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4-Aminoquinoline-pyrimidine-aminoalkanols: Synthesis, *in vitro* antimalarial activity, docking studies and ADME predictions

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Supplementary Information

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1. Experimental Protocol for Computational Studies

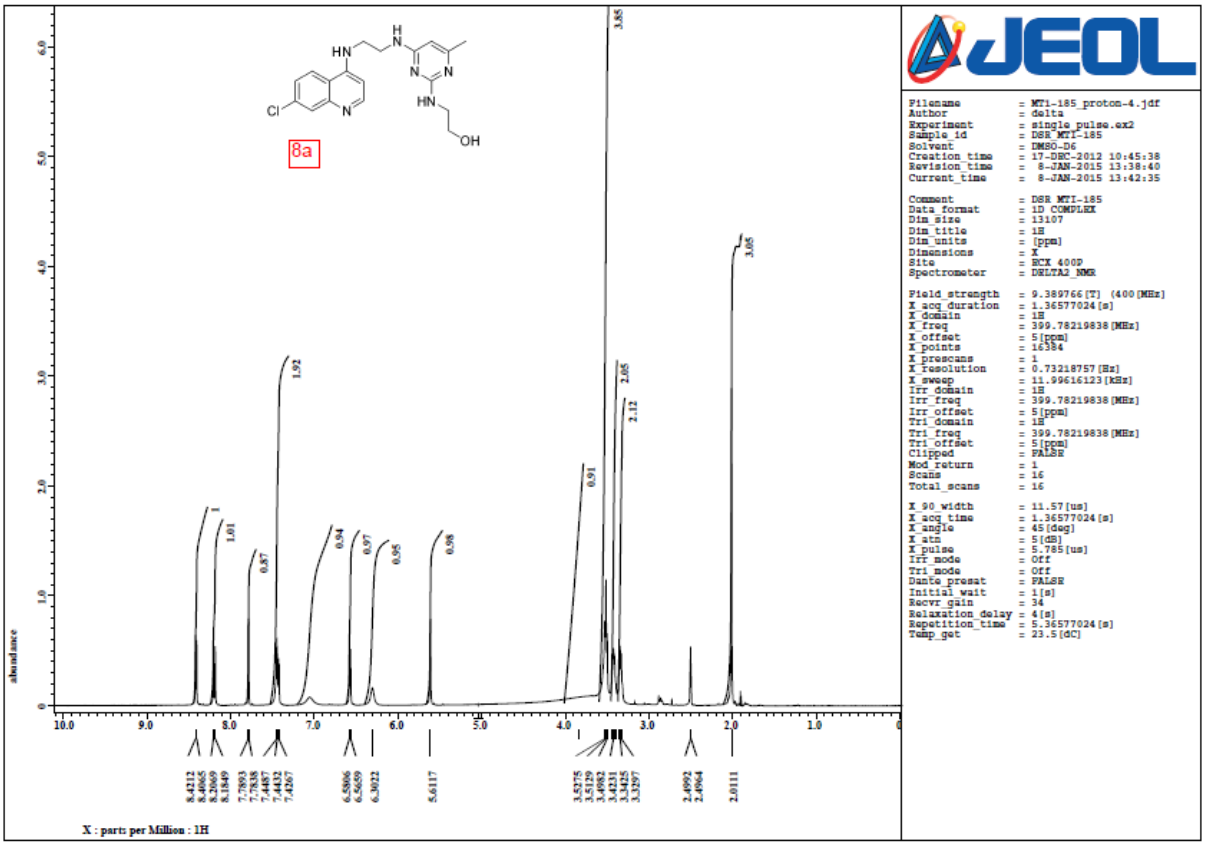
1.1 Docking studies

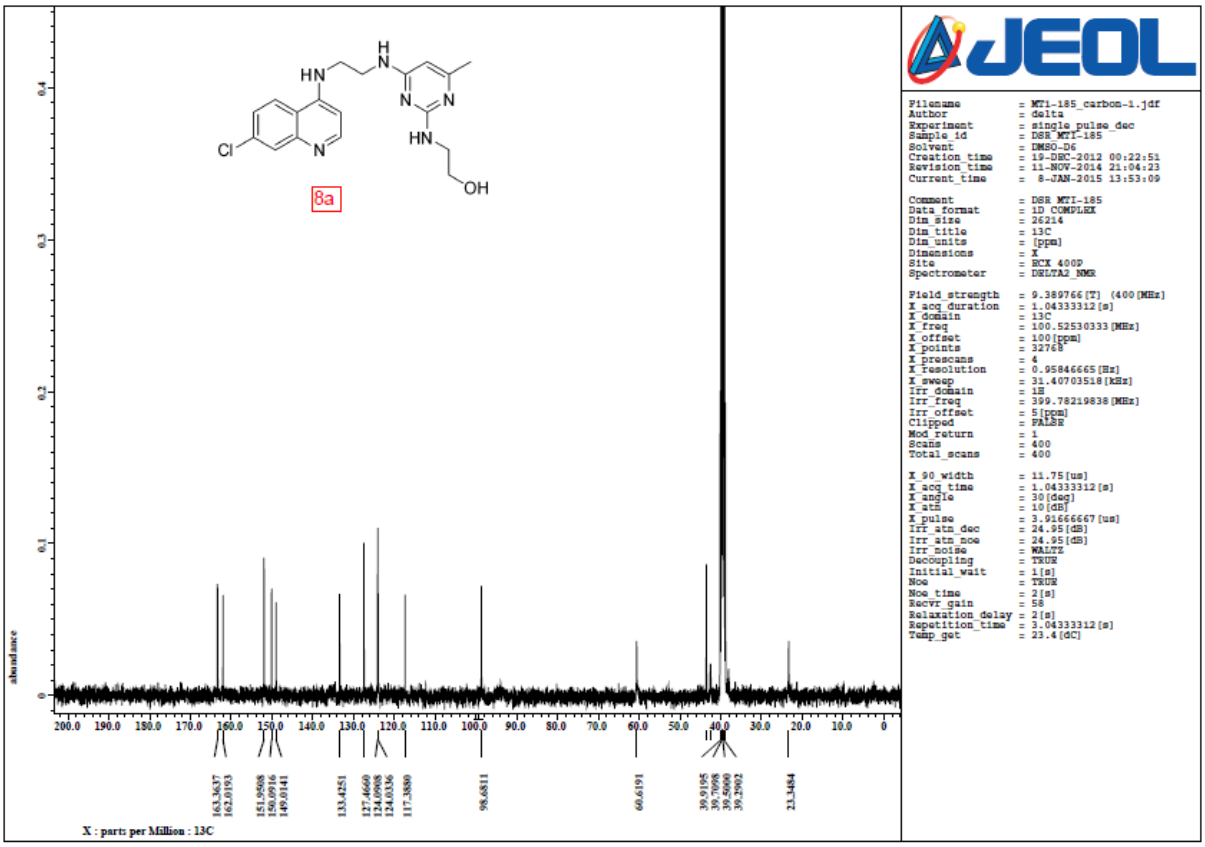
The 2D structures of the test compounds were generated using ChemBioDraw Ultra 12.0 (www.cambridgesoft.com) and the Ligprep module in Schrodinger was used to generate energy-minimized 3D structures. Partial atomic charges were computed using the OPLS_2005 force field. The correct Lewis structure, tautomers and ionization states (pH 7.0 $\pm$ 2.0) for each of these ligands were generated and optimized with default settings (Ligprep 2.5, Schro¨dinger, LLC, New York, NY, 2012). The 3D crystal structures of wild type PfDHFR-TS (PDB ID: 3QGT; resolution 2.30 Å) and quadruple mutant (N51I + C59R + S108N + I164L) PfDHFR-TS (PDB ID: 3QG2; resolution: 2.30 Å) were retrieved from the protein data bank (www.rcsb.org). The proteins were prepared for docking using the Protein Preparation Wizard (Maestro 10.0 Schro¨dinger, LLC, New York, NY, 2012). Water molecules within 5 Å of the protein structures were considered. Bond order and formal charges were assigned and hydrogen atoms were added to the crystal structure. To further refine the structure, an OPLS-2005 force field parameter was used to alleviate steric clashes and the minimization was terminated when RMSD reached a maximum cutoff value of 0.30 Å. The location of co-crystallized ligand pyrimethamine in both wild and mutant protein structures was used to choose the center and size of the receptor grid, which was generated using Glide 5.8 (Schro¨dinger, LLC, New York, NY, 2012) with default settings for all parameters. The grid size was chosen to be sufficiently large so as to include all active site residues involved in substrate binding. The cofactor NADH in the PfDHFR-TS wild and mutant structures was also considered as part of the receptor protein. All ligand conformers were docked to each of the receptor grid files (PfDHFR-TS wild and mutant structures) using Glide extra precision (XP)-mode. Default settings were used for the refinement and scoring.

