

Supporting Information

for

Synthesis, Binding Mode, and Anti-hyperglycemic Activity of Potent and Selective (5-imidazol-2-yl-4-phenylpyrimidin-2-yl)[2-(2-pyridylamino)ethyl]amine Inhibitors of Glycogen Synthase Kinase 3

Allan S. Wagman[†], Rustum S. Boyce[†], Sean P. Brown[†], Dane Goff[†], Johanna Jansen, Vincent P. Le[†], Barry H. Levine[†], Simon C. Ng[†], Zhi-Jie Ni[†], John M. Nuss[†], Keith B. Pfister, Savithri Ramurthy, Paul A. Renhowe[†], David B. Ring[†], Wei Shu, Sharadha Subramanian, Cynthia M. Shafer, Xiaohui A. Zhou, Stephen D. Harrison[†], Kirk W. Johnson[†] and Dirksen E. Bussiere*

Global Discovery Chemistry, Novartis Institutes for BioMedical Research, 5300 Chiron Way, Emeryville, California 94608

- 1) Table S1 for crystallographic refinement.
- 2) ¹H and ¹³C NMR spectra, HPLC and LCMS traces for compounds 1, 2, 8, 16, 17, 18a, 18d, 20, 25a, 25u, 26, 30a, 30b, 31b, 32, 33, 35a, 36a, 36b, 36c, 37b, 46b, 46c, 46d, 46e, 46f, 49, 51b, 51d, 60a, 60b, 60c, 60k, 60m, 60n, 60p, 60q, 60r, 60s, 60t, and 61r.

*To whom correspondence and compound requests should be addressed. Phone: (510)879-9505. E-mail: dirksen.bussiere@novartis.com.

[†]No longer at Novartis Institutes for BioMedical Research-Emeryville, formerly Chiron Corporation

Table S1. Data collection and refinement statistics

Data collection	GSK3:CHIR-911
Resolution (Å)	25.00-2.595 (2.69-2.595)*
Space group	P2 ₁
Cell dimension	
a, b, c (Å)	56.747, 65.070, 57.336
α , β , γ (°)	90.000, 110.526, 90.000
Total reflections	58415 (5548)
Unique reflections	12763 (1261)
Multiplicity	4.6 (4.4)
Completeness (%)	99.7 (99.4)
I/ σ (I)	12.4 (3.6)
R _{merge} of intensities	0.115 (0.455)
CC1/2	(0.896)
CC*	(0.972)
Refinement	
R _{work}	0.2121
R _{free}	0.2466
Number of non-H atoms	3018
macromolecules	2987
ligands	31
Protein	
RMSD bonds (Å)	0.010
RMSD angles (°)	1.240
Ramachandran favored (%)	93.20
Ramachandran allowed (%)	5.32
Ramachandran outliers (%)	1.48
Clashscore	18.06
Mean B-factor (Å ²)	38.99
macromolecules	39.59
ligands	26.35

*Values in parentheses are for highest-resolution shell. Two separate crystal data sets were merged to refine this structure.

**R_{work} and R_{free} were calculated from the working and test reflection sets, respectively. The test set contained 5% of the total reflections available.

SampleName kpc155HCL

Injection Volume 12.00 ul

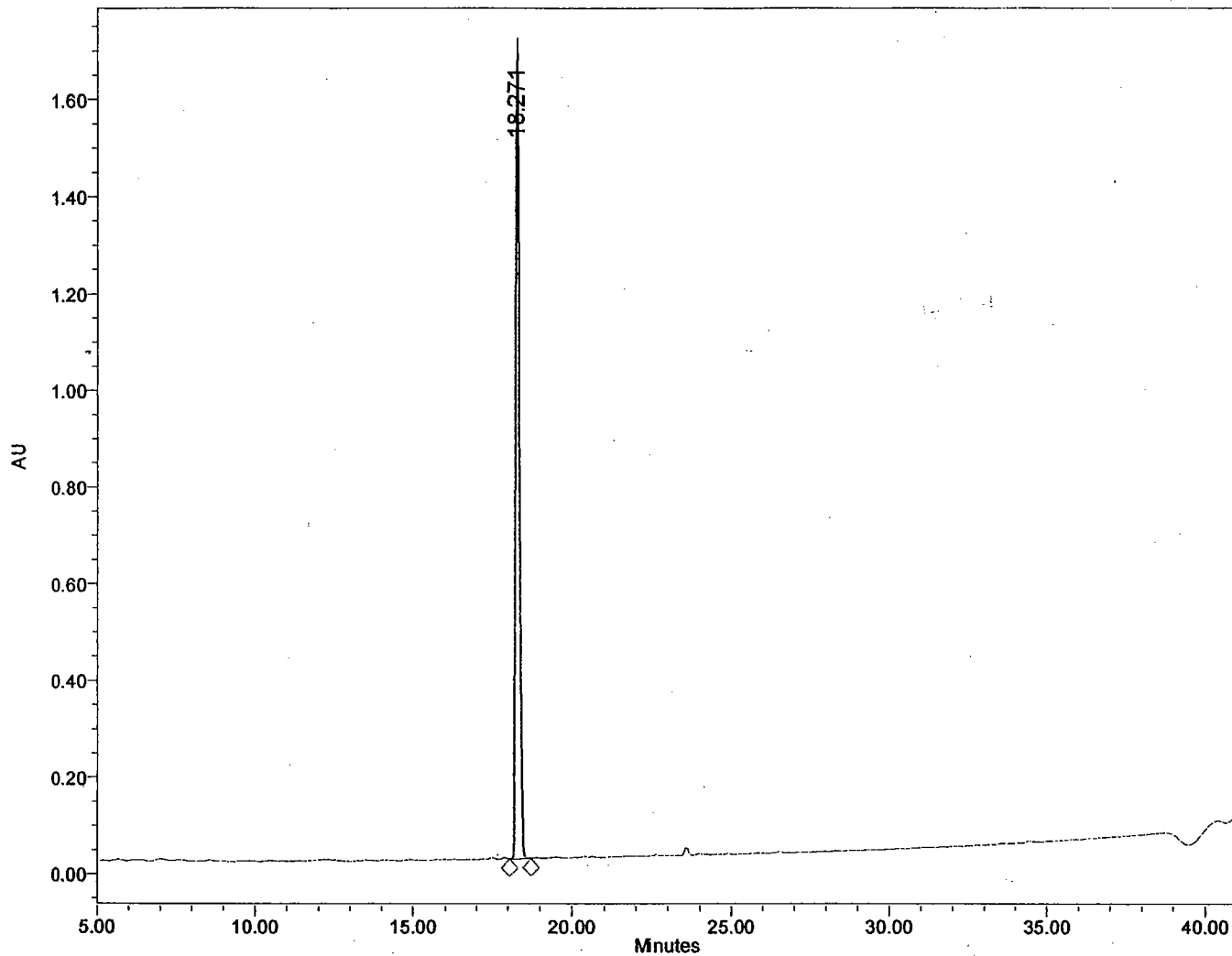
Date Acquired 4/13/99 6:19:56 F

Vial 1

Channel Description PDA 221

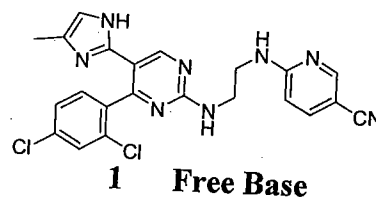
Acq Method Set 5100

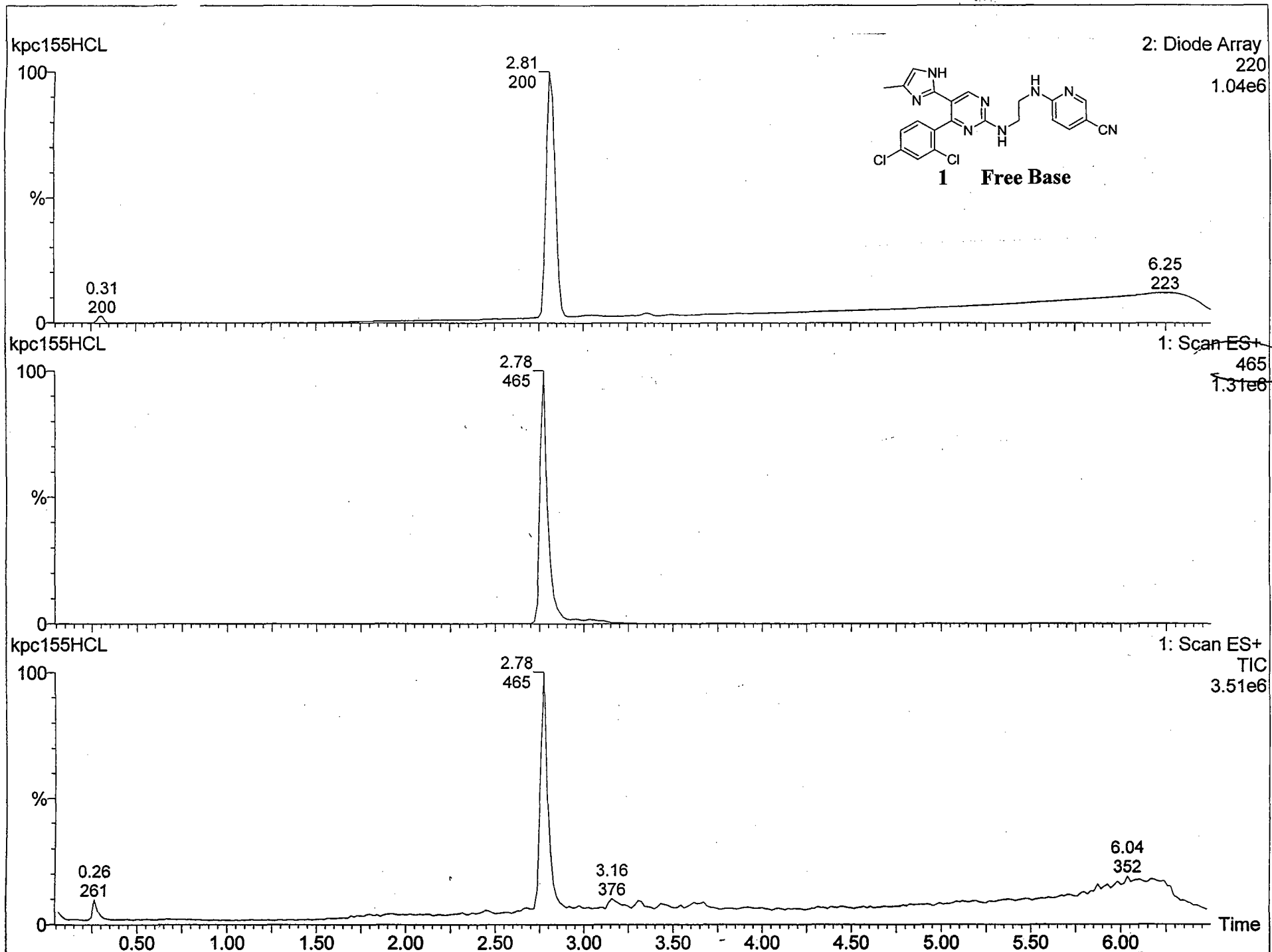
Auto-Scaled Chromatogram



Peak Results

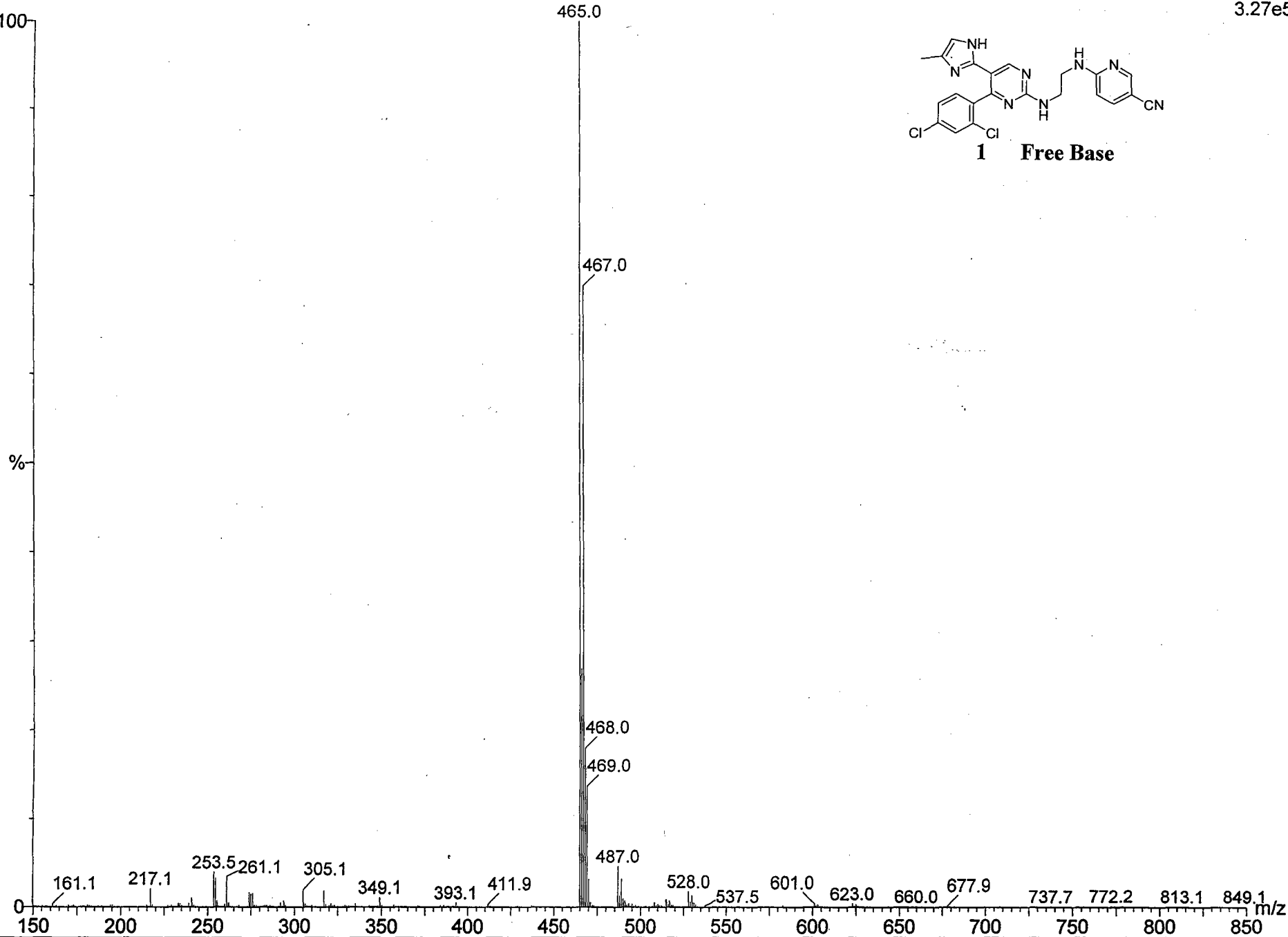
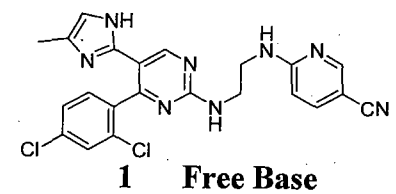
	Name	RT	Start Time	End Time	% Height	% Area
1		18.271	18.072	18.738	100.00	100.00





kpc155HCL 150 (2.775) Cm (146:156)

1: Scan ES+
3.27e5



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Relax. delay 1.000 sec

Pulse 37.5 degrees

Acq. time 1.998 sec

Width 4500.5 Hz

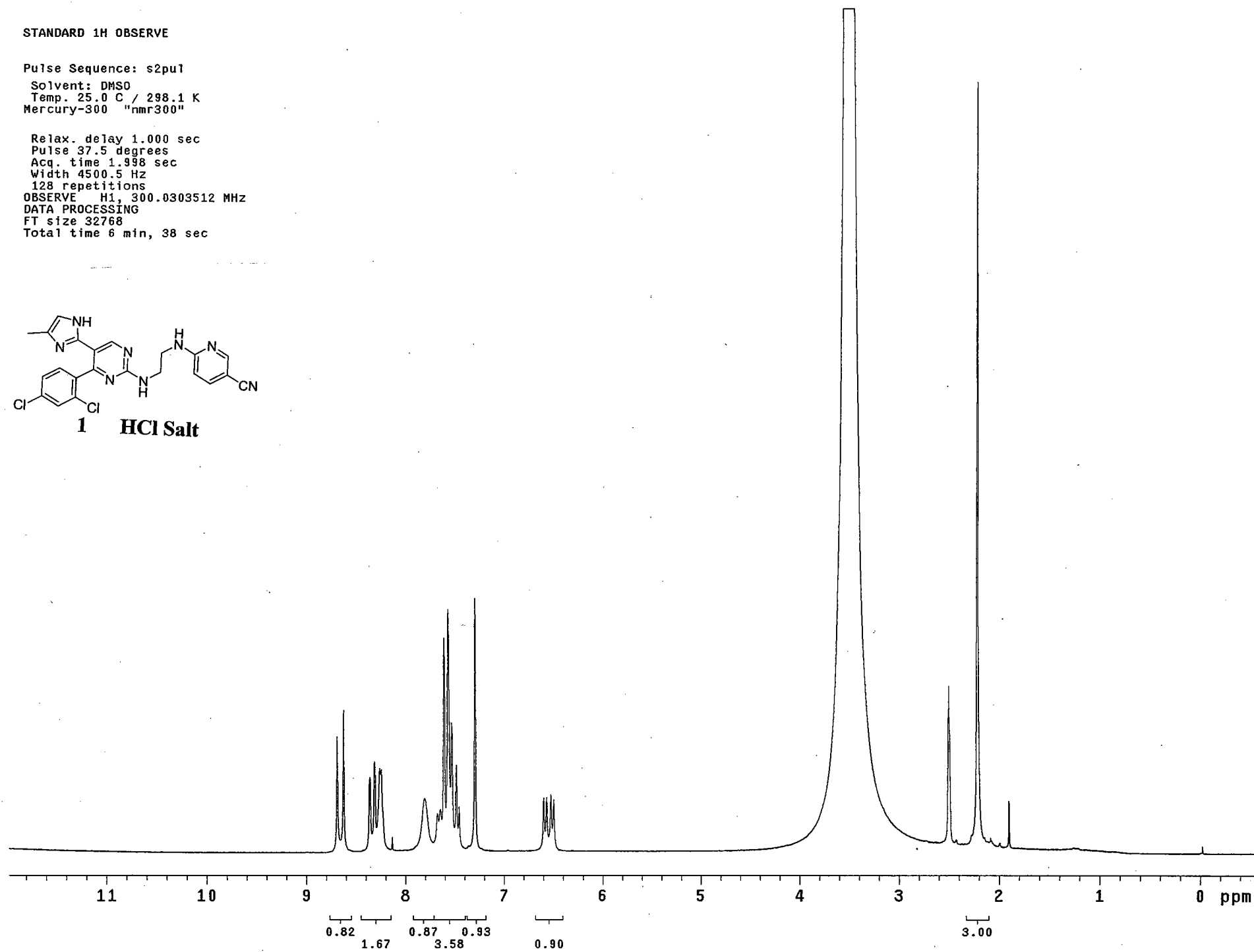
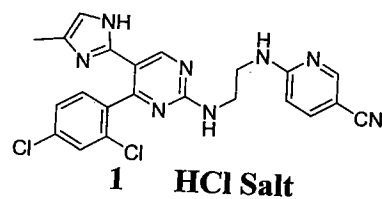
128 repetitions

OBSERVE H1, 300.0303512 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 38 sec



13C OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Pulse 54.2 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

2272 repetitions

OBSERVE C13, 75.4427175 MHz

DECOUPLE H1, 300.0318890 MHz

Power 45 dB

continuously on

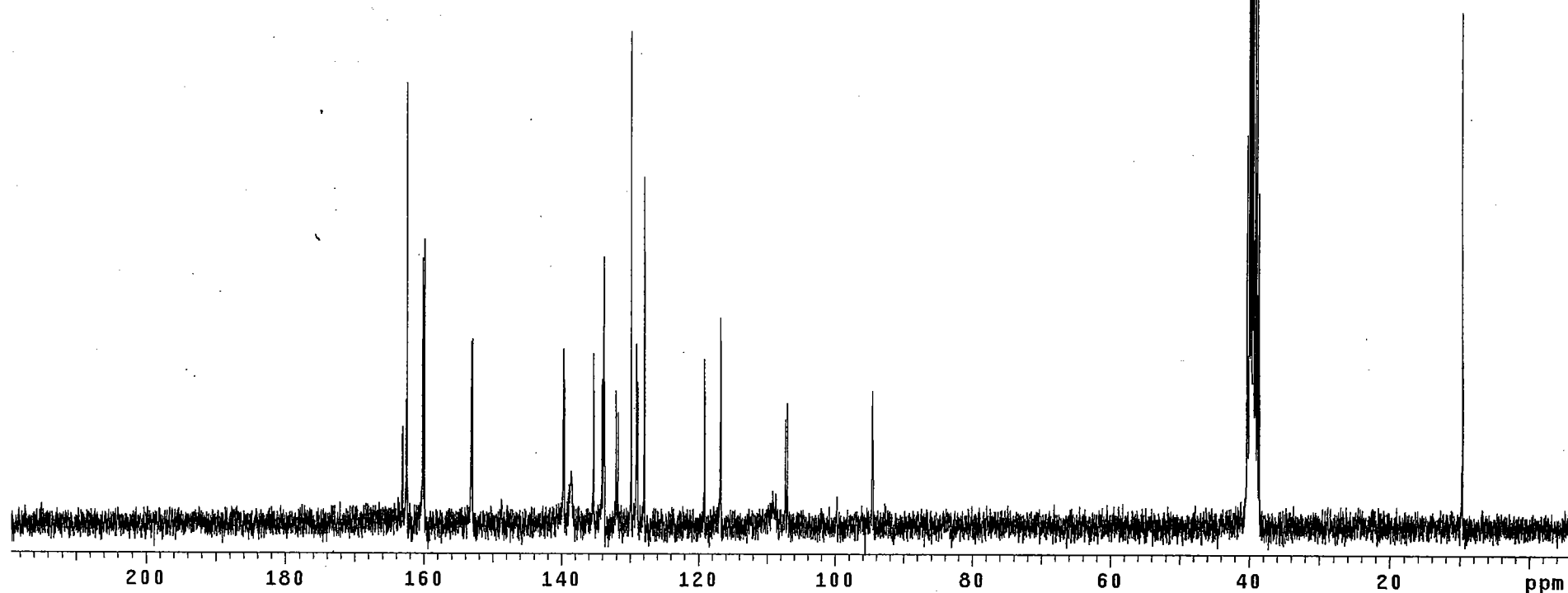
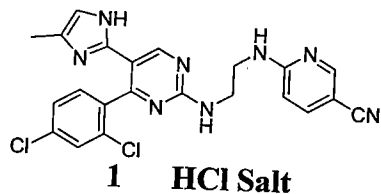
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 586 hr, 42 min, 3 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Relax. delay 1.000 sec

Pulse 37.5 degrees

Acq. time 1.998 sec

Width 4500.5 Hz

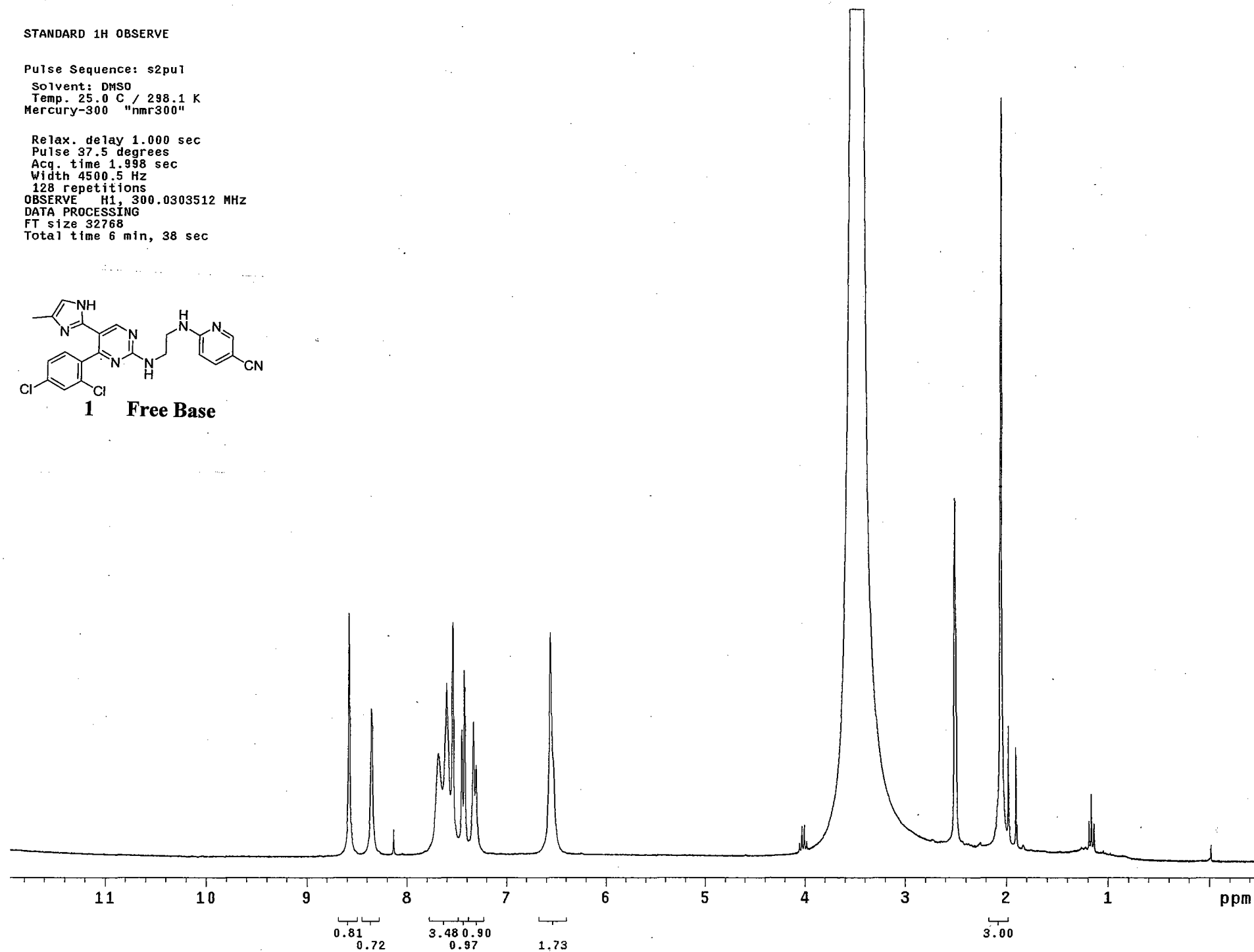
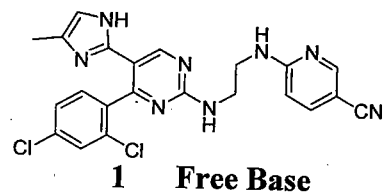
128 repetitions

OBSERVE H1, 300.0303512 MHz

DATA PROCESSING

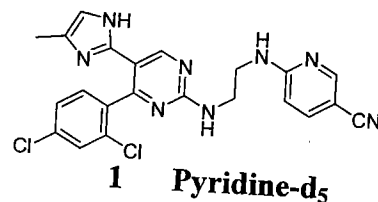
FT size 32768

Total time 6 min, 38 sec



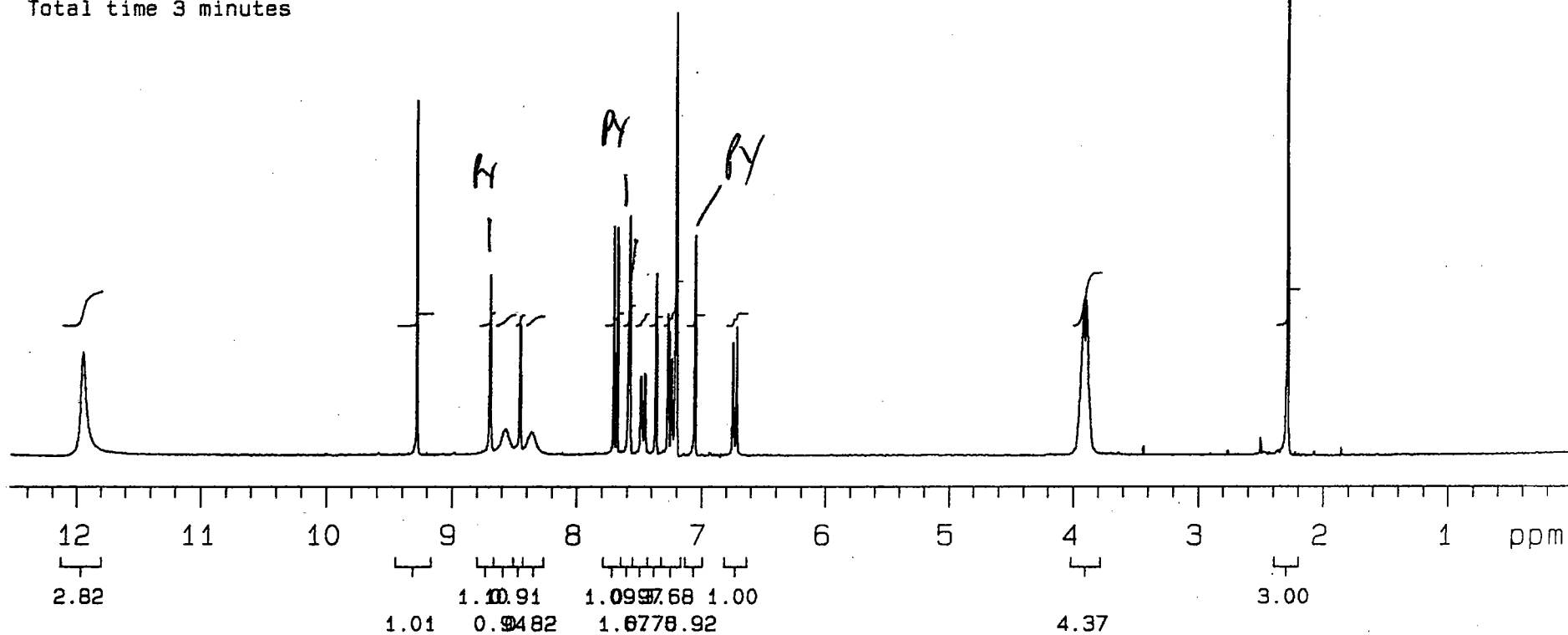
STANDARD 1H OBSERVE

Solvent: *pyridine-d₅*
 Temp. 70.0 C / 343.1 K
 Mercury-300 "nmr300"



PULSE SEQUENCE

Relax. delay arrayed
 1st pulse arrayed
 2nd pulse 45.0 degrees
 Acq. time 2.000 sec
 Width 3775.5 Hz
 Arrayed repetitions
 OBSERVE H1, 300.0369535 MHz
 DATA PROCESSING
 FT size 16384
 Total time 3 minutes



13C OBSERVE

Pyridine-d₅

Solvent:

Temp. 70.0 C / 343.1 K

Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed

1st pulse arrayed

2nd pulse 30.0 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

Arrayed repetitions

OBSERVE C13, 75.4443256 MHz

DECOUPLE H1, 300.0389129 MHz

Power 47 dB

continuously on

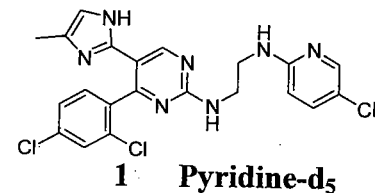
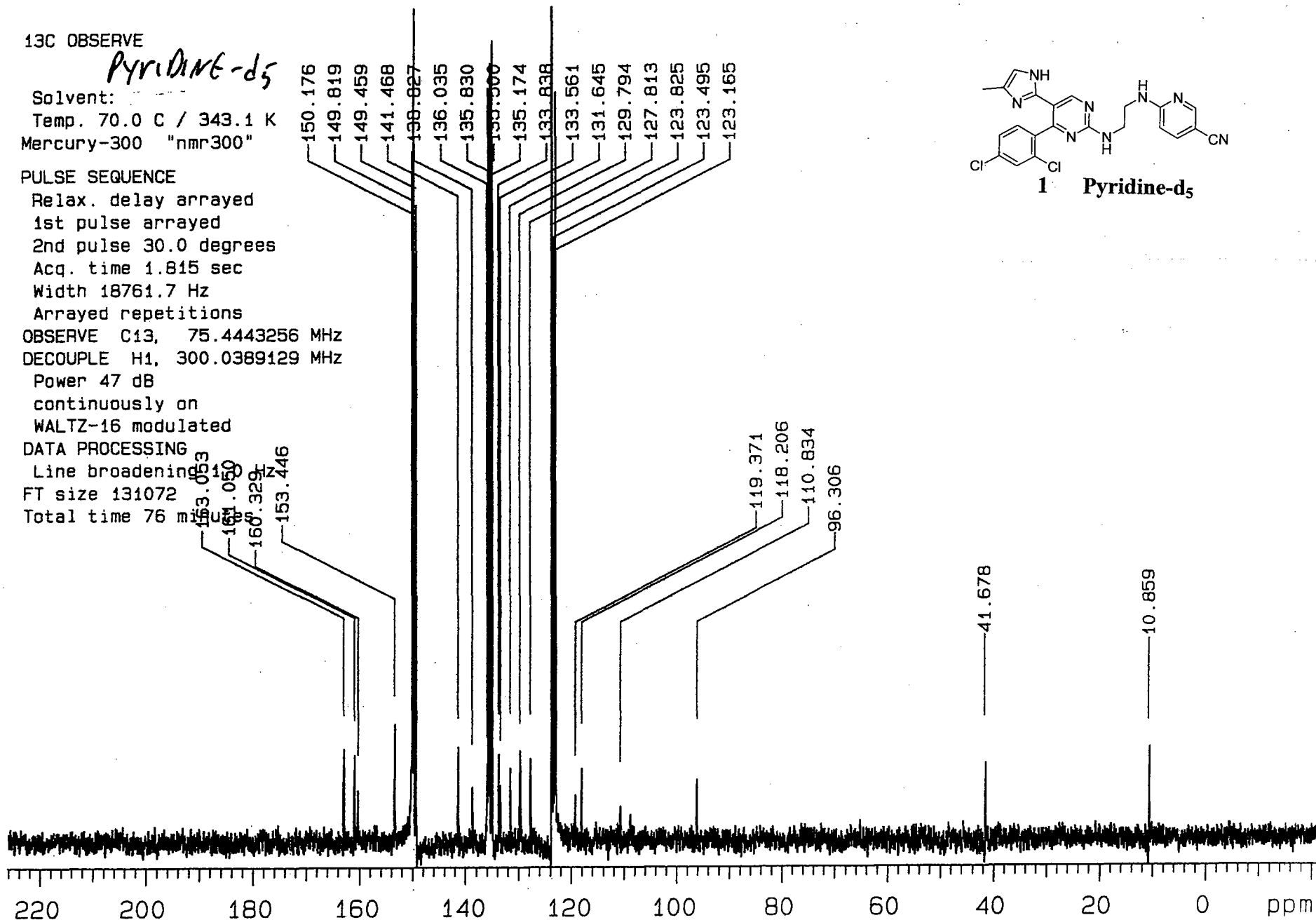
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.10

FT size 131072

Total time 76 min



CHIRON Technologies S M D D R Medicinal & Organic Chemistry Group

Sample Name: az3061

System Name: Shana

Project Name: GSK_3

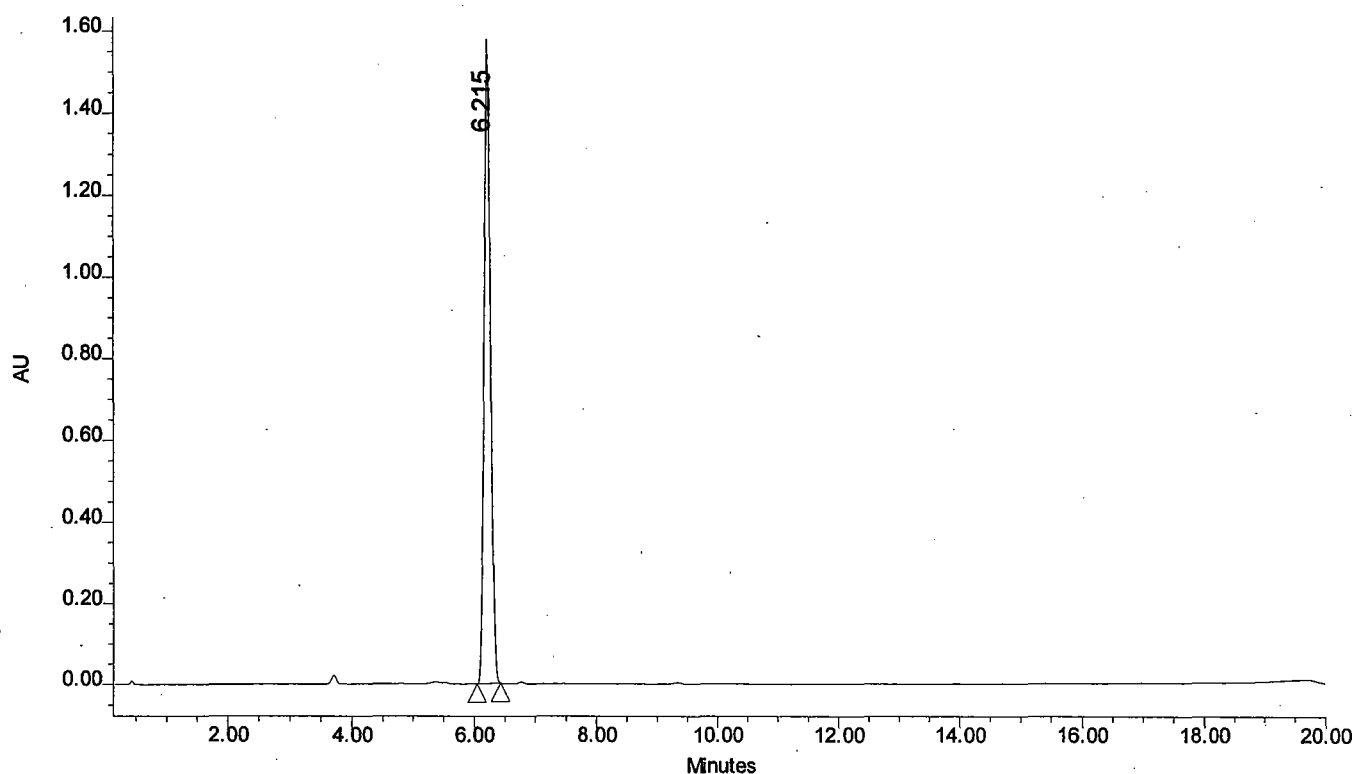
Label:

Acq Method Set: Rabbit20

Date Acquired: 8/7/98 5:39:34 PM

Injection Volume- 10.00 ul

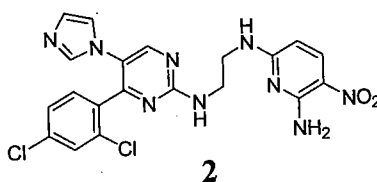
Vial # 30



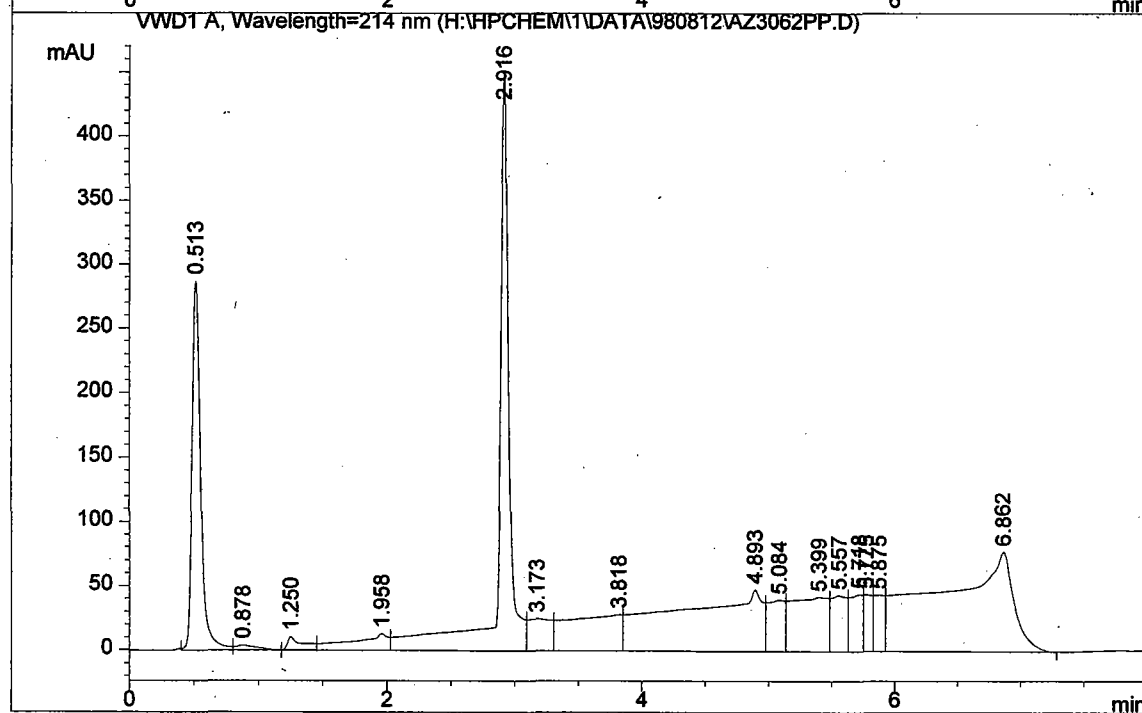
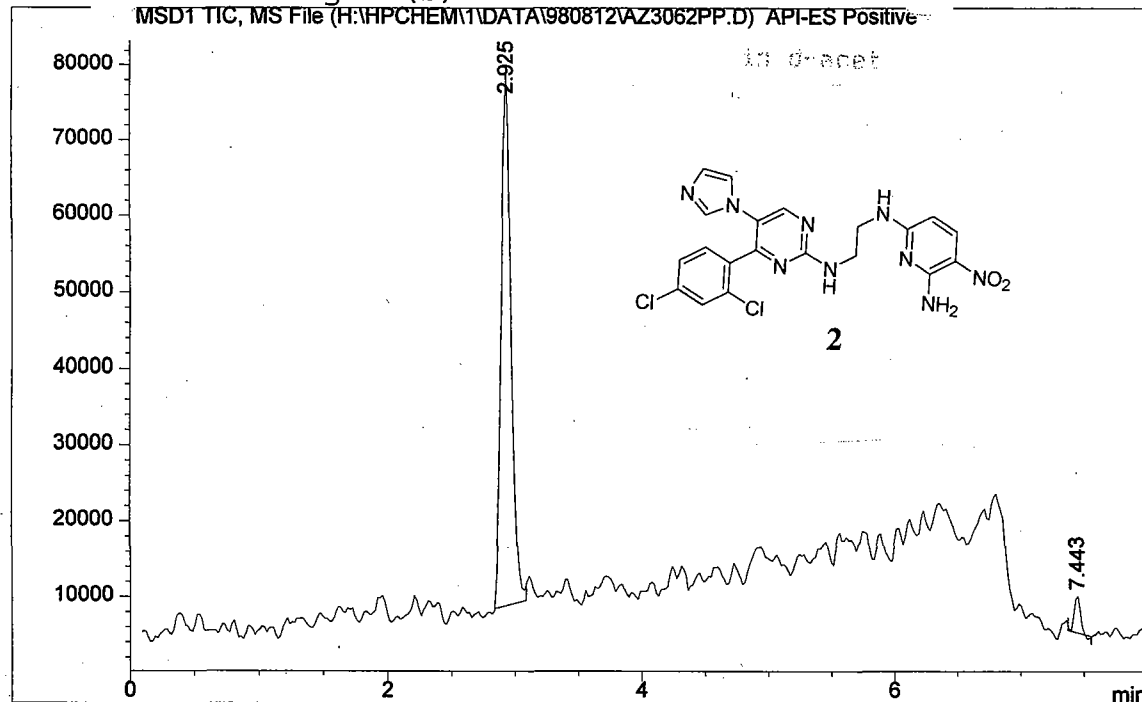
Peak Results

	Retention Time	Start Time	End Time	% Area
1	6.215	6.047	6.430	100.00

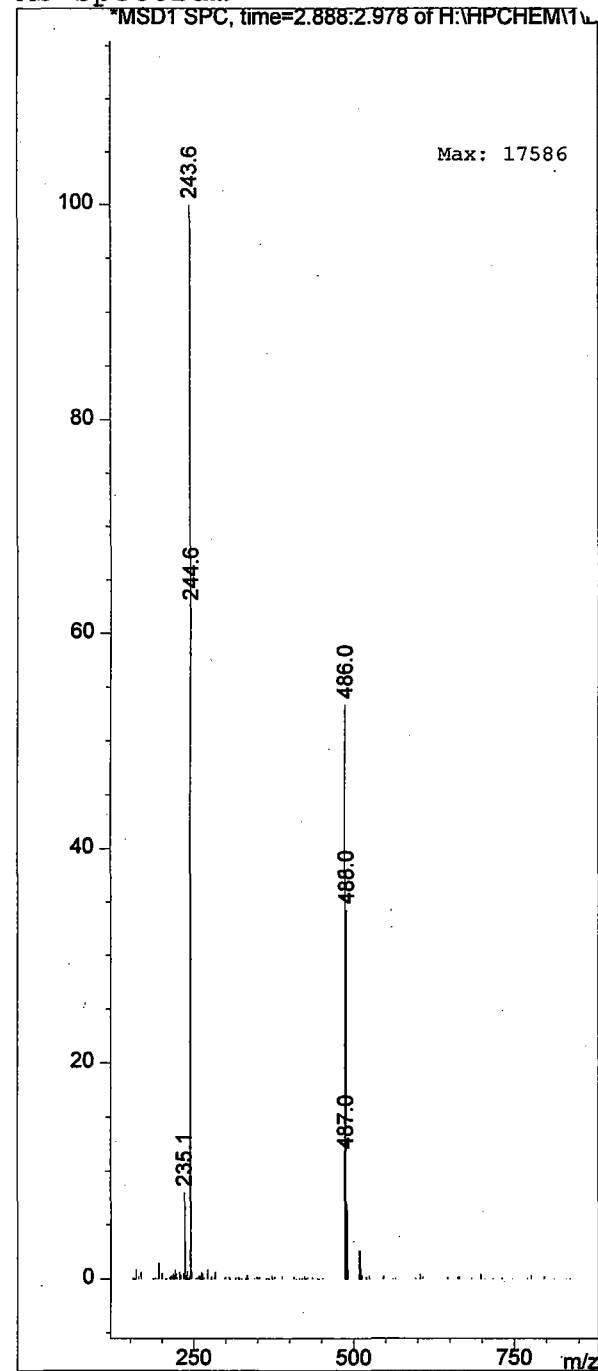
in D-ACET



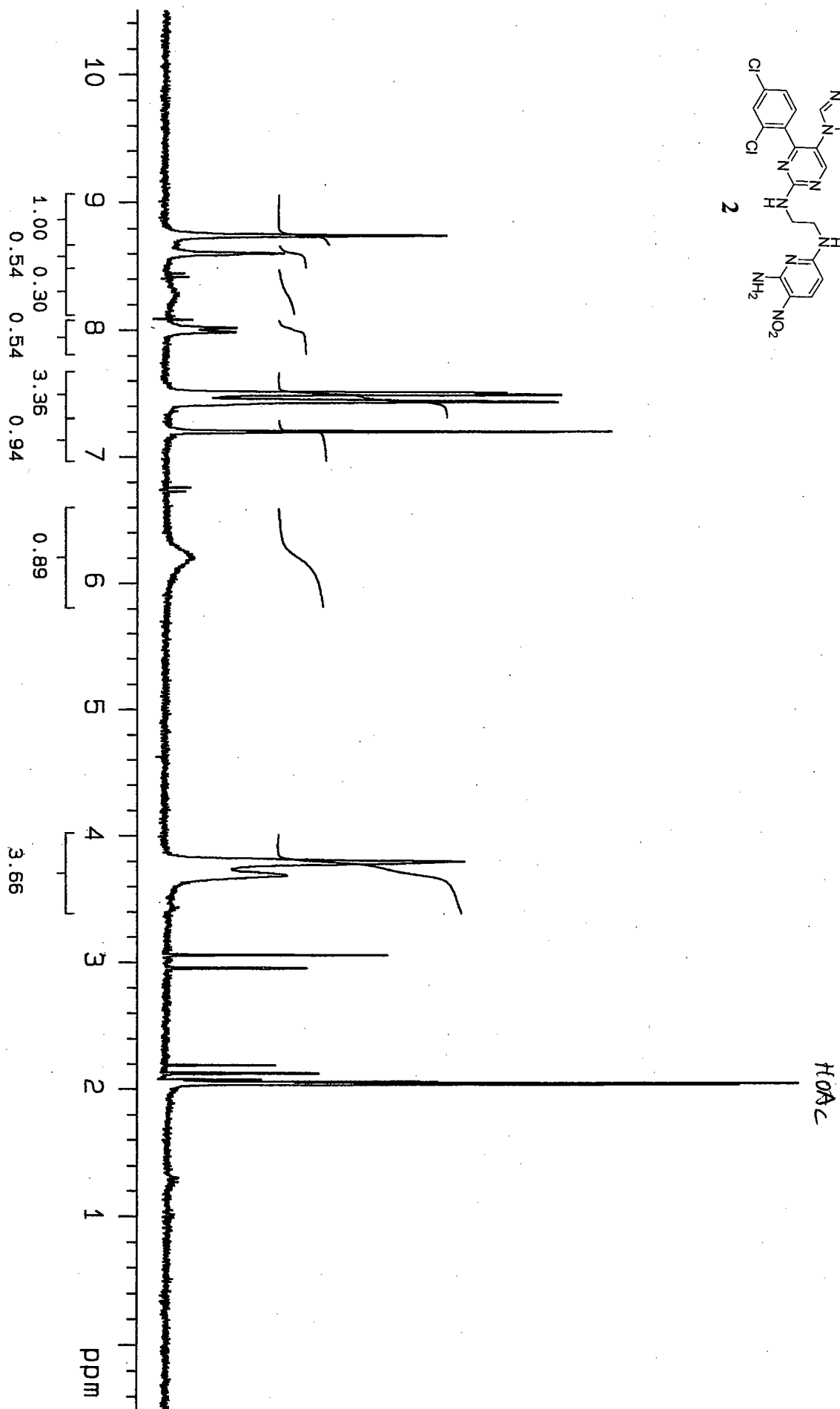
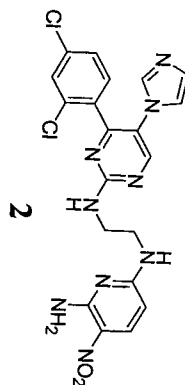
Chromatogram(s)



MS Spectrum



az3062pp in d-acetic acid



SampleName kpc16-2

Injection Volume 10.00 ul

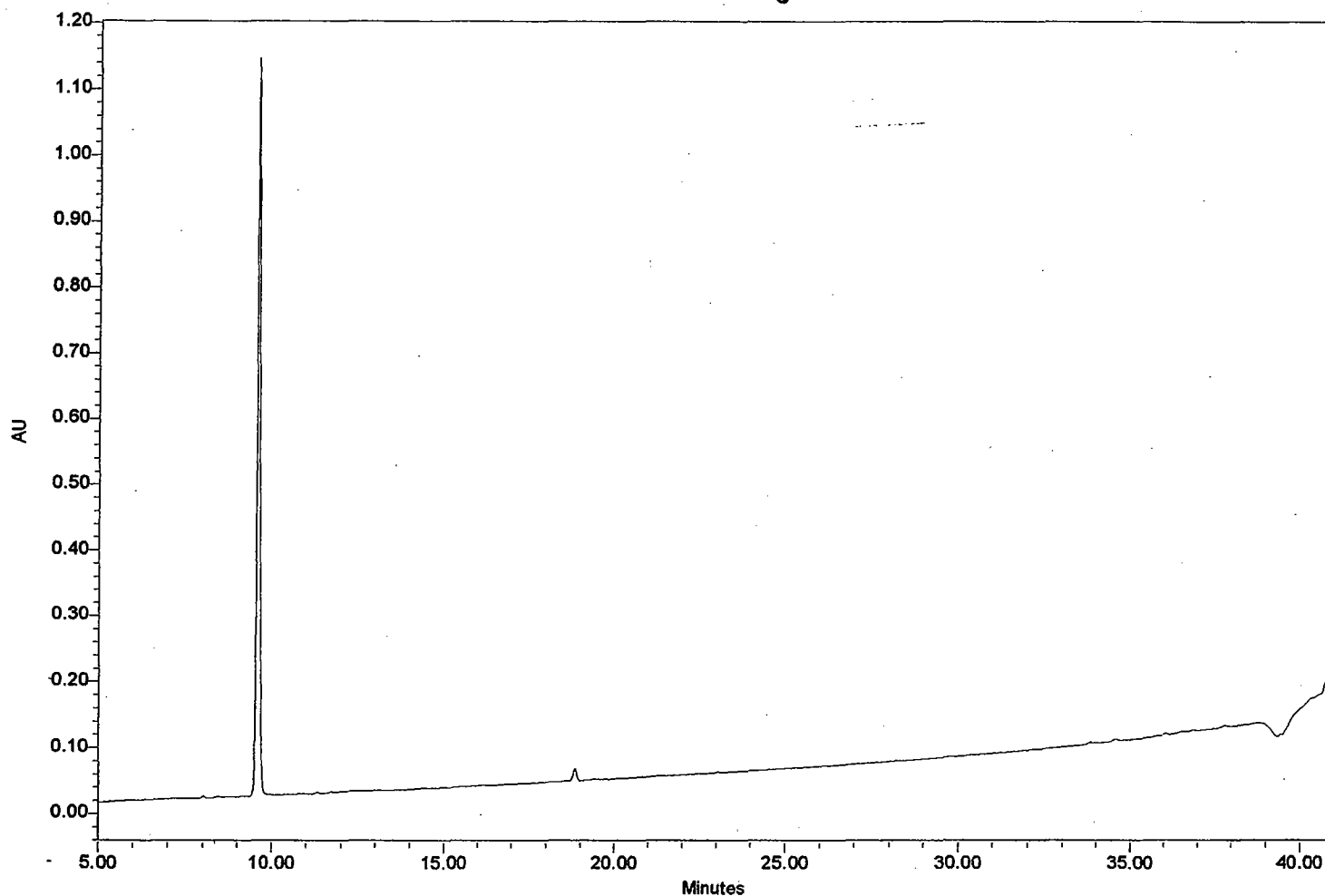
Date Acquired 2/10/99 3:40:14 PM

Vial 22

Channel Description PDA 220.0 nm

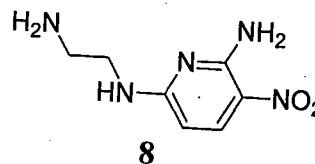
Acq Method Set 5100

Auto-Scaled Chromatogram



Peak Results

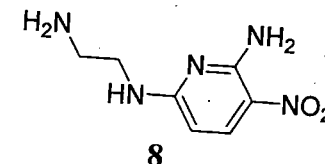
	RT	Start Time	End Time	% Height	% Area
1					



=====

Injection Date : 2/11/99 12:35:03 PM Seq. Line : 18
Sample Name : kpc16n2 Vial : 18
Acq. Operator : ntg Inj : 1
Inj Volume : Inj prog

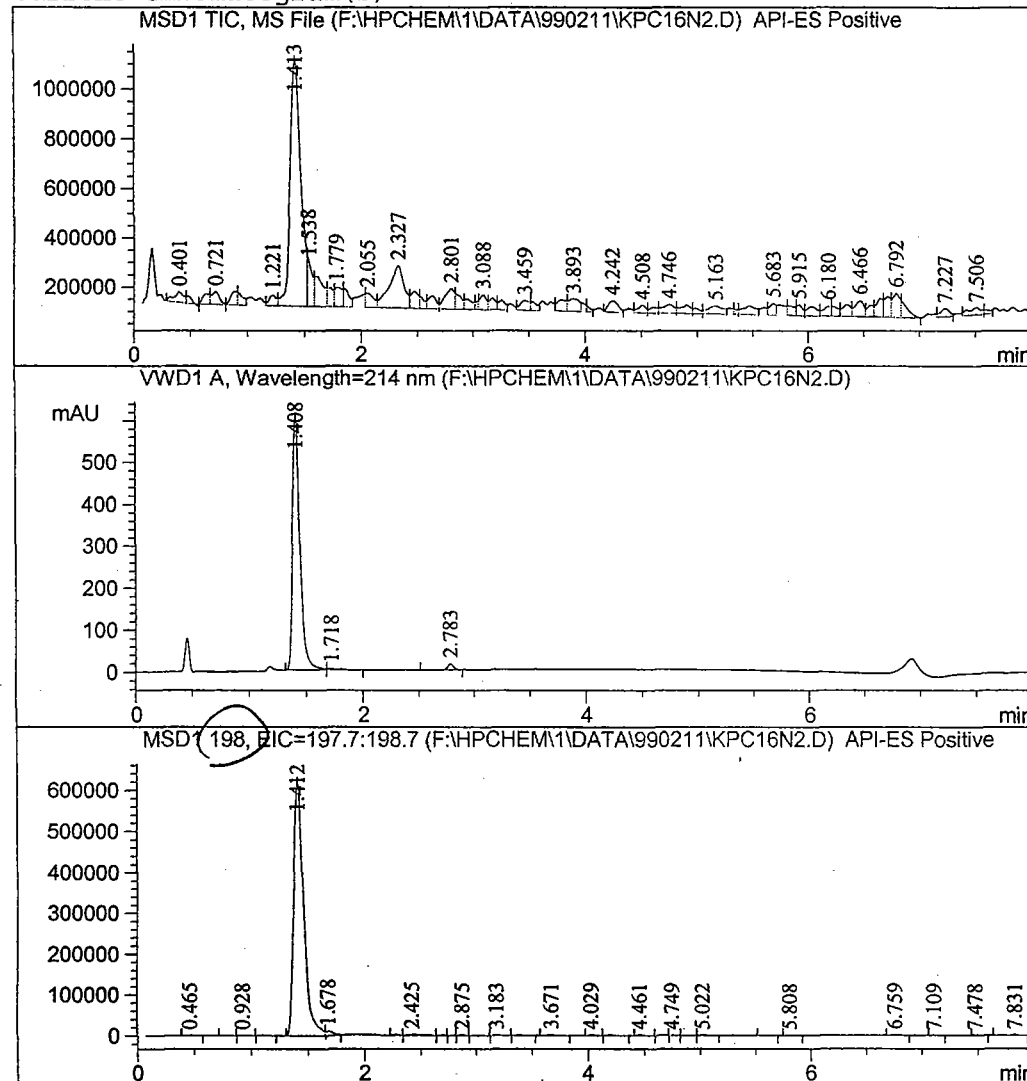
Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
Last changed : 9/17/98 11:16:18 AM by ntg
Analysis Method : C:\HPCHEM\1\METHODS\ALICE.M
Last changed : 2/11/99 4:58:05 PM
(modified after loading)



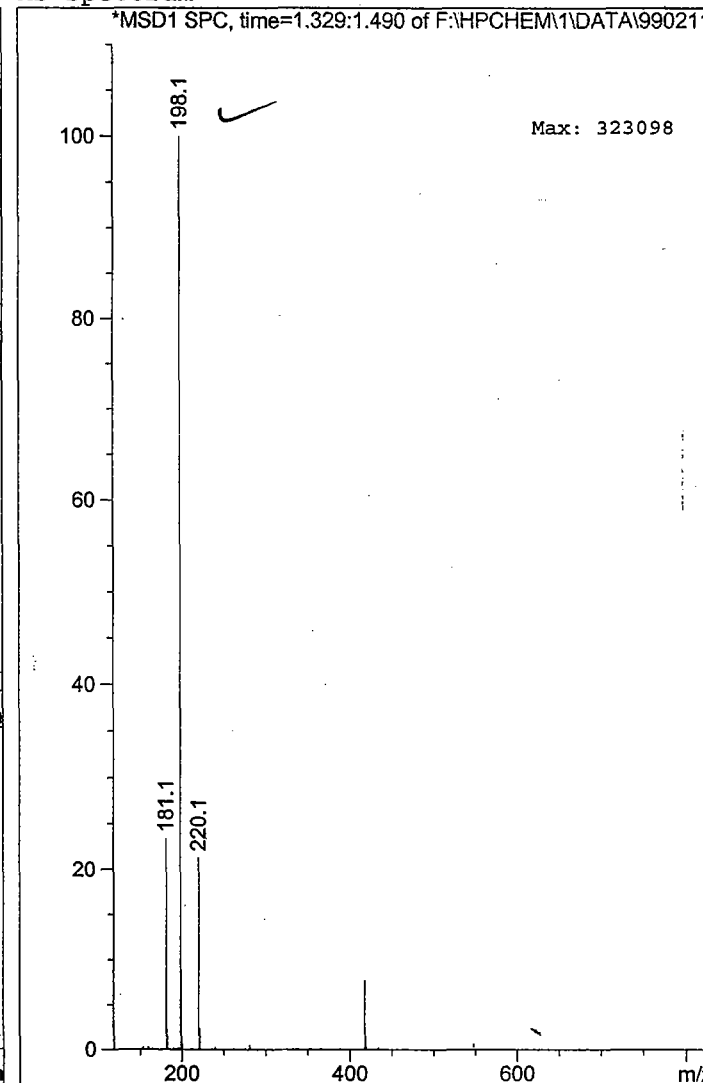
kpc16-2

LC/MSD method. Flow rate:0.4 mL/min, 1-95% B in 6 min. 2 min for equilibration. condense scan. Solvent A:H2O+0.05%TFA, B:ACN +0.05%TFA. Column Temp. is 30. 150-850, 50 V

