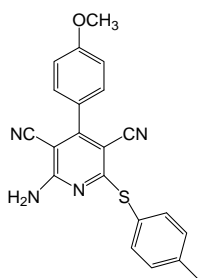
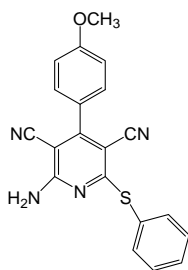


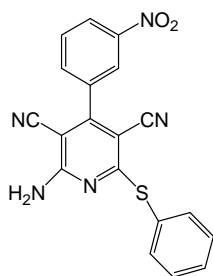
Supplementary data



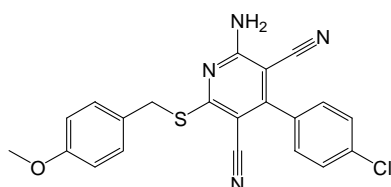
2-Amino-4-(4-methoxyphenyl)-6-(p-tolylthio)pyridine-3,5-dicarbonitrile (5a). Yellow solid; mp 229–231 °C; FT-IR (KBr): ($\nu_{\max}/\text{cm}^{-1}$): 3462, 3332, 2218, 1632, 1544; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.43 (s, 3H, CH_3), 3.88 (s, 3H, OCH_3), 5.47 (s, 2H, NH_2), 7.04–7.06 (d, 2H, $J = 8$ Hz, Ar-H), 7.28 (d, 2H, Ar-H), 7.42 (d, 2H, $J = 7.8$ Hz, ArH), 7.51–7.53 (d, 2H, $J = 8$ Hz, ArH); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 21.4, 55.6, 87.1, 94.8, 114.3, 115.6, 124.1, 126.1, 130.3, 130.4, 135.3, 139.7, 158.2, 160.2, 161.2, 165.1, 167.4; **MS (EI, 70 eV): m/z 372 (M^+)**, Anal. Calcd for $\text{C}_{21}\text{H}_{16}\text{N}_4\text{OS}$: C, 67.72; H, 4.33; N, 15.04%. Found: C, 67.62; H, 4.39; N, 15.14%.



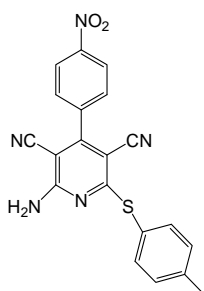
2-Amino-4-(4-methoxyphenyl)-6-(phenylthio)pyridine-3,5-dicarbonitrile (5b). Yellow solid; mp 240–242 °C; FT-IR (KBr): ($\nu_{\max}/\text{cm}^{-1}$): 3438, 3329, 2217, 1640, 1545; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 3.86 (s, 3H, OCH_3), 6.81 (s, 2H, NH_2), 7.04 (d, 2H, $J = 7.6$ Hz, Ar-H), 7.42–7.51 (m, 5H, Ar-H), 7.54 (d, 2H, $J = 7.6$ Hz, Ar-H), ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 55.5, 86.3, 93.6, 114.2, 115.6, 129.3, 129.6, 130.8, 131.1, 133.2, 135.7, 157.6, 158.9, 159.9, 161.4, 166.9; **MS (EI, 70 eV): m/z 358 (M^+)**, Anal. Calcd for $\text{C}_{20}\text{H}_{14}\text{N}_4\text{OS}$: C, 67.02, H, 3.94; N, 15.63 %. Found: C, 67.11; H, 3.85; N, 15.52%.



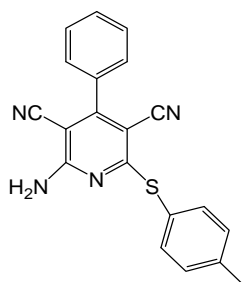
2-Amino-4-(3-nitrophenyl)-6-(phenylsulfanyl)-3,5-pyridine dicarbonitrile (5c). Yellow solid, mp 218–220 °C; FT-IR (KBr): ($\nu_{\max}/\text{cm}^{-1}$): 3447, 3315, 2218, 1626, 1523, 1349; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 5.38 (s, 2H, NH_2), 7.50–7.57 (m, 5H, Ar-H), 7.38–7.72 (m, 3H, Ar-H), 8.44 (s, 1H, ArH); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 87.4, 95.9, 114.8, 115.2, 127.1, 128.4, 129.3, 129.9, 131.2, 133.2, 135.8, 136.1, 137.2, 158.4, 159.3, 164.1, 169.5; MS (EI, 70 eV): m/z 373 (M^+), Anal. Calcd for $\text{C}_{19}\text{H}_{11}\text{N}_5\text{O}_2\text{S}$: C, 61.12; H, 2.97; N, 18.76%. Found: C, 61.21; H, 2.91; N, 18.68%. HR MS calc. for $\text{C}_{19}\text{H}_{11}\text{N}_5\text{O}_2\text{S}$: 373.0633, found: 373.0631;



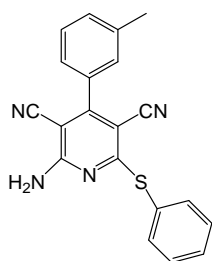
2-Amino-4-(4-chlorophenyl)-6-((4-methoxybenzyl)thio)-3,5-pyridinedicarbonitrile (5d). Yellow solid, mp 237–239 °C; FT-IR (KBr): ($\nu_{\max}/\text{cm}^{-1}$): 3322, 2214, 1626, 1543, 1482, 1243; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ (ppm) 3.71 (s, 3H, OCH_3), 4.43 (s, 2H, CH_2), 6.84–6.86 (d, $J=8.4$, 2H, Ar-H), 7.41–7.43 (d, $J=8.2$, 2H, Ar-H), 7.54–7.56 (d, $J=8.4$, 2H, Ar-H), 7.61–7.63 (d, $J=8.2$, 2H, Ar-H), 8.06 (s, 2H, NH_2). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ (ppm) 33.3, 55.5, 86.3, 93.6, 114.2, 114.9, 115.6, 129.3, 129.6, 130.8, 131.1, 133.2, 135.7, 157.6, 158.9, 159.9, 169.8 MS (EI, 70 eV): m/z 406 (M^+), Anal. Calcd for $\text{C}_{21}\text{H}_{15}\text{ClN}_4\text{OS}$: C, 61.99; H, 3.72; N, 13.77%. Found: C, 61.83; H, 3.80; N, 13.86%.



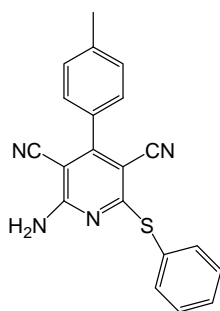
2-Amino-4-(4-nitrophenyl)-6-(p-tolylthio)pyridine-3,5-dicarbonitrile (5e). Yellow solid, mp 301–303 °C; FT-IR (KBr): ($\nu_{\max}/\text{cm}^{-1}$): 3472, 3332, 3218, 2215, 1626, 1541, 1509, 1344, 1262, ^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.40 (s, 3H, CH_3), 5.50 (s, 2H, NH_2), 7.26–7.28 (d, $J=7.6$, 2H, Ar-H), 7.43–7.45 (d, $J=7.8$, 2H, Ar-H), 7.66–7.68 (d, $J=7.6$, 2H, Ar-H), 8.39–8.41 (d, $J=7.8$, 2H, Ar-H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 18.9, 86.8, 96.2, 115.1, 116.9, 125.3, 131.3, 132.9, 134.1, 134.9, 135.5, 136.2, 137.3, 156.1, 158.2, 165.1. MS (EI, 70 eV): m/z 387 (M^+), Anal. Calcd for $\text{C}_{20}\text{H}_{13}\text{N}_5\text{O}_2\text{S}$: C, 62.01; H, 3.38; N, 18.08%. Found: C, 61.83; H, 3.26; N, 18.15%.



