

Supporting Information

Synthesis of highly diversified 1,2,3-triazole derivatives via domino [3+2] azide cycloaddition and denitration reaction sequence

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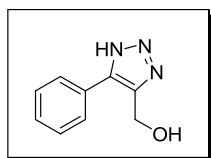
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Experimental Section

General Remarks: Commercial reagents were used without further purification. Melting points were recorded on a Superfit (India) capillary melting point apparatus and were uncorrected. IR spectra were recorded on a Perkin Elmer-FTIR spectrometer using solid samples as KBr plates. For compounds ^1H NMR (300 MHz, CDCl_3) and ^{13}C NMR (75 MHz, CDCl_3) spectra were recorded in deuteriochloroform (CDCl_3) on a Bruker 300 MHz spectrometer using tetramethylsilane (TMS, $\delta = 0$) as an internal standard at room temperature. Mass spectra were recorded on Agilent 1200 LC/MS-6110 mass spectrometer.

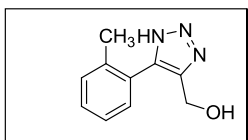
Typical experimental procedure for the synthesis of (5-phenyl-1H-1,2,3-triazol-4-yl)methanol (**3a**)

To a stirred solution of (*E*)-2-nitro-3-phenylprop-2-en-1-ol (**1a**) (0.36g, 2 mmol) in DMSO (3 ml), sodium azide (**2**) (0.39g, 6 mmol) was added and the reaction mixture was kept at 80 °C for 10 min. After completion of the reaction as indicated by TLC, the reaction mixture was diluted with water (10 ml) and extracted with ethylacetate (20 ml). The organic layer thus obtained was washed with brine solution (10 ml). The crude sample was purified by column chromatography (20%, EtOAc / hexanes) to provide the desired pure product **3a** as colorless solid in 87% (0.30g) yield.



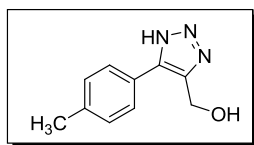
(5-Phenyl-1H-1,2,3-triazol-4-yl)methanol (**3a**)

Colourless solid Yield : 87% M. P : 121-123 °C IR (KBr) : 3450, 3185, 1730, 1620 cm^{-1} ^1H NMR (CDCl_3 + (2 drops) DMSO-d_6 , 300 MHz): δ 4.75 (d, $J = 5.1\text{Hz}$ 2H), 5.16 (s, 1H), 5.53 (s, 1H), 7.35-7.91 (m, 5H). ^{13}C NMR (CDCl_3 + (2 drops) DMSO-d_6 , 75 MHz) : δ 59.5, 132.2, 132.7, 133.5, 133.5, 142.8, 149.8. MS (m/z) : 176 ($\text{M}^+ + 1$). Elemental Analysis for $\text{C}_9\text{H}_9\text{N}_3\text{O}$ Calculated : C, 61.70; H, 5.18; N, 23.99. Found : C, 61.75; H, 5.16; N, 23.96.



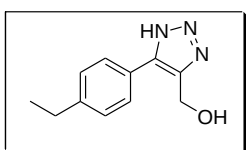
(5-o-Tolyl-1H-1,2,3-triazol-4-yl)methanol (**3b**)

Colourless solid Yield : 91% M. P : 110-112 °C IR (KBr): 3422, 3224, 1740, 1624 cm^{-1} ^1H NMR (CDCl_3 , 300 MHz) : δ 2.23 (s, 3H), 2.99 (s, 1H), 4.70 (s, 2H), 7.16-7.36 (m, 5H). ^{13}C NMR (CDCl_3 , 75 MHz) : δ 19.2, 54.8, 127.0, 129.9, 130.3, 132.0, 133.3, 140.1, 143.8, 146.7. MS (m/z) : 190 ($\text{M}^+ + 1$). Elemental Analysis for $\text{C}_{10}\text{H}_{11}\text{N}_3\text{O}$ Calculated: C, 63.48; H, 5.86; N, 22.21. Found: C, 63.44; H, 5.91; N, 22.29.



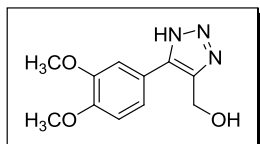
(5-*p*-Tolyl-1H-1,2,3-triazol-4-yl)methanol (3c)

Colourless solid Yield: 82% M. P: 127-129 °C IR (KBr): 3425, 3224, 1706, 1627 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 2.24 (s, 1H), 2.41 (s, 3H), 4.93 (s, 2H), 7.26-7.67 (m, 4H), 11.94 (s, 1H). ¹³C NMR (75 MHz): δ 21.2, 55.0, 127.3, 129.4, 129.5, 138.2, 142.4, 144.5. MS (m/z): 190 (M⁺+1). Elemental Analysis for C₁₀H₁₁N₃O Calculated : C, 63.48; H, 5.86; N, 22.21. Found : C, 63.55; H, 5.83; N, 22.27.



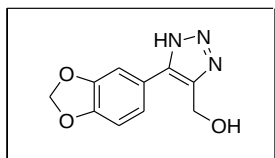
(5-(4-Ethylphenyl)-1H-1,2,3-triazol-4-yl)methanol (3d)

Colourless solid Yield : 92% M. P : 98-100 °C IR (KBr) : 3321, 3198, 1715, 1628 cm⁻¹ ¹H NMR (CDCl₃ + (2 drops) DMSO-d₆, 300 MHz): δ 1.21 (t, *J* = 7.5Hz, 3H), 2.65 (q, *J* = 7.5Hz, 2H), 4.63 (s, 2H), 5.36 (s, 1H), 7.30-7.74 (m, 4H), 14.77 (s, 1H). ¹³C NMR (CDCl₃ + (2 drops) DMSO-d₆, 300 MHz) : δ 15.5, 27.9, 54.3, 127.1, 128.1, 131.0, 138.2, 141.0, 144.3. MS (m/z) : 204 (M⁺+1). Elemental Analysis for C₁₁H₁₃N₃O Calculated: C, 65.01; H, 6.45; N, 20.68 Found: C, 65.06; H, 6.42; N, 20.77.



(5-(3,4-Dimethoxyphenyl)-1H-1,2,3-triazol-4-yl)methanol (3e)

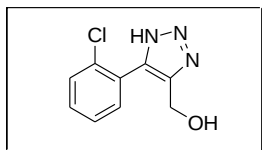
Colourless solid Yield : 80% M. P : 106-108 °C IR (KBr): 3422, 3234, 1727, 1625 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 3.89 (s, 3H), 3.91 (s, 3H), 4.82 (s, 2H), 5.74 (s, 1H), 6.88-7.38 (m, 4H). ¹³C NMR (CDCl₃, 75 MHz) : δ 55.9, 56.0, 56.2, 110.7, 111.3, 120.2, 120.4, 134.8, 144.8, 146.7, 149.3. MS (m/z): 236 (M⁺+1). Elemental Analysis for C₁₁H₁₃N₃O₃ Calculated: C, 56.16; H, 5.57; N, 17.86. Found: C, 56.20; H, 5.61; N, 17.90.



(5-(Benzo[d][1,3]dioxol-6-yl)-1H-1,2,3-triazol-4-yl)methanol (3f)

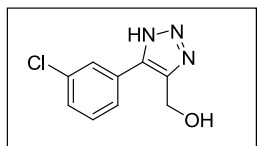
Colourless solid Yield : 92% M. P : 151-153 °C IR (KBr) : 3431, 3224, 1715, 1602 cm⁻¹ ¹H NMR (CDCl₃ + (2 drops) DMSO-d₆, 300 MHz) : δ 4.63 (s, 2H), 5.48, (s, 1H), 6.07 (s, 2H), 7.01-7.38 (m, 3H), 15.04 (s, 1H). ¹³C NMR (CDCl₃ + (2 drops) DMSO-d₆, 75 MHz) : δ 53.8, 101.1, 107.3, 108.6, 120.9,

124.3, 132.1, 142.1, 147.1, 147.6. MS (m/z): 220 (M^+ +1). Elemental Analysis for $C_{10}H_9N_3O_3$ Calculated: C, 54.79; H, 4.14; N, 19.17. Found : C, 54.82; H, 4.20; N, 19.22.



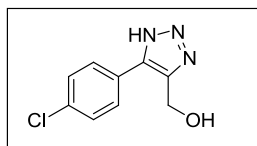
(5-(2-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methanol (3g)

Colourless solid Yield : 80% M. P: 140-142 $^{\circ}C$ IR (KBr): 3433, 3225, 1735, 1615 cm^{-1} 1H NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 300 MHz): δ 4.68 (s, 2H), 5.49 (s, 1H), 7.45-7.92 (m, 4H), 14.96 (s, 1H). ^{13}C NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 75 MHz) : δ 54.2, 125.5, 126.5, 127.7, 130.6, 133.1, 133.5, 143.0, 143.9. MS (m/z): 209 (M^+), 211 (M^+ +2). Elemental Analysis for $C_9H_8ClN_3O$ Calculated : C, 51.56; H, 3.85; N, 20.04 Found: C, 51.61; H, 3.78; N, 20.12.



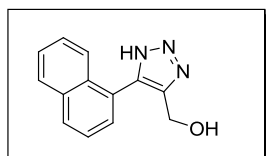
(5-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methanol (3h)

Colourless solid Yield : 81% M. P : 138-140 $^{\circ}C$ IR (KBr): 3424, 3217, 1740, 1620 cm^{-1} 1H NMR ($CDCl_3$, 300 MHz) : δ 4.66 (s, 2H), 5.33 (s, 1H), 5.75 (s, 1H), 7.21-7.39 (m, 4H). ^{13}C NMR ($CDCl_3$, 75 MHz) : δ 55.03, 126.93, 127.00, 129.87, 130.33, 131.99, 133.32, 140.38, 143.91. MS (m/z) : 209 (M^+), 211 (M^+ +2). Elemental Analysis for $C_9H_8ClN_3O$ Calculated : C, 51.56; H, 3.85; N, 20.04. Found: C, 51.51; H, 3.87; N, 20.13.



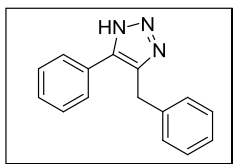
(5-(4-Chlorophenyl)-1H-1,2,3-triazol-4-yl)methanol (3i)

Colourless solid Yield : 83% M. P: 131-133 $^{\circ}C$ IR (KBr): 3425, 3219, 1710, 1634 cm^{-1} 1H NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 300 MHz): δ 2.91 (s, 1H), 4.59 (s, 1H), 4.82 (s, 2H), 7.39-7.85 (m, 4H). ^{13}C NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 75 MHz) : δ 60.2, 131.8, 133.5, 134.6, 138.4, 145.5, 148.5. MS (m/z): 209 (M^+), 211 (M^+ +2). Elemental Analysis for $C_9H_8ClN_3O$ Calculated : C, 51.56; H, 3.85; N, 20.04. Found: C, 51.59; H, 3.92; N, 20.09.



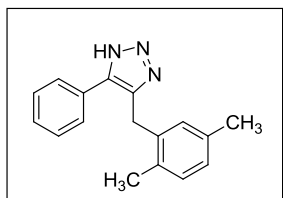
5-(Naphthalen-1-yl)-1H-1,2,3-triazol-4-yl)methanol (3j)

Colourless solid Yield : 85% M. P : 127-129 °C IR (KBr) : 3421, 3214, 1720, 1610 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 4.67 (s, 2H), 5.86 (s, 1H), 7.33-7.88 (m, 8H). ¹³C NMR (CDCl₃, 75 MHz) : δ 55.3, 125.1, 125.2, 126.3, 126.9, 128.4, 128.5, 129.6, 131.7, 133.7, 137.0, 142.1, 145.5. MS (m/z) : 226 (M⁺+1). Elemental Analysis for C₁₃H₁₁N₃O Calculated : C, 69.32; H, 4.92; N, 18.66. Found : C, 69.33; H, 4.96; N, 18.93.



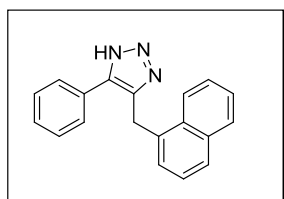
4-Benzyl-5-phenyl-1H-1,2,3-triazole (7)

Colourless solid Yield : 84% M. P: 116-118 °C IR (KBr): 3426, 3228, 1719, 1635 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 1.86 (s, 1H), 4.25 (s, 2H), 7.21-7.64 (m, 10H). ¹³C NMR (CDCl₃, 75 MHz) : δ 31.0, 126.6, 127.6, 128.4, 128.5, 128.7, 128.8, 130.2, 138.2, 141.0, 143.7. MS (m/z) : 236 (M⁺+1). Elemental Analysis for C₁₅H₁₃N₃ Calculated : C, 76.57; H, 5.57; N, 17.86. Found : C, 76.60; H, 5.65; N, 17.87.



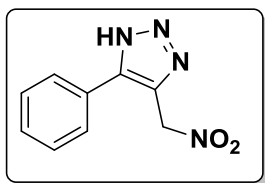
4-(2,5-dimethylbenzyl)-5-phenyl-1H-1,2,3-triazole (8)

Colourless solid Yield : 81% M. P : 120-122 °C IR (KBr) : 3431, 3223, 1715, 1630 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 2.20 (s, 3H), 2.23 (s, 3H), 2.21 (s, 1H), 4.14 (s, 2H), 6.83-7.65 (m, 8H). ¹³C NMR (CDCl₃, 75 MHz) : δ 19.1, 21.0, 29.0, 127.5, 127.7, 128.3, 128.8, 129.7, 130.3, 130.5, 133.0, 135.8, 135.9, 140.6, 144.2. MS (m/z) : 264 (M⁺+1). Elemental Analysis for C₁₇H₁₇N₃ Calculated : C, 77.54; H, 6.51; N, 15.96. Found : C, 77.55; H, 6.48; N, 15.98.



4-(Naphthalen-1-ylmethyl)-5-phenyl-1H-1,2,3-triazole (9)

Colourless solid Yield : 83% M. P : 123-125 °C IR (KBr) : 3411, 3204, 1712, 1609 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 4.67 (s, 2H), 7.17-7.96 (m, 12H), 11.85 (s, 1H). ¹³C NMR (CDCl₃, 75 MHz) : δ 28.6, 123.5, 125.6, 125.8, 126.1, 126.3, 126.4, 126.8, 127.5, 127.6, 128.4, 128.8, 130.3, 131.7, 133.8, 140.3, 144.0. MS (m/z) : 286 (M⁺+1). Elemental Analysis for C₁₉H₁₅N₃ Calculated : C, 79.98; H, 5.30; N, 14.73. Found : C, 79.93; H, 5.36; N, 14.74.

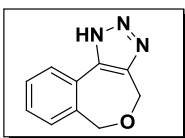


4-(nitromethyl)-5-phenyl-1H-1,2,3-triazole (16)

Brown Colour Solid Yield : 81% M. P : 145-147 °C IR (KBr) : 3411, 3215, 1731, 1622, 1530 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) : δ 4.76 (s, 2H), 7.28-7.50 (m, 5H), 7.65 (s, 1H). ¹³C NMR (CDCl₃, 100 MHz) : δ 62.8, 129.3, 130.4, 131.2, 132.4, 140.0, 163.7; MS (m/z) : 205 (M⁺+1). Elemental Analysis for C₉H₈N₄O₂ Calculated : C, 52.94; H, 3.95; N, 27.44; O, 15.67. Found : C, 52.85; H, 3.98; N, 27.49; O, 15.66.

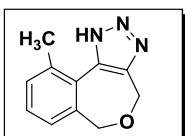
Typical experimental procedure for the synthesis of benzoxepino-1,2,3-triazol (11a)

To a stirred solution of 4-nitro-1,3-dihydrobenzo[c]oxepine (**10a**) (0.38g, 2 mmol) in DMSO (3 ml), sodium azide (**2**) (0.39g, 2mmol) was added and the reaction mixture was kept at 80 °C for 0.5 h. After completion of the reaction as indicated by TLC, the reaction mixture was diluted with water (10 ml) and extracted with ethylacetate (20 ml). The organic layer thus obtained was washed with brine solution (10 ml). The crude sample was purified by column chromatography (20%, EtOAc / hexanes) to provide the desired pure product **11a** as colorless solid in 96% (0.36g) yield.



4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11a)

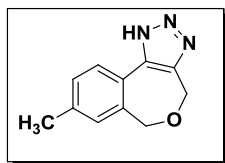
Colourless solid Yield : 96% M. P : 129-131 °C IR (KBr) : 3205, 1720, 1610 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 3.73 (s, 1H), 4.81 (s, 2H), 5.20 (s, 2H), 7.22-7.44 (m, 3H), 8.15-8.18 (m, 1H). ¹³C NMR (CDCl₃, 75 MHz) : δ 68.8, 74.4, 126.6, 128.4, 128.6, 128.9, 129.0, 137.7, 142.7, 144.4. MS (m/z): 188 (M⁺+1). Elemental Analysis for C₁₀H₉N₃O Calculated: C, 64.16; H, 4.85; N, 22.45. Found: C, 64.24; H, 4.87; N, 22.46.



10-methyl-4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11b)

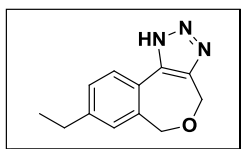
Colourless solid Yield : 90% M. P : 132-134 °C IR (KBr) : 3148, 1698, 1622 cm⁻¹ ¹H NMR (CDCl₃, 300 MHz) : δ 2.69 (s, 3H), 4.58 (s, 2H), 5.15 (s, 2H), 7.17-7.33 (m, 3H), 12.93 (s, 1H). ¹³C NMR (CDCl₃ + (2 drops) DMSO-d₆, 75 MHz) : δ 27.1, 71.1, 76.1, 131.5, 132.2, 133.9, 136.3, 141.9, 143.6, 147.4, 149.2.

MS (m/z) : 202 ($M^+ + 1$). Elemental Analysis for $C_{11}H_{11}N_3O$ Calculated : C, 65.66; H, 5.51; N, 20.88. Found : C, 65.69; H, 5.55; N, 20.95.