Current Chromatogram(s)

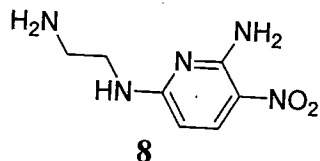


MS Spectrum



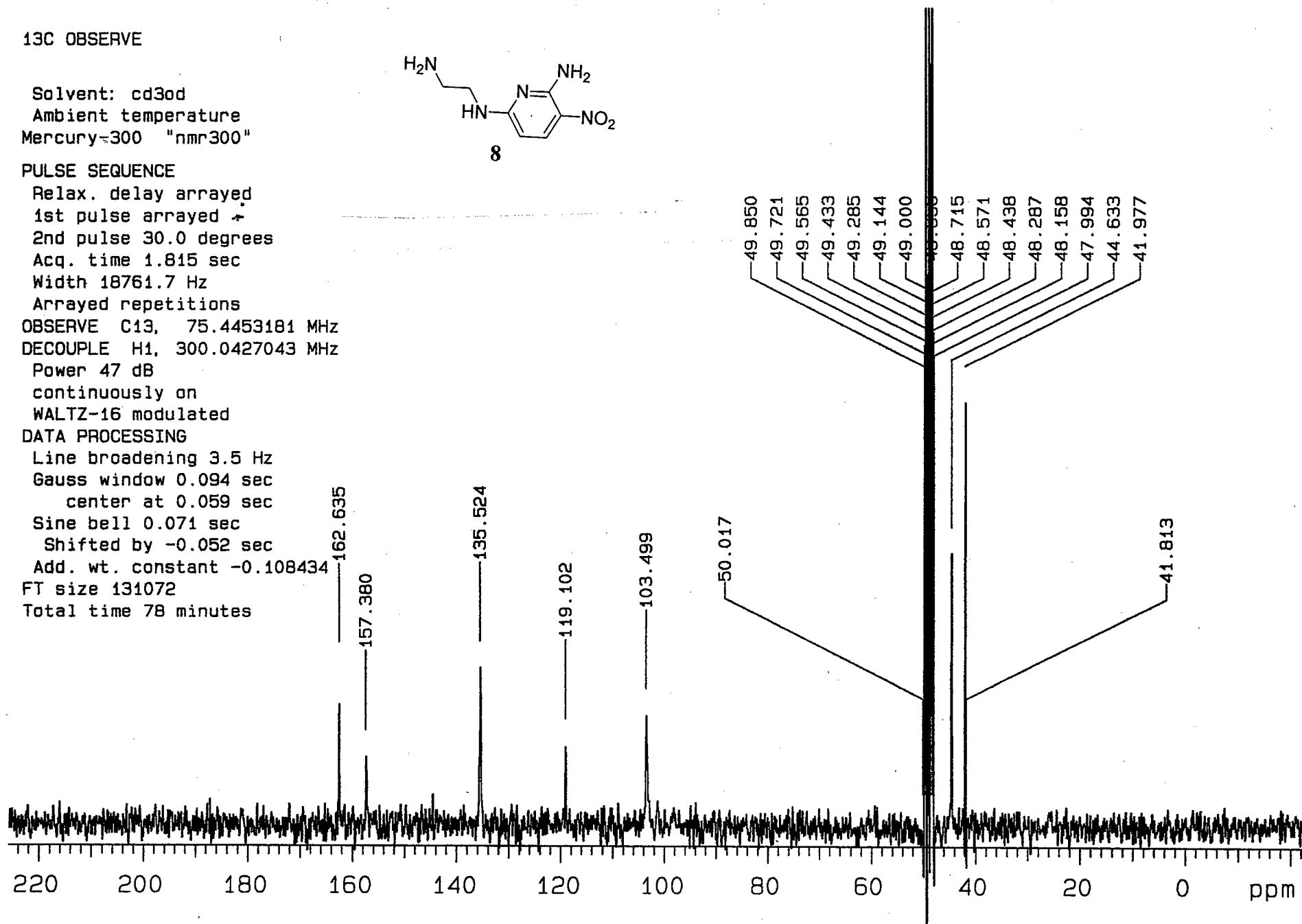
13C OBSERVE

Solvent: cd3od
Ambient temperature
Mercury-300 "nmr300"



PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed +
2nd pulse 30.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
Arrayed repetitions
OBSERVE C13, 75.4453181 MHz
DECOUPLE H1, 300.0427043 MHz
Power 47 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.5 Hz
Gauss window 0.094 sec
center at 0.059 sec
Sine bell 0.071 sec
Shifted by -0.052 sec
Add. wt. constant -0.108434
FT size 131072
Total time 78 minutes

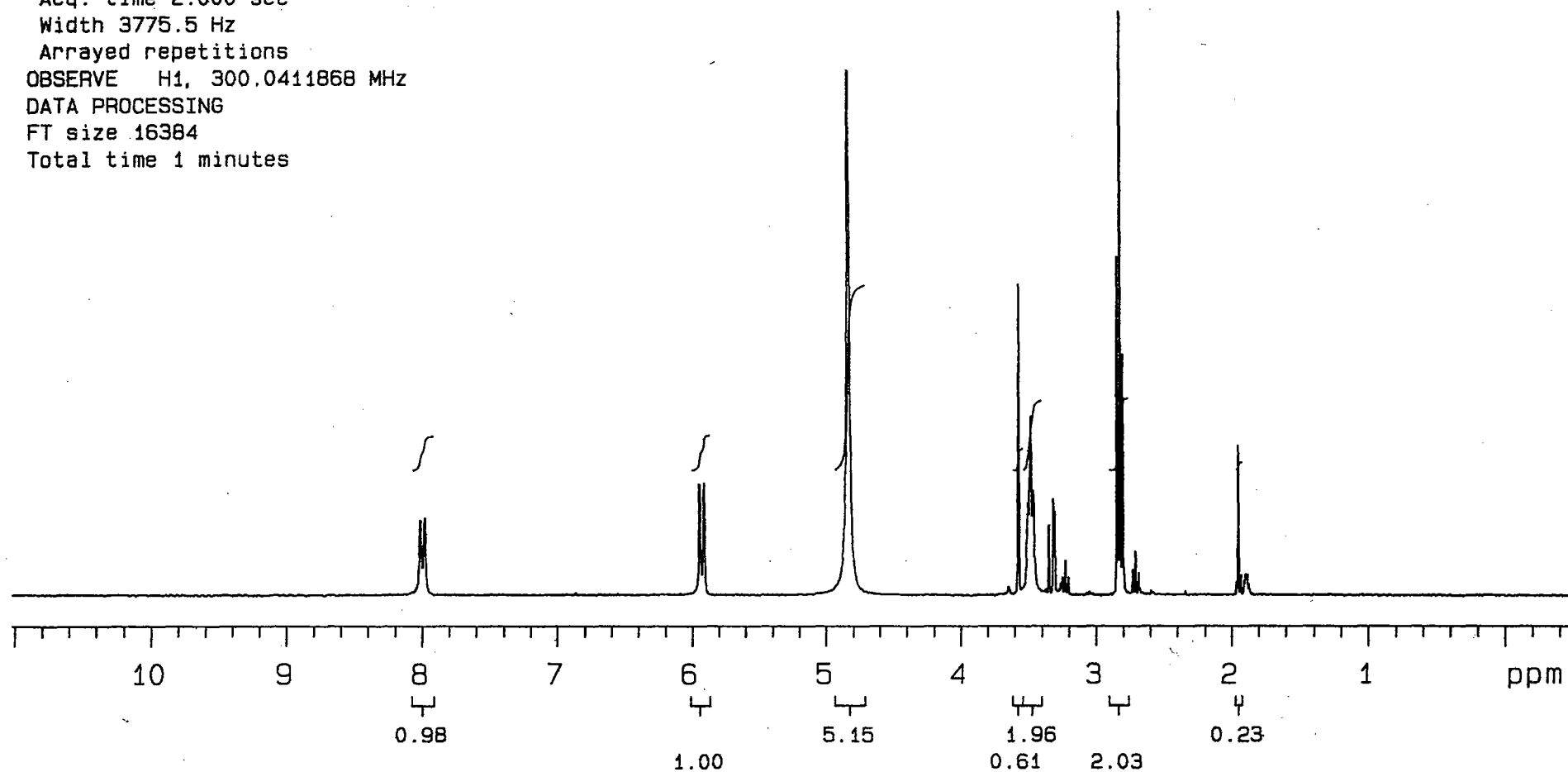
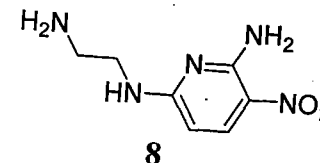


STANDARD 1H OBSERVE

Solvent: cd3od
Ambient temperature
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed →
2nd pulse 19.4 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.0411868 MHz
DATA PROCESSING
FT size 16384
Total time 1 minutes



SampleName SU3-007 rock

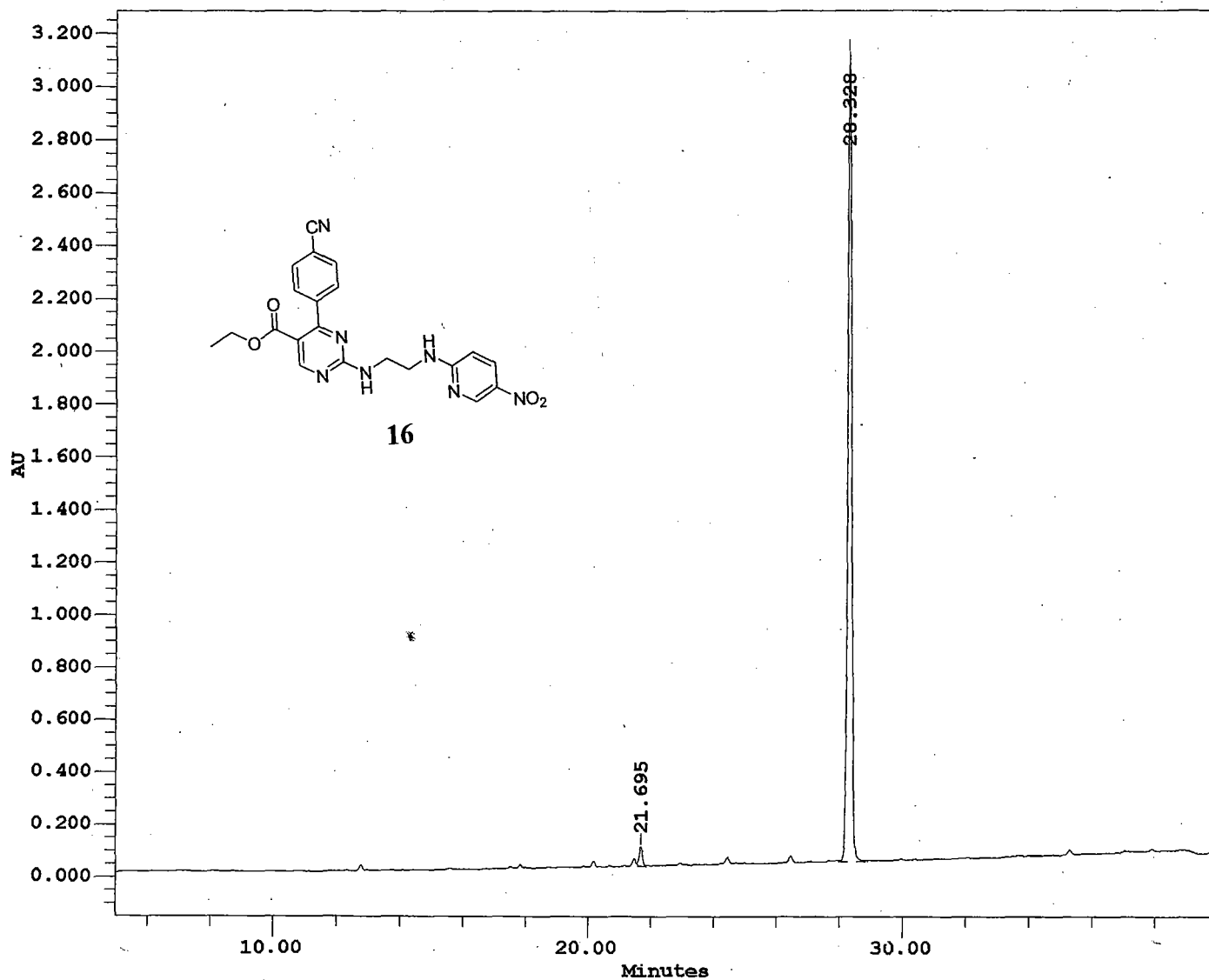
Volume: 10

Date Acquired: 12/15/97 09:13:04 PM

Vial 2

Channel Descr. PDA 220.0 nm

Acq Meth Set: 5100



Peak Results

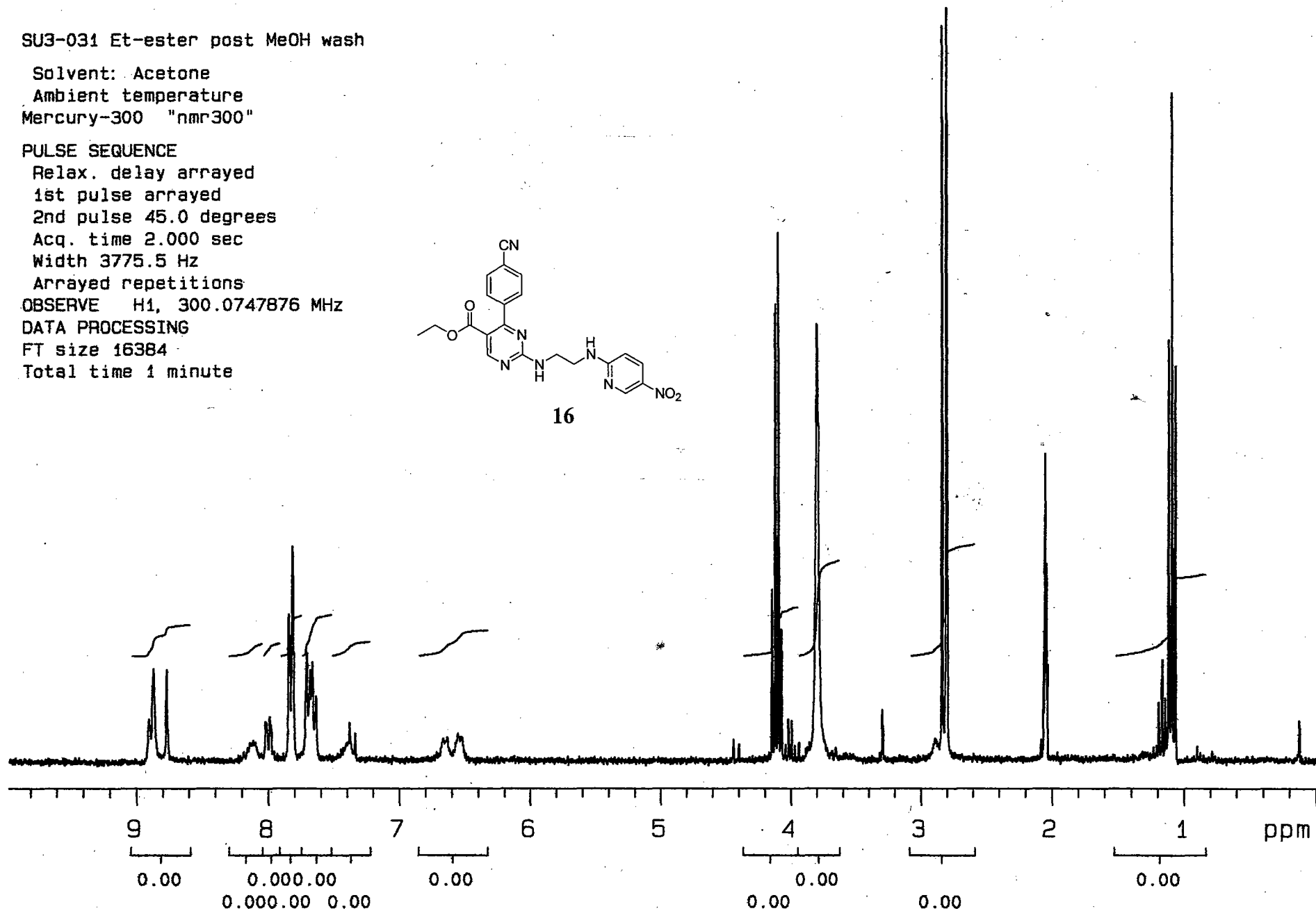
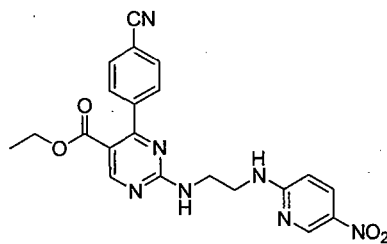
#	Name	Ret Time (min)	Start Time (min)	End Time (min)	% Height	% Area
1		21.695	21.578	22.012	2.41	2.12
2		28.328	27.978	28.895	97.59	97.88

SU3-031 Et-ester post MeOH wash

Solvent: Acetone
Ambient temperature
Mercury-300 "nmr300"

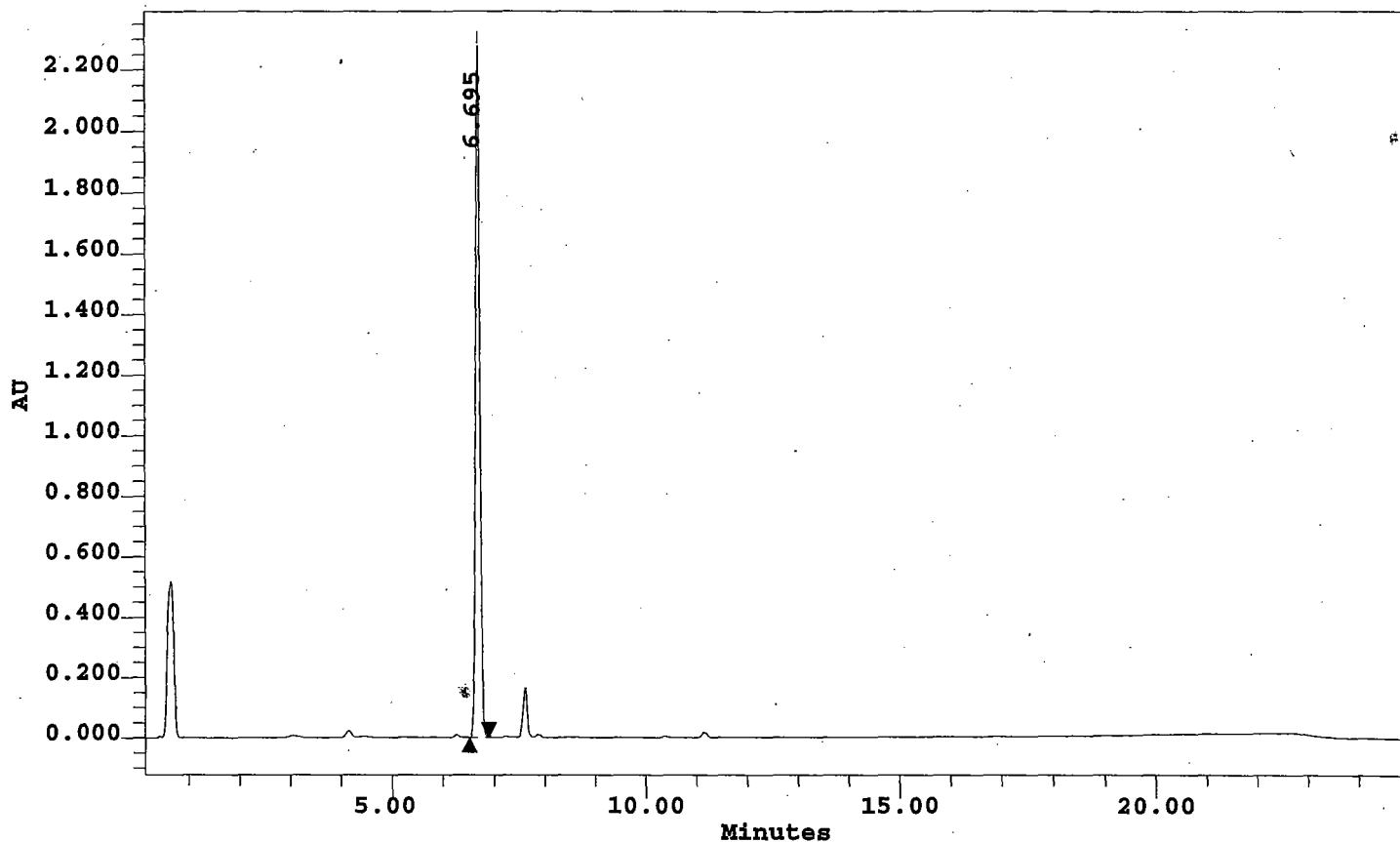
PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 45.0 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.074786 MHz
DATA PROCESSING
FT size 16384
Total time 1 minute



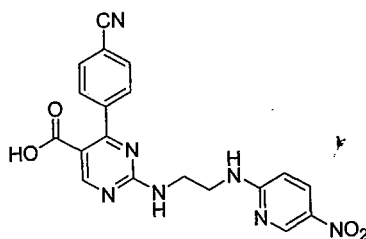
Sample Name: SU3-033 Acid
 SamDes Acid frm TFA of t-Bu
 Date Acquired: 02/10/98 10:47:46 AM
 Channel Descr. PDA 254.0

Volume: 10.00
 Vial: 26
 Acq Meth Set: Rabbit25
 Project Name: Jordan



Peak Results

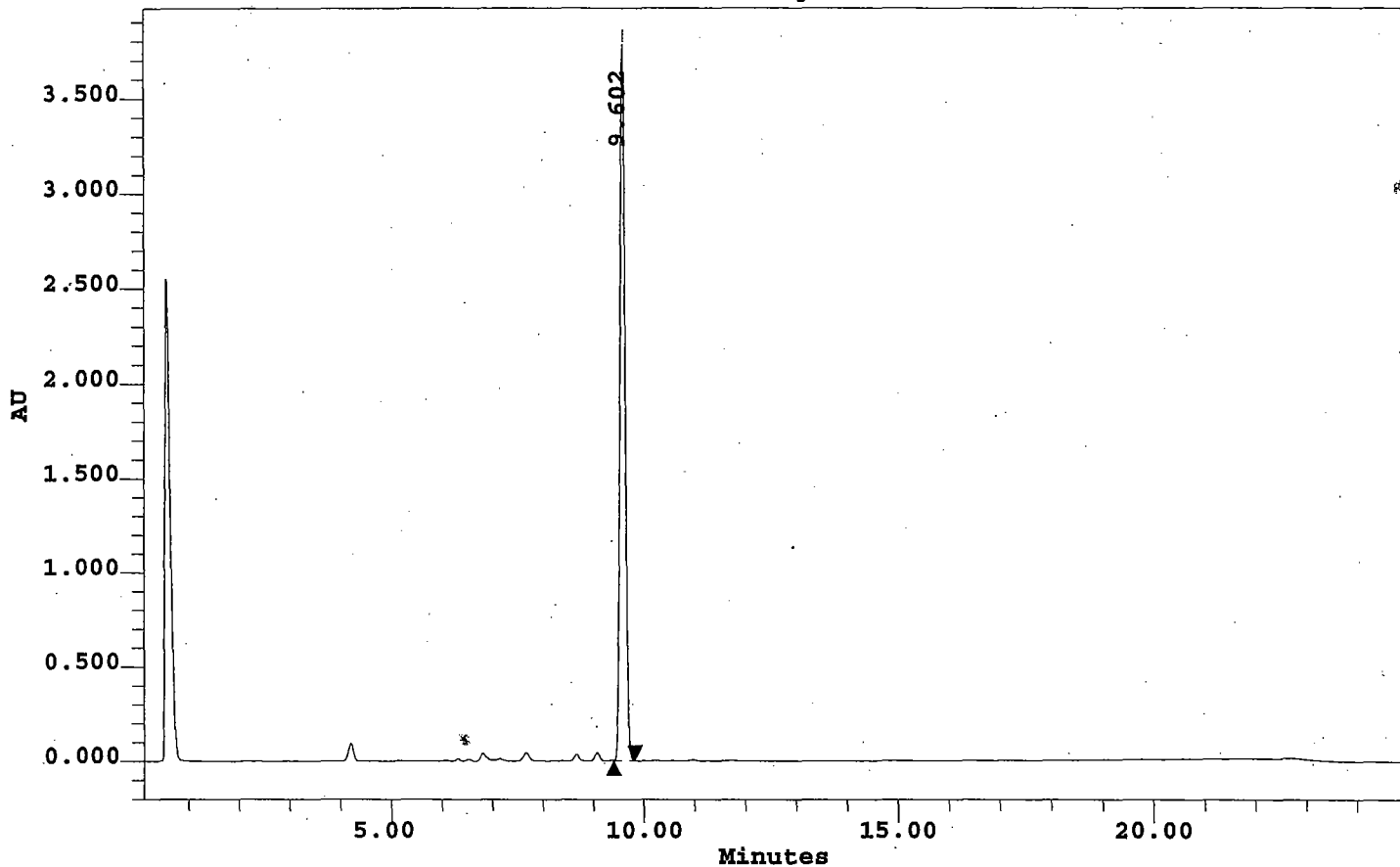
#	Ret Time (min)	Start Time (min)	End Time (min)	% Area	% Height	Int Type
1	6.695	6.512	6.895	100.00	100.00	BB



17

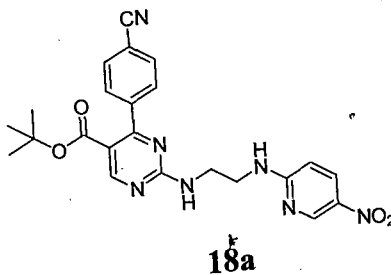
Sample Name: SU3
 SamDes MeOH Wash
 Date Acquired: 02/05/98 12:32:00 PM
 Channel Descr. PDA 254.0

Volume: 5.00
 Vial: 2
 Acq Meth Set: Rabbit25
 Project Name: Jordan



Peak Results

#	Name	Ret Time (min)	Start Time (min)	End Time (min)	% Area	% Height	Int Type
1		9.602	9.402	9.818	100.00	100.00	BB

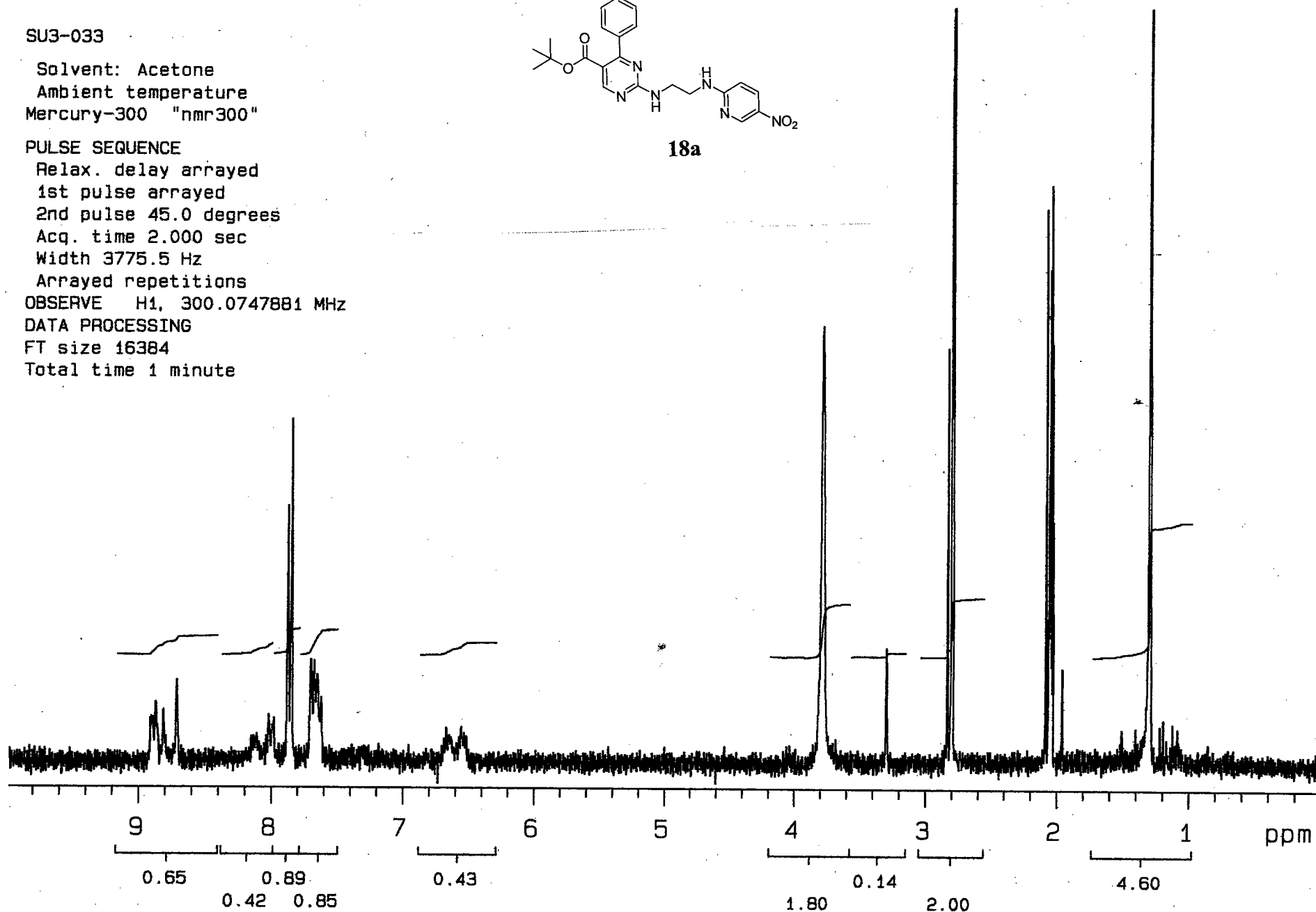
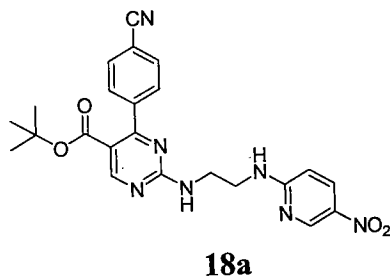


SU3-033

Solvent: Acetone
Ambient temperature
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 45.0 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.0747881 MHz
DATA PROCESSING
FT size 16384
Total time 1 minute



SampleName 38131purified

Volume:

10

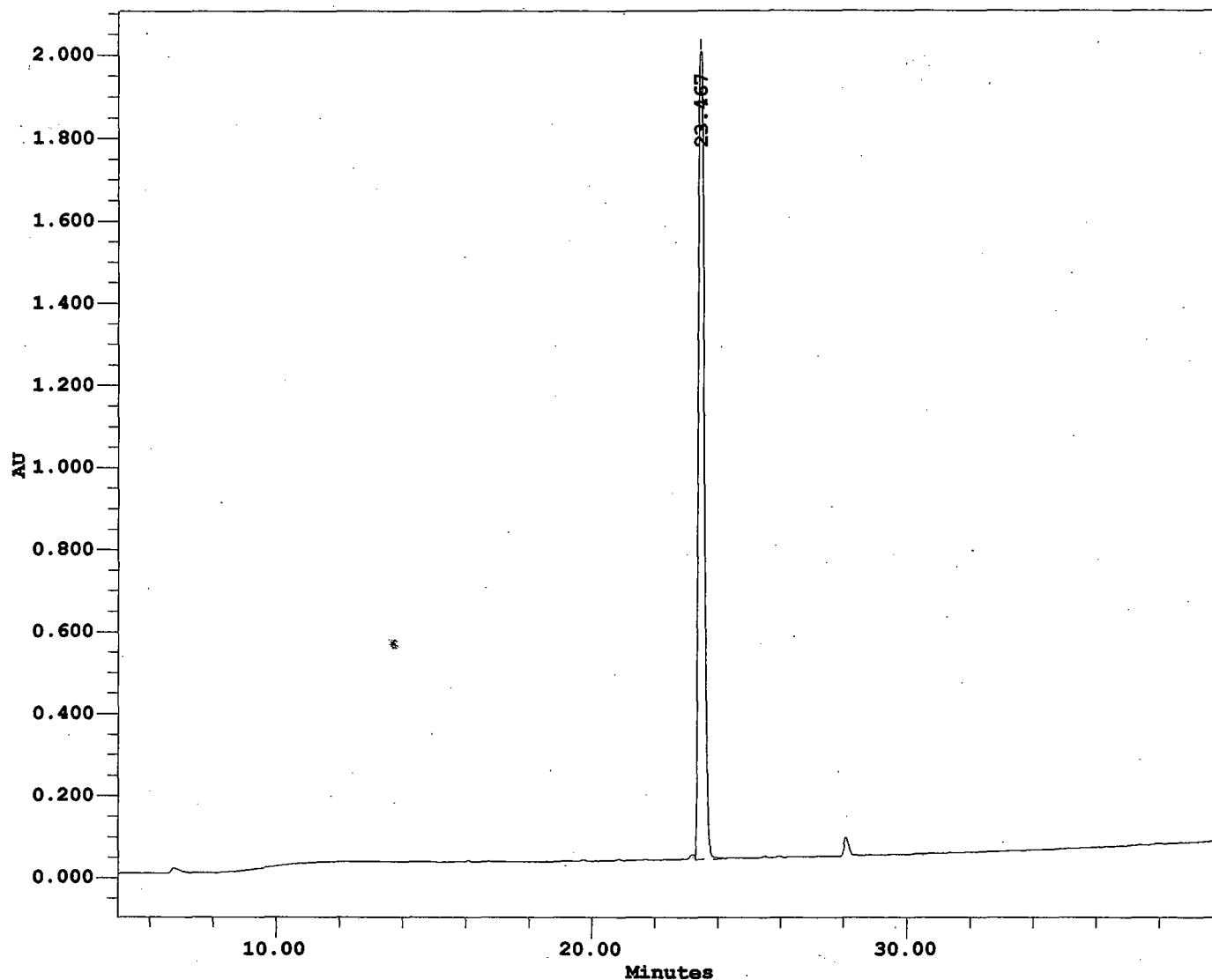
Date Acquired: 01/27/98 07:20:42 PM

Vial 1

hannel Descr. 220 nm

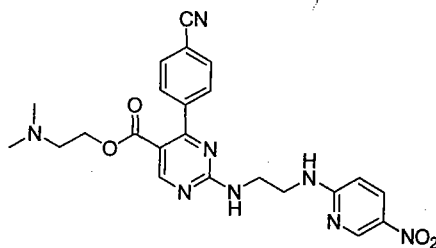
Acq Meth Set:

5100_220



Peak Results

#	Name	Ret Time (min)	Start Time (min)	End Time (min)	% Height	% Area
1		23.467	23.283	24.250	100.00	100.00



18d

38131

Solvent: Acetone
Ambient temperature
Mercury-300 "nmr300"

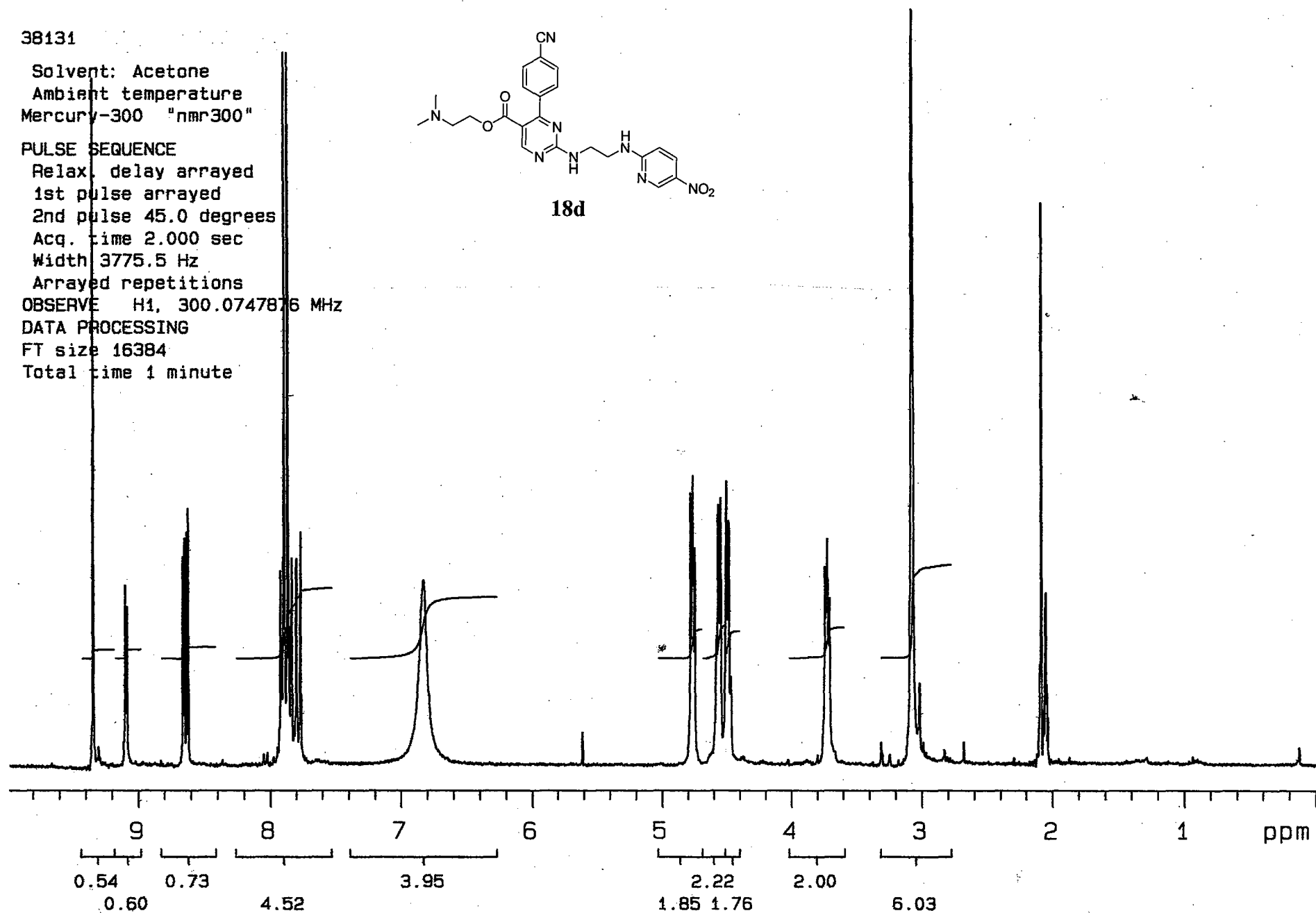
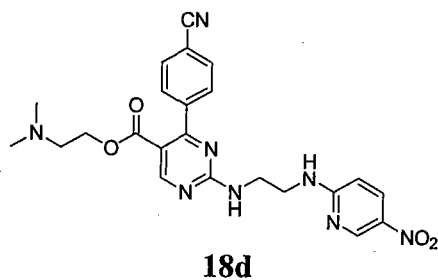
PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 45.0 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions

OBSERVE H1, 300.0747876 MHz

DATA PROCESSING

FT size 16384
Total time 1 minute



SampleName

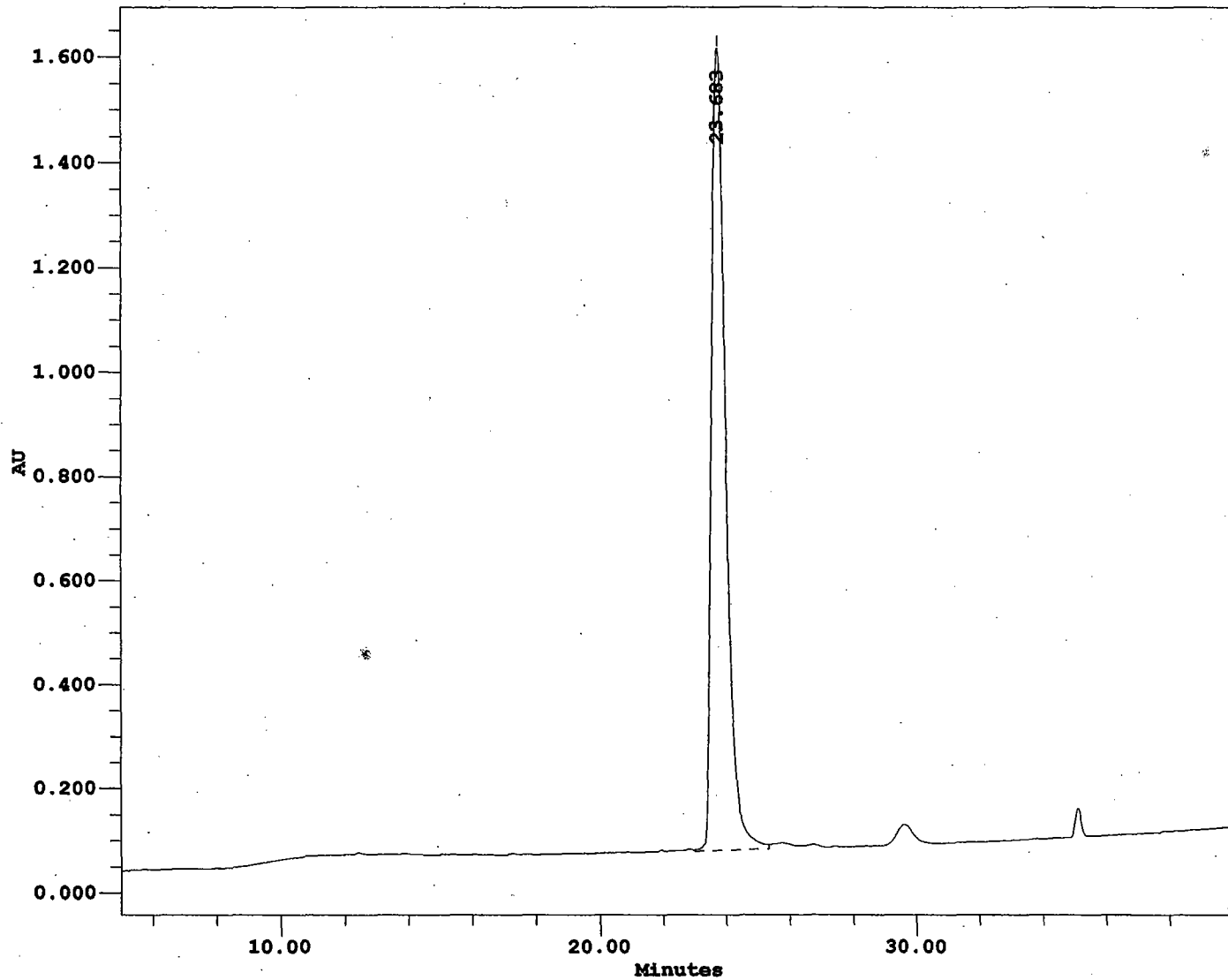
Volume: 10

Date Acquired: 01/29/98 12:22:47 PM

Vial 6

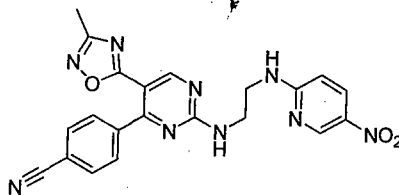
Channel Descr. 220 nm

Acq Meth Set: 5100_220



Peak Results

#	Name	Ret Time (min)	Start Time (min)	End Time (min)	% Height	% Area
1		23.683	22.983	25.333	100.00	100.00



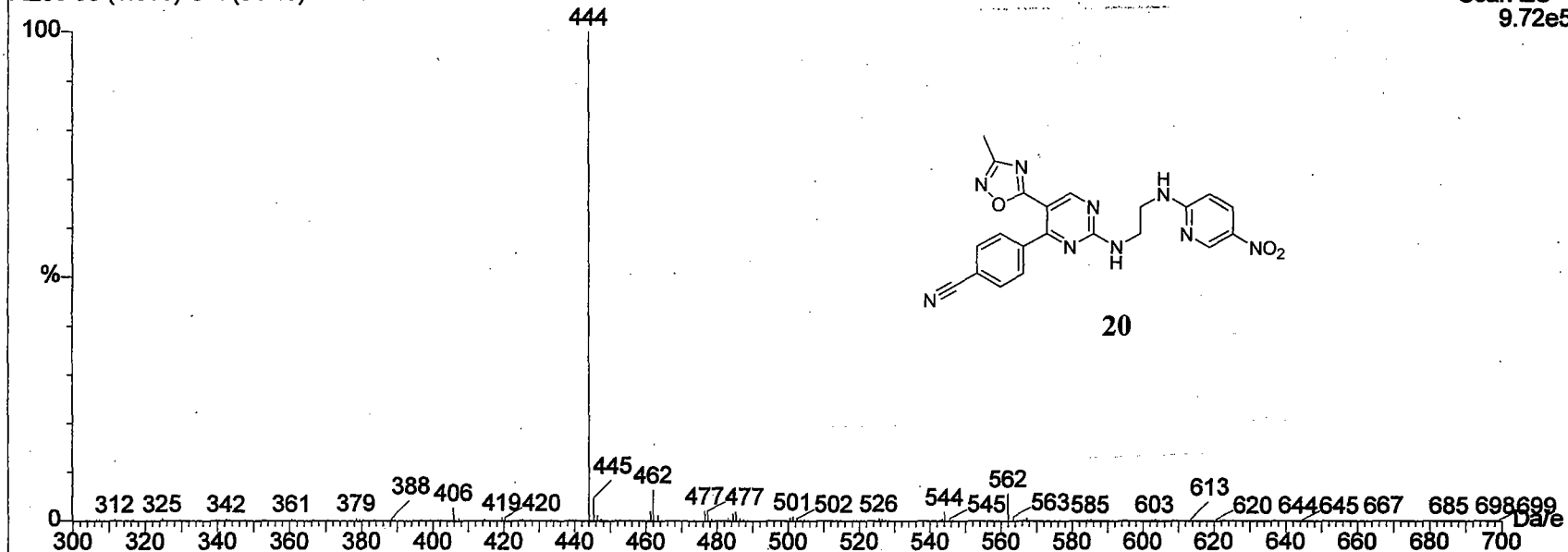
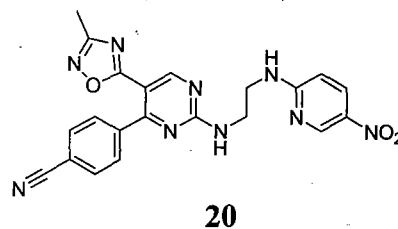
20

Oxadiazole

15-Jan-1998

AZ05 38 (1.355) Cm (34:45)

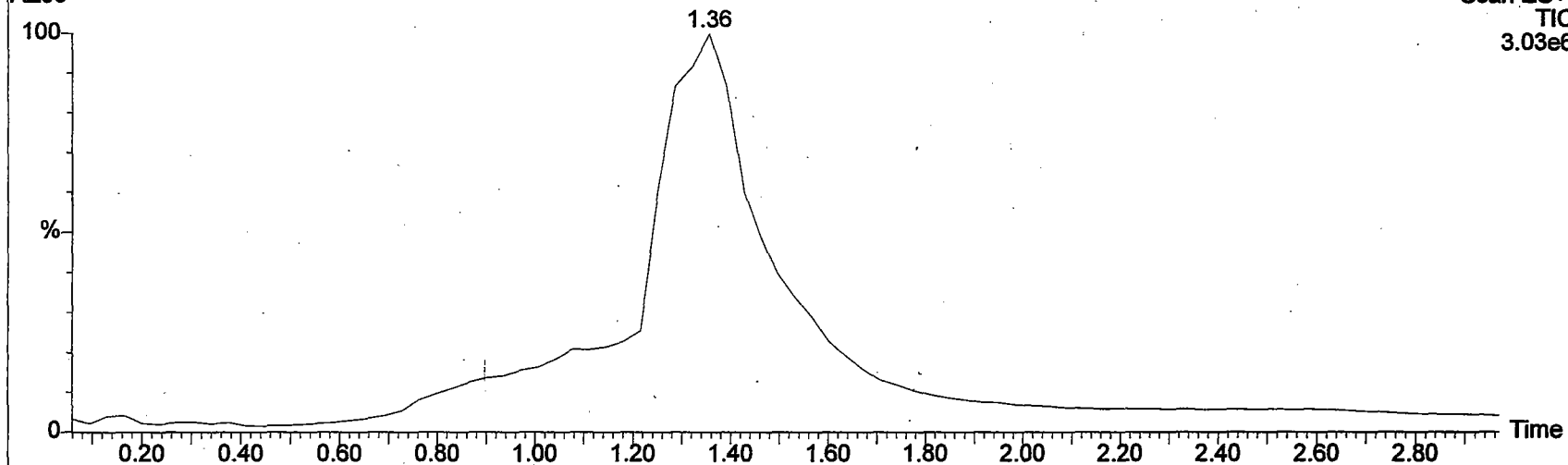
Scan ES+
9.72e5



15-Jan-1998

AZ05

Scan ES+
TIC
3.03e6



CHIRON Technologies S M D D R Medicinal & Organic Chemistry Group

Sample Name: SU3-158 Crop 1

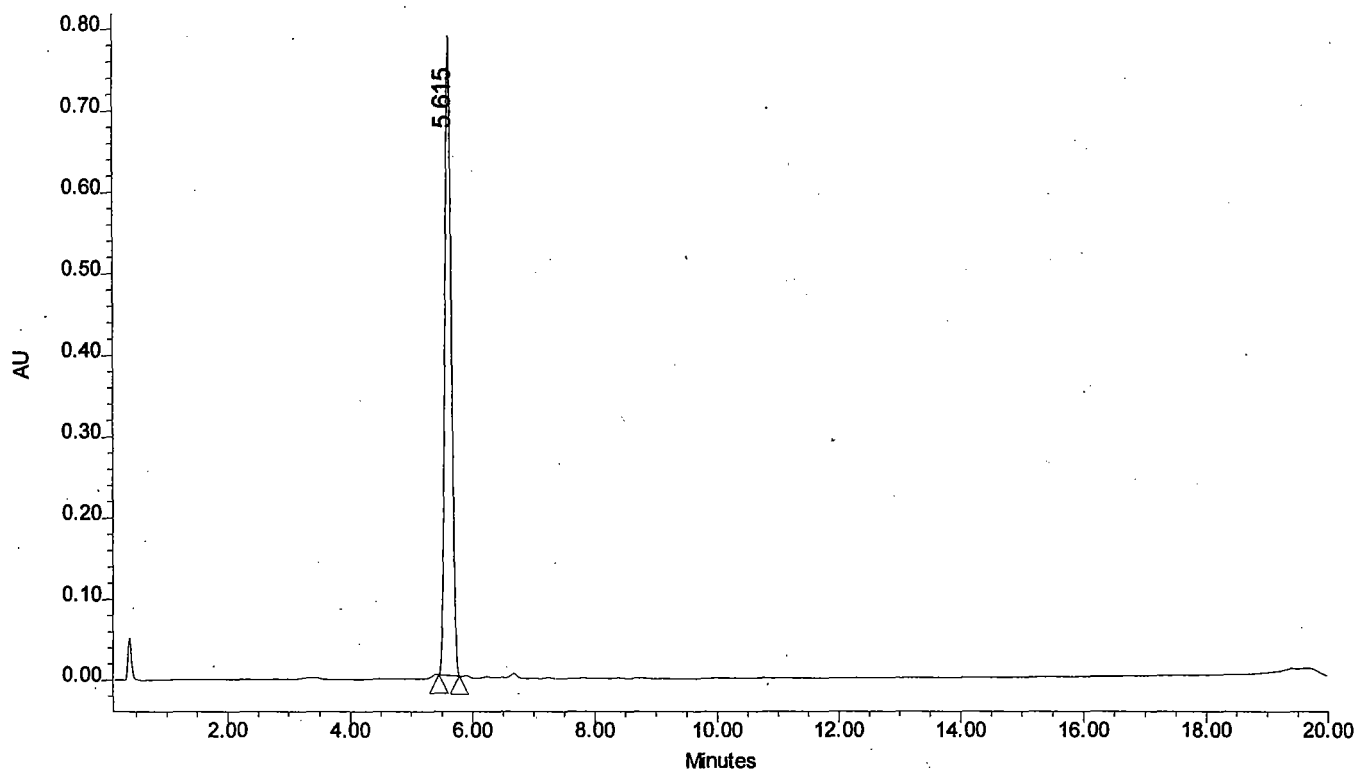
System Name: Shana Project Name: GSK_3

Label: NMR 50302 Crystals

Acq Method Set: Rabbit20

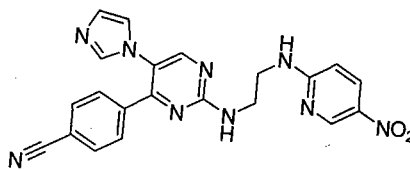
Date Acquired: 8/6/98 1:50:35 PM

Injection Volume- 10.00 ul Vial # 6



Peak Results

	Retention Time	Start Time	End Time	% Area
1	5.615	5.453	5.787	100.00



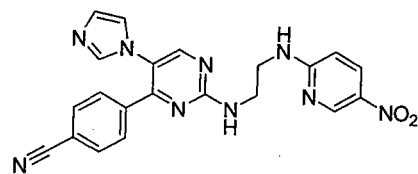
25a HCl Salt

STANDARD 1H OBSERVE

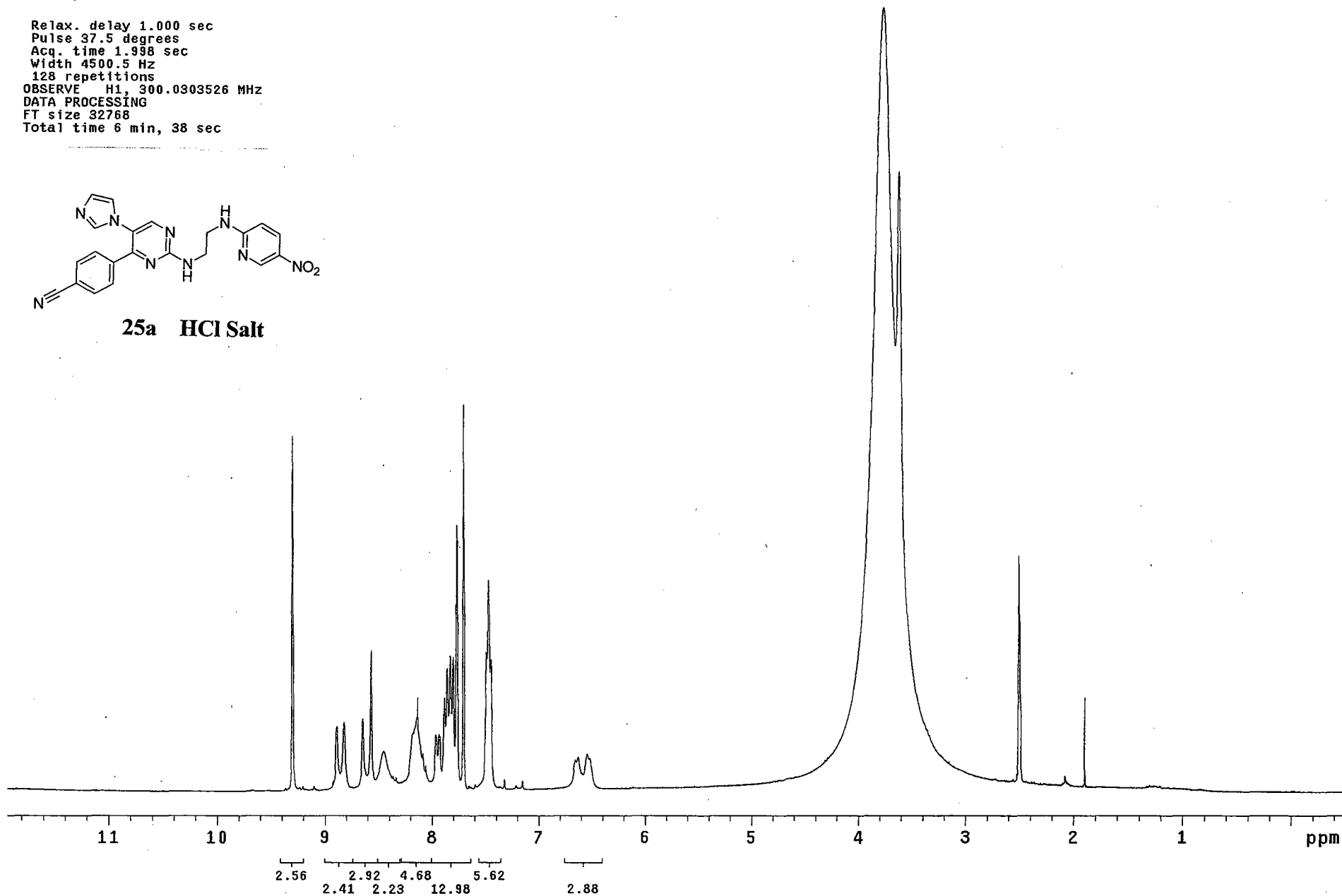
Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 25.0 C / 298.1 K
Mercury-300 "nmr300"

Relax. delay 1.000 sec
Pulse 37.5 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
128 repetitions
OBSERVE H1, 300.0303526 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 38 sec



25a HCl Salt



SU3-158 Crop 1 Crystals from Acetone

Solvent: DMSO

Ambient temperature

Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed

1st pulse arrayed

2nd pulse 45.0 degrees

Acq. time 2.000 sec

Width 3775.5 Hz

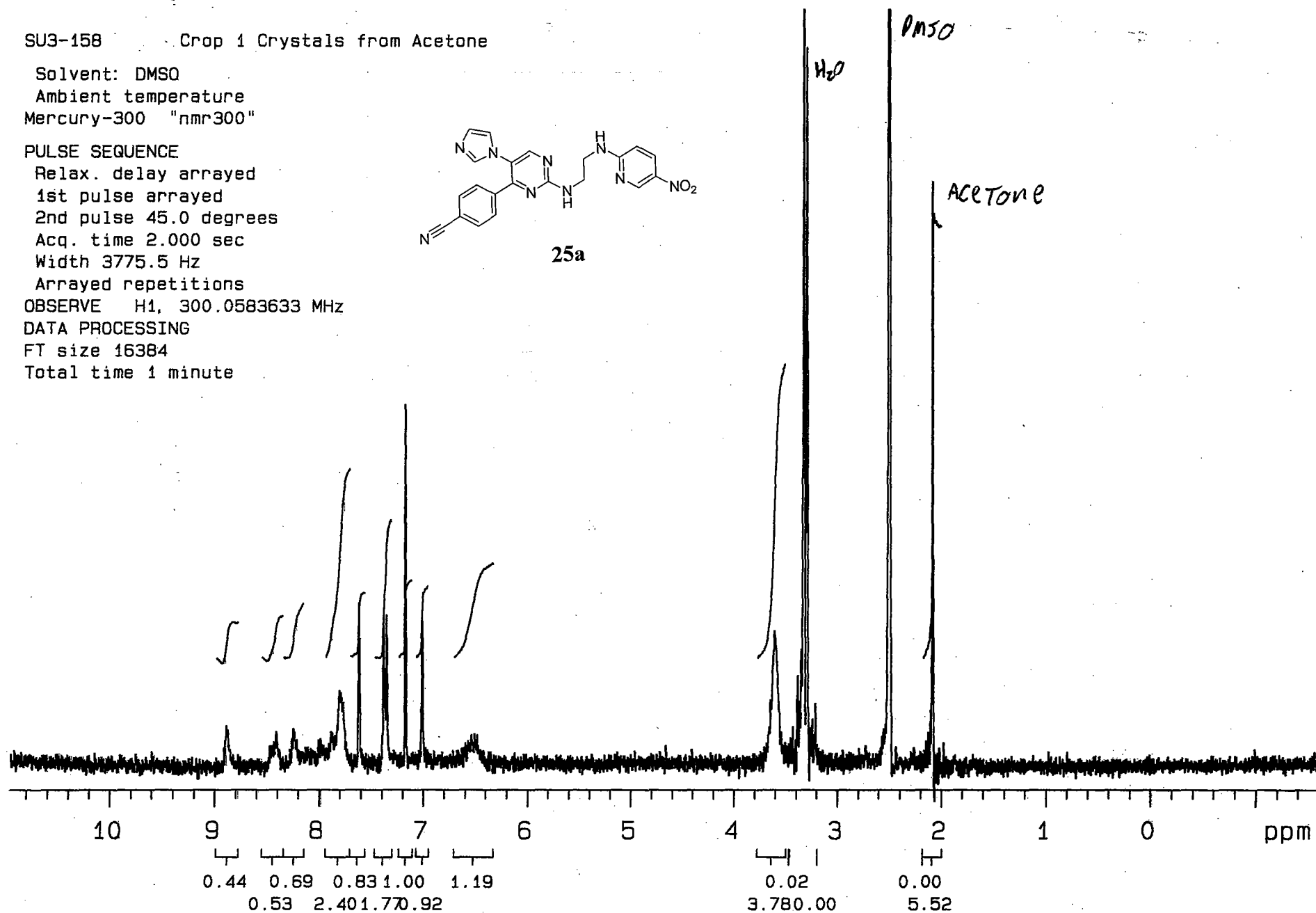
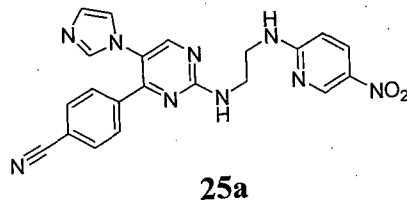
Arrayed repetitions