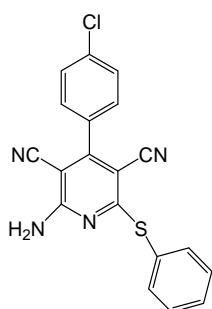
2-Amino-4-phenyl-6-(*p*-tolylthio) pyridine-3,5-dicarbonitrile (5f). Yellow solid, mp 248–250 °C; FT-IR (KBr): ($\nu_{\max}/\text{cm}^{-1}$): 3446, 3314, 2219, 1627, 1522; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ (ppm) 2.34 (s, 3H, CH_3), 7.27 (d, $J = 7.9$, 2H, Ar-H), 7.45 (d, 2H, $J = 7.9$, Ar-H), 7.49 (m, 5H, Ar-H), 7.80 (s, 2H, NH_2); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ (ppm) 21.4, 87.2, 95.7, 114.8, 115.2, 123.5, 128.4, 129.9, 130.1, 130.9, 133.2, 135.6, 140.3, 158.3, 159.3, 169.5, **MS (EI, 70 eV): m/z 342 (M^+)**, Anal. Calcd for $\text{C}_{20}\text{H}_{14}\text{N}_4\text{S}$: C, 70.15; H, 4.12; N, 16.36%. Found: C, 70.09; H, 4.21; N, 16.31%. **HR MS calc. for $\text{C}_{20}\text{H}_{14}\text{N}_4\text{S}$: 342.0939; found: 342.0949;**



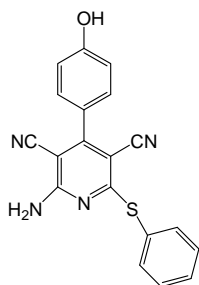
2-amino-6-(phenylthio)-4-*m*-tolylpyridine-3,5-dicarbonitrile (5g). Colorless solid; mp 278–280 °C, IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3420, 3339, 3219, 2214, 1621; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ (ppm) δ 2.44 (s, 3H), 7.32–7.74 (m, 6H), 7.45–7.55 (m, 3H) 7.63 (s, 2H, NH_2), ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ (ppm) 15.1, 87.6, 94.1, 115.9, 116.0, 126.0, 128.1, 129.7, 130.1, 130.3, 130.5, 131.3, 133.5, 135.6, 142.7, 158.6, 160.6. **MS (EI, 70 eV): m/z 342 (M^+)**, Anal. Calcd for $\text{C}_{20}\text{H}_{14}\text{N}_4\text{S}$: C, 70.15; H, 4.12; N, 16.36%. Found: C, 70.18; H, 4.15; N 16.32%.



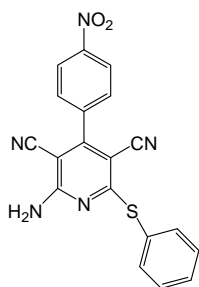
2-Amino-6-phenylsulfanyl-4-*p*-tolyl-pyridine-3,5-dicarbonitrile (5h) Colourless solid, mp 206–207 °C, IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3441, 3339, 3216, 2214, 1627, 1544, 1522, 1265; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ (ppm) 2.52 (s, 3H), 7.33–7.75 (m, 6H), 7.46–7.55 (m, 3H), 7.63 (s, 2H, NH_2), ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ (ppm) 14.9, 87.6, 94.1, 115.9, 116.0, 126.0, 126.2, 128.1, 129.7, 130.1, 130.3, 130.5, 135.6, 142.7, 158.6, 160.6. **MS (EI, 70 eV): m/z 342 (M^+)**, Anal. Calcd for $\text{C}_{20}\text{H}_{14}\text{N}_4\text{S}$: C, 70.15; H, 4.12; N, 16.36%. Found: C, 70.17; H, 4.18; N, 16.39%.



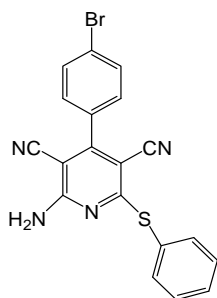
2-Amino-4-(4-chlorophenyl)-6-phenylsulfanylpyridine-3,5-dicarbonitrile (5i) Colourless solid, mp 221-222°C, IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3487, 3344, 3222, 2926, 2214, 1633, 1545; ^1H NMR (400 MHz, DMSO- d_6): δ (ppm) 7.45–7.50 (m, 3H, Ar-H), 7.57 (d, 2H, $J=8.0\text{Hz}$, Ar-H), 7.59 (d, 2H, $J=8.0\text{Hz}$, Ar-H), 7.64 (d, 2H, $J=8.0\text{Hz}$, Ar-H) 7.83 (s, 2H, NH_2); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 87.5, 93.7, 115.2, 115.5, 127.3, 129.2, 129.5, 129.8, 130.8, 133.1, 135.2, 135.7, 157.8, 159.9, 166.6. **MS (EI, 70 eV):** m/z 362 (M^+), Anal. Calcd for $\text{C}_{19}\text{H}_{11}\text{ClN}_4\text{S}$: C, 62.89; H, 3.06; N, 15.44; S, 8.84 %. Found: C, 62.85; H, 3.11; N 15.48 %. **HRMS m/z (ESI) calcd for $\text{C}_{19}\text{H}_{12}\text{N}_4\text{SCl}$ ($\text{M}+\text{H}$) $^+$ 363.0471, found 363.0481.**



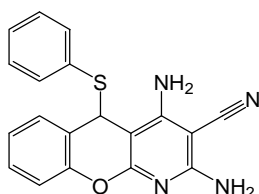
2-Amino-4-(4-hydroxy-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (5j) Colourless solid, mp 315-317°C, IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3648, 3498, 3367, 3237, 2222, 2217, 1632; ^1H NMR (400 MHz, DMSO- d_6): δ (ppm) δ 6.94 (d, $J=8.5\text{ Hz}$, 2H), 7.39 (d, $J=8.5\text{ Hz}$, 2H), 7.52 (m, 3H), 7.60 (m, 2H), 7.69 (s, 2H), 10.05 (bs, 1H, OH); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 93.7, 96.9, 115.6, 115.9, 116.0, 124.5, 127.5, 129.8, 130.1, 130.7, 135.2, 159.1, 159.8, 160.3, 166.5; **MS (EI, 70 eV):** m/z 344 (M^+), Anal. Calcd for $\text{C}_{19}\text{H}_{12}\text{N}_4\text{OS}$: C, 66.26; H, 3.51; N, 16.27%. Found: C, 66.10; H, 3.62; N, 16.22 %.



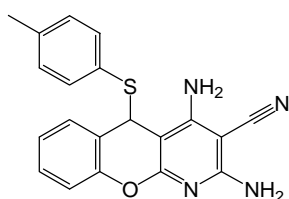
2-Amino-4-(4-nitro-phenyl)-6-phenylsulfanyl-pyridine-3,5-dicarbonitrile (5k) Colourless solid, mp 289-290 °C, IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3407, 3328, 3235, 2228, 2214, 1645, 1555; ^1H NMR (400 MHz, DMSO- d_6): δ (ppm) 7.47-7.49 (m, 3H), 7.56-7.59 (m, 2H), 7.85 (d, $J=8.5\text{ Hz}$, 2H), 7.91 (s, 2H, NH_2), 8.39 (d, $J=8.5\text{ Hz}$, 2H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 87.2, 93.3, 114.9, 115.3, 124.2, 127.2, 129.8, 130.1, 130.5, 135.1, 140.5, 148.9, 157.0, 159.8, 166.5; **MS (EI, 70 eV):** m/z 373 (M^+), Anal. Calcd for $\text{C}_{19}\text{H}_{11}\text{N}_5\text{O}_2\text{S}$: C, 61.12; H, 2.97; N, 18.76% Found: C, 61.05; H, 2.78; N, 18.91%.



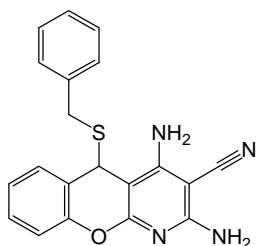
2-Amino-4-(4-bromophenyl)-6-phenylsulphanylpyridine-3,5-dicarbonitrile (5l) Colourless solid, mp 255-257 °C; IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3442, 3338, 3222, 2219, 1629, 1555, 1531, 1459; ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ (ppm) 7.54–7.62 (m, 5H), 7.80–7.82 (m, 4H), 7.87 (s, 2H, NH_2); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ (ppm) 85.6, 92.1, 113.5, 113.4, 120.6, 125.9, 127.1, 128.0, , 129.5, 131.9, 133.5, 134.3, 158.3, 159.8, 166.5; MS (EI, 70 eV): m/z 405 (M^+), Anal. Calcd for $\text{C}_{19}\text{H}_{11}\text{BrN}_4\text{S}$: C, 56.03; H, 2.72; N, 13.76; S 7.87%. Found: C, 56.08; H, 2.78; N 13.68, S 7.81 %. HRMS calc. for $\text{C}_{19}\text{H}_{11}\text{BrN}_4\text{S}$: 405.9888, found: 405.9885.



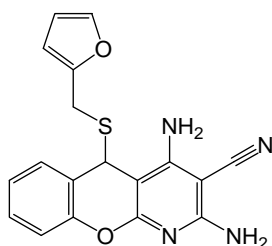
2,4-Diamino-5-phenylsulfanyl-5H-chromeno [2,3-b] pyridine- 3-carbonitrile(6a). Yellow solid, mp 220-222°C, IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3355, 3429, 2203, 1400-1623; ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 5.73 (s, 1H), 6.50 (2H, s), 6.74-6.78 (3H, m), 6.94 (s, 2H), 7.05-7.11 (3H, m), 7.15-7.30 (m, 3H); ^{13}C NMR (100MHz, $\text{DMSO-}d_6$): δ (ppm) 43.12, 70.8, 86.90, 116.01, 116.5, 121.5, 123.9, 128.60, 128.64, 129.50, 129.70, 134.2, 137.7, 150.90, 156.40, 159.7, 160.90. MS (EI, 70 eV): m/z 346 (M^+), Anal. Calcd. For $\text{C}_{19}\text{H}_{14}\text{N}_4\text{OS}$: C, 65.88; H, 4.074; N, 16.17; S, 9.26 %. Found C 65. 82, H 4.09, N 16.07%. HRMS m/z (ESI) calcd for $\text{C}_{19}\text{H}_{15}\text{N}_4\text{OS}$ ($\text{M}+\text{H}^+$) 347.0966, found 347.0958.



