Supplementary Information

Novel 4-aminoquinoline-pyrimidine based hybrids with improved *in vitro* and *in vivo* antimalarial activity

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List of Contents

Experimental

Chemistry

All of the chemicals used in the synthesis were purchased from Sigma-Aldrich and were used as such. Thin layer chromatography was used to monitor the progress of the reactions and checked by precoated TLC plates (E. Merck Kieselgel 60 F_{254}) with spots being visualized by iodine vapors. Compounds were purified over silica gel (60-120 mesh) column or recrystallized with suitable solvents. Solvents were distilled before using for purification purposes. Meting points were recorded on an ERS automated melting point apparatus and are uncorrected. IR spectra were recorded using Perkin-Elmer and Bruker FT-IR and the values are expressed as λ_{max} cm^{-1}. Mass spectral data were recorded on a Jeol-AccuTOF JMS-T100LC and micromass LCT Mass Spectrometer/Data system. The ^{1}H NMR and ^{13}C NMR spectra were recorded on Jeol Spectrospin spectrometer at 400 MHz and 100 MHz respectively using TMS as an internal standard. The chemical shift values are recorded on δ scale and the coupling constants (J) are in Hz. HPLC was done using Waters HPLC system, 25 cm C18 column, and a run time of 60 min.

General procedure for the synthesis of compounds 6a-d and 7a-d

To a well stirred solution of 2,4-dichloro-6-methyl-pyrimidine (2.0 g, 12.2 mmol) and triethylamine (2.48 g, 24.5 mmol) in ethanol (50 ml) at room temperature was added diamines **5a-d** (12.2 mmol). The reaction mixture was allowed to stir overnight at room temperature. After completion of reaction as evident by TLC, reaction mixture was poured into ice cold water (250 ml) and precipitate thus formed was filtered and washed with excess of water at vaccum pump. The crude precipitate was then dried, dissolved in 100 ml of $CHCl_3$ and extracted with water (2 × 500 ml) and finally with brine. Excess of solvent was evaporated to dryness under vaccum and the crude product thus obtained was purified by SiO_2 column using MeOH/$CHCl_3$ as eluent to yield respective compounds **6a-d** and **7a-d**.

N-(2-chloro-6-methyl-pyrimidin-4-yl)-N'-(7-chloro-quinolin-4-yl)-ethane-1,2-diamine (6a): White solid; Yield: 75 %; mp 220-222 ^{o}C; IR (cm^{-1}, KBr): 3269, 2954, 1581, 1434, 1234, 1105, 848; ^{1}H NMR (400 MHz, DMSO-d_6): 2.20 (s, 3H), 3.39-3.46 (m, 4H), 6.57 (s, 1H), 6.71 (d, 1H, J = 5.5 Hz), 7.37 (brs, 1H), 7.41 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.65 (brs, 1H), 7.74 (d, 1H, J = 2.3 Hz), 8.15 (d, 1H, J = 8.7 Hz), 8.37 (d, 1H, J = 5.5 Hz); ESI-MS

(m/z): 348.10 $(M+H)^+$; Anal. Calcd for $C_{16}H_{15}Cl_2N_5$: C, 55.19; H, 4.34; N, 20.11; Found: C, 55.28; H, 4.30; N, 20.13. HPLC purity: 98.6 %

N-(2-Chloro-6-methyl-pyrimidin-4-yl)-N'-(7-chloro-quinolin-4-yl)-propane-1,3-diamine (6b): Pale yellow solid; Yield: 78 %; mp 192-194 ^oC; IR (cm^{-1}, KBr): 3263, 3062, 2963, 1583, 1363, 1280, 1100, 848; ^1H NMR (400 MHz, DMSO-d_6): 1.88 (quin, 2H), 2.18 (s, 3H), 3.28-3.33 (m, 4H), 6.44 (d, 1H, J = 5.4 Hz), 6.53 (s, 1H), 7.28 (brs, 1H), 7.42 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.63 (brs, 1H), 7.75 (d, 1H, J = 2.3 Hz), 8.23 (d, 1H, J = 9.1 Hz), 8.35 (d, 1H, J = 5.5 Hz); ^{13}C NMR (100 MHz, DMSO-d_6): 24.48, 28.16, 39.80, 41.05, 99.58, 108.78, 118.39, 124.94, 124.98, 128.39, 134.30, 149.96, 150.94, 152.76, 160.84, 163.03, 170.59; ESI-MS (m/z): 362.11 $(M+H)^+$; Anal. Calcd for $C_{17}H_{17}Cl_2N_5$: C, 56.36; H, 4.73; N, 19.33 Found: C, 56.42; H, 4.74; N, 19.38; HPLC purity: 98.4 %

N-(2-Chloro-6-methyl-pyrimidin-4-yl)-N'-(7-chloro-quinolin-4-yl)-butane-1,4-diamine (6c): White solid; Yield: 70 %; mp 156-158 ^oC; IR (cm^{-1}, KBr): 3286, 2955, 1581, 1367, 1290, 1137, 1102, 871; ^1H NMR (400 MHz, $CDCl_3$): 1.73-1.87 (m, 4H), 2.28 (s, 3H), 3.37 (q, 2H), 3.52 (q, 2H), 5.13 (brs, 1H), 5.30 (brs, 1H), 6.41 (d, 1H, J = 5.5 Hz), 6.45 (s, 1H), 7.34 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.66 (d, 1H, J = 8.7 Hz), 7.95 (d, 1H, J = 2.3 Hz), 8.52 (d, 1H, J = 5.5 Hz); ESI-MS (m/z): 376.33 $(M+H)^+$; Anal. Calcd for $C_{18}H_{19}Cl_2N_5$: C, 57.45; H, 5.09; N, 18.61 Found: C, 57.39; H, 5.16; N, 18.62; HPLC purity: 99.0 %

N-(2-Chloro-6-methyl-pyrimidin-4-yl)-N'-(7-chloro-quinolin-4-yl)-hexane-1,6-diamine (6d): Off white solid; Yield: 80 %; mp 103-105 ^oC; IR (cm^{-1}, KBr): 3277, 3065, 2937, 1581, 1366, 1291, 1078, 849, 797; ^1H NMR (400 MHz, $CDCl_3$): 1.45-1.55 (m, 4H), 1.60-1.67 (m, 2H), 1.73-1.81 (m, 2H), 2.29 (s, 3H), 3.31 (q, 4H), 3.43 (q, 4H), 4.96 (brs, 1H), 5.14 (brs, 1H), 6.41 (d, 1H, J = 5.5 Hz), 6.43 (s, 1H), 7.36 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.65 (d, 1H, J = 8.7 Hz), 7.96 (d, 1H, J = 2.3 Hz), 8.53 (d, 1H, J = 5.5 Hz); ESI-MS (m/z): 404.11 $(M+H)^+$; Anal. Calcd for $C_{20}H_{23}Cl_2N_5$: C, 59.41; H, 5.73; N, 17.32 Found: C, 59.44; H, 5.71; N, 17.31; HPLC purity: 97.1 %

N-(4-chloro-6-methyl-pyrimidin-2-yl)-N'-(7-chloro-quinolin-4-yl)-ethane-1,2-diamine (7a): White solid; Yield: 22 %; mp 208-210 ^oC; IR (cm^{-1}, KBr): 3257, 2969, 1584, 1432, 1368, 1248, 1140, 973; ^1H NMR (400 MHz, DMSO-d_6): 2.13 (s, 3H), 3.41-3.48 (m, 4H), 6.25 (s, 1H), 6.70 (d, 1H, J = 5.4 Hz), 7.32 (brs, 1H), 7.41 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.74 (d, 1H, J = 2.3 Hz), 7.91 (brs, 1H), 8.16 (d, 1H, J = 8.7 Hz), 8.37 (d, 1H, J = 5.5 Hz); ^{13}C NMR (100 MHz, DMSO-d_6): 22.87, 38.29, 41.33, 98.89, 102.94, 117.44, 124.00, 124.17, 127.42, 133.49, 148.95, 150.11, 151.80, 159.46, 164.05, 165.43; ESI-MS (m/z): 348.10

$(M+H)^+$; Anal. Calcd for $C_{16}H_{15}C_{l2}N_5$: C, 55.19; H, 4.34; N, 20.11; Found C, 55.15; H, 4.32; N, 20.21; HPLC purity: 98.7 %

N-(4-Chloro-6-methyl-pyrimidin-2-yl)-N'-(7-chloro-quinolin-4-yl)-propane-1,3-diamine (7b): Pale yellow solid; Yield: 15 %; mp 172-174 ^oC; IR (cm^{-1}, KBr): 3264, 3063, 2964, 1583, 1364, 1280, 1100, 863; ^1H NMR (400 MHz, DMSO-d_6): 1.89 (quin, 2H), 2.14 (s, 3H), 3.24-3.35 (m, 4H), 6.25 (s, 1H), 6.46 (d, 1H, J = 5.4 Hz), 7.28 (brs, 1H), 7.43 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.76 (d, 1H, J = 2.3 Hz), 7.81 (brs, 1H), 8.25 (d, 1H, J = 9.1 Hz), 8.37 (d, 1H, J = 9.1 Hz); ^{13}C NMR (100 MHz, DMSO-d_6): 22.85, 27.22, 38.01, 40.12, 98.71, 102.79, 117.48, 124.09, 127.46, 133.43, 149.03, 150.04, 151.84, 159.51, 164.00, 165.04, 167.75; ESI-MS (m/z): 362.12 $(M+H)^+$; Anal. Calcd for $C_{17}H_{17}C_{l2}N_5$: C, 56.36; H, 4.73; N, 19.33; Found: C, 56.37; H, 4.76; N, 19.41.

N-(4-Chloro-6-methyl-pyrimidin-2-yl)-N'-(7-chloro-quinolin-4-yl)-butane-1,4-diamine (7c): White solid; Yield: 25 %; mp 175-177 ^oC; IR (cm^{-1}, KBr): 3251, 3127, 2957, 1589, 1367, 1234, 1139, 972, 847; ^1H NMR (400 MHz, $CDCl_3$): 1.79-1.82 (m, 4H), 2.31 (s, 3H), 3.36-3.40 (m, 4H), 5.13 (brs, 1H), 5.30 (brs, 1H), 6.06 (s, 1H), 6.39 (d, 1H, J = 5.5 Hz), 7.35 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.66 (d, 1H, J = 8.7 Hz), 7.95 (d, 1H, J = 2.3 Hz), 8.51 (d, 1H, J = 5.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 22.71, 24.83, 25.97, 41.88, 97.93, 102.13, 116.81, 122.29, 123.74, 127.18, 133.63, 148.36, 149.67, 151.09, 159.26, 163.55, 164.25; ESI-MS (m/z): 376.16 $(M+H)^+$; Anal. Calcd for $C_{18}H_{19}C_{l2}N_5$: C, 57.45; H, 5.09; N, 18.61; Found: C, 57.50; H, 5.10; N, 18.67.

N-(4-Chloro-6-methyl-pyrimidin-2-yl)-N'-(7-chloro-quinolin-4-yl)-hexane-1,6-diamine (7d): White solid; Yield: 18 %; mp 99-101 ^oC; IR (cm^{-1}, KBr): 3108, 2941, 1580, 1366, 1280, 1221, 1163, 972; ^1H NMR (400 MHz, $CDCl_3$): 1.41-1.53 (m, 4H), 1.59-1.67 (m, 2H), 1.73- 1.79 (m, 2H), 2.30 (s, 3H), 3.27-3.32 (m, 4H), 4.97 (brs, 1H), 5.16 (brs, 1H), 6.04 (s, 1H), 6.39 (d, 1H, J = 5.5 Hz), 7.34 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.64 (d, 1H, J = 8.7 Hz), 7.94 (d, 1H, J = 2.3 Hz), 8.51 (d, 1H, J = 5.5 Hz); ESI-MS (m/z): 404.38 $(M+H)^+$; Anal. Calcd for $C_{20}H_{23}C_{l2}N_5$: C, 59.41; H, 5.73; N, 17.32; Found: C, 59.35; H, 5.80; N, 17.31; HPLC purity: 98.1 %

General Procedure for the synthesis of compounds 8a-n

In a 100 ml round bottom flask, compound **6a-d** (1 eq.) was taken and dissolved in 10 ml of DMF. To this, a solution of respective amine (3 eq.) in DMF (5 ml) was added dropwise. Reaction mixture was allowed to stir at 100-120 ^oC for 10 hours monitored by TLC. After completion, water (50 ml) was added to reaction mixture and it was extracted with EtOAc (2 × 25 ml). Organic layer was then collected, washed with water (2 × 100 ml) and brine, dried

over Na_2SO_4 and finally excess of solvent was evaporated under vaccum. The crude residue thus obtained was purified by SiO_2 column using MeOH/$CHCl_3$ as eluent to afford respective compounds **8a-n.**

N-(7-chloro-quinolin-4-yl)-N'-(6-methyl-2-piperidin-1-yl-pyrimidin-4-yl)-ethane-1,2-diamine (8a): White solid. Yield: 85 %; mp 177-179 ^oC; IR (cm^{-1}, KBr): 3385, 3344, 2941, 1580, 1447, 1331, 1237, 1141, 790; ^1H NMR (400 MHz, DMSO-d_6): 1.36-1.49 (m, 6H), 2.02 (s, 3H), 3.31-3.41 (m, 8H), 5.85 (s, 1H), 6.56-6.72 (m, 2H), 7.34 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.41 (brs, 1H), 7.68 (d, 1H, J =2.3 Hz); 8.07 (d, 1H, J = 8.7 Hz), 8.28 (d, 1H, J = 5.5 Hz); ESI-MS (m/z): 397.22 $(M+H)^+$; Anal. Calcd for $C_{21}H_{25}ClN_6$: C, 63.55; H, 6.35; N, 21.17; Found: C, 63.53; H, 6.39; N, 21.26; HPLC purity: 99.7 %

N-(7-Chloro-quinolin-4-yl)-N'-(6-methyl-2-piperidin-1-yl-pyrimidin-4-yl)-propane-1,3-diamine (8b): Pale yellow solid; Yield: 82 %; mp 194-196 ^oC; IR (cm^{-1}, KBr): 3241, 3079, 1940, 1615, 1587, 1361, 1208, 1001, 804; ^1H NMR (400 MHz, $CDCl_3$): 1.46-1.56 (m, 6H), 1.87 (quin, 2H), 2.16 (s, 3H), 3.36 (q, 2H), 4.45 (t, 4H), 3.49 (q, 2H), 4.86 (brs, 1H), 5.72 (s, 1H), 5.92 (brs, 1H), 6.32 (d, 1H, J = 5.4 Hz), 7.22 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.66 (d, 1H, J = 8.7 Hz), 7.85 (d, 1H, J = 2.3 Hz), 8.41 (d, 1H, J = 5.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 24.36, 24.67, 25.45, 29.06, 38.55, 40.34, 44.89, 92.36, 98.86, 117.43, 121.55, 124.83, 128.53, 134.63, 149.18, 149.91, 151.96, 162.42, 162.84, 165.62; ESI-MS (m/z): 411.23 $(M+H)^+$; Anal. Calcd for $C_{22}H_{27}ClN_6$: C, 64.30; H, 6.62; N, 20.45; Found: C, 64.42; H, 6.68; N, 20.41; HPLC purity: 99.1 %

N-(7-Chloro-quinolin-4-yl)-N'-(6-methyl-2-piperidin-1-yl-pyrimidin-4-yl)-butane-1,4-diamine (8c): White solid; Yield: 88 %; mp 187-189 ^oC; IR (cm^{-1}, KBr): 3247, 3067, 2935, 1581, 1364, 1210, 1079, 848; ^1H NMR (400 MHz, $CDCl_3$): 1.49-1.65 (m, 6H), 1.73-1.79 (m, 2H), 1.83-1.89 (m, 2H), 2.17 (s, 3H), 3.35 (q, 2H), 3.45-3.52 (m, 6H), 4.79 (brs, 1H), 5.25 (brs, 1H), 5.76 (s, 1H), 6.38 (d, 1H, J = 5.5 Hz), 7.31 (dd, 1H, J = 11.0 Hz, 2.0 Hz), 7.63 (d, 1H, J = 8.7 Hz), 7.93 (d, 1H, J = 2.3 Hz), 8.50 (d, 1H, J = 5.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 24.09, 24.67, 25.43, 25.75, 27.64, 40.64, 43.02, 44.87, 91.91, 98.92, 117.14, 121.21, 125.04, 128.56, 134.66, 149.05, 149.76, 151.93, 162.17, 162.90, 165.67; ESI-MS (m/z): 425.31 $(M+H)^+$; Anal. Calcd for $C_{23}H_{29}ClN_6$: C, 65.00; H, 6.88; N, 19.78; Found: C, 64.98; H, 6.90; N, 19.81; HPLC purity: 97.9 %

N-(7-Chloro-quinolin-4-yl)-N'-(6-methyl-2-piperidin-1-yl-pyrimidin-4-yl)-hexane-1,6-diamine (8d): Light brown solid; Yield: 82 %; mp 97-99 ^oC; IR (cm^{-1}, KBr): 3314, 2933, 1579, 1368, 1232, 1134, 983, 853, 789; ^1H NMR (400 MHz, $CDCl_3$): 1.47-1.64 (m, 12H), 1.72-1.79 (m,2H), 2.17 (s, 3H), 3.29 (q, 2H), 3.39 (q, 2H), 3.54 (t, 4H), 4.76 (brs, 1H), 5.07

(brs, 1H), 5.74 (s, 1H), 6.39 (d, 1H, *J* = 5.5 Hz), 7.34 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.67 (d, 1H, *J* = 8.7 Hz), 7.95 (d, 1H, *J* = 2.3 Hz), 8.51 (d, 1H, *J* = 5.5 Hz); ESI-MS (m/z): 453.35 $(M+H)^+$; Anal. Calcd for $C_{25}H_{33}ClN_6$: C, 66.28; H, 7.34; N, 18.55; Found: C, 66.32; H, 7.35; N, 18.49; HPLC purity: 96.9 %

N-(7-Chloro-quinolin-4-yl)-N'-(6-methyl-2-morpholin-4-yl-pyrimidin-4-yl)-ethane-1,2-diamine (8e): Pale yellow solid; Yield: 86 %; mp 165-167 ^oC; IR (cm^{-1}, KBr): 3391, 3245, 2954, 1585, 1438, 1228, 1110, 993; ^1H NMR (400 MHz, DMSO-d_6): 2.09 (s, 3H), 3.35-3.48 (m, 8H), 3.57 (t, 4H), 5.91 (s, 1H), 6.62-6.70 (m, 2H), 7.41 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.44 (brs, 1H), 7.74 (d, 1H, *J* = 2.3 Hz), 8.14 (d, 1H, *J* = 9.1 Hz), 8.35 (d, 1H, *J* = 5.5 Hz); ESI-MS (m/z): 399.20 $(M+H)^+$; Anal. Calcd for $C_{20}H_{23}ClN_6O$: C, 60.22; H, 5.81; N, 21.07; Found: C, 60.34; H, 5.79; N, 21.09; HPLC purity: 90.8 %

N-(7-Chloro-quinolin-4-yl)-N'-(6-methyl-2-morpholin-4-yl-pyrimidin-4-yl)-propane-1,3-diamine (8f): White solid; Yield: 82 %; mp 165-167 ^oC; IR (cm^{-1}, KBr): 3233, 3063, 2954, 1576, 1366, 1247, 1123, 791; ^1H NMR (400 MHz, $CDCl_3$): 1.92 (quin, 2H), 2.20 (s, 3H), 3.39 (q, 2H), 3.47 (t, 4H), 3.52 (q, 2H), 3.66 (t, 4H), 5.22 (brs, 1H), 5.71 (s, 1H), 5.95 (brs, 1H), 6.34 (d, 1H, *J* = 5.4 Hz), 7.25 (dd, 1H, *J* = 11.0 Hz, 2.2 Hz), 7.72 (d, 1H, *J* = 8.7 Hz), 7.89 (d, 1H, *J* = 2.3 Hz), 8.44 (d, 1H, *J* = 5.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 24.10, 28.85, 38.56, 40.34, 44.09, 66.46, 92.27, 98.85, 117.35, 121.52, 124.93, 128.46, 134.73, 149.06, 149.90, 151.83, 161.87, 163.27, 165.70; ESI-MS (m/z): 413.21 $(M+H)^+$; Anal. Calcd for $C_{21}H_{25}ClN_6O$: C, 61.08; H, 6.10; N, 20.35; Found: C, 61.12; H, 6.17; N, 20.40; HPLC purity: 99.5 %

N-(7-Chloro-quinolin-4-yl)-N'-(6-methyl-2-morpholin-4-yl-pyrimidin-4-yl)-butane-1,4-diamine (8g): White solid; Yield: 80 %; mp 214-216 ^oC; IR (cm^{-1}, KBr): 3256, 3066, 2964, 1583, 1367, 1245, 1122, 994, 790; ^1H NMR (400 MHz, $CDCl_3$): 1.72-1.80 (m, 2H), 1.83-1.91 (m, 2H), 2.20 (s, 3H), 3.36 (q, 2H), 3.48 (q, 2H), 3.52 (t, 4H), 3.71 (t, 4H), 4.83 (brs, 1H), 5.19 (brs,1H), 5.75 (s, 1H), 6.40 (d, 1H, *J* = 5.5 Hz), 7.32 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.63 (d, 1H, *J* = 8.7 Hz), 7.95 (d, 1H, *J* = 2.3 Hz), 8.51 (d, 1H, *J* = 5.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 22.75, 24.18, 25.83, 41.39, 42.69, 64.93, 89.96, 97.19, 122.10, 122.28, 122.80, 126.34, 132.68, 147.77, 149.11, 150.43, 160.69, 161.99, 164.64; ESI-MS (m/z): 427.29 $(M+H)^+$; Anal. Calcd for $C_{22}H_{27}ClN_6O$: C, 61.89; H, 6.37; N, 19.68; Found: C, 61.99; H, 6.45; N, 19.70; HPLC purity: 96.2 %

N-(7-Chloro-quinolin-4-yl)-N'-(6-methyl-2-morpholin-4-yl-pyrimidin-4-yl)-hexane-1,6-diamine (8h): Pale yellow solid; Yield: 90 %; mp 107-109 ^oC; IR (cm^{-1}, KBr): 3245, 2935, 2855, 1579, 1366, 1220, 1123, 994, 789; ^1H NMR (400 MHz, $CDCl_3$): 1.44-1.46 (m, 4H),

1.55-1.62 (m, 2H), 1.69-1.74 (m, 2H), 2.20 (s, 3H), 3.27 (q, 2H), 3.36 (q, 2H), 3.54 (t, 4H), 3.78 (t, 4H), 4.88 (brs, 1H), 5.26 (brs, 1H), 5.73 (s, 1H), 6.37 (d, 1H, *J* = 5.1 Hz), 7.31 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.70 (d, 1H, *J* = 8.7 Hz), 7.93 (d, 1H, *J* = 2.2 Hz), 8.50 (d, 1H, *J* = 5.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 24.13, 26.62, 26.82, 28.66, 29.60, 41.04, 43.06, 44.09, 66.53, 91.58, 98.93, 117.07, 121.00, 125.08, 128.62, 134.67, 149.04, 149.68, 151.94, 162.00, 163.45, 166.31; ESI-MS (m/z): 456.21 $(M+H)^+$; Anal. Calcd for $C_{24}H_{31}ClN_6O$: C, 63.35; H, 6.87; N, 18.47; Found: C, 63.29; H, 6.91; N, 18.46; HPLC purity: 99.5 %

N-(7-Chloro-quinolin-4-yl)-N'-[6-methyl-2-(4-methyl-piperazin-1-yl)-pyrimidin-4-yl]-ethane-1,2-diamine (8i): White solid 83 %; Yield: ; mp 134-136 ^oC; IR (cm^{-1}, KBr): 3385, 3066, 2940, 1581, 1445, 1305, 1139, 997, 793; ^{1}H NMR (400 MHz, $CDCl_3$): 2.29 (s, 3H), 2.30 (s, 3H), 2.42 (t, 4H), 3.41 (q, 2H), 3.62 (t, 4H), 3.84 (q, 2H), 5.51 (brs, 1H), 5.87 (s, 1H), 6.30 (d, 1H, *J* = 5.5 Hz), 6.90 (brs, 1H), 7.21 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.55 (d, 1H, *J* = 8.7 Hz), 7.89 (d, 1H, *J* = 2.3 Hz), 8.46 (d, 1H, *J* = 5.5 Hz); ESI-MS (m/z): 412.26 $(M+H)^+$; Anal. Calcd for $C_{21}H_{26}ClN_7$: C, 61.23; H, 6.36; N, 23.80; Found: C, 61.18; H, 6.51; N, 23.85; HPLC purity: 99.4 %

N-(7-Chloro-quinolin-4-yl)-N'-[6-methyl-2-(4-methyl-piperazin-1-yl)-pyrimidin-4-yl]-propane-1,3-diamine (8j): Off white solid; Yield: 80 %; mp 176-178 ^oC; IR (cm^{-1}, KBr): 3257, 3065, 2938, 1580, 1369, 1236, 1142, 1001, 789; ^{1}H NMR (400 MHz, $CDCl_3$): 1.94 (quin, 2H), 2.21 (s, 3H), 2.28 (s, 3H), 2.36 (t, 4H), 3.42 (q, 2H), 3.52-3.56 (m, 6H), 5.32 (brs, 1H), 5.74 (s, 1H), 6.01 (brs, 1H), 6.37 (d, 1H, *J* = 5.4 Hz), 7.27 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.75 (d, 1H, *J* = 8.7 Hz), 7.91 (d, 1H, *J* = 2.3 Hz), 8.46 (d, 1H, *J* = 5.5 Hz); ESI-MS (m/z): 426.32 $(M+H)^+$; Anal. Calcd for $C_{22}H_{28}ClN_7$: C, 62.03; H, 6.63; N, 23.02; Found: C, 62.11; H, 6.68; N, 22.95; HPLC purity: 99.3 %

