Supporting Information

Counteranion-directed structural consequences in silver-adenine N-oxide complexes

Rajneesh Kumar Prajapati, Jitendra Kumar and Sandeep Verma*
Department of Chemistry, Indian Institute of Technology-Kanpur
Kanpur-208016 (UP), India

General Procedures: ^{1}H and ^{13}C NMR spectra were obtained on a JEOL-DELTA2 500 model spectrometer operating at 500MHz. The spectra were recorded in DMSO-d_6 solution and the chemical shifts were referenced with respect to tetramethylsilane. High resolution (ESI$^+$ mode) mass spectra were obtained on Waters, Q-Tof Premier Micromass HAB 213 mass spectrometer, Department of Chemistry, IIT Kanpur, India. Solvents were evaporated using rotary evaporator under reduce pressure.

Synthesis of 9-Propyladenine: Experimental details for the synthesis of 9-Propyladenine have been reported earlier.[1] A similar protocol was followed and the purity of product so obtained was confirmed by spectroscopic analysis.

Synthesis of 9-Propyladenine-*N¹*-oxide (1): 9-Propyladenine (2 g, 1 eq.) was dissolved in hot glacial acetic acid (30 mL) followed by heating at reflux temperature under N_2 atmosphere 24 hours with constant stirring and progress of reaction was observed by TLC. After this acetic acid was evaporated under high vacuum and compound was purified by column chromatography eluting with methanol/Chloroform (2:98) to afford white powder**.** (1.5 g, 68.80% Yield). HRMS: $(M+1)^+$ calculated: 194.1042, Found: 194.1041; M.P.211-216°C; ^{1}H NMR (500 MHz, DMSO-d_6, 25°C): δ(ppm) 0.78-0.81 (t, 3H, CH_3), 1.75-1.81 (m, 2H, CH_2), 4.07-4.09 (t, 2H, N-CH_2), 8.27 (s, 1H, C8-H), 8.57 (s, 1H, C2-H); ^{13}C NMR (125 MHz, DMSO-d_6, 25°C): δ (ppm) 11.42, 23.18, 45.25, 118.93, 142.68, 143.55, 144.50, 148.63.

Synthesis and characterization of complex 1: In a 25 ml round bottom flask, wrapped with aluminum foil, the ligand (0.02 g) was dissolved in methanol and to this added silver nitrate solution in water drop wise with constant stirring. The white complex started precipitating out with the addition of silver salt solution. Stirring was continued for another one hour. After this time, the precipitate was filtered carefully to avoid direct light, washed with water (4x 5 mL) and methanol (4 x 5 mL) to remove any traces of unreacted metal salt and ligand. The product so obtained was dried under high vacuum. The yield was almost quantitative. HRMS: $(M+Ag)^+$ calculated: 300.0015, 302.0011 Found: 300.0015, 302.0032 ; M.P. >260.

Synthesis and characterization of complex 2: In a 25 ml round bottom flask, wrapped with aluminum foil, the ligand (0.02 g) was dissolved in methanol and to this added silver tetrafluoroborate solution in water (prepared in situ by the 1:1 addition of silver carbonate and HBF_4 in water) drop wise with constant stirring. The white complex started precipitating out with the addition of silver salt solution. Stirring was continued for another one hour. After this time, the precipitate was filtered carefully to avoid direct light, washed with water (4x 5 mL) and methanol (4 x 5 mL) to remove any traces of unreacted metal salt and ligand. The product so obtained was dried under high vacuum. The yield was almost quantitative. HRMS: $(M+Ag+MeCN)^+$ calculated: 341.0280, 343.0277, Found: 341.0296, 343.0294; M.P. >260.

Synthesis and characterization of complex 3: In a 25 ml round bottom flask, wrapped with aluminum foil, the ligand (0.02 g) was dissolved in methanol and to this added silver hexafluorophosphate solution in acetonitrile (prepared in situ by the 1:1 addition of silver nitrate and ammonium hexafluorophosphate in acetonitrile) drop wise with constant stirring. Stirring was continued for another one hour. After this time, the solvent was evaporated under high vacuum by avoiding direct light; the white precipitate so obtained was washed with water (4x 5 mL) and methanol (4 x 5 mL) to remove any traces of unreacted metal salt and ligand. The product so obtained was dried under high vacuum. The yield was almost quantitative. HRMS: $(M+Ag)^+$ calculated: 300.0015, 302.0011 Found: 300.0021, 302.0019 $(M+Ag+MeCN)^+$ calculated: 341.0280, Found: 341.0287, M.P. >260.

Synthesis and characterization of complex 4: In a 25 ml round bottom flask, wrapped with aluminum foil, the ligand (0.02 g) was dissolved in methanol and to this added silver triflate solution in water (prepared in situ by the 1:1 addition of silver carbonate and triflic acid in water) drop wise with constant stirring. The white complex started precipitating out with the addition of silver salt solution. Stirring was continued for another one hour. After this time, the precipitate was filtered carefully to avoid direct light, washed with water (4x 5 mL) and methanol (4 x 5 mL) to remove any traces of unreacted metal salt and ligand. The product so obtained was dried under high vacuum. The yield was almost quantitative. HRMS: $(M+Ag+MeCN)^+$ calculated: 341.0280, 343.0277, Found: 341.0296, 343.0295, M.P. >260.

Synthesis and characterization of complex 5: In a 25 ml round bottom flask, wrapped with aluminum foil, the ligand (0.02 g) was dissolved in methanol and to this added silver perchlorate solution in water (prepared in situ by the 1:1 addition of silver carbonate and perchloric acid in water) drop wise with constant stirring. The white complex started precipitating out with the addition of silver salt solution. Stirring was continued for another one hour. After this time, the precipitate was filtered carefully to avoid direct light, washed with water (4x 5 mL) and methanol (4 x 5 mL) to remove any traces of unreacted metal salt and ligand. The product so obtained was dried under high vacuum. The yield was almost quantitative. HRMS: $M+Ag+MeCN)^+$ calculated: 341.0280, 343.0277, Found: 341.0293, 343.0298, M.P. >260.

Crystal structure refinement details for 1, 2 and 3: Single Crystal of **1, 2**, **3, 4** and **5** were coated with light hydrocarbon oil and mounted in the 100 K dinitrogen stream of a Bruker SMART APEX CCD diffractometer equipped with CRYO Industries low-temperature apparatus and intensity data were collected using graphite-monochromated Mo KR radiation. The data integration and reduction were processed with the SAINT software.[2] An absorption correction was applied.[3] Structures were solved by the direct method using SHELXS-97 and refined on *F*2 by a full-matrix least-squares technique using the SHELXL-97 program package.[4] Non-hydrogen atoms were refined anisotropically. In the refinement, hydrogens were treated as riding atoms using the SHELXL default parameters. Crystal structure refinement parameters are given in Table S1 whereas H-bonding parameters are provided in Table S2. CCDC contains the supplementary crystallographic data for this paper with a deposition number of CCDC **943526**, **943527**, **943528**, **943529 and 943530** for complexes **1**, **2, 3, 4** and **5** respectively. Copies of this information can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK. [Fax: +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

In the crystal lattice of **2**, **3** and **4**, and **5** water molecules are present and hydrogen atoms are not located on Fourier map due to which 'A' level alerts appears, quoting "isolated oxygen atoms", in the check-cif report. We have included the hydrogen atoms corresponding to water molecules during refinement which causes few 'C' level alerts quoting "Calc. and Reported SumFormula Strings Differ" and "Reported F000 Differs from Calcd (or Missing)" in the check-cif report. Other alert indicates that "coordinates do not form properly connected set" which is common for coordination polymers.

Table S1:

Identification Code	**Complex 1**	**Complex 2**	**Complex 3**	**Complex 4**	**Complex 5**
Empirical Formula	$C_{16}H_{28}AgN_{11}O_8$	$C_{16}H_{24}AgBF_4N_{10}O_{4.}$	$C_{16}H_{24}AgF_6N_{10}O_3P$	$C_{17}H_{26}AgF_3N_{10}O_7S$	$C_{16}H_{28}Ag_2Cl_2N_{10}O_{13}$
Mr	610.36	615.13	657.29	679.41	855.12
Data Collection Temperature (K)	100(2)	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	Monoclinic
Space group	*P 21/c*	*P21/c*	*P 21/c*	*P 21/n*	*P 21*
a/Å	6.616(5)	6.720(5)	16.106(5)	20.150(5)	12.7023(17)
b/ Å	11.643(5)	11.611(5)	6.901(5)	6.903(5)	9.2602(12)
c/ Å	30.632(5)	30.232(5)	21.480(5)	20.342(5)	13.3792(17)
$\alpha/^o$	90.000	90.000	90.000	90.000	90.000
$\beta/^o$	95.291(5)	95.504(5)	93.470(5)	116.516(5)	117.315(2)
$\gamma/^o$	90.000	90.000	90.000	90.000	90.000
Volume/A^3	2350(2)	2348(2)	2383(2)	2532(2)	1398.3(3)
Z	4	4	4	4	2
Dx /Mg m^{-3}	1.726	1.740	1.832	1.777	2.031
F(000)	1248	1240	1320	1368	852
μ/ mm^{-1}	0.926	0.937	1.002	0.961	1.673
θ range for data collection/ °	2.20−24.16	1.35−26.00	1.27−26.00	2.24−26.00	2.85-26.00
Limiting indices	-6<=h<=7, -13<=k<=12, -35<=l<=35	-8<=h<=8, -11<=k<=14, -37<=l<=37	-19<=h<=19, -8<=k<=7, -26<=l<=21	-27<=h<=24, -8<=k<=8, -20<=l<=25	-11<=h<=15, -11<=k<=10, -16<=l<=16
Reflections collected	14286	12938	12514	16832	7677
Unique reflections	3771	4587	4671	4996	4884
R(int)	0.0317	0.0438	0.0605	0.0741	0.0273
Completeness to θ	99.8 %	99.3 %	99.6 %	100 %	99.2 %
T_{max} / T_{min}	0.8813-0.8365	0.8646−0.8065	0.8724-0.8247	0.8614-0.8022	0.7756-0.7308
Data/restraints/ parameters	3771 / 4 / 349	4587 / 0/ 325	4671 / 0 / 334	4996 / 0 / 360	4884 / 0 / 389
Goodness-of-fit on F^2	1.048	1.044	1.099	1.039	1.081
*R*1 and *R*2 [$I>2\sigma(I)$]	0.0278, 0.0583	0.0574, 0.1546	0.0701, 0.1750	0.0588, 0.1349	0.0400, 0.1039
*R*1 and *R*2 (all data)	0.0408, 0.0627	0.0816, 0.1939	0.1013, 0.2180	0.949, 0.1551	0.0416, 0.1059