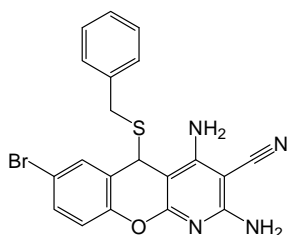
2,4-Diamino-5-(4-methylphenylsulfanyl)-5H-chromeno[2,3-b] pyridine-3-carbonitrile (6b). Yellow solid, mp 223–225 °C; IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3457, 3349, 2198, 1400-1623. ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 2.19 (s, 3H), 5.66 (s, 1H), 6.46 (br s, 2H), 6.61 (d, $J=7.9\text{Hz}$, 2H), 6.79 (d, $J=7.9\text{Hz}$, 1H), 6.90 (m, 4H), 7.11; (d, $J=6.8\text{Hz}$, 1H), 7.19 (d, $J=7.3\text{Hz}$, 2H). ^{13}C NMR (100MHz, $\text{DMSO-}d_6$): δ (ppm) 21.2, 43.11, 70.8, 86.3, 115.7, 116.4, 121.8, 123.6, 127.0, 128.2, 128.6, 129.8, 136.9, 138.3, 151.33, 156.3, 160.08, 160.25 MS (EI, 70 eV): m/z 360 (M^+), Anal. Calcd. For $\text{C}_{20}\text{H}_{16}\text{N}_4\text{OS}$: C 66.64, H 4.47, N 15.54, S 8.90%. Found C 66.59, H 4.51, N 15.48 %. HR MS ESI [$\text{M}+\text{H}^+$] calcd. for $\text{C}_{20}\text{H}_{17}\text{N}_4\text{OS}$ 361.1123; found 361.1132.



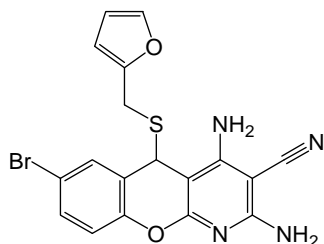
2,4-Diamino-5-(benzylthio)-5H-chromeno[2,3-b]pyridine-3-carbonitrile (6c). Yellow solid, mp 173–175 °C; IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3377, 3439, 2200, 1400, 1605; ^1H NMR (400 MHz, DMSO- d_6): δ 3.49 (ABq, 2H, $J=12\text{Hz}$), 5.48 (1H), 6.55 (bs, 2H), 6.83 (bs, 2H), 7.03–7.21 (m, 7H), 7.33 (m, 2H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 35.02, 44.01, 70.90, 87.01, 117.6, 118.3, 119.3, 122.8, 124.2, 124.3, 129.6, 133.2, 133.3, 136.6, 143.7, 152.9, 159.9, 160.2. **MS (EI, 70 eV): m/z 360 (M^+),** Anal. Calcd For $\text{C}_{20}\text{H}_{16}\text{N}_4\text{OS}$: C, 66.64; H, 4.47; N, 15.54; Found C, 66.48; H, 4.58; N, 15.39%. **HRMS m/z (ESI) calcd for $\text{C}_{20}\text{H}_{17}\text{N}_4\text{OS}$ ($M+H$) $^+$ 361.1123, found 361.1129.**



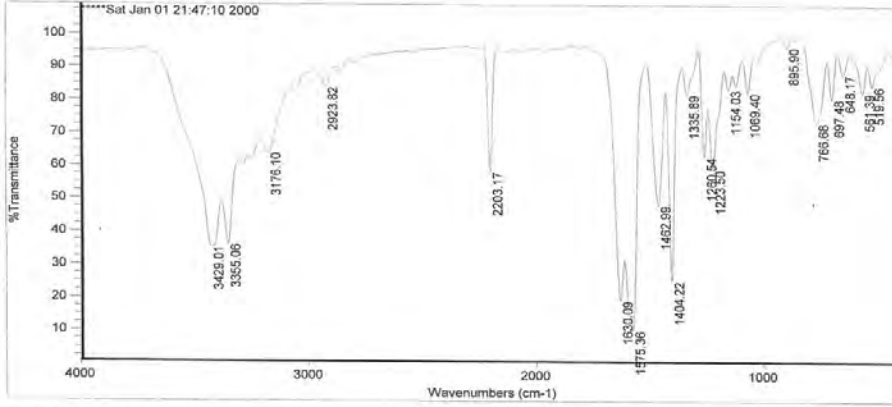
5-(furan-2-yl)methylthio-2,4-diamino-5H-chromeno[2,3-b]pyridine-3-carbonitrile (6d). Yellow solid, mp 200–201 °C; IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3386, 3440, 2203, 1397, 1612; ^1H NMR (400 MHz, DMSO- d_6): δ 3.51 (ABq, 2H, $J=12\text{Hz}$), 5.46 (1H), 5.99 (1H), 6.23 (s, 1H), 6.55 (bs, 2H), 6.79 (bs, 2H), 7.10 (d, 1H, $J=8\text{Hz}$), 7.17 (t, 1H, $J=8\text{Hz}$), 7.24 (s, 1H), 7.31 (t, 2H, $J=8\text{Hz}$); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 25.9, 36.03, 71.0, 87.9, 107.8, 111.0, 116.5, 116.9, 129.0, 129.7, 133.8, 142.7, 149.4, 151.2, 157.1, 160.03, 160.10. **MS (EI, 70 eV): m/z 350 (M^+),** Anal. Calcd For $\text{C}_{18}\text{H}_{14}\text{N}_4\text{O}_2\text{S}$: C 61.70, H 4.03, N 15.99 Found C 61.62, H 4.10, N 15.91%. **HRMS m/z (ESI) calcd for $\text{C}_{18}\text{H}_{15}\text{N}_4\text{O}_2\text{S}$ ($M+H$) $^+$ 351.0915, found 351.0913.**



2,4-Diamino-5-(benzylthio)-7-bromo-5H-chromeno[2,3-b]pyridine-3-carbonitrile (6e). Yellow solid, mp 206–208 °C, IR (KBr) ($\nu_{\max}/\text{cm}^{-1}$): 3315, 3441, 2189, 1403, 1653; ^1H NMR (400 MHz, DMSO- d_6): δ 4.06–4.45 (ABq, 2H, $J=12\text{Hz}$), 4.67 (1H), 6.48 (s, 1H), 6.88–6.90 (m, 5H), 7.37 (m, 6H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 33.34, 35.78, 71.21, 87.22, 116.46, 118.79, 120.90, 121.60, 124.41, 128.60, 129.79, 131.05, 137.53, 137.96, 148.22, 152.75, 160.44, 160.80. **MS (EI, 70 eV): m/z 439 (M^+),** Anal. Calcd For $\text{C}_{20}\text{H}_{15}\text{N}_4\text{OSBr}$: C 54.68, H 3.44, N 12.75 Found C 54.55, H 3.52, N 12.61%.



5-((furan-2-yl)methylthio)-2,4-diamino-7-bromo-5H-chromeno[2,3-b]pyridine-3-carbonitrile (6f). Yellow solid. mp 225–227 °C, IR (KBr)($\nu_{\max}/\text{cm}^{-1}$): 3311, 3442, 2194, 1404, 1655; ^1H NMR (400 MHz, DMSO- d_6) δ 4.14–4.56 (ABq, 2H, $J=12\text{Hz}$), 4.89 (1H), 6.34 (s, 1H), 6.46 (d, $J=8.3\text{Hz}$, 1H), 6.78–6.95 (m, 6H), 7.39 (d, 1H, $J=9\text{Hz}$), 7.62 (d, 1H); ^{13}C NMR (100 MHz, DMSO- d_6) δ (ppm) 28.64, 36.31, 54.27, 84.86, 108.77, 111.49, 116.50, 118.87, 119.41, 124.14, 125.50, 131.12, 131.89, 143.26, 148.21, 150.72, 155.24, 160.5. MS (EI, 70 eV): m/z 429 (M^+). Anal. Calcd For $\text{C}_{18}\text{H}_{13}\text{N}_4\text{O}_2\text{SBr}$: C 50.39, H 3.05, N 13.06 Found C 50.35, H 2.97, N 13.01%.



