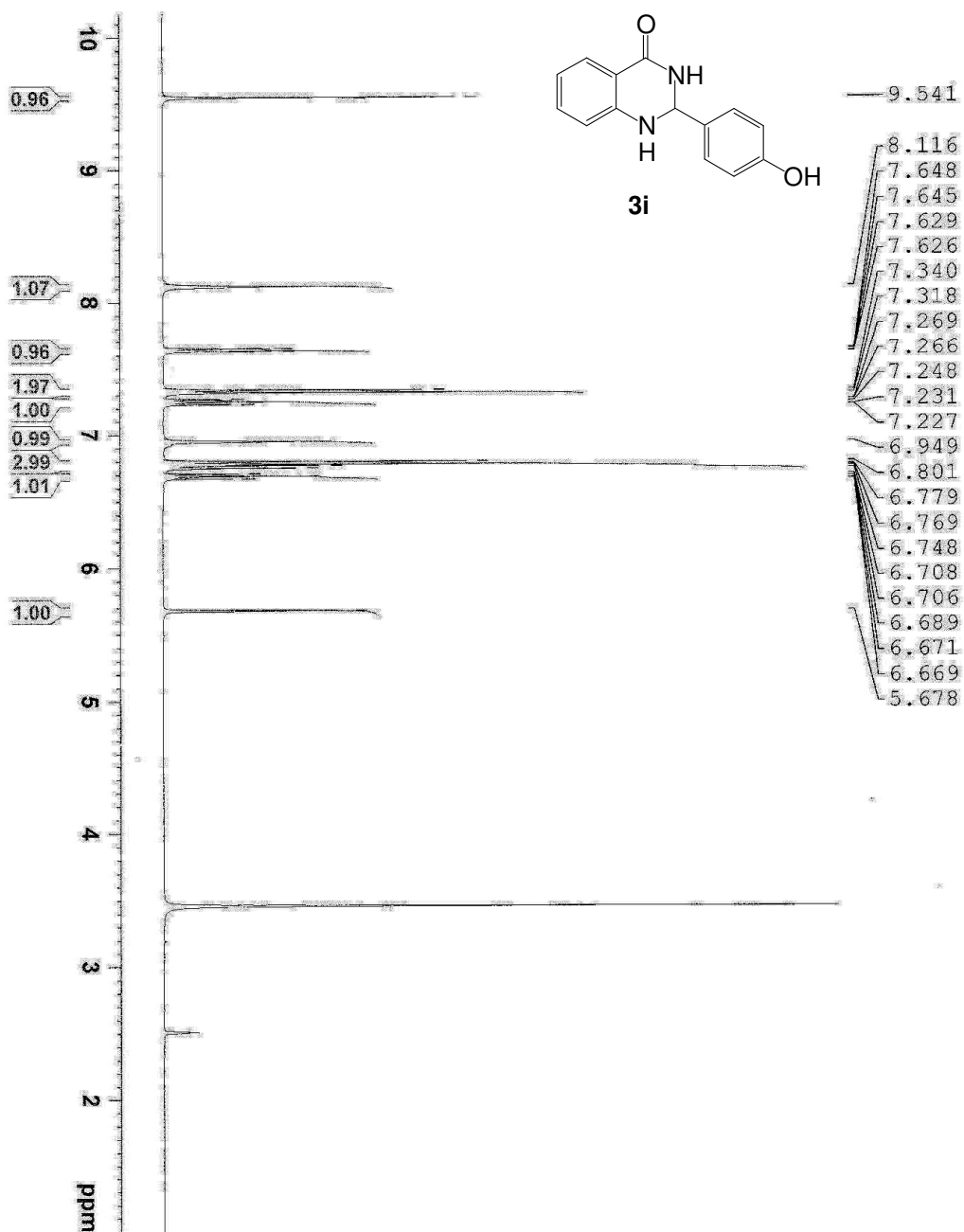
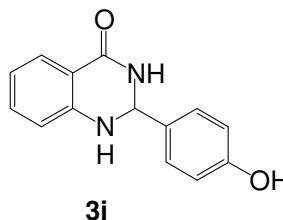


13C--4-CN-CHO



Current Data Parameters
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110423
 Time 13:15
 INSTRUM spect
 PROBRD 5 FT DABO 36/
 PULPROG zgpg30
 FIDRES 0.5534
 T2 0.5534
 SOLVENT DMSO
 NS 400
 DS 4
 SWH 2403.461 Hz
 FIDRES 0.36678 Hz
 AQ 1.363198 sec
 RG 200.65
 DW 20.900 USEC
 DE 0.550000
 TE 298.1 K
 d11 2.0000000 sec
 d11 0.0300000 sec
 PC 0.5989998 sec
 P1 13C
 P1 16.06 USEC
 P1 32.0000000 sec
 P1 100.628285 MHz
 CPMPCP2
 KOC2 1H
 P1M12 12.0010000 sec
 P1M12 0.5563001 sec
 P1M12 0.5563001 sec
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 SF 100.614590 MHz
 AQC DM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.60

1H - 4-OH

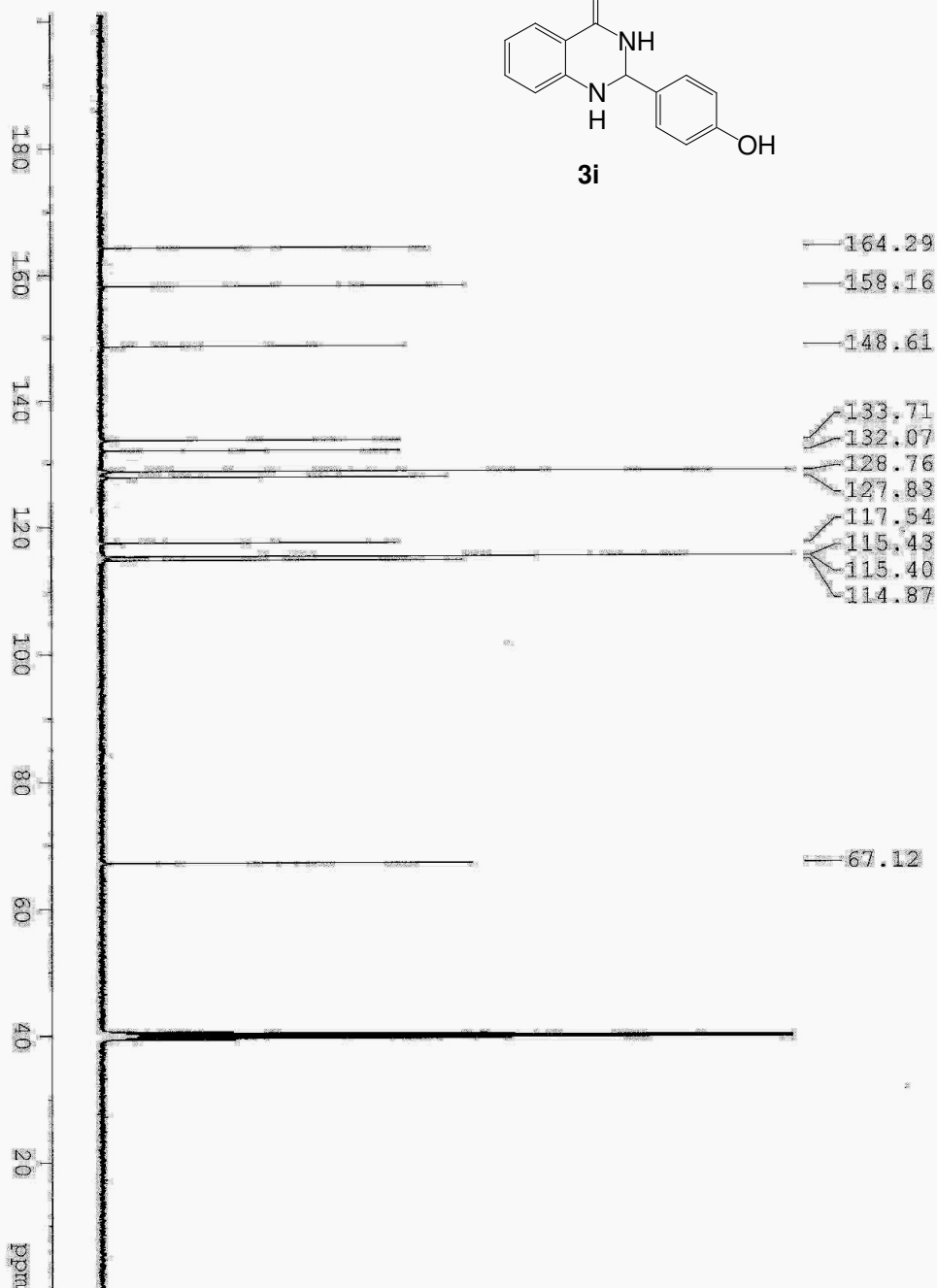
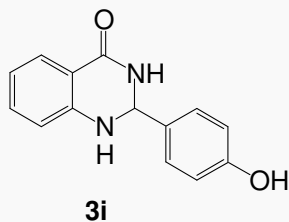


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7.318
7.269
7.266
7.248
7.231
7.227
6.949
6.801
6.779
6.769
6.748
6.708
6.706
6.689
6.671
6.669
5.678