N-(7-Chloro-quinolin-4-yl)-N'-[6-methyl-2-(4-methyl-piperazin-1-yl)-pyrimidin-4-yl]-butane-1,4-diamine (8k): White solid; Yield: 87 %; mp 183-185 ^oC; IR (cm^{-1}, KBr): 3248, 3072, 2927, 1581, 1367, 1280, 1139, 997, 790; ^{1}H NMR (400 MHz, $CDCl_3$): 1.75-1.91 (m, 4H), 2.19 (s, 3H), 2.29 (s, 3H), 2.39 (t, 4H), 3.36 (q, 2H), 3.48 (q, 2H), 3.56 (t, 4H), 4.86 (brs, 1H), 5.23 (brs, 1H), 5.77 (s, 1H), 6.39 (d, 1H, *J* = 5.5 Hz), 7.32 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.64 (d, 1H, *J* = 8.7 Hz), 7.94 (d, 1H, *J* = 2.3 Hz), 8.51 (d, 1H, *J* = 5.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 24.15, 25.79, 27.65, 40.65, 43.04, 43.64, 46.10, 54.61, 92.00, 98.97, 117.12, 121.09, 125.09, 128.69, 134.67, 149.11, 149.68, 151.99, 162.13, 163.16, 166.16; ESI-MS (m/z): 440.33 $(M+H)^+$; Anal. Calcd for $C_{23}H_{30}ClN_7$: C, 62.79; H, 6.87; N, 22.28; Found: C, 62.80; H, 6.85; N, 22.30; HPLC purity: 97.0 %

N-(7-Chloro-quinolin-4-yl)-N'-[6-methyl-2-(4-methyl-piperazin-1-yl)-pyrimidin-4-yl]-hexane-1,6-diamine (8l): Light brown solid; Yield: 85 %; mp 152-154 ^{o}C; IR (cm^{-1}, KBr): 3266, 3068, 2931, 1580, 1367, 1279, 1164, 993, 789; ^{1}H NMR (400 MHz, $CDCl_3$): 1.46-1.55 (m, 4H), 1.59-1.61 (m, 2H), 1.74-1.77 (m, 2H), 2.19 (s, 3H), 2.30 (s, 3H), 2.42-2.44 (m, 4H), 3.29 (q, 2H), 3.38 (q, 2H), 3.60 (t, 4H), 4.77 (brs, 1H), 5.02 (brs, 1H), 5.75 (s, 1H), 6.40 (d, 1H, *J* = 5.5 Hz), 7.35 (dd, 1H, *J* = 11.0 Hz, 2.1 Hz), 7.66 (d, 1H, *J* = 8.7 Hz), 7.95 (d, 1H, *J* = 2.3 Hz), 8.51 (d, 1H, *J* = 5.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 24.14, 26.62, 26.82, 28.70, 29.63, 41.05, 43.10, 43.64, 46.12, 54.67, 91.72, 98.98, 117.08, 120.96, 125.14, 128.70, 134.71, 149.07, 149.67, 151.98, 162.05, 163.21, 166.09; ESI-MS (m/z): 468.32 $(M+H)^+$; Anal. Calcd for $C_{25}H_{34}ClN_7$: C, 64.15; H, 7.32; N, 20.95; Found: C, 64.09; H, 7.31; N, 20.98; HPLC purity: 99.0 %

N-(7-Chloro-quinolin-4-yl)-N'-[2-(4-ethyl-piperazin-1-yl)-6-methyl-pyrimidin-4-yl]-propane-1,3-diamine (8m): White solid; Yield: 82 %; mp 184-186 ^{o}C; IR (cm^{-1}, KBr): 3233, 2967, 2812, 1579, 1366, 1250, 1132, 998; ^{1}H NMR (400 MHz, $CDCl_3$): 1.10 (t, 3H), 1.95 (quin, 2H), 2.24 (s, 3H), 2.40-2.44 (m, 6H), 3.43 (q, 2H), 3.55-3.59 (m, 6H), 4.94 (brs, 1H), 5.78 (s, 1H), 5.92 (brs, 1H), 6.40 (d, 1H, *J* = 5.4 Hz), 7.30 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.73 (d, 1H, *J* = 8.7 Hz), 7.93 (d, 1H, *J* = 2.3 Hz), 8.49 (d, 1H, *J* = 5.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 11.86, 24.38, 29.05, 38.50, 40.31, 43.64, 52.26, 52.34, 92.35, 98.85, 117.38, 121.47, 124.84, 128.53, 134.61, 149.15, 149.84, 151.94, 162.34, 163.04, 166.03; ESI-MS (m/z): 440.16 $(M+H)^+$; Anal. Calcd for $C_{23}H_{30}ClN_7$: C, 62.79; H, 6.87; N, 22.28; Found: C, 62.75; H, 6.89; N, 22.20; HPLC purity: 99.6 %

N-(7-Chloro-quinolin-4-yl)-N'-[2-(4-ethyl-piperazin-1-yl)-6-methyl-pyrimidin-4-yl]-butane-1,4-diamine (8n): White solid; Yield: 86 %; mp 101-103 ^{o}C; IR (cm^{-1}, KBr): 3255, 2939, 2813, 1583, 1372, 1249, 1127, 994, 791; ^{1}H NMR (400 MHz, $CDCl_3$): 1.09 (t, 3H), 1.73-1.80 (m, 2H), 1.84-1.91 (m, 2H), 2.19 (s, 3H), 2.38-2.43 (m, 6H), 3.35 (q, 2H), 3.48 (q, 2H), 3.57 (t, 4H), 4.83 (brs, 1H), 5.23 (brs, 1H), 5.77 (s, 1H), 6.39 (d, 1H, *J* = 5.5 Hz), 7.31 (dd, 1H, *J* = 11.0 Hz, 2.0 Hz), 7.64 (d, 1H, *J* = 8.7 Hz), 7.94 (d, 1H, *J* = 2.3 Hz), 8.51 (d, 1H, *J* = 5.5 Hz); ESI-MS (m/z): 454.35 $(M+H)^+$; Anal. Calcd for $C_{24}H_{32}ClN_7$: C, 63.49; H, 7.10; N, 21.60; Found: C, 63.59; H, 7.18; N, 21.63; HPLC purity: 99.6 %

Assay for *in vitro* antimalarial activity and cytotoxicity

The antimalarial activity was determined by measuring plasmodial LDH activity as described earlier.[1] A suspension of red blood cells infected with D6 or W2 strain of *P. falciparum* (200

μL, with 2% parasitemia and 2% hematocrit in RPMI 1640 medium supplemented with 10% human serum and 60 μg/mL amikacin) was added to the wells of a 96- well plate containing 10 μL of serially diluted test samples. The plate was flushed with a gas mixture of 90% N_2, 5% O_2, and 5% CO_2 and incubated at 37 ºC, for 72 h in a modular incubation chamber (Billups-Rothenberg, CA). Parasitic LDH activity was determined according to the procedure of Makler and Hinrichs.[2] Briefly, 20 μL of the incubation mixture was mixed with 100 μL of the Malstat™ reagent (Flow Inc., Portland, OR) and incubated at room temperature for 30 min. Twenty microliters of a 1:1 mixture of NBT/PES (Sigma, St. Louis, MO) was then added and the plate is further incubated in the dark for 1 h. The reaction was then stopped by the addition of 100 μL of a 5% acetic acid solution. The plate was read at 650 nm. Artemisinin and chloroquine were included in each assay as antimalarial drug controls. IC_{50} values were computed from the dose response curves. To determine the selectivity index of antimalarial activity of compounds there *in vitro* cytotoxicity to mammalian cells was also determined. The assay was performed in 96-well tissue culture-treated plates as described earlier.[3] Vero cells (monkey kidney fibroblasts) or PK1(pig kidney epithelial cells) or HepG2 (human hepatoma cells) were seeded to the wells of 96-well plate at a density of 25,000 cells/well and incubated for 24 h. Samples at different concentrations were added and plates were again incubated for 48 h. The number of viable cells was determined by Neutral Red assay. IC_{50} values were obtained from dose response curves. Doxorubicin was used as a positive control for cytotoxicity.

Crystallographic Data

Single crystal X-ray diffraction intensities for compound **8f** was collected on an Oxford CCD diffractometer having Xcalibur, sapphire diffraction measurement device at 293 K, using graphite-monochromated Mo-Ka radiation (λ = 0.71073 Å).[4] The multi-scan absorption correction was applied using CrysalisPRO. The crystal structures were solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on F^2 using SHELXL97. Hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using WinGX software.[5] CCDC 838496 contains the supplementary crystallographic data for compound **8f**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

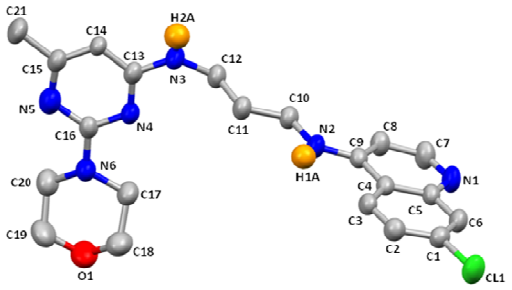


Figure 2: Crystal structure of compound **8f** with partial numbering scheme**.** Thermal ellipsoidal are drawn at 40% probability level**.** Hydrogen atoms attached only to nitrogen atoms are shown for more clarity. Selected bond lengths [Å]: C9-N2 1.344(3), C10-N2 1.452(4), C12-N3 1.449(4), C13-N3 1.351(4), C16-N4 1.340(4), C16-N6 1.379(4), C16-N5 1.403(4); Selected bond angles [deg]: N4-C16-N6 116.2(3), N6-C16-N5 122.5(3), C9-N2-C10 121.9(2), C13-N3-C12 124.1(3).

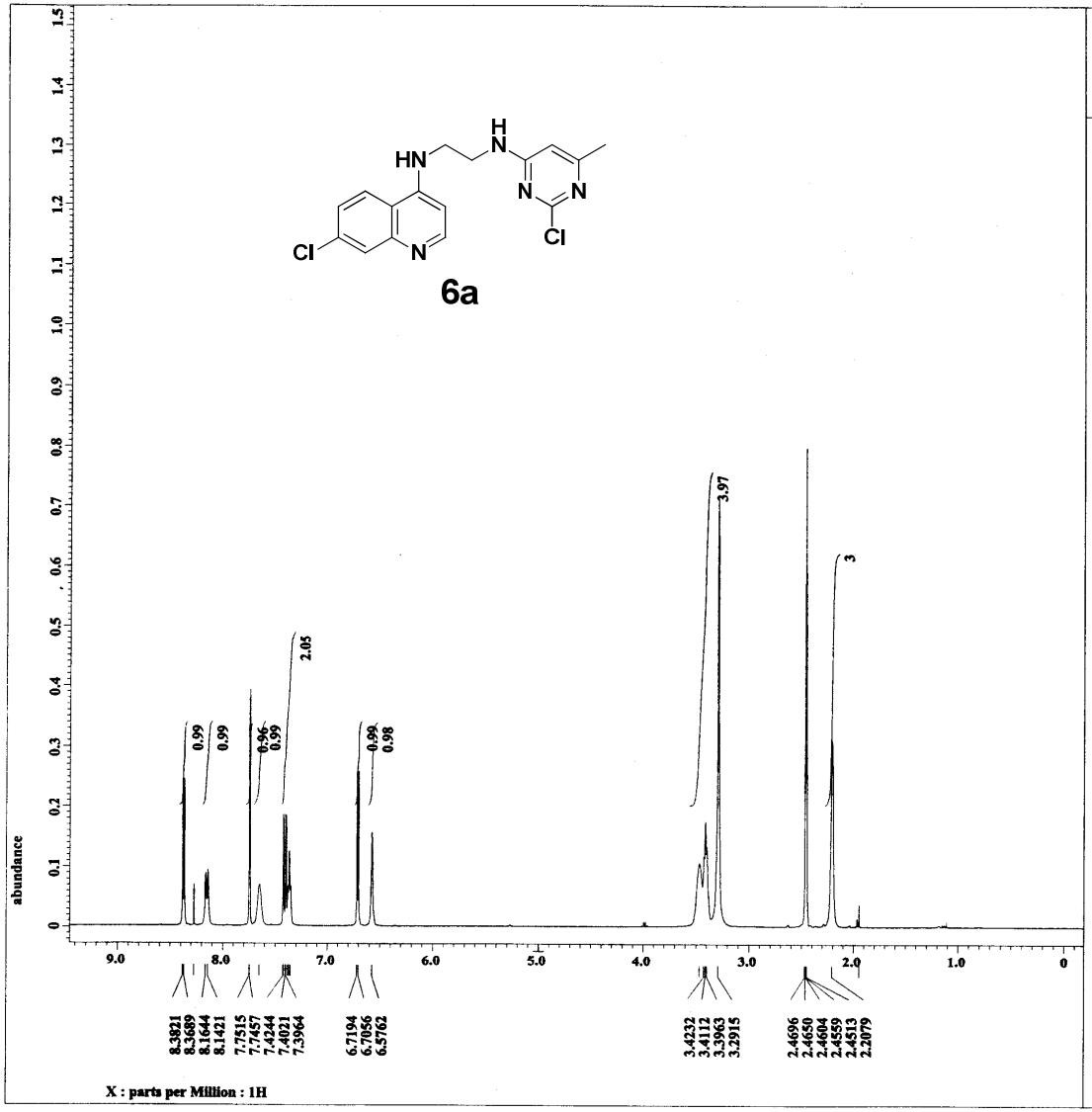
	Compound 8f
Molecular formula	$C_{21}H_{25}ClN_6O$ ($CHCl_3.H_2O$)
Formula Weight	546.27
Temperature (K)	298(2)
Crystal system	triclinic
Space group	P -1
a (Å)	9.1519(5)
b (Å)	9.4906(4)
c (Å)	16.1562(8)
α [°]	74.799(4)
β [°]	75.567(5)
γ [°]	78.317(4)
V ($Å_3$)	1297.25(11)
Z	2
d (g cm^{-3})	1.399
F(000)	564
Goodness of fit (F^2)	1.031
R_1, wR_2[I >2 (I)][a]	R_1 = 0.0686, wR_2= 0.2009
R_1, wR_2[all data][b]	R_1 = 0.0816, wR_2= 0.2174

[a] $R = \sum(||F_o| - |F_c||)/\sum|F_o|$

[b] $R_w = \{\sum[w(F^2_o - F^2_c)^2]/\sum[w(F^2_o)^2]\}^{1/2}$

References

1. M. Jain, S. I. Khan, B. L. Tekwani, M. R. Jacob, S. Singh, P. P. Singh and R. Jain, Bioorg. *Med. Chem.*, 2005, **13**, 4458-4466.
2. M. T. Makler and D. J. Hinrichs, *Am. J. Trop. Med. Hyg.*, 1993, **48**, 205-210.
3. J. Mustafa, S. I. Khan, G. Ma, L. A. Walker and I. A. Khan, *Lipids*, 2004, **39**, 167-172.
4. *CrysAlisPro*, Oxford Diffraction Ltd., version 1.171.33.49b, 2009.
5. L. J. Farrugia, *WinGX*, version 1.64, *An Integrated System of Windows Programs for the Solution, Refinement and Analysis of Single-Crystal X-ray Diffraction Data*, Department of Chemistry, University of Glasgow, 2003.



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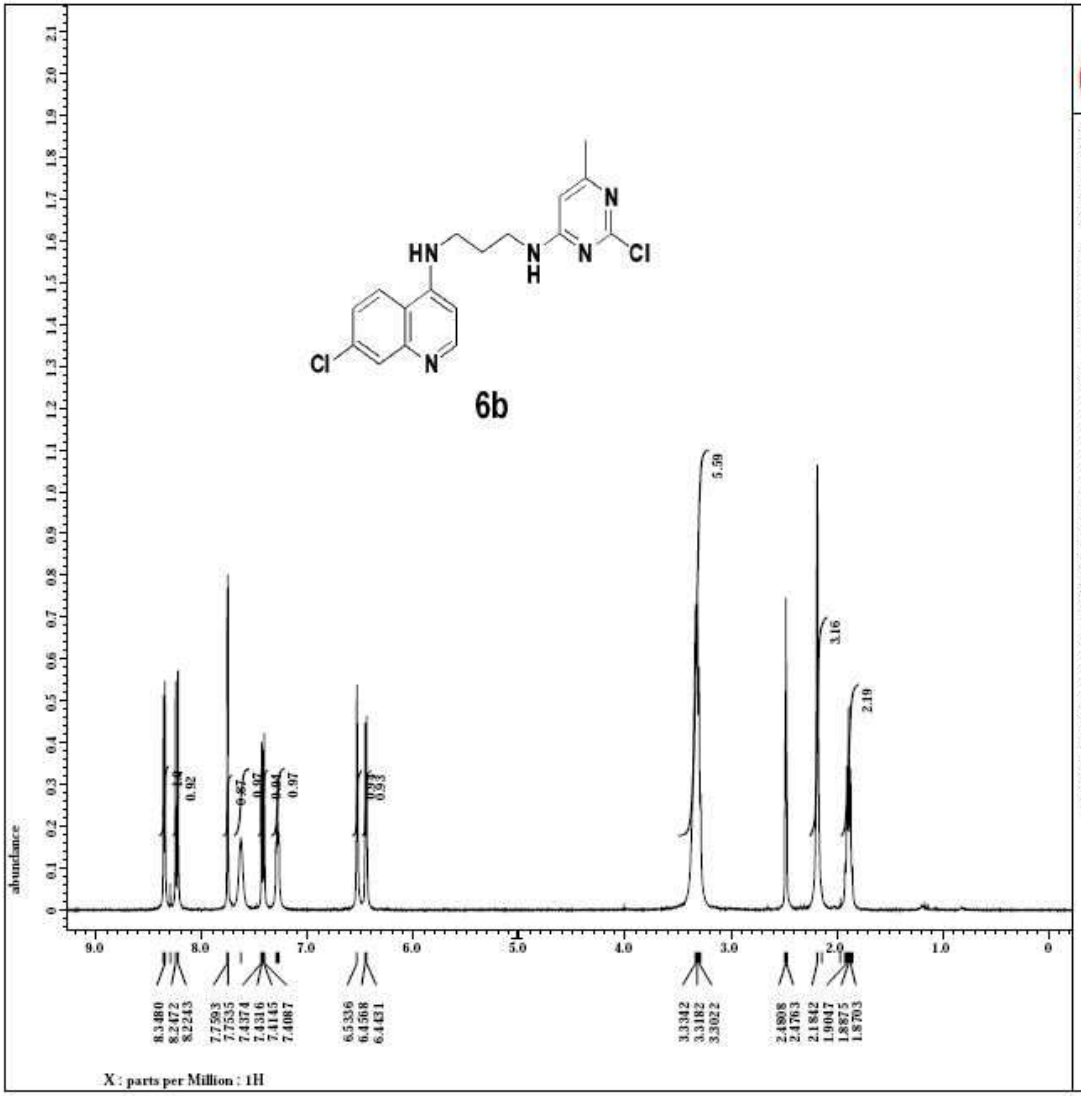

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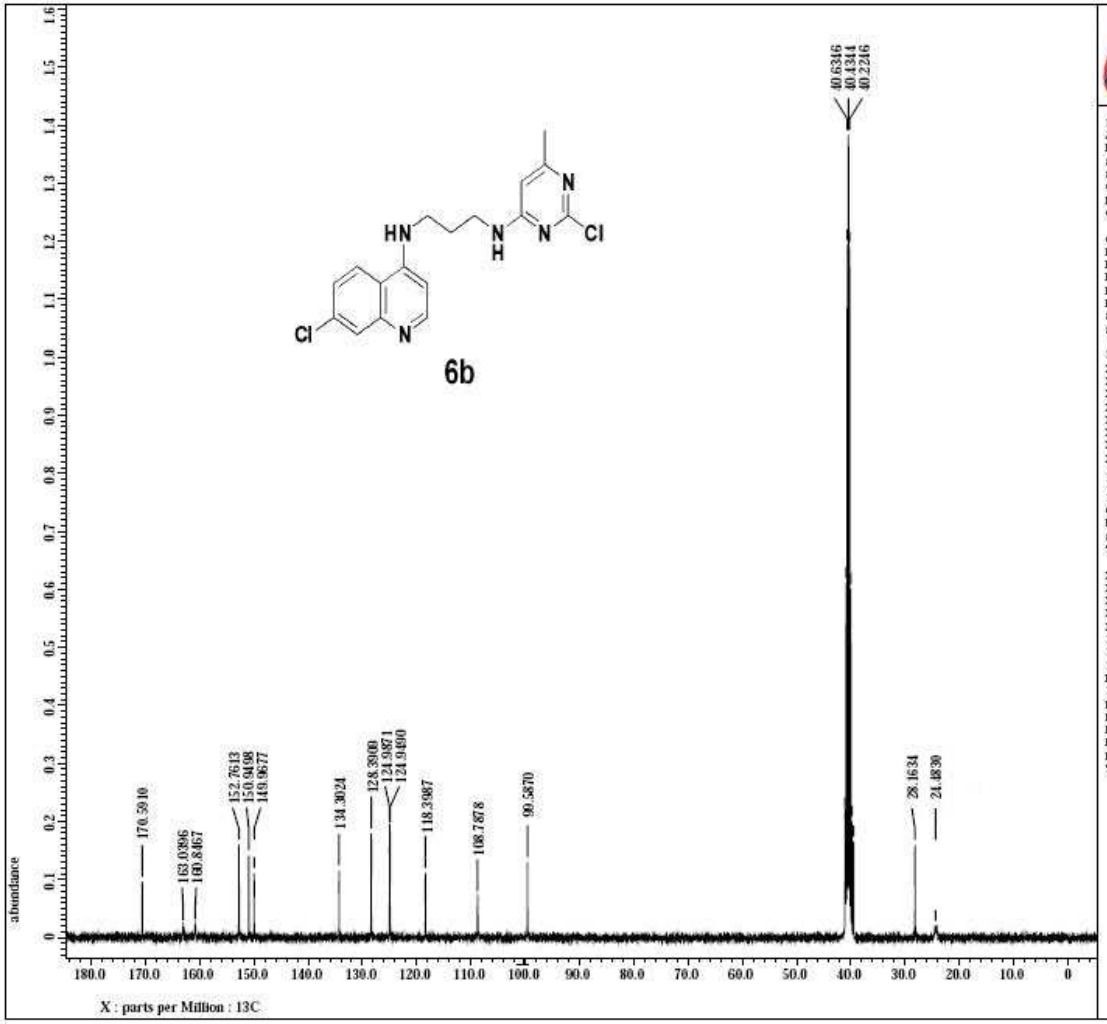

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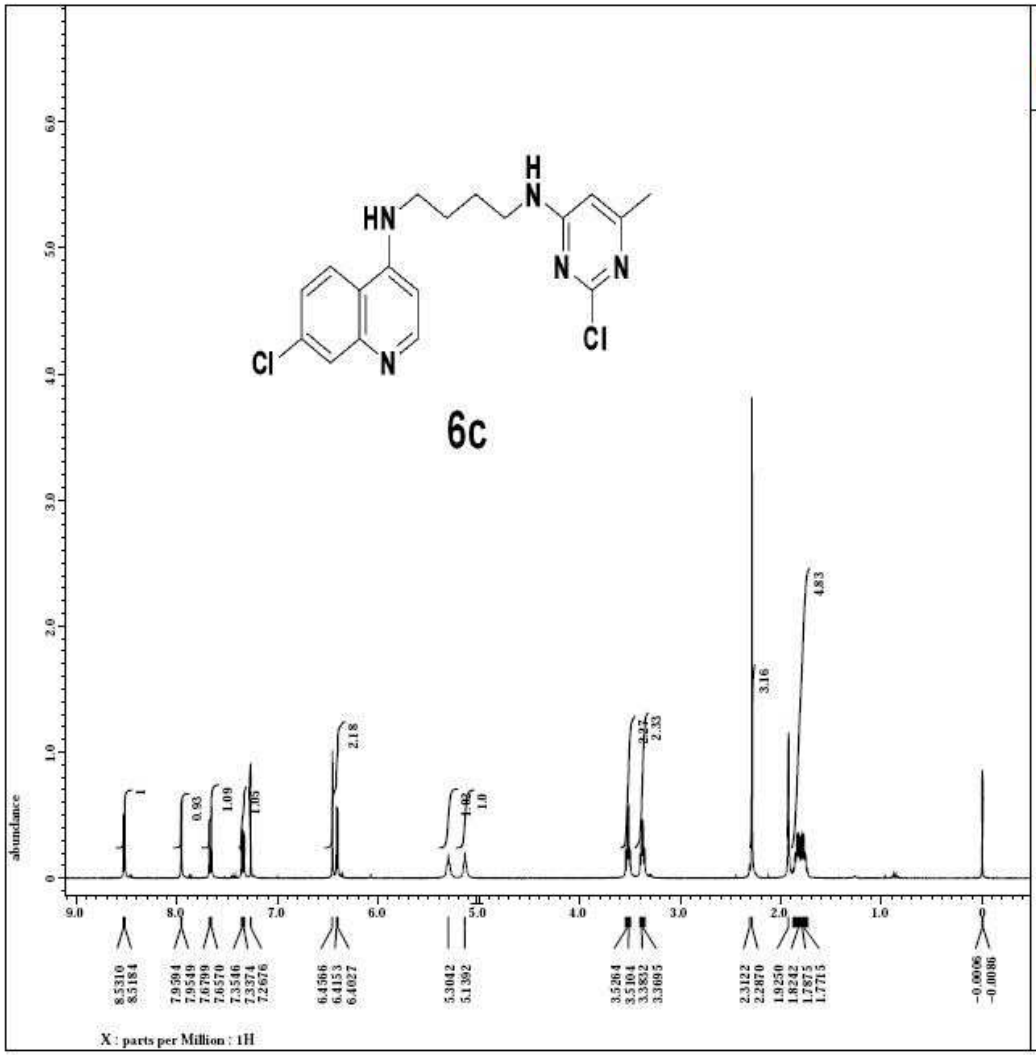