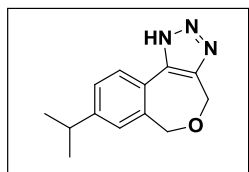
8-methyl-4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11c)

Colourless solid Yield : 94% M. P: 127-129 $^{\circ}C$ IR (KBr) : 3178, 1710, 1620 cm^{-1} 1H NMR ($CDCl_3$, 300 MHz) : δ 2.38 (s, 3H), 4.78 (s, 2H) 5.18 (s, 2H), 7.04-7.26 (m, 2H), 8.03 (d, $J = 8.1$, 1H), 11.87 (s, 1H). ^{13}C NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 75 MHz) : δ 20.6, 67.7, 73.5, 126.0, 128.7, 128.9, 131.7, 137.1, 137.5, 141.6, 144.4. MS (m/z) : 202 ($M^+ + 1$). Elemental Analysis for $C_{11}H_{11}N_3O$ Calculated : C, 65.66; H, 5.51; N, 20.88. Found : C, 65.67; H, 5.47; N, 20.90.



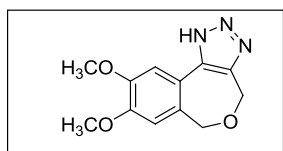
8-ethyl-4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11d)

Colourless solid Yield : 96% M. P : 131-133 $^{\circ}C$ IR (KBr) : 3225, 1740, 1640 cm^{-1} 1H NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 300 MHz) : δ 1.19 (t, $J = 7.5Hz$, 3H), 2.61 (q, $J = 7.5Hz$, 2H), 4.76 (s, 2H), 5.06 (s, 2H), 7.13-8.10 (m, 3H), 14.98 (s, 1H). ^{13}C NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 75 MHz) : δ 15.4, 27.8, 68.2, 73.7, 125.9, 127.0, 127.5, 127.7, 137.8, 142.0, 143.4, 144.0. MS (m/z) : 216 ($M^+ + 1$). Elemental Analysis for $C_{12}H_{13}N_3O$ Calculated : C, 66.96; H, 6.09; N, 19.52. Found : C, 66.94; H, 6.14; N, 19.59.



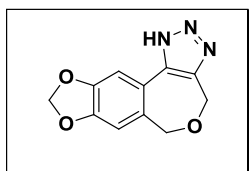
8-isopropyl-4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11e)

Colourless solid Yield : 96% M. P : 135-137 $^{\circ}C$ IR (KBr) : 3157, 1712, 1618 cm^{-1} 1H NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 75 MHz) : δ 1.27 (d, $J = 6.9Hz$, 6H), 1.78 (s, 1H), 2.93 (sep, $J = 6.9Hz$, 1H), 4.80 (s, 2H), 5.19 (s, 2H), 7.08 (s, 1H), 7.29 (s, 1H), 8.06 (d, $J = 7.8Hz$, 1H). ^{13}C NMR ($CDCl_3$ + (2 drops) $DMSO-d_6$, 300 MHz) : δ 28.7, 38.5, 73.8, 79.4, 128.1, 131.1, 132.3, 137.0, 142.3, 147.4, 148.8, 153.3. MS (m/z) : 230 ($M^+ + 1$). Elemental Analysis for $C_{13}H_{15}N_3O$ Calculated : C, 68.10; H, 6.59; N, 18.33. Found : C, 68.14; H, 6.63; N, 18.38.



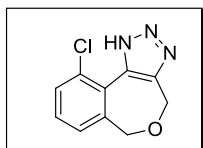
8,9-dimethoxy-4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11f)

Colourless solid Yield : 82% M. P : 167-169⁰C IR (KBr) : 3195, 1715, 1620 cm⁻¹ ¹H NMR (CDCl₃ + (2 drops) DMSO-d₆, 300 MHz) : δ 3.91 (s, 3H), 3.96 (s, 3H), 4.73 (s, 2H), 5.14 (s, 2H), 6.73 (s, 1H), 7.45 (s, 1H), 7.71 (s, 1H). ¹³C NMR (CDCl₃ + (2 drops) DMSO-d₆, 75 MHz) : δ 55.0, 55.2, 70.8, 73.1, 108.7, 110.6, 119.2, 127.8, 123.0, 147.4, 147.8, 148.2. MS (m/z) : 248 (M⁺+1). Elemental Analysis for C₁₂H₁₃N₃O₃ Calculated : C, 58.29; H, 5.30; N, 17.00. Found : C, 58.30; H, 5.35; N, 17.09.



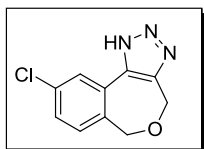
4,6-dihydro-1H-[1,3]dioxolo[4'',5'':4',5']benzo[1',2':5,6]oxepino[3,4-d][1,2,3]triazole (11g)

Colourless solid Yield : 81% M. P : 154-156⁰C IR (KBr) : 3178, 1714, 1609 cm⁻¹ ¹H NMR (CDCl₃ + (2 drops) DMSO-d₆, 300 MHz) : δ 4.69 (s, 2H), 5.16 (s, 2H), 6.01 (s, 2H), 6.71 (s, 1H), 7.29 (s, 1H), 7.62 (s, 1H). ¹³C NMR (CDCl₃ + (2 drops) DMSO-d₆, 75 MHz) : δ 73.5, 78.4, 106.3, 111.2, 113.6, 128.9, 137.1, 147.1, 148.4, 151.9, 152.4. MS (m/z) : 232(M⁺+1). Elemental Analysis for C₁₁H₉N₃O₃ Calculated : C, 57.14; H, 3.92; N, 18.17. Found : C, 57.20; H, 3.89; N, 18.25.



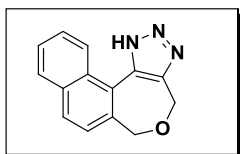
10-chloro-4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11h)

Colourless solid Yield : 82% M. P : 144-146⁰C IR (KBr) : 3167, 1715, 1602 cm⁻¹ ¹H NMR (CDCl₃ + (2 drops) DMSO-d₆, 300 MHz) : δ 1.80 (s, 1H), 4.76 (s, 2H), 5.17 (s, 2H), 7.13-7.27 (m, 2H), 8.19 (d, J = 2.1Hz, 1H). ¹³C NMR (CDCl₃ + (2 drops) DMSO-d₆, 75 MHz) : δ 68.9, 73.8, 126.6, 127.8, 129.1, 129.6, 131.1, 134.4, 136.0, 144.3. MS (m/z) : 222 (M⁺+1), 223 (M⁺+2). Elemental Analysis for C₁₀H₈ClN₃O Calculated : C, 54.19; H, 3.64; N, 18.96. Found : C, 54.16; H, 3.69; N, 18.97.



9-chloro-4,6-dihydro-1H-benzo[5,6]oxepino[3,4-d][1,2,3]triazole (11i)

Colourless solid Yield : 86% M. P : 130-132⁰C IR (KBr): 3215, 1710, 1600 cm⁻¹ ¹H NMR (CDCl₃ + (2 drops) DMSO-d₆, 300 MHz) : δ 4.48 (s, 2H), 4.74 (s, 1H), 5.08 (s, 2H), 7.17-7.45 (m, 3H). ¹³C NMR (CDCl₃, 75 MHz) : δ 65.7, 70.1, 126.4, 126.8, 127.9, 129.3, 130.0, 131.1, 140.0, 143.4. MS (m/z) : 222 (M⁺+1), 223 (M⁺+2). Elemental Analysis for C₁₀H₈ClN₃O Calculated : C, 54.19; H, 3.64; N, 18.96. Found : C, 54.25; H, 3.60; N, 18.98.



4,6-dihydro-1H-naphtho[1',2':5,6]oxepino[3,4-d][1,2,3]triazole (11j)

Colourless solid Yield : 92% M. P : 140-142 °C IR (KBr): 3189, 1715, 1620 cm^{-1} ^1H NMR (CDCl_3 , 300 MHz) : δ 4.71 (s, 2H), 5.15 (s, 2H), 7.45-7.92 (m, 5H); 9.00 (d, $J = 8.4\text{Hz}$, 1H), 12.24 (s, 1H). ^{13}C NMR (CDCl_3 , 75 MHz) : δ 65.8, 71.1, 126.3, 126.3, 127.1, 127.2, 127.2, 128.4, 129.2, 129.3, 130.8, 133.9, 137.2, 145.7. MS (m/z) : 238 ($\text{M}^+ + 1$). Elemental Analysis for $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}$ Calculated : C, 70.87; H, 4.67; N, 17.71. Found : C, 70.89; H, 4.61; N, 17.79.

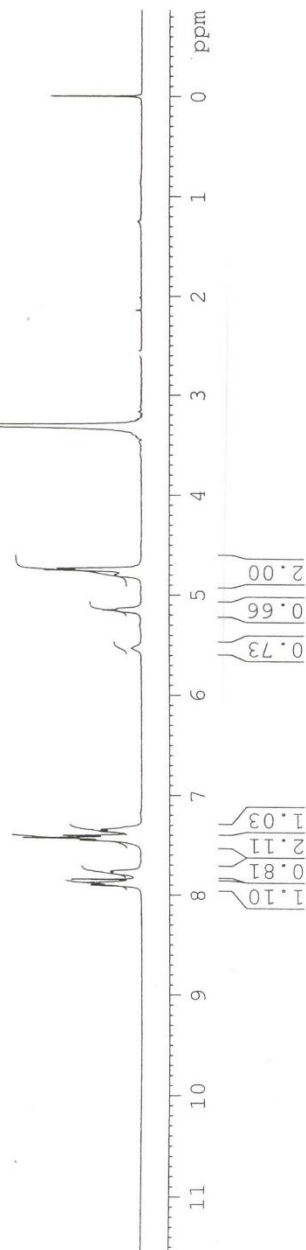
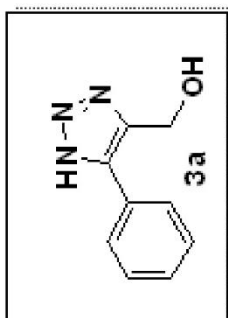


Current Data Parameters
 NAME NSK-X-OH-Ph-N3
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20100711
 Time 9.08
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 SMH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 228.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 1H
 PL1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1314047 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00

3.311

5.534
5.157
4.757
4.740

7.906
7.882
7.847
7.787
7.765
7.459
7.435
7.410
7.369
7.346





Current Data Parameters
 NAME NSK-X-PH-OH-N3
 EXENO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100724
 Time_ 22.54
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1014
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

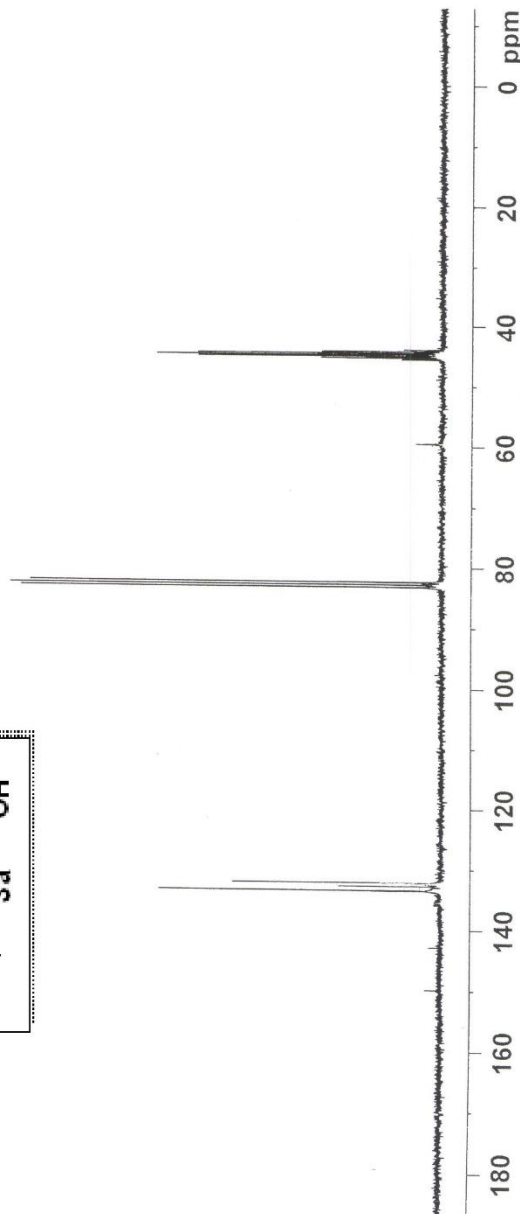
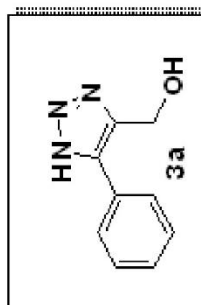
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.86 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

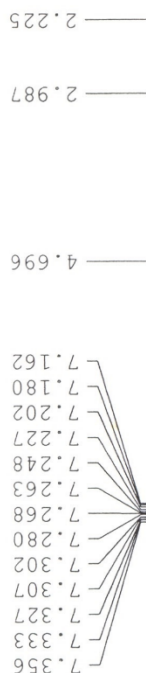
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

59.51
 45.58
 45.30
 45.02
 44.74
 44.47
 44.19
 43.91

83.20
 82.77
 82.34

149.79
 142.84
 133.54
 133.46
 132.74
 132.17

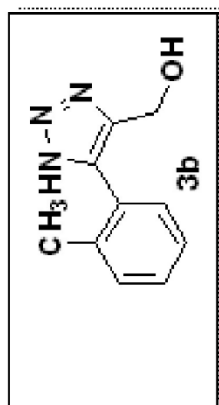




4.696

2.987

2.225

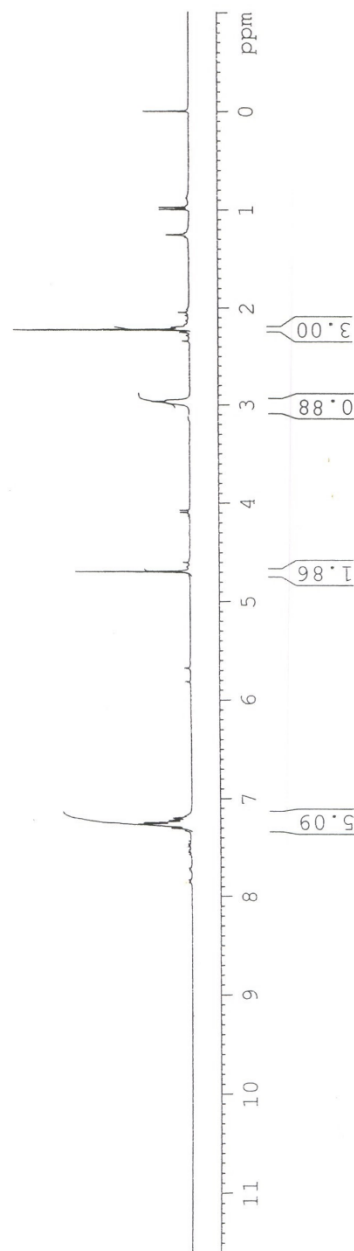


Current Data Parameters
NAME NSK-X-171
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100316
Time_ 15.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 203.2
DM 81.000 usec
DE 30.0 usec
TE 300.0 K
D1 1.00000000 sec
D11 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.40 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300058 MHz
WDW EM
SSB 0
CB 0
GB 0
PC 1.00





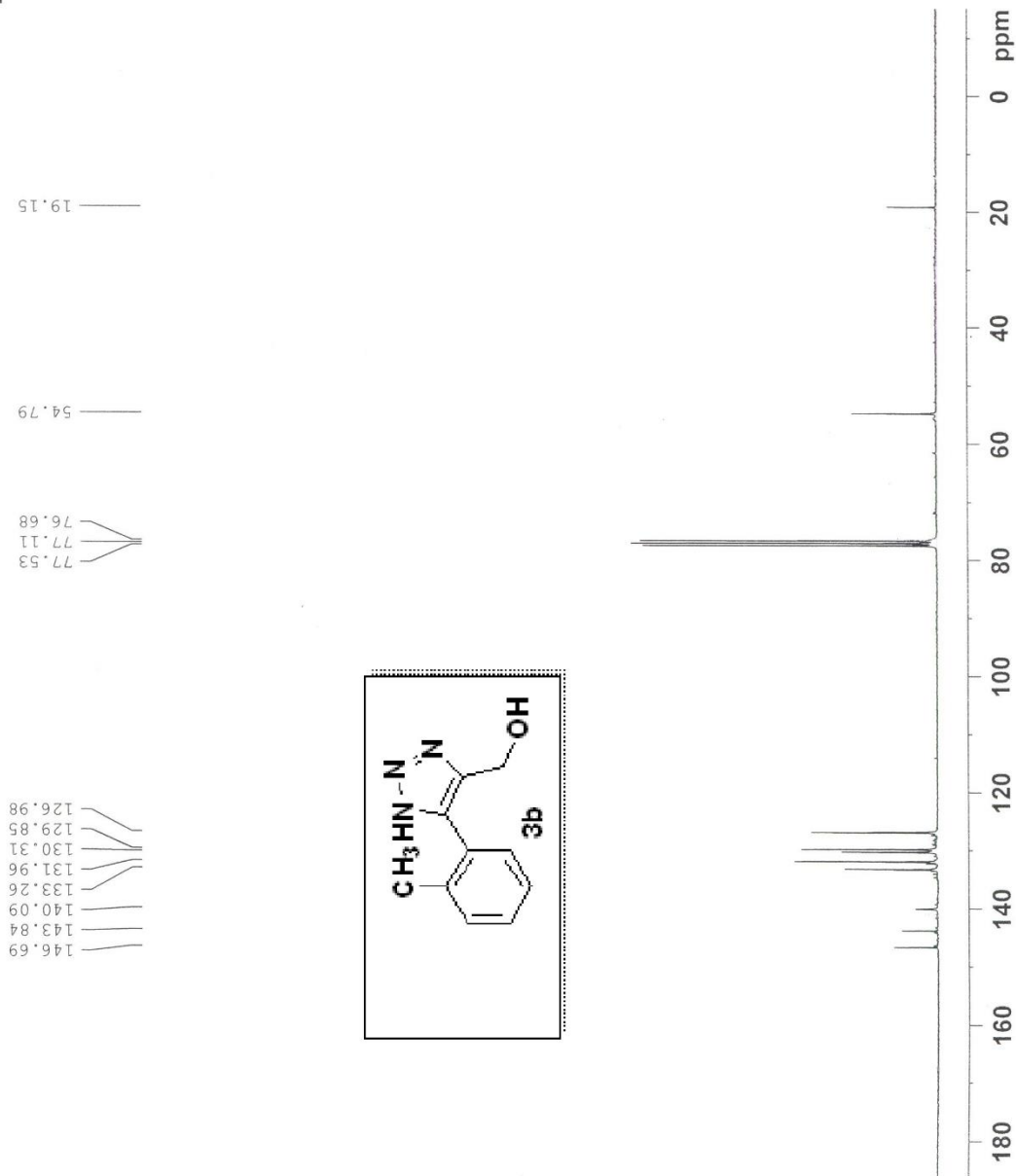
Current Data Parameters
 NAME NSR-X-2CH3OHN2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110223
 Time_ 8.43
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 6536
 SOLVENT CDC13
 NS 6920
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 812.7
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