OBSERVE H1, 300.0583633 MHz

DATA PROCESSING

FT size 16384

Total time 1 minute



CHIRON Technologies S M D D R Medicinal & Organic Chemistry Group

Sample Name: SU3-166 Crop 1

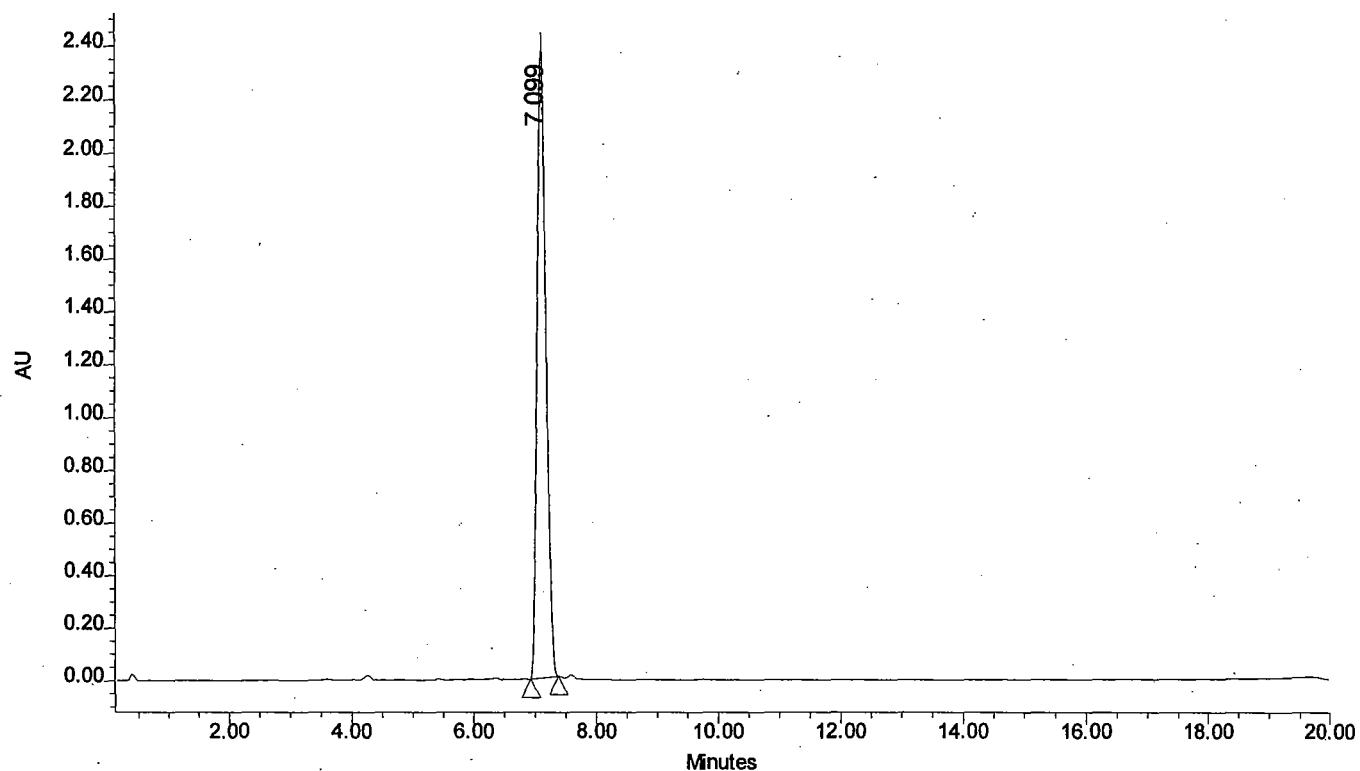
System Name: Shana Project Name: GSK_3

Label: ppt

Acq Method Set: Rabbit20

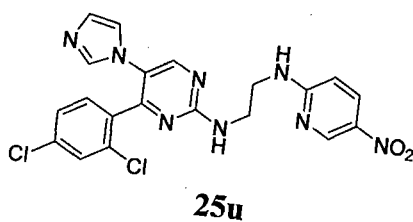
Date Acquired: 8/6/98 1:29:47 PM

Injection Volume- 5.00 ul Vial # 5



Peak Results

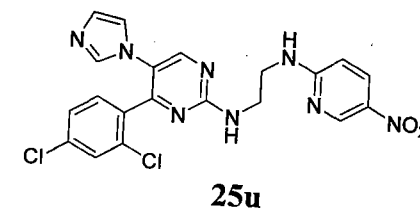
	Retention Time	Start Time	End Time	% Area
1	7.099	6.933	7.383	100.00



Injection Date : 8/6/98 1:06:25 PM
 Sample Name : CROP 1
 Acq. Operator : ntg

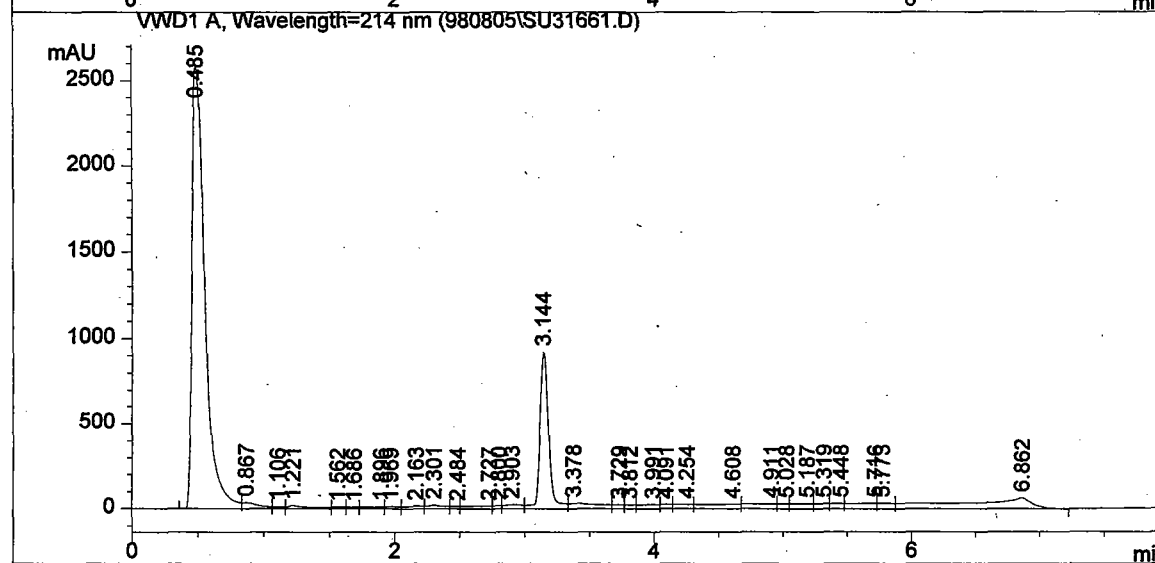
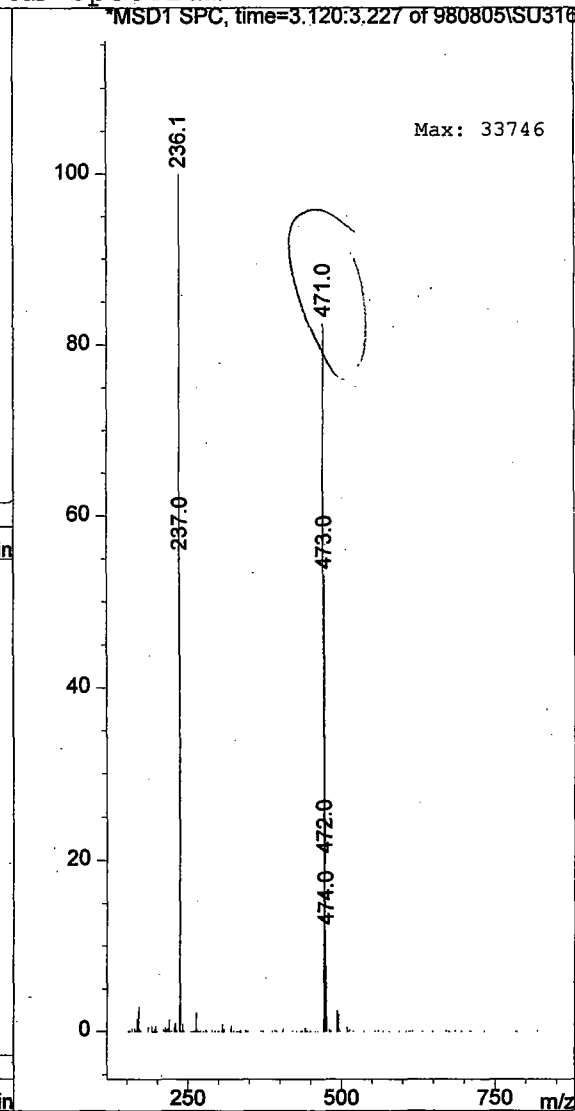
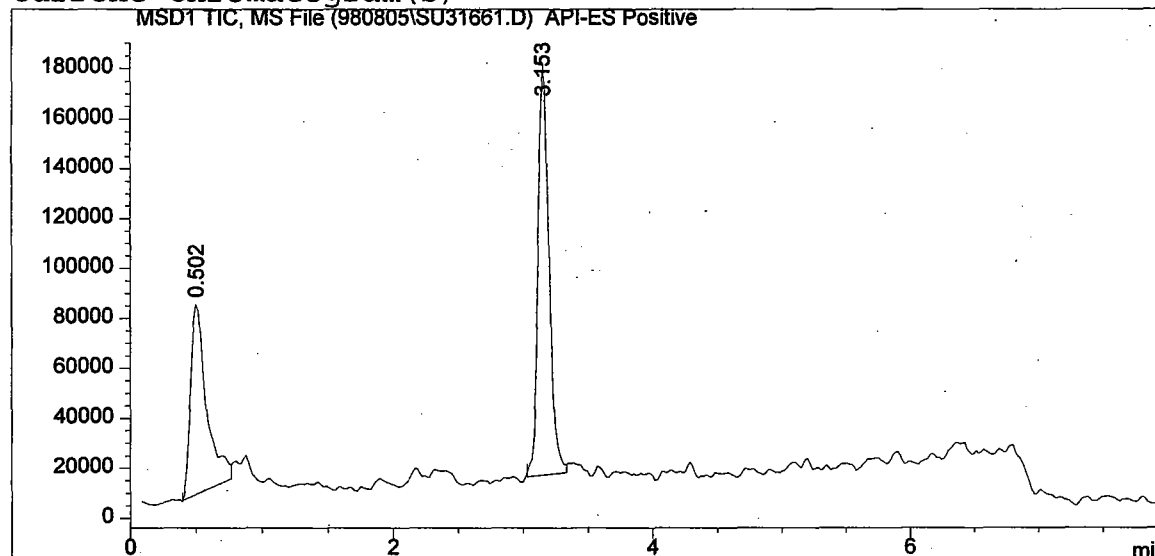
Seq. Line : 21
 Vial : 14
 Inj : 1
 Inj Volume : Inj prog

Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
 Last changed : 7/31/98 9:32:14 AM by ntg
 Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
 Last changed : 8/6/98 4:26:16 PM by chemist
 (modified after loading)



Current Chromatogram(s)

MS Spectrum

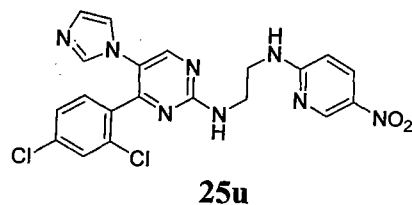


SU3-166 4 Crop 1

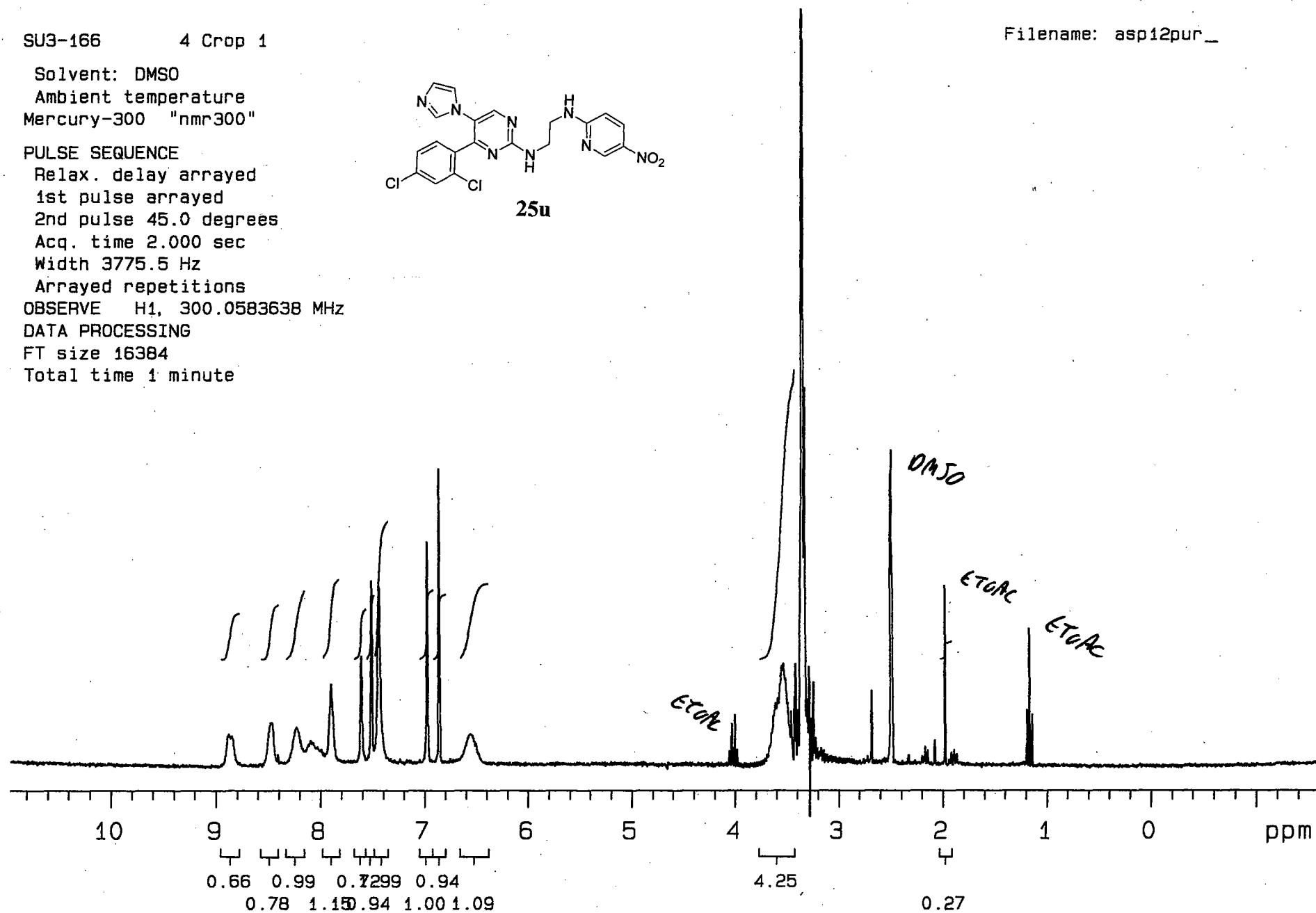
Solvent: DMSO
Ambient temperature
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 45.0 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.0583638 MHz
DATA PROCESSING
FT size 16384
Total time 1 minute



Filename: asp12pur_



CHIRON Technologies SMDR Medicinal & Organic Chemistry Group

Sample Name: ss140apu

System Name: Shana

Project Name: GSK4

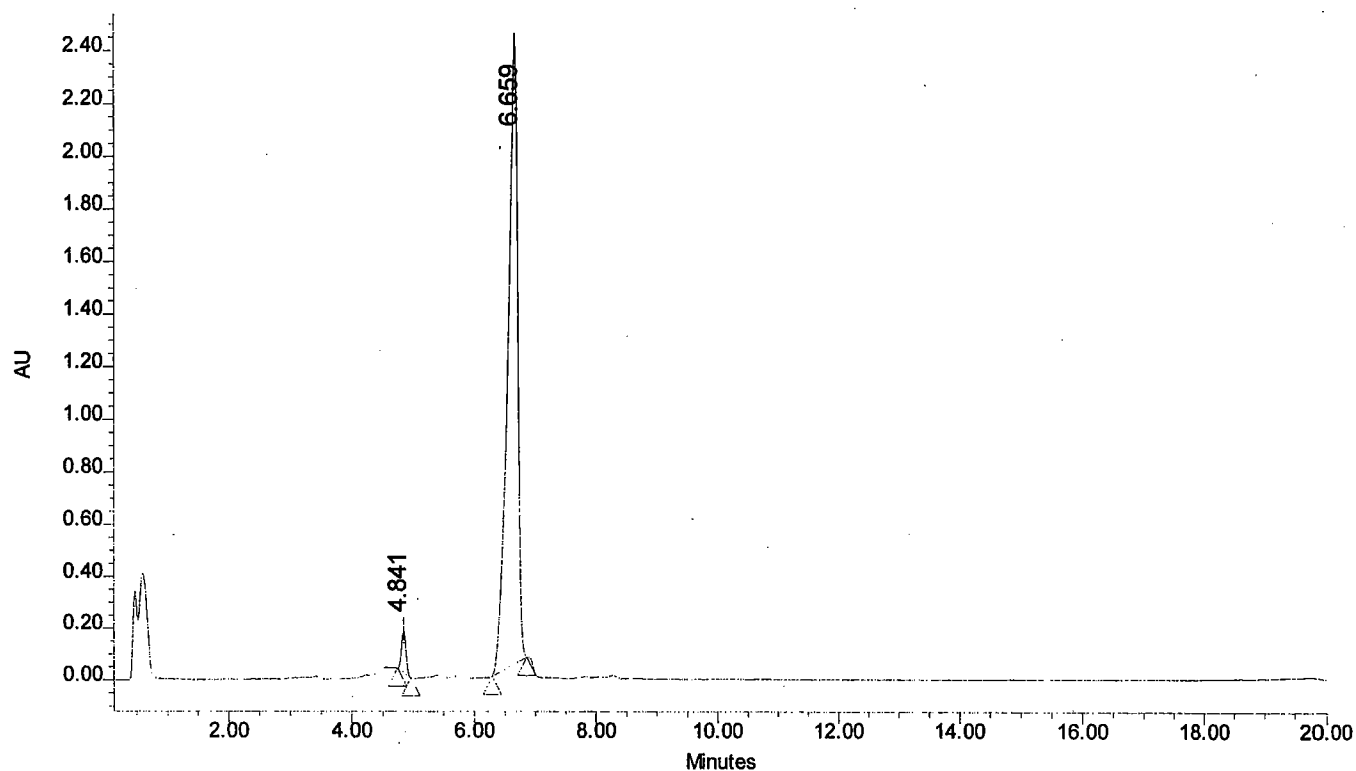
Label:

Acq Method Set: Rabbit20

Date Acquired: 9/21/99 3:23:44 PM

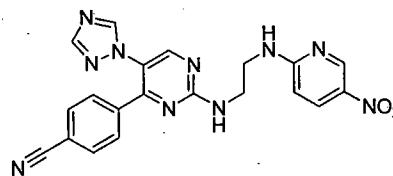
Injection Volume- 20.00 ul

Vial # 1



Peak Results

	Retention Time	Start Time	End Time	% Area
1	4.841	4.738	4.955	3.01
2	6.659	6.288	6.855	96.99



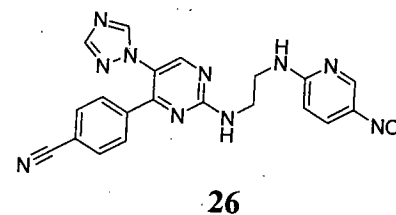
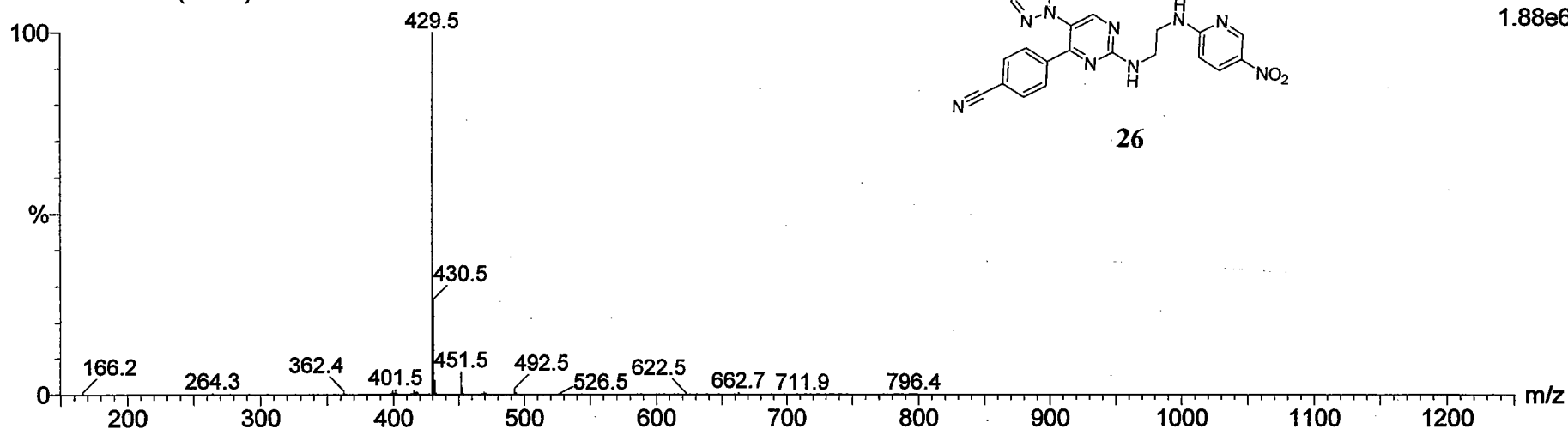
26

21-Sep-1999

16:17:23

SS1450APU 86 (3.035)

1: Scan ES+
1.88e6

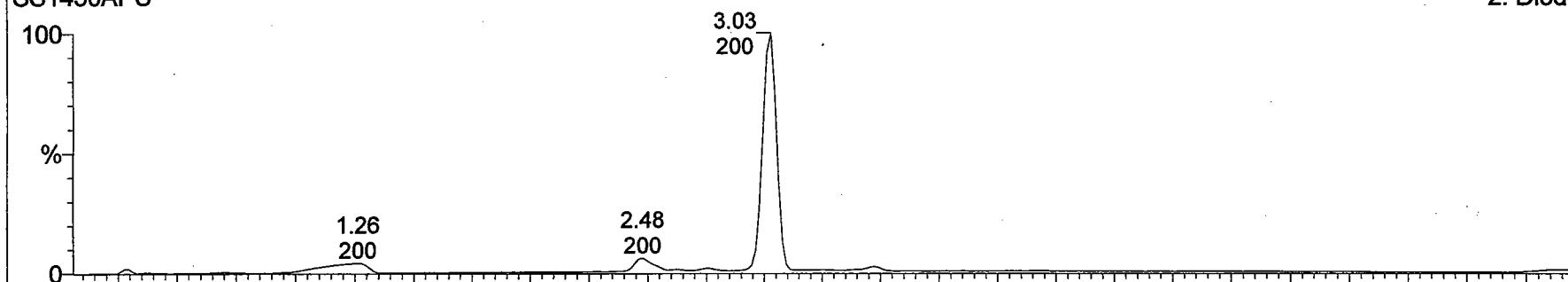


21-Sep-1999

16:17:23

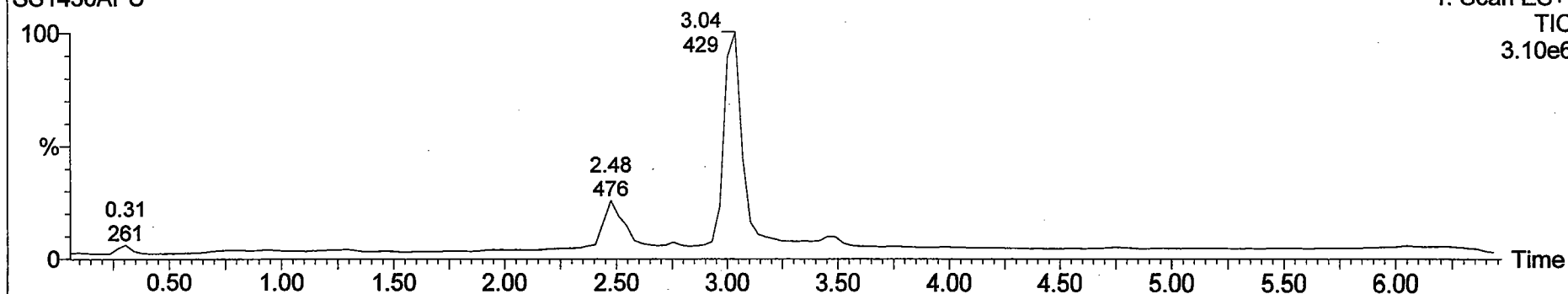
SS1450APU

2: Diode Array
214
2.21e6



SS1450APU

1: Scan ES+
TIC
3.10e6



SampleName kp106

Injection Volume 10.00 ul

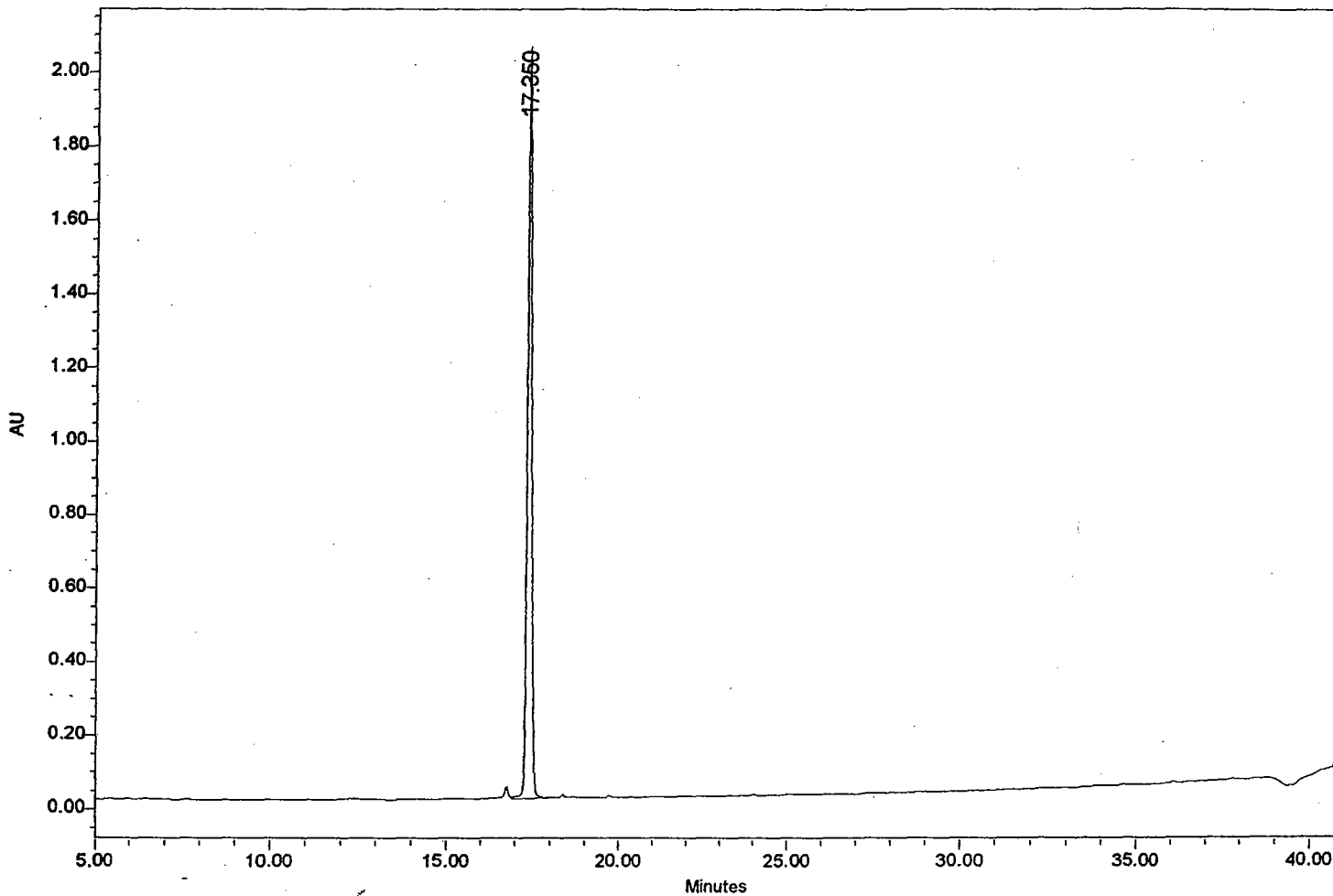
Date Acquired 2/7/99 9:03:07 PM

Vial 2

Channel Description PDA 220.0 nm

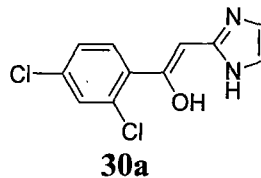
Acq Method Set 5100

Auto-Scaled Chromatogram



Peak Results

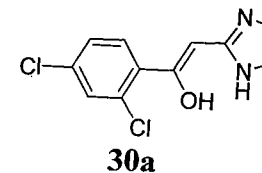
Peak	RT	Start Time	End Time	% Height	% Area
1	17.350	16.883	17.950	100.00	100.00



=====

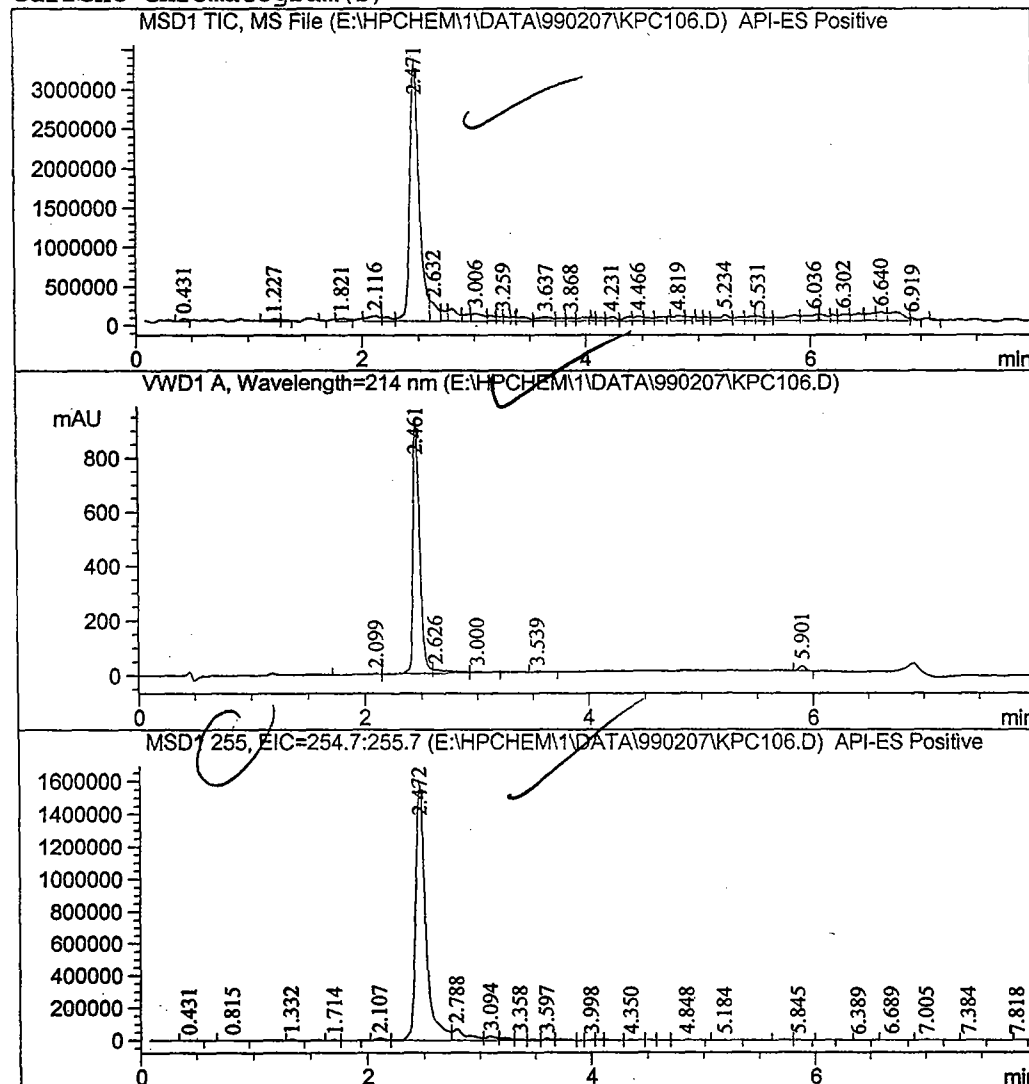
Injection Date	: 2/8/99 12:22:28 PM	Seq. Line	: 19
Sample Name	: kpc106	Vial	: 19
Acq. Operator	:	Inj	: 1
Acq. Instrument	: HP LCMS System	Inj Volume	: Inj prog
Acq. Method	: C:\HPCHEM\1\METHODS\POS_MODE.M		
Last changed	: 1/27/99 9:46:31 AM by ntg		
Analysis Method	: C:\HPCHEM\1\METHODS\ALICE.M		
Last changed	: 2/8/99 3:56:50 PM		

(modified after loading)

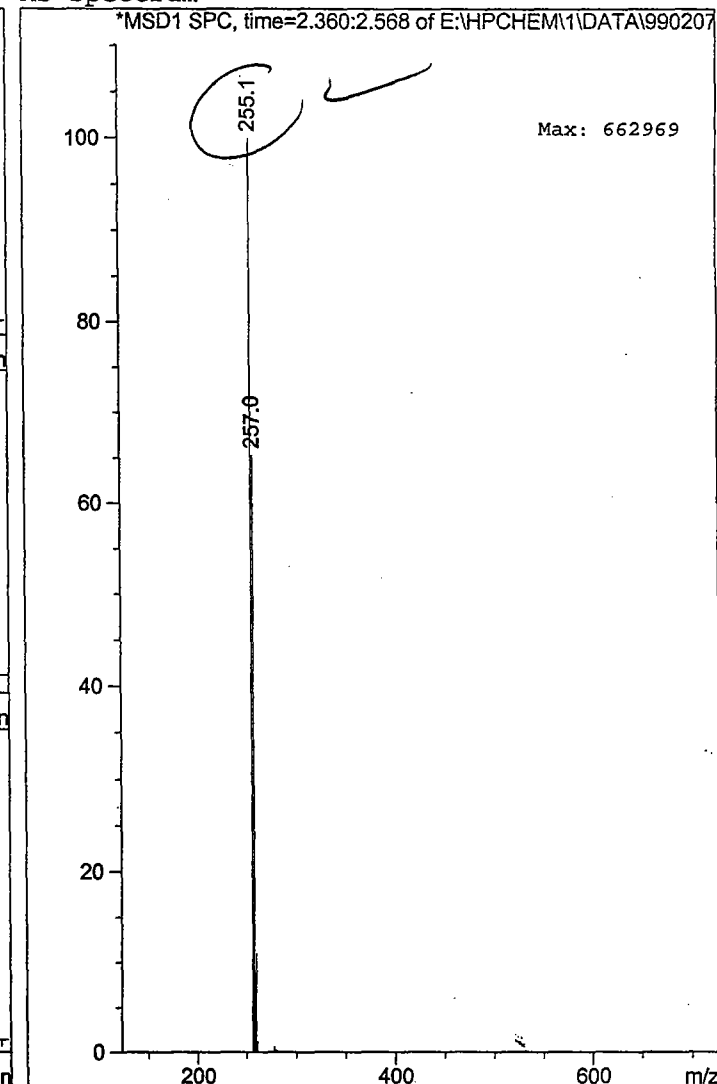


LC/MSD method. Flow rate: 0.4 mL/min, 1-95% B in 6 min. 2 min for equilibration. condense scan. Solvent A: H₂O + 0.05% TFA, B: ACN + 0.05% TFA. Column Temp. is 30. 150-850, 50 V

Current Chromatogram(s)



MS Spectrum



STANDARD 1H OBSERVE

Solvent: DMSO
Ambient temperature
Mercury-300 "nmr300"

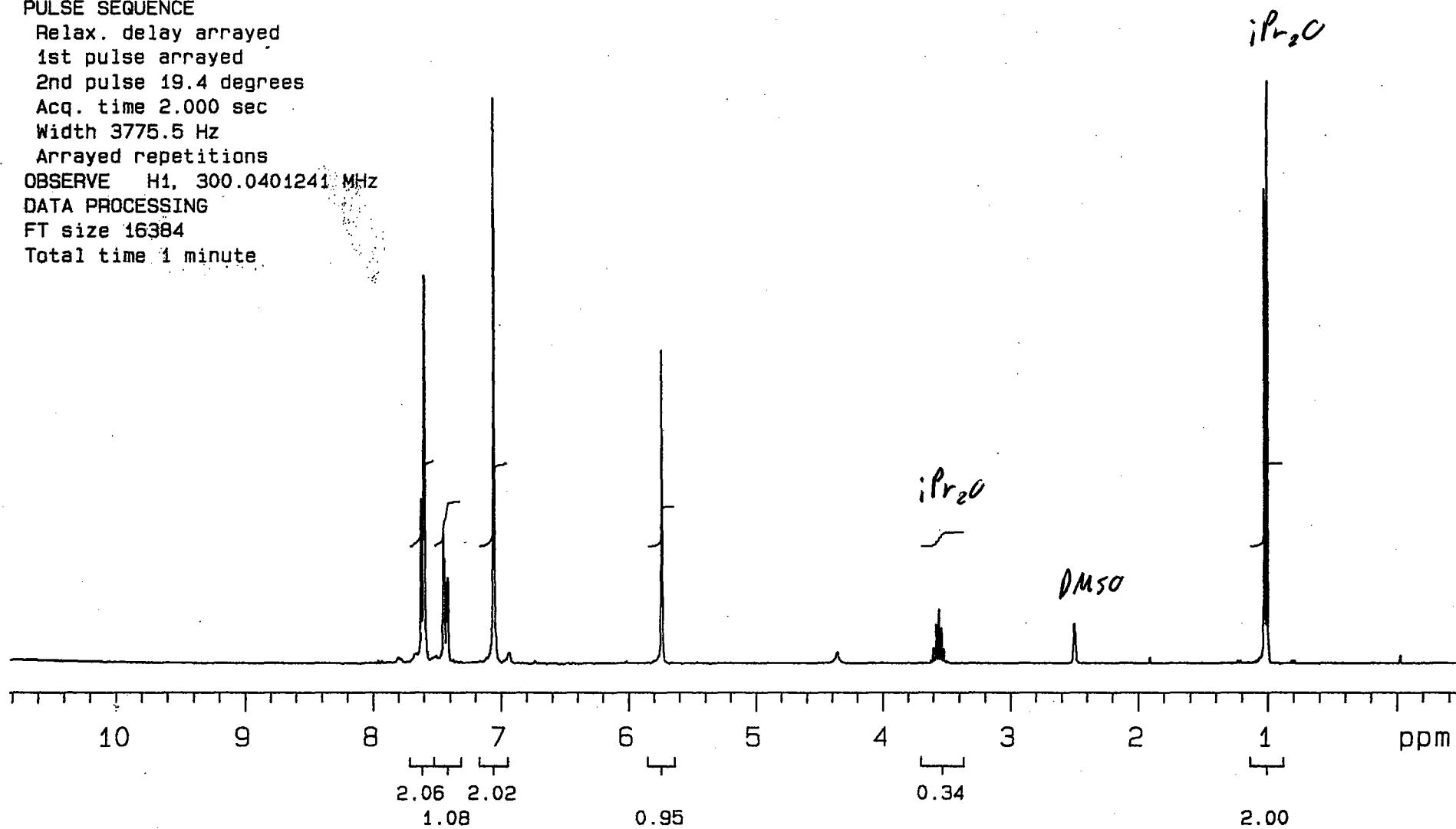
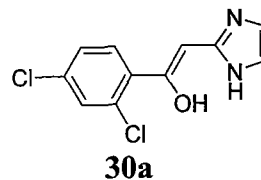
PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 19.4 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions

OBSERVE H1, 300.0401241 MHz

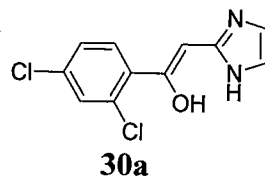
DATA PROCESSING

FT size 16384
Total time 1 minute



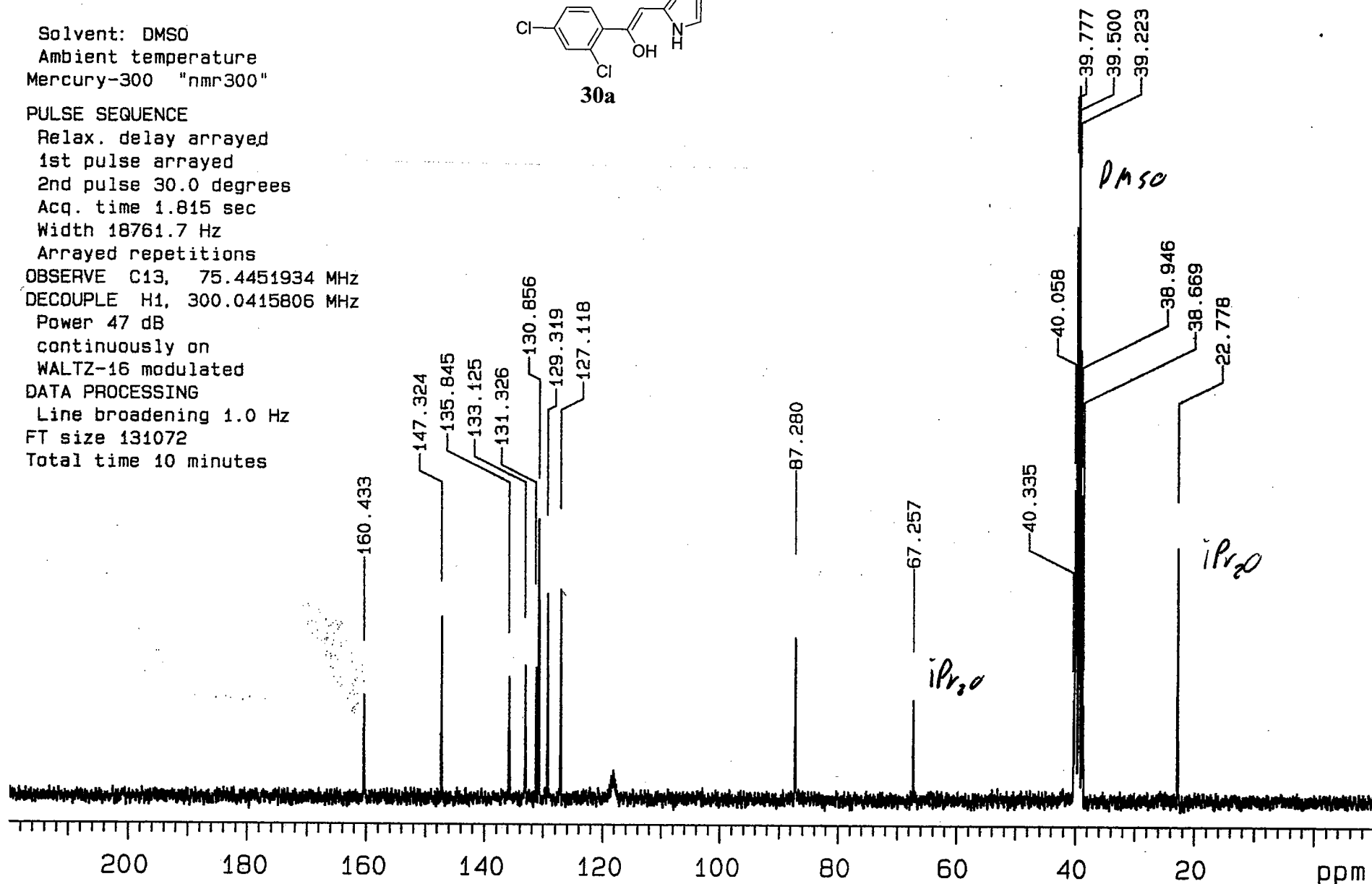
13C OBSERVE

Solvent: DMSO
Ambient temperature
Mercury-300 "nmr300"



PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 30.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
Arrayed repetitions
OBSERVE C13, 75.4451934 MHz
DECOUPLE H1, 300.0415806 MHz
Power 47 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 10 minutes



SampleName KPC62PROD

Injection Volume 10.00 ul

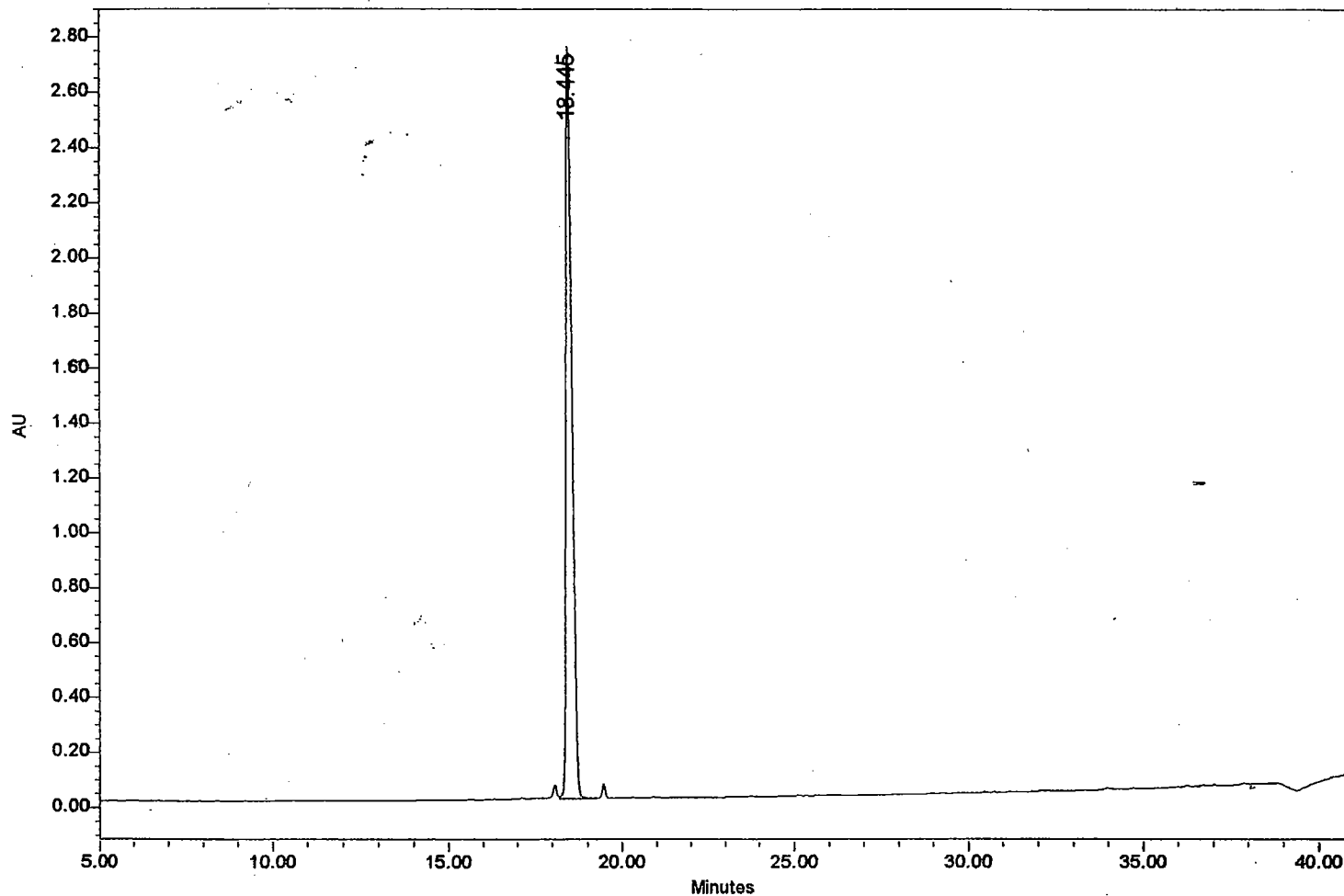
Date Acquired 12/9/98 5:28:31 PM

Vial 3

Channel Description FDA 220.0 nm

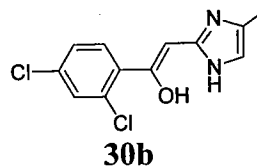
Acq Method Set 5100

Auto-Scaled Chromatogram



Peak Results

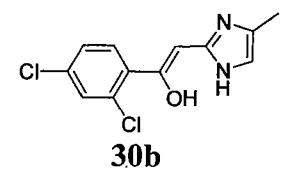
	RT	Start Time	End Time	% Height	% Area
1	18.445	18.200	19.250	100.00	100.00



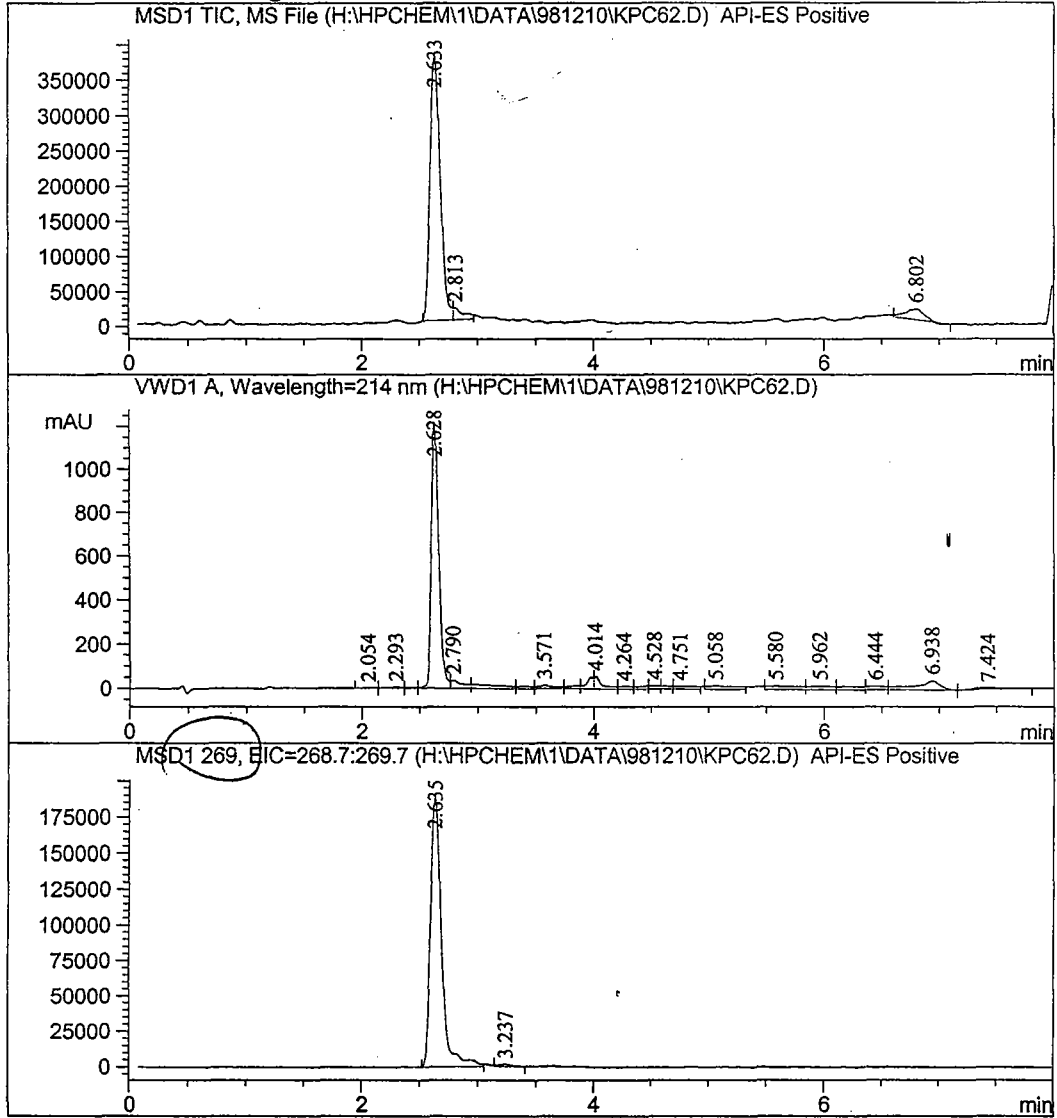
=====

Injection Date	: 12/10/98 9:56:24 AM	Seq. Line	: 5
Sample Name	: KPC62	Vial	: 5
Acq. Operator	: ntg	Inj	: 1
		Inj Volume	: Inj prog

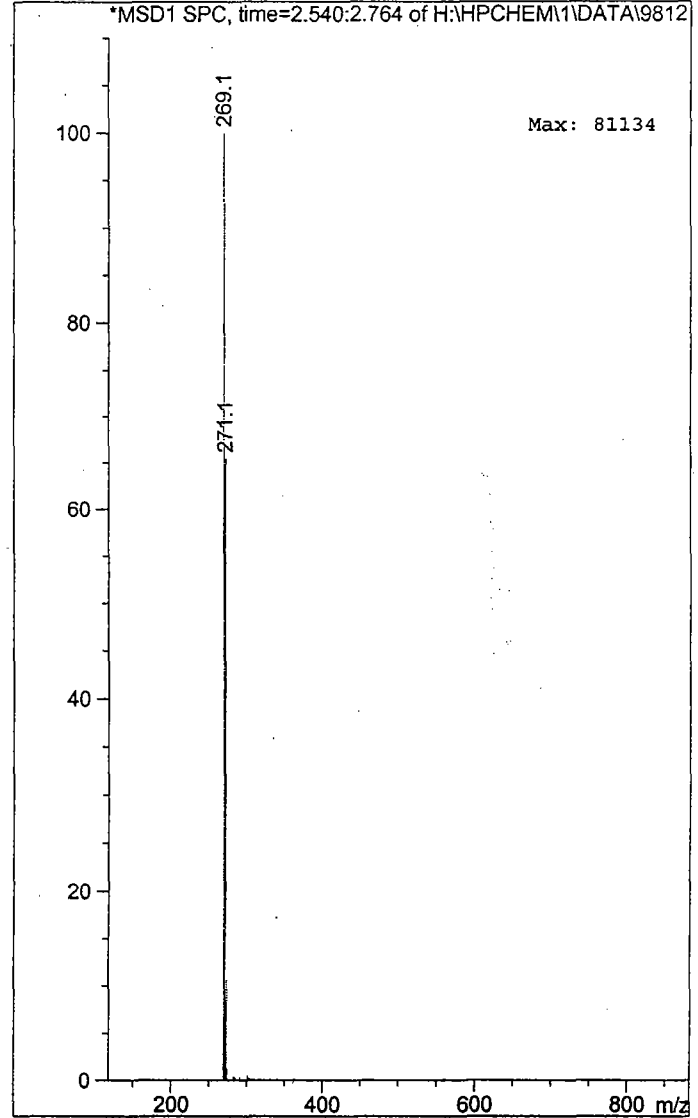
Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
Last changed : 11/10/98 1:09:54 PM by ntg
Analysis Method : C:\HPCHEM\1\METHODS\ALICE.M
Last changed : 9/3/98 2:14:14 PM by ntg
LC/MSD method. Flow rate:0.4 mL/min, 1-95% B in 6 min. 2 min for equilibration. condense scan. Solvent A:H2O+0.05%TFA, B:ACN +0.05%TFA. Column Temp. is 30. 150-850, 50 V



Current Chromatogram(s)

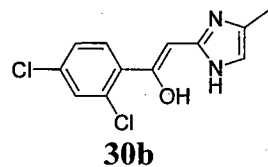


MS Spectrum



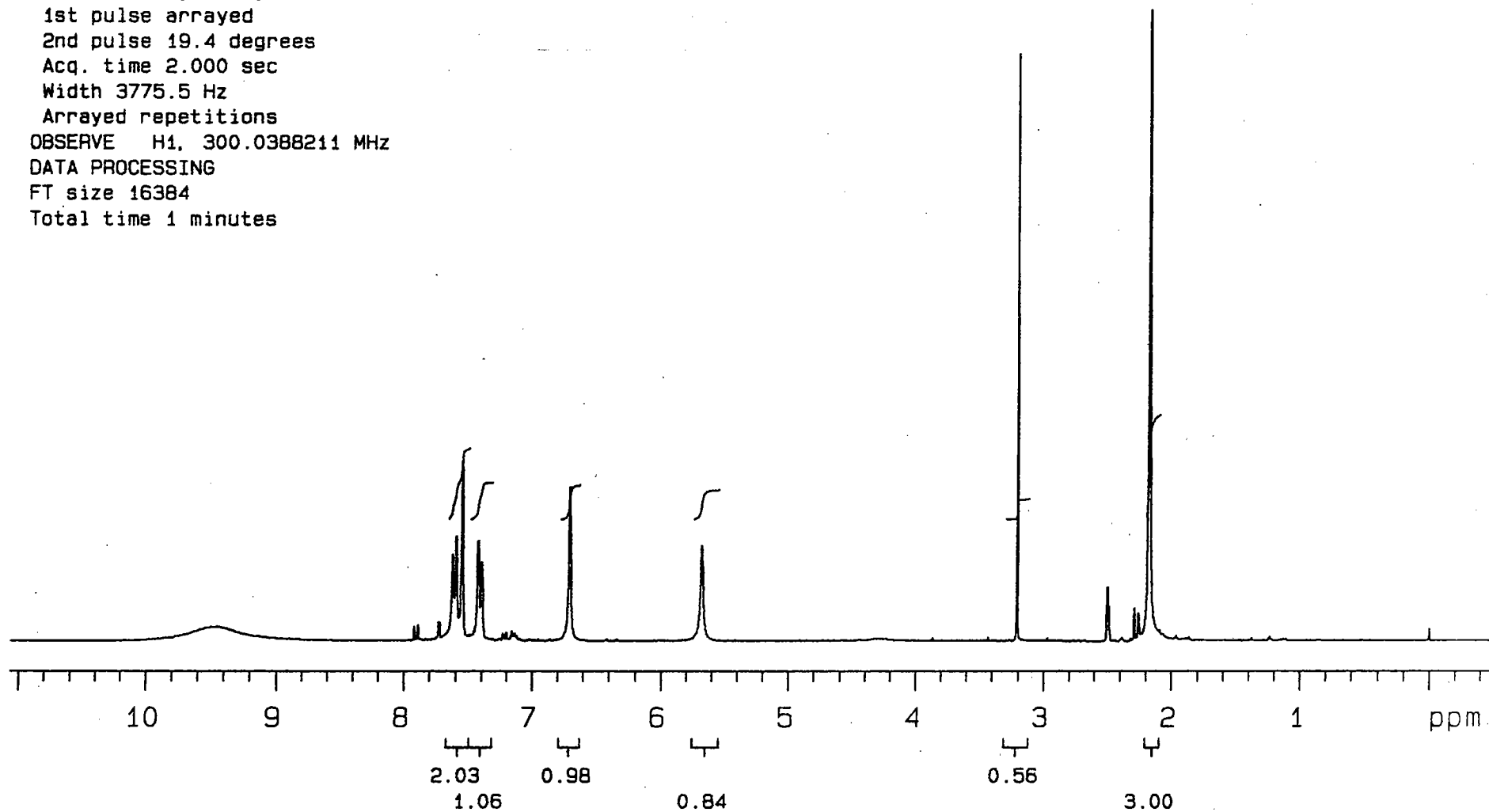
STANDARD 1H OBSERVE

Solvent: DMSO
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"



PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 19.4 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.0388211 MHz
DATA PROCESSING
FT size 16384
Total time 1 minutes