Sat Jan 01 21:51:51 2000

FIND PEAKS:

Spectrum: *****Sat Jan 01 21:47:10 2000

Region: 4000.00 400.00

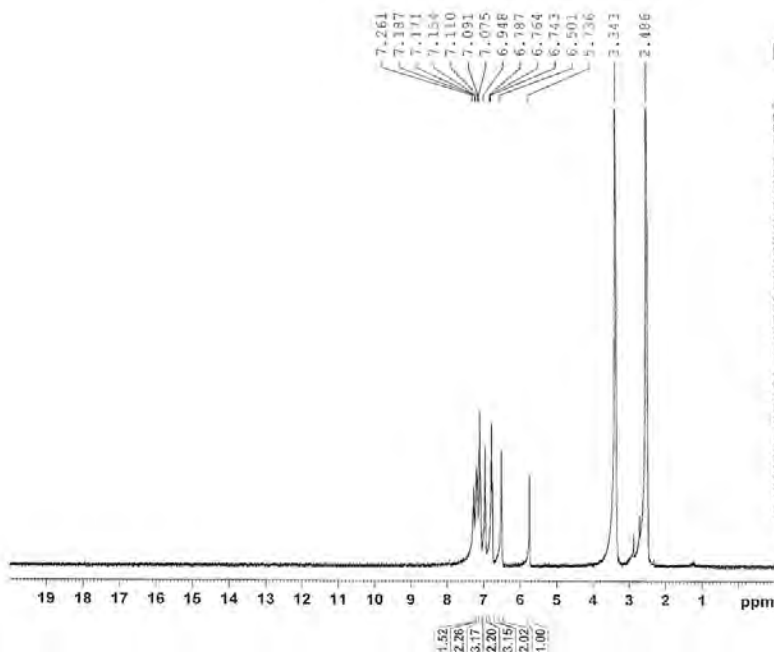
Absolute threshold: 99.069

Sensitivity: 50

Peak list:

Position:	1575.38	Intensity:	9.996
Position:	1630.09	Intensity:	15.224
Position:	1404.22	Intensity:	52.352
Position:	3428.01	Intensity:	28.292
Position:	3355.06	Intensity:	35.220
Position:	1462.99	Intensity:	42.114
Position:	2203.17	Intensity:	59.164

Position:	895.90	Intensity:	98.416
Position:	648.17	Intensity:	88.192
Position:	519.56	Intensity:	84.651
Position:	2923.82	Intensity:	83.811
Position:	1194.03	Intensity:	83.388
Position:	561.39	Intensity:	82.513
Position:	1069.40	Intensity:	82.440
Position:	1335.89	Intensity:	81.886
Position:	697.49	Intensity:	80.637
Position:	766.68	Intensity:	73.366
Position:	3176.10	Intensity:	63.811
Position:	1260.54	Intensity:	63.026
Position:	1223.50	Intensity:	59.034

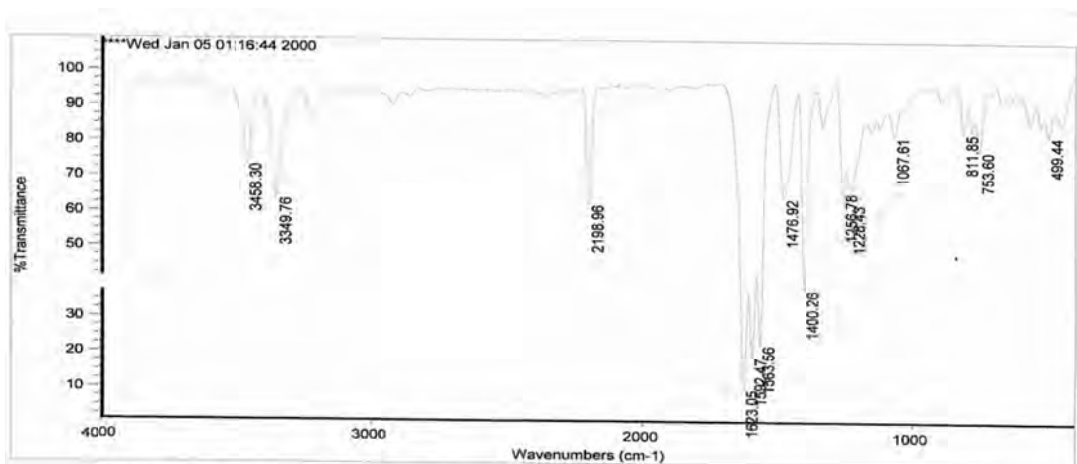
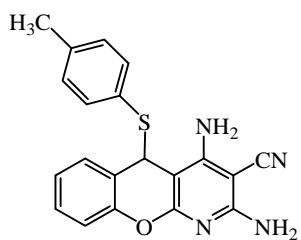


Current Data Parameters
NAME 3H
EXPNO 315
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120116
Time 15:10
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg
TD 32768
SOLVENT HMSD
NS 1
DS 0
SWH 11674.074 Hz
FIDRES 0.35313 Hz
AQ 1.4156276 sec
RG 360
RW 43.200 usec
DE 6.00 usec
TE 300.0 K
D1 5.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -0.00 dB
SFO1 100.1324710 MHz

F2 - Processing parameters
ST 32768
SF 100.1306045 MHz
HFWD EM
SBB 0
GB 0.30 Hz
GB 0
BC 1.00

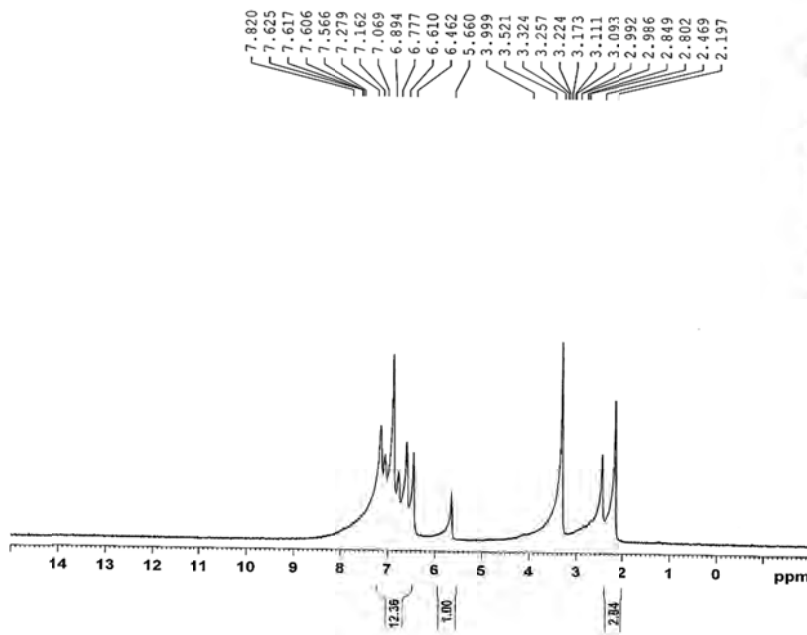
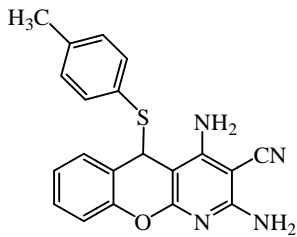


Wed Jan 05 01:19:11 2000

FIND PEAKS:

Spectrum: ****Wed Jan 05 01:16:44 2000
 Region: 4000.00 400.00
 Absolute threshold: 83.345
 Sensitivity: 50
 Peak list:

Position	Intensity
1623.05	9.873
1592.47	19.015
1563.56	22.568
1476.92	64.146
1228.43	62.517
3349.76	63.590



```

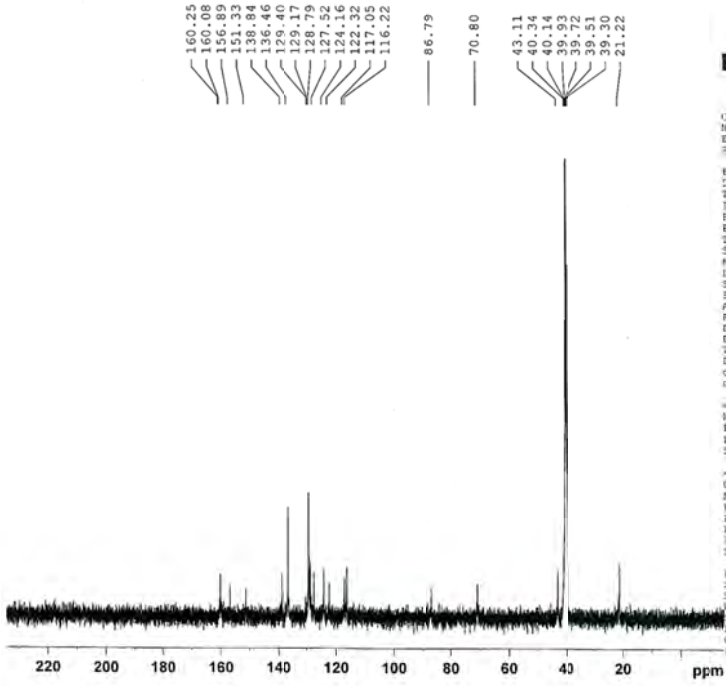
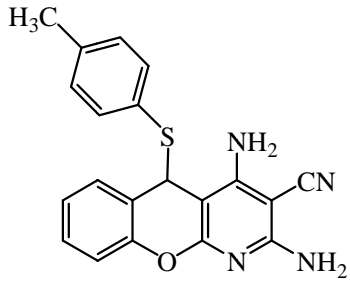
Current Data Parameters
NAME      3H
EXPRO    1328
PROCNO   1

F2 - Acquisition Parameters
Date     20130826
TIME     16.18
INSTRUM  spect
PROBHD   5 mm Multinucl
PULPROG  zg
TD       32768
SOLVENT  DMSO
NS       1
DS       0
SWH      11574.074 Hz
FIDRES   0.353213 Hz
AQ       1.4156276 sec
RG       181
DM       43.200 usec
DE       6.00 usec
TE       300.0 K
D1       5.0000000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       3.00 usec
PL1      -6.00 dB
SFO1     400.1324710 MHz

F2 - Processing parameters
SI       32768
SF       400.1300005 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