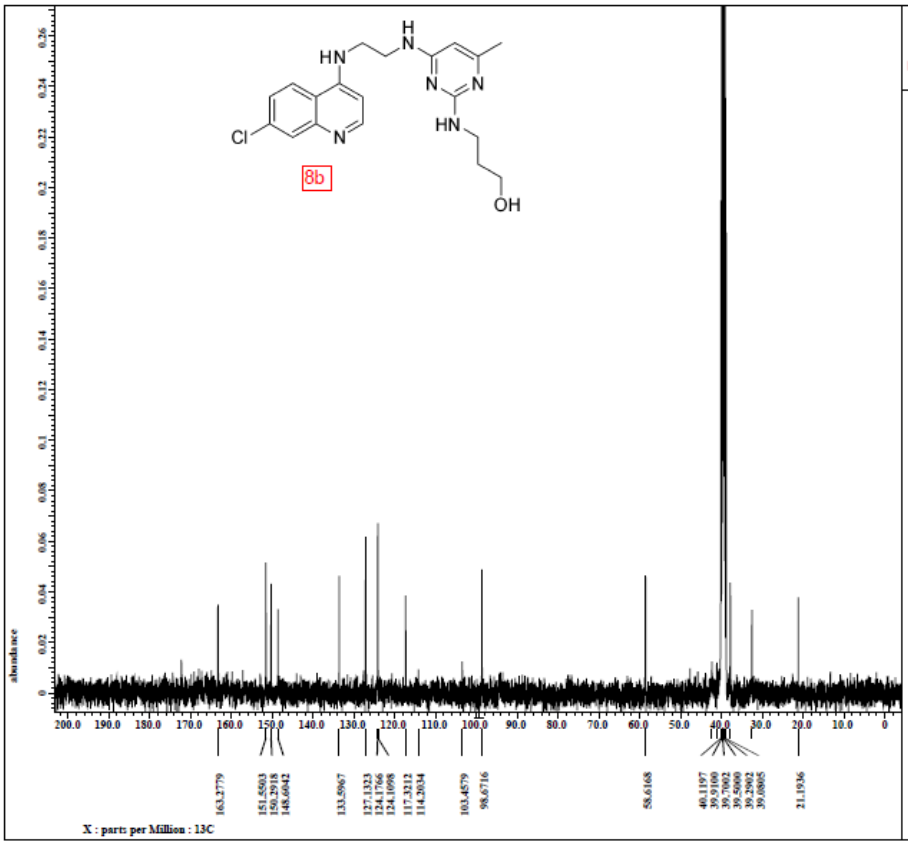
1.2 *In silico* ADMET prediction

All the 3D structures of the test compounds as prepared above by using LigPrep were used for the calculation of pharmacokinetic properties by QikProp v3.5. The program QikProp, utilizes the method of Jorgensen to compute pharmacokinetic properties and descriptors such as octanol/water partitioning coefficient, aqueous solubility, brain/blood partition coefficient, intestinal wall permeability, plasma protein binding and others.