13C OBSERVE

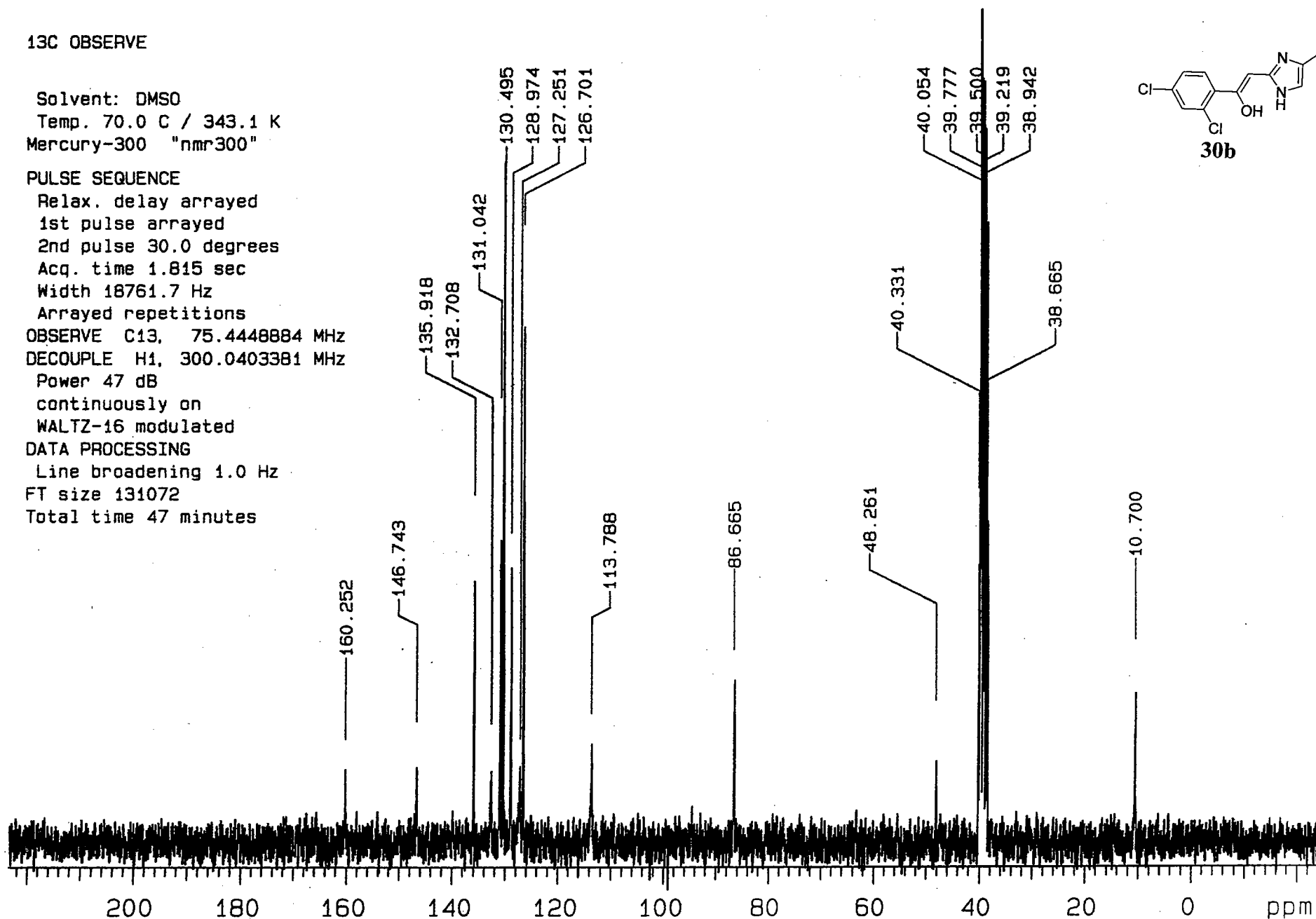
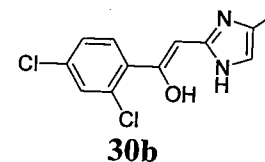
Solvent: DMSO
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 30.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
Arrayed repetitions
OBSERVE C13, 75.4448884 MHz
DECOUPLE H1, 300.0403381 MHz
Power 47 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz
FT size 131072
Total time 47 minutes



SampleName KPC64 *a*

Injection Volume 3.00 ul

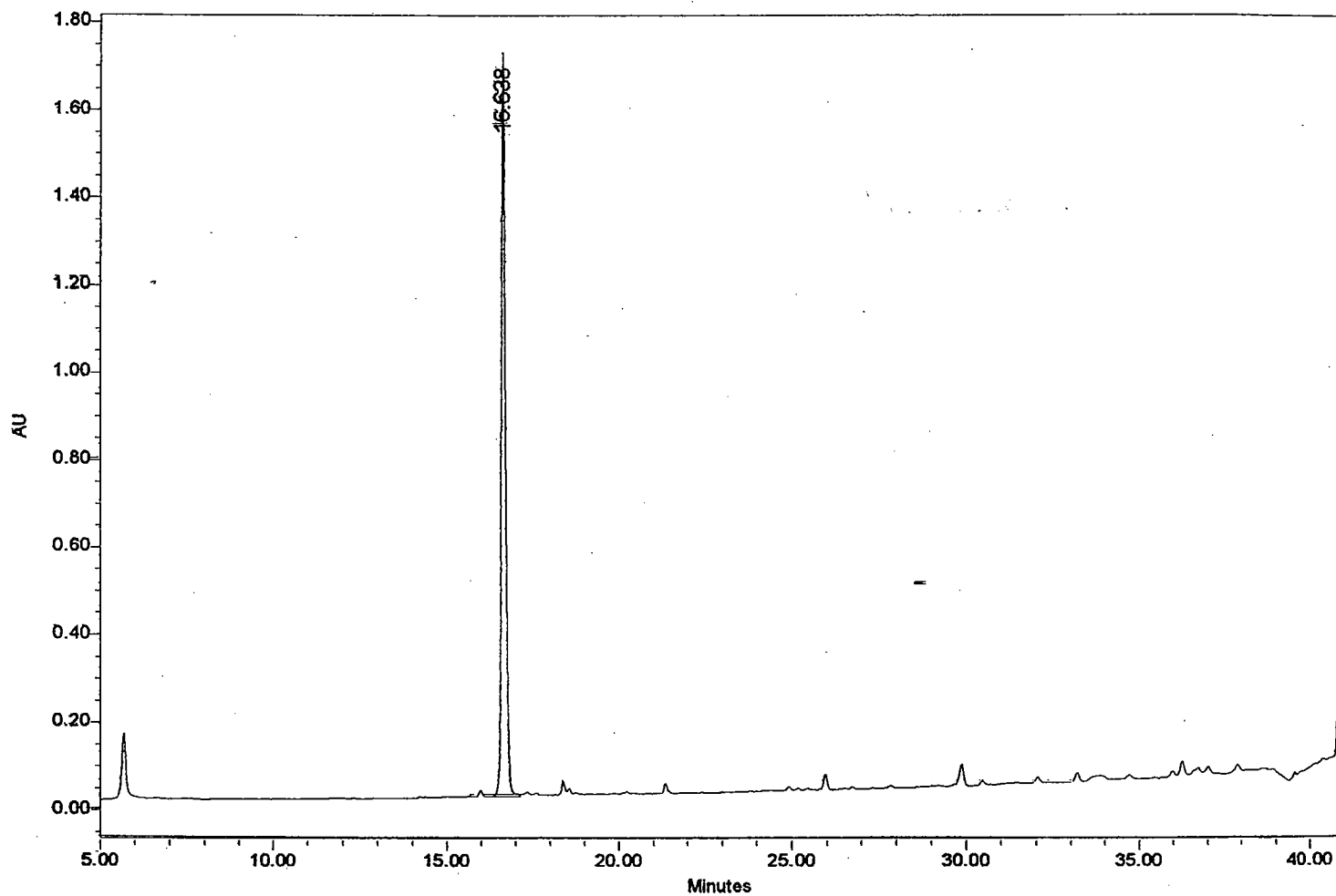
Date Acquired 12/10/98 6:03:10 PM

Vial 28

Channel Description PDA 220.0 nm

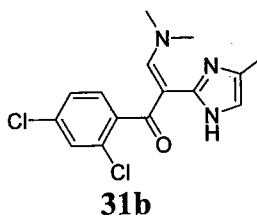
Acq Method Set 5100

Auto-Scaled Chromatogram



Peak Results

	RT	Start Time	End Time	% Height	% Area
1	16.638	16.317	17.133	100.00	100.00

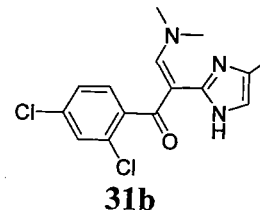


Injection Date : 12/10/98 10:00:17 PM Seq. Line : 33
 Sample Name : kpc64a Vial : 33
 Acq. Operator : ntg Inj : 1
 Inj Volume : Inj prog

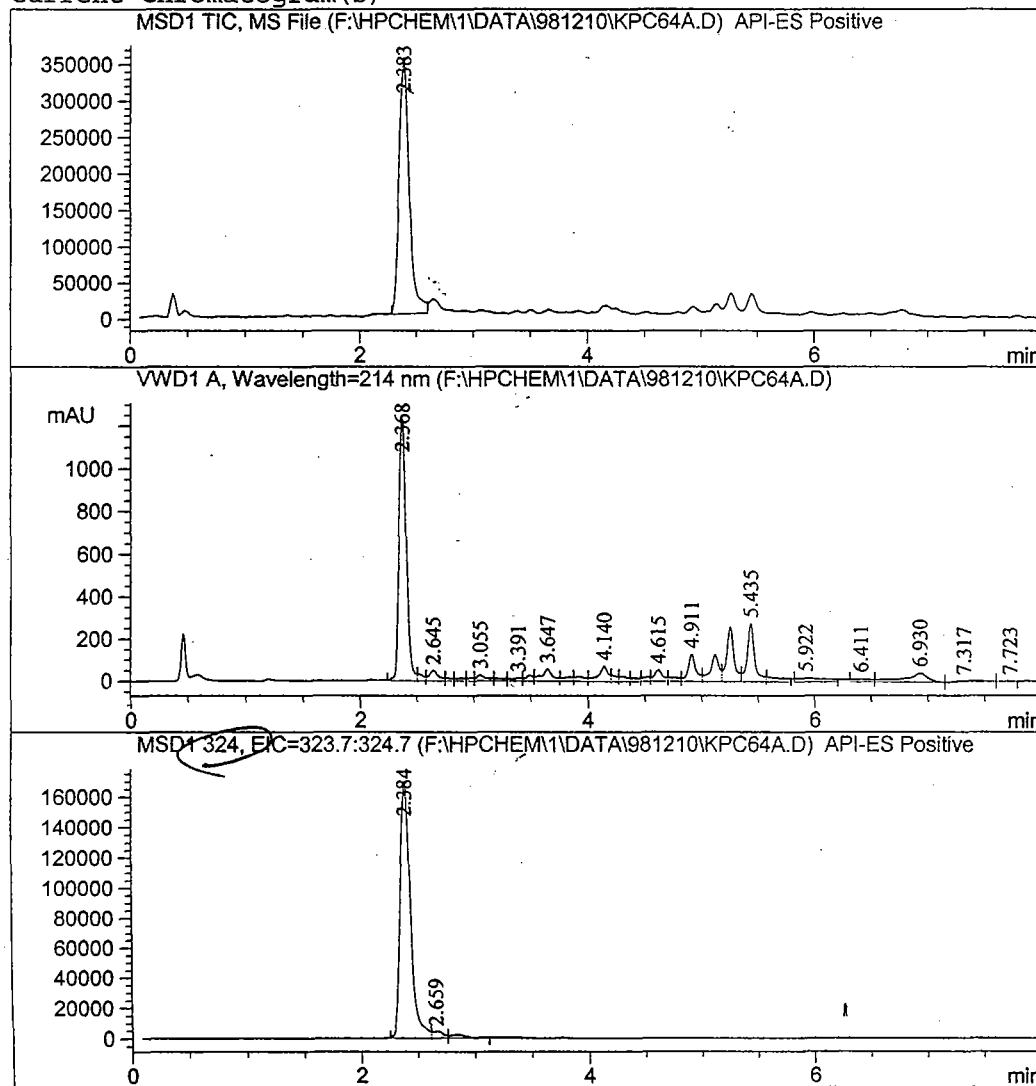
Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
 Last changed : 11/10/98 1:09:54 PM by ntg
 Analysis Method : C:\HPCHEM\1\METHODS\ALICE.M
 Last changed : 12/10/98 2:01:08 PM

(modified after loading)

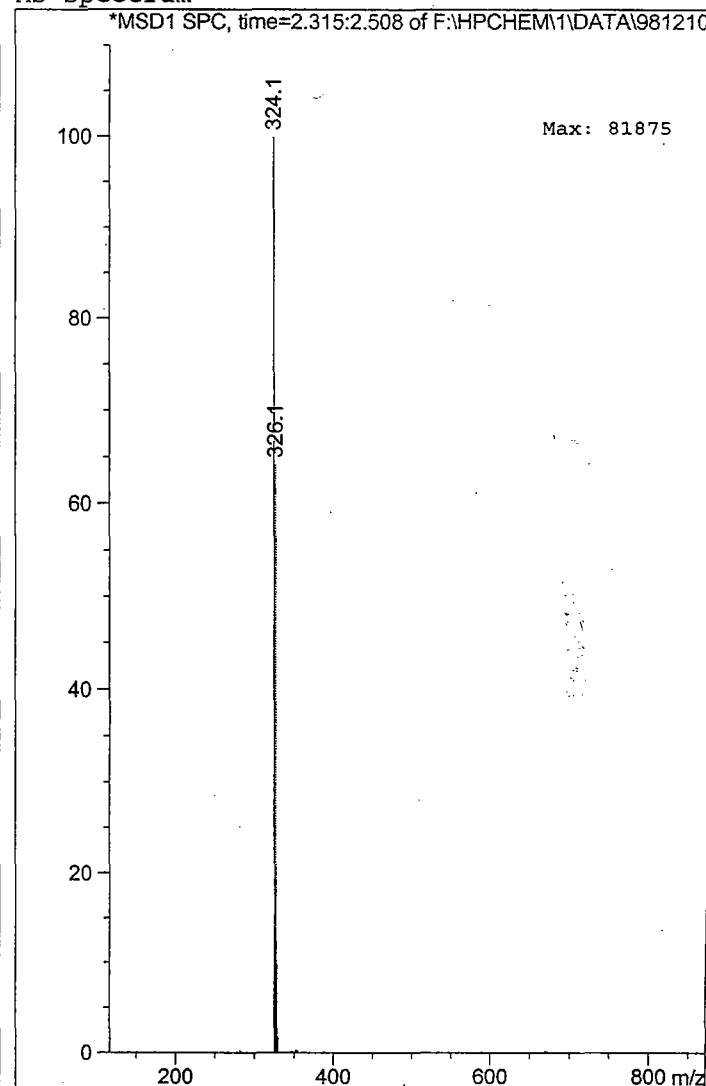
LC/MSD method. Flow rate:0.4 mL/min, 1-95% B in 6 min. 2 min for equilibration. condense scan. Solvent A:H2O+0.05%TFA, B:ACN +0.05%TFA. Column Temp. is 30. 150-850, 50 V



Current Chromatogram(s)



MS Spectrum



SampleName kpc92

Injection Volume 10.00 ul

Date Acquired 2/10/99 4:29:17 PM

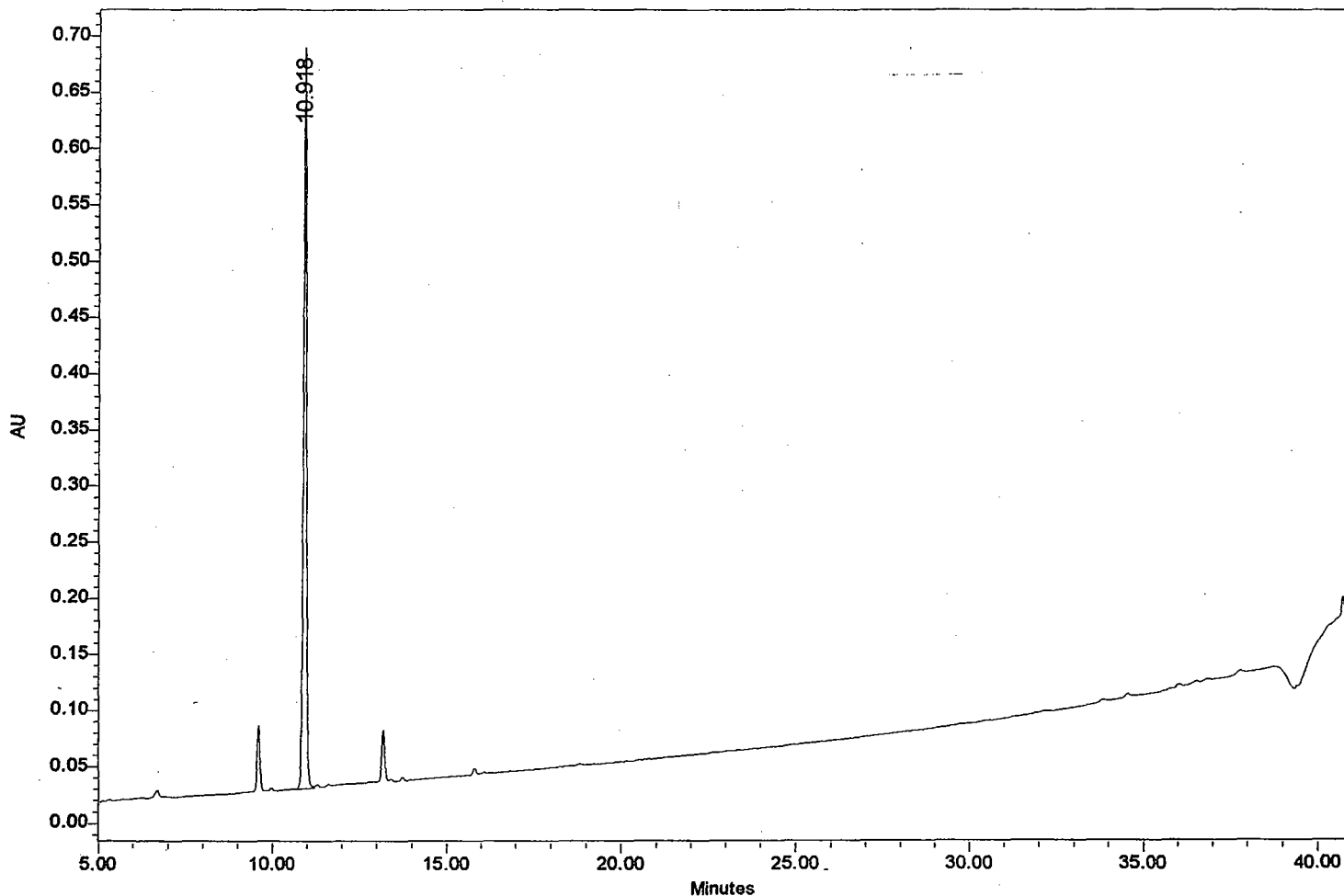
Vial 23

Channel Description PDA 220.0 nm

Acq Method Set 5100

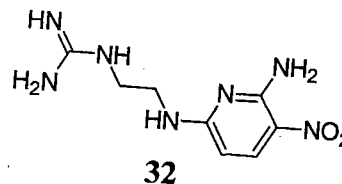
KPC92

Auto-Scaled Chromatogram



Peak Results

	RT	Start Time	End Time	% Height	% Area
1	10.918	10.683	11.200	100.00	100.00



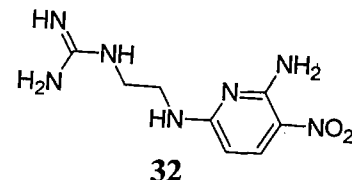
=====

Injection Date : 2/11/99 12:44:55 PM	Seq. Line : 19
Sample Name : kpc92	Vial : 19
Acq. Operator : ntg	Inj : 1
	Inj Volume : Inj prog

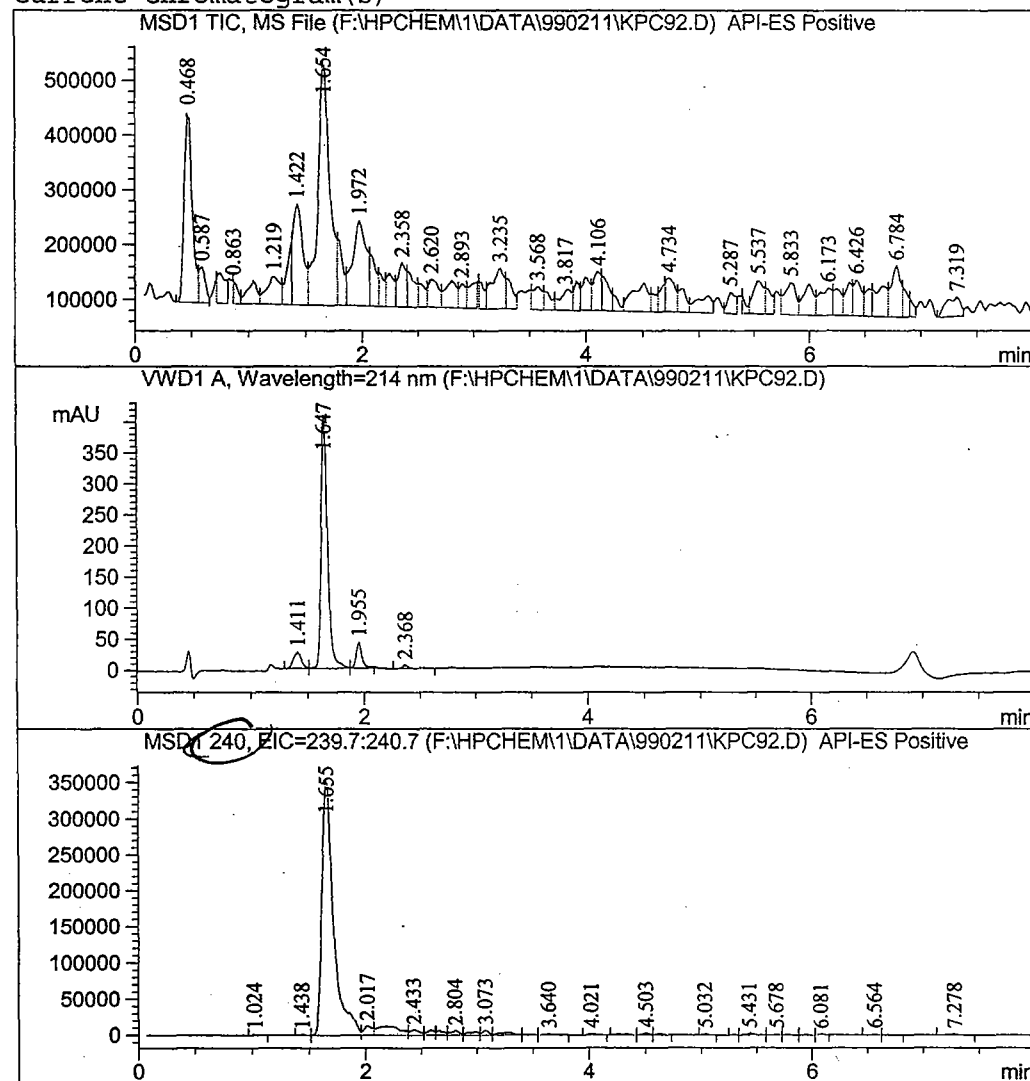
Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
 Last changed : 9/17/98 11:16:18 AM by ntg
 Analysis Method : C:\HPCHEM\1\METHODS\ALICE.M
 Last changed : 2/11/99 4:58:05 PM
 (modified after loading)

LC/MSD method. Flow rate: 0.4 mL/min, 1-95% B in 6 min. 2 min for equilibration. Condense scan. Solvent A: H₂O+0.05%TFA, 3: ACN +0.05%TFA. Column Temp. is 30. 150-850, 50 V

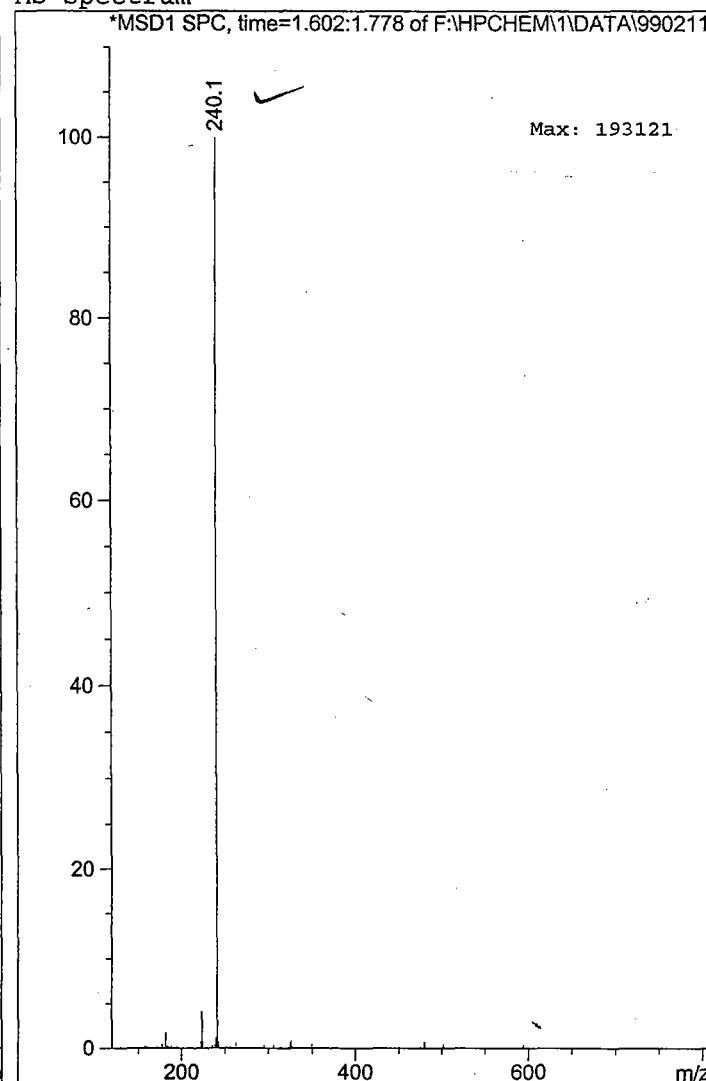
KPC92



Current Chromatogram(s)



MS Spectrum



STANDARD 1H OBSERVE

Solvent: DMSO *d*₂O
Ambient temperature
Mercury-300 "nmr300"

PULSE SEQUENCE

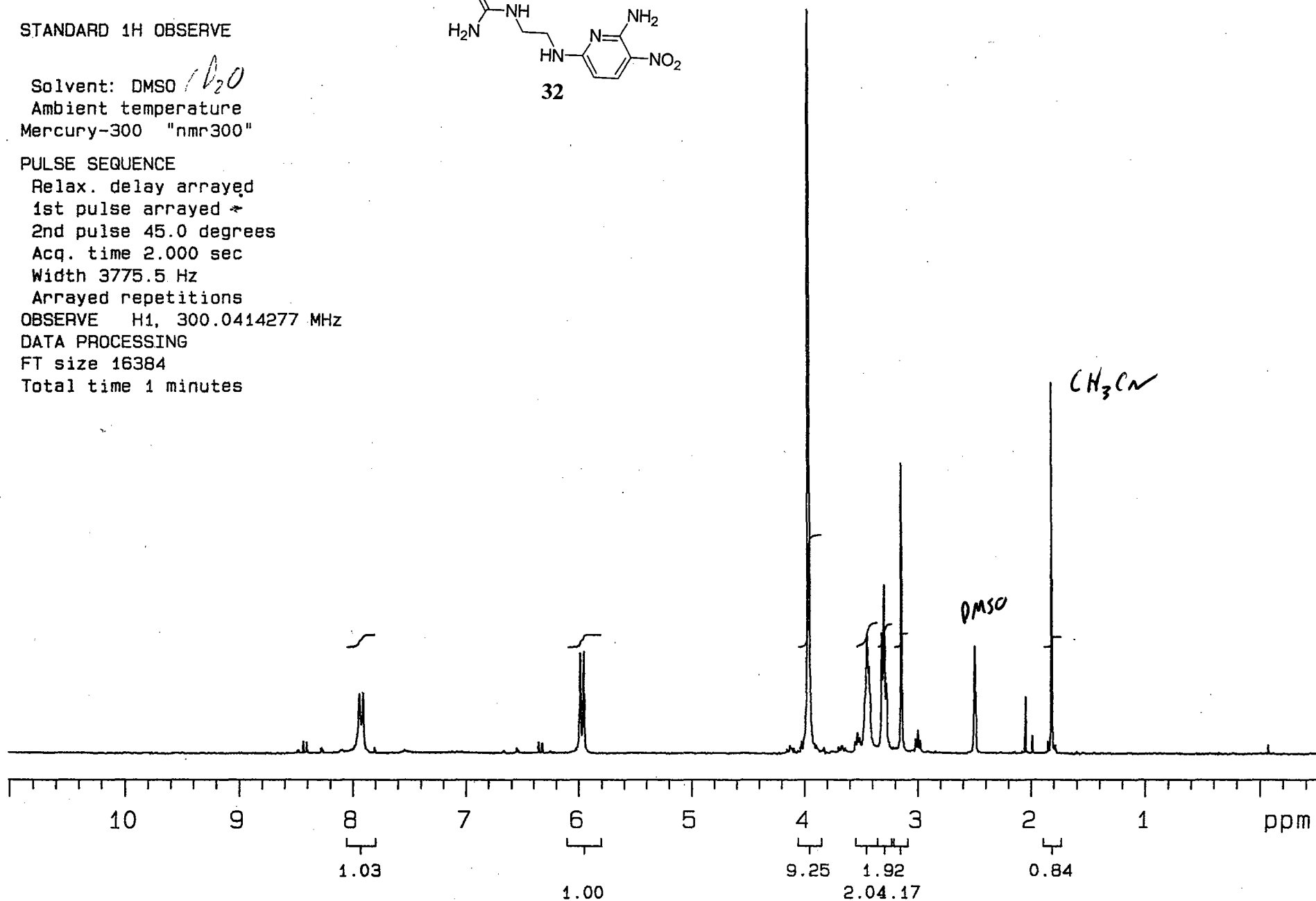
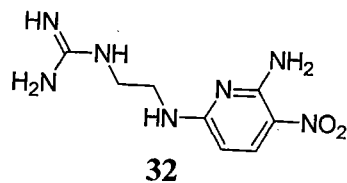
Relax. delay arrayed
1st pulse arrayed →
2nd pulse 45.0 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions

OBSERVE H1, 300.0414277 MHz

DATA PROCESSING

FT size 16384

Total time 1 minutes



SampleName kpc16-1

Injection Volume 10.00 ul

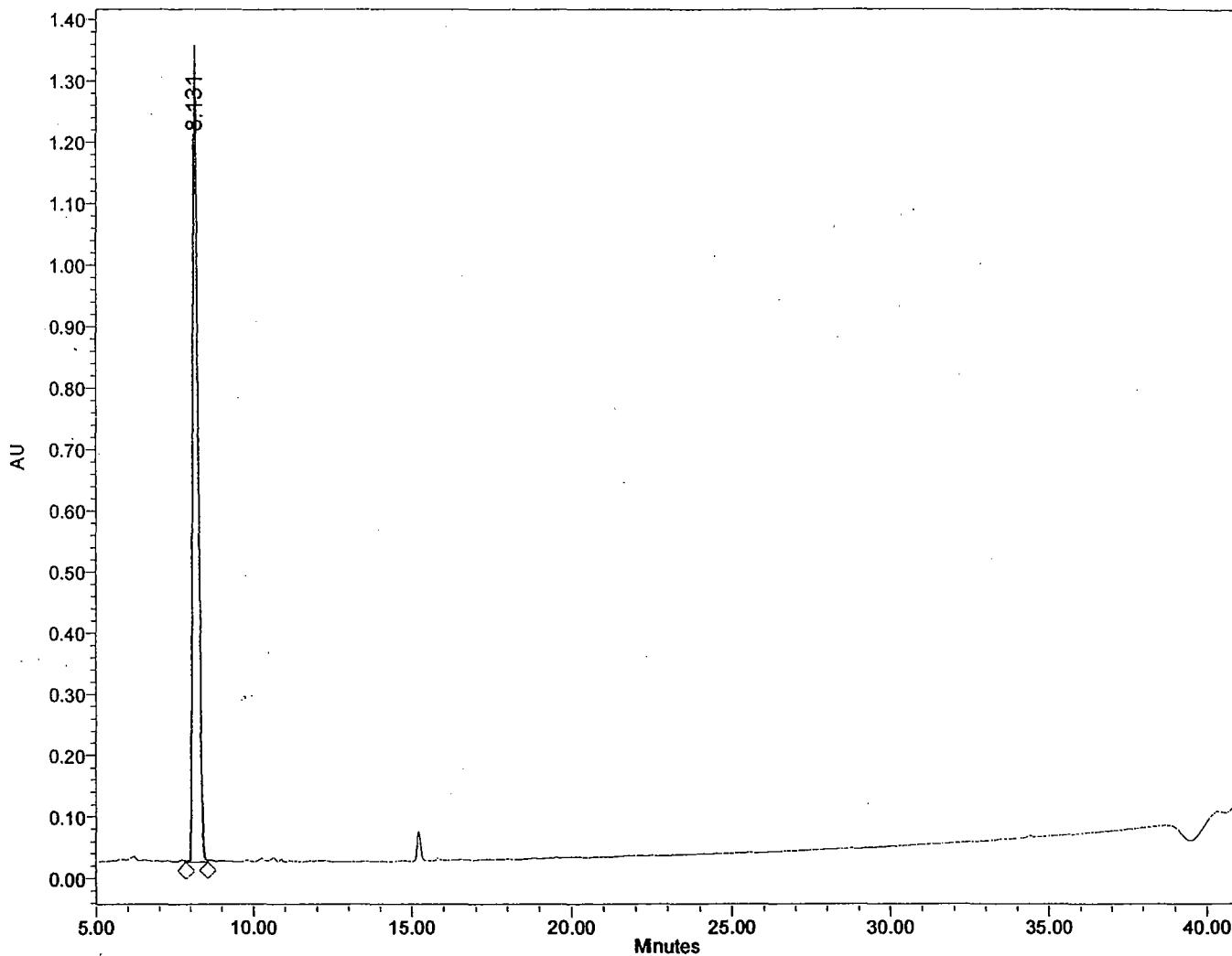
Date Acquired 4/15/99 9:22:24 A

Vial 10

Channel Description PDA 220

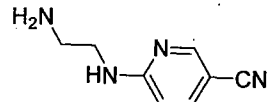
Acq Method Set 5100

Auto-Scaled Chromatogram



Peak Results

	Name	RT	Start Time	End Time	% Height	% Area
1		8.131	7.893	8.577	100.00	100.00



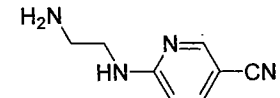
6-(2-Amino-ethylamino)-
nicotinonitrile

=====

Injection Date	: 4/15/99 11:27:13 AM	Seq. Line	: 5
Sample Name	: kpc16-1	Vial	: 5
Acq. Operator	: Manager	Inj	: 1
		Inj Volume	: Inj prog

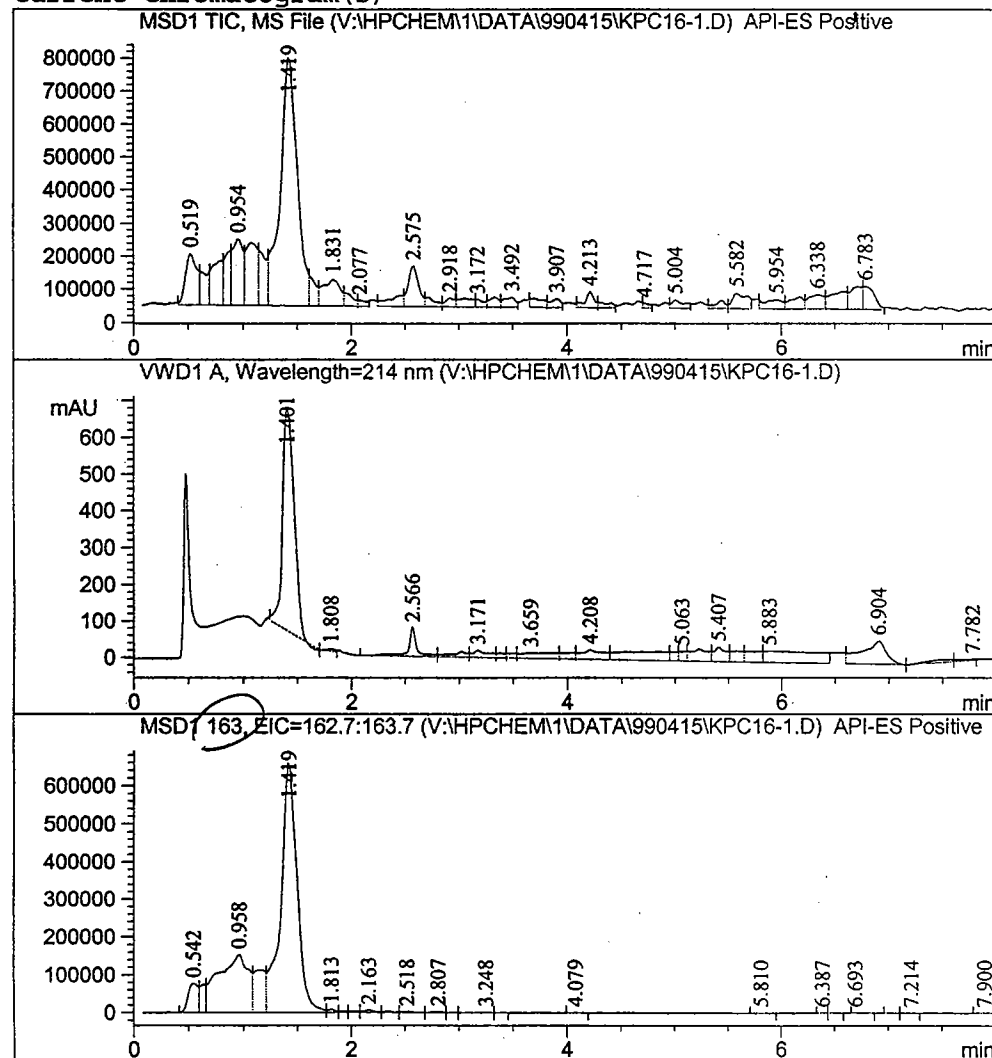
Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
Last changed : 3/4/99 1:46:07 PM by Manager
Analysis Method : C:\HPCHEM\1\METHODS\ALICE.M
Last changed : 4/15/99 10:14:07 AM
(modified after loading)

C/MSD method. Flow rate:0.4 mL/min, 1-95% B in 6 min. 2 min for equilibration. condense scan. Solvent A:H2O+0.05%TFA, B:ACN +0.5%TFA. Column Temp. is 30. 150-850, 50 V

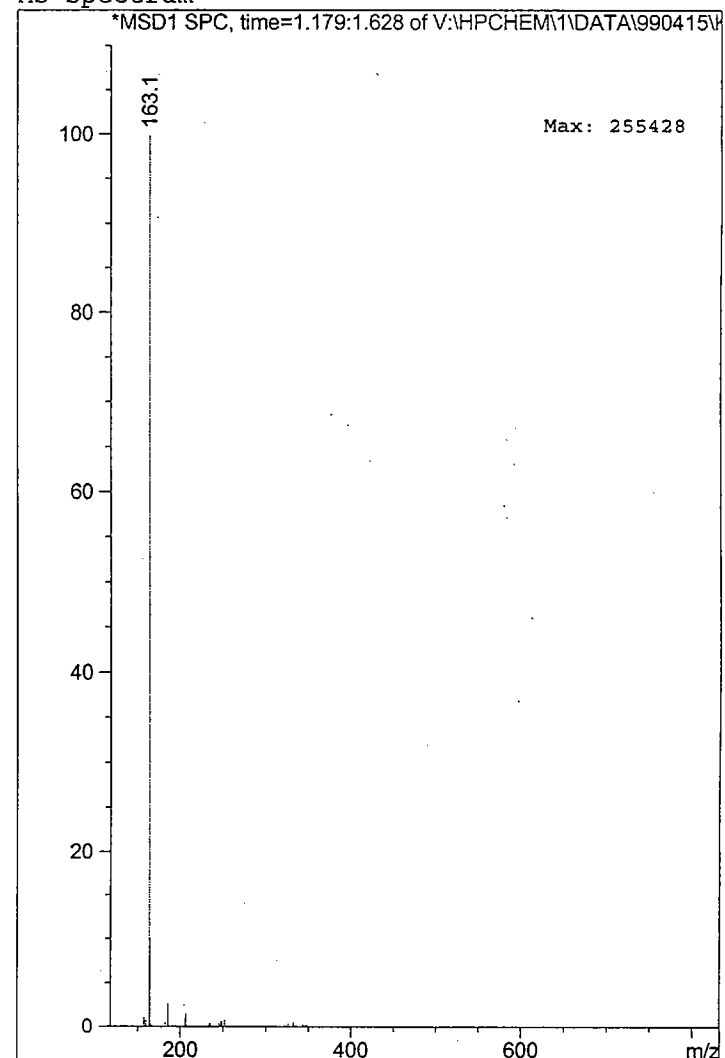


**6-(2-Amino-ethylamino)-
nicotinonitrile**

Current Chromatogram(s)



MS Spectrum



STANDARD 1H OBSERVE

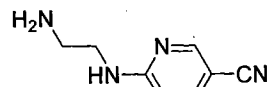
Solvent: DMSO
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"

PULSE SEQUENCE

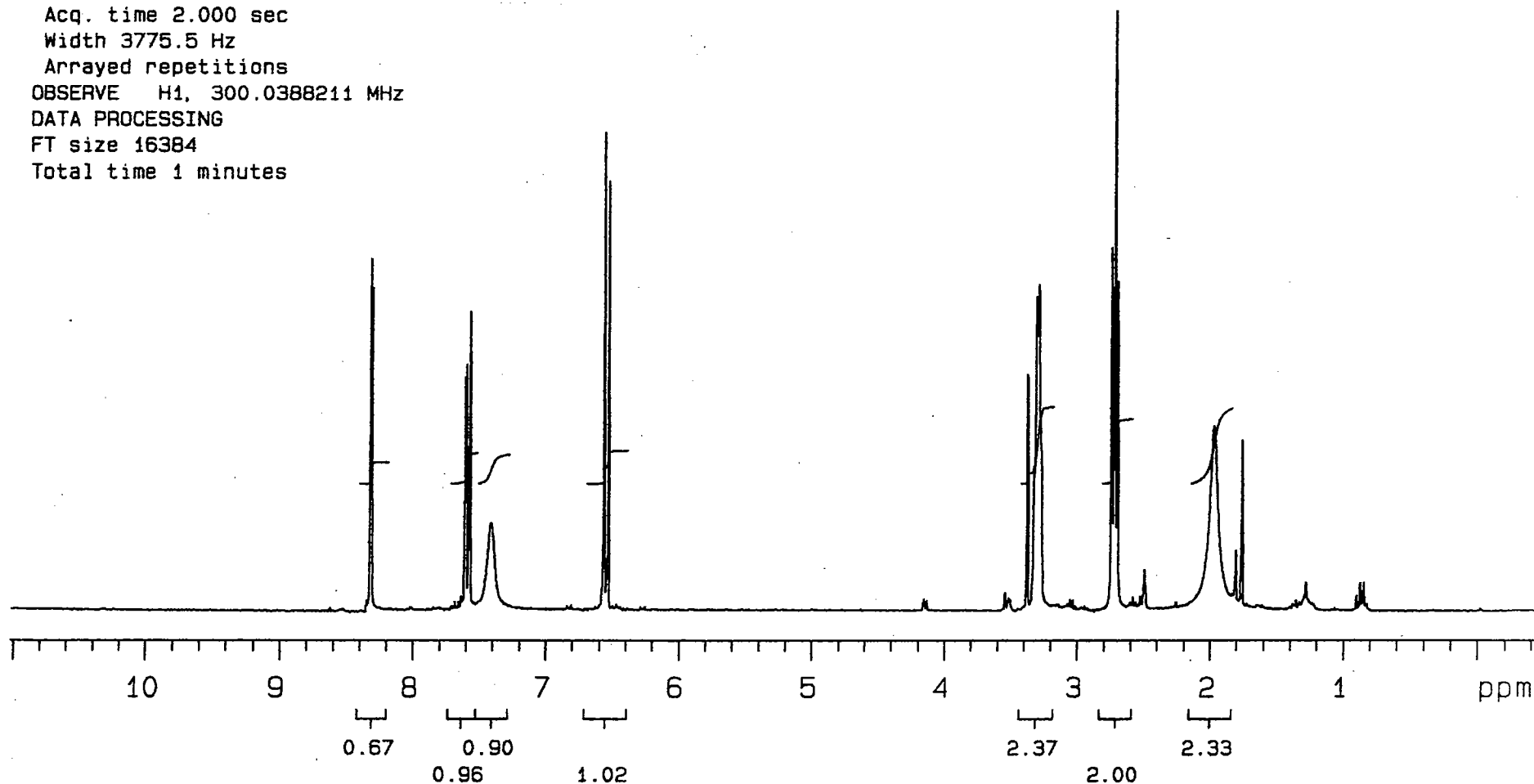
Relax. delay arrayed
1st pulse arrayed
2nd pulse 45.0 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.0388211 MHz

DATA PROCESSING

FT size 16384
Total time 1 minutes



**6-(2-Amino-ethylamino)-
nicotinonitrile**

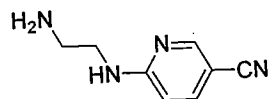


13C OBSERVE

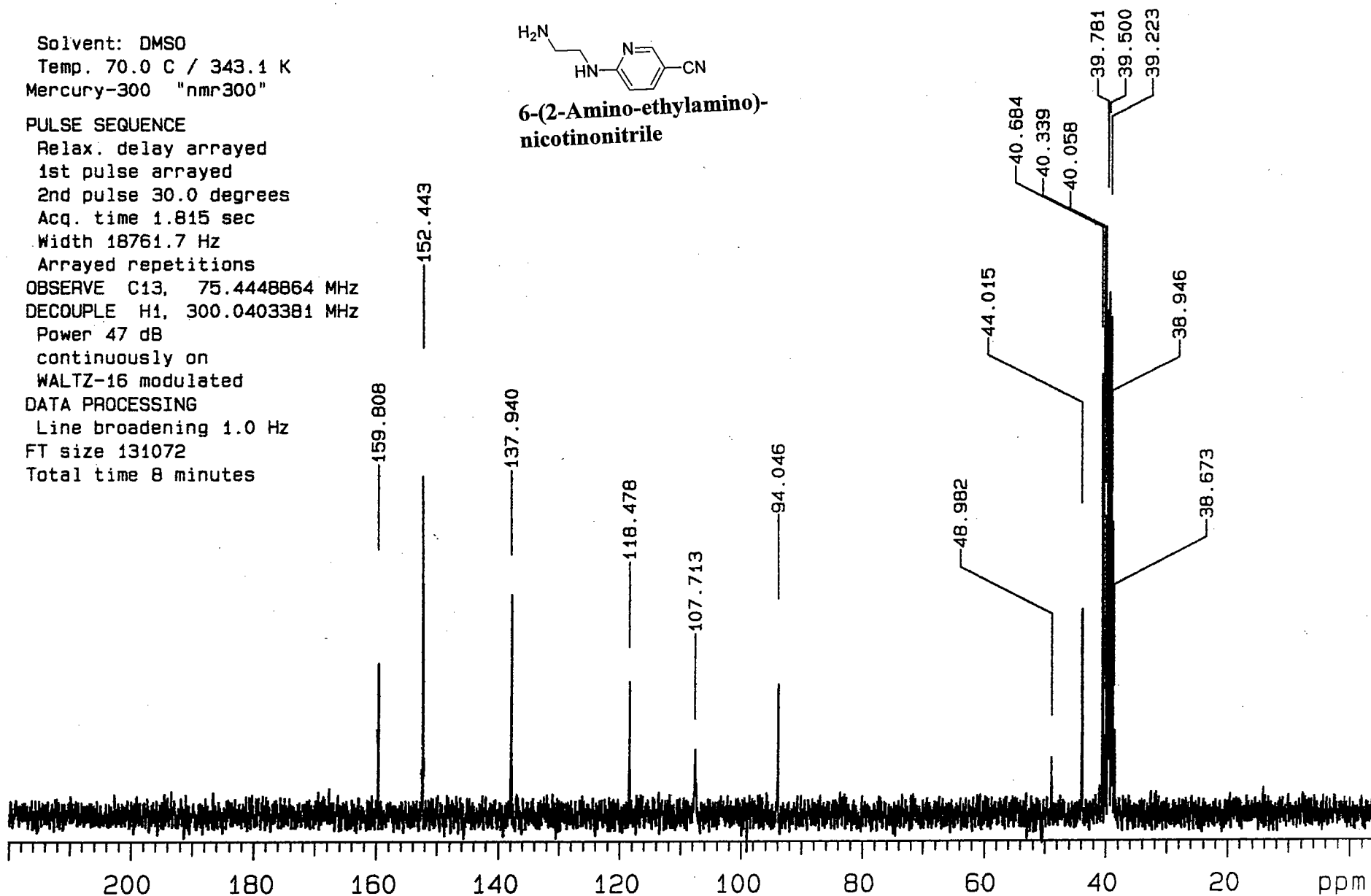
Solvent: DMSO
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 30.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
Arrayed repetitions
OBSERVE C13, 75.4448864 MHz
DECOUPLE H1, 300.0403381 MHz
Power 47 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 8 minutes



6-(2-Amino-ethylamino)-
nicotinonitrile



SampleName kpc60-1

Injection Volume 30.00 ul

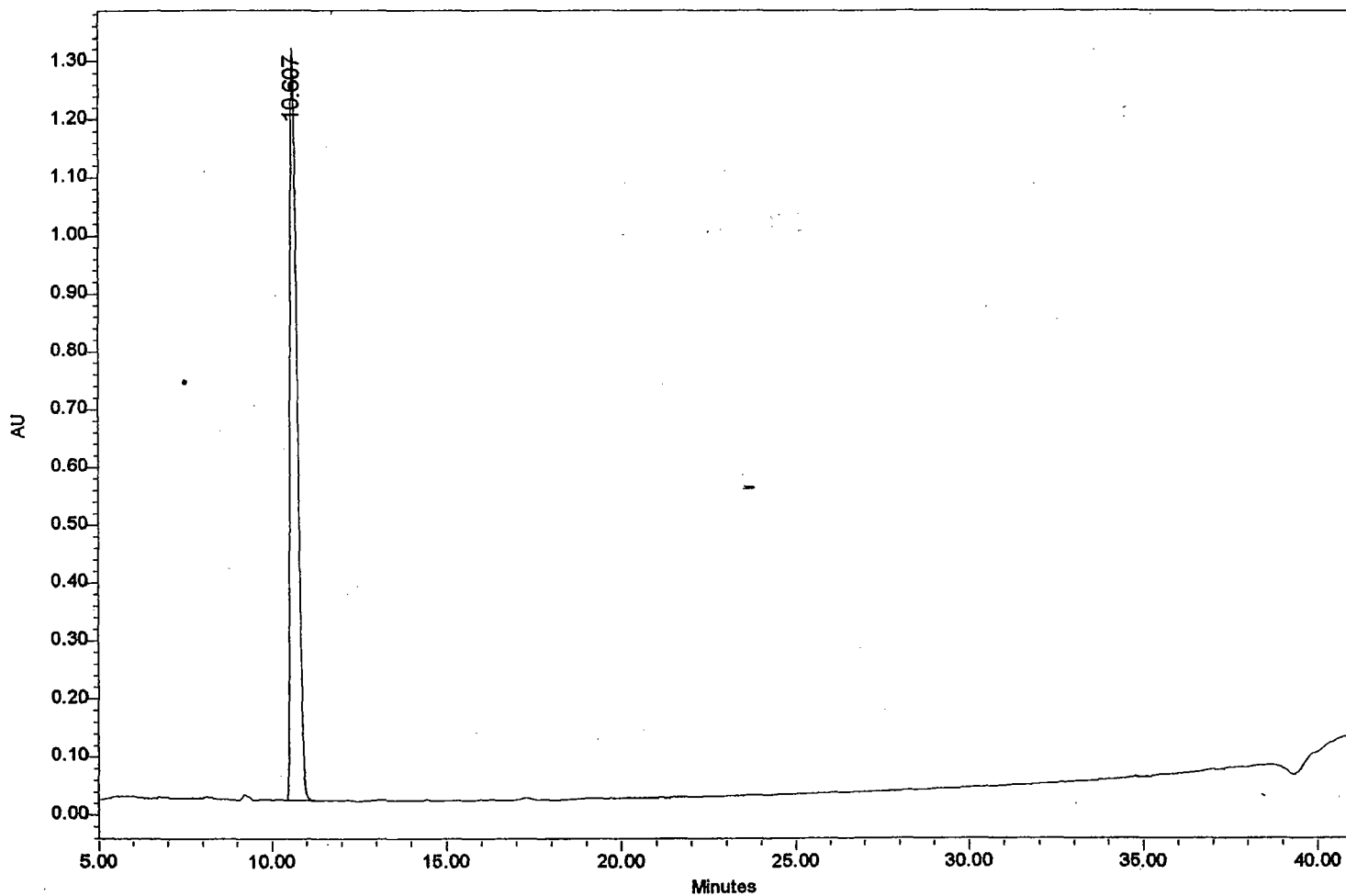
Date Acquired 4/14/99 7:09:24 PM

Vial 4

Channel Description PDA 220.0 nm

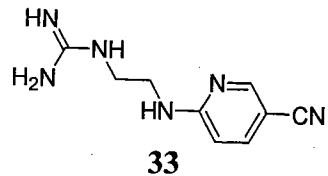
Acq Method Set 5100

Auto-Scaled Chromatogram

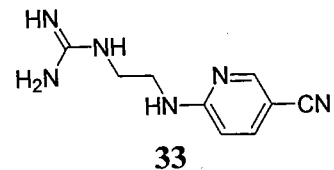


Peak Results

	RT	Start Time	End Time	% Height	% Area
1	10.607	10.433	11.450	100.00	100.00

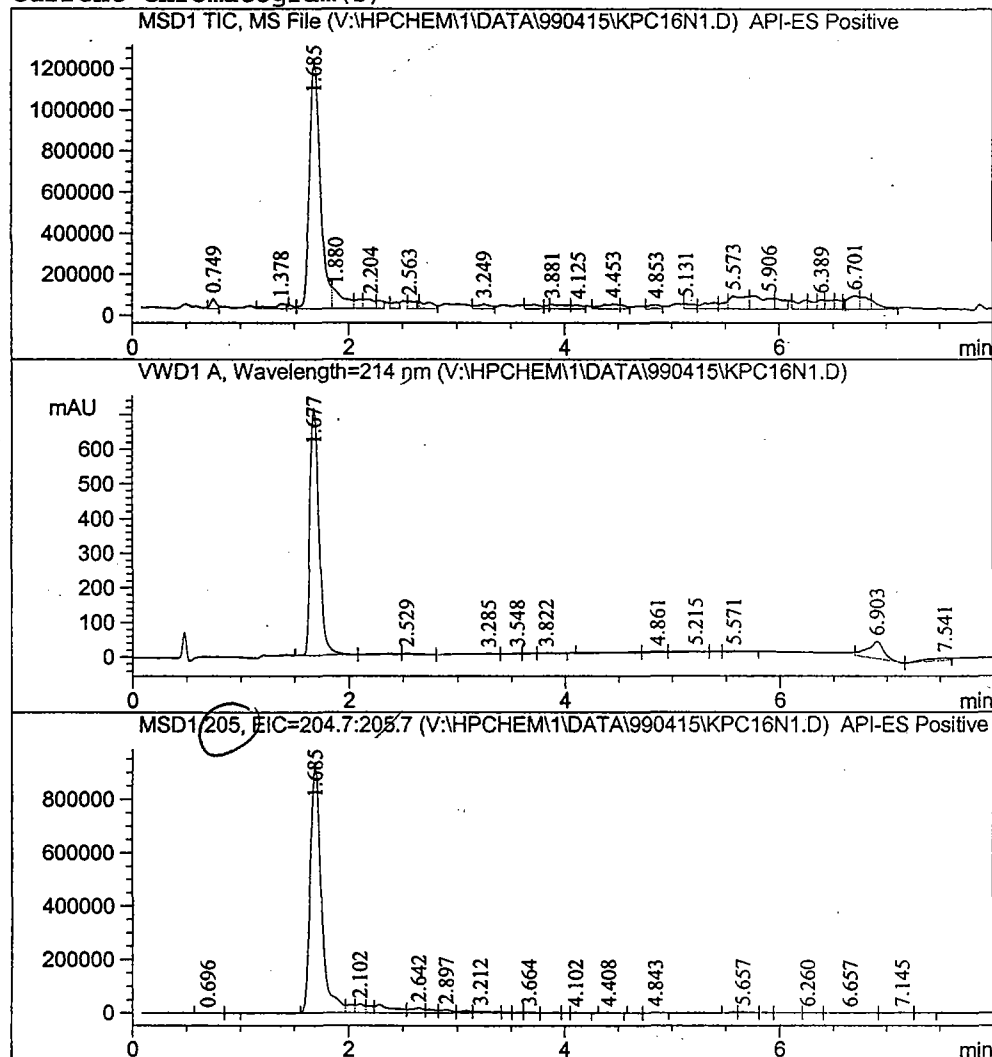


Injection Date : 4/15/99 12:36:48 PM Seq. Line : 12
 Sample Name : kpc60n1 Vial : 12
 Acq. Operator : Manager Inj : 1
 Inj Volume : Inj prog
 Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
 Last changed : 3/4/99 1:46:07 PM by Manager
 Analysis Method : C:\HPCHEM\1\METHODS\ALICE.M
 Last changed : 4/15/99 10:14:07 AM
 (modified after loading)

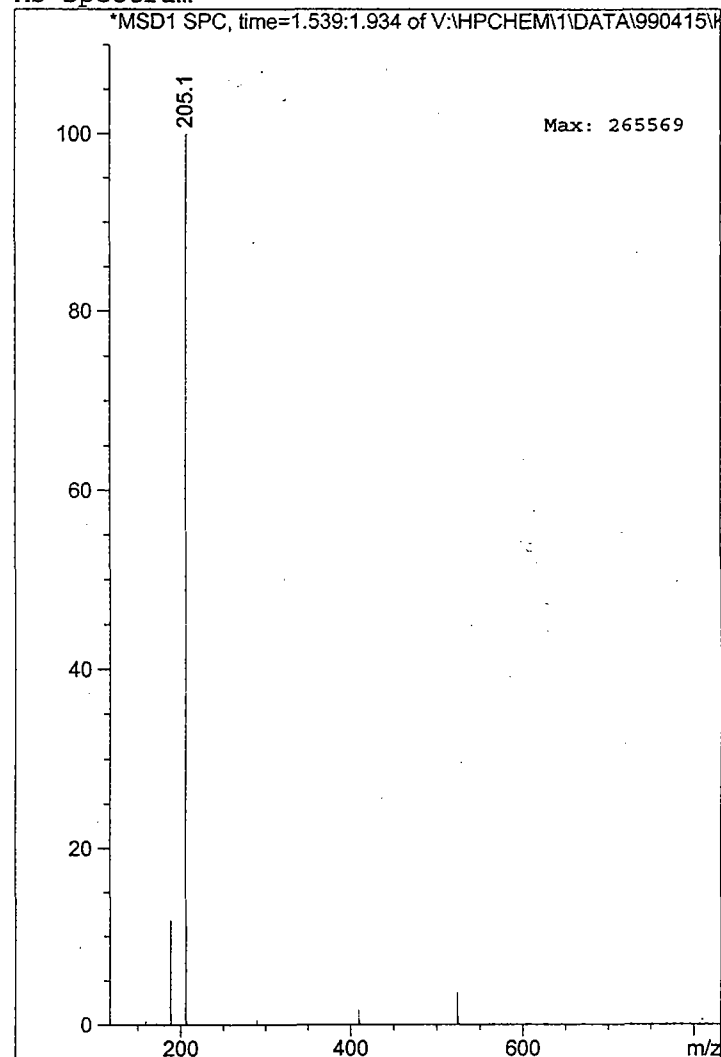


LC/MSD method. Flow rate: 0.4 mL/min, 1-95% B in 6 min. 2 min for equilibration. condense scan. Solvent A: H₂O+0.05%TFA,
 B: ACN +0.05%TFA. Column Temp. is 30. 150-850, 50 V

Current Chromatogram(s)



MS Spectrum



STANDARD 1H OBSERVE

Solvent: DMSO
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"