Current: 600 MHz Parameters
NAME: 0610-031, 10
EXNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 201107
Time: 13:41
INSTRUM: spect
PROBHD: 5 mm PABBO BB/
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 16
DS: 2
SWH: 8012.820 Hz
FIDRES: 0.122266 Hz
AQ: 0.081731 sec
RG: 409.57 Hz
CWM: 62.400 usec
DS: 6.50 usec
TS: 258.2 K
D1: 1.00000000 sec
d11: 1
===== CHANNEL f1 =====
SFO1: 400.1324710 MHz
NUC1: 15 N
P1: 15.00 usec
PL1: 0 dB
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SF: 400.1300000 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

¹³C -4-OH

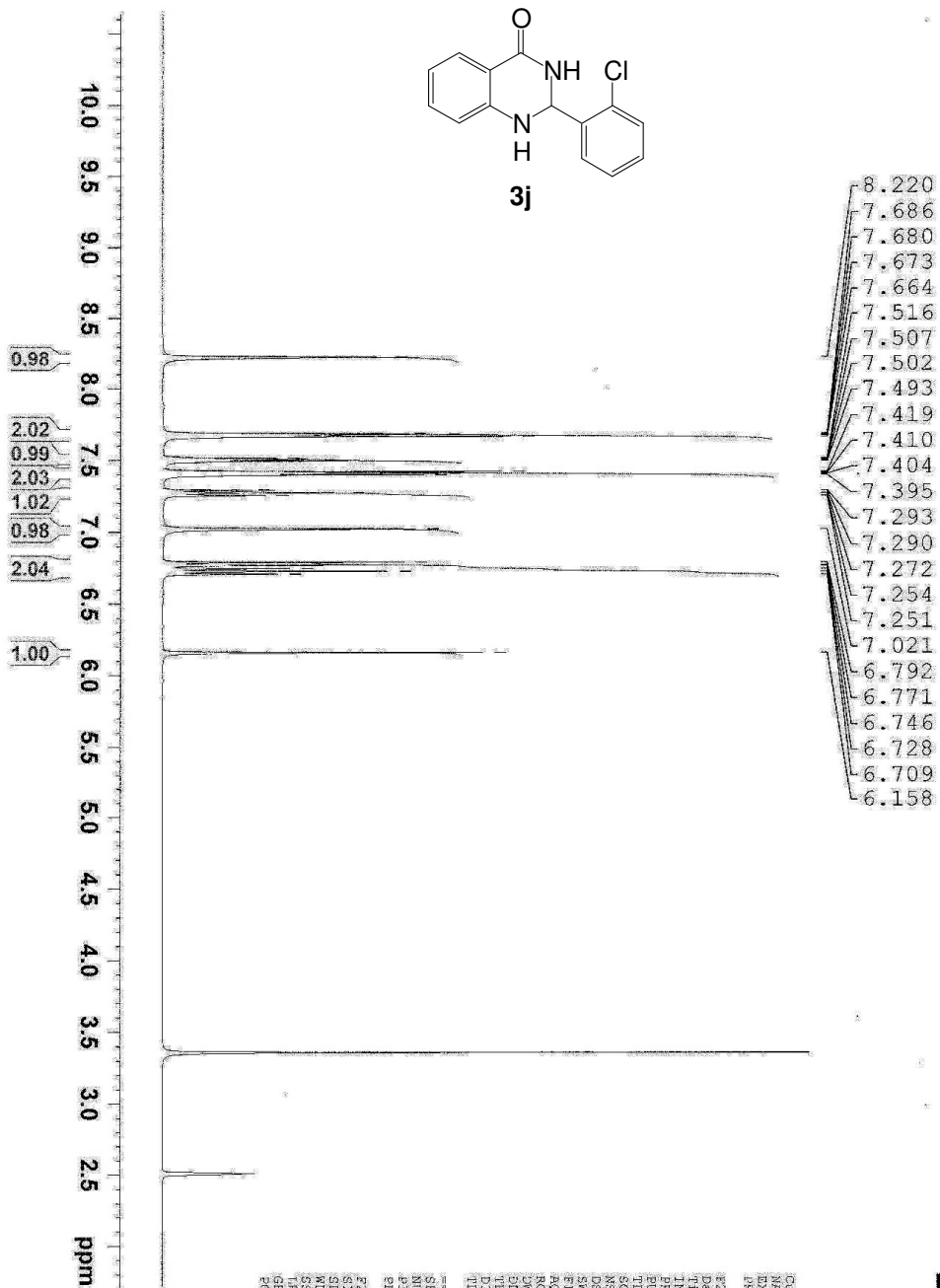
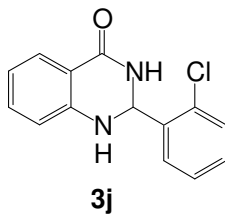


Current Data Parameters
NAME Octid-2014_RatH101-CH
EXPNO 11
PROCNO 1
P2 - Acquisition Parameters
Date_ 20141116
Time 15:06
F2 - Processing parameters
SI 32768
SF 100.617690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
EC 1.40

Acquisition Parameters
Date_ 20141116
Time 15:06
F2 - Processing parameters
SI 32768
SF 100.617690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
EC 1.40

Acquisition Parameters
Date_ 20141116
Time 15:06
F2 - Processing parameters
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SF 100.617690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
EC 1.40

1H-2-Cl-CHO



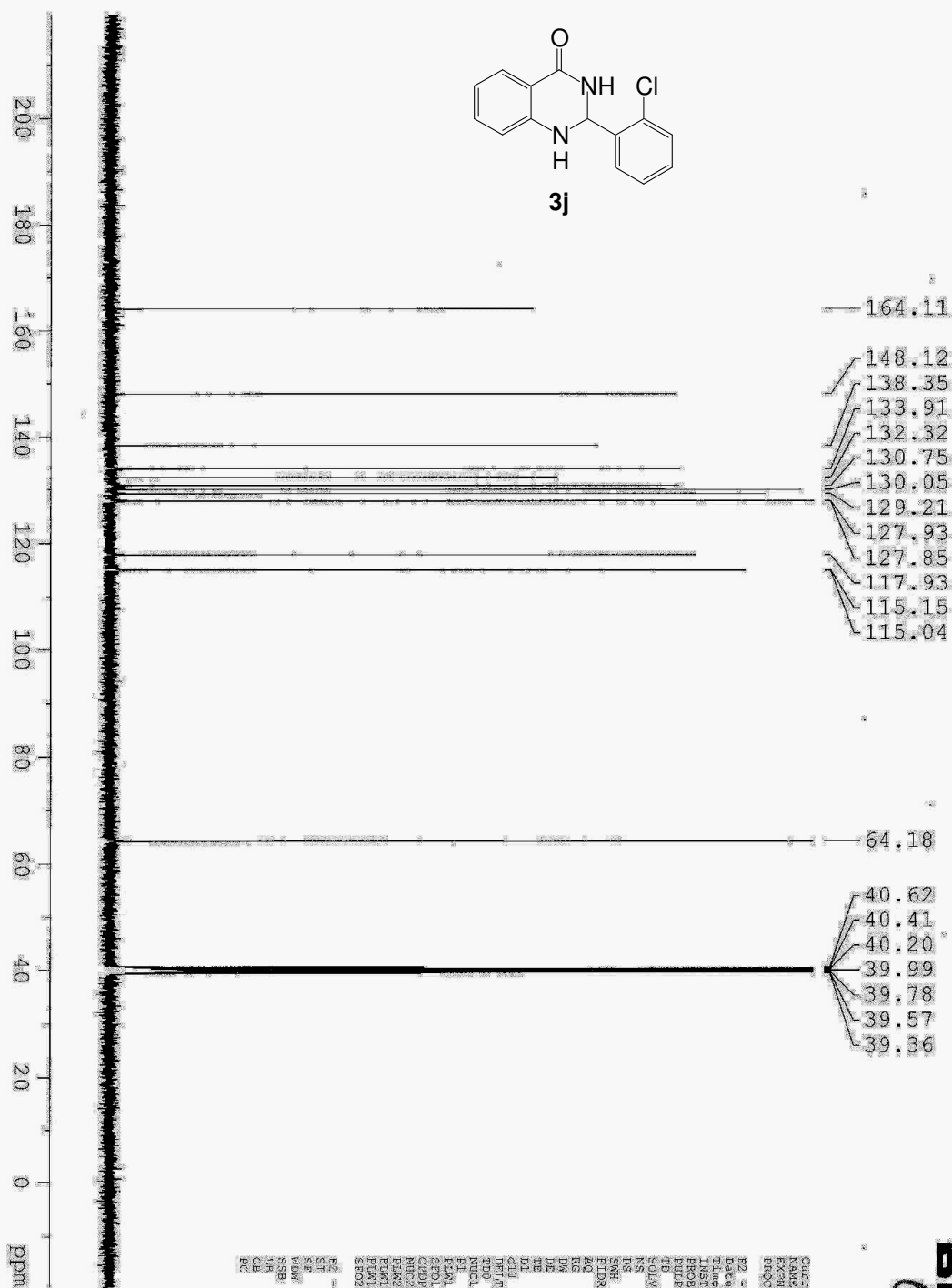
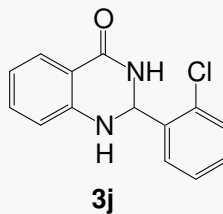
Current Data Parameters
NAME Sep18-2014, Mutar-2-Cl
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140918
Time 11:08
INSTRUM spect
PROBHD 5 mm BBO-5H/1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6013.820 MHz
FIDRES 0.123280 Hz
AQ 4.084569 sec
RG 99.75
BW 62.400 usec
GB 5.50 usec
HY 298.1 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.132410 MHz
NUC1 1H
P1 15.50 usec
PL1 0.0000000 dB
ELW1 12.0000000 W