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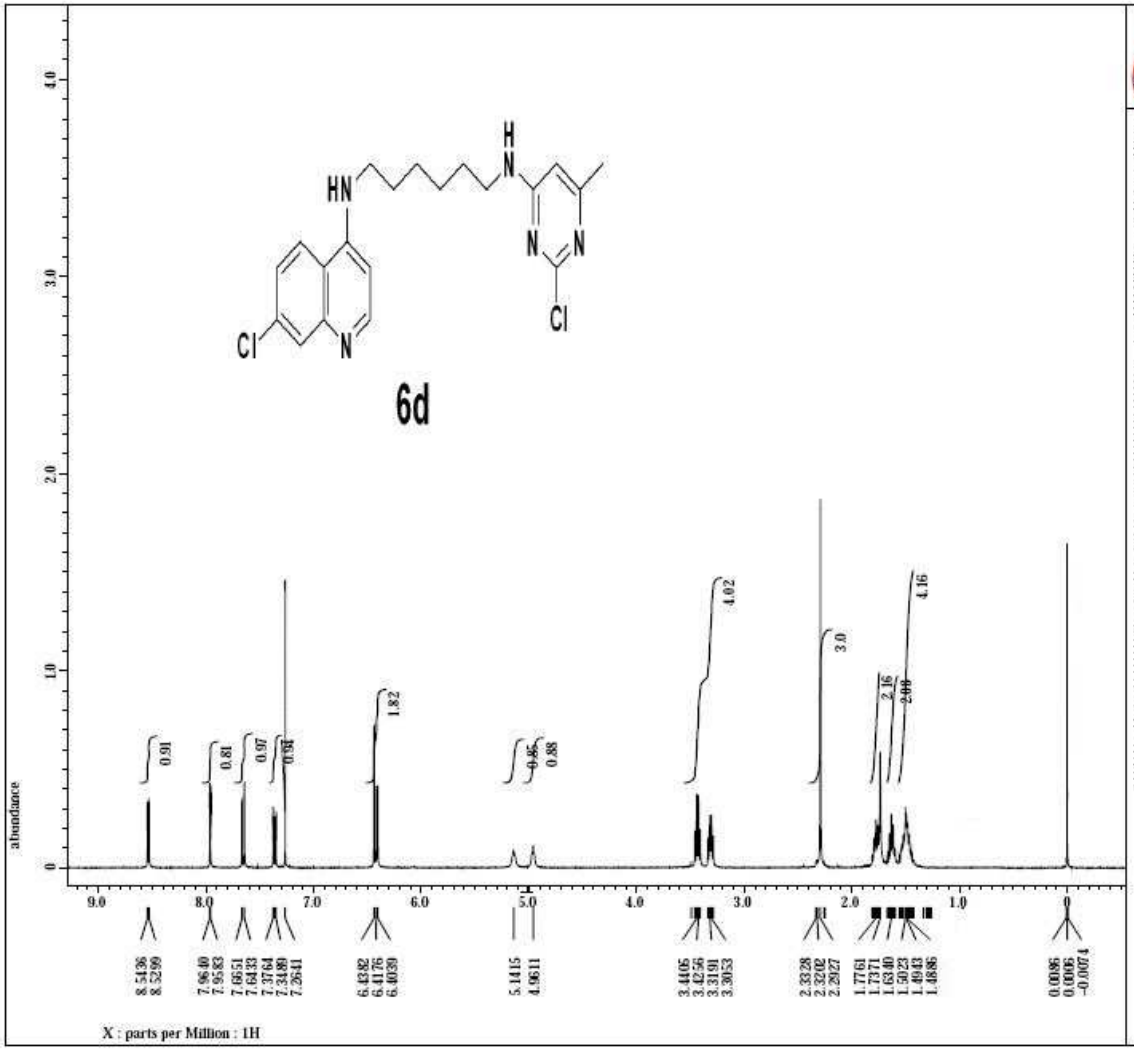

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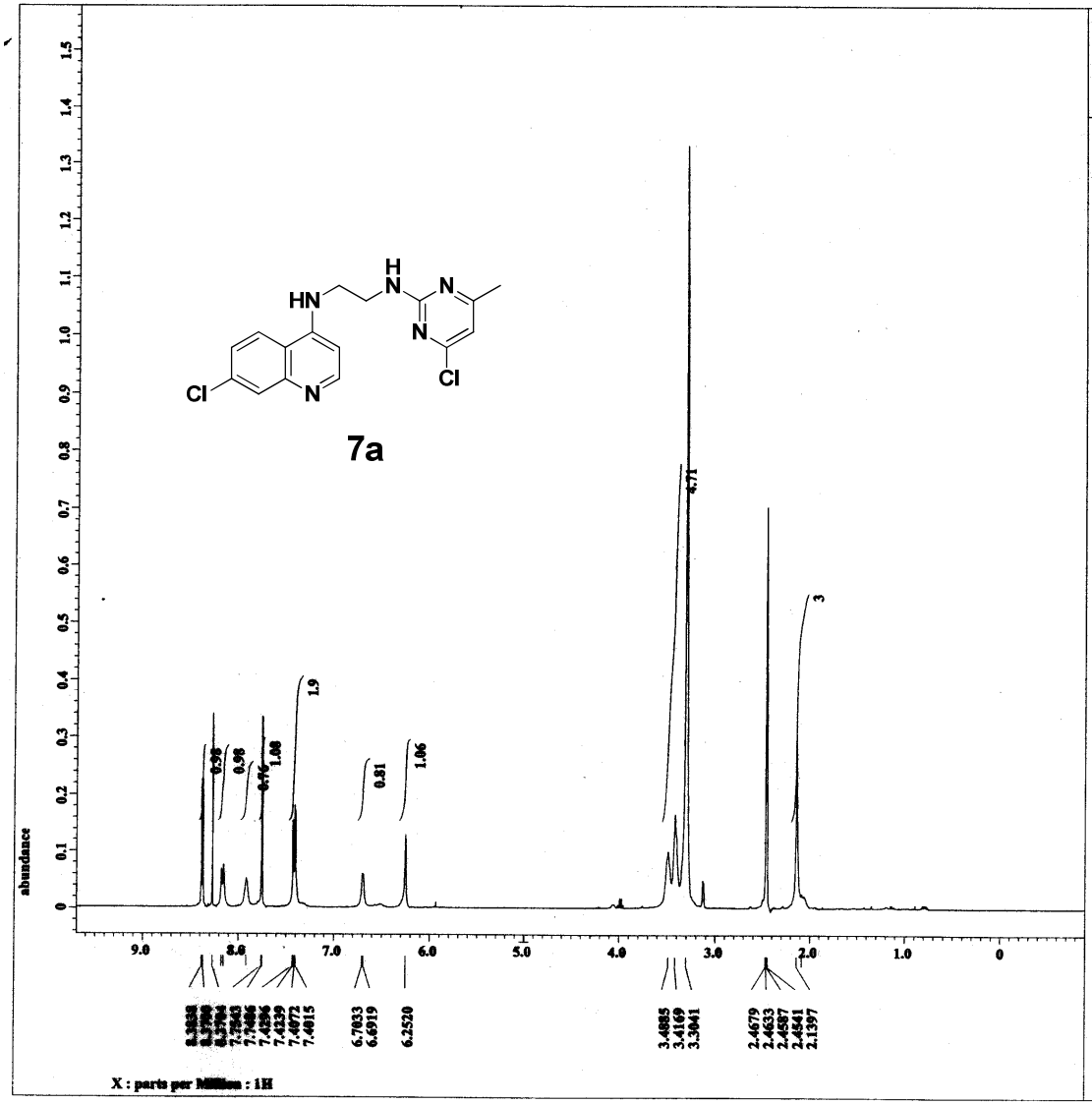
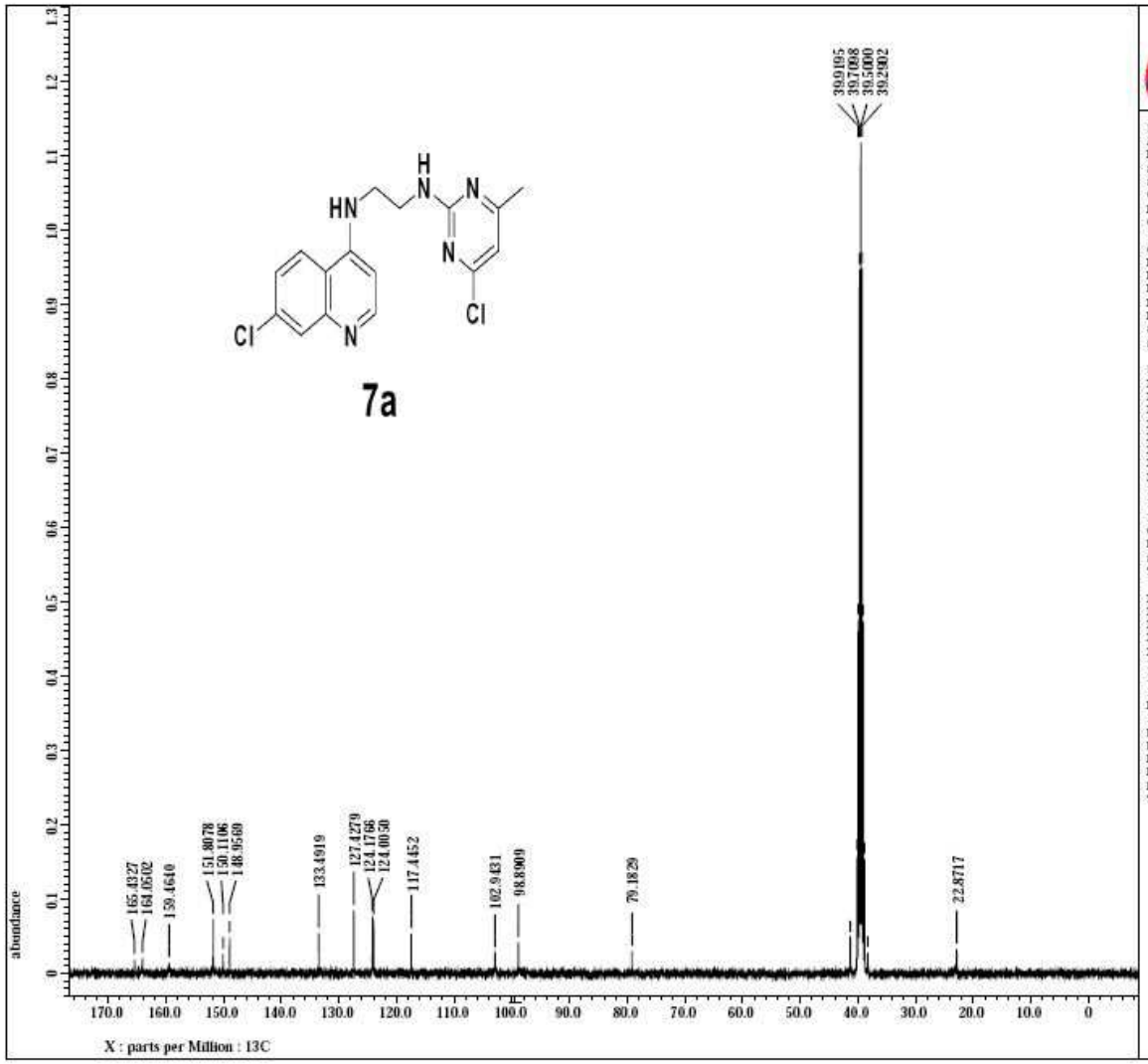
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 40
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 23.7[dC]



JEOL

Filename	= RK 58B-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= RK 58B
Solvent	= DMSO-D6
Creation_time	= 25-MAY-2010 19:23:52
Revision_time	= 25-MAY-2010 17:09:46
Current_time	= 25-MAY-2010 17:09:54
Comment	= RK 58B
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 4.36731904[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 5[ppm]
X_points	= 32768
X_prescans	= 1
X_resolution	= 0.22897343[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.5[us]
X_acq_time	= 4.36731904[s]
X_angle	= 45[deg]
X_atn	= 0.99[dB]
X_pulse	= 5.75[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 40
Relaxation_delay	= 5[s]
Repetition_time	= 9.36731904[s]
Temp_get	= 24.4[dC]

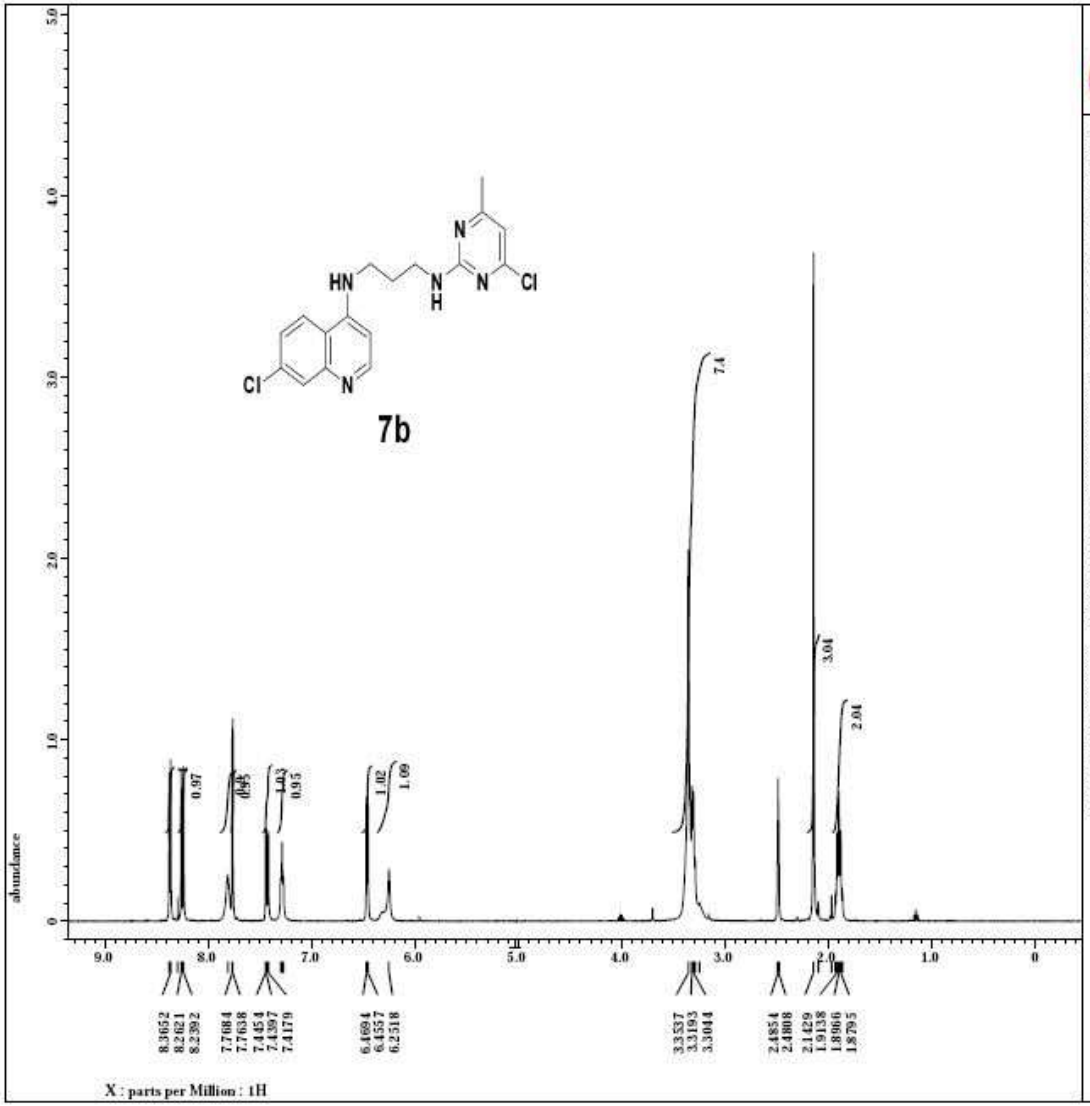


Filename - DSR_SM-488B_CARBON-5.
Author - delta
Experiment - single_pulse_dec
Sample_id - DSR_SM-488B
Solvent - DMSO-D6
Creation_time - 27-NOV-2010 05:21:38
Revision_time - 1-DEC-2010 22:15:19
Current_time - 1-DEC-2010 22:26:32

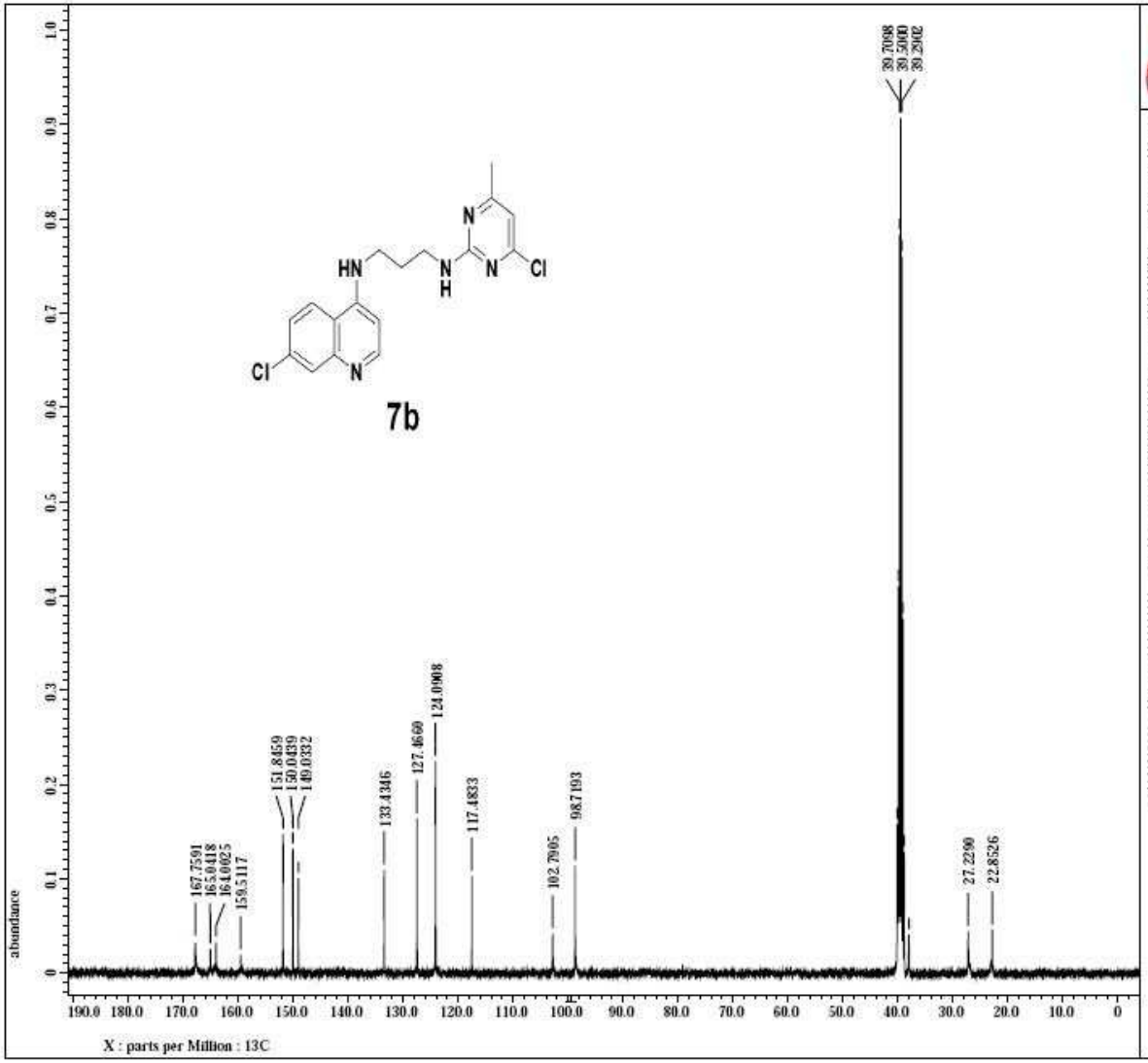
Comment - DSR SM-488B
Data_format - 1D COMPLEX
Dim_size - 26214
Dim_title - 13C
Dim_units - [ppm]
Dimensions - X
Site - ECX 400P
Spectrometer - DELTA2_NMR

Field_strength - 9.389766[T] (400[MHz])
X_acq_duration - 1.04333312[s]
X_domain - 13C
X_freq - 100.52530333[MHz]
X_offset - 100[ppm]
X_points - 32768
X_prescans - 4
X_resolution - 0.95846665[Hz]
X_sweep - 31.40703518[kHz]
Irr_domain - 1H
Irr_freq - 399.78219838[MHz]
Irr_offset - 5[ppm]
Clipped - FALSE
Mod_return - 1
Scans - 750
Total_scans - 750

X_90_width - 11.75[us]
X_acq_time - 1.04333312[s]
X_angle - 30[deg]
X_atn - 10[dB]
X_pulse - 3.91666667[us]
Irr_atn_dec - 24.95[dB]
Irr_atn_noe - 24.95[dB]
Irr_noise - WALTZ
Decoupling - TRUE
Initial_wait - 1[s]
Noe - TRUE
Noe_time - 2[s]
Recvr_gain - 58
Relaxation_delay - 2[s]
Repetition_time - 3.04333312[s]
Temp_get - 22.2[dC]



Filename	- RK_54B_PROTON-5.jdf
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- RK_54B
Solvent	- DMSO-D6
Creation_time	- 3-JUN-2010 17:06:23
Revision_time	- 3-JUN-2010 16:38:15
Current_time	- 3-JUN-2010 16:38:39
Comment	- RK 54B
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 36
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 24[dC]

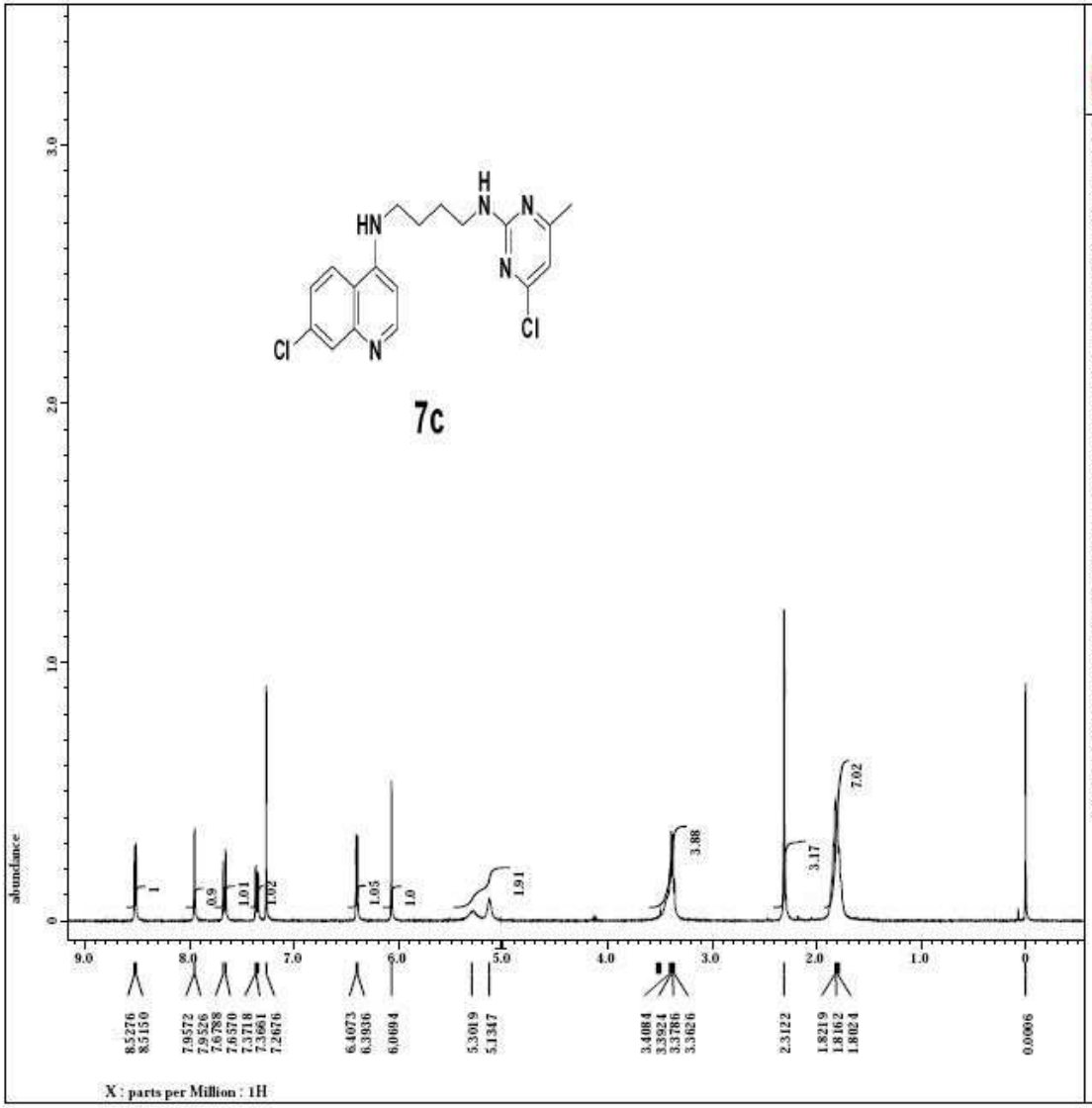


Filename = DSR_SM-484B_CARBON-5.
Author = delta
Experiment = single_pulse_dec
Sample_id = DSR_SM-484B
Solvent = DMSO-D6
Creation_time = 24-NOV-2010 08:13:08
Revision_time = 29-NOV-2010 21:46:44
Current_time = 29-NOV-2010 21:48:08