```



```

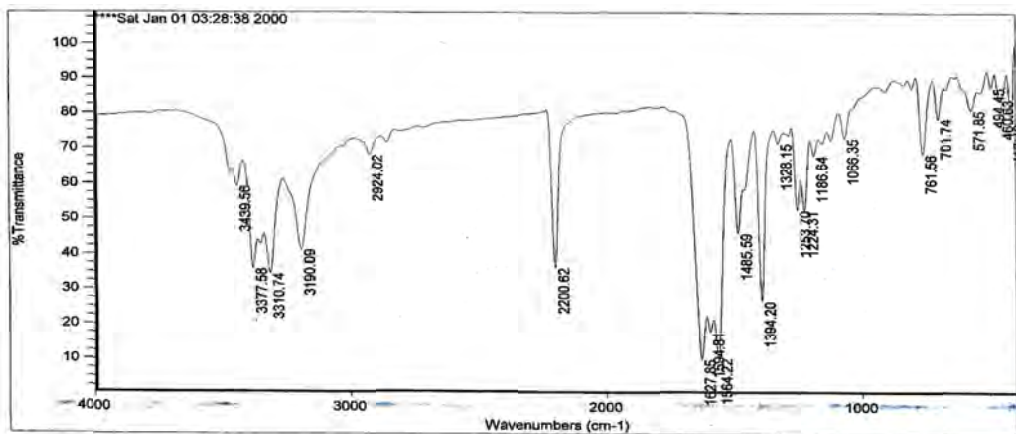
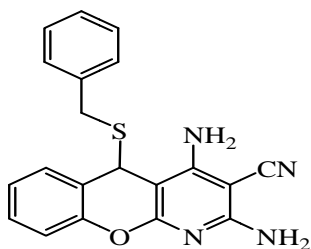
Current Data Parameters
NAME      Carbon13
EXPNO    2388
PROCNO   3

F2 - Acquisition Parameters
Date_    20130507
Time     16.17
INSTRUM spect
PROBHD   5 mm MaltAvuc1
PULPROG zgpg30
TD        65536
SOLVENT  DMSO
NS        500
DS        4
SWH       40404.039 Hz
FIDRES    0.616517 Hz
AQ        0.8110580 sec
RG        32768
DM        1.375 usec
DE        6.00 usec
TE        300.0 K
D1        1.00000000 sec
d11       0.00000000 sec
d12       0.00002000 sec

===== CHANNEL f1 =====
NUC1      13C
P1        7.50 usec
PL1       -2.00 dB
SFO1     100.6204965 MHz

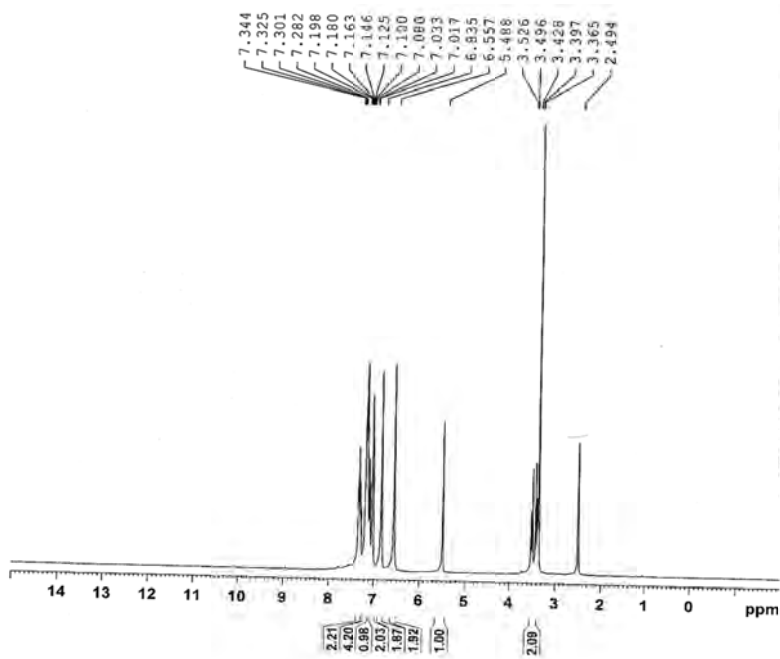
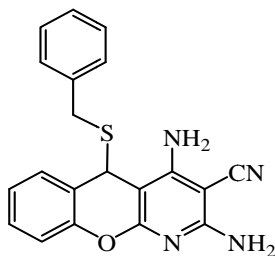
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       4.00 dB
PL12     18.50 dB
PL13     18.50 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI        32768
SF        100.6217690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



Sat Jan 01 03:31:07 2000
 FIND PEAKS:
 Spectrum: ****Sat Jan 01 03:28:38 2000
 Region: 4000.00 400.00
 Absolute threshold: 91.621
 Sensitivity: 50
 Peak list:

Position	Intensity	Position	Intensity
494.45	87.683	1186.64	68.130
460.63	84.347	1186.64	68.382
571.85	81.238	1224.31	62.703
701.74	79.825	1328.15	59.235
417.49	77.547	1394.20	52.658
73.313	73.313	1564.22	36.233
71.854	71.854	1627.85	9.996
1328.15	68.859	1627.85	9.996
761.56	68.859	1627.85	9.996
1186.64	68.382	1627.85	9.996
2824.02	68.130	1627.85	9.996
3439.58	59.235	1627.85	9.996
1224.31	62.703	1627.85	9.996
1224.31	52.658	1627.85	9.996
1224.31	52.658	1627.85	9.996
1485.69	46.129	1627.85	9.996
3190.09	41.136	1627.85	9.996



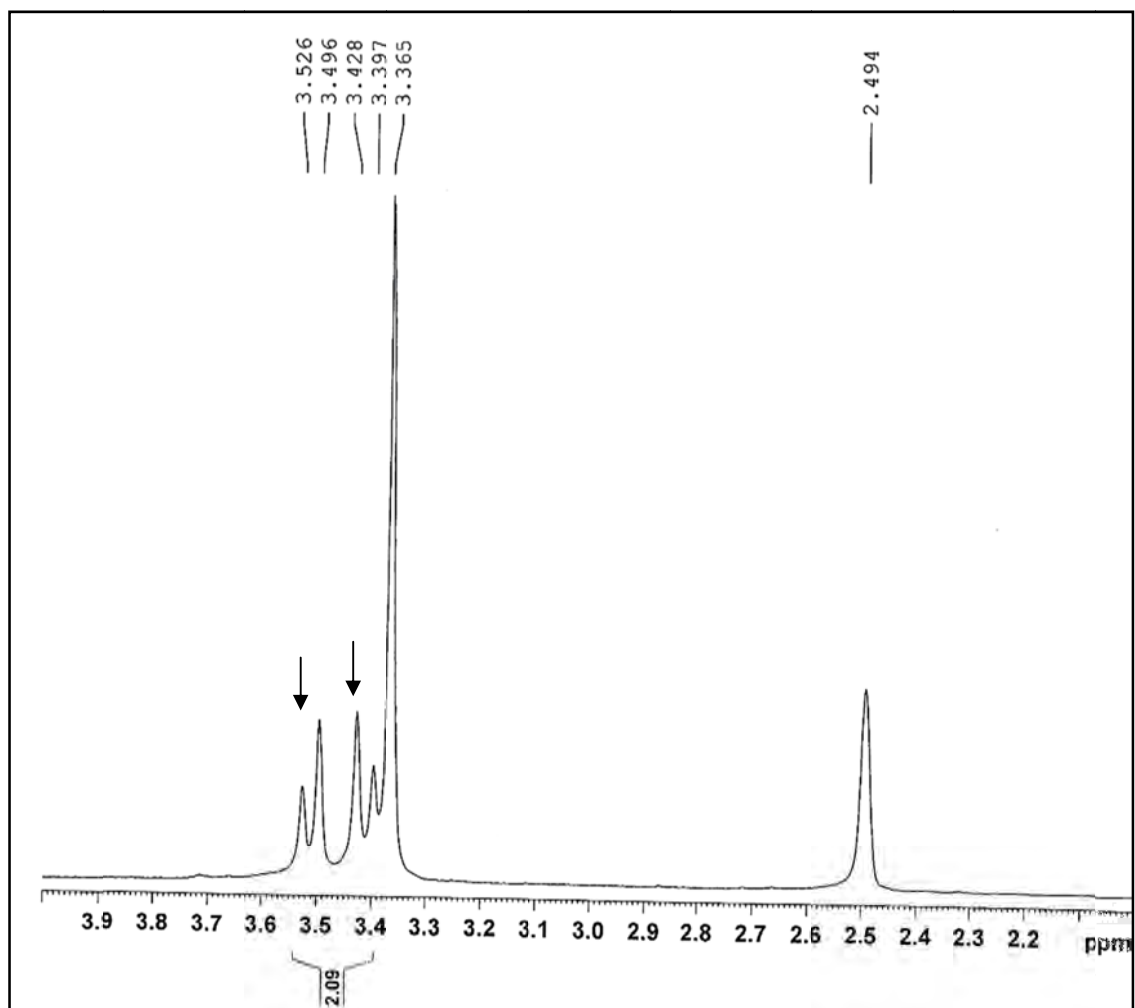
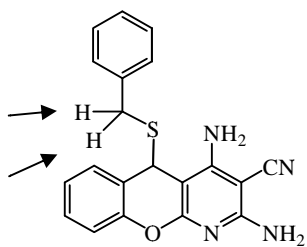
```