Largest diff. peak and hole/e.A^{-3}	0.400−0.258	1.843−1.232	2.887−1.537	2.811−1.065	2.043-0.650
CCDC No.	**943526**	**943527**	**943528**	**943529**	**943530**

Table S2:

D—H…A	**Symmetry for A**	**H…A**	**D…A**	**D—H…A**
Complex-1				
N6A —H6A1…O1A	----------	2.25	2.603(3)	104
N6A—H6A1…O1B	x,1+y,z	2.08	2.816(4)	144
O2W—H1W2…O1C	----------	2.05(4)	2.837(4)	154(3)
O2W—H2W2…O2C	-1+x,y,z	2.54(4)	3.221(4)	147(3)
O2W—H2W2…O3C	-1+x,y,z	2.24(4)	2.913(4)	145(4)
N6A —H6A2…O1W	----------	1.96	2.766(4)	156
O1W—H1W1…O1A	1-x,-1/2+y,1/2-z	1.88(3)	2.675(3)	168(3)
O1W- H2W1….O1C	----------	2.02(3)	2.888(3)	169(3)
N6B —H6B1 ...O1A	x,-1+y,z	2.03	2.765(3)	142
N6B—H6B1...O1B	----------	2.25	2.604(3)	105
N6B —H6B2. ..O3W	1-x,-1/2+y,1/2-z	1.94	2.751(4)	156
O3W —H1W3...O1B	-1+x,1+y,z	1.91(3)	2.707(4)	160(3)
O3W—H2W3...O2W	----------	2.05(3)	2.808(4)	166(4)
C2B—H2B...O2C	x,-1+y,z	2.41	3.315(4)	164
C9B—H9B1...O3C	----------	2.51	3.154(4)	124
C8A—H8A...O1C	1-x,-1/2+y,1/2-z	2.57	3.313(4)	137
C8A—H8A...O3W	1-x,-1/2+y,1/2-z	2.47	3.065(4)	122
C8B —H8B. ..O1W	----------	2.48	3.083(4)	123
	Complex-2			
N6A—H6A1...O1	x,1+y,z	2.06	2.795(7)	142
N6A—H6A1...O1A	----------	2.26	2.610(6)	104
N6A —H6A2. ..O2W	1-x,1/2+y,1/2-z	1.97	2.783(7)	157
N6—H6A...O1	----------	2.23	2.580(6)	104
N6—H6A...O1A	x,-1+y,z	2.08	2.828(7)	145
N6—H6B...O1W	1+x,1+y,1+z	2.00	2.782(7))	150
C2—H2...F4	1-x,-1/2+y,1/2-z	2.28	3.130(12)	151
C8 —H8...F3	1-x,1/2+y,1/2-z	2.53	3.335(9)	144
C8—H8...O2W	1-x,1/2+y,1/2-z	2.57	3.158(8)	121
C8A—H8A...O1W	----------	2.46	3.052(8)	122
C10A —H10B...F4	1+x,y,z	2.44	3.333(13)	152
	Complex-3			
N6A—H6A1...O1A	----------	2.26	2.608(8)	104
N6A—H6A2...O1	1-x,1/2+y,1/2-z	1.92	2.770(8)	168
N6—H6A...O1	----------	2.28	2.625(6)	104
N6—H6A...O1W	1-x,-1/2+y,1/2-z	2.04	2.838(8)	154
N6—H6B...O1A	1-x,1-y,1-z	1.97	2.821(6)	171
C2A—H2A...O1W	x,3/2-y,1/2+z	2.43	3.343(9)	166
C8—H8...F5	x,3/2-y,1/2+z	2.31	3.135(11)	148
C8A—H8A...F3	x,3/2-y,1/2+z	2.54	2.992(10)	110
C8A— H8A...F6	1-x,1/2+y,1/2-z	2.31	3.213(9)	164
C10A—H10B...F4	x,1+y,z	2.44	3.324(11)	151

C12—H12A...F1	-x,-1/2+y,1/2-z	2.45	3.375(15)	161
C12— H12C...N9	----------	2.59	2.914(13)	100
C12A—H12F...F5	----------	2.51	3.417(14)	158
Complex 4				
N6A—H6A2...O1	----------	2.27	2.611(7)	104
N6A—H6A1...O1W	x,1+y,z	2.07	2.858(8)	153
O1W—H1W...O1	----------	1.93(11)	2.721(7)	175(13)
N6A—H6A2...O1	-x,2-y,-z	1.95	2.807(7)	171
O1W—H2W...O4	1/2-x,-1/2+y,1/2-z	1.94(10)	2.791(9)	169(8)
N6—H6A...O1	----------	2.27	2.613(7)	104
N6 —H6A...N7	1/2-x,1/2+y,1/2-z	2.59	3.229(8)	132
N6—H6B...O1A	1/2-x,-1/2+y,1/2-z	1.91	2.751(7)	165
C2—H2...O1W	-x,1-y,-z	2.43	3.338(9)	166
C2A—H2A...O3	----------	2.54	3.260(9)	135
C8A—H8A...O2	1/2-x,1/2+y,1/2-z	2.26	3.174(8)	166
C12A —H12F...O2W	-1/2+x,3/2-y,-1/2+z	2.31	3.17(2)	150
Complex 5				
N6A—H6A1...O1A	----------	2.28	2.6260	104
N6A—H6A1...O2	1-x,1/2+y,1-z	2.54	3.0776	122
N6A—H6A1...O3	1-x,1/2+y,1-z	2.26	3.0411	151
N6A —H6A2...O1W	----------	2.11	2.9660	174
N6—H6A...O1	----------	2.25	2.6124	105
N6 —H6A...O4	1-x,-1/2+y,1-z	2.09	2.8916	156
N6 —H6B...O2W	----------	2.12	2.9787	174
C2 —H2 ..O4	----------	2.50	3.4262	172
C2A—H2A...O3	x,y,-1+z	2.57	3.4418	157
C8A —H8A...O9	x,-1+y,z	2.43	3.1547	135
C10A—H10A...O9	x,-1+y,z	2.47	3.3443	150
C10A —H10B...O3	1-x,-1/2+y,1-z	2.55	3.3078	135

Figure S1: Tetrahedral coordination environment of silver (a) in complex **3** (b) in complex **4**

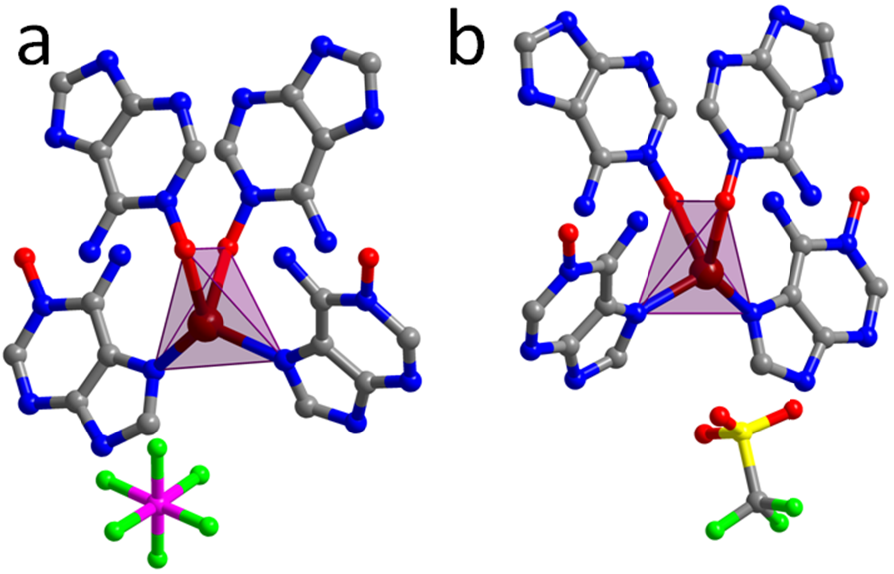


Figure S2: Intermolecular hydrogen bonding of exocyclic amino group with perchlorate and water oxygen