2. ^{1}H and ^{13}C NMR of representative compounds



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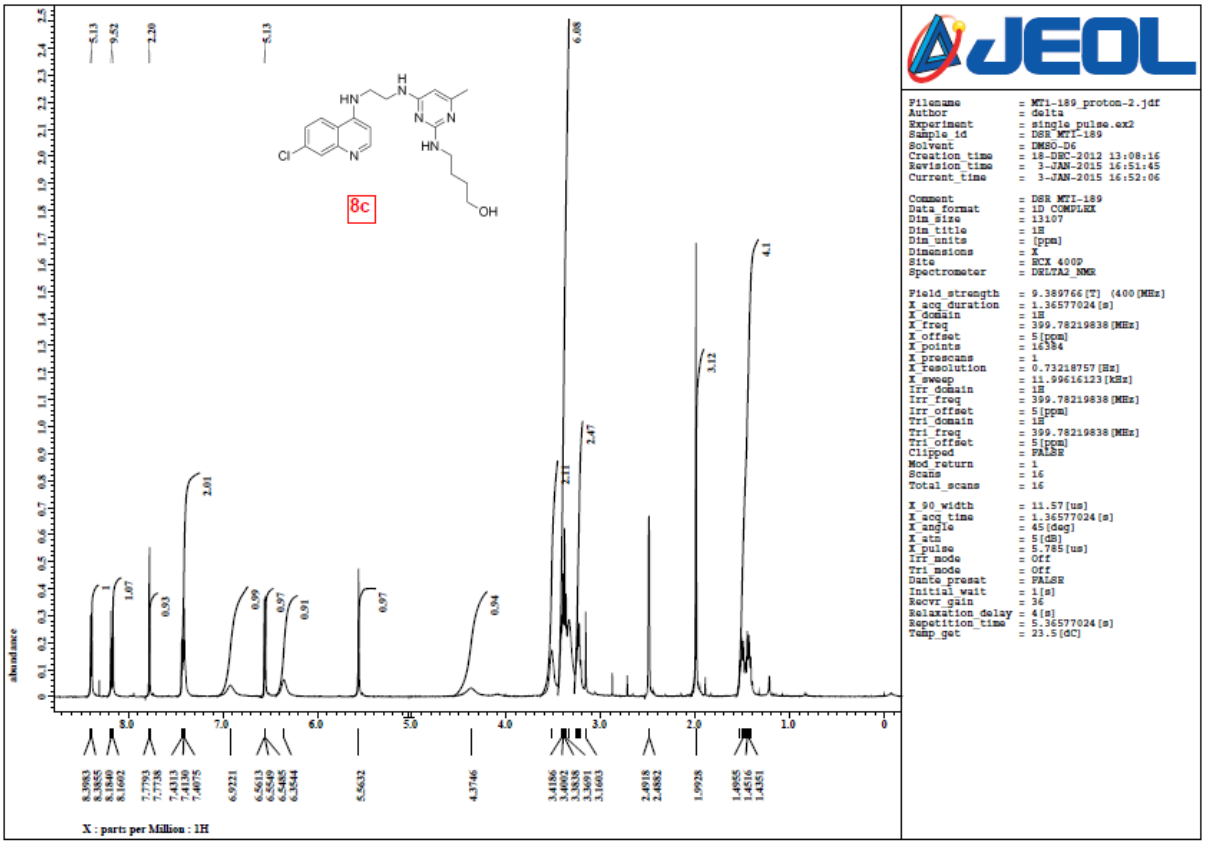
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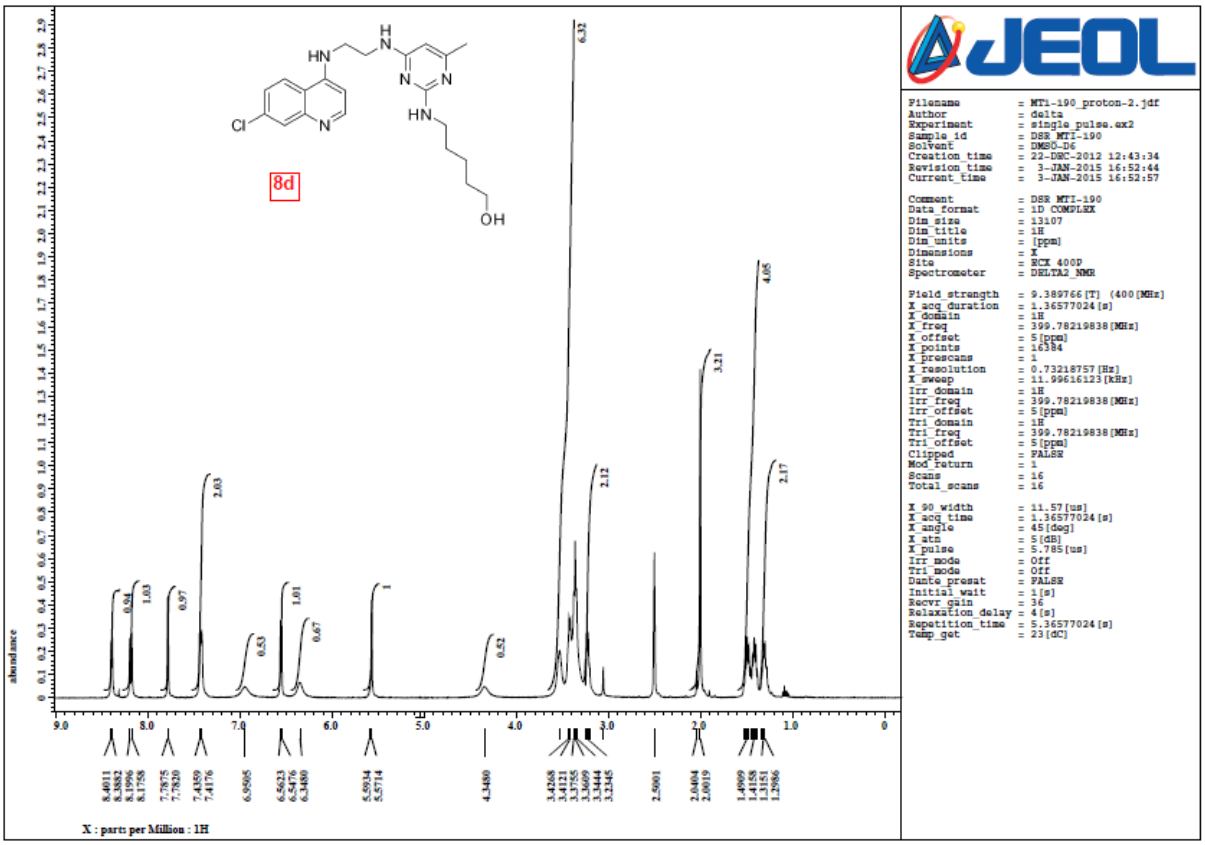
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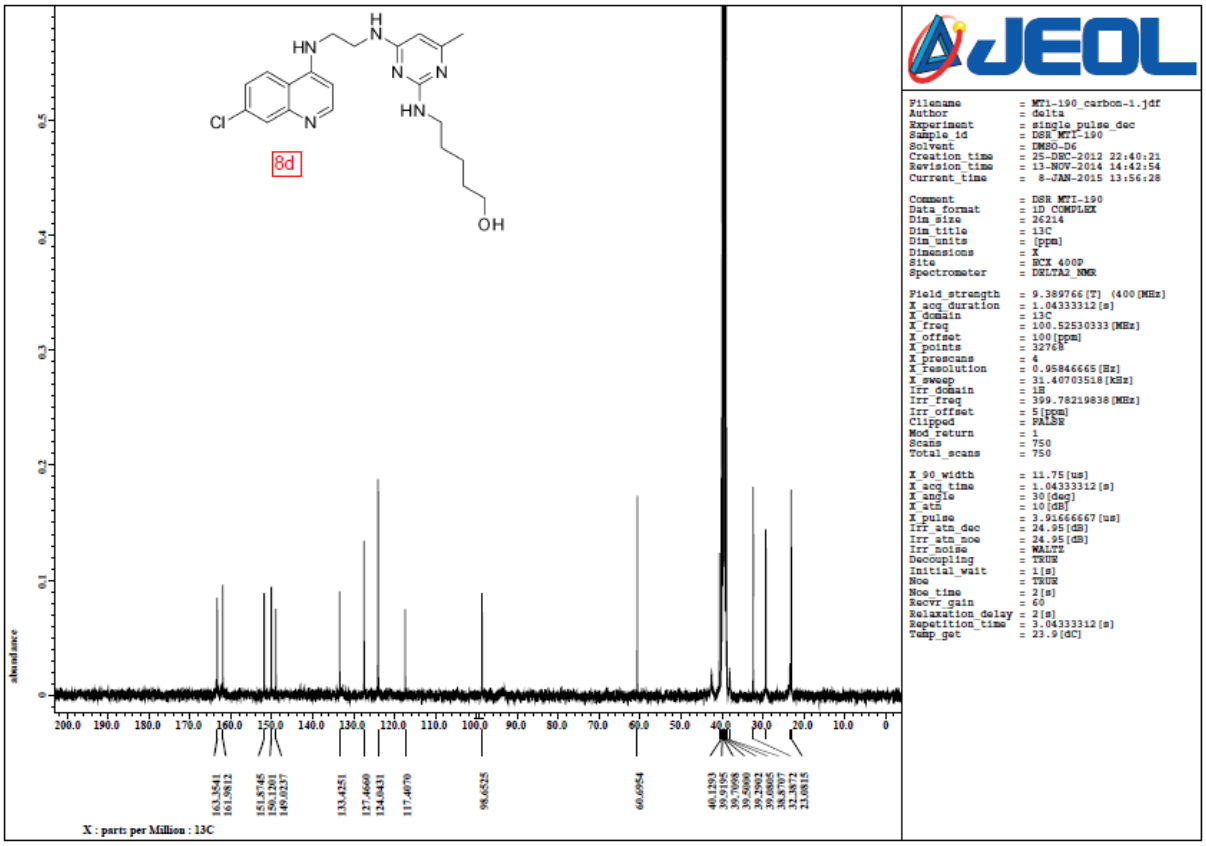
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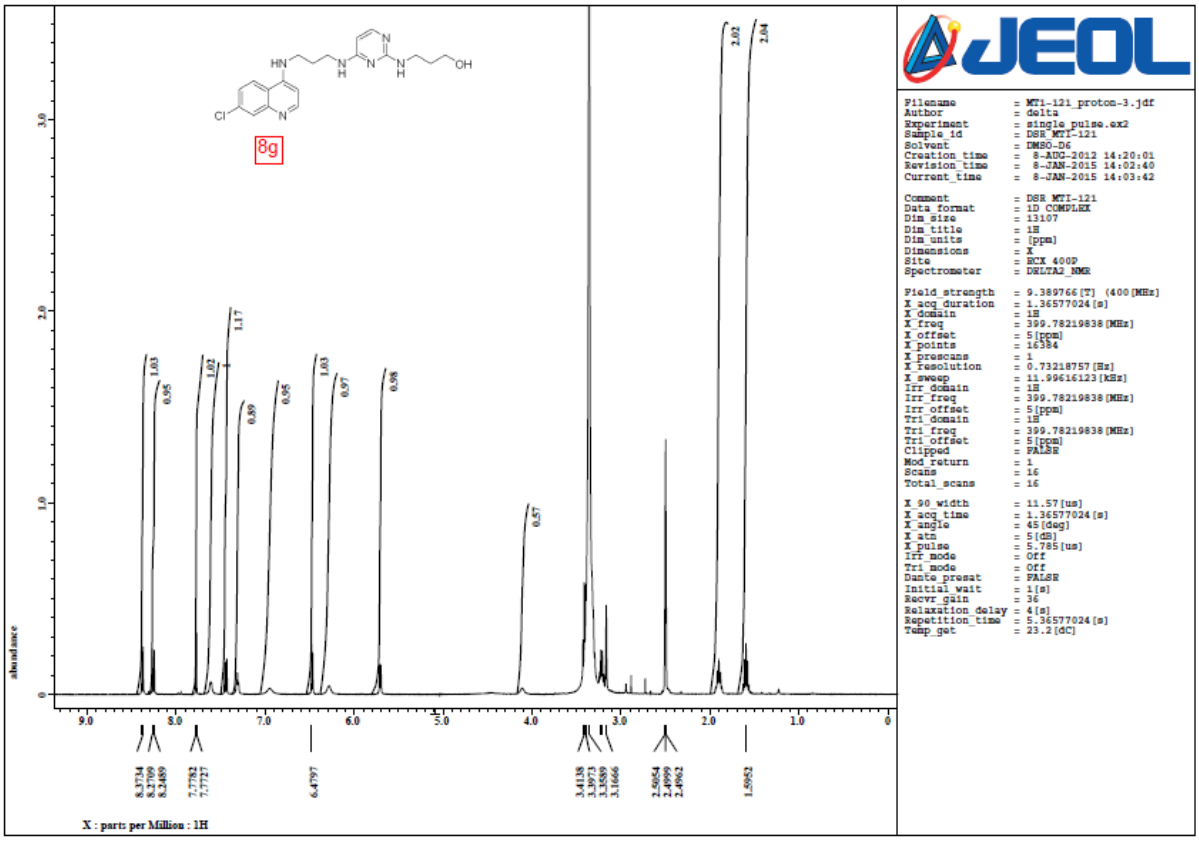
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Irr_mode = Off
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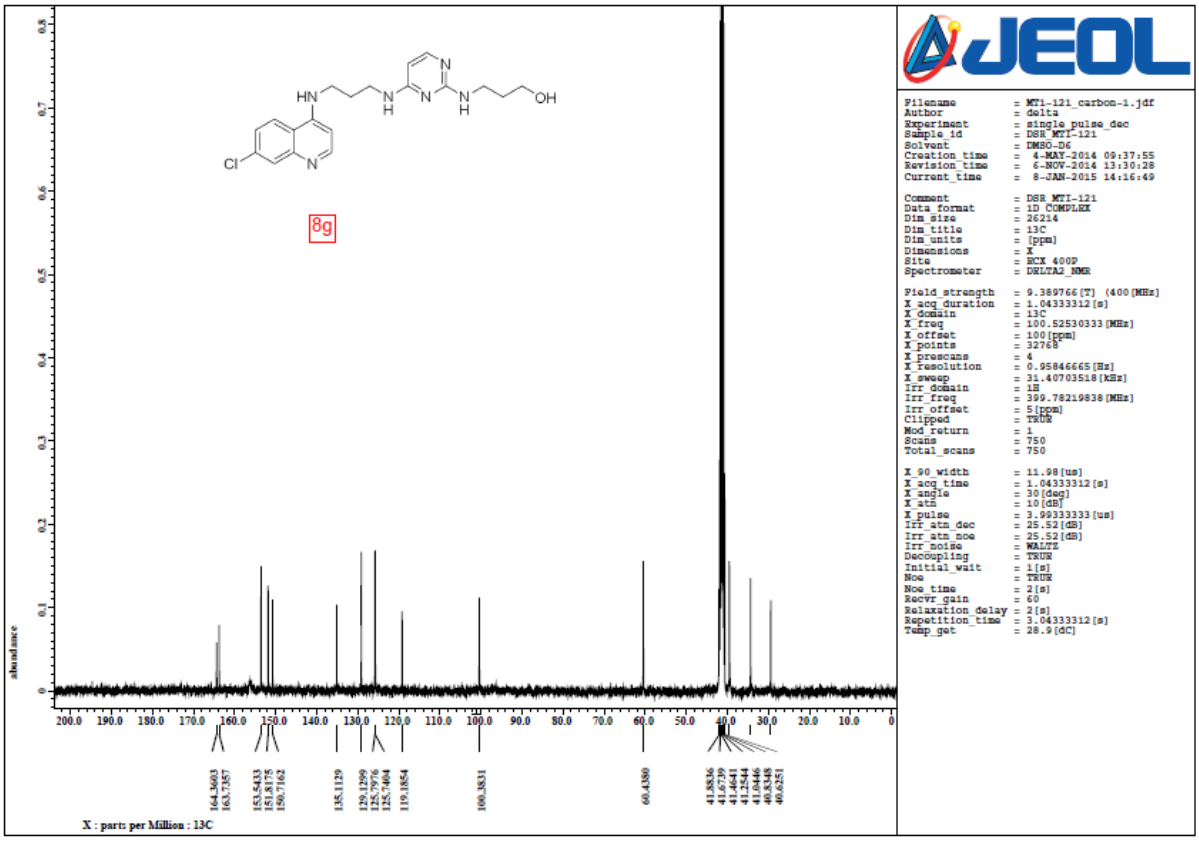
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Irr_atn_dec = 25.52[dB]
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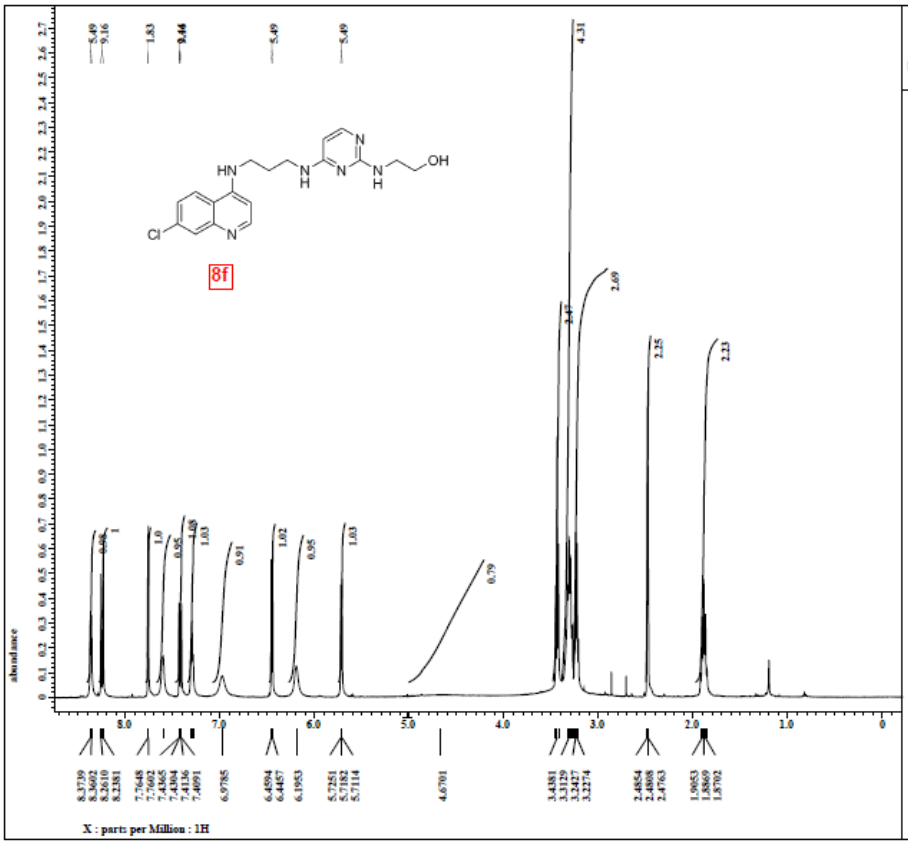