PULSE SEQUENCE

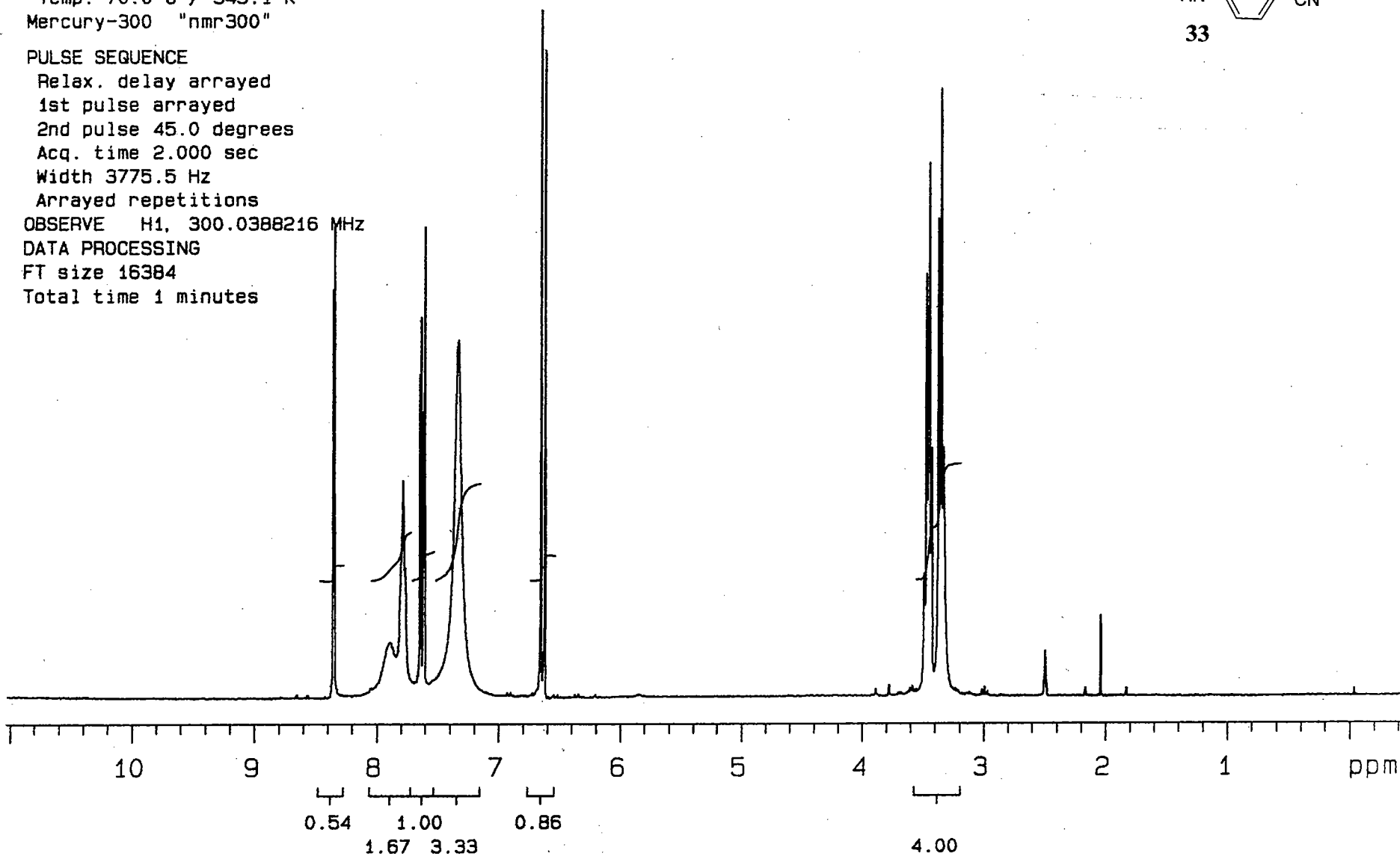
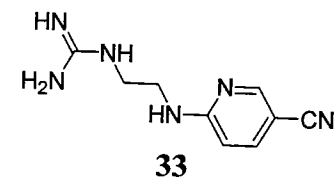
Relax. delay arrayed
1st pulse arrayed
2nd pulse 45.0 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions

OBSERVE H1, 300.0388216 MHz

DATA PROCESSING

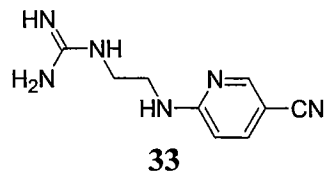
FT size 16384

Total time 1 minutes



¹³C OBSERVE

Solvent: DMSO
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"



PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 30.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
Arrayed repetitions

OBSERVE C13, 75.4448841 MHz

DECOUPLE H1, 300.0403381 MHz

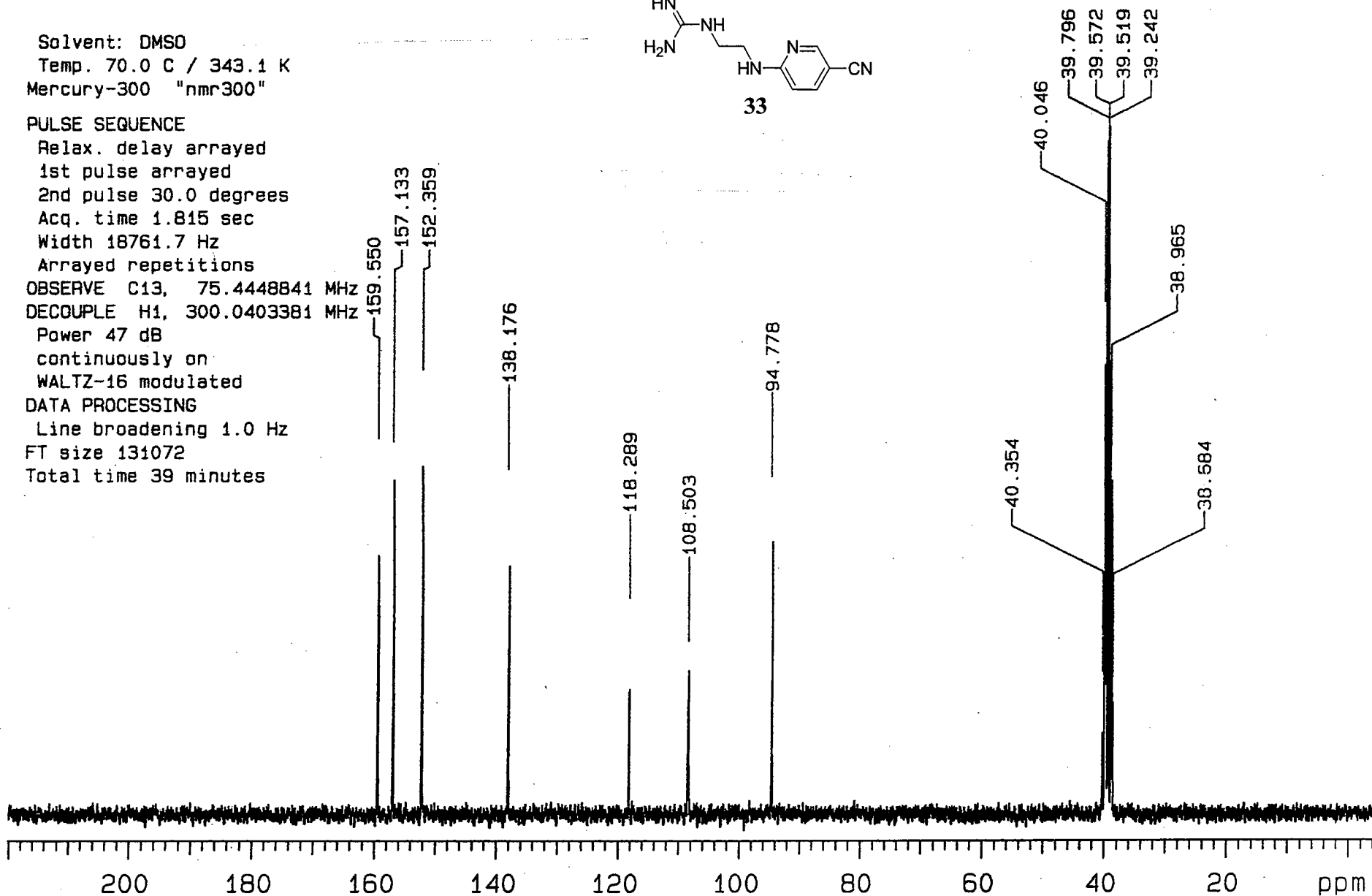
Power 47 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 39 minutes



SampleName AZ21551

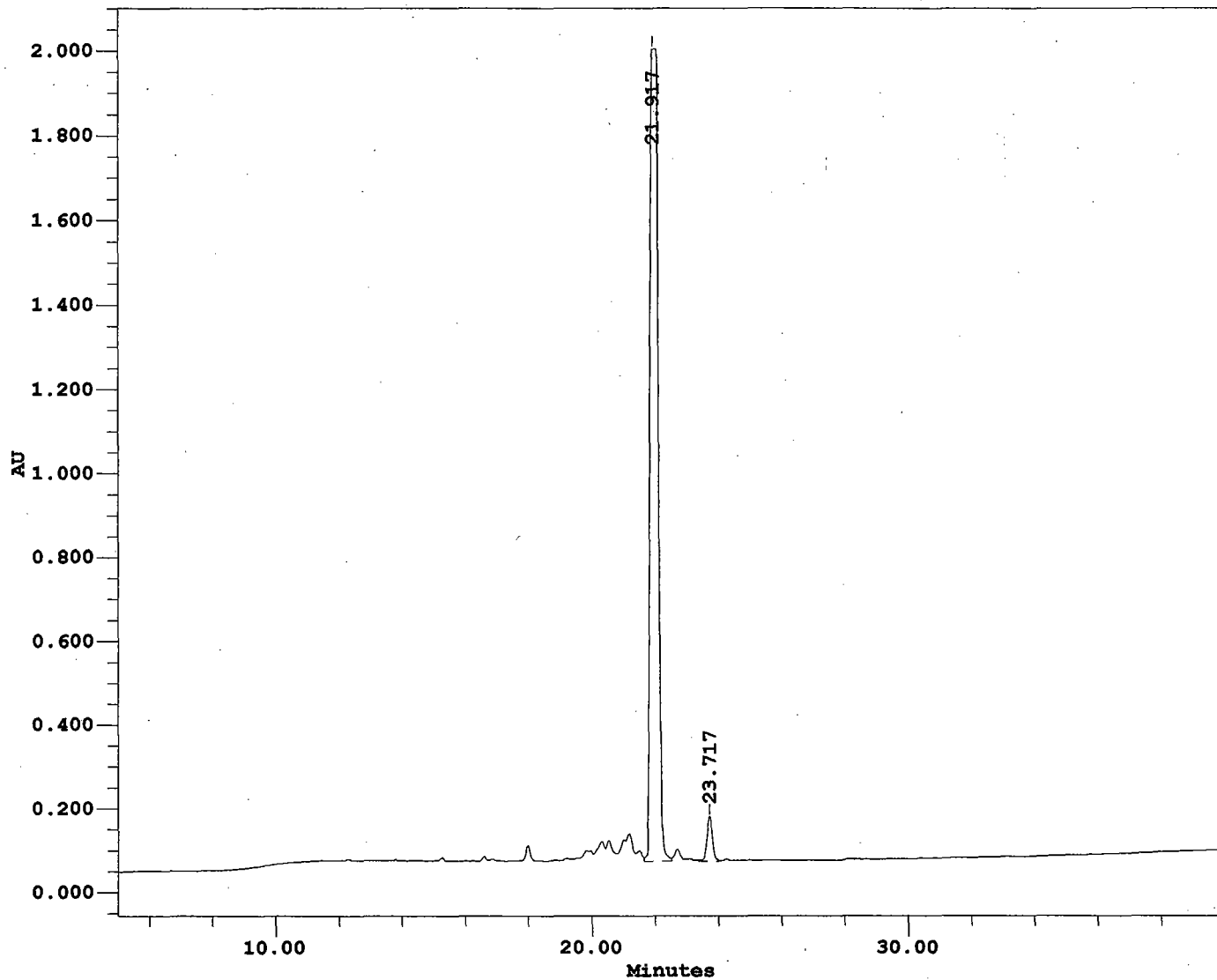
Volume: 10

Date Acquired: 03/10/98 01:51:40 PM

Vial 2

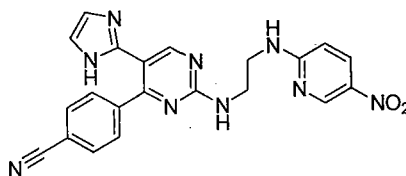
Channel Descr. 220 nm

Acq Meth Set: 5100_220



Peak Results

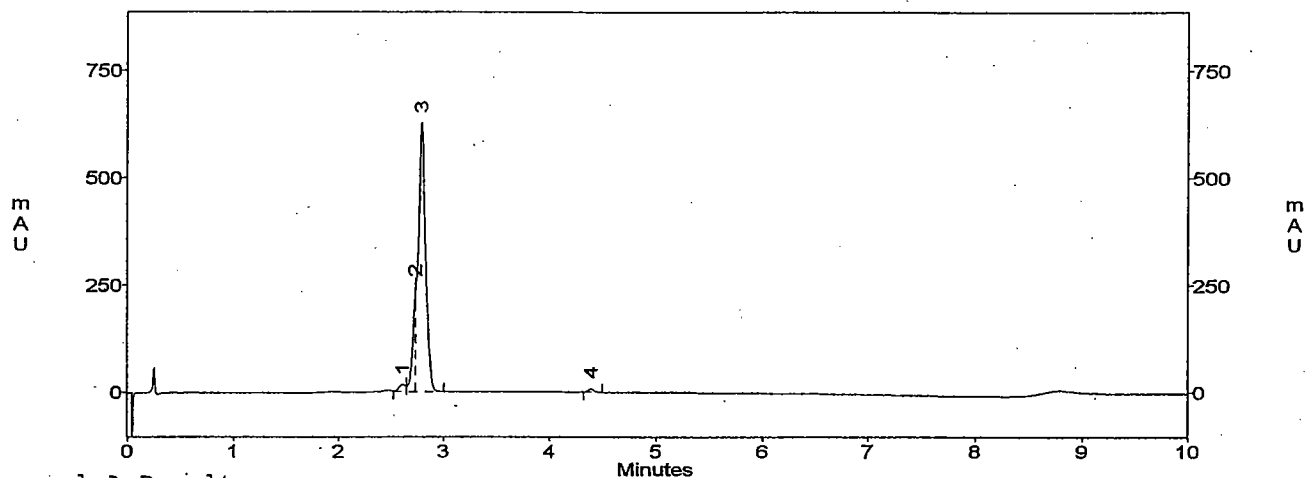
#	Name	Ret Time (min)	Start Time (min)	End Time (min)	% Height	% Area
1		21.917	21.650	22.500	94.83	96.44
2		23.717	23.350	24.067	5.17	3.56



35a

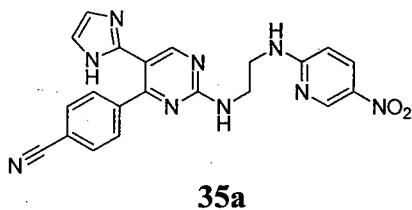
File : c:\ezchrom2\chrom\1998-03\Az51f2qc.ez2
Method : c:\ezchrom2\methods\200ul.met\M06m595w.met
Sample ID : mg2-10ul
Acquired : Mar 03, 1998 13:49:41

c:\ezchrom2\chrom\1998-03\Az51f2qc.ez2 -- Channel A



Channel A Results

Peak	Time	Area	Area %	Height	Height %
1	2.62	74761	2.1	16653	1.9
2	2.74	437060	12.5	244865	27.3
3	2.79	2940904	84.4	626083	69.9
4	4.39	31136	0.9	7848	0.9
Totals :		3483861	100.0	895449	100.0

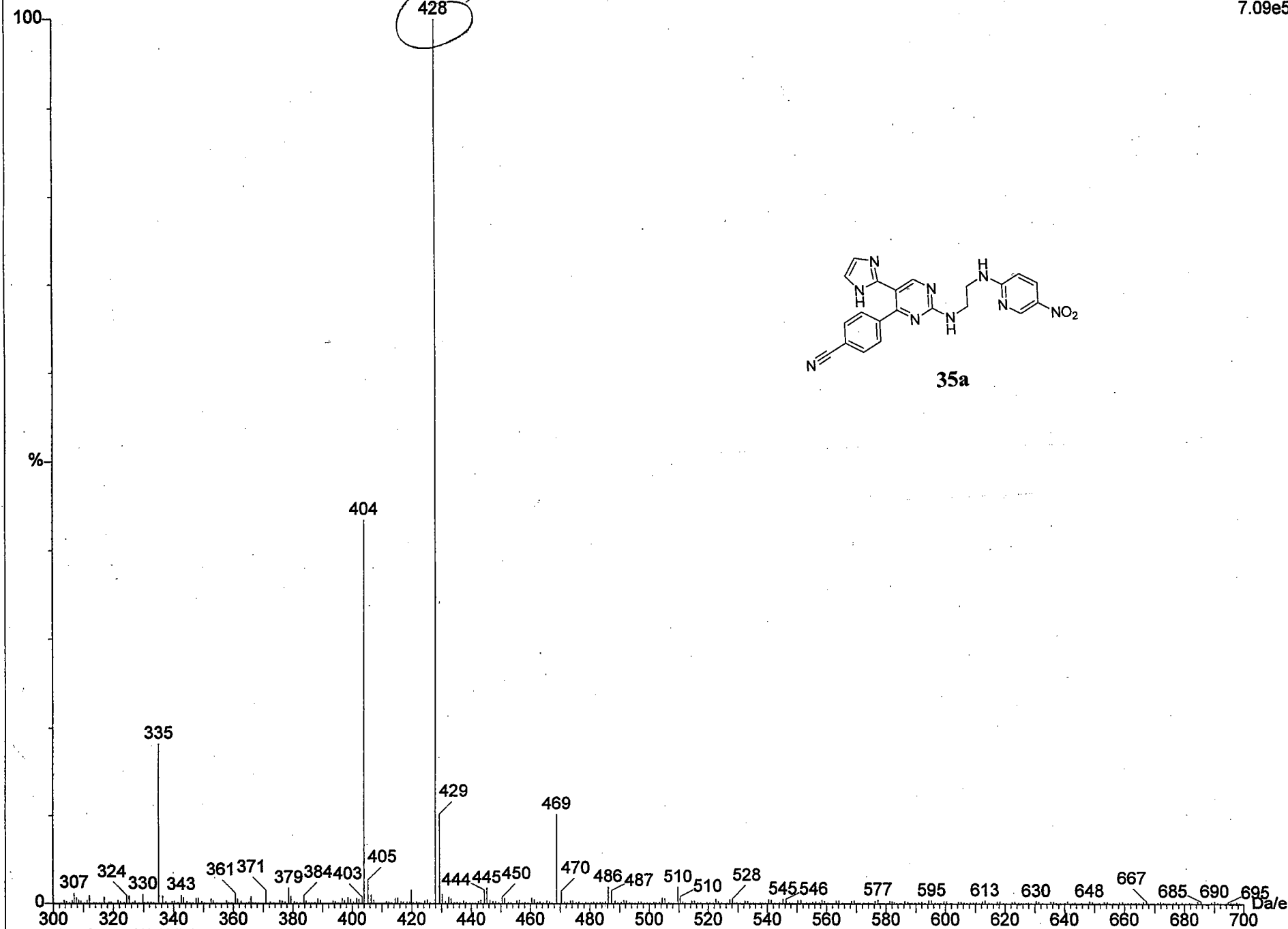


427, 50UL

AZ51F2QC 36 (1.285) Cm (34:37)

04-Mar-1998

Scan ES+
7.09e5



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Relax. delay 1.000 sec

Pulse 37.5 degrees

Acq. time 1.998 sec

Width 4500.5 Hz

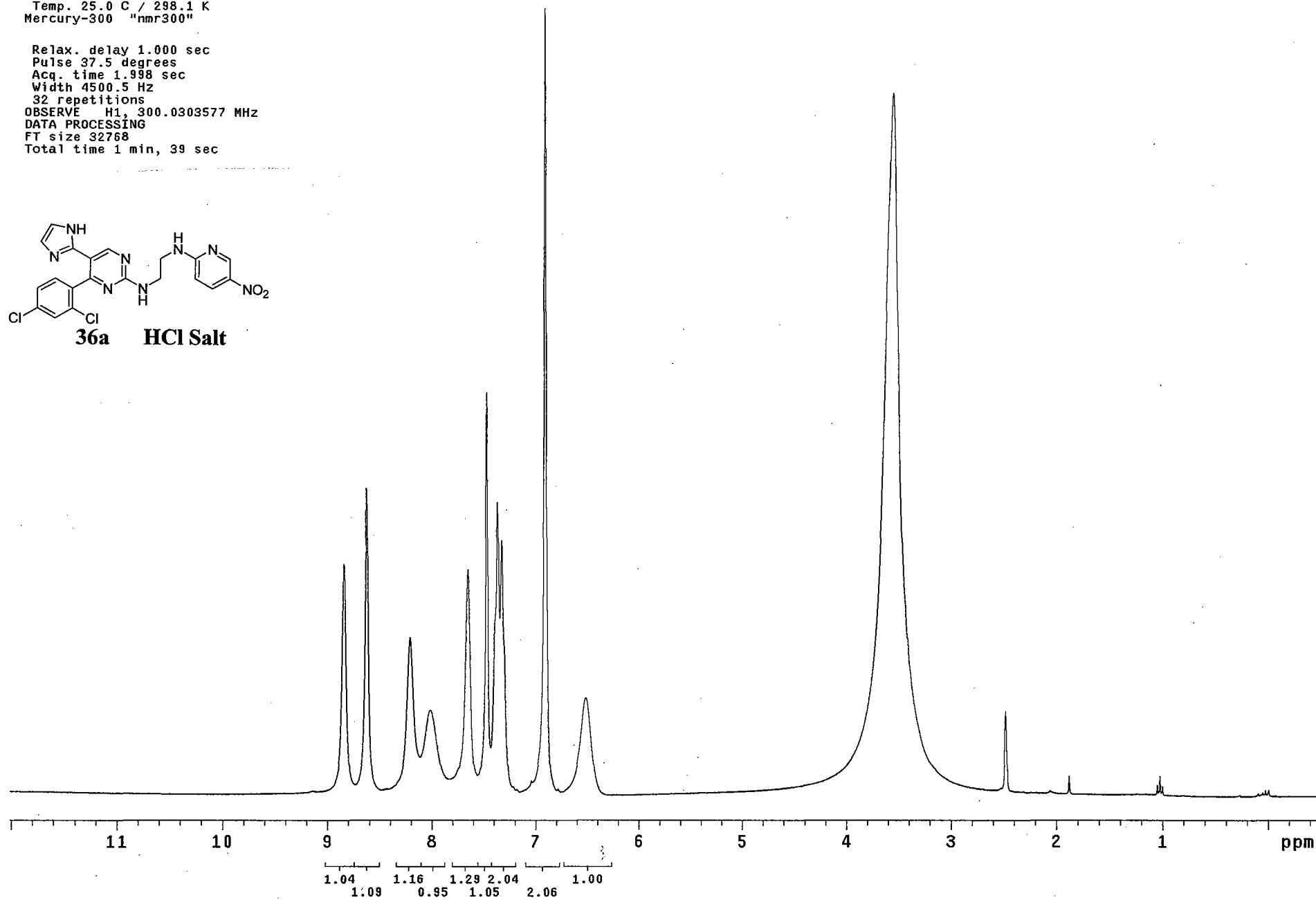
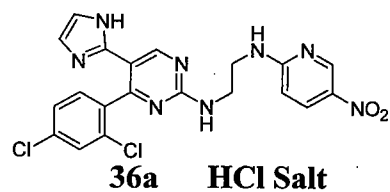
32 repetitions

OBSERVE H1, 300.0303577 MHz

DATA PROCESSING

FT size 32768

Total time 1 min, 39 sec



13C OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Pulse 54.2 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

1776 repetitions

OBSERVE C13, 75.4427150 MHz

DECOUPLE H1, 300.0318890 MHz

Power 45 dB

continuously on

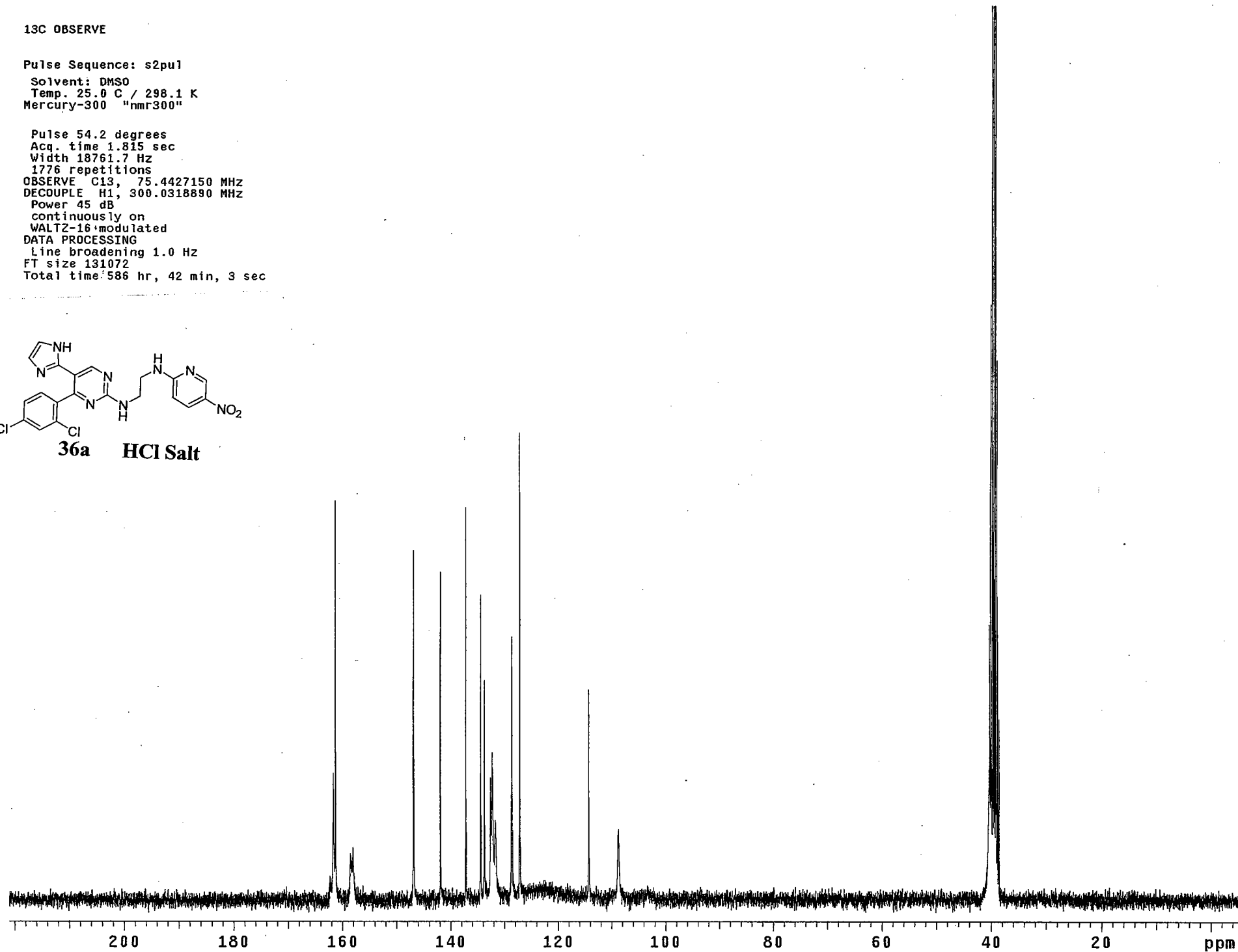
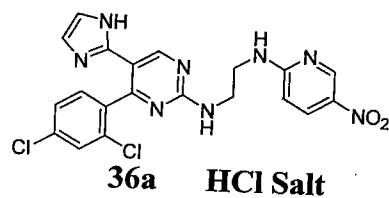
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 586 hr, 42 min, 3 sec



SampleName kpc90prod

Injection Volume 20.00 ul

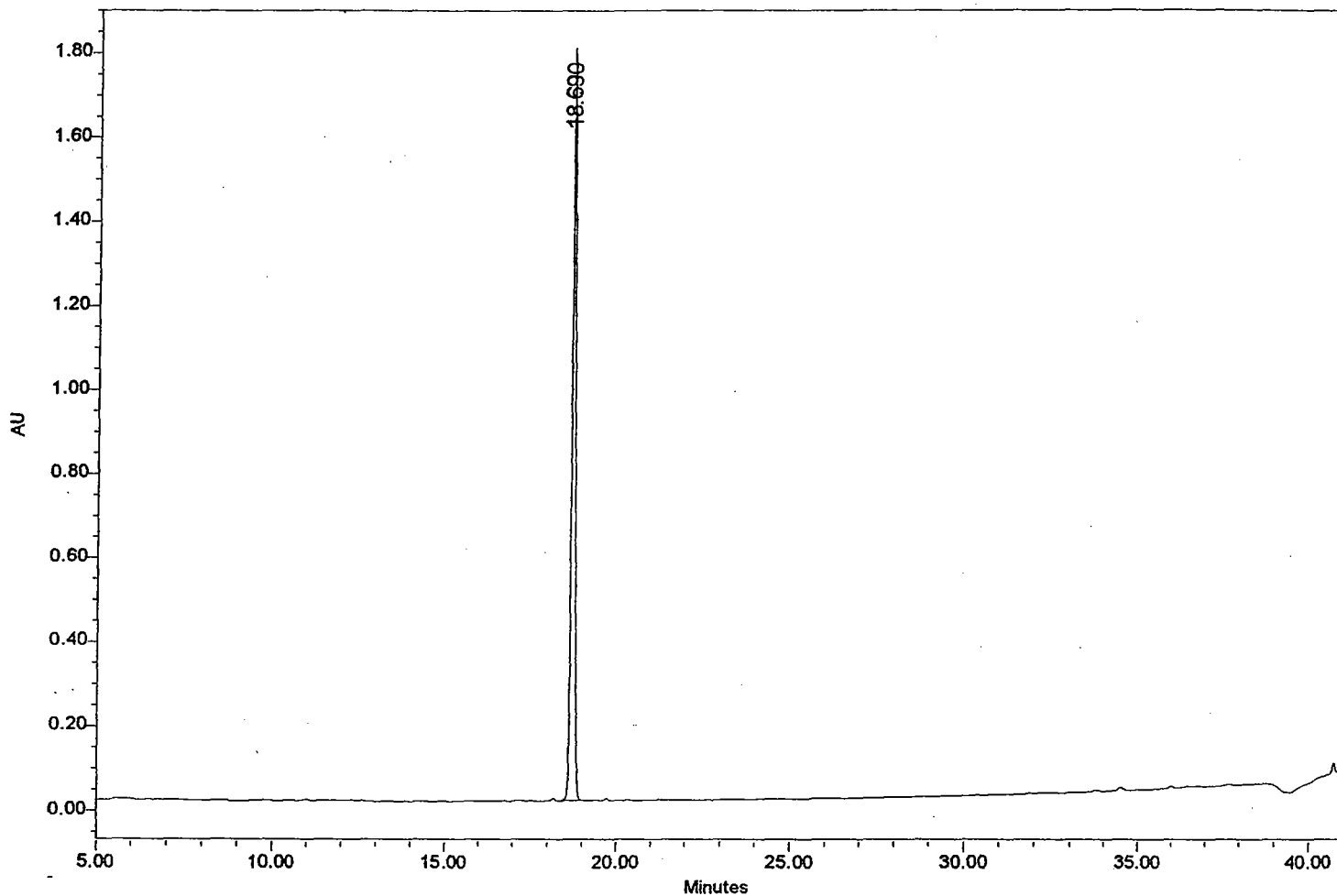
Date Acquired 1/18/99 7:42:07 PM

Vial 11

Channel Description FDA 220.0 nm

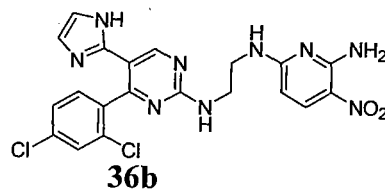
Acq Method Set 5100

Auto-Scaled Chromatogram



Peak Results

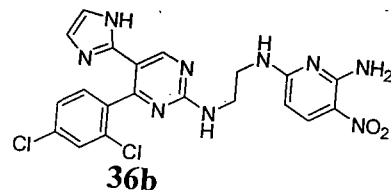
	RT	Start Time	End Time	% Height	% Area
1	18.690	18.317	19.200	100.00	100.00



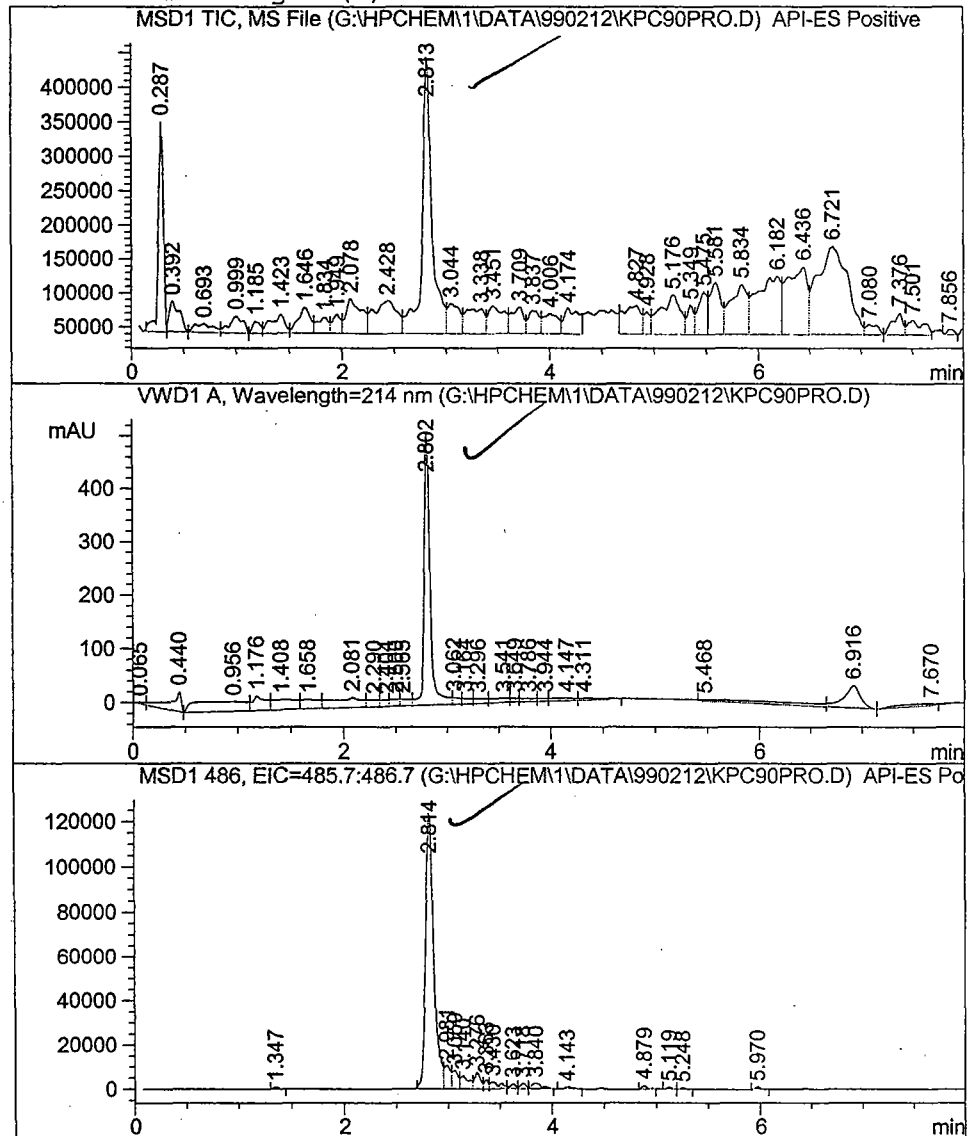
Print of all graphic windows

=====

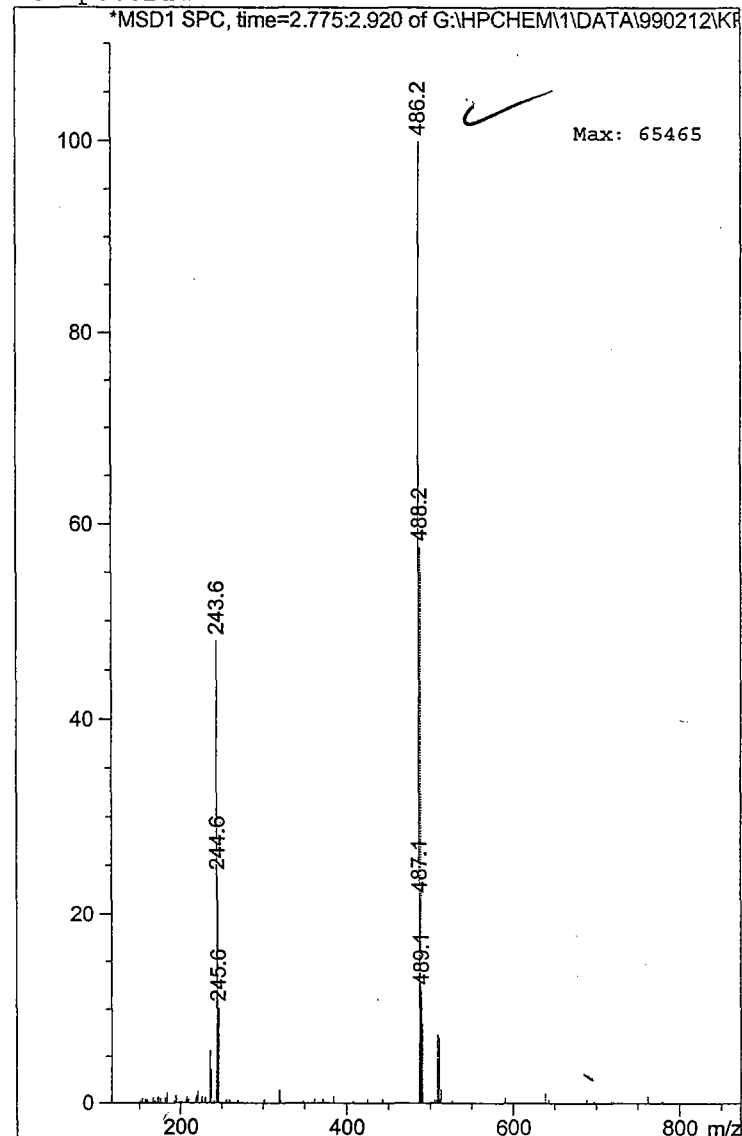
Injection Date	: 2/12/99 11:36:04 AM	Seq. Line	: 16
Sample Name	: kpc90prod	Vial	: 16
Acq. Operator	: ntg	Inj	: 1
		Inj Volume	: Inj prog
Acq. Method	: C:\HPCHEM\1\METHODS\POS_MODE.M		
Last changed	: 9/17/98 11:16:18 AM by ntg		
Analysis Method	: C:\HPCHEM\1\METHODS\ALICE.M		
Last changed	: 2/12/99 5:38:08 PM		
	(modified after loading)		



Current Chromatogram(s)



MS Spectrum

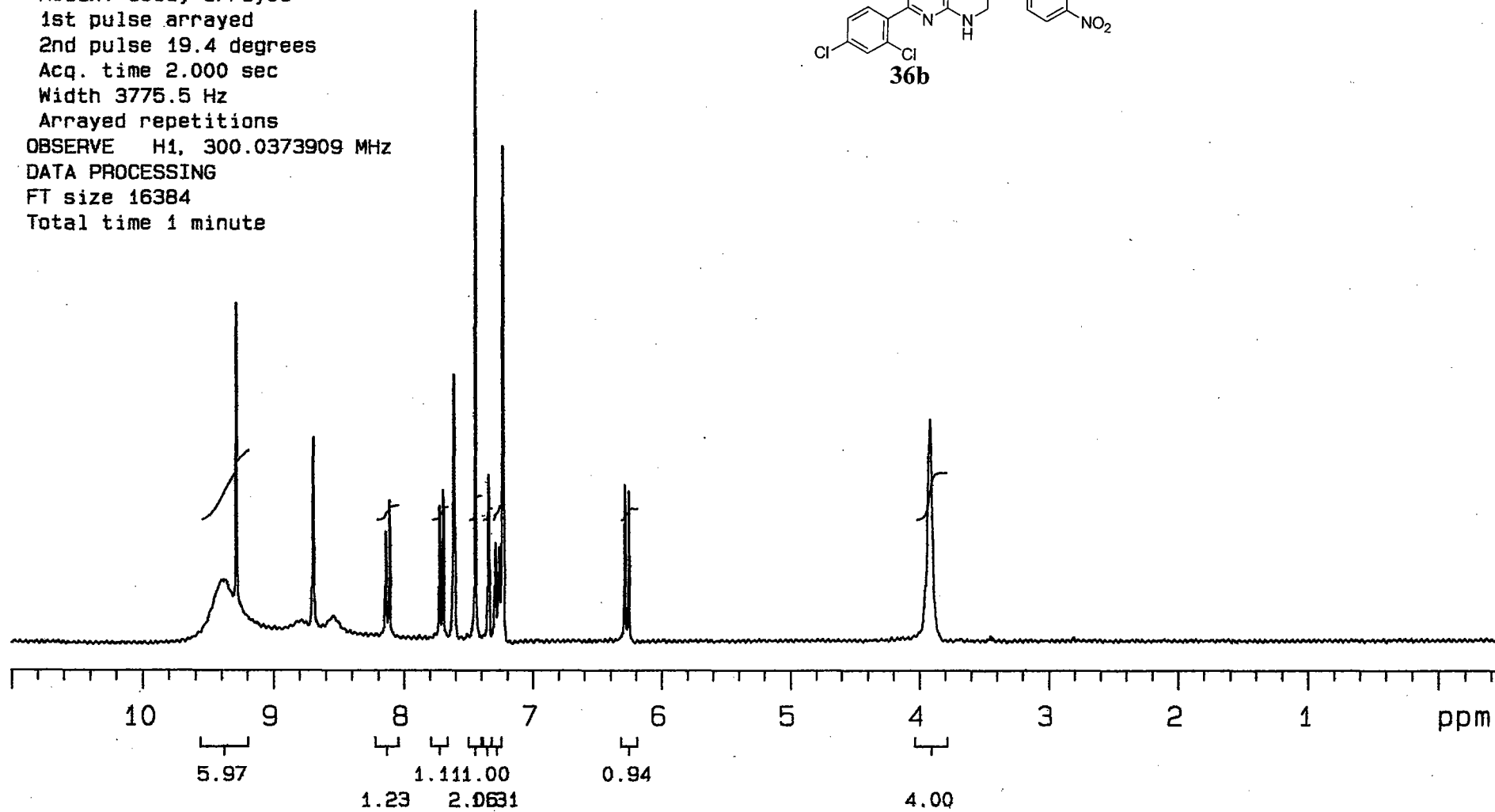
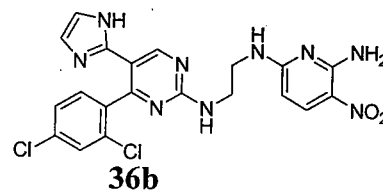


STANDARD 1H OBSERVE

Solvent: CDCl₃
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 19.4 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.0373909 MHz
DATA PROCESSING
FT size 16384
Total time 1 minute

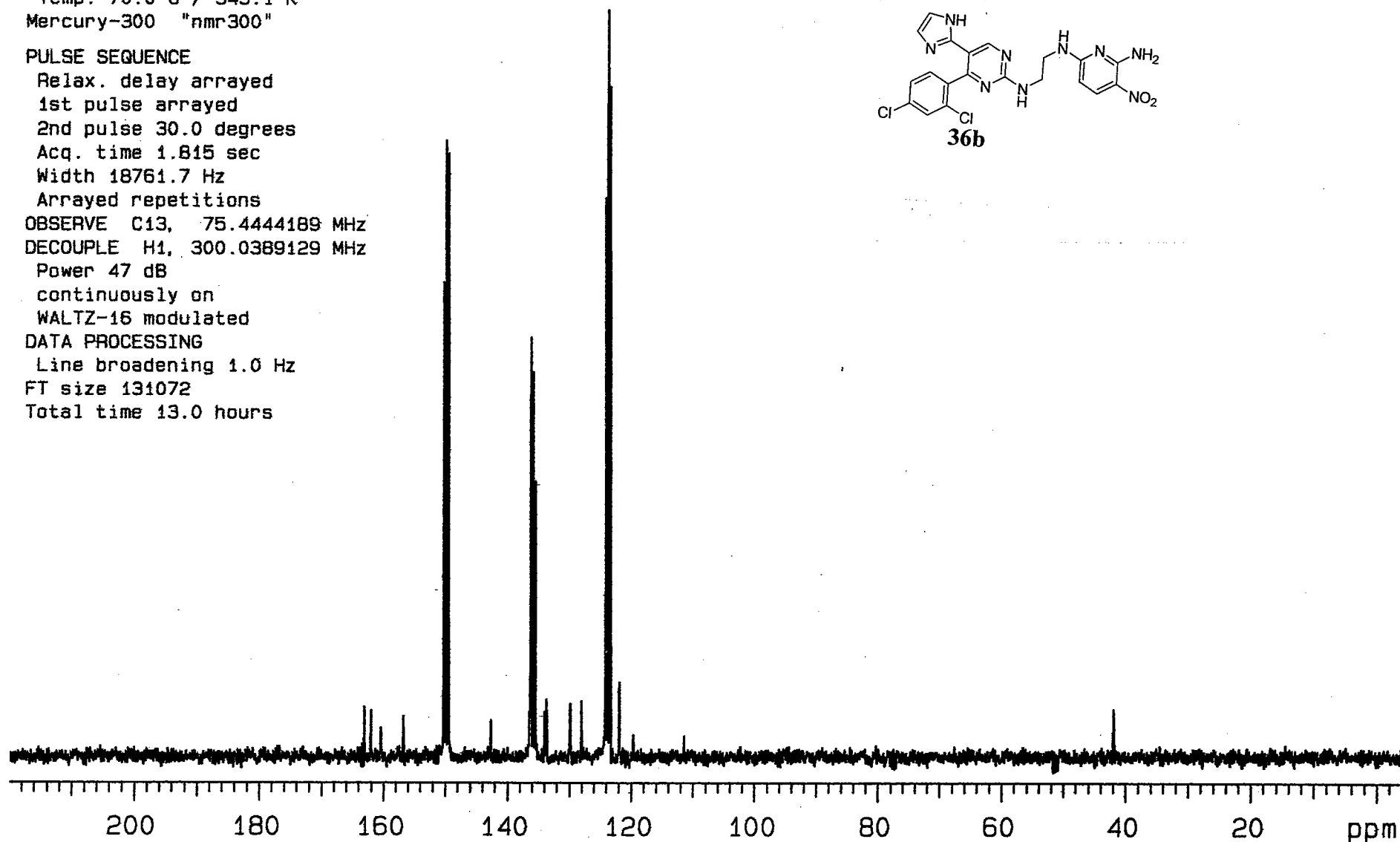
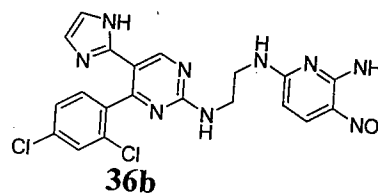


13C OBSERVE

Solvent: CDC13
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 30.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
Arrayed repetitions
OBSERVE C13, 75.4444189 MHz
DECOUPLE H1, 300.0389129 MHz
Power 47 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 13.0 hours

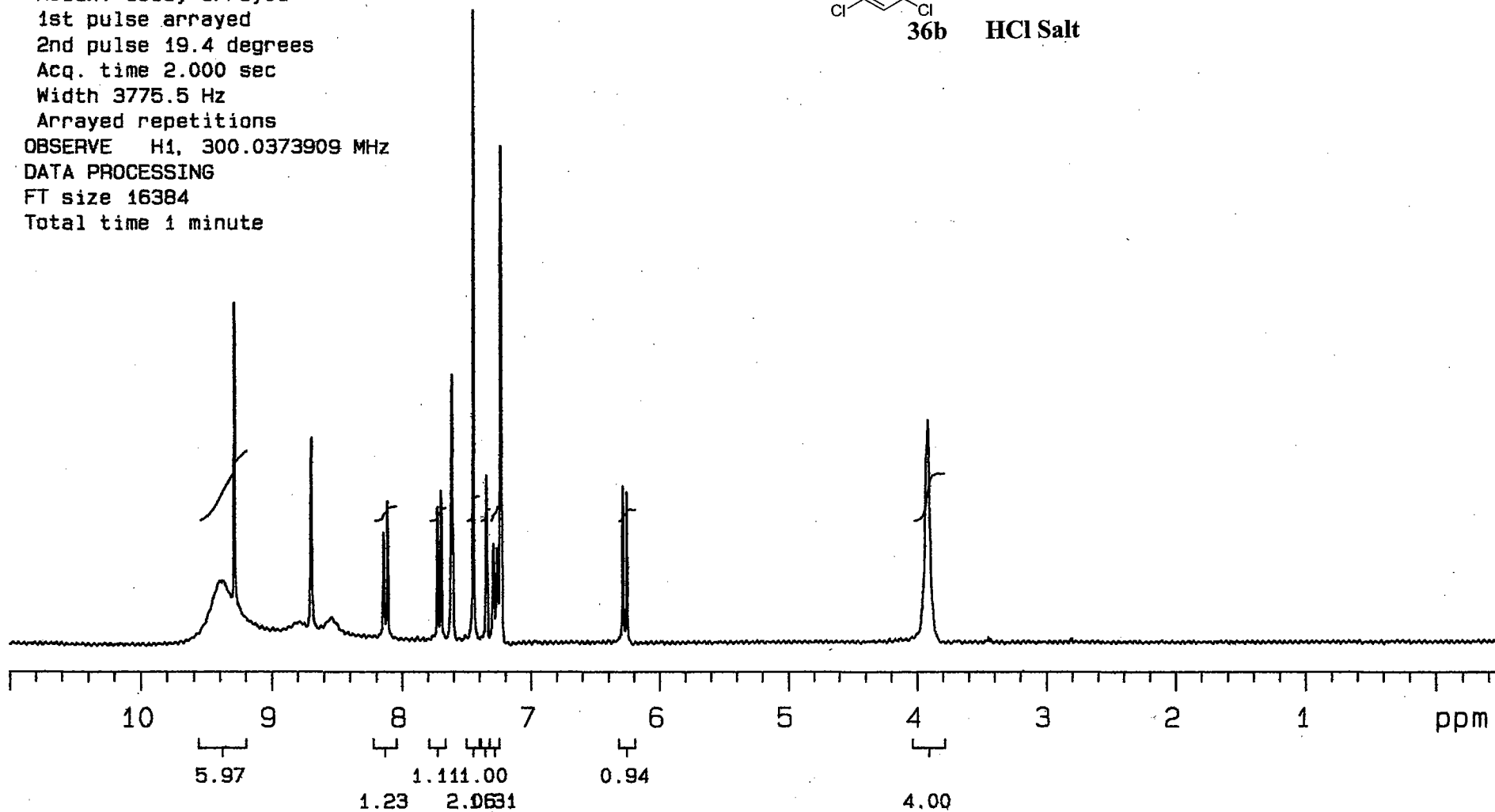
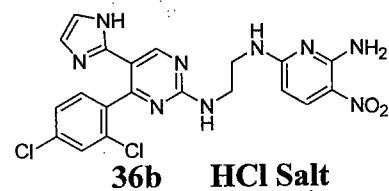


STANDARD 1H OBSERVE

Solvent: CDCl3
Temp. 70.0 C / 343.1 K
Mercury-300 "nmr300"

PULSE SEQUENCE

Relax. delay arrayed
1st pulse arrayed
2nd pulse 19.4 degrees
Acq. time 2.000 sec
Width 3775.5 Hz
Arrayed repetitions
OBSERVE H1, 300.0373909 MHz
DATA PROCESSING
FT size 16384
Total time 1 minute

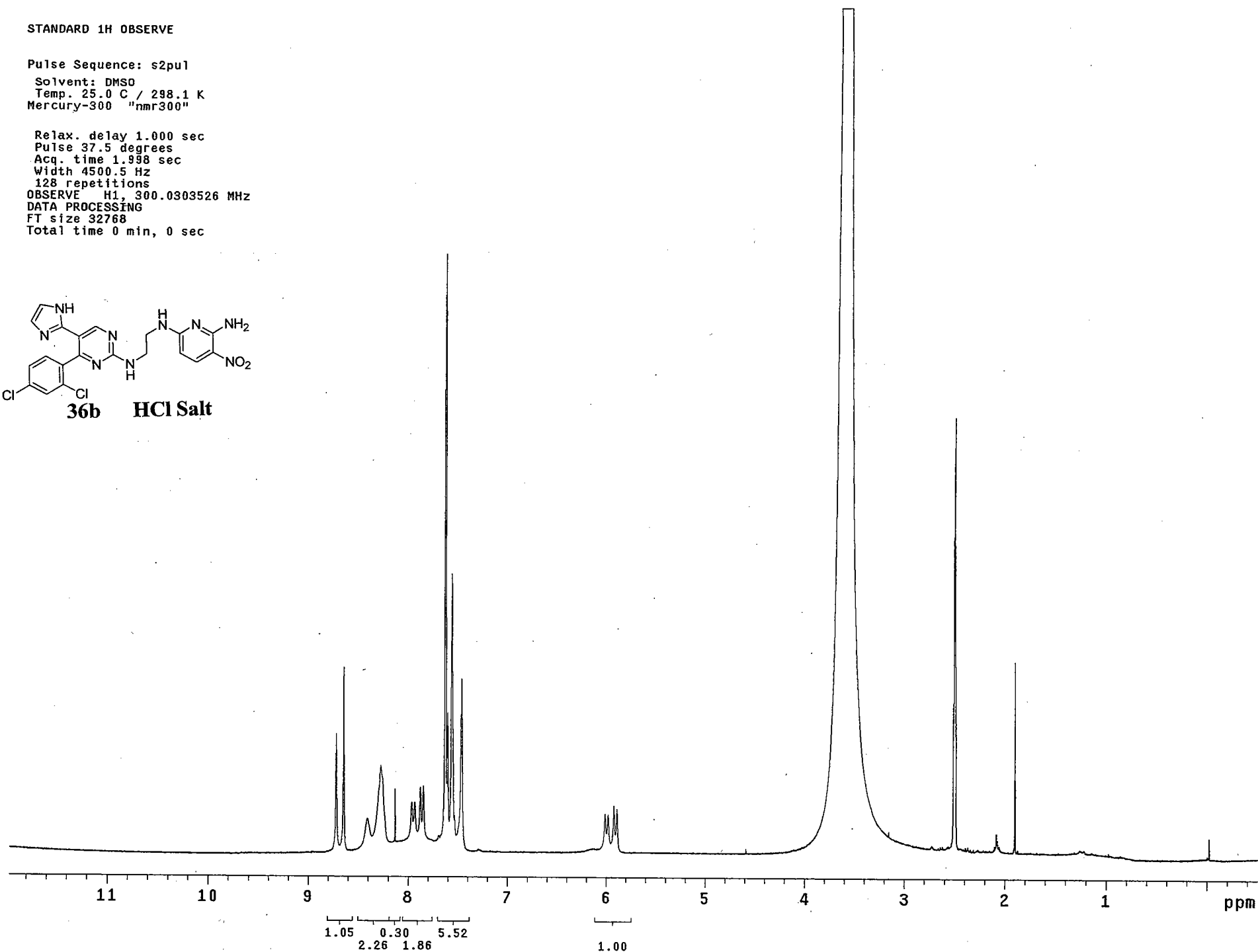
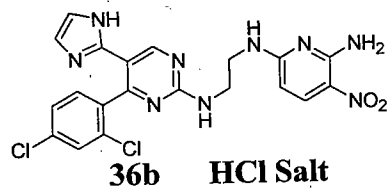


STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 25.0 C / 298.1 K
Mercury-300 "nmr300"

Relax. delay 1.000 sec
Pulse 37.5 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
128 repetitions
OBSERVE H1, 300.0303526 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Relax. delay 1.000 sec

Pulse 37.5 degrees

Acq. time 1.998 sec

Width 4500.5 Hz

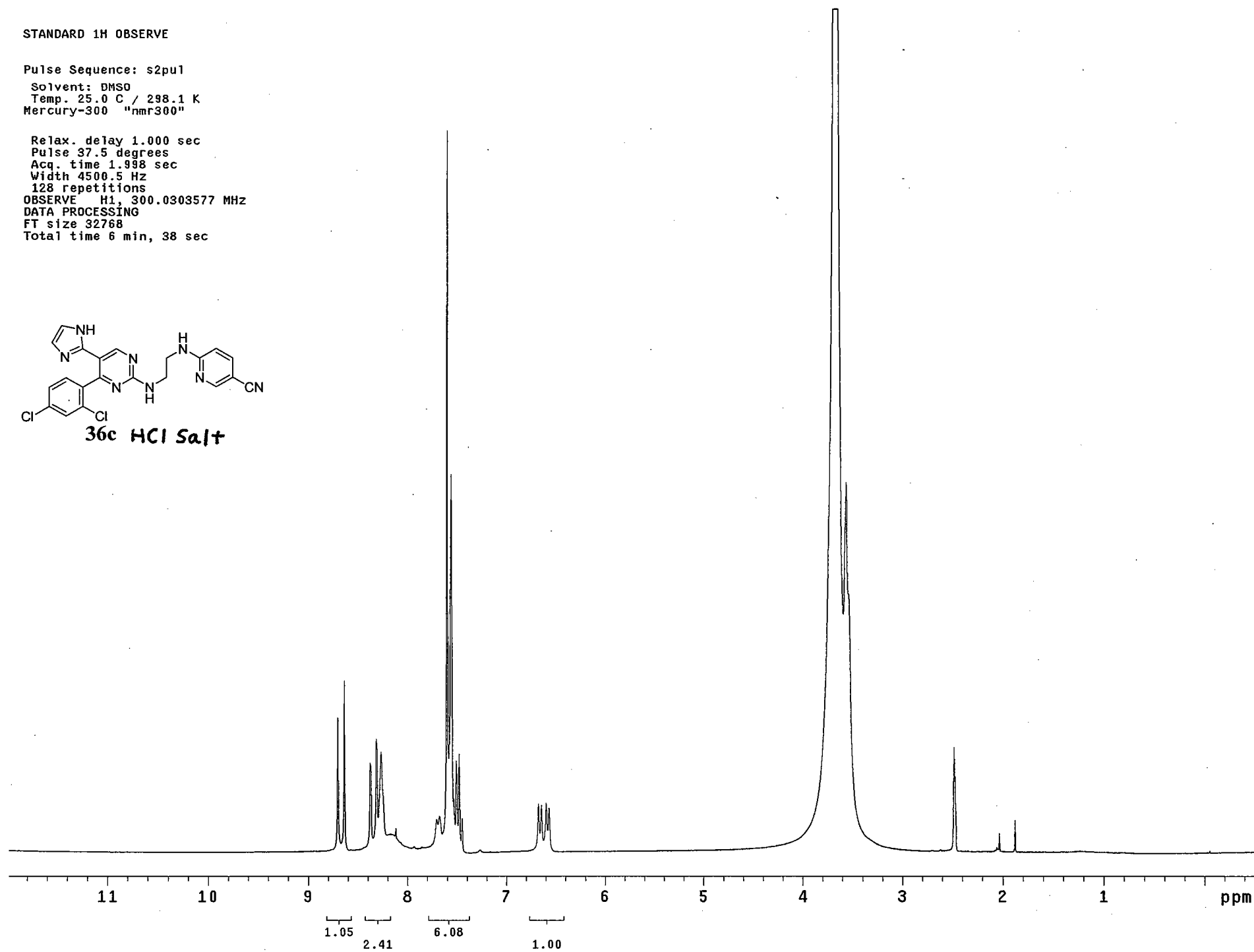
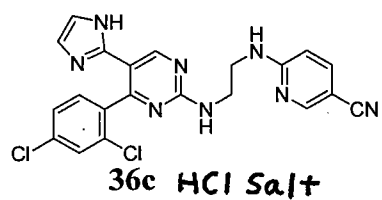
128 repetitions

OBSERVE H1, 300.0303577 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 38 sec



13C OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Pulse 54.2 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