F2 - Processing parameters
SI 32768
SF 400.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
EC 1.00

¹³C-2-Cl-CHO



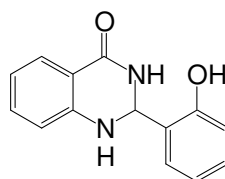
Current Data Parameters
 NAME Sep18-2010, NMR1-2-Cl
 EXNO 11
 PROCNO 1

F2 - Acquisition Parameters
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 Time 11:32
 INSTRUM spect
 PULPROG zgpg30
 PROCNO 5
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 TD 65536
 SFO 125.76
 SOLVENT DMSO
 NS 400
 DS 4
 SWH 24038.463 Hz
 FIDRES 0.366798 Hz
 AQ 1.361968 sec
 RG 204.63
 DW 20.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89299998 sec
 TD 1
 NUC1 13C
 P1 10.00 usec
 PL1 52.0000000 W
 SE1 100.622293 MHz
 CQDPRG2 1H
 F2 125.7600000 MHz
 PL2 0.3265001 W
 SE2 100.622293 MHz
 FID1 0.2830001 W
 SFO2 400.1316005 MHz

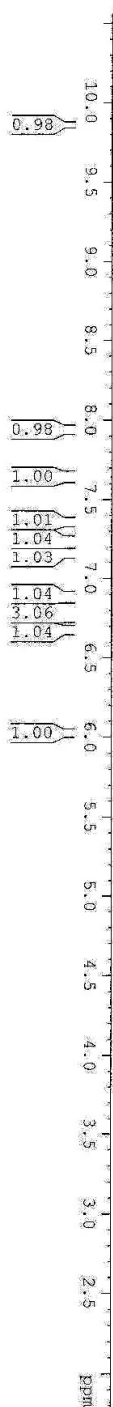
F2 - Processing parameters
 SI 32768
 SF 100.622440 MHz
 WDE 32
 SSB 0
 GB 0
 PC 1.40

¹H, saltsaldehyde

7.946
7.654
7.634
7.371
7.352
7.249
7.231
7.214
7.211
7.180
7.161
7.145
7.142
6.893
6.872
6.829
6.810
6.796
6.776
6.757
6.697
6.679
6.660
6.028



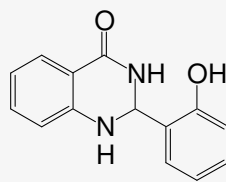
3k



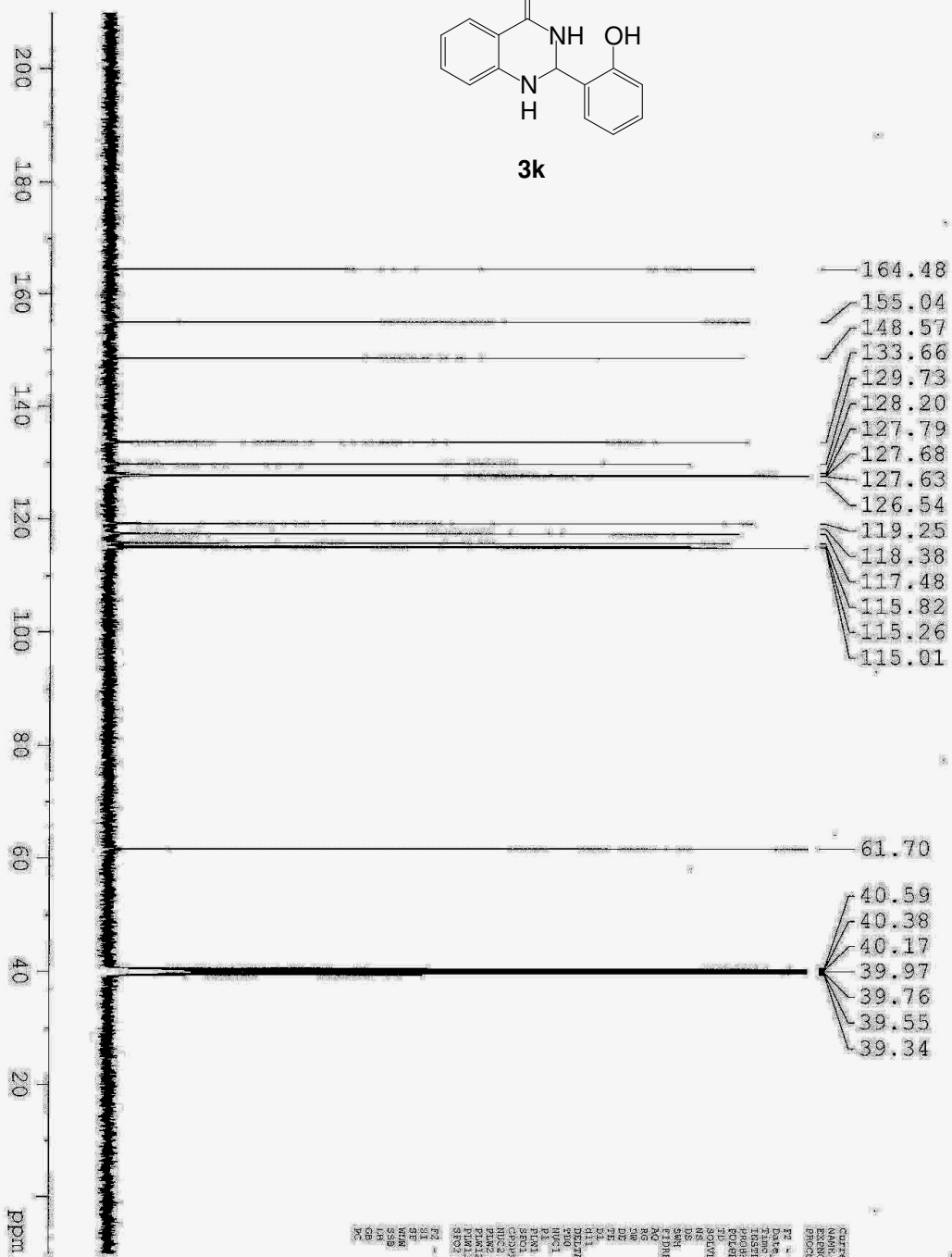
Current Data Parameters
NAME Sep12-2014_MetNur_SaltsalD3
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140912
Time 11.43
INSTRUM spect
PROBHD 5 mm PRBBO-430
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 12
DS 2
SWH 4012.820 Hz
AQ 0.122266 Hz
RG 4.089196 sec
SFO 89.403 MHz
NUC1 13C
NUC2 1H
TE 298.2 K
DE 1.0000000 sec
SFO 400.1136710 MHz
NAME 3k
EXPNO 10
PROCNO 1
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
GB 0
PC 1.006



¹³C, salisaldehyde



3k

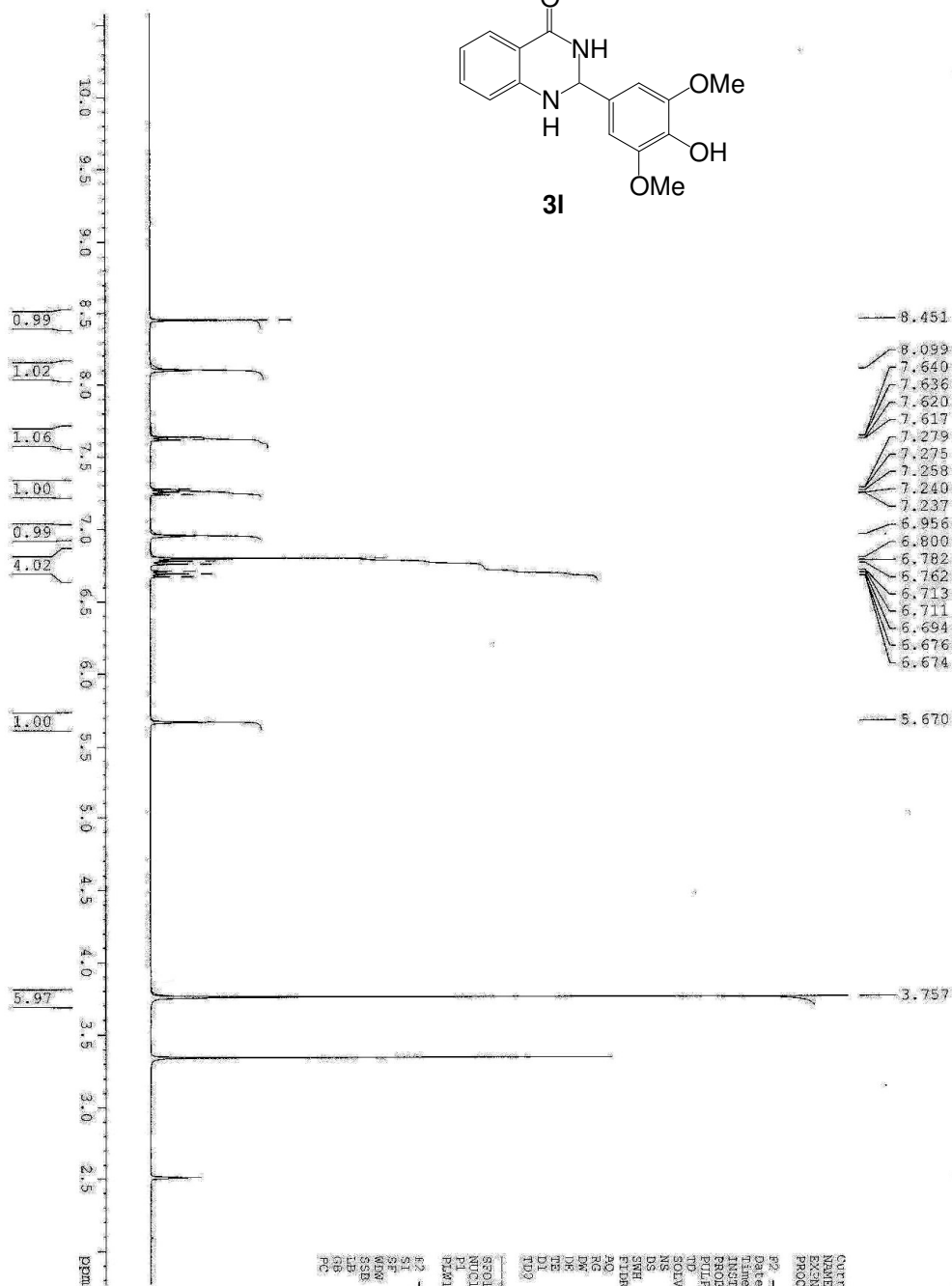
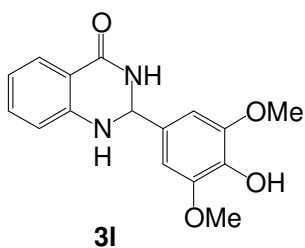