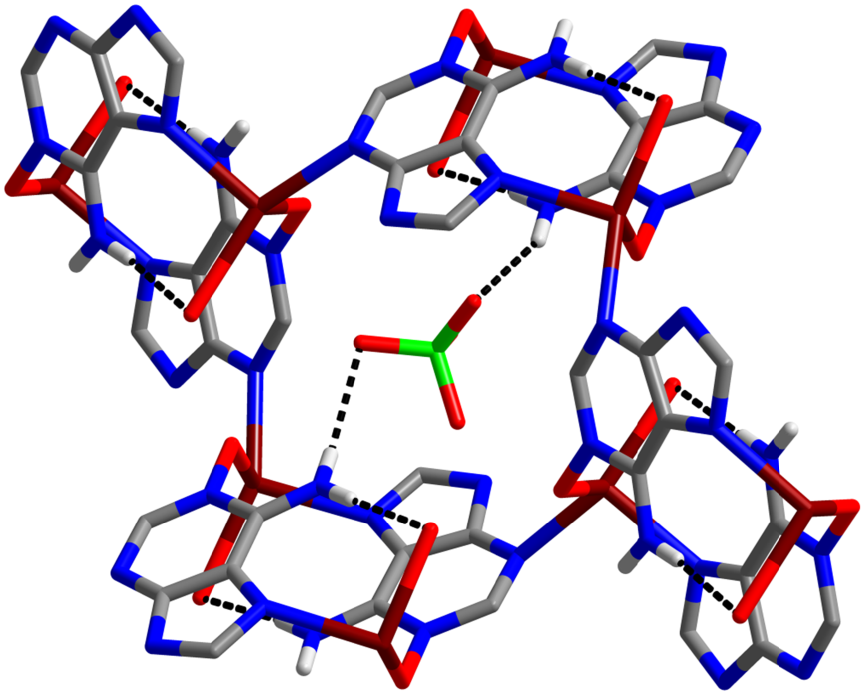


Figure S3: Ortep diagram of complex **1** drawn at 50% ellipsoid probability.

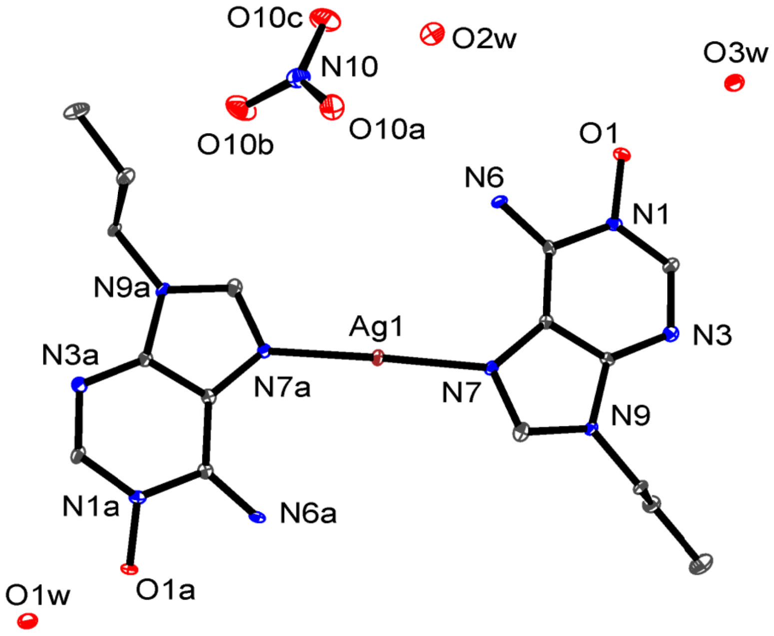


Figure S4: Ortep diagram of complex **2** drawn at 50% ellipsoid probability.

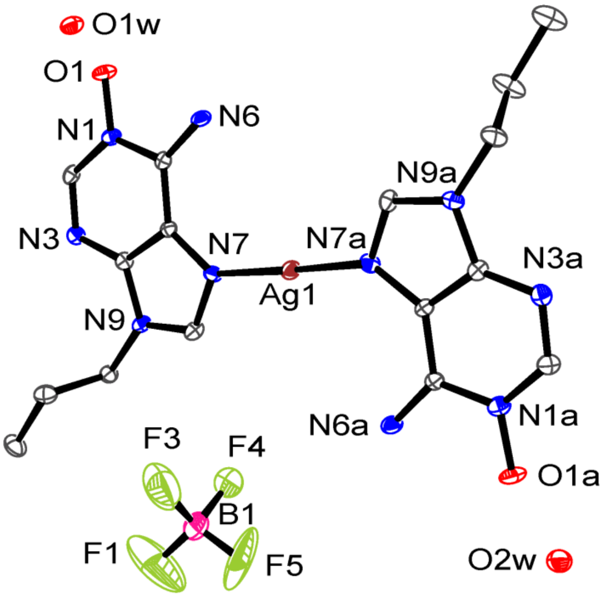


Figure S5: Ortep diagram of complex **3** drawn at 50% ellipsoid probability.

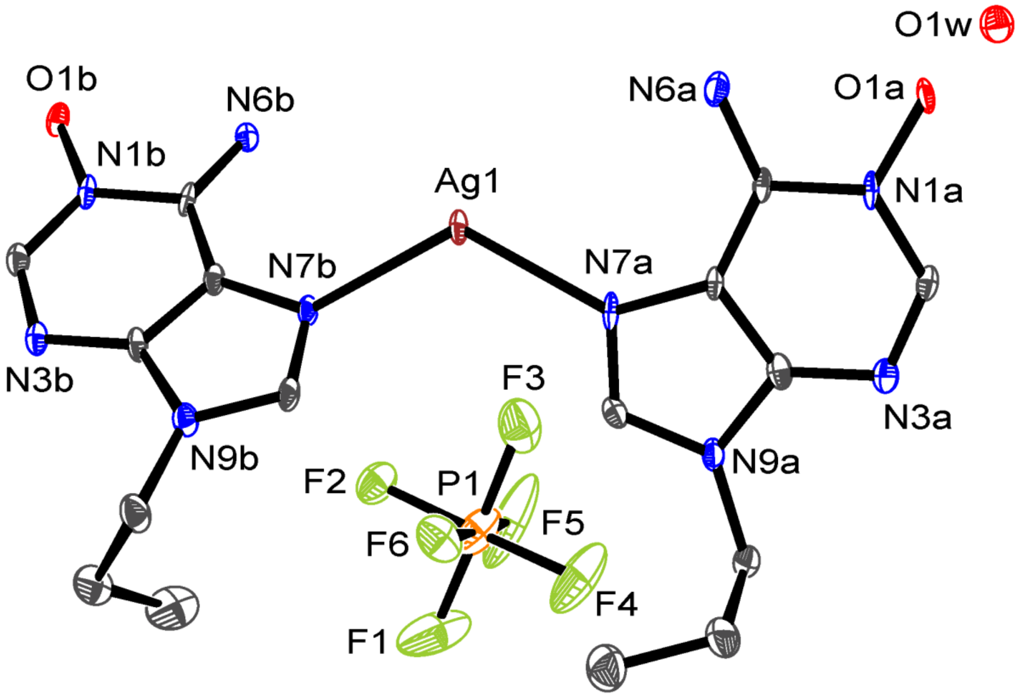


Figure S6: Ortep diagram of complex **4** drawn at 50% ellipsoid probability.

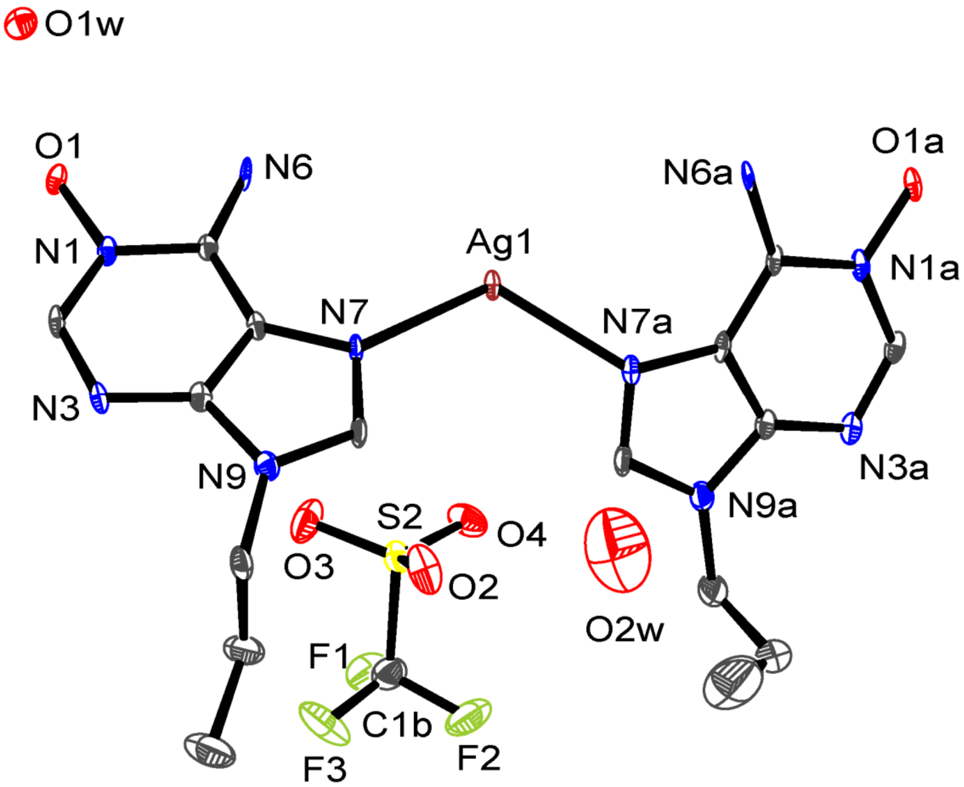


Figure S7: Ortep diagram of complex **5** drawn at 50% ellipsoid probability.