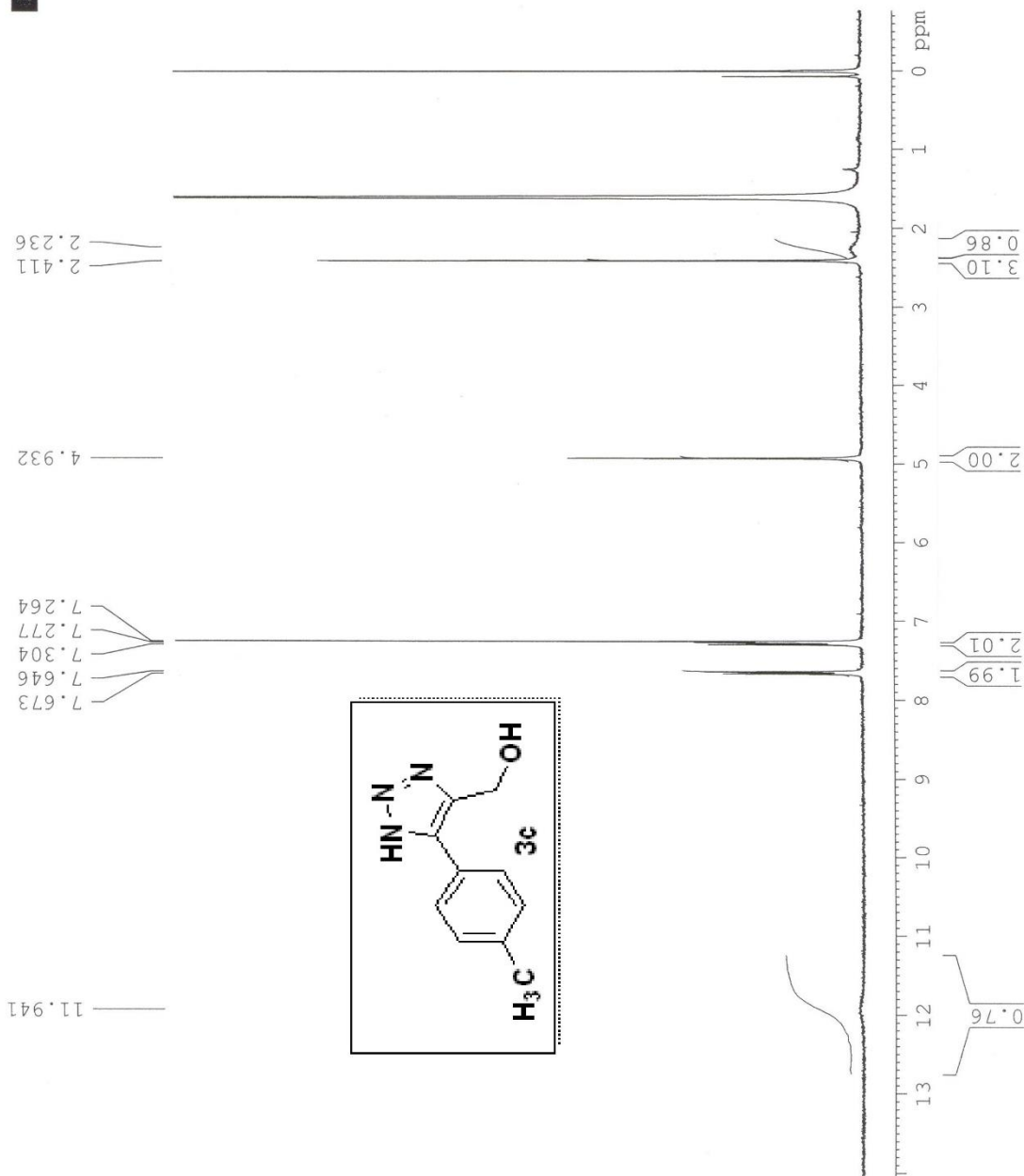
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing Parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME NSK-X-172
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20100302
 Time 13.00
 INSTRUM spect
 PROHD 5 mm BUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 1
 SH 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 645.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1
 CHANNEL f1
 NUC1 1H
 P1 12.40 usec
 PL1 0.00 dB
 SFO1 300.1318594 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300052 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME NSK-4Me-N3-OH
 EXENO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101215
 Time_ 0.42
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1668
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 512
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SF01 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SF02 300.1312005 MHz

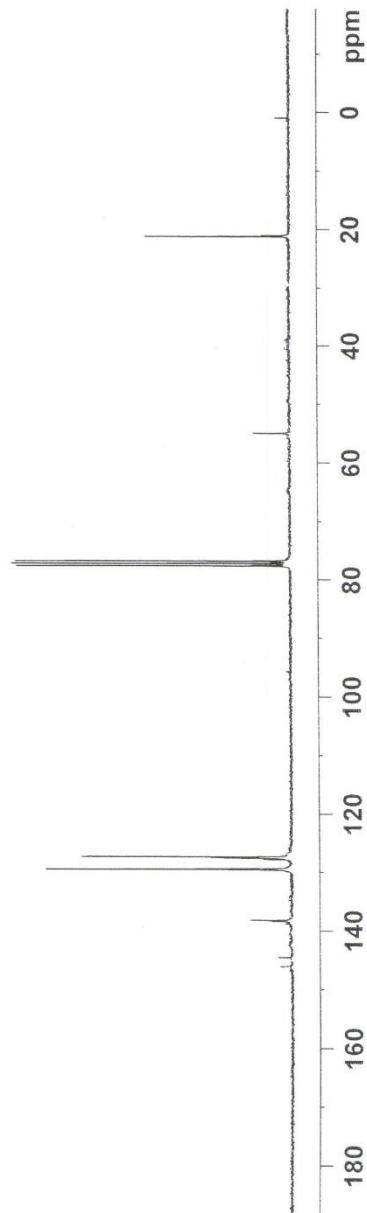
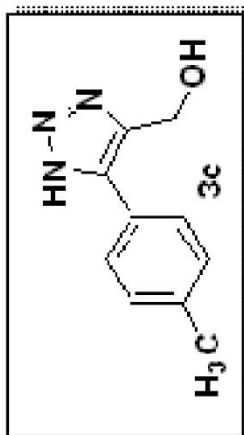
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EM
 WDW 0
 SSB 1.00 Hz
 LB 0
 GB 0
 PC 1.40

21.20

55.00

77.64
77.21
76.79

144.51
142.42
138.17
129.50
129.39
127.33

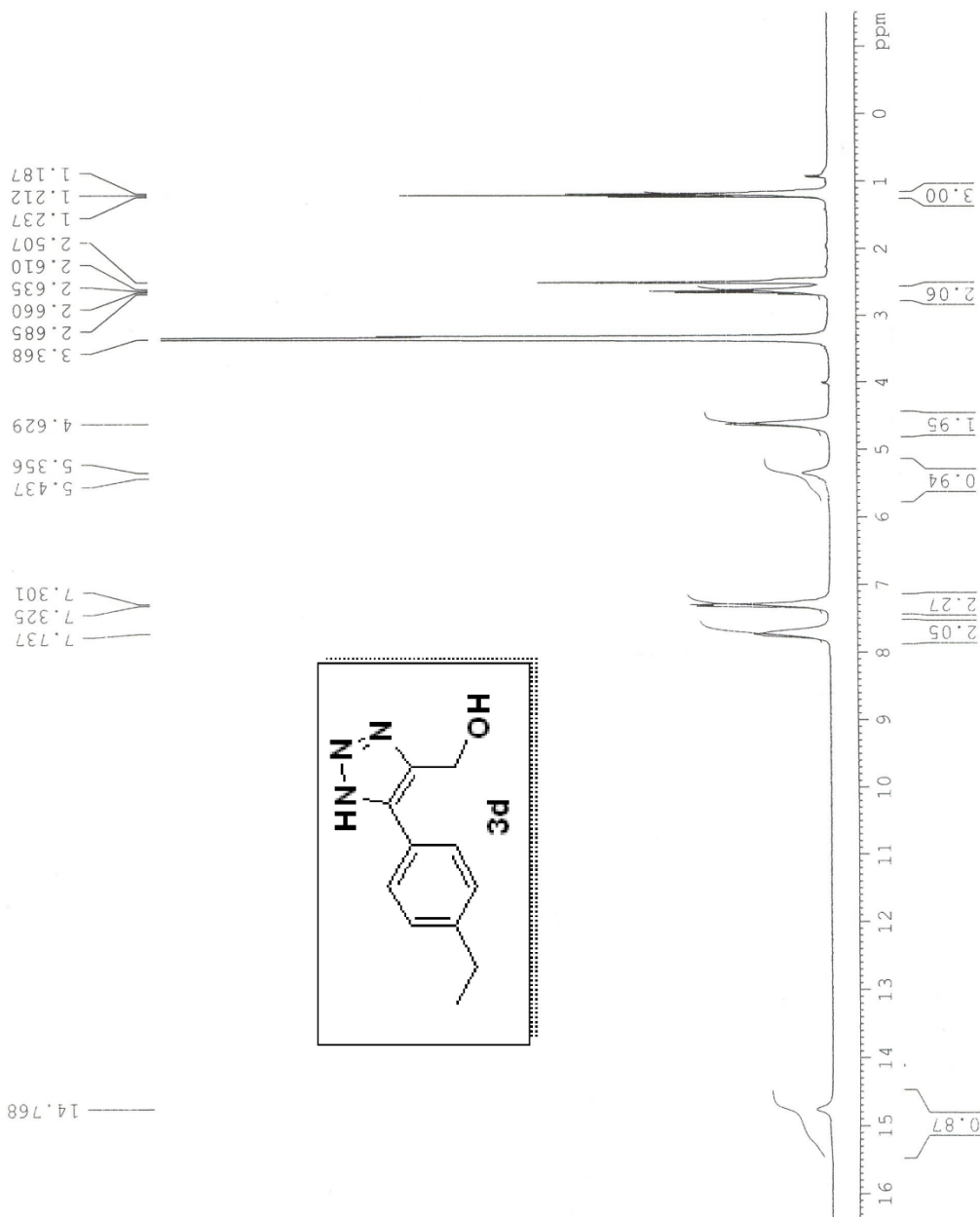




Current Data Parameters
 NAME nsk-x-193
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100714
 Time 0.20
 INSTRUM spect
 PROBU 5 mm DUL 130C1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 228.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME NSK-X-193
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100711
 Time 20.55
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 5000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 574.7
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

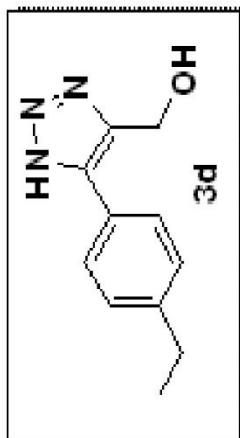
===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

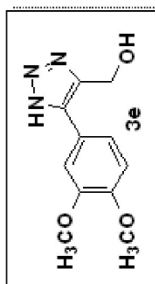
F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 EM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

54.25
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 39.49
 39.21
 38.94
 38.66
 27.89
 15.49

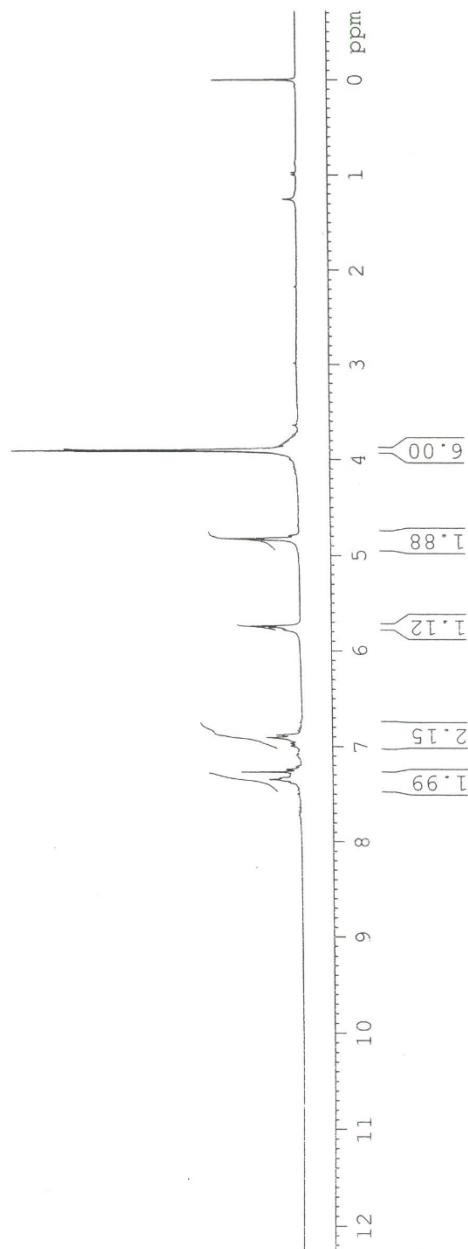
144.32
 141.04
 138.21
 130.97
 128.07
 127.06



ppm



Current Data Parameters
 NAME NSK-X-dich3-OH-N3
 EXNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date 20101130
 Time 20.53
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 228.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 1H
 PL 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300042 MHz
 EM 0
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





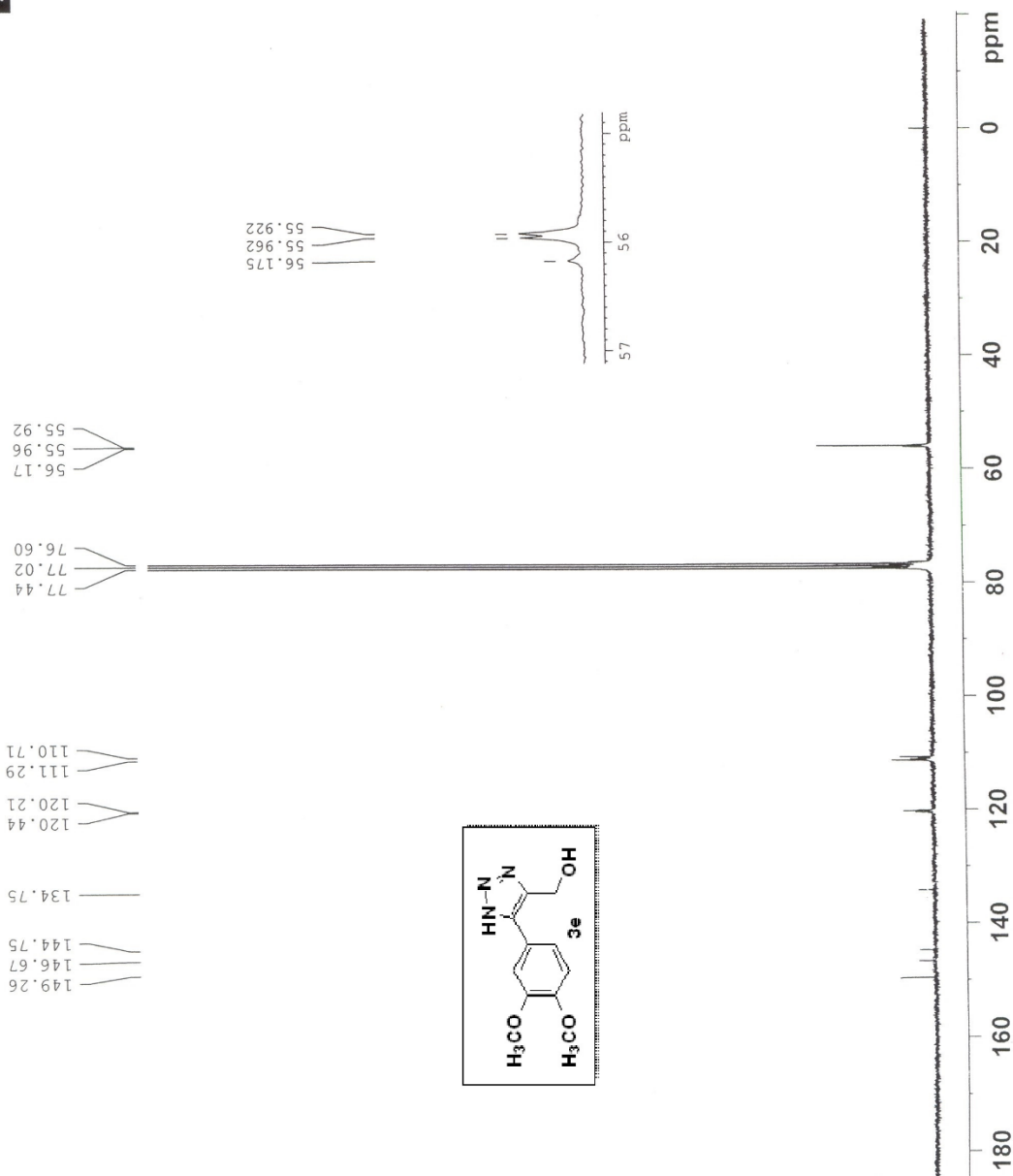
Current Data Parameters
 NAME NSK-X-diome-OH-N3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101201
 Time 8.12
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 5476
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 574.7
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing Parameters
 SI 32768
 SF 75.4677490 MHz
 EM 0
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





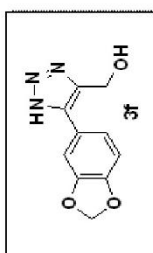
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 NAME NSK-X-152
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100720
 Time 22.25
 INSTRUM spect
 PROHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 4
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 57
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 TD0 1