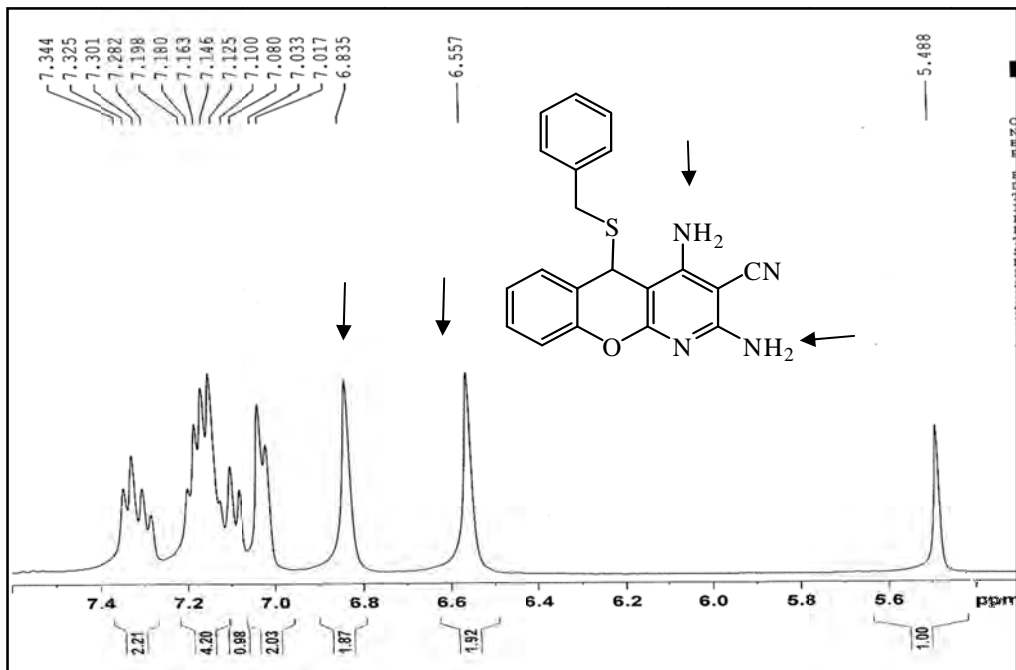
Current Data Parameters
NAME      3H
EXPNO    1355
PROCNO   1

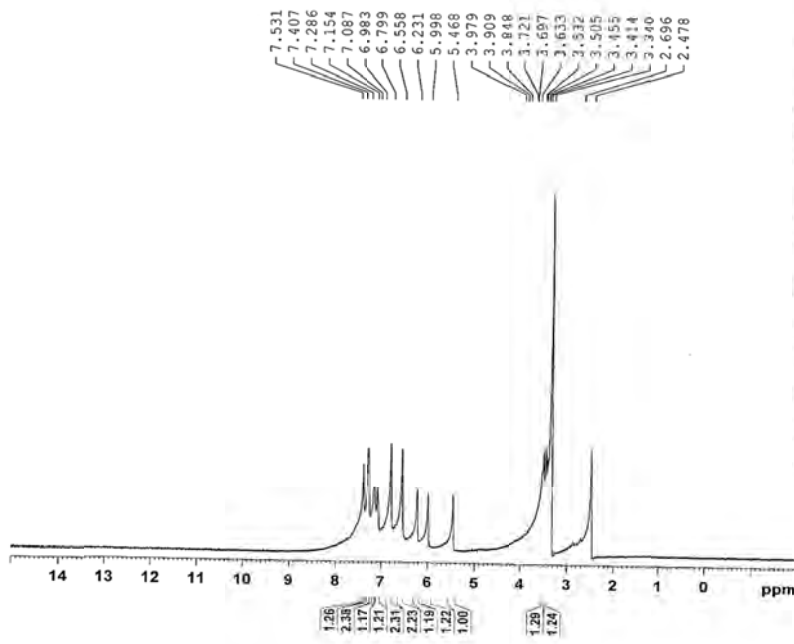
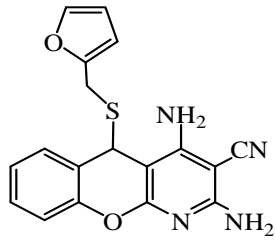
F2 - Acquisition Parameters
Date_    20130828
Time     15.46
INSTRUM spect
PROBHD   5 mm Multinuc1
PULPROG zg
TD       32768
SOLVENT DMSO
NS       1
DS       0
SWH      11574.074 Hz
FIDRES   0.353213 Hz
AQ       1.4196276 sec
RG       114
EM       43.200 usec
DE       6.00 usec
TE       300.0 K
SI       5.00000000 sec

----- CHANNEL f1 -----
NUC1     1H
P1       9.00 usec
PL1     -6.00 dB
SFO1    400.1324710 MHz