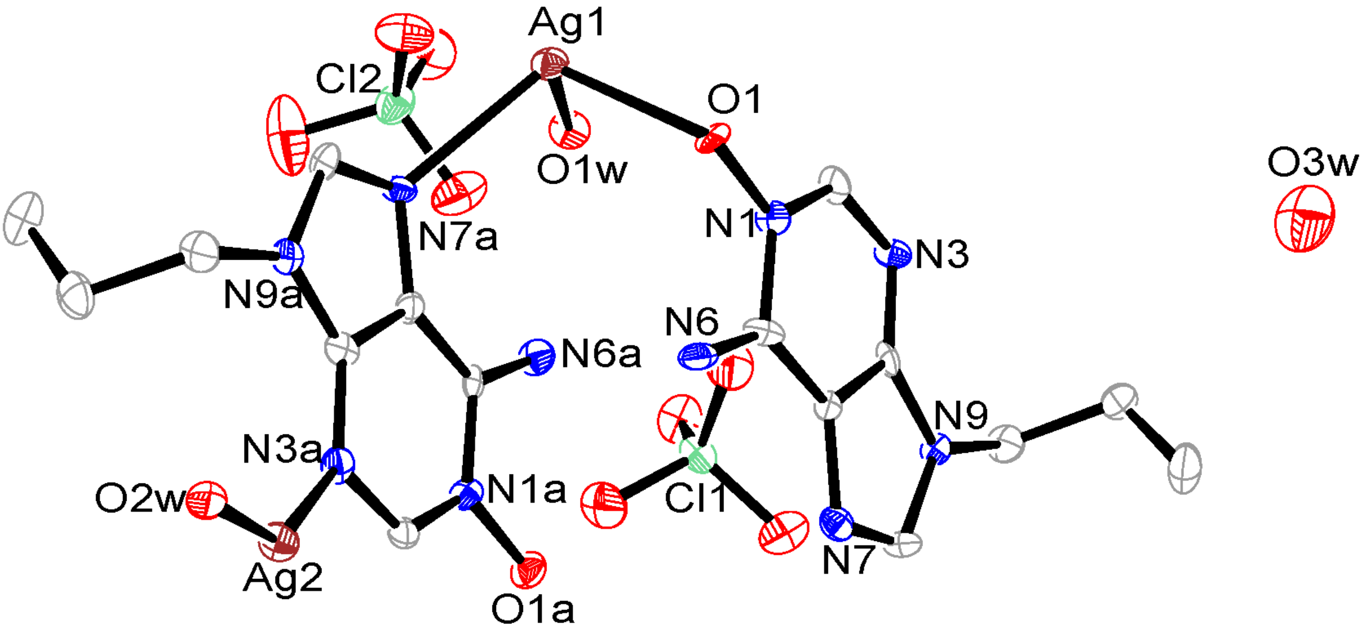
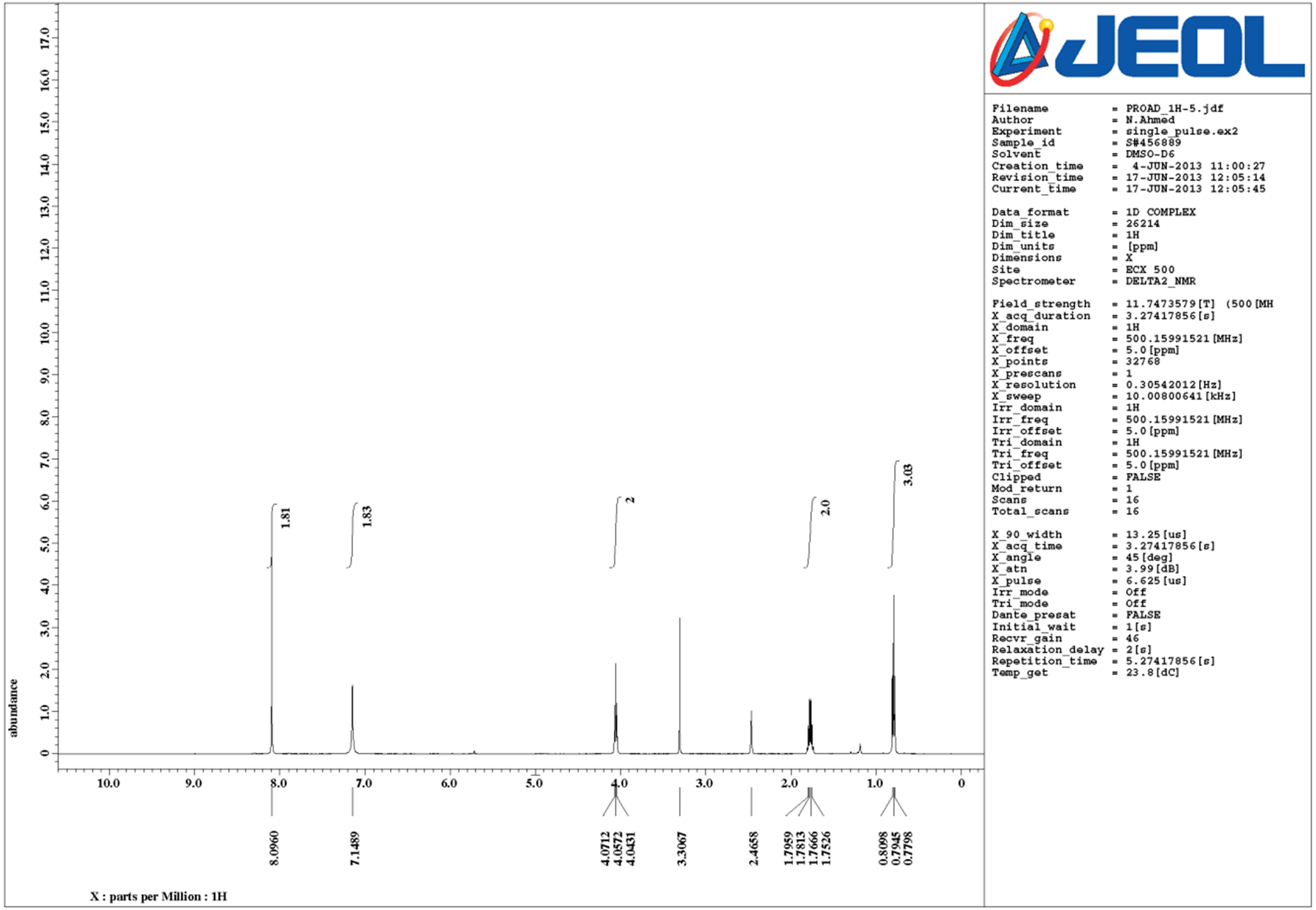


Figure S8: ^{1}H NMR spectra of N9-propyladenine.



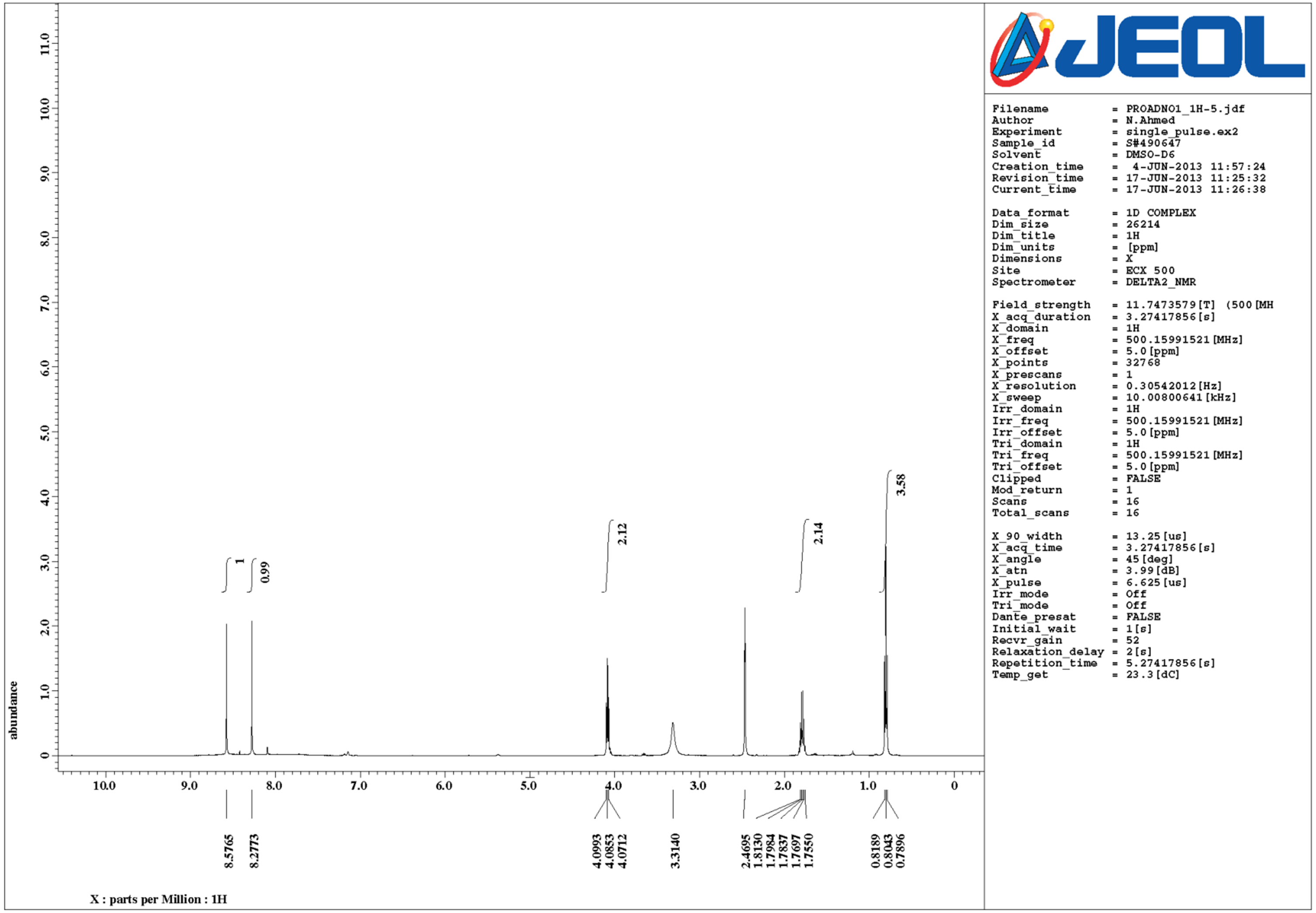
```
Filename          = PROAD_1H-5.jdf
Author            = N.Ahmed
Experiment        = single_pulse.ex2
Sample_id         = S#456889
Solvent           = DMSO-D6
Creation_time     =  4-JUN-2013 11:00:27
Revision_time     = 17-JUN-2013 12:05:14
Current_time      = 17-JUN-2013 12:05:45

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 3.27417856[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 32768
X_prescans        = 1
X_resolution      = 0.30542012[Hz]
X_sweep           = 10.00800641[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 13.25[us]
X_acq_time        = 3.27417856[s]
X_angle           = 45[deg]
X_atn             = 3.99[dB]
X_pulse           = 6.625[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 46
Relaxation_delay  = 2[s]
Repetition_time   = 5.27417856[s]
Temp_get          = 23.8[dC]
```