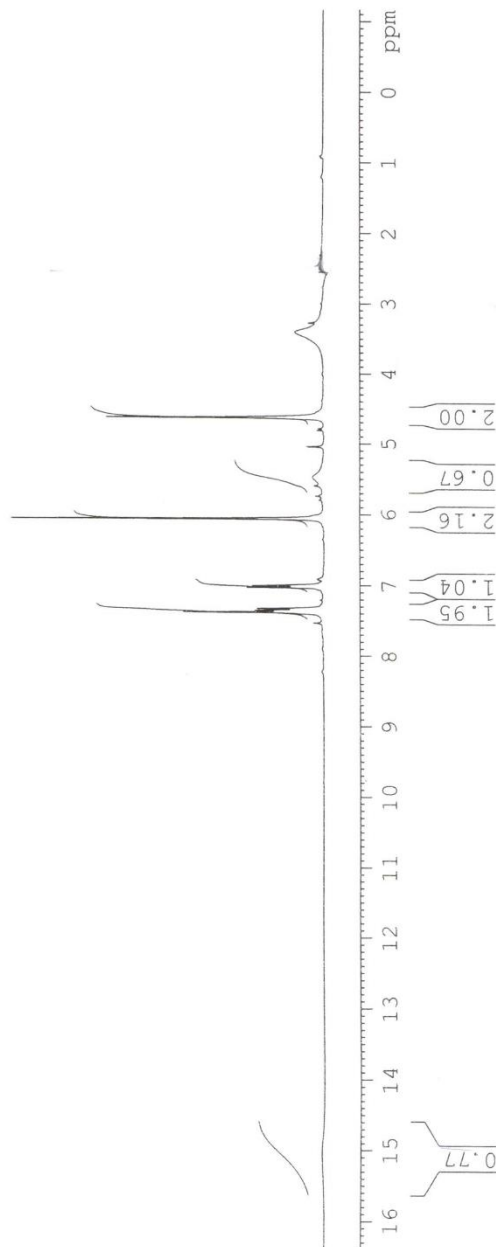
===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing Parameters
 SI 32768
 SF 300.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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 7.331
 7.033
 7.007
 6.066
 5.477
 4.630



15.042





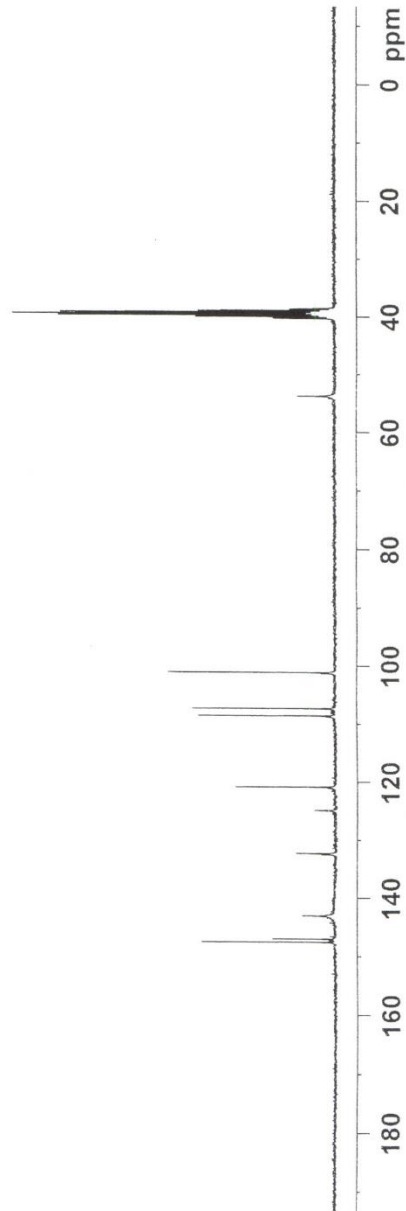
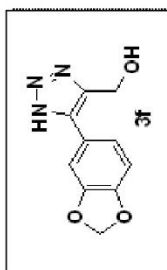
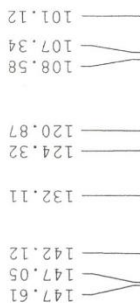
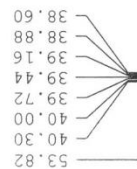
Current Data Parameters
 NAME NSK-X-152
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100720
 Time_ 22.30
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 810
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 724.1
 DM 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999999 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

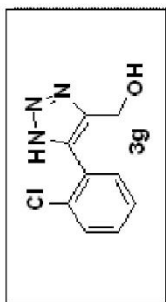
F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 EM 0
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



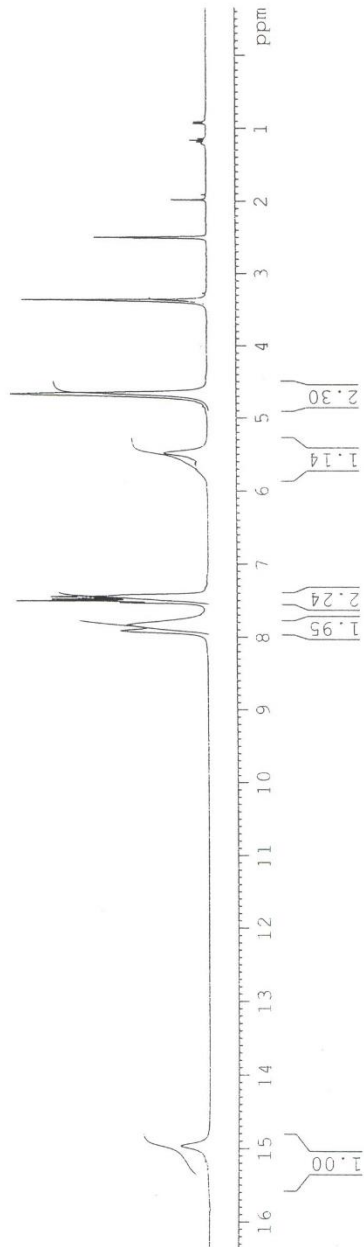


Current Data Parameters
 NAME nsk-x-199
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date 20100630
 Time 7.04
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 143.7
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.921
 7.838
 7.537
 7.511
 7.485
 7.454
 5.486
 4.675
 3.365



14.965





Current Data Parameters
 NAME NSK-X-199
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20100704
 Time 22.28
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1925
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DE 27.800 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====

NUC1 13C
 PL 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====

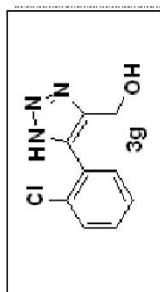
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768
 SF 75.4677867 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

54.23
 40.30
 40.02
 39.74
 39.47
 39.19
 38.91
 38.63

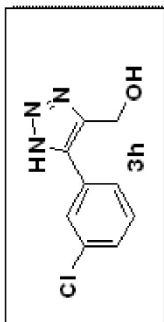
143.89
 143.01
 133.48
 133.13
 130.62
 127.66
 126.54
 125.52



180 160 140 120 100 80 60 40 20 0 ppm



7.393
7.366
7.339
7.324
7.299
7.273
7.266
7.251
7.234
7.211
5.755
5.741
5.330
4.662

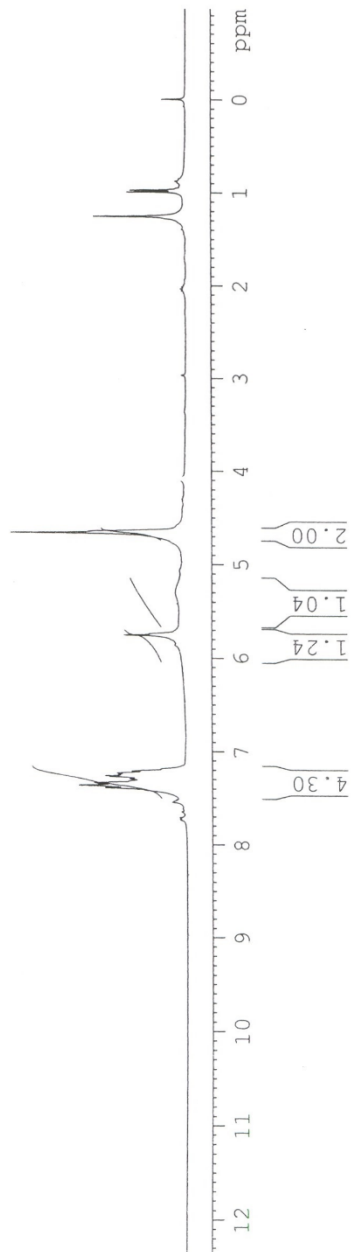


Current Data Parameters
NAME NSK-X-3Cl-OH-N3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101211
Time 17.59
INSTRUM spect
PROBHD 5 mm DUL 15C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 101.6
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300047 MHz
WDW EM
SSB 0
GB 0
PC 1.00





Current Data Parameters
 NAME NSK-3Cl-OH-N3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101211
 Time 21.44
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 819
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.6219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SF01 75.4752953 MHz

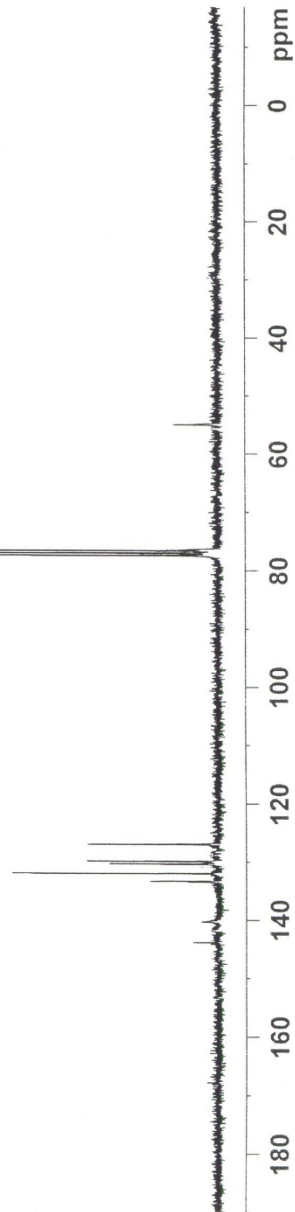
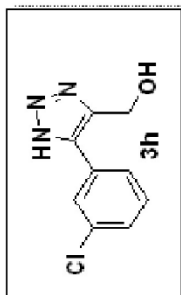
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

55.03

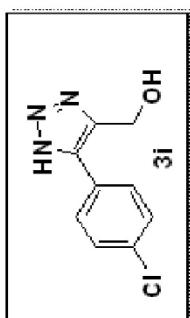
77.47
77.05
76.62

143.91
140.38
133.32
131.99
130.33
129.87
127.00
126.93

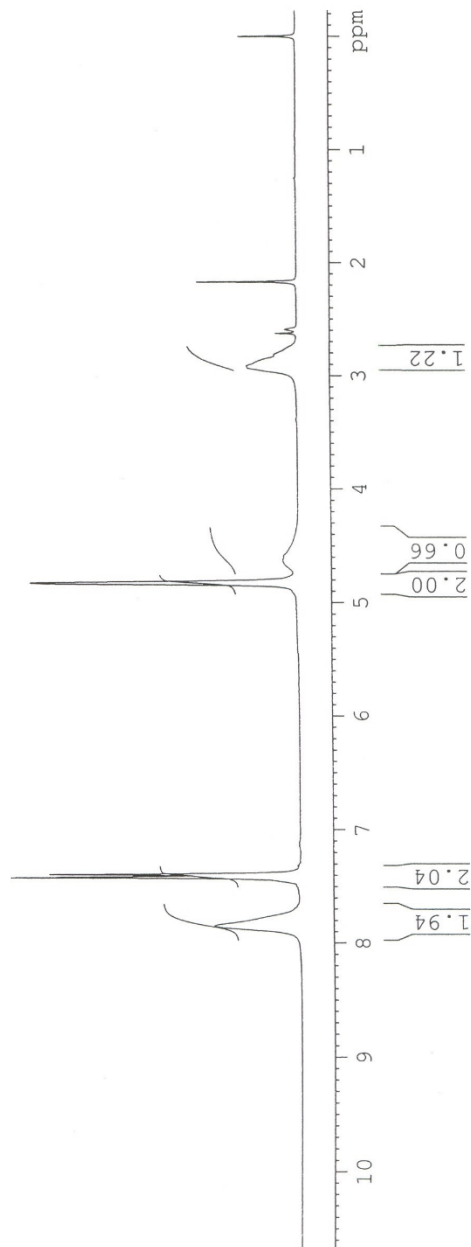




7.848 —
7.420 —
7.392 —
4.824 —
4.634 —
4.586 —
2.914 —
2.171 —



Current Data Parameters
NAME NSK-X-4Cl-OH-Azide
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100728
Time 12.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 203.2
DM 81.000 usec
DE 3.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1314007 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





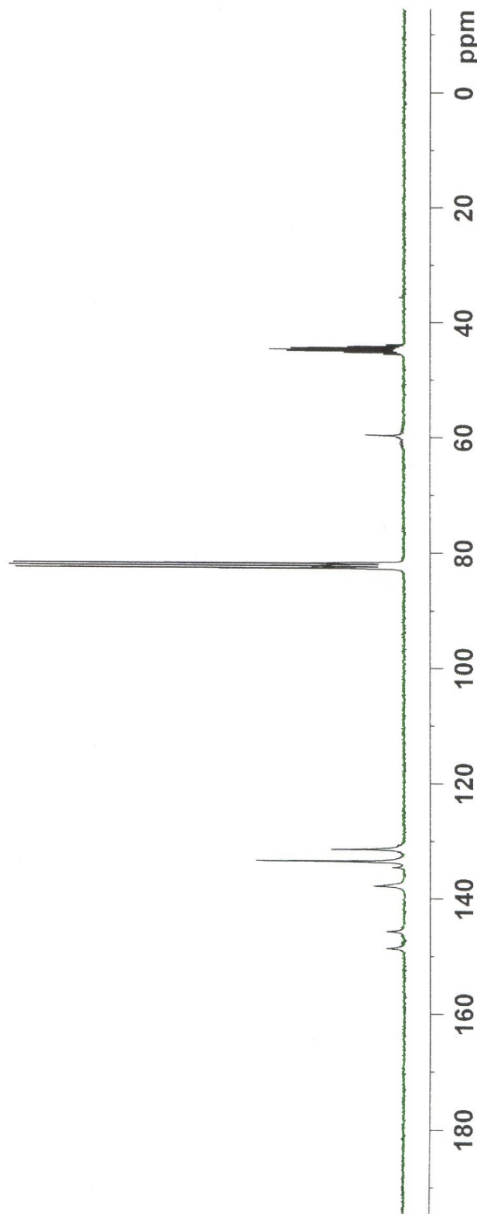
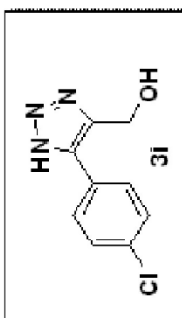
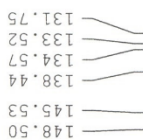
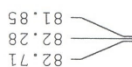
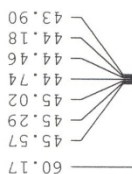
Current Data Parameters
 NAME NSK-X4Cl-OH-Azide
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100728
 Time 1.31
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65336
 SOLVENT CDCl3
 NS 7151
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 645.1
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EM 0
 WDW 0
 SSB 1.00 Hz
 LB 0
 GB 0
 PC 1.40





Current Data Parameters
 NAME NSK-X-Naph-OH-N3
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101130
 Time_ 21.02
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 11
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 2260
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

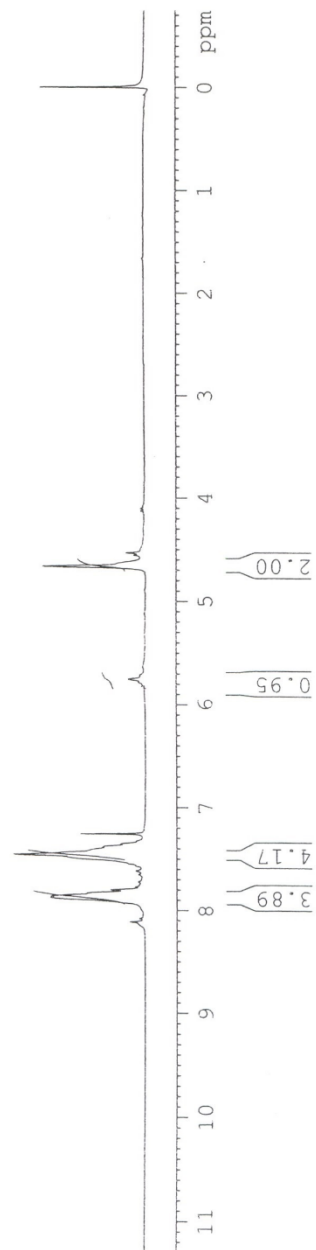
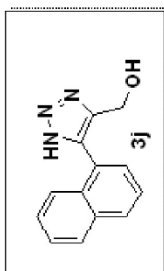
===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300065 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.880
 7.866
 7.837
 7.803
 7.775
 7.620
 7.461
 7.385
 7.355
 7.329