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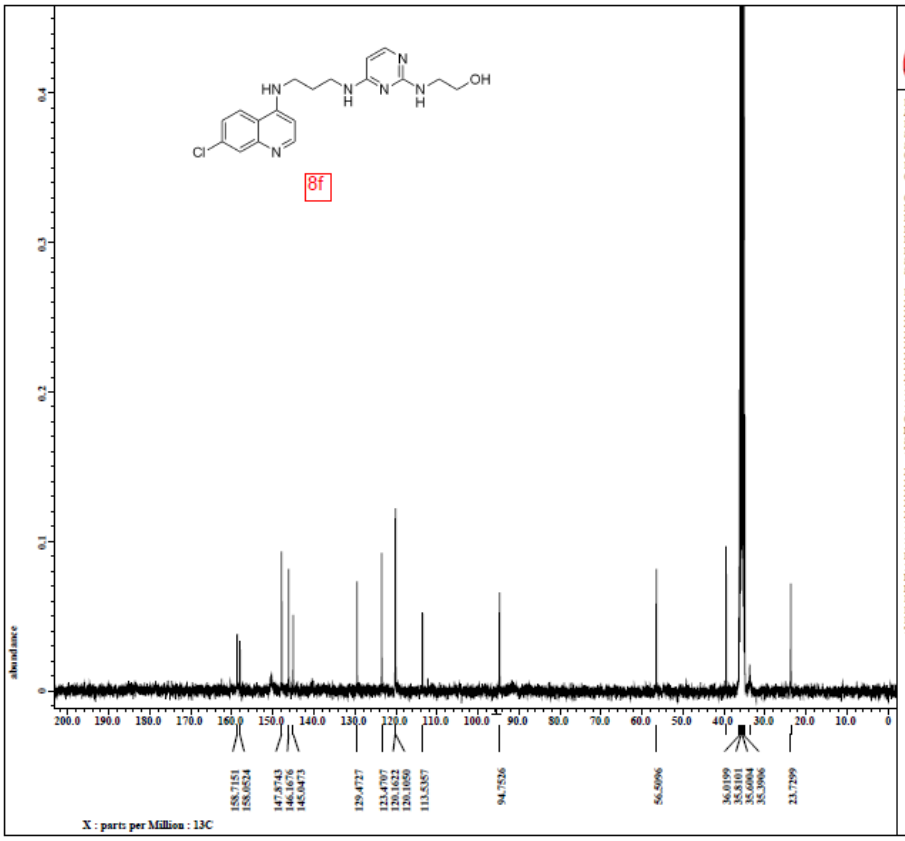


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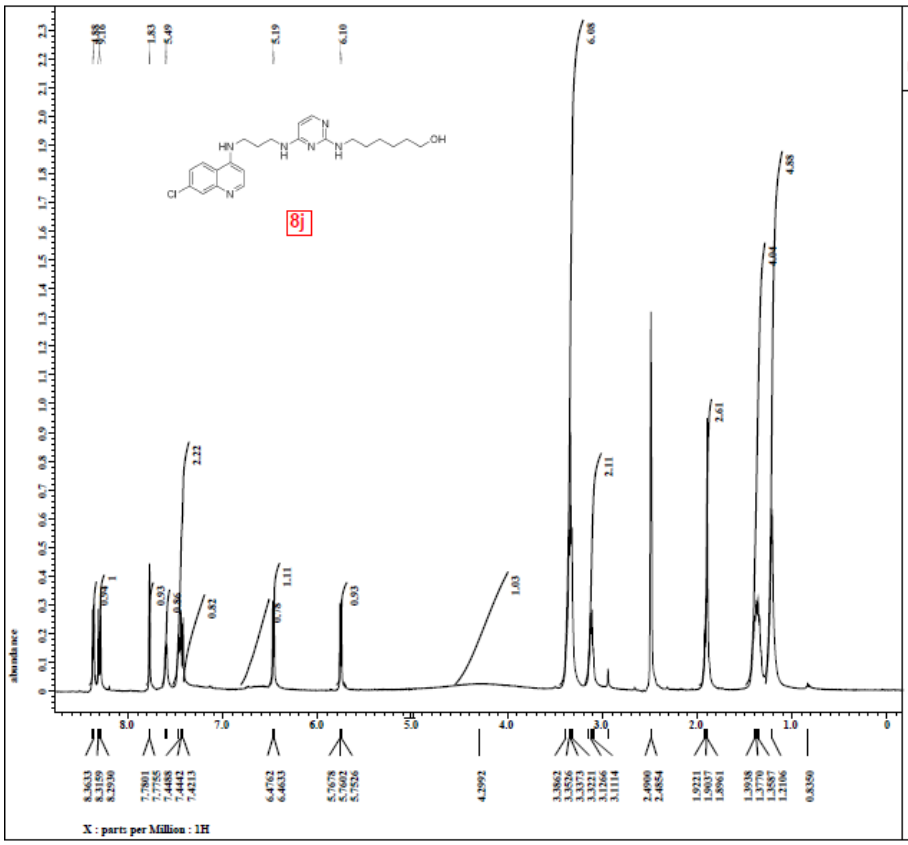


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Mod_return        = 1
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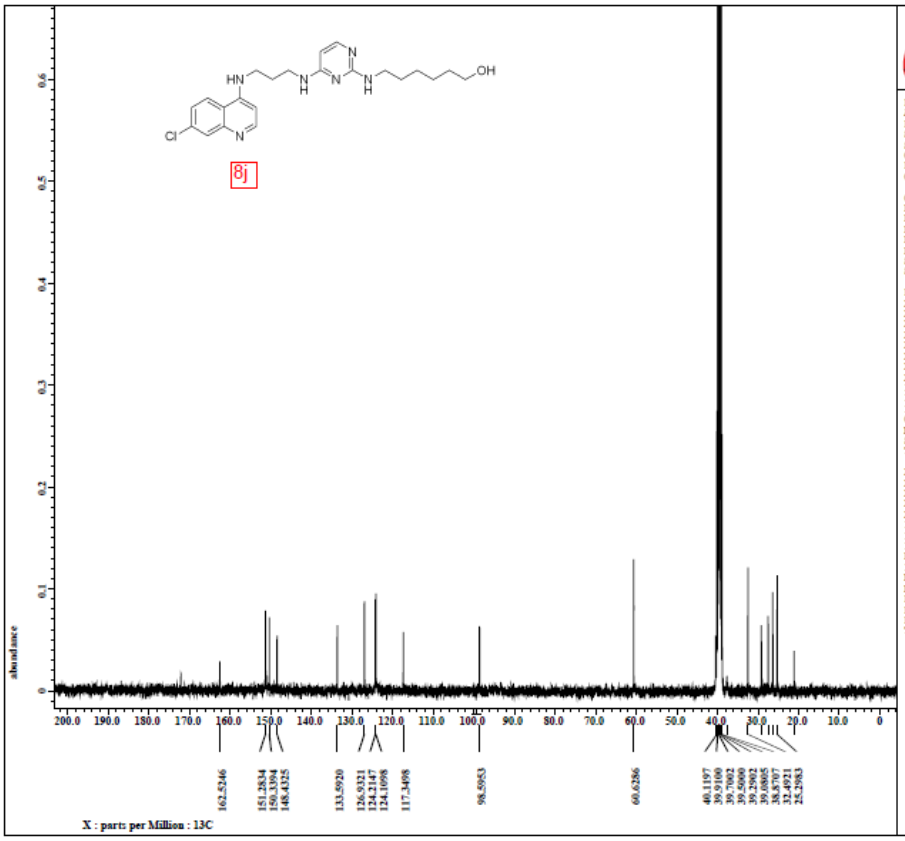


