Supporting Information

Microwave-Promoted Efficient Synthesis of C6-cyclo Secondary Amine Substituted Purine Analogues in Neat Water

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General:

All reagents and solvents were purchased from commercial sources and used without further purification. For thin layer chromatography (TLC), silica gel plates VWR GL60 F254 were used. Melting points were determined with an XRC-1 micro melting point apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded in DMSO-d_6 solutions on a Bruker DPX-400 spectrometer (at 400 MHz and 100 MHz, respectively) using TMS as internal standard. Chemical shifts (δ) were expressed in ppm and coupling constants (J) were given in Hz. IR spectra were recorded for KBr tablets on a Bruker Vector 22 spectrometer with absorptions expressed in cm^{-1}. High resolution mass spectra were obtained on the electrospray ionization (ESI) mass spectrometer. The nucleobase were obtained from Xinxiang Tuoxin Biochemical Technology & Science Co. Ltd, P. R. China for free.

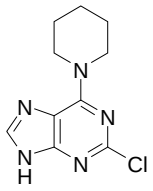
All microwave irradiation experiments were carried out in the cavity of a commercially available single-mode microwave synthesis apparatus equipped with a high sensitivity infrared sensor for temperature control and measurement (MAS-I, Sineo Microwave Chemical Technology Co. Ltd., Shanghai, P. R. of China) with continuous irradiation power from 0 to 600 W. The reactions were carried out in 5 mL open glass vials. The temperature was measured with an IR sensor on the outer surface of the process vial.

General Procedure:

Method **a**: 6-dichloropurine derivatives **1** (1 mmol) and piperidine **2a** or 1-ethylpiperazine **2d** (4 mmol) were mixed in water (2 mL). The mixture was put into microwave synthesis apparatus (MAS-I, sineo Microwave Chemical Techology Co.Ltd., Shanghai, China) and irradiated at 400 w (100 ^{o}C). The reaction was monitored by TLC. 8 minutes later, the starting material disappeared and the reaction mixture was cooled to the room temperature. For 3a and 6a-6c, the reactions were filtered, washed by water, dried in air and the pure products were obtained. For 3b-3j and 6d-6f, the reactions were purified by flash column chromatography (ethyl acetate/petroleum ether) to afford pure products.

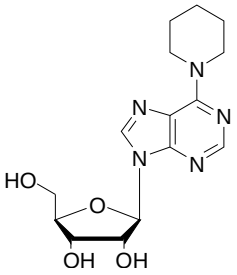
Method **b**: 6-dichloropurine derivatives **1** (1 mmol) and pyrrolidine **2b** or morpholine **2e**, or thiomorpholine **2f** (1.2 mmol) were mixed in water (2 mL), and then NaOH (2 mmol) was added. The mixture was put into microwave synthesis apparatus and irradiated at 400 w (100 ^{o}C). The reaction was monitored by TLC. 8 minutes later, the starting material disappeared and the reaction mixture was cooled to the room temperature. For 4a-4c, 7a and 8a-8c, the reactions were filtered, washed by water, dried in air and the pure products were obtained. For 4b-4i, 7b-7j and 8d-8f, the reactions were purified by flash column chromatography (ethyl acetate/petroleum ether) to afford pure products.

2-Chloro-6-piperidin-1-yl-9*H*-purine (3a).



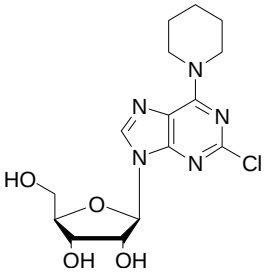
Pale white crystal. mp 282-284 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.56-1.67 (m, 6H), 3.93-4.28 (m, 4H), 8.10 (s, 1H), 13.12 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.5, 25.8, 45.7, 118.8, 137.9, 151.6, 152.0, 153.1. IR (KBr) ν_{max} /cm^{-1}: 782, 1126, 1361, 1464, 1590, 2856, 2941, 3107, 3456. HRMS: calcd for $C_{10}H_{13}ClN_5$ [M+H$^+$] 238.0859, found. 238.0850.

6-piperidino-9-*β*-furanosyl purine (3b). [1]



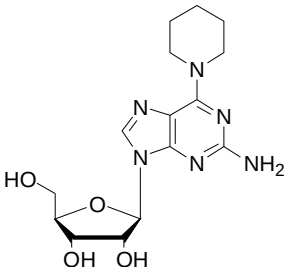
White powder. mp 179-181 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.57-1.68 (m, 6H), 3.53-3.58 (m, 1H), 3.64-3.69 (m, 1H), 3.95-3.97 (m, 1H), 4.13-4.20 (m, 4H), 4.56-4.60 (m, 1H), 5.17-5.18 (m, 1H), 5.34-5.45 (m, 1H), 5.75-5.91 (m, 1H), 8.21 (s, 1H), 8.37 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.4, 25.9, 45.9, 61.7, 70.7, 73.7, 86.0, 88.0, 120.0, 138.7, 150.3, 152.0, 153.3. IR (KBr) ν_{max}/cm^{-1}: 789, 1131, 1344, 1466, 1483, 1590, 2864, 2939, 3406. HRMS: calcd for $C_{15}H_{22}N_5O_4$ [M+H$^+$] 336.1672, found 336.1669.

2-chloro-6-piperidino-9-*β*-furanosyl purine (3c). [2]



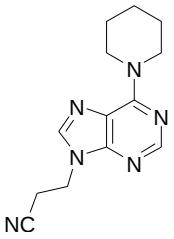
White powder. mp 196-198 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.59-1.68 (m, 6H), 3.55-3.57 (m, 1H), 3.63-3.67 (m, 1H), 3.92-3.95 (m, 1H), 4.11-4.14 (m, 1H), 4.47-4.51 (m, 1H), 5.04-5.07 (m, 1H), 5.20-5.21 (m, 1H), 5.47-5.49 (m, 1H), 5.83-5.85 (m, 1H), 8.05 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.2, 25.8, 61.4, 70.5, 73.9, 85.8, 87.5, 118.4, 138.7, 151.7, 152.9, 153.4. IR (KBr) ν_{max}/cm^{-1}: 782, 1153, 1363, 1442, 1480, 1527, 1600, 2863, 2942, 3111, 3424. HRMS: calcd for $C_{15}H_{21}ClN_5O_4$ [M+H$^+$] 370.1282, found 370.1286.

2-amino-6-piperidino-9-*β*-furanosyl purine (3d). [3]



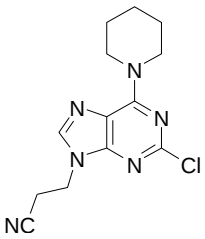
White powder. mp 120-122 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.55-1.65 (m, 6H), 3.50-3.55 (m, 1H), 3.60-3.65 (m, 1H), 3.88-3.89 (m, 1H), 4.08-4.11 (m, 1H), 4.45-4.49 (m, 1H), 5.08-5.10 (m, 1H), 5.32-5.36 (m, 1H), 5.74-5.76 (m, 1H), 5.79 (s, 2H), 7.94 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.6, 25.9, 45.5, 61.8, 70.8, 73.4, 85.6, 87.0, 113.9, 135.1, 152.9, 153.7, 159.5. IR (KBr) ν_{max}/cm^{-1}: 786, 1126, 1375, 1490, 1580, 1620, 2855, 2933, 3378. HRMS: calcd for $C_{15}H_{23}N_6O_4$ [M+H$^+$] 351.1781, found 351.1780.

3-(6-Piperidin-1-yl-purin-9-yl)propionitrile (3e).



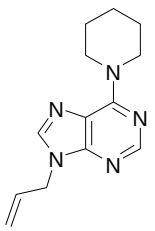
White powder; mp 118-120 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.58-1.68 (m, 6H), 3.16 (t, 2H, *J* = 6.4 Hz), 4.19 (brs, 4H), 4.45 (t, 2H, *J* = 6.4 Hz), 8.21 (s, 1H), 8.23 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 18.1, 24.0, 25.6, 45.1, 117.6, 117.8, 140.1, 151.6, 152.7, 153.3. IR (KBr) ν_{max} /cm^{-1}: 790, 1070, 1343, 1481, 1587, 1592, 2250, 2862, 2939. HRMS: calcd for $C_{13}H_{17}N_6$ [M+H$^+$] 257.1514, found 257.1521.

3-(2-Chloro-6-piperidin-1-yl-purin-9-yl)propionitrile (3f).



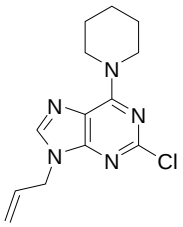
white powder; mp 136-138 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.59-1.74 (m, 6H), 3.13 (t, 2H, *J* = 6.4 Hz), 3.87-4.14 (m, 4H), 4.41 (t, 2H, *J* = *6.4* Hz), 8.23 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 18.2, 24.1, 25.7, 117.9, 118.3, 140.0, 151.7, 152.9, 153.3. IR (KBr) ν_{max}/cm^{-1}: 790, 1120, 1385, 1481, 1483, 1582, 2270, 2876, 2921. HRMS: *m/z* calcd for $C_{13}H_{15}ClN_6$: 290.1047; found: 290.1057.

9-Allyl-6-piperidin-1-yl-9H-purine (3g).



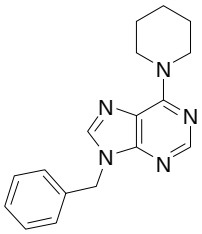
white powder; mp 54-56 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.57-1.67 (m, 2H), 4.19 (brs, 4H), 4.79 (d, 2H, J = 4.8 Hz), 5.05 (d, 1H, J =7.2 Hz), 5.20 (d, 1H, J = 7.2 Hz), 6.00-6.08 (m, 1H), 8.12 (s, 1H), 8.20 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.3, 25.7, 44.9, 45.6, 117.5, 118.8, 133.4, 139.4, 150.4, 151.9, 153.2. IR (KBr) ν_{max} /cm^{-1}: 792, 1120, 1370, 1479, 1585, 2852, 2936, 3080. HRMS: *m/z* calcd for $C_{13}H_{17}N_5$: 243.1484; found: 243.1476.

9-Allyl-2-chloro-6-piperidin-1-yl-9*H*-purine (3h).



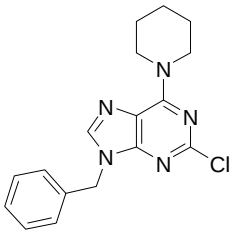
white powder; mp 56-57 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.59-1.67 (m, 6H), 4.00-4.34 (m, 4H), 4.75 (d, 2H, J = 5.2 Hz), 5.04 (d, 1H, J = 9.6 Hz), 5.21 (d, 1H, J = 9.6 Hz), 5.98-6.08 (m, 1H), 8.14 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.0, 25.6, 45.1, 117.6, 117.8, 133.0, 140.1, 151.6, 152.7, 153.3. IR (KBr) ν_{max} /cm^{-1}: 798, 1112, 1450, 1608, 2862, 2930, 3078. HRMS: *m/z* calcd for $C_{13}H_{16}ClN_5$: 277.1094; found: 277.1085.

9-Benzyl-6-piperidin-1-yl-9*H*-purine (3i). [4]



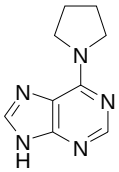
white powder; mp 66-68 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ ppm 1.56 (s, 4H), 1.67 (s, 2H), 4.18 (brs, 4H), 5.37 (s, 2H), 7.27-7.31 (m, 5H), 8.21 (s, 1H), 8.27 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d$_6$): δ ppm 24.3, 25.7, 45.5, 46.2, 118.9, 127.6, 127.7, 128.7, 137.1, 139.6, 150.5, 152.0, 153.2. IR (KBr) ν_{max}/cm^{-1}: 704, 732, 791, 1130, 1334, 1479, 1585, 2830, 2926, 3115. HRMS: *m/z* calcd for $C_{17}H_{19}N_5$: 293.1640; found: 293.1649.

9-Benzyl-2-chloro-6-piperidin-1-yl-9*H*-purine (3j).



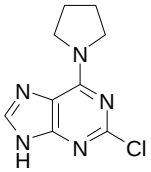
white powder; mp 96-98 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.58 (s 4H), 1.65-1.74 (m, 2H), 3.93-4.36 (m, 4H), 5.34 (s, 2H), 7.03-7.37 (m, 5H), 8.27 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.0, 25.6, 46.3, 117.9, 127.4, 127.8, 128.7, 136.7, 140.1, 151.7, 152.9, 153.3. IR (KBr) ν_{max}/cm^{-1}: 702, 745, 783, 1106, 1369, 1458, 1495, 1596, 2823, 2939, 3100. HRMS: *m/z* calcd for $C_{17}H_{18}ClN_5$: 327.1251; found: 327.1262.

6-pyrrolidyl purine (4a). [5]



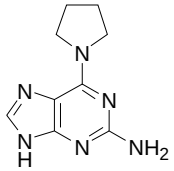
White powder. mp 284-286 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ ppm 1.95 (s, 4H), 3.63-4.05 (m, 4H), 8.05 (s, H), 8.16 (s, H), 12.88 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δppm 25.0, 47.7, 119.2, 138.2, 150.8, 152.2, 152.6. IR (KBr) ν_{max}/cm^{-1}:781, 1130, 1258, 1335, 1454, 1496, 1628, 2862, 3362. HRMS: calcd for $C_9H_{12}N_5$ [M+H$^+$] 190.1092, found 190.1090.

2-chloro-6-pyrrolidyl purine (4b). [6]



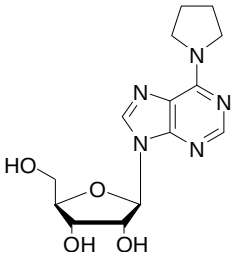
White powder. mp 288-289 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ ppm 1.83-1.98 (m, 4H), 3.57-4.05 (m, 4H), 8.07 (s, H), 13.06 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 25.7, 47.2, 118.2, 138.9, 151.7, 152.7, 152.8. IR (KBr) ν_{max}/cm^{-1}: 784, 1127, 1383, 1457, 1492, 1601, 2869, 2976, 3464. HRMS: calcd for $C_9H_{11}ClN_5$ [M+H$^+$] 224.0703, found 224.0709.

2-amino-6-pyrrolidyl purine (4c). [7]



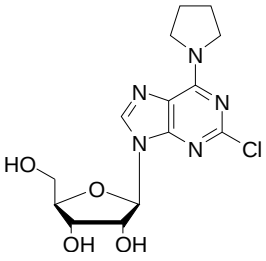
White needle crystal. mp 268-270 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.90 (s, 4H), 3.51-3.92 (m, 4H), 5.61 (s, 2H), 7.61 (s, 1H), 12.04 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.7, 47.2, 113.8, 134.9, 153.0, 159.9. IR (KBr) ν_{max} /cm^{-1}: 782, 1110, 1259, 1347, 1449, 1483, 1586, 2974, 3350. HRMS: calcd for $C_9H_{13}N_6$ [M+H$^+$] 205.1201, found 205.1206.

6-pyrrolidyl-9-*β*-furanosyl purine (4d). [8]



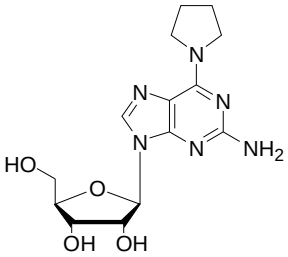
white powder**.** mp 112-114 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.94-1.97 (m, 4H), 3.45-3.57 (m, 2H), 3.65-3.70 (m, 2H), 3.95-3.97 (m, 1H), 4.05-4.10 (m, 1H), 4.13-4.16 (m, 1H), 4.55-4.69 (m, 1H), 5.16-5.18 (m, 1H), 5.35-5.44 (m, 2H), 5.85-5.91 (m, 1H), 8.20 (s, 1H), 8.37 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 25.1, 47.6, 62.0, 71.0, 73.9, 86.2, 88.3, 120.4, 139.5, 150.0, 152.5, 153.0. IR (KBr) ν_{max}/cm^{-1}: 788, 1110, 1383, 1469, 1481, 1572, 1603, 2885, 2930, 3113, 3595. HRMS: calcd for $C_{14}H_{20}N_5O_4$ [M+H$^+$] 322.1515, found 322.1508.

2-chloro-6-pyrrolidyl-9-*β*-furanosyl purine (4e). [9]



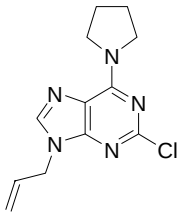
White pale crystal. mp 216-218 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.88-2.02 (m, 4H), 3.46-3.69 (m, 4H), 3.93-3.96 (m, 1H), 4.02-4.06 (m, 1H), 4.11-4.14 (m, 1H), 4.47-4.52 (m, 1H), 5.04-5.07 (m, 1H), 5.19-5.20 (m, 1H), 5.46-5.49 (m, 1H), 5.83-5.85（m, 1H）, 8.41 （d, 1H, *J = 7.6 Hz*）. ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 25.5, 47.8, 61.7, 70.7, 74.2, 86.1, 87.8, 119.3, 139.1, 151.6, 153.2, 154.9. IR (KBr) ν_{max}/cm^{-1}: 783, 1127, 1353, 1403, 1534, 1603, 2850, 2929, 3342. HRMS: calcd for $C_{14}H_{19}ClN_5O_4$ [M+H$^+$] 356.1125, found 356.1129.

2-amino-6--pyrrolidyl-9-β-furanosyl purine (4f). [10]



White column crystal. mp 125-127 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.91 (s, 4H), 3.51-3.68 (m, 4H), 3.88-3.89 (m, 2H), 4.08-4.11 (m, 1H), 4.44-4.47 (m, 1H), 5.08-5.10 (m, 1H), 5.34-5.35 (m, 2H), 5.74-5.79 (m, 3H), 7.94 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 24.2, 47.6, 62.1, 71.0, 73.7, 85.8, 87.3, 114.4, 135.5, 152.9, 153.5, 159.6. IR (KBr) ν_{max} /cm^{-1}: 785, 1123, 1349, 1456, 1494, 1698, 2861, 2929, 3321, 3377. HRMS: calcd for $C_{14}H_{21}N_6O_4$ [M+H$^+$] 337.1624, found 337.1627.

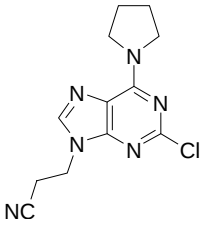
9-Allyl-2-chloro-6-pyrrolidin-1-yl-9*H*-purine (4g).



white powder; mp 65-66 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δppm 1.91-1.98 (m, 4H), 3.58 (s, 2H), 4.04 (s, 2H), 4.75 (d, 2H, J = 4.8 Hz), 5.02 (d, 1H, *J* = 7.2 Hz), 5.20 (d, 1H, *J* = 7.2 Hz), 5.99-6.09 (m, 1H), 8.08 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 25.6, 45.0, 47.3, 117.5, 118.4, 133.1, 140.6, 150.8, 152.8, 152.9. IR (KBr) ν_{max} /cm^{-1}: 784, 1123, 1360, 1456,

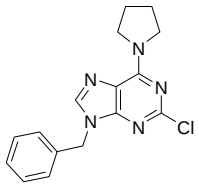
1475, 1596, 2875, 2972, 3084. HRMS: *m/z* calcd for $C_{12}H_{14}ClN_5$: 263.0938; found: 263.0949.

3-(2-Chloro-6-pyrrolidin-1-yl-purin-9-yl)propionitrile (4h).



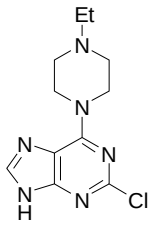
white needle crystal; mp 176-178 ^oC; ^1H NMR (400 MHz, DMSO-d_6): δ ppm 1.89-1.98 (m, 4H), 3.11 (t, 2H, J = 6.4 Hz), 3.56-3.64 (m, 2H), 4.03 (t, 2H, J = 6.4 Hz), 4.41 (t, 2H, J = 6.4 Hz), 8.19 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ ppm 18.9, 26.1, 39.7, 47.7, 116.6, 117.3, 138.4, 150.9, 153.4, 154.4. IR (KBr) ν_{max} /cm^{-1}: 1119, 1362, 1417, 1604, 2252, 2887, 2910. HRMS: *m/z* calcd for $C_{12}H_{13}ClN_6$: 276.0890; found: 276.0899.

9-Benzyl-2-chloro-6-pyrrolidin-1-yl-9*H*-purine (4i).



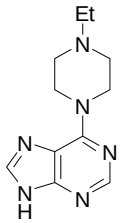
white column crystal; mp 98-100 ^oC. ^1H NMR (400 MHz, DMSO-d_6): δ ppm 1.89-1.96 (m, 4H), 3.57 (s, 2H), 4.03 (s, 2H), 5.34 (s, 2H), 7.25-7.34 (m, 5H), 8.20 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 25.7, 46.3, 47.4, 118.5, 127.4, 127.9, 128.7, 136.8, 140.7, 151.0, 152.9, 153.1. IR (KBr) ν_{max}/cm^{-1}: 703, 761, 1122, 1377, 1458, 1594, 2854, 2955. HRMS: *m/z* calcd for $C_{16}H_{16}ClN_5$: 313.1094; found: 313.1102.

2-Chloro-6-(4-ethyl-piperazin-1-yl)-9*H*-purine (6a).



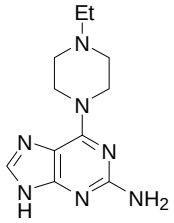
white needle crystal; mp 210-211 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.02 (t, 3H, J = 7.2 Hz), 2.35 (q, 2H, J = 7.2 Hz), 2.45-2.50 (m, 4H), 4.00-4.56 (m, 4H), 8.13 (s, 1H), 13.16 (brs, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 11.9, 51.6, 52.3, 117.7, 138.8, 152.5, 152.6, 153.3. IR (KBr) ν_{max}/cm^{-1}: 635, 762, 1110, 1381, 1480, 1490, 1584, 2817, 2980, 3103, 3440. HRMS: *m/z* calcd for $C_{11}H_{15}ClN_6$: 266.1047; found: 266.1051.

6-(4-Ethyl-piperazin-1-yl)-9*H*-purine (6b). [11]



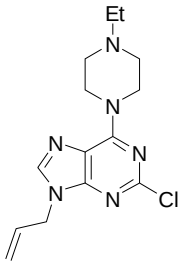
White needle crystal. mp 254-255 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.01 (t, 3H, J = *7.2 Hz*), 2.32 (q, 2H, J = *7.2 Hz*), 2.42-2.49 (m, 4H), 4.19 (s, 4H), 8.10 (s, 1H), 8.18 (s,1H), 13.03 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 12.1, 44.7, 51.9, 52.6, 119.0, 138.3, 151.6, 152.0, 153.3. IR (KBr) ν_{max}/cm^{-1}: 791, 1110, 1378, 1481, 1490, 1518, 1584, 2808, 2974, 3072, 3457. HRMS: calcd for $C_{11}H_{17}N_6$ [M+H$^+$] 233.1514, found 233.1516.

6-(4-Ethyl-piperazin-1-yl)-9*H*-purin-2-ylamine (6c).



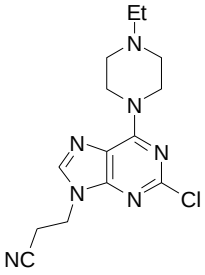
white powder; mp 196-198 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.02 (t, 3H, J = 7.2 Hz), 2.34 (q, 2H, J =7.2 Hz), 2.41-2.50 (m, 4H), 4.10 (brs, 4H), 5.70 (s, 2H), 7.65 (s, 1H), 12.14 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d$_6$): δ ppm 11.9, 44.3, 51.7, 52.5, 113.3, 134.7, 153.6, 153.8, 159.5. IR (KBr) ν_{max} /cm^{-1}: 788, 1123, 1276, 1303, 1487, 1574, 2851, 2966, 3220, 3309. HRMS: calcd for $C_{11}H_{18}N_7$ [M+H$^+$] 248.1623, found 248.1629.

9-Allyl-2-chloro-6-(4-ethyl-piperazin-1-yl)-9*H*-purine (6d).



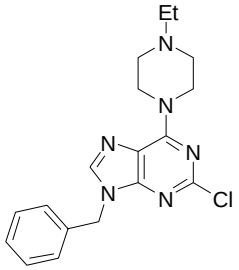
yellow oil. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.03 (t, 3H, J = 7.2 Hz), 2.38 (q, 2H, J = 7.2 Hz), 2.49 (brs, 4H), 4.18 (brs, 4H), 4.76 (d, 2H, J = 5.2 Hz), 5.06 (d, 1H, J = 10 Hz), 5.22 (d, 1H, J = 10 Hz), 5.99-6.08 (m, 1H), 8.14 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 11.8, 45.1, 51.5, 52.2, 117.7, 117.9, 133.0, 140.4, 151.7, 152.7, 153.4. IR (KBr) ν_{max} /cm^{-1}: 784, 1136, 1380, 1453, 1678, 1588, 2813, 2972, 3087, 3450. HRMS: *m/z* calcd for $C_{14}H_{19}ClN_6$: 306.1360; found: 306.1367.

3-[2-Chloro-6-(4-ethyl-piperazin-1-yl)purin-9-yl]propionitrile (6e).



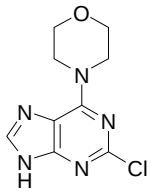
white powder; mp 100-102 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm1.01 (t, 3H, J = 6.8 Hz), 2.30 (q, 2H, J = 6.8 Hz), 2.47-2.48 (m, 4H), 3.11 (t, 2H, J = 6.4 Hz), 3.85 (brs, 4H), 4.40 (t, 2H, J = 6.4 Hz), 8.24 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ ppm 11.7, 18.8, 36.2, 44.5, 52.2, 52.6, 117.8, 118.3, 138.2, 151.7, 153.8, 154.1. IR (KBr) ν_{max} /cm^{-1}: 763, 1115, 1359, 1420, 1589, 1679, 2252, 2883, 3406. HRMS: calcd for $C_{14}H_{19}ClN_7$ [M+H^{+}] 320.1390, found 320.1377.

9-Benzyl-2-chloro-6-(4-ethyl-piperazin-1-yl)-9*H*-purine (6f).



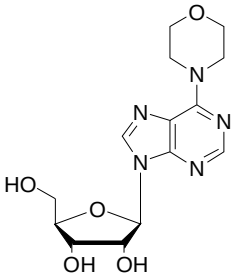
yellow oil. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 1.02 (t, 3H, J = 6.8 Hz), 2.36 (q, 2H, J = 6.8 Hz), 2.46 (brs, 4H), 4.18 (brs, 4H), 5.35 (s, 2H), 7.26-7.36 (m, 5H), 8.27 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 11.91, 48.3, 51.5, 52.2, 118.0, 127.4, 127.8, 128.7, 136.6, 140.5, 151.8, 152.8, 153.4. IR (KBr) ν_{max} /cm^{-1}: 710, 730, 763, 1120, 1469, 1587, 1665, 2832, 2981, 3436. HRMS: *m/z* calcd for $C_{18}H_{21}ClN_6$: 356.1516; found: 356.1523.

2-Chloro-6-morpholin-4-yl-9*H*-purine (7a). [12]



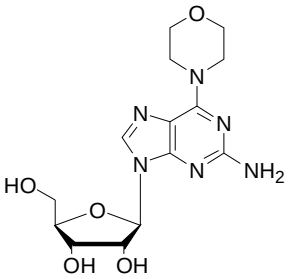
Pale white crystal. mp > 300 ^{o}C. ^{1}H NMR (400MHz, DMSO-d$_6$): δ ppm 3.64-3.72 (m, 4H), 4.15-4.17 (m, 4H), 8.15 (s, 1H), 13.19 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 45.5, 66.2, 118.0, 139.1, 152.6, 152.8, 153.6. IR (KBr) ν_{max} /cm^{-1}: 759, 1113, 1270, 1374, 1449, 1603, 2823, 2972, 3450. HRMS: calcd for $C_9H_{11}ClN_5O$ [M+H^{+}] 240.0652, found 240.0660.

6-morpholinyl-9-*β*-furanosyl purine (7b). [13]



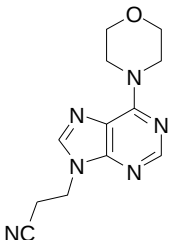
White needel crystal. mp 136-138 °C. ^{1}H NMR (400MHz, DMSO-d_6): δ ppm 3.11-3.14 (m, 2H), 3.21-3.24 (m, 2H), 3.30-3.32 (m, 4H), 3.81-3.82 (m, 1H), 3.83-3.84 (m, 1H), 3.93-3.94 (m, 1H), 3.97-3.98 (m, 1H), 4.01-4.10 (m, 4H), 7.03 (s, 1H), 7.14 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 44.5, 61.6, 66.0, 70.3, 73.1, 85.3, 86.8, 117.7, 132.0, 145.4, 151.7. 152.3. IR (KBr) ν_{max} /cm^{-1}: 786, 1137, 1259, 1390, 1480, 1523, 1595, 2871, 2939, 3024, 3397, 3487. HRMS: calcd for $C_{14}H_{20}N_5O_5$ [M+H$^+$] 338.1464, found 338.1457.

2-amino-6-morpholinyl-9-*β*-furanosyl purine (7c). [9]



White powder. mp 152-154 °C. ^{1}H NMR (400MHz, DMSO-d_6): δ ppm 3.51-3.54 (m, 2H), 3.62-3.67 (m, 4H), 3.89 (s, 1H), 4.11 (s, 4H), 4.46-4.47 (m, 1H), 5.07-5.08 (m, 1H), 5.25 (s, 1H), 5.33-5.34 (m, 1H), 5.76 (d, 1H, *J = 6 Hz*), 5.88 (s, 2H), 7.98 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 45.2, 61.8, 66.4, 70.7, 73.5, 85.5, 87.0, 113.9, 135.5, 153.2, 153.8, 159.5. IR (KBr) ν_{max}/cm^{-1}: 786, 1119, 1241, 1332, 1450, 1489, 1584, 2858, 2923, 3506, 3389. HRMS: calcd for $C_{14}H_{21}N_6O_5$ [M+H$^+$] 353.1573, found 353.1566.

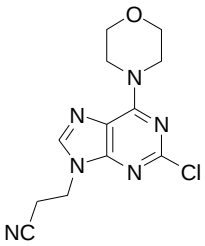
3-(6-Morpholin-4-yl-purin-9-yl)propionitrile (7d).



white needle crystal; mp 116-118 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 3.17 (t, 2H, *J* = 6.4 Hz), 3.71-3.73 (m, 4H), 4.21-4.33 (m, 4H), 4.47 (t, 2H, *J* = 6.4 Hz), 8.26 (s, 1H), 8.29 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ ppm 18.8, 39.8, 45.6, 67.0, 116.6, 120.1, 127.8, 150.6,

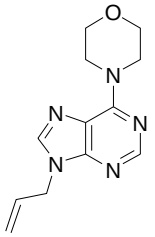
152.6, 154.0. IR (KBr) ν_{max} /cm^{-1}: 796, 1120, 1386, 1448, 1476, 1586, 2270, 2856, 2926, 3050. HRMS: calcd for $C_{12}H_{15}N_6O$ [M+H$^+$] 259.1307 found 259.1298.

3-(2-Chloro-6-morpholin-4-yl-purin-9-yl)propionitrile (7e).



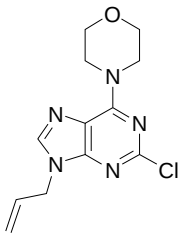
white column crystal; mp 168-170 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 3.13 (t, 2H, J = 6.4 Hz), 3.70 (t, 6H), 4.21 (brs, 2H), 4.41 (t, 2H, J = 6.4 Hz), 8.21 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d$_6$): δ ppm 18.3, 45.2, 66.2, 118.1, 118.4, 139.1, 151.8, 152.8, 153.5. IR (KBr) ν_{max} /cm^{-1}: 784, 1117, 1266, 1358, 1448, 1469, 1583, 2260, 2868, 2940. HRMS: *m/z* calcd for $C_{12}H_{13}ClN_6O$: 292.0839; found: 292.0831.

9-Allyl-6-morpholin-4-yl-9*H*-purine (7f).



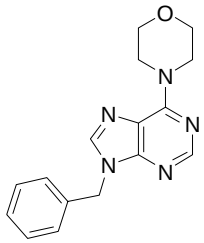
white powder; mp 122-124 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 3.70-3.75 (m, 4 H), 4.20 (brs, 4H), 4.80 (d, 2H, J =5.6 Hz), 5.04 (dd, 1H, J = 16 Hz, 1.2 Hz), 5.20 (d, 1H, J = 10.4 Hz), 6.01-6.10 (m, 1H), 8.18 (s, 1H), 8.25 (d, 1H, J = 5.6 Hz). ^{13}C NMR (100 MHz, DMSO-d$_6$): δ ppm 45.0, 66.2, 117.5, 119.1, 133.4, 140.1, 150.1, 151.9, 153.3. IR (KBr) ν_{max} /cm^{-1}: 779, 1114, 1251, 1332, 1476, 1587, 2866, 2965, 3073. HRMS: calcd for $C_{12}H_{16}N_5O$ [M+H$^+$] 246.1355, found 246.1348.

9-Allyl-2-chloro-6-morpholin-4-yl-9*H*-purine (7g).



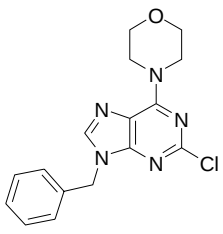
white powder; mp 128-130 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 3.70-3.77 (m, 4H), 4.25 (brs, 4H), 4.76 (d, 2H, J = 5.2 Hz), 5.03 (dd, 1H, J = 17.2 Hz, 1.2 Hz), 5.21 (dd, 1H, J = 17.2 Hz, 1.2 Hz), 5.99-6.08 (m, 1H), 8.18 (s, 1H).^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 45.1, 66.1, 117.6, 118.0, 133.0, 140.6, 151.7, 152.6, 153.4. IR (KBr) ν_{max} /cm^{-1}: 779, 1110, 1245, 1332, 1470, 1590, 2866, 2975, 3050. HRMS: *m/z* calcd for $C_{12}H_{14}ClN_5O$: 279.0887; found: 279.0879.