5.863

4.667





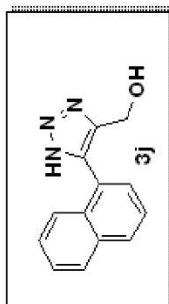
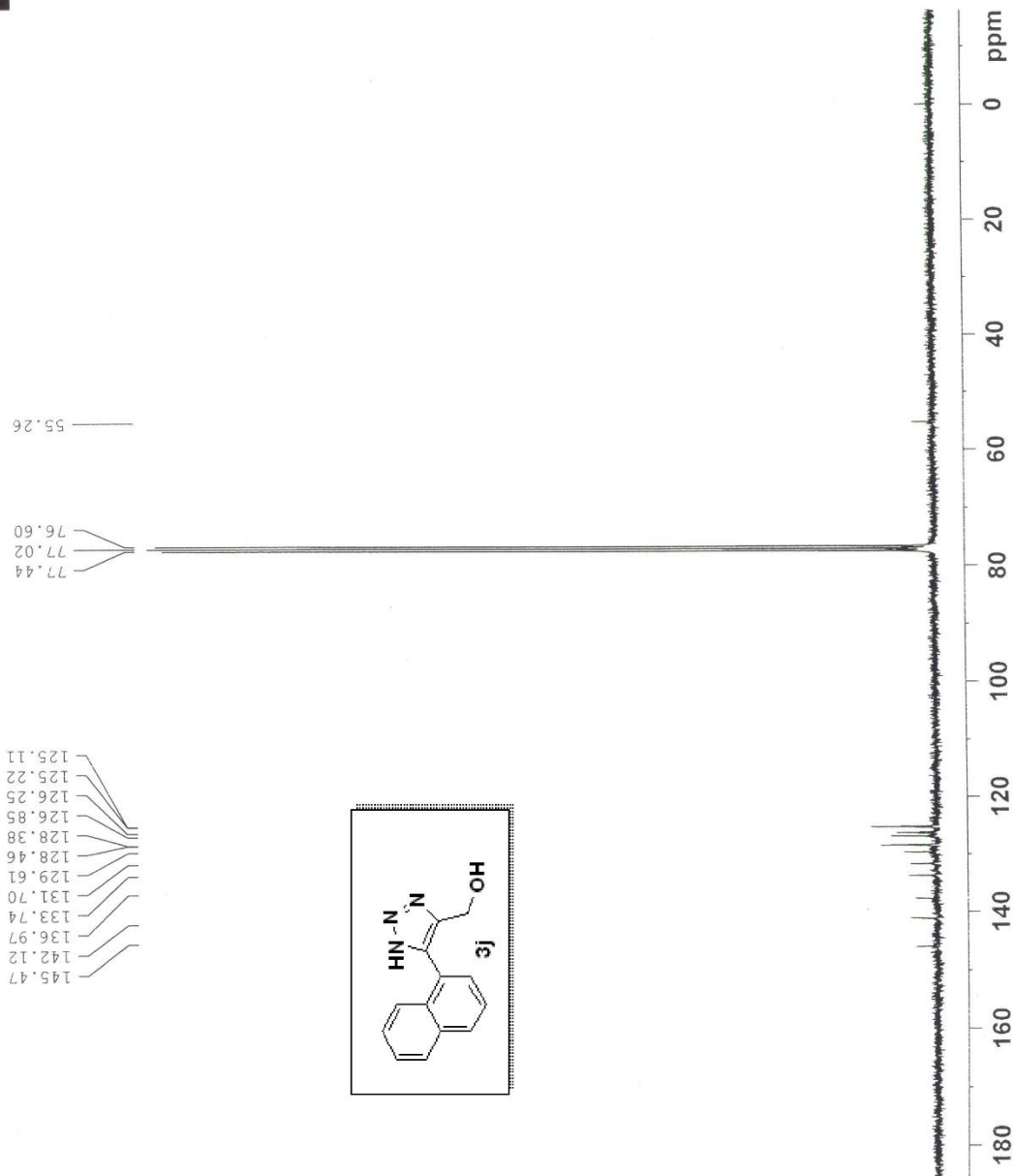
Current Data Parameters
 NAME NSK-X-Naph-OH-N3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101201
 Time 2.11
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1152
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 512
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677450 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



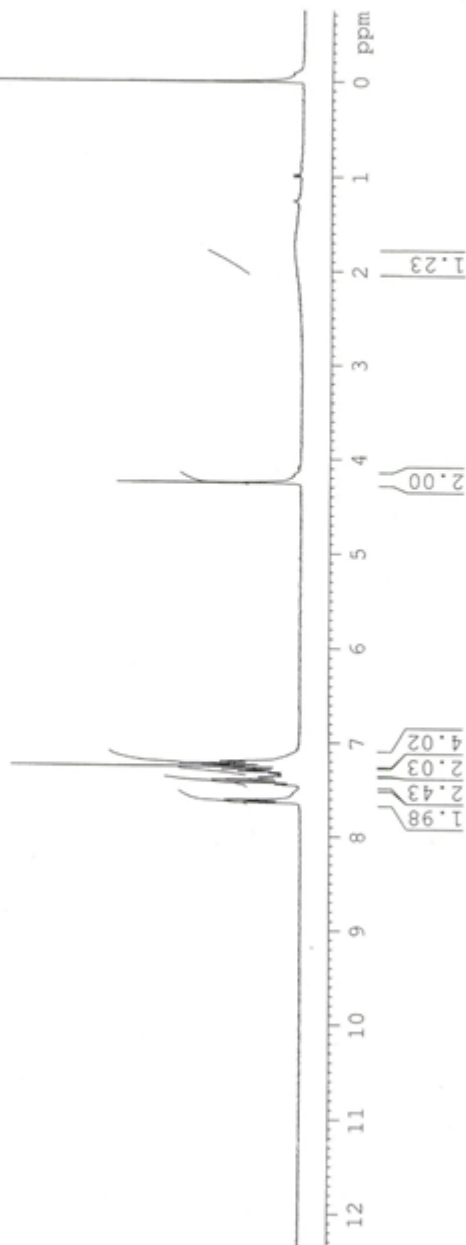
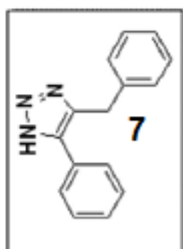


Current Data Parameters
 NAME NSK-X-202
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20100403
 Time 11:19
 INSTRUM spect
 PROCNO 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SNR 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 812.7
 CW 81.000 usec
 PC 6.00 usec
 TT 300.0 K
 DI 1.00000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 12.40 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300064 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz
 GC 0
 PC 1.00

1.857

4.255

7.644
7.638
7.617
7.612
7.612
7.449
7.427
7.422
7.401
7.395
7.390
7.372
7.334
7.311
7.287
7.261
7.231
7.226
7.205





Current Data Parameters
 NAME NSK-PH-NM3FC
 EXFNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101013
 Time 1:52
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1999
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

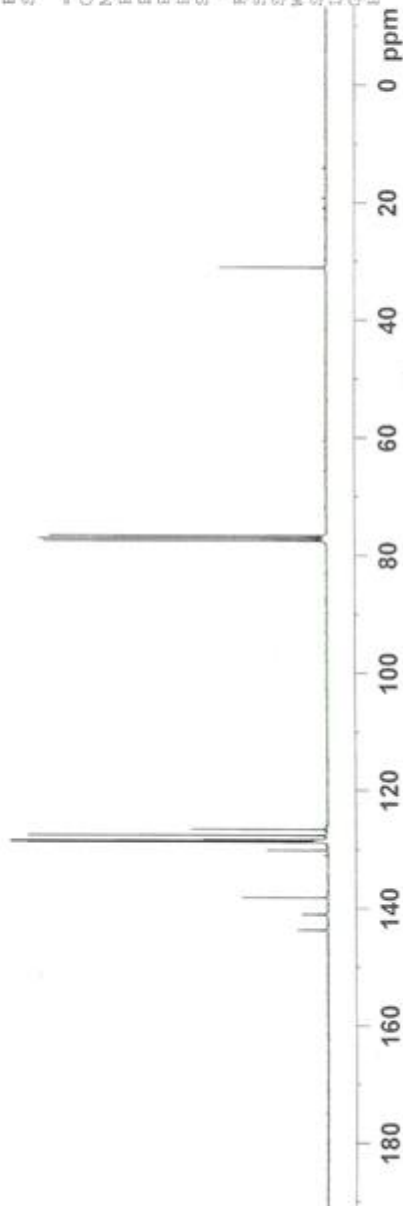
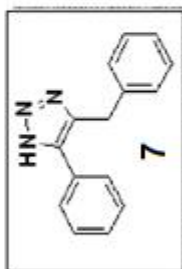
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

31.04

77.51
77.09
76.67

143.71
141.02
138.16
130.18
128.79
128.69
128.52
128.37
127.63
126.62





Current Data Parameters
 NAME NSK-X-207
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100701
 Time 18.29
 INSTRUM spect
 PROBRD 5 mm DOL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 9.305860 sec
 RG 327.1
 DW 81.000 usec
 DE 6.000 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

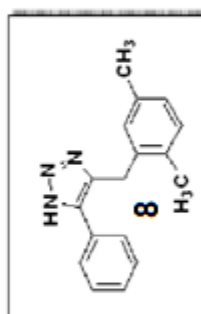
===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300083 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

2.226
2.196

4.143

7.651
7.646
7.623
7.620
7.457
7.450
7.428
7.403
7.393
7.380
7.370
7.351
7.346
7.255
7.090
7.065
6.986
6.961
6.829





Current Data Parameters
 NAME NSK-X-207
 EXFNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100721
 Time 1.09
 INSTRUM spect
 PROBD 5 mm DOL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 351
 DS 4
 SMH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DM 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

CHANNEL f1
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

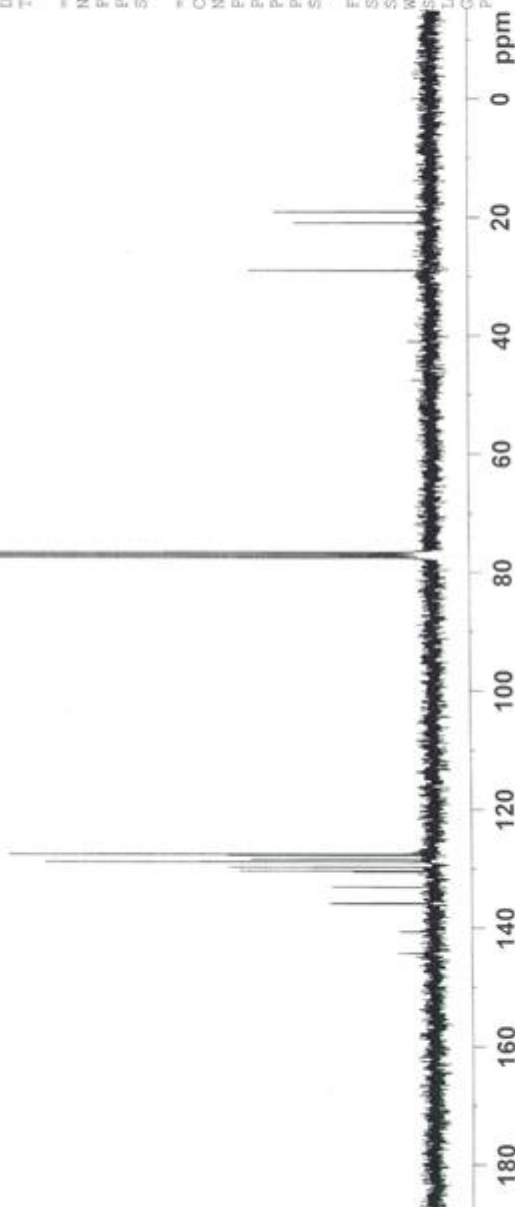
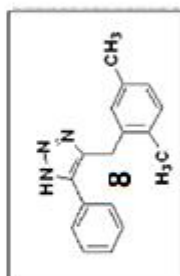
CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 60.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EQ 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

28.99
 20.97
 19.11

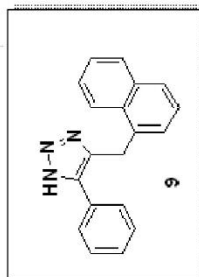
77.45
 77.03
 76.61

144.24
 140.61
 135.89
 135.78
 133.05
 130.52
 130.34
 129.68
 129.79
 128.31
 127.69
 127.50





11.852
7.955
7.935
7.923
7.901
7.887
7.869
7.790
7.763
7.681
7.676
7.655
7.626
7.598
7.508
7.495
7.482
7.476
7.458
7.440
7.430
7.426
7.410
7.399
7.386
7.375
7.348
7.259
7.194
7.170
4.670

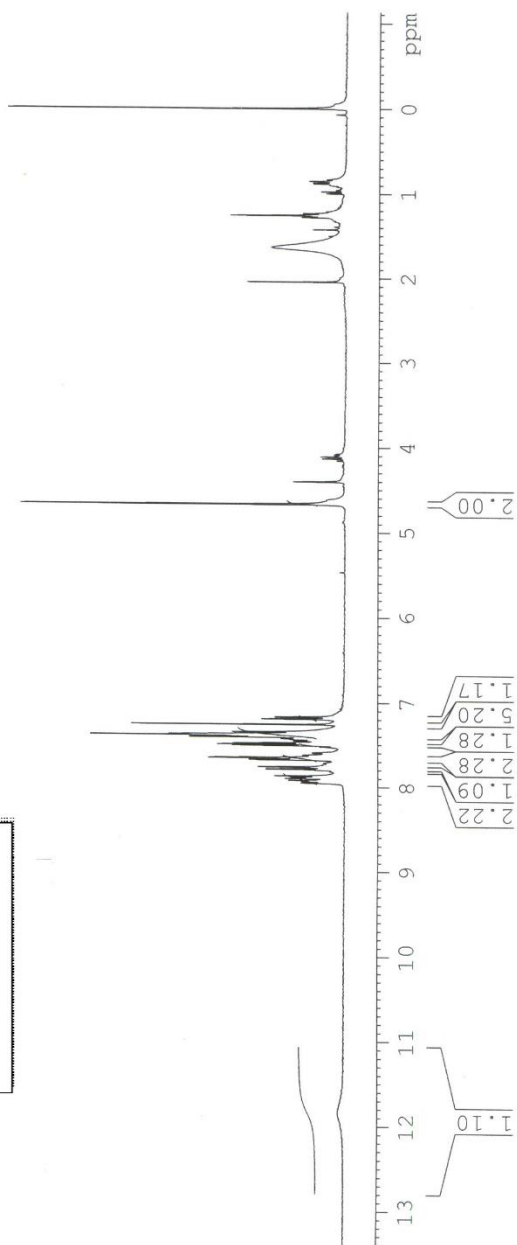


Current Data Parameters
NAME NSK-X-206
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100508
Time 16.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.308660 sec
RG 300.00
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.40 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300069 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.00





Current Data Parameters
 NAME nsk-Naph-FC-N3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110222
 Time 22.47
 INSTRUM spect
 PROHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1659
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SF01 75.4752953 MHz

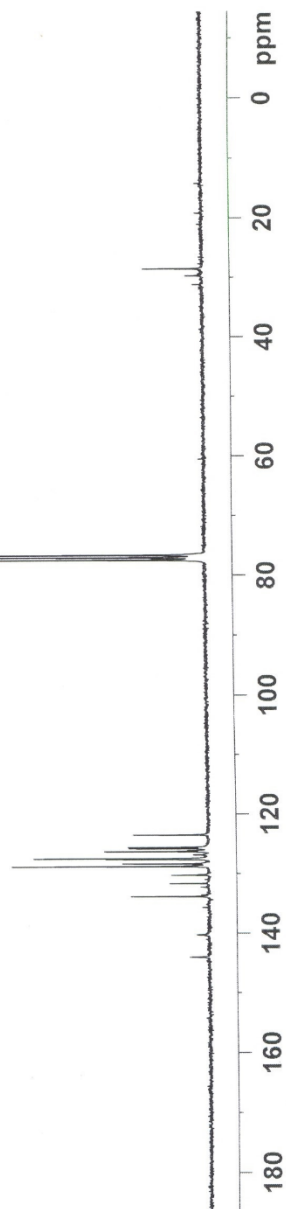
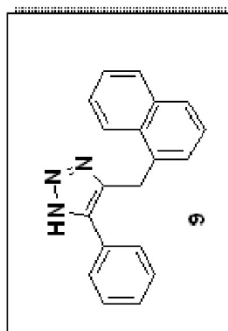
===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SF02 300.1312005 MHz

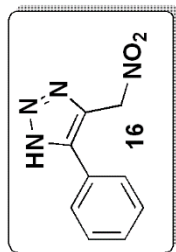
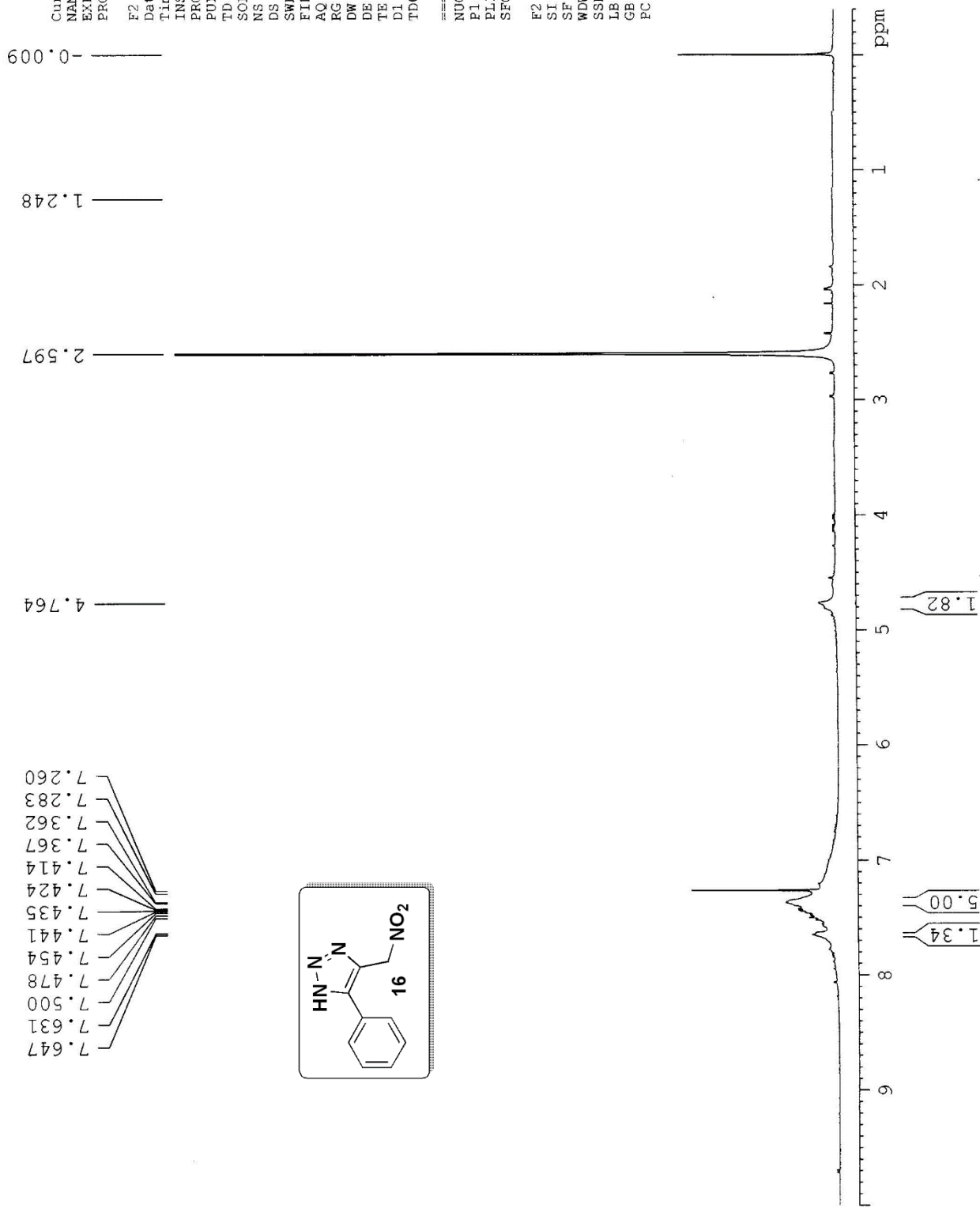
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EM 0
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