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X_sweep           = 31.40703518[kHz]
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Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
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X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
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X_pulse           = 3.99333333[us]
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Irr_atn_noe       = 25.52[dB]
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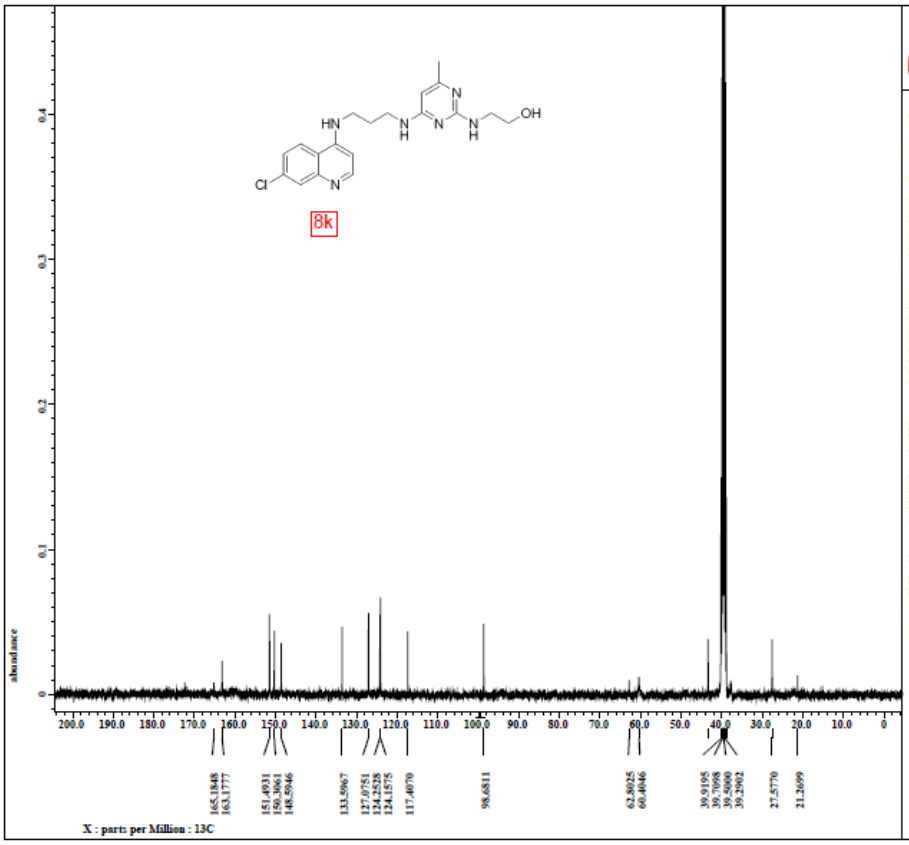
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 27.1[dC]
```

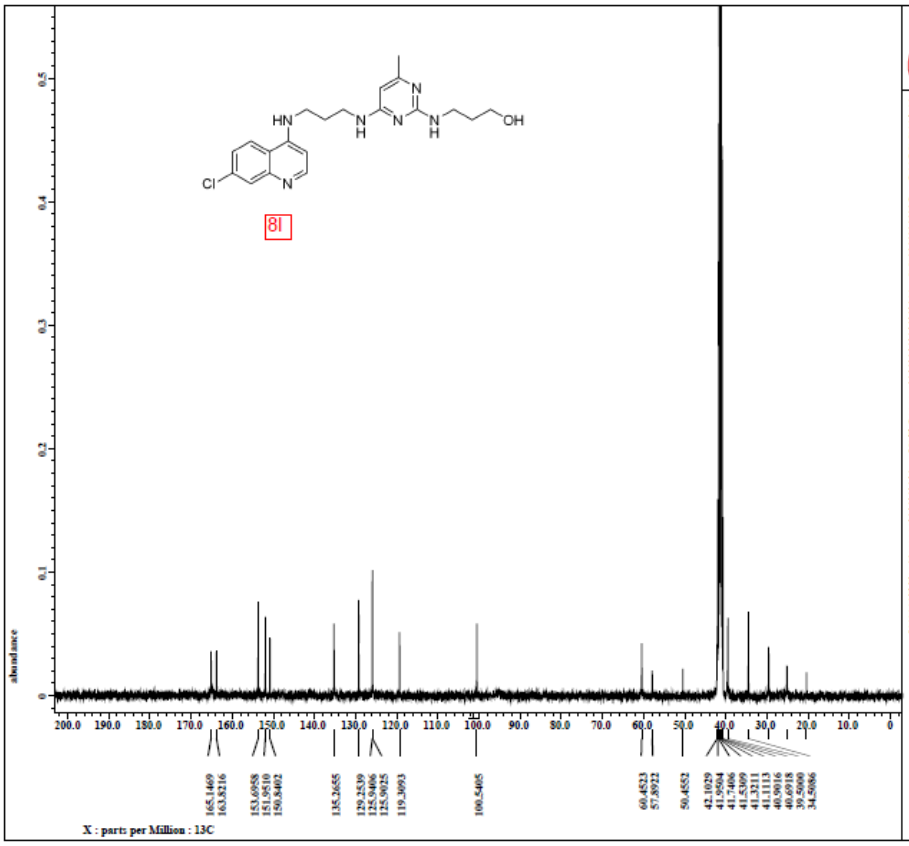



```
Filename          = MTI-145_carbon-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = DSR_MTI-145
Solvent           = DMSO-D6
Creation_time     = 14-SEP-2012 15:48:28
Revision_time     =  8-JAN-2015 14:22:20
Current_time      =  8-JAN-2015 14:23:20

Comment           = DSR MTI-145
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX 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        = 54
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 22.5[dC]
```

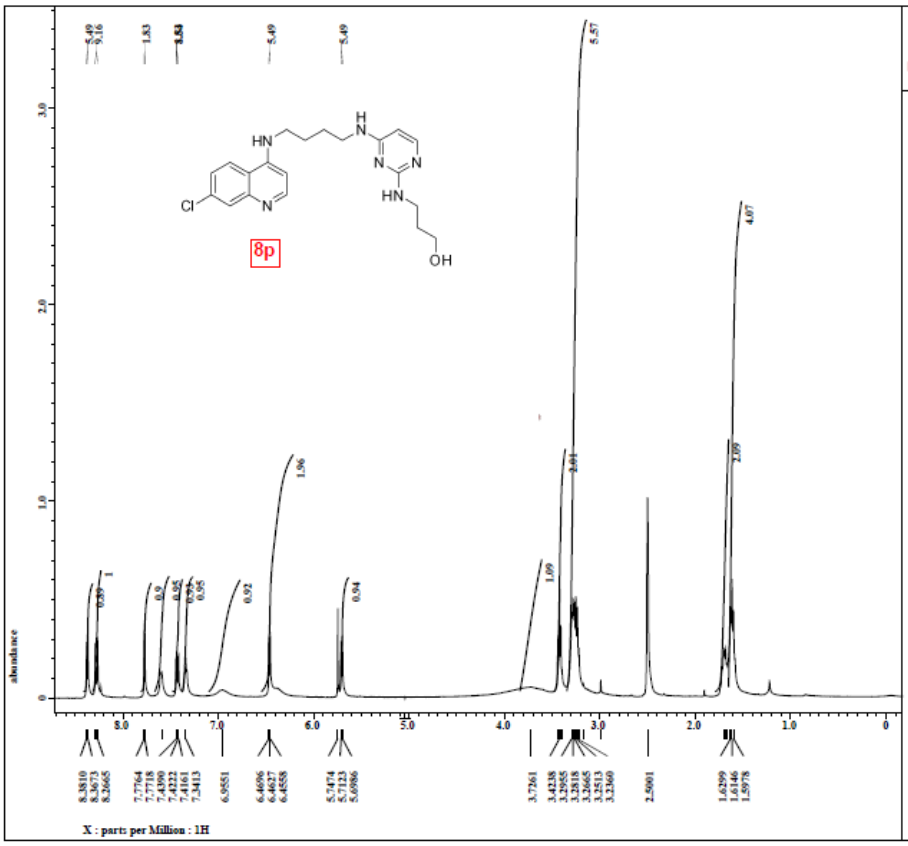



```
Filename          = MTI-146_carbon-1.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = DSR_MTI-146_A
Solvent           = DMSO-D6
Creation_time     = 21-SEP-2012 20:32:40
Revision_time     =  6-NOV-2014 19:11:42
Current_time      =  8-JAN-2015 14:25:09

Comment           = DSR MTI-146 A
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX 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          = 23.5[dC]
```

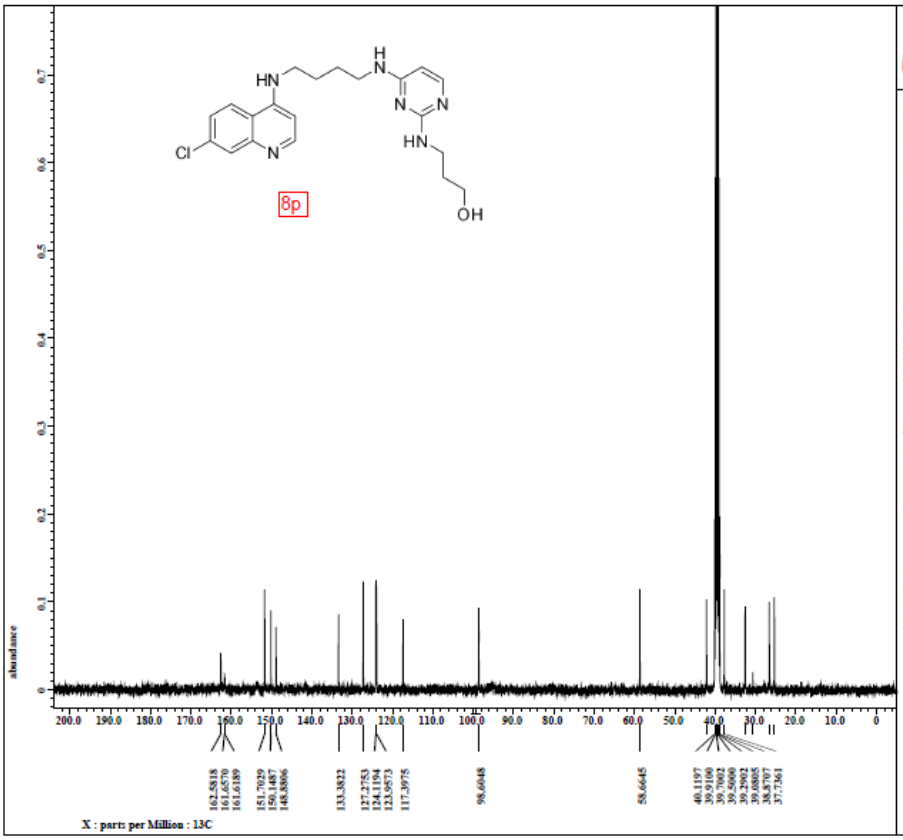