9-Benzyl-6-morpholin-4-yl-9*H*-purine (7h). [14]



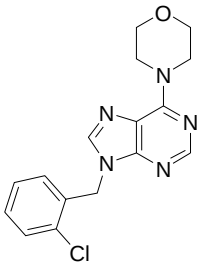
White powder, mp 82-83 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 3.70-3.72 (m, 4H), 4.06-4.35 (m, 4H), 5.40 (s, 2H), 7.22-7.35 (m, 5H), 8.27 (m, 1H), 8.34 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm: 45.2, 46.3, 66.2, 119.1, 127.6, 127.8, 128.7, 137.1, 140.2, 150.7, 152.0, 153.3. IR (KBr) ν_{max} /cm^{-1}: 697, 778, 793, 1111, 1263, 1380, 1476, 1496, 1588, 2857, 2974, 3108. HRMS: calcd for $C_{16}H_{18}N_5O$ [M+H$^+$] 296.1511, found 296.1515.

9-Benzyl-2-chloro-6-morpholin-4-yl-9*H*-purine (7i). [15]



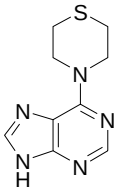
White powder, mp 108-110 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 3.70-3.72 (m, 4H), 3.90-4.20 (m, 4H), 5.35 (s, 2H), 7.25-7.36 (m, 5H), 8.30 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 46.4, 66.1, 118.1, 127.4, 127.9, 128.8, 136.6, 140.7, 151.8, 152.8, 153.5. IR (KBr) ν_{max} /cm^{-1}: 708, 807, 1110, 1250, 1340, 1454, 1486, 1591, 2820, 2940, 3070. HRMS: calcd for $C_{16}H_{17}ClN_5O$ [M+H$^+$] 330.1121, found 330.1120.

9-(2-Chloro-benzyl)-6-morpholin-4-yl-9*H*-purine (7j).



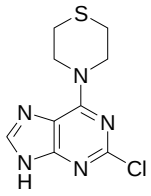
White needle crystal, mp 138-140 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 3.71-3.73 (m, 4H), 4.21 (brs, 4H,), 5.49 (s, 2H,), 6.96 (d, 1H, J = 7.2 Hz), 7.26-7.36 (m, 2H), 7.50 (d, 1H, J = 7.6 Hz), 8.24 (s, 1H), 8.26 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 44.3, 45.2, 66.2, 119.0, 127.6, 129.2, 129.6, 129.7, 132.0, 134.0, 140.4, 150.8, 152.1, 153.3. IR (KBr) ν_{max} /cm^{-1}: 757, 794, 1110, 1197, 1331, 1420, 1481, 1600, 2854, 2971, 3009. HRMS: calcd for $C_{16}H_{17}ClN_5O$ [M+H$^+$] 330.1121, found 330.1121.

6-Thiomorpholin-4-yl-9*H*-purine (8a).



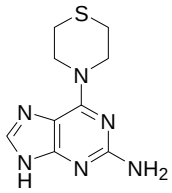
white powdwr; mp 285-287 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 2.66 (m, 4H), 4.49 (brs, 4H), 8.13 (s, 1H), 8.21 (s, 1H), 13.07 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 26.5, 117.8, 138.9, 152.4, 152.8, 153.2. IR (KBr) ν_{max} /cm^{-1}: 1149, 1258, 1336, 1455, 1513, 1576, 1604, 2804, 2960, 3070, 3451. HRMS: *m/z* calcd for $C_9H_{11}N_5S$: 221.0735; found: 221.0746.

2-chloro-6-thiomorpholinyl purine (8b). [6]



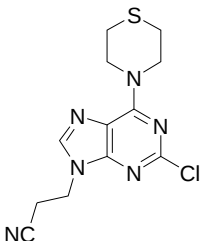
White needle crystal. mp 248-249 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 2.70-2.71 (m, 4 H), 4.08-4.78 (m, 4 H), 8.16 (s, 1 H), 13.20 (s, 1 H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 26.6, 47.5, 119.1, 138.5, 151.7, 152.0, 153.1. IR (KBr) ν_{max} /cm^{-1}: 635, 757, 938, 1148, 1261, 1360, 1460, 1571, 2980, 3420. HRMS: calcd for $C_9H_{11}ClN_5S$ [M+H$^+$] 256.0423, found 256.0420.

6-Thiomorpholin-4-yl-9*H*-purin-2-ylamine (8c).



white column crystal; mp 250-251 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 2.63-2.65 (m, 4H), 4.41 (brs, 4H), 5.70 (s, 2H), 7.67 (s, 1H), 13.17 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 26.4, 47.0, 113.2, 134.9, 153.3, 154.0, 159.6. IR (KBr) ν_{max} /cm^{-1}: 785, 932, 1135, 1396, 1479, 1568, 1620, 2845, 2916, 3093, 3348, 3452. HRMS: calcd for $C_9H_{13}N_6S$ [M+H$^+$] 237.0922, found 237.0913.

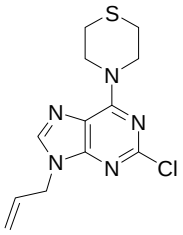
3-(2-Chloro-6-thiomorpholin-4-yl-purin-9-yl)propionitrile (8d).



white needle crystal; mp 130-132 ^{o}C. ^{1}H NMR (400 MHz, DMSO- d_6): δ ppm 2.70-2.78 (m,

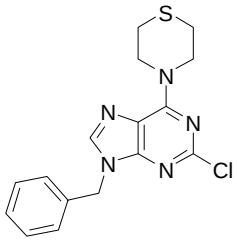
4H), 3.12 (t, 2H, *J* = 6.4 Hz), 4.20 (brs, 2H), 4.41 (t, 2H, *J* = 6.4 Hz), 4.60 (brs, 2H), 8.27 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 18.1, 18.2, 26.7, 48.1, 118.2, 118.4, 140.6, 151.9, 152.8, 153.4. IR (KBr) ν_{max} /cm^{-1}: 763, 958, 124, 1479, 1583, 2252, 2823, 2980, 3428. HRMS: *m/z* calcd for $C_{12}H_{13}ClN_6S$: 308.0611; found: 308.0602.

9-Allyl-2-chloro-6-thiomorpholin-4-yl-9*H*-purine (8e).



white needle crystal; mp 88-89 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 2.71-2.72 (m, 4H), 4.45 (brs, 4H), 4.77 (d, 2H, *J* = 4.8 Hz), 5.07 (d, 1H, *J* = 7.2 Hz), 5.21 (d, 1H, *J* = 7.2 Hz), 5.99-6.09 (m, 1H), 8.18 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 26.5, 45.2, 117.8, 118.1, 132.9, 140.6, 151.8, 152.6, 153.3. IR (KBr) ν_{max} /cm^{-1}: 780, 956, 1123, 1373, 1469, 1479, 1595, 2922, 3010. HRMS: *m/z* calcd for $C_{12}H_{14}ClN_5S$: 295.0658; found: 295.0665.

9-Benzyl-2-chloro-6-thiomorpholin-4-yl-9*H*-purine (8f).



white powder; mp 46-48 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ ppm 2.69 (brs, 4H), 4.18-4.69 (m, 4H), 5.34 (s, 2H), 7.26-7.35 (m, 5H), 8.32 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ ppm 26.7, 46.5, 118.2, 127.6, 128.0, 128.9, 136.7, 140.8, 152.0, 152.9, 153.4. IR (KBr) ν_{max} /cm^{-1}: 687, 733, 784, 1122, 1368, 1477, 1496, 1595, 2918, 2957, 3090. HRMS: calcd for $C_{16}H_{17}ClN_5S$ [M+H$^+$] 346.0893, found: 346.0891.

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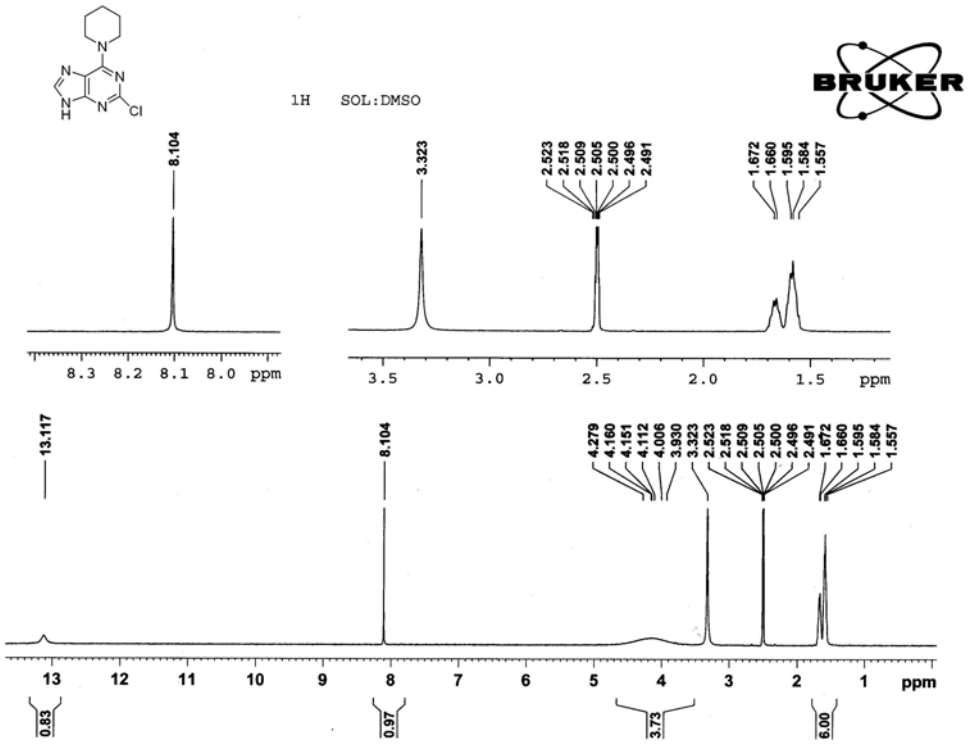
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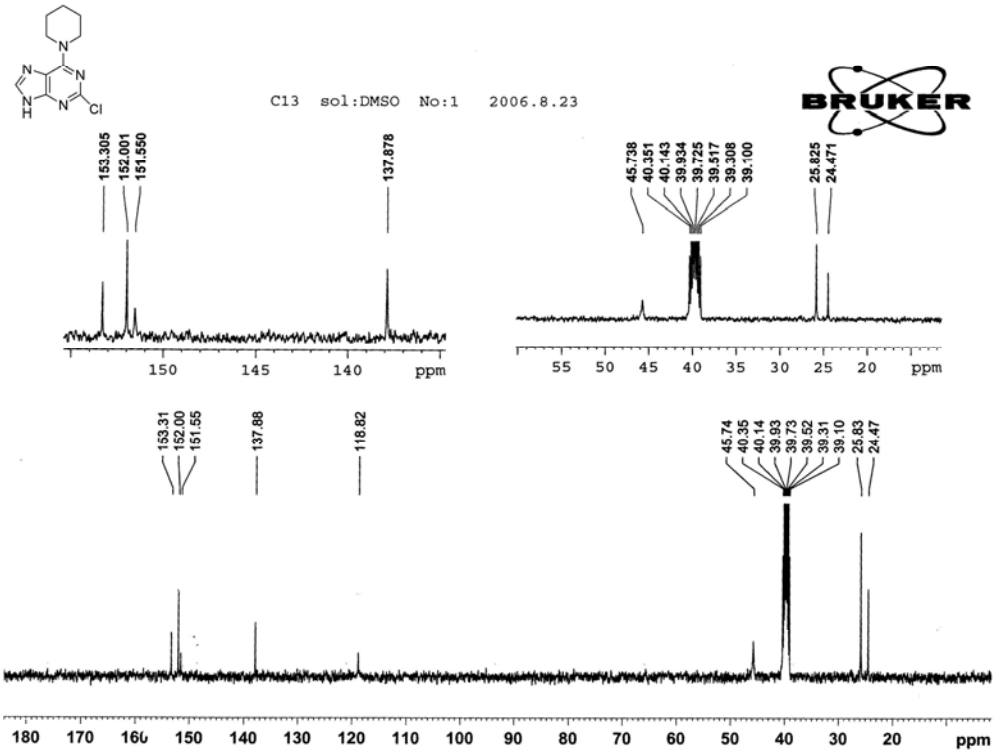
BRUKER
8.104
3.323
2.523
2.518
2.509
2.505
2.500
2.496
2.491
1.672
1.660
1.595
1.584
1.557
8.3 8.2 8.1 8.0 ppm
3.5 3.0 2.5 2.0 1.5 ppm
13.117
8.104
4.279
4.160
4.151
4.112
4.006
3.930
3.323
2.523
2.518
2.509
2.505
2.500
2.496
2.491
1.672
1.660
1.595
1.584
1.557
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.83
0.97
3.73
6.00


C13 sol:DMSO No:1 2006.8.23
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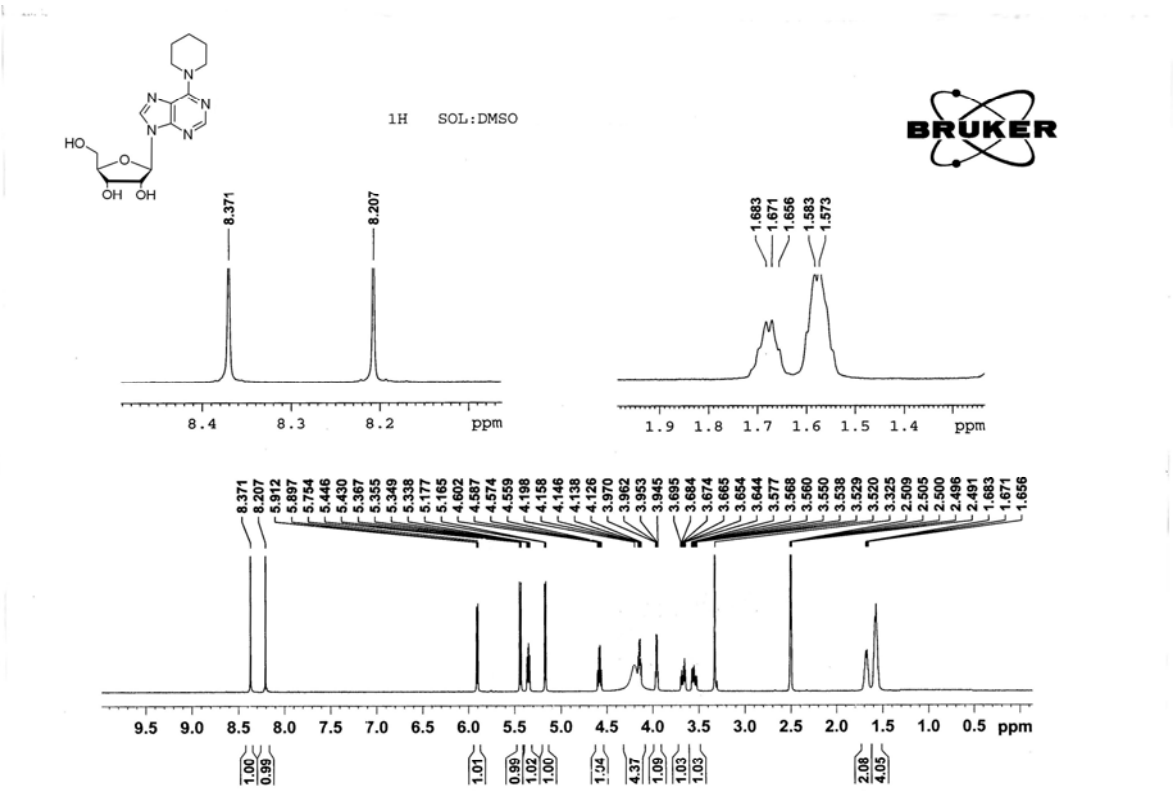
151.550
137.878
45.738
40.351
40.143
39.934
39.725
39.517
39.308
39.100
25.825
24.471
150 145 140 ppm
55 50 45 40 35 30 25 20 ppm
153.31
152.00
151.55
137.88
118.82
45.74
40.35
40.14
39.93
39.73
39.52
39.31
39.10
25.83
24.47
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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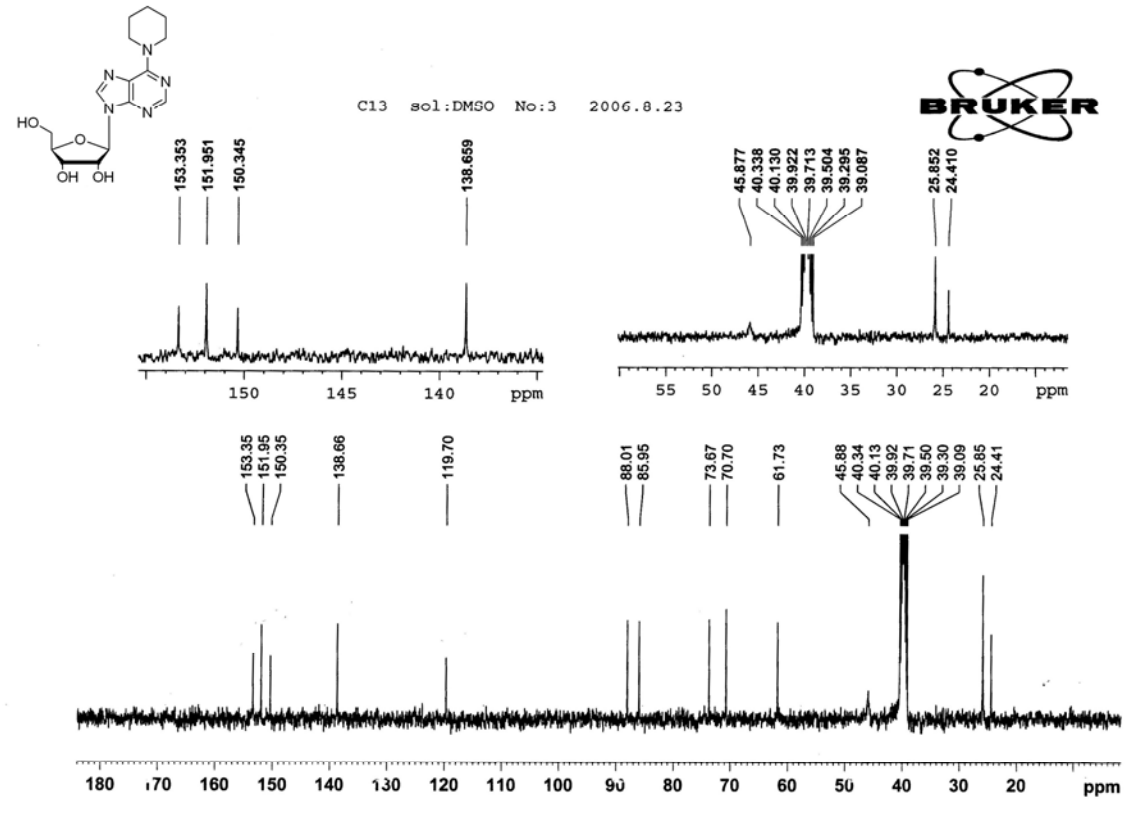
1.583
1.573
ppm


C13 sol:DMSO No:3 2006.8.23
BRUKER
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151.951
150.345
138.659
45.877
40.338
40.130
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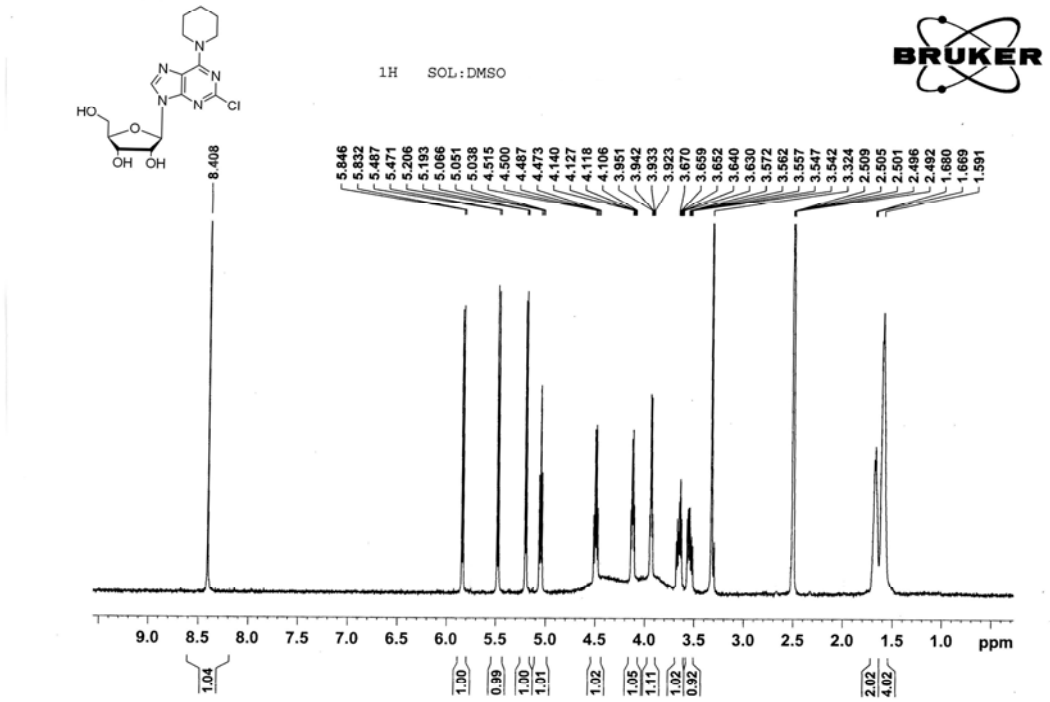
39.713
39.504
39.295
39.087
25.852
24.410
ppm


1H SOL:DMSO
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HO
OH OH
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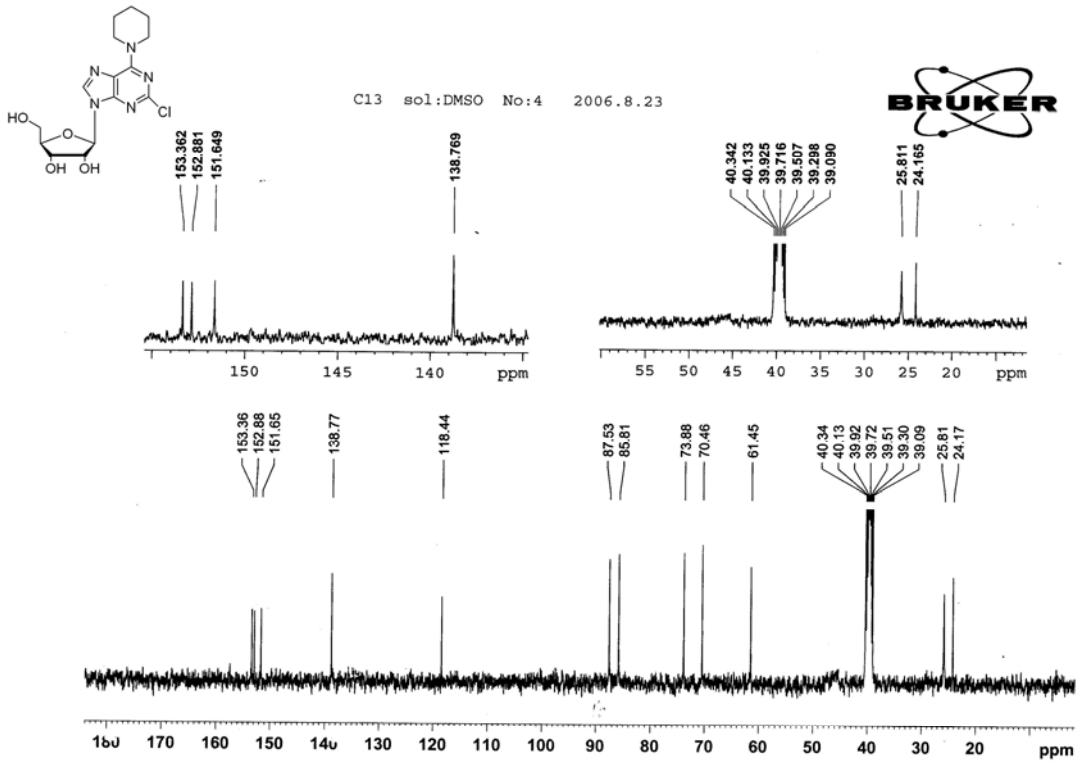
5.487
5.471
5.206
5.193
5.066
5.051
5.038
4.515
4.500
4.487
4.473
4.140
4.127
4.118
4.106
3.951
3.942
3.933
3.923
3.670
3.659
3.652
3.640
3.630
3.572
3.562
3.557
3.547
3.542
3.324
2.509
2.505
2.501
2.496
2.492
1.680
1.669
1.591
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.04
1.00
0.99
1.00
1.01
1.02
1.05
1.11
1.02
0.32
2.02
4.02


C13 sol:DMSO No:4 2006.8.23
BRUKER
HO
OH OH
Cl
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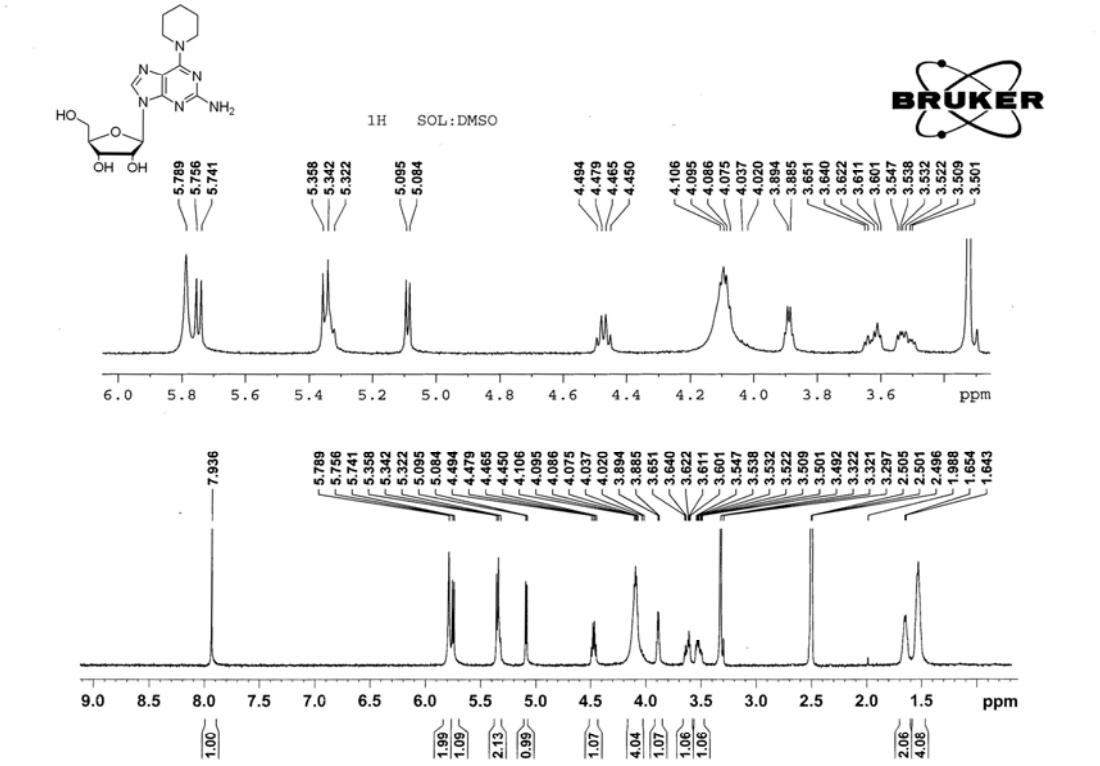
151.649
138.769
40.342
40.133
39.925
39.716
39.507
39.298
39.090
25.811
24.165
150 145 140 ppm
55 50 45 40 35 30 25 20 ppm
153.36
152.88
151.65
138.77
118.44
87.53
85.81
73.88
70.46
61.45
40.34
40.13
39.92
39.72
39.51
39.30
39.09
25.81
24.17
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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BRUKER
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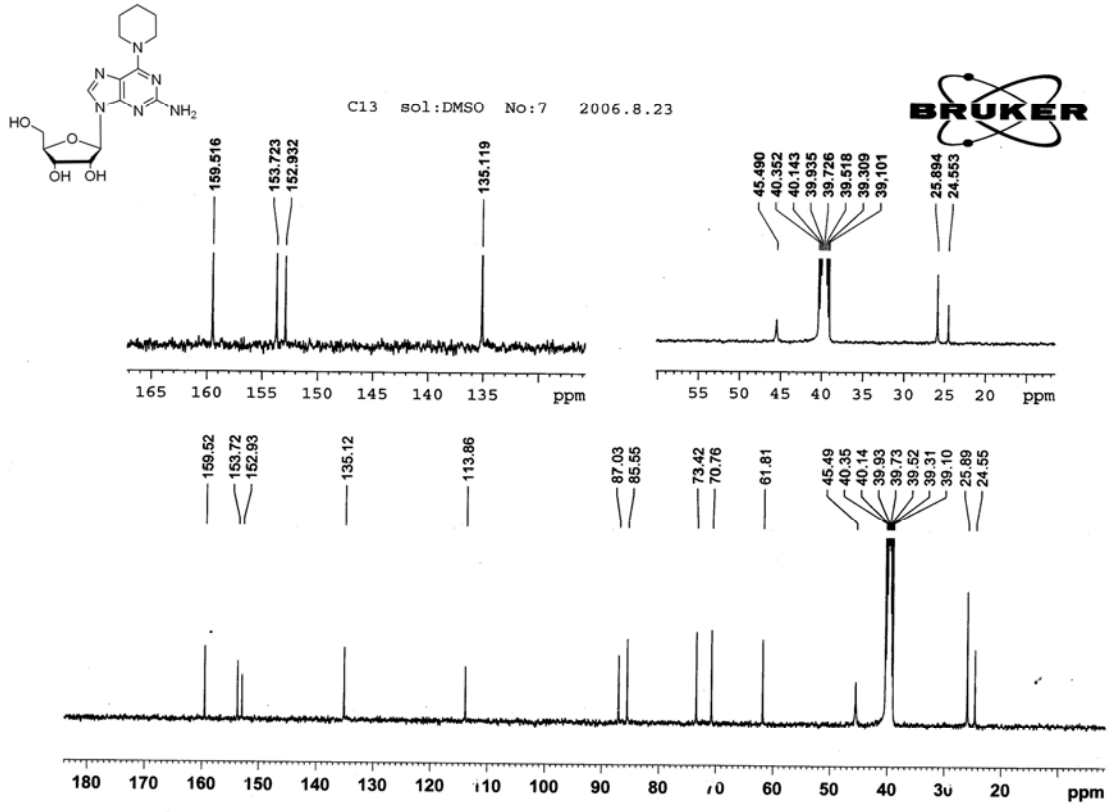
6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 ppm
7.936
5.789 5.756 5.741 5.358 5.342 5.322 5.095 5.084 4.494 4.479 4.465 4.450 4.106 4.095 4.086 4.075 4.037 4.020 3.894 3.885 3.651 3.640 3.622 3.611 3.601 3.547 3.538 3.532 3.522 3.509 3.501 3.492 3.322 3.321 3.297 2.505 2.501 2.496 1.988 1.654 1.643
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.00 1.99 1.09 2.13 0.99 1.07 4.04 1.07 1.06 1.06 2.06 4.08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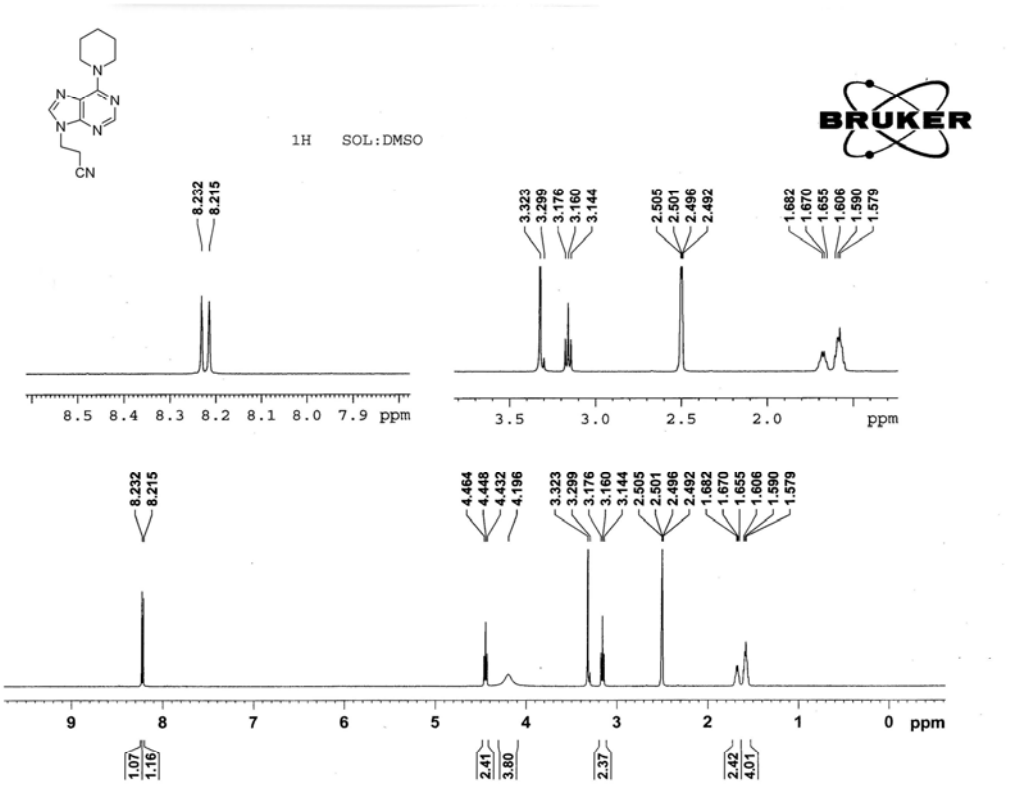
165 160 155 150 145 140 135 ppm
45.490 40.352 40.143 39.935 39.726 39.518 39.309 39.101 25.894 24.553
55 50 45 40 35 30 25 20 ppm
159.52 153.72 152.93 135.12 113.86 87.03 85.55 73.42 70.76 61.81 45.49 40.35 40.14 39.93 39.73 39.52 39.31 39.10 25.89 24.55
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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3.176
3.160
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2.505
2.501
2.496
2.492
1.682
1.670
1.655
1.606
1.590
1.579
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4.432
4.196
1.07
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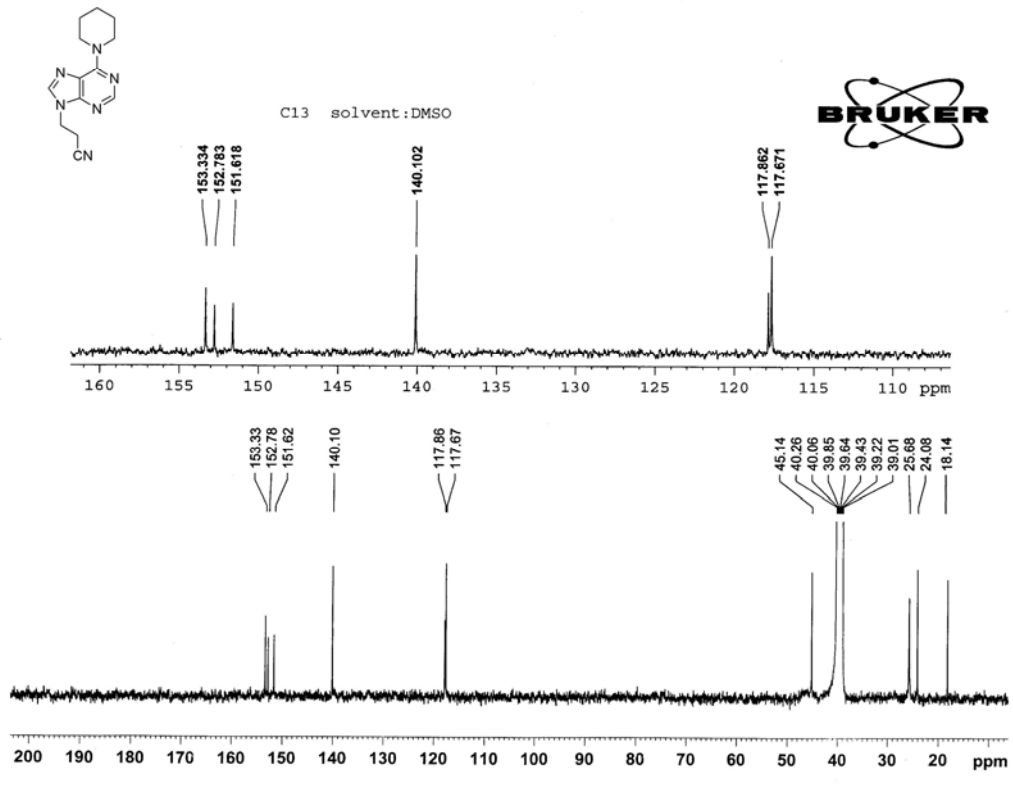
3.80
2.37
2.42
4.01
ppm