144.01
 140.26
 133.84
 131.68
 130.28
 128.84
 128.36
 127.62
 127.50
 126.84
 126.32
 126.30
 126.13
 125.82
 125.59
 123.52

77.49
 77.07
 76.65

28.57





7.647
7.631
7.500
7.478
7.454
7.441
7.435
7.424
7.414
7.367
7.362
7.283
7.260

4.764

2.597

1.248

0.009

Current Data Parameters
 NAME PVK-NO2-A2-CYC
 EXPNO 1
 PROCNO 1

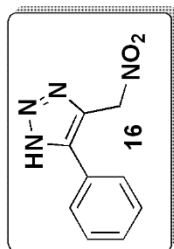
F2 - Acquisition Parameters
 Date_ 20150923
 Time 17.10
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 181
 DW 60.800 usec
 DE 6.00 usec
 TE 297.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.42 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300051 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

163.67
140.07
132.37
131.28
130.41
129.33

77.45
77.13
76.82
62.83



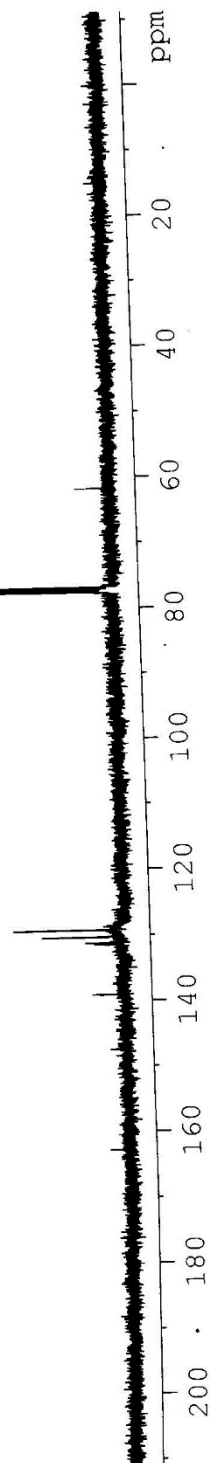
Current Data Parameters
NAME PVK-BH-NO2-AZ-CYL-VII
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150923
Time 15.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DE 20.800 usec
TE 6.00 usec
297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127568 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
NAME NSK-X-131
EXPNO 1
PROCNO 1

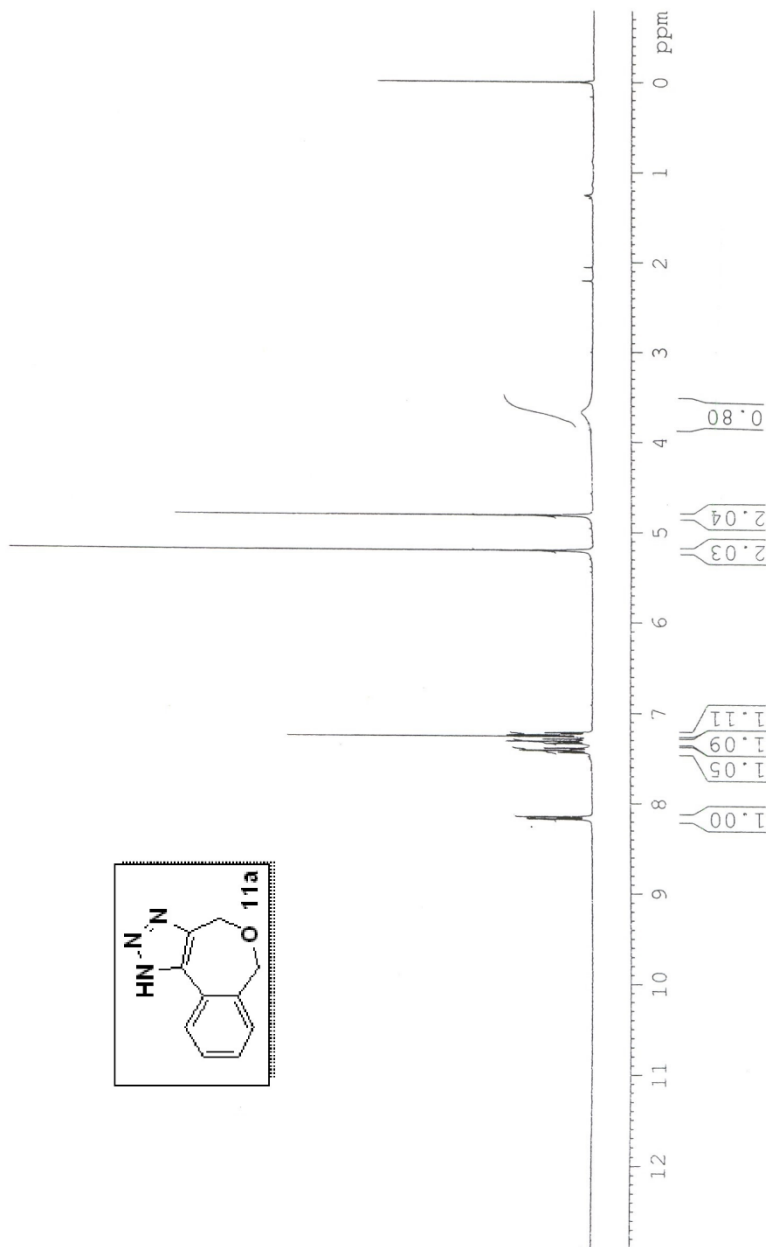
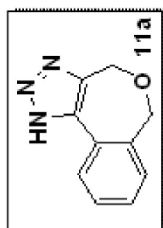
F2 - Acquisition Parameters
Date_ 20091022

Time 11.34
INSTRUM spect
PROBHD 5 mm DUL 125-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 11
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DM 81.000 usec
DE 8.000 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.40 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.178
8.175
8.152
8.149
7.444
7.440
7.420
7.415
7.394
7.389
7.343
7.339
7.318
7.314
7.294
7.289
7.263
7.247
7.243
7.222
7.218
5.204
4.814
3.734





Current Data Parameters
 NAME NSK-X-131
 EXPNO 5
 PROCNO 1

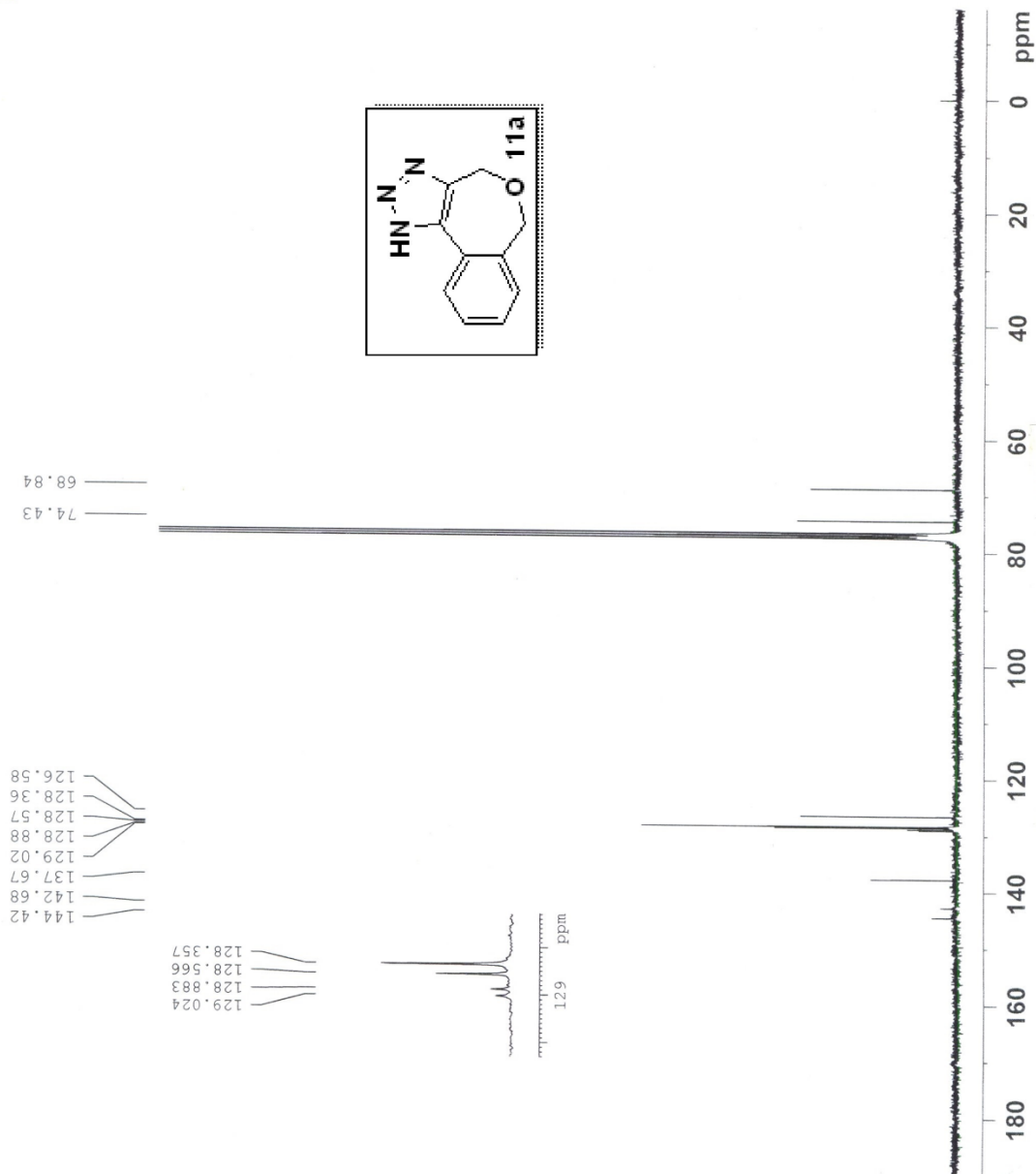
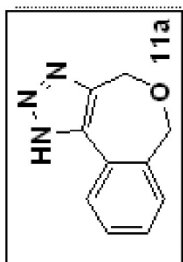
F2 - Acquisition Parameters

Date_ 20091026
 Time_ 6.23
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 2896.3
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.10 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 16.19 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677504 MHz
 EM 0
 WDW 0
 SSB 1.00 Hz
 LB 0
 GB 0
 PC 1.40





Current Data Parameters
 NAME NSR-X-138
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20091107
 Time 18.33
 INSTRUM spect
 PROBHD 5 mm DUI-13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 3
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 181
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 PL 12.40 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing Parameters
 SI 32768
 SF 300.130062 MHz
 EX 0
 SCB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

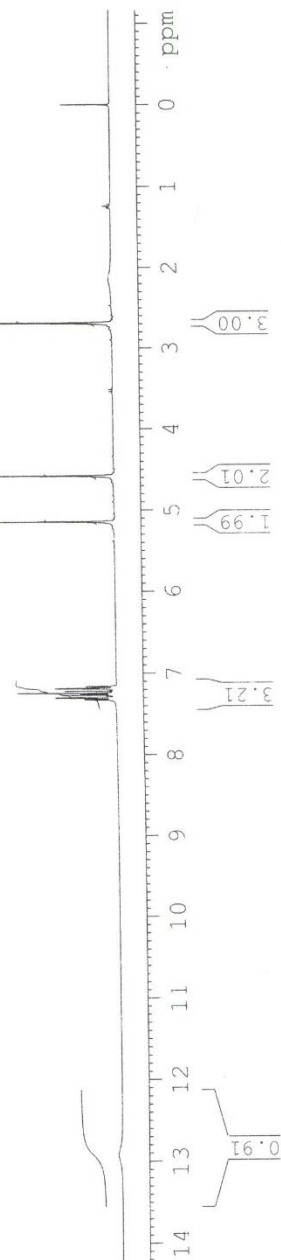
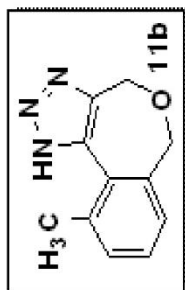
2.688

4.578

5.145

7.326
7.304
7.301
7.270
7.259
7.246
7.221
7.190
7.186
7.166

12.925





Current Data Parameters
 NAME NSK-X-138
 EXPNO 1
 PROCNO 1

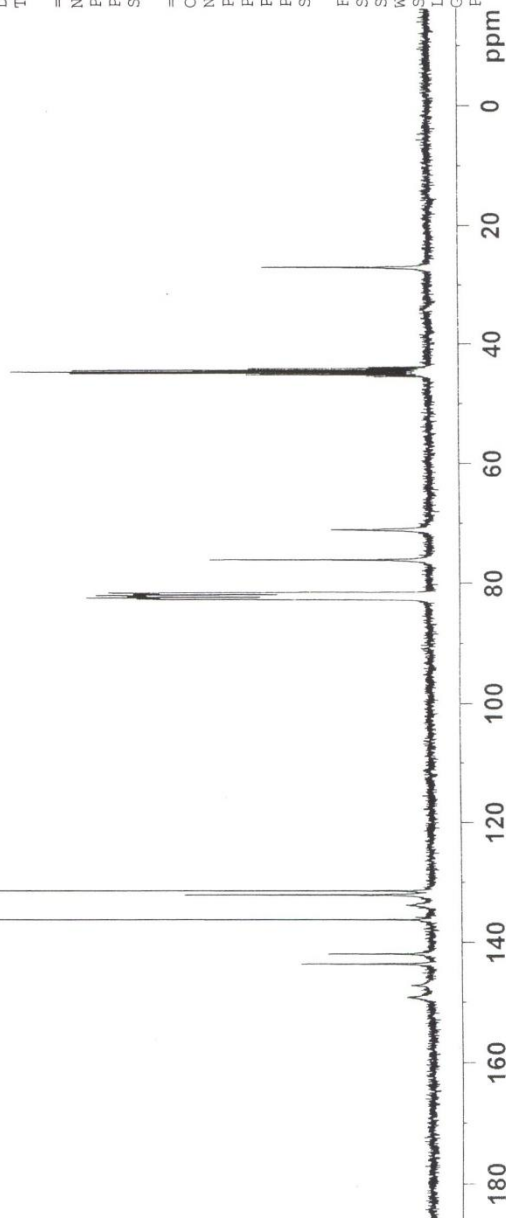
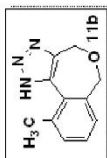
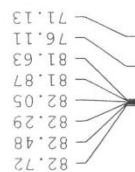
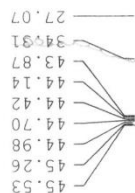
F2 - Acquisition Parameters
 Date_ 20100801
 Time_ 0.59

INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 7006
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

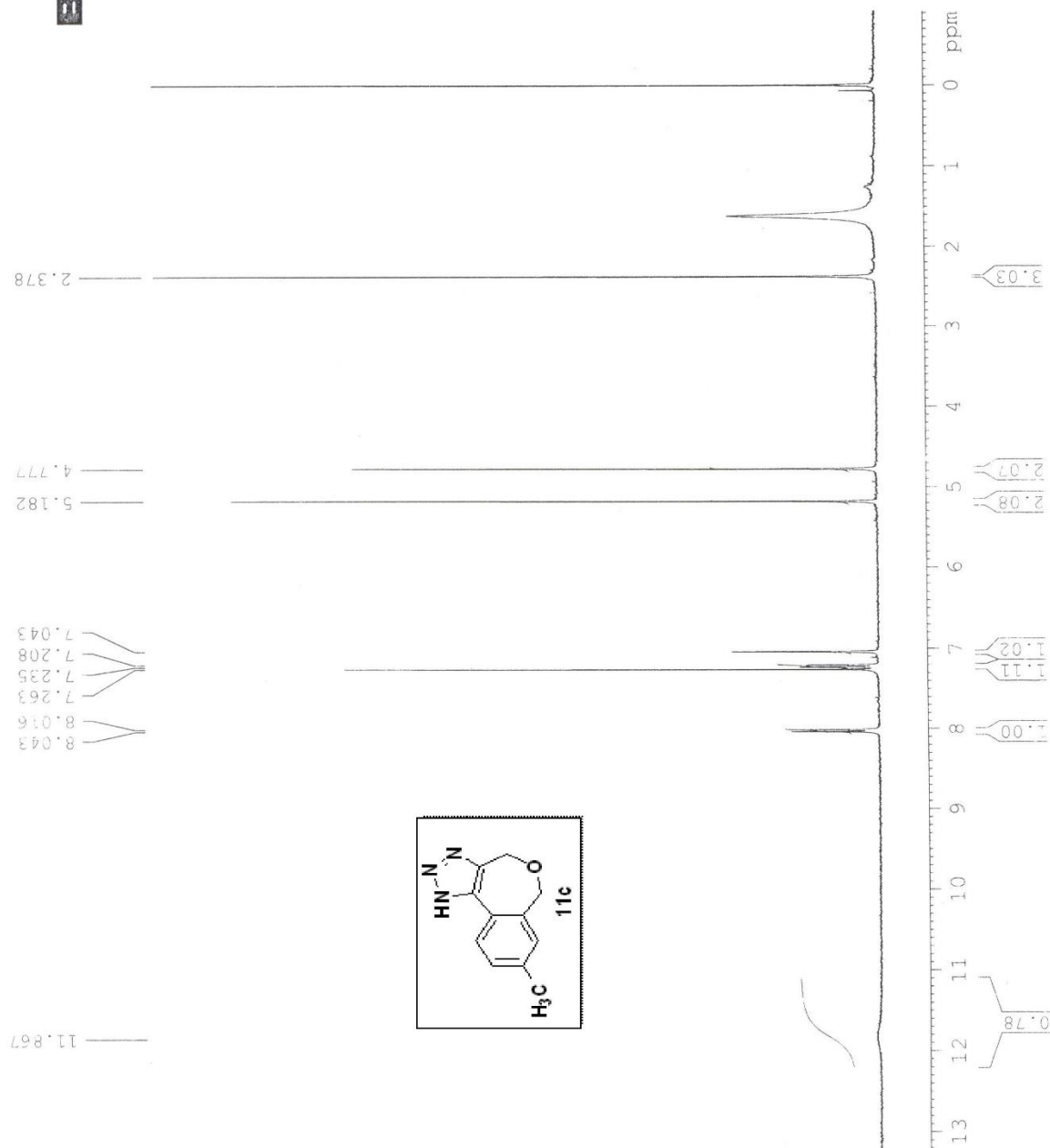
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME NSK-155
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date 20091110
 Time 20.33
 INSTRUM spect
 PROBHD 5 mm BBO 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 SS 16
 SWH 6172.839 Hz
 FIDRES 0.394190 Hz
 AQ 5.3064660 sec
 RG 645.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1
 ===== CHANNEL F1 =====
 NUC1 1H
 P1 12.40 usec
 PL1 0.00 dB
 SFO1 300.131854 MHz
 F2 - Processing parameters
 SI 300.1300048 MHz
 SF 32768
 WTW 0
 SSR 0
 LB 0
 GB 0
 PC 1.00