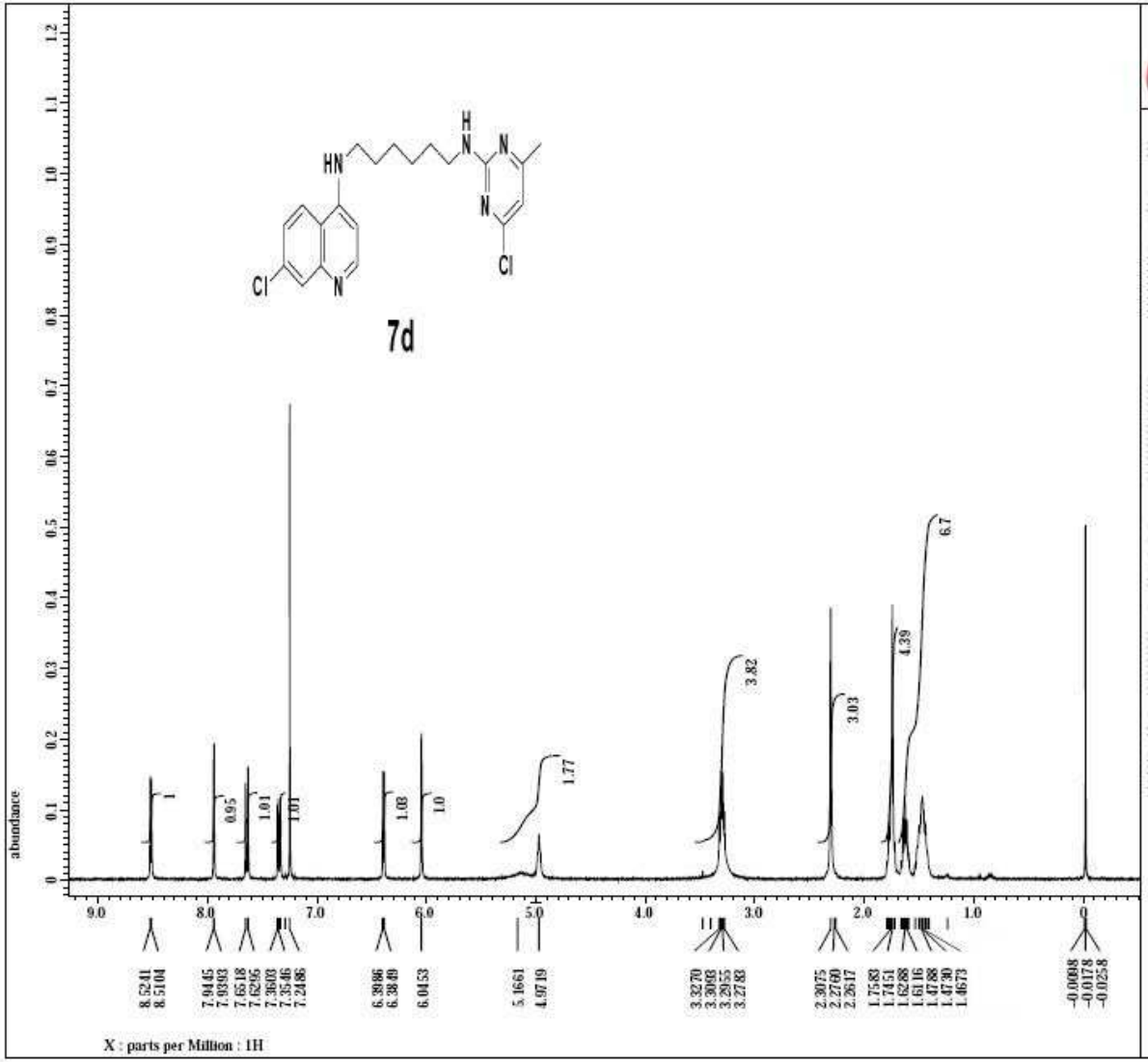
Comment = DSR_SM-484B
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = BCX 400P
Spectrometer = DELTA2_NMR

Field_strength = 9.389766[T] (400[MHz])
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 750
Total_scans = 750

X_90_width = 11.75[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 10[dB]
X_pulse = 3.91666667[us]
Irr_atn_dec = 24.95[dB]
Irr_atn_noe = 24.95[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 56
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 21.5[dC]

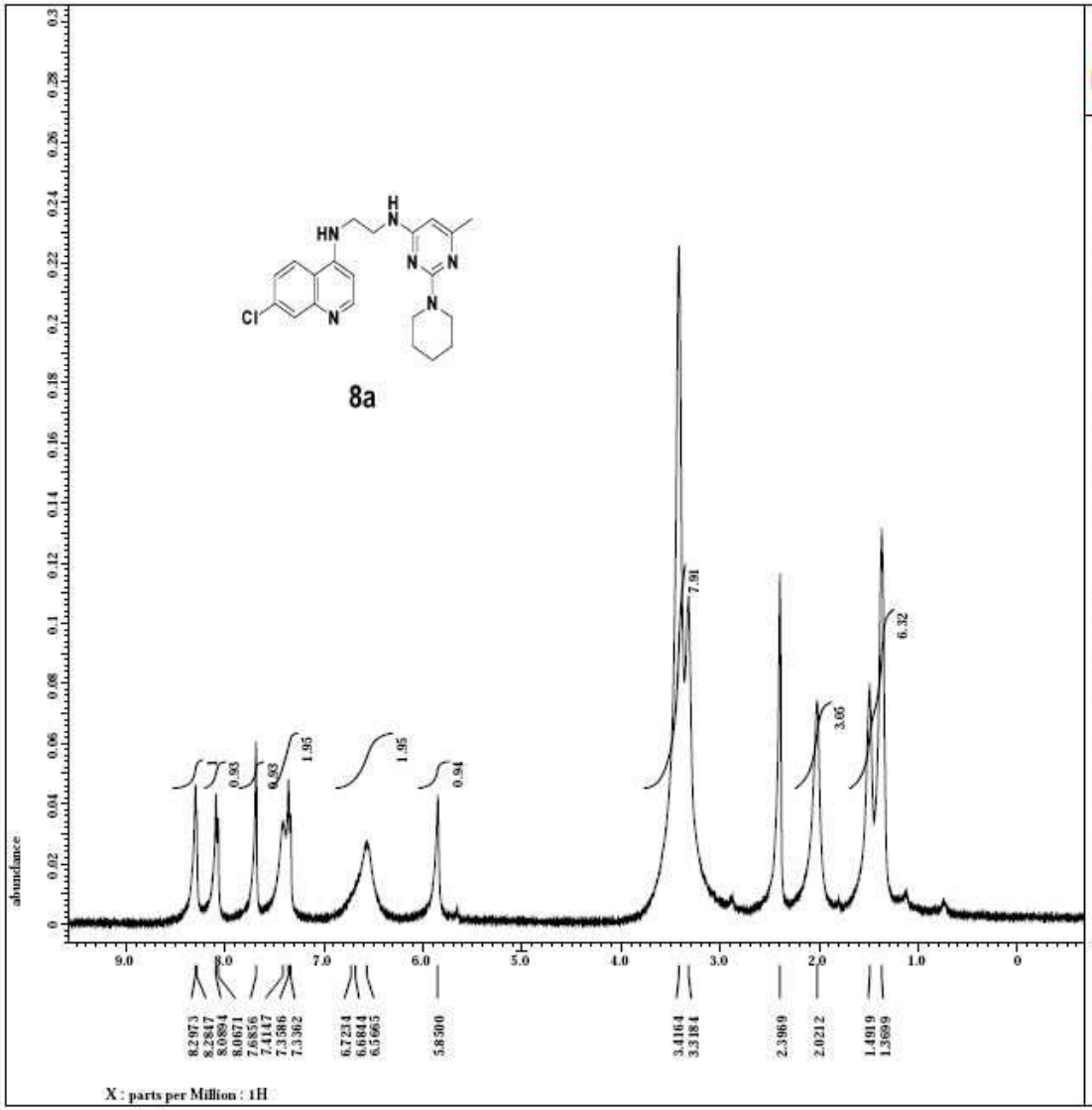


Filename	- DSR_SM-448B_PROTON-5.
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SM-448B
Solvent	- CHLOROFORM-D
Creation_time	- 16-JUN-2010 13:25:50
Revision_time	- 16-JUN-2010 15:34:06
Current_time	- 16-JUN-2010 15:34:49
Comment	- DSR SM-448B
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 42
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 21.7[dC]

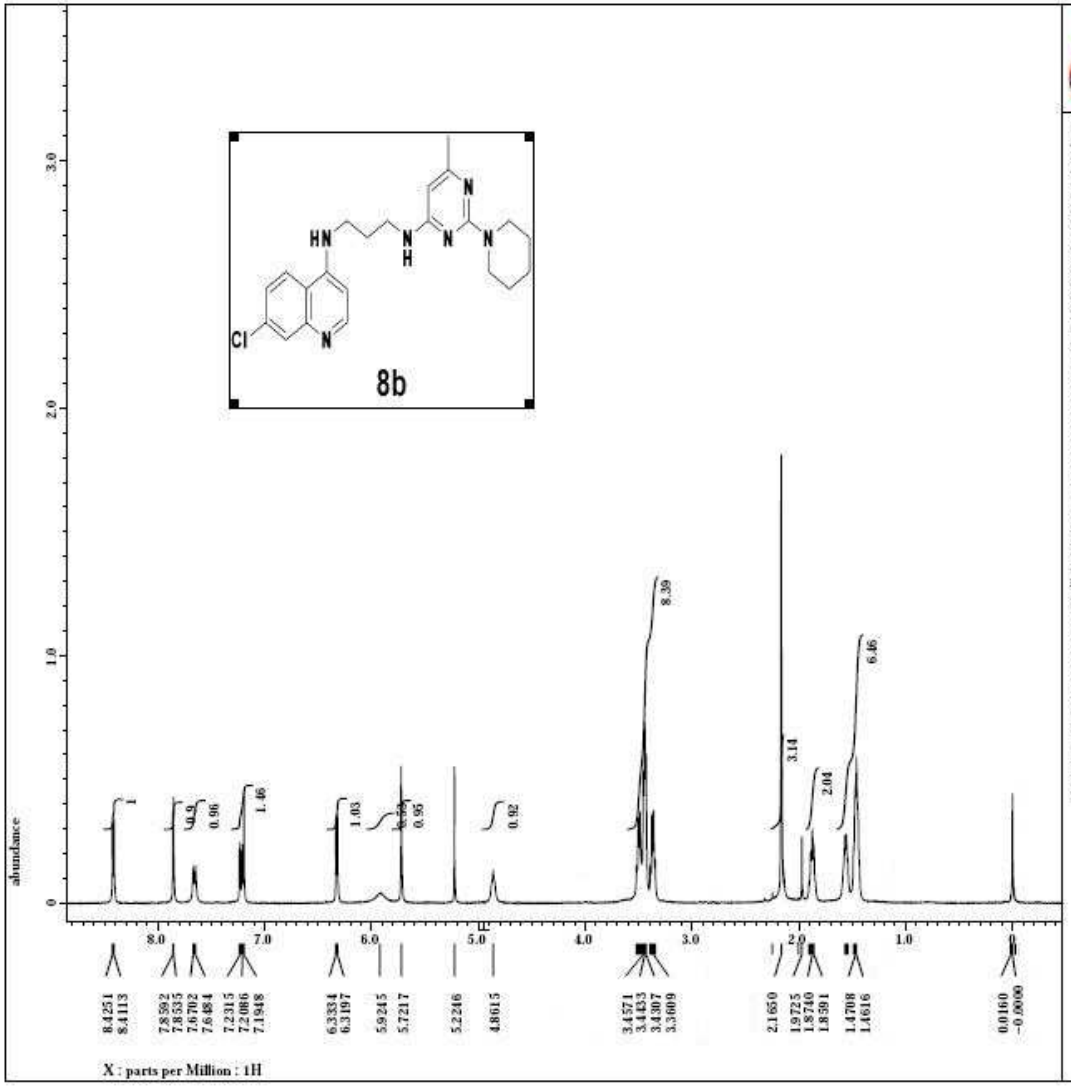


JEOL

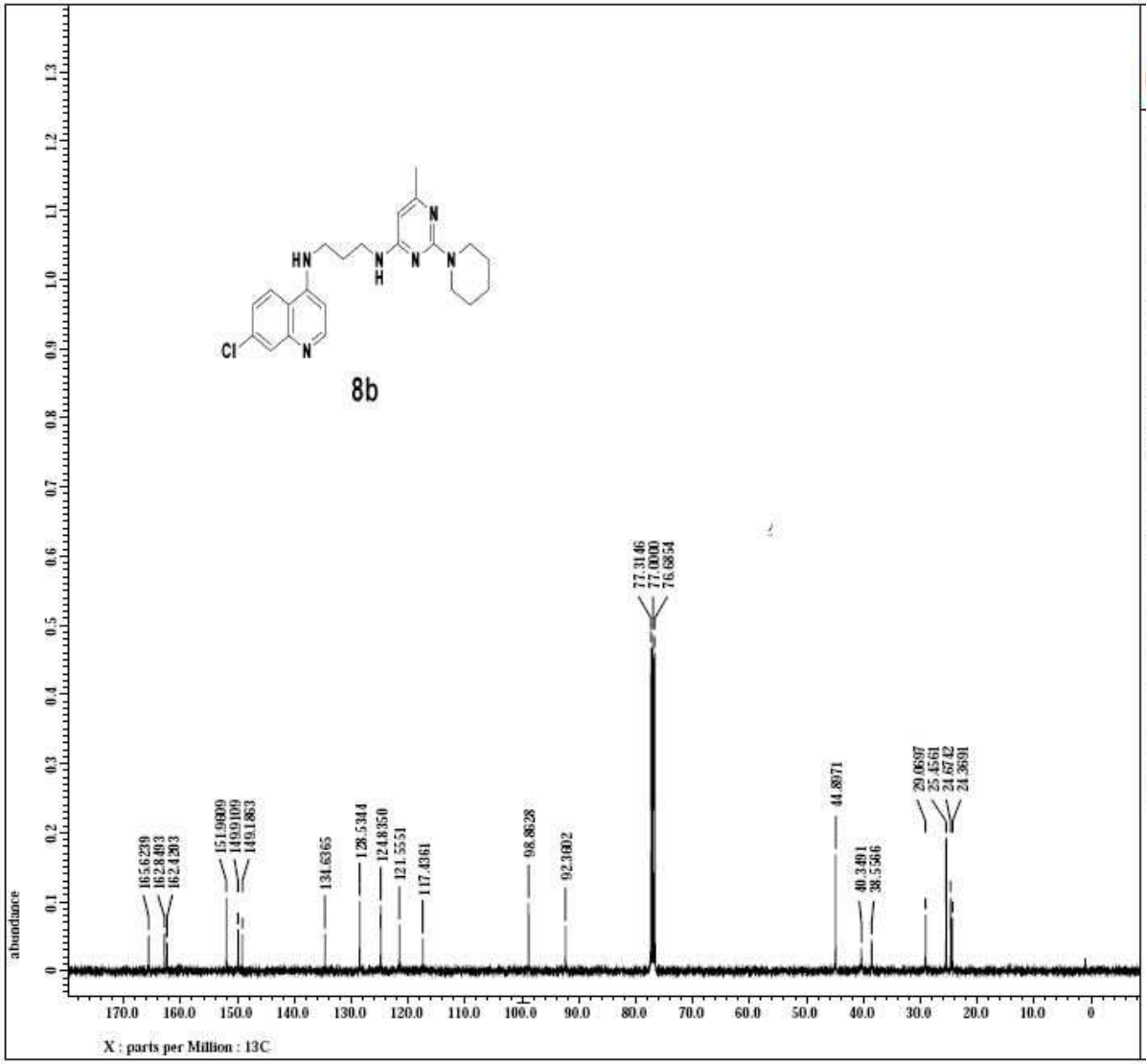
Filename	- DSR SM-504B-4.jdf
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR SM-504B
Solvent	- CHLOROFORM-D
Creation_time	- 24-JUN-2010 07:55:44
Revision_time	- 28-JUN-2010 10:32:20
Current_time	- 28-JUN-2010 10:32:51
Comment	- single_pulse
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 4.36731904[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 32768
X_prescans	- 1
X_resolution	- 0.22897343[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 4.36731904[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 42
Relaxation_delay	- 5[s]
Repetition_time	- 9.36731904[s]
Temp_get	- 21.9[dC]



Filename	= DSR SN-490-3.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= DSR SN-490
Solvent	= DMSO-D6
Creation_time	= 31-MAY-2010 17:00:31
Revision_time	= 31-MAY-2010 17:53:08
Current_time	= 31-MAY-2010 17:53:41
Comment	= DSR SN-490
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 4.36731904[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 5[ppm]
X_points	= 32768
X_prescans	= 1
X_resolution	= 0.22897343[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.5[us]
X_acq_time	= 4.36731904[s]
X_angle	= 45[deg]
X_atn	= 0.99[dB]
X_pulse	= 5.75[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 5[s]
Repetition_time	= 9.36731904[s]
Temp_get	= 21.3[dC]

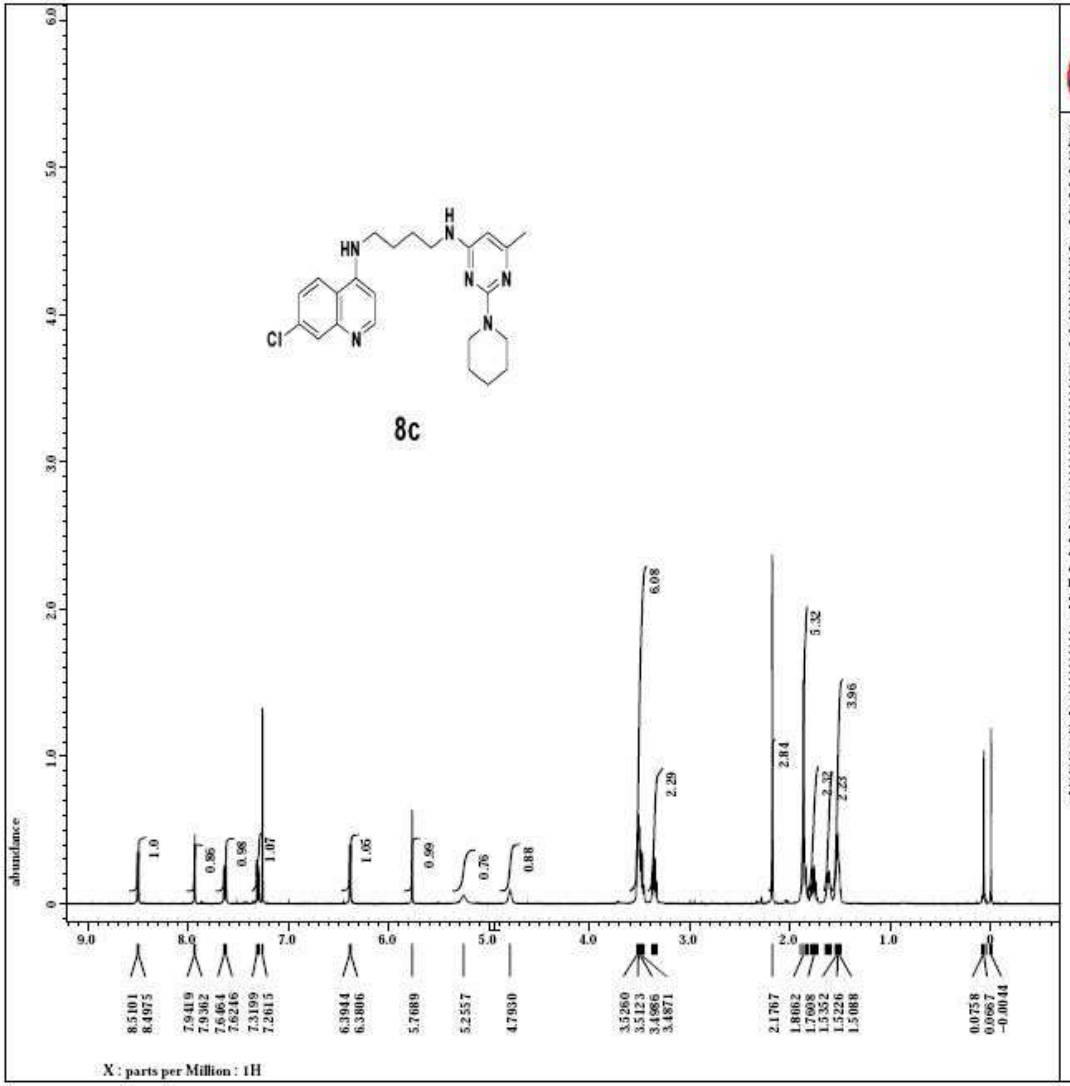


Filename	- DSR_SM-485_PROTON-5.j
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SM-485
Solvent	- CHLOROFORM-D
Creation_time	- 9-JUN-2010 14:02:36
Revision_time	- 9-JUN-2010 16:53:22
Current_time	- 9-JUN-2010 16:53:46
Comment	- DSR_SM-485
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 36
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 23.4[dC]



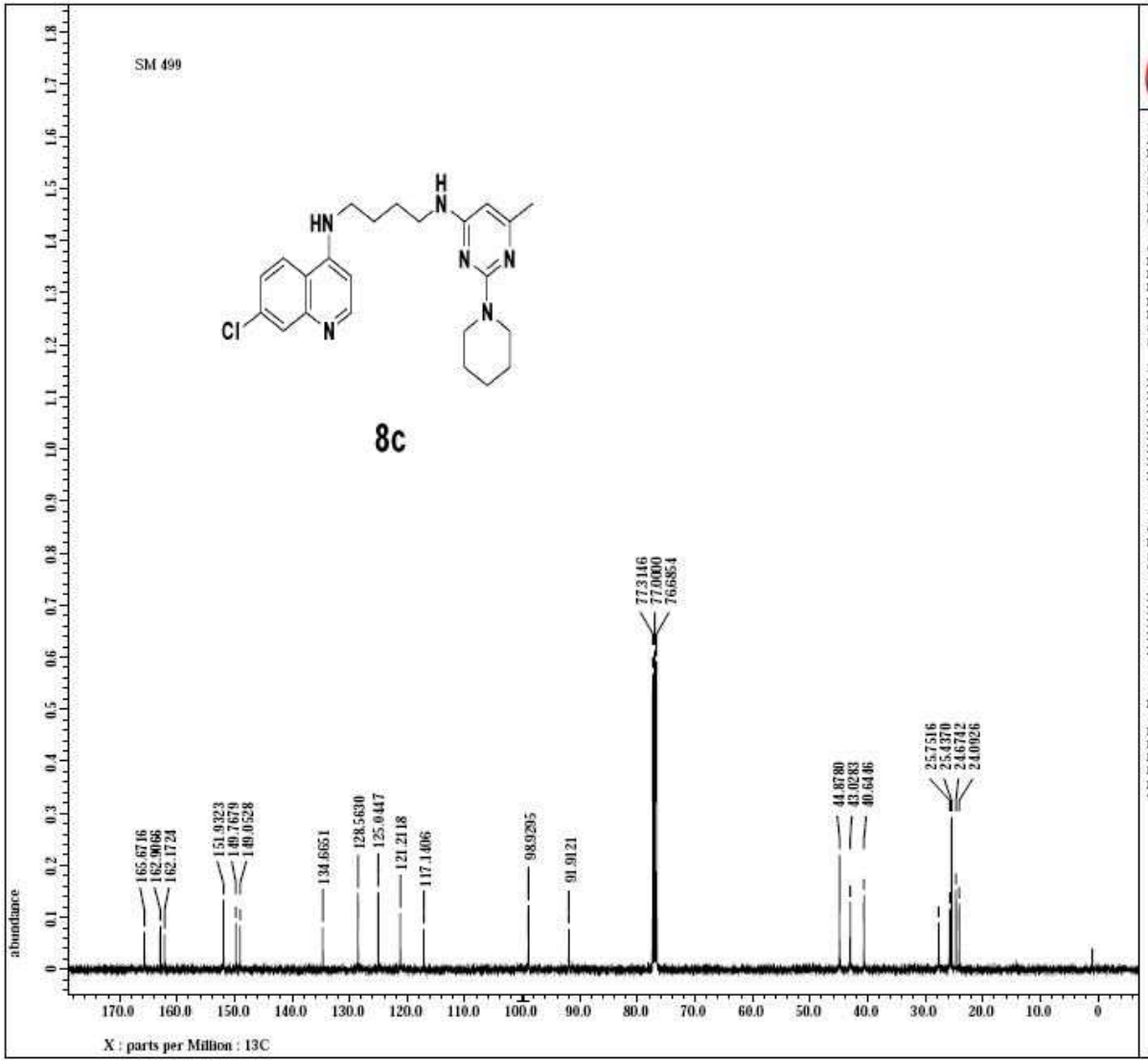
JEOL

Filename	- DSR_SM-485_CARBON-3.j
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- DSR_SM-485
Solvent	- CHLOROFORM-D
Creation_time	- 24-NOV-2010 22:42:45
Revision_time	- 24-NOV-2010 19:13:14
Current_time	- 29-NOV-2010 21:30:17
Comment	- DSR SM-485
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32768
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 1000
Total_scans	- 1000
X_90_width	- 11.75[us]
X_acq_time	- 1.04333312[s]
X_angle	- 30[deg]
X_atn	- 10[dB]
X_pulse	- 3.91666667[us]
Irr_atn_dec	- 24.95[dB]
Irr_atn_noe	- 24.95[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 58
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 22.1[dC]