Current Data Parameters
 Name: Sep12-2014, NMR1, Salisaldehyde
 Date: 12/13
 Time: 12:13
 Instrument: spect
 Processor: 3
 F2: 100.625000 MHz
 F1: 400.146005 MHz
 AQ: 1.00 Hz
 RG: 32768
 DE: 1.00 Hz
 CB: 0
 PC: 1.40

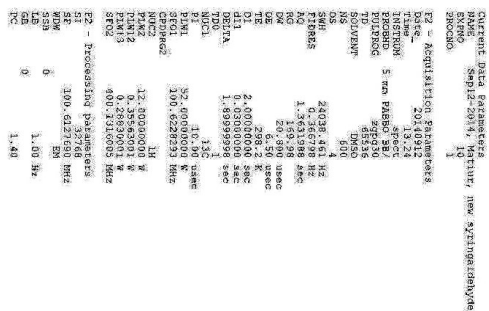
Processing parameters
 SI: 32768
 SF: 100.625000 MHz
 WW: 400.146005 MHz
 FWHM: 1.00 Hz
 GB: 0
 PC: 1.40

Acquisition parameters
 P1: 10.00 sec
 P2: 0.00 sec
 P3: 0.00 sec
 P4: 0.00 sec
 P5: 0.00 sec
 P6: 0.00 sec
 P7: 0.00 sec
 P8: 0.00 sec
 P9: 0.00 sec
 P10: 0.00 sec
 P11: 0.00 sec
 P12: 0.00 sec
 P13: 0.00 sec
 P14: 0.00 sec
 P15: 0.00 sec
 P16: 0.00 sec
 P17: 0.00 sec
 P18: 0.00 sec
 P19: 0.00 sec
 P20: 0.00 sec
 P21: 0.00 sec
 P22: 0.00 sec
 P23: 0.00 sec
 P24: 0.00 sec
 P25: 0.00 sec
 P26: 0.00 sec
 P27: 0.00 sec
 P28: 0.00 sec
 P29: 0.00 sec
 P30: 0.00 sec
 P31: 0.00 sec
 P32: 0.00 sec
 P33: 0.00 sec
 P34: 0.00 sec
 P35: 0.00 sec
 P36: 0.00 sec
 P37: 0.00 sec
 P38: 0.00 sec
 P39: 0.00 sec
 P40: 0.00 sec
 P41: 0.00 sec
 P42: 0.00 sec
 P43: 0.00 sec
 P44: 0.00 sec
 P45: 0.00 sec
 P46: 0.00 sec
 P47: 0.00 sec
 P48: 0.00 sec
 P49: 0.00 sec
 P50: 0.00 sec
 P51: 0.00 sec
 P52: 0.00 sec
 P53: 0.00 sec
 P54: 0.00 sec
 P55: 0.00 sec
 P56: 0.00 sec
 P57: 0.00 sec
 P58: 0.00 sec
 P59: 0.00 sec
 P60: 0.00 sec
 P61: 0.00 sec
 P62: 0.00 sec
 P63: 0.00 sec
 P64: 0.00 sec
 P65: 0.00 sec
 P66: 0.00 sec
 P67: 0.00 sec
 P68: 0.00 sec
 P69: 0.00 sec
 P70: 0.00 sec
 P71: 0.00 sec
 P72: 0.00 sec
 P73: 0.00 sec
 P74: 0.00 sec
 P75: 0.00 sec
 P76: 0.00 sec
 P77: 0.00 sec
 P78: 0.00 sec
 P79: 0.00 sec
 P80: 0.00 sec
 P81: 0.00 sec
 P82: 0.00 sec
 P83: 0.00 sec
 P84: 0.00 sec
 P85: 0.00 sec
 P86: 0.00 sec
 P87: 0.00 sec
 P88: 0.00 sec
 P89: 0.00 sec
 P90: 0.00 sec
 P91: 0.00 sec
 P92: 0.00 sec
 P93: 0.00 sec
 P94: 0.00 sec
 P95: 0.00 sec
 P96: 0.00 sec
 P97: 0.00 sec
 P98: 0.00 sec
 P99: 0.00 sec
 P100: 0.00 sec

¹H, 3,5-Di-OMe



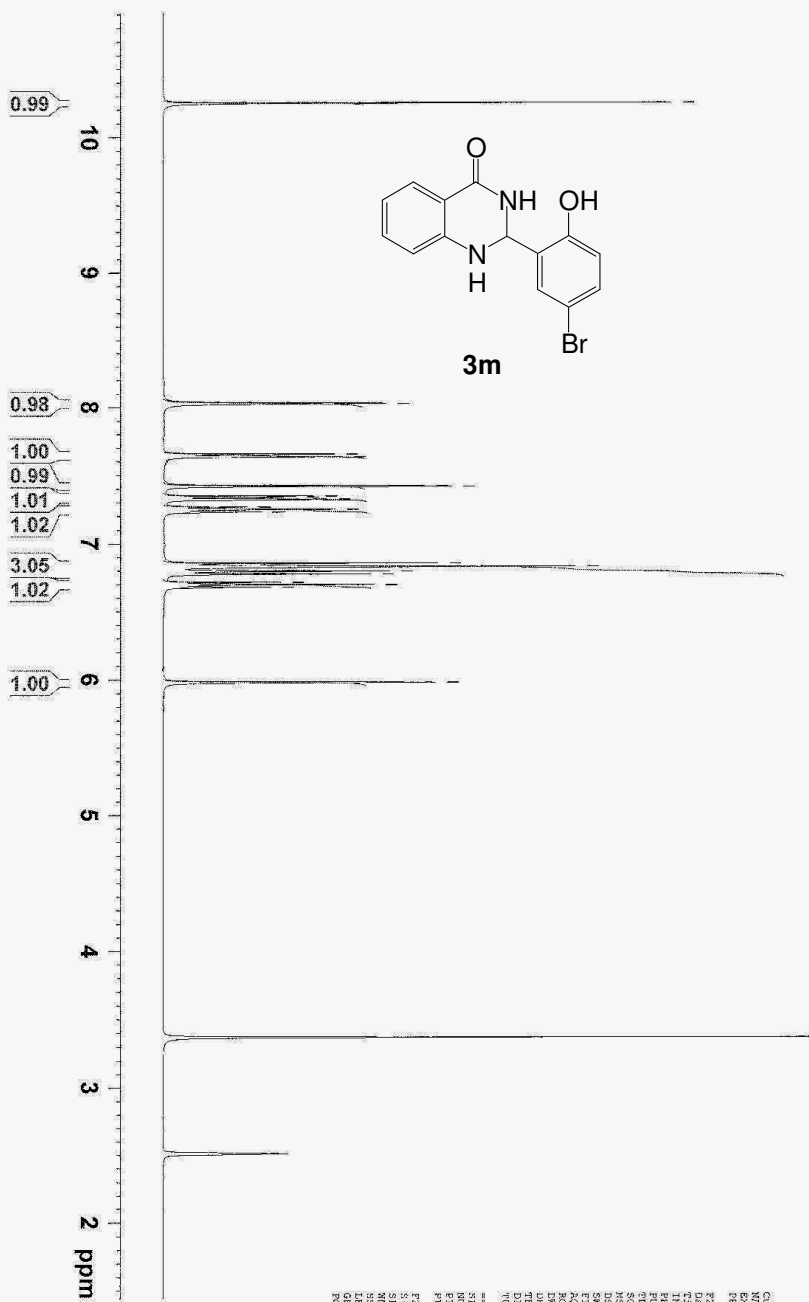
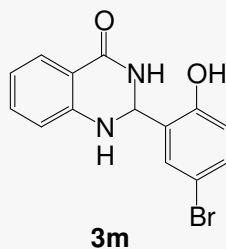
Current Data Parameters
 NAME Sep03-2014_Matior 3,5-di-OMe
 EXNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20140903
 Time_ 15.13
 INSTRUM spect
 PROBNM 5 mm PABO Bb/
 PULPROG zgpg30
 TOU 63936
 SOLVENT DMF
 NS 12
 DS 2
 SWH 8012.820 HZ
 FIDRES 0.122266 HZ
 AQ 4.084966 sec
 RG 138.31
 IN 62.401 usec
 DE 254.11 usec
 TE 298.15 K
 DI 1.0000000 sec
 TD0 1
 =====
 CHANNEL f1
 SOL 400.132410 MHz
 NUC1 1H
 P1 15.50 usec
 PL1 0.0000000 W
 FWH 12.0000000 W
 F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 GB 0.30 HZ
 RB 0
 PC 1.00