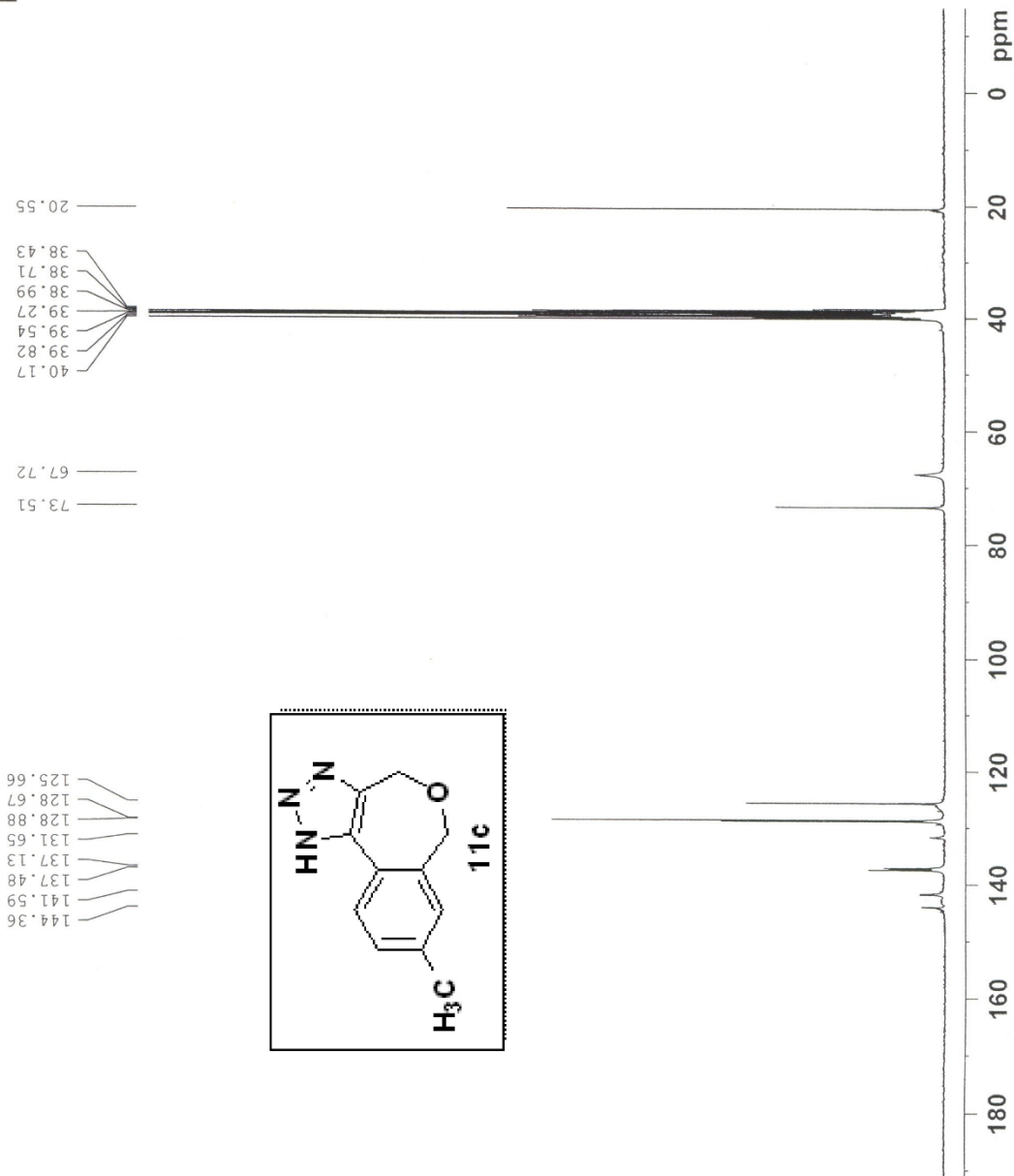
Current Data Parameters
 NAME NSK-4-Me-N3-Ben
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101024
 Time 23.53
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 13000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 724.1
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME: nsk-3-11-9
 EXPNO: 2
 PROCNO: 1

F2 Acquisition Parameters
 Date_: 20100630
 Time: 7.26
 INSTRUM: spect
 PROHD: 5 mm DUL 13C-1
 PULPROG: zg30
 TD: 65536
 SOLVENT: DMSO
 NS: 16
 DS: 4
 SWH: 6172.839 Hz
 FIDRES: 0.094130 Hz
 AQ: 5.3084660 sec
 RG: 161.3
 DW: 81.000 usec
 DE: 6.00 usec
 TF: 300.0 K
 D1: 1.0000000 sec
 TDO: 1

===== CHANNEL f1 =====
 NUC1: 13
 P1: 13.00 usec
 PL1: 0.00 dB
 SFO: 300.1318534 MHz

F2 Processing parameters
 SI: 32768
 SF: 300.1300000 MHz
 WDW: EM
 SSF: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

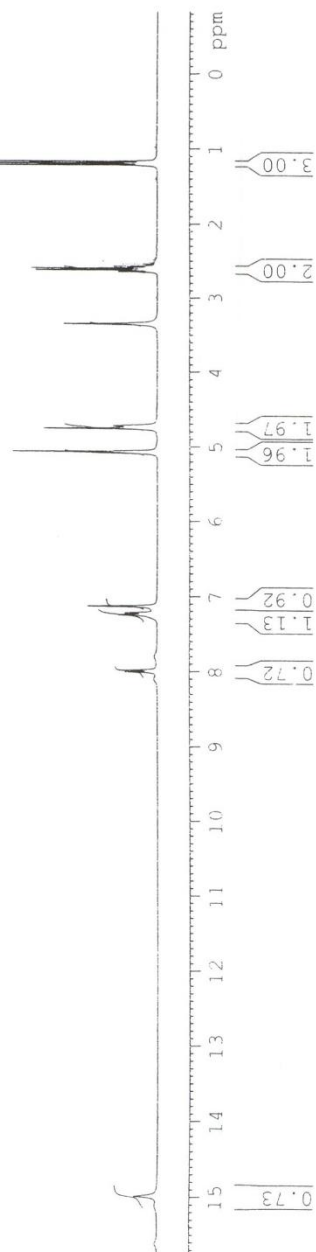
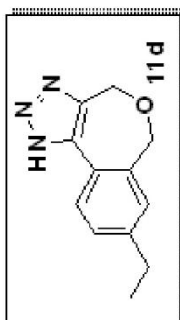
1.218
1.193
1.168

3.351
2.650
2.625
2.599
2.574
2.544
2.510

5.066
4.759

8.009
7.983
7.248
7.222
7.133

14.983





Current Data Parameters
 NAME NSK-X-149
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100711
 Time_ 19.43
 INSTRUM spect
 PROHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 658
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 574.7
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 EM
 WDW 0
 SSB 1.00 Hz
 LB 0
 GB 0
 FC 1.40

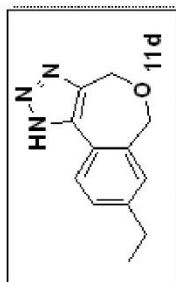
15.37

27.75

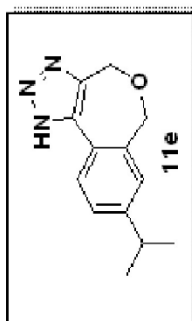
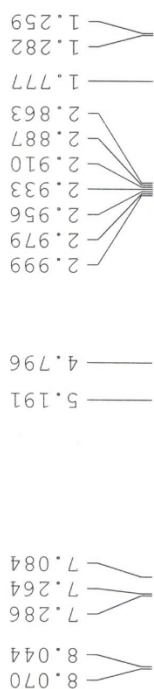
68.21

73.69

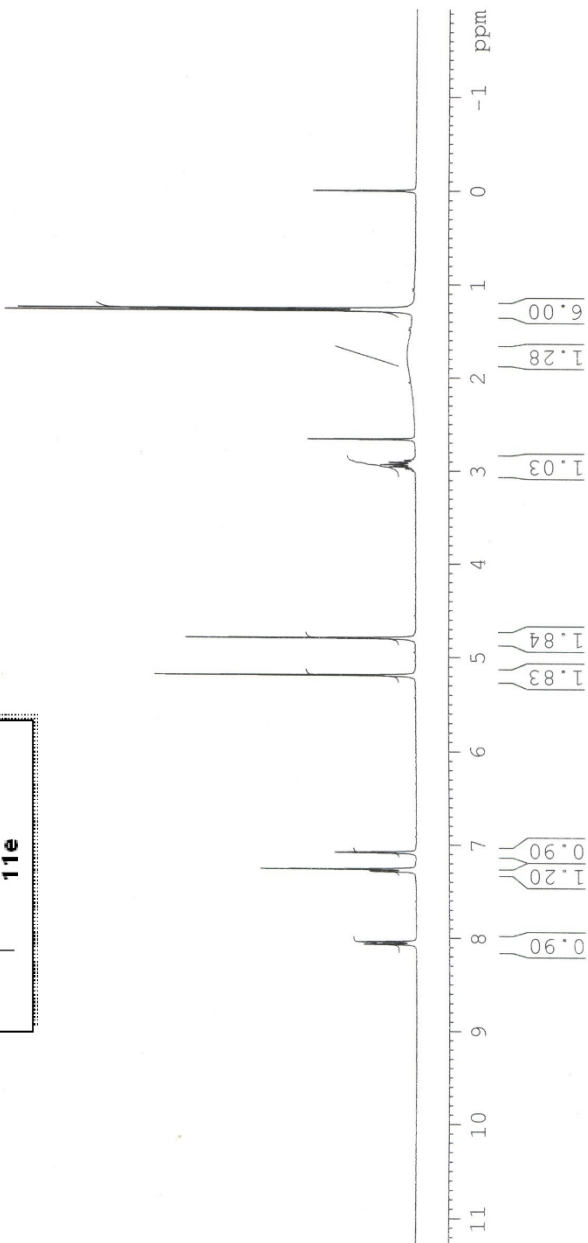
125.95
 126.95
 127.48
 127.66
 137.81
 142.00
 143.40
 144.03



180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters
 NAME NSK-PTC-11-10
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20100416
 Time 17:25
 INSTRUM spect
 PROBHD 5 mm DULS-BB-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 162
 DS 6472.839 Hz
 SWH 6472.839 Hz
 FIDRES 0.000100 Hz
 AQ 5.308400 sec
 RG 327.680
 DW 81.000 usec
 DE 6.000 usec
 TE 300.2 K
 D1 1.0000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 100.626126 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.626126 MHz
 WDW 3000
 SSB 0
 LB 0.00 Hz
 GB 0.00 Hz
 PC 1.000





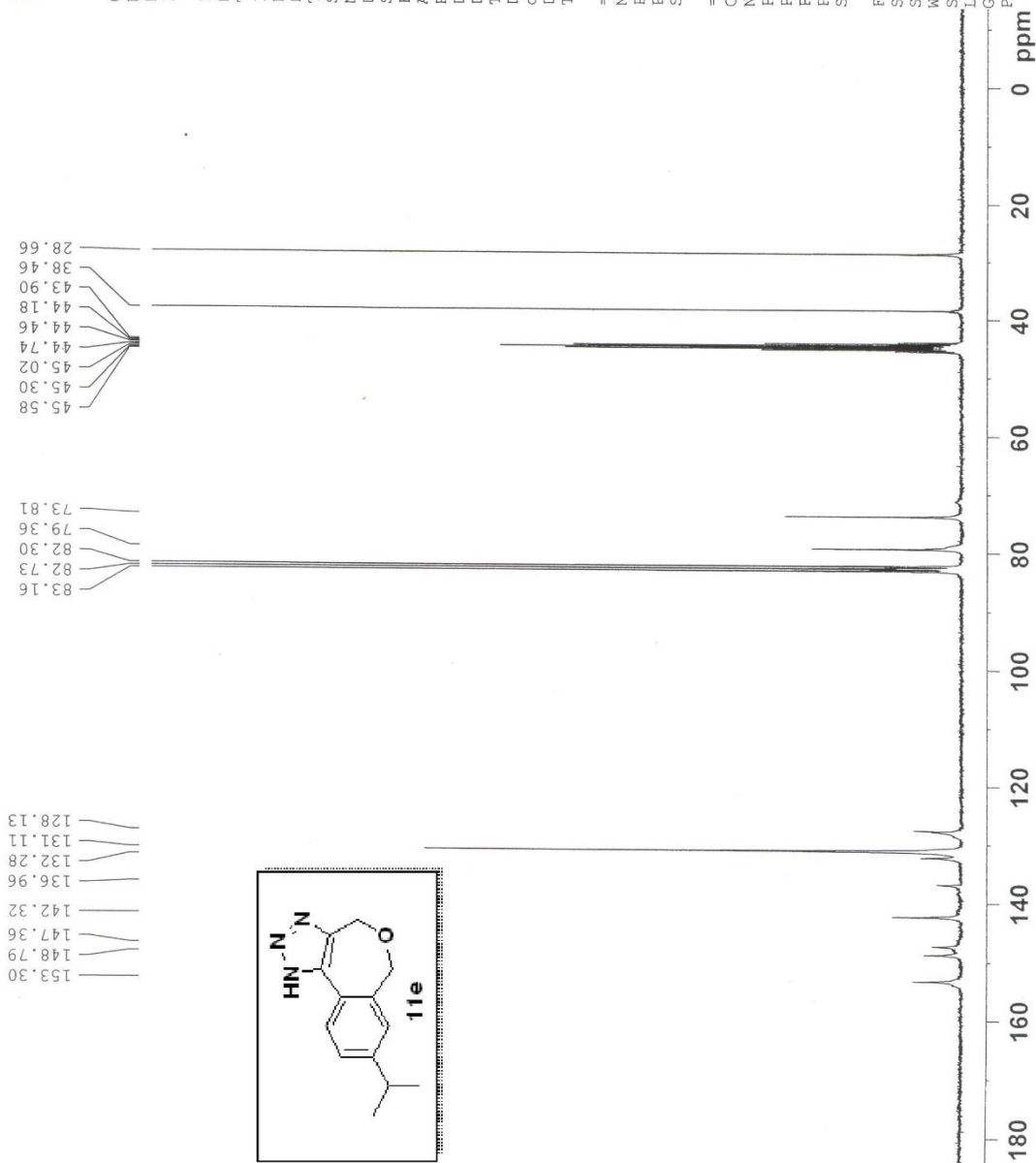
Current Data Parameters
NAME NSK-X-219-4-Iso-N3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101020
Time 9.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8531
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 362
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





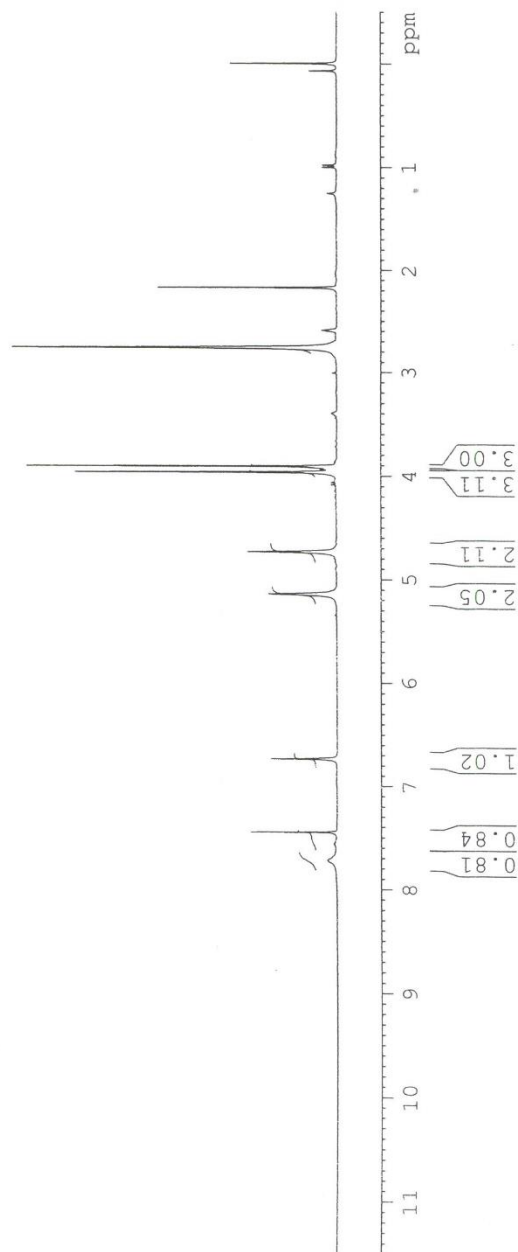
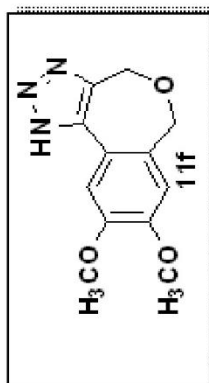
Current Data Parameters
 NAME: NSK-X-168
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20100801
 Time: 9.53
 NSRUM: spect
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 6172.839 Hz
 FIDRES: 0.094190 Hz
 AQ: 5.3084660 sec
 RG: 406.4
 DW: 81.000 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 1.00000000 sec
 T1D0: 1

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 13.15 usec
 PL1: 0.00 dB
 SFO1: 300.1318534 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1314003 MHz
 WFM: 0
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

7.712
 7.449
 6.733
 5.141
 4.733
 3.964
 3.907
 2.758





Current Data Parameters
 NAME NSK-DIOME-N3-BEN
 EXNO 1
 PROCNO 1

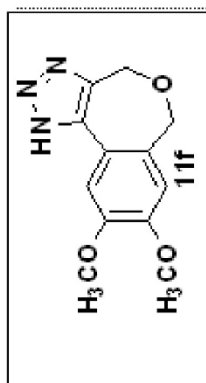
F2 - Acquisition Parameters
 Date_ 20110228
 Time_ 8.19
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8867
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4678191 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