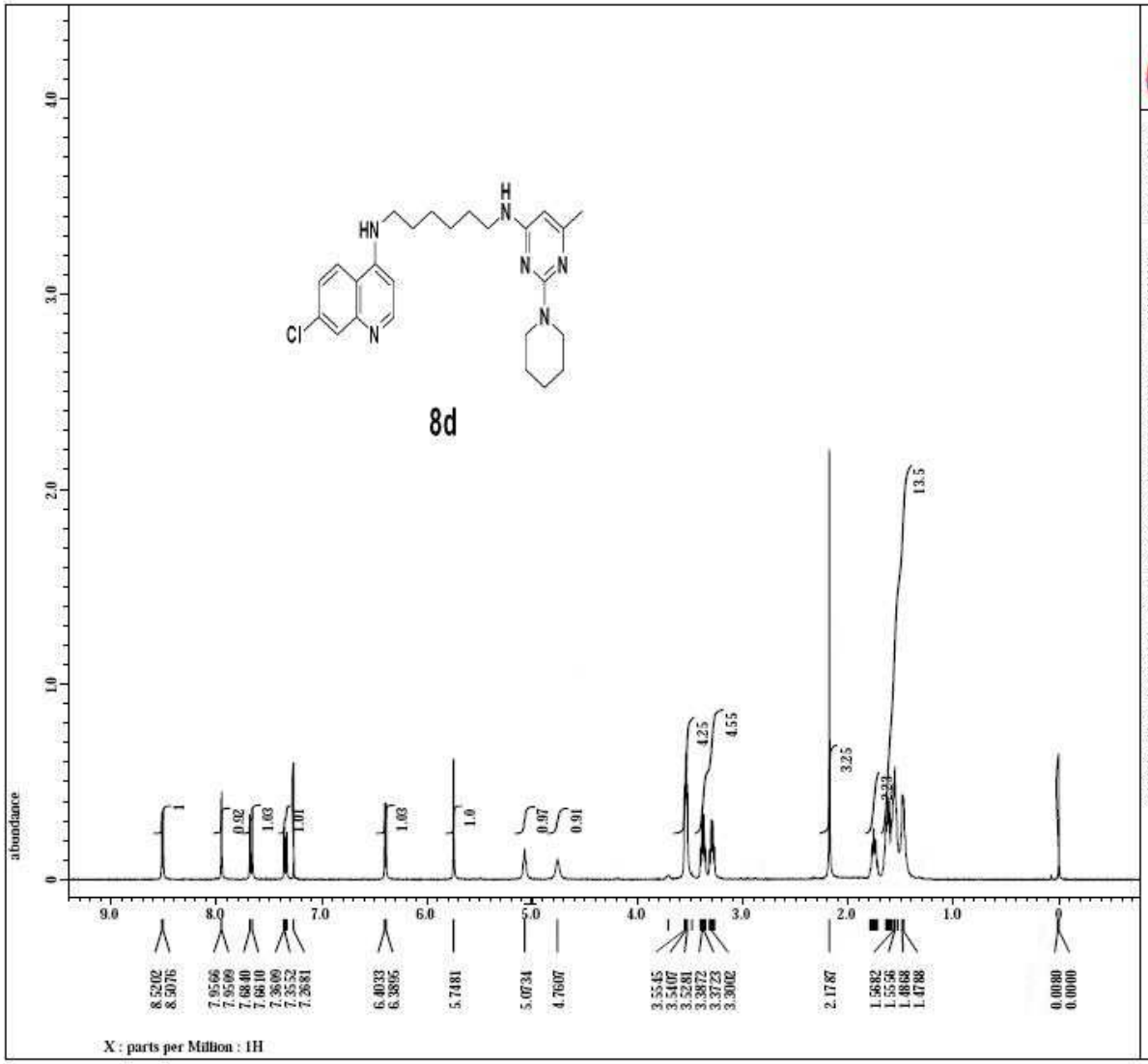
JEOL

Filename	- DSR_SM-499_PROTON-5.j
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SM-499
Solvent	- CHLOROFORM-D
Creation_time	- 15-JUN-2010 15:12:18
Revision_time	- 15-JUN-2010 16:20:59
Current_time	- 15-JUN-2010 16:21:14
Comment	- DSR SM-499
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 40
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 24.4[dC]



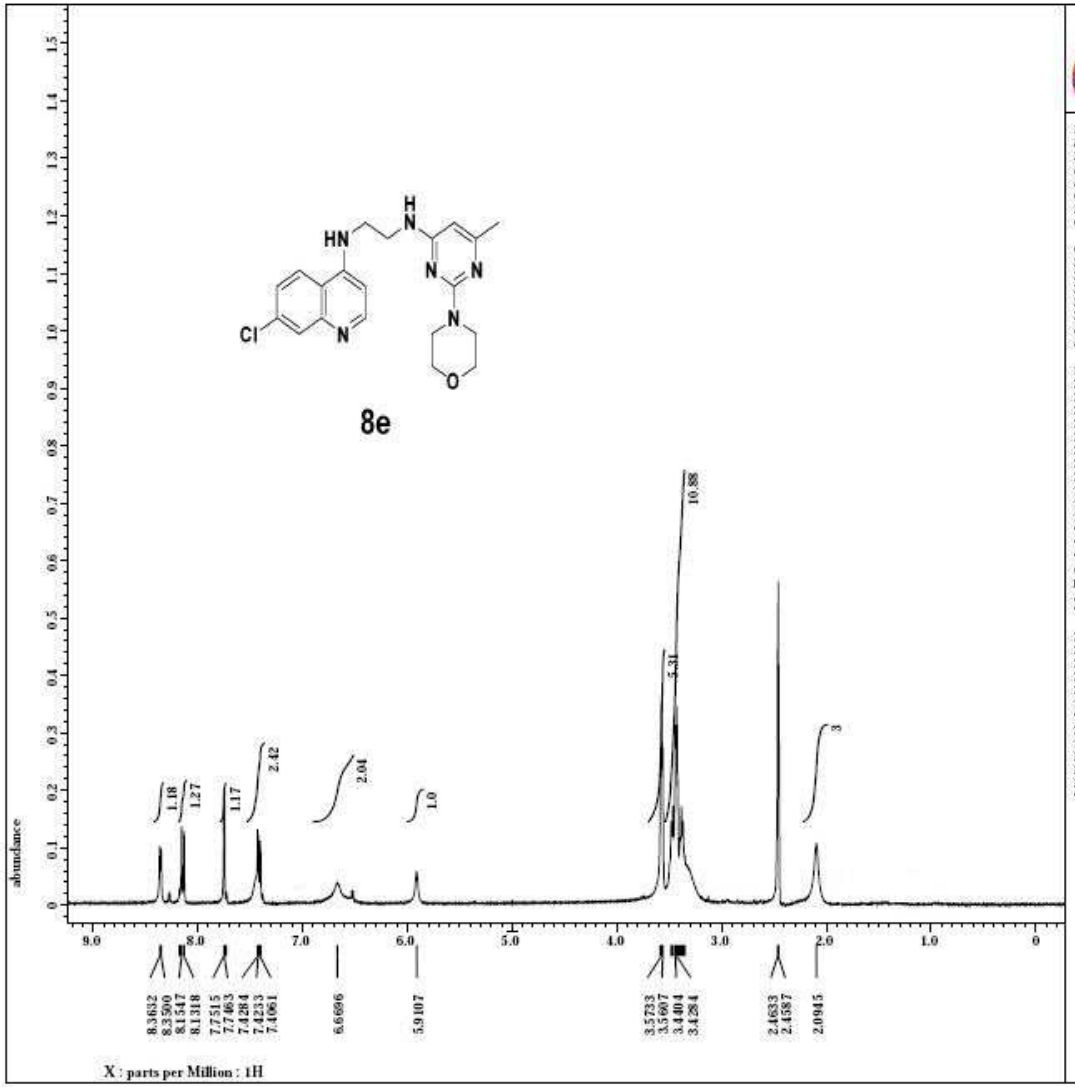
JEOL

Filename	- DSR_SM-499_CARBON-4.j
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- DSR_SM-499
Solvent	- CHLOROFORM-D
Creation_time	- 2-DEC-2010 05:39:05
Revision_time	- 3-DEC-2010 22:08:13
Current_time	- 3-DEC-2010 22:08:25
Comment	- DSR SM-499
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32768
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 1000
Total_scans	- 1000
X_90_width	- 11.75[us]
X_acq_time	- 1.04333312[s]
X_angle	- 30[deg]
X_atn	- 10[dB]
X_pulse	- 3.91666667[us]
Irr_atn_dec	- 24.95[dB]
Irr_atn_noe	- 24.95[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 60
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 21.8[dC]



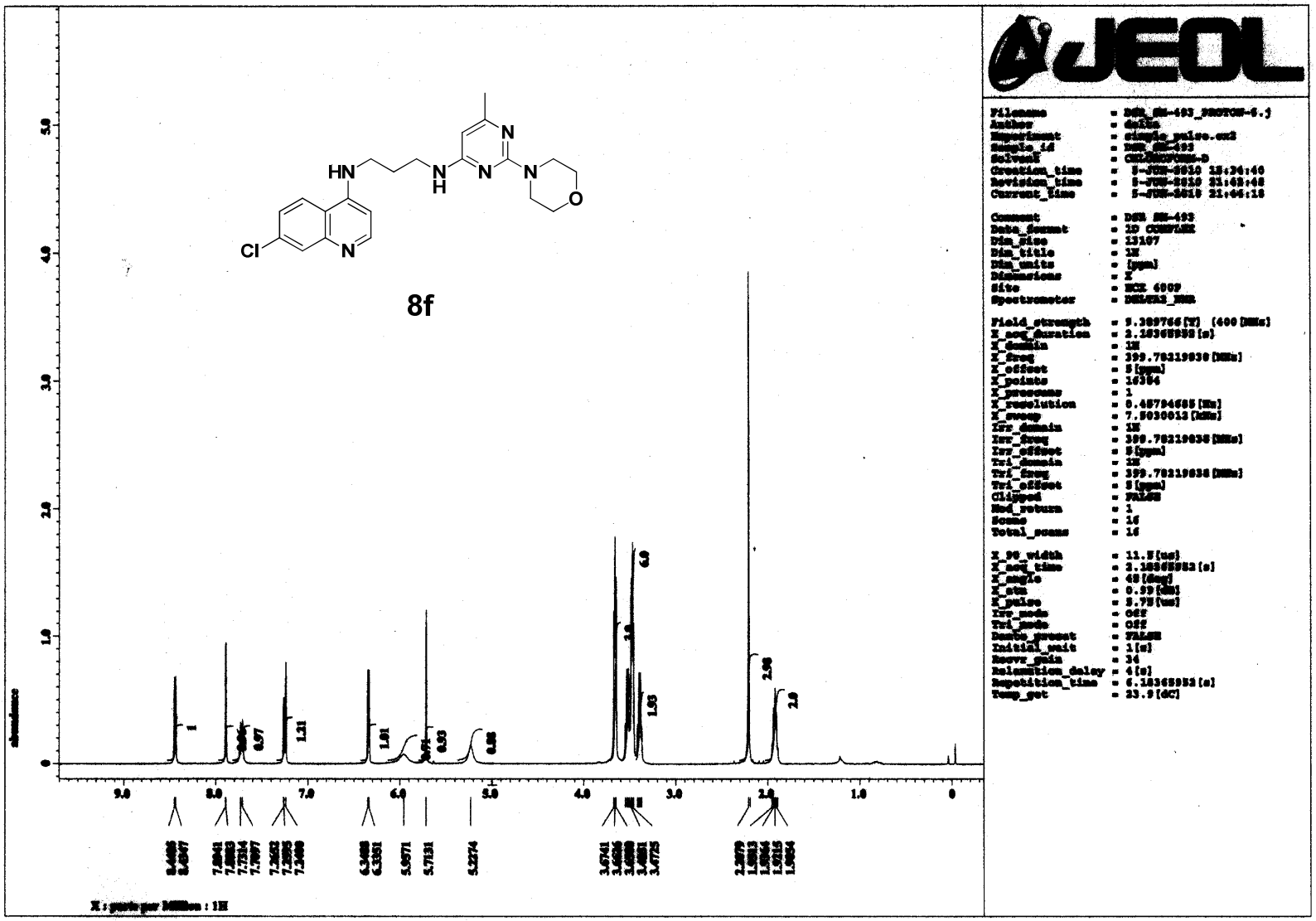
JEOL

Filename	- DSR_SM-505_PROTON-5.j
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SM-505
Solvent	- CHLOROFORM-D
Creation_time	- 23-JUN-2010 14:20:42
Revision_time	- 28-JUN-2010 10:53:25
Current_time	- 28-JUN-2010 10:53:44
Comment	- DSR SM-505
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 40
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 24[dC]



JEOL

Filename	- DSR SM-489-3.jdf
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR SM-489
Solvent	- DMSO-D6
Creation_time	- 26-MAY-2010 14:01:27
Revision_time	- 26-MAY-2010 15:56:40
Current_time	- 26-MAY-2010 15:56:57
Comment	- DSR SM-489
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 4.36731904[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 32768
X_prescans	- 1
X_resolution	- 0.22897343[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 4.36731904[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 40
Relaxation_delay	- 5[s]
Repetition_time	- 9.36731904[s]
Temp_get	- 23.5[dC]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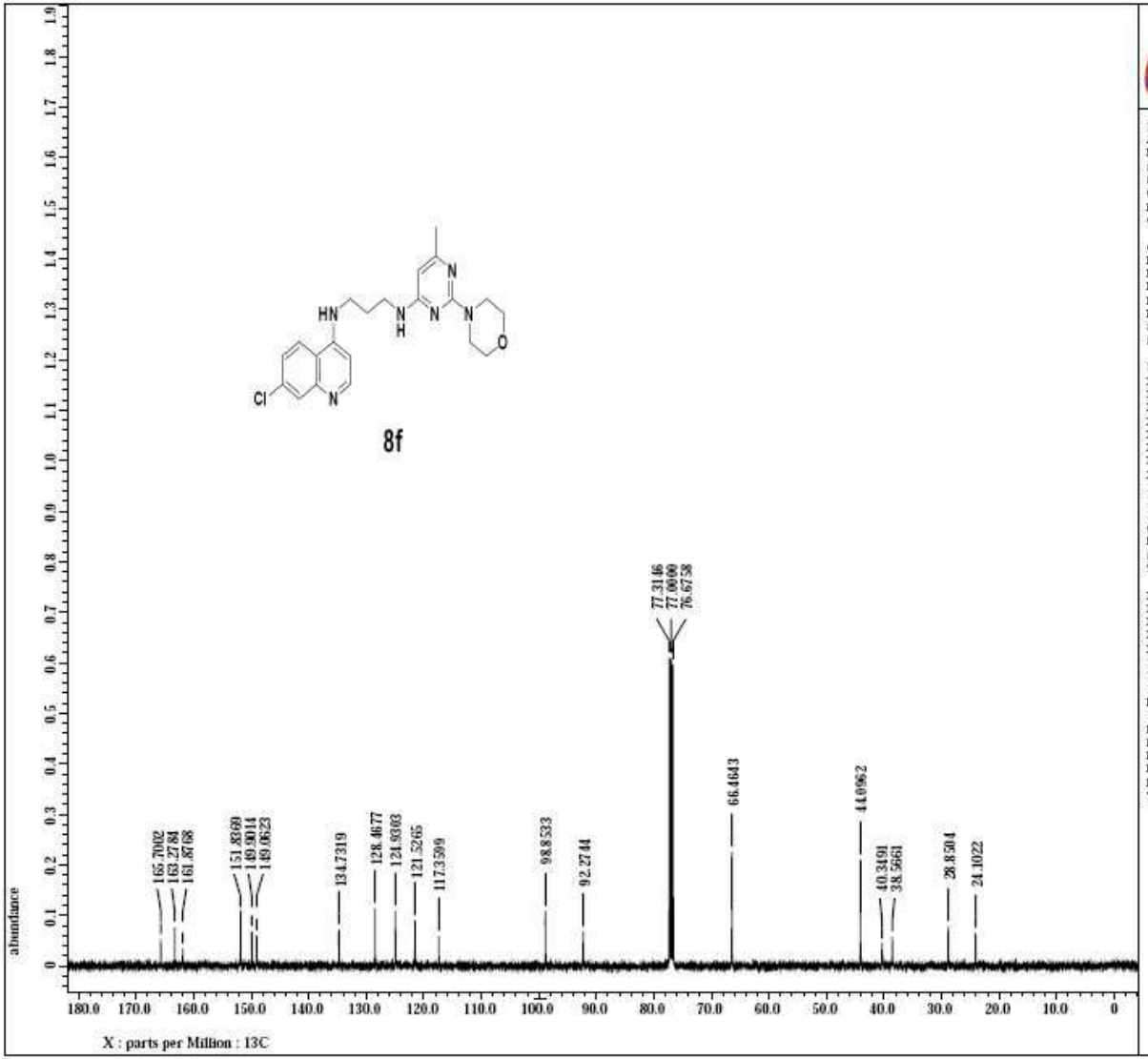
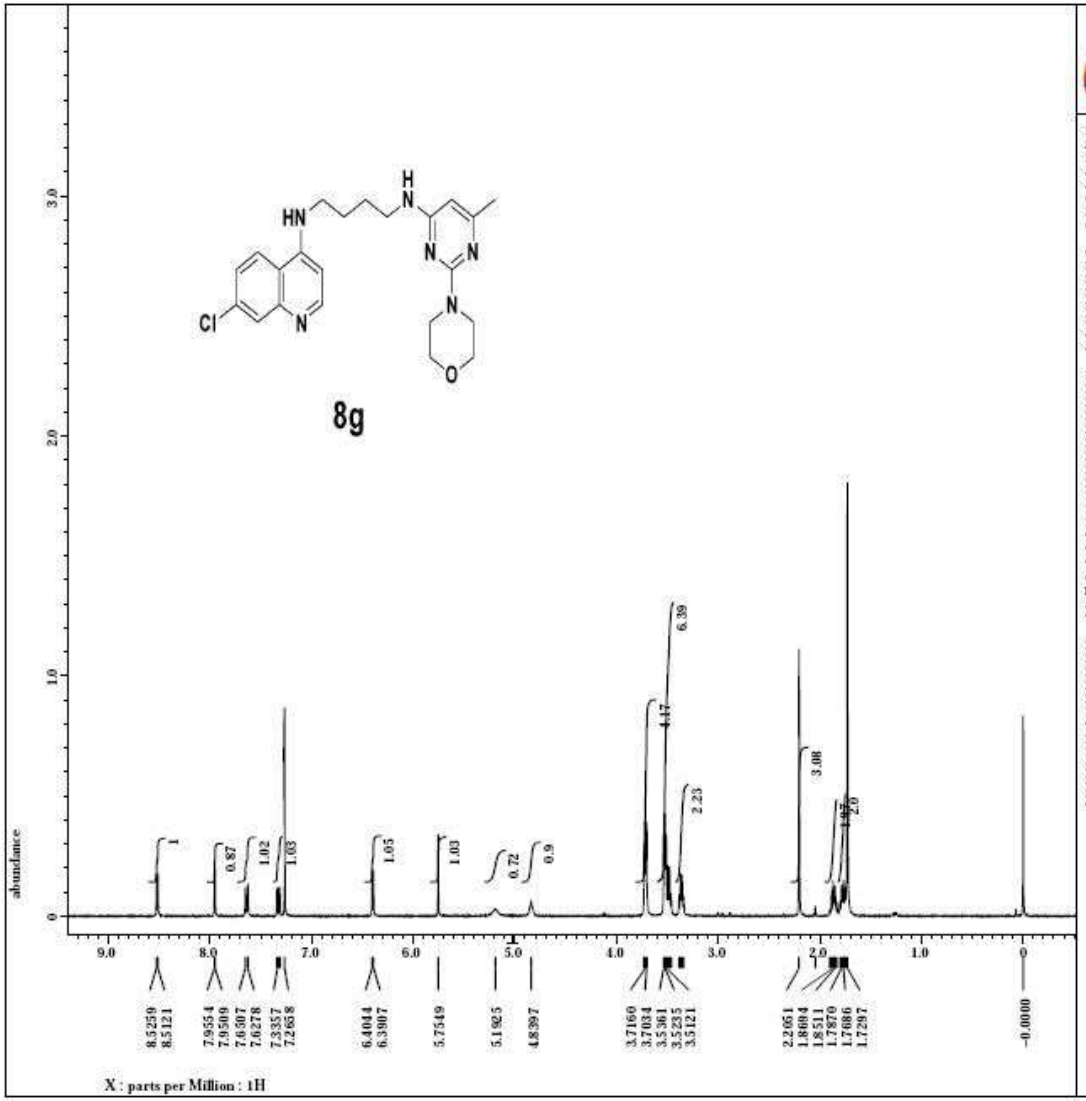
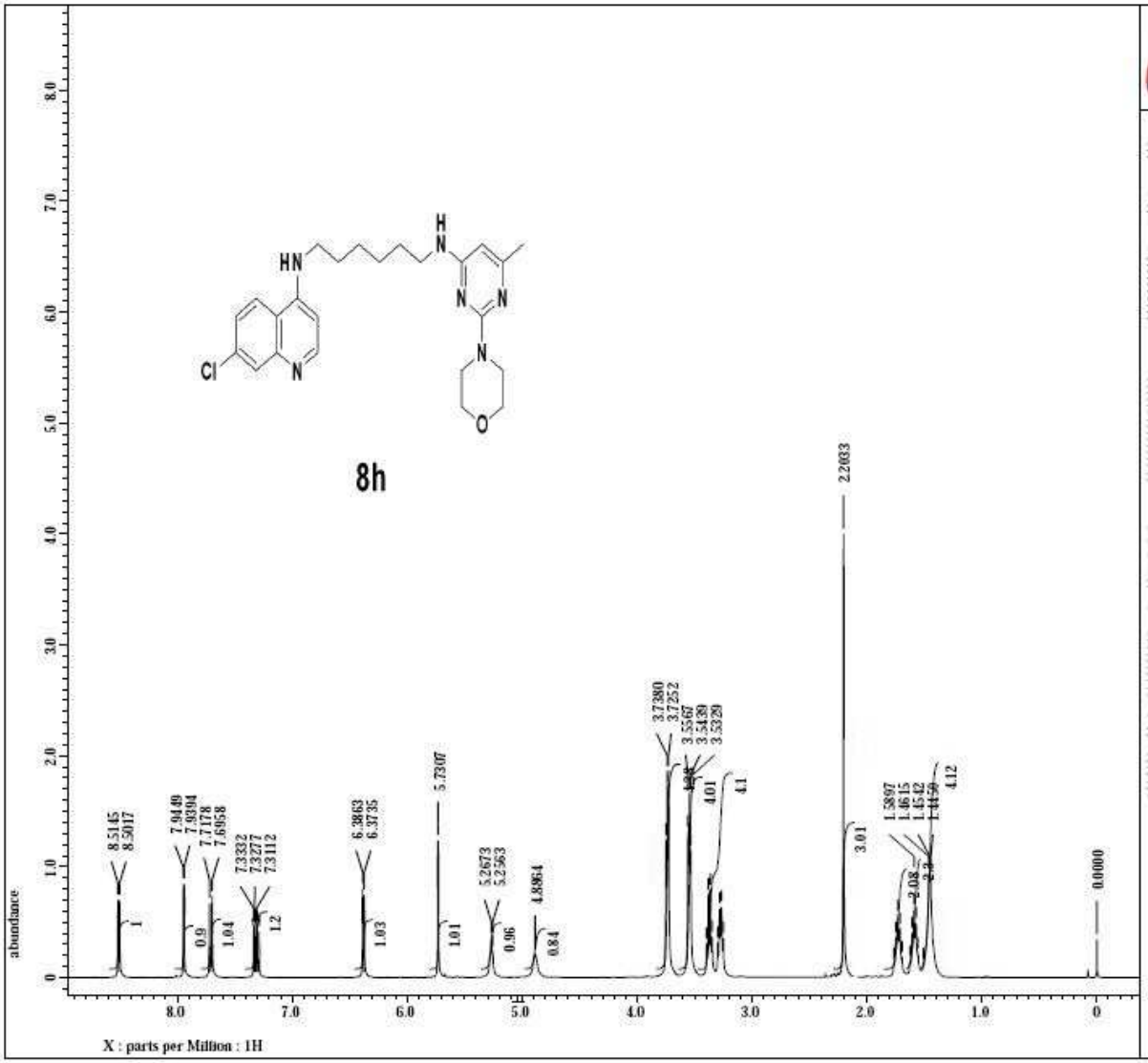


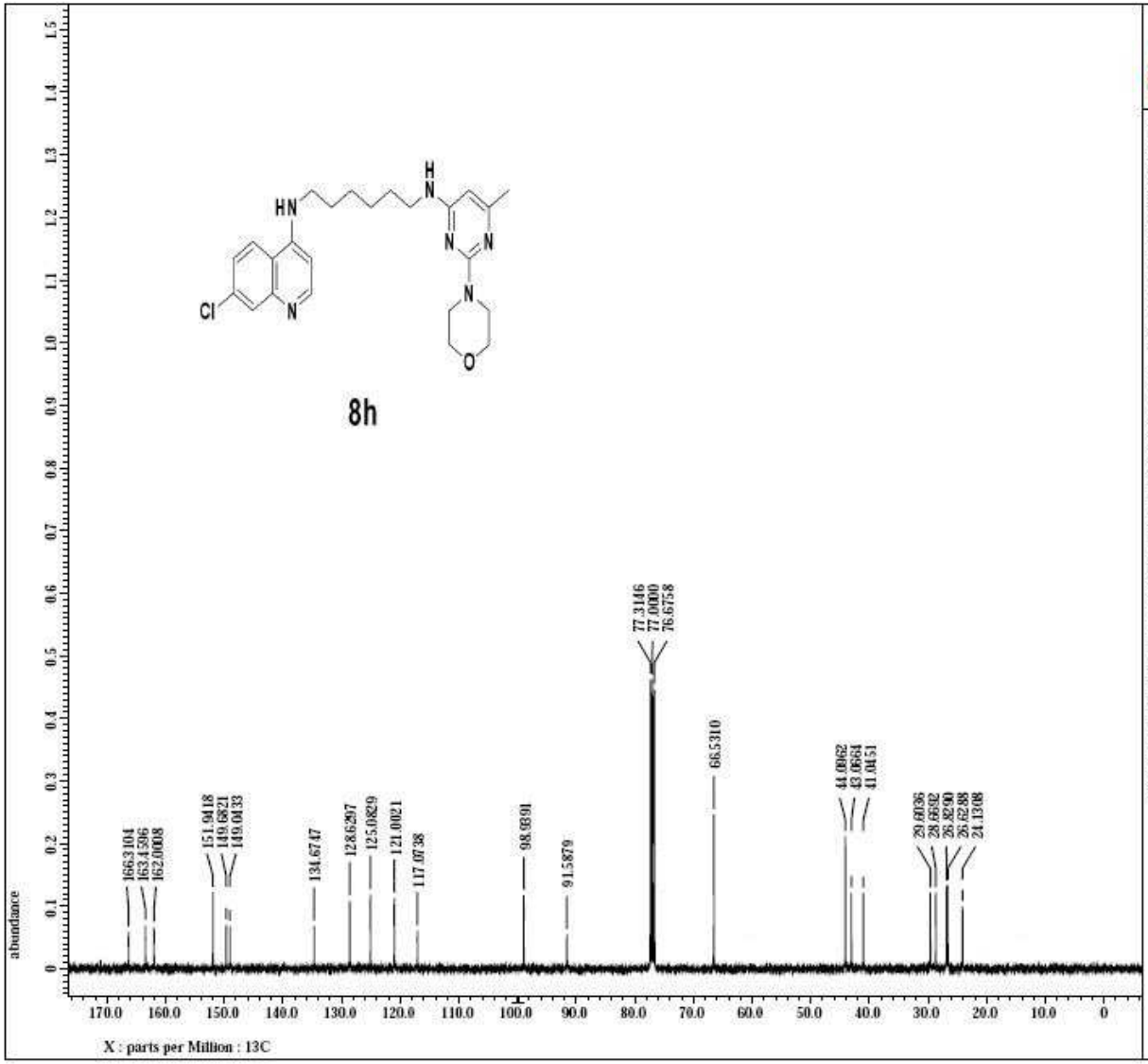
Filename	- DSR_SM-493_CARBON-4.j
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- DSR_SM-493
Solvent	- CHLOROFORM-D
Creation_time	- 29-NOV-2010 20:17:17
Revision_time	- 1-DEC-2010 22:17:46
Current_time	- 1-DEC-2010 22:19:13
Comment	- DSR SM-493
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32768
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 750
Total_scans	- 750
X_90_width	- 11.75[us]
X_acq_time	- 1.04333312[s]
X_angle	- 30[deg]
X_atn	- 10[dB]
X_pulse	- 3.91666667[us]
Irr_atn_dec	- 24.95[dB]
Irr_atn_noe	- 24.95[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 60
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 24.3[dC]