20992 repetitions

OBSERVE C13, 75.4427164 MHz

DECOUPLE H1, 300.0318890 MHz

Power 45 dB

continuously on

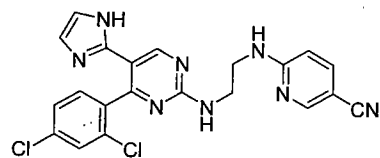
WALTZ-16 modulated

DATA PROCESSING

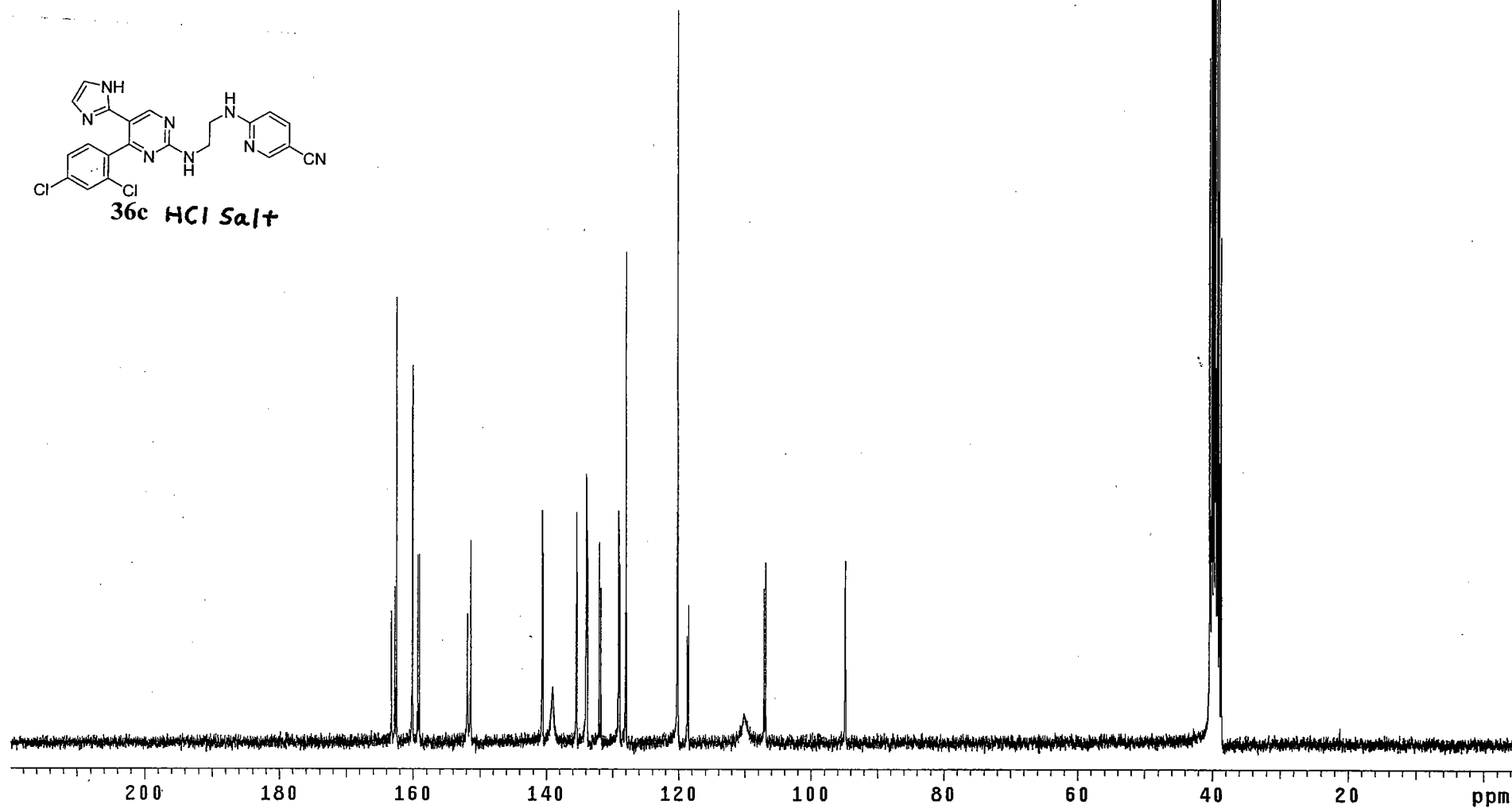
Line broadening 1.0 Hz

FT size 131072

Total time 586 hr, 42 min, 3 sec



36c HCl Salt

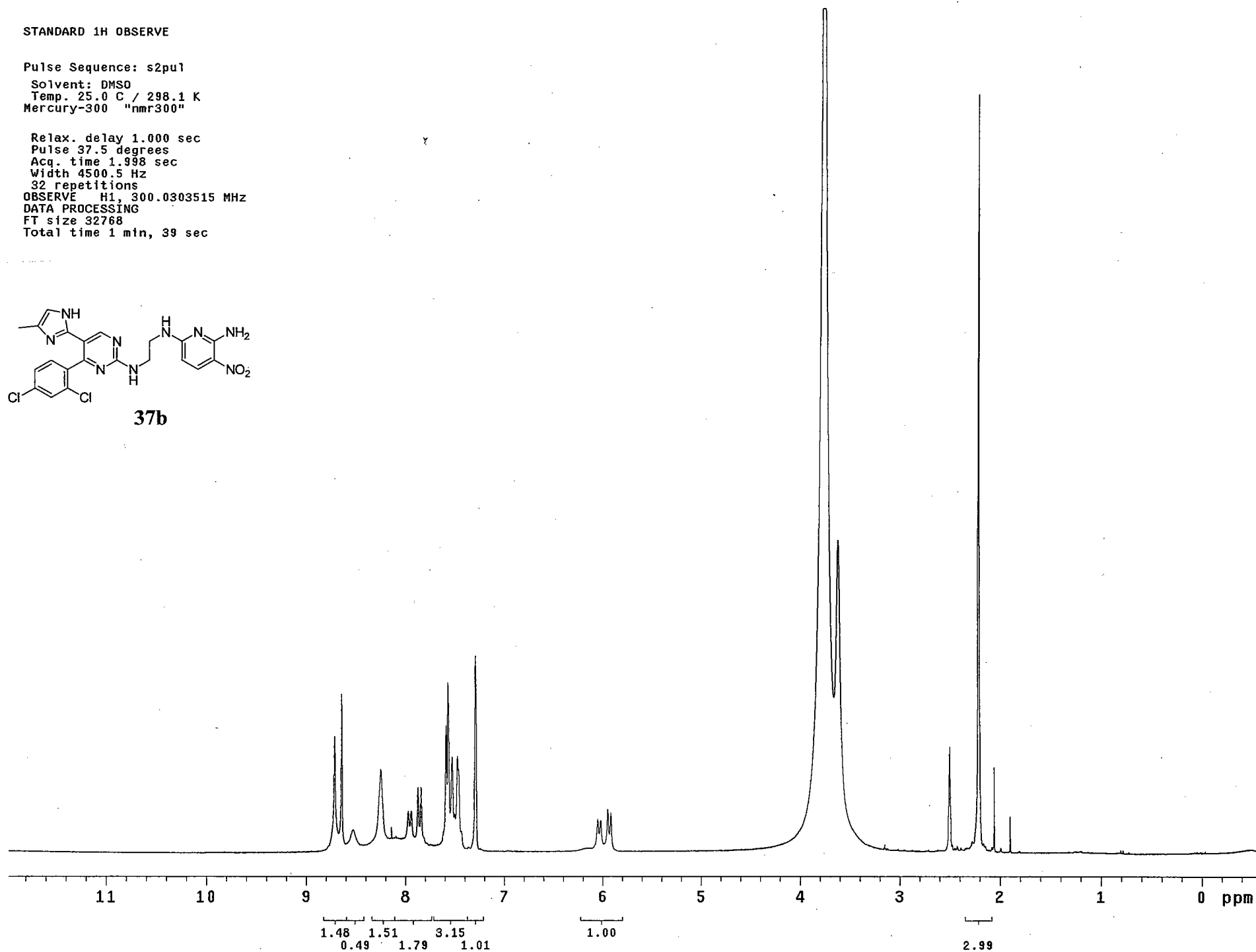
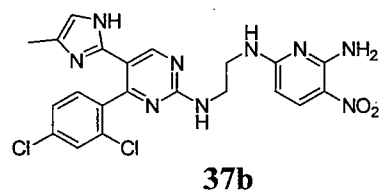


STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 25.0 C / 298.1 K
Mercury-300 "nmr300"

Relax. delay 1.000 sec
Pulse 37.5 degrees
Acq. time 1.998 sec
Width 4500.5 Hz
32 repetitions
OBSERVE H1, 300.0303515 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 39 sec



13C OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Pulse 54.2 degrees

Acq. time 1.815 sec

Width 18761.7 Hz

2000 repetitions

OBSERVE C13, 75.4426754 MHz

DECOUPLE H1, 300.0318890 MHz

Power 45 dB

continuously on

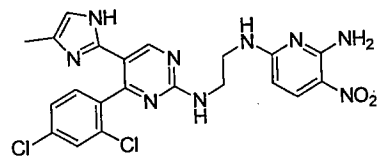
WALTZ-16 modulated

DATA PROCESSING

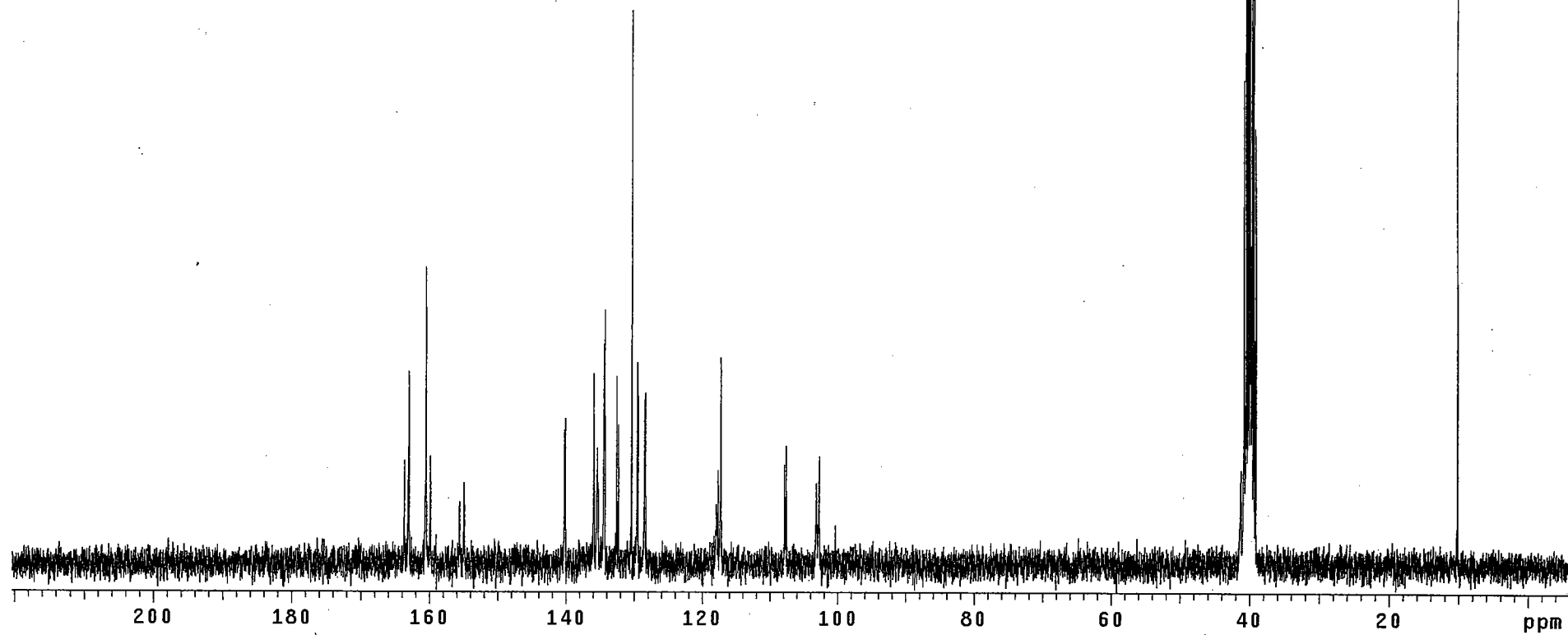
Line broadening 1.0 Hz

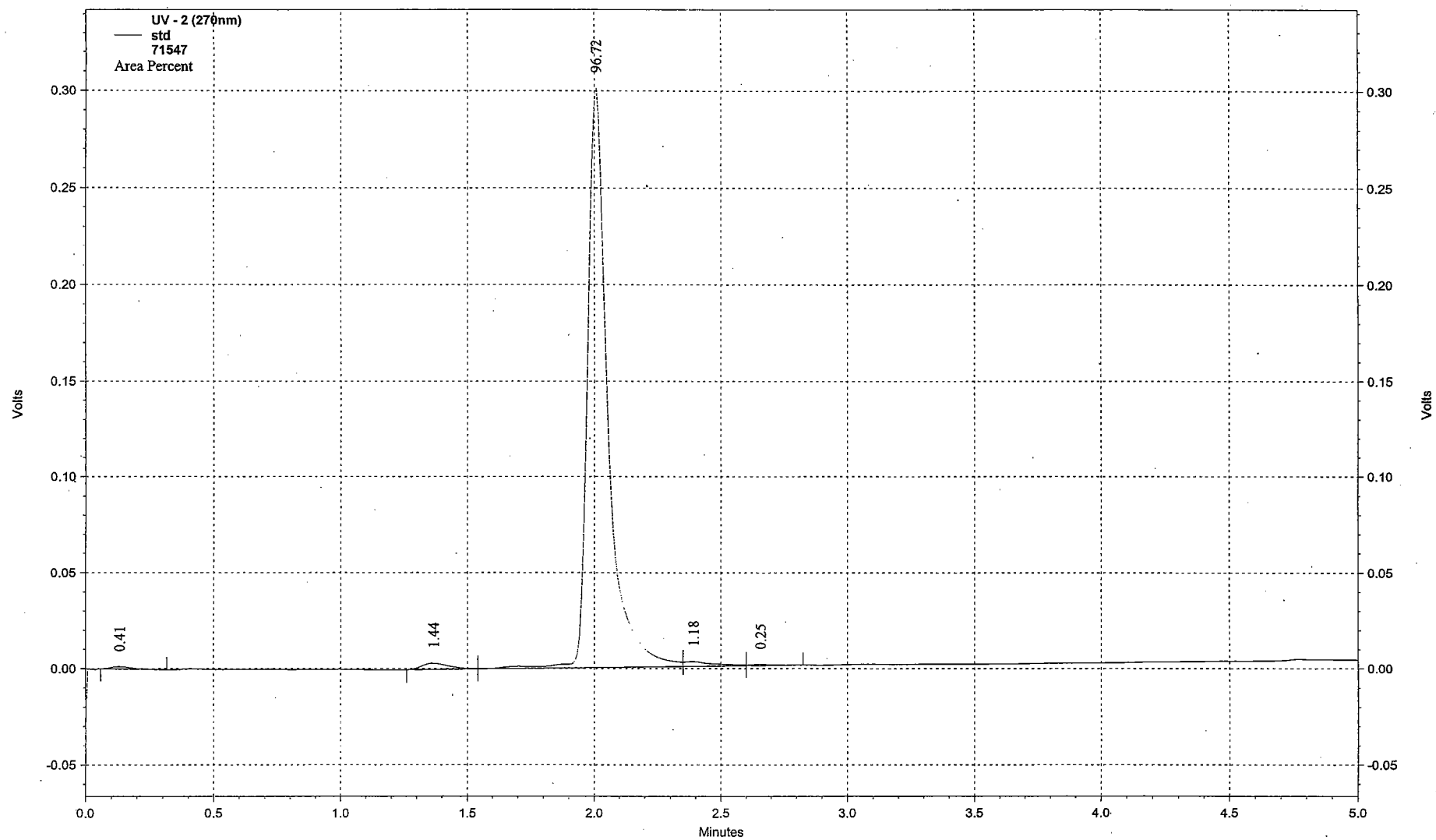
FT size 131072

Total time 5867 hr, 36 sec

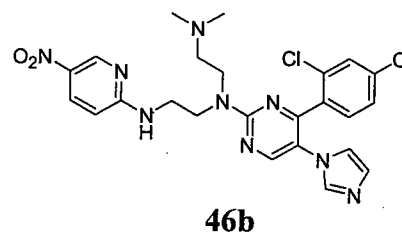


37b

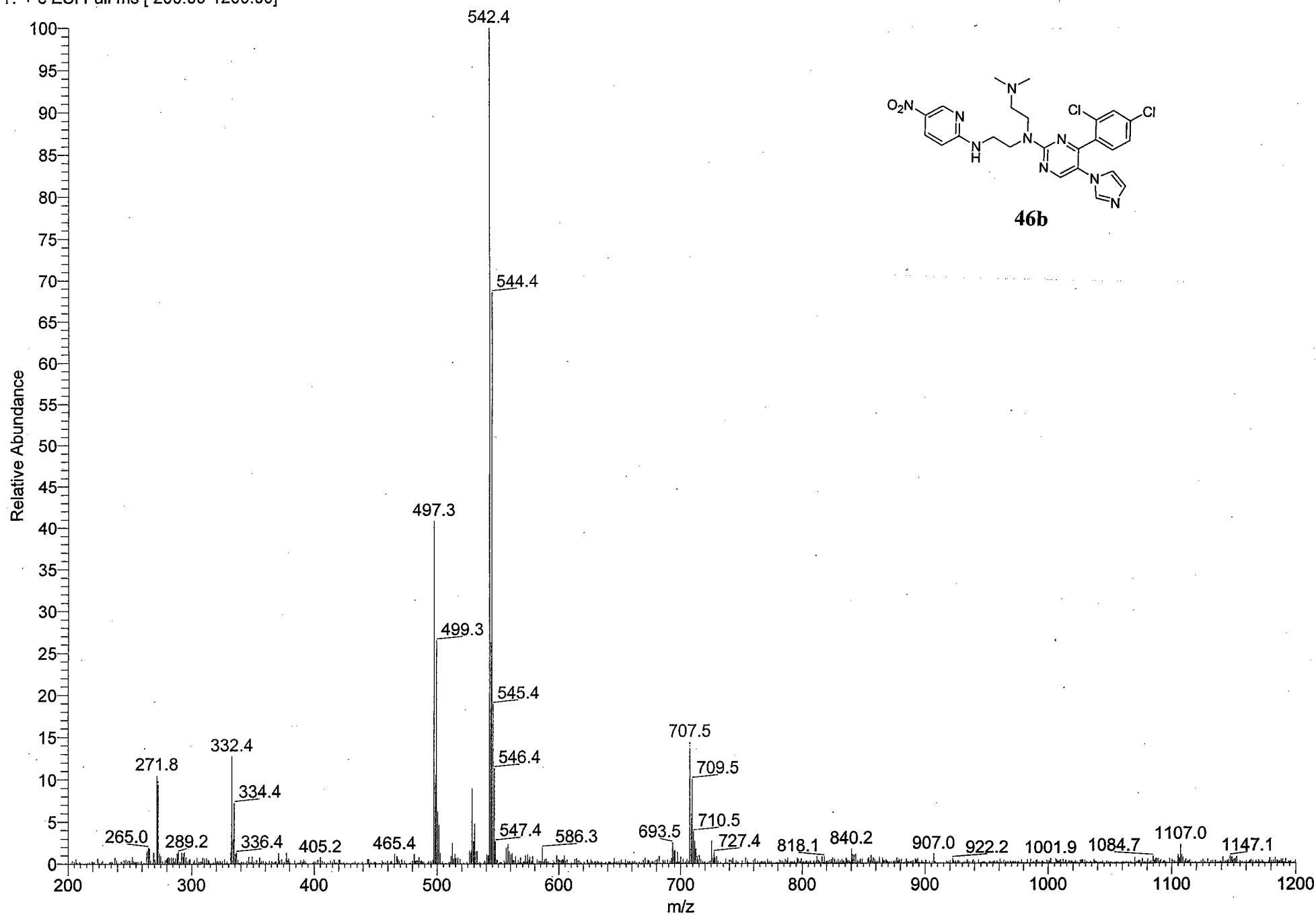




C:\Class-up\041203_ssRR\71547, UV - 2 (270nm)



71547_2 #125-130 RT: 3.17-3.29 AV: 6 NL: 1.10E6
T: + c ESI Full ms [200.00-1200.00]



CHIRON Technologies SMDR Medicinal & Organic Chemistry Group

Sample Name: ss73pu1.

System Name: Shana

Project Name: GSK4

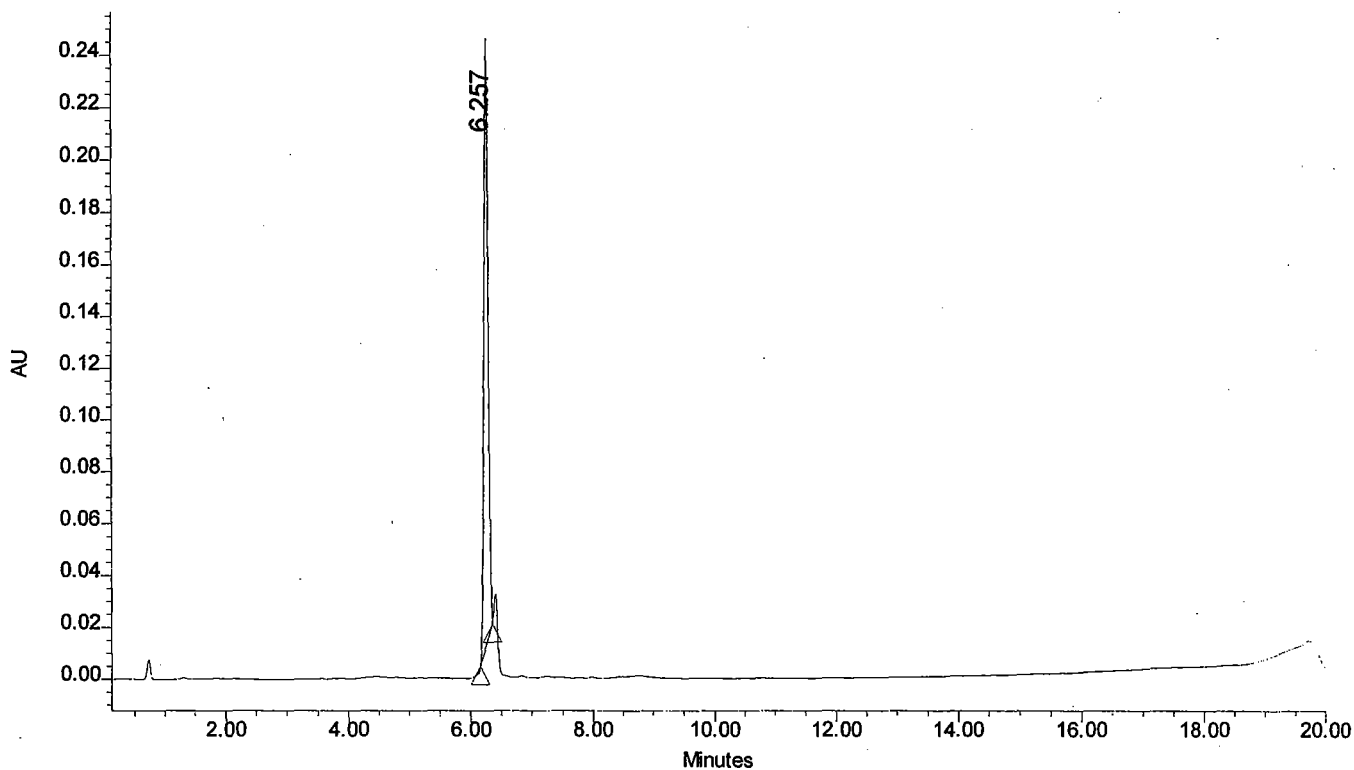
Label:

Acq Method Set: Rabbit20

Date Acquired: 2/3/2000 4:34:19 PM

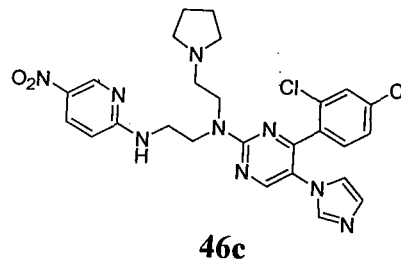
Injection Volume- 10.00 ul

Vial # 1



Peak Results

	Retention Time	Start Time	End Time	% Area
1	6.257	6.155	6.355	100.00

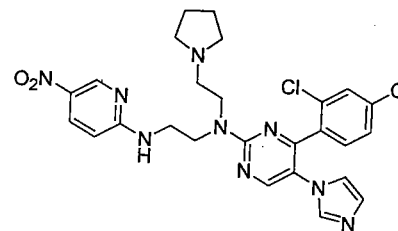


Print of all graphic windows

```

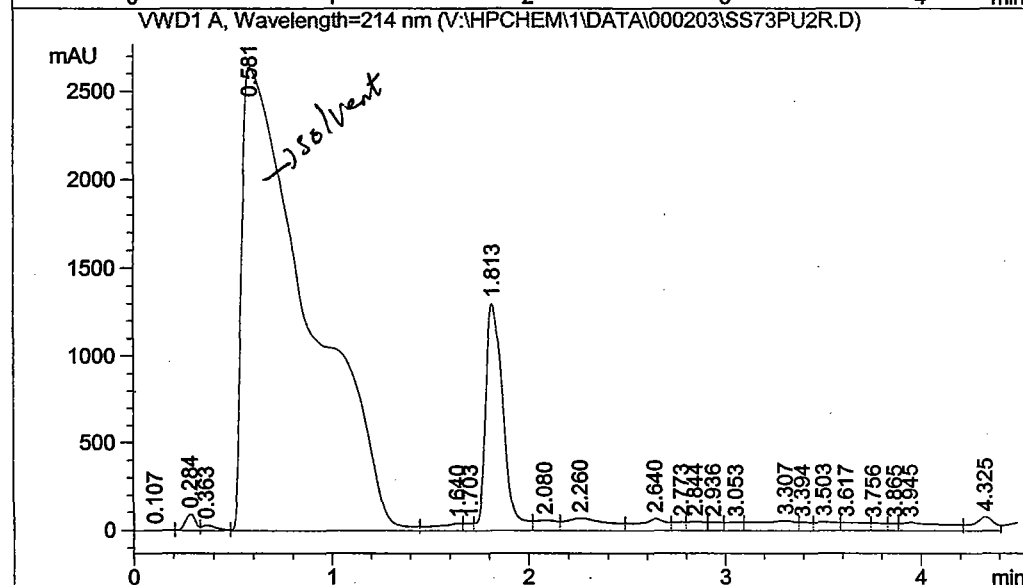
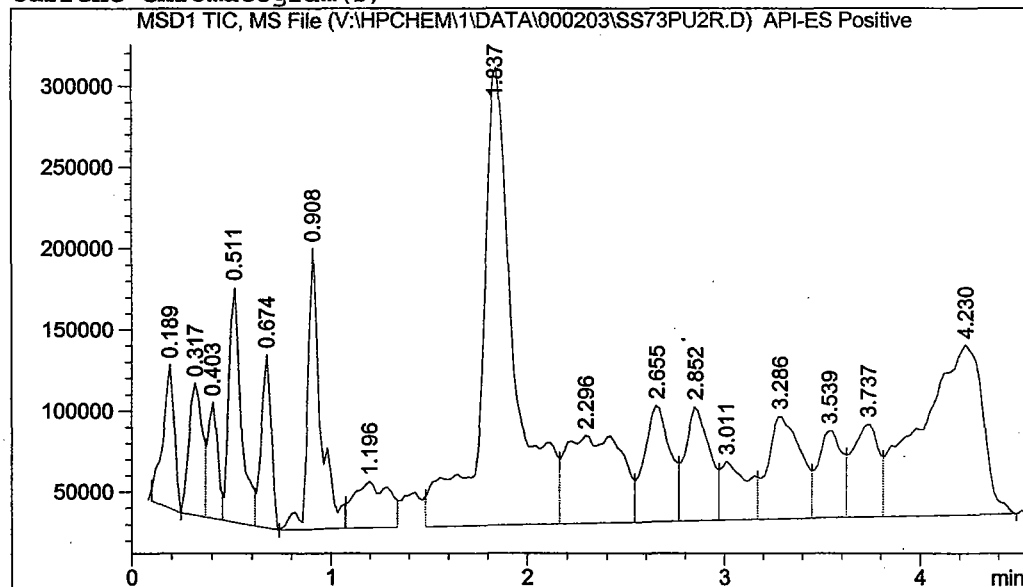
=====
Injection Date   : 2/3/00 4:51:19 PM      Seq. Line :    5
Sample Name     : SS73PU2R                Vial       :   55
Acq. Operator   : Manager                 Inj        :    1
                                           Inj Volume : Inj prog

Acq. Method     : C:\HPCHEM\1\METHODS\POS_MODE.M
Last changed    : 1/12/00 11:50:39 AM by Manager
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC1.M
Last changed    : 1/5/00 3:07:44 PM
    
```

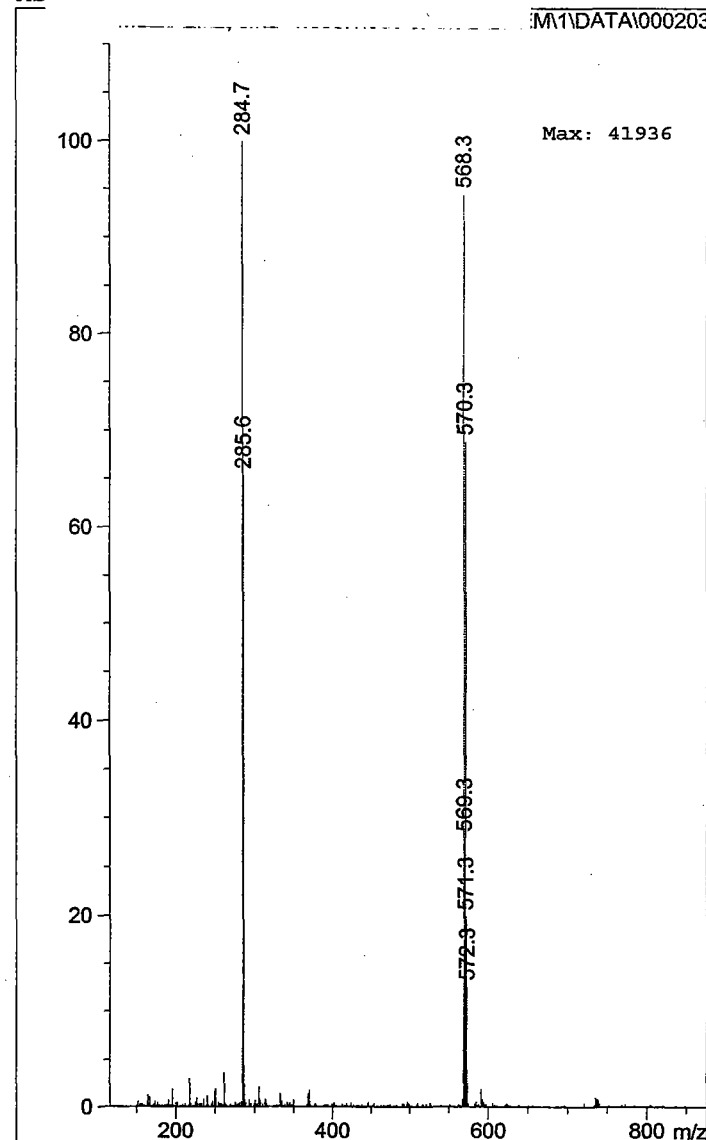


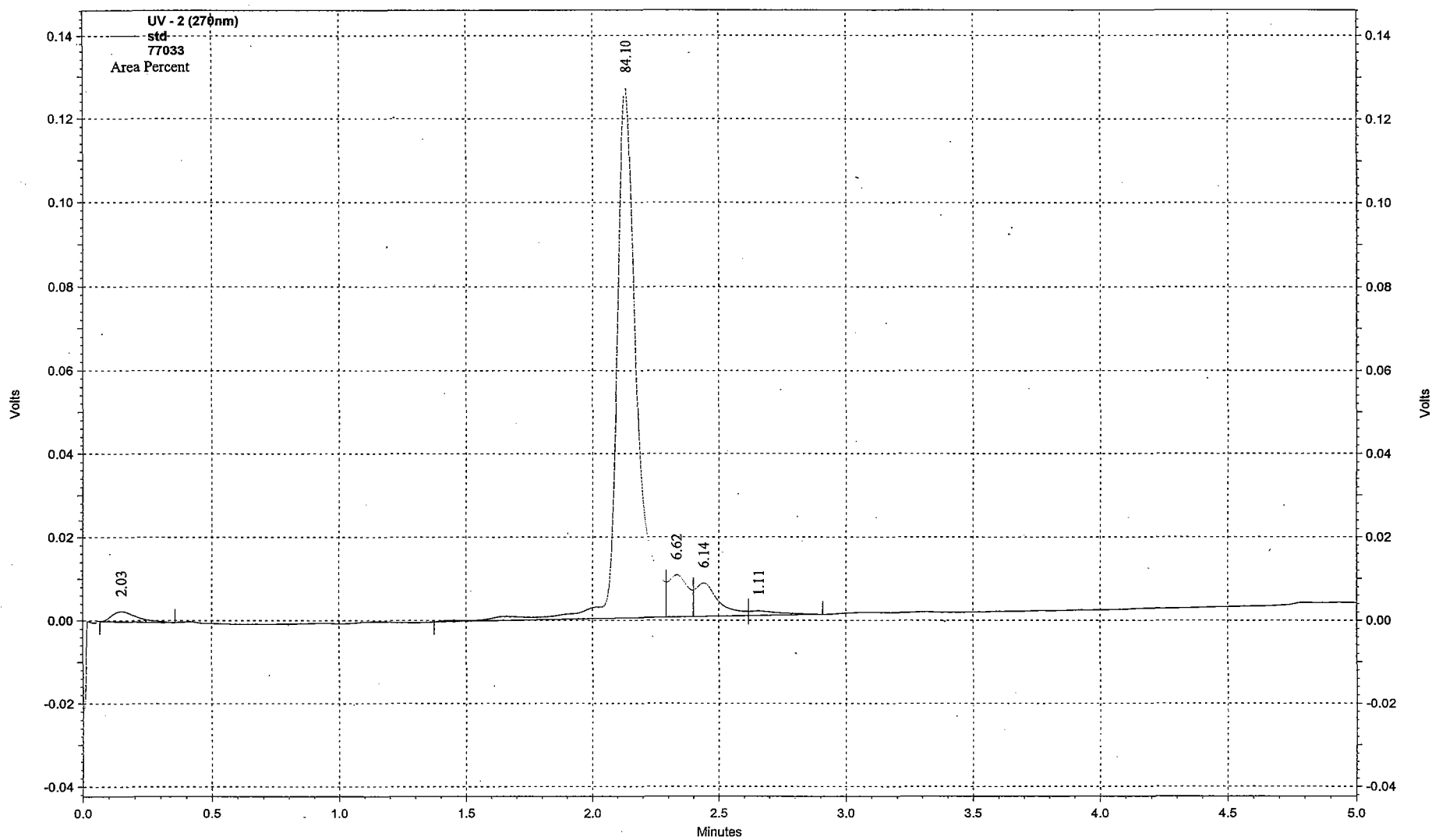
46c

Current Chromatogram(s)

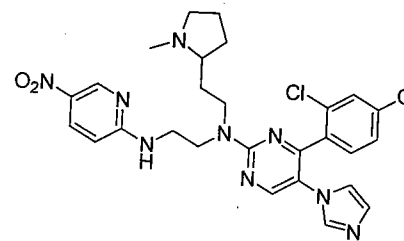


MS





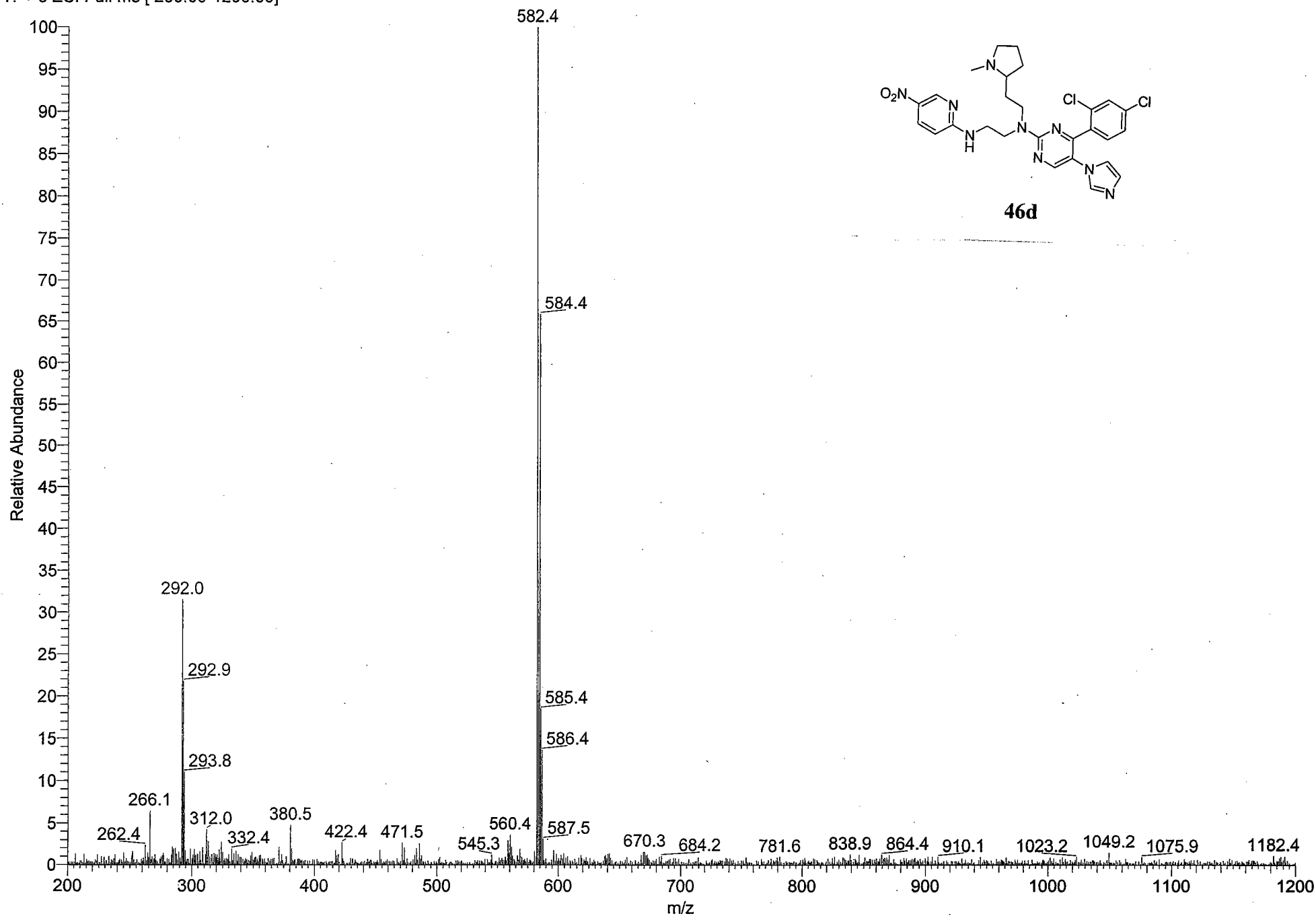
— C:\Class-up\041203_ssRR\77033, UV - 2 (270nm)

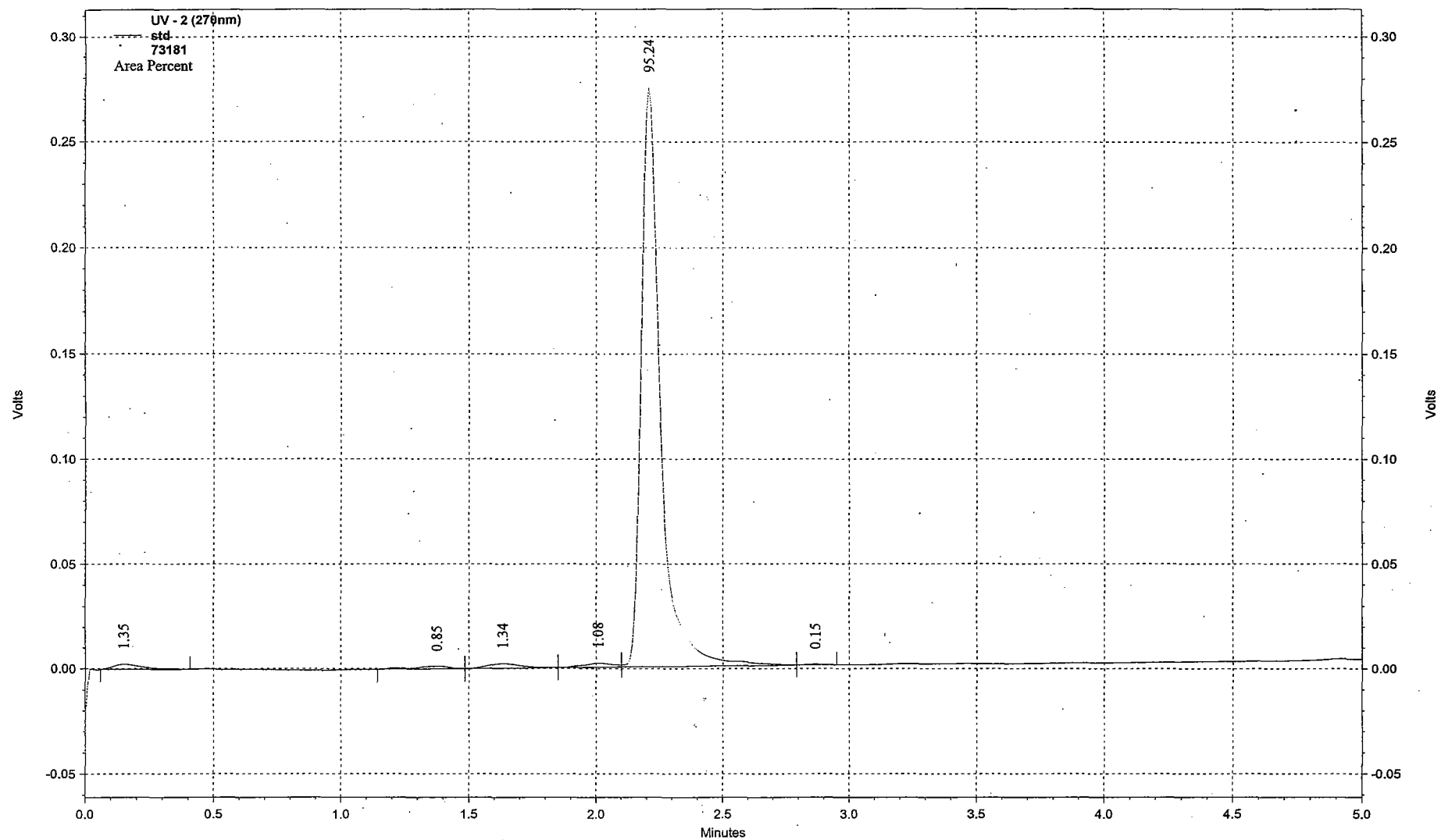


46d

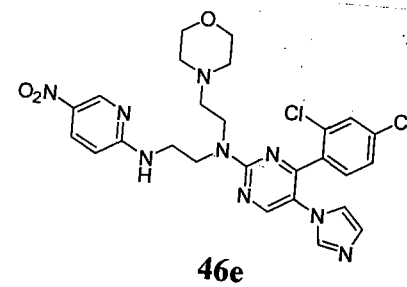
77033_1 #128-135 RT: 3.27-3.45 AV: 8 NL: 4.78E5

T: + c ESI Full ms [200.00-1200.00]



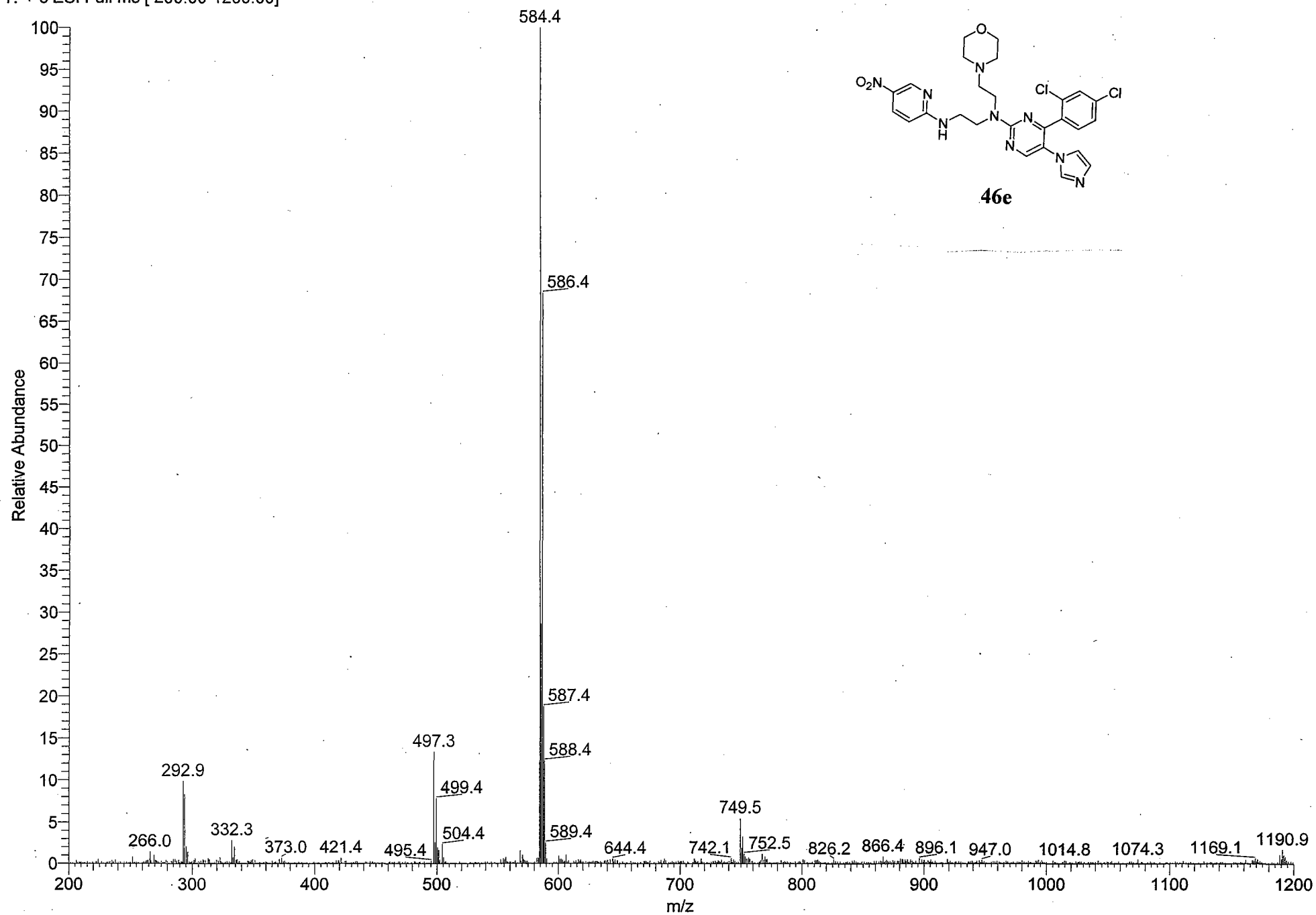


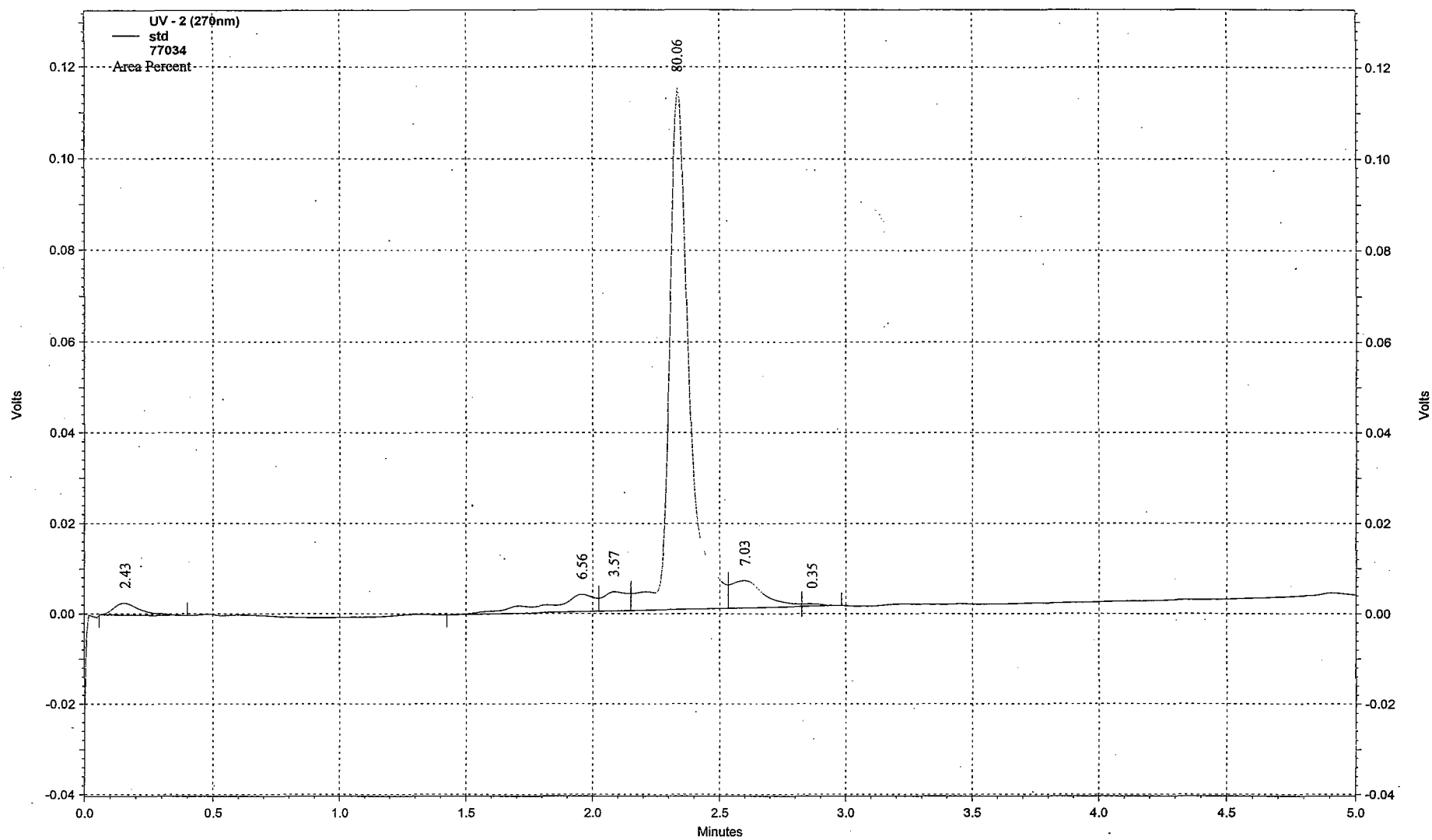
C:\Class-up\041203_ssRR\73181, UV - 2 (270nm)



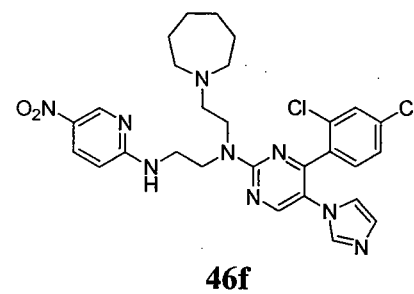
73181_2 #131-138 RT: 3.33-3.49 AV: 8 NL: 1.60E6

T: + c ESI Full ms [200.00-1200.00]



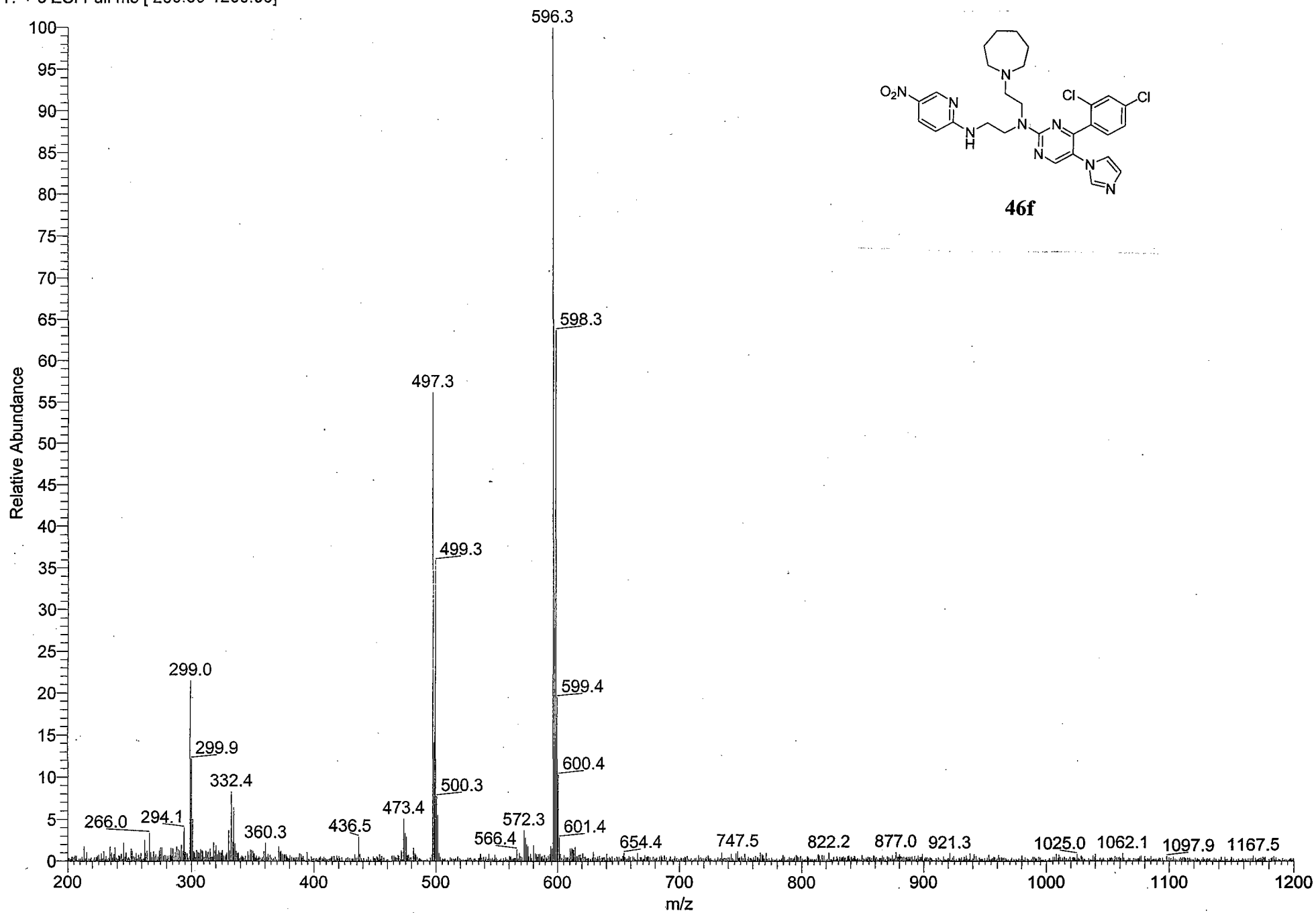


C:\Class-up\041203_ssRR\77034, UV - 2 (270nm)



77034_1 #137-145 RT: 3.48-3.68 AV: 9 NL: 6.56E5

T: + c ESI Full ms [200.00-1200.00]



SampleName az2172pp

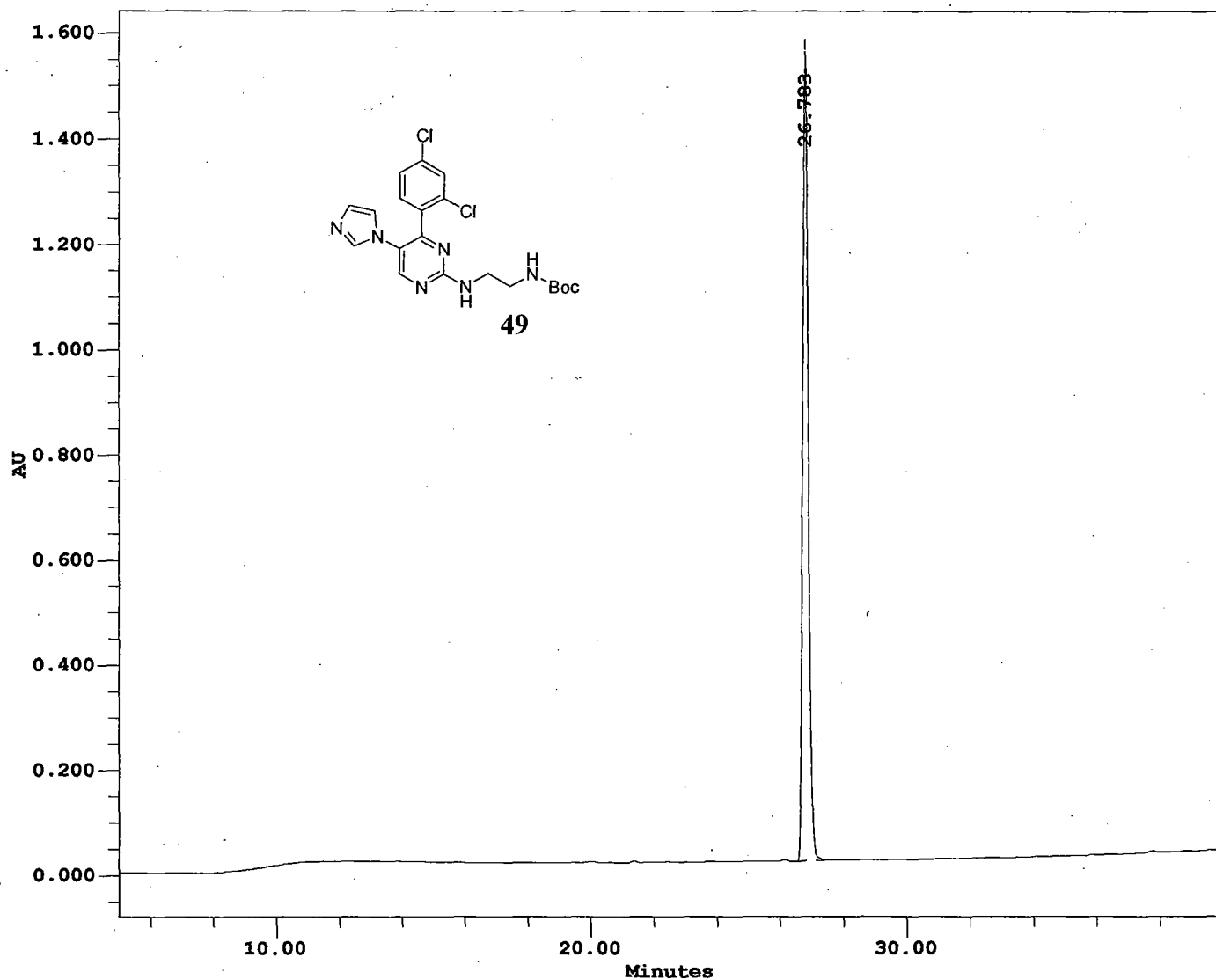
Volume: 10

Date Acquired: 03/27/98 03:02:51 PM

Vial 7

Channel Descr. 220 nm

Acq Meth Set: 5100_220



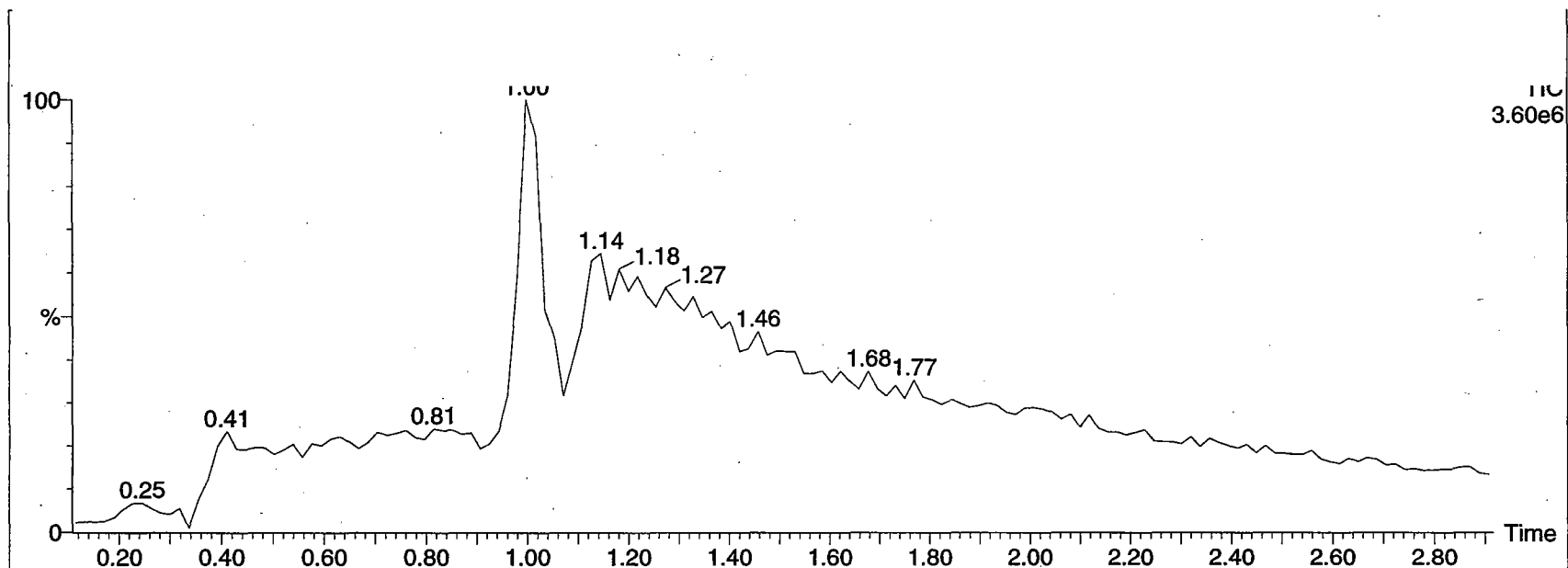
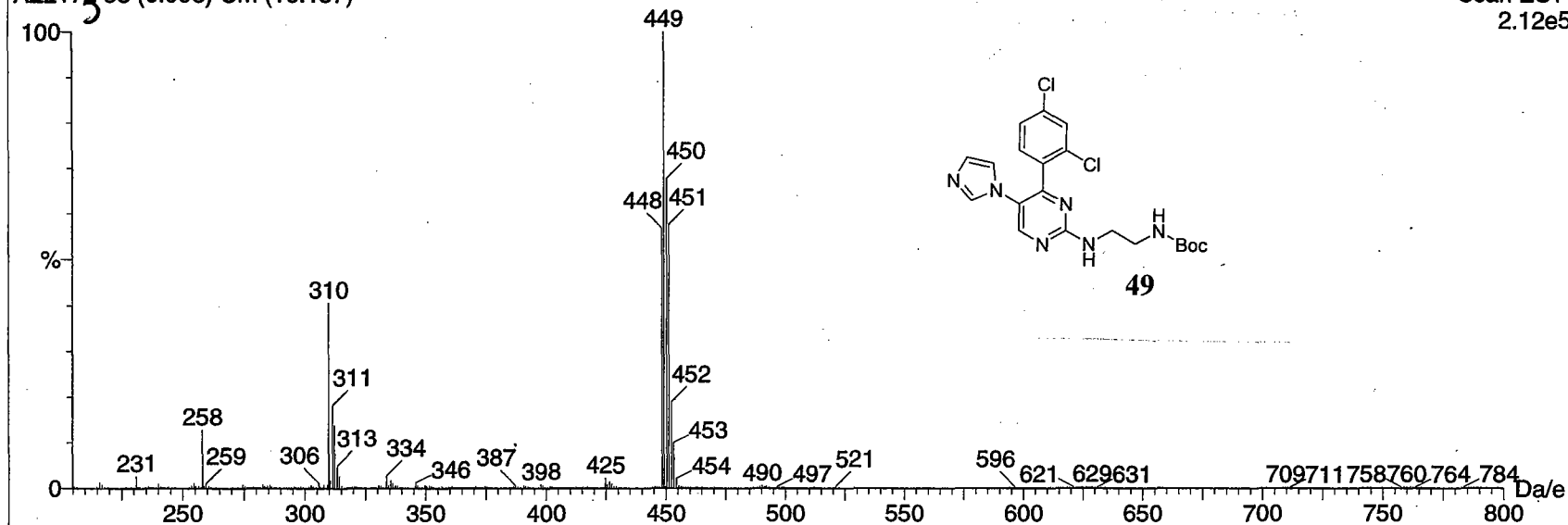
Peak Results