F1 - Processing parameters
SI       32768
SF      400.130045 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
  
```





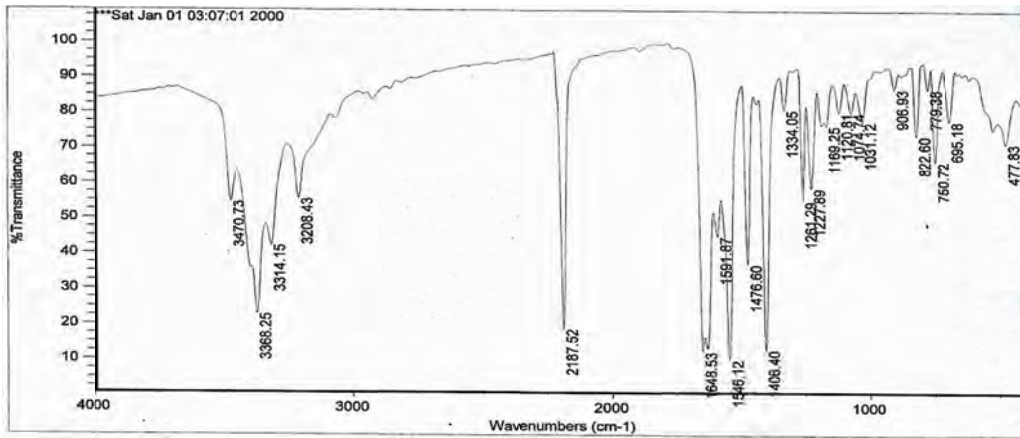
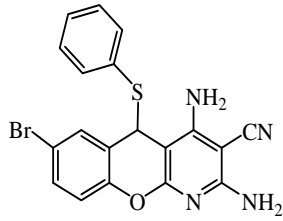


Current Data Parameters
 NAME SU
 EXPNO 1205
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130729
 Time 12.31
 INSTRUM spect
 PROBHD 5 mm Multinuc1
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 11574.074 Hz
 FIDRES 0.353213 Hz
 AQ 1.4184236 sec
 RG 181
 SW 43.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 5.00000000 sec

===== CHANNEL f2 =====
 NUC1 1H
 P1 9.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130045 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Sat Jan 01 03:09:34 2000

FIND PEAKS:

Spectrum: ****Sat Jan 01 03:07:01 2000

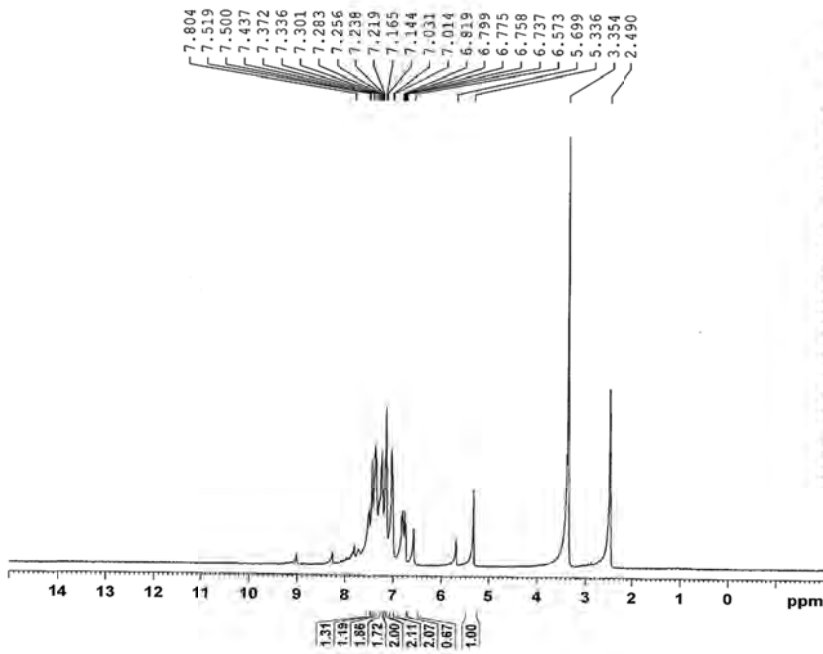
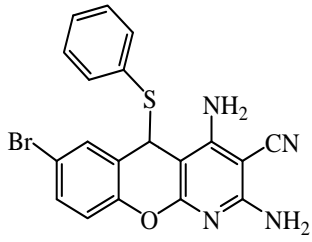
Region: 4000.00 400.00

Absolute threshold: 94.103

Sensitivity: 50

Peak list:

Position	Intensity	Position	Intensity
1591.87	45.033	1031.12	35.000
1546.12	9.931	1020.91	35.000
1476.60	42.146	1000.00	35.000
1408.40	37.361	906.93	45.000
1334.05	54.543	822.60	35.000
1261.28	55.123	775.35	35.000
1227.89	58.428	760.72	35.000
1189.25	66.628	695.16	35.000
1170.91	71.898	600.00	35.000
1100.00	75.899	500.00	35.000
1090.91	77.790	400.00	35.000
1031.12	77.844	300.00	35.000
1020.91	77.844	200.00	35.000
906.93	77.790	100.00	35.000
822.60	78.723	0.00	35.000
775.35	79.723		
760.72	79.723		
695.16	79.723		
600.00	79.723		
500.00	79.723		
400.00	79.723		
300.00	79.723		
200.00	79.723		
100.00	79.723		
0.00	79.723		

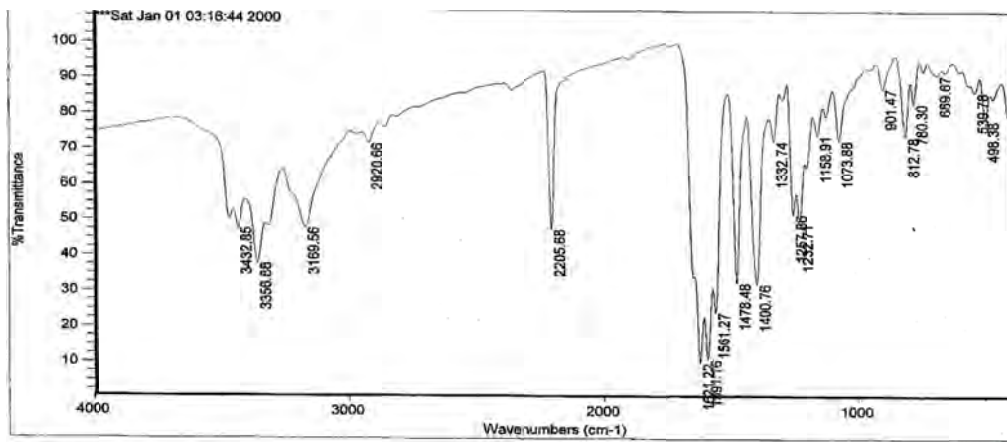
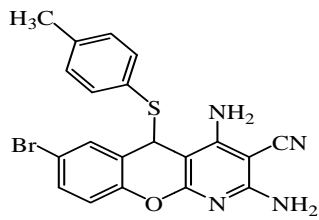


Current Data Parameters
NAME 3H
EXPNO 1356
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130828
Time 15.52
INSTRUM spect
PROBHD 5 mm Multinuc1
PULPROG zg
TD 32768
SOLVENT DMSO
NS 1
DS 0
SWH 11574.074 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 181
AQ 43.200 usec
DE 6.00 usec
TE 300.0 K
D1 5.0000000 sec

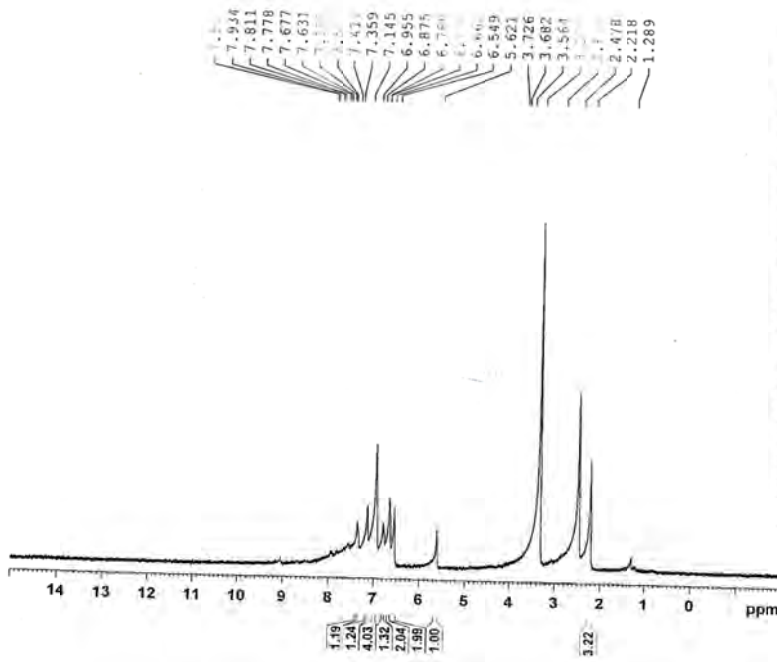
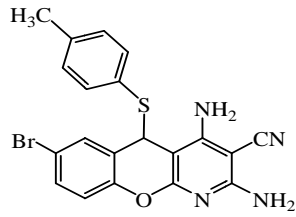
----- CHANNEL f1 -----
NUC1 1H
P1 9.00 usec
PL1 -6.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300045 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Sat Jan 01 03:21:46 2000
 FIND PEAKS:
 Spectrum: *** Sat Jan 01 03:16:44 2000
 Region: 4000.00 - 400.00
 Absolute threshold: 94.531
 Sensitivity: 50
 Peak list:

Position	Intensity
3432.85	47.671
3356.88	49.420
3169.56	3169.56
2920.86	2920.86
2205.68	2205.68
1621.73	1621.73
1581.27	1581.27
1478.48	1478.48
1400.76	1400.76
1332.74	1332.74
1257.86	1257.86
1159.91	1159.91
1073.88	1073.88
901.47	901.47
812.79	812.79
80.30	80.30
699.67	699.67
539.78	539.78
489.36	489.36
469.36	469.36
409.36	409.36



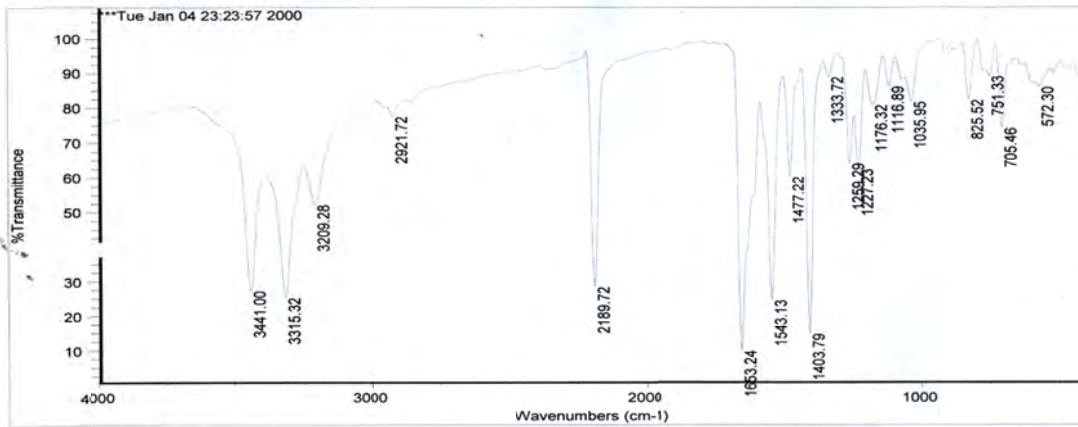
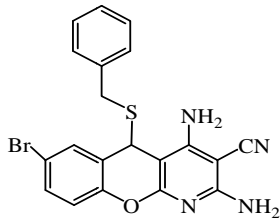
BRUKER

Current Data Parameters
 NAME 3H
 EXPNO 1073
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130715
 Time 10.58
 INSTRUM spect
 PROBHD 5 mm Multinucl
 FOLPROG zg
 ID 32768
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 11574.074 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 382
 DW 43.200 usec
 DE 6.00 usec
 TE 300.2 K
 D1 5.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 9.00 usec
 PL1 -6.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300045 MHz
 WMW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



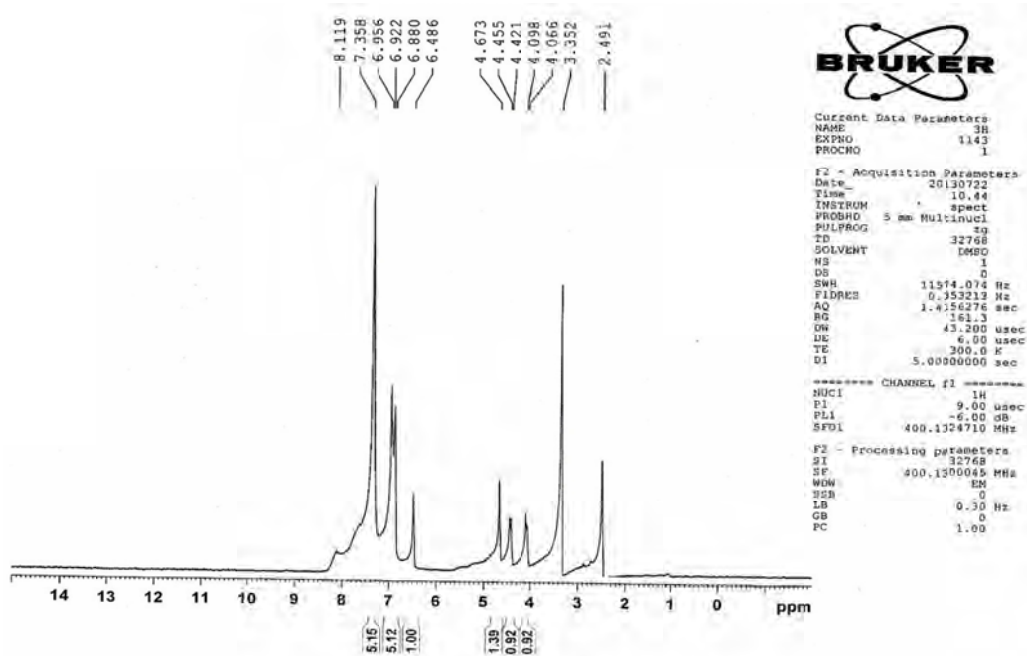
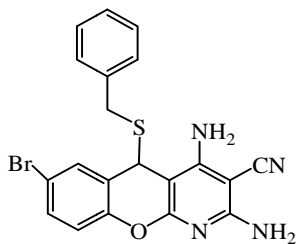
Wed Jan 05 01:16:41 2000

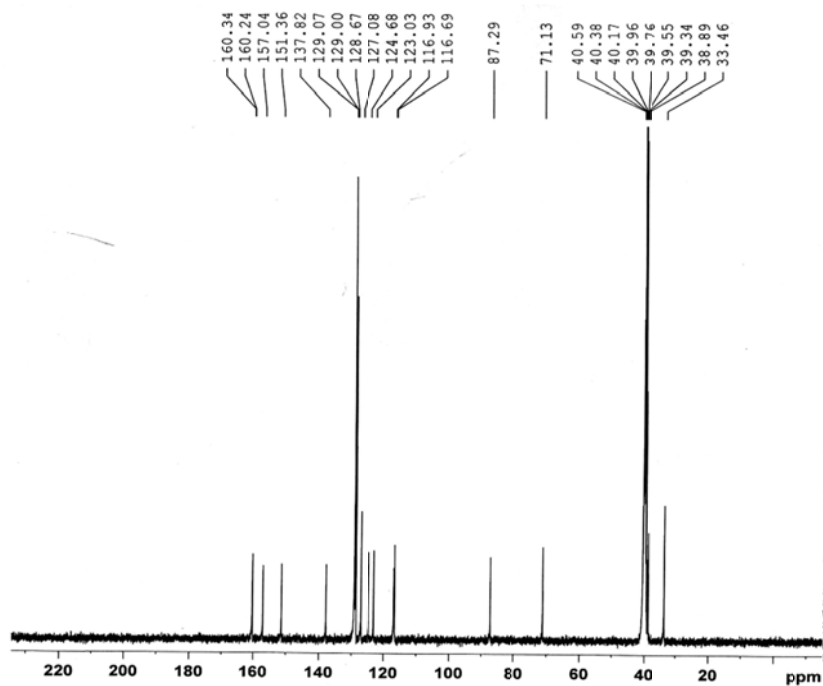
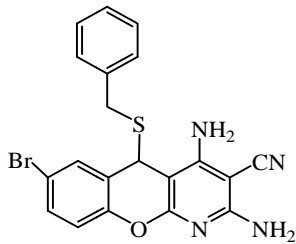
FIND PEAKS:

Spectrum: ***Tue Jan 04 23:23:57 2000
 Region: 4000.00 400.00
 Absolute threshold: 99.897
 Sensitivity: 50

Peak list:

Position	Intensity
1653.24	9.909
1403.79	14.758
1543.13	24.671
1477.22	60.227
2189.72	52.251
3209.28	52.251
1477.22	60.227