C13 solvent:DMSO
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CN
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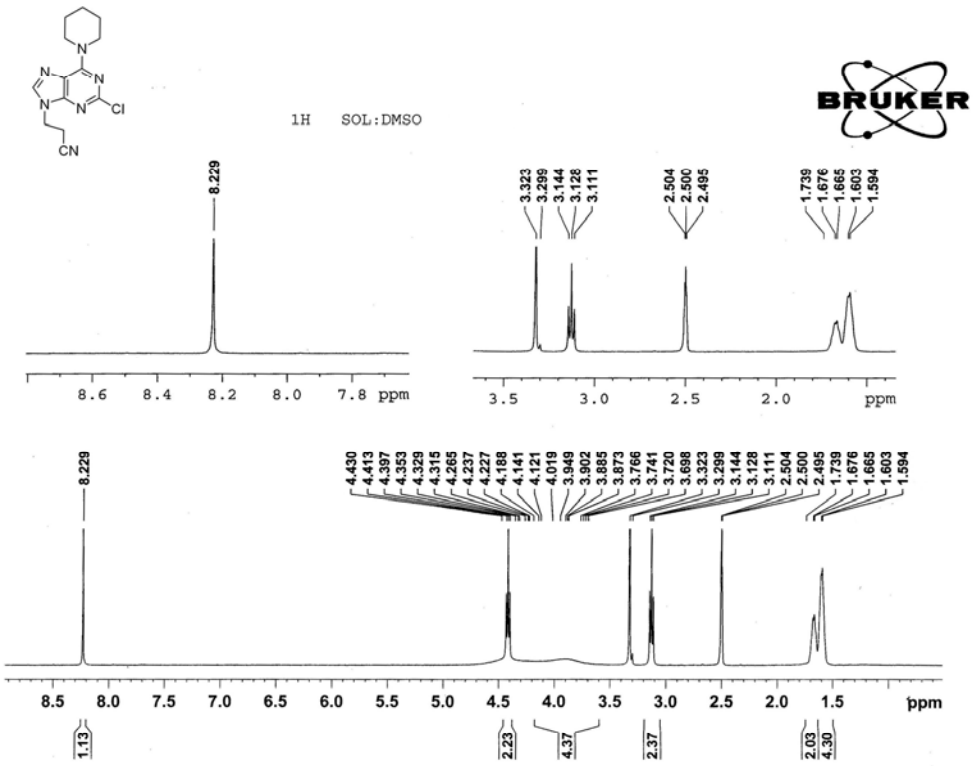
152.783
151.618
140.102
117.862
117.671
153.33
152.78
151.62
140.10
117.86
117.67
45.14
40.26
40.06
39.85
39.64
39.43
39.22
39.01
25.68
24.08
18.14
ppm


1H SOL:DMSO
BRUKER
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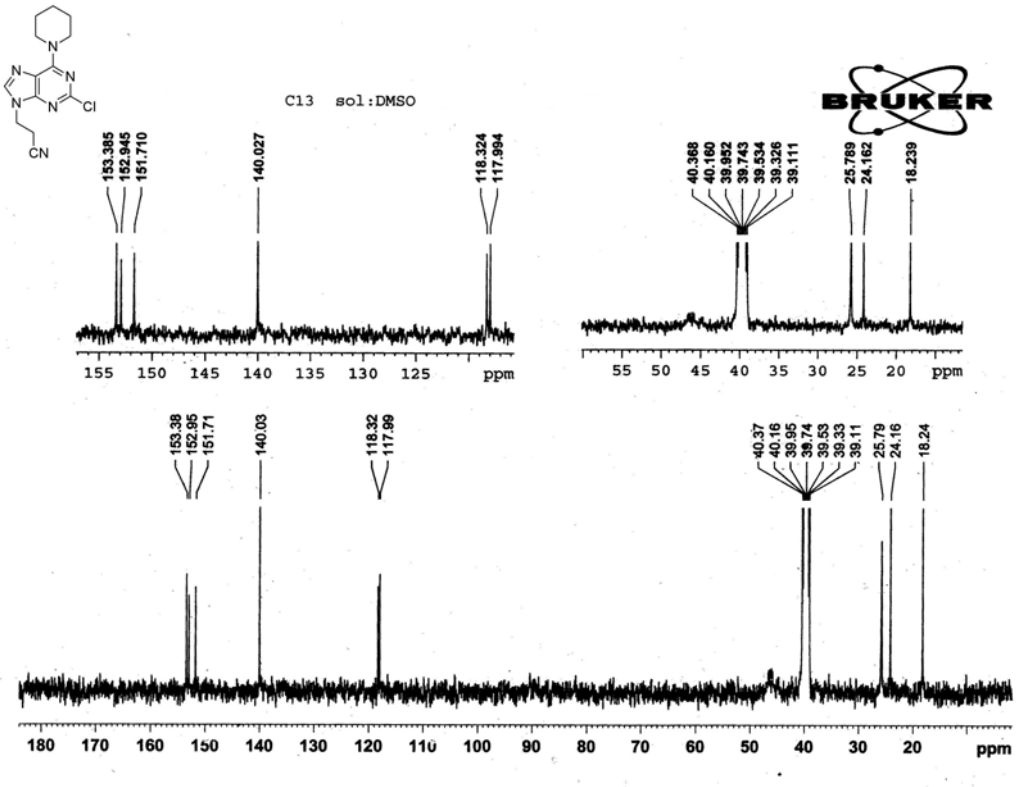
3.128
3.111
2.504
2.500
2.495
1.739
1.676
1.665
1.603
1.594
8.6 8.4 8.2 8.0 7.8 ppm
3.5 3.0 2.5 2.0 ppm
4.430
4.413
4.397
4.353
4.329
4.315
4.265
4.237
4.227
4.188
4.141
4.121
4.019
3.949
3.902
3.885
3.873
3.766
3.741
3.720
3.698
3.323
3.299
3.144
3.128
3.111
2.504
2.500
2.495
1.739
1.676
1.665
1.603
1.594
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.13
2.23
4.37
2.37
2.03
4.30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151.710
140.027
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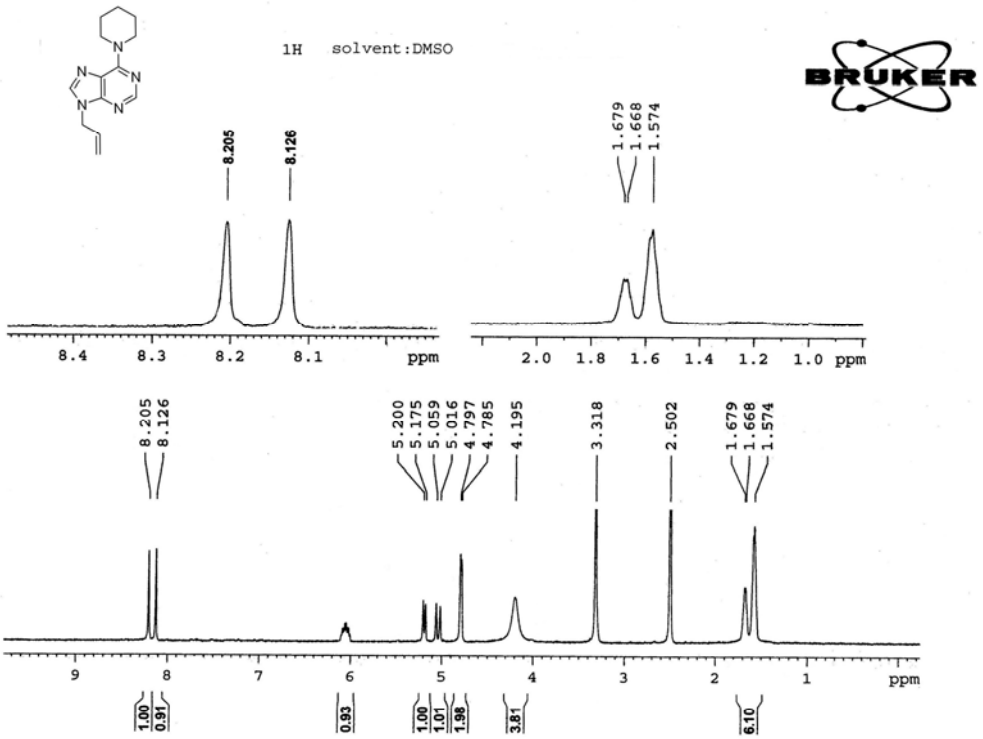
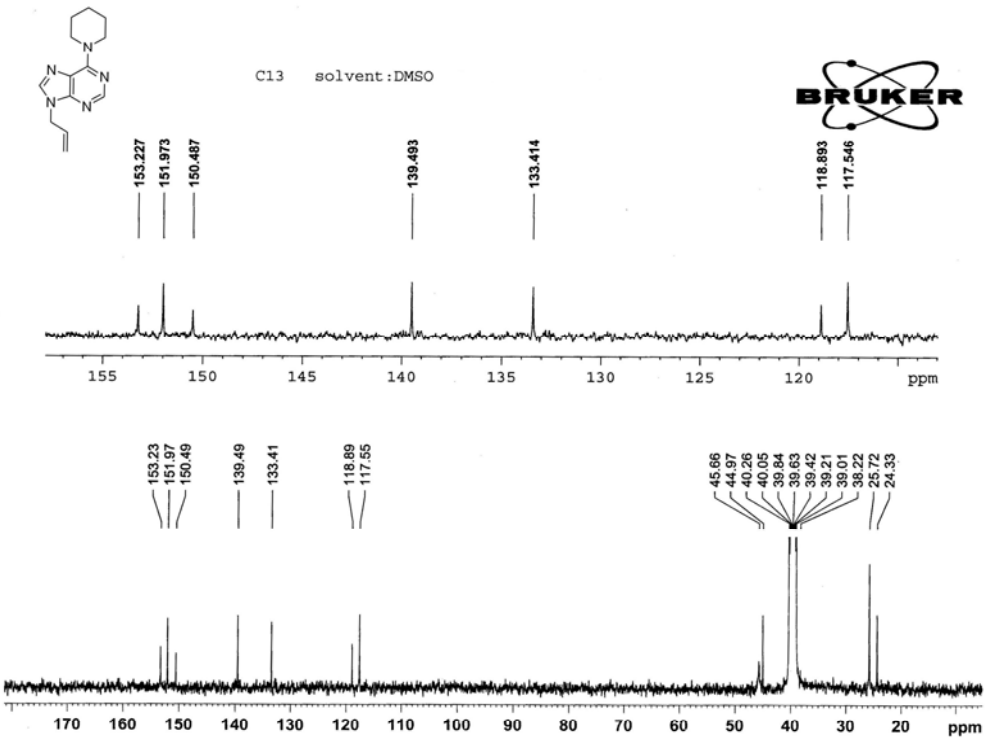
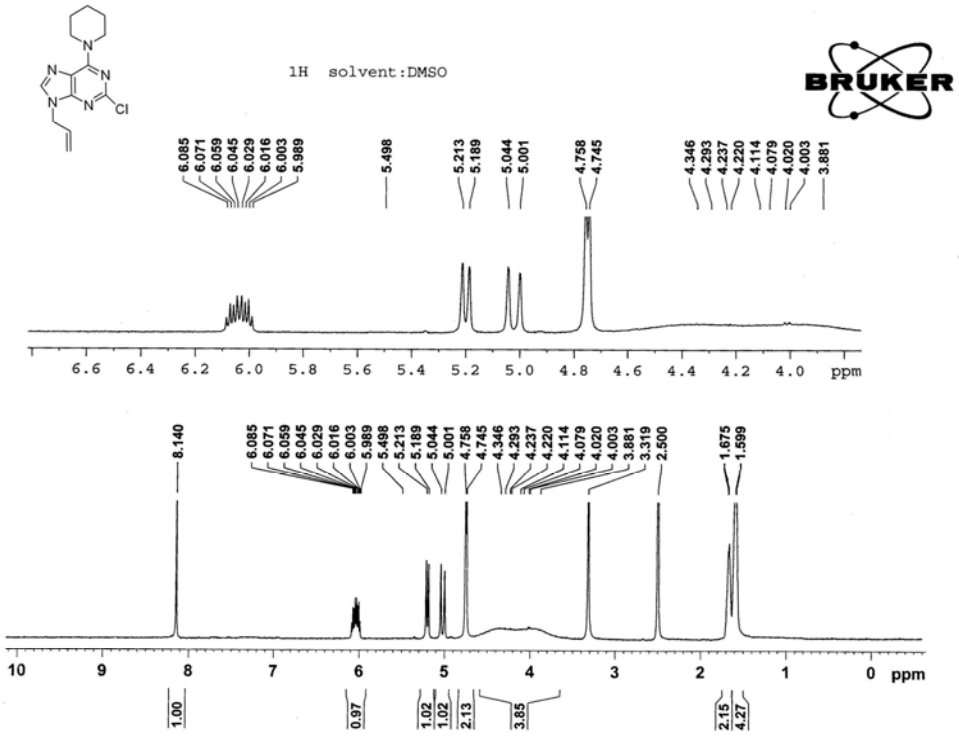
117.994
40.368
40.160
39.952
39.743
39.534
39.326
39.111
25.789
24.162
18.239
155 150 145 140 135 130 125 ppm
55 50 45 40 35 30 25 20 ppm
153.38
152.95
151.71
140.03
118.32
117.99
40.37
40.16
39.95
39.74
39.53
39.33
39.11
25.79
24.16
18.24
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


1H solvent:DMSO
BRUKER
8.205
8.126
1.679
1.668
1.574
8.4 8.3 8.2 8.1 ppm
2.0 1.8 1.6 1.4 1.2 1.0 ppm
8.205
8.126
5.200
5.175
5.059
5.016
4.797
4.785
4.195
3.318
2.502
1.679
1.668
1.574
9 8 7 6 5 4 3 2 1 ppm
1.00
0.91
0.93
1.00
1.01
1.98
3.81
6.10


C13 solvent:DMSO
BRUKER
153.227
151.973
150.487
139.493
133.414
118.893
117.546
155 150 145 140 135 130 125 120 ppm
153.23
151.97
150.49
139.49
133.41
118.89
117.55
45.66
44.97
40.26
40.05
39.84
39.63
39.42
39.21
39.01
38.22
25.72
24.33
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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BRUKER
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6.071
6.059
6.045
6.029
6.016
6.003
5.989
5.498
5.213
5.189
5.044
5.001
4.758
4.745
4.346
4.293
4.237
4.220
4.114
4.079
4.020
4.003
3.881
8.140
3.319
2.500
1.675
1.599
ppm
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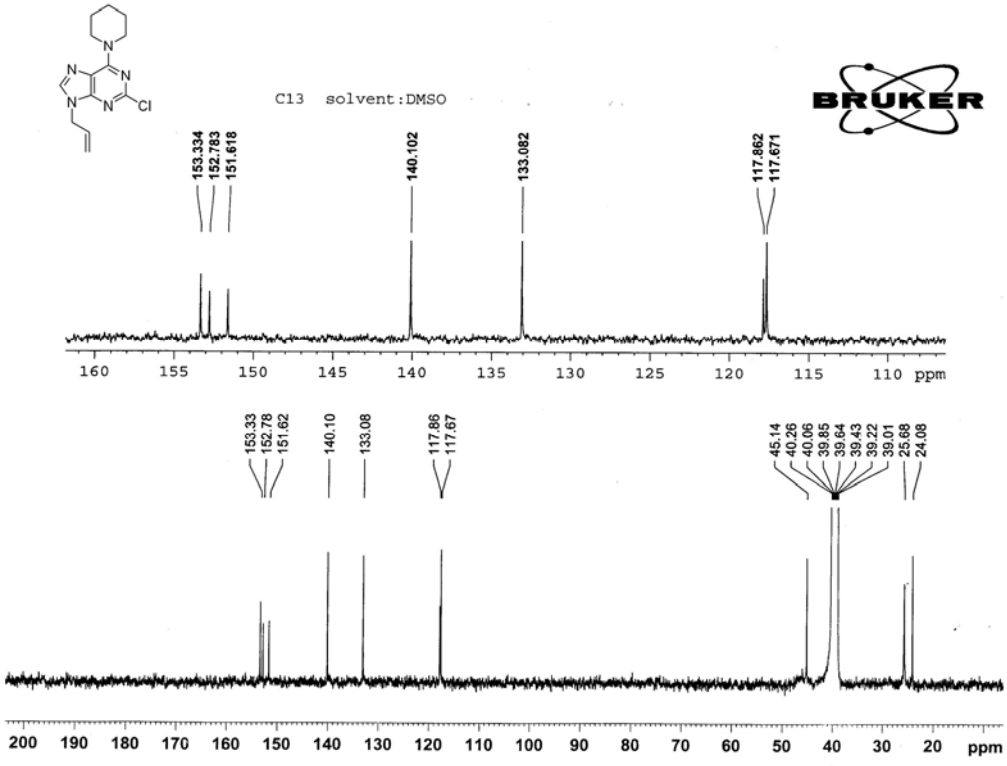
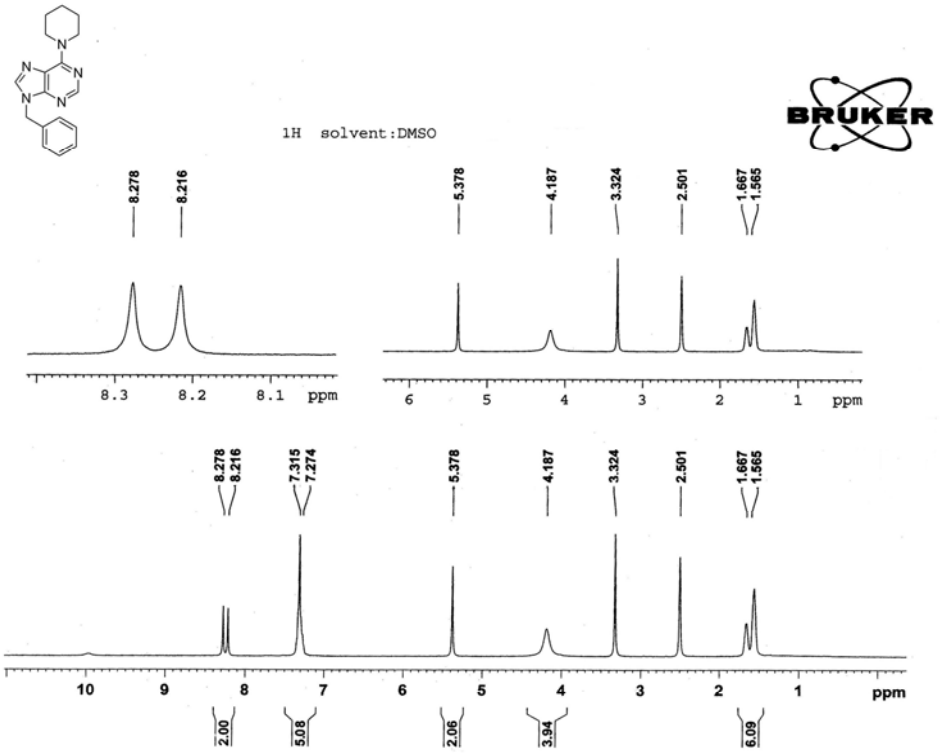
0.97
1.02
1.02
2.13
3.85
2.15
4.27


C13 solvent:DMSO
BRUKER
153.334
152.783
151.618
140.102
133.082
117.862
117.671
110 ppm
153.33
152.78
151.62
140.10
133.08
117.86
117.67
45.14
40.26
40.06
39.85
39.64
39.43
39.22
39.01
25.68
24.08
ppm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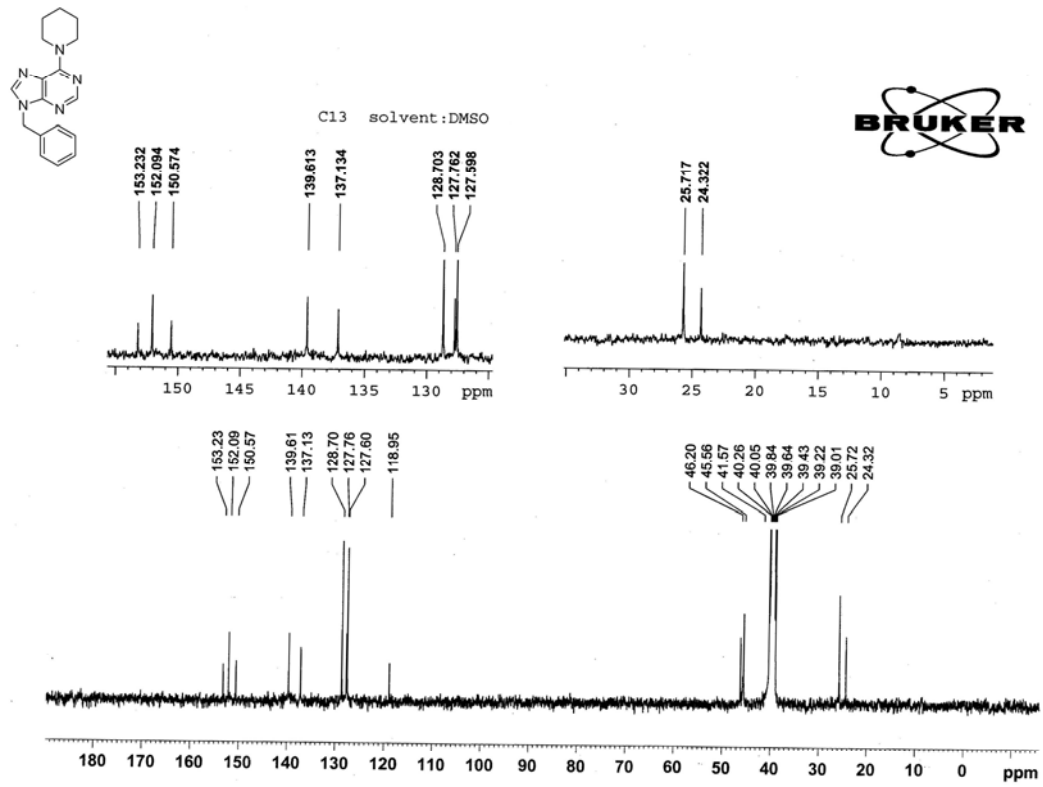
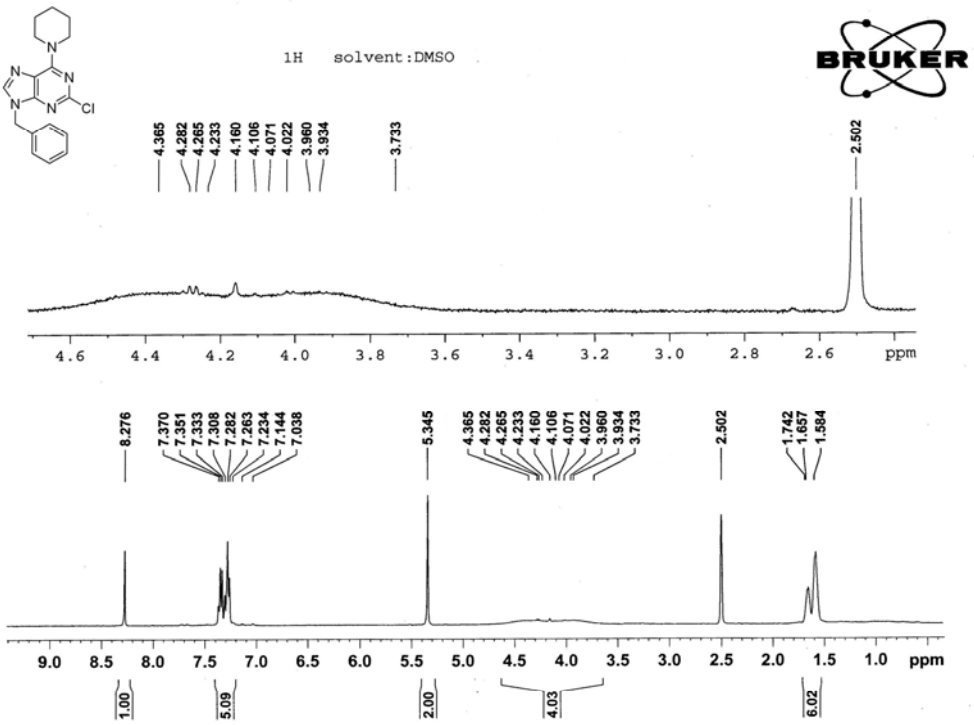
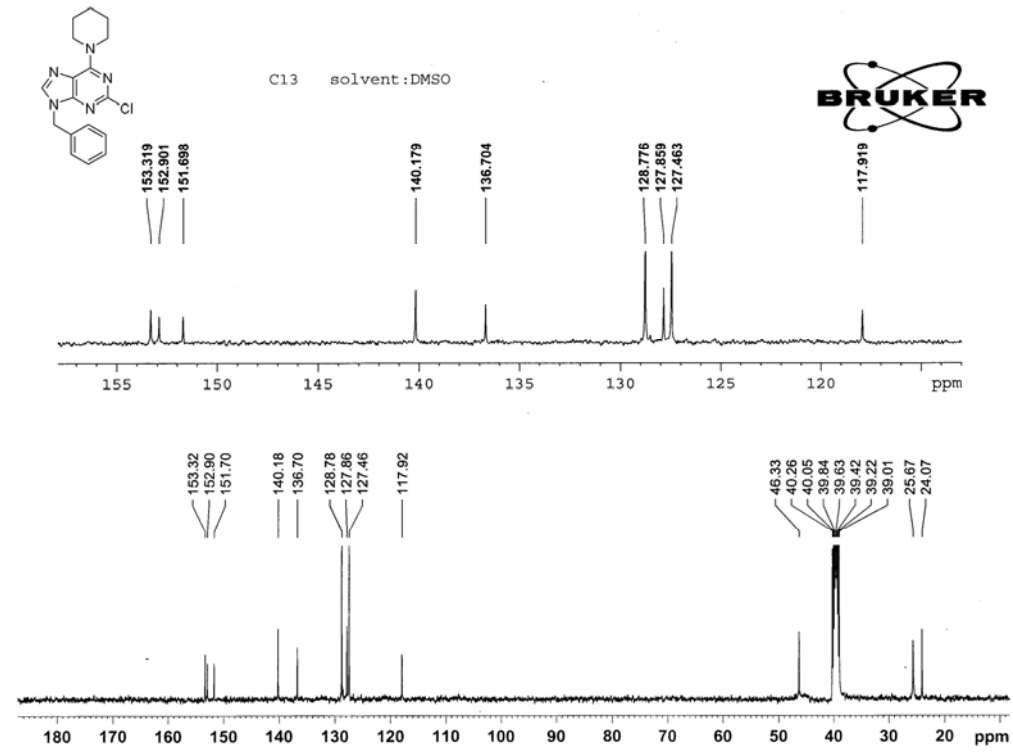
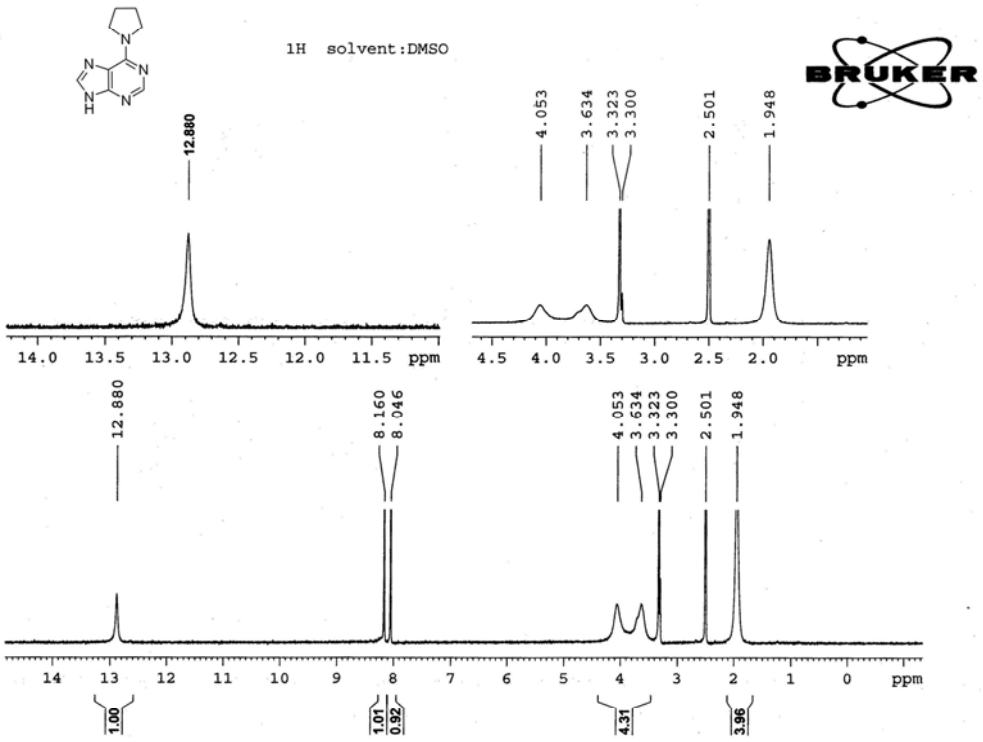
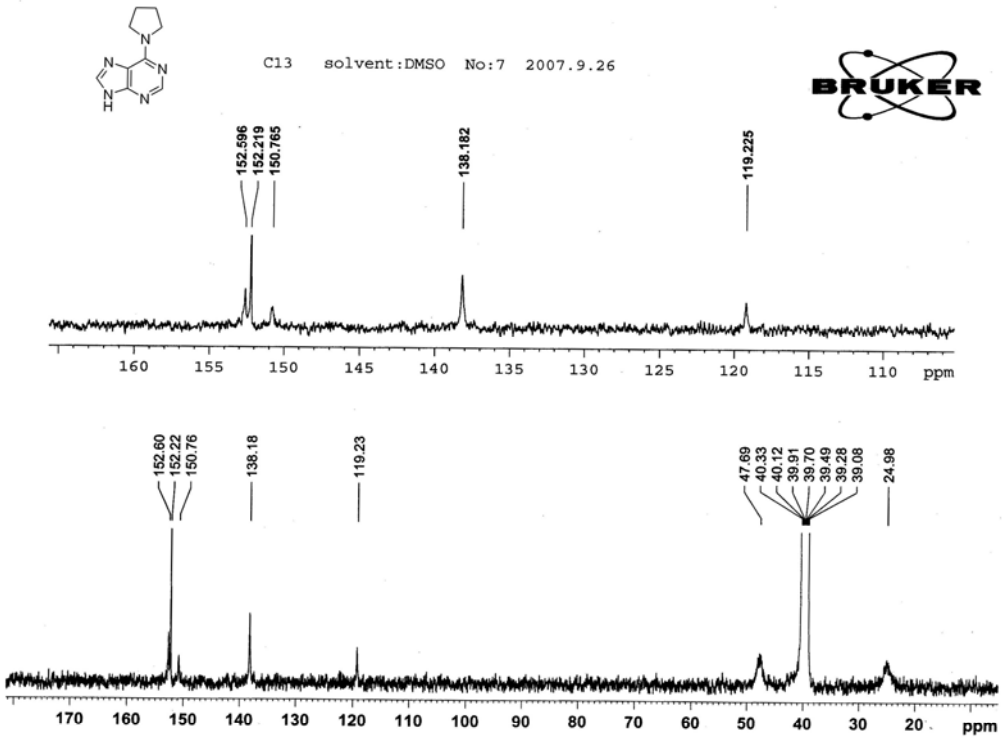
8.278
8.216
5.378
4.187
3.324
2.501
1.667
1.565
7.315
7.274
8.3
8.2
8.1
ppm
6
5
4
3
2
1
10
9
8
7
2.00
5.08
2.06
3.94
6.09