Filename	- DSR_SM-500_PROTON-5.j
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SM-500
Solvent	- CHLOROFORM-D
Creation_time	- 18-JUN-2010 14:27:02
Revision_time	- 18-JUN-2010 16:24:44
Current_time	- 18-JUN-2010 16:25:07
Comment	- DSR SM-500
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 42
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 22.8[dC]

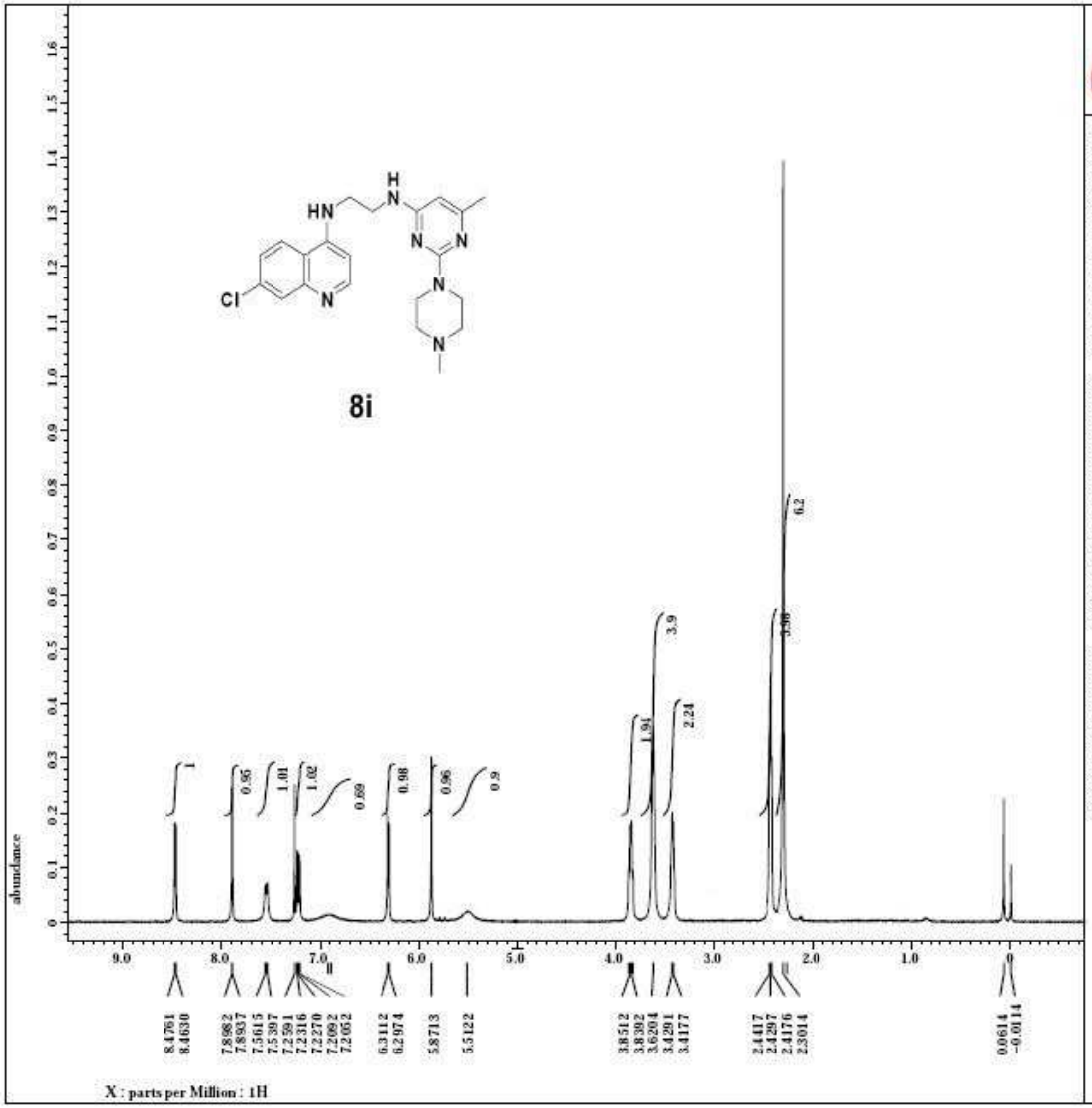


Filename	- DSR_SM-506_PROTON-5.j
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SM-506
Solvent	- CHLOROFORM-D
Creation_time	- 10-DEC-2010 13:56:08
Revision_time	- 23-JUN-2011 23:44:58
Current_time	- 23-JUN-2011 23:45:58
Comment	- DSR SM-506
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.36577024[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.73218757[Hz]
X_sweep	- 11.99616123[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.57[us]
X_acq_time	- 1.36577024[s]
X_angle	- 45[deg]
X_atn	- 5[dB]
X_pulse	- 5.785[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 28
Relaxation_delay	- 4[s]
Repetition_time	- 5.36577024[s]
Temp_get	- 20.9[dc]

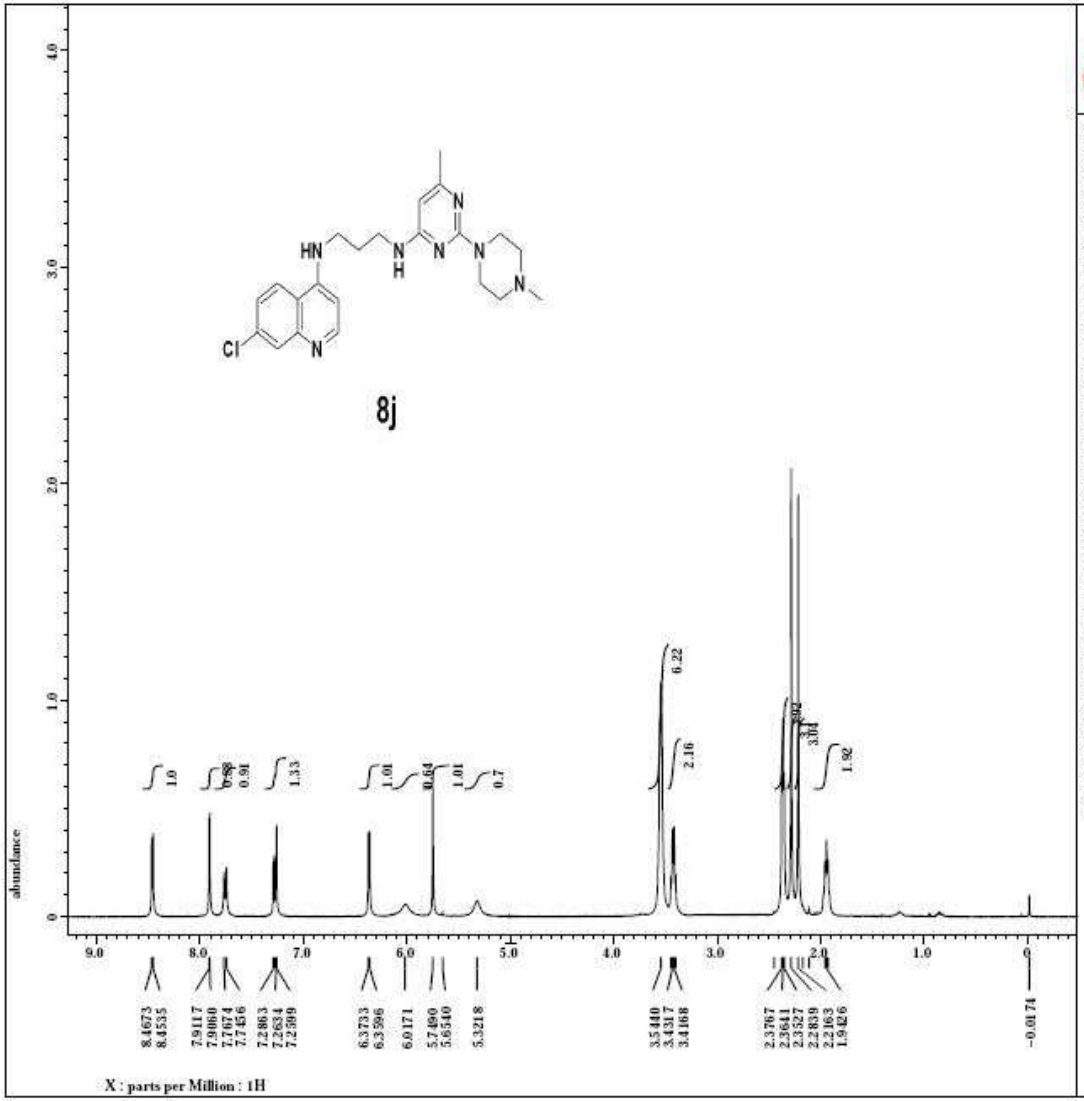


JEOL

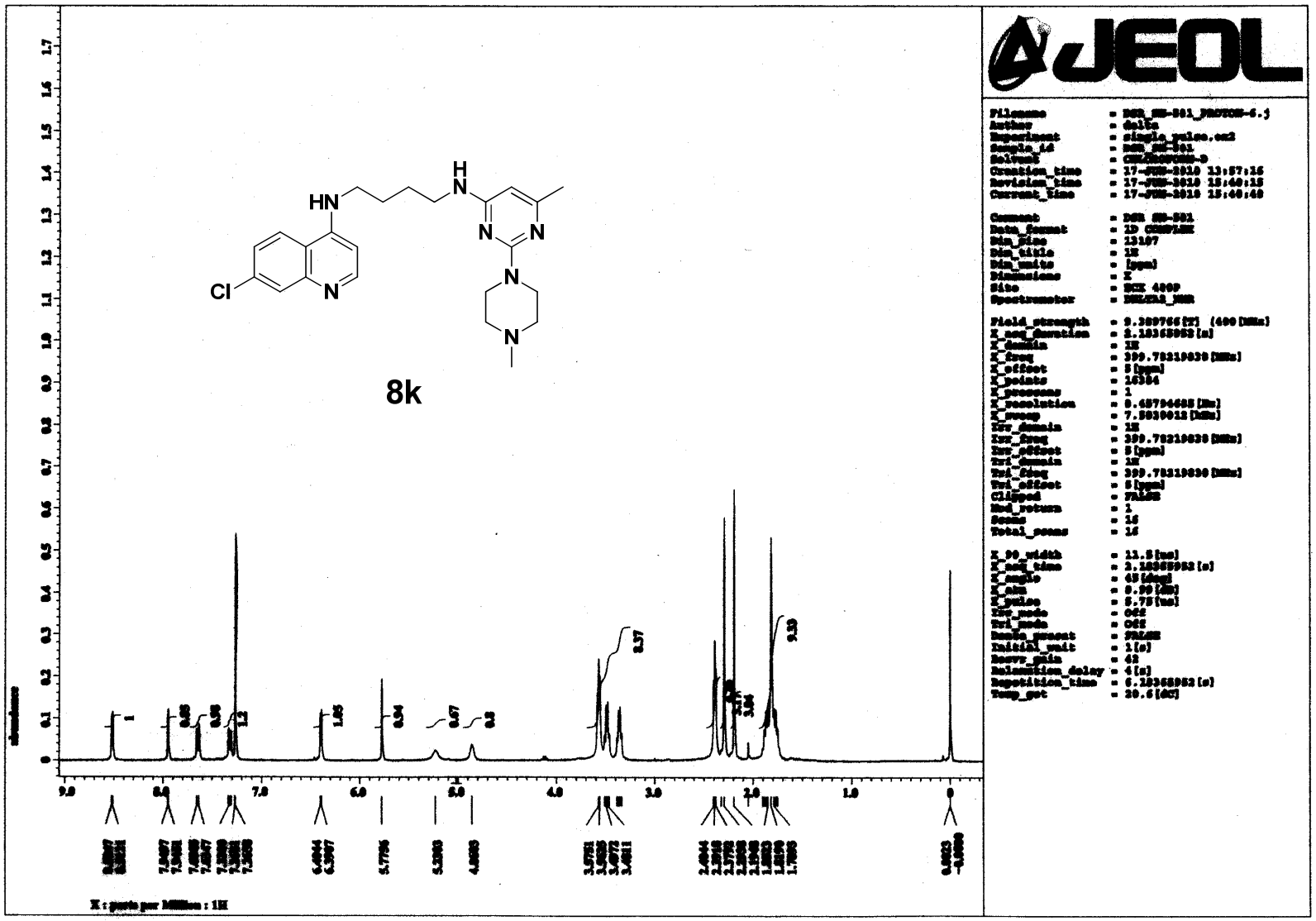
Filename	- DSR_SM-506_CARBON-4.j
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- DSR_SM-506
Solvent	- CHLOROFORM-D
Creation_time	- 9-DEC-2010 00:18:00
Revision_time	- 23-JUN-2011 23:20:22
Current_time	- 23-JUN-2011 23:22:00
Comment	- DSR SM-506
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32768
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 750
Total_scans	- 750
X_90_width	- 11.75[us]
X_acq_time	- 1.04333312[s]
X_angle	- 30[deg]
X_atn	- 10[dB]
X_pulse	- 3.91666667[us]
Irr_atn_dec	- 24.95[dB]
Irr_atn_noe	- 24.95[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 58
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 21.4[dC]



Filename	- DSR SM-491-3.jdf
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR SM-491
Solvent	- CHLOROFORM-D
Creation_time	- 1-JUN-2010 14:14:28
Revision_time	- 1-JUN-2010 12:38:55
Current_time	- 1-JUN-2010 12:39:14
Comment	- DSR SM-491
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 4.36731904[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 32768
X_prescans	- 1
X_resolution	- 0.22897343[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 4.36731904[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 36
Relaxation_delay	- 5[s]
Repetition_time	- 9.36731904[s]
Temp_get	- 24[dC]



Filename	- DSR_SM-494_PROTON-5.j
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SM-494
Solvent	- CHLOROFORM-D
Creation_time	- 8-JUN-2010 15:47:54
Revision_time	- 8-JUN-2010 14:52:54
Current_time	- 8-JUN-2010 14:54:02
Comment	- DSR SM-494
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 34
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 23.6[dC]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0.85
1.12
1.05
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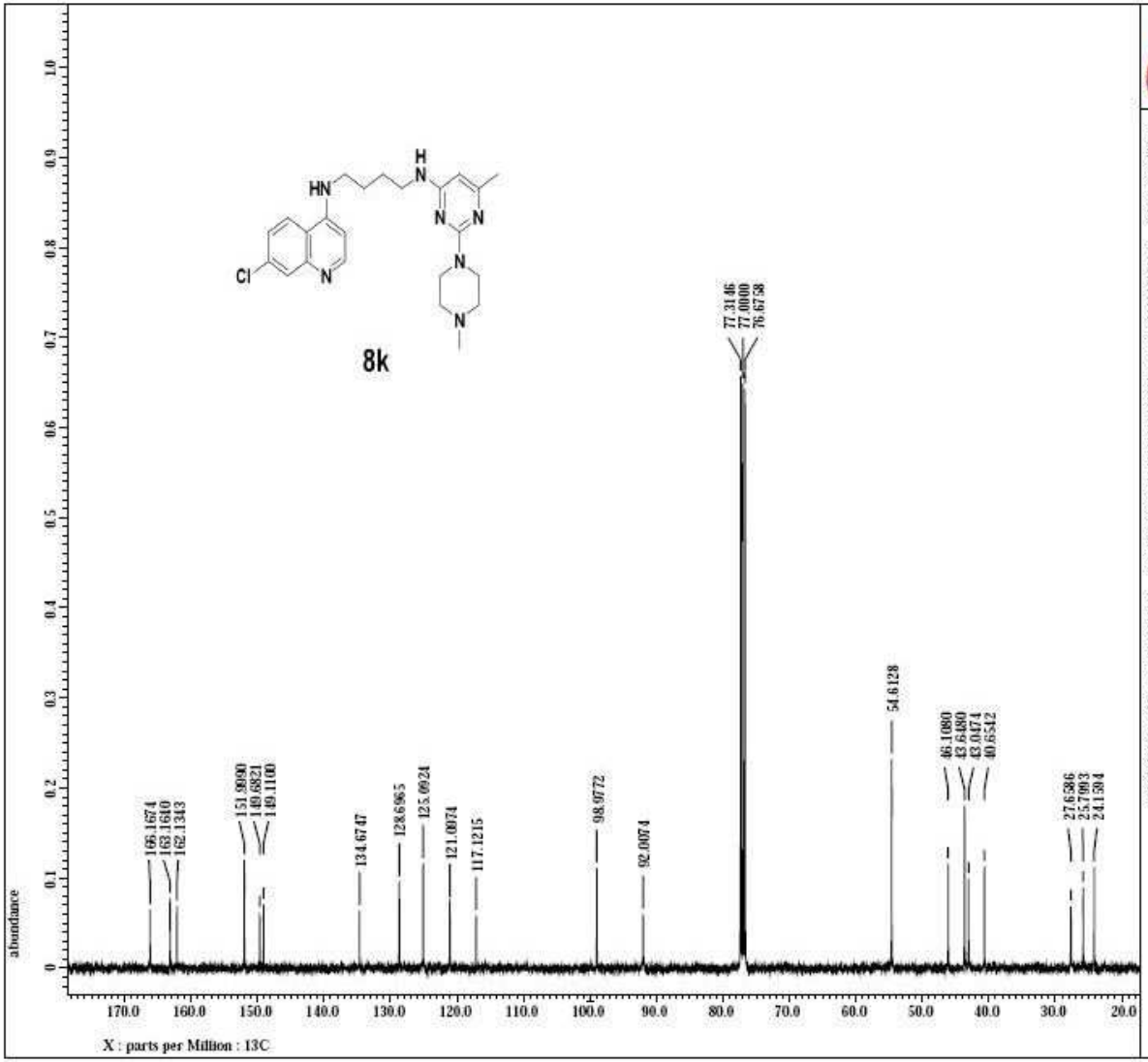
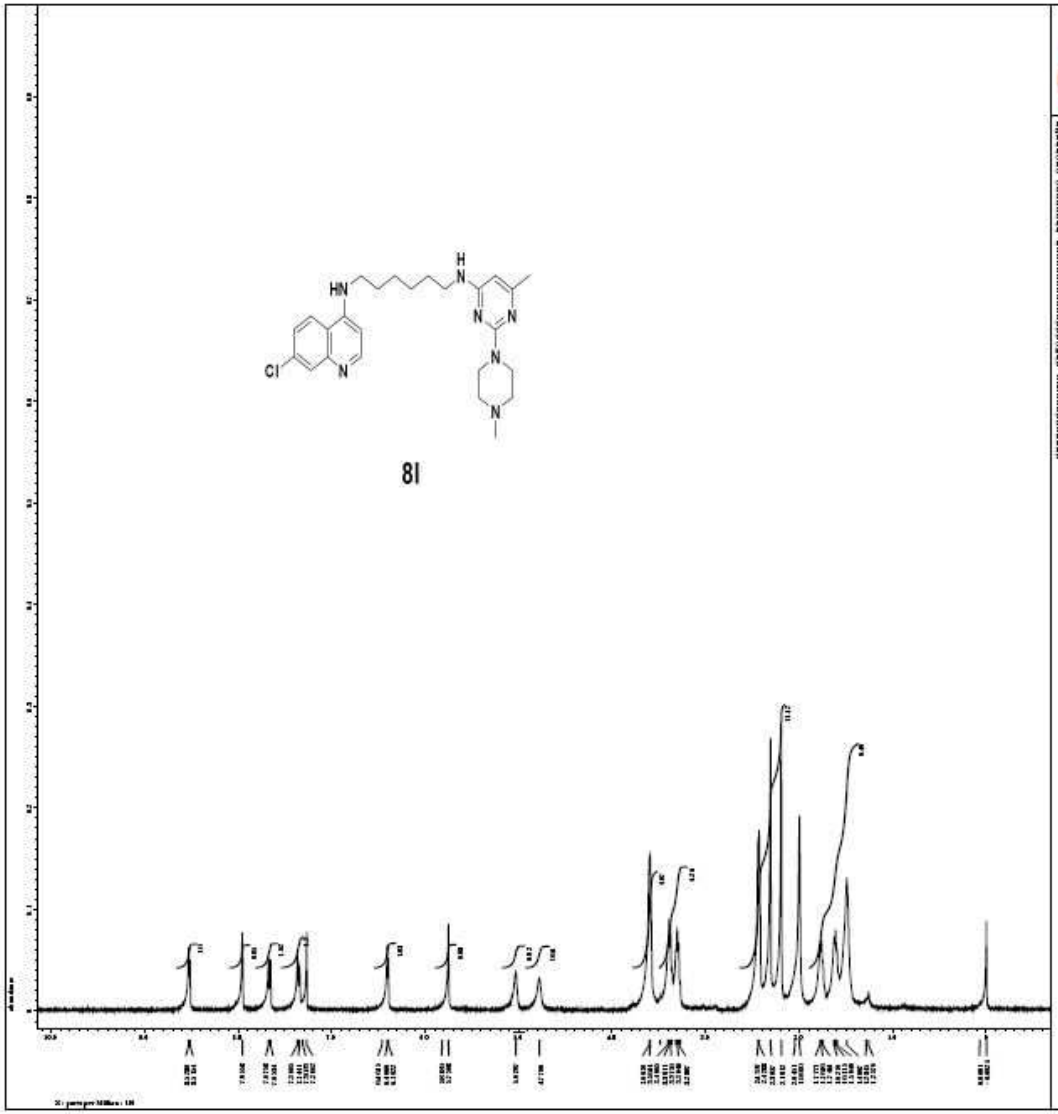
0.87
0.8
3.57
3.39
3.04
X : parts per Million : 1H



JEOL

Filename	- DSR_SM-501_CARBON-3.j
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- DSR_SM-501
Solvent	- CHLOROFORM-D
Creation_time	- 4-DEC-2010 02:56:53
Revision_time	- 3-DEC-2010 23:27:09
Current_time	- 23-JUN-2011 23:09:16
Comment	- DSR SM-501
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32768
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 750
Total_scans	- 750
X_90_width	- 11.75[us]
X_acq_time	- 1.04333312[s]
X_angle	- 30[deg]
X_atn	- 10[dB]
X_pulse	- 3.91666667[us]
Irr_atn_dec	- 24.95[dB]
Irr_atn_noe	- 24.95[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 60
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 22.1[dC]