```
Filename          = MTI-157_proton-1.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = DSR_MTI-157
Solvent           = DMSO-D6
Creation_time     = 16-MAY-2014 13:38:44
Revision_time     =  7-NOV-2014 17:16:00
Current_time      =  3-JAN-2015 16:44:49

Comment           = DSR_MTI-157
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T]  (400[MHz]
X_acq_duration    = 1.6384[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.61035156[Hz]
X_sweep           = 10[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        = 10.1[us]
X_acq_time        = 1.6384[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.05[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 4[s]
Repetition_time   = 5.6384[s]
Temp_get          = 409.9[dC]
```

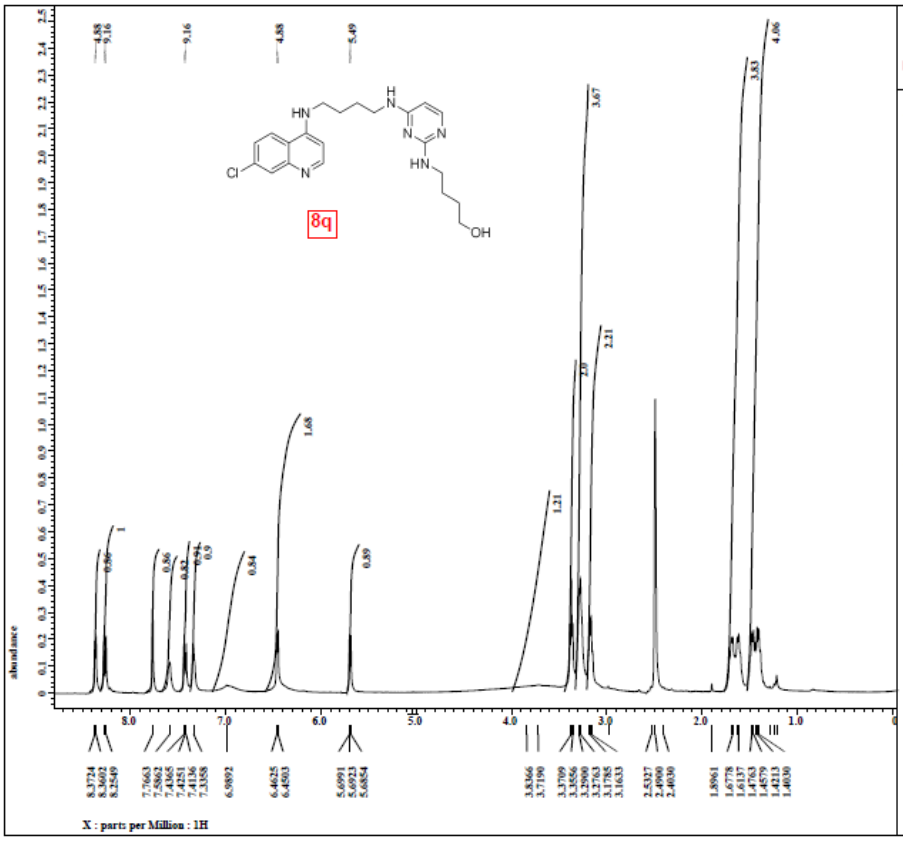



```
Filename          = MTI-157_carbon-1.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = DSR_MTI-157
Solvent           = DMSO-D6
Creation_time     = 15-MAY-2014 19:21:22
Revision_time     =  7-NOV-2014 17:19:21
Current_time      =  8-JAN-2015 14:30:24

Comment           = DSR_MTI-157
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX 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           = TRUE
Mod_return        = 1
Scans             = 512
Total_scans       = 512

X_90_width        = 11.98[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 10[dB]
X_pulse           = 3.99333333[us]
Irr_atn_dec       = 25.52[dB]
Irr_atn_noe       = 25.52[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          = 409.6[dC]
```

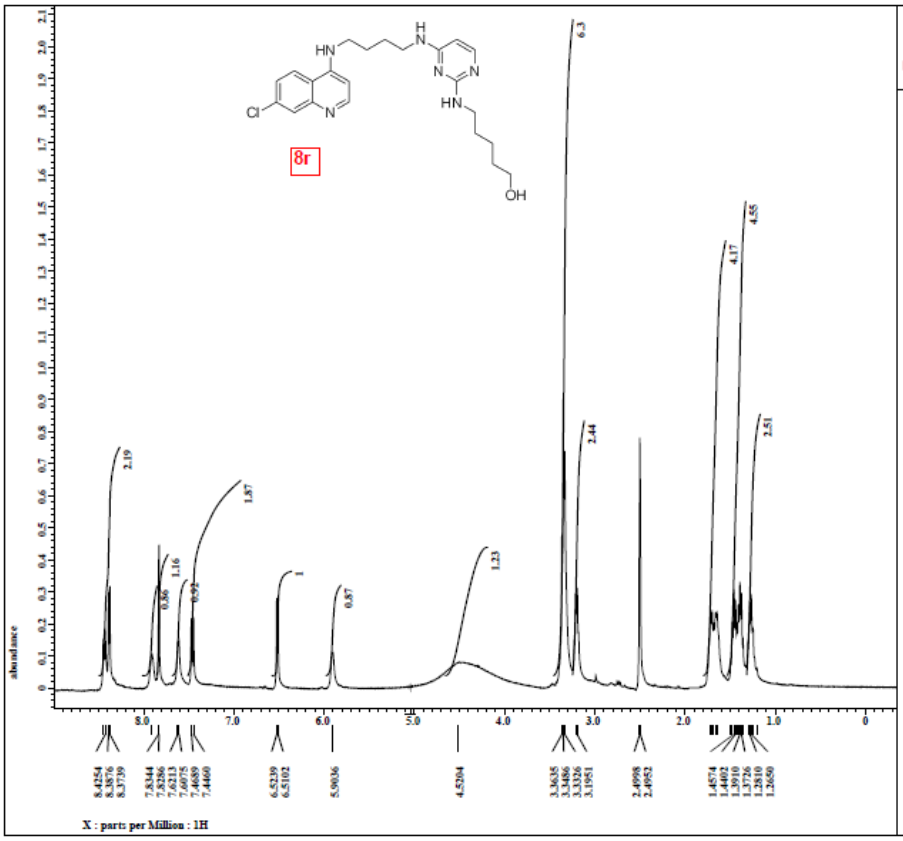



```
Filename          = MTI-158_proton-1.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = DSR_MTI-158
Solvent           = DMSO-D6
Creation_time     = 16-MAY-2014 13:45:13
Revision_time     =  7-NOV-2014 17:30:13
Current_time      =  3-JAN-2015 16:45:42