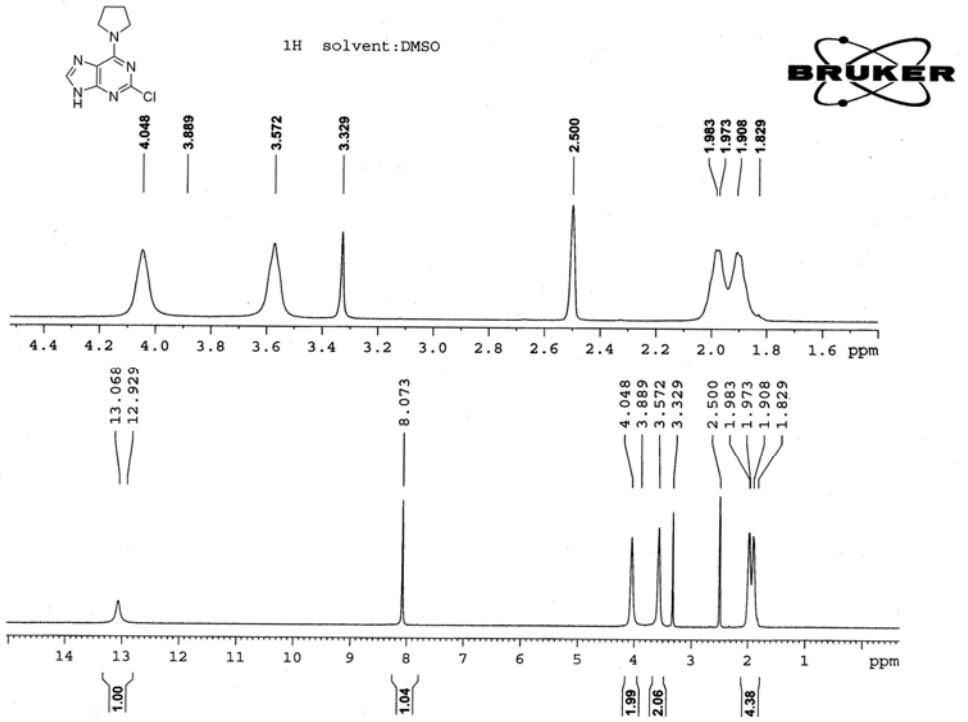

C13 solvent:DMSO
153.232
152.094
150.574
139.613
137.134
128.703
127.762
127.598
25.717
24.322
150
145
140
135
130
ppm
30
25
20
15
10
5
153.23
152.09
150.57
139.61
137.13
128.70
127.76
127.60
118.95
46.20
45.56
41.57
40.26
40.05
39.84
39.64
39.43
39.22
39.01
25.72
24.32
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

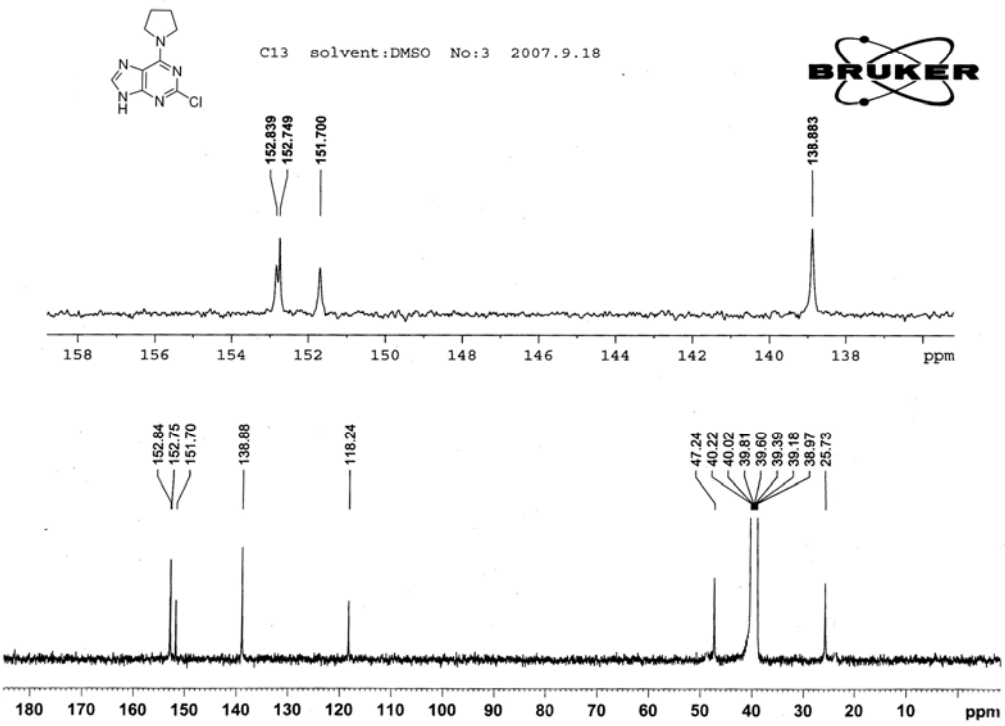

1H solvent:DMSO
BRUKER
4.365
4.282
4.265
4.233
4.160
4.106
4.071
4.022
3.960
3.934
3.733
2.502
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
ppm
8.276
7.370
7.351
7.333
7.308
7.282
7.263
7.234
7.144
7.038
5.345
4.365
4.282
4.265
4.233
4.160
4.106
4.071
4.022
3.960
3.934
3.733
2.502
1.742
1.657
1.584
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
5.09
2.00
4.03
6.02

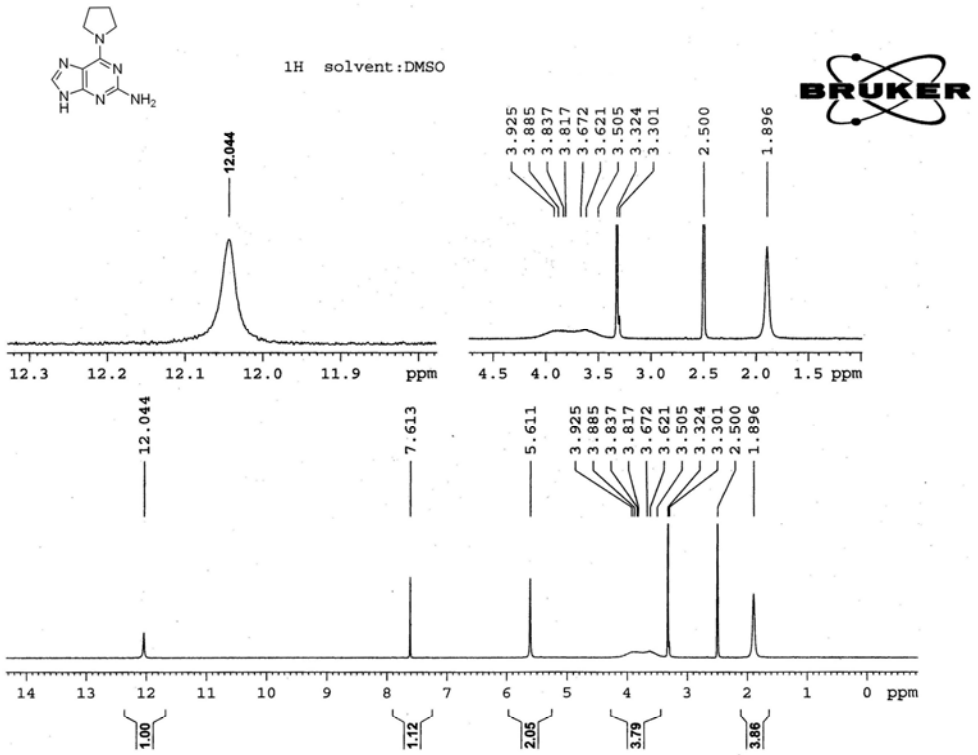

C13 solvent:DMSO
BRUKER
153.319
152.901
151.698
140.179
136.704
128.776
127.859
127.463
117.919
155
150
145
140
135
130
125
120
ppm
153.32
152.90
151.70
140.18
136.70
128.78
127.86
127.46
117.92
46.33
40.26
40.05
39.84
39.63
39.42
39.22
39.01
25.67
24.07
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

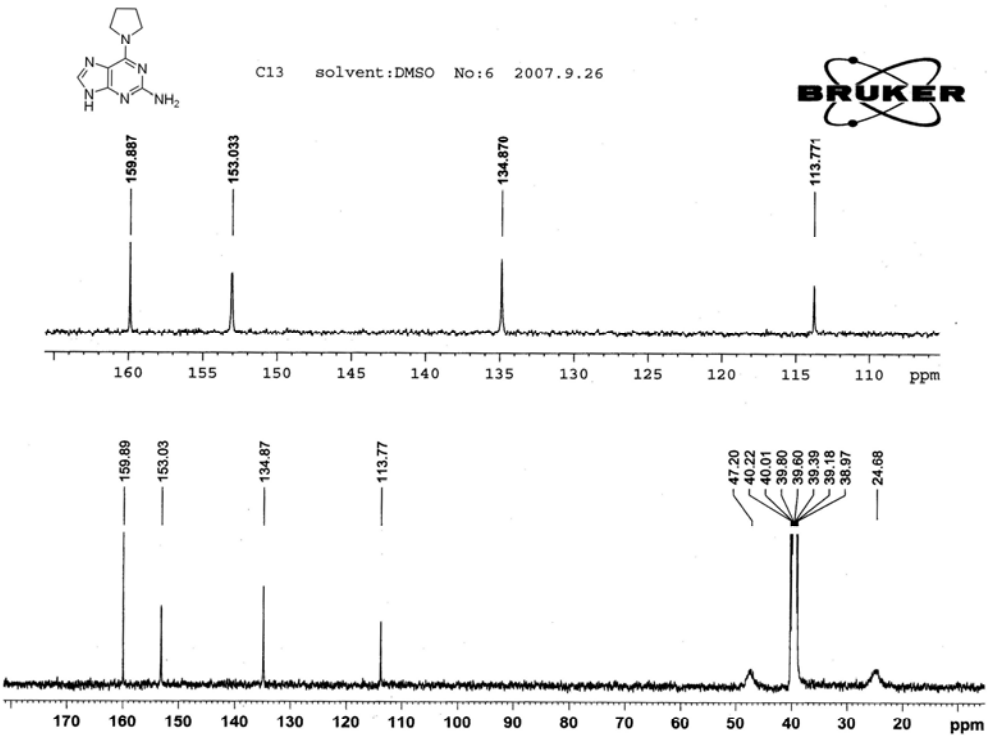

1H solvent:DMSO
BRUKER
12.880
4.053
3.634
3.323
3.300
2.501
1.948
8.160
8.046
ppm
1.00
1.01
0.92
4.31
3.96

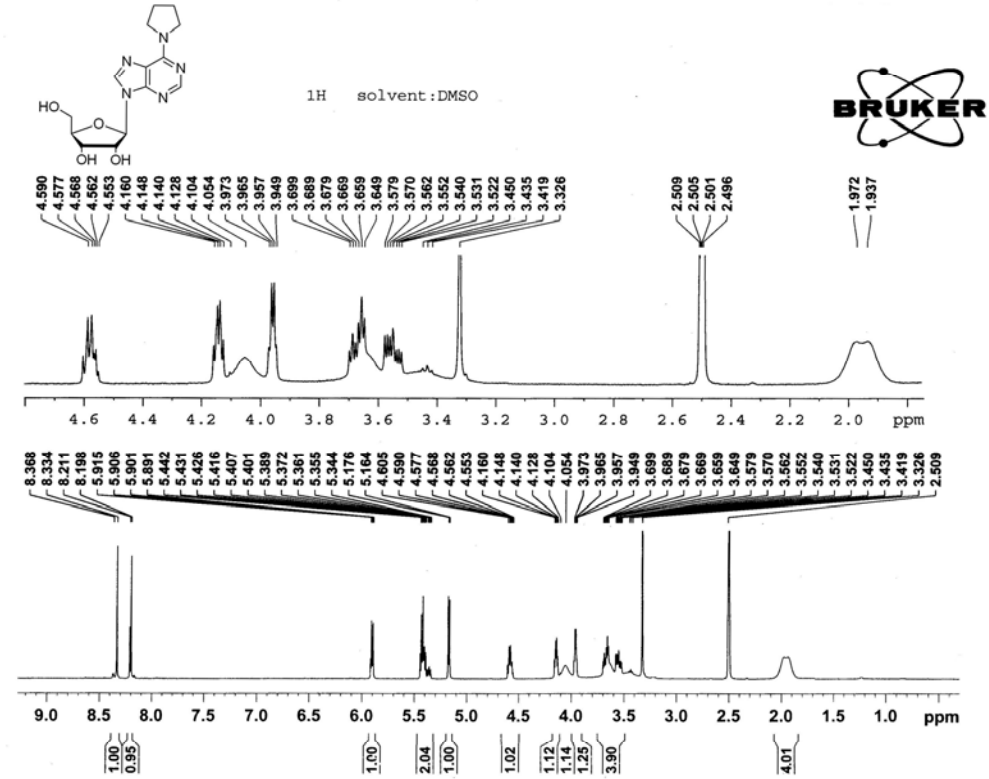

C13 solvent:DMSO No:7 2007.9.26
BRUKER
152.596
152.219
150.765
138.182
119.225
152.60
152.22
150.76
138.18
119.23
47.69
40.33
40.12
39.91
39.70
39.49
39.28
39.08
24.98
ppm

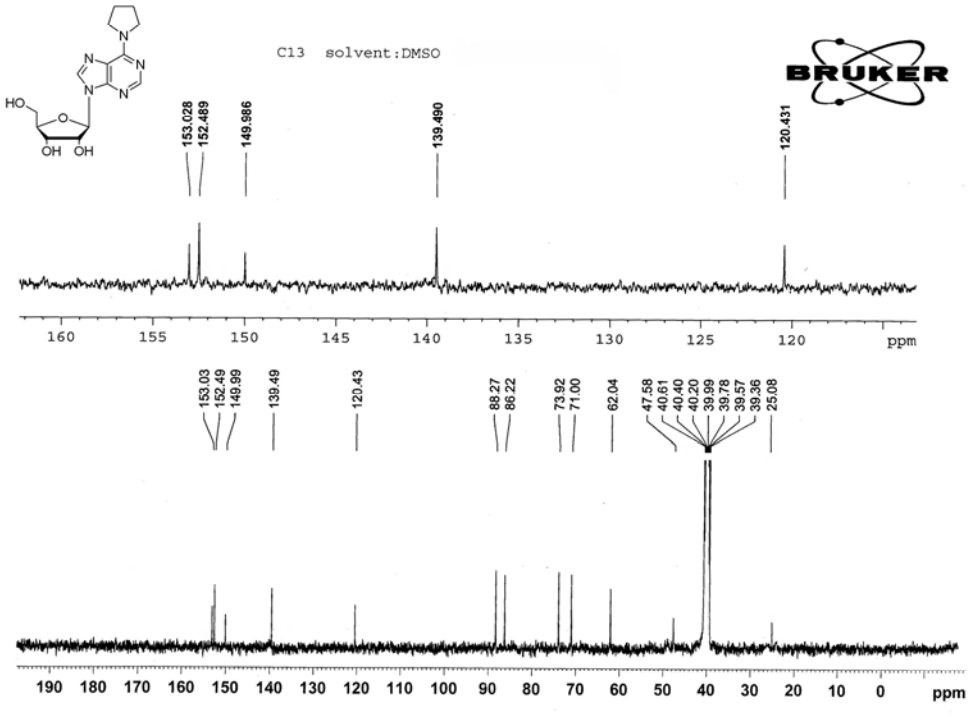

1H solvent:DMSO
BRUKER
4.048
3.889
3.572
3.329
2.500
1.983
1.973
1.908
1.829
4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 ppm
13.068
12.929
8.073
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.04
1.99
2.06
4.38

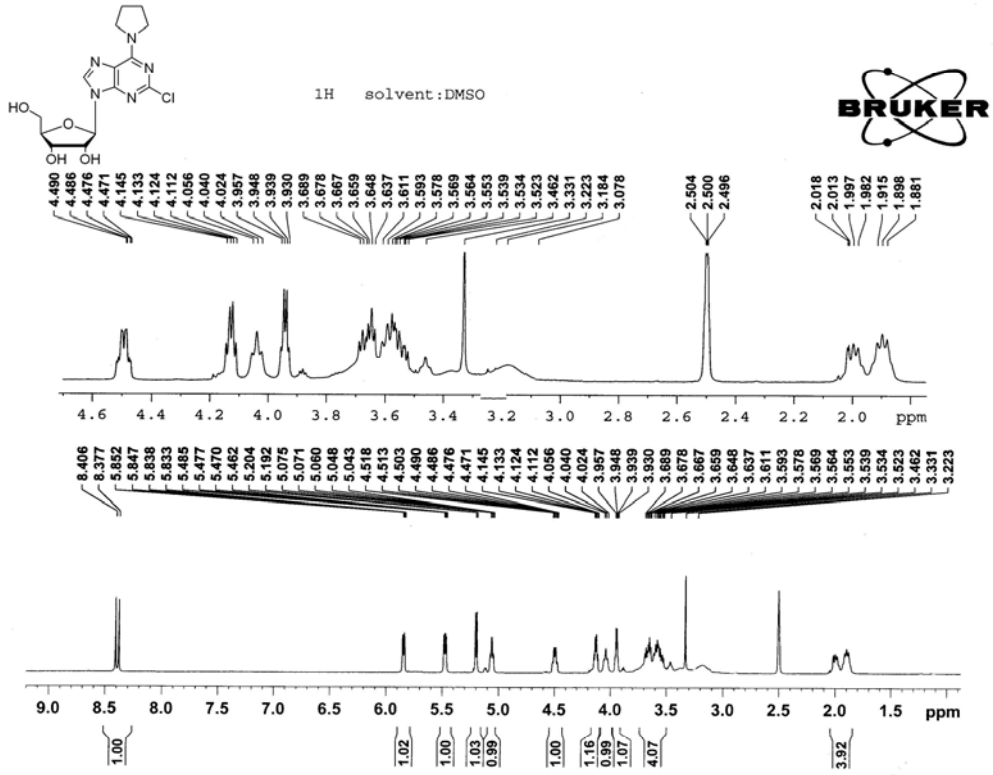

C13 solvent:DMSO No:3 2007.9.18
BRUKER
152.839
152.749
151.700
138.883
158 156 154 152 150 148 146 144 142 140 138 ppm
152.84
152.75
151.70
138.88
118.24
47.24
40.22
40.02
39.81
39.60
39.39
39.18
38.97
25.73
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

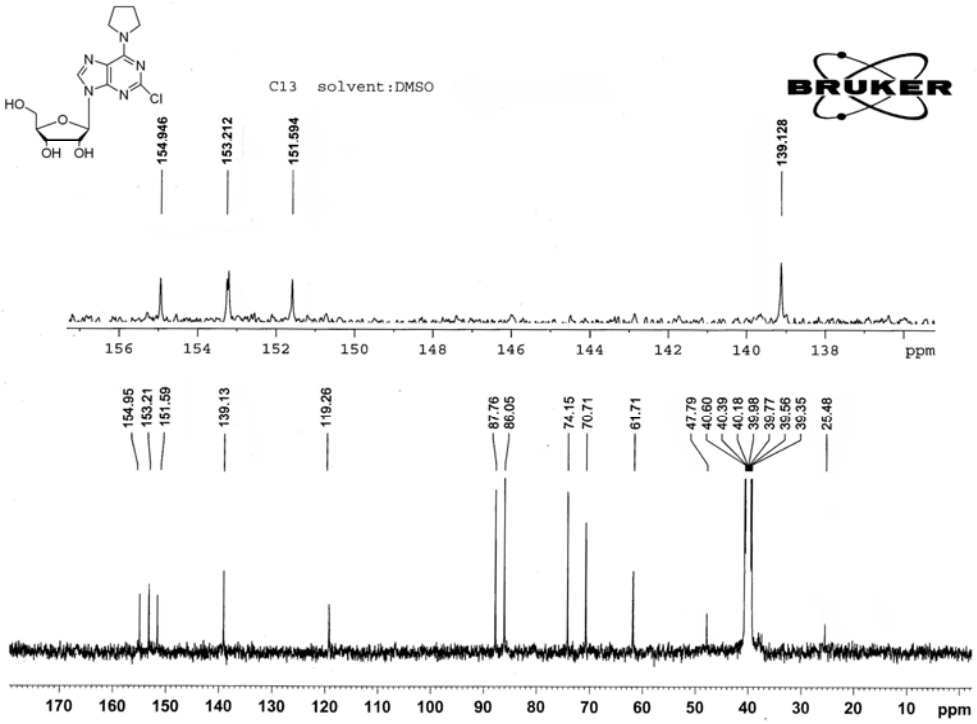

1H solvent:DMSO
BRUKER
12.044
3.925
3.885
3.837
3.817
3.672
3.621
3.505
3.324
3.301
2.500
1.896
12.3 12.2 12.1 12.0 11.9 ppm
4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
12.044
7.613
5.611
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.12
2.05
3.79
3.86

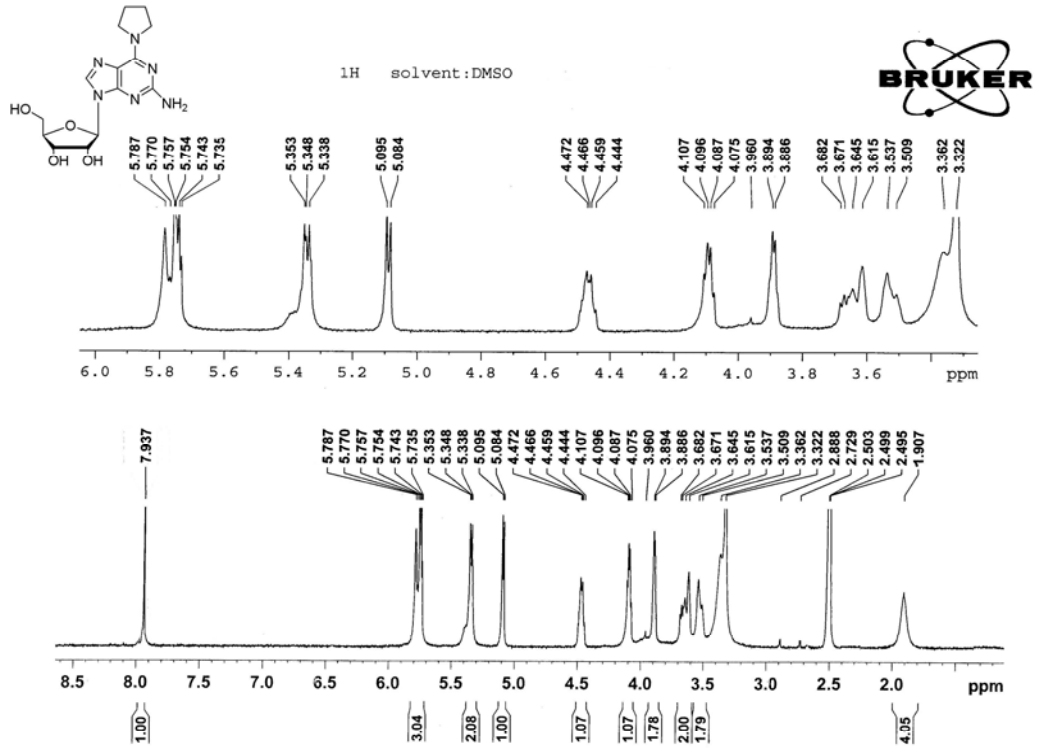

C13 solvent:DMSO No:6 2007.9.26
BRUKER
159.887
153.033
134.870
113.771
160 155 150 145 140 135 130 125 120 115 110 ppm
159.89
153.03
134.87
113.77
47.20
40.22
40.01
39.80
39.60
39.39
39.18
38.97
24.68
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

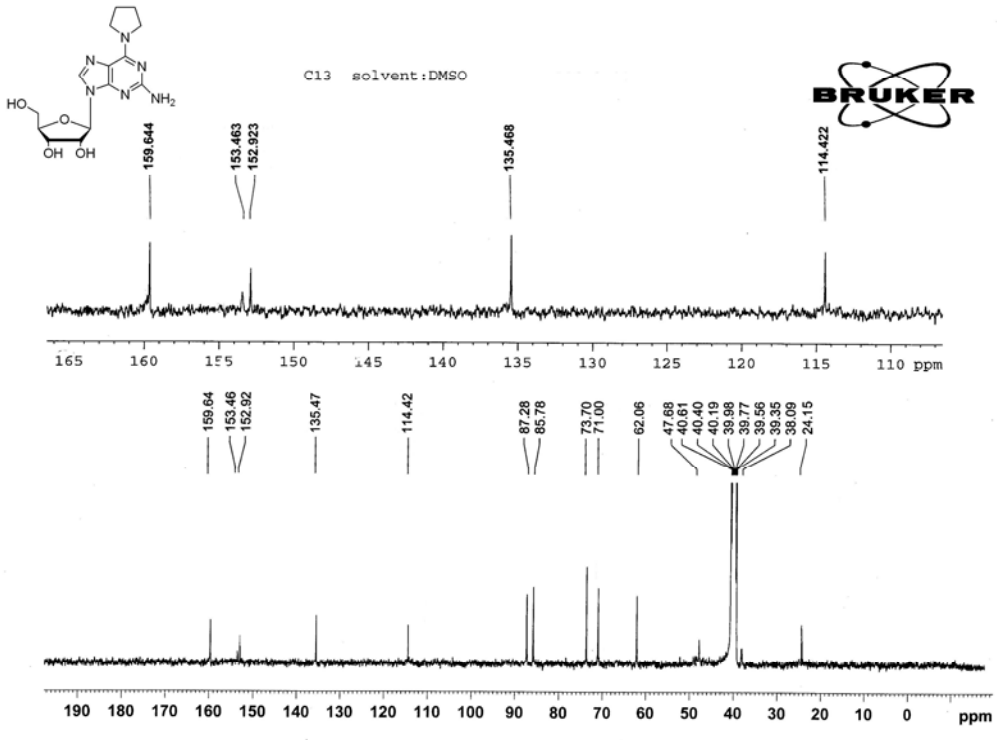

1H solvent:DMSO
BRUKER
HO
OH OH
4.590 4.577 4.568 4.562 4.553 4.160 4.148 4.140 4.128 4.104 4.054 3.973 3.965 3.957 3.949 3.699 3.689 3.679 3.669 3.659 3.649 3.579 3.570 3.562 3.552 3.540 3.531 3.522 3.450 3.435 3.419 3.326
2.509 2.505 2.501 2.496
1.972 1.937
4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 ppm
8.368 8.334 8.211 8.198 5.915 5.906 5.901 5.891 5.442 5.431 5.426 5.416 5.407 5.401 5.389 5.372 5.361 5.355 5.344 5.176 5.164 4.605 4.590 4.577 4.568 4.562 4.553 4.160 4.148 4.140 4.128 4.104 4.054 3.973 3.965 3.957 3.949 3.699 3.689 3.679 3.669 3.659 3.649 3.579 3.570 3.562 3.552 3.540 3.531 3.522 3.450 3.435 3.419 3.326 2.509
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00 0.95 1.00 2.04 1.00 1.02 1.12 1.14 1.25 3.90 4.01

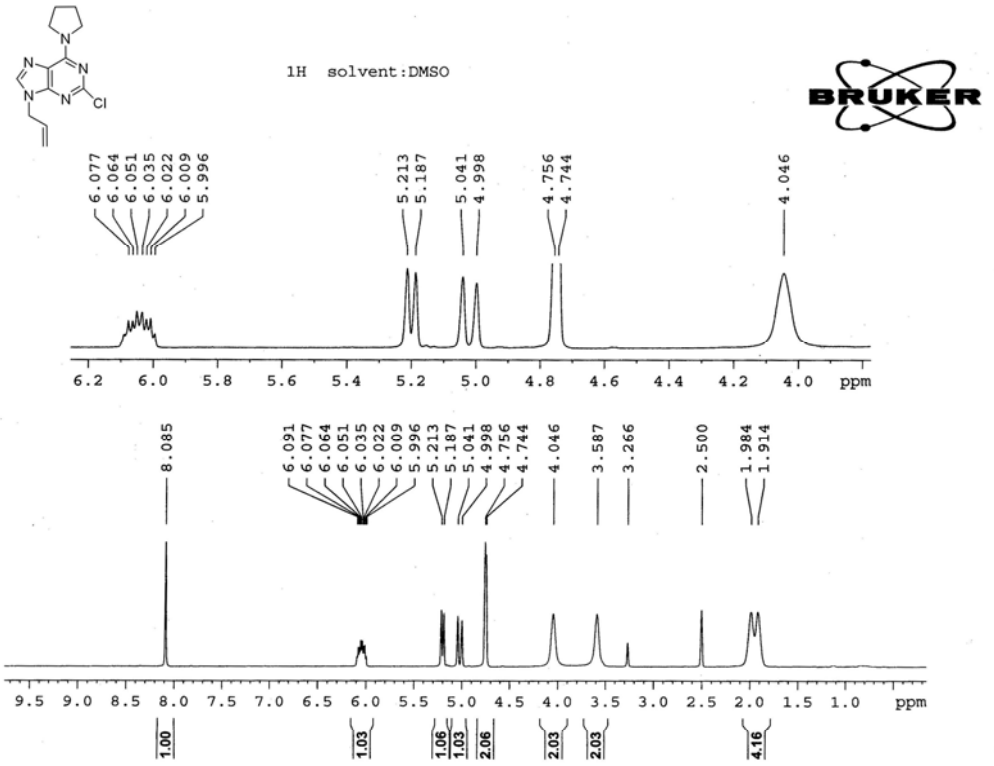

C13 solvent:DMSO
BRUKER
HO
OH OH
153.028 152.489 149.986 139.490 120.431
160 155 150 145 140 135 130 125 120 ppm
153.03 152.49 149.99 139.49 120.43 88.27 86.22 73.92 71.00 62.04 47.58 40.61 40.40 40.20 39.99 39.78 39.57 39.36 25.08
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

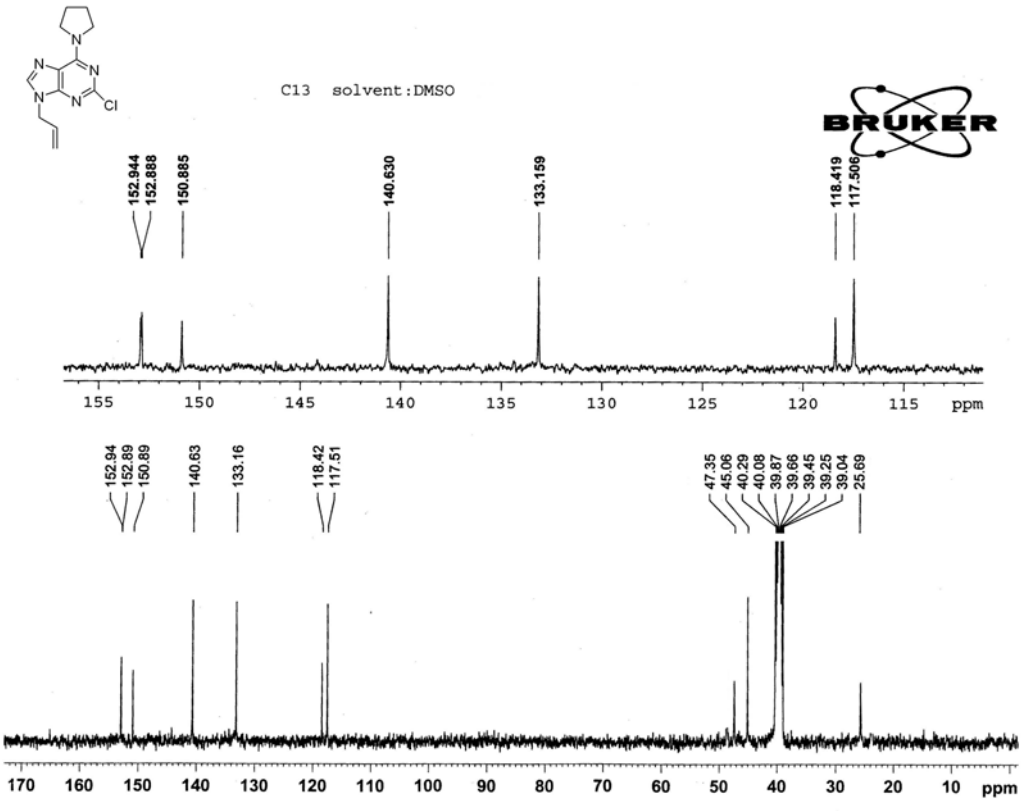

1H solvent:DMSO
BRUKER
HO
OH OH
Cl
4.490 4.486 4.476 4.471 4.145 4.133 4.124 4.112 4.056 4.040 4.024 3.957 3.948 3.939 3.930 3.689 3.678 3.667 3.659 3.648 3.637 3.611 3.593 3.578 3.569 3.564 3.553 3.539 3.534 3.523 3.462 3.331 3.223 3.184 3.078
2.504 2.500 2.496
2.018 2.013 1.997 1.982 1.915 1.898 1.881
4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 ppm
8.406 8.377 5.852 5.847 5.838 5.833 5.485 5.477 5.470 5.462 5.204 5.192 5.075 5.071 5.060 5.048 5.043 4.518 4.513 4.503 4.490 4.486 4.476 4.471 4.145 4.133 4.124 4.112 4.056 4.040 4.024 3.957 3.948 3.939 3.930 3.689 3.678 3.667 3.659 3.648 3.637 3.611 3.593 3.578 3.569 3.564 3.553 3.539 3.534 3.523 3.462 3.331 3.223
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.00 1.02 1.00 1.03 0.99 1.00 1.16 0.99 1.07 4.07 3.92