```

Current Data Parameters
NAME          Carbon13
EXPNO        2395
PROCNO       1

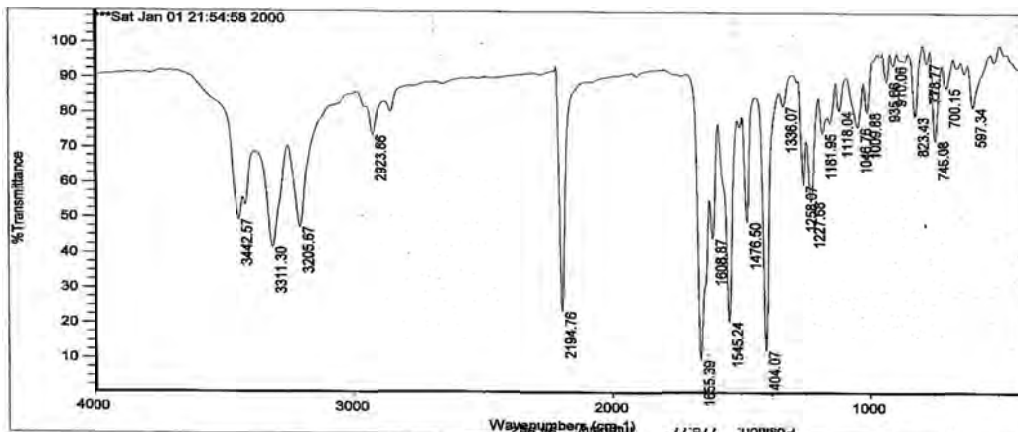
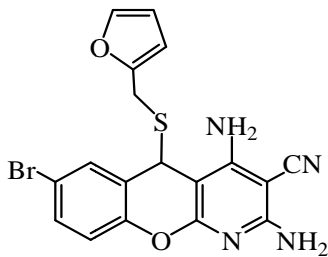
F2 - Acquisition Parameters
Date_        20130926
Time         1.20
INSTRUM     spect
PROBHD      5 mm Multinucl
PULPROG     zgpg30
TD          65536
SOLVENT     DMSO
NS          2000
DS          4
SWH         40404.039 Hz
FIDRES     0.616517 Hz
AQ         0.8110580 sec
RG         32768
DW         12.375 usec
DE         6.00 usec
TE         300.0 K
d1         1.0000000 sec
d11        0.0300000 sec
d12        0.0000200 sec

===== CHANNEL f1 =====
NUC1        13C
P1         7.50 usec
PL1        -2.00 dB
SFO1       100.6204965 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      80.00 usec
PL2        -4.00 dB
PL12       18.50 dB
PL13       18.50 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



Sat Jan 01 22:02:43 2000

FIND PEAKS:

Spectrum: ****Sat Jan 01 21:54:58 2000
 Region: 4000.00 400.00
 Absolute threshold: 100.724
 Sensitivity: 50
 Peak list:

Position	Intensity
1655.39	9.843
1404.07	12.614
1545.24	21.074
2194.76	23.631
3311.30	41.589
1608.87	44.979
3205.67	47.418

Position	Intensity
49.275	49.432
82.305	80.973
82.658	79.789
76.659	78.789
74.965	76.659
73.710	74.965
72.936	72.936
58.914	58.914
55.269	55.269
49.432	49.432
1476.50	1476.50
1476.50	1476.50
1009.88	1009.88
1118.04	1118.04
597.34	597.34
1338.07	1338.07
700.15	700.15
823.43	823.43
810.09	810.09
775.77	775.77