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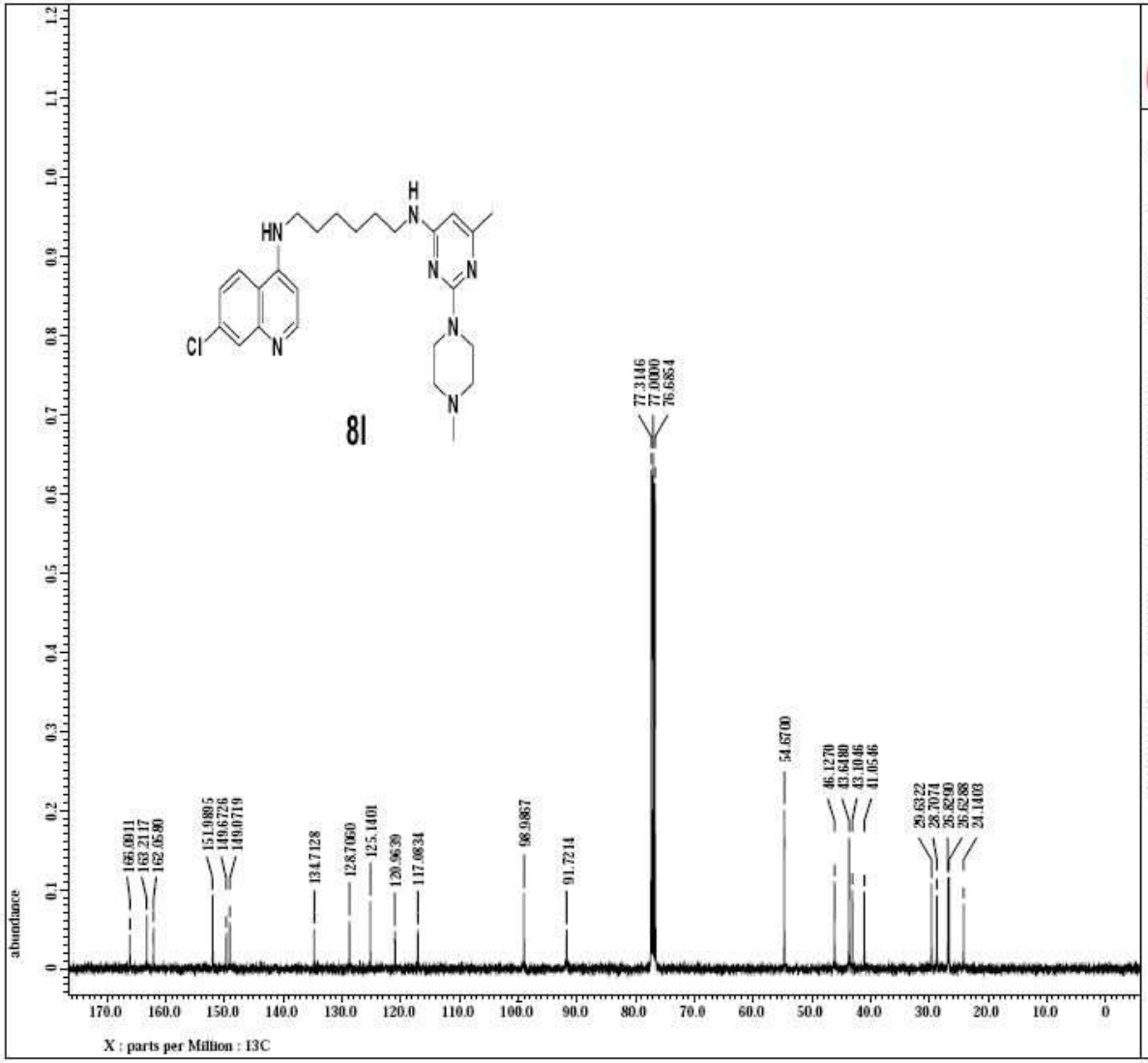
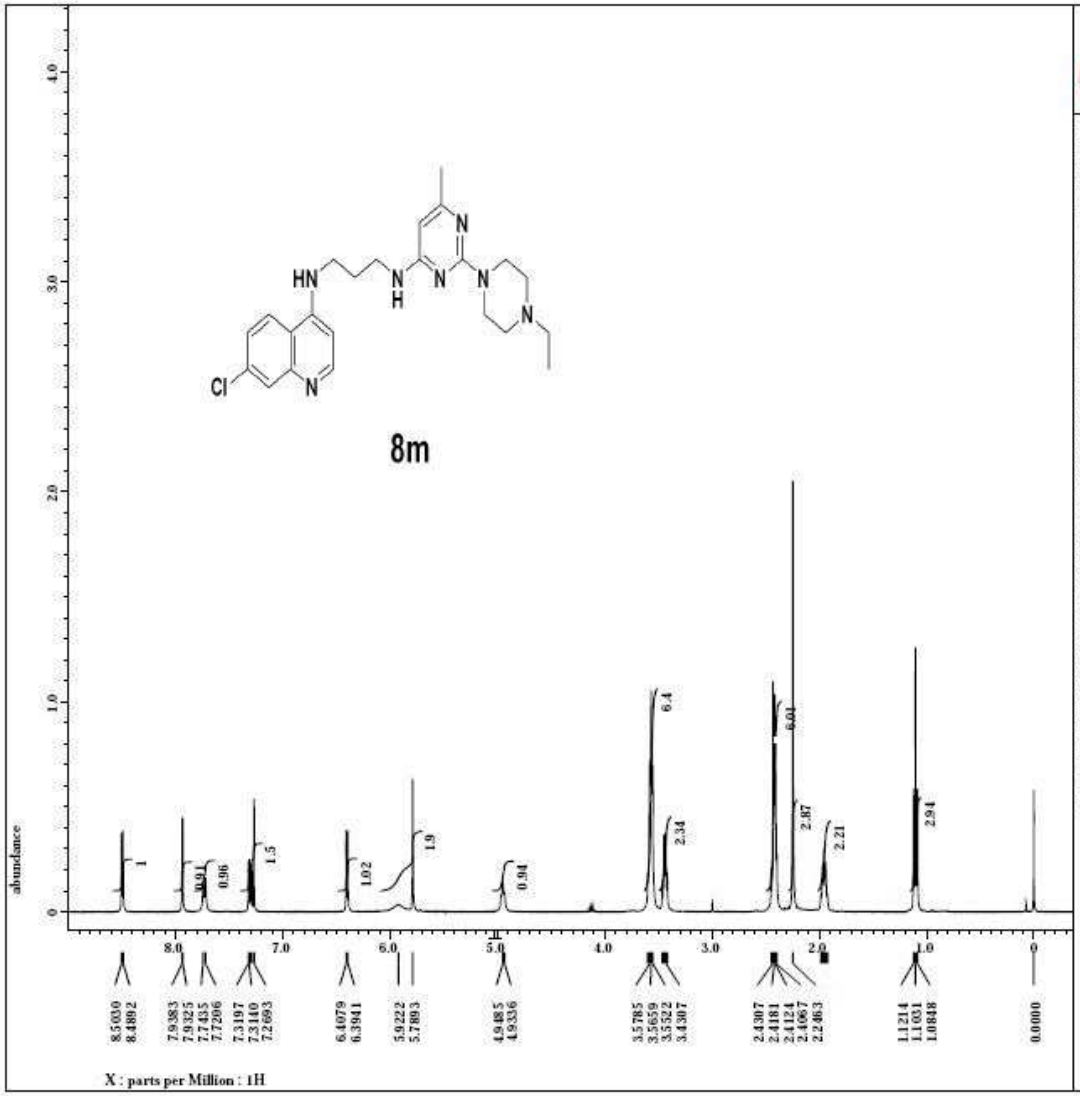