Figure S9: ^{1}H NMR spectra of N9-propyladenine N^1-oxide.



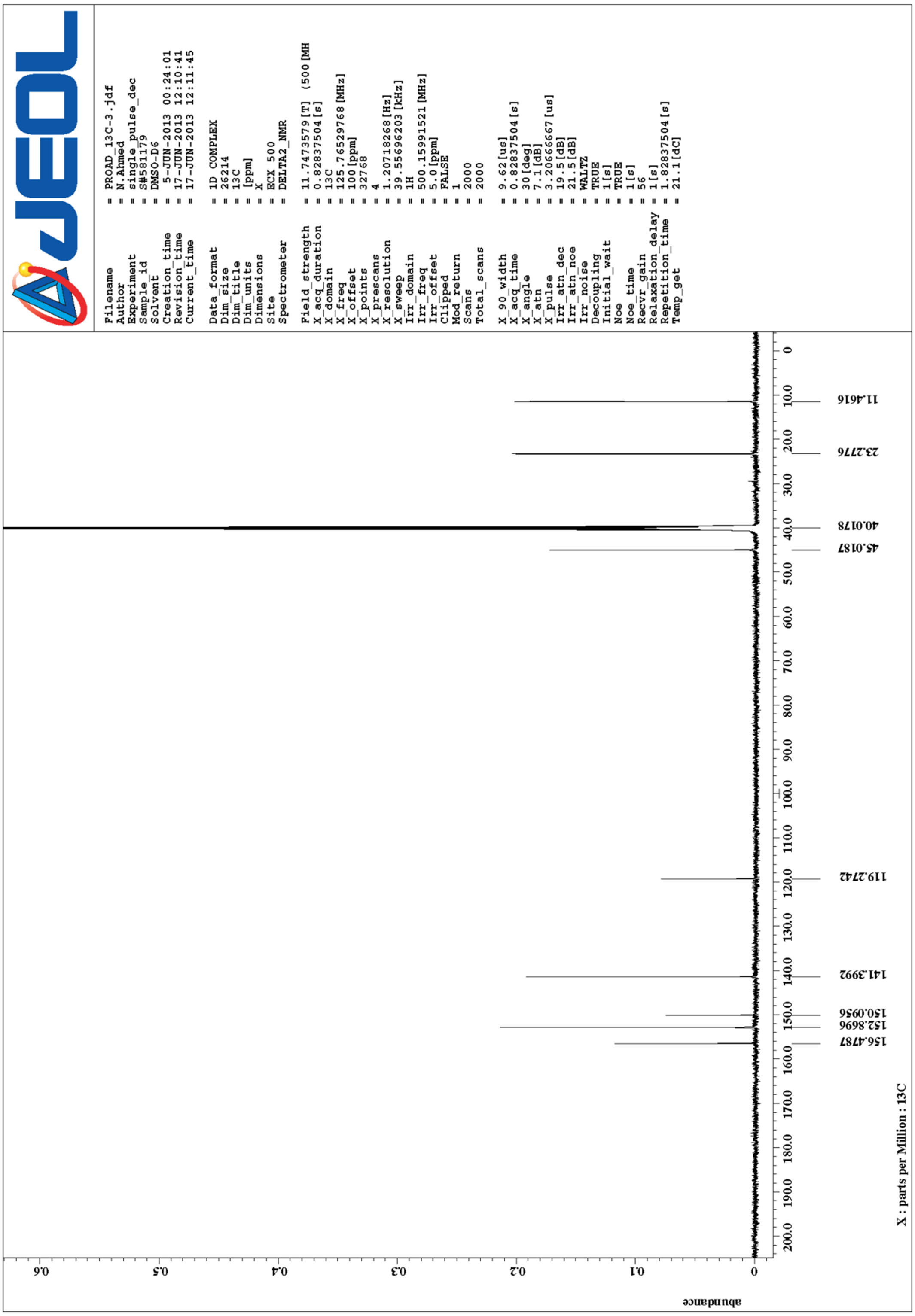
```
Filename          = PROADNO1_1H-5.jdf
Author            = N.Ahmed
Experiment        = single_pulse.ex2
Sample_id         = S#490647
Solvent           = DMSO-D6
Creation_time     =  4-JUN-2013 11:57:24
Revision_time     = 17-JUN-2013 11:25:32
Current_time      = 17-JUN-2013 11:26:38

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T]  (500[MH
X_acq_duration    = 3.27417856[s]
X_domain          = 1H
X_freq            = 500.15991521[MHz]
X_offset          = 5.0[ppm]
X_points          = 32768
X_prescans        = 1
X_resolution      = 0.30542012[Hz]
X_sweep           = 10.00800641[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Tri_domain        = 1H
Tri_freq          = 500.15991521[MHz]
Tri_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 13.25[us]
X_acq_time        = 3.27417856[s]
X_angle           = 45[deg]
X_atn             = 3.99[dB]
X_pulse           = 6.625[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 52
Relaxation_delay  = 2[s]
Repetition_time   = 5.27417856[s]
Temp_get          = 23.3[dC]
```

Figure S10: ^{13}C NMR spectra of N9-propyladenine.