148.16
 147.80
 147.35
 129.97
 127.81
 119.20
 110.59
 108.70
 76.70
 76.28
 75.85
 73.13
 70.77
 55.15
 55.02
 39.83
 39.55
 39.27
 38.99
 38.71
 38.43
 38.16



180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters
NAME NSK-X-152
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081113
Time 8:14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 812.7
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.40 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300045 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.595

4.688

5.156

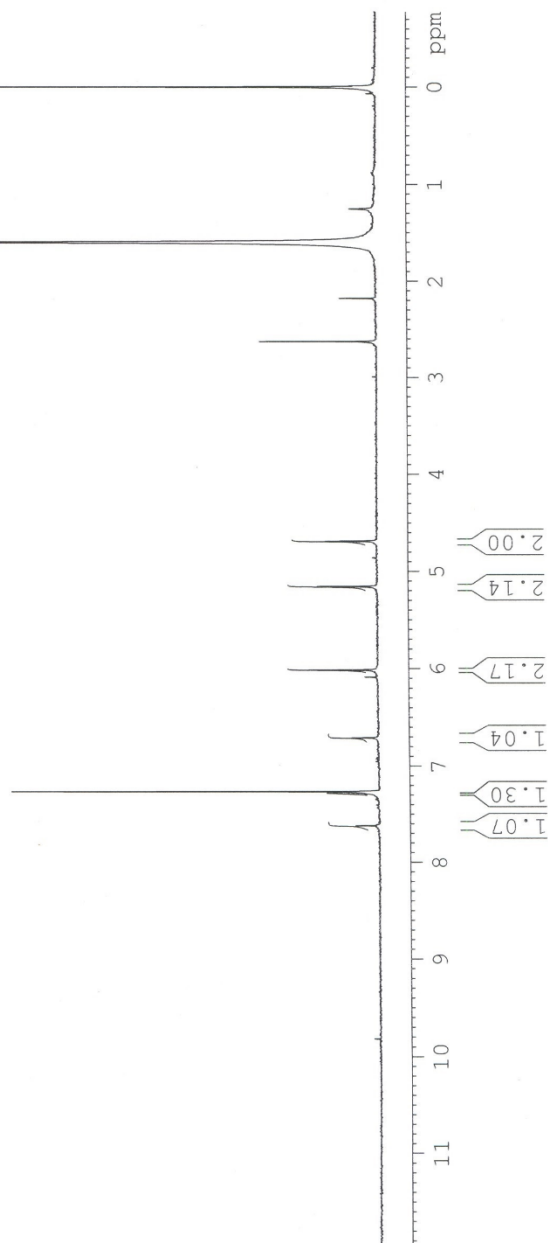
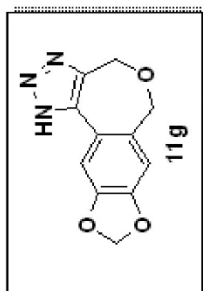
6.014

6.711

7.264

7.289

7.621





Current Data Parameters
 NAME NSK-X-152
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100811
 Time 8.13
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 7000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 512
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

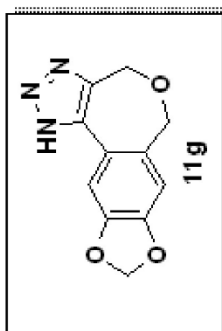
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EM
 WDW 0
 SSB 1.00 Hz
 LB 0
 GB 0
 PC 1.40

43.97
 44.25
 44.53
 44.81
 45.09
 45.37
 45.65

73.47
 78.38
 83.22
 83.66
 84.09

106.25
 111.23
 113.56

128.93
 137.08
 147.14
 148.43
 151.86
 152.38



180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters
 NAME NSK-150
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091111
 Time 20.26
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 362
 DW 81.000 usec
 DE 6.00 usec
 TE 300.2 K
 FL 300.000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 PL 12.40 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

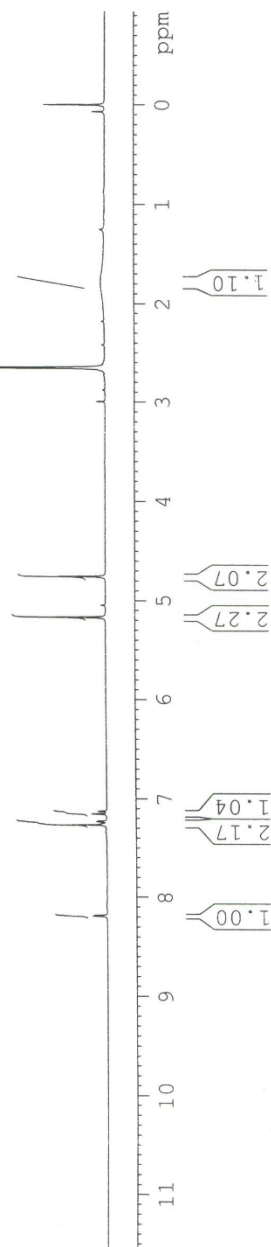
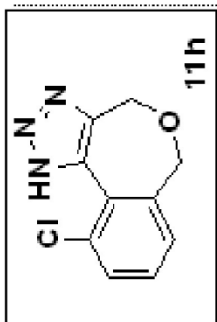
F2 - Processing parameters
 SI 32768
 SF 300.1300028 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1.798

4.758

5.171

7.130
 7.157
 7.230
 7.237
 7.257
 7.270
 8.188
 8.195





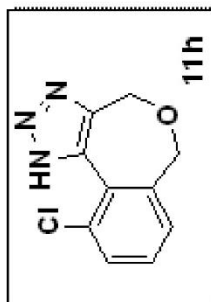
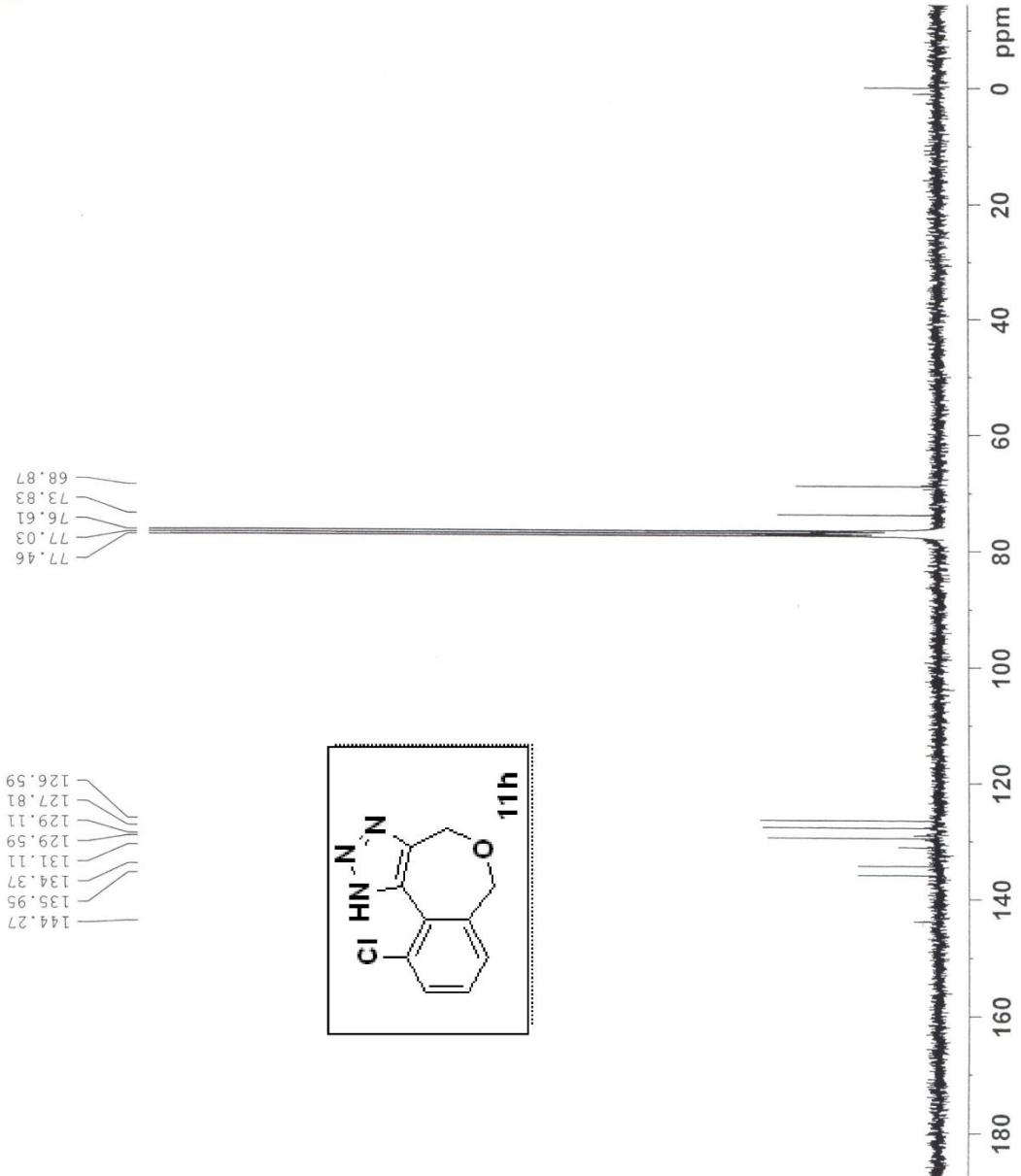
Current Data Parameters
 NAME NSK-X-150
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091118
 Time 8.26
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 9000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 20642.5
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.10 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 16.19 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677479 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME NSK-X-3C1-OH-N3
 EXPNO 2
 PROCNO 1

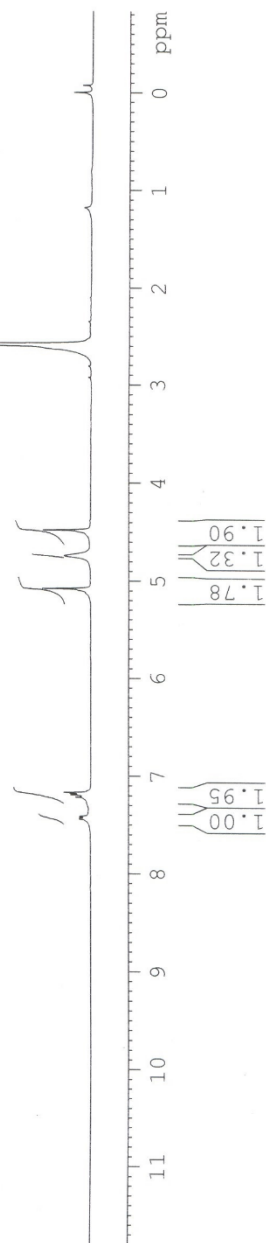
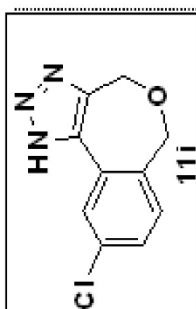
F2 - Acquisition Parameters
 Date_ 20101130
 Time 22.10
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.084190 Hz
 AQ 5.300000 sec
 RG 320.000
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300179 MHz
 RGW EM
 SSB 0
 FB 0.30 Hz
 GB 0
 PC 1.00

5.082
 4.744
 4.481

7.445
 7.437
 7.423
 7.414
 7.220
 7.196
 7.180
 7.173





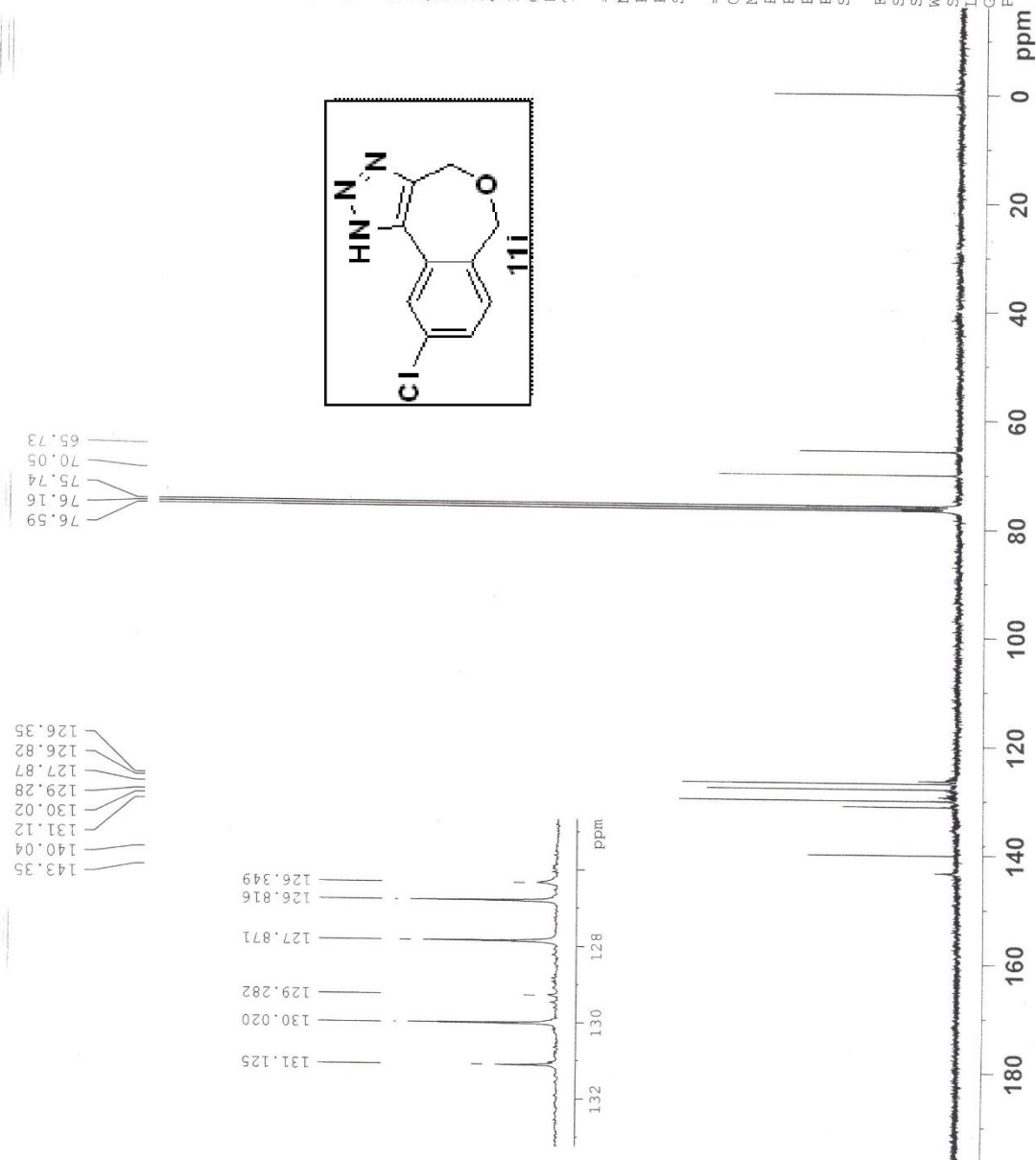
Current Data Parameters
 NAME NSK-3Cl-Ben-N3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101205
 Time_ 18.19
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1168
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

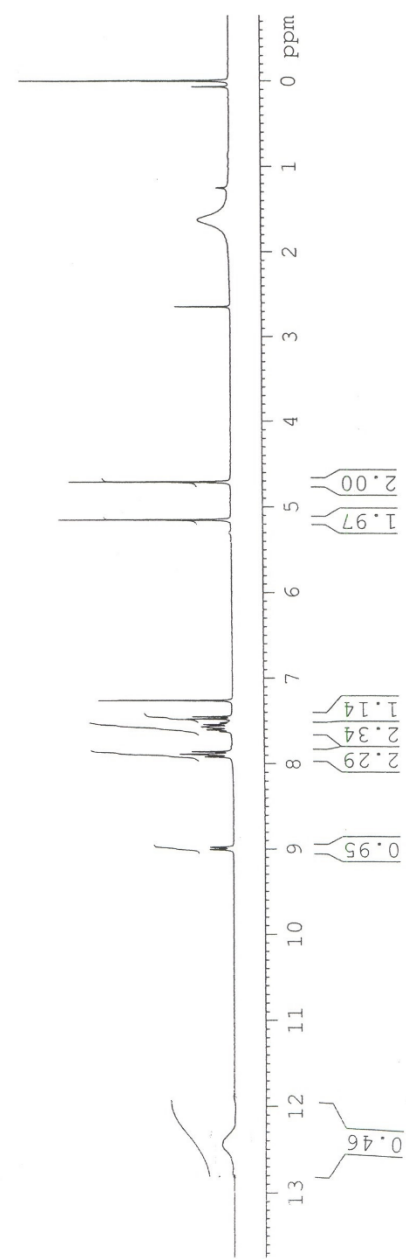
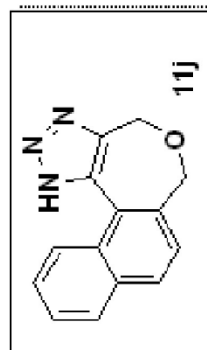
F2 - Processing parameters
 SI 32768
 SF 75.4678235 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME: NSK-Naph-Ben-N3
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20101205
 Time: 19.19
 INSTRUM: spect
 PROBHD: 5 mm DUL 13C-1
 PULPROG: zg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 12
 DS: 4
 SFO1: 6172.839 Hz
 SFO2: 0.054190 Hz
 FIDRES: 5.3084660 sec
 AQ: 645.1
 RG: 81.000 usec
 DW: 6.00 usec
 DE: 300.0 K
 TE: 1.00000000 sec
 D1: 1
 TDO: 1
 CHANNEL f1
 NUC1: 13
 P1: 13.15 usec
 PL1: 0.00 dB
 SFO1: 300.1318534 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 300.1300057 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

9.011
 8.983
 7.923
 7.891
 7.861
 7.627
 7.608
 7.604
 7.581
 7.572
 7.544
 7.522
 7.479
 7.451
 5.151
 4.712
 12.241





Current Data Parameters
 NAME NSK-Naph-Ben-N3
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101206
 Time_ 1.58
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

145.71
 137.23
 133.94
 130.83
 129.27
 129.21
 128.44
 127.22
 127.17
 127.08
 126.34
 126.26

77.43
 77.01
 76.59
 71.05
 65.81