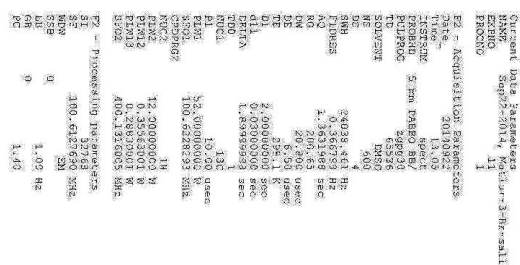
1H-3-Br-sal1



10.246
8.028
7.652
7.633
7.422
7.416
7.346
7.340
7.324
7.318
7.269
7.267
7.249
7.231
7.229
6.857
6.835
6.798
6.777
6.716
6.697
6.679
5.979

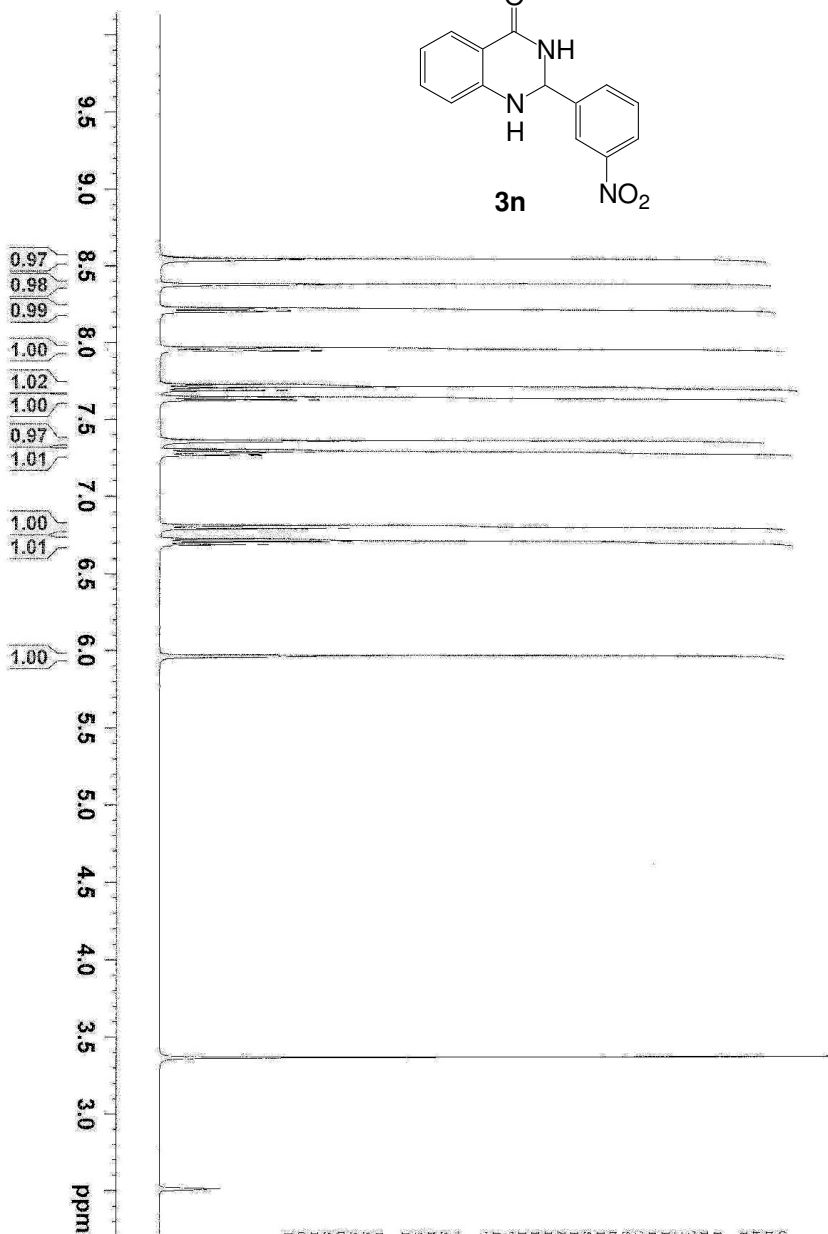
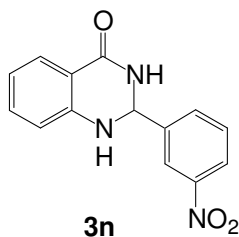


Current Data Parameters
NAME Sep22-2014_1H-3-Br-sal1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140922
Time 12.29
INSTRUM spect
PROBHD 5 mm
PULPROG zgpg30
FIDRES 0.32
AQ 0.0894966 sec
RG 125.93
DE 4.50 usec
TE 298.1 K
TD 1.00000000 sec
F2 - Processing parameters
SI 65536
SF 400.136000 MHz
WDW EM
SSB 0
GB 0
PC 1.00



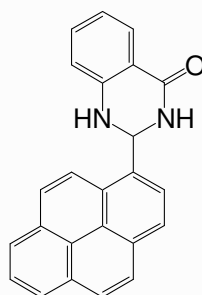
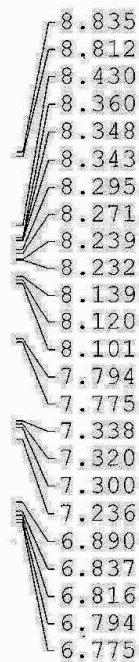
1H, 3-NO2

8.540
8.377
8.223
8.219
8.217
8.202
8.198
7.965
7.946
7.724
7.704
7.684
7.641
7.622
7.353
7.303
7.299
7.282
7.265
7.261
6.812
6.792
6.726
6.707
6.688
5.962

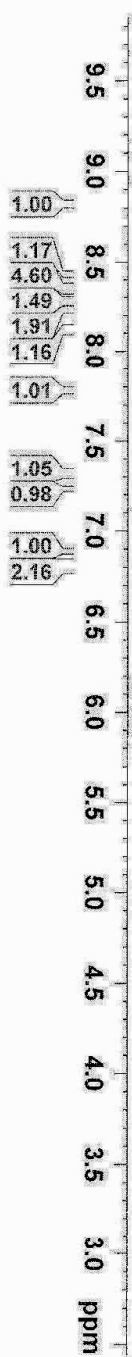


Current Data Parameters
NAME Sep12-2013_1H-3-NO2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140912
Time 11:02
INSTRUM spect
PROBHD 5 mm PABBO BBI
PULPROG zgpg30
TD 65536
FIDRES 0.000000
SOLVENT DMSO
NS 12
DS 4
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0934966 sec
RG 89.00
IN 62.400 usec
TS 4.50 usec
TE 298.1 K
D1 1.00000000 sec
RNO 1
===== CHANNEL f1 =====
SECT1 400.134710 MHz
NUC1 1H
P1 15.50 usec
PL1 0.00000000 dB
FWD1 12.00000000 N
===== CHANNEL f2 =====
P2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-Pyrene-CHO

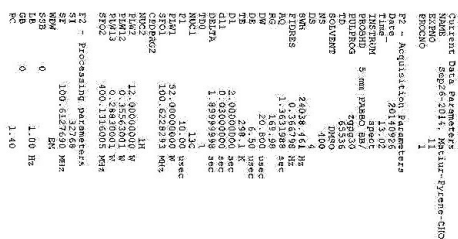


30

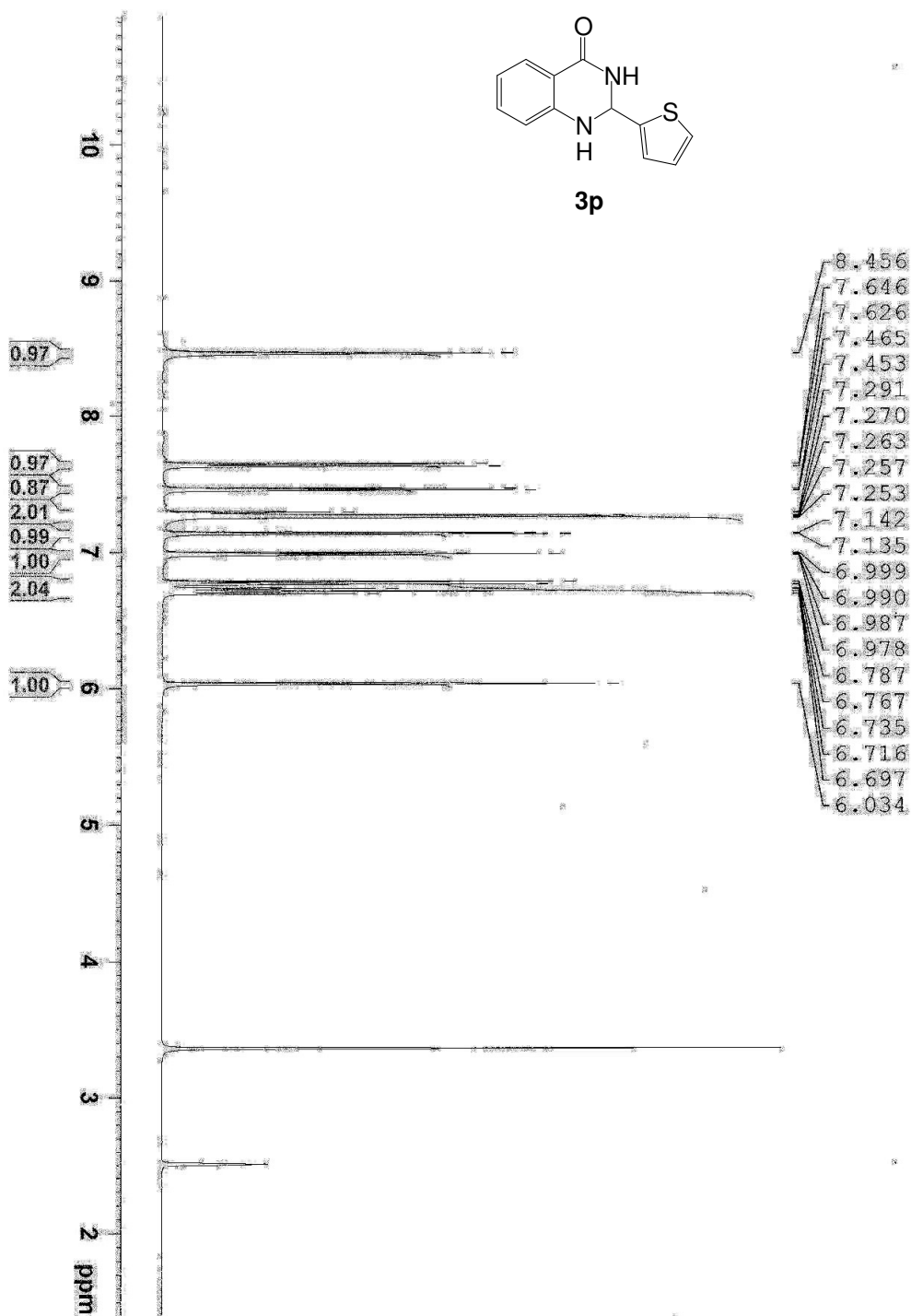
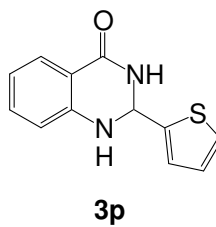