Filename	- DSR_SM-507_CARBON-3.j
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- DSR_SM-507
Solvent	- CHLOROFORM-D
Creation_time	- 8-DEC-2010 01:59:14
Revision_time	- 7-DEC-2010 22:29:22
Current_time	- 23-JUN-2011 23:24:51
Comment	- DSR SM-507
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32769
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 750
Total_scans	- 750
X_90_width	- 11.75[us]
X_acq_time	- 1.04333312[s]
X_angle	- 30[deg]
X_atn	- 10[dB]
X_pulse	- 3.91666667[us]
Irr_atn_dec	- 24.95[dB]
Irr_atn_noe	- 24.95[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 60
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 21.4[dC]




```
Filename          - DSR_SM-497A_PROTON-6.
Author            - delta
Experiment        - single_pulse.ex2
Sample_id         - DSR_SM-497A
Solvent           - CHLOROFORM-D
Creation_time     - 14-JUN-2010 16:31:05
Revision_time     - 14-JUN-2010 15:58:30
Current_time      - 14-JUN-2010 15:58:59

Comment           - DSR SM-497A
Data_format       - 1D COMPLEX
Dim_size          - 13107
Dim_title         - 1H
Dim_units         - [ppm]
Dimensions        - X
Site              - ECX 400P
Spectrometer      - DELTA2_NMR

Field_strength    - 9.389766[T] (400[MHz]
X_acq_duration    - 2.18365952[s]
X_domain          - 1H
X_freq            - 399.78219838[MHz]
X_offset          - 5[ppm]
X_points          - 16384
X_prescans        - 1
X_resolution      - 0.45794685[Hz]
X_sweep           - 7.5030012[kHz]
Irr_domain        - 1H
Irr_freq          - 399.78219838[MHz]
Irr_offset        - 5[ppm]
Tri_domain        - 1H
Tri_freq          - 399.78219838[MHz]
Tri_offset        - 5[ppm]
Clipped           - FALSE
Mod_return        - 1
Scans             - 16
Total_scans       - 16

X_90_width        - 11.5[us]
X_acq_time        - 2.18365952[s]
X_angle           - 45[deg]
X_atn             - 0.99[dB]
X_pulse           - 5.75[us]
Irr_mode          - Off
Tri_mode          - Off
Dante_presat      - FALSE
Initial_wait      - 1[s]
Recvr_gain        - 36
Relaxation_delay  - 4[s]
Repetition_time   - 6.18365952[s]
Temp_get          - 24.5[dC]
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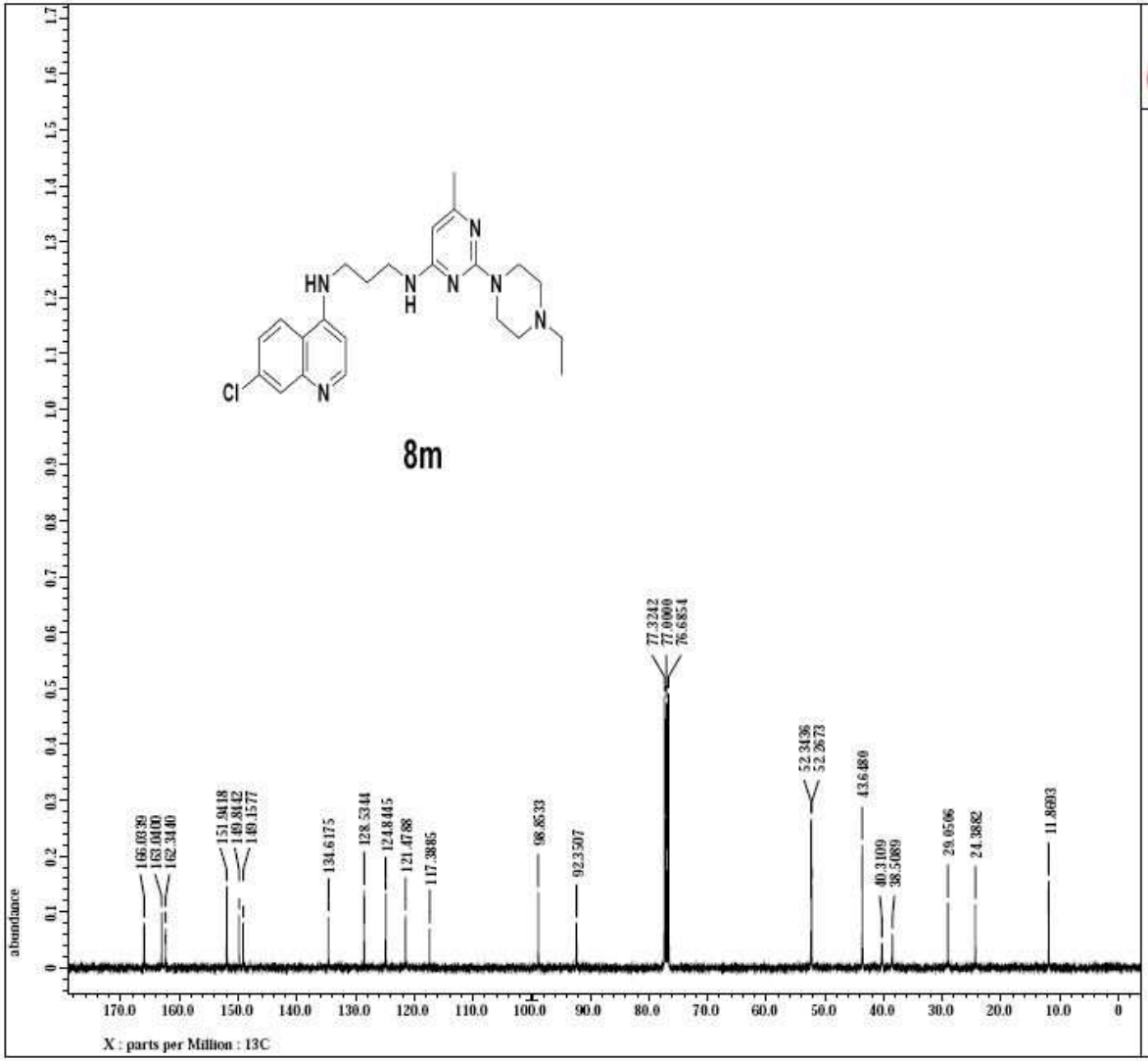
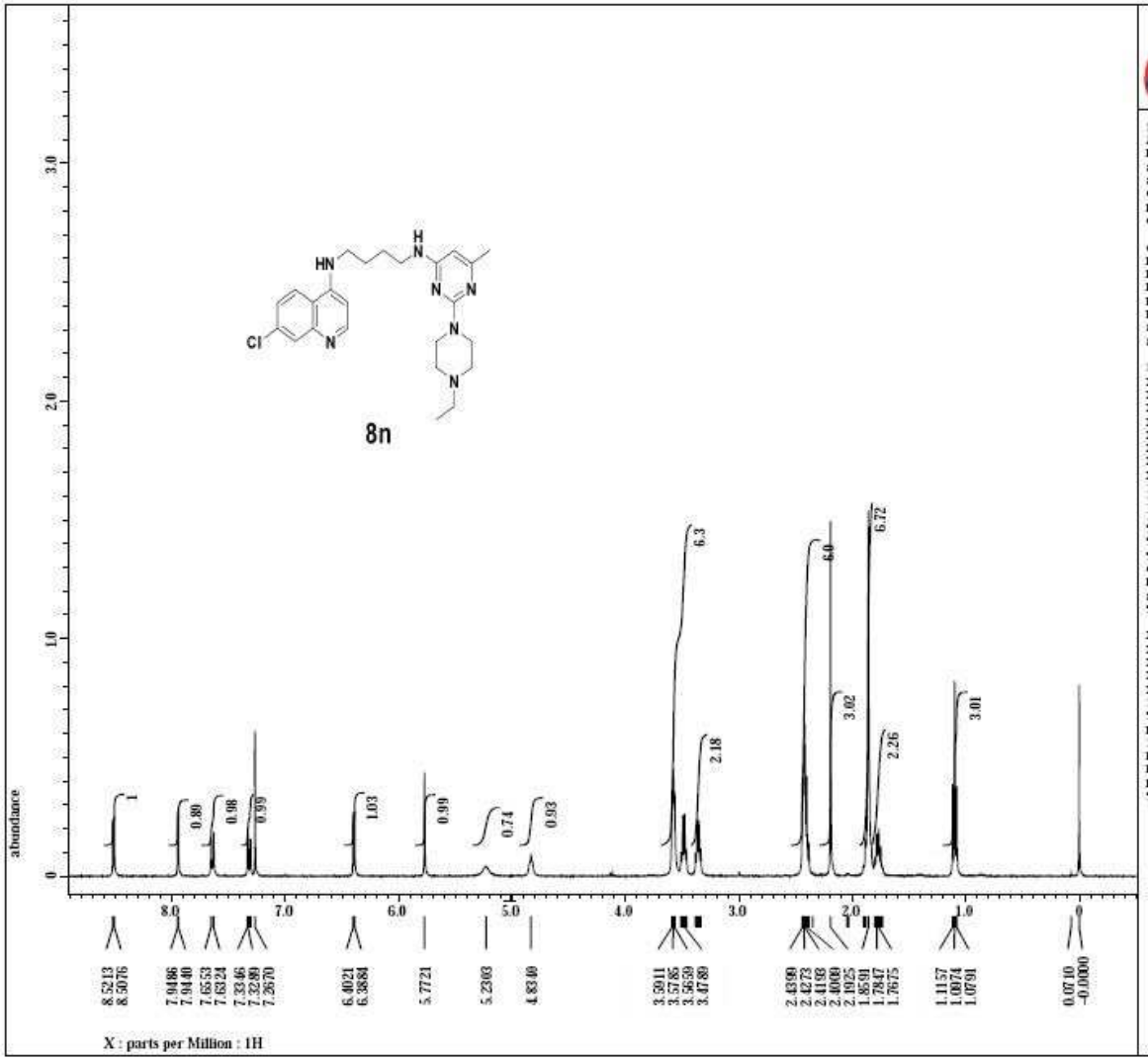


JEOL

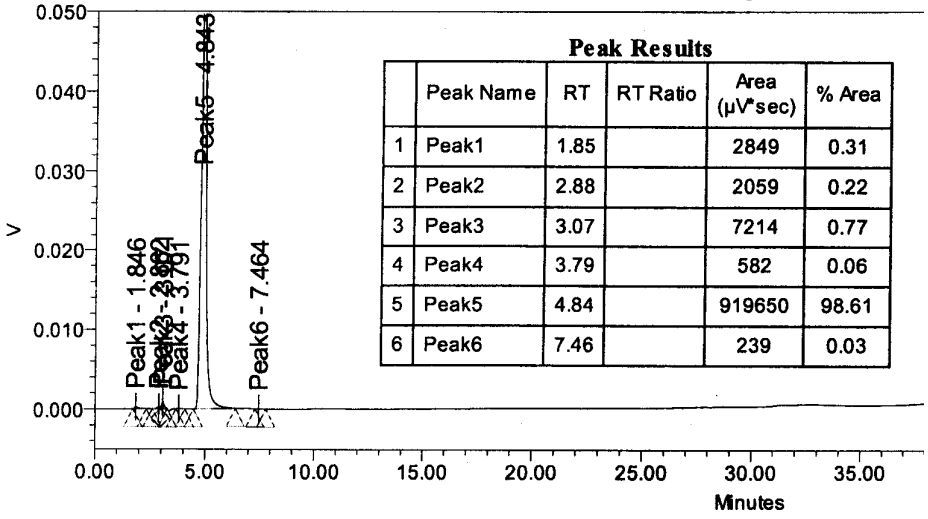
Filename	- DSR_SM-497_CARBON-4.j
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- DSR_SM-497
Solvent	- CHLOROFORM-D
Creation_time	- 30-NOV-2010 21:46:36
Revision_time	- 1-DEC-2010 22:20:11
Current_time	- 1-DEC-2010 22:20:59
Comment	- DSR SM-497
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DELTA2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32768
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 750
Total_scans	- 750
X_90_width	- 11.75[us]
X_acq_time	- 1.04333312[s]
X_angle	- 30[deg]
X_atn	- 10[dB]
X_pulse	- 3.91666667[us]
Irr_atn_dec	- 24.95[dB]
Irr_atn_noe	- 24.95[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 58
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 22.4[dC]



JEOL

Filename	- DSR_SN-502_PROTON-5.j
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- DSR_SN-502
Solvent	- CHLOROFORM-D
Creation_time	- 21-JUN-2010 13:49:54
Revision_time	- 28-JUN-2010 10:44:36
Current_time	- 28-JUN-2010 10:44:58
Comment	- DSR SN-502
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- ECX 400P
Spectrometer	- DEL7A2_NMR
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 2.18365952[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 5[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.45794685[Hz]
X_sweep	- 7.5030012[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 16
Total_scans	- 16
X_90_width	- 11.5[us]
X_acq_time	- 2.18365952[s]
X_angle	- 45[deg]
X_atn	- 0.99[dB]
X_pulse	- 5.75[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 42
Relaxation_delay	- 4[s]
Repetition_time	- 6.18365952[s]
Temp_get	- 21.7[dC]

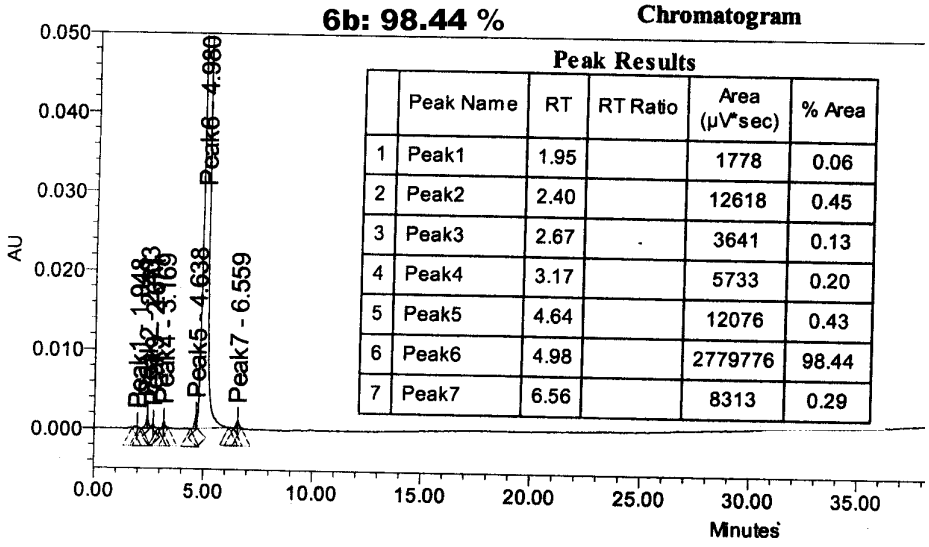
6a; 98.61 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.85		2849	0.31
2	Peak2	2.88		2059	0.22
3	Peak3	3.07		7214	0.77
4	Peak4	3.79		582	0.06
5	Peak5	4.84		919650	98.61
6	Peak6	7.46		239	0.03

6b: 98.44 % **Chromatogram**

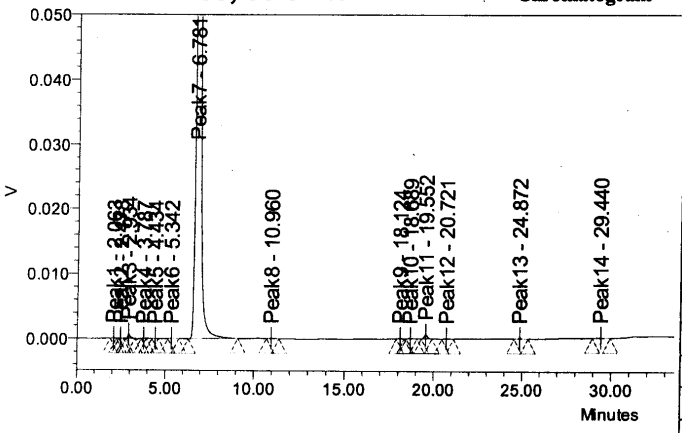


Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.95		1778	0.06
2	Peak2	2.40		12618	0.45
3	Peak3	2.67		3641	0.13
4	Peak4	3.17		5733	0.20
5	Peak5	4.64		12076	0.43
6	Peak6	4.98		2779776	98.44
7	Peak7	6.56		8313	0.29

6c; 99.02 %

Chromatogram

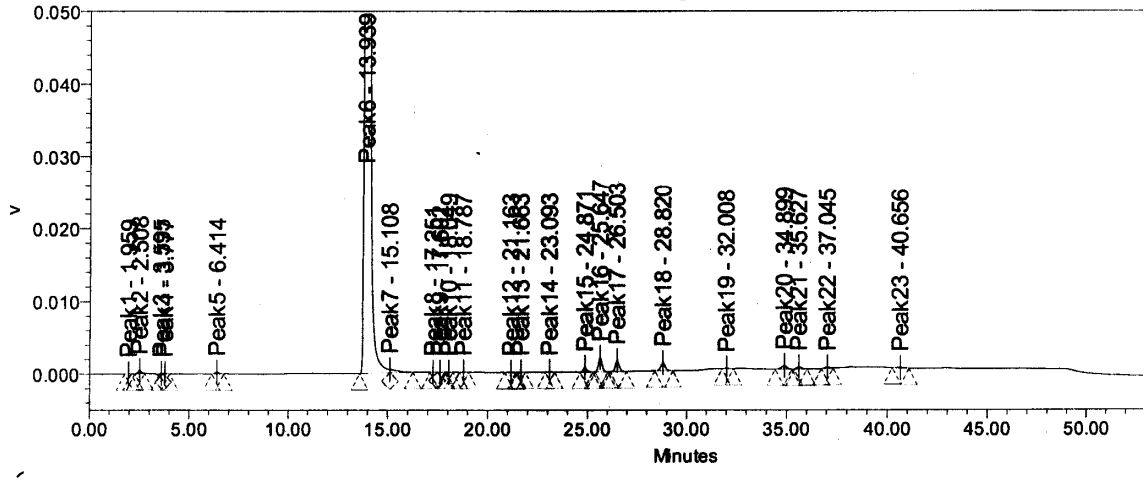


Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	2.06		664	0.03
2	Peak2	2.48		186	0.01
3	Peak3	2.93		5624	0.27
4	Peak4	3.79		166	0.01
5	Peak5	4.43		210	0.01
6	Peak6	5.34		577	0.03
7	Peak7	6.78		2064967	99.02
8	Peak8	10.96		564	0.03
9	Peak9	18.12		857	0.04
10	Peak10	18.69		624	0.03
11	Peak11	19.55		8048	0.39
12	Peak12	20.72		627	0.03
13	Peak13	24.87		1285	0.06
14	Peak14	29.44		1036	0.05

6d; 97.17 %

Chromatogram

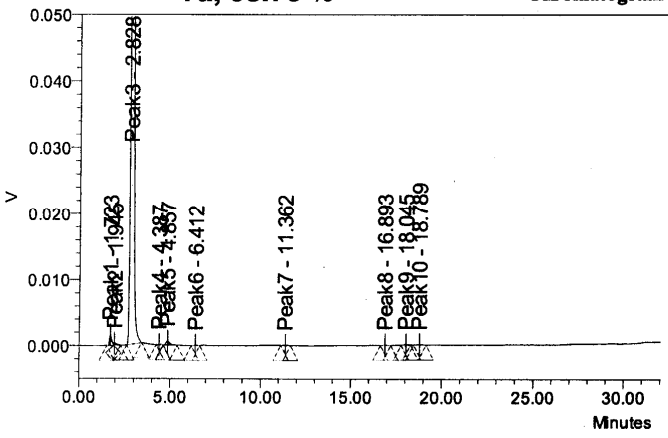


Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.96		296	0.01
2	Peak2	2.51		4703	0.12
3	Peak3	3.60		665	0.02
4	Peak4	3.78		833	0.02
5	Peak5	6.41		3240	0.08
6	Peak6	13.94		3829961	97.17
7	Peak7	15.11		12004	0.30
8	Peak8	17.25		192	0.00
9	Peak9	17.60		283	0.01
10	Peak10	18.05		204	0.01
11	Peak11	18.79		526	0.01
12	Peak12	21.16		576	0.01
13	Peak13	21.66		425	0.01
14	Peak14	23.09		299	0.01

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
15	Peak15	24.87		7383	0.19
16	Peak16	25.65		24543	0.62
17	Peak17	26.50		20190	0.51
18	Peak18	28.82		16687	0.42
19	Peak19	32.01		615	0.02
20	Peak20	34.90		8828	0.22
21	Peak21	35.63		4569	0.12
22	Peak22	37.05		2684	0.07
23	Peak23	40.66		1633	0.04

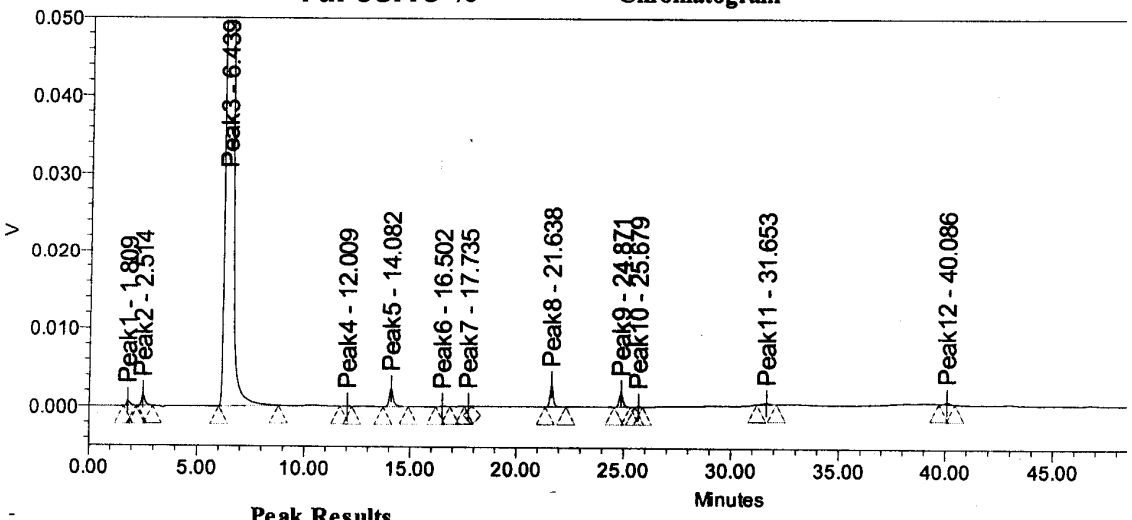
7a; 98.76 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.72		13108	0.60
2	Peak2	1.95		3551	0.16
3	Peak3	2.83		2153620	98.76
4	Peak4	4.39		478	0.02
5	Peak5	4.86		7907	0.36
6	Peak6	6.41		355	0.02
7	Peak7	11.36		261	0.01
8	Peak8	16.89		321	0.01
9	Peak9	18.04		376	0.02
10	Peak10	18.79		746	0.03

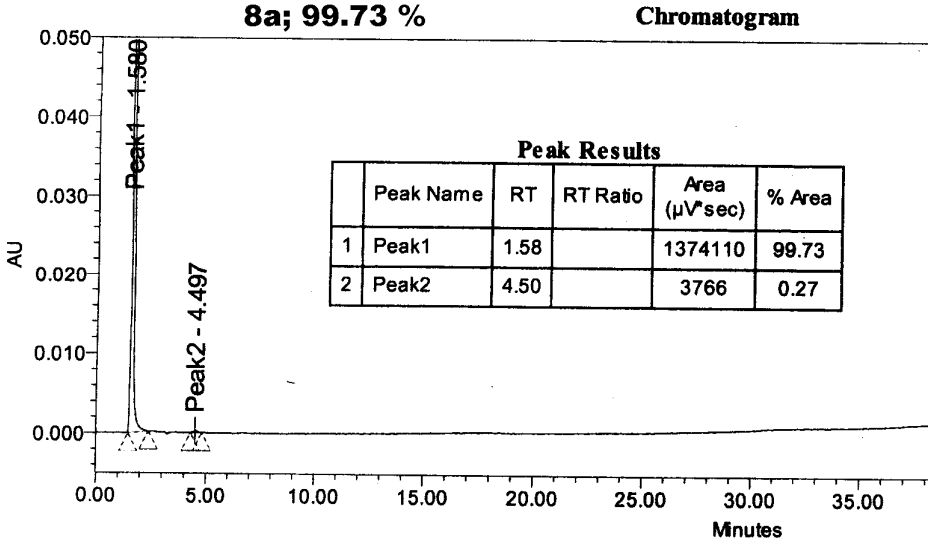
7d: 98.16 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.81		6690	0.11
2	Peak2	2.51		15914	0.26
3	Peak3	6.44		6017415	98.16
4	Peak4	12.01		612	0.01
5	Peak5	14.08		31038	0.51
6	Peak6	16.50		321	0.01
7	Peak7	17.74		320	0.01
8	Peak8	21.64		29870	0.49
9	Peak9	24.87		20706	0.34
10	Peak10	25.68		207	0.00
11	Peak11	31.65		3044	0.05
12	Peak12	40.09		3972	0.06

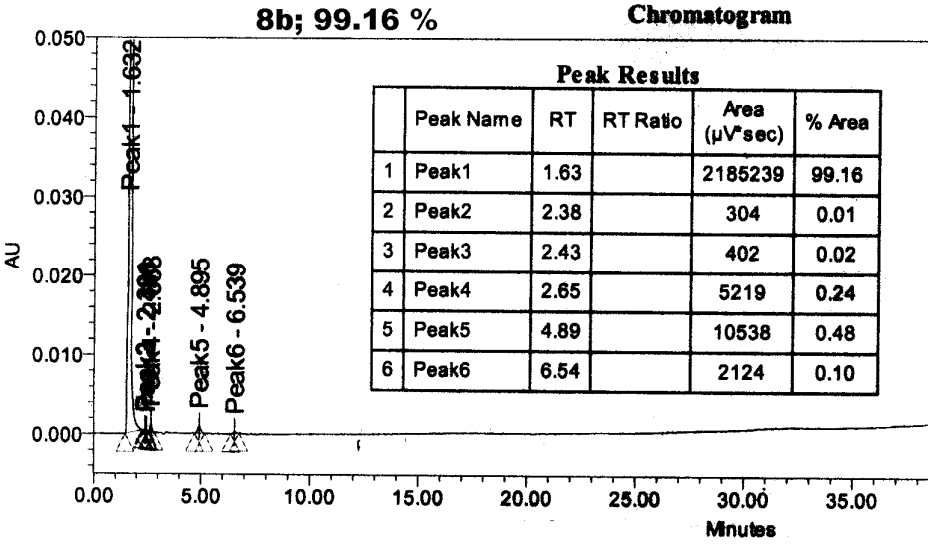
8a; 99.73 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.58		1374110	99.73
2	Peak2	4.50		3766	0.27

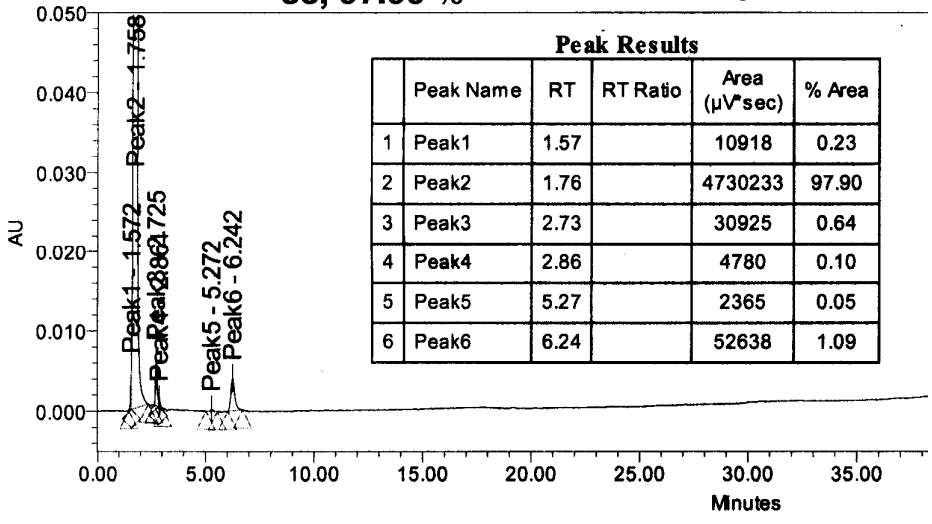
8b; 99.16 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.63		2185239	99.16
2	Peak2	2.38		304	0.01
3	Peak3	2.43		402	0.02
4	Peak4	2.65		5219	0.24
5	Peak5	4.89		10538	0.48
6	Peak6	6.54		2124	0.10

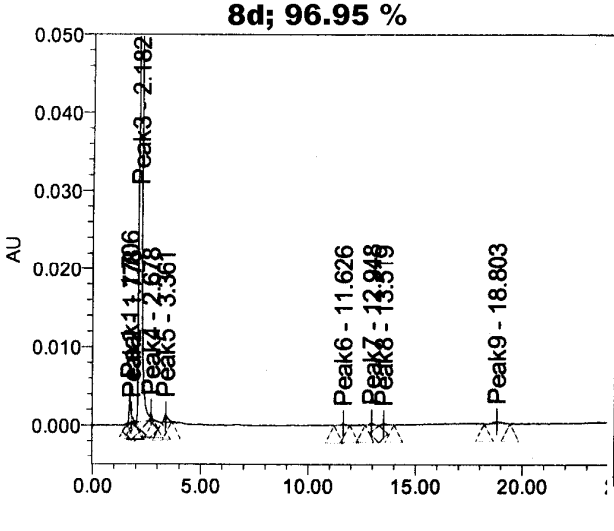
8c; 97.90 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.57		10918	0.23
2	Peak2	1.76		4730233	97.90
3	Peak3	2.73		30925	0.64
4	Peak4	2.86		4780	0.10
5	Peak5	5.27		2365	0.05
6	Peak6	6.24		52638	1.09

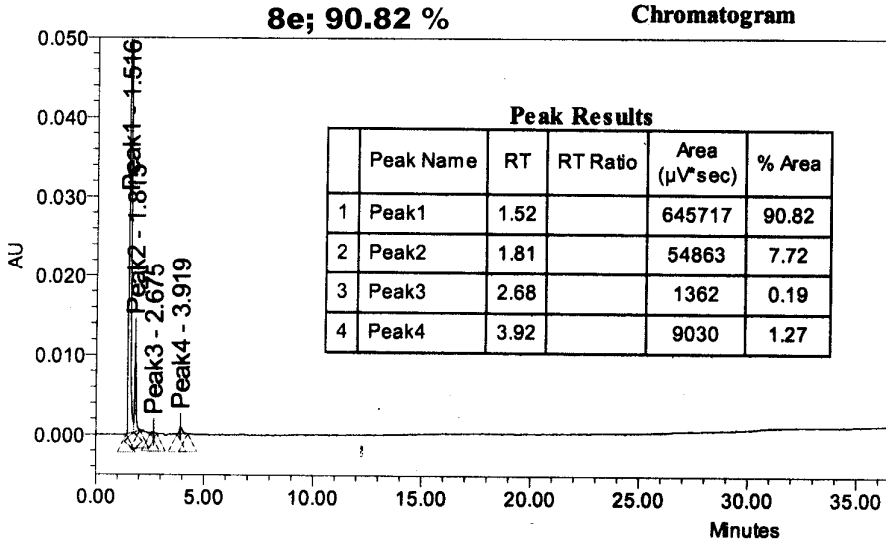
8d; 96.95 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.71		15687	0.95
2	Peak2	1.78		3095	0.19
3	Peak3	2.18		1608654	96.95
4	Peak4	2.68		6264	0.38
5	Peak5	3.36		10584	0.64
6	Peak6	11.63		2143	0.13
7	Peak7	12.95		3093	0.19
8	Peak8	13.52		2515	0.15
9	Peak9	18.80		7200	0.43

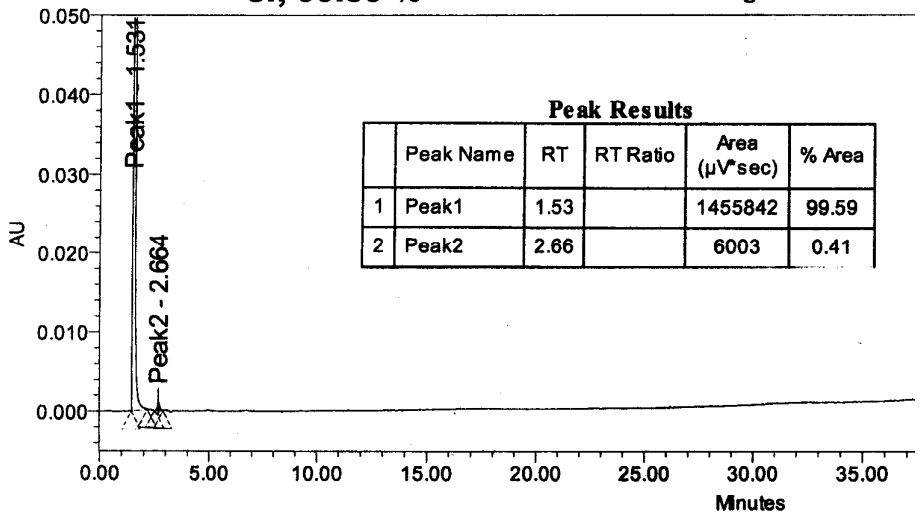
8e; 90.82 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.52		645717	90.82
2	Peak2	1.81		54863	7.72
3	Peak3	2.68		1362	0.19
4	Peak4	3.92		9030	1.27

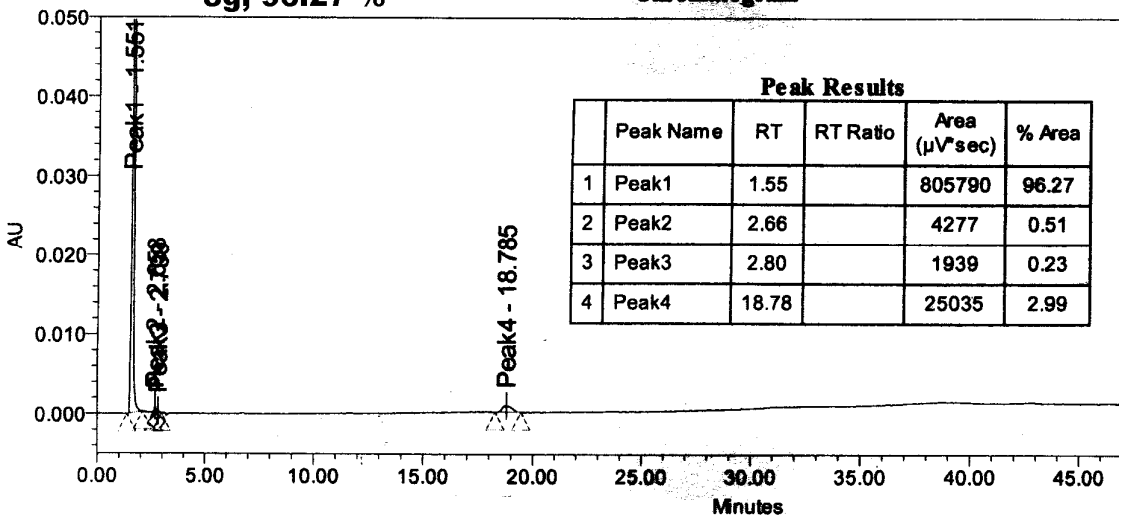
8f; 99.59 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.53		1455842	99.59
2	Peak2	2.66		6003	0.41

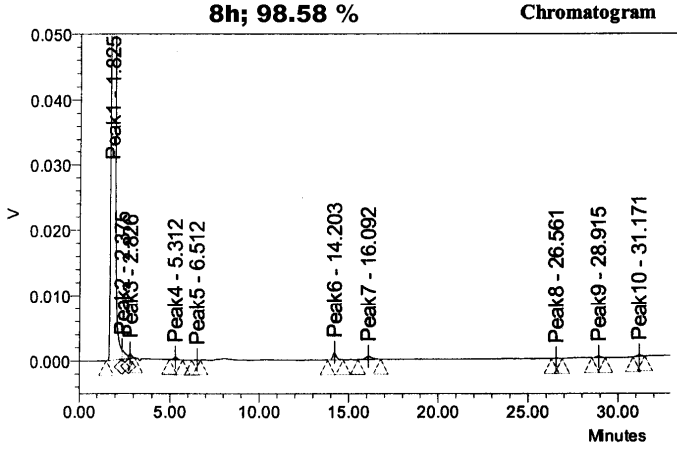
8g; 96.27 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.55		805790	96.27
2	Peak2	2.66		4277	0.51
3	Peak3	2.80		1939	0.23
4	Peak4	18.78		25035	2.99

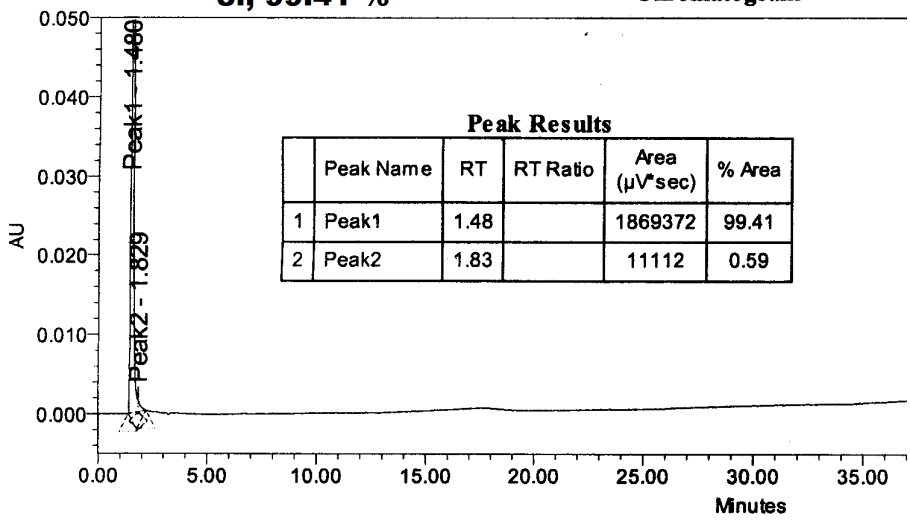
8h; 98.58 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.83		4574316	98.58
2	Peak2	2.38		18656	0.40
3	Peak3	2.83		8219	0.18
4	Peak4	5.31		4662	0.10
5	Peak5	6.51		722	0.02
6	Peak6	14.20		15023	0.32
7	Peak7	16.09		11664	0.25
8	Peak8	26.56		904	0.02
9	Peak9	28.92		3204	0.07
10	Peak10	31.17		3070	0.07

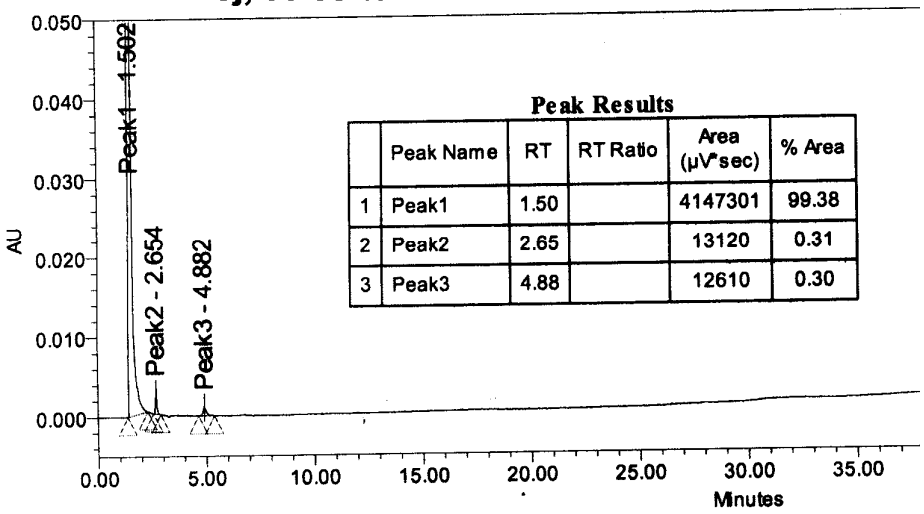
8i; 99.41 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.48		1869372	99.41
2	Peak2	1.83		11112	0.59

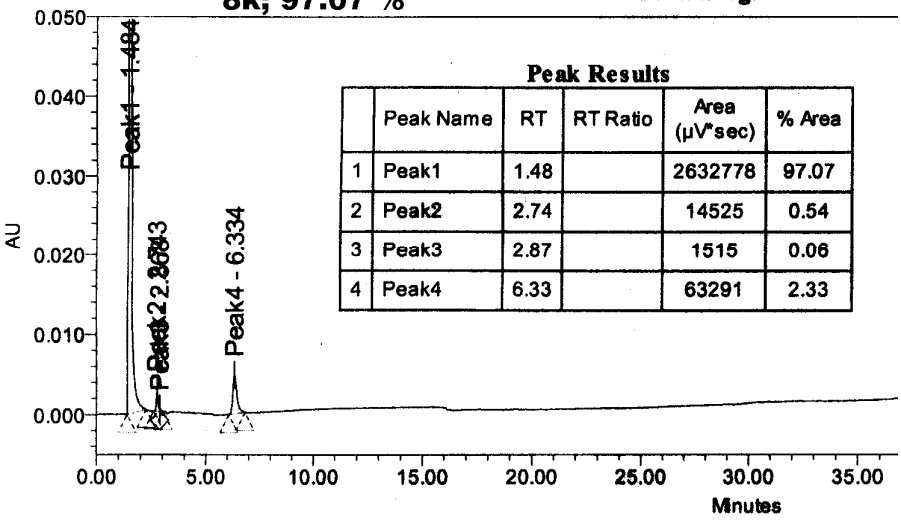
8j; 99.38 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.50		4147301	99.38
2	Peak2	2.65		13120	0.31
3	Peak3	4.88		12610	0.30

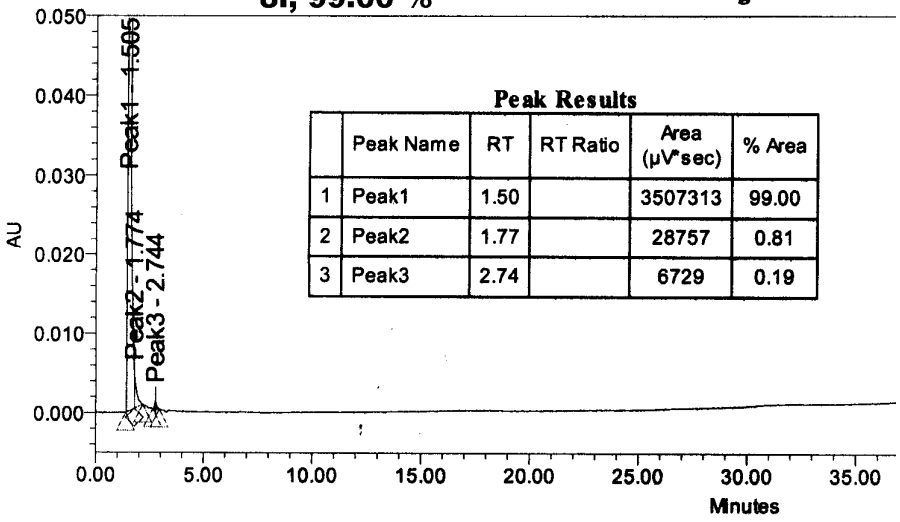
8k; 97.07 % **Chromatogram**



Peak Results

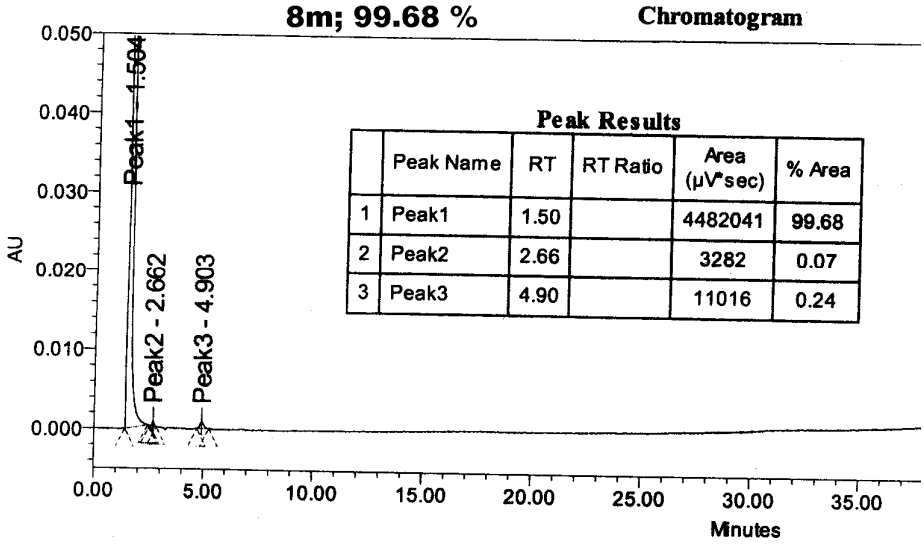
	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.48		2632778	97.07
2	Peak2	2.74		14525	0.54
3	Peak3	2.87		1515	0.06
4	Peak4	6.33		63291	2.33

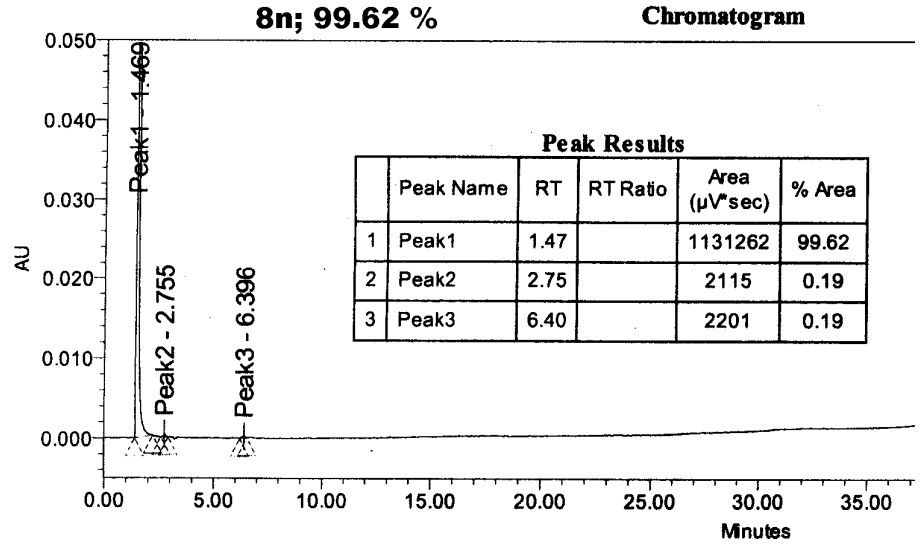
8l; 99.00 % **Chromatogram**



Peak Results

	Peak Name	RT	RT Ratio	Area (µV*sec)	% Area
1	Peak1	1.50		3507313	99.00
2	Peak2	1.77		28757	0.81
3	Peak3	2.74		6729	0.19


8m; 99.68 %
Chromatogram
Peak Results
Peak Name | RT | RT Ratio | Area (µV*sec) | % Area
1 | Peak1 | 1.50 | | 4482041 | 99.68
2 | Peak2 | 2.66 | | 3282 | 0.07
3 | Peak3 | 4.90 | | 11016 | 0.24
Peak1 - 1.504
Peak2 - 2.662
Peak3 - 4.903
AU
0.050
0.040
0.030
0.020
0.010
0.000
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
Minutes


8n; 99.62 %
Chromatogram
Peak Results
Peak Name | RT | RT Ratio | Area (µV*sec) | % Area
1 | Peak1 | 1.47 | | 1131262 | 99.62
2 | Peak2 | 2.75 | | 2115 | 0.19
3 | Peak3 | 6.40 | | 2201 | 0.19
Peak1 - 1.469
Peak2 - 2.755
Peak3 - 6.396
AU
0.050
0.040
0.030
0.020
0.010
0.000
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
Minutes