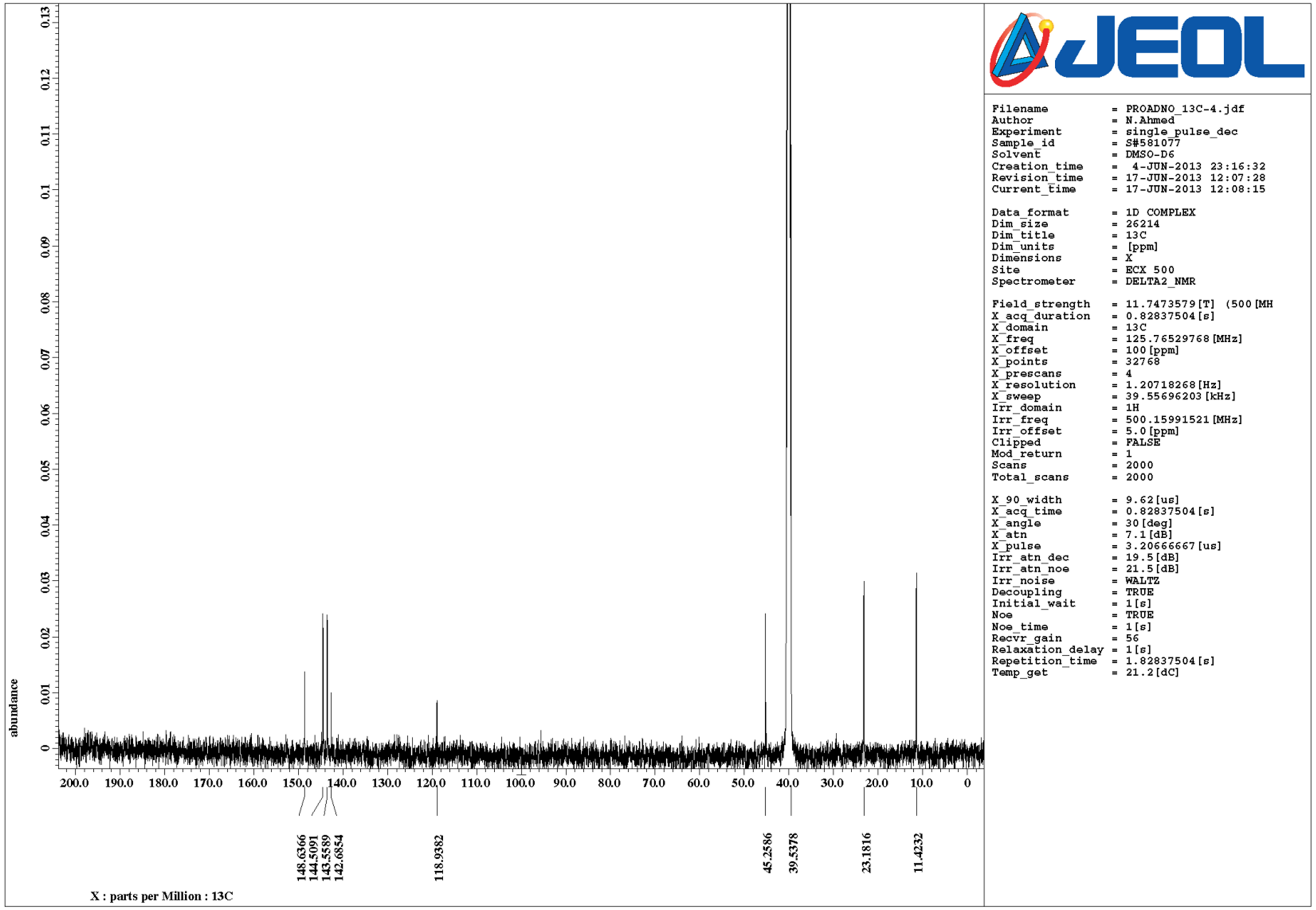
```
Filename            = PROAD_13C-3.jdf
Author              = N.Ahmed
Experiment          = single_pulse_dec
Sample_id           = S#581179
Solvent             = DMSO-D6
Creation_time       =  5-JUN-2013 00:24:01
Revision_time       = 17-JUN-2013 12:10:41
Current_time        = 17-JUN-2013 12:11:45

Data_format         = 1D COMPLEX
Dim_size            = 26214
Dim_title           = 13C
Dim_units           = [ppm]
Dimensions          = X
Site                = ECX 500
Spectrometer        = DELTA2_NMR

Field_strength      = 11.7473579[T] (500[MH
X_acq_duration      = 0.82837504[s]
X_domain            = 13C
X_freq              = 125.76529768[MHz]
X_offset            = 100[ppm]
X_points            = 32768
X_prescans          = 4
X_resolution        = 1.20718268[Hz]
X_sweep             = 39.55696203[kHz]
Irr_domain          = 1H
Irr_freq            = 500.15991521[MHz]
Irr_offset          = 5.0[ppm]
Clipped             = FALSE
Mod_return          = 1
Scans               = 2000
Total_scans         = 2000

X_90_width          = 9.62[us]
X_acq_time          = 0.82837504[s]
X_angle             = 30[deg]
X_atn               = 7.1[dB]
X_pulse             = 3.20666667[us]
Irr_atn_dec         = 19.5[dB]
Irr_atn_noe         = 21.5[dB]
Irr_noise           = WALTZ
Decoupling          = TRUE
Initial_wait        = 1[s]
Noe                 = TRUE
Noe_time            = 1[s]
Recvr_gain          = 56
Relaxation_delay    = 1[s]
Repetition_time     = 1.82837504[s]
Temp_get            = 21.1[dC]
```

Figure S11: ^{13}C NMR spectra of N9-propyladenine *N*^{1}-oxide.



```
Filename          = PROADNO_13C-4.jdf
Author            = N.Ahmed
Experiment        = single_pulse_dec
Sample_id         = S#581077
Solvent           = DMSO-D6
Creation_time     =  4-JUN-2013 23:16:32
Revision_time     = 17-JUN-2013 12:07:28
Current_time      = 17-JUN-2013 12:08:15

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 500
Spectrometer      = DELTA2_NMR

Field_strength    = 11.7473579[T] (500[MH
X_acq_duration    = 0.82837504[s]
X_domain          = 13C
X_freq            = 125.76529768[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.20718268[Hz]
X_sweep           = 39.55696203[kHz]
Irr_domain        = 1H
Irr_freq          = 500.15991521[MHz]
Irr_offset        = 5.0[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 2000
Total_scans       = 2000

X_90_width        = 9.62[us]
X_acq_time        = 0.82837504[s]
X_angle           = 30[deg]
X_atn             = 7.1[dB]
X_pulse           = 3.20666667[us]
Irr_atn_dec       = 19.5[dB]
Irr_atn_noe       = 21.5[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 1[s]
Recvr_gain        = 56
Relaxation_delay  = 1[s]
Repetition_time   = 1.82837504[s]
Temp_get          = 21.2[dC]
```

Figure S12: HRMS of N9-propyladenine N^1-oxide.

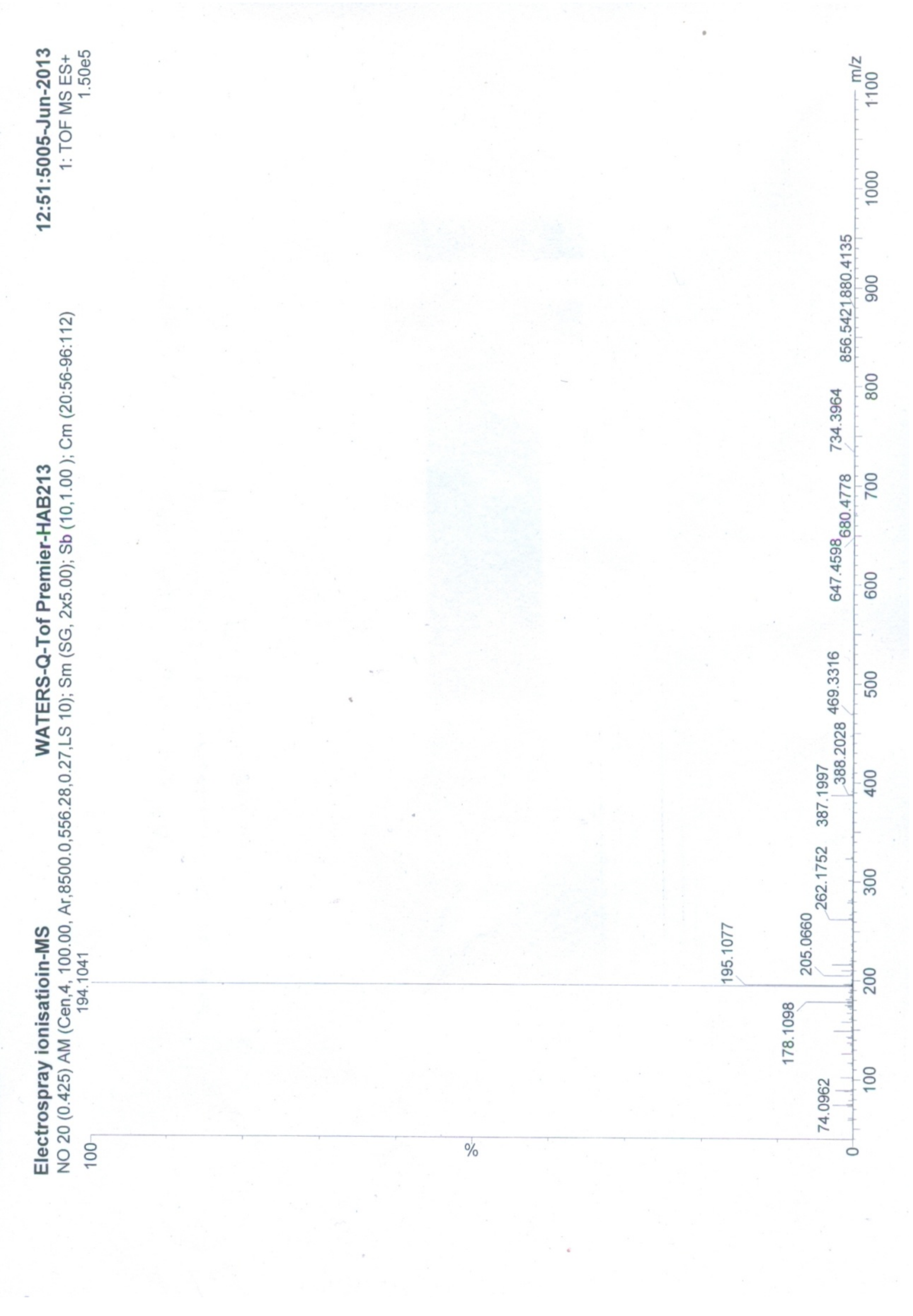


Figure S13: HRMS of complex **1**.