#	Name	Ret Time (min)	Start Time (min)	End Time (min)	% Height	% Area
1		26.783	26.550	27.583	100.00	100.00

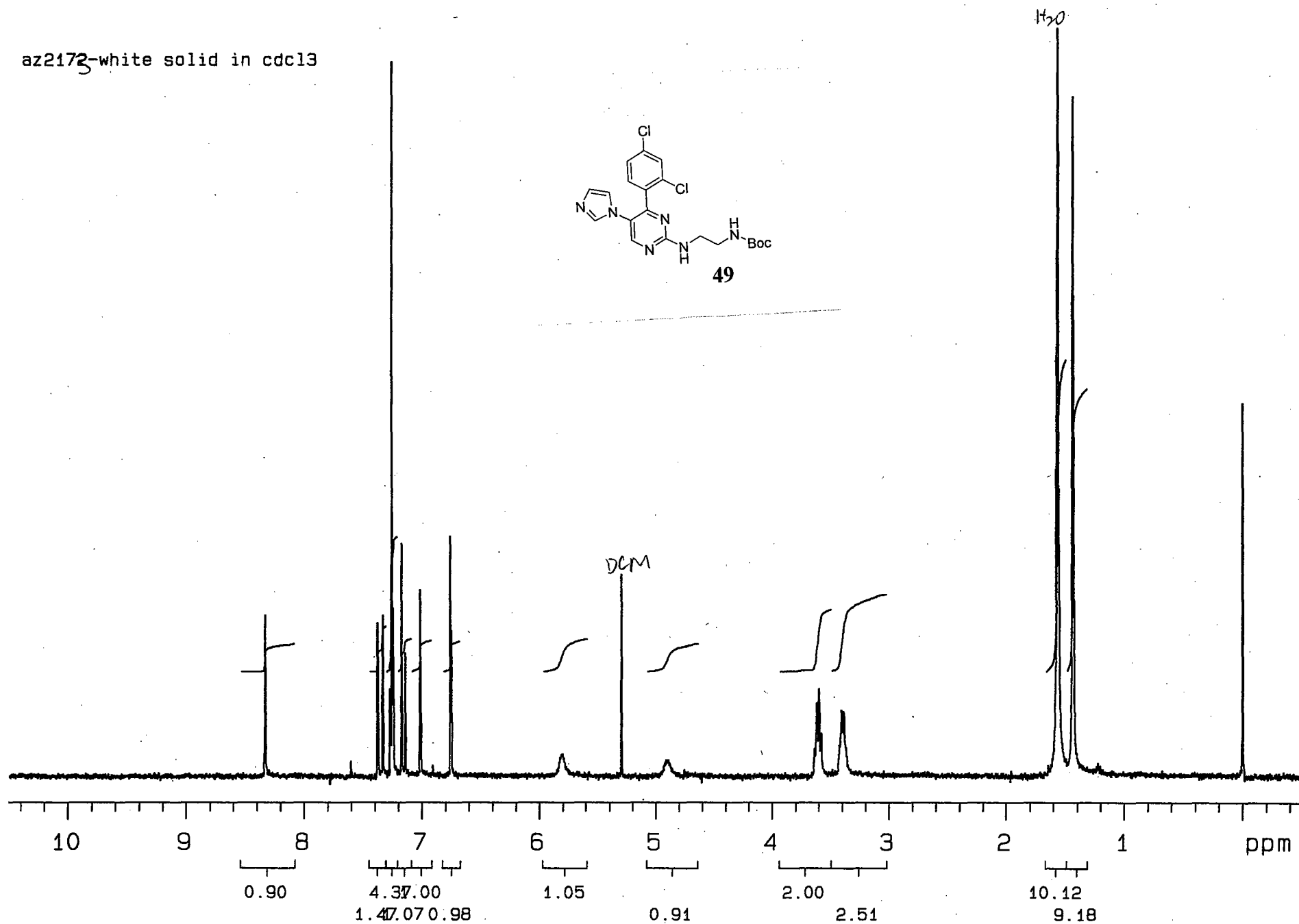
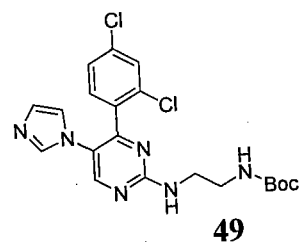
MW449

AZ2172 53 (0.998) Cm (16:157)

Scan ES+
2.12e5



az2173-white solid in cdcl3



CHIRON Technologies S M D D R Medicinal & Organic Chemistry Group

Sample Name: az30

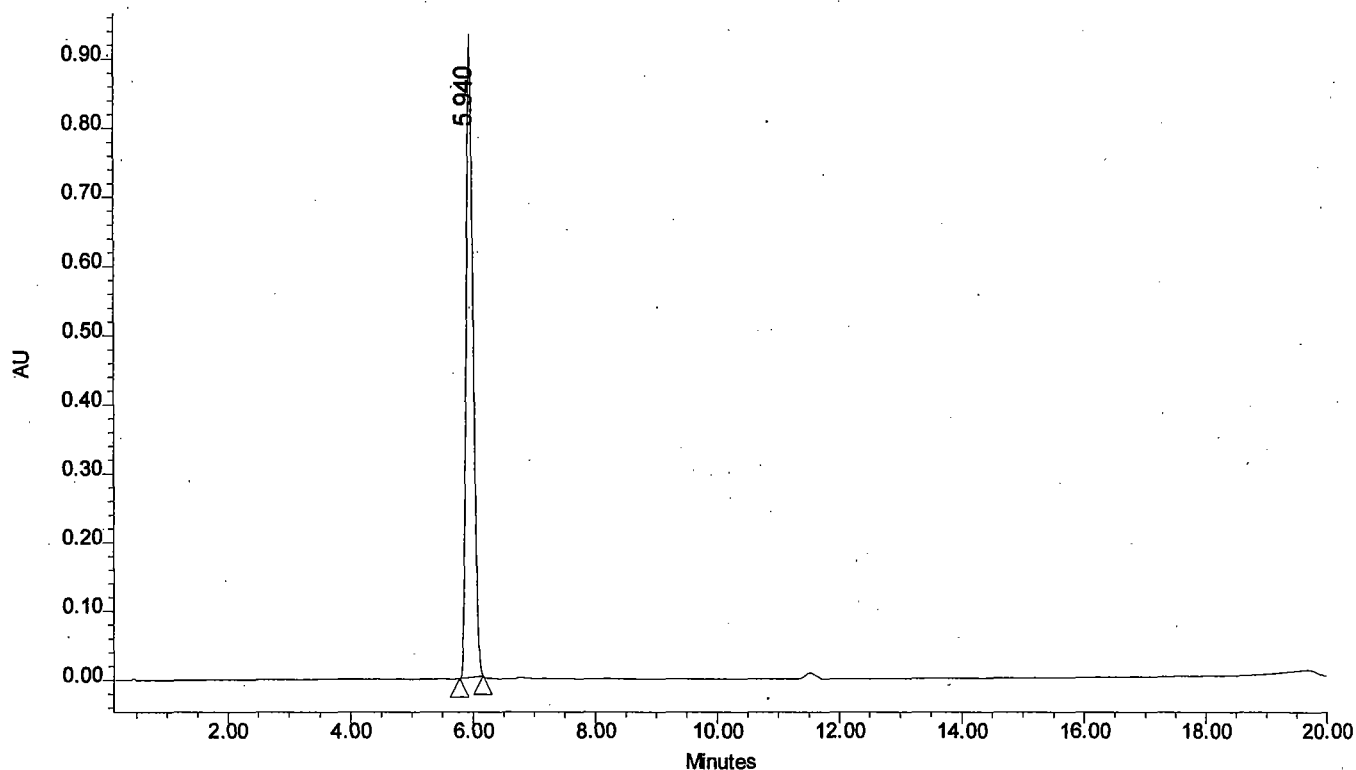
System Name: Shana Project Name: GSK_3

Label:

Acq Method Set: Rabbit20

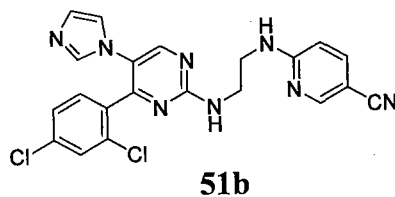
Date Acquired: 8/17/98 3:12:07 PM

Injection Volume- 10.00 ul Vial # 41



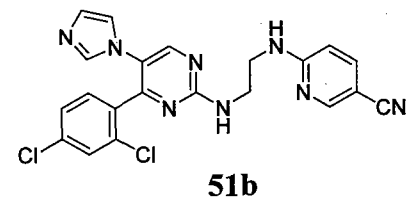
Peak Results

	Retention Time	Start Time	End Time	% Area
1	5.940	5.772	6.155	100.00

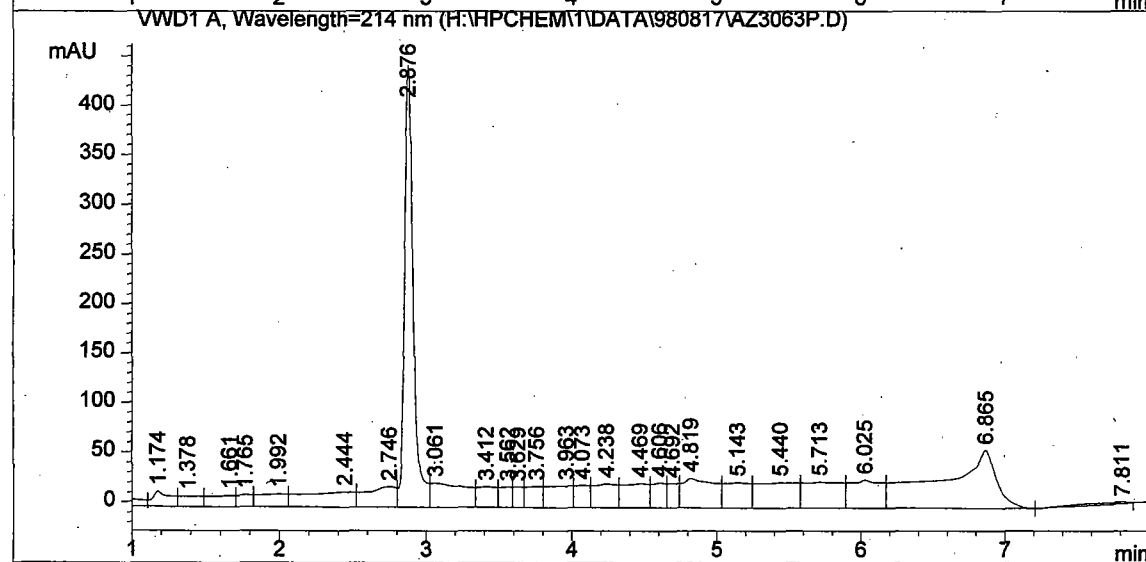
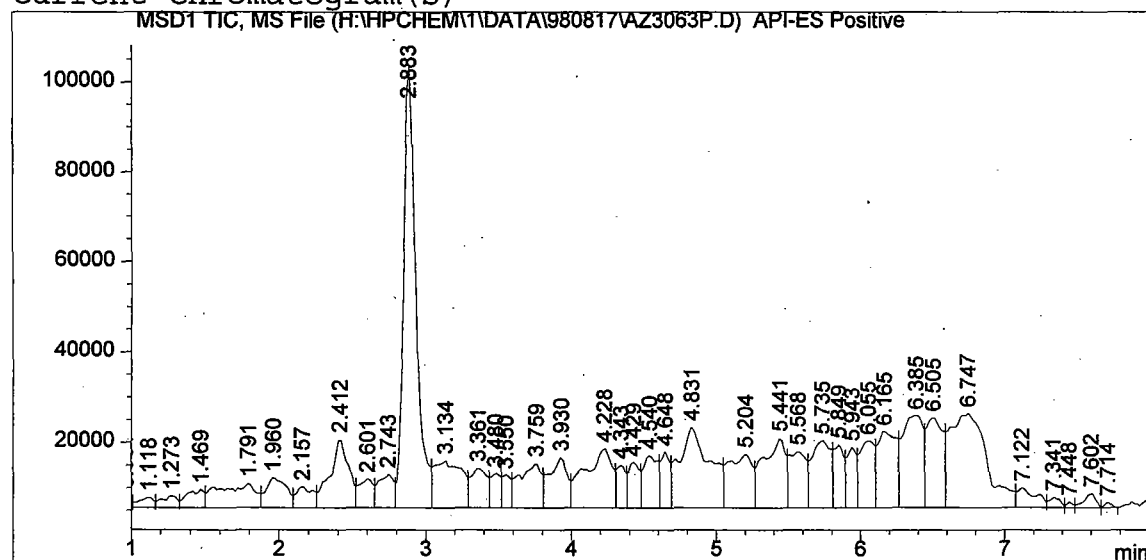


```
=====
Injection       : 8/17/98 5:49:47 PM      Seq. line : 35
Sample Name     : AZ3063P                Vial       : 37
Acq. Operator   : ntg                    Inj        : 1
                                           Inj Volume : Inj prog

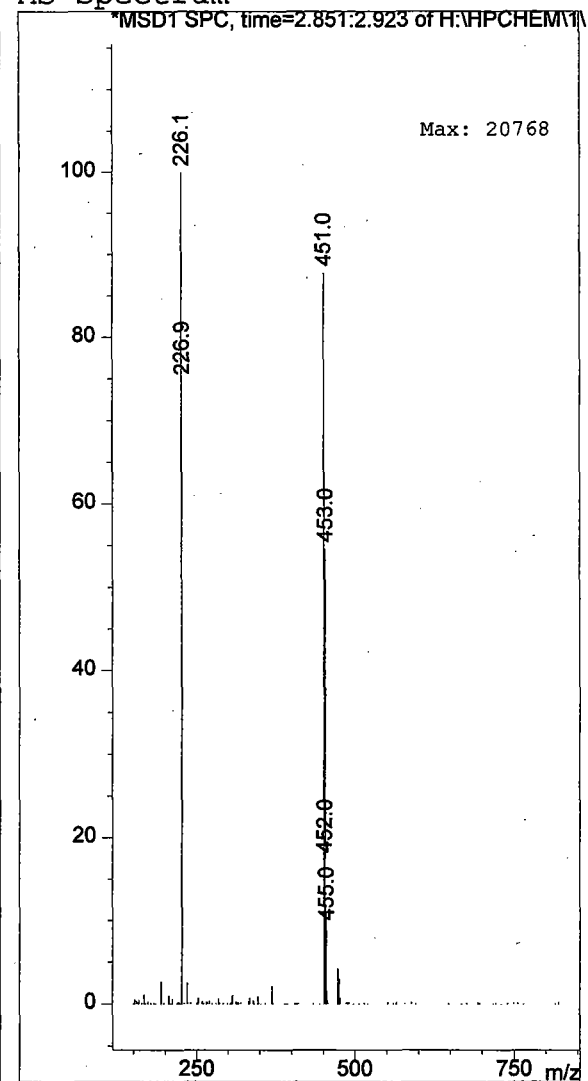
Acq. Method     : C:\HPCHEM\1\METHODS\POS_MODE.M
Last changed    : 7/31/98 9:32:14 AM by ntg
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M
Last changed    : 8/17/98 3:19:24 PM by chemist
                  (modified after loading)
=====
```



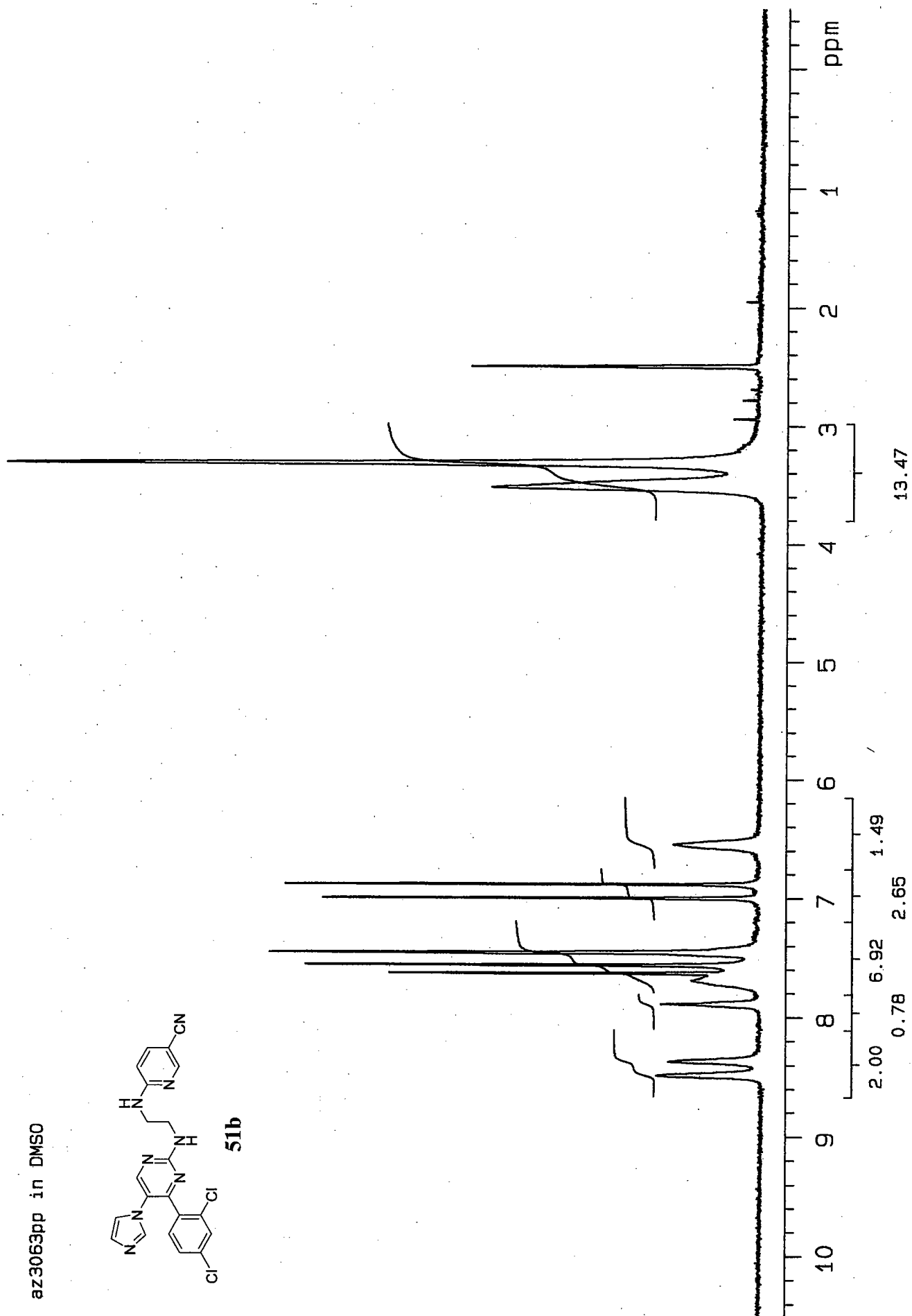
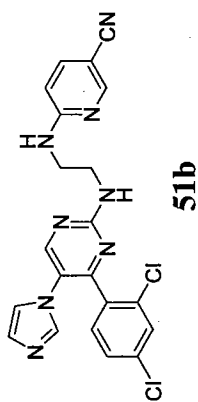
Current Chromatogram(s)



MS Spectrum



az3063pp in DMSO



SampleName SR6

Injection Volume 5.00 ul

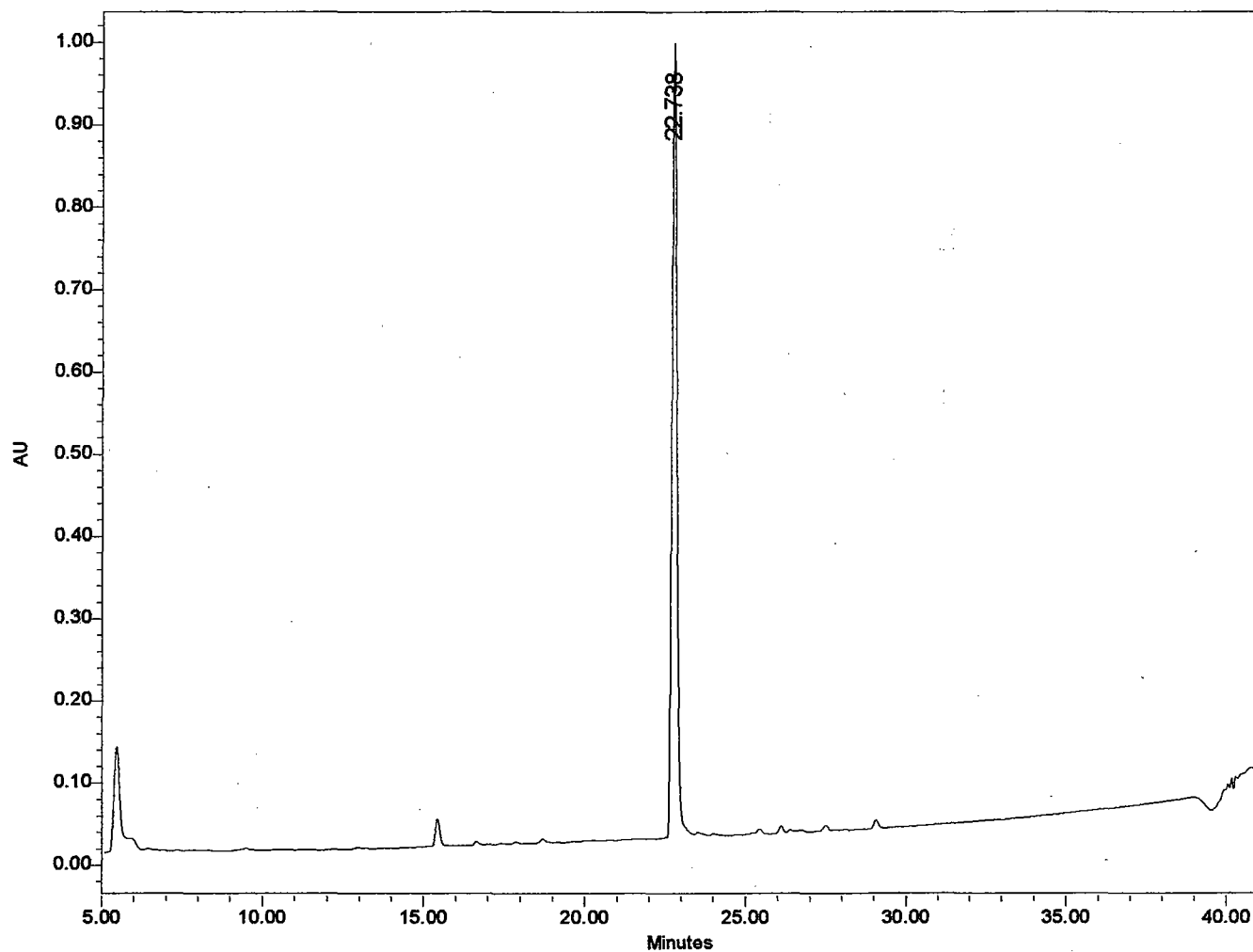
Date Acquired 2/8/99 1:09:47 PM

Vial 3

Channel Description FDA 220.0

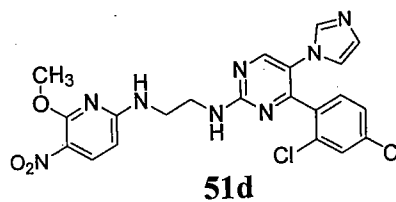
Acq Method Set 5100

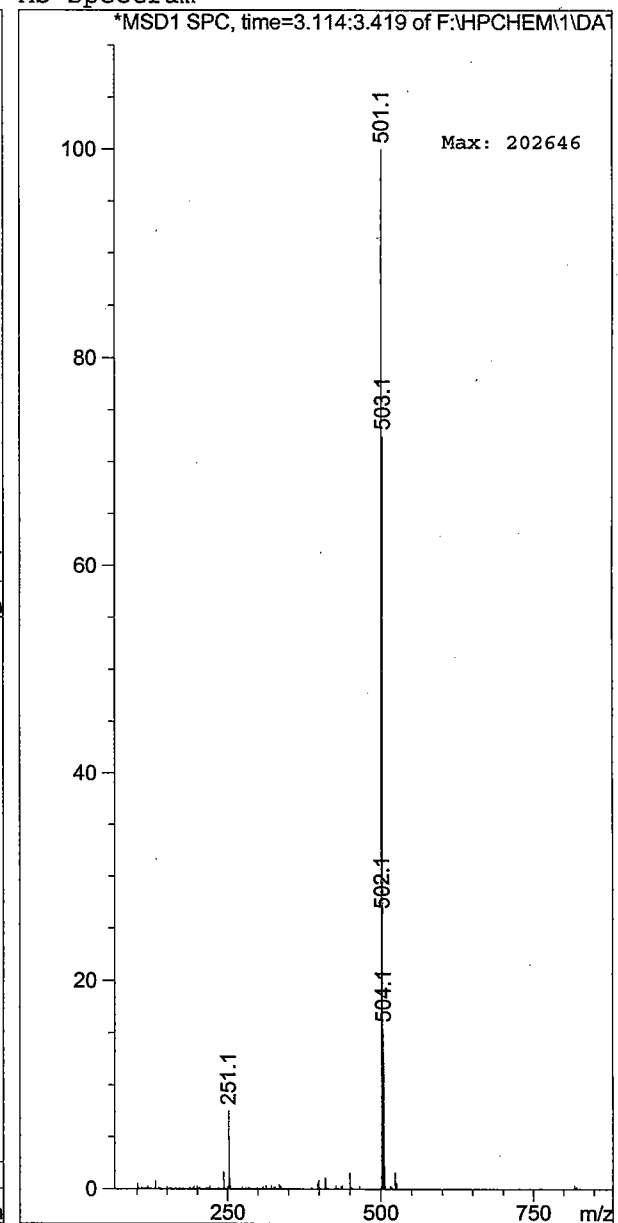
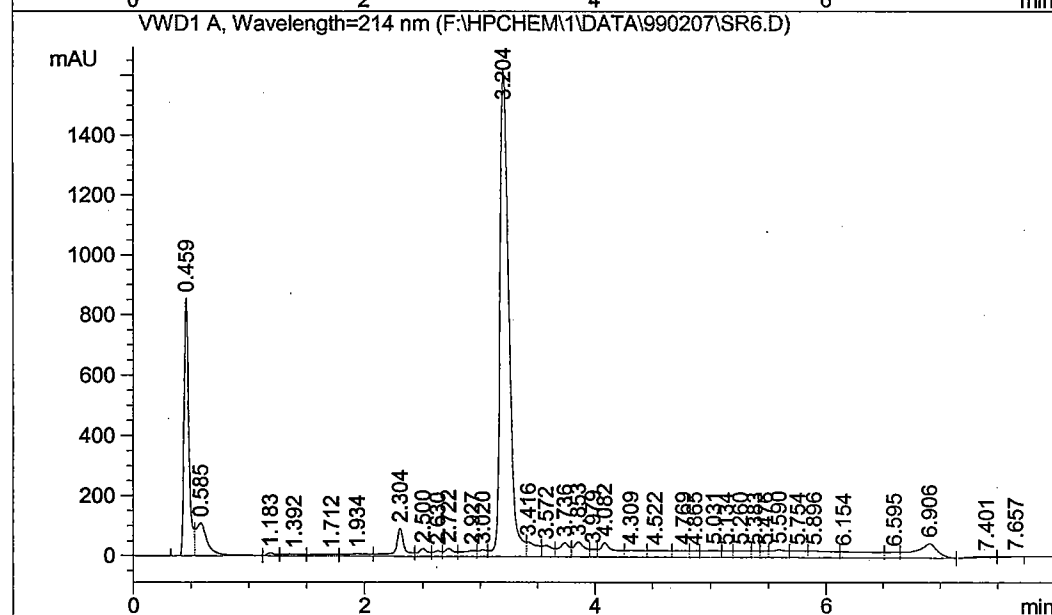
Auto-Scaled Chromatogram

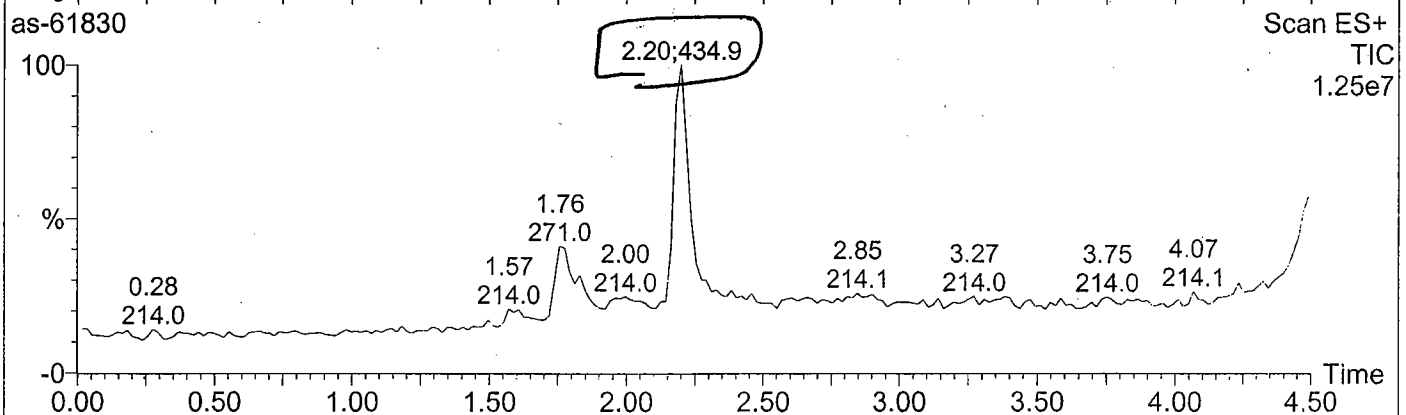
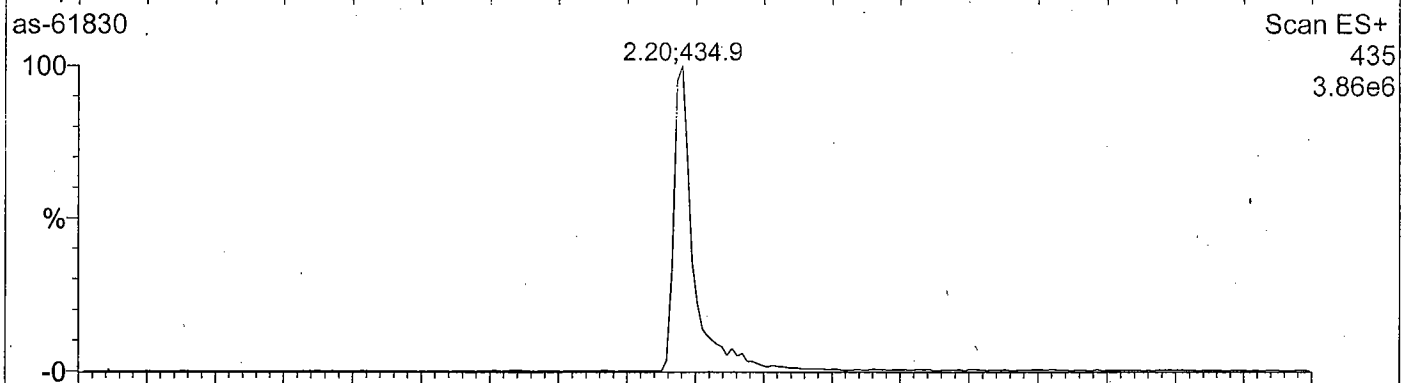
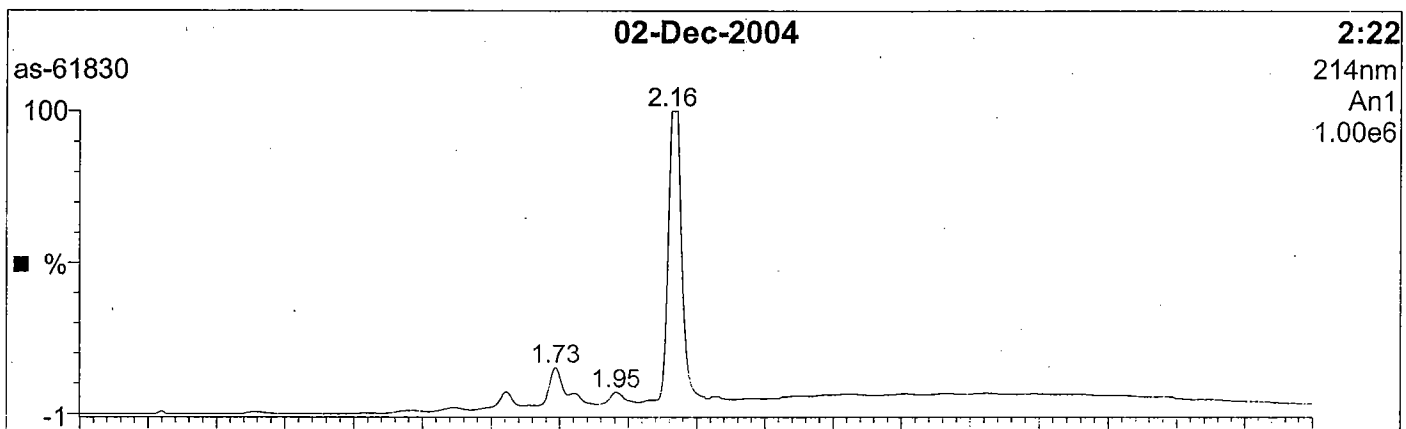
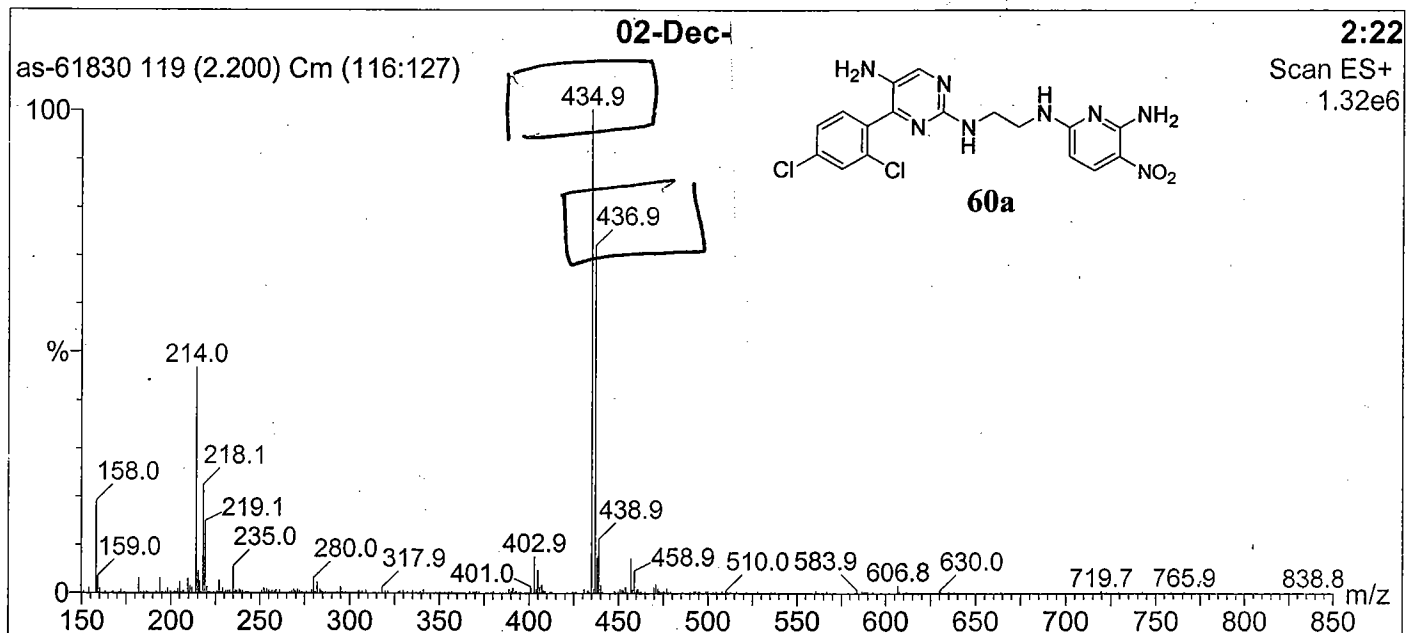


Peak Results

	Name	RT	Start Time	End Time	% Height	% Area
1		22.738	22.383	23.383	100.00	100.00



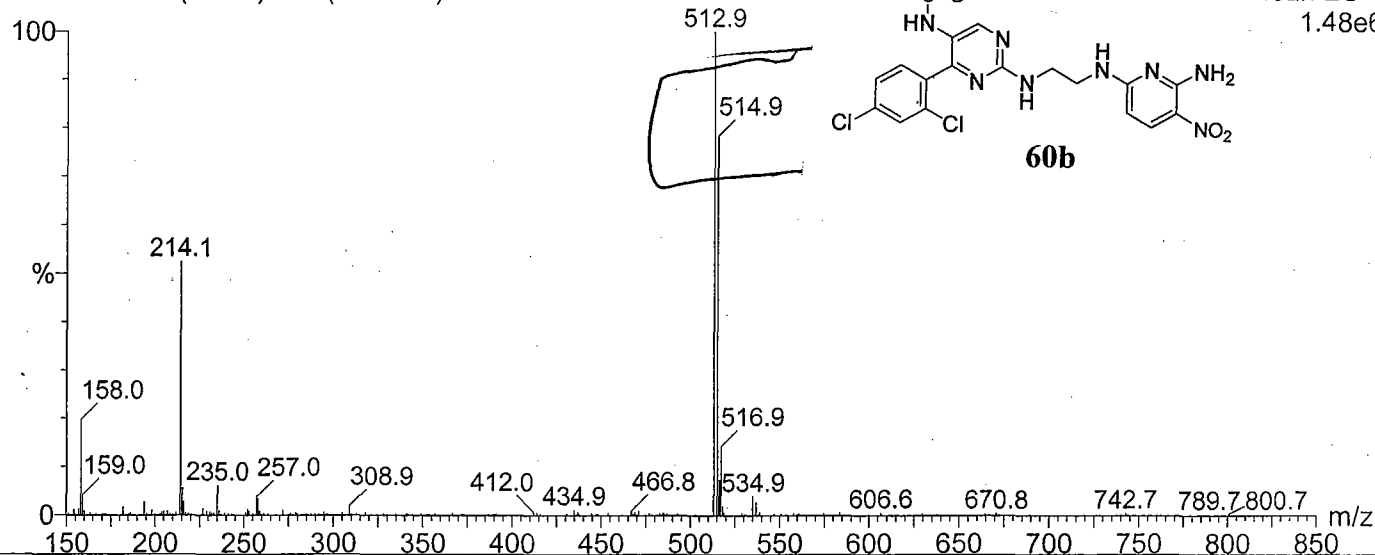




03-Dec-2004

1:12

as-85229 130 (2.403) Cm (126:135)

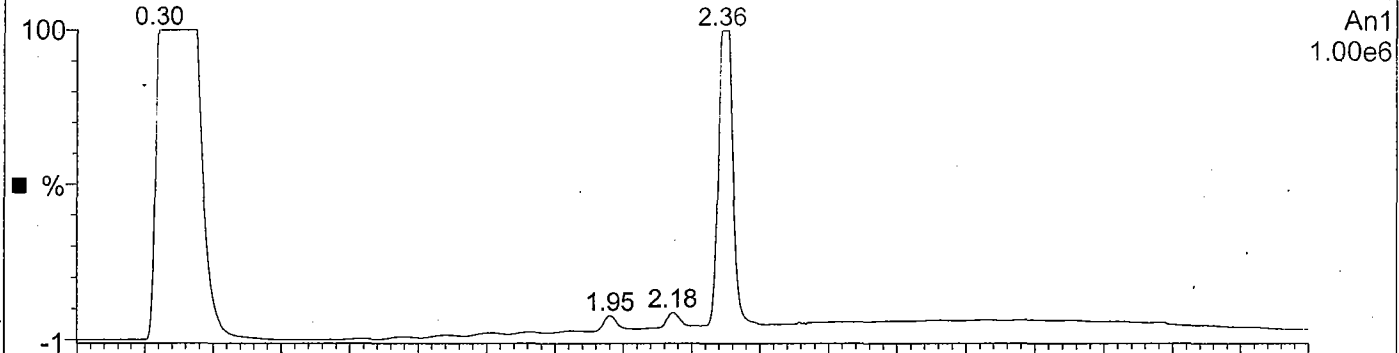
Scan ES+
1.48e6

03-Dec-2004

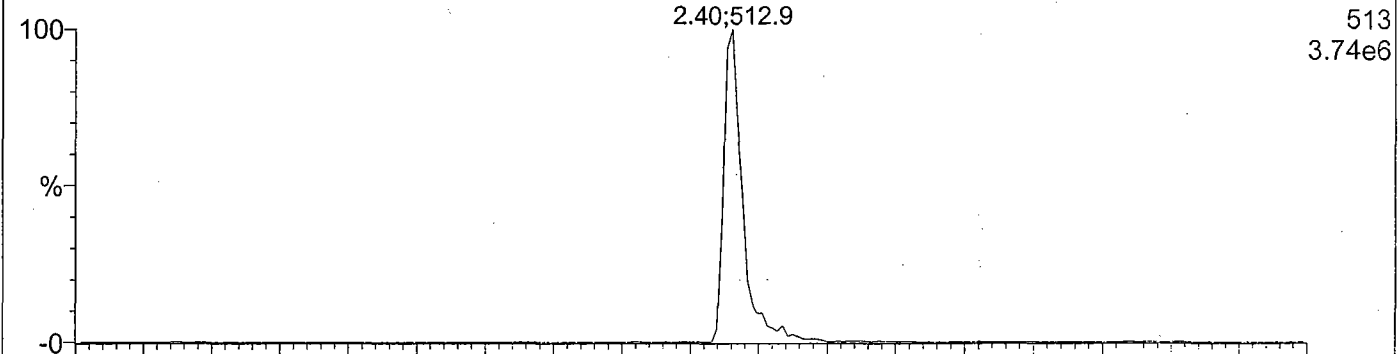
1:12

as-85229

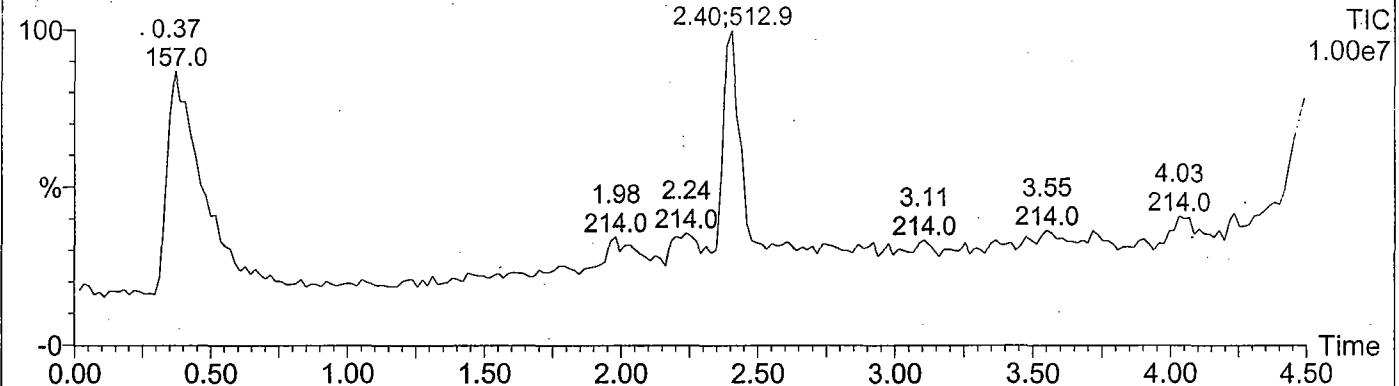
214nm



as-85229

Scan ES+
513
3.74e6

as-85229

Scan ES+
TIC
1.00e7

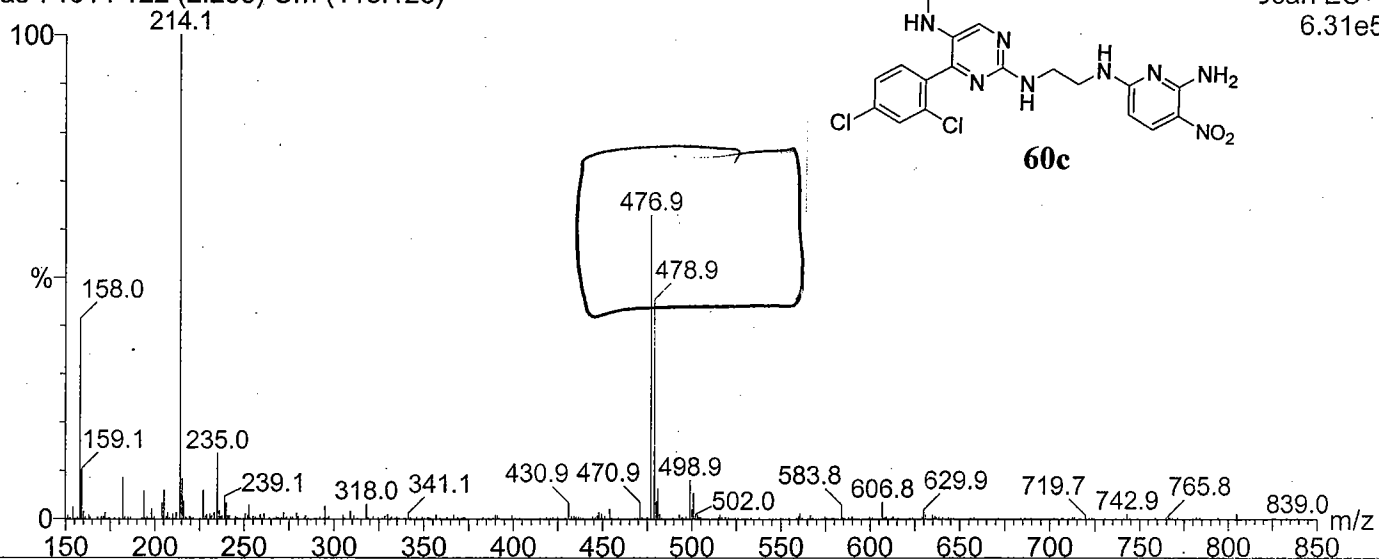
02-Dec-2004

2:19

as-71514 122 (2.255) Cm (118:128)

Scan ES+

6.31e5



02-Dec-2004

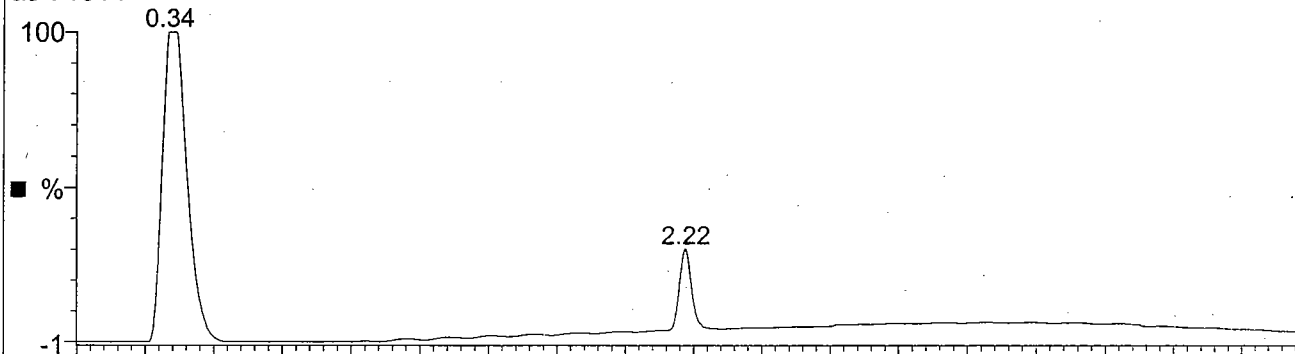
2:19

as-71514

214nm

An1

1.00e6

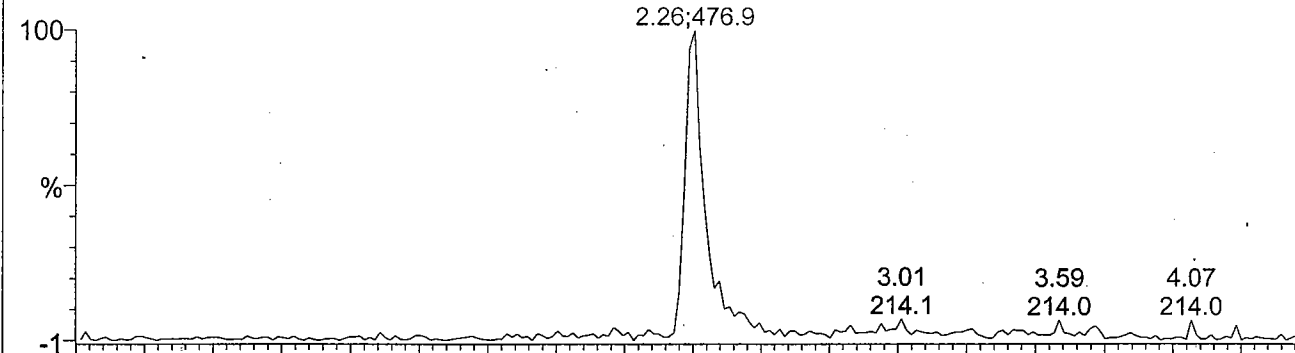


as-71514

Scan ES+

477

9.92e5

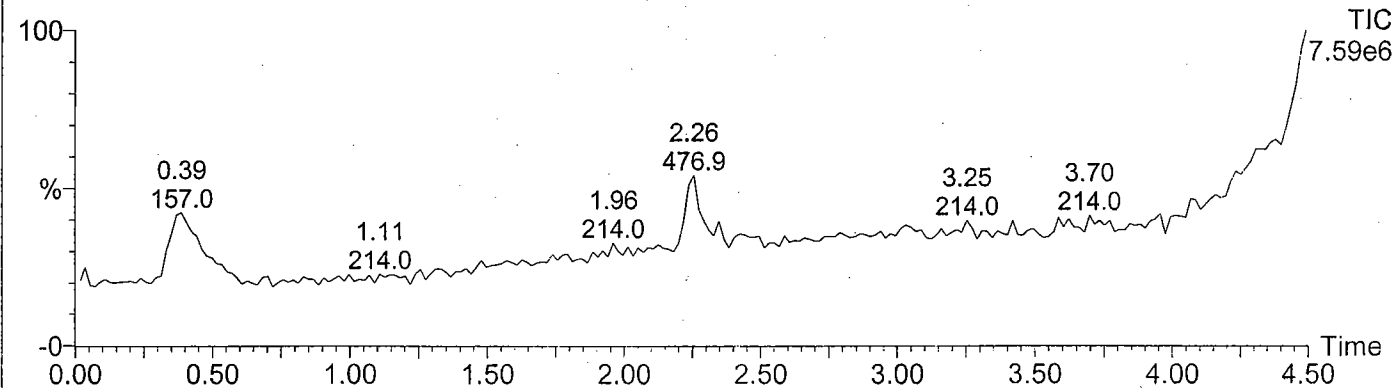


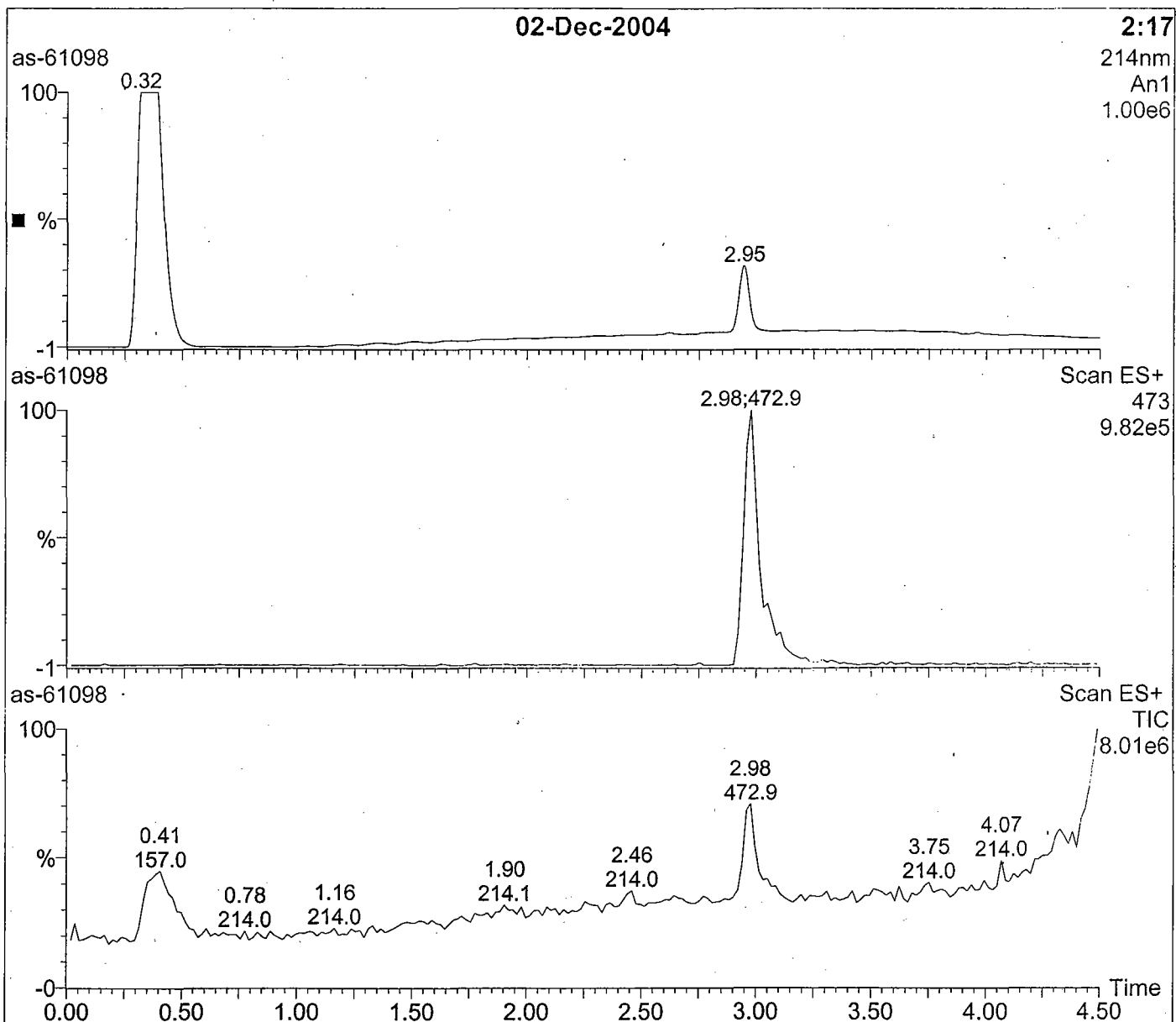
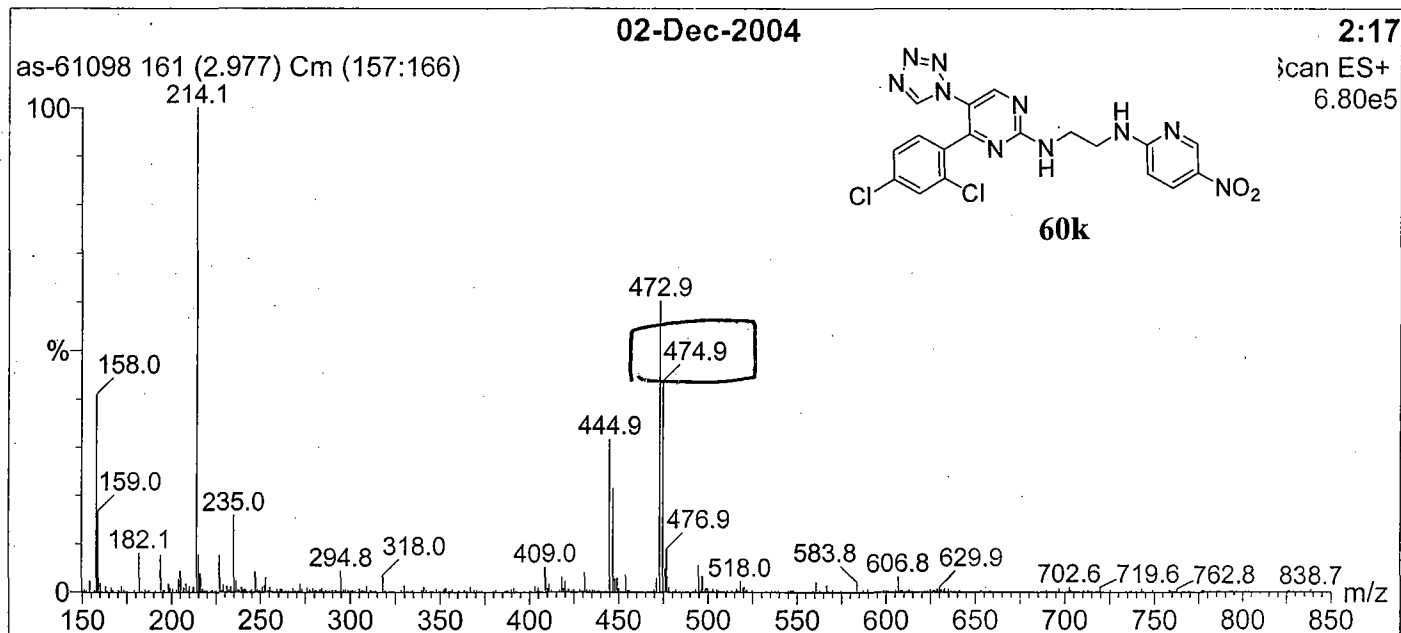
as-71514

Scan ES+

TIC

7.59e6





Chiron Drug Discovery Research

System Name: Chiron Project 45

Data File name: C:\HPCHEM\1\DATA\000126\122.D

Method name: C:\HPCHEM\1\METHODS\5TO95.M

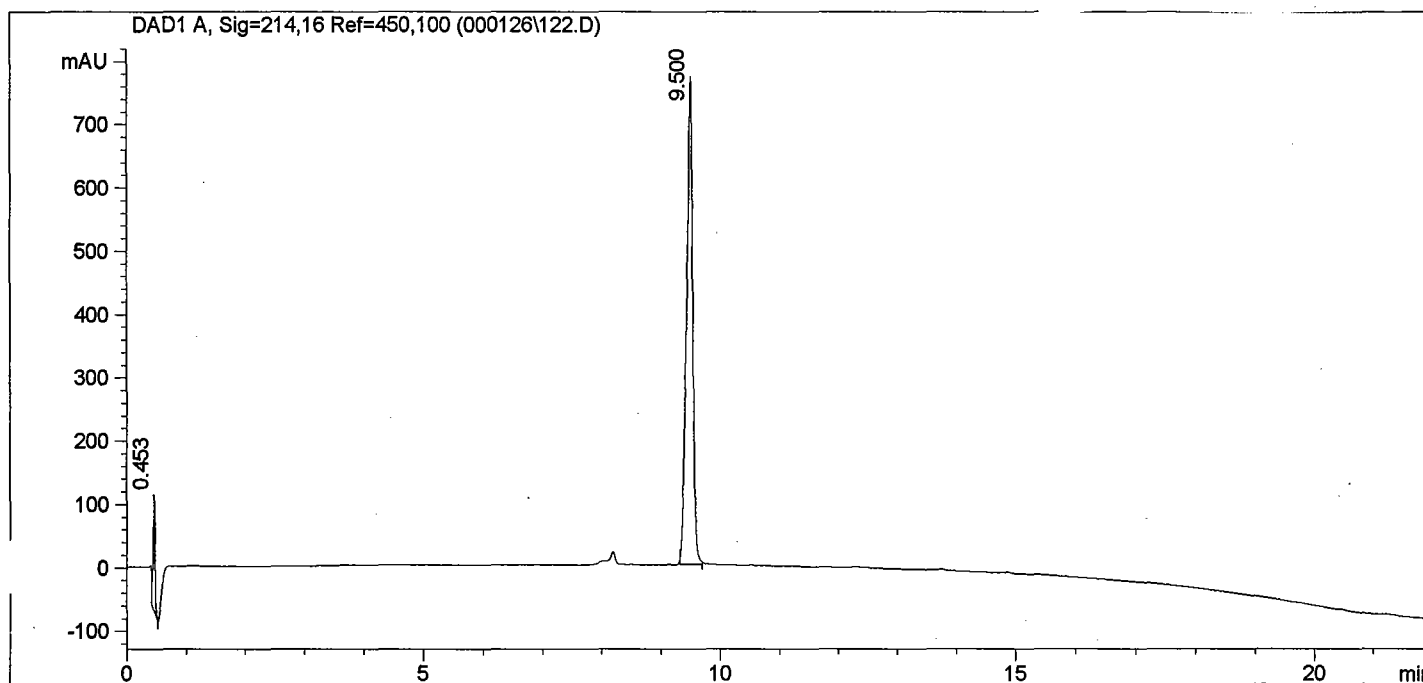
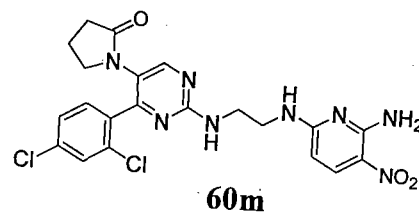
Sample Name : 122