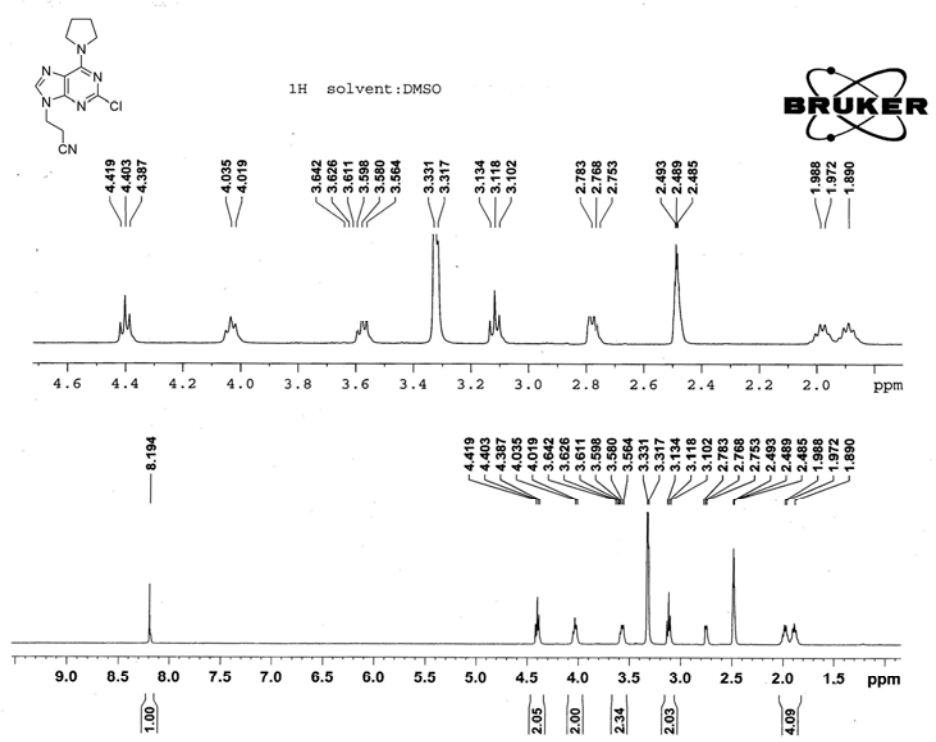

C13 solvent:DMSO
BRUKER
HO
OH OH
Cl
154.946 153.212 151.594 139.128
156 154 152 150 148 146 144 142 140 138 ppm
154.95 153.21 151.59 139.13 119.26 87.76 86.05 74.15 70.71 61.71 47.79 40.60 40.39 40.18 39.98 39.77 39.56 39.35 25.48
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

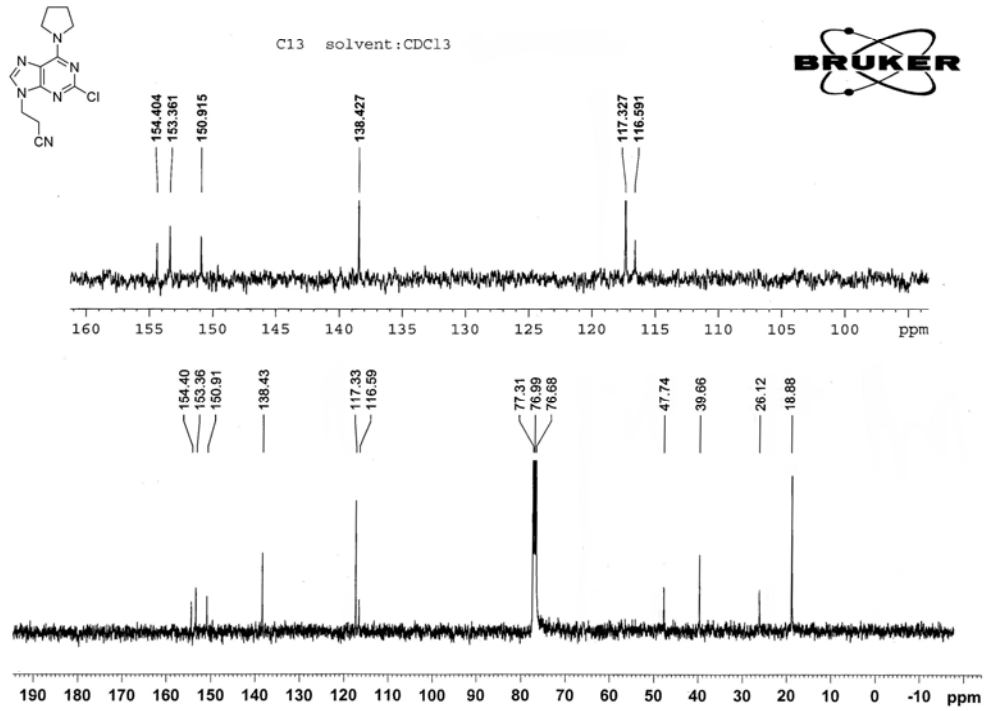

1H solvent:DMSO
BRUKER
HO
OH OH
NH2
5.787 5.770 5.757 5.754 5.743 5.735
5.353 5.348 5.338
5.095 5.084
4.472 4.466 4.459 4.444
4.107 4.096 4.087 4.075
3.960
3.894
3.886
3.682 3.671 3.645 3.615 3.537 3.509
3.362 3.322
6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 ppm
7.937
5.787 5.770 5.757 5.754 5.743 5.735 5.353 5.348 5.338 5.095 5.084 4.472 4.466 4.459 4.444 4.107 4.096 4.087 4.075 3.960 3.894 3.886 3.682 3.671 3.645 3.615 3.537 3.509 3.362 3.322 2.888 2.729 2.503 2.499 2.495 1.907
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
1.00 3.04 2.08 1.00 1.07 1.07 1.78 2.00 1.79 4.05

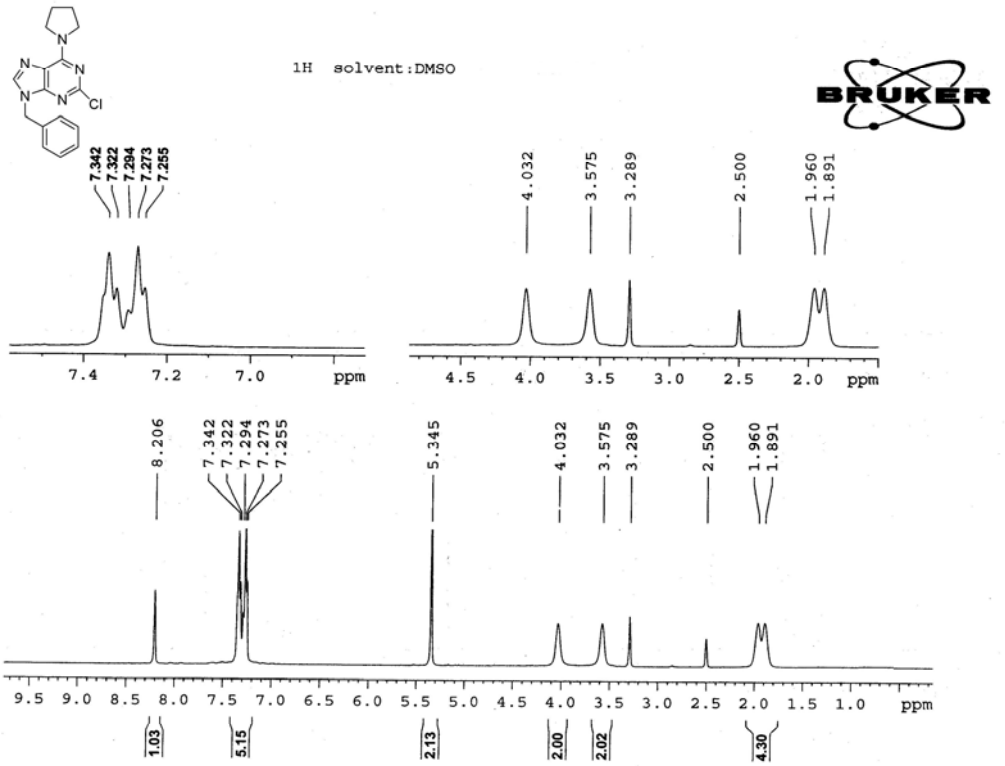

C13 solvent:DMSO
BRUKER
HO
OH OH
NH2
159.644
153.463
152.923
135.468
114.422
165 160 155 150 145 140 135 130 125 120 115 110 ppm
159.64
153.46
152.92
135.47
114.42
87.28
85.78
73.70
71.00
62.06
47.68
40.61
40.40
40.19
39.98
39.77
39.56
39.35
38.09
24.15
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

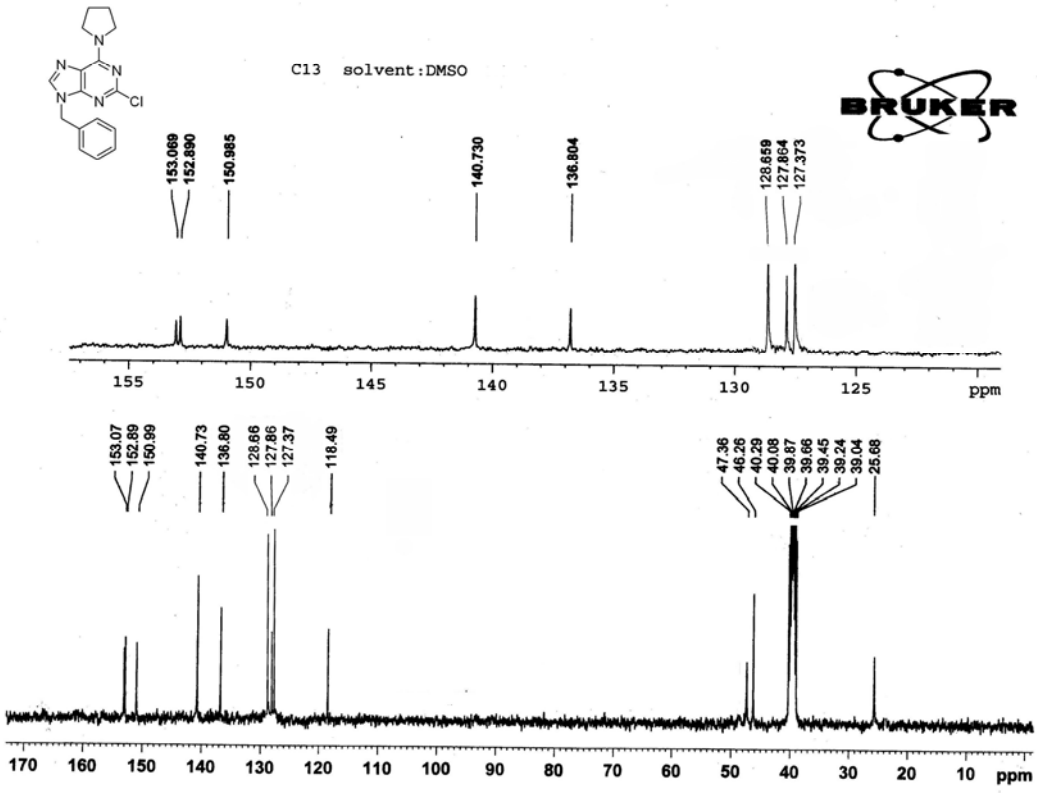

1H solvent:DMSO
BRUKER
6.077
6.064
6.051
6.035
6.022
6.009
5.996
5.213
5.187
5.041
4.998
4.756
4.744
4.046
6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 ppm
8.085
6.091
6.077
6.064
6.051
6.035
6.022
6.009
5.996
5.213
5.187
5.041
4.998
4.756
4.744
4.046
3.587
3.266
2.500
1.984
1.914
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.03
1.06
1.03
2.06
2.03
2.03
4.16

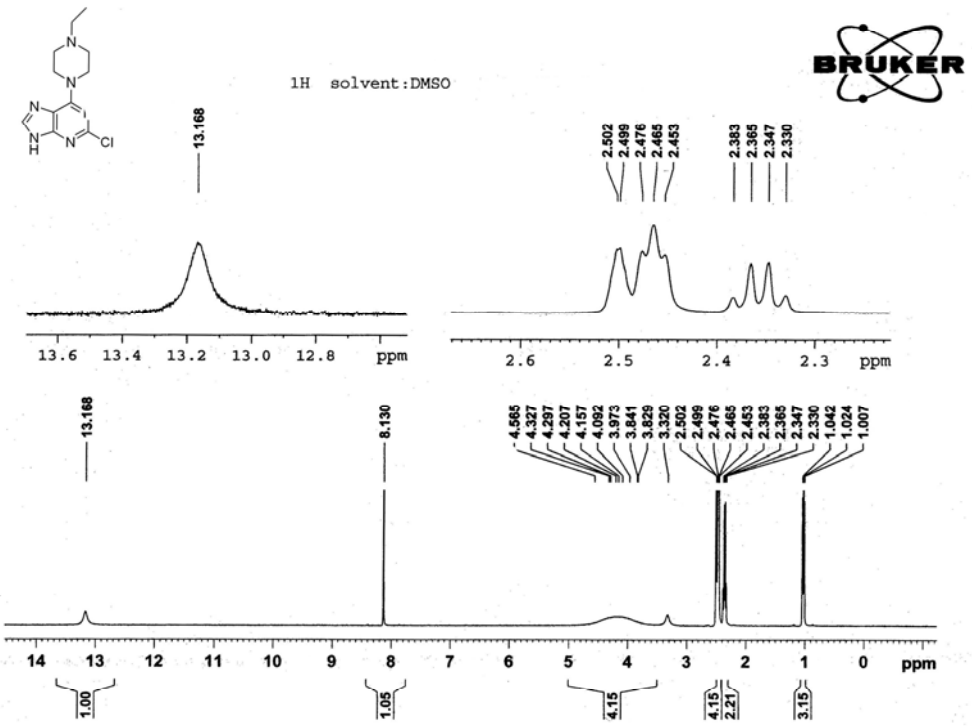

C13 solvent:DMSO
BRUKER
152.944
152.888
150.885
140.630
133.159
118.419
117.506
155 150 145 140 135 130 125 120 115 ppm
152.94
152.89
150.89
140.63
133.16
118.42
117.51
47.35
45.06
40.29
40.08
39.87
39.66
39.45
39.25
39.04
25.69
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

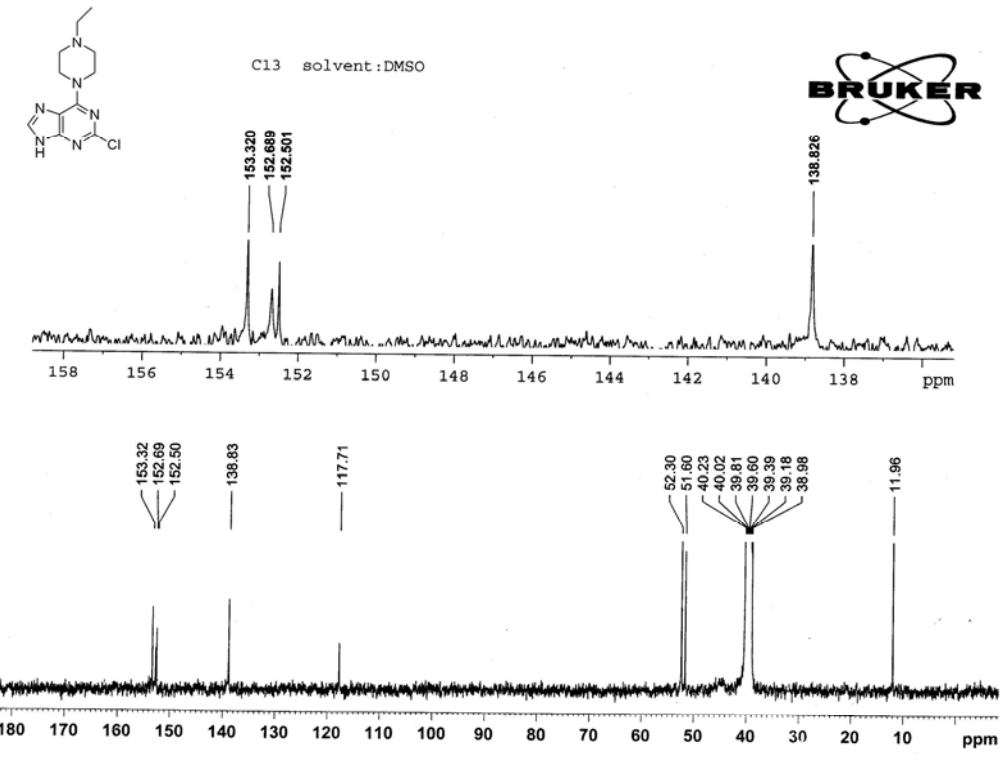

1H solvent:DMSO
BRUKER
4.419
4.403
4.387
4.035
4.019
3.642
3.626
3.611
3.598
3.580
3.564
3.331
3.317
3.134
3.118
3.102
2.783
2.768
2.753
2.493
2.489
2.485
1.988
1.972
1.890
ppm
8.194
1.00
2.05
2.00
2.34
2.03
4.09

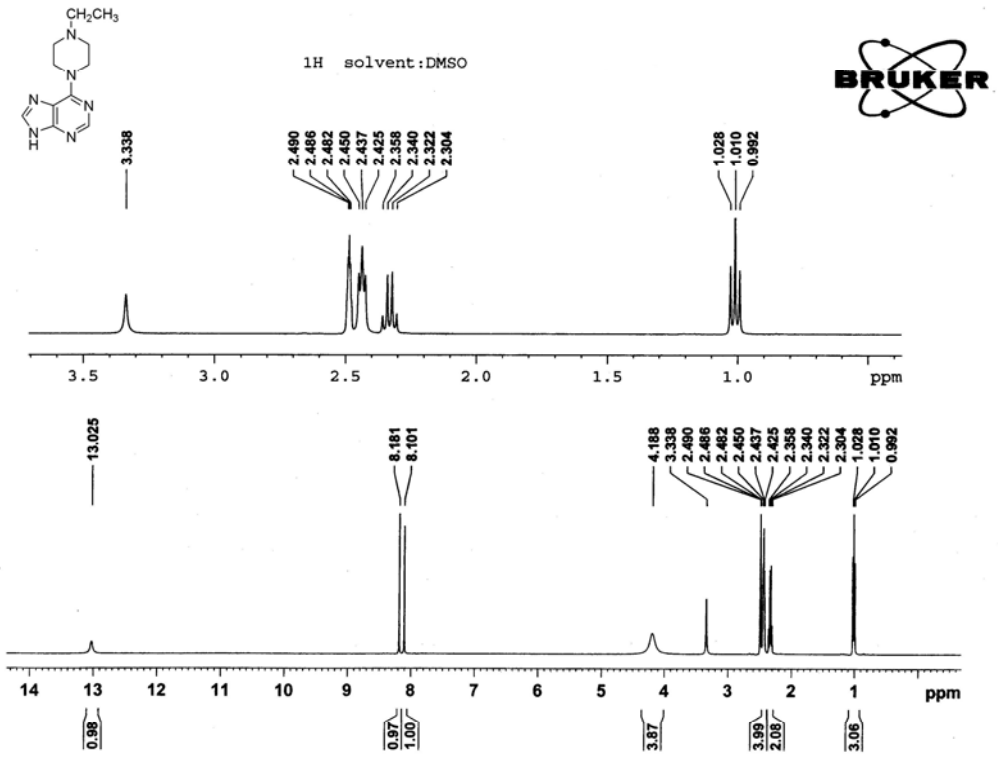

C13 solvent:CDCl3
BRUKER
154.404
153.361
150.915
138.427
117.327
116.591
ppm
154.40
153.36
150.91
138.43
117.33
116.59
77.31
76.99
76.68
47.74
39.66
26.12
18.88

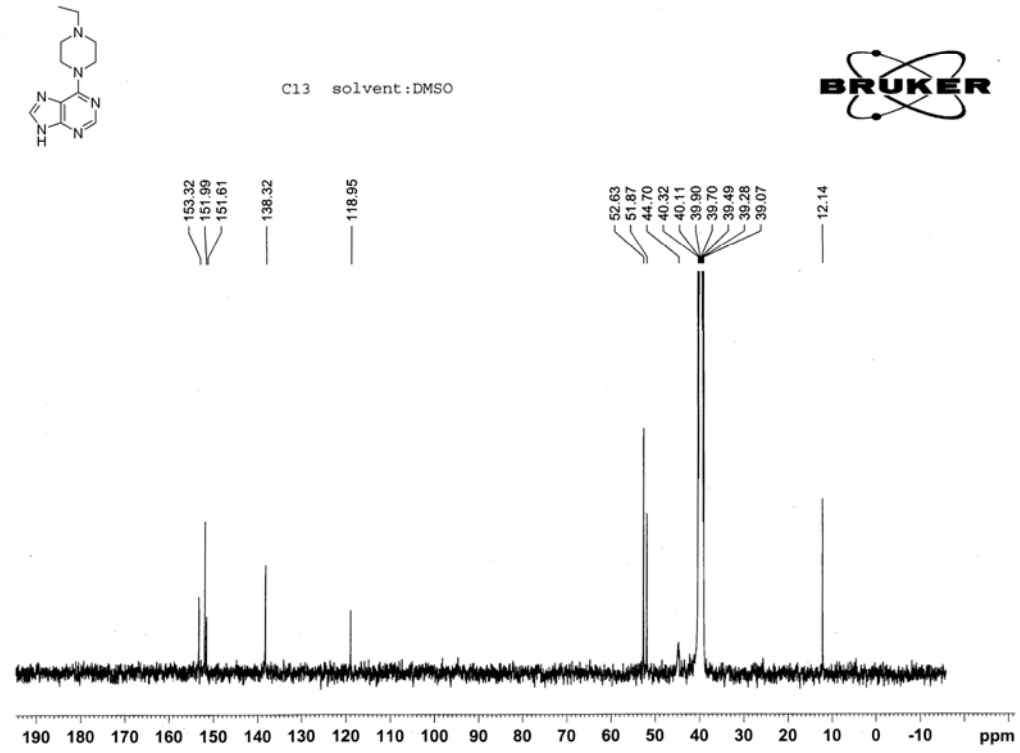

1H solvent:DMSO
BRUKER
7.342
7.322
7.294
7.273
7.255
4.032
3.575
3.289
2.500
1.960
1.891
8.206
5.345
1.03
5.15
2.13
2.00
2.02
4.30
ppm

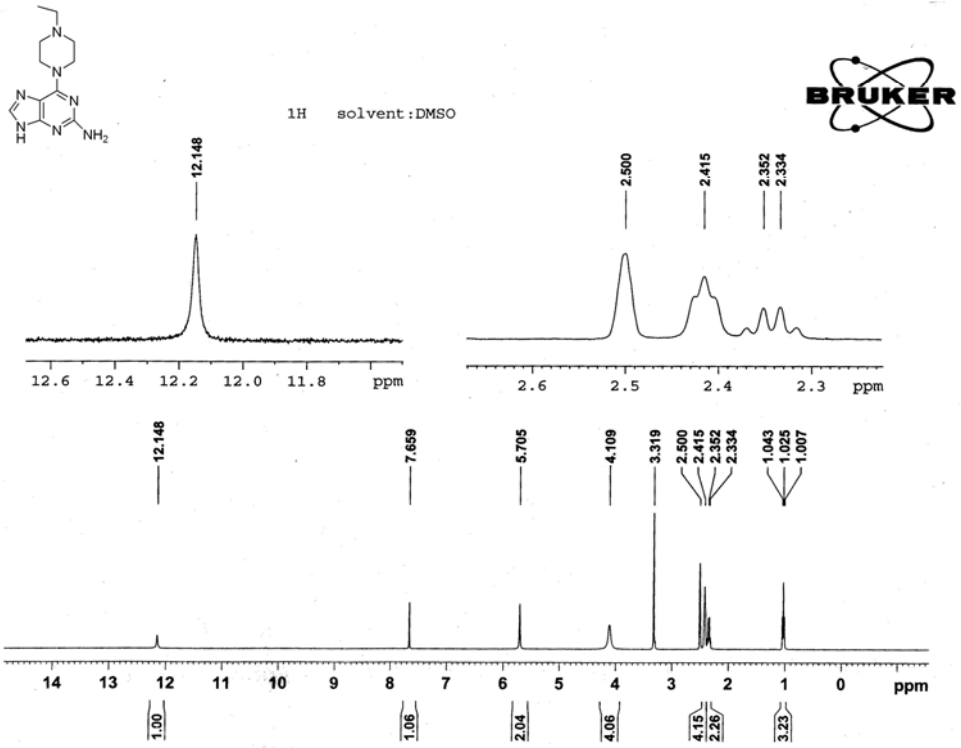

C13 solvent:DMSO
BRUKER
153.069
152.890
150.985
140.730
136.804
128.659
127.864
127.373
153.07
152.89
150.99
140.73
136.80
128.66
127.86
127.37
118.49
47.36
46.26
40.29
40.08
39.87
39.66
39.45
39.24
39.04
25.68
ppm

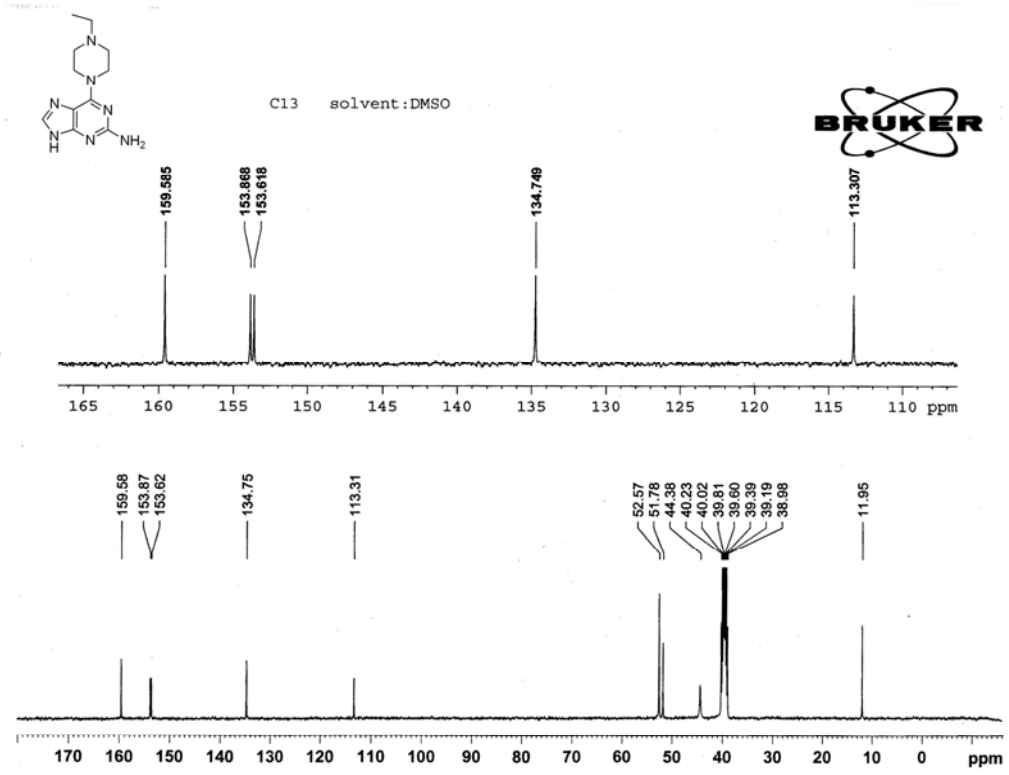

1H solvent:DMSO
BRUKER
13.168
2.502
2.499
2.476
2.465
2.453
2.383
2.365
2.347
2.330
13.6 13.4 13.2 13.0 12.8 ppm
2.6 2.5 2.4 2.3 ppm
13.168
8.130
4.565
4.327
4.297
4.207
4.157
4.092
3.973
3.841
3.829
3.320
2.502
2.499
2.476
2.465
2.453
2.383
2.365
2.347
2.330
1.042
1.024
1.007
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.05
4.15
4.15
2.21
3.15

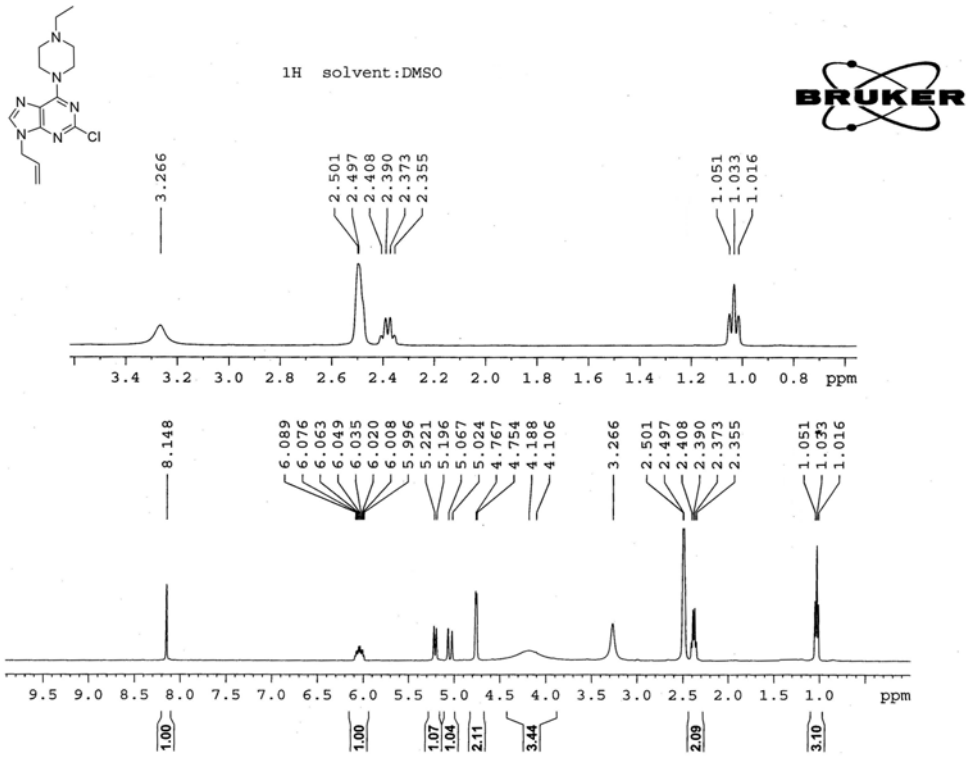

C13 solvent:DMSO
BRUKER
153.320
152.689
152.501
138.826
158 156 154 152 150 148 146 144 142 140 138 ppm
153.32
152.69
152.50
138.83
117.71
52.30
51.60
40.23
40.02
39.81
39.60
39.39
39.18
38.98
11.96
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

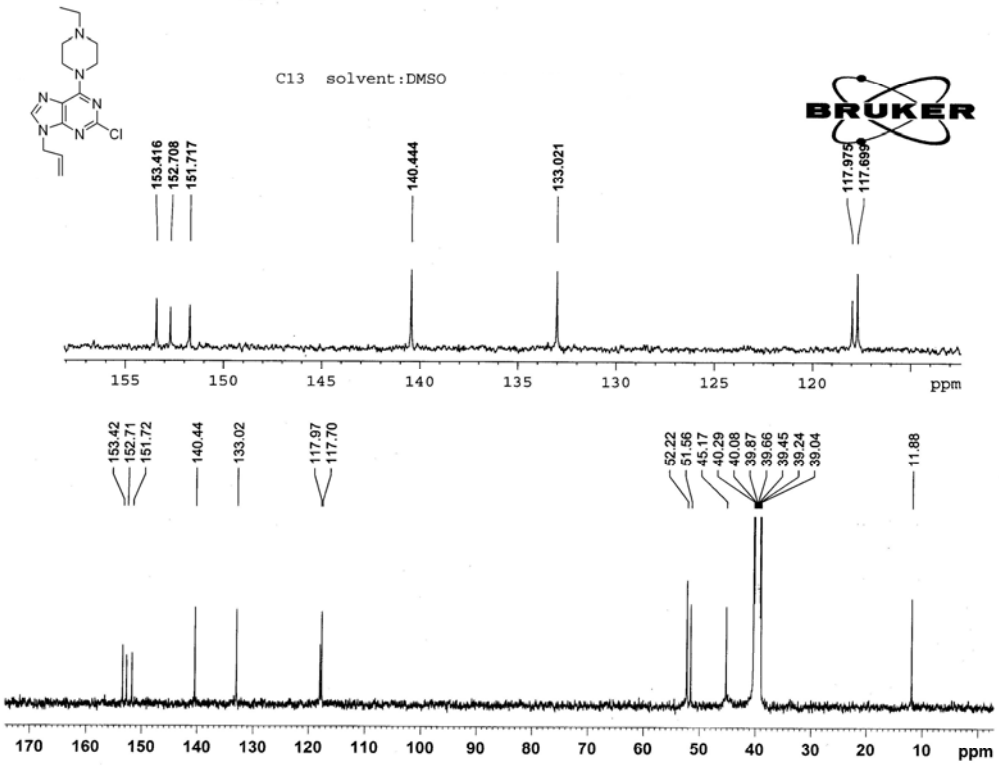

1H solvent:DMSO
BRUKER
3.338
2.490
2.486
2.482
2.450
2.437
2.425
2.358
2.340
2.322
2.304
1.028
1.010
0.992
ppm
13.025
8.181
8.101
4.188
0.98
0.97
1.00
3.87
3.99
2.08
3.06