Current Data Parameters
NAME Sep23-2014, 1H-Pyrene-CHO
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140925
Time 11:20
INSTRUM spect
PROBHD 5 mm PABBO 5B/
PULPROG zgpg30
TD 65536
SFO 400.136000
AQ 0.050000
RG 32
DS 2
SWH 8013.320 Hz
FIDRES 0.000466 Hz
AQRES 4.009466 sec
RG 107.78
RG 67.106 usec
DE 263.90 usec
TE 300.2 K
D1 1.00000000 sec
D13 1
===== CHANNEL f1 =====
SFO1 400.1364710 MHz
NUC1 1H
P1 15.50 usec
PL1 12.000000000 W
F2 - Processing parameters
SI 65536
SF 400.1360000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
EC 1.00



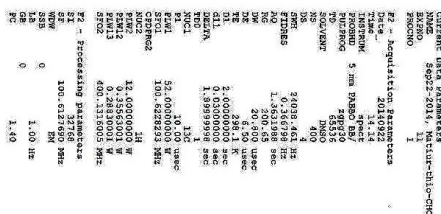


1H-Thio-CHO

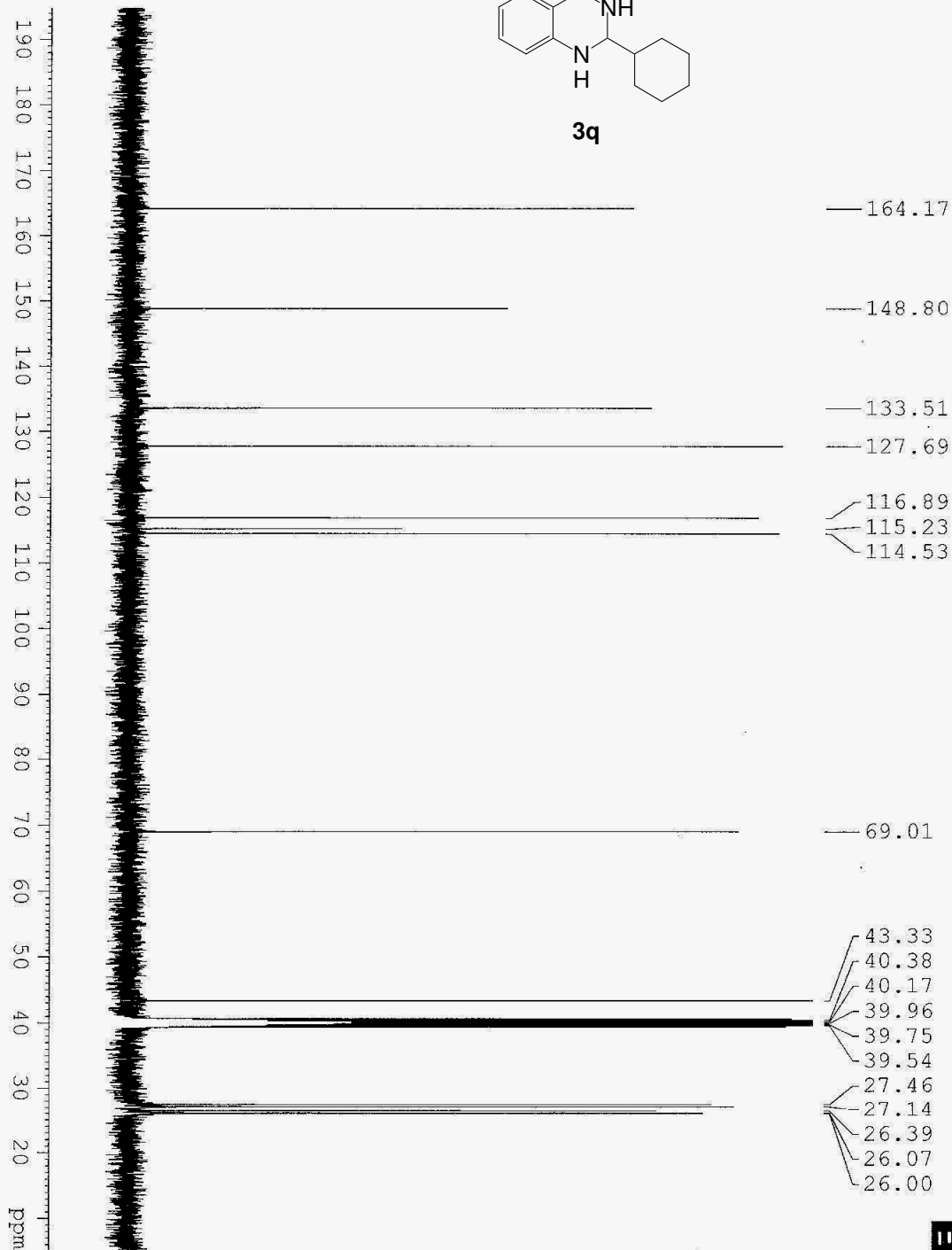
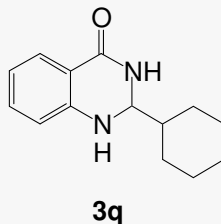


Current: 10.000000
Date: 2012-01-10
Time: 10:10:10
F1: Acquisition Parameters
F2: 2012-01-10
F3: 10:10:10
F4: 10:10:10
F5: 10:10:10
F6: 10:10:10
F7: 10:10:10
F8: 10:10:10
F9: 10:10:10
F10: 10:10:10
F11: 10:10:10
F12: 10:10:10
F13: 10:10:10
F14: 10:10:10
F15: 10:10:10
F16: 10:10:10
F17: 10:10:10
F18: 10:10:10
F19: 10:10:10
F20: 10:10:10
F21: 10:10:10
F22: 10:10:10
F23: 10:10:10
F24: 10:10:10
F25: 10:10:10
F26: 10:10:10
F27: 10:10:10
F28: 10:10:10
F29: 10:10:10
F30: 10:10:10
F31: 10:10:10
F32: 10:10:10
F33: 10:10:10
F34: 10:10:10
F35: 10:10:10
F36: 10:10:10
F37: 10:10:10
F38: 10:10:10
F39: 10:10:10
F40: 10:10:10
F41: 10:10:10
F42: 10:10:10
F43: 10:10:10
F44: 10:10:10
F45: 10:10:10
F46: 10:10:10
F47: 10:10:10
F48: 10:10:10
F49: 10:10:10
F50: 10:10:10
F51: 10:10:10
F52: 10:10:10
F53: 10:10:10
F54: 10:10:10
F55: 10:10:10
F56: 10:10:10
F57: 10:10:10
F58: 10:10:10
F59: 10:10:10
F60: 10:10:10
F61: 10:10:10
F62: 10:10:10
F63: 10:10:10
F64: 10:10:10
F65: 10:10:10
F66: 10:10:10
F67: 10:10:10
F68: 10:10:10
F69: 10:10:10
F70: 10:10:10
F71: 10:10:10
F72: 10:10:10
F73: 10:10:10
F74: 10:10:10
F75: 10:10:10
F76: 10:10:10
F77: 10:10:10
F78: 10:10:10
F79: 10:10:10
F80: 10:10:10
F81: 10:10:10
F82: 10:10:10
F83: 10:10:10
F84: 10:10:10
F85: 10:10:10
F86: 10:10:10
F87: 10:10:10
F88: 10:10:10
F89: 10:10:10
F90: 10:10:10
F91: 10:10:10
F92: 10:10:10
F93: 10:10:10
F94: 10:10:10
F95: 10:10:10
F96: 10:10:10
F97: 10:10:10
F98: 10:10:10
F99: 10:10:10
F100: 10:10:10