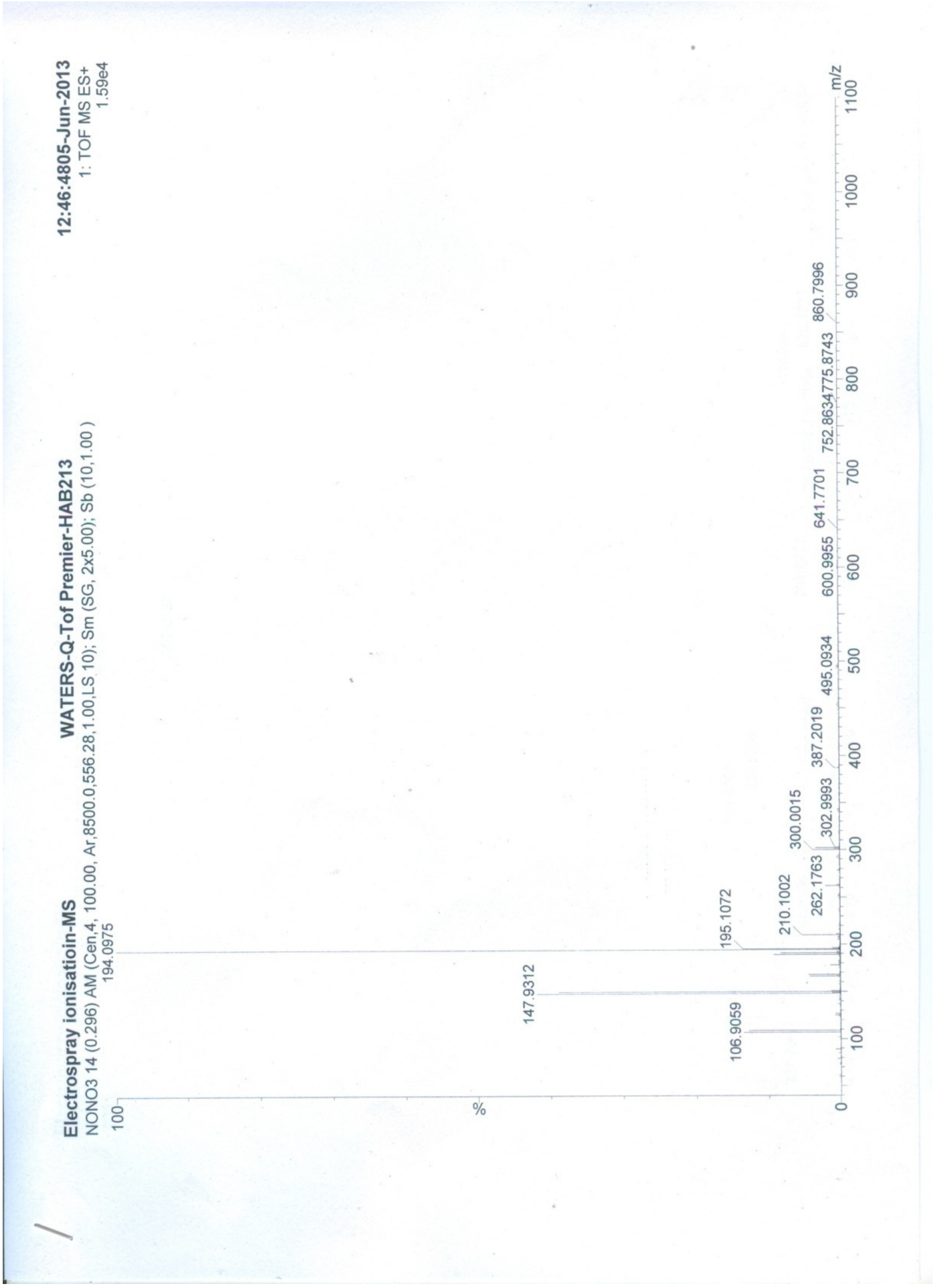


Figure S14: HRMS of complex **2**.

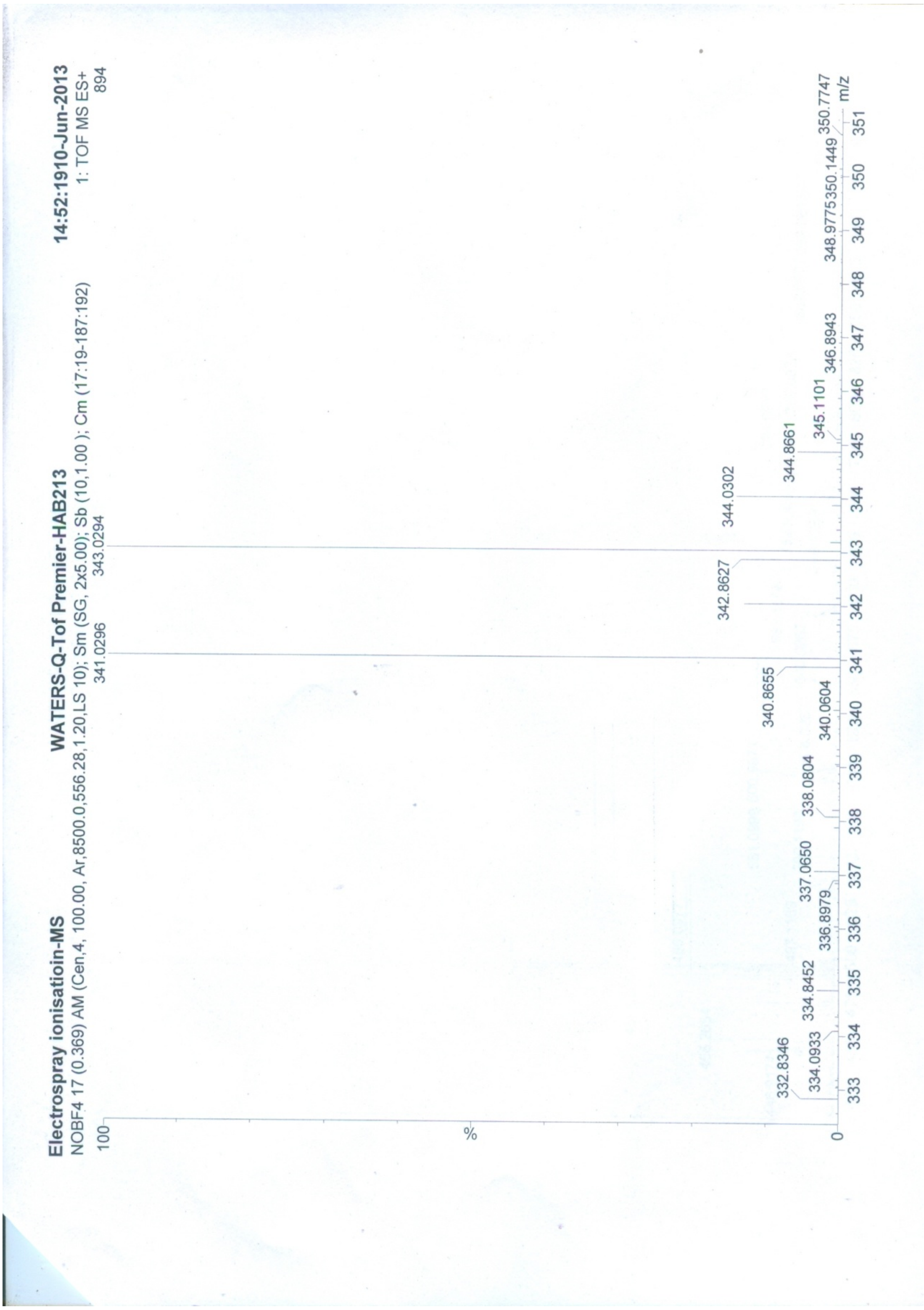


Figure S15: HRMS of complex **3**.

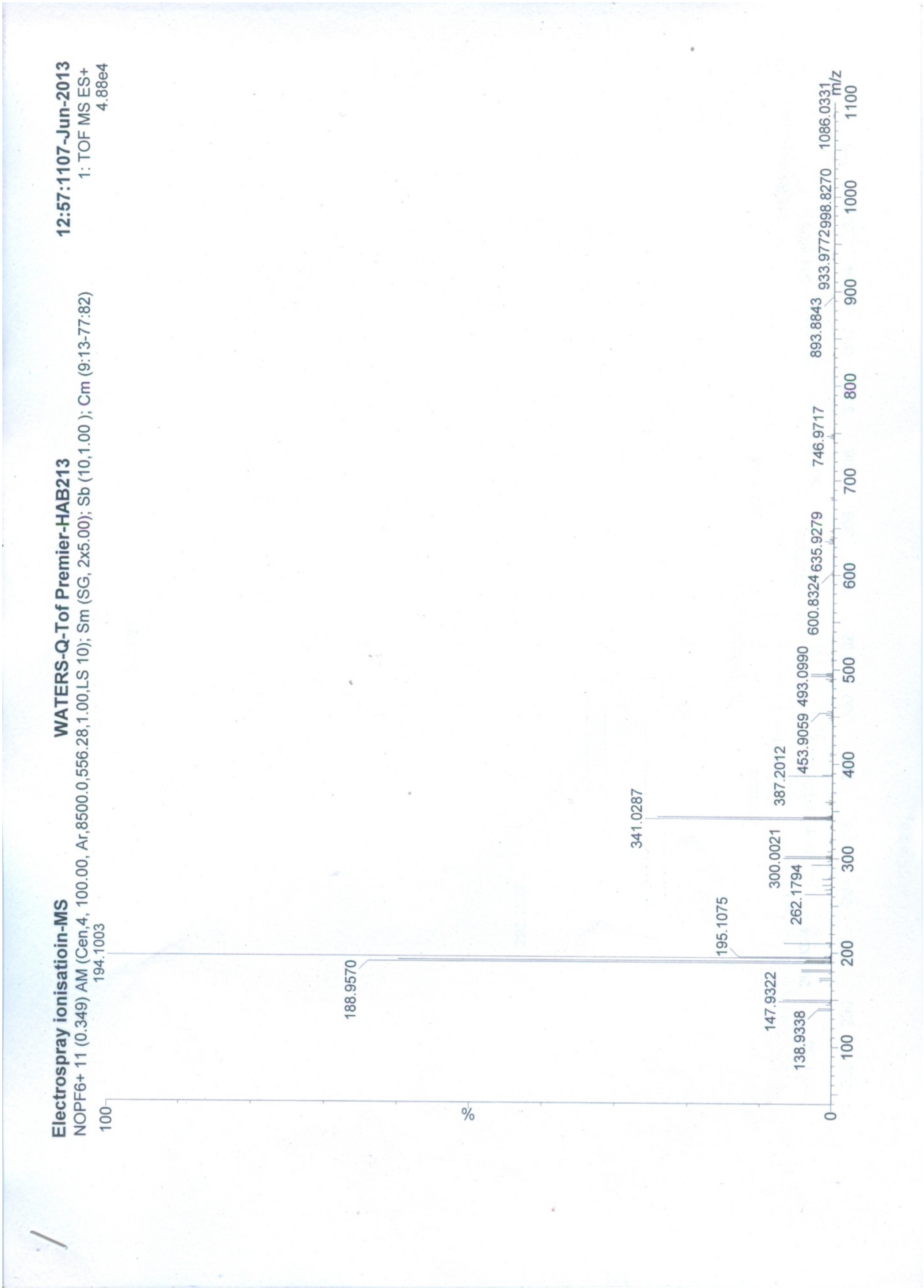


Figure S16: HRMS of complex **4**.