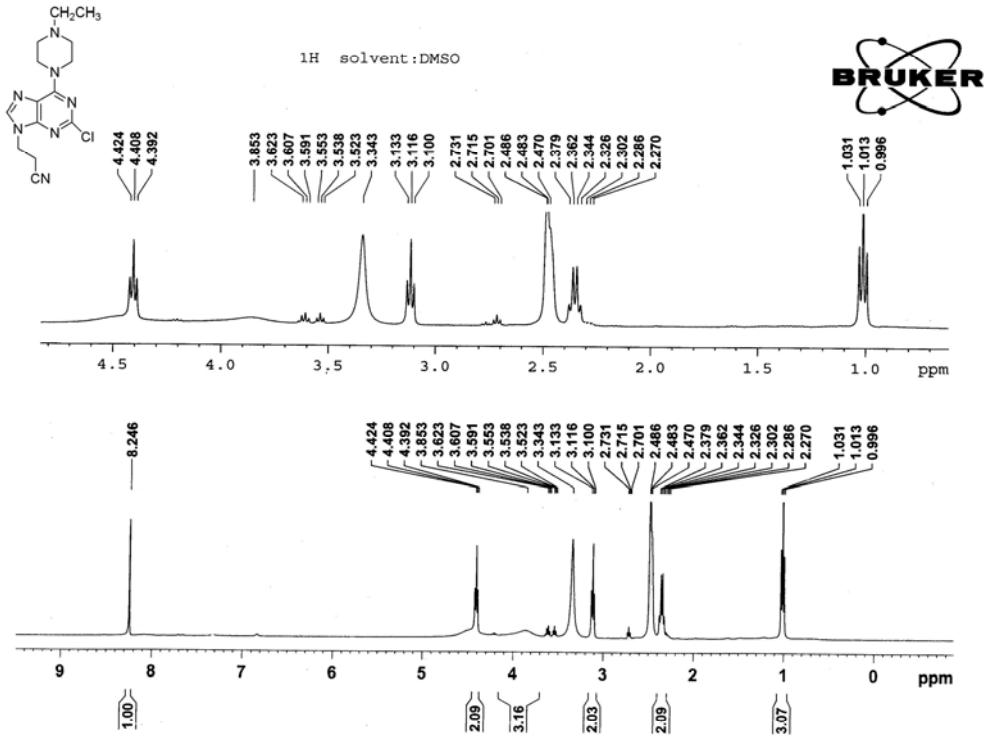

C13 solvent:DMSO
BRUKER
153.32
151.99
151.61
138.32
118.95
52.63
51.87
44.70
40.32
40.11
39.90
39.70
39.49
39.28
39.07
12.14
ppm

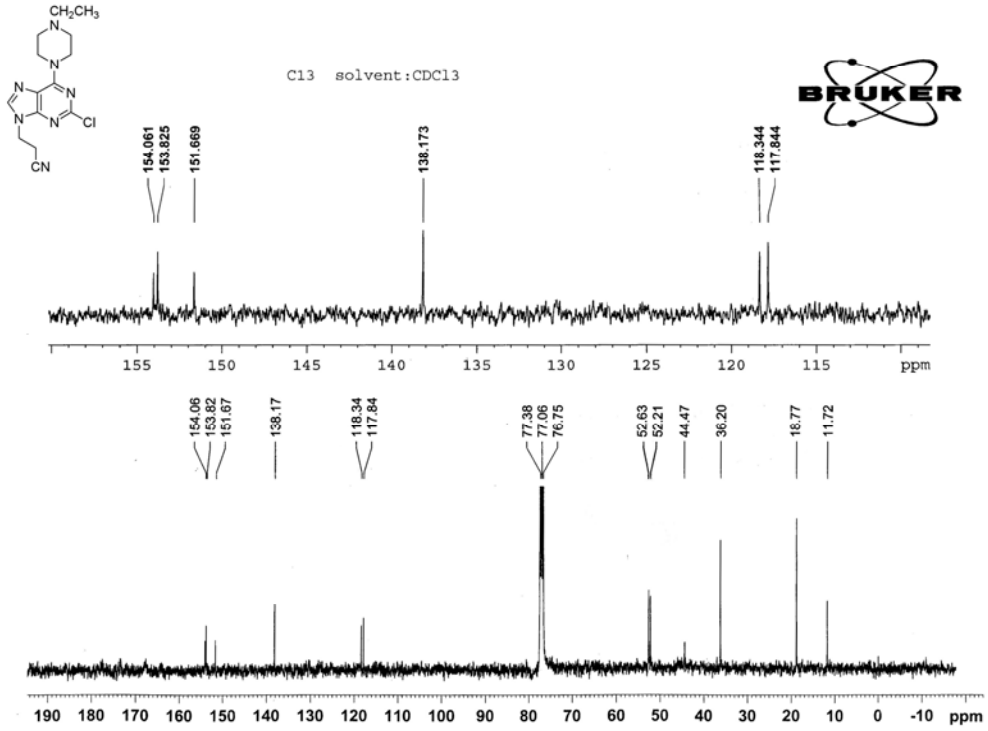

1H solvent:DMSO
BRUKER
12.148
2.500
2.415
2.352
2.334
12.6 12.4 12.2 12.0 11.8 ppm
2.6 2.5 2.4 2.3 ppm
12.148
7.659
5.705
4.109
3.319
2.500
2.415
2.352
2.334
1.043
1.025
1.007
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.06
2.04
4.06
4.15
2.26
3.23

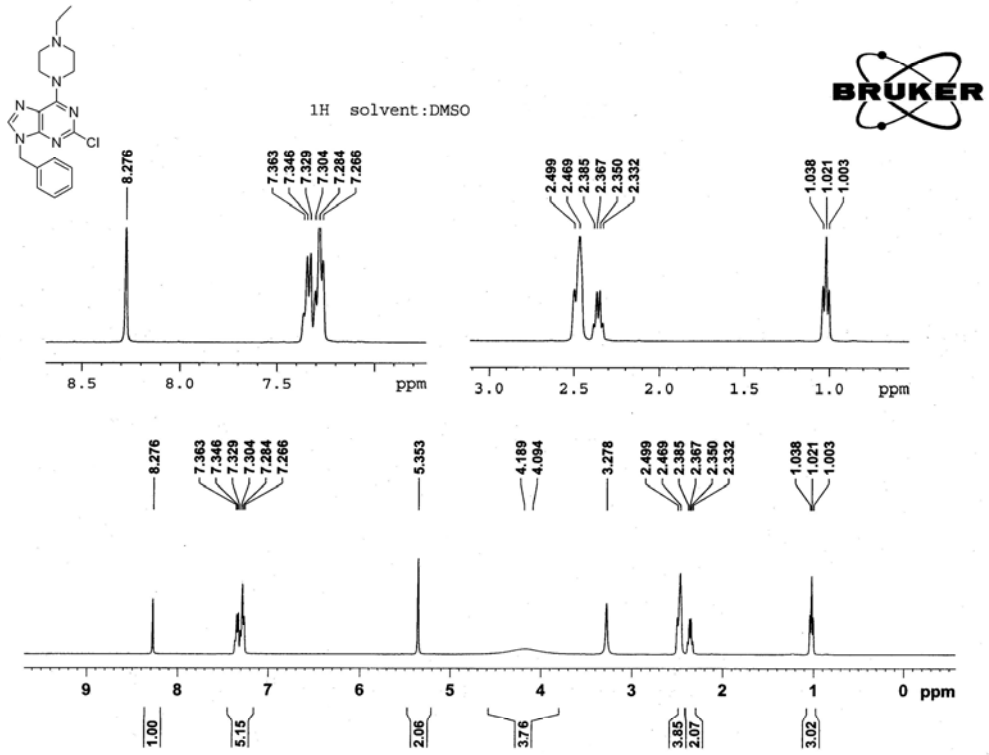

C13 solvent:DMSO
BRUKER
159.585
153.868
153.618
134.749
113.307
165 160 155 150 145 140 135 130 125 120 115 110 ppm
159.58
153.87
153.62
134.75
113.31
52.57
51.78
44.38
40.23
40.02
39.81
39.60
39.39
39.19
38.98
11.95
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

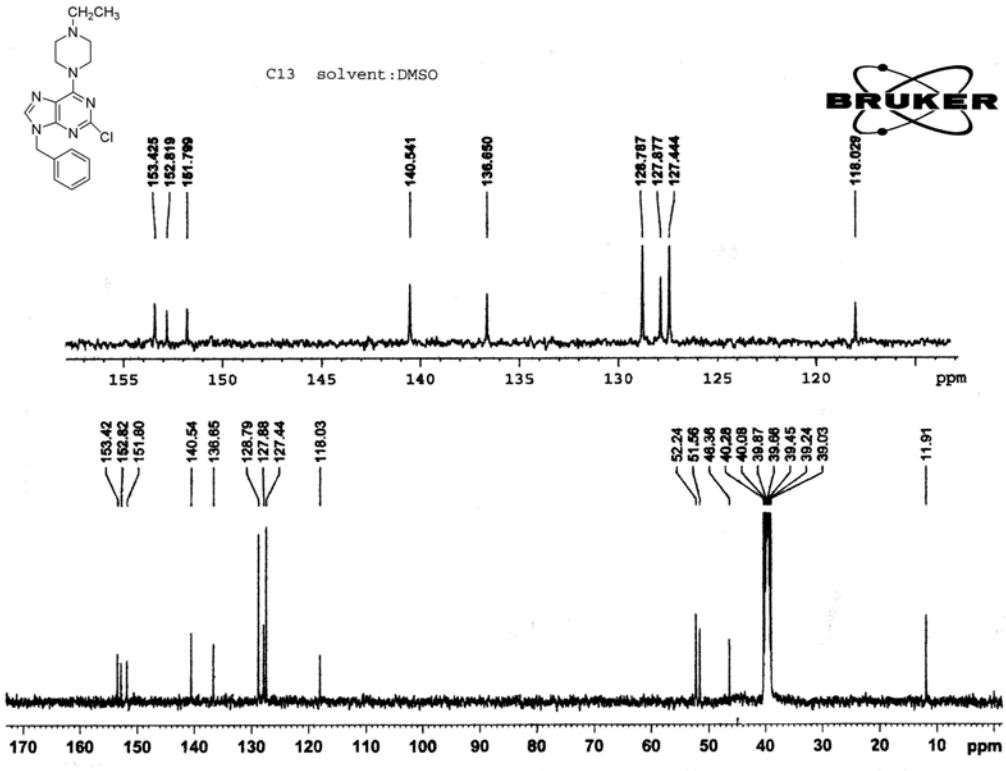

1H solvent:DMSO
BRUKER
3.266
2.501
2.497
2.408
2.390
2.373
2.355
1.051
1.033
1.016
ppm
8.148
6.089
6.076
6.063
6.049
6.035
6.020
6.008
5.996
5.221
5.196
5.067
5.024
4.767
4.754
4.188
4.106
1.00
1.00
1.07
1.04
2.11
3.44
2.09
3.10

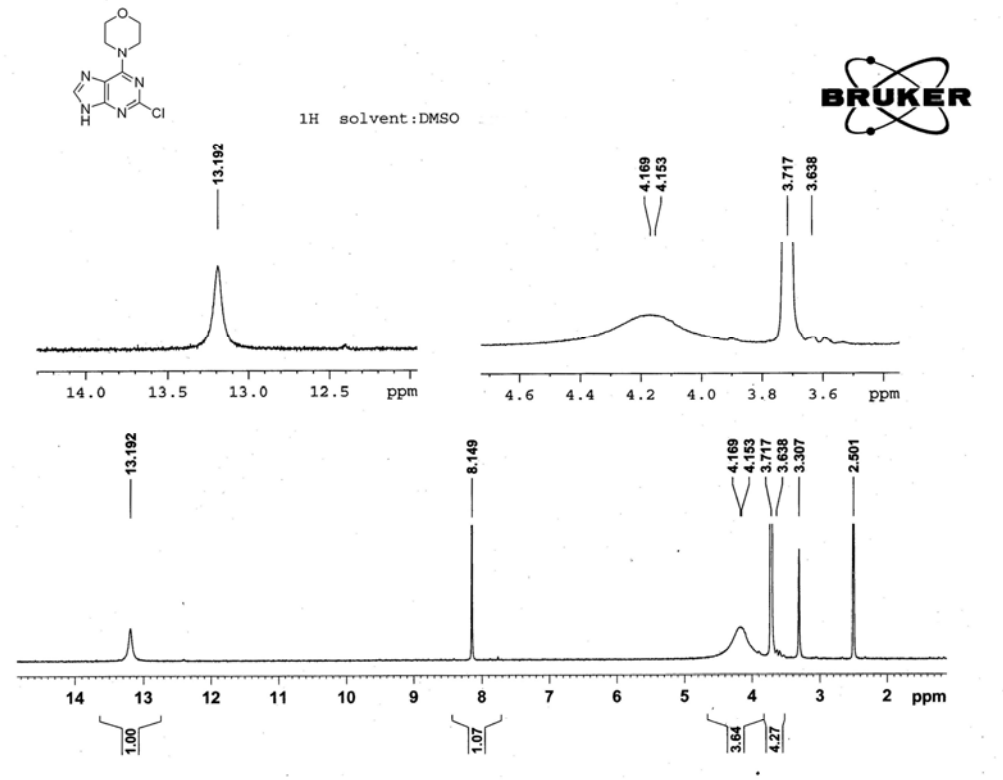

C13 solvent:DMSO
BRUKER
153.416
152.708
151.717
140.444
133.021
117.975
117.699
ppm
153.42
152.71
151.72
140.44
133.02
117.97
117.70
52.22
51.56
45.17
40.29
40.08
39.87
39.66
39.45
39.24
39.04
11.88
ppm

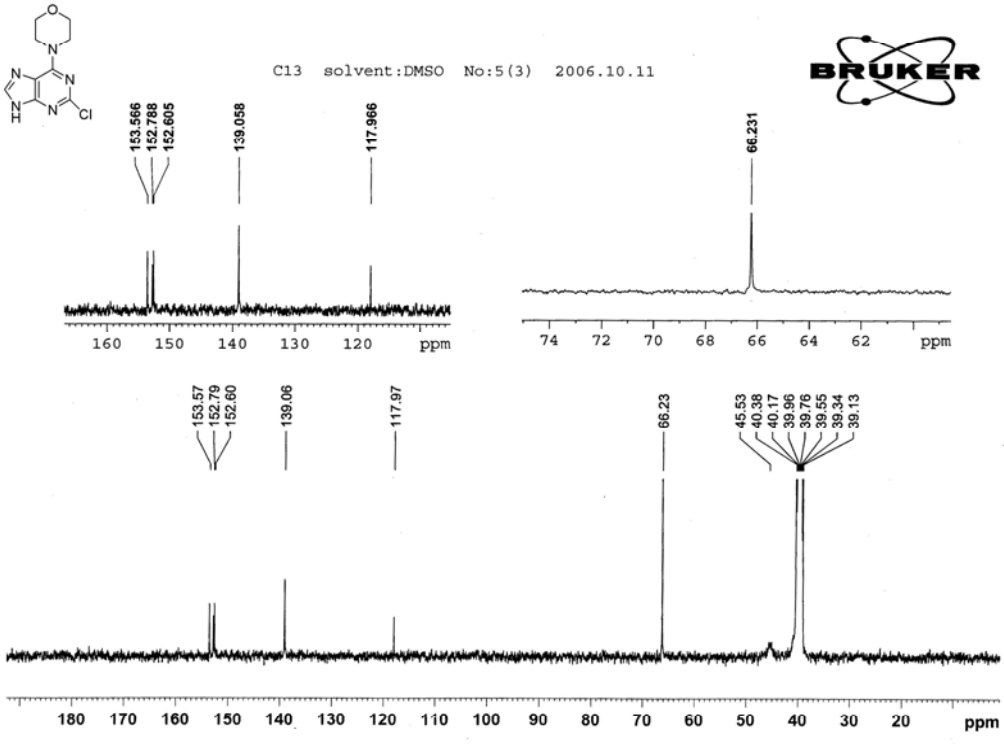

1H solvent:DMSO
BRUKER
4.424
4.408
4.392
3.853
3.623
3.607
3.591
3.553
3.538
3.523
3.343
3.133
3.116
3.100
2.731
2.715
2.701
2.486
2.483
2.470
2.379
2.362
2.344
2.326
2.302
2.286
2.270
1.031
1.013
0.996
8.246
ppm
1.00
2.09
3.16
2.03
2.09
3.07

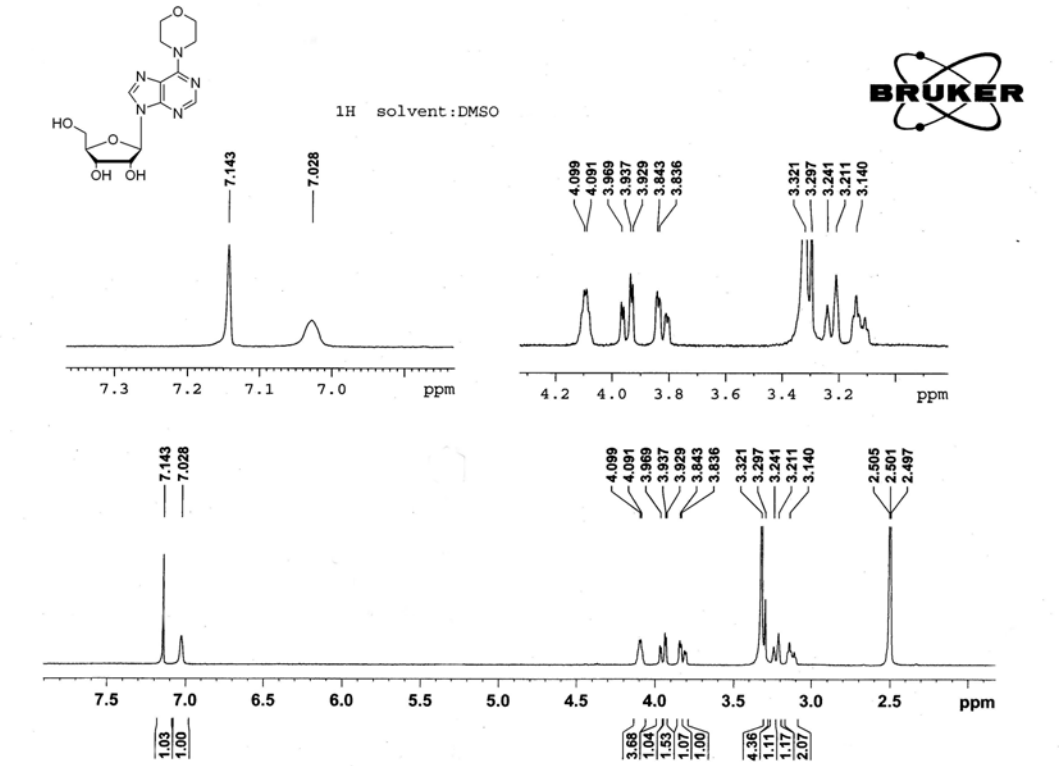

C13 solvent:CDCl3
BRUKER
154.061
153.825
151.669
138.173
118.344
117.844
ppm
154.06
153.82
151.67
138.17
118.34
117.84
77.38
77.06
76.75
52.63
52.21
44.47
36.20
16.77
11.72

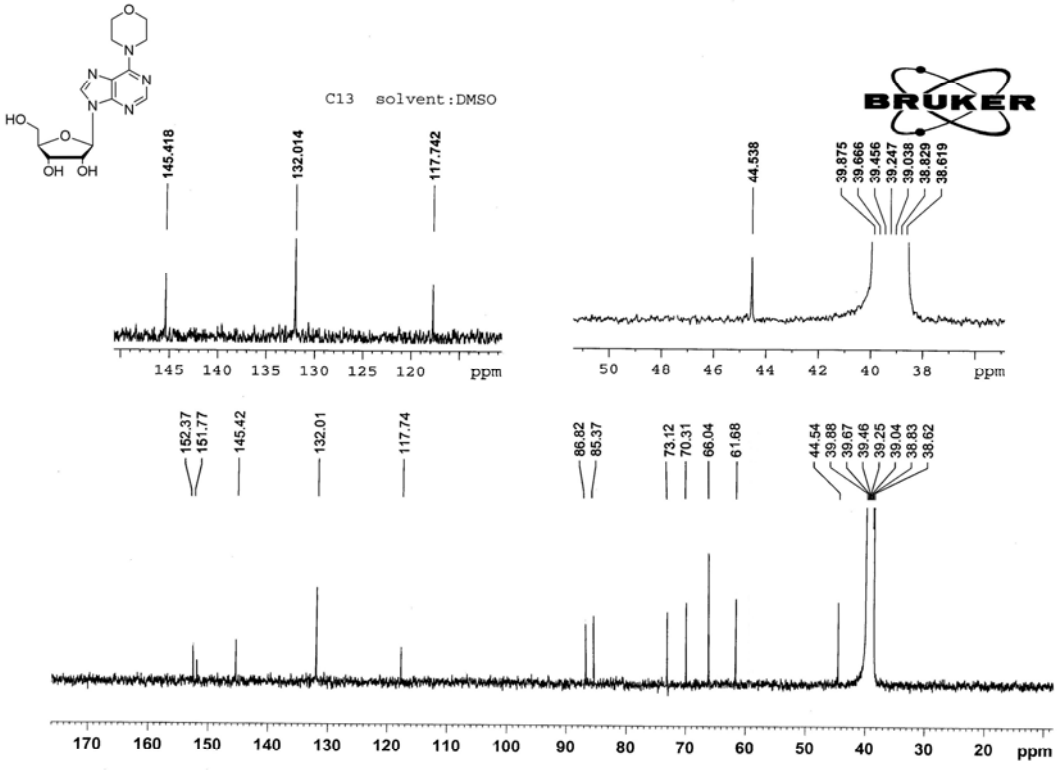

1H solvent:DMSO
BRUKER
8.276
7.363
7.346
7.329
7.304
7.284
7.266
2.499
2.469
2.385
2.367
2.350
2.332
1.038
1.021
1.003
5.353
4.189
4.094
3.278
ppm
1.00
5.15
2.06
3.76
3.85
2.07
3.02

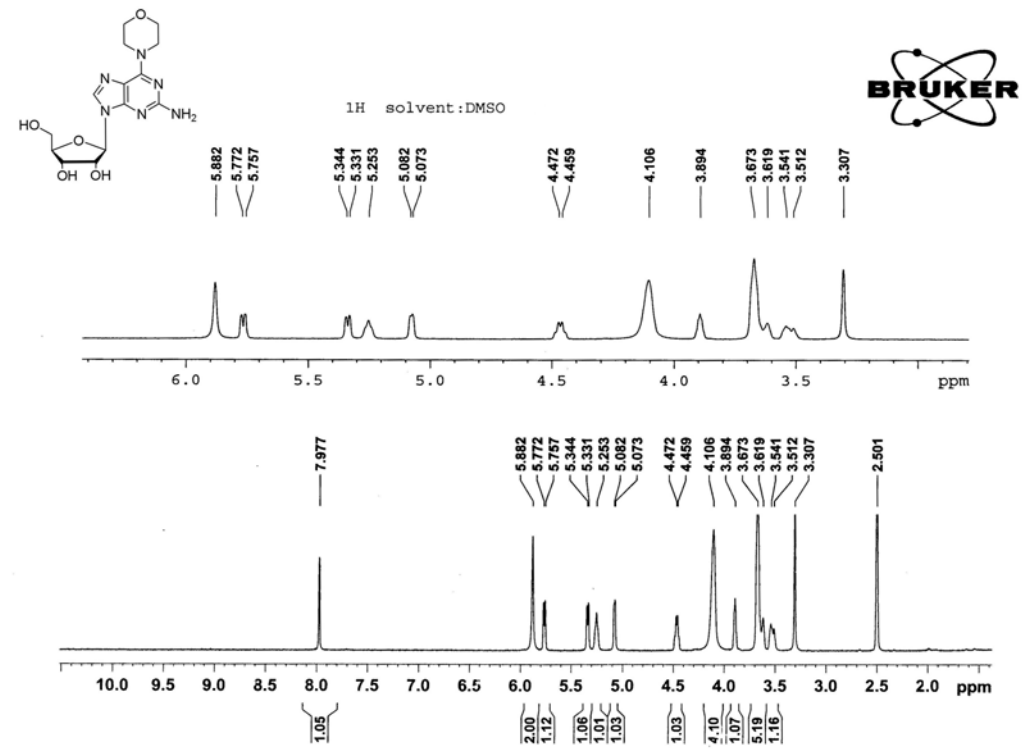

C13 solvent:DMSO
BRUKER
153.425
152.819
151.799
140.541
136.650
128.787
127.877
127.444
118.029
ppm
153.42
152.82
151.80
140.54
136.65
128.79
127.88
127.44
118.03
52.24
51.56
48.36
40.28
40.08
39.87
39.66
39.45
39.24
39.03
11.91

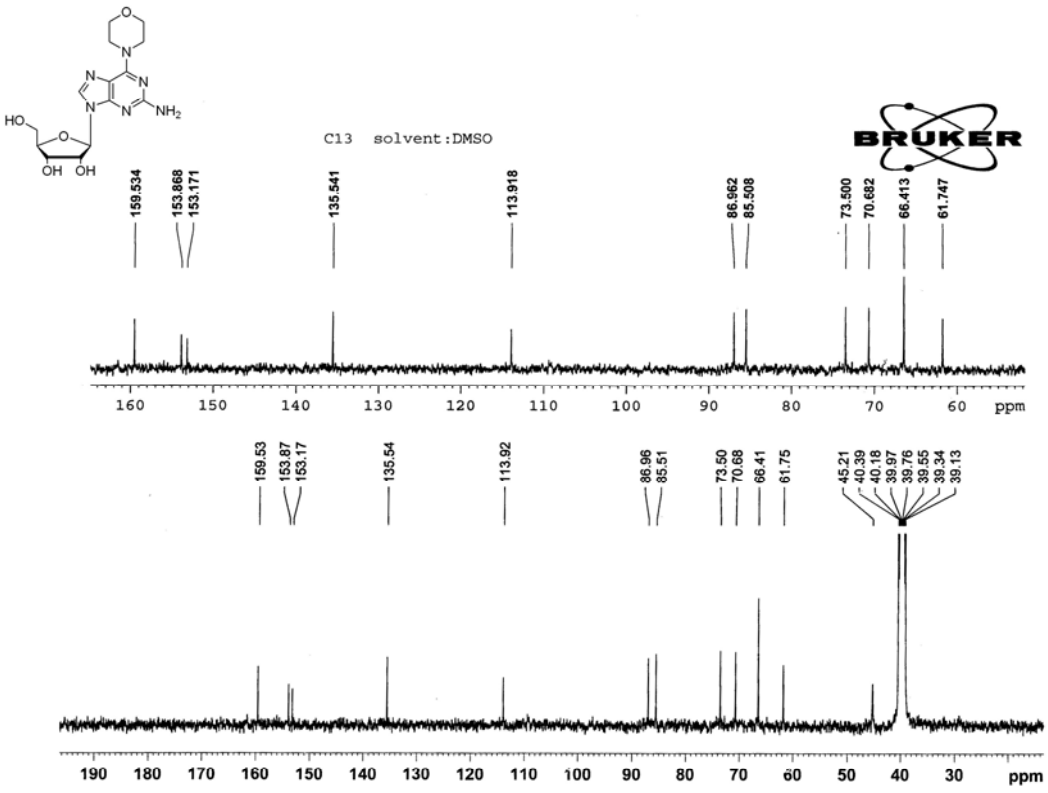

1H solvent:DMSO
13.192
4.169
4.153
3.717
3.638
8.149
3.307
2.501
1.00
1.07
3.64
4.27
ppm

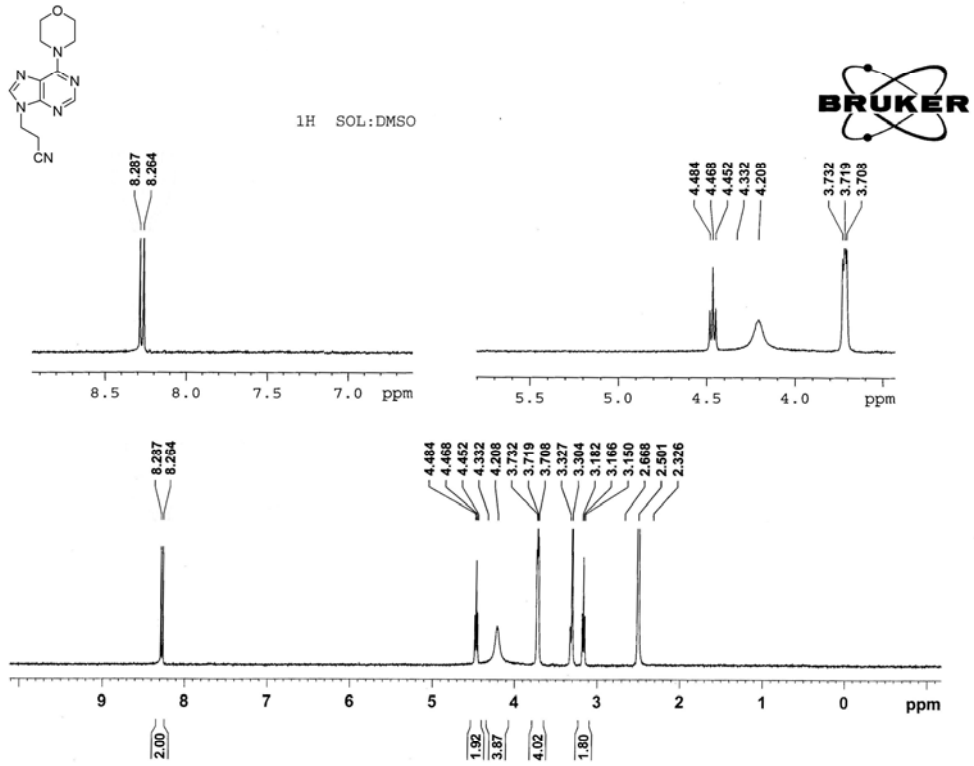

C13 solvent:DMSO No:5(3) 2006.10.11
153.566
152.788
152.605
139.058
117.966
66.231
153.57
152.79
152.60
139.06
117.97
66.23
45.53
40.38
40.17
39.96
39.76
39.55
39.34
39.13
ppm

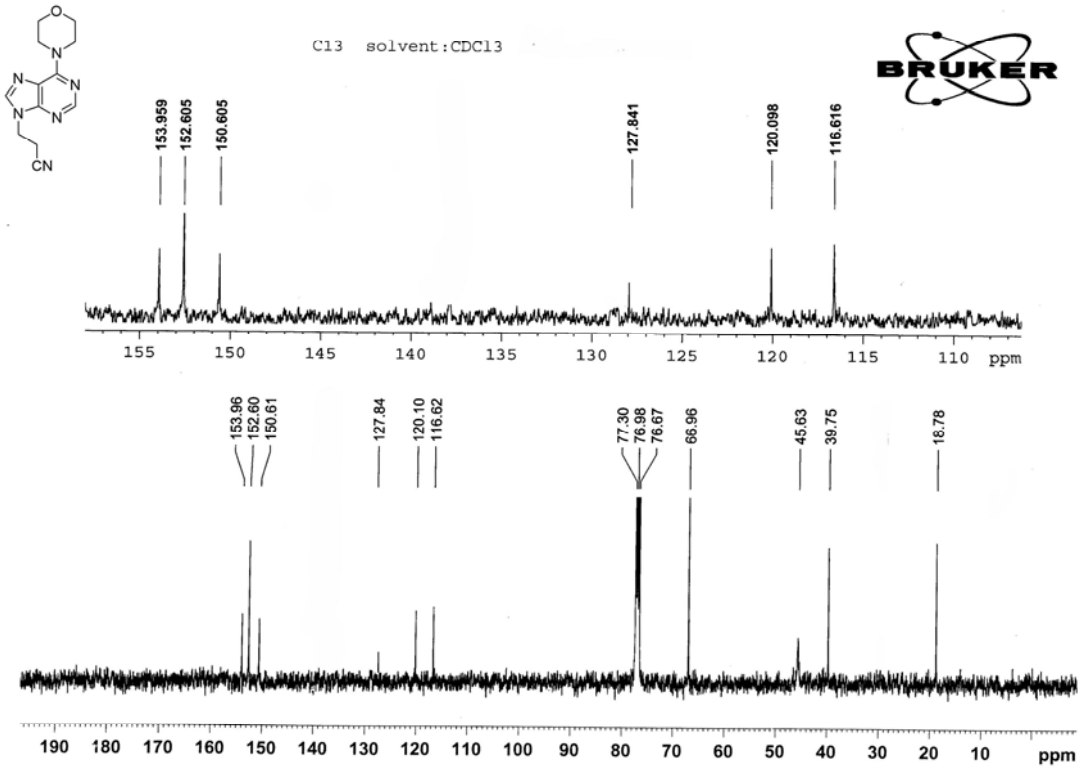

1H solvent:DMSO
7.143
7.028
4.099
4.091
3.969
3.937
3.929
3.843
3.836
3.321
3.297
3.241
3.211
3.140
2.505
2.501
2.497
ppm