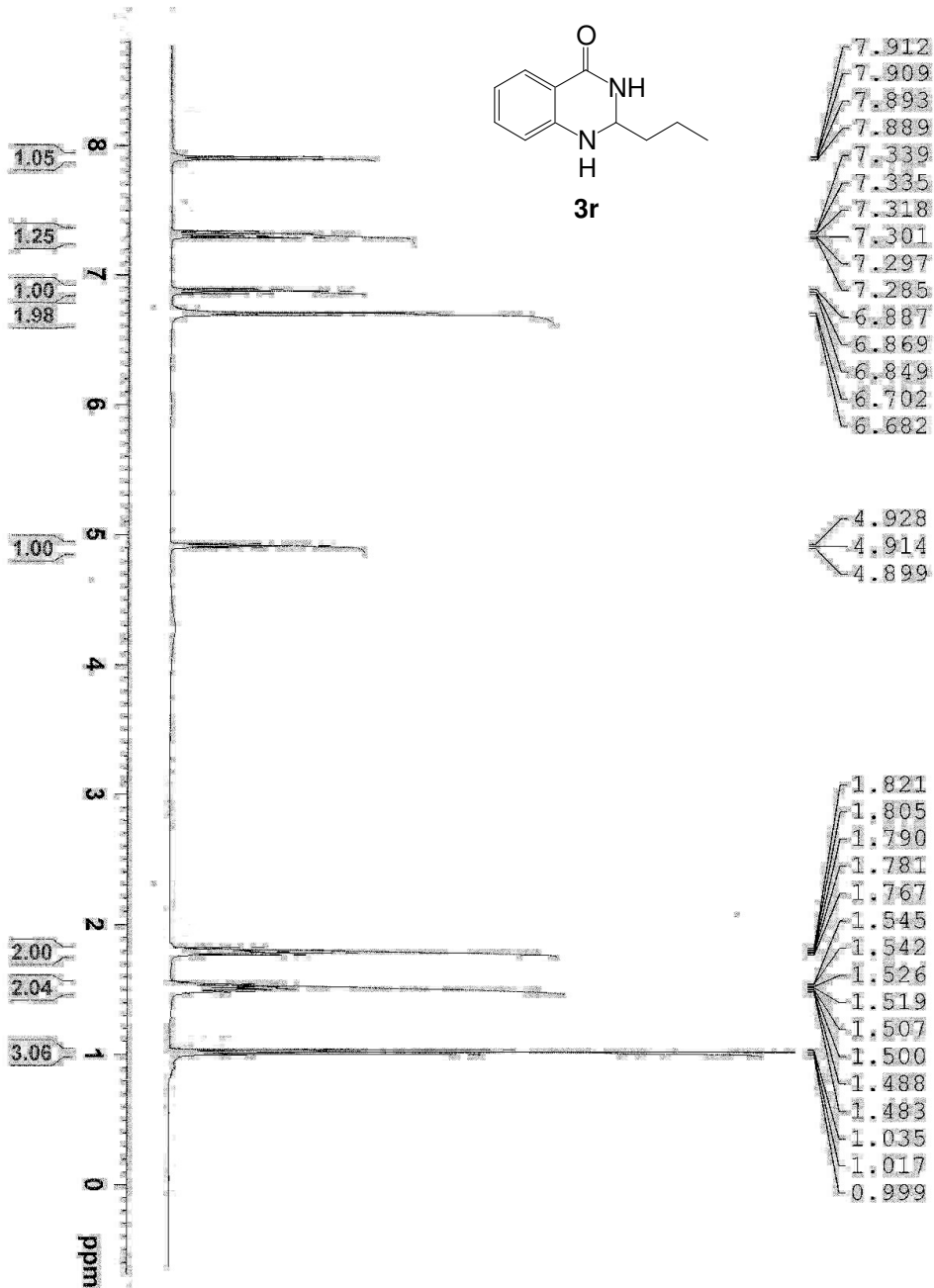
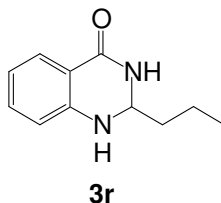


¹³C-Cyclohexanone



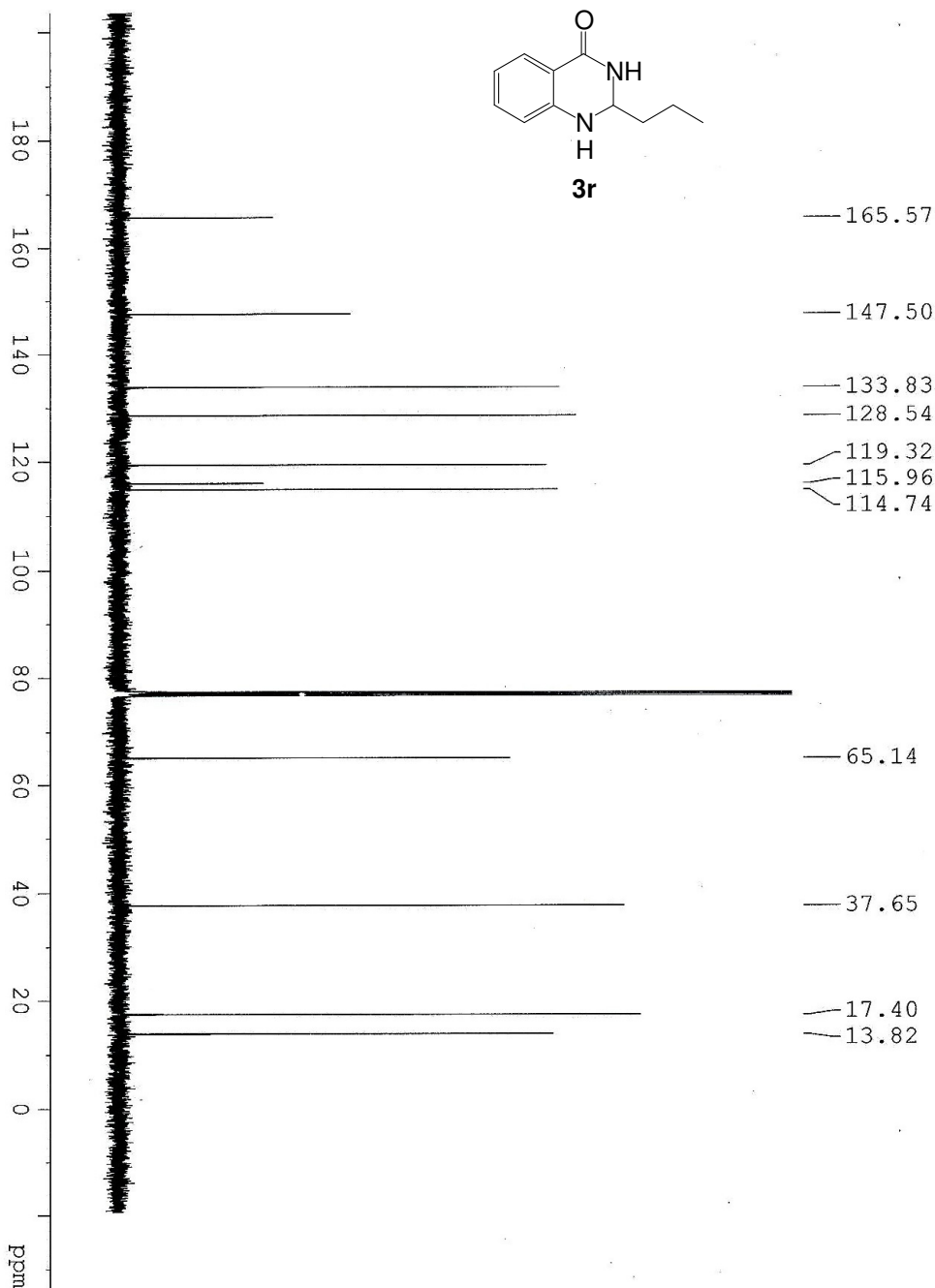
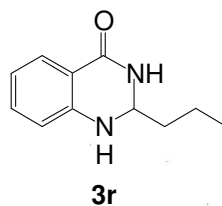
Current Data Parameters
 Name: 13C-Cyclohexanone
 ExpNo: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20140922
 Time: 14.54
 Instrument: spect
 PROBHD: 5 mm BBOBO MM/5
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: DMSO
 NS: 600
 DS: 4
 SWH: 24038.461 Hz
 FIDRES: 0.330000 Hz
 AQRES: 1.333988 sec
 RG: 200.65
 DB: 20.600 usec
 TE: 298.1 K
 D1: 8.000000 sec
 d11: 0.030000 sec
 DELTA: 1.0999998 sec
 INJ1: 130
 INJ2: 10.00 usec
 F1: 100.626125 MHz
 F2: 125.000000 MHz
 C1PULSE2: 12.00000000 usec
 P1: 0.3550001 sec
 P2: 0.2881001 sec
 P3: 0.2550001 sec
 SFO: 500.1361995 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 100.6127690 MHz
 SW: 24038.461 Hz
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1H-aliphatic



Name: 3r
 Date: 20111117
 Time: 15.13
 File: 3r_1513
 F2 - Acquisition parameters
 Date: 20111117
 Time: 15.13
 File: 3r_1513
 F2 - Processing parameters
 SI: 65535
 SF: 100.130000
 EQ: 10.00
 CB: 0.00
 PC: 1.00