Comment           = DSR_MTI-158
Data_format       = 1D REAL
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    = 1.6384[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.61035156[Hz]
X_sweep           = 10[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        = 10.1[us]
X_acq_time        = 1.6384[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.05[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 4[s]
Repetition_time   = 5.6384[s]
Temp_get          = 409.9[dC]
```

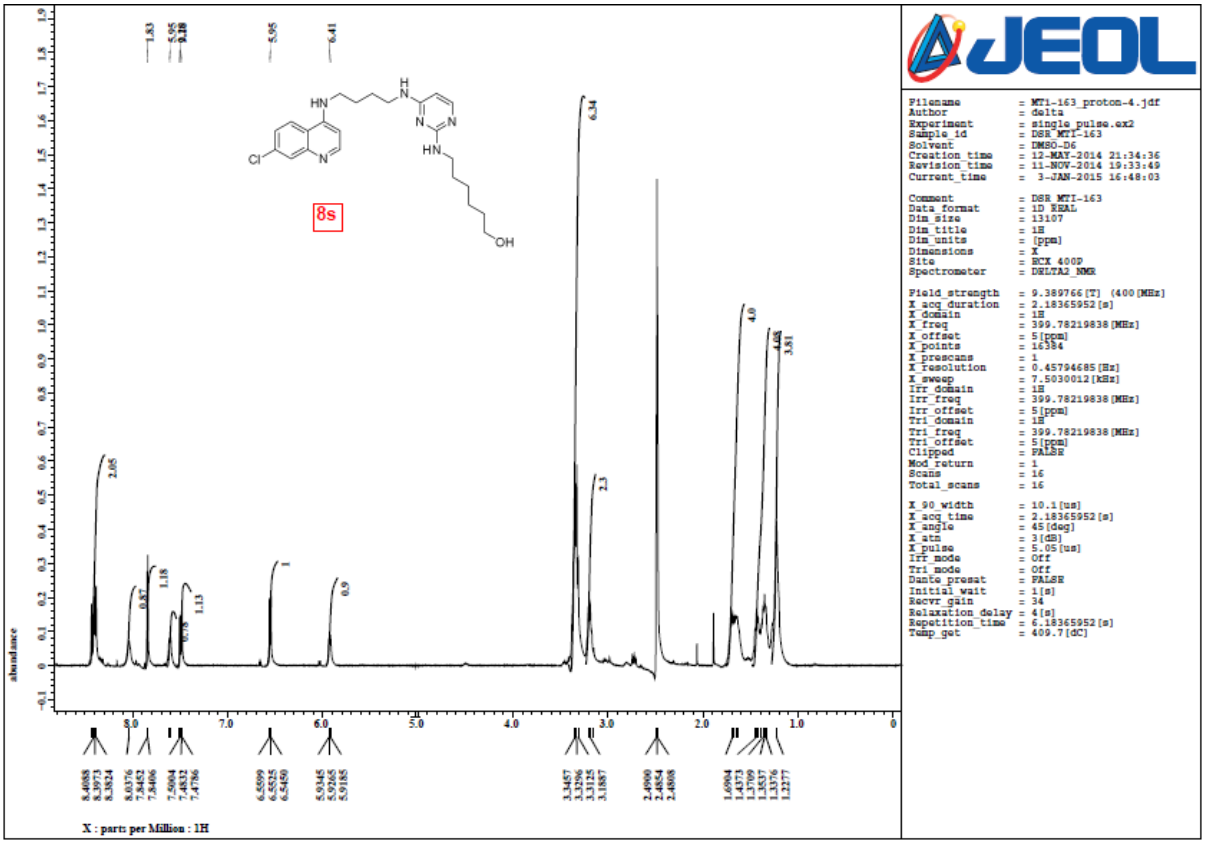


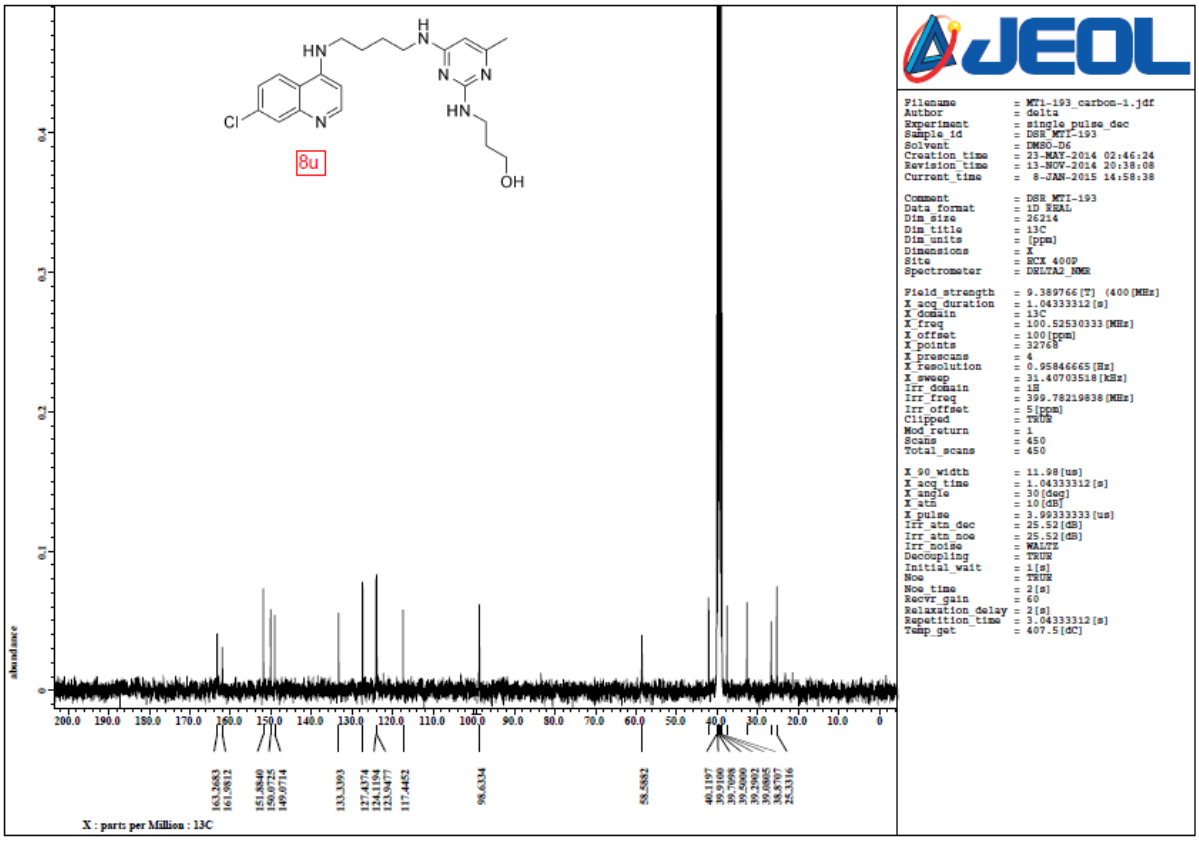

```
Filename          = MTI-162_proton-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = DSR_MTI-162
Solvent           = DMSO-D6
Creation_time     = 12-MAY-2014 21:01:23
Revision_time     = 11-NOV-2014 19:09:10
Current_time      =  3-JAN-2015 16:46:51

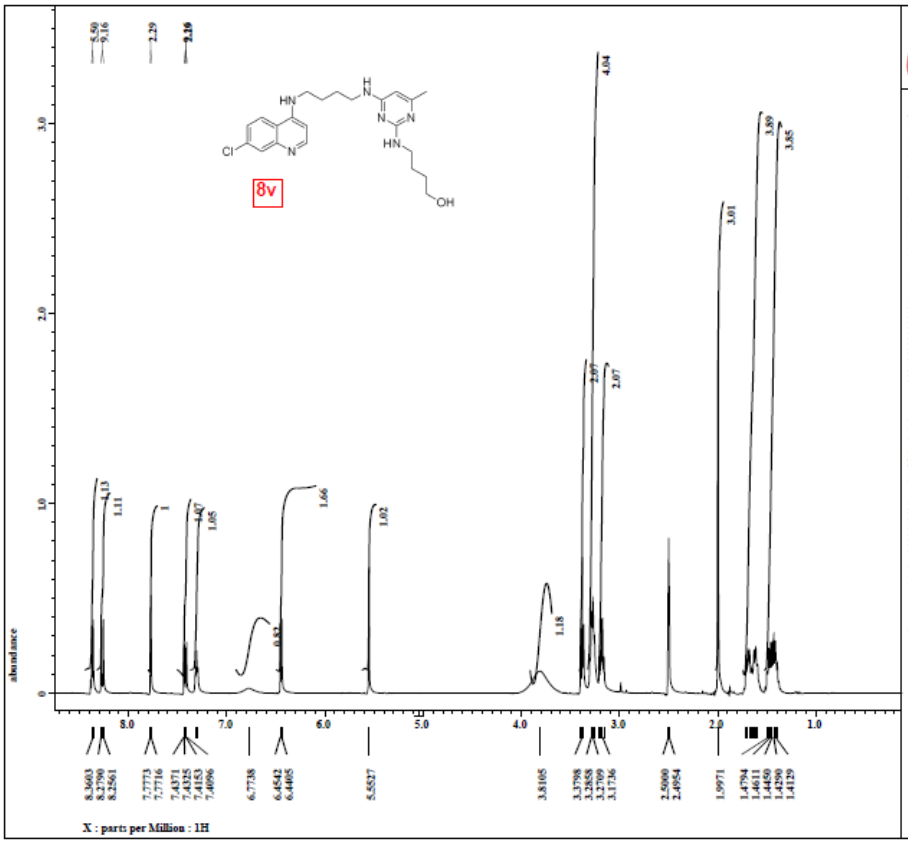
Comment           = DSR_MTI-162
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