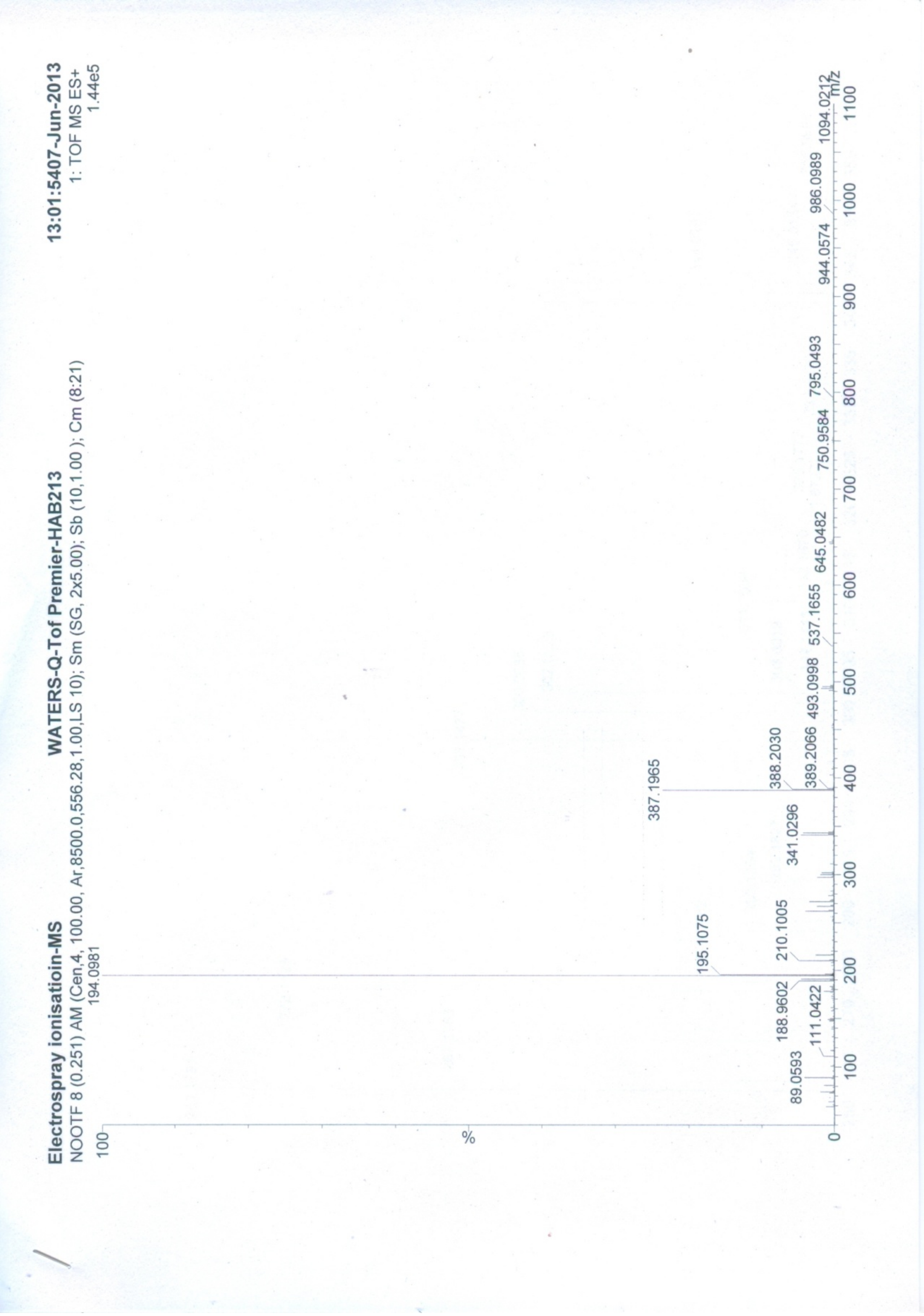
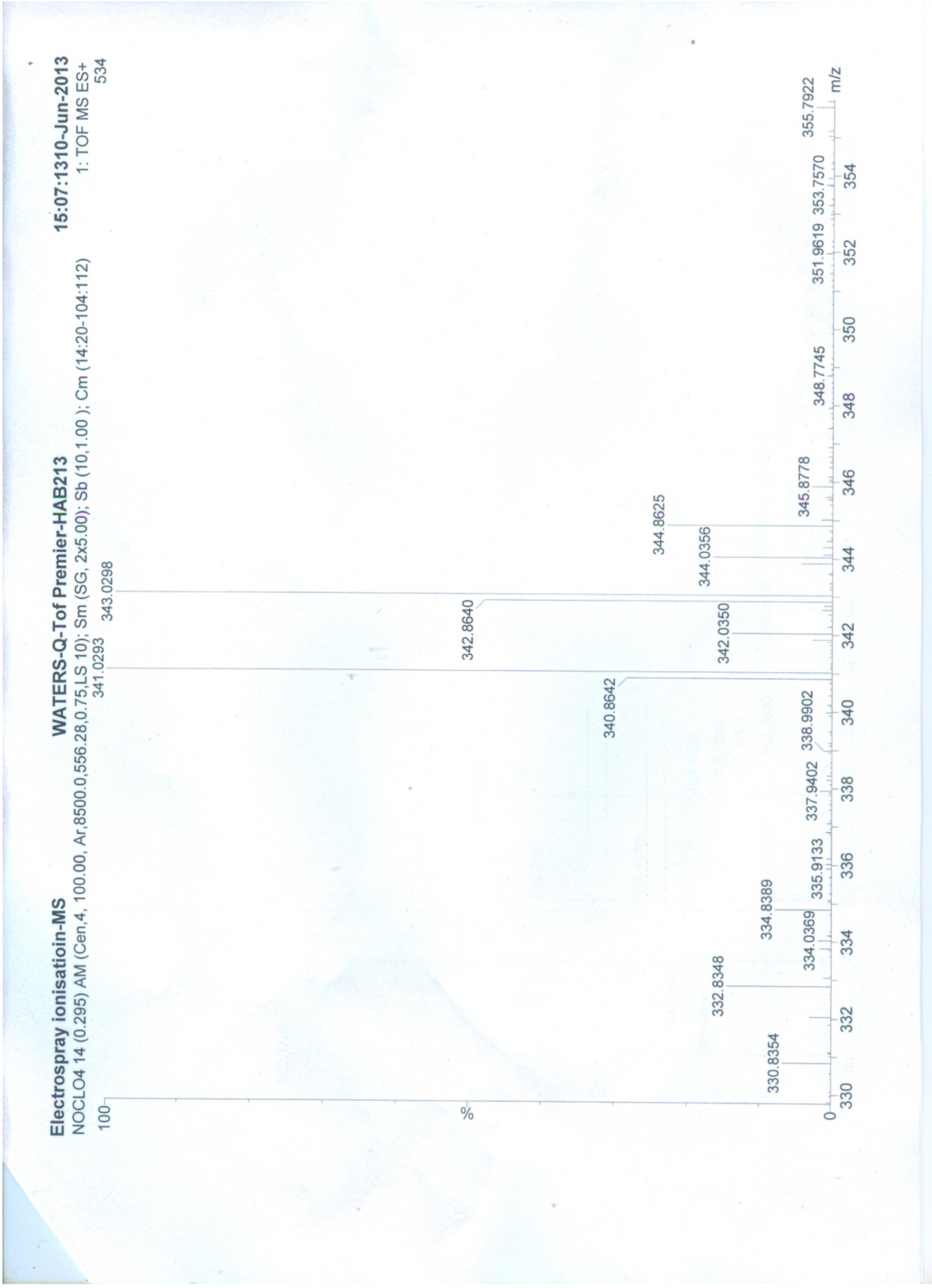


Figure S17: HRMS of complex **5**.



References:

1. C. S. Purohit, A. K. Mishra, S. Verma, *Inorg. Chem.,* 2007, **46**, 8493
2. SAINT+, 6.02 ed.; Bruker AXS, Madison, WI, **1999**.
3. Sheldrick, G. M. SADABS 2.0; University of Göttingen: Göttingen, Germany, **2000**.
4. Sheldrick, G. M. SHELXL-97: Program for Crystal Structure Refinement; University of Göttingen: Göttingen, Germany, **1997**.