On: Wed, 26. Jan. 2000

Injection Time : 02:07

Vial # 6.000

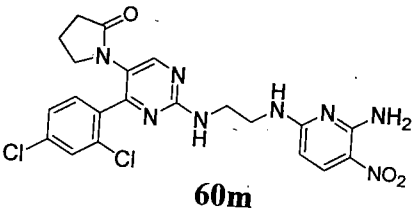
Injection Volume : 8.0ul



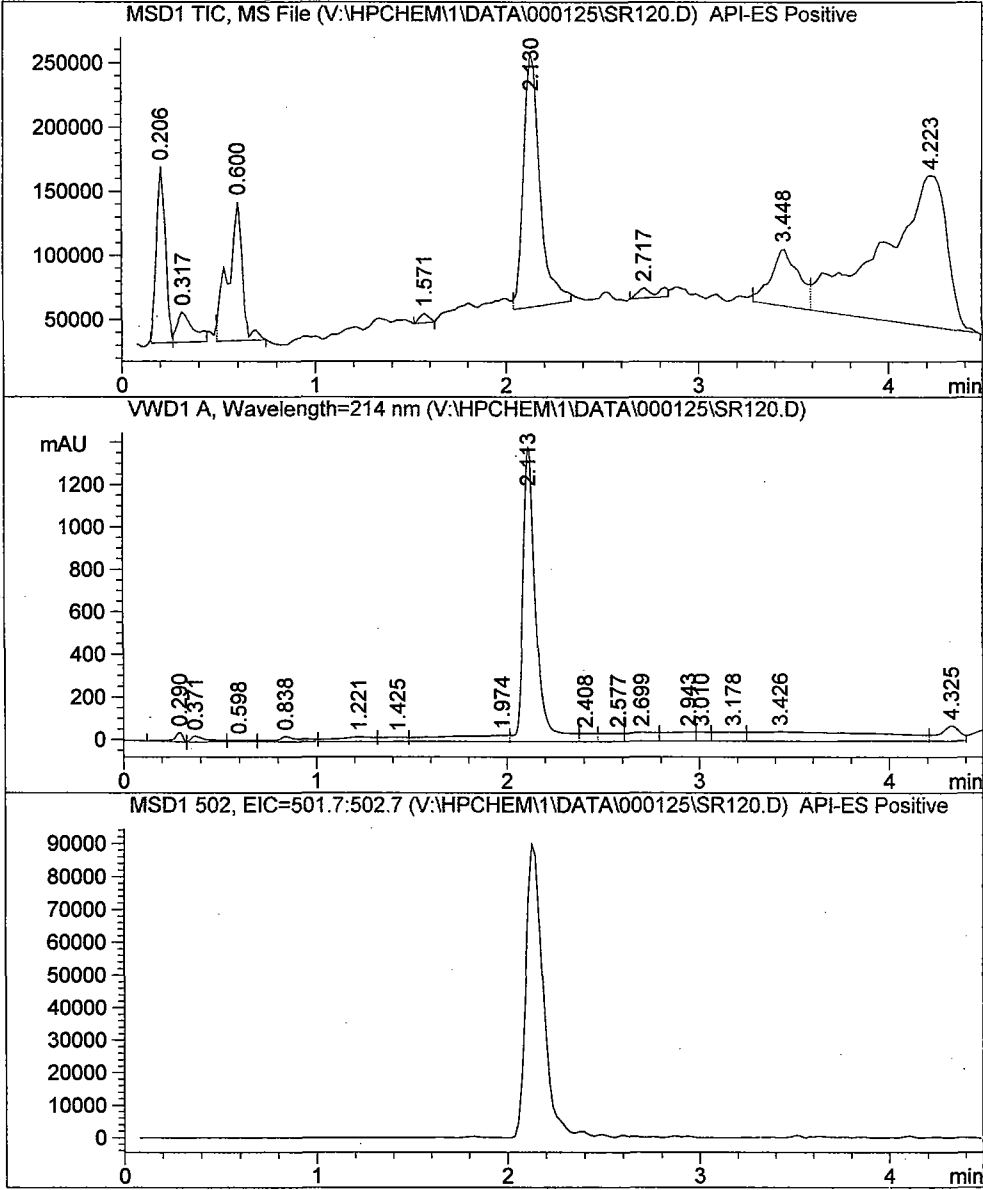
Peak Results

#	Meas.RT	Main Height%	Main Area%
1	0.453	18.980	6.955
2	9.500	81.020	93.045

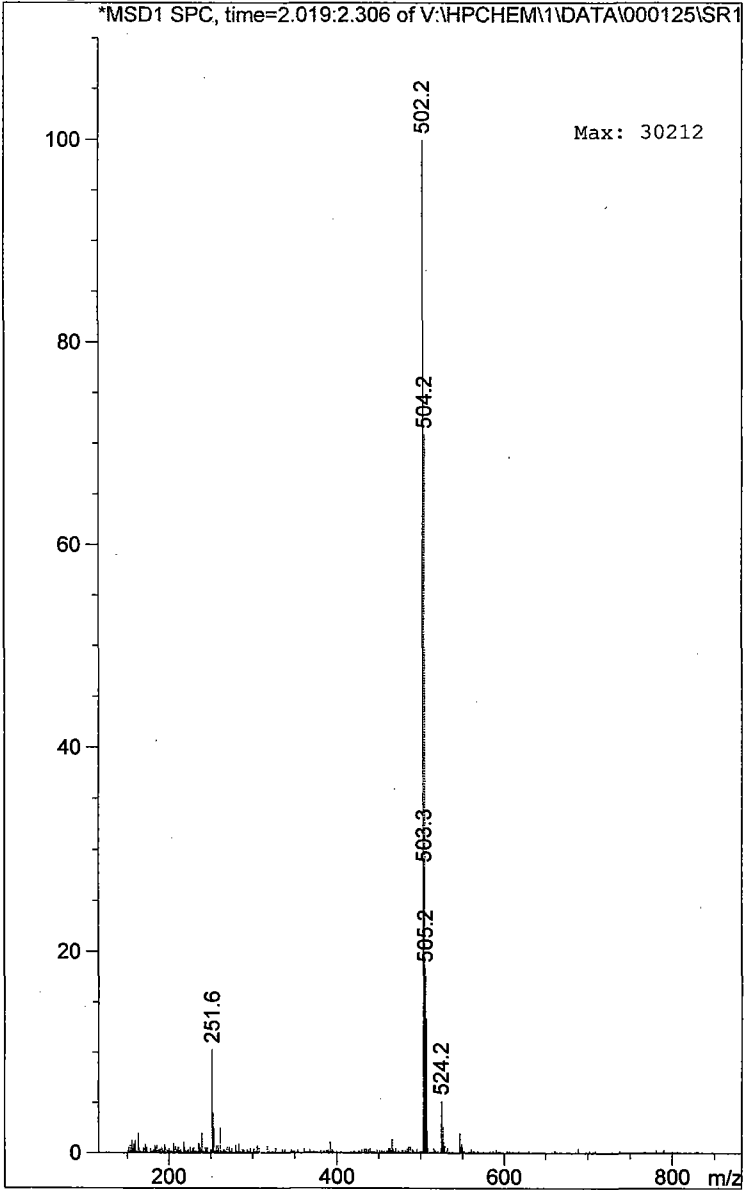
Injection Date : 1/25/00 9:00:24 AM Seq. Line : 3
Sample Name : SR120 Vial : 3
Acq. Operator : Manager Inj : 1
Inj Volume : Inj prog
Acq. Method : C:\HPCHEM\1\METHODS\POS_MODE.M
Last changed : 1/12/00 11:50:39 AM by Manager
Analysis Method : C:\HPCHEM\1\METHODS\DEF_LC.M

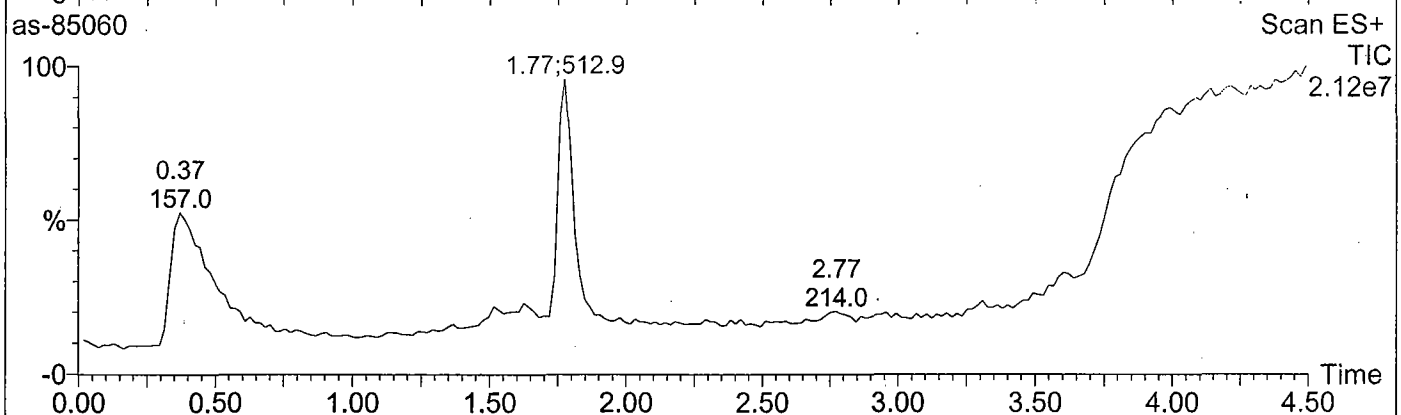
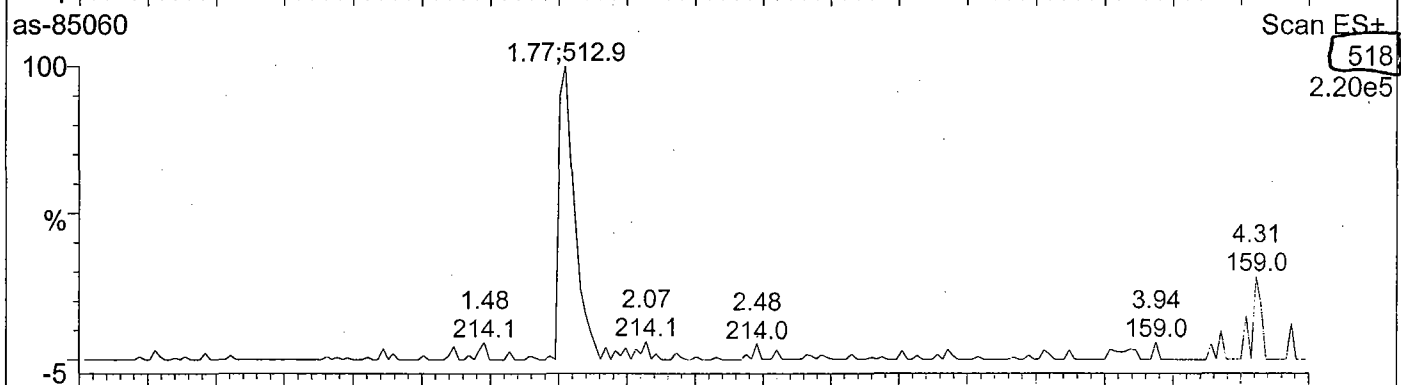
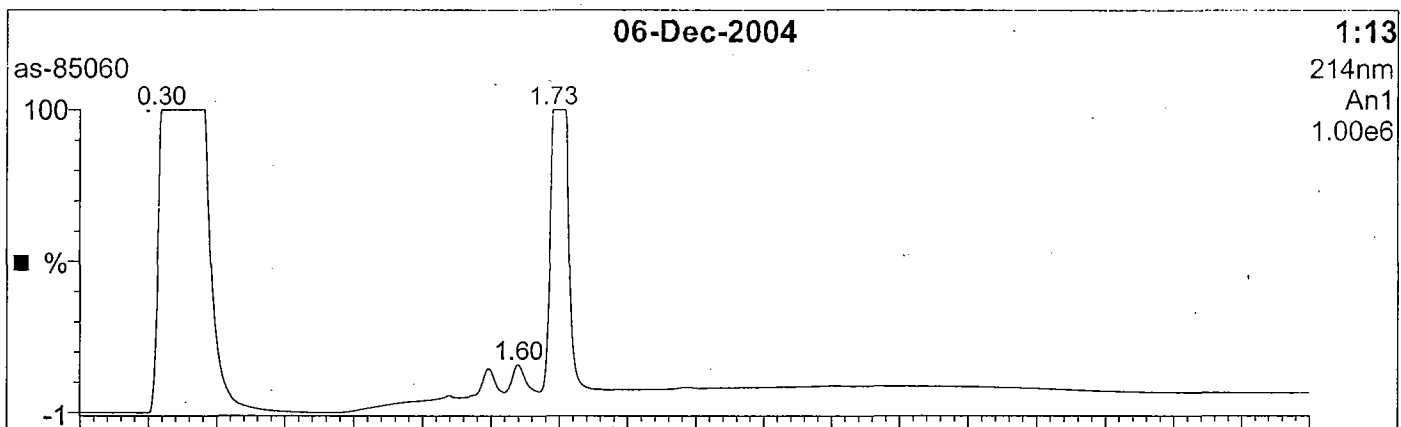
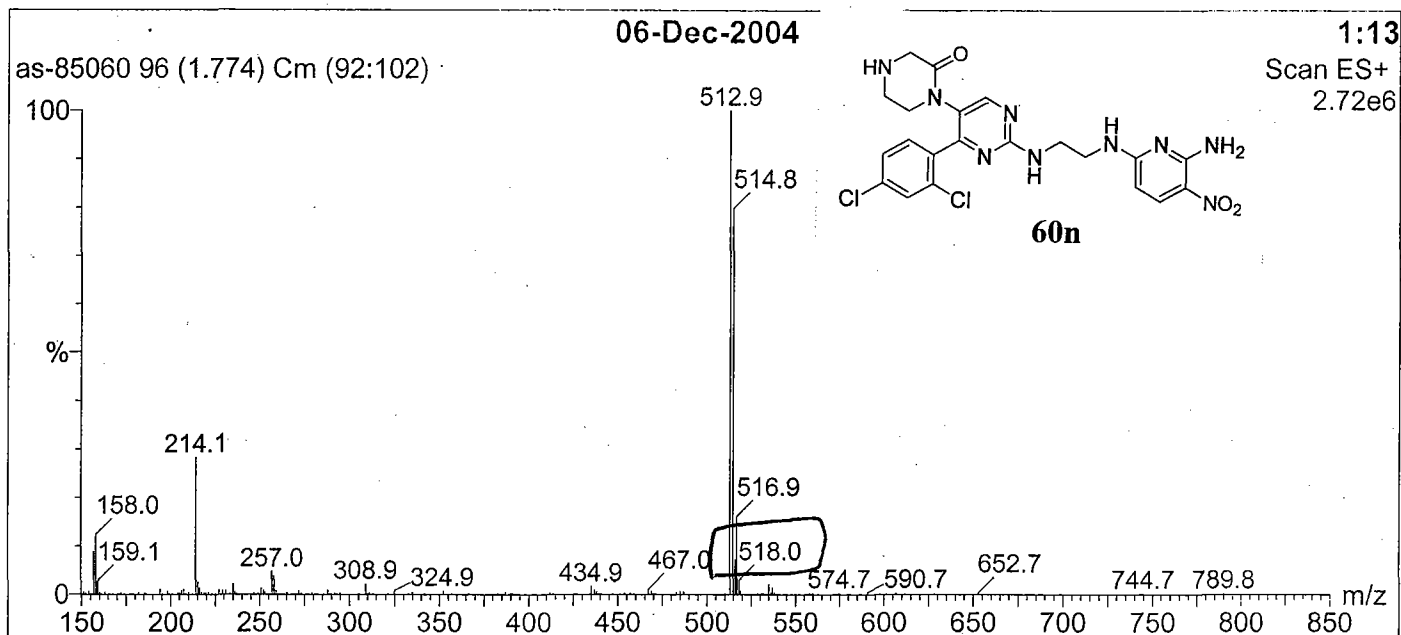


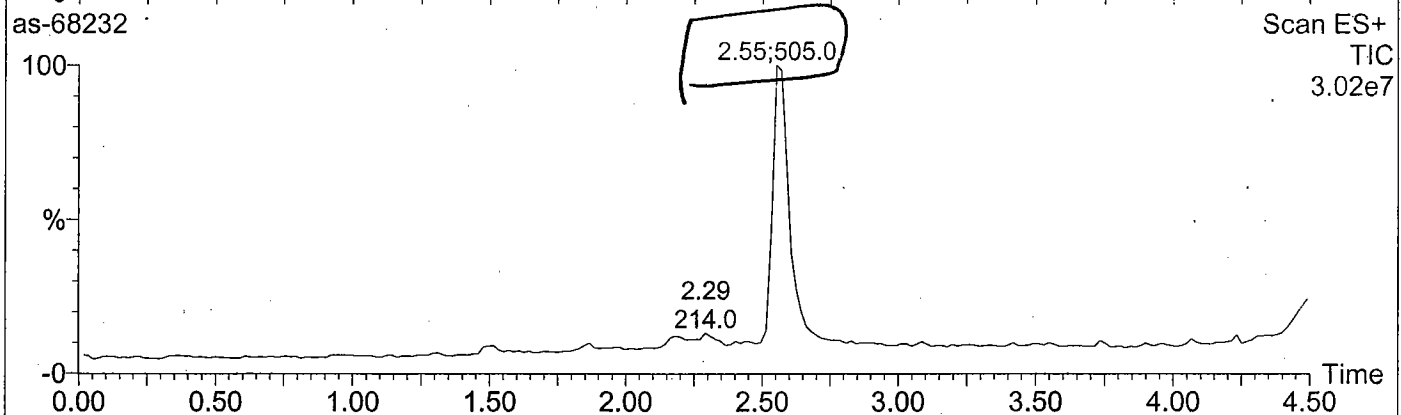
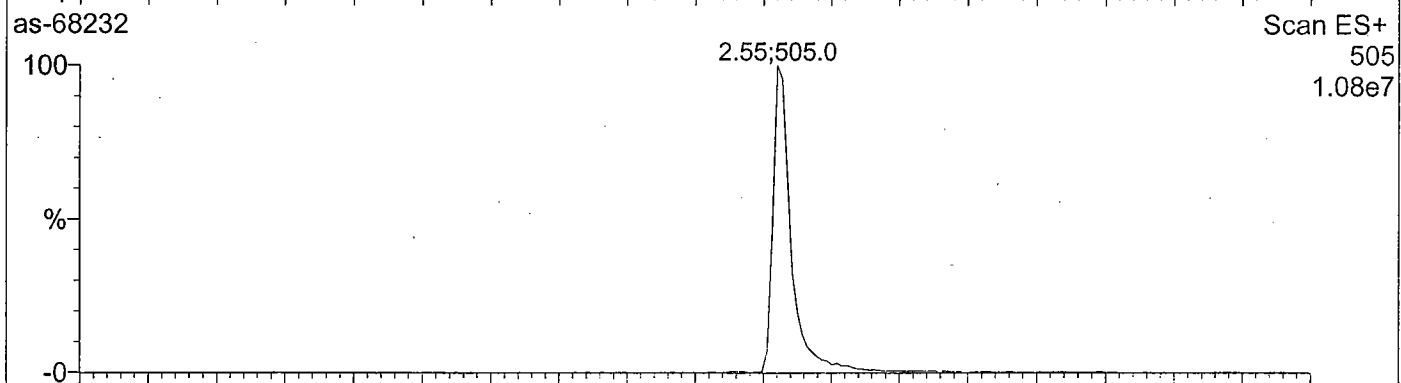
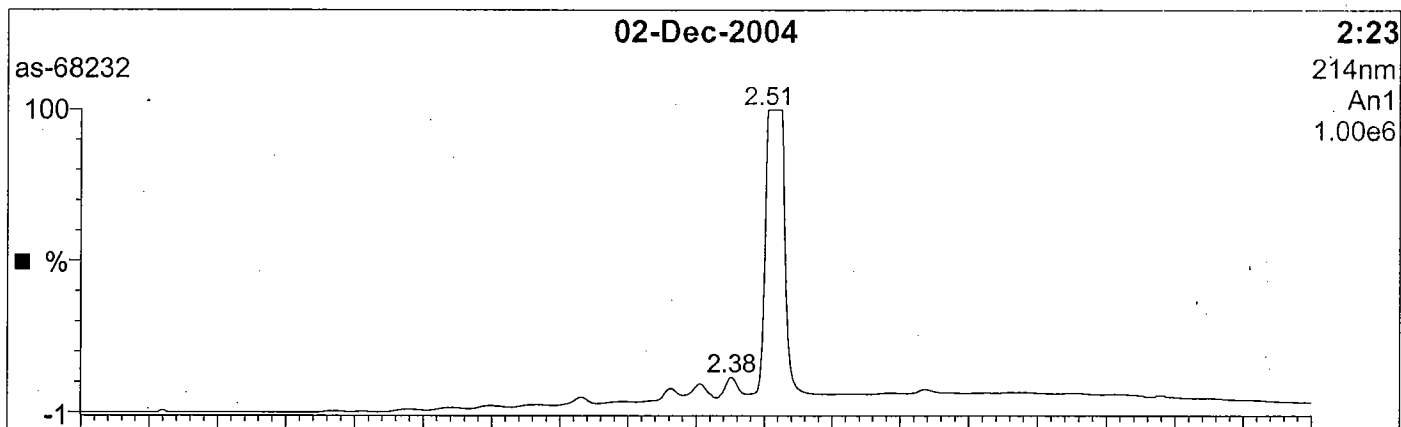
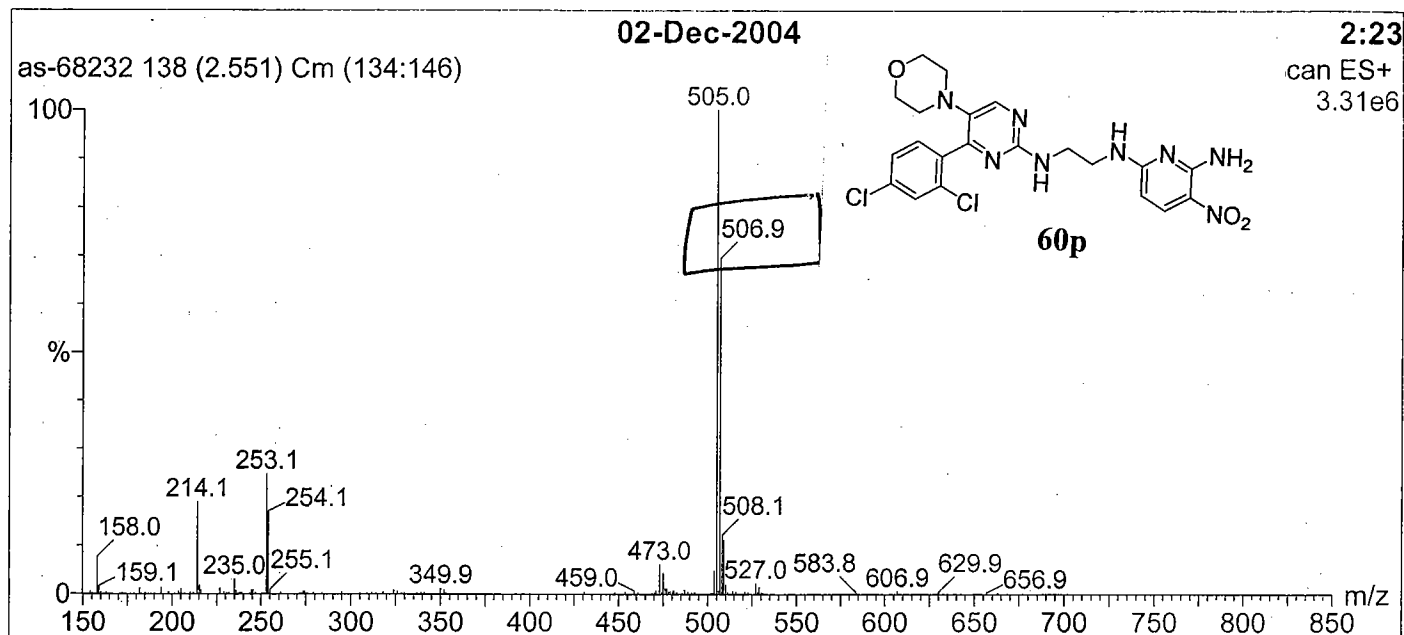
Current Chromatogram(s)



MS Spectrum



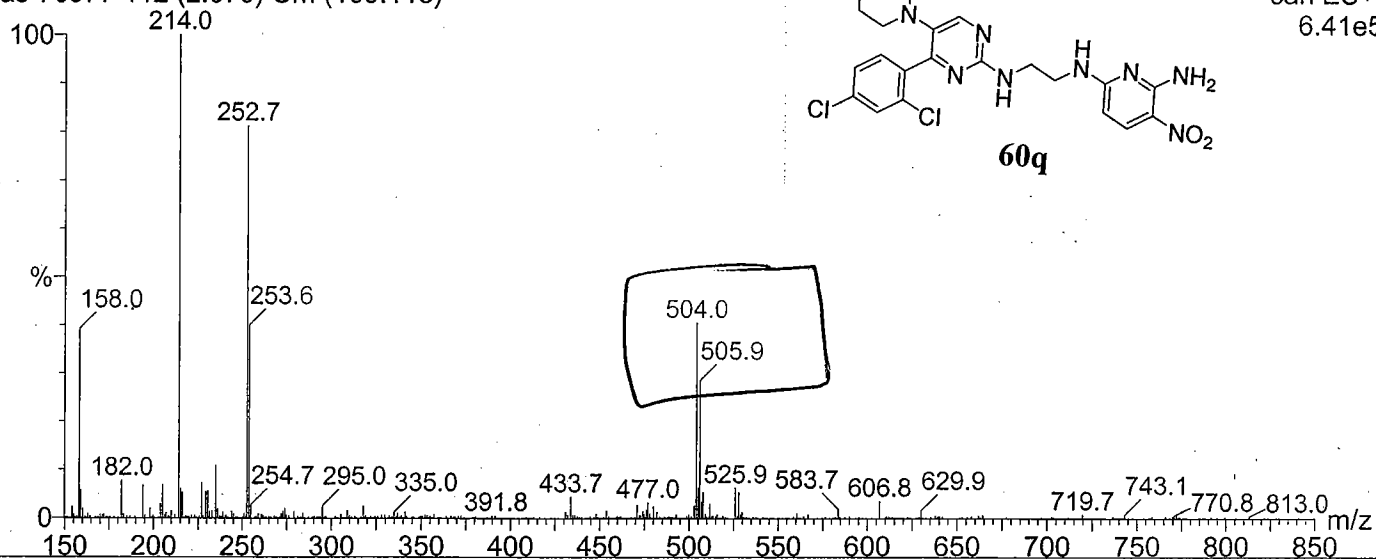




02-Dec-2004

2:16

as-70977 112 (2.070) Cm (109:118)

can ES+
6.41e5

02-Dec-2004

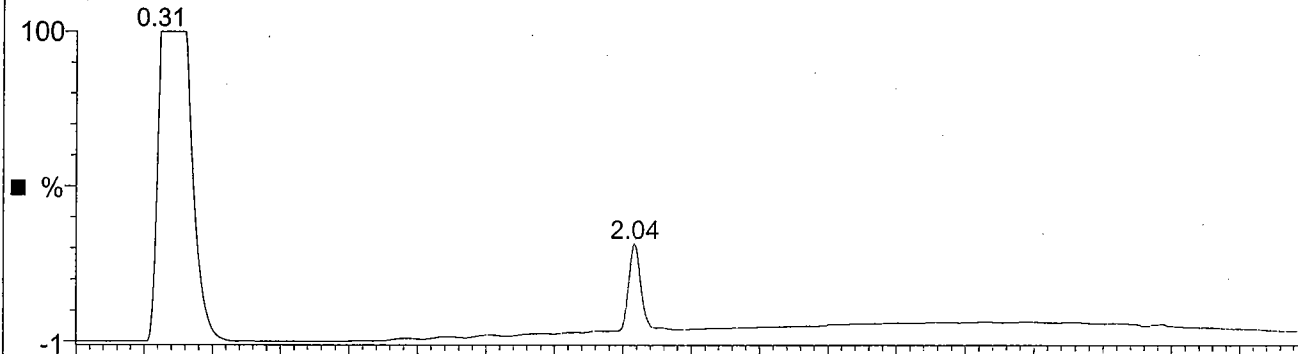
2:16

as-70977

214nm

An1

1.00e6



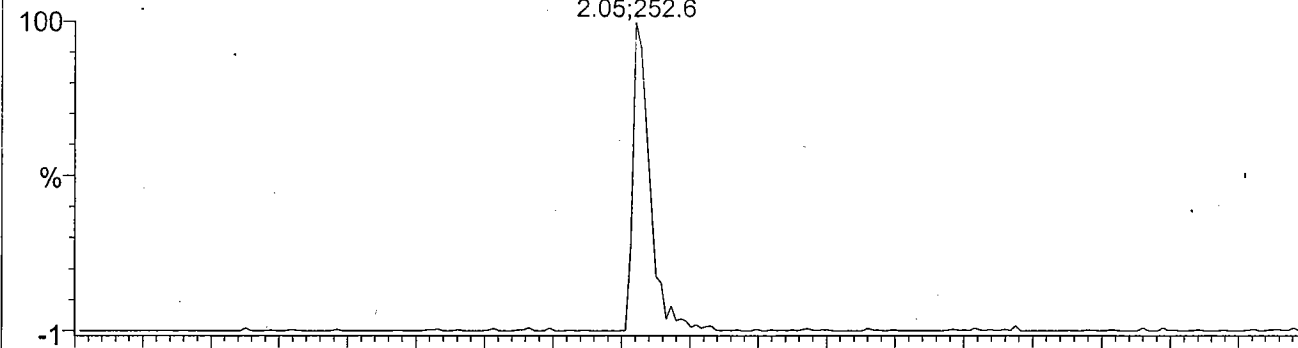
as-70977

Scan ES+

2.05;252.6

504

7.03e5

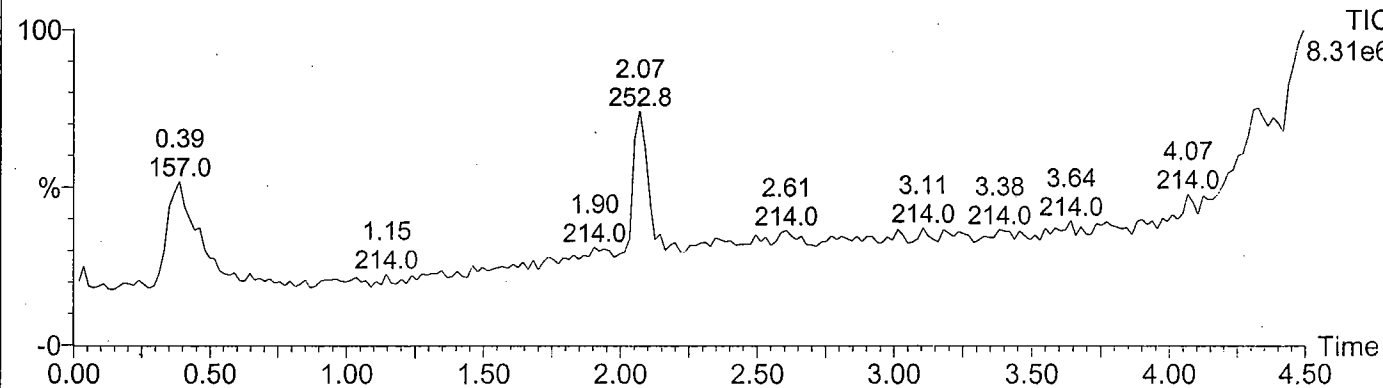


as-70977

Scan ES+

TIC

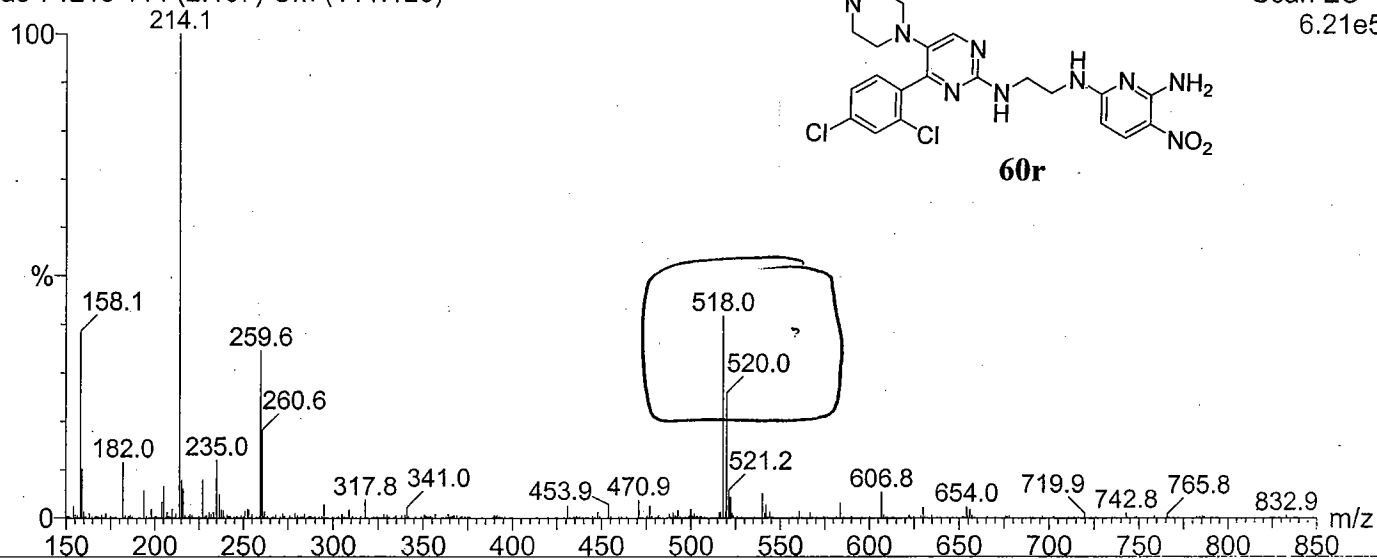
8.31e6



02-Dec-2004

2:21

as-71219 114 (2.107) Cm (111:120)

Scan ES+
6.21e5

02-Dec-2004

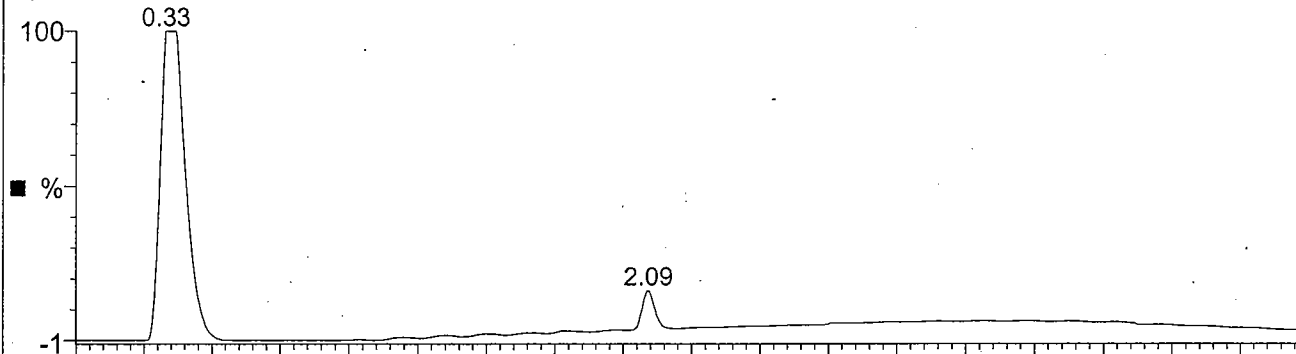
2:21

as-71219

214nm

An1

1.00e6

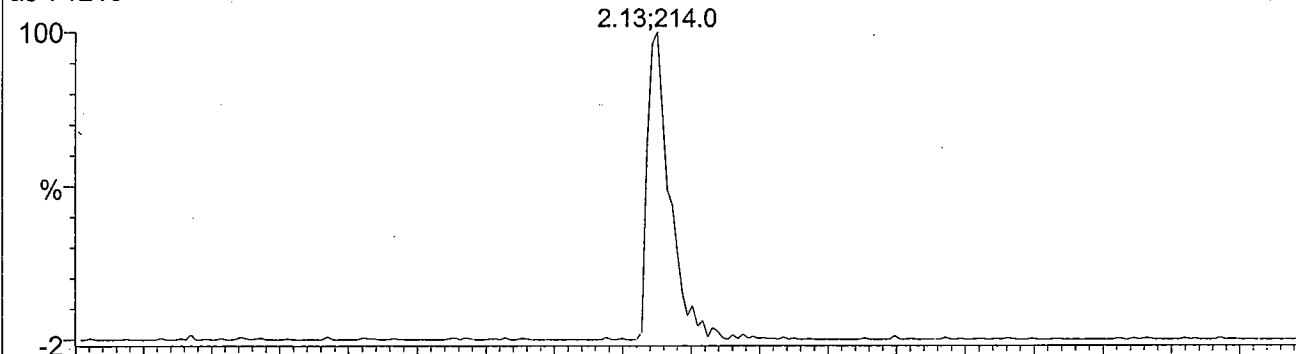


as-71219

Scan ES+

518

5.46e5

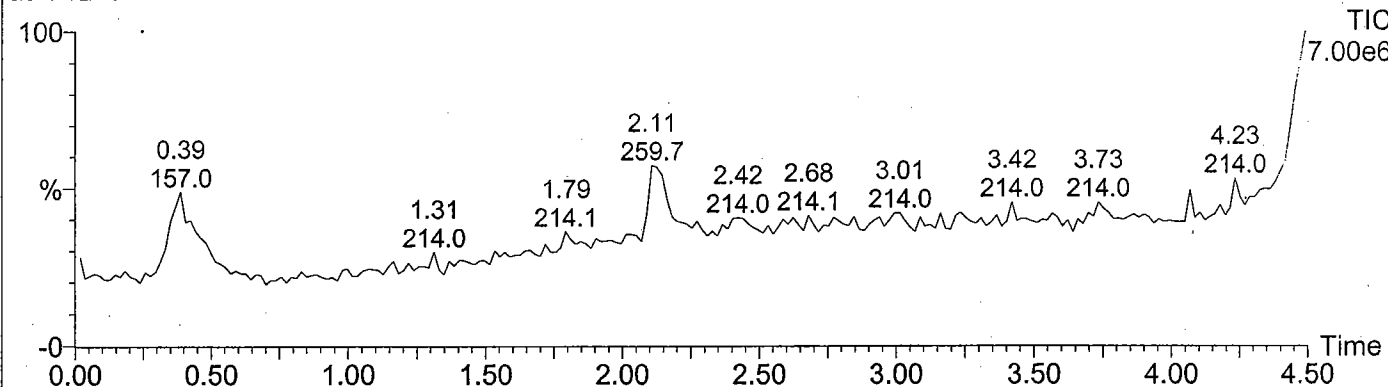


as-71219

Scan ES+

TIC

7.00e6



Sample Name zn230-35xHCl

Injection Volume 20.00 µl

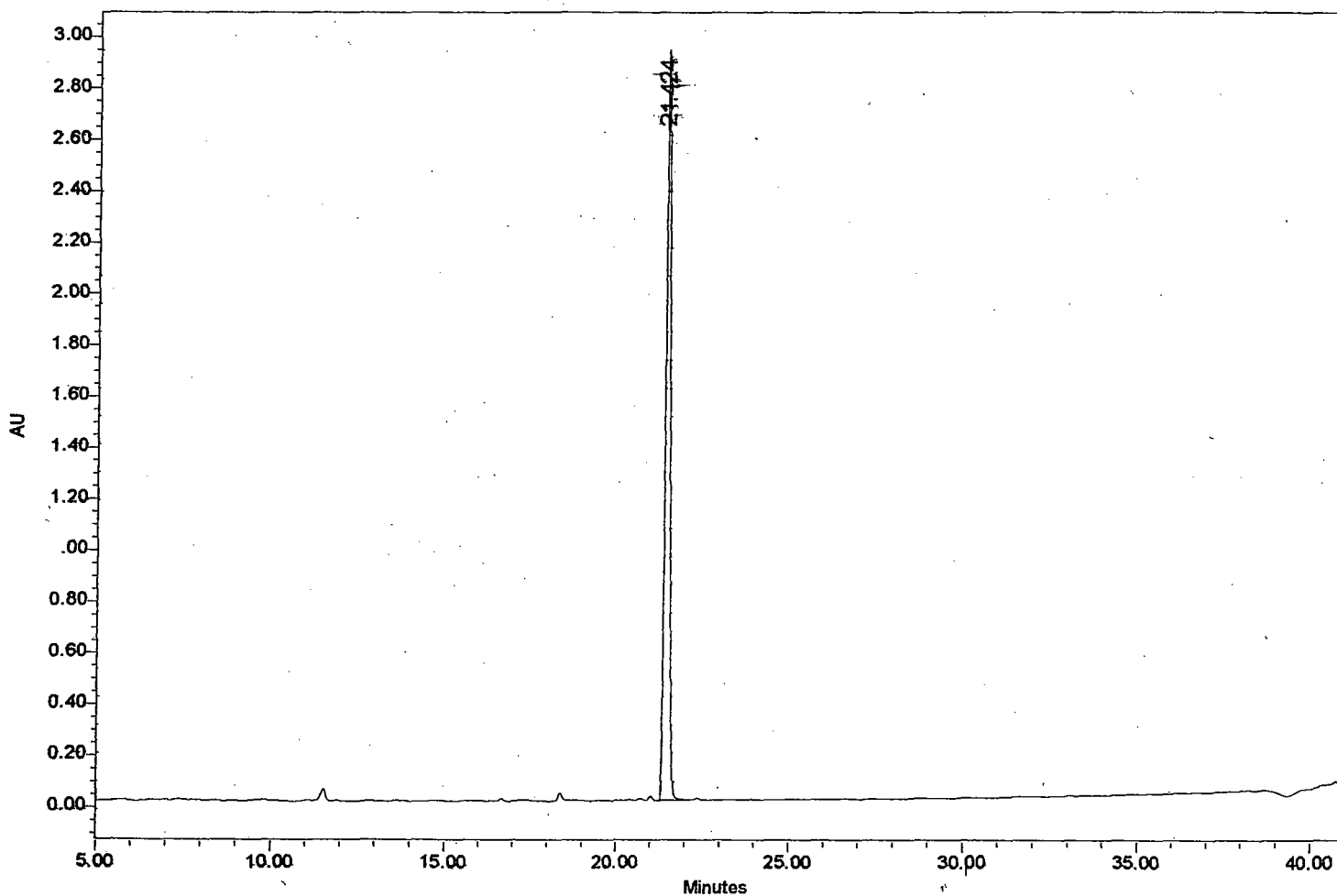
Date Acquired 10/27/99 12:34:15 PM

Vial 1

Channel Description PDA 220.0 nm

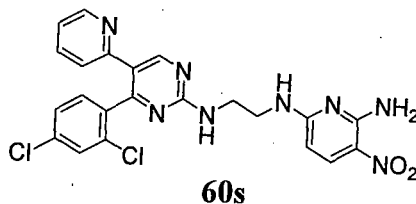
Acq Method Set 5100

~~Auto-1-1-1 Chromatogram~~



Peak Results

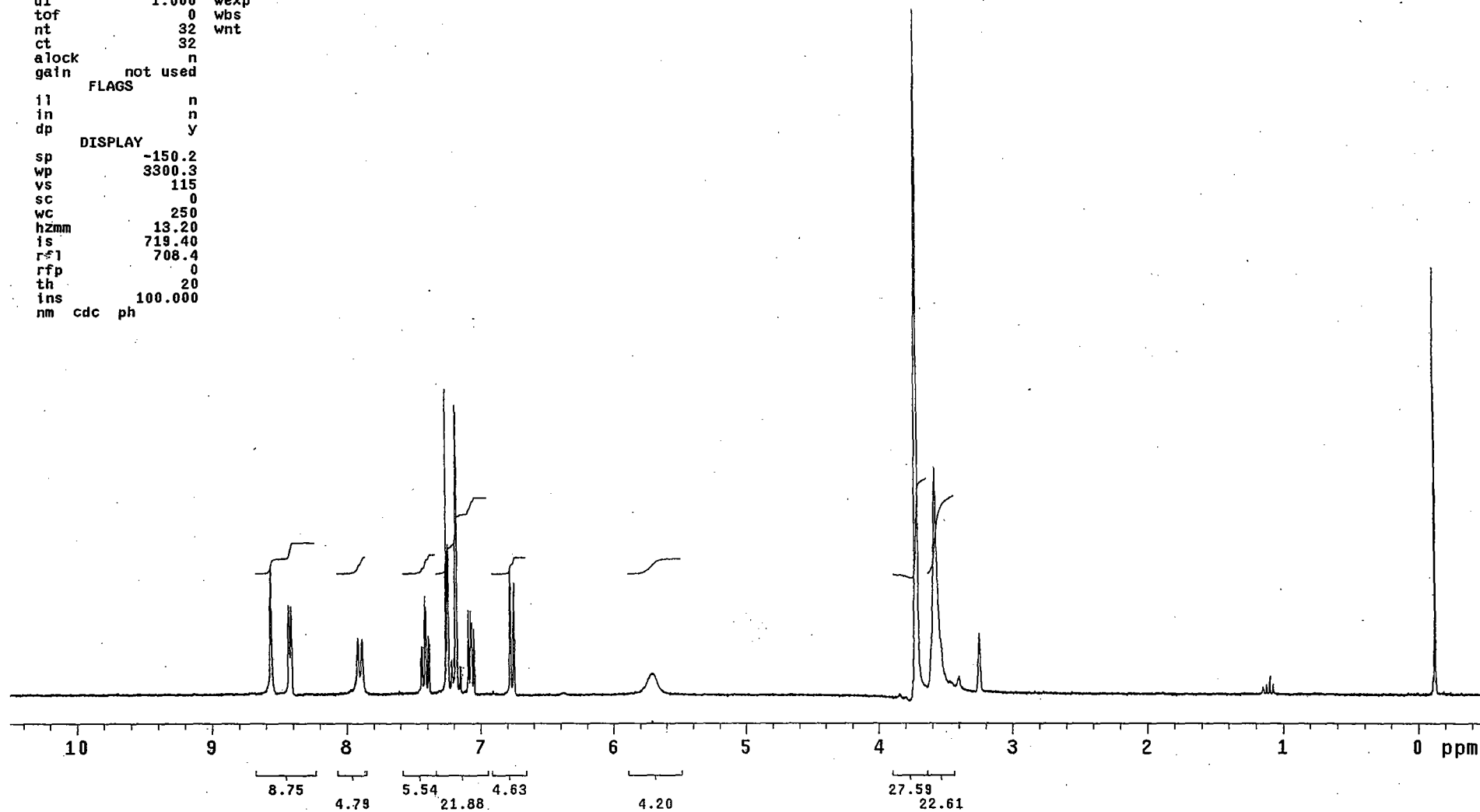
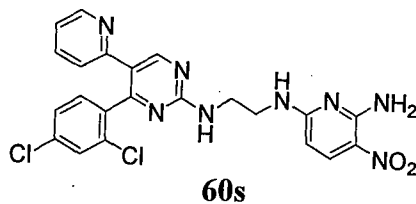
	RT	Start Time	End Time	% Height	% Area
1	21.424	21.183	22.167	100.00	100.00



zn230-35p-

exp1 std1h

SAMPLE		DEC. & VT	
date	Nov 8 1999	dfrq	300.038
solvent	CDCl3	dn	H1
file	exp	dpwr	47
ACQUISITION		dof	0
sfrq	300.038	dm	nnn
tn	H1	dmm	c
at	1.998	dmf	11500
np	17984	PROCESSING	
sw	4500.5	wtfile	
fb	2600	proc	ft
bs	4	fn	not used
tpwr	62		
pw	8.4	werr	
d1	1.000	wexp	
tof	0	wbs	
nt	32	wnt	
ct	32		
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-150.2		
wp	3300.3		
vs	115		
sc	0		
wc	250		
hzmm	13.20		
is	719.40		
rfl	708.4		
rff	0		
th	20		
ins	100.000		
nm	cdc ph		



SampleName kpD98HCL

Injection Volume 15.00 μ l

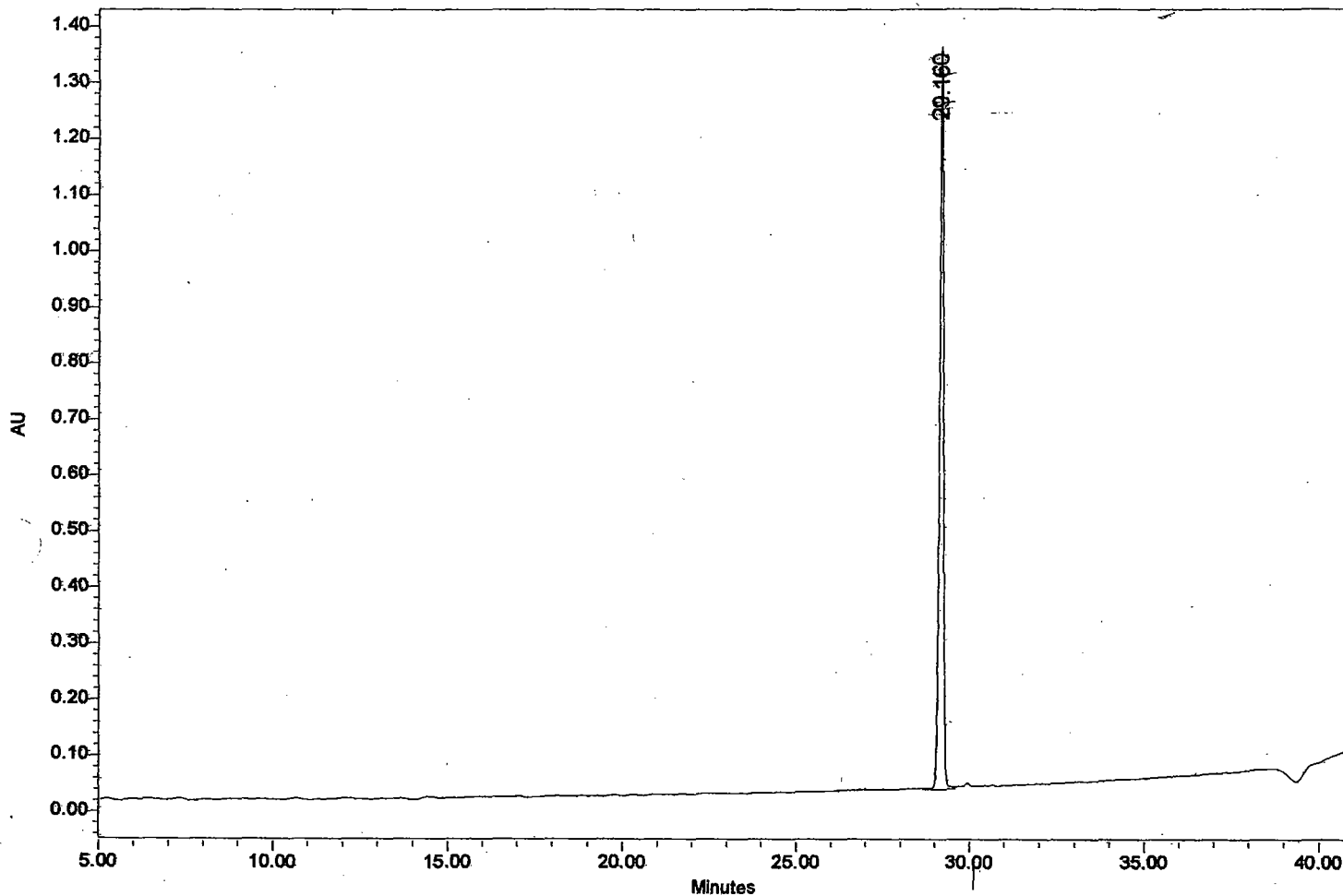
Date Acquired 10/6/99 5:50:29 PM

Vial 31

Channel Description PDA 220.0 nm

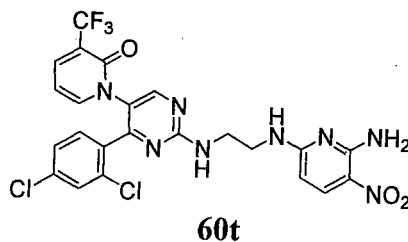
Acq Method Set 5100

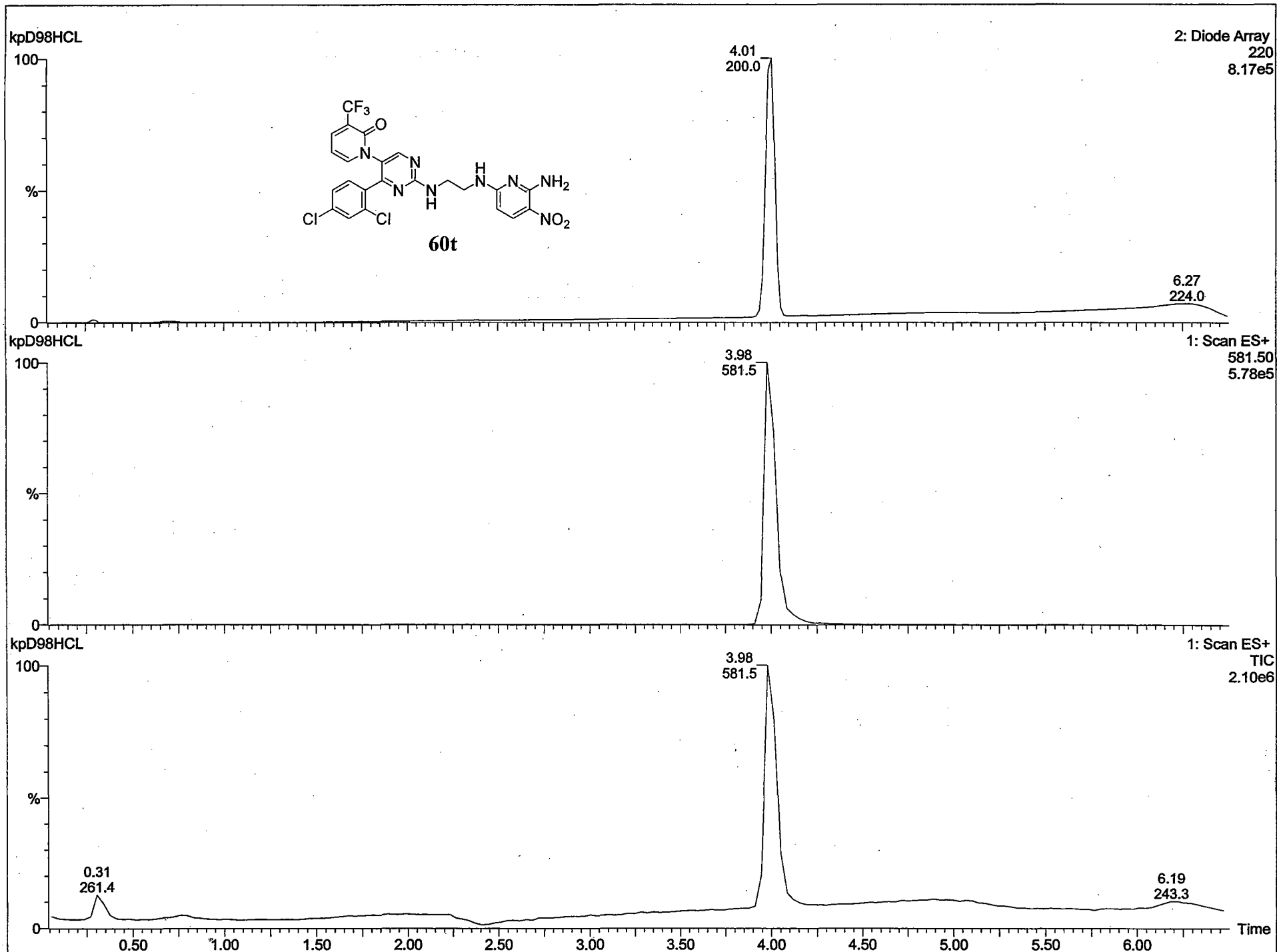
~~Auto-Scaled Chromatogram~~



Peak Results

	RT	Start Time	End Time	% Height	% Area
1	29.160	28.650	29.583	100.00	100.00

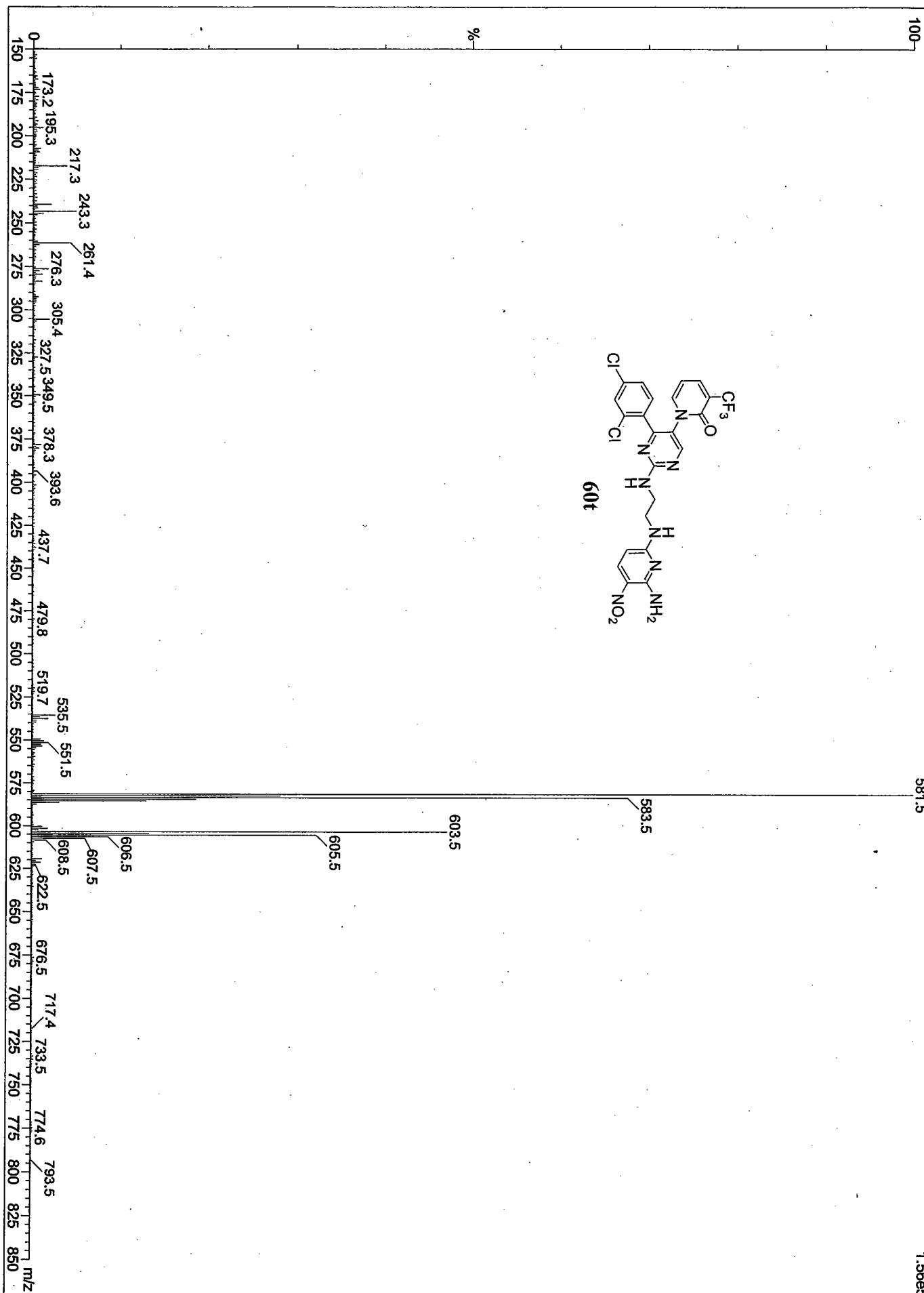
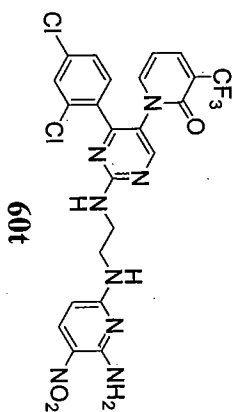




KPD98HCL 113 (3.980) Cm (11:1:118)

581.5

1: Scan ES+
1.56e5



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1

Solvent: DMSO

Temp. 25.0 C / 298.1 K

Mercury-300 "nmr300"

Relax. delay 1.000 sec

Pulse 37.5 degrees

Acq. time 1.998 sec

Width 4500.5 Hz

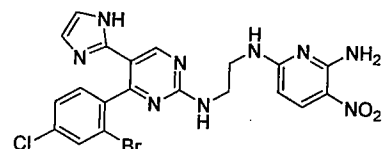
128 repetitions

OBSERVE H1, 300.0303526 MHz

DATA PROCESSING

FT size 32768

Total time 6 min, 38 sec



61r HCl Salt