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        = 10.1[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.05[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 32
Relaxation_delay  = 4[s]
Repetition_time   = 6.18365952[s]
Temp_get          = 409.7[dC]
```


8s
X : parts per Million : 1H
abundance
JEOL
Filename = MTI-163_proton-4.jdf
Author = delta
Experiment = single_pulse.ex2
Sample_id = DSR_MTI-163
Solvent = DMSO-D6
Creation_time = 12-MAY-2014 21:34:36
Revision_time = 11-NOV-2014 19:33:49
Current_time = 3-JAN-2015 16:48:03
Comment = DSR MTI-163
Data_format = 1D REAL
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = RCX 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 = 10.1[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 5.05[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 = 409.7[dC]


8u
X : parts per Million : 13C
abundance
JEOL
Filename = MTI-193_carbon-1.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = DSR_MTI-193
Solvent = DMSO-D6
Creation_time = 23-MAY-2014 02:46:24
Revision_time = 13-NOV-2014 20:38:08
Current_time = 8-JAN-2015 14:58:38
Comment = DSR MTI-193
Data_format = 1D REAL
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = RCX 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 = TRUE
Mod_return = 1
Scans = 450
Total_scans = 450
X_90_width = 11.98[us]
X_acq_time = 1.04333312[s]
X_angle = 30[deg]
X_atn = 10[dB]
X_pulse = 3.99333333[us]
Irr_atn_dec = 25.52[dB]
Irr_atn_noe = 25.52[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 = 407.5[dC]

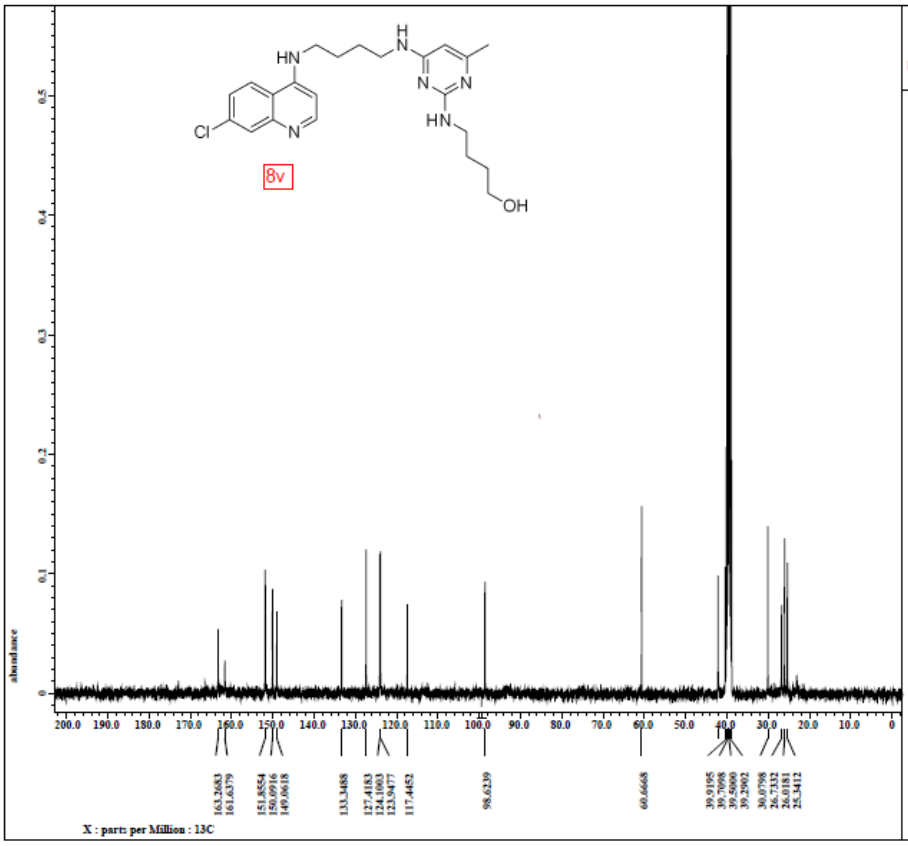



```
Filename          = MTi-194_proton-3.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = DSR_MTI-194
Solvent           = DMSO-D6
Creation_time     = 25-MAY-2014 15:46:53
Revision_time     = 13-NOV-2014 21:00:20
Current_time      =  3-JAN-2015 17:00:31

Comment           = DSR_MTI-194
Data_format       = 1D REAL
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX_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        = 10.1[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.05[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 30
Relaxation_delay  = 4[s]
Repetition_time   = 6.18365952[s]
Temp_get          = 408.5[dC]
```

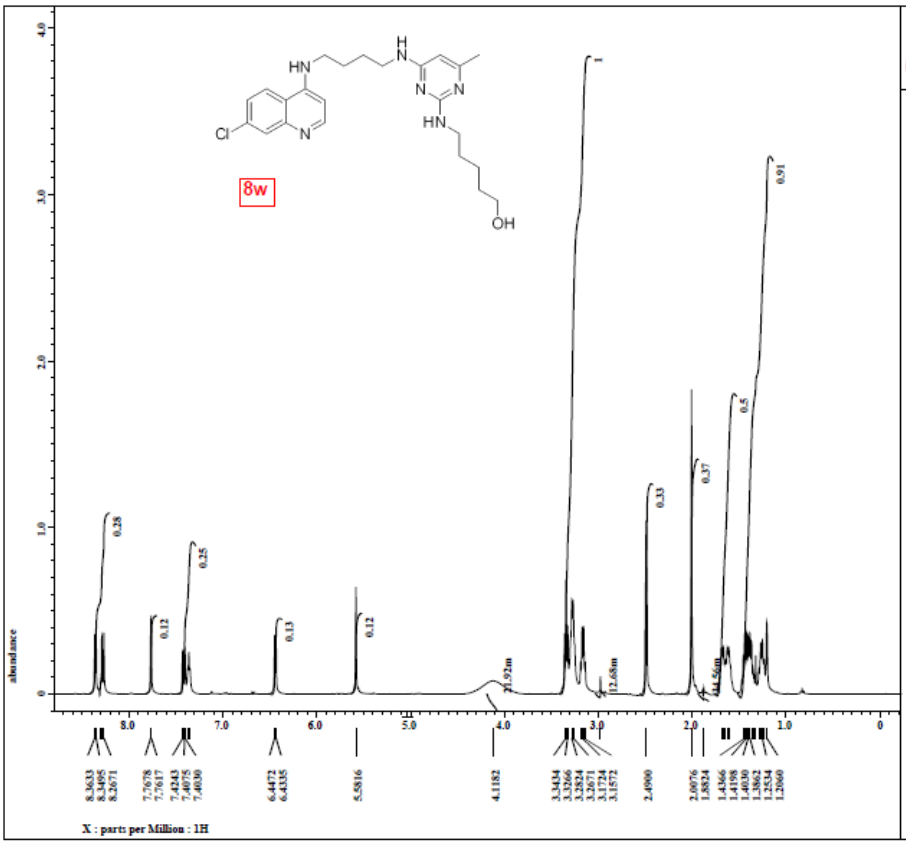



```
Filename          = MTi-194_carbon-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = DSR_MTI-194
Solvent           = DMSO-D6
Creation_time     = 25-MAY-2014 16:13:53
Revision_time     = 14-NOV-2014 14:04:06
Current_time      =  8-JAN-2015 15:00:17

Comment           = DSR_MTI-194
Data_format       = 1D REAL
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX_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           = TRUE
Mod_return        = 1
Scans             = 512
Total_scans       = 512

X_90_width        = 11.98[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 10[dB]
X_pulse           = 3.99333333[us]
Irr_atn_dec       = 25.52[dB]
Irr_atn_noe       = 25.52[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          = 408.5[dC]
```

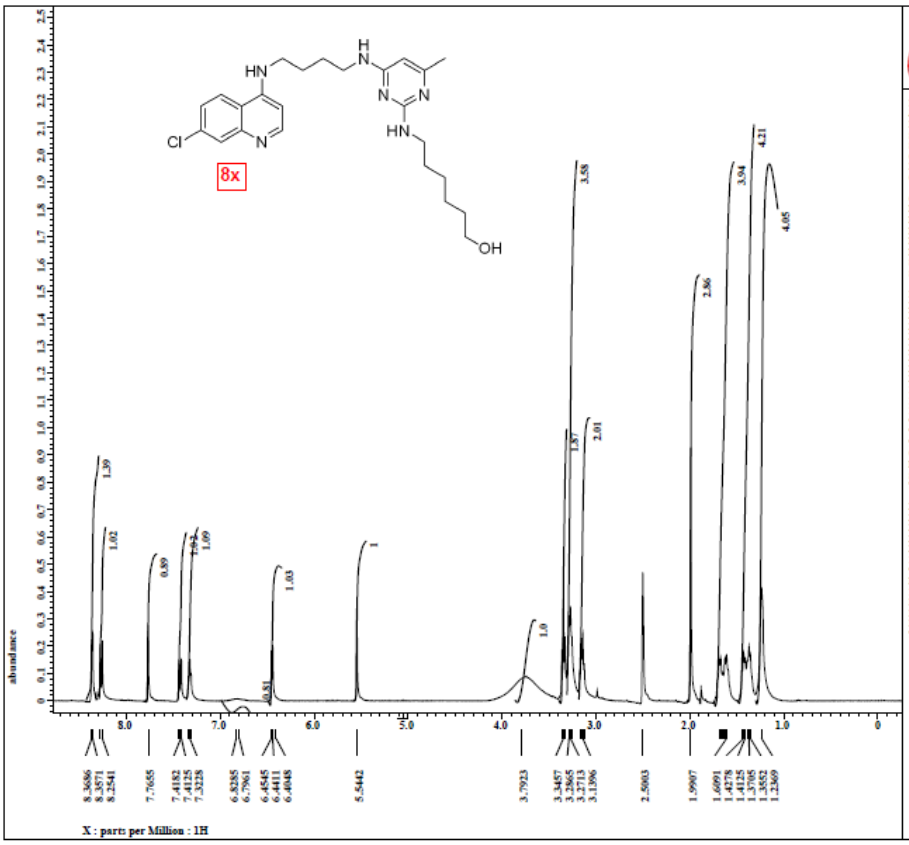



```
Filename          = MTi-195_proton-1.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = DSR_MTI-195
Solvent           = DMSO-D6
Creation_time     = 22-MAY-2014 18:58:56
Revision_time     = 14-NOV-2014 15:36:10
Current_time      =  3-JAN-2015 17:01:13

Comment           = DSR_MTI-195
Data_format       = 1D REAL
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.6384[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.61035156[Hz]
X_sweep           = 10[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        = 10.1[us]
X_acq_time        = 1.6384[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.05[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 32
Relaxation_delay  = 4[s]
Repetition_time   = 5.6384[s]
Temp_get          = 407.9[dC]
```




```
Filename          = MTi-196_proton-8.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = DSR_MTI-196
Solvent           = DMSO-D6
Creation_time     = 15-NOV-2014 13:25:53
Revision_time     = 18-NOV-2014 13:13:07
Current_time      =  3-JAN-2015 17:03:06

Comment           = DSR_MTI-196
Data_format       = 1D REAL
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = RCX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.31072[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.76293945[Hz]
X_sweep           = 12.5[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        = 10.1[us]
X_acq_time        = 1.31072[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.05[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 32
Relaxation_delay  = 4[s]
Repetition_time   = 5.31072[s]
Temp_get          = 22[dC]
```