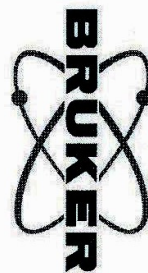
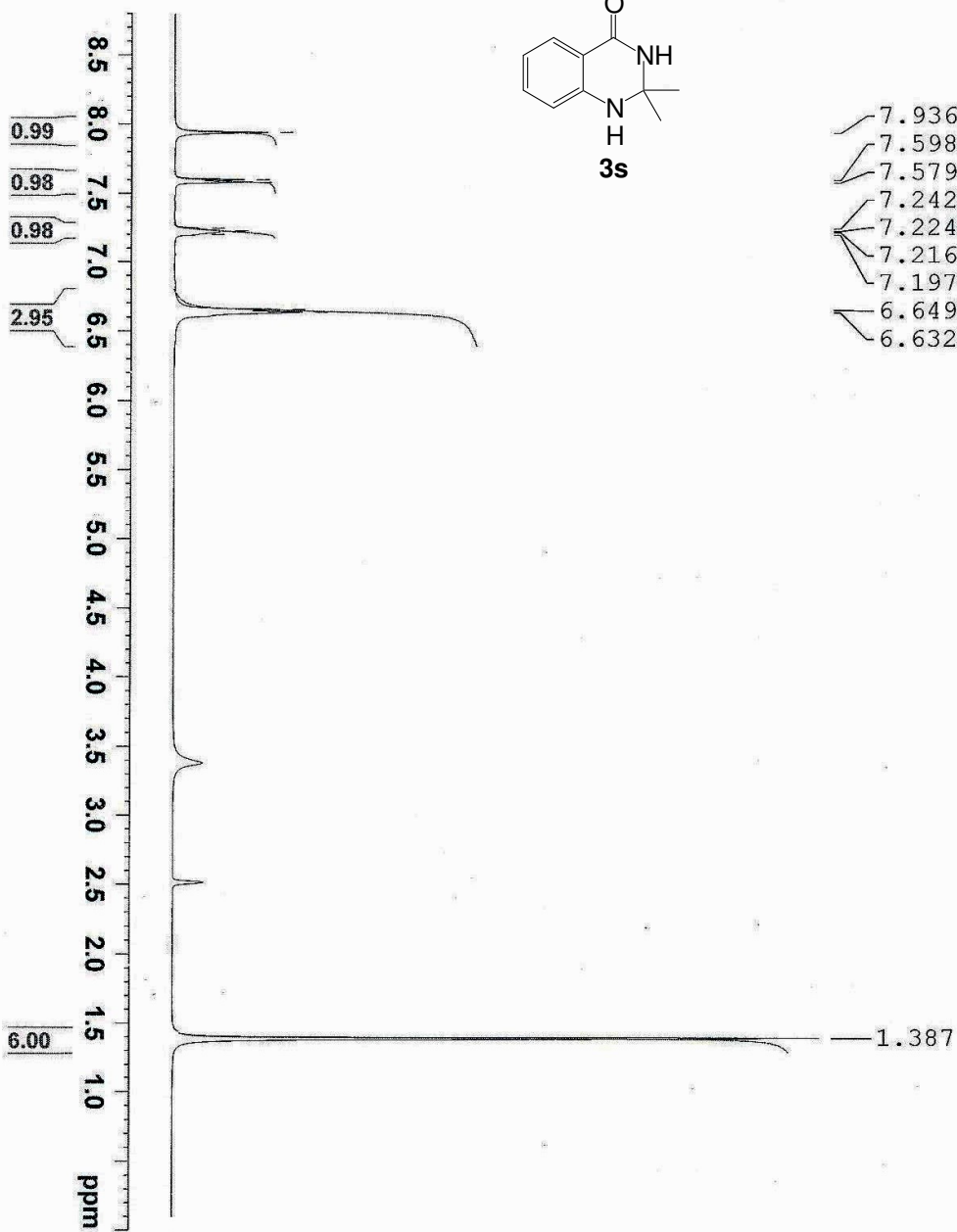
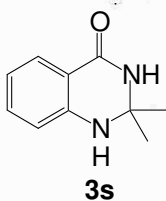
¹³C -aliphatic



Current Data Parameters
 NAME: 20141010
 EXPNO: 11
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20141010
 Time: 11.11
 INSTRUM: spect
 PROBRD: 5 mm PABBO B1/
 PULPROG: zgpg30
 F4: 400.133
 SOLVENT: CDCl3
 NS: 400
 DS: 4
 SWH: 24038.461 Hz
 FIDRES: 0.366798 Hz
 AQ: 1.361678 sec
 RG: 327.674
 IN: 20.800 usec
 DE: 6.50 usec
 TE: 300.2 K
 DELTA: 2.0000000 sec
 DI: 0.0300000 sec
 TPO: 1.8999996 sec
 F1: 100.628393 MHz
 F2: 400.133 MHz
 SFO1: 100.628393 MHz
 CDEP662
 NU1: 14
 P1: 12.0000000 W
 P1A2: 0.3552001 W
 P1A3: 0.2893001 W
 SFO2: 400.1330000 MHz
 F2 - Processing Parameters
 SI: 32768
 SF: 100.627690 MHz
 WDW: EM
 SSB: 0
 GB: 0
 PC: 1.40

¹H-Acetone

7.936
7.598
7.579
7.242
7.224
7.216
7.197
6.649
6.632



Current Data Parameters
NAME Sep30-2014, Matur-Acetic
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

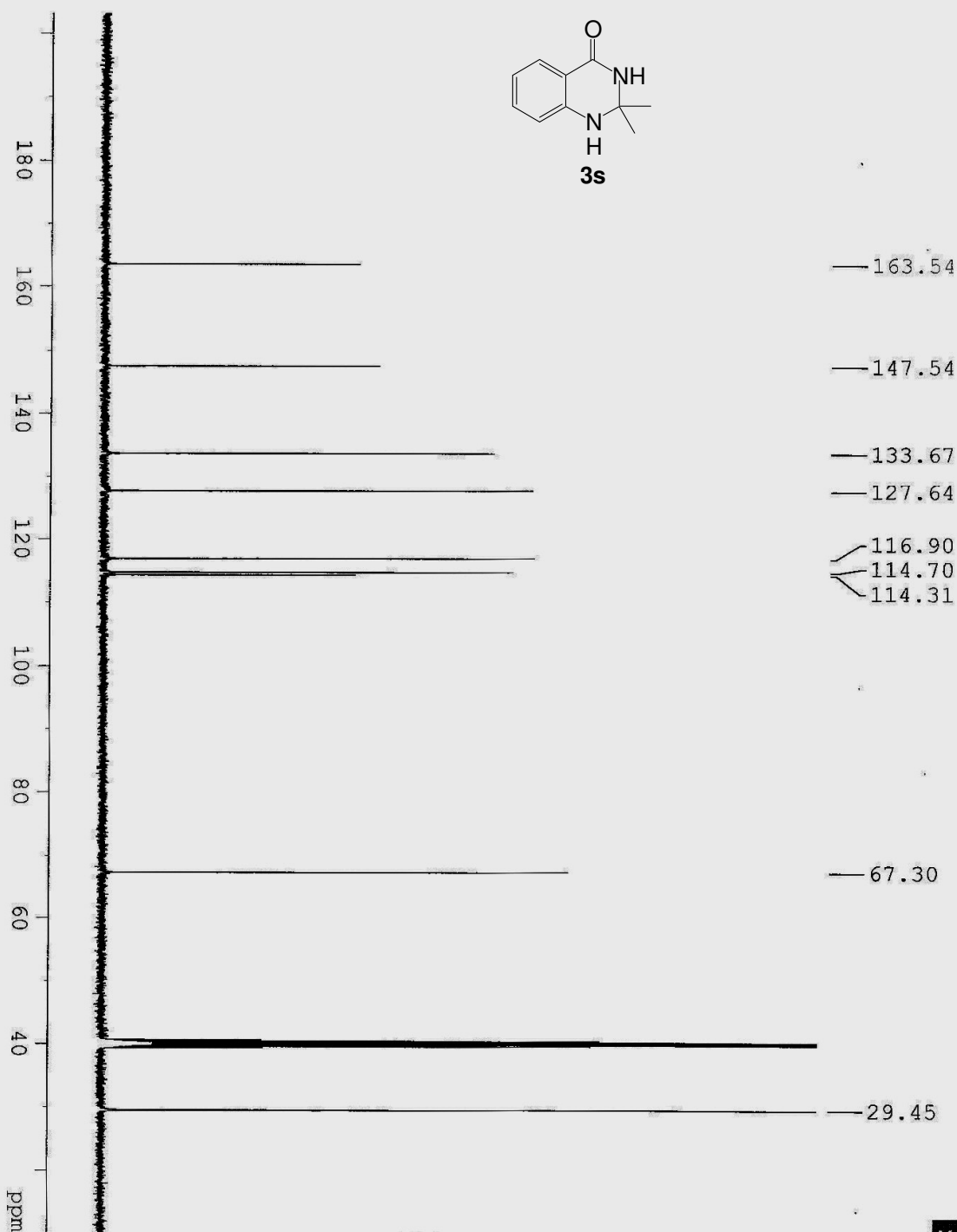
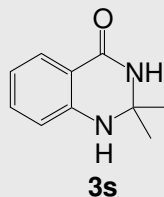
Date_ 20140930
Time 12.05
INSTRUM spect
PROBHD 5 mm PABO B1/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 80.05
DM 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

CHANNEL f1

SCF1 400.1324710 MHz
NUC1 1H
P1W1 15.50 usec
PLW1 12.00000000 W

F2 - Processing Parameters

SI 65536
SF 400.130000 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.00

[illegible]