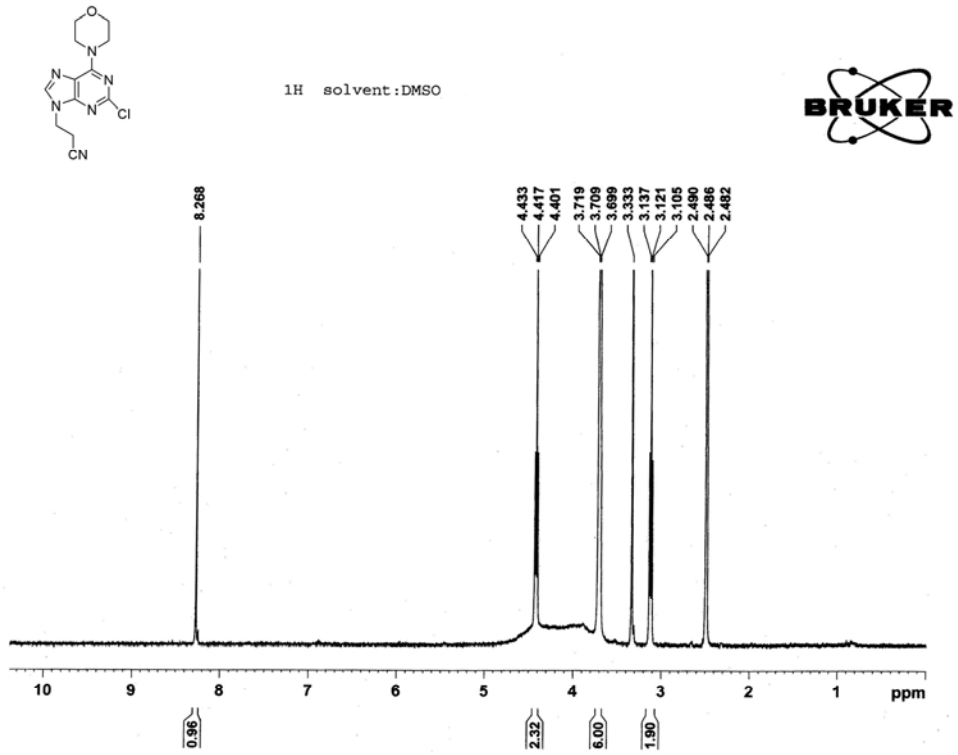

C13 solvent:DMSO
145.418
132.014
117.742
44.538
39.875
39.666
39.456
39.247
39.038
38.829
38.619
152.37
151.77
145.42
132.01
117.74
86.82
85.37
73.12
70.31
66.04
61.68
44.54
39.88
39.67
39.46
39.25
39.04
38.83
38.62
ppm

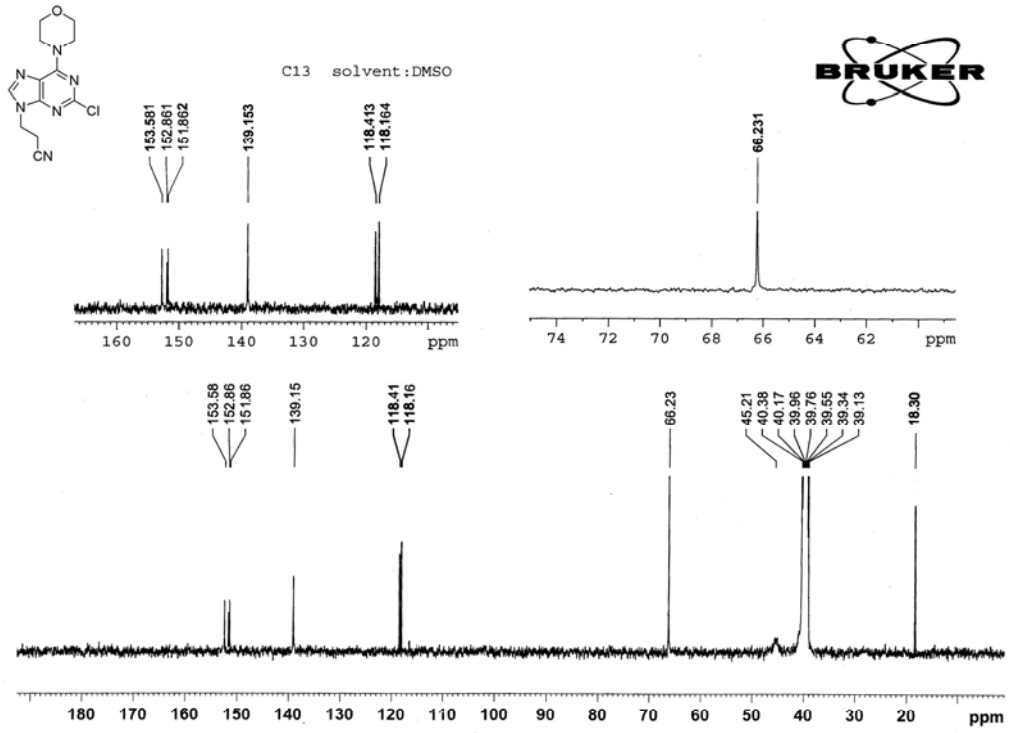

1H solvent:DMSO
BRUKER
5.882
5.772
5.757
5.344
5.331
5.253
5.082
5.073
4.472
4.459
4.106
3.894
3.673
3.619
3.541
3.512
3.307
6.0
5.5
5.0
4.5
4.0
3.5
ppm
7.977
2.501
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.05
2.00
1.12
1.06
1.01
1.03
1.03
4.10
1.07
5.19
1.16

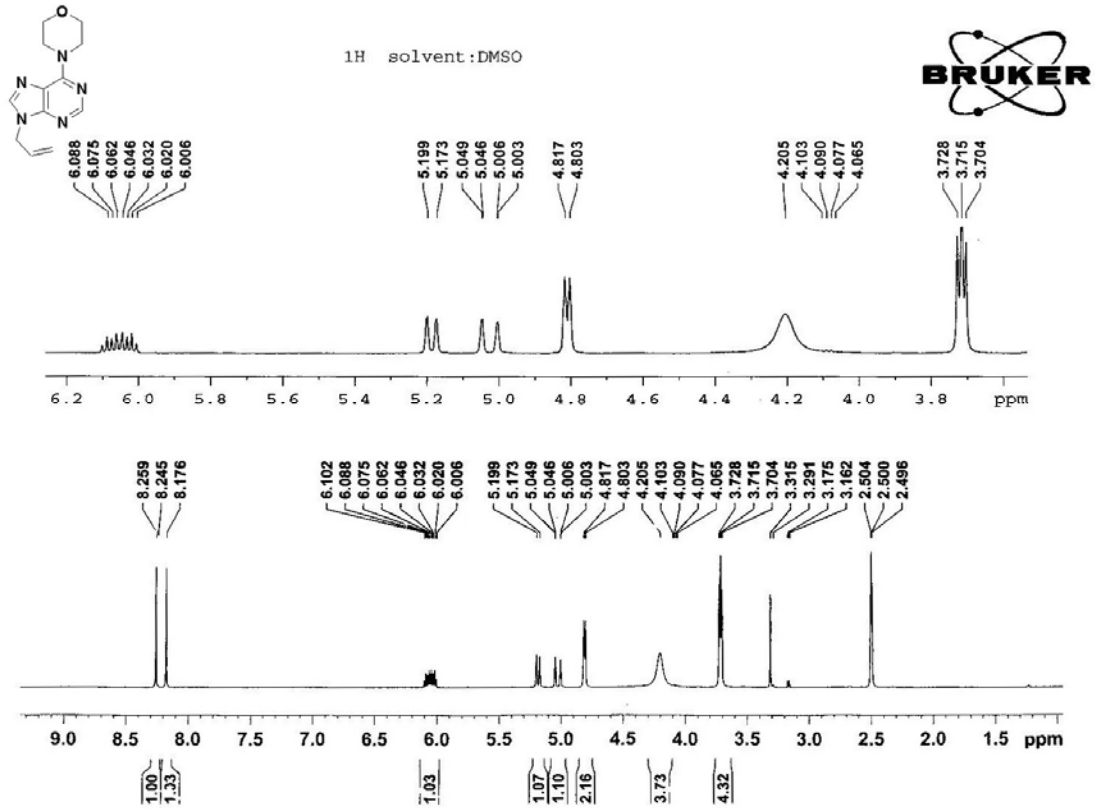

C13 solvent:DMSO
BRUKER
159.534
153.868
153.171
135.541
113.918
86.962
85.508
73.500
70.682
66.413
61.747
160
150
140
130
120
110
100
90
80
70
60
ppm
159.53
153.87
153.17
135.54
113.92
86.96
85.51
73.50
70.68
66.41
61.75
45.21
40.39
40.18
39.97
39.76
39.55
39.34
39.13
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

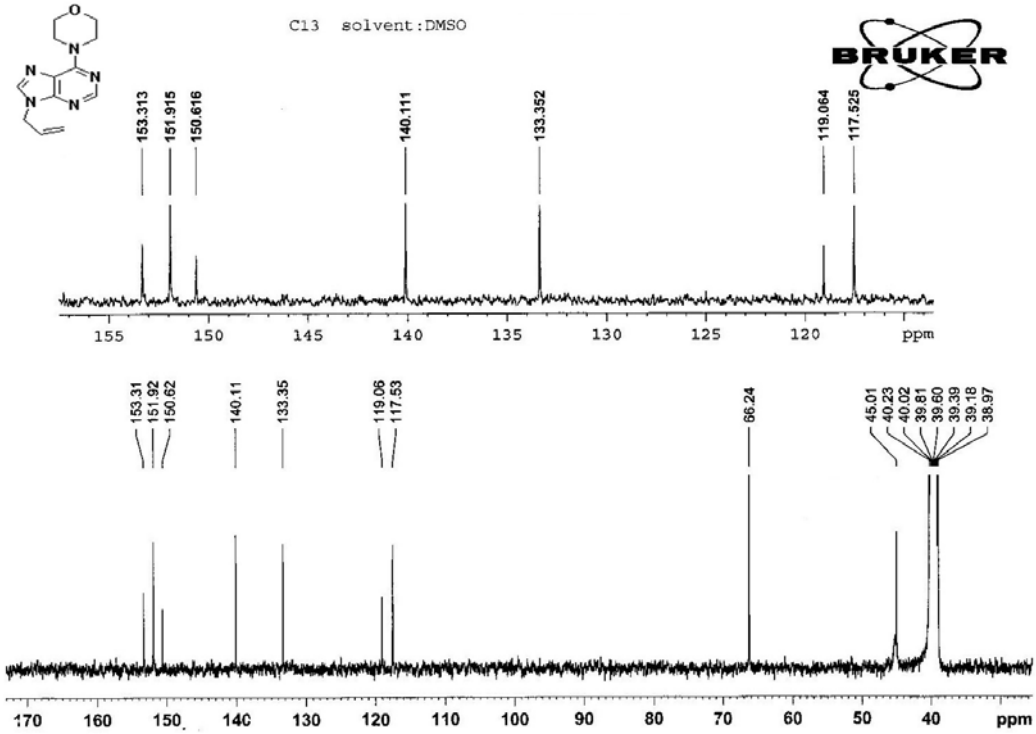

1H SOL:DMSO
BRUKER
8.287
8.264
4.484
4.468
4.452
4.332
4.208
3.732
3.719
3.708
8.5
8.0
7.5
7.0
ppm
5.5
5.0
4.5
4.0
ppm
8.237
8.264
4.484
4.468
4.452
4.332
4.208
3.732
3.719
3.708
3.327
3.304
3.182
3.166
3.150
2.668
2.501
2.326
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.92
3.87
4.02
1.80

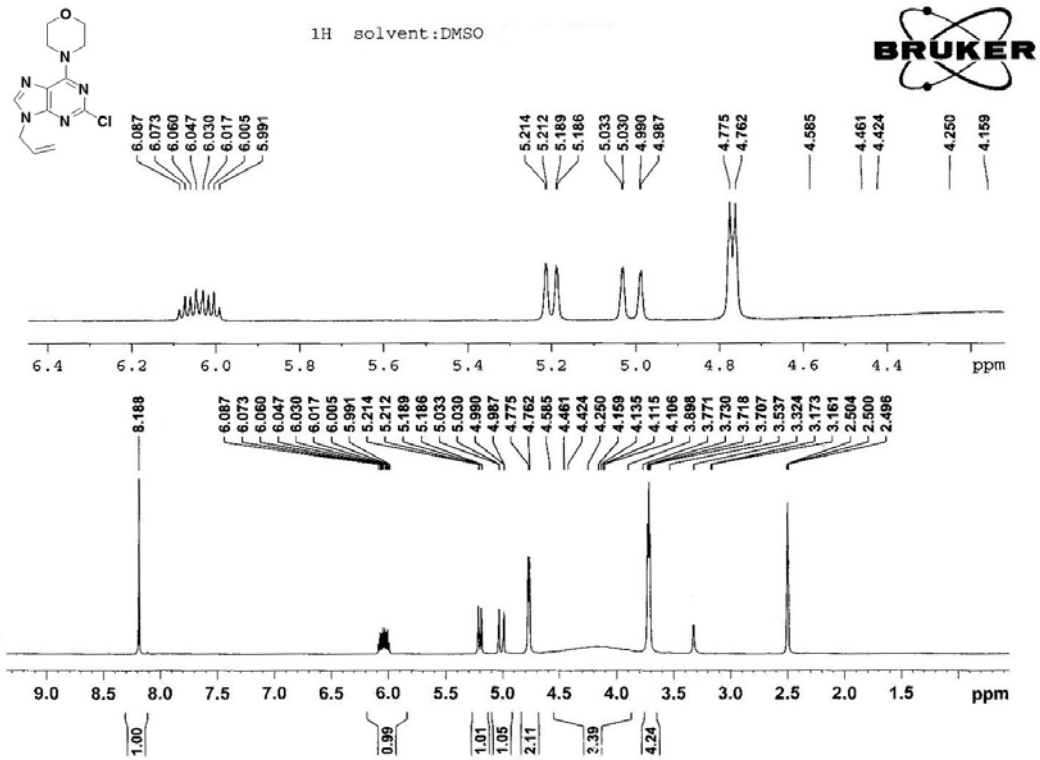

C13 solvent:CDCl3
BRUKER
153.959
152.605
150.605
127.841
120.098
116.616
155
150
145
140
135
130
125
120
115
110
ppm
153.96
152.60
150.61
127.84
120.10
116.62
77.30
76.98
76.67
66.96
45.63
39.75
18.78
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

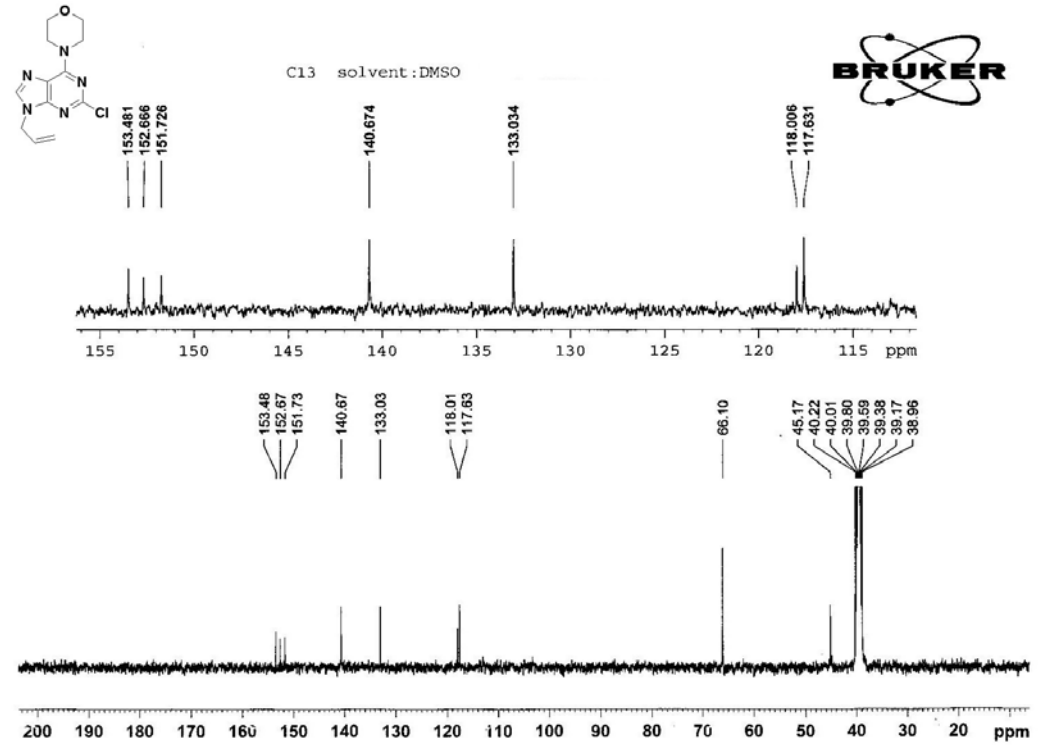

1H solvent:DMSO
8.268
4.433
4.417
4.401
3.719
3.709
3.699
3.333
3.137
3.121
3.105
2.490
2.486
2.482
10 9 8 7 6 5 4 3 2 1 ppm
0.96
2.32
6.00
1.90

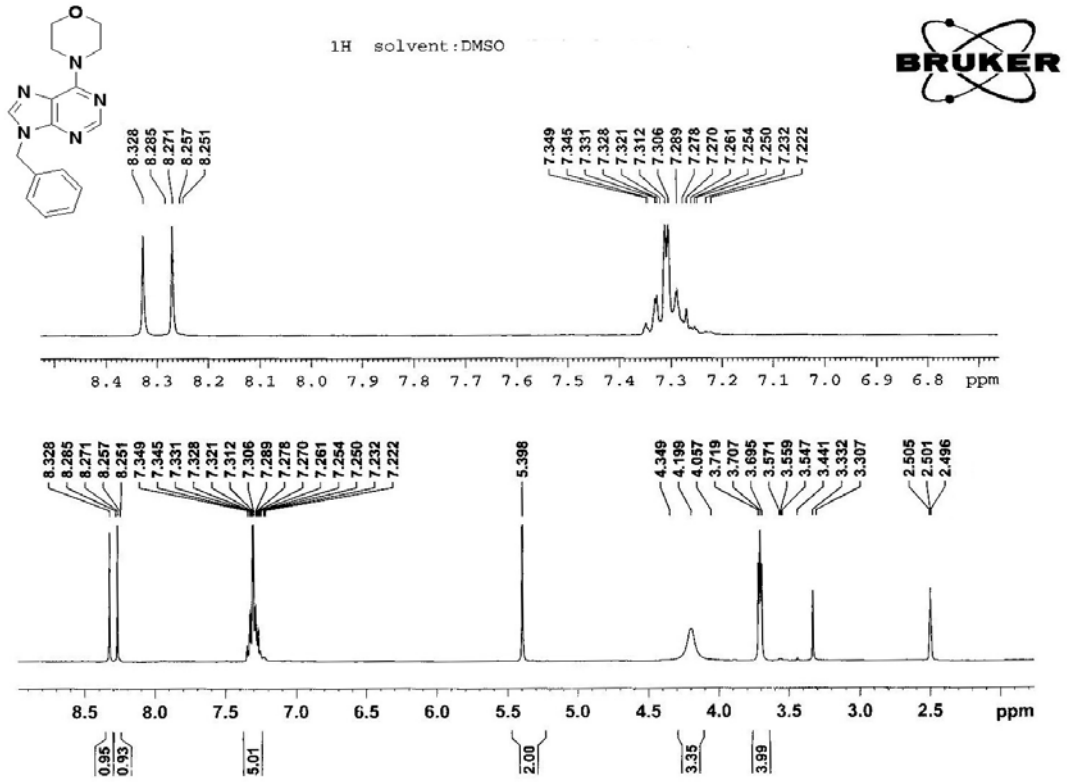

C13 solvent:DMSO
153.581
152.861
151.862
139.153
118.413
118.164
66.231
160 150 140 130 120 ppm
74 72 70 68 66 64 62 ppm
153.58
152.86
151.86
139.15
118.41
118.16
66.23
45.21
40.38
40.17
39.96
39.76
39.55
39.34
39.13
18.30
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

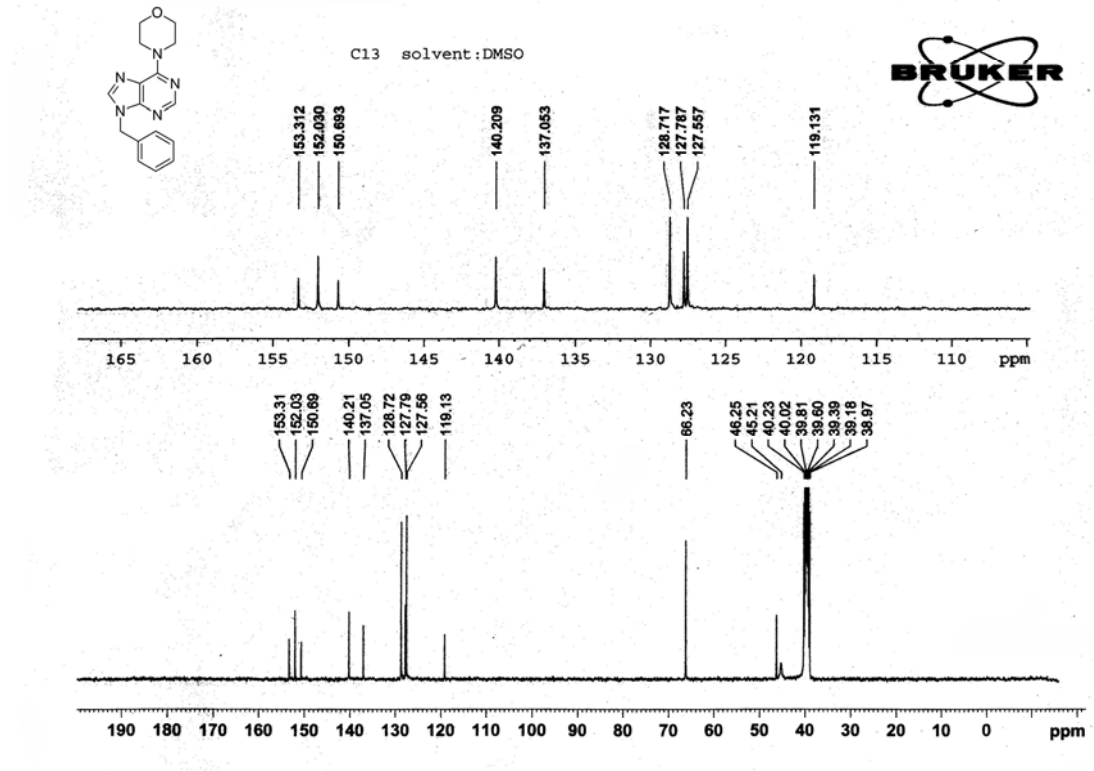

1H solvent:DMSO
BRUKER
6.088
6.075
6.062
6.046
6.032
6.020
6.006
5.199
5.173
5.049
5.046
5.006
5.003
4.817
4.803
4.205
4.103
4.090
4.077
4.065
3.728
3.715
3.704
6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 ppm
8.259
8.245
8.176
6.102
6.088
6.075
6.062
6.046
6.032
6.020
6.006
5.199
5.173
5.049
5.046
5.006
5.003
4.817
4.803
4.205
4.103
4.090
4.077
4.065
3.728
3.715
3.704
3.315
3.291
3.175
3.162
2.504
2.500
2.496
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.00
1.33
1.03
1.07
1.10
2.16
3.73
4.32

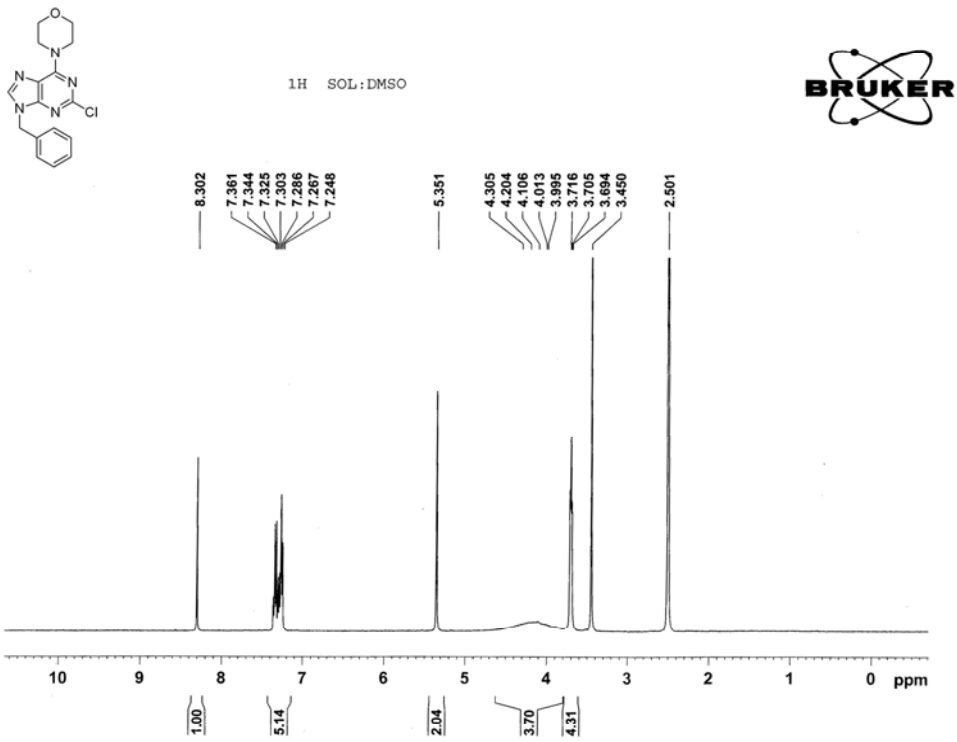

C13 solvent:DMSO
BRUKER
153.313
151.915
150.616
140.111
133.352
119.064
117.525
155 150 145 140 135 130 125 120 ppm
153.31
151.92
150.62
140.11
133.35
119.06
117.53
66.24
45.01
40.23
40.02
39.81
39.60
39.39
39.18
38.97
170 160 150 140 130 120 110 100 90 80 70 60 50 40 ppm

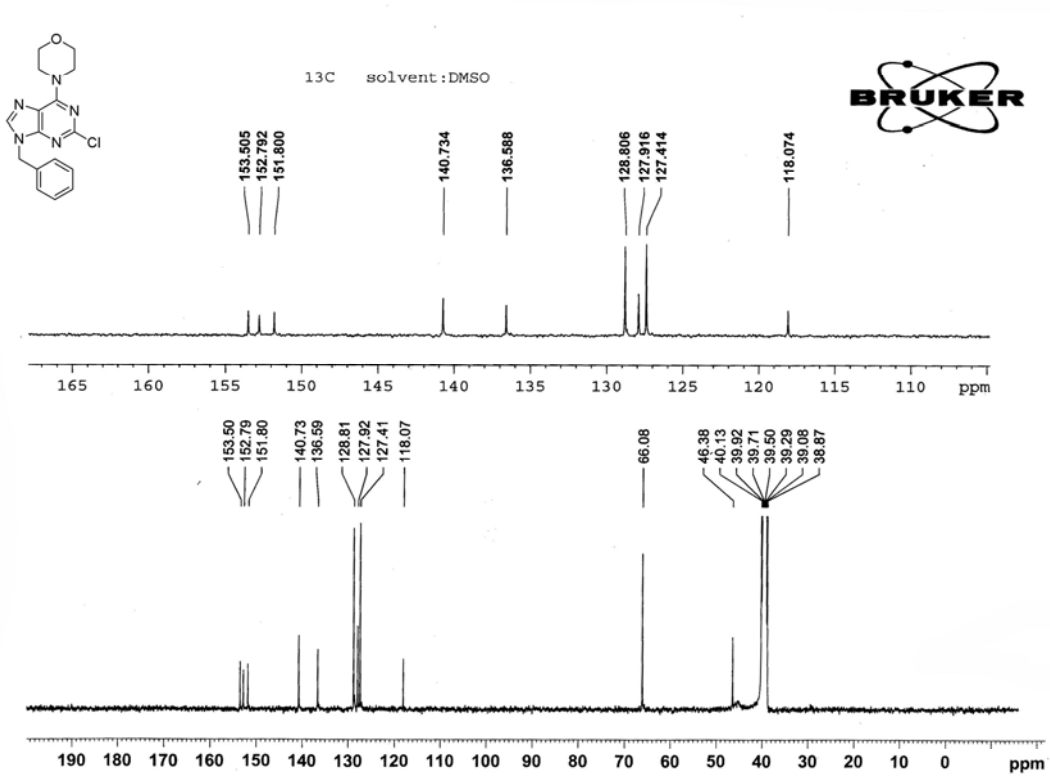

1H solvent:DMSO
BRUKER
6.087
6.073
6.060
6.047
6.030
6.017
6.005
5.991
5.214
5.212
5.189
5.186
5.033
5.030
4.990
4.987
4.775
4.762
4.585
4.461
4.424
4.250
4.159
ppm
8.188
4.135
4.115
4.106
3.898
3.771
3.730
3.718
3.707
3.537
3.324
3.173
3.161
2.504
2.500
2.496
1.00
0.99
1.01
1.05
2.11
2.39
4.24

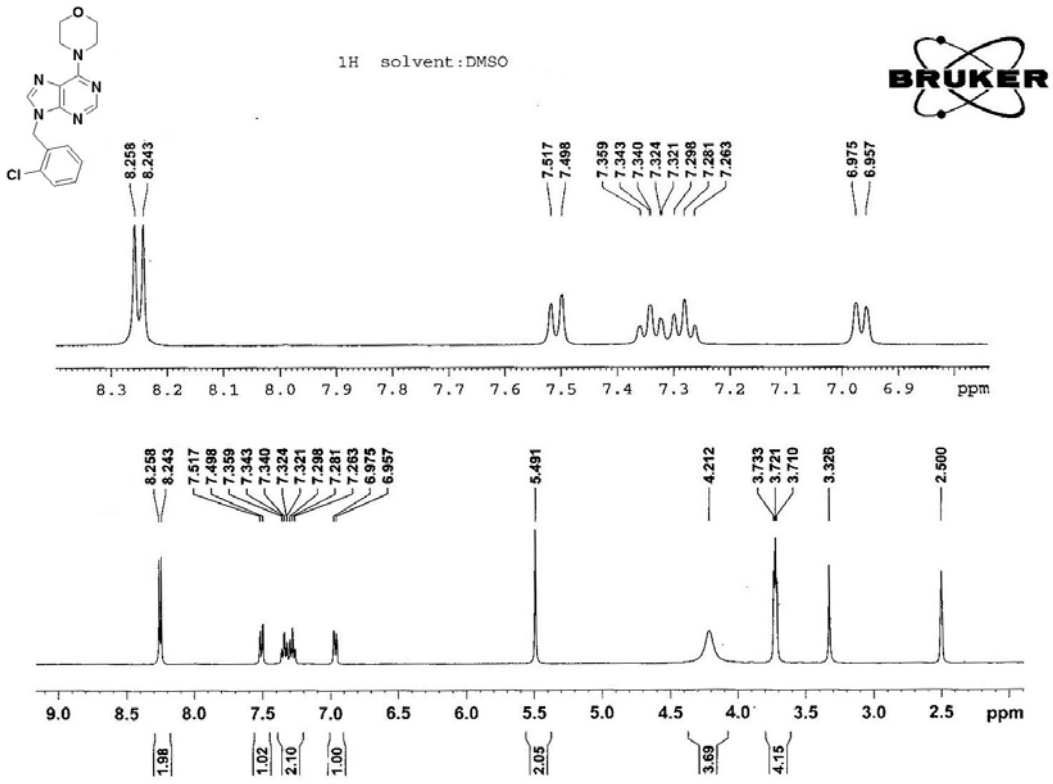

C13 solvent:DMSO
BRUKER
153.481
152.666
151.726
140.674
133.034
118.006
117.631
ppm
153.48
152.67
151.73
140.67
133.03
118.01
117.63
66.10
45.17
40.22
40.01
39.80
39.59
39.38
39.17
38.96

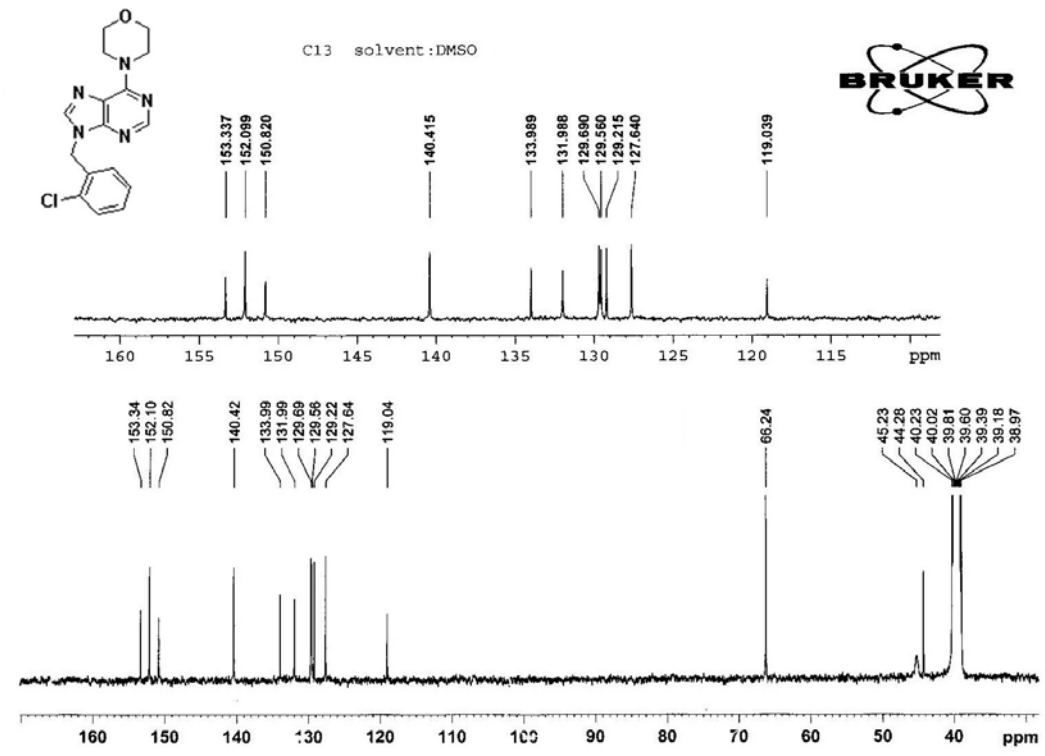

1H solvent:DMSO
BRUKER
8.328
8.285
8.271
8.257
8.251
7.349
7.345
7.331
7.328
7.321
7.312
7.306
7.289
7.278
7.270
7.261
7.254
7.250
7.232
7.222
5.398
4.349
4.199
4.057
3.719
3.707
3.695
3.571
3.559
3.547
3.441
3.332
3.307
2.505
2.501
2.496
ppm
0.95
0.93
5.01
2.00
3.35
3.99

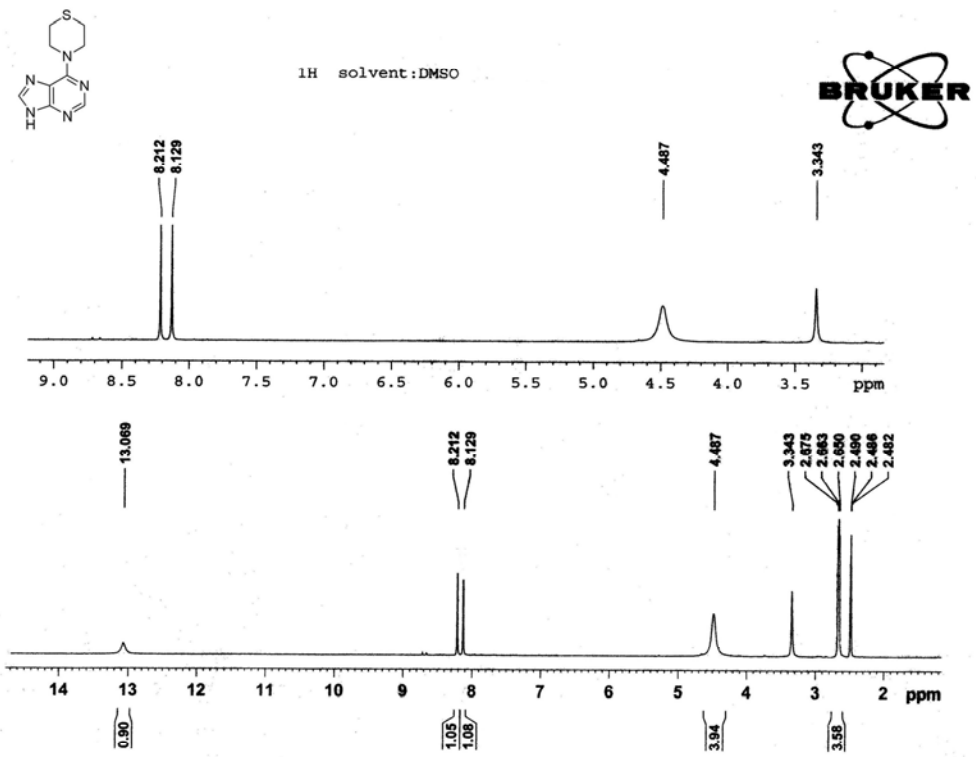

C13 solvent:DMSO
BRUKER
153.312
152.030
150.693
140.209
137.053
128.717
127.787
127.557
119.131
ppm
153.31
152.03
150.69
140.21
137.05
128.72
127.79
127.56
119.13
66.23
46.25
45.21
40.23
40.02
39.81
39.60
39.39
39.18
38.97
ppm

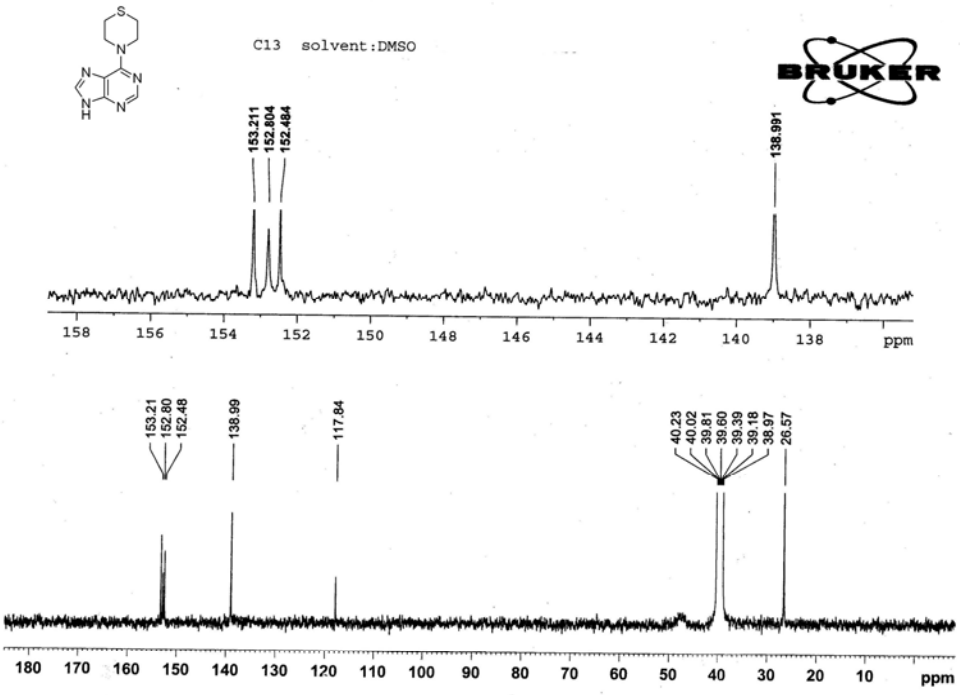

1H SOL:DMSO
BRUKER
8.302
7.361
7.344
7.325
7.303
7.286
7.267
7.248
5.351
4.305
4.204
4.106
4.013
3.995
3.716
3.705
3.694
3.450
2.501
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
5.14
2.04
3.70
4.31

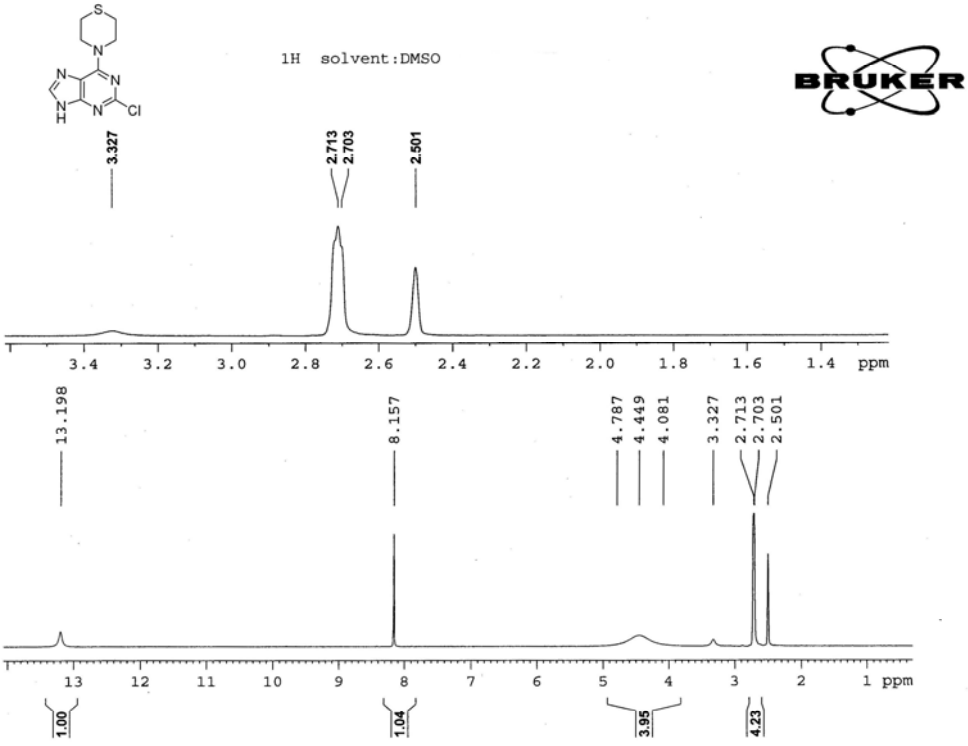

13C solvent:DMSO
BRUKER
153.505
152.792
151.800
140.734
136.588
128.806
127.916
127.414
118.074
165 160 155 150 145 140 135 130 125 120 115 110 ppm
153.50
152.79
151.80
140.73
136.59
128.81
127.92
127.41
118.07
66.08
46.38
40.13
39.92
39.71
39.50
39.29
39.08
38.87
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

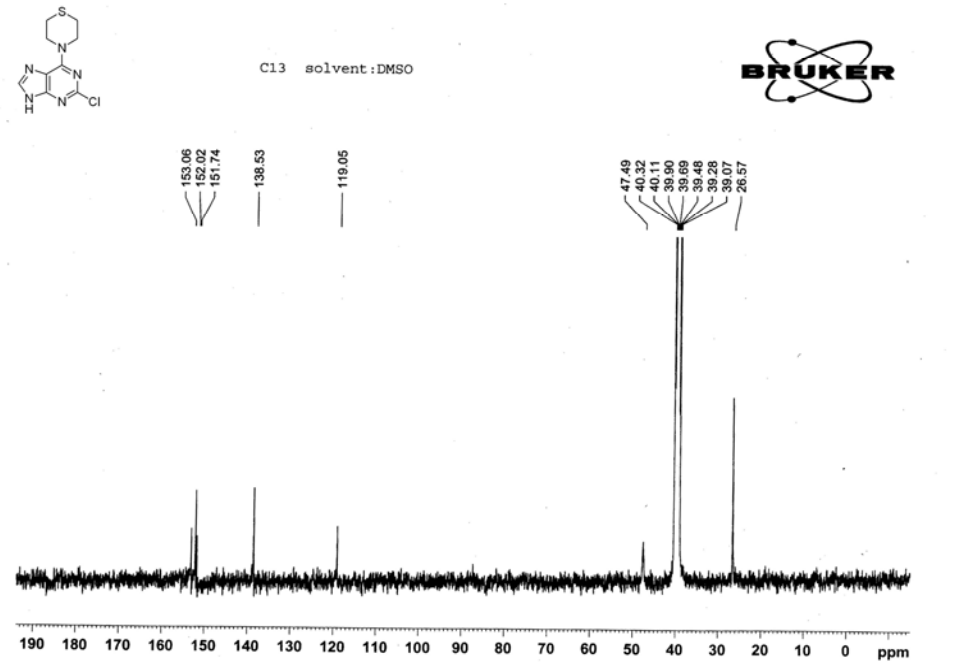

1H solvent:DMSO
BRUKER
8.258
8.243
7.517
7.498
7.359
7.343
7.340
7.324
7.321
7.298
7.281
7.263
6.975
6.957
5.491
4.212
3.733
3.721
3.710
3.326
2.500
ppm
1.98
1.02
2.10
1.00
2.05
3.69
4.15

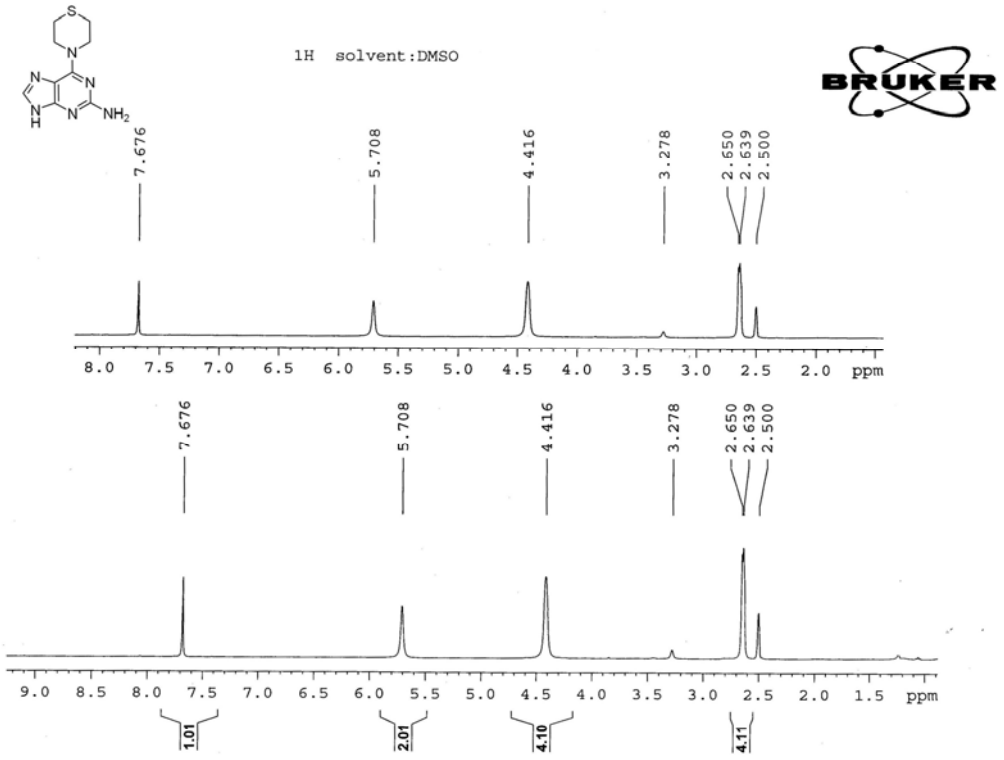

C13 solvent:DMSO
BRUKER
153.337
152.099
150.820
140.415
133.989
131.988
129.690
129.560
129.215
127.640
119.039
ppm
153.34
152.10
150.82
140.42
133.99
131.99
129.69
129.56
129.22
127.64
119.04
66.24
45.23
44.26
40.23
40.02
39.81
39.60
39.39
39.18
38.97
ppm

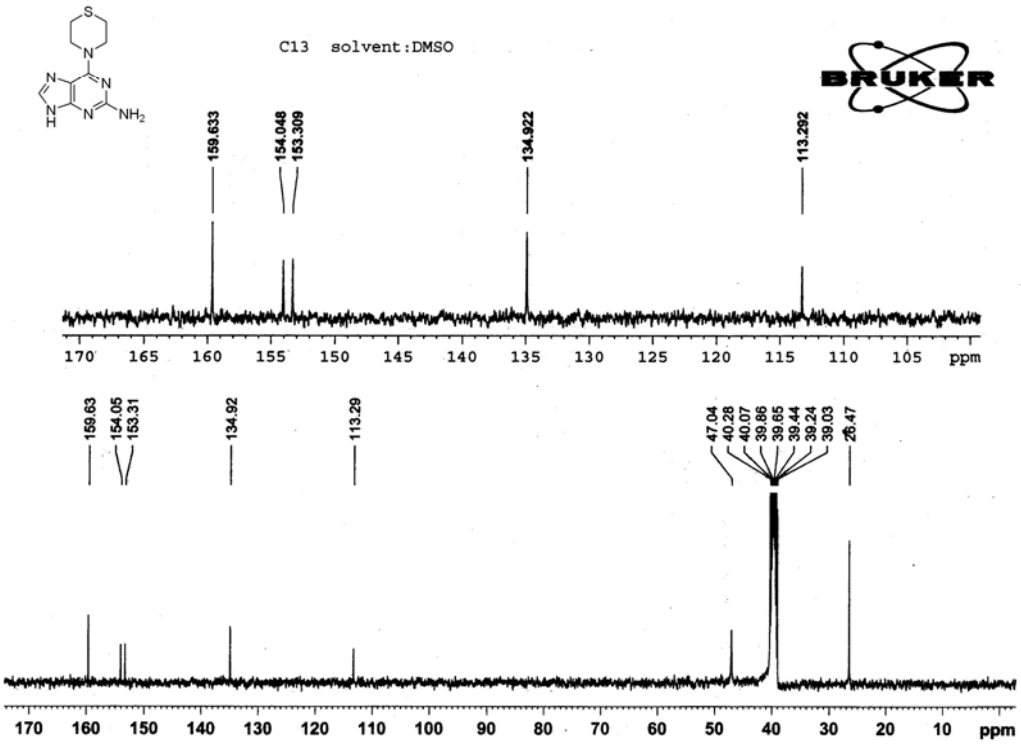

1H solvent:DMSO
BRUKER
8.212
8.129
4.487
3.343
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 ppm
13.069
8.212
8.129
4.487
3.343
2.675
2.663
2.650
2.496
2.486
2.482
14 13 12 11 10 9 8 7 6 5 4 3 2 ppm
0.90
1.05
1.08
3.94
3.56

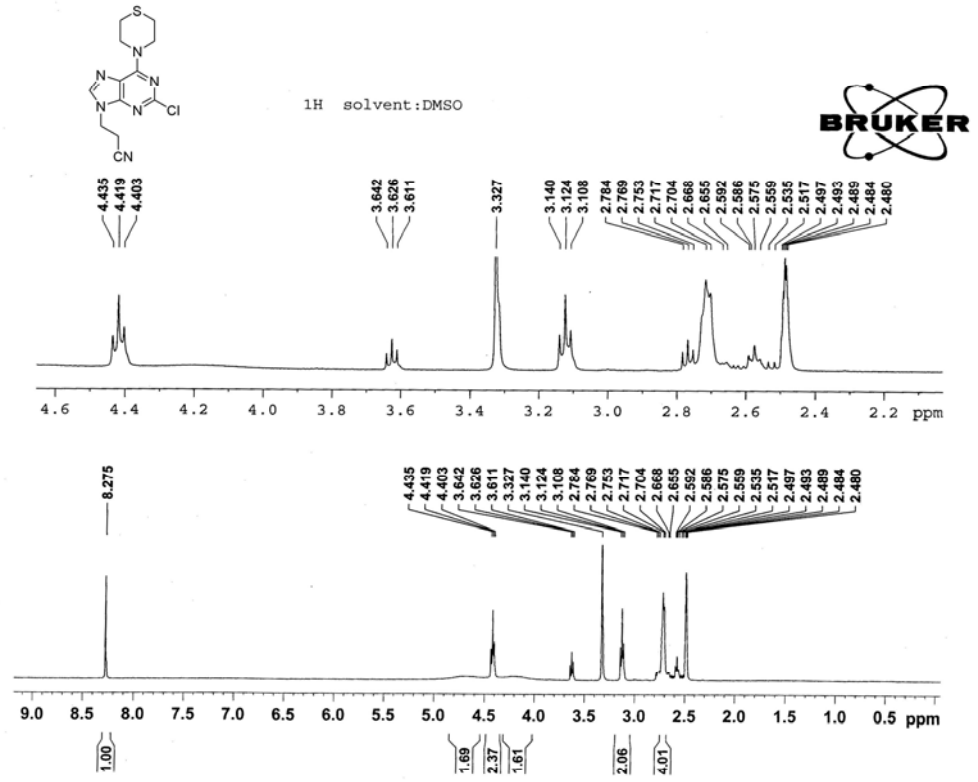

C13 solvent:DMSO
BRUKER
153.211
152.804
152.484
138.991
158 156 154 152 150 148 146 144 142 140 138 ppm
153.21
152.80
152.48
138.99
117.84
40.23
40.02
39.81
39.60
39.39
39.18
38.97
26.57
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

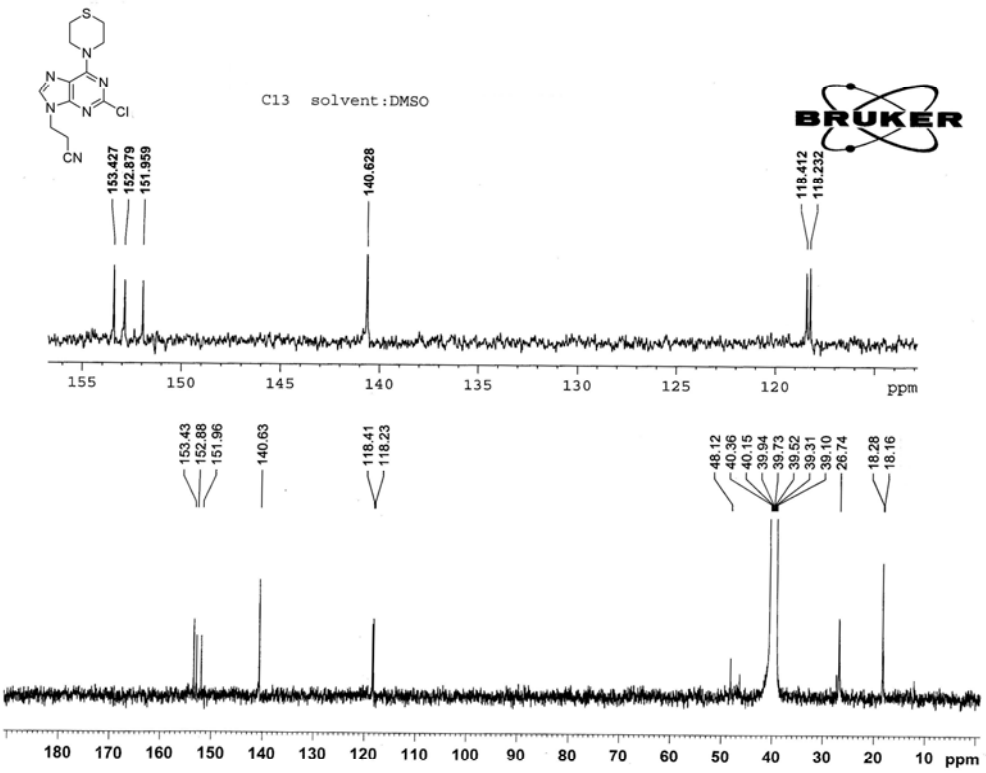

1H solvent:DMSO
BRUKER
3.327
2.713
2.703
2.501
3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 ppm
13.198
8.157
4.787
4.449
4.081
3.327
2.713
2.703
2.501
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.04
3.95
4.23

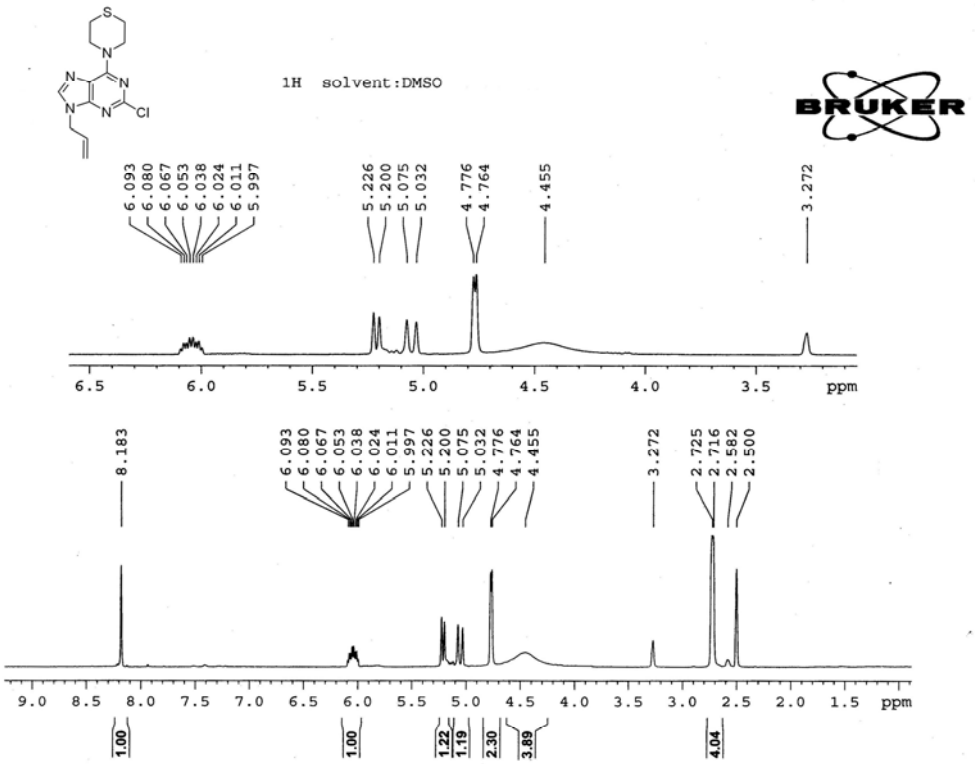

C13 solvent:DMSO
BRUKER
153.06
152.02
151.74
138.53
119.05
47.49
40.32
40.11
39.90
39.69
39.48
39.28
39.07
26.57
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

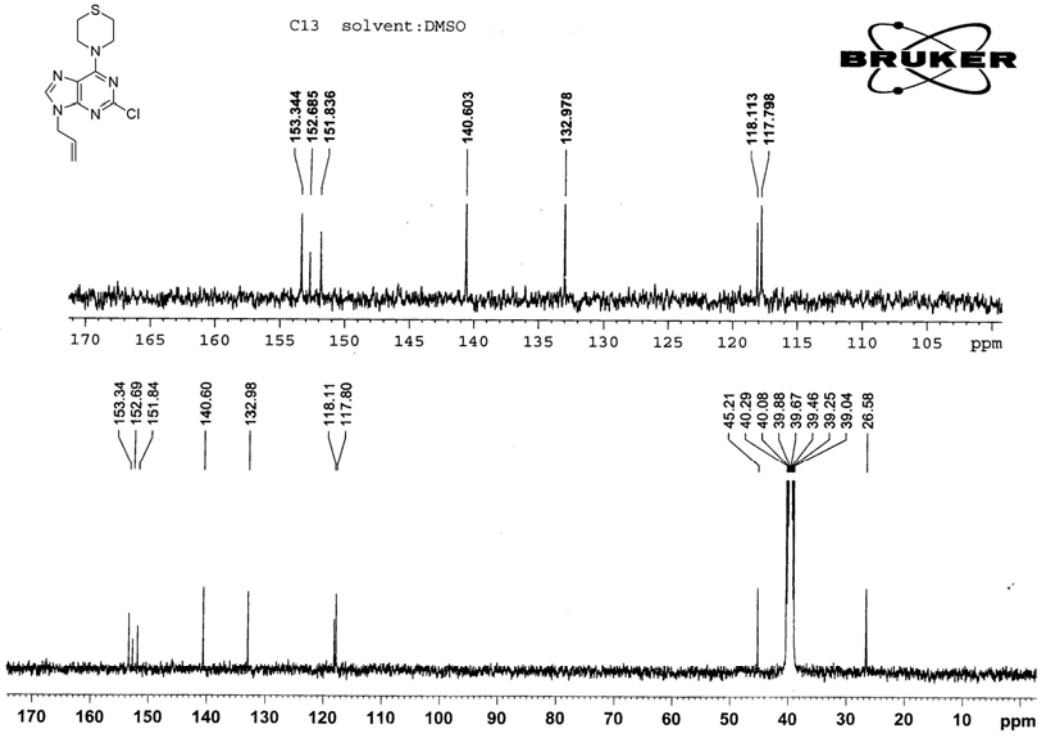

1H solvent:DMSO
BRUKER
7.676
5.708
4.416
3.278
2.650
2.639
2.500
ppm
1.01
2.01
4.10
4.11

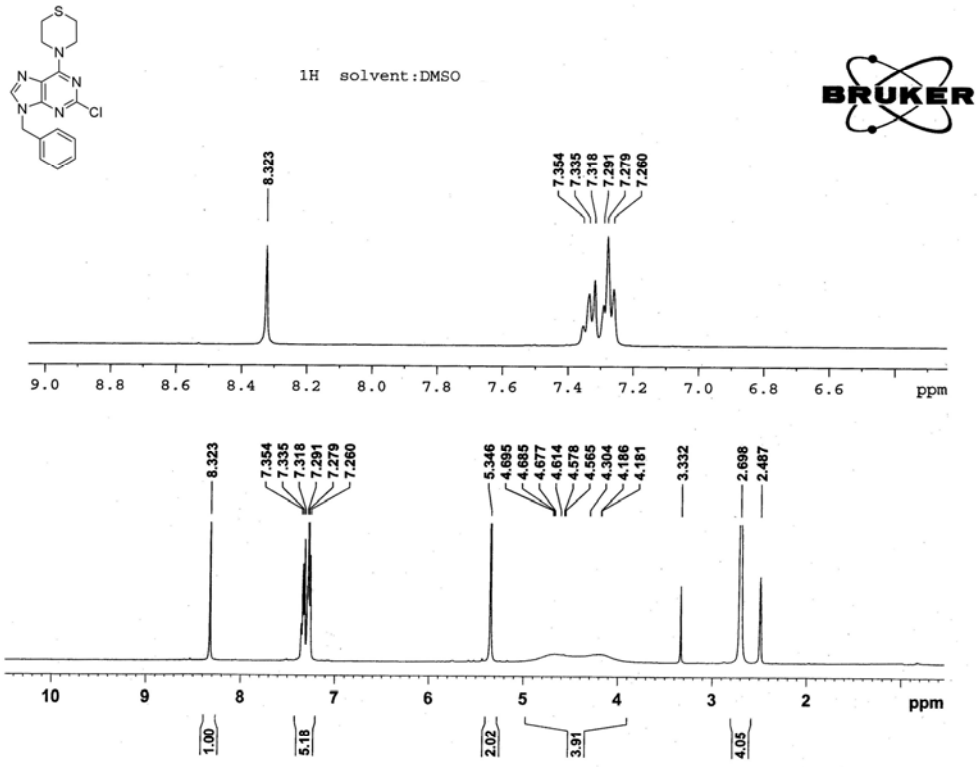

C13 solvent:DMSO
BRUKER
159.633
154.048
153.309
134.922
113.292
ppm
159.63
154.05
153.31
134.92
113.29
47.04
40.28
40.07
39.86
39.65
39.44
39.24
39.03
26.47

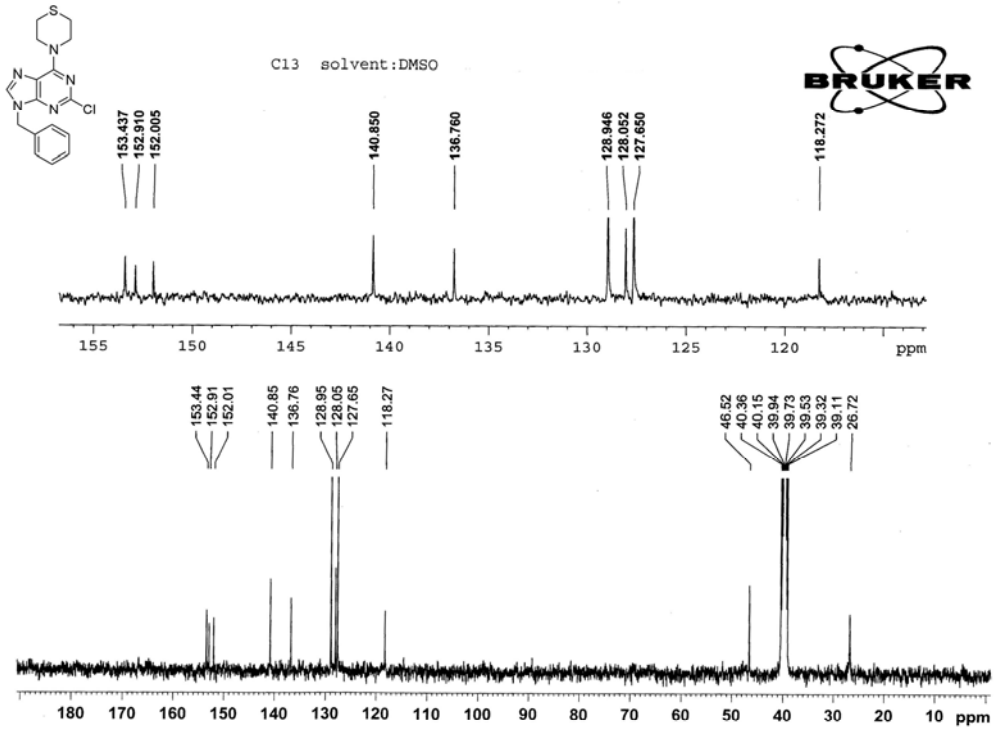

1H solvent:DMSO
BRUKER
4.435
4.419
4.403
3.642
3.626
3.611
3.327
3.140
3.124
3.108
2.784
2.769
2.753
2.717
2.704
2.668
2.655
2.592
2.586
2.575
2.559
2.535
2.517
2.497
2.493
2.489
2.484
2.480
8.275
ppm
1.00
1.69
2.37
1.61
2.06
4.01


C13 solvent:DMSO
BRUKER
153.427
152.879
151.959
140.628
118.412
118.232
ppm
153.43
152.88
151.96
140.63
118.41
118.23
48.12
40.36
40.15
39.94
39.73
39.52
39.31
39.10
26.74
18.28
18.16
ppm


1H solvent:DMSO
BRUKER
6.093
6.080
6.067
6.053
6.038
6.024
6.011
5.997
5.226
5.200
5.075
5.032
4.776
4.764
4.455
3.272
8.183
2.725
2.716
2.582
2.500
ppm
1.00
1.00
1.22
1.19
2.30
3.89
4.04


C13 solvent:DMSO
BRUKER
153.344
152.685
151.836
140.603
132.978
118.113
117.798
153.34
152.69
151.84
140.60
132.98
118.11
117.80
45.21
40.29
40.08
39.88
39.67
39.46
39.25
39.04
26.58
ppm


1H solvent:DMSO
BRUKER
8.323
7.354
7.335
7.318
7.291
7.279
7.260
9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 ppm
8.323
7.354
7.335
7.318
7.291
7.279
7.260
5.346
4.695
4.685
4.677
4.614
4.578
4.565
4.304
4.186
4.181
3.332
2.698
2.487
10 9 8 7 6 5 4 3 2 ppm
1.00
5.18
2.02
3.91
4.05


C13 solvent:DMSO
BRUKER
153.437
152.910
152.005
140.850
136.760
128.946
128.052
127.650
118.272
155 150 145 140 135 130 125 120 ppm
153.44
152.91
152.01
140.85
136.76
128.95
128.05
127.65
118.27
46.52
40.36
40.15
39.94
39.73
39.53
39.32
39.11
26.72
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm