

Supporting Informations

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Contents:

1. Instrumentation and Chemicals
2. Crystallographic description.
3. Spectra of all compounds

Instrumentation and Chemicals

All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulfate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F₂₅₄ (0.25mm). Melting points were recorded on melting point apparatus and are uncorrected. IR spectra were recorded on IR spectrophotometer. NMR spectra were recorded in CDCl₃ with tetramethylsilane as the internal standard for ¹H NMR (400 MHz) CDCl₃ solvent as the internal standard for ¹³C NMR (100 MHz.) MS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat. ¹H and ¹³C NMR spectra were recorded on Varian 400 and Bruker 600 spectrometer by using TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm).

Elemental analyses were carried out using analyzer. Column chromatographic separations were performed using Merck silica gel (60-120 mesh).

Crystallographic Description

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoK α radiation ($\lambda = 0.71073 \text{ \AA}$) at 298 K. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. The structure was solved by direct methods implemented in SHELX-97 program and refined by full-matrix least-squares methods on F². All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions.

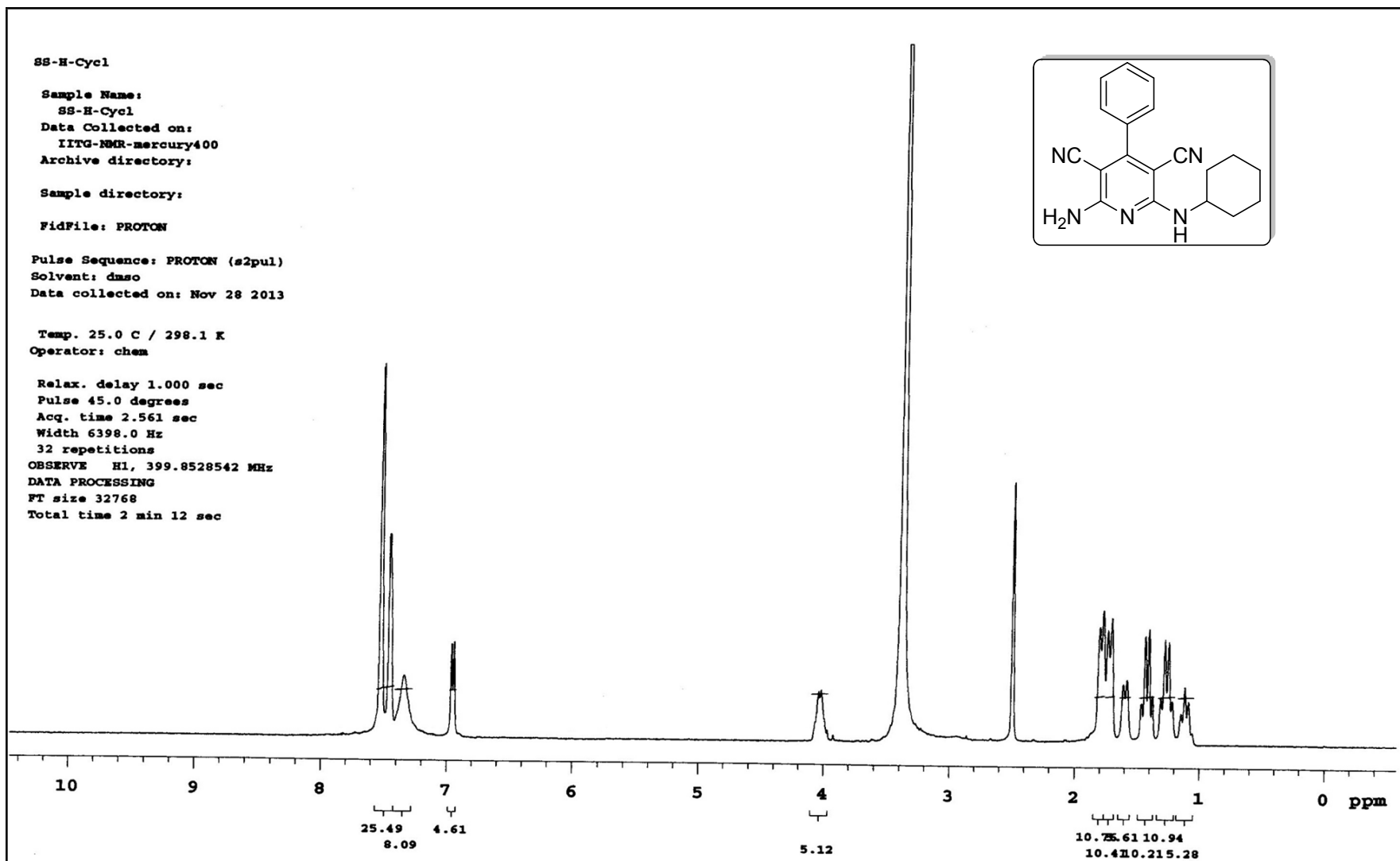
Table S1. Crystal data and structure refinement for **4a** and **6d**. For atomic coordinates and equivalent isotropic displacement parameters and bond angles, please check the CIF.

	Compound (CCDC)	Compound (CCDC)
Identification code	SS- 4a	SS- 6d
Empirical formula	'C ₁₉ H ₁₉ N ₅ '	'C ₂₀ H ₁₆ ClN ₅ '
Formula weight	318.1719	362.1172
Temperature	298(2) K	296(2) K
Wavelength	0.71073 \AA	0.71073 \AA
Crystal system	Triclinic	Monoclinic
Space group	P-1	P 21/n

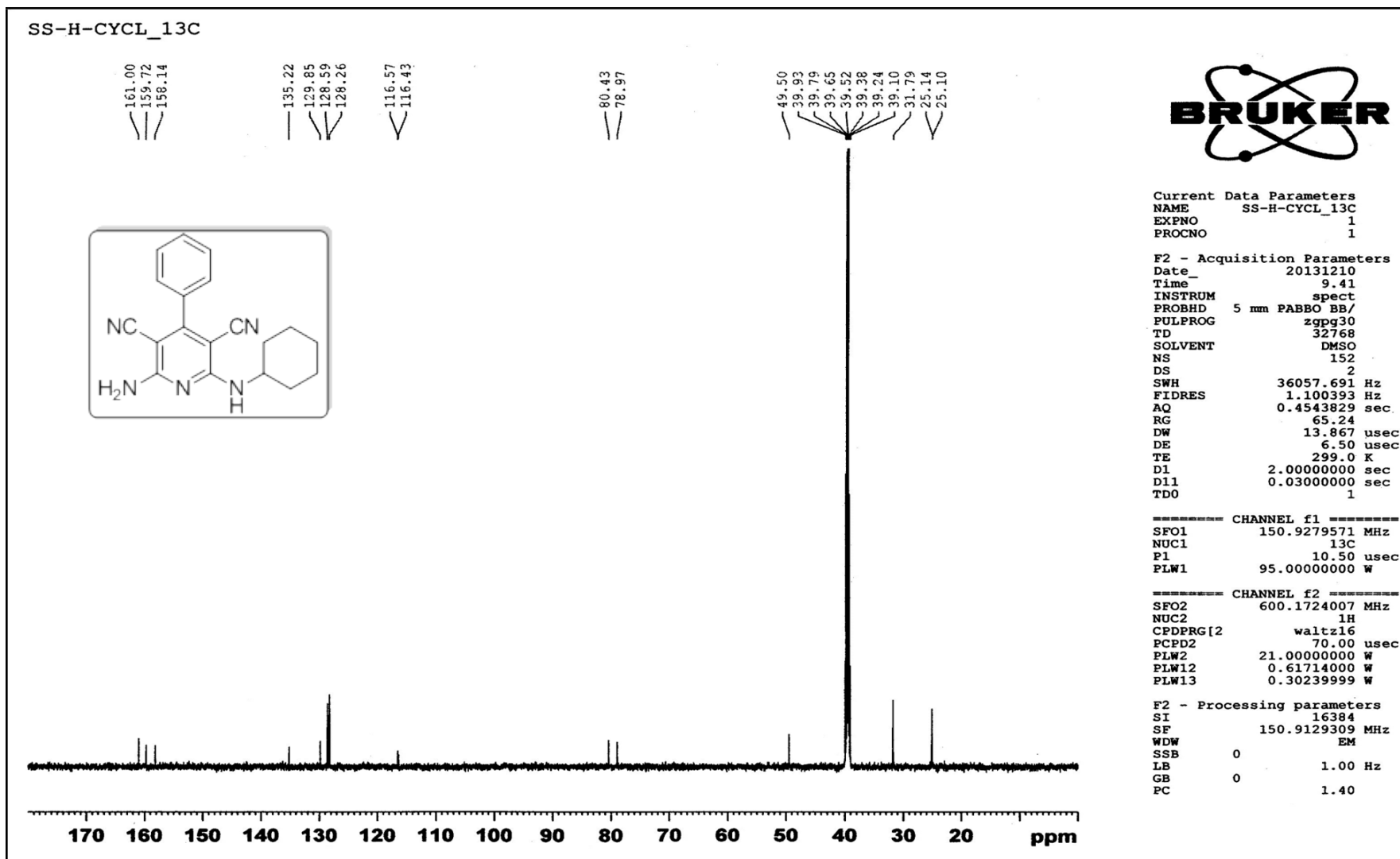
Unit cell dimensions		
a	8.5845(3) Å	12.968(2)Å
b	10.8223(3) Å	10.2902(18)Å
c	12.5073(4) Å	13.385(2)Å
α	84.207(2) °	90.00°
β	72.287(2) °	98.889(12)°
γ	75.180(2) °	90.00°
Volume	1069.73(6) Å ³	1764.7(5)Å ³
Z	2	4
Density (calculated)	1.228 g/cm ³	1.362g/cm ³
Absorption coefficient	0.172 mm ⁻¹	0.230 mm ⁻¹
F(000)	420.0	752
Theta range for data collection	1.71 to 28.42 °	2.04 to 24.99 °
Index ranges	-11<=h<=11, -13<=k<=13, -16<=l<=14	-15<=h<=15, -11<=k<=12, -15<=l<=15
Reflections collected	13065	12046
Independent reflections	5294 R _{int} = 0.0606	2962 R _{int} = 0.1004
Completeness to θ°	98.3 % ($\theta = 28.42^\circ$)	95.4% ($\theta = 24.99^\circ$)
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2

Data / restraints / parameters	5294 / 0 / 268	2962 / 0 / 237
Goodness-of-fit on F2	1.086	1.010
Final R indices [$>2\sigma(I)$]	$R_{\text{obs}} = 0.0772$, $wR_{\text{obs}} = 0.2353$	$R_{\text{obs}} = 0.1537$, $wR_{\text{obs}} = 0.3668$
R indices (all data)	$R_{\text{all}} = 0.0952$, $wR_{\text{all}} = 0.2513$	$R_{\text{all}} = 0.1914$, $wR_{\text{all}} = 0.3821$
Largest diff. peak and hole	1.109 and $-1.204\text{e}\cdot\text{\AA}^{-3}$	0.964 and $-0.525\text{e}\cdot\text{\AA}^{-3}$

¹H-NMR spectra of compound 4a

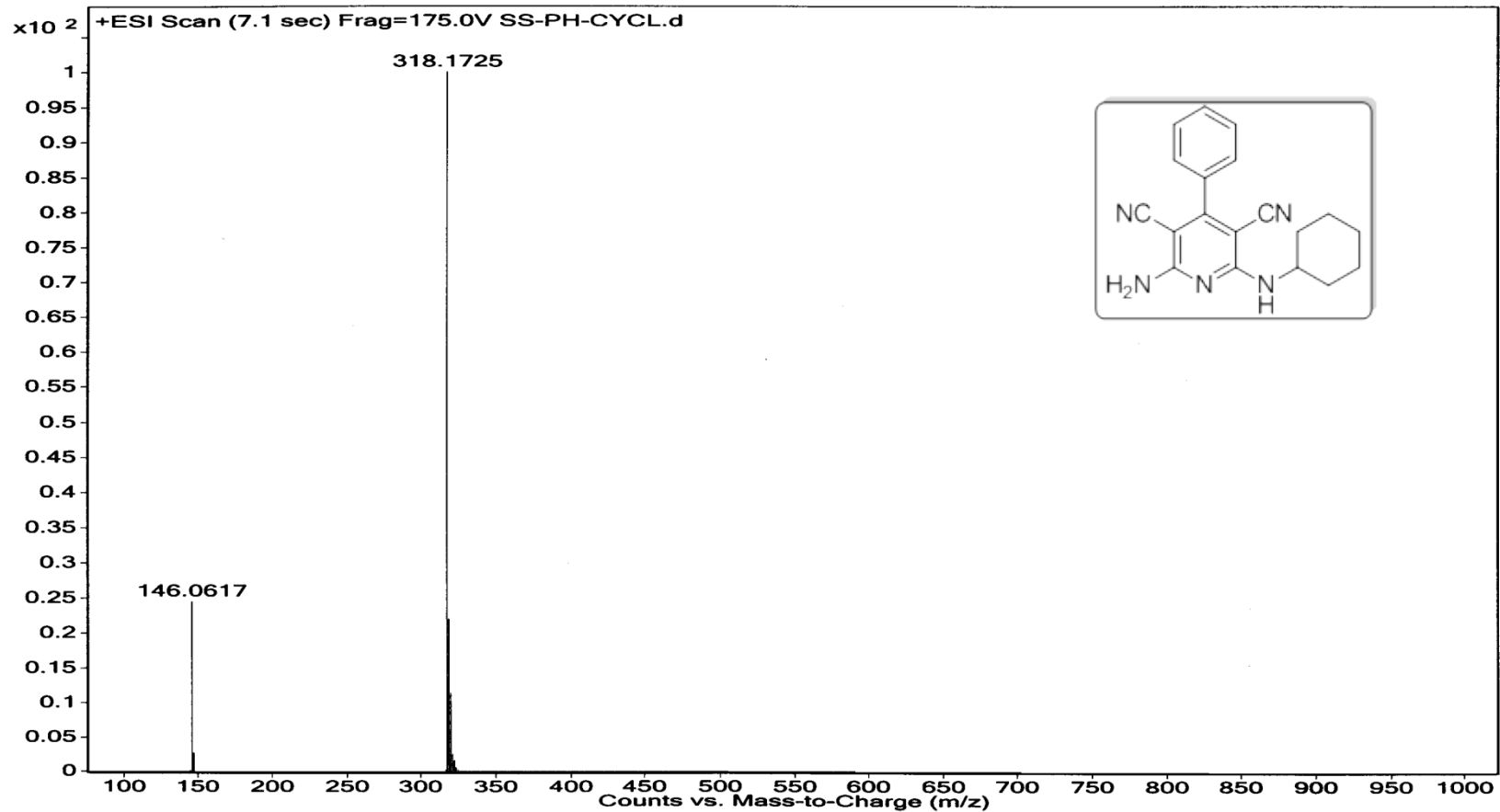


¹³C-NMR spectra of compound 4a

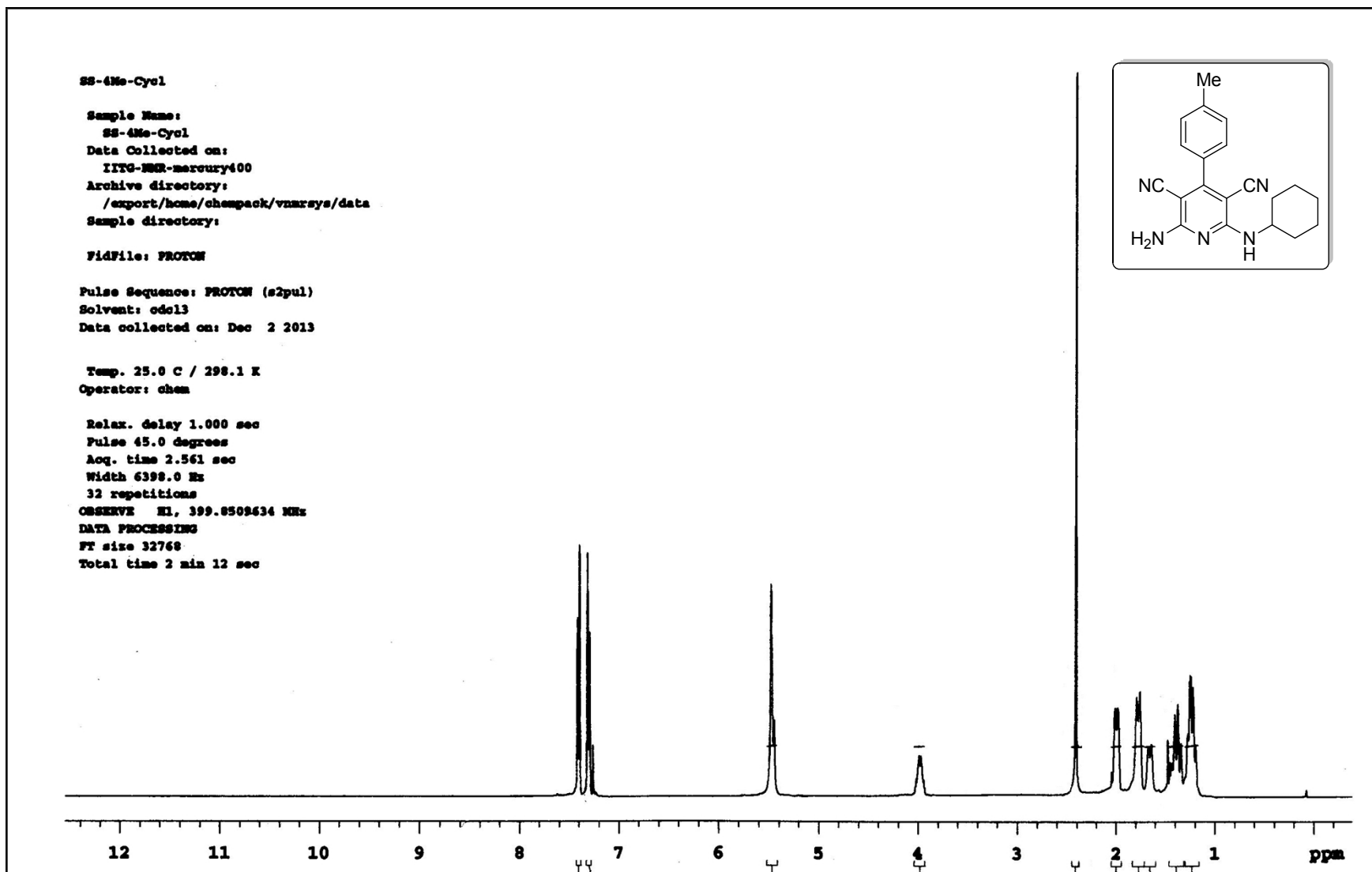


HRMS spectra of compound 4a

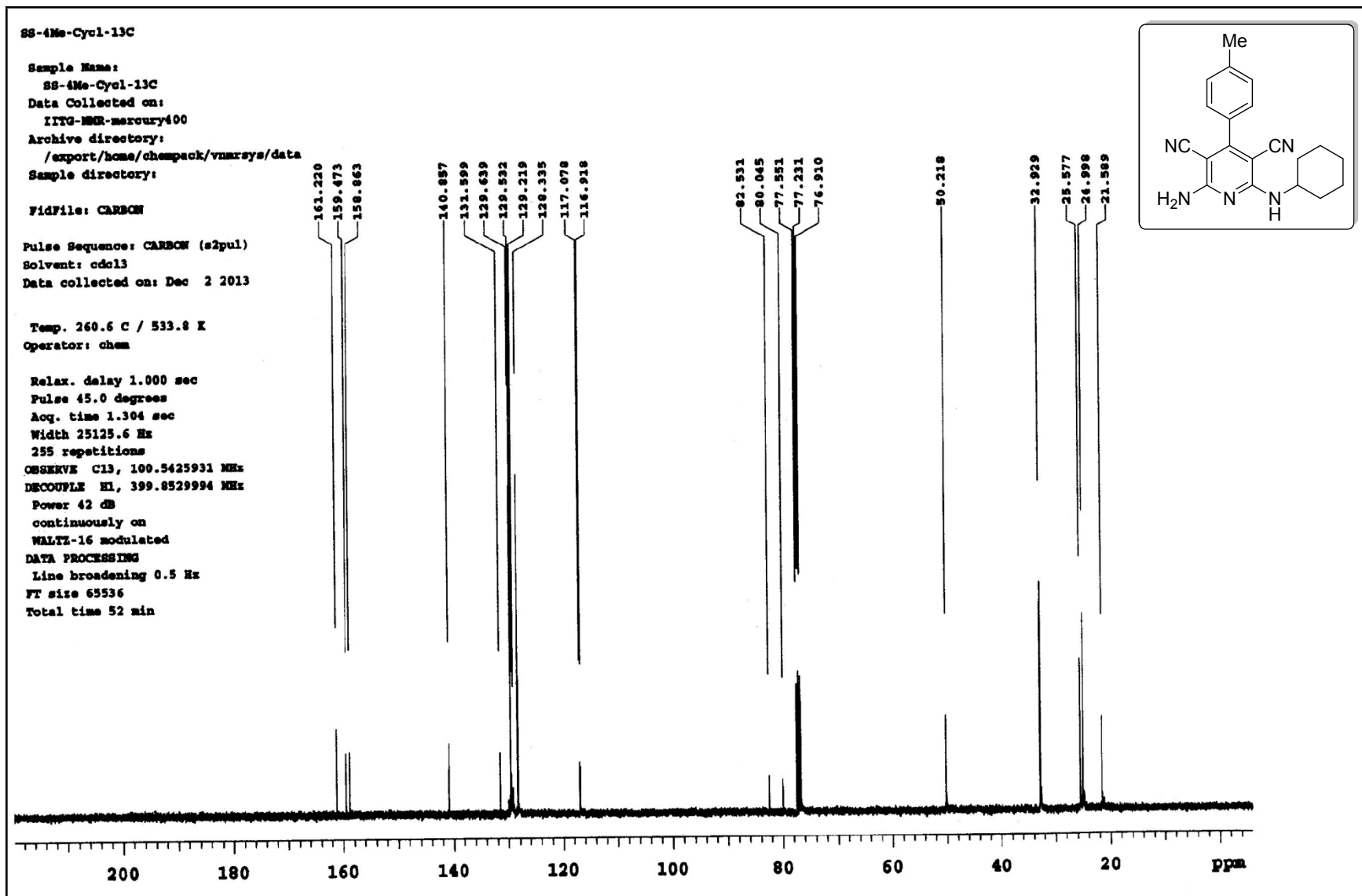
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¹H-NMR spectra of compound 4b



13C-NMR spectra of compound 4b



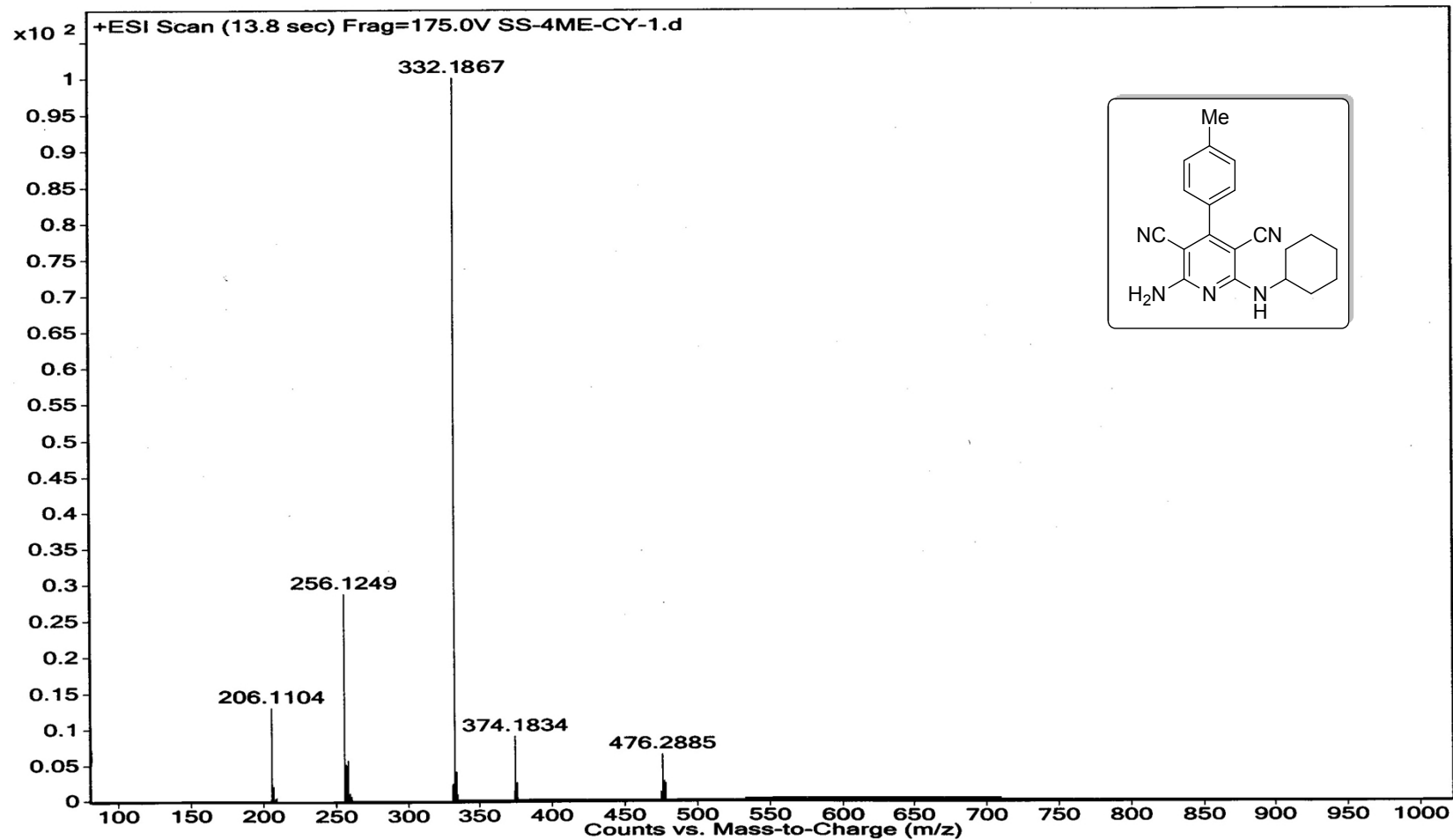
HRMS spectra of compound 4b

Sample Name
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Data Filename

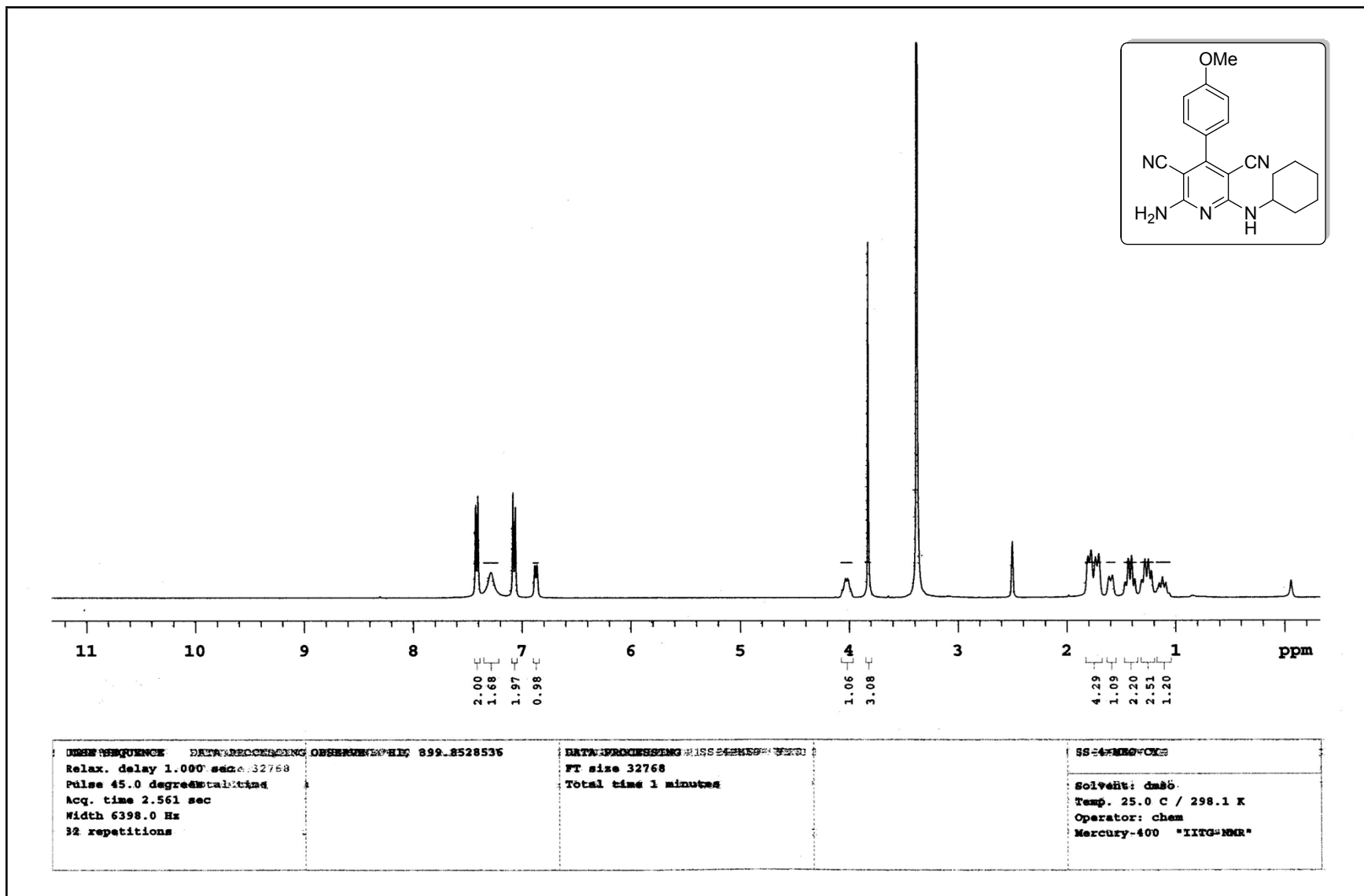
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Instrument Name
SampleType
Comment

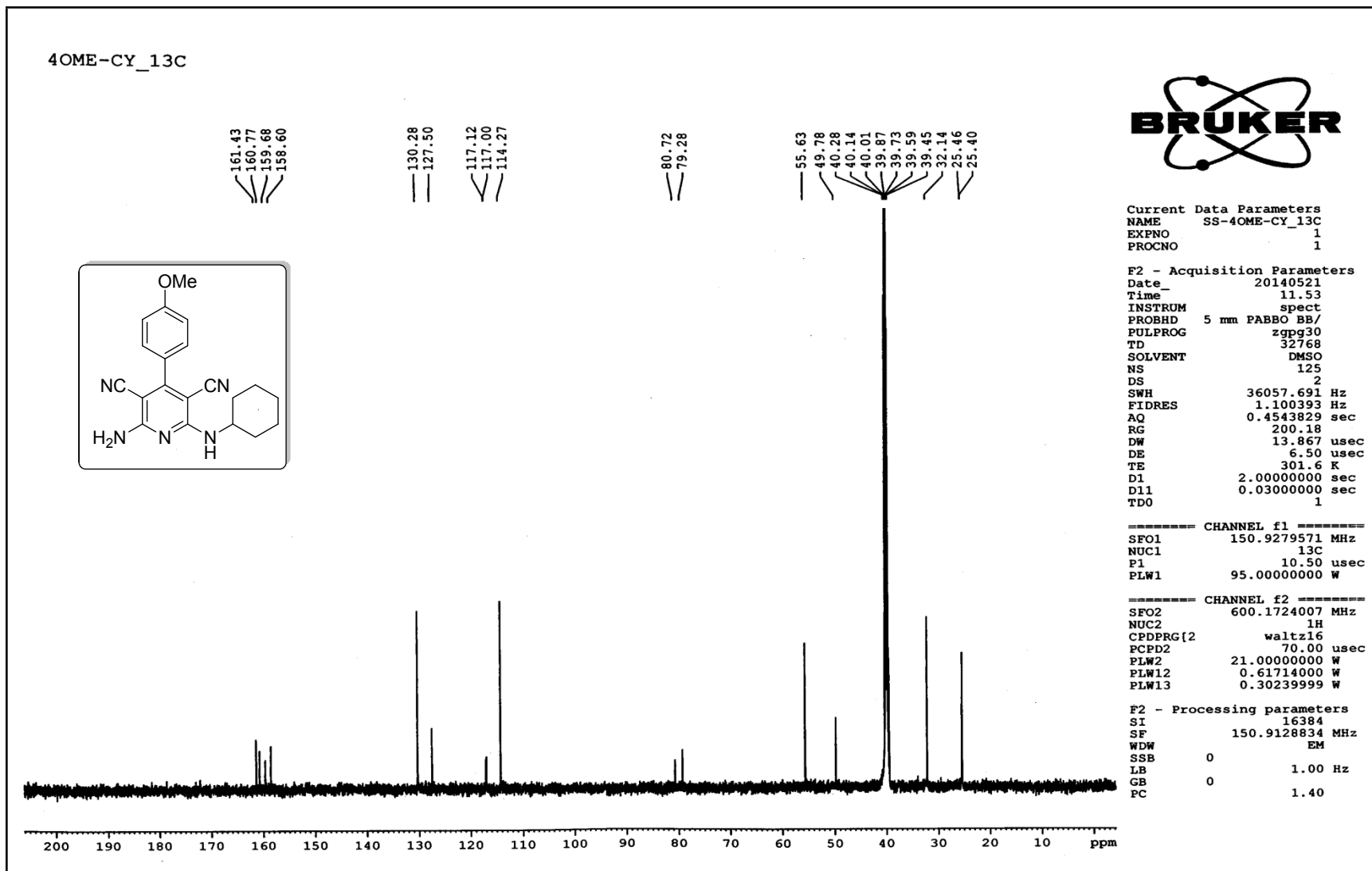
User Name
IRM Calibration Status
Acquired Time



¹H-NMR spectra of compound 4c

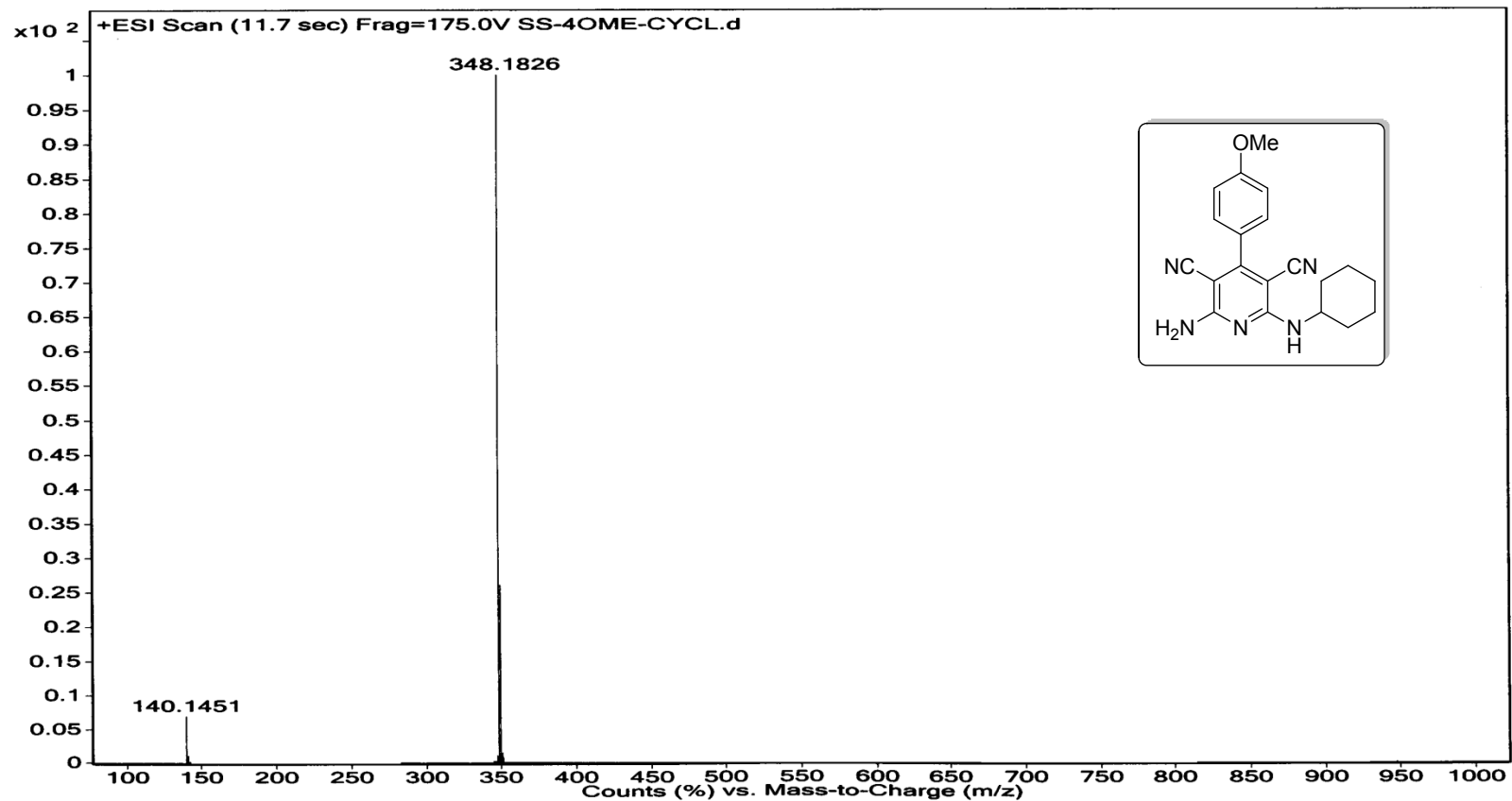


¹³C-NMR spectra of compound 4c

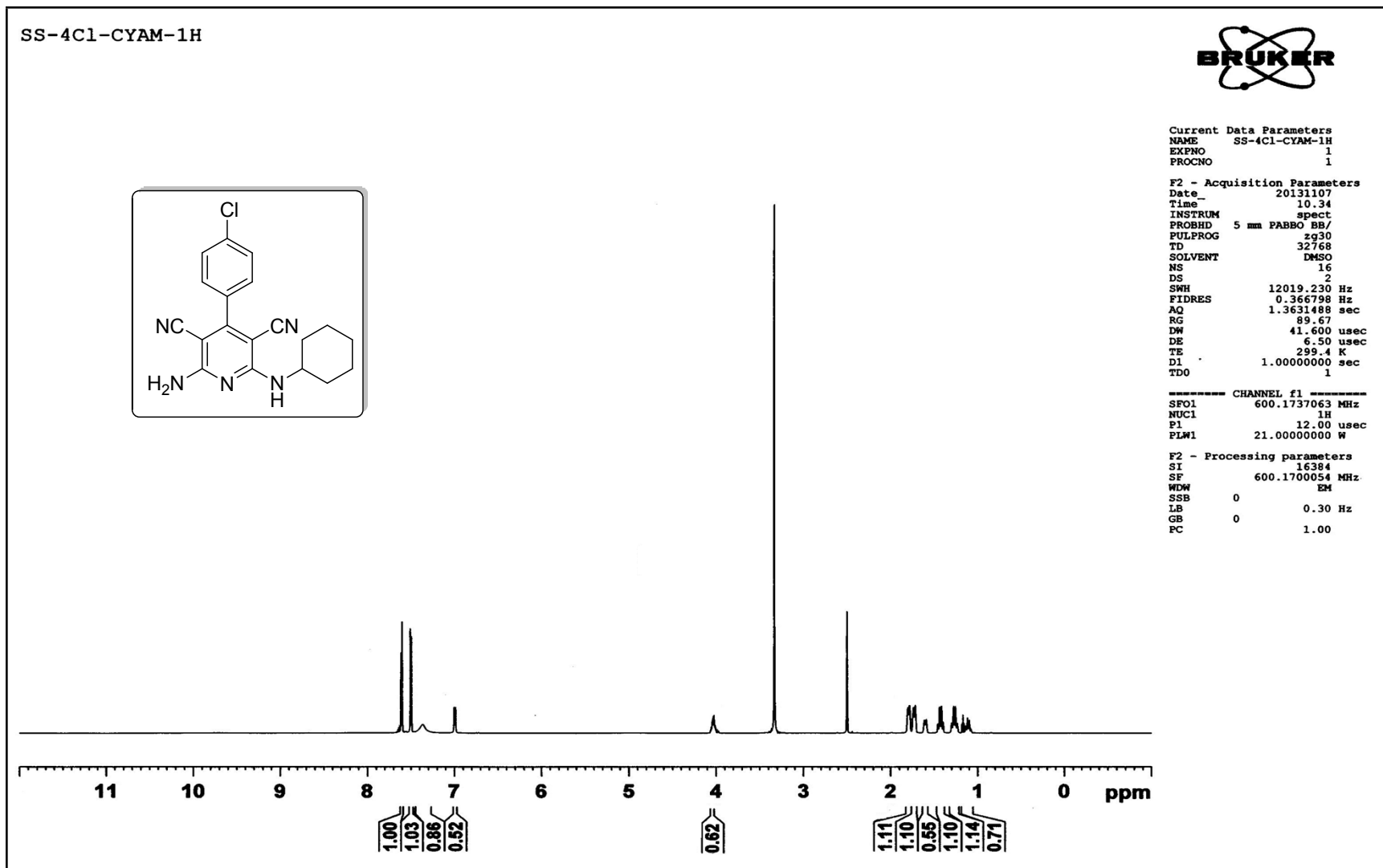


HRMS-spectra of compound 4c

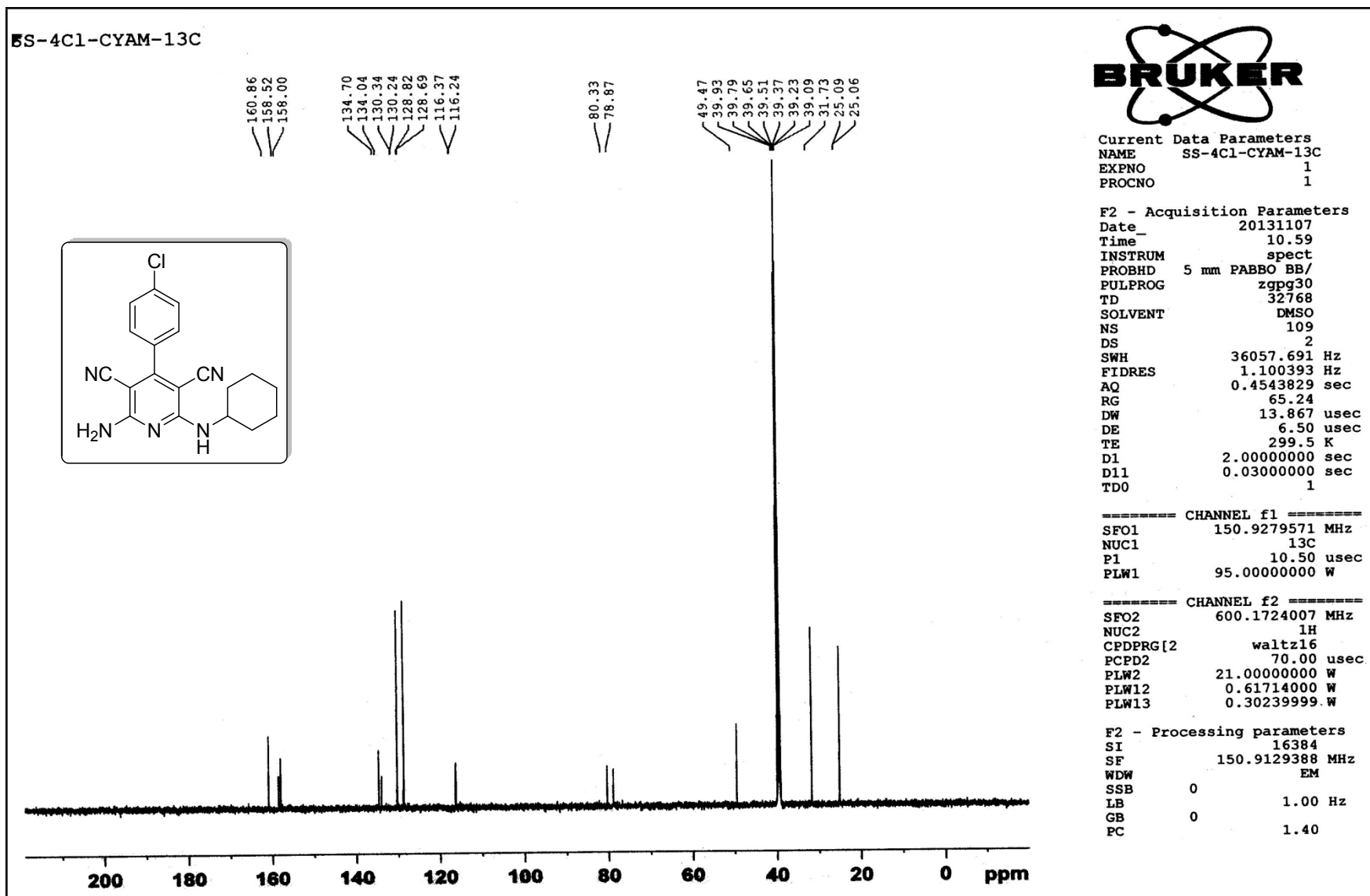
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¹H-NMR spectra of compound **4d**

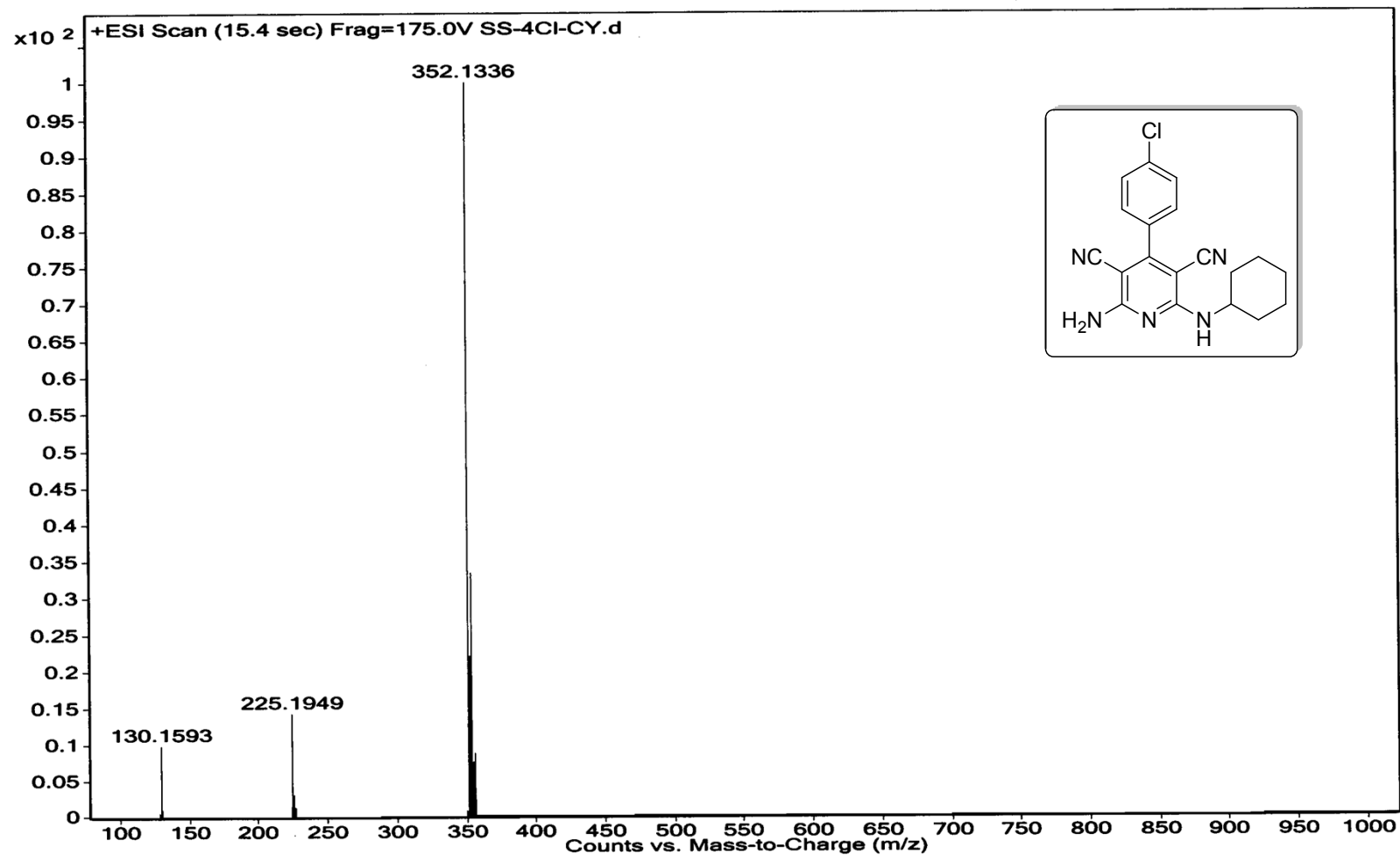


¹³C-NMR spectra of compound 4d

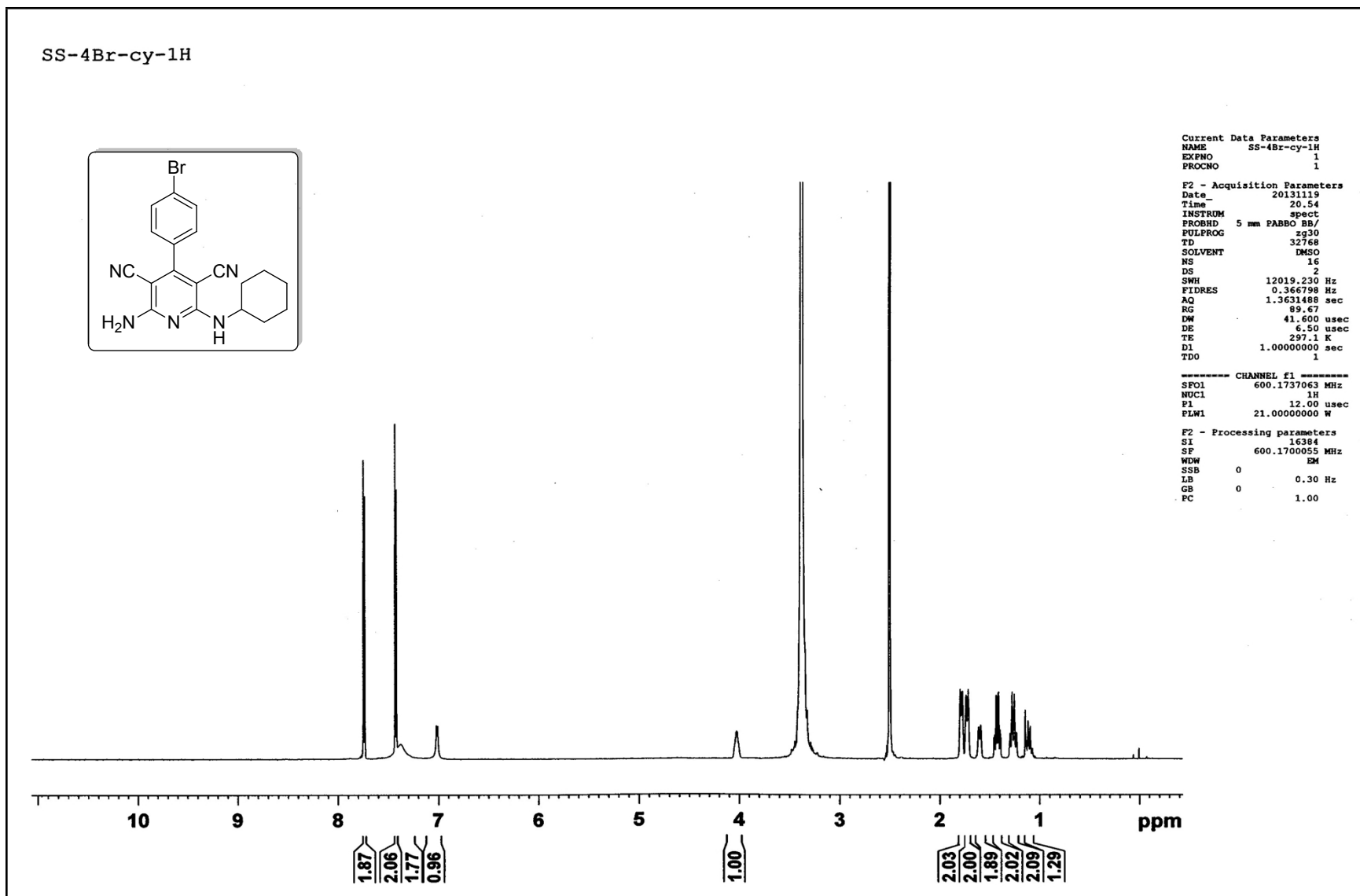


HRMS spectra of compound 4d

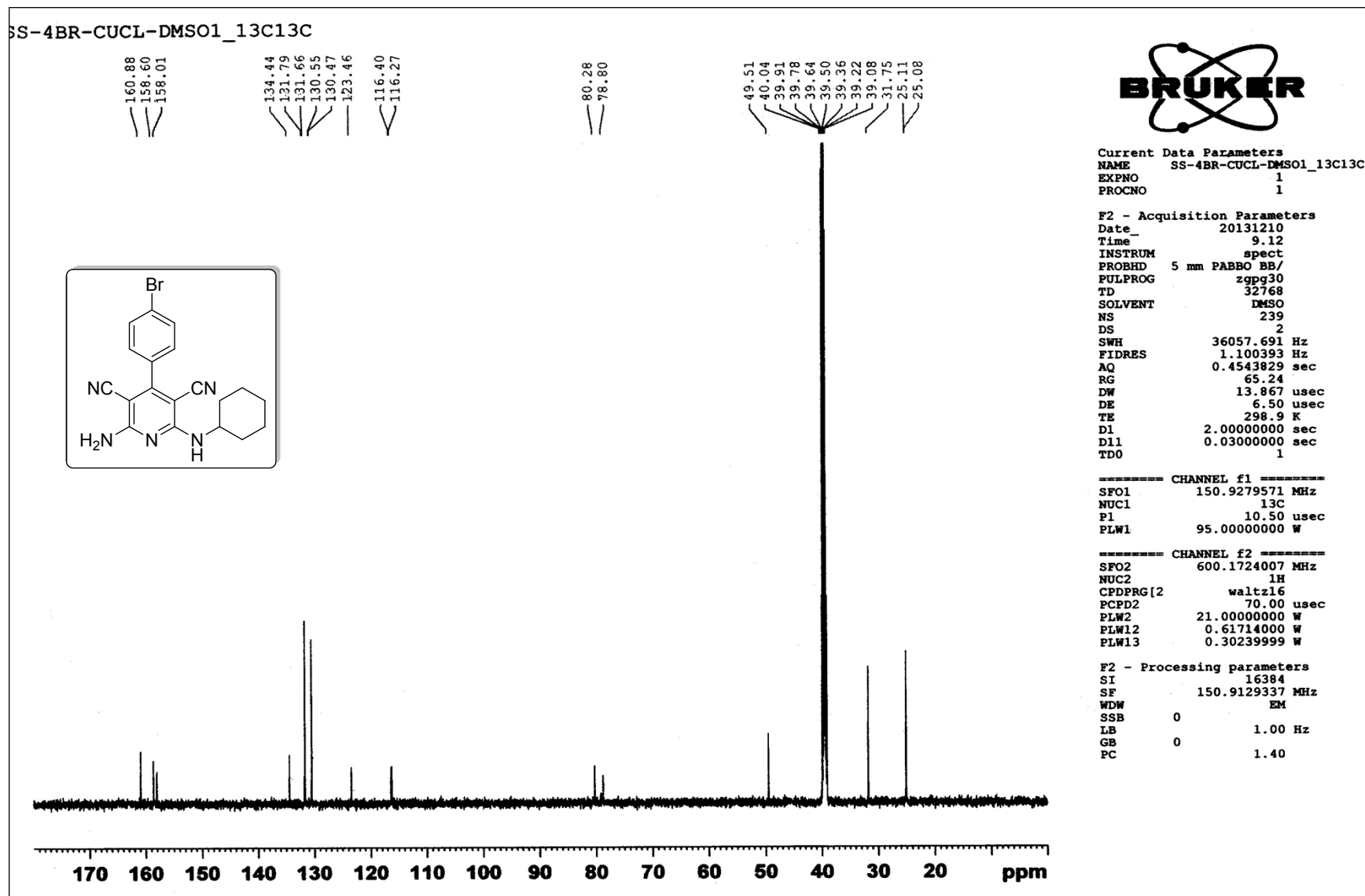
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¹H-NMR spectra of compound 4e

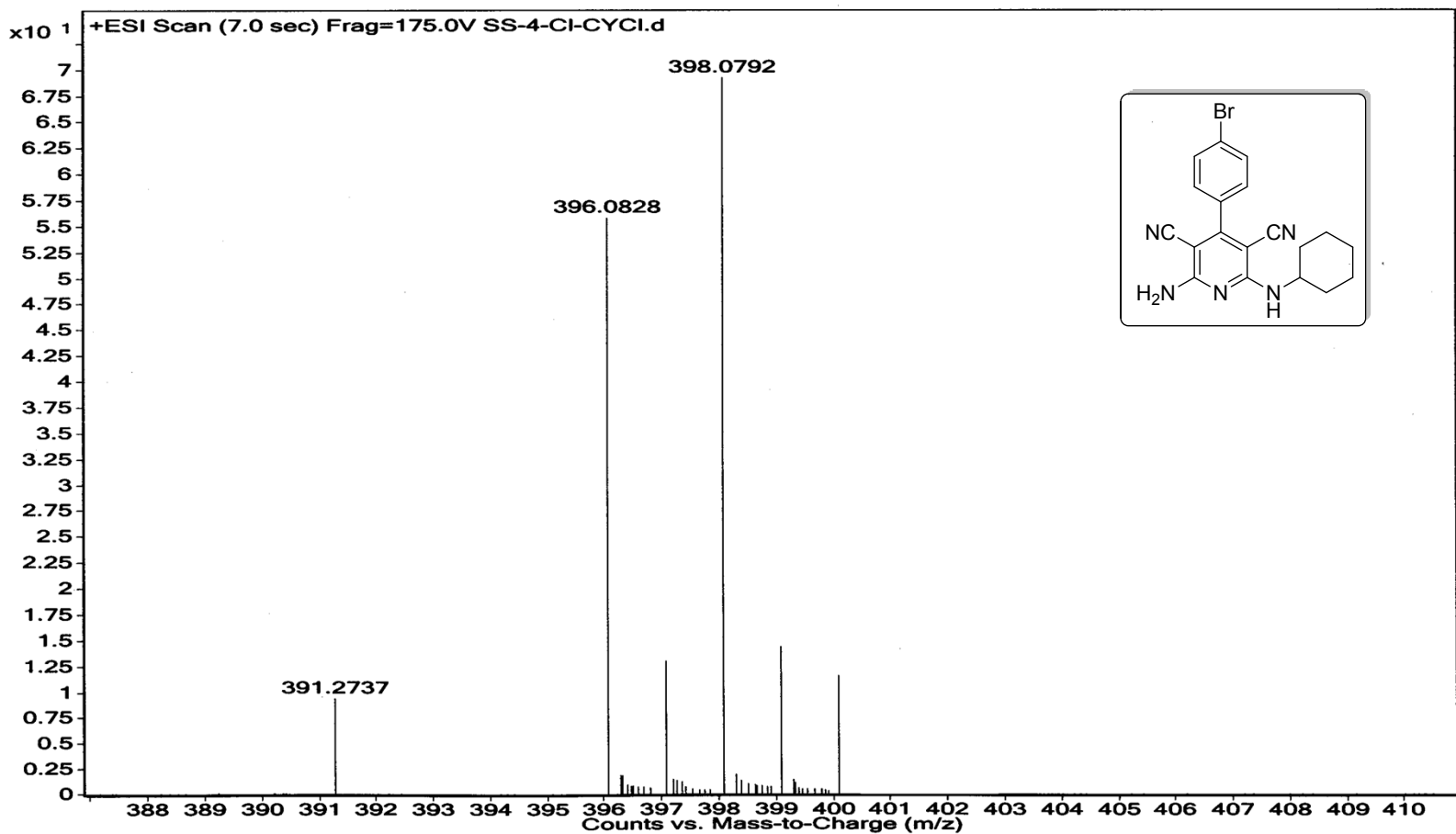


¹³C-NMR spectra of compound 4e



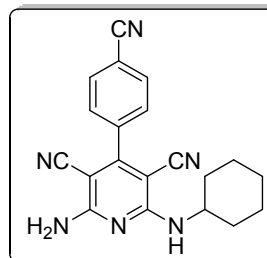
HRMS-spectra of compound 4e

Sample Name	SS-4-Cl-CYCl	Position	-1	Instrument Name	Instrument 1	User Name	
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¹H-NMR spectra of compound **4g**

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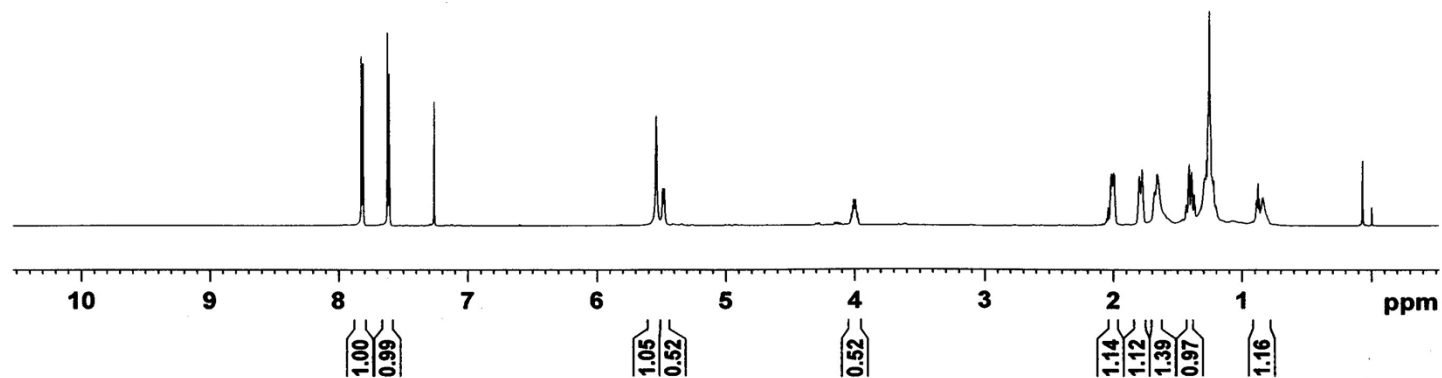


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PROCNO    1

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PULPROG   zg30
TD         32768
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FIDRES     0.366798 Hz
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D1         1.00000000 sec
TDO        1

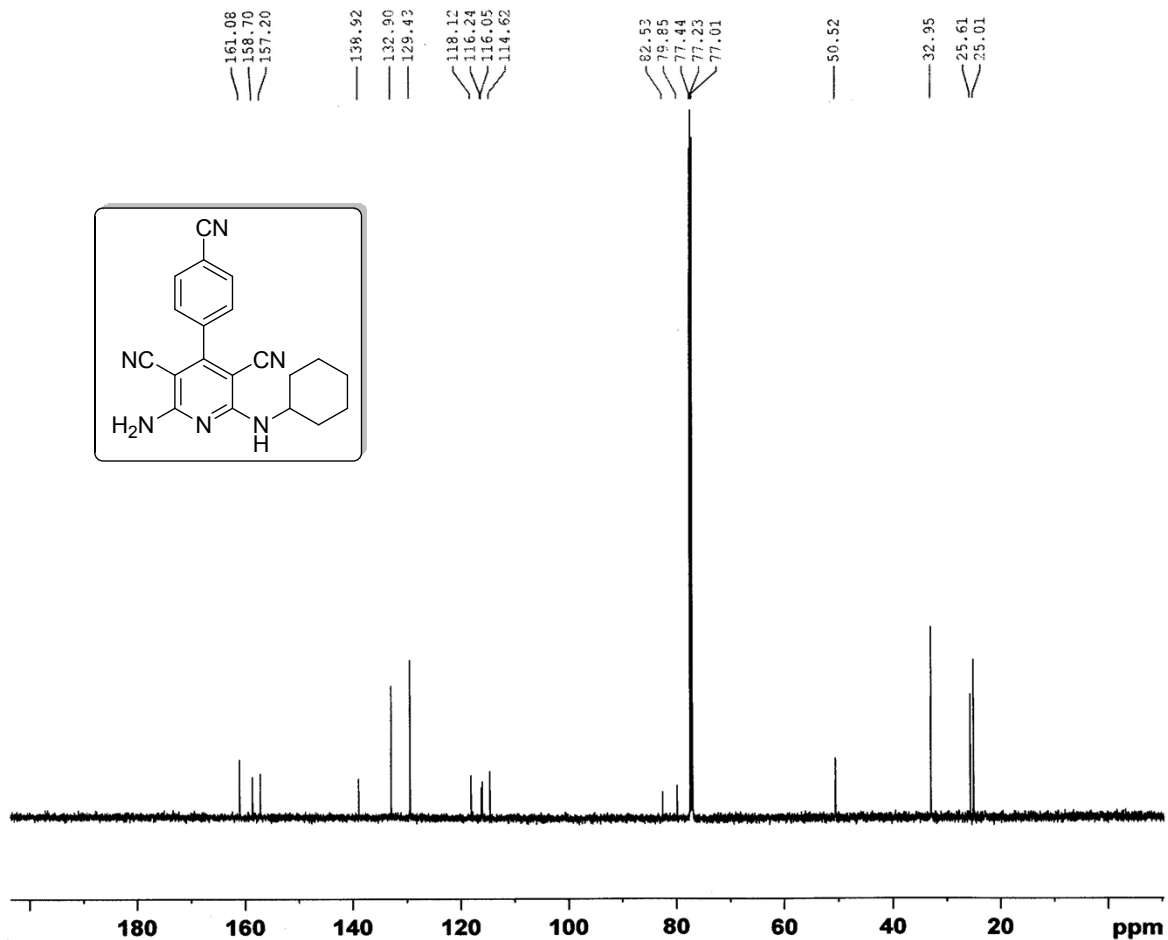
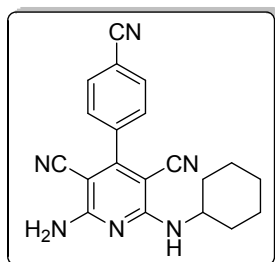
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¹³C-NMR spectra of compound 4g

4CN-CY-13C



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 PROCNO 1

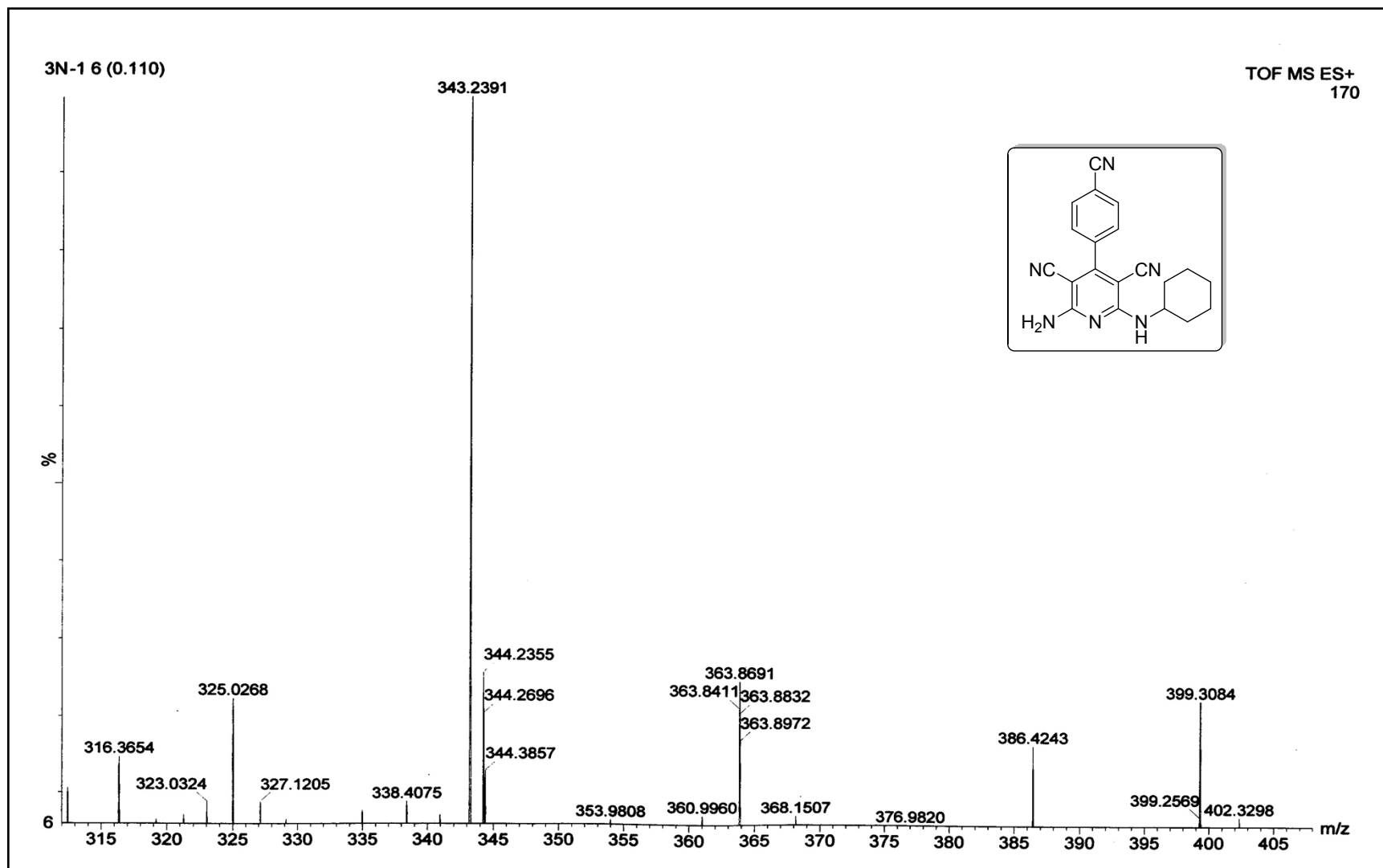
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 AQ 0.4543829 sec
 RG 65.24
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 TE 300.3 K
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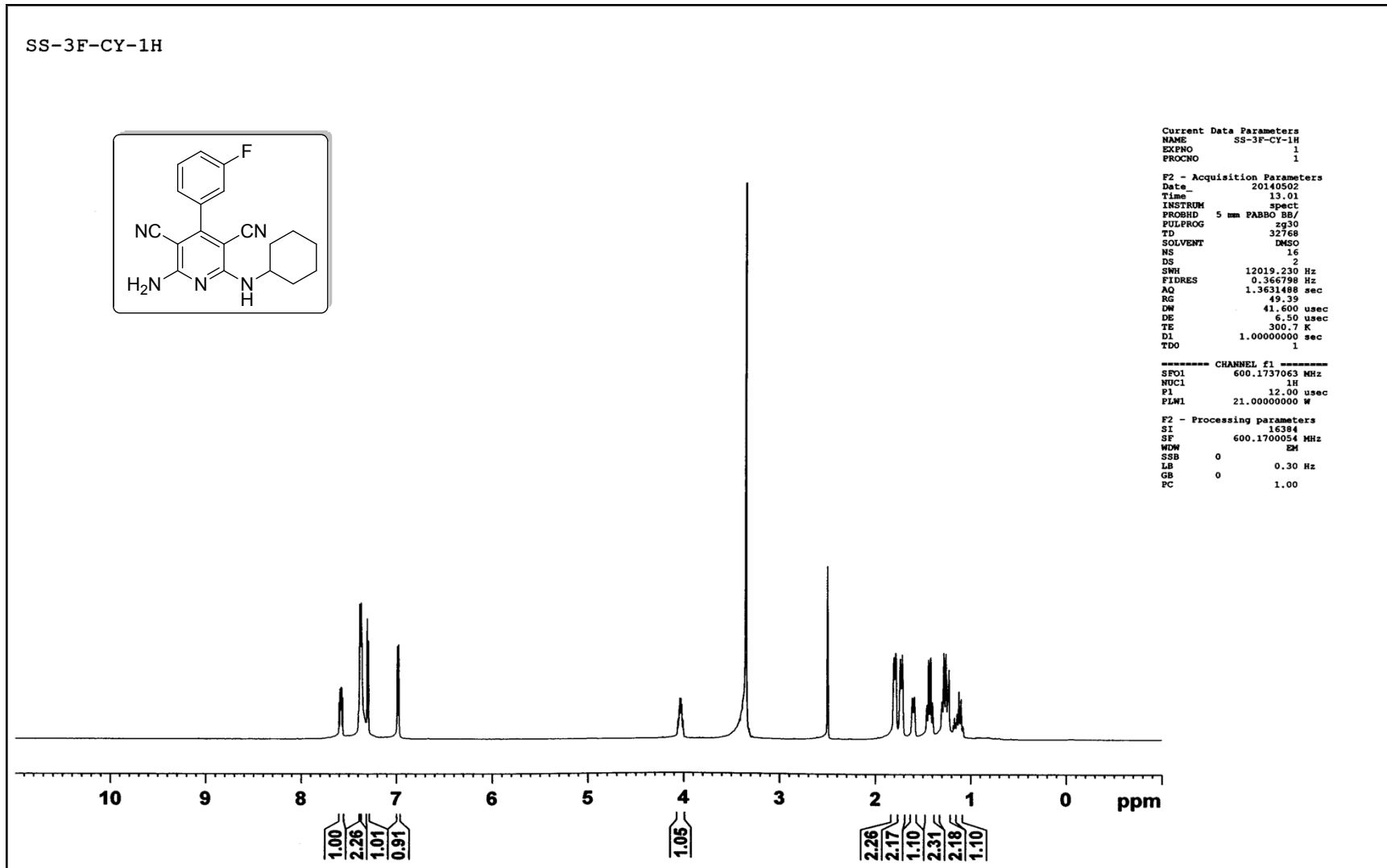
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 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
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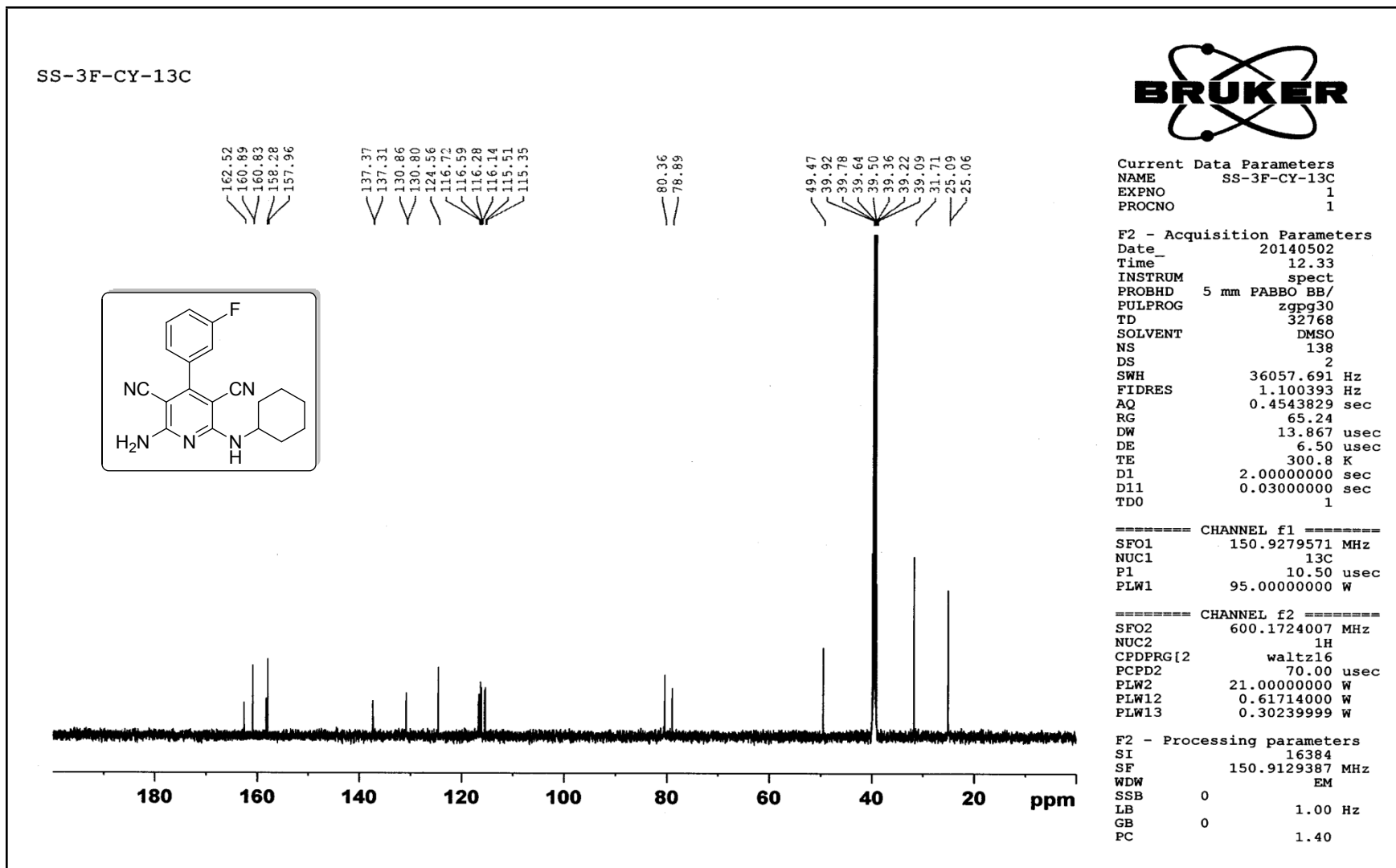
HRMS spectra of compound 4g



¹H-NMR spectra of compound **4h**

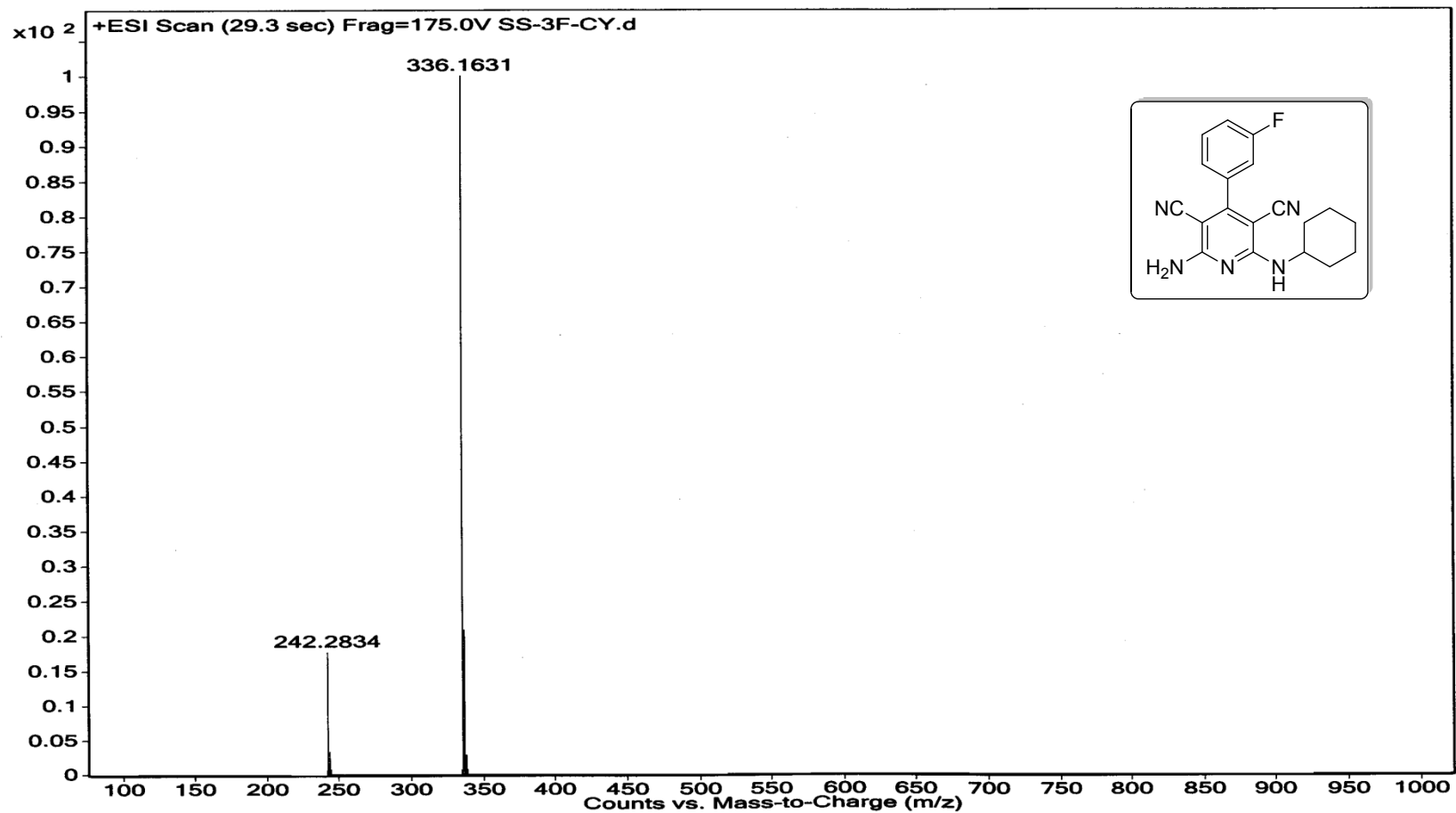


¹³C-NMR spectra of compound 4h

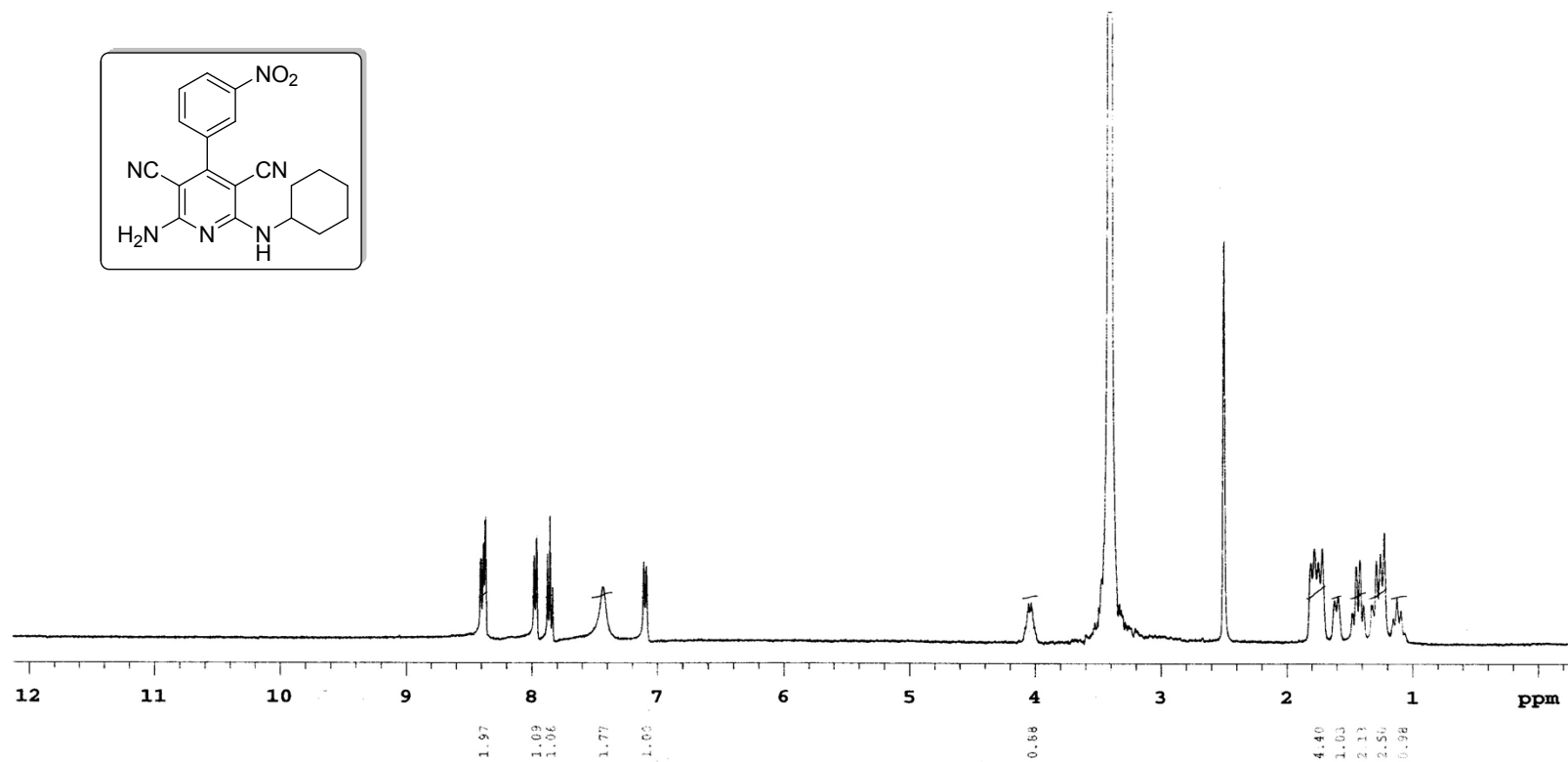
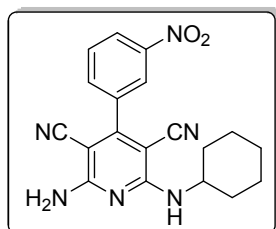


HRMS-spectra of compound 4h

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



¹H-NMR spectra of compound **4i**



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Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions

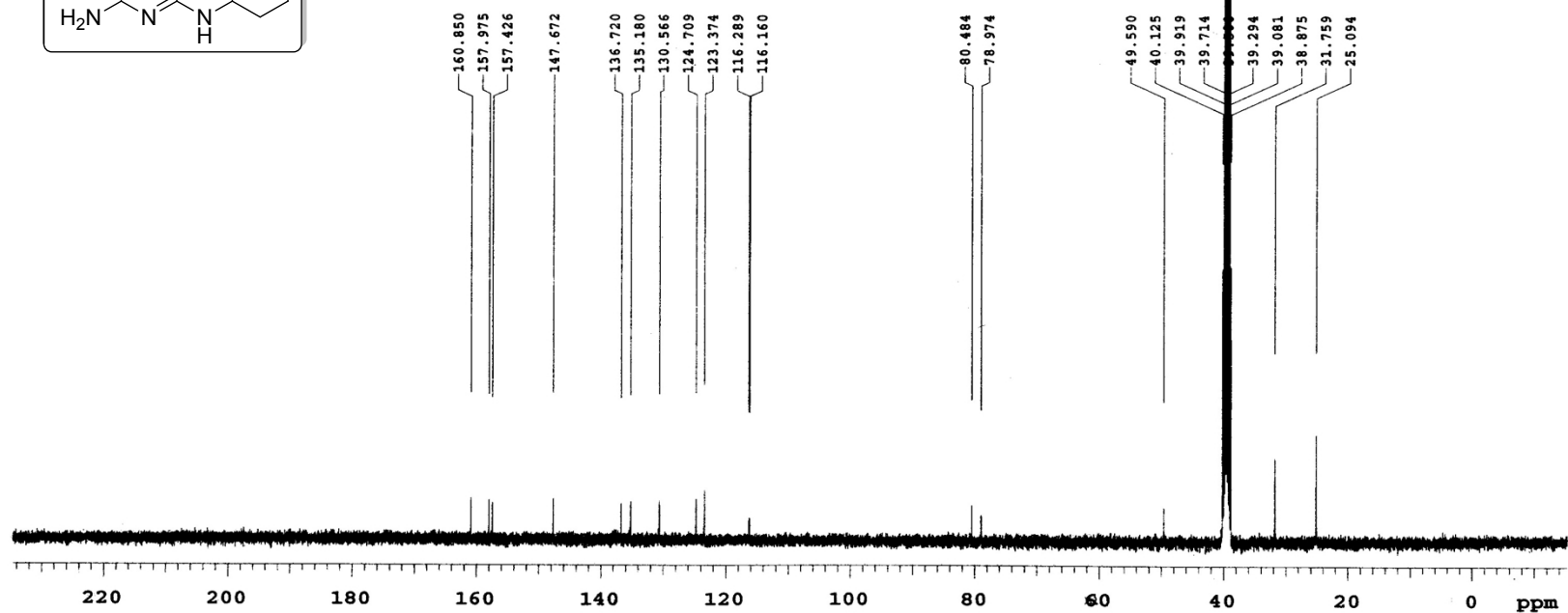
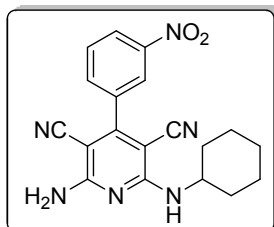
OBSERVE H1, 399.8528520

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FT size 32768
Total time 1 minutes

SS-3NO2-Cy-1H

Solvent: dmsc
Temp. 25.0 C / 298.1 K
Operator: chem
Mercury-400 "IITG-NMR"

¹³C-NMR spectra of compound 4i



SEQUENCE
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 Acq. time 1.304 sec
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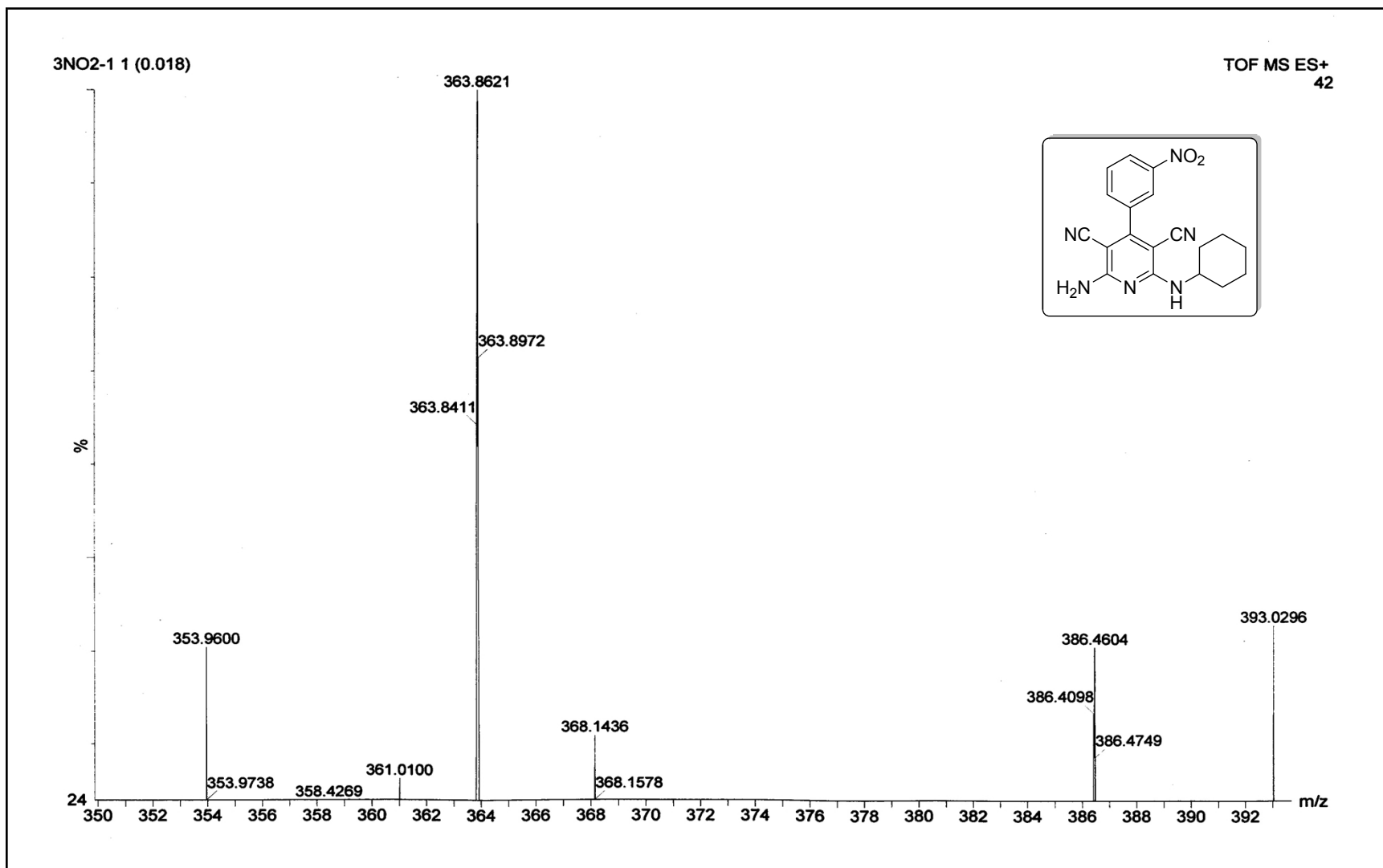
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 Power 42 dB
 continuously on
 WALTZ-16 modulated

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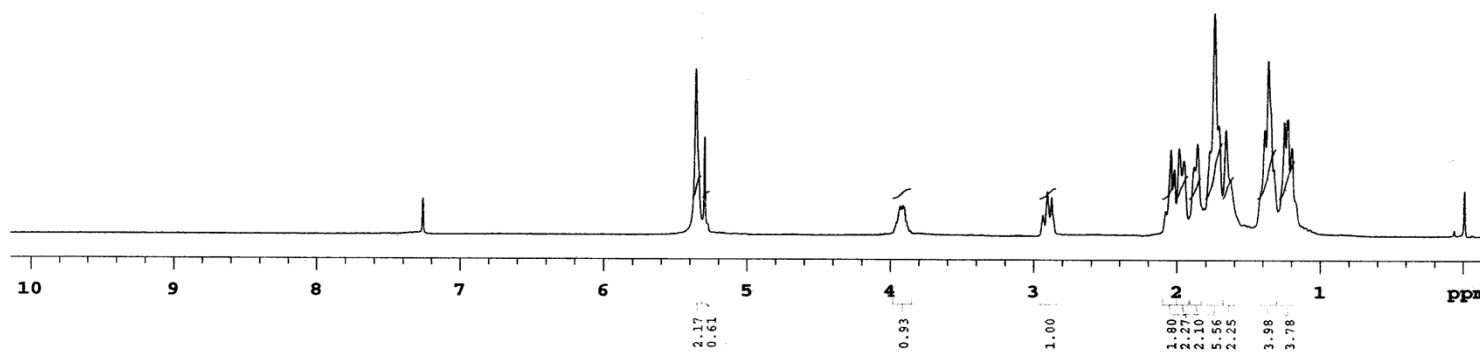
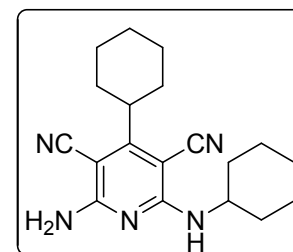
SS-3NO2-cy-13C

Solvent: dmsd
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 Mercury-400 "IITG-NMR"

HRMS spectra of compound **4i**



¹H-NMR spectra of compound **4j**

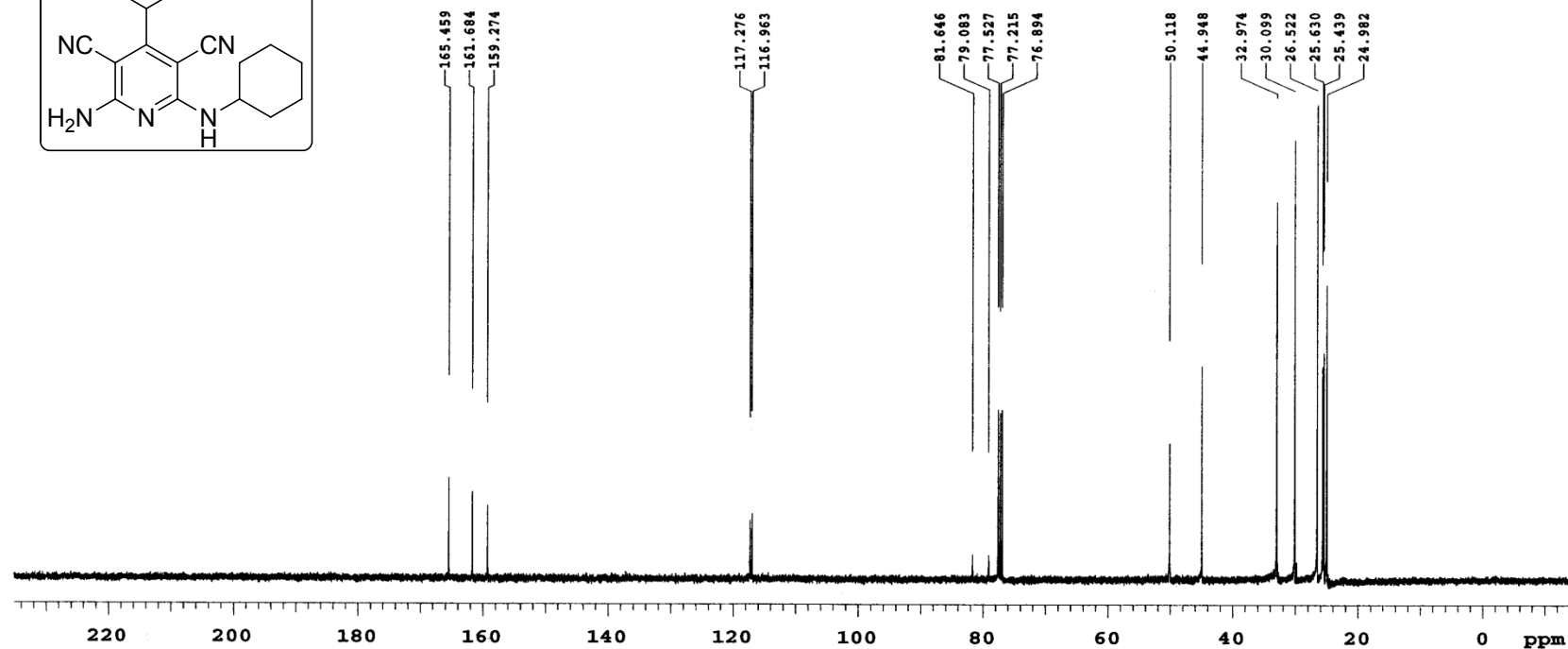
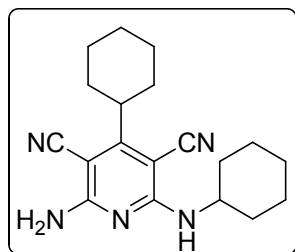


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32 repetitions

DATE: 08/25/2011 10:54:59 AM
FT size 32768
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Solvent: cdc13
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Operator: chem
Mercury 400 "1H-NMR"

¹³C-NMR spectra of compound 4j



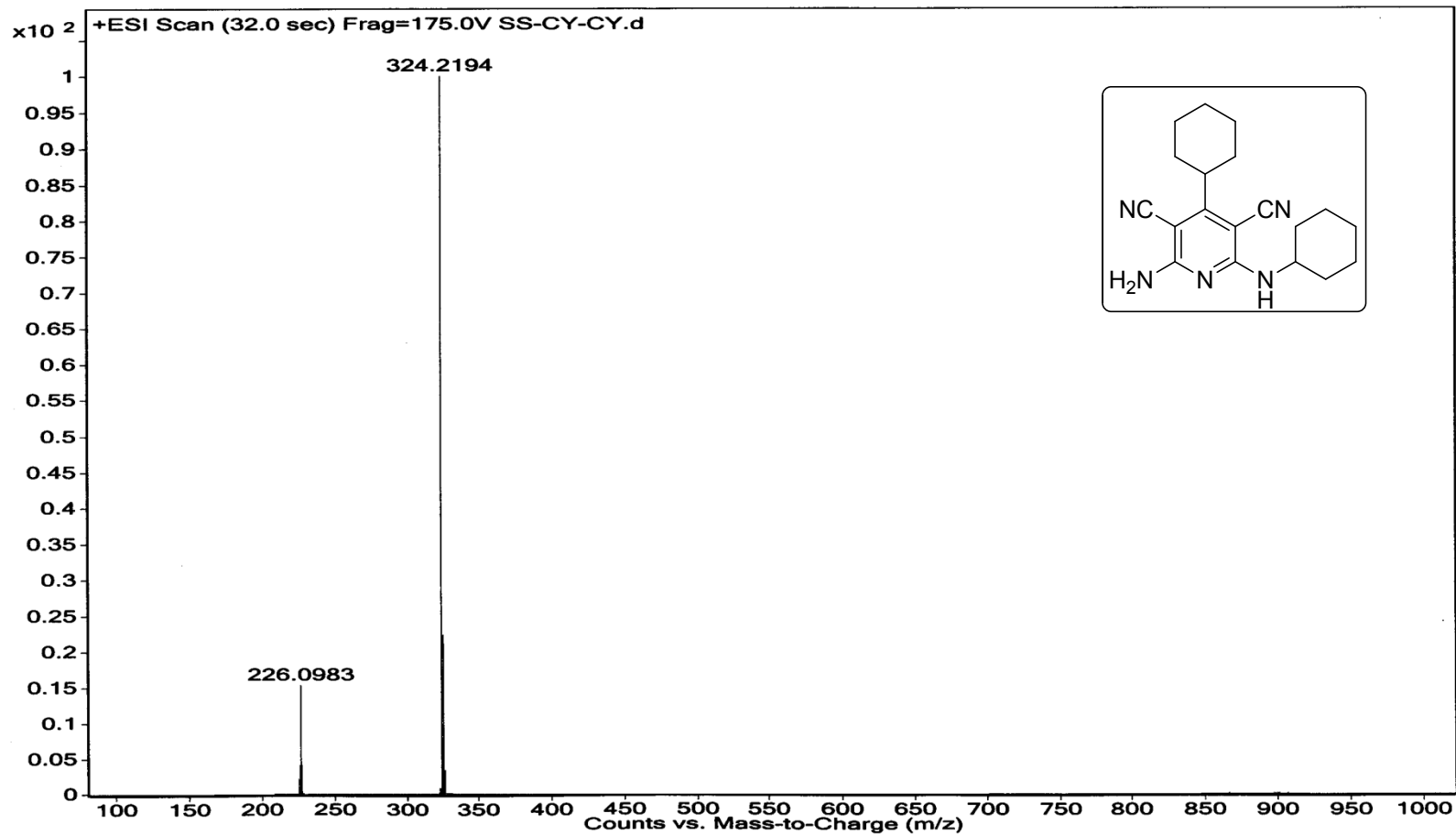
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Pulse 45.0 degree: size 65538:Power:42 dB
Acq. time 1.304 sec continuously on
Width 25125.6 Hz WALTZ-16 modulated
980 repetitions

DATA PROCESSING:GSEACQ:13C
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FT size 65536
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Operator: chem
Mz:Bruker-400 "IITG-NMR"

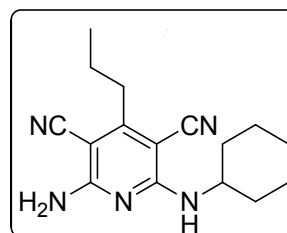
HRMS-spectra of compound 4j

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



¹H-NMR spectra of compound **4k**

SS-Bu-Cy-1H

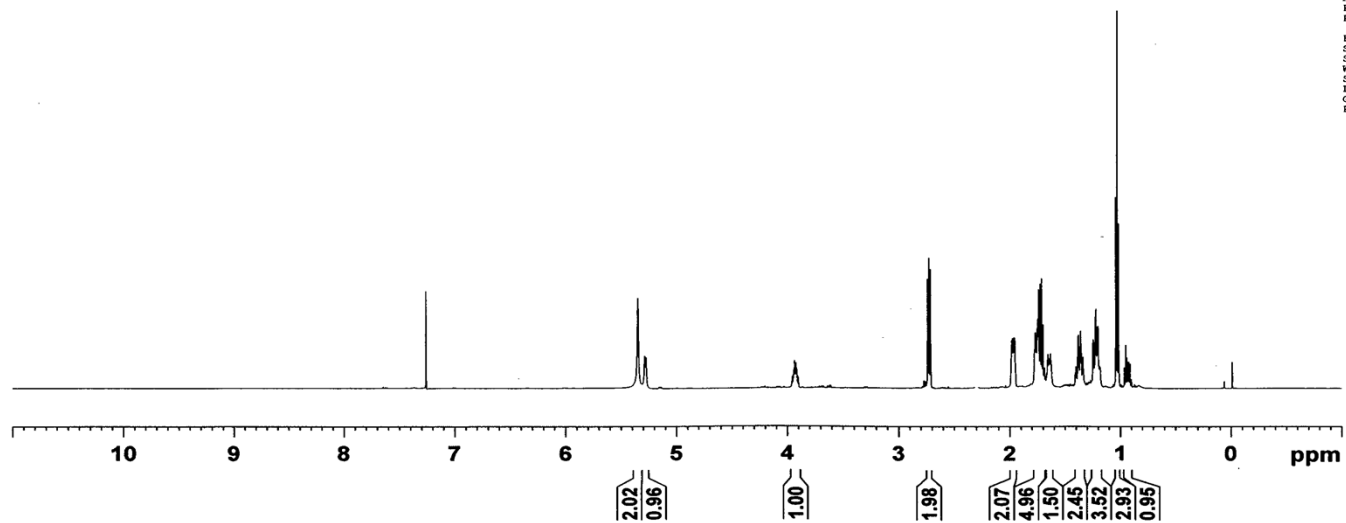


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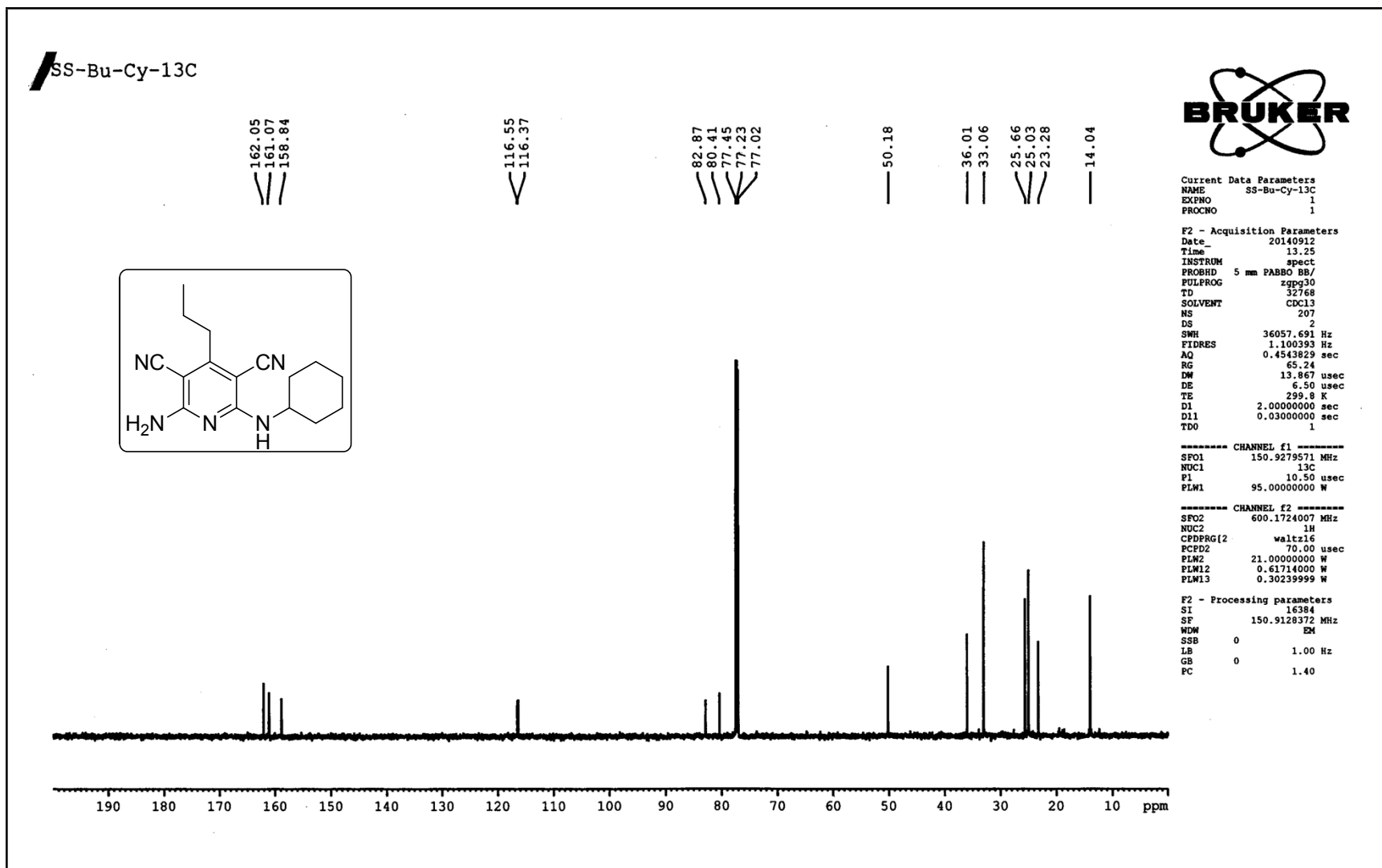
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FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         49.39
DN         41.600 usec
DE         6.50 usec
TE         298.7 K
D1         1.00000000 sec
TDO        1

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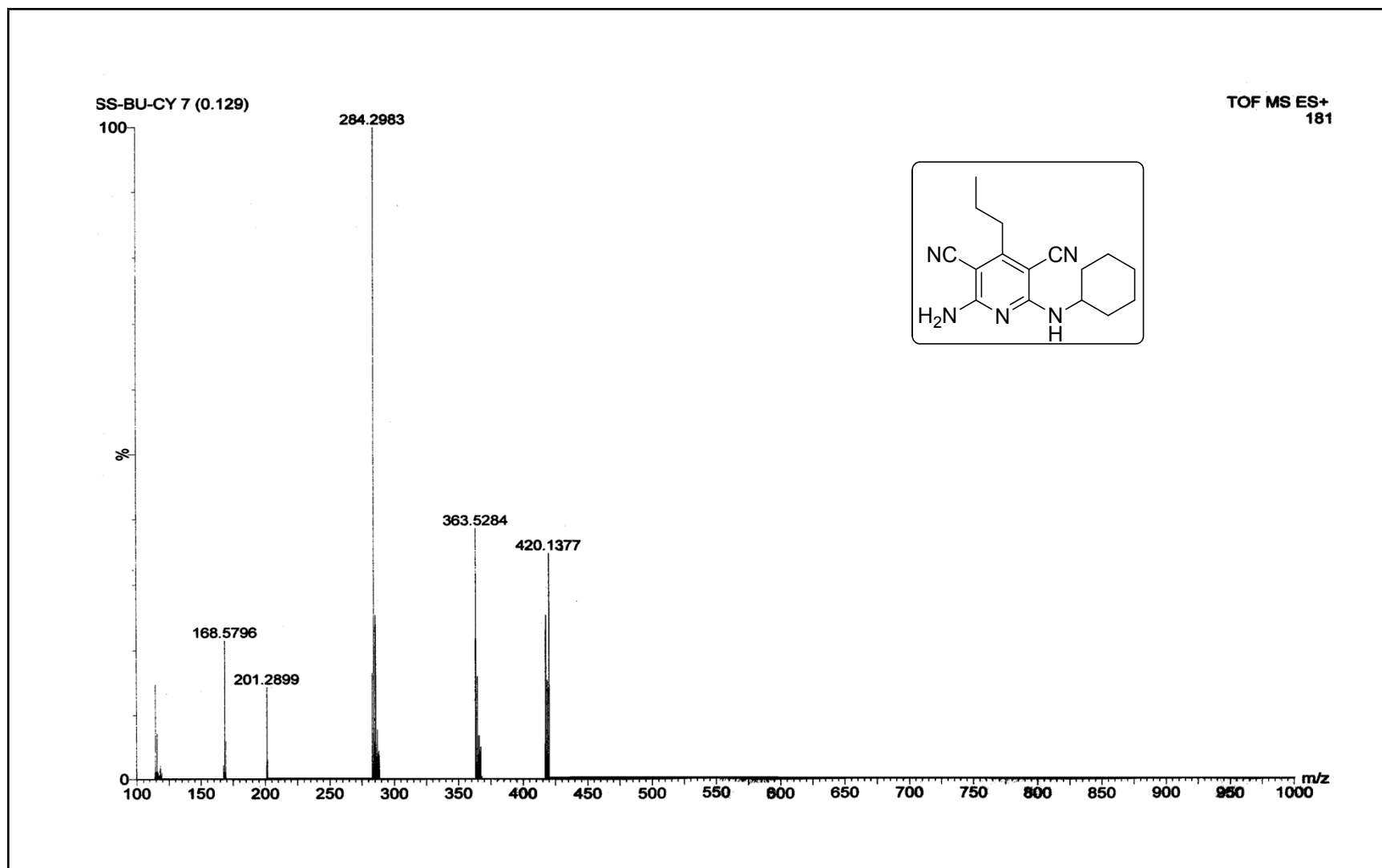
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¹³C-NMR spectra of compound 4k

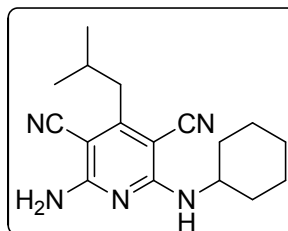


HRMS-spectra of compound 4k



¹H-NMR spectra of compound 4I

SS-3MeBu-Cy_1H



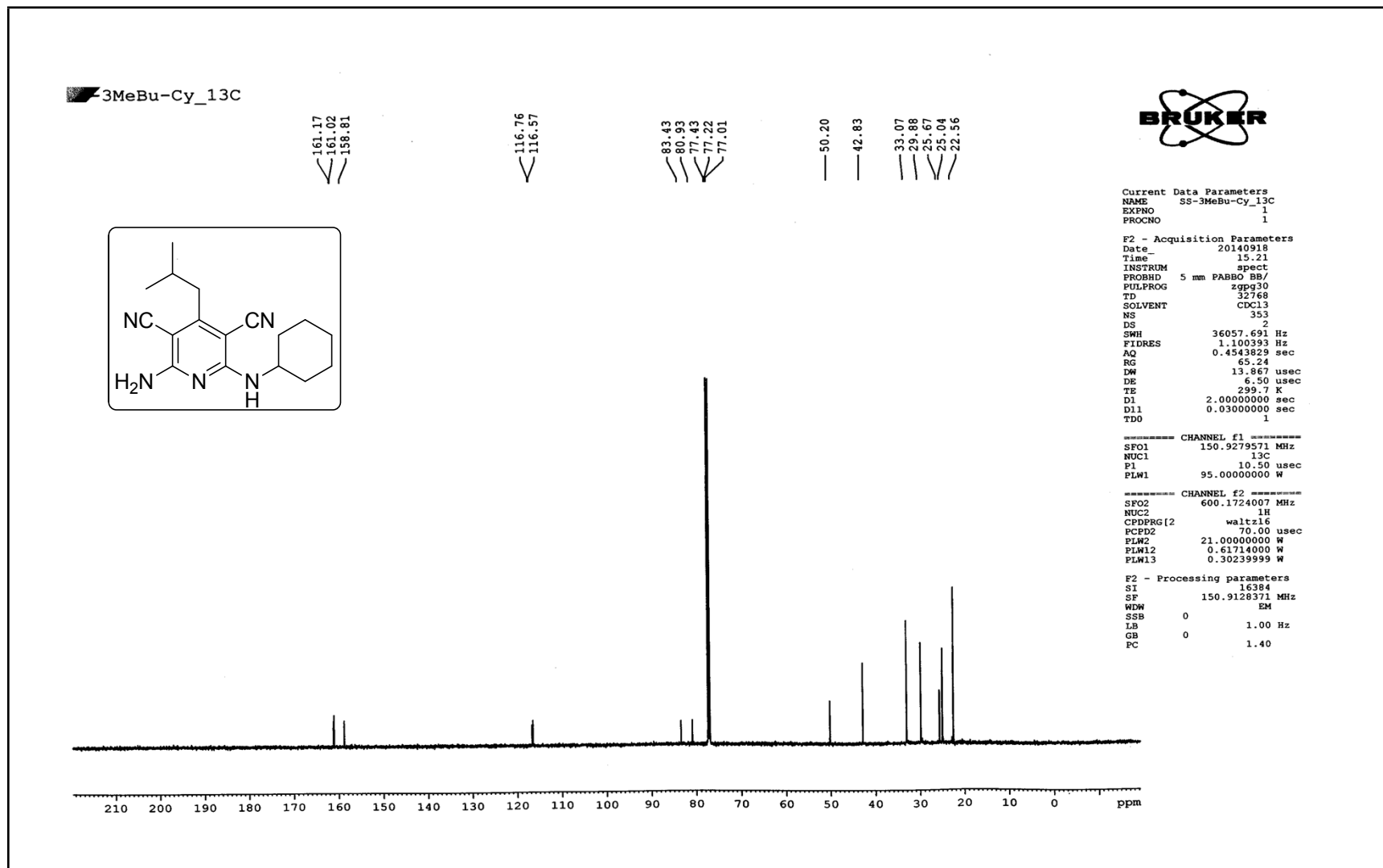
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EXPNO 1
PROCNO 1

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PULPROG zg30
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NS 16
DS 2
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D1 1.00000000 sec
TDO 1

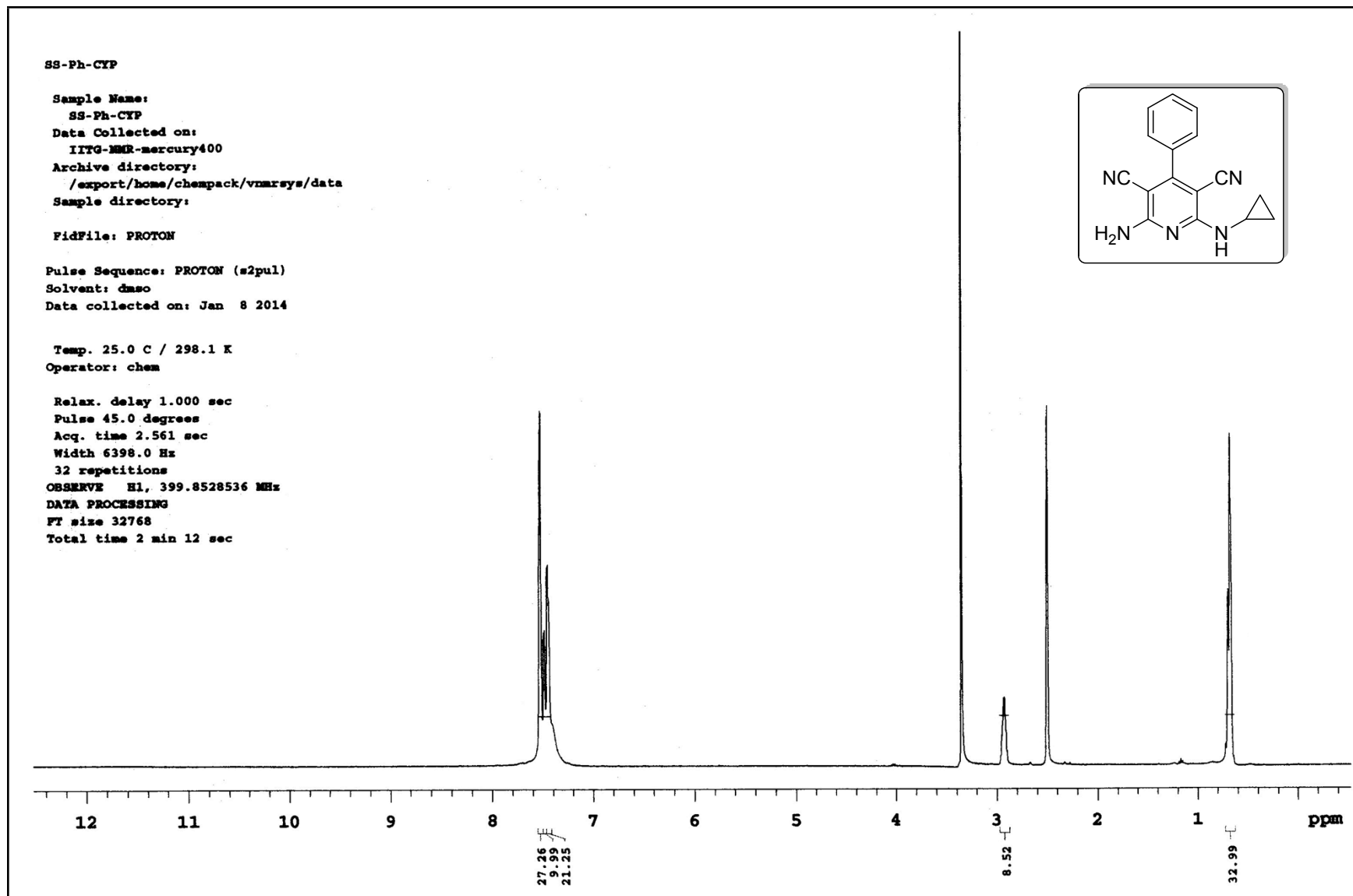
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F2 - Processing parameters
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LB 0.30 Hz
GB 0
PC 1.00

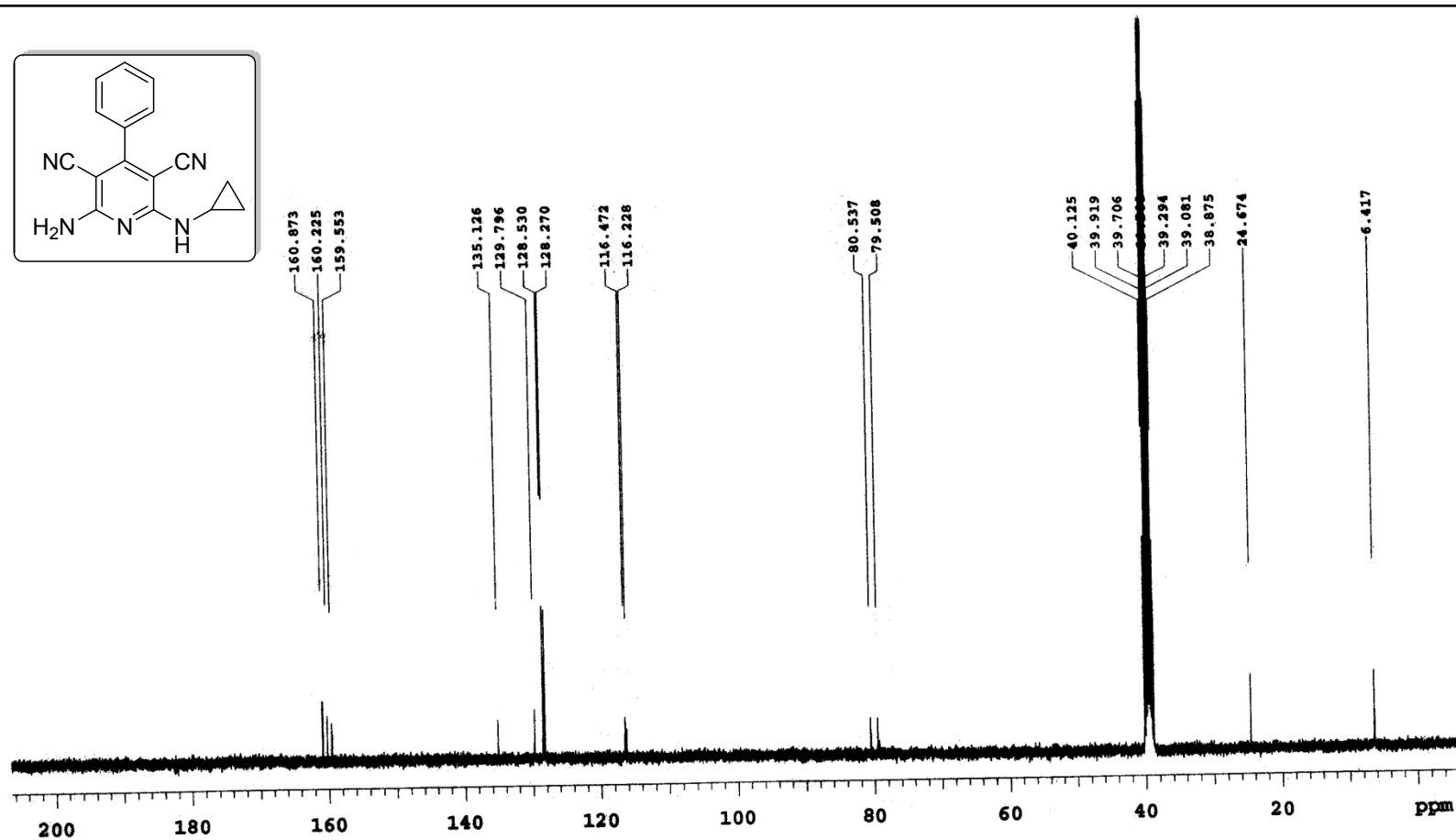
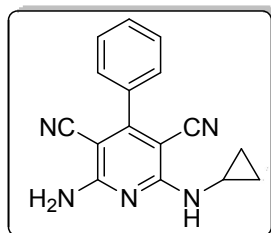
¹³C-NMR spectra of compound 4l



¹H-NMR spectra of compound 4m



¹³C-NMR spectra of compound 4m



PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.304 sec
 Width 25125.6 Hz
 5240 repetitions

OBSERVE C13, 100.5431285
DECOUPLE H1, 399.8548987
 Power 42 dB
 continuously on
 WALTZ-16 modulated

DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 3.4 hours

SS-Ph-CyP-13C
 Solvent: dmsc
 Temp. 25.0 C / 298.1 K
 Operator: chem
 Mercury-400 "IITG-NMR"

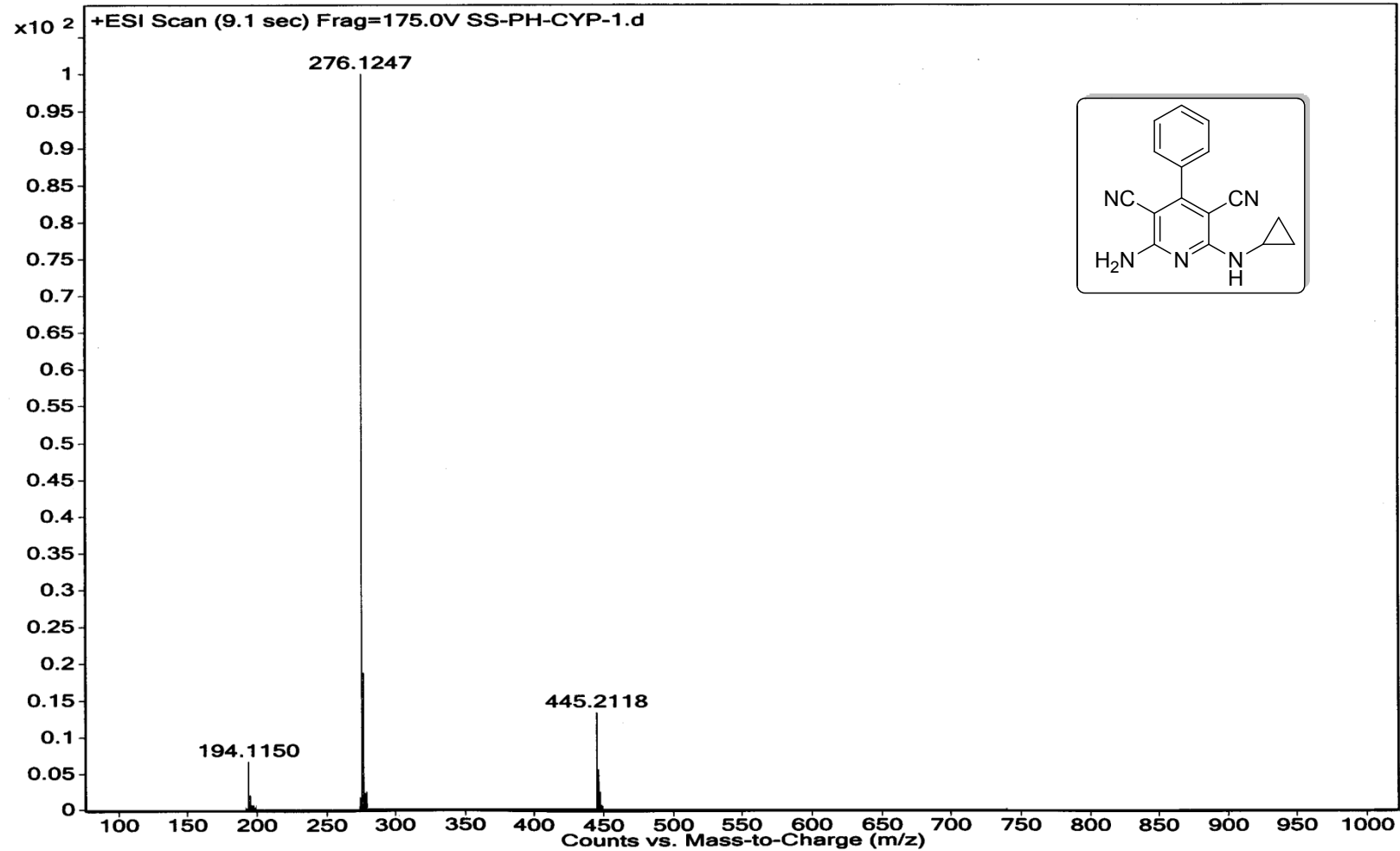
HRMS-spectra of compound **4m**

Sample Name
Inj Vol
Data Filename

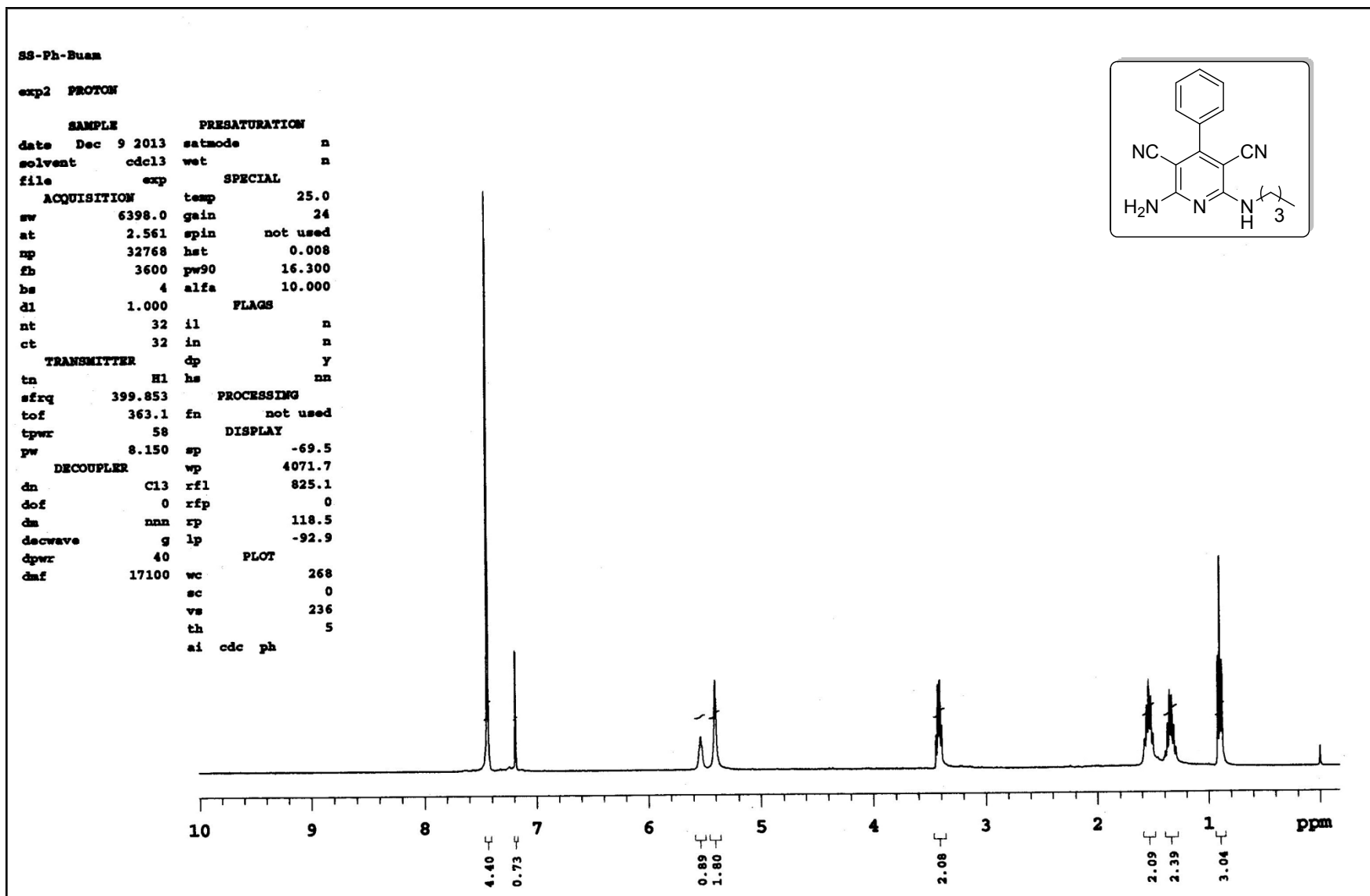
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ACQ Method

Instrument Name
SampleType
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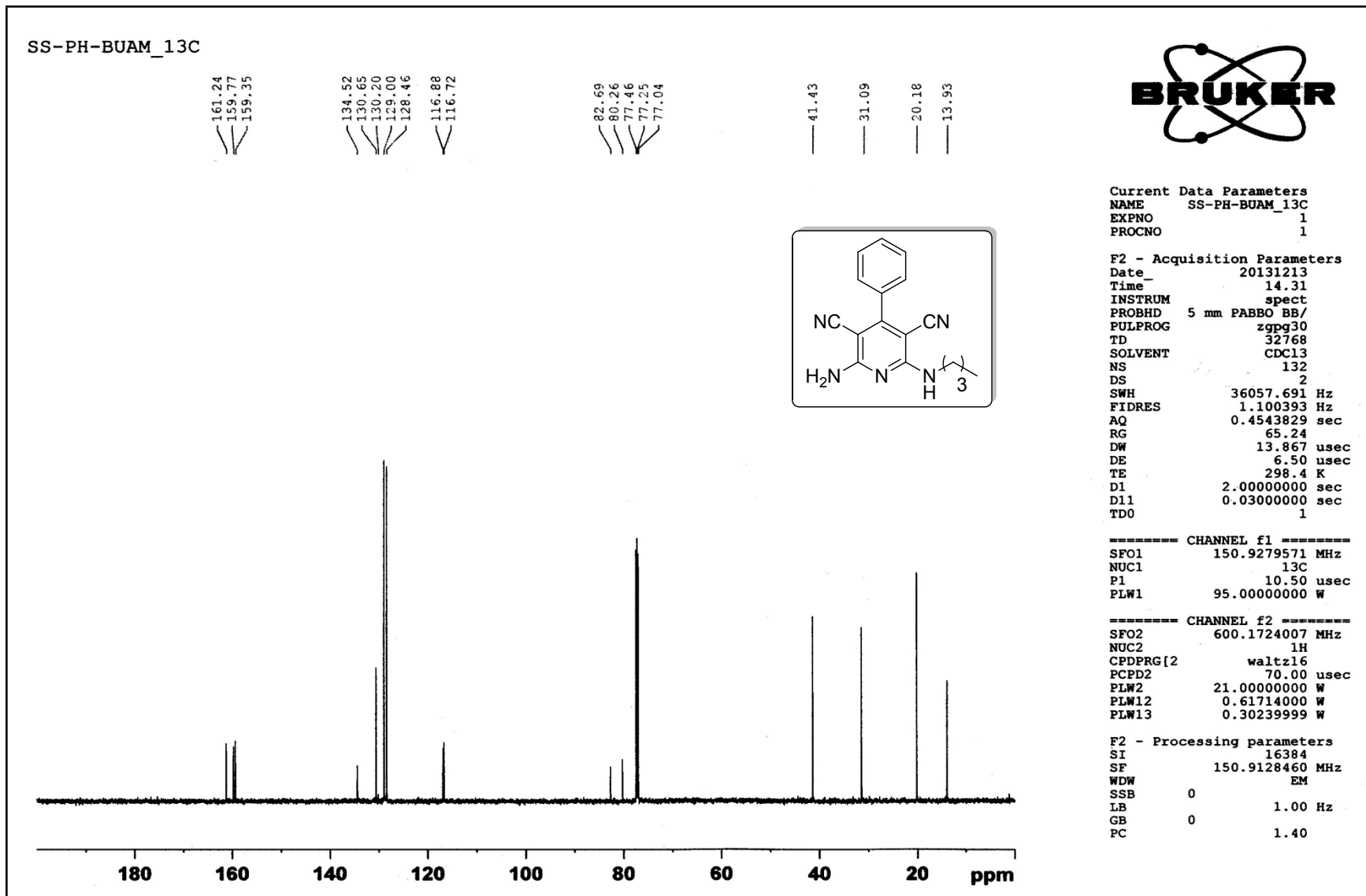
User Name
IRM Calibration Status
Acquired Time



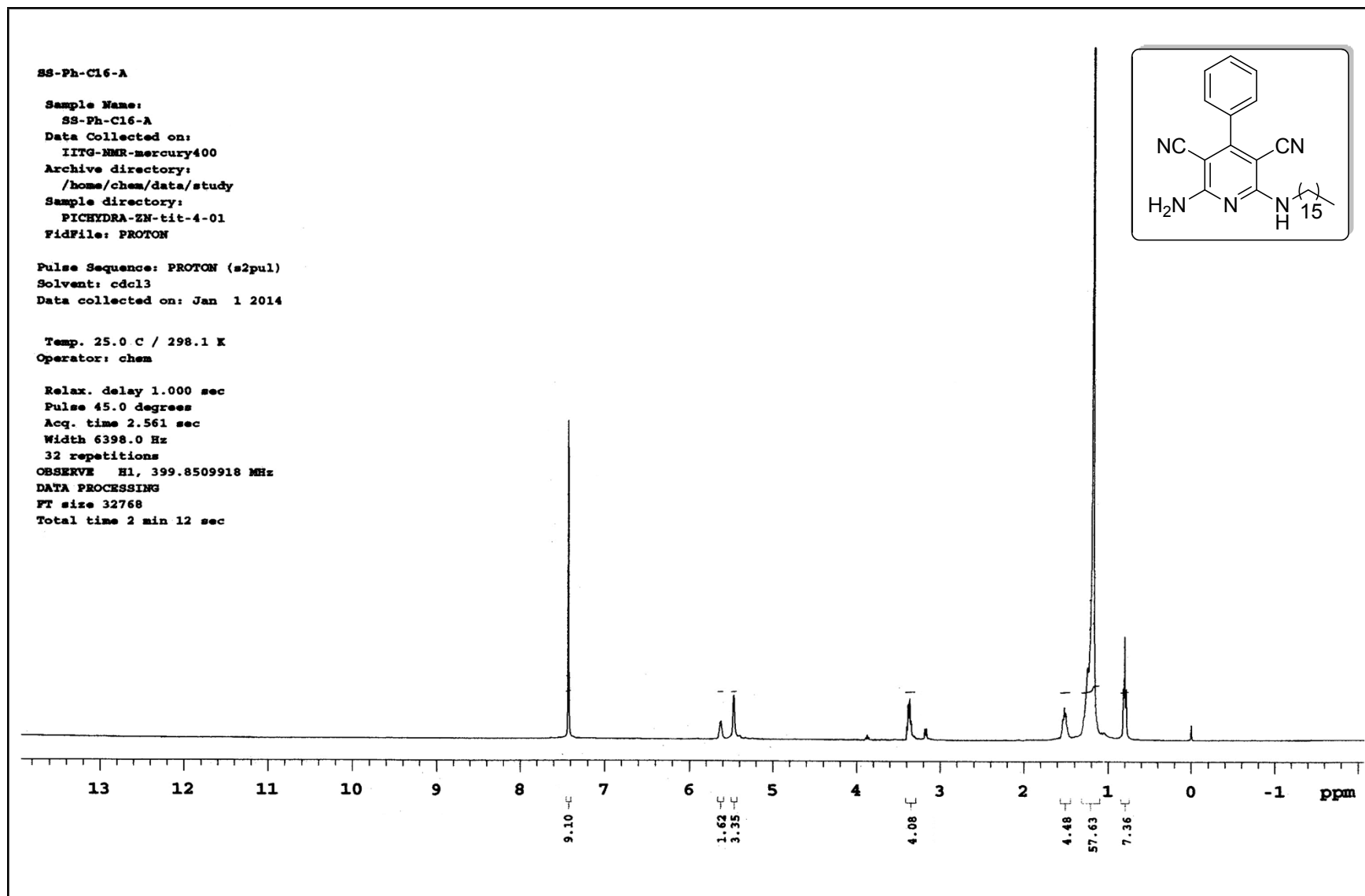
¹H-NMR spectra of compound 4n



¹³C-NMR spectra of compound 4n

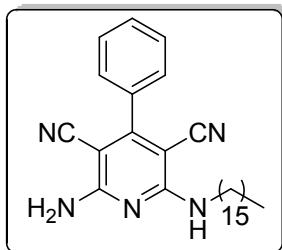


¹H-NMR spectra of compound **4o**



¹³C-NMR spectra of compound **4o**

SS-Ph-C16-A_13C



161.22
159.72
159.29

134.52
129.34
129.28
128.94
128.84
128.43
116.84
116.68

82.62
80.19
77.44
77.23
77.02

41.71
36.74
32.05
29.82
29.74
29.67
29.49
29.44
29.37
27.00
25.10
22.81
14.25

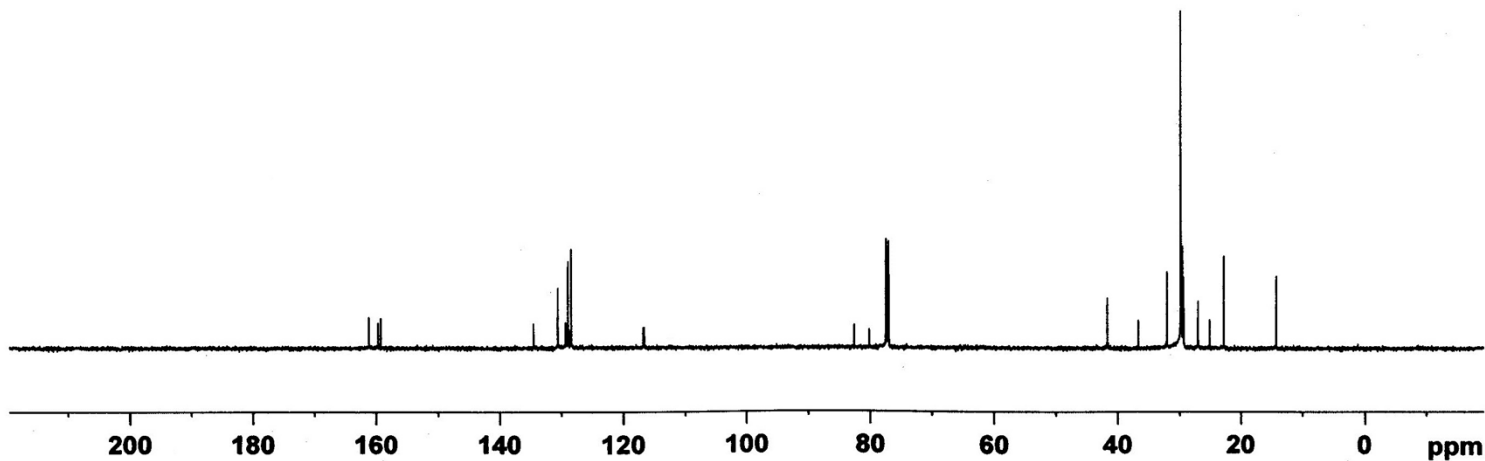
Current Data Parameters
NAME SS-Ph-C16-A_13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140116
Time 13.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

----- CHANNEL f2 -----
SFO2 600.1724007 MHz
NUC2 1H
CPCPDS2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9128496 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



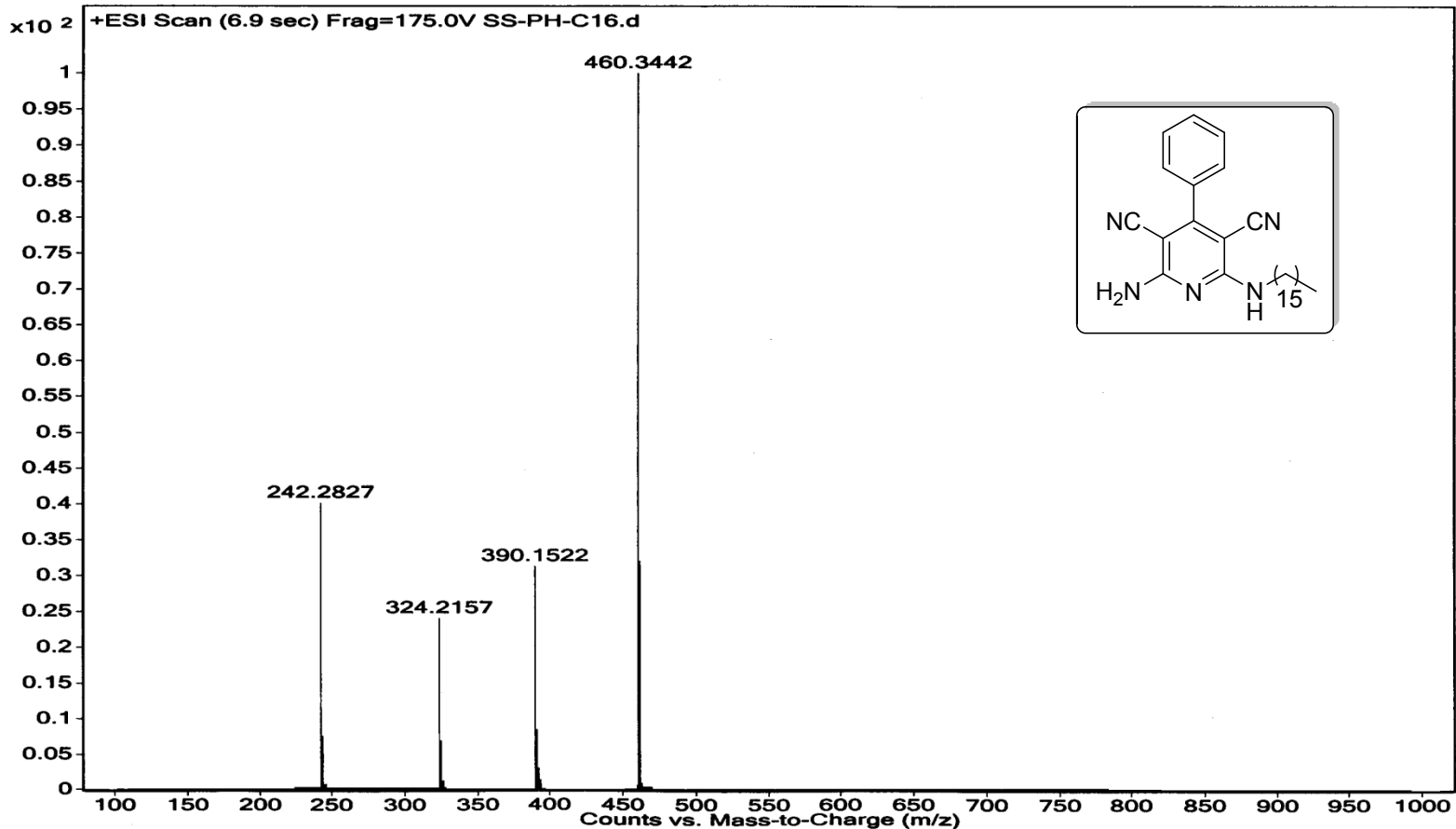
HRMS-spectra of compound 4o

Sample Name
Inj Vol
Data Filename

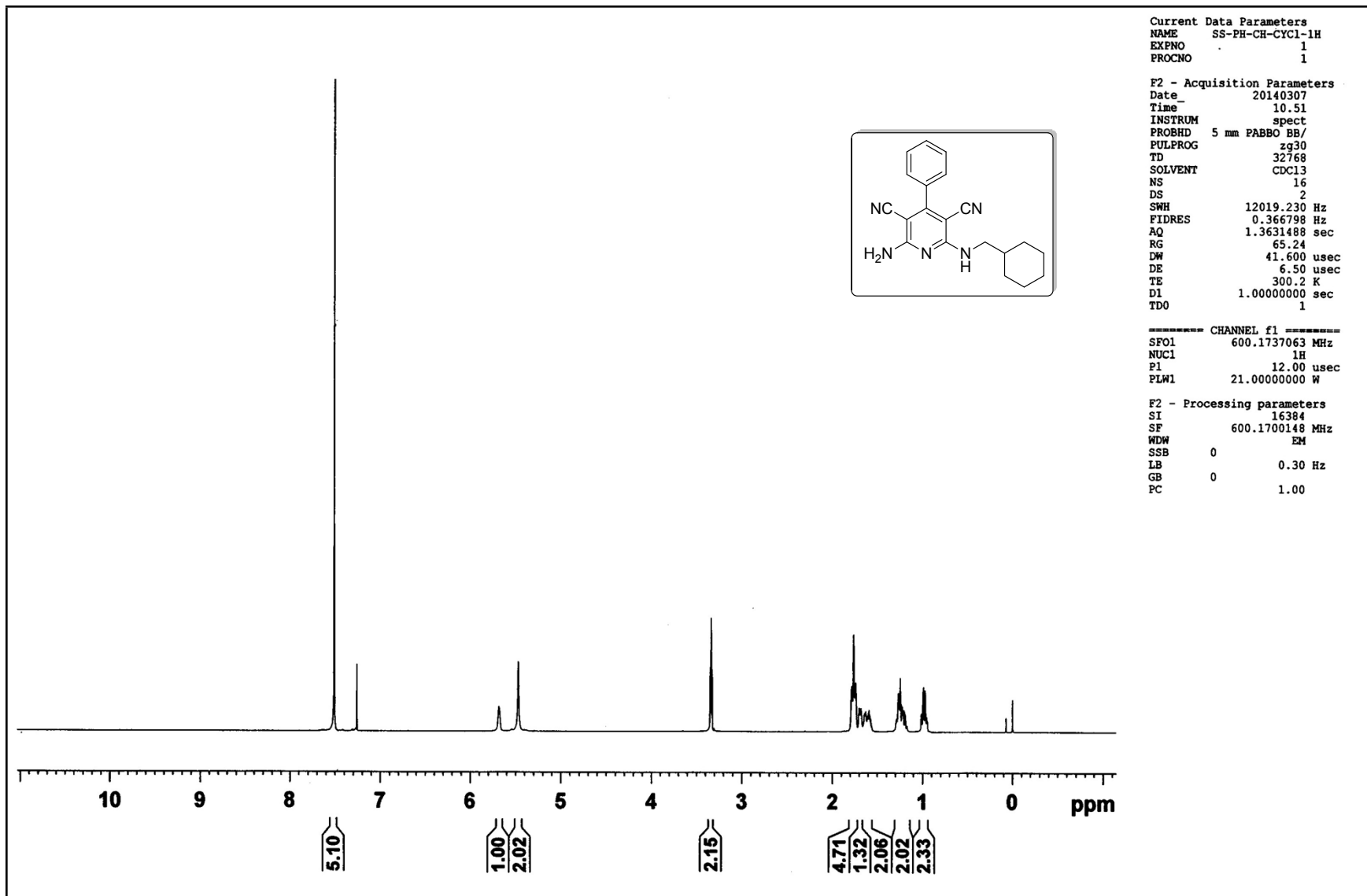
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

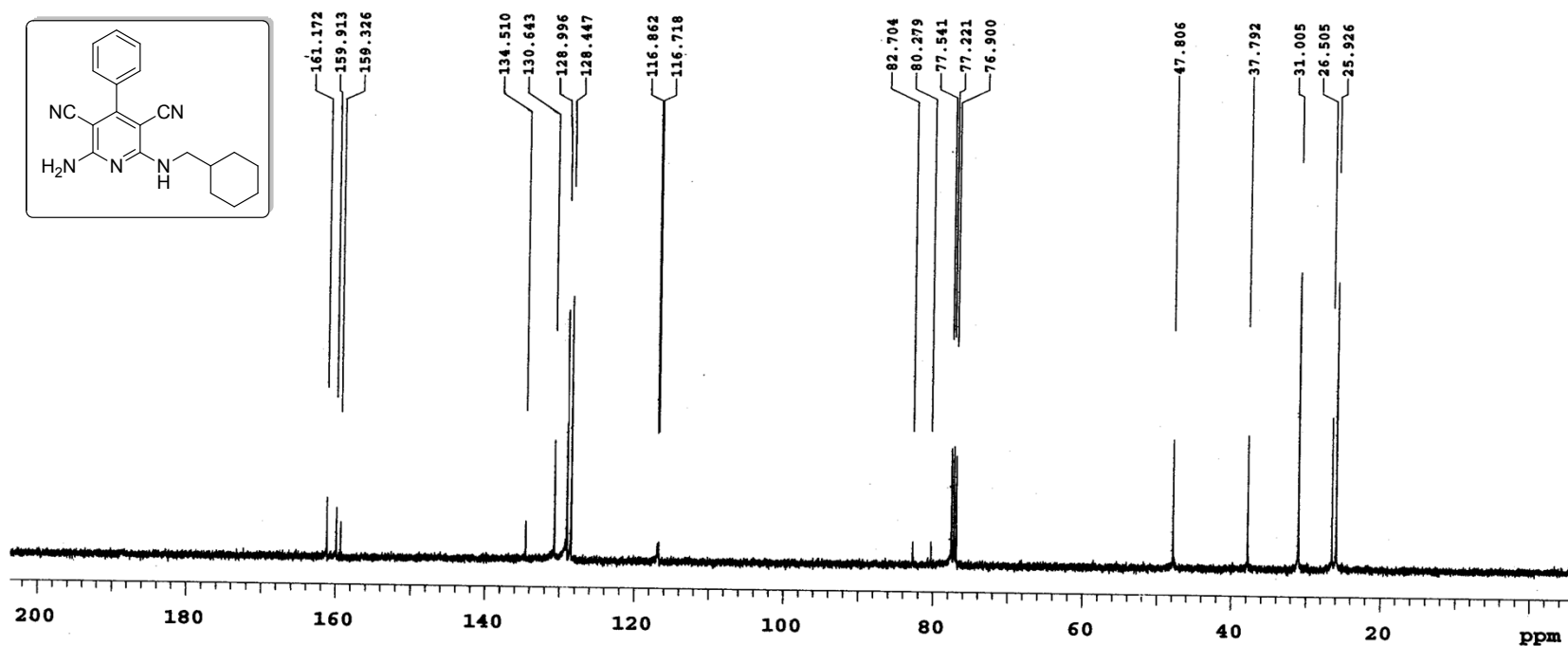
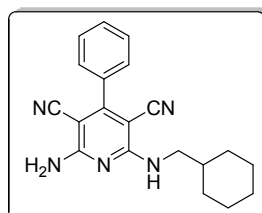
User Name
IRM Calibration Status
Acquired Time



¹H-NMR spectra of compound 4p



¹³C-spectra of compound 4p



PULSE SEQUENCE:

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.304 sec
Width 25125.6 Hz
1180 repetitions

OBSERVE C13, 100.5425887
DECOUPLE H1, 399.8529994
Power 42 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz
FT size 65536
Total time 45 minutes

SS-Ph-CH-Cycl-13C

Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: chem
Mercury-400 "IITG-NMR"

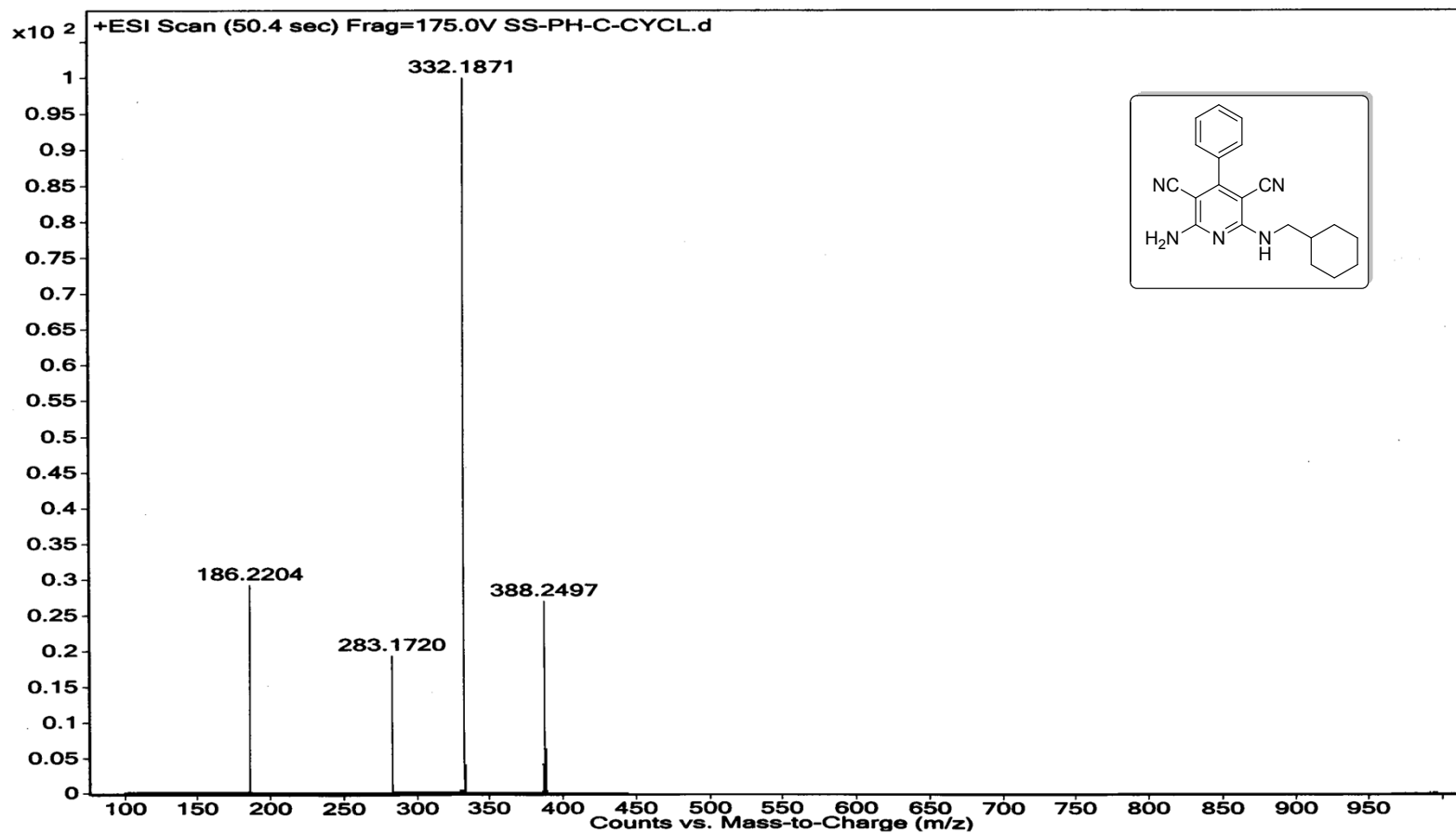
HRMS-spectra of compound 4p

Sample Name
Inj Vol
Data Filename

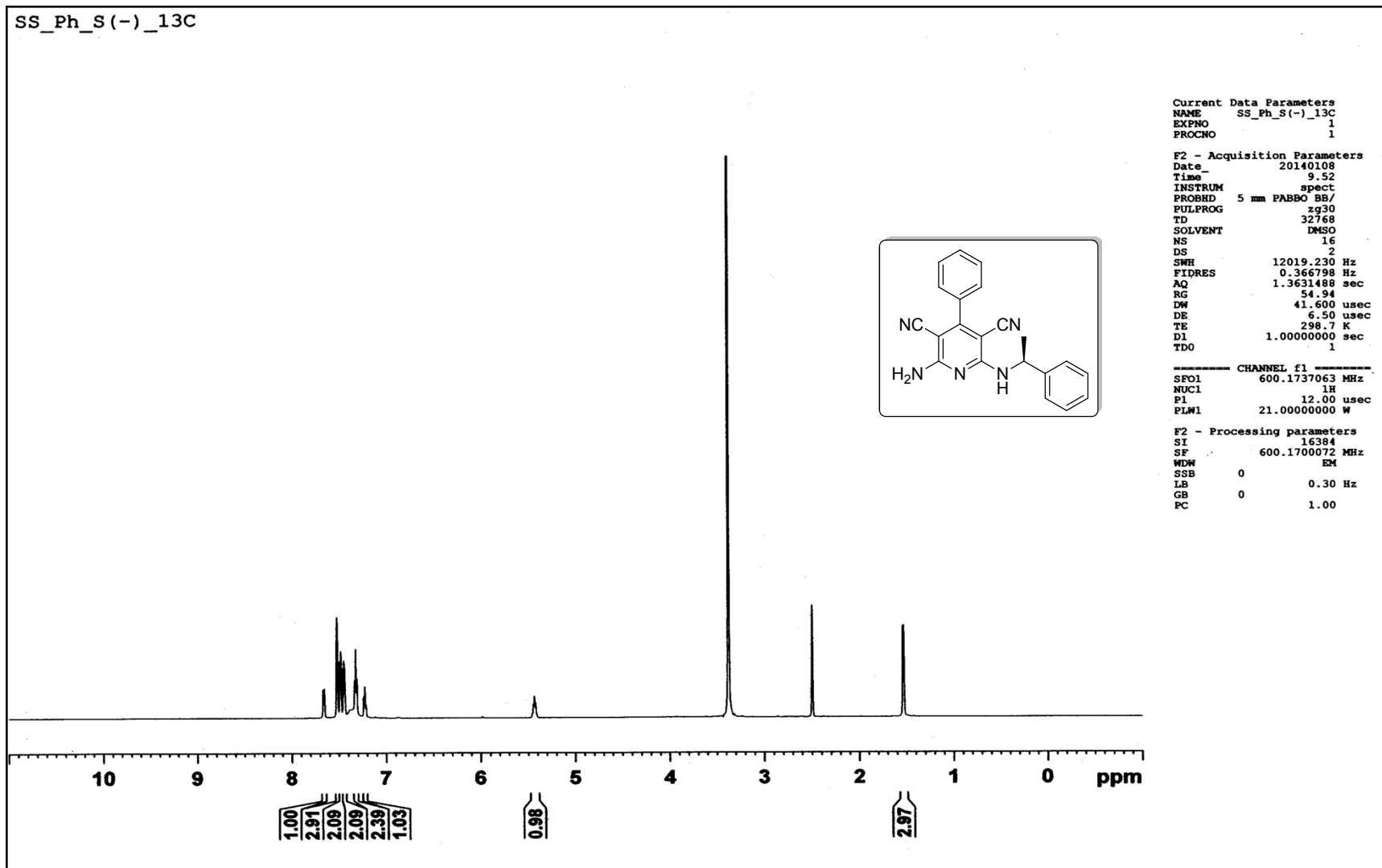
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

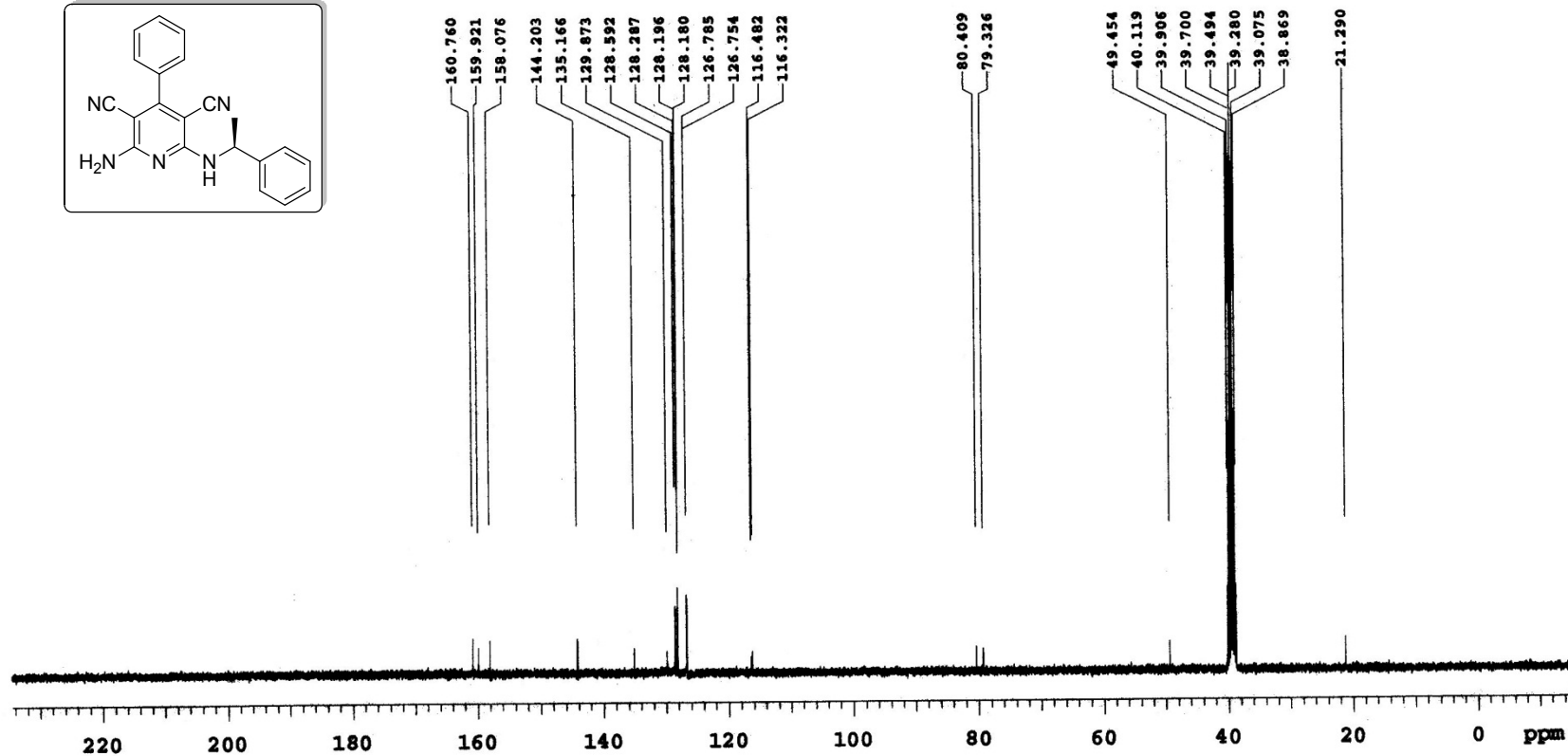
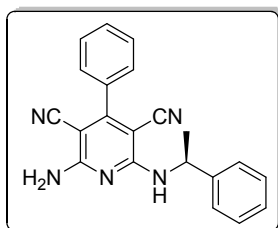
User Name
IRM Calibration Status
Acquired Time



¹H-NMR spectra of compound 4q



¹³C-NMR spectra of compound 4q



PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.304 sec
 Width 25125.6 Hz
 1775 repetitions

OBSERVE C13, 100.5431230
DECOUPLE H1, 399.8548987
 Power 42 dB
 continuously on
WALTZ-16 modulated

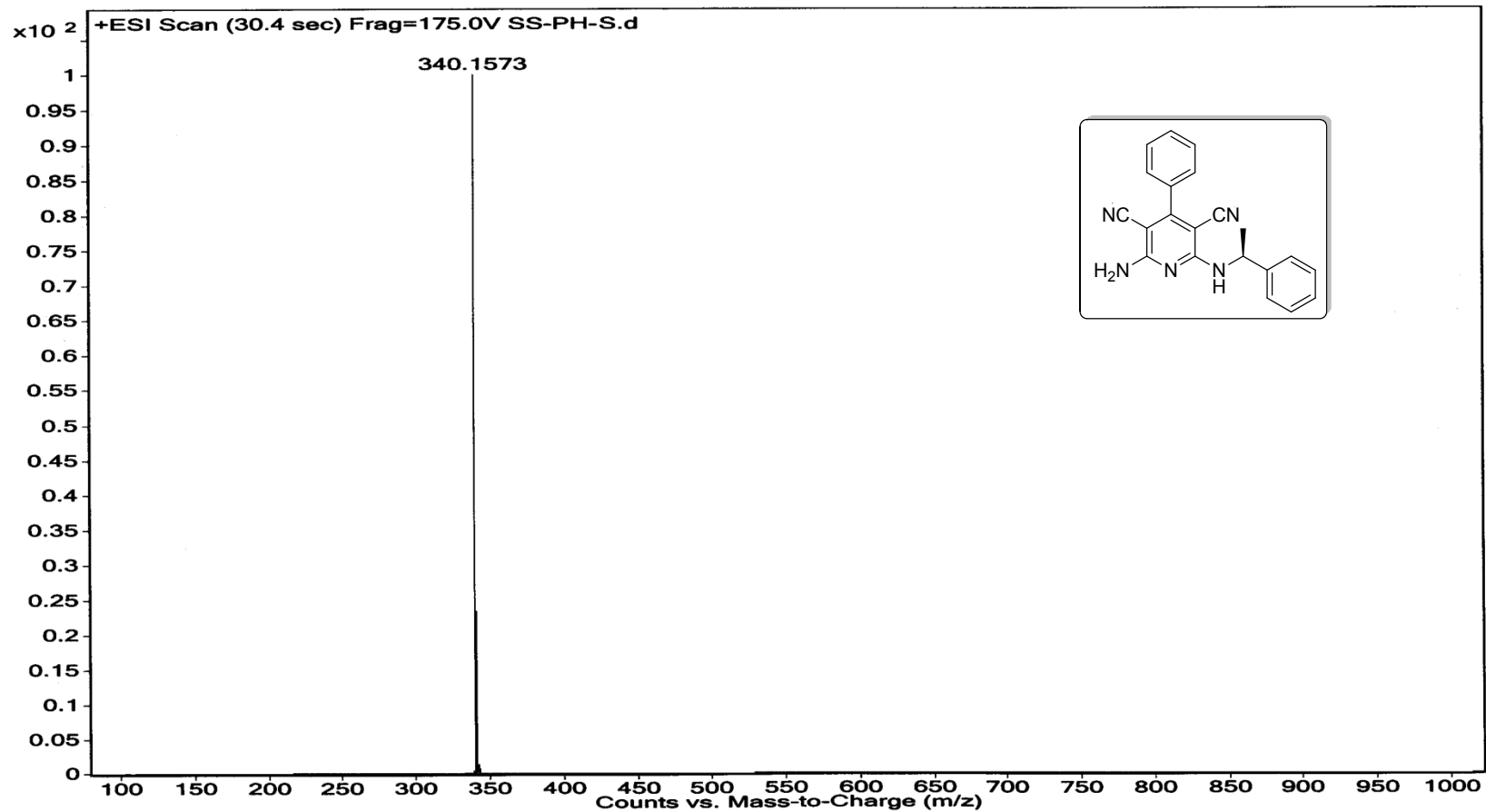
DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 68 minutes

SS-Ph-S(-)-13C

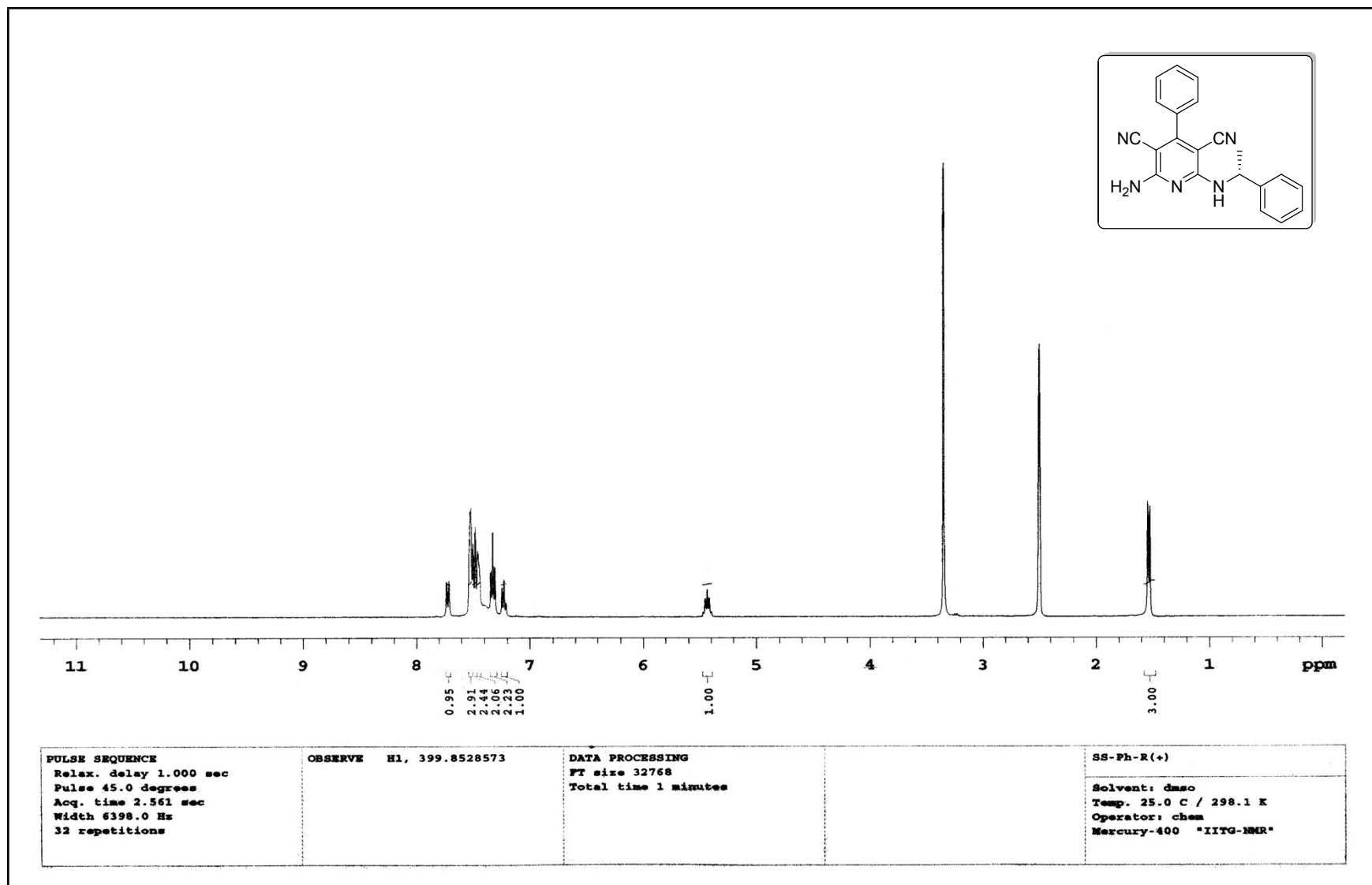
Solvent: dmso
 Temp. 25.0 C / 298.1 K
 Operator: chem
 Mercury-400 "IITG-NMR"

HRMS-spectra of compound 4q

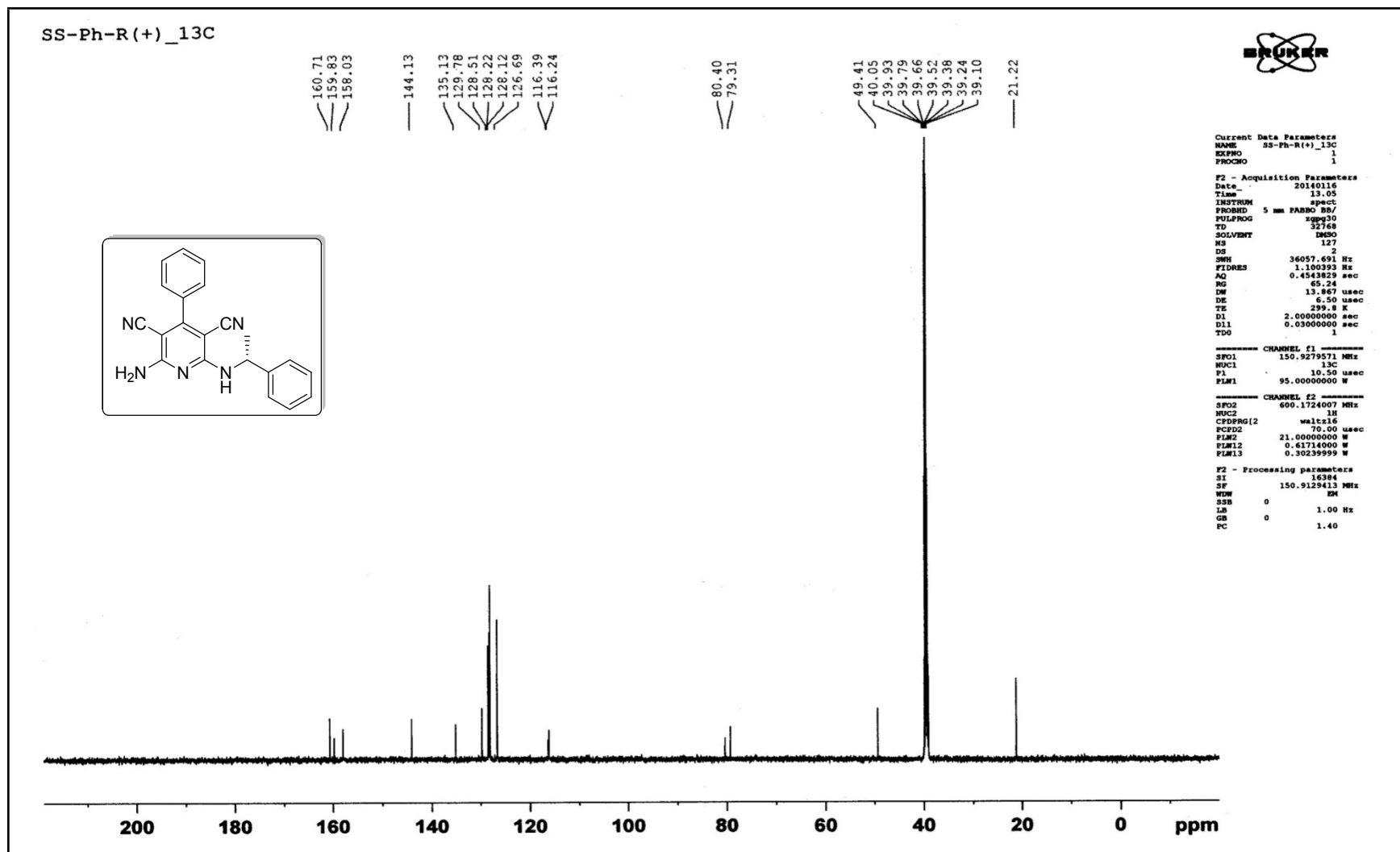
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



¹H-NMR spectra of compound 4r



¹³C-NMR spectra of compound 4r



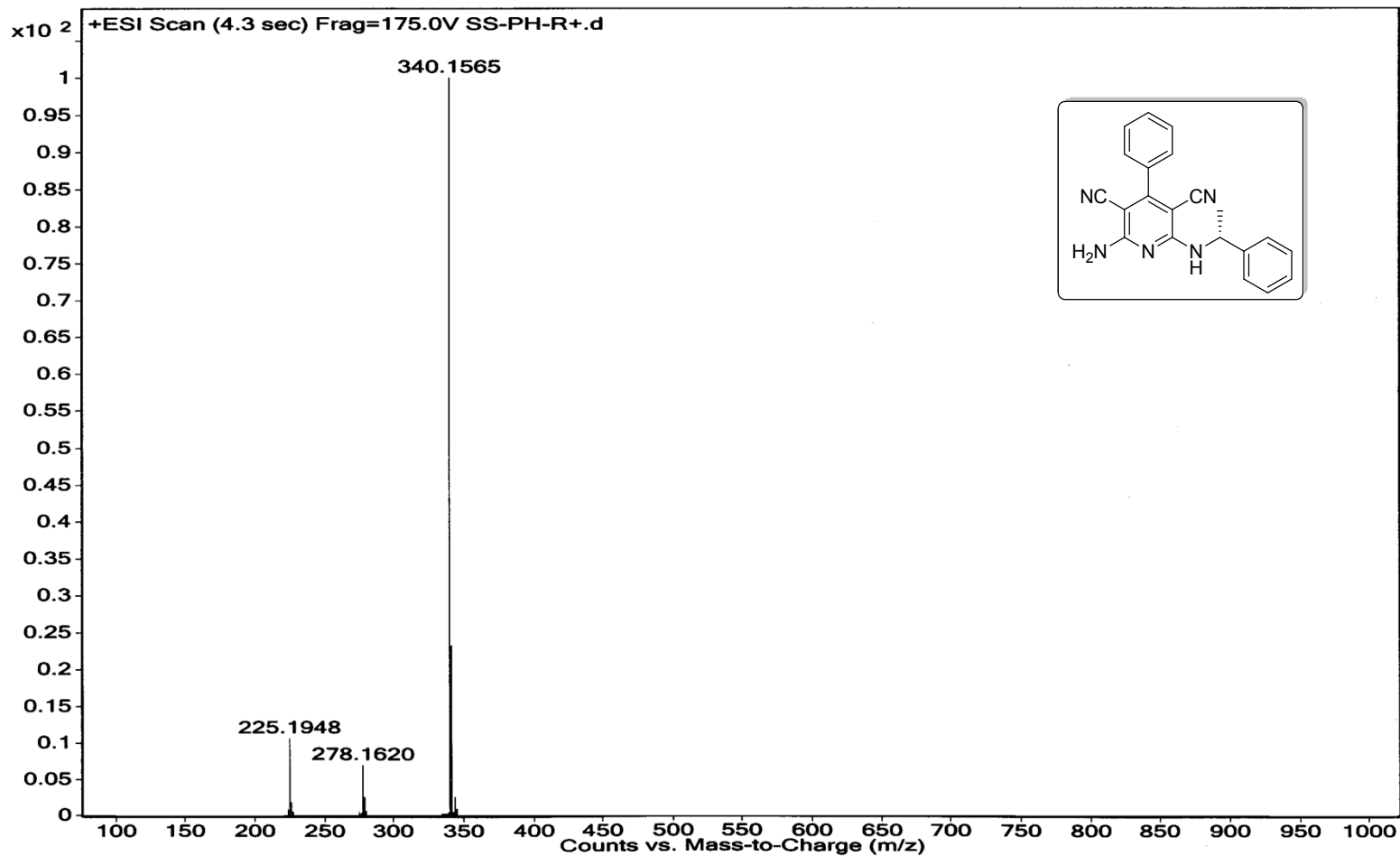
HRMS-spectra of compound 4r

Sample Name SS-PH-R+
Inj Vol -10
Data Filename SS-PH-R+.d

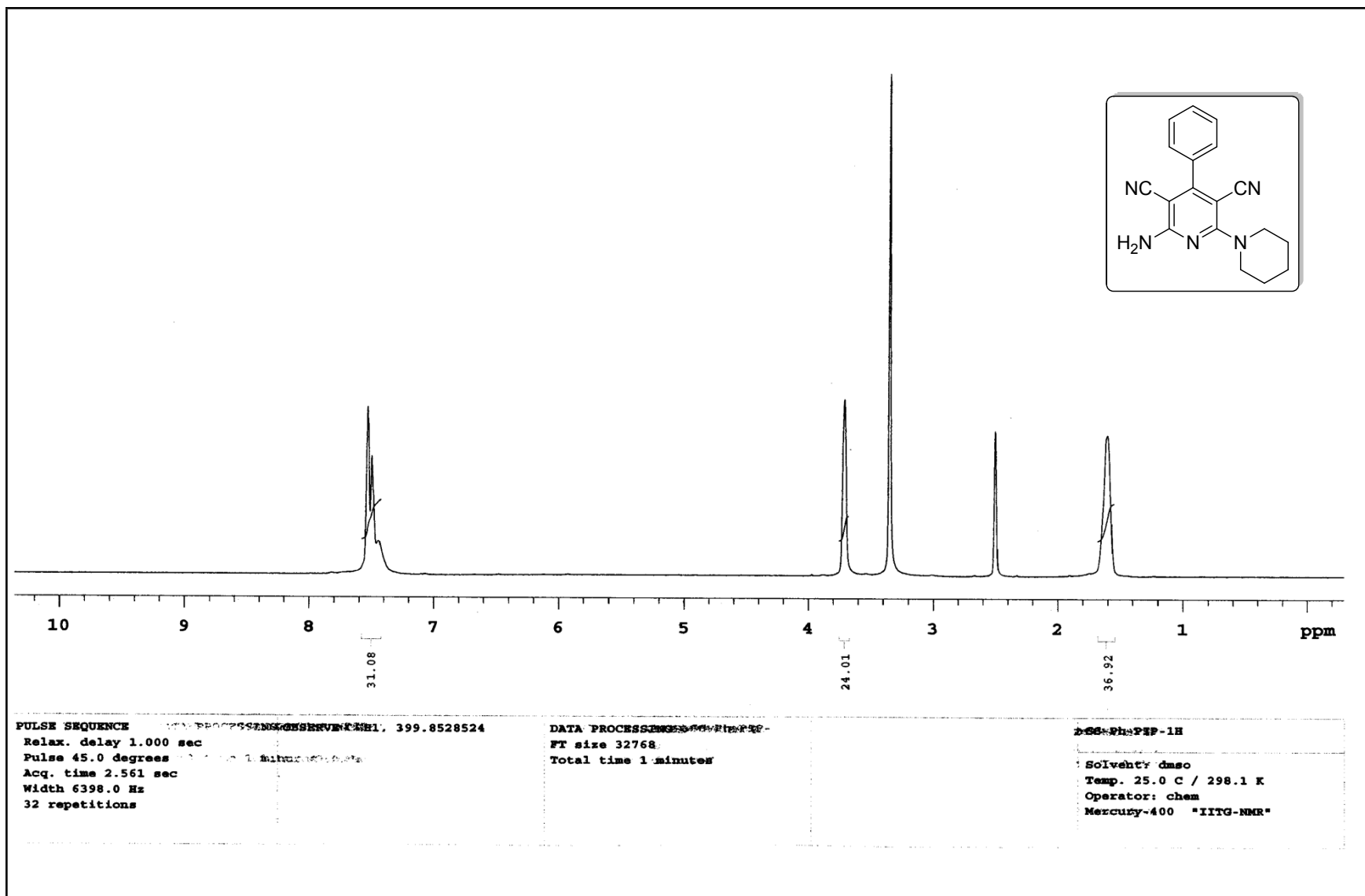
Position -1
InjPosition
ACQ Method

Instrument Name Instrument 1
SampleType Sample
Comment

User Name
IRM Calibration Status Success
Acquired Time 4/10/2014 11:37:59 AM



¹H-NMR spectra of compound 4s



¹³C-NMR spectra of compound 4s

SS_PH_PIP_13C

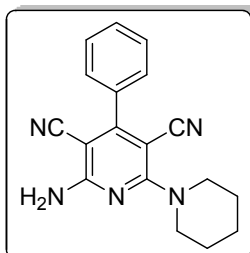
Current Data Parameters

F2 - Acquisition Parameters
Date_ 20140319
Time_ 10.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 220
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 301.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.0000000 W

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 21.0000000 W
PLW12 0.6171400 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9129420 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



161.76
160.66
159.70

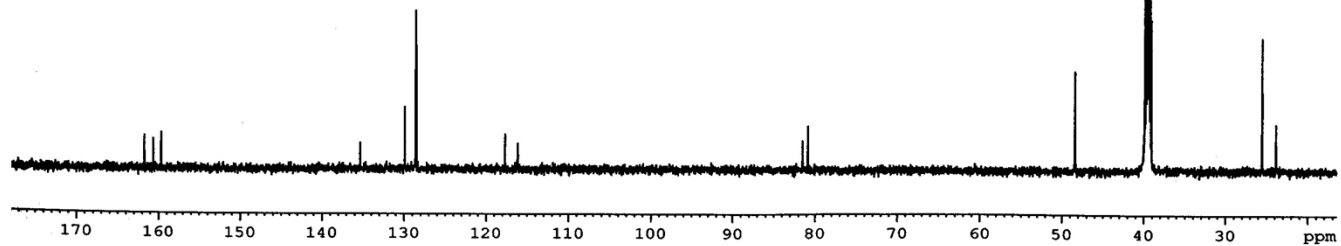
135.35
129.91
128.61
128.50

117.72
116.16

81.50
80.85

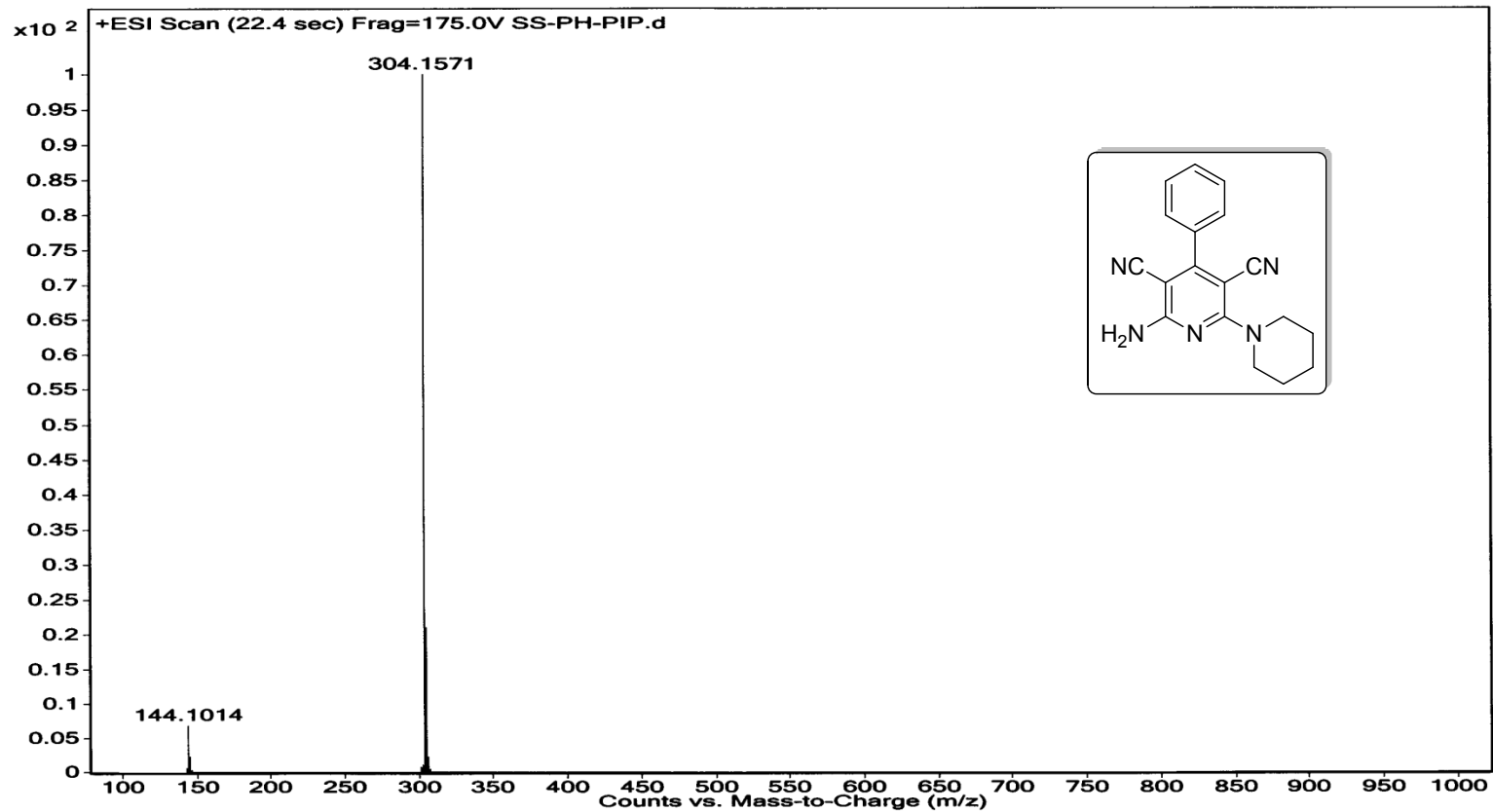
48.41
39.93
39.79
39.65
39.51
39.37
39.23
39.09

25.54
23.87

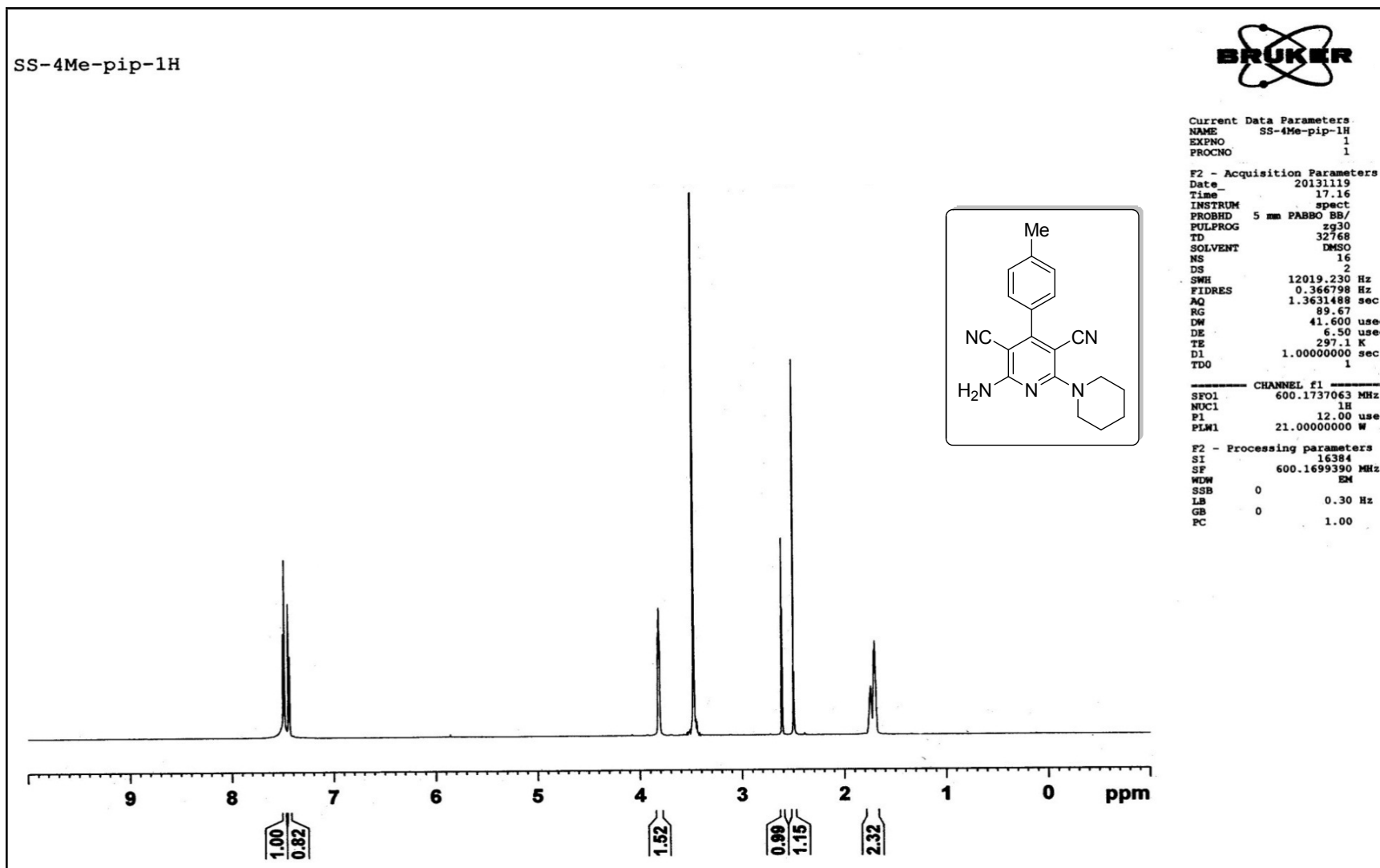


HRMS-spectra of compound 4s

Sample Name	SS-PH-PIP	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SS-PH-PIP.d	ACQ Method		Comment		Acquired Time	3/24/2014 12:08:31 PM

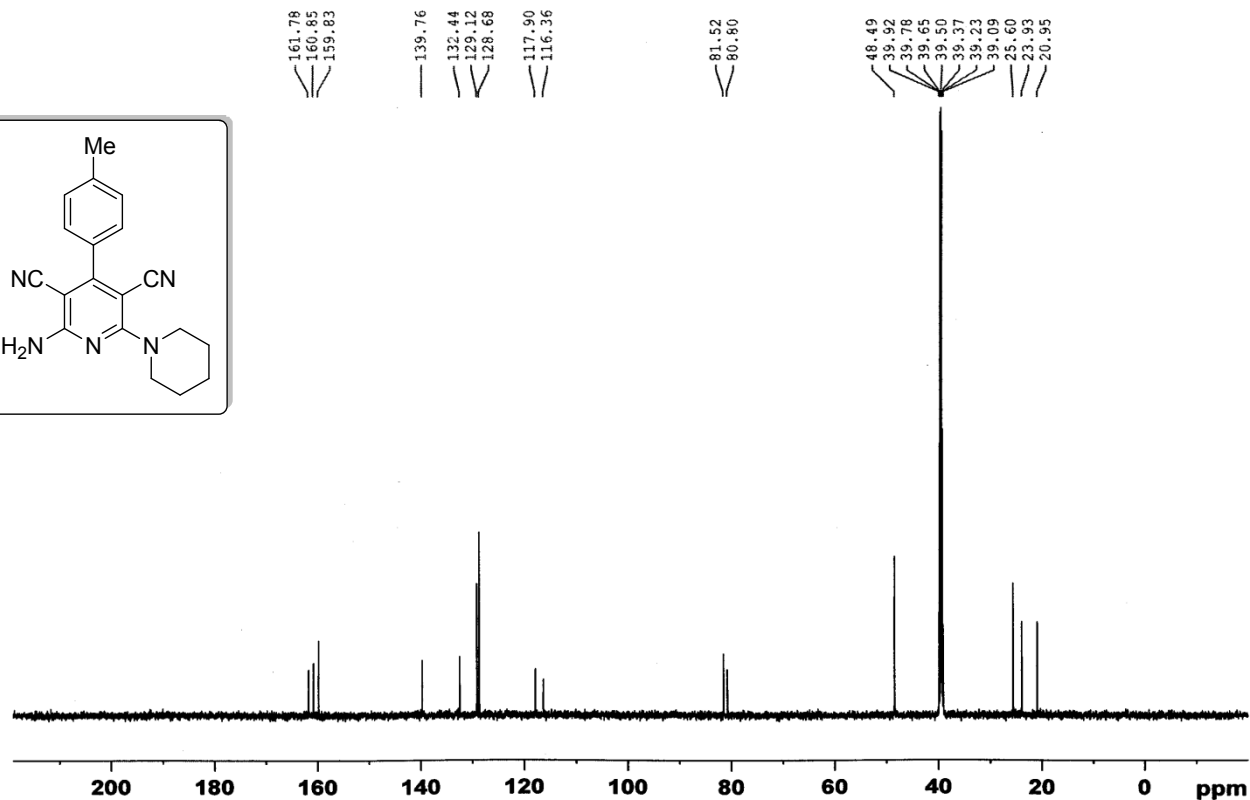
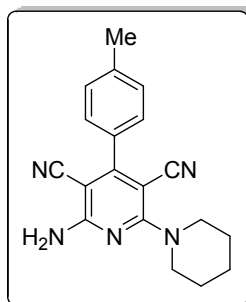


¹H-NMR spectra of compound 4t



¹³C-NMR spectra of compound 4t

SS-4Me-pip-13C



Current Data Parameters
 NAME SS-4Me-pip-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131125
 Time 8.59
 INSTRUM spect
 PROBHD 5 mm PABCO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 52
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543829 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 297.9 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 95.0000000 W

----- CHANNEL f2 -----
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 21.0000000 W
 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
 SI 16384
 SF 150.9129342 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

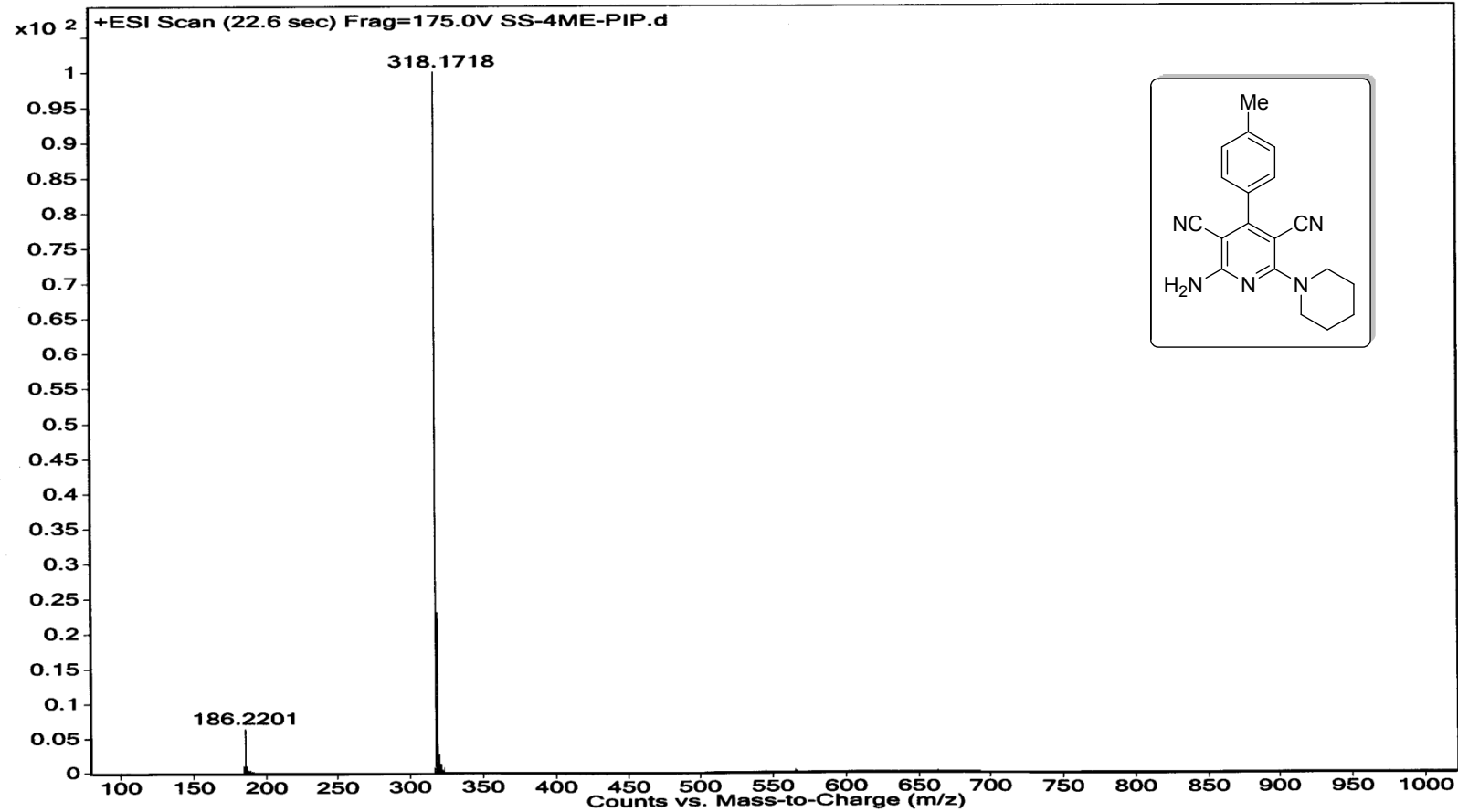
HRMS-spectra of compound 4t

Sample Name
Inj Vol
Data Filename

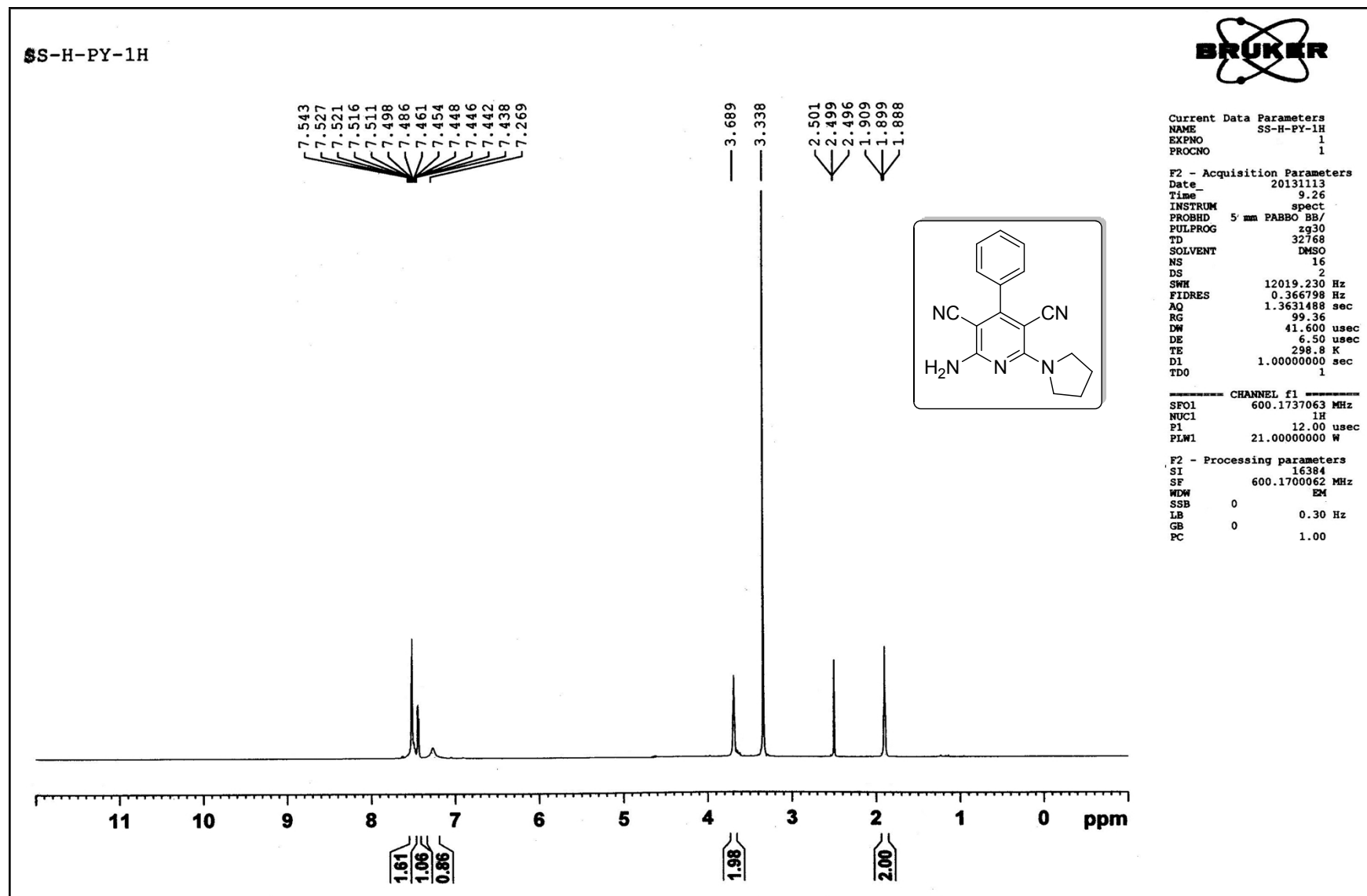
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time

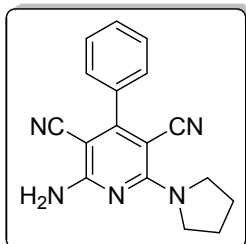


¹H-NMR spectra of compound **4u**



¹³C-NMR spectra of compound **4u**

SS-H-Py-13C

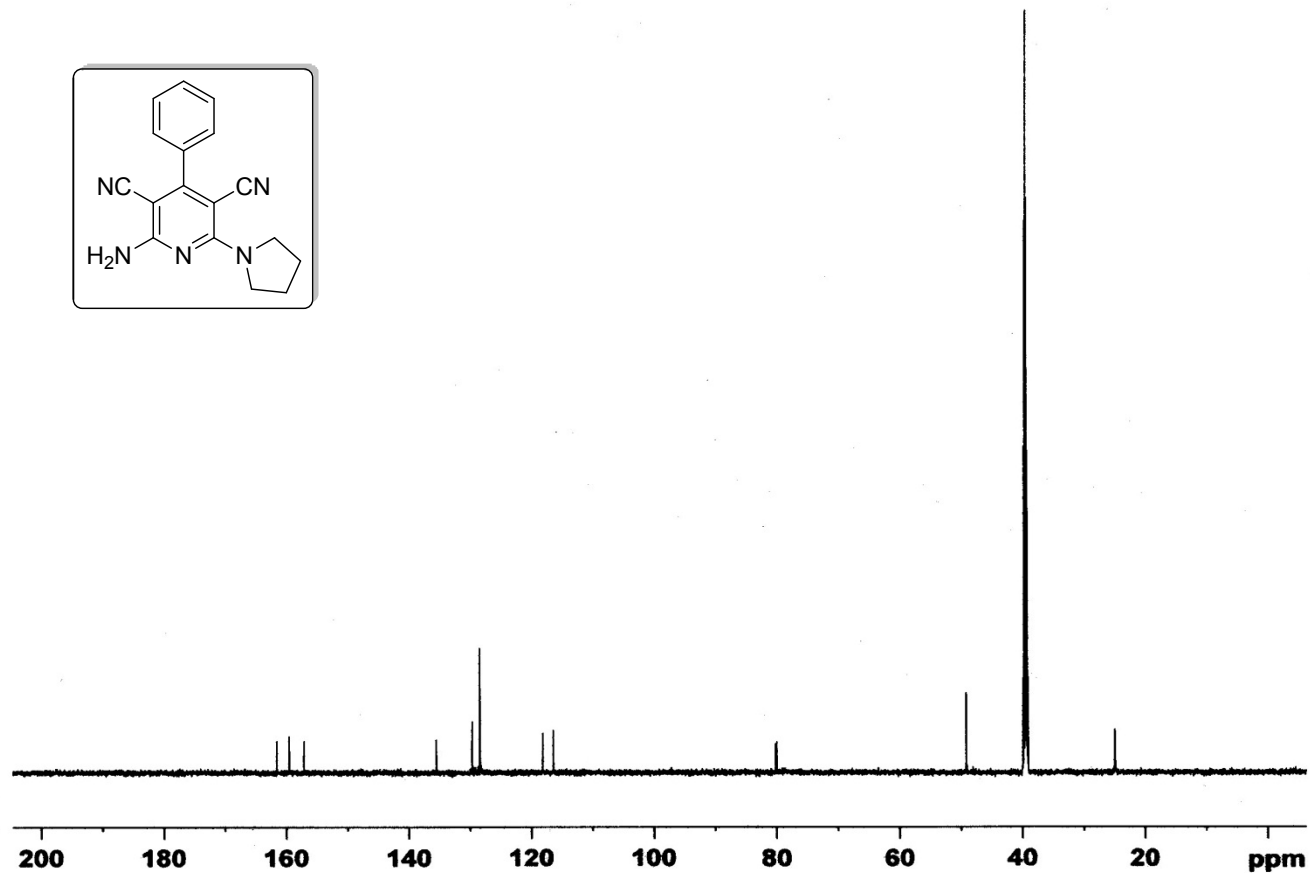


161.59
159.59
157.19

135.57
129.74
128.50
128.45
118.18
116.47

80.17
80.01

49.15
39.91
39.78
39.64
39.50
39.36
39.22
39.08
24.92



Current Data Parameters
NAME SS-H-Py-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131118
Time_ 10.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 139
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

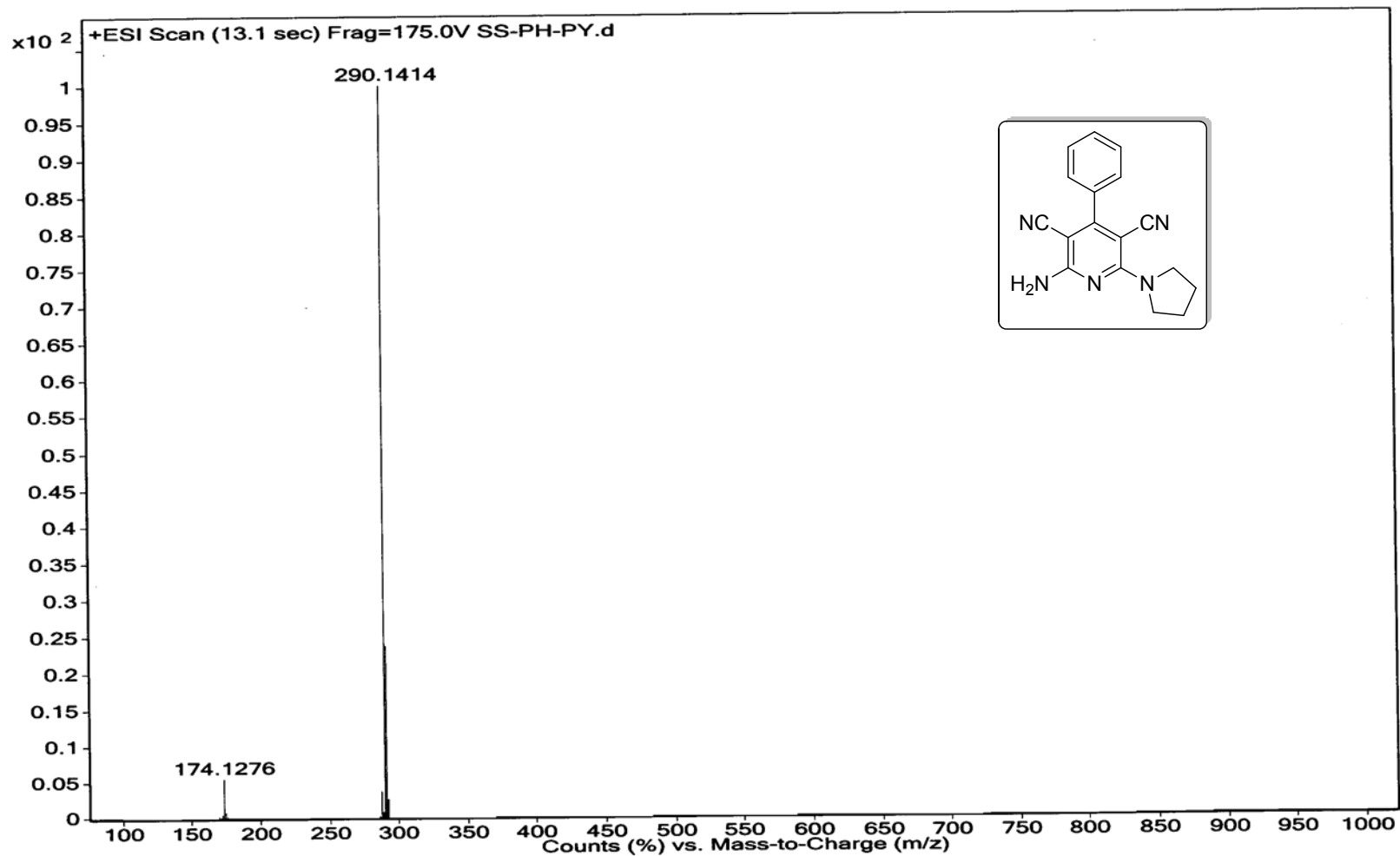
===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9129343 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS-spectra of compound 4u

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	SS-PH-PY.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



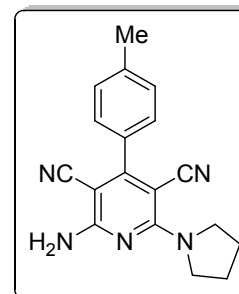
¹H-NMR spectra of compound 4v

SS-4Me-PhCHO-PY-1H



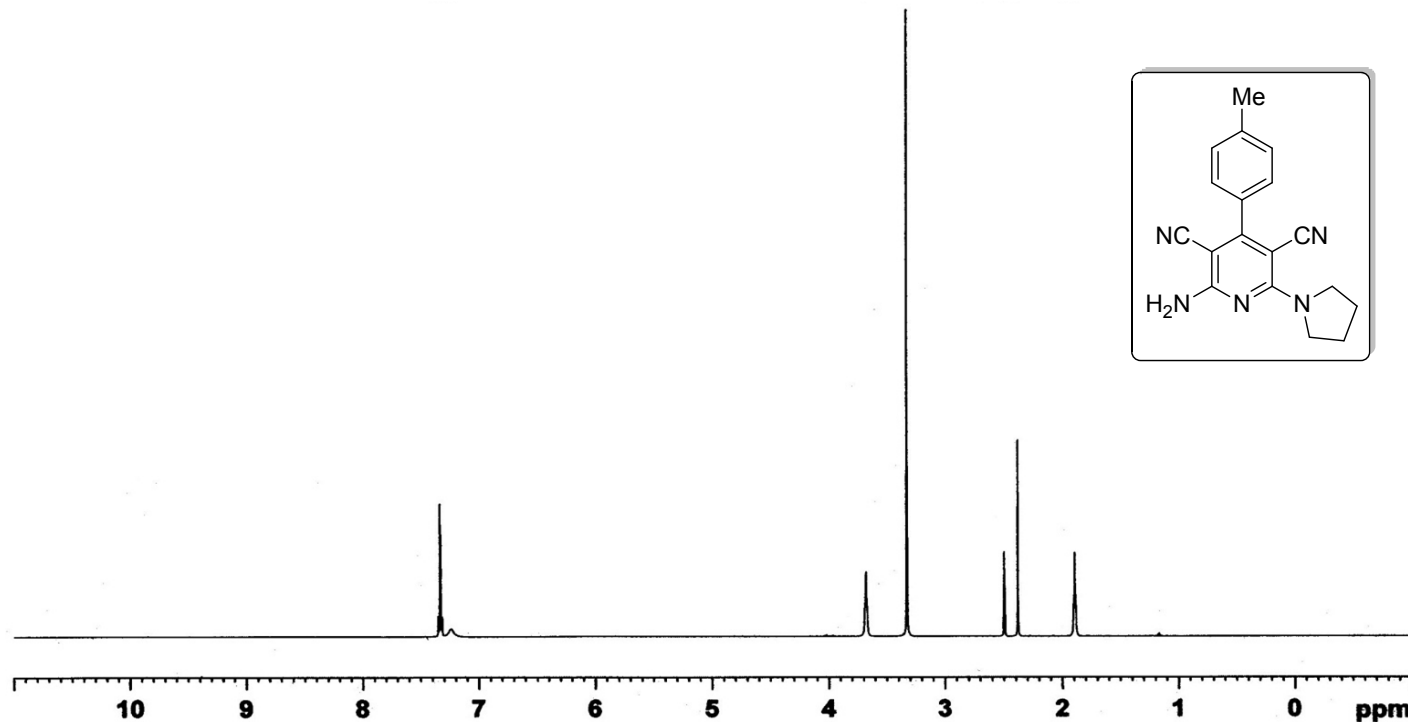
Current Data Parameters
NAME SS-4Me-PhCHO-PY-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20131107
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 80.22
DW 41.600 usec
DE 6.50 usec
TE 299.3 K
D1 1.0000000 sec
TD0 1

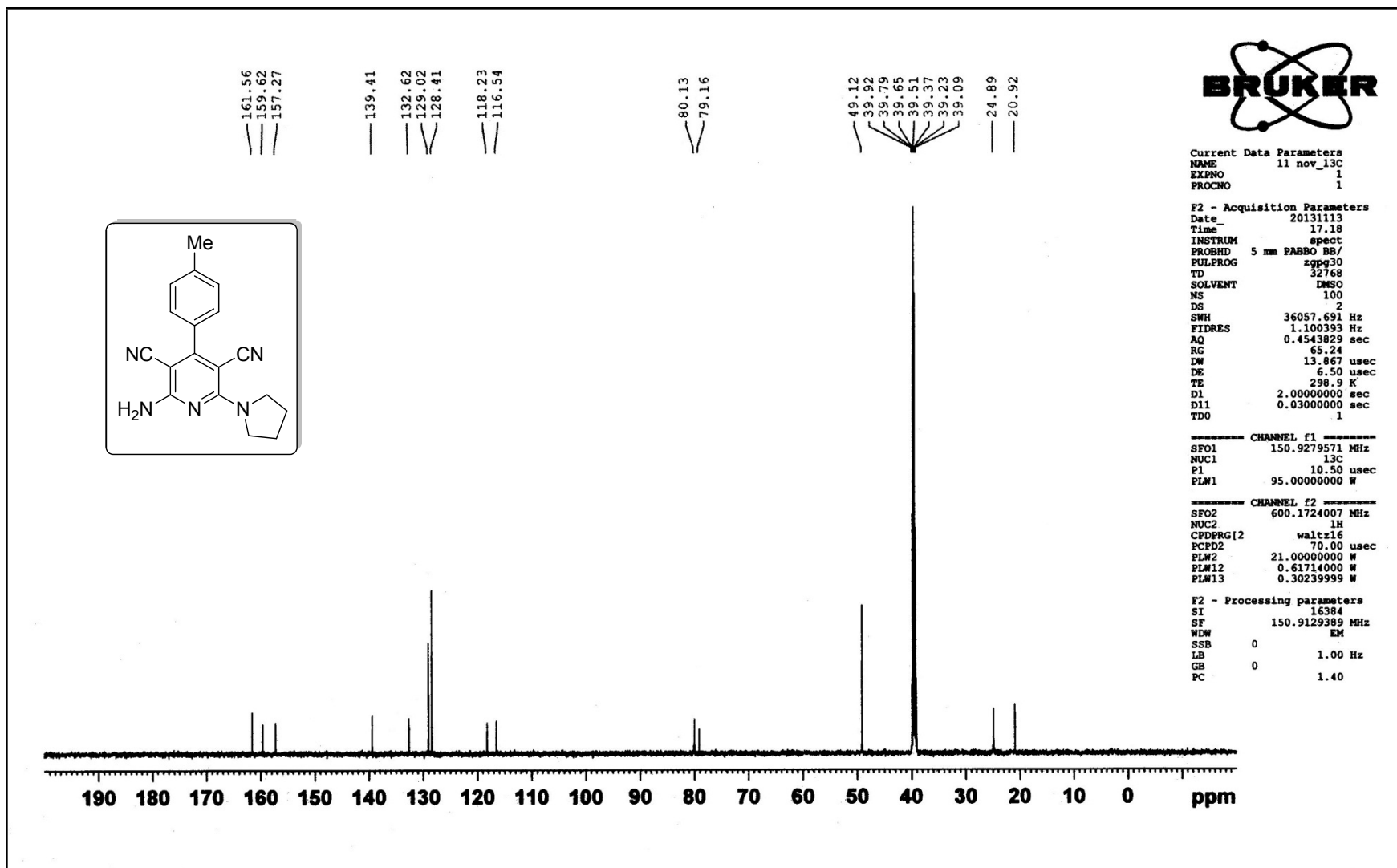


----- CHANNEL f1 -----
SF01 600.1737063 MHz
NUC1 1H
P1 12.00 usec
PLW1 21.0000000 W

F2 - Processing parameters
SI 16384
SF 600.1700054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C-NMR spectra of compound 4v



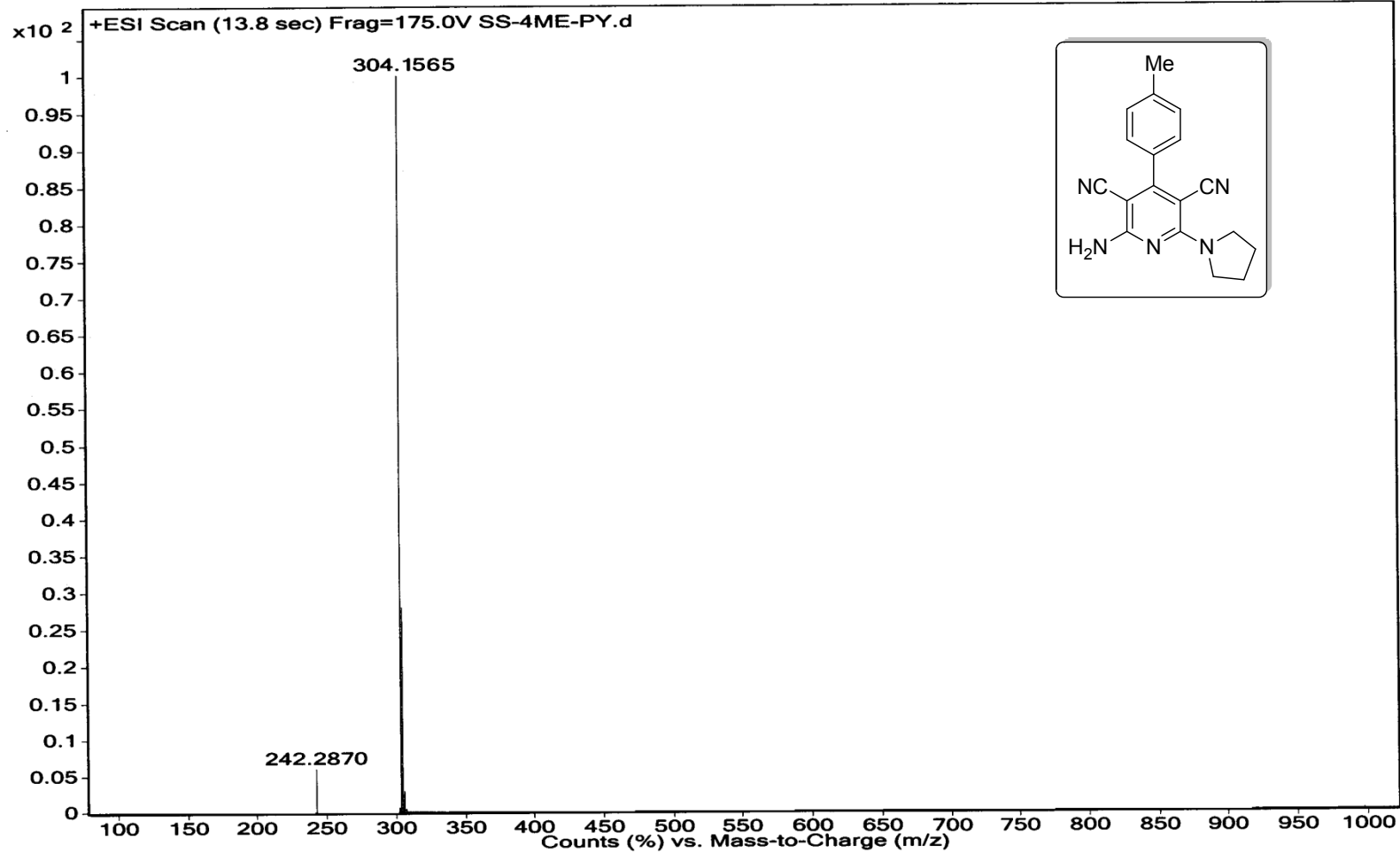
HRMS-spectra of compound 4v

Sample Name SS-4ME-PY
Inj Vol -10
Data Filename SS-4ME-PY.d

Position -1
InjPosition
ACQ Method

Instrument Name Instrument 1
SampleType Sample
Comment

User Name
IRM Calibration Status Success
Acquired Time 3/7/2014 11:48:18 AM



¹H-NMR spectra of compound **6a**

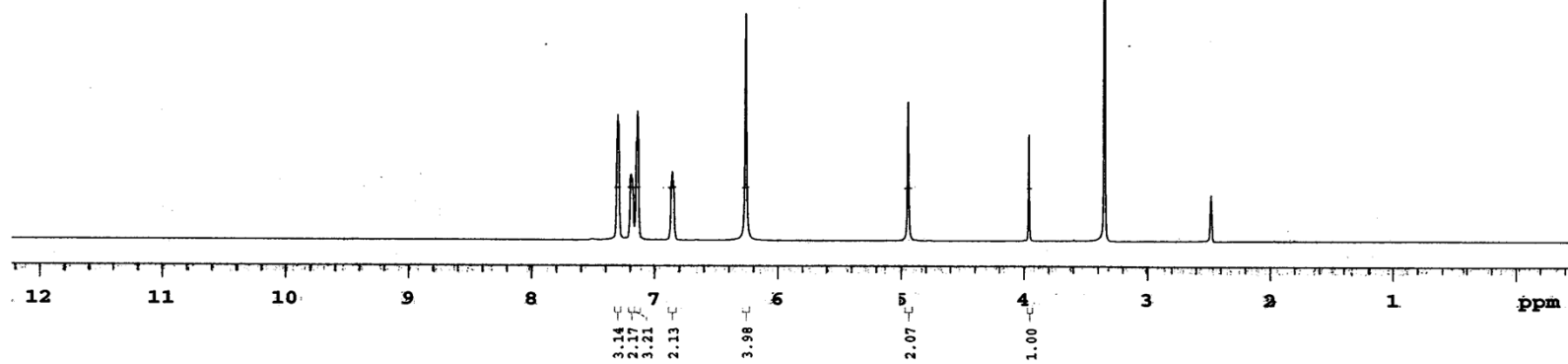
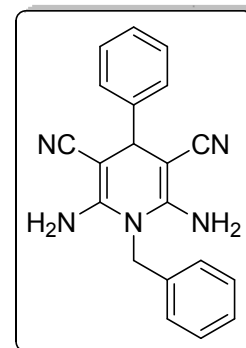
SS-Ph-BA

Sample Name:
SS-Ph-BA
Data Collected on:
IITG-NMR-mercury400
Archive directory:
/home/chem/data/study
Sample directory:
MR-CM-Li-S-THR-F1-01
Fidfile: PROTON

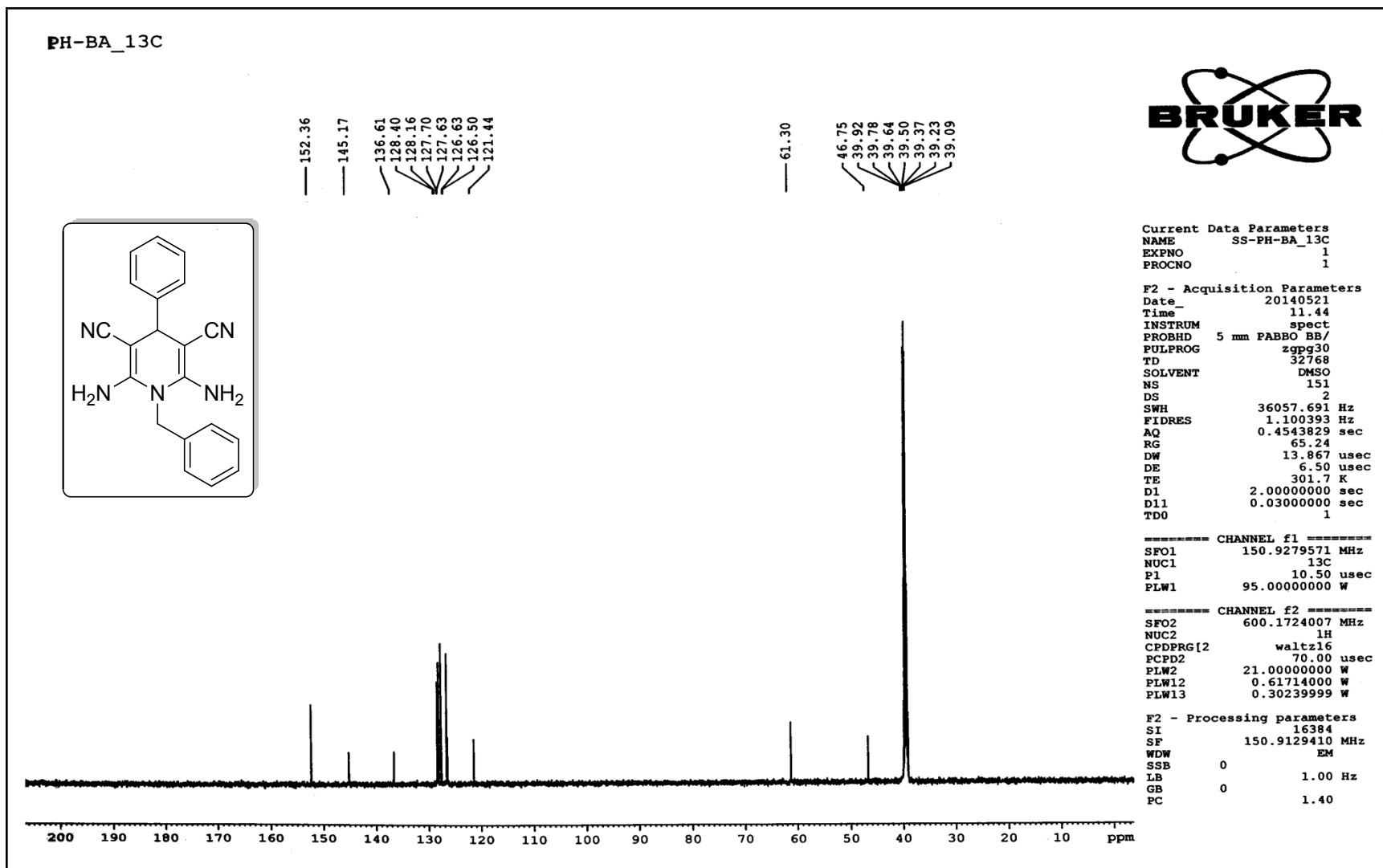
Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: May 20 2014

Temp. 25.0 C / 298.1 K
Operator: chem

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions
OBSERVE H1, 399.8528627 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 12 sec

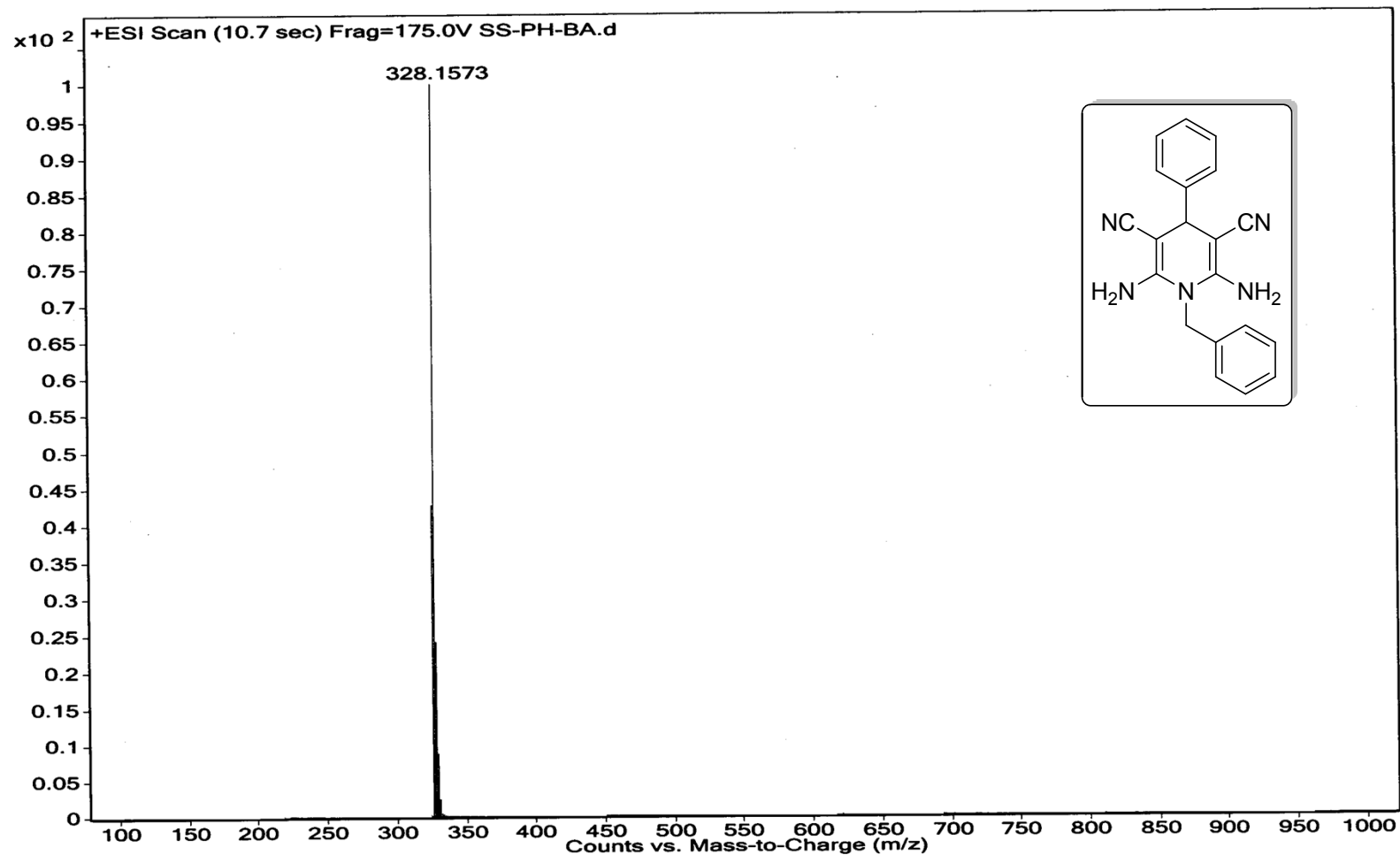


¹³C-NMR spectra of compound 6a

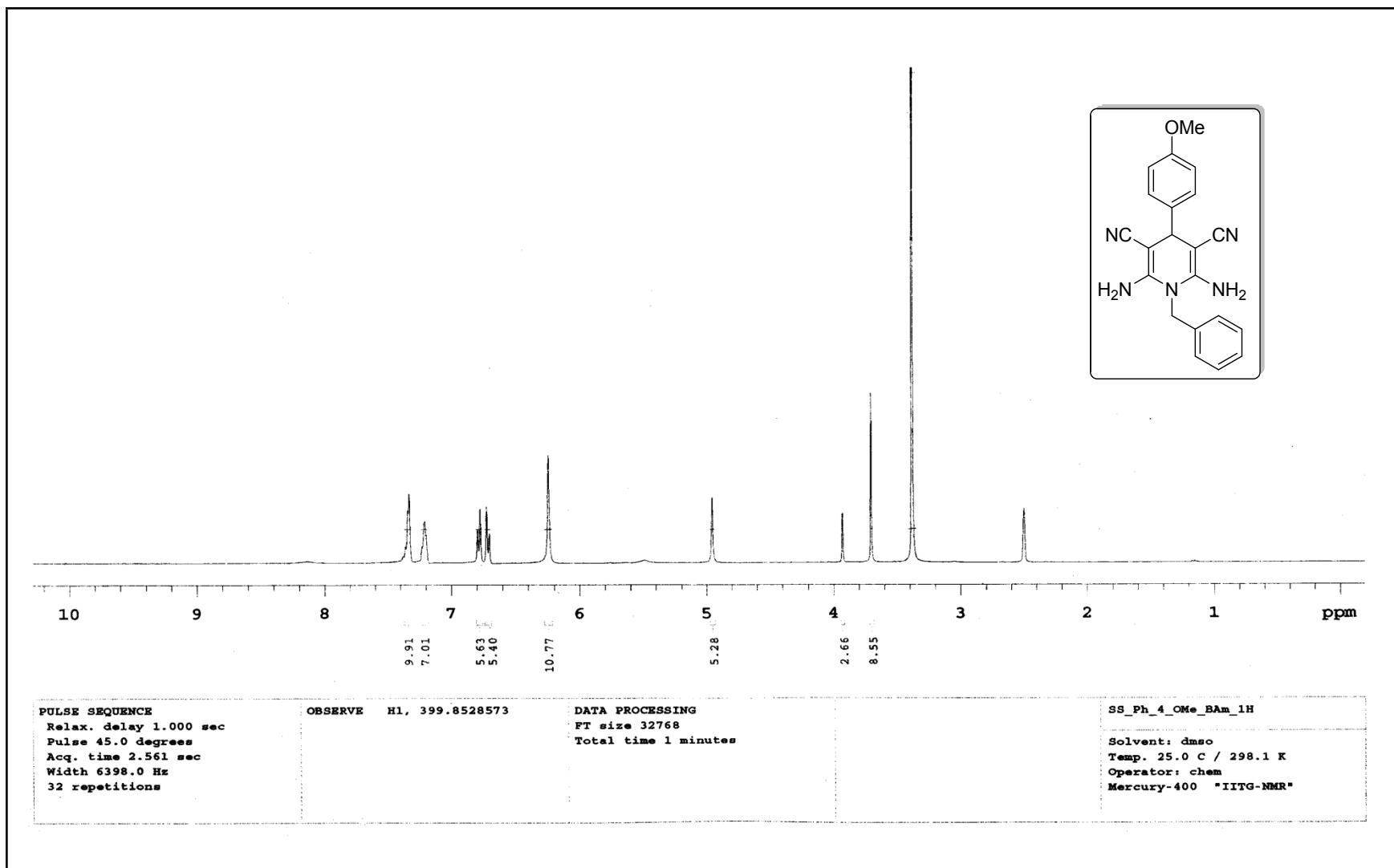


HRMS-spectra of compound 6a

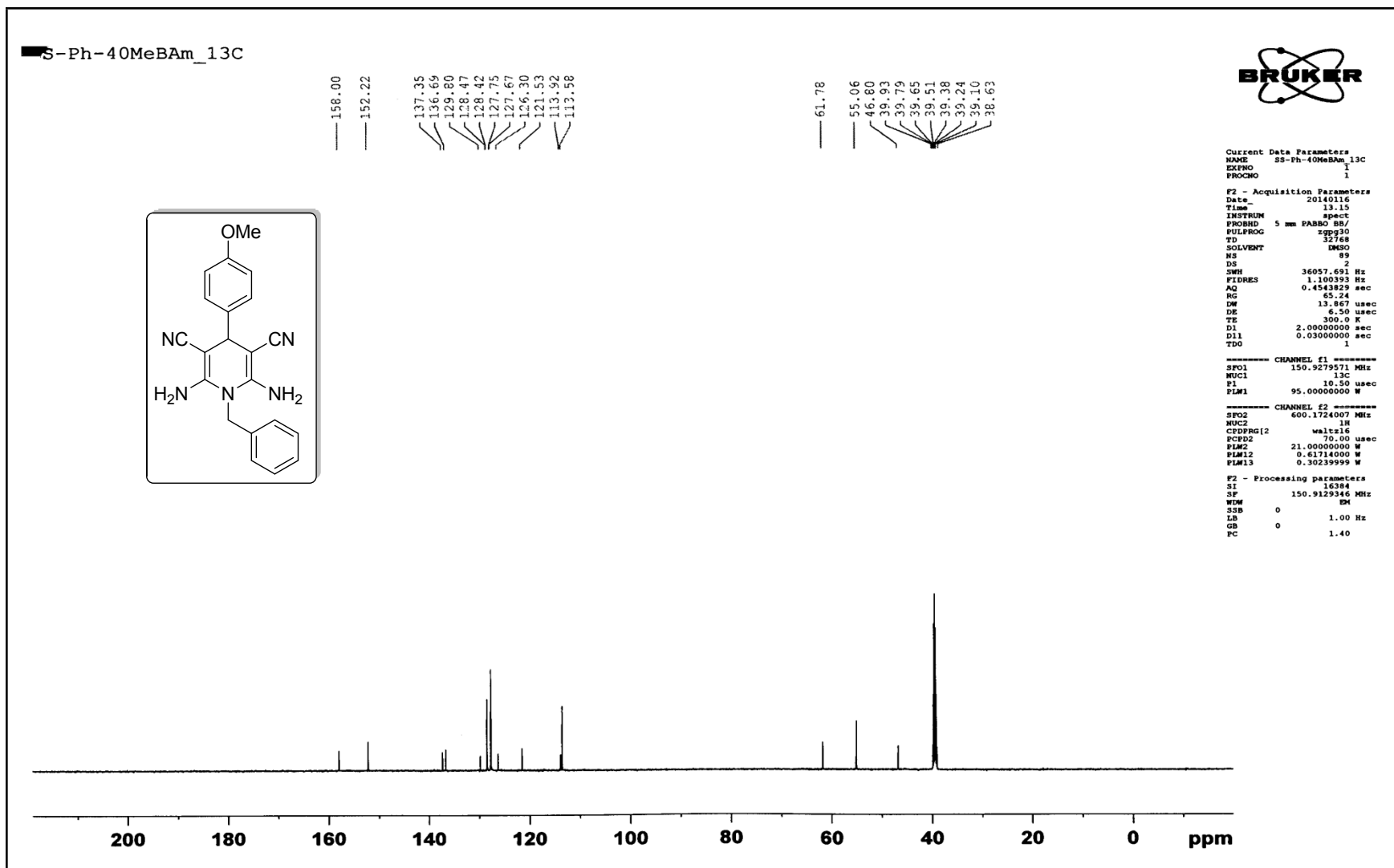
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	SS-PH-BA.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H-NMR spectra of compound **6b**



¹³C-NMR spectra of compound **6b**



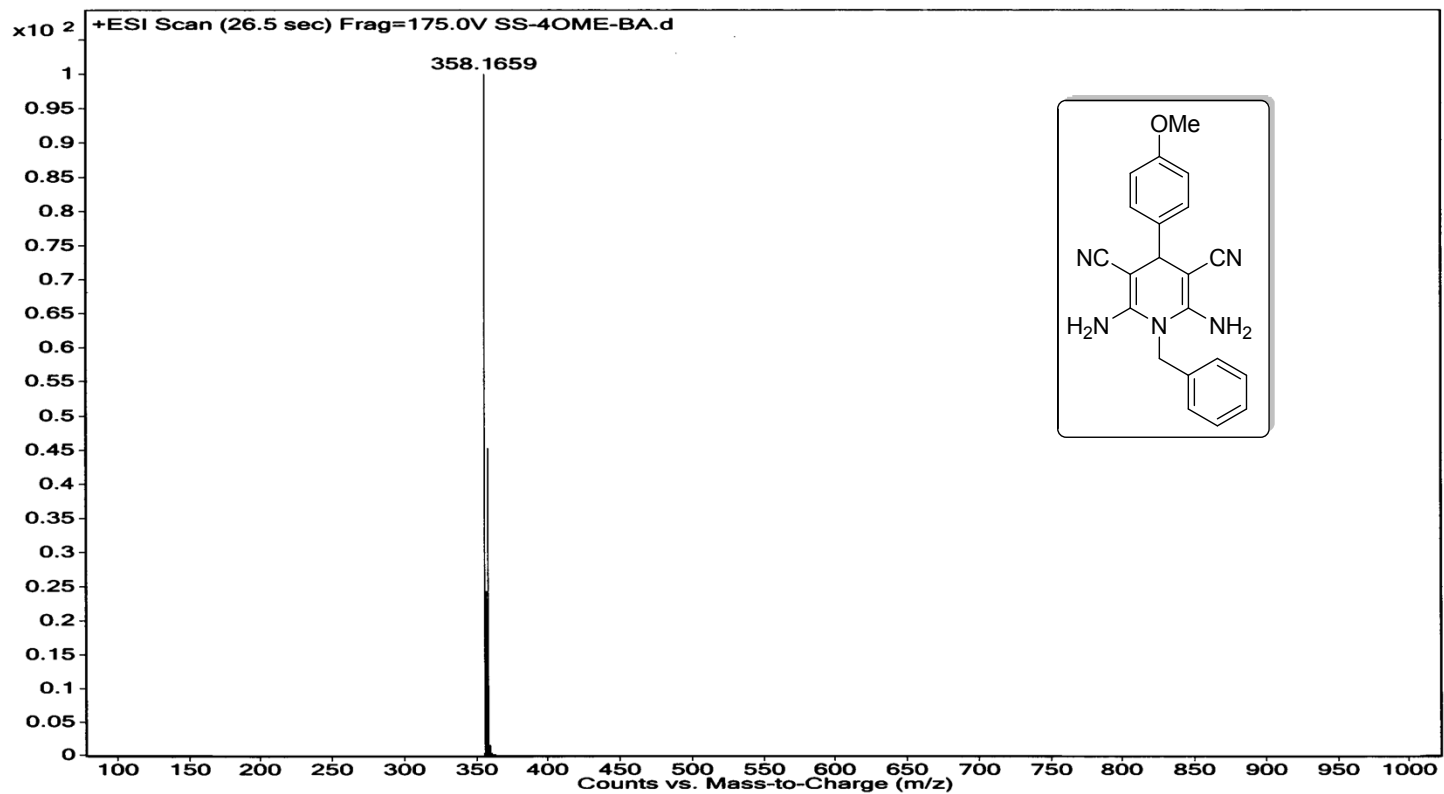
HRMS-spectra of compound **6b**

Sample Name SS-4OME-BA
Inj Vol -10
Data Filename SS-4OME-BA.d

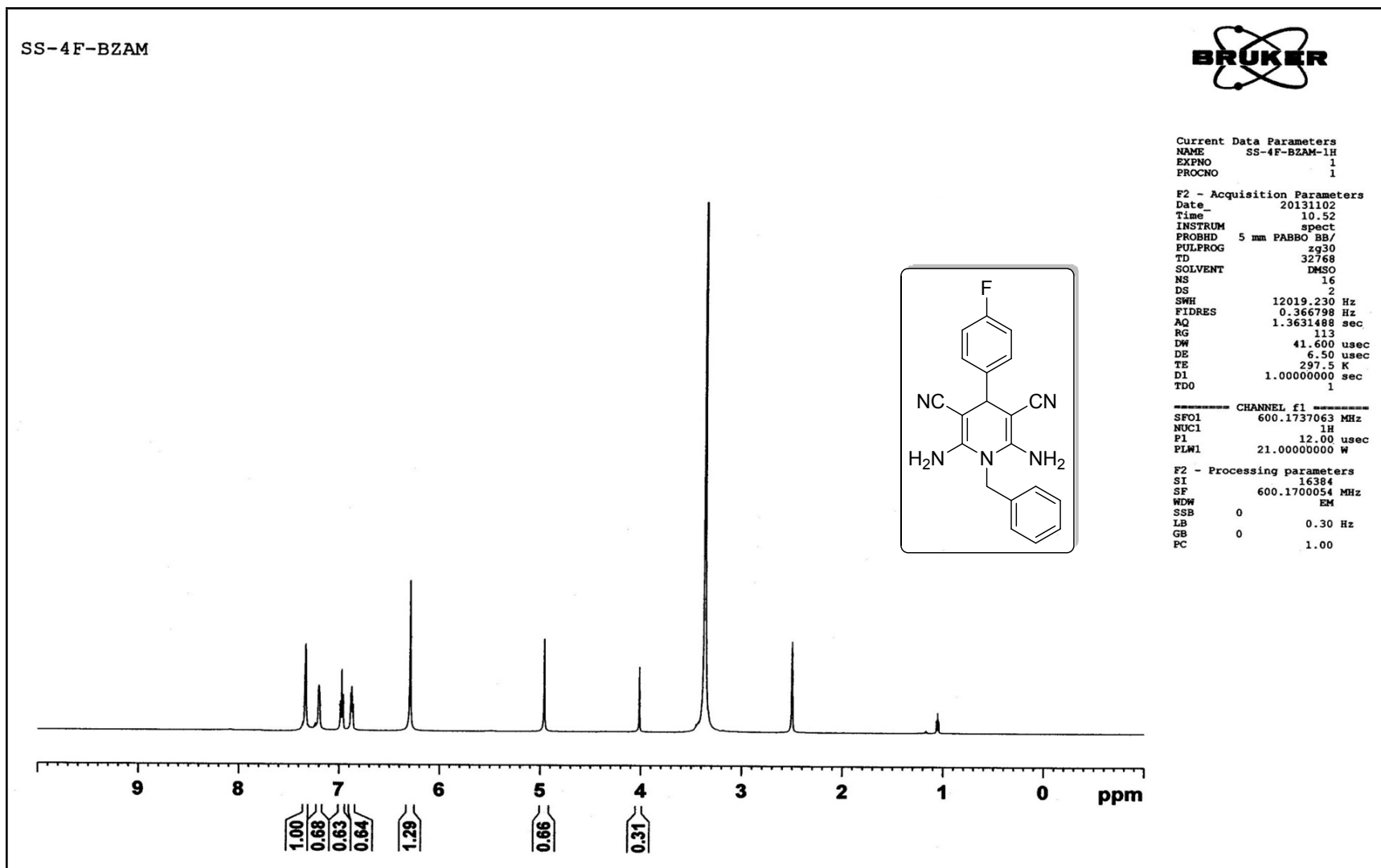
Position -1
InjPosition
ACQ Method

Instrument Name Instrument 1
SampleType Sample
Comment

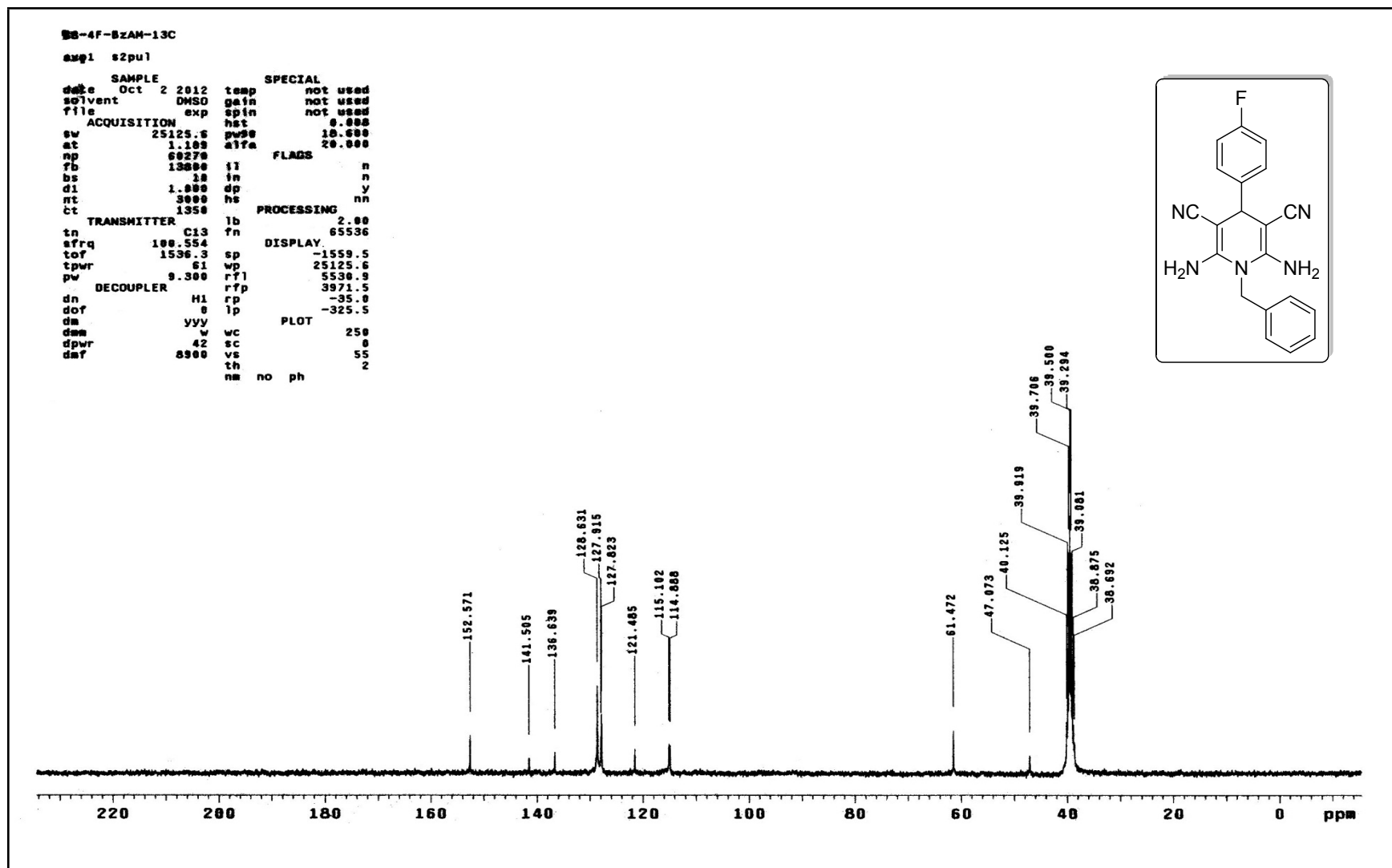
User Name
IRM Calibration Status Success
Acquired Time 3/24/2014 12:06:48 PM



¹H-NMR spectra of compound 6c



¹³C-NMR spectra of compound 6c



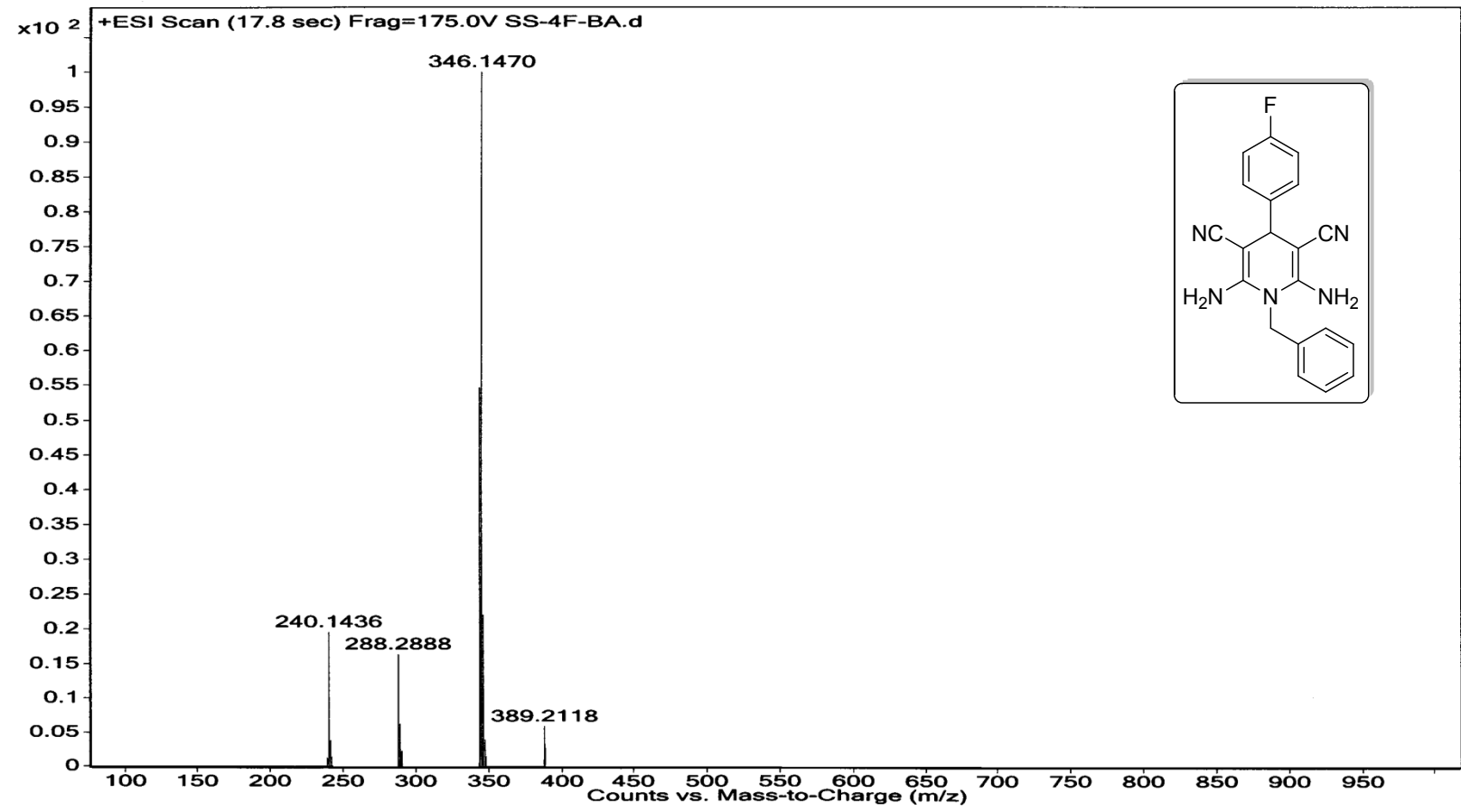
HRMS-spectra of compound 6c

Sample Name SS-4F-BA
Inj Vol -10
Data Filename SS-4F-BA.d

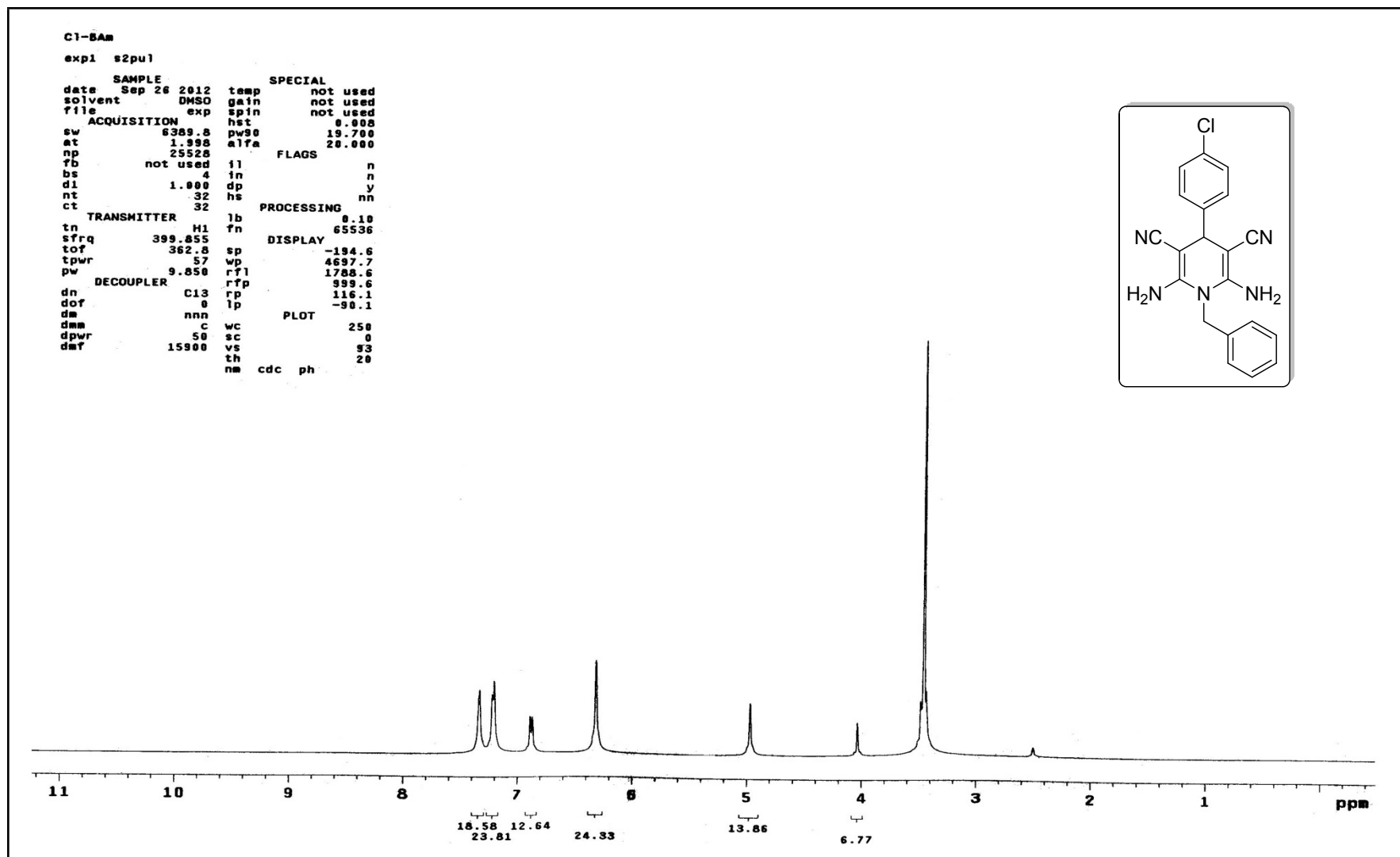
Position -1
InjPosition
ACQ Method

Instrument Name Instrument 1
SampleType Sample
Comment

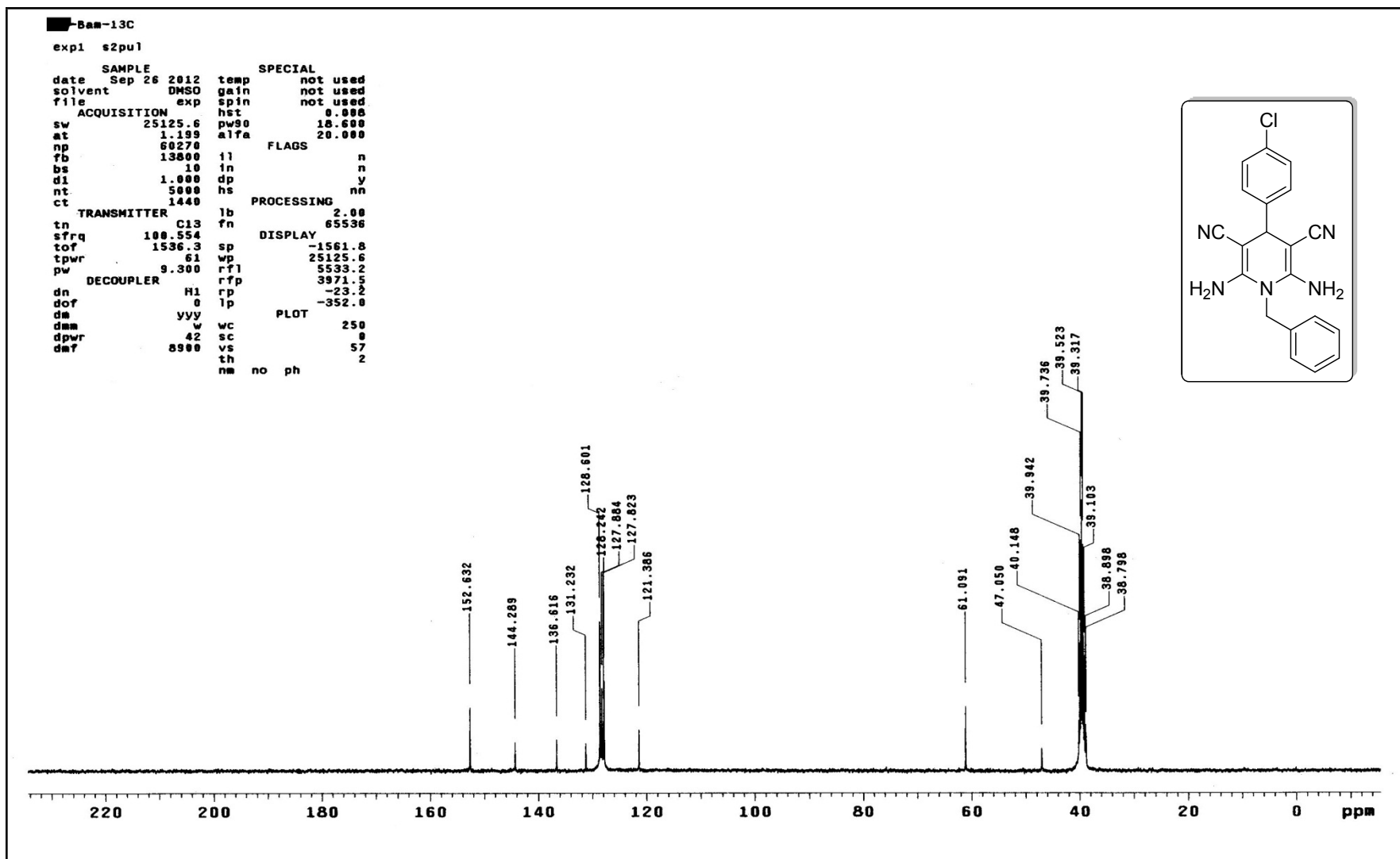
User Name
IRM Calibration Status Success
Acquired Time 4/10/2014 11:34:47 AM



¹H-NMR spectra of compound **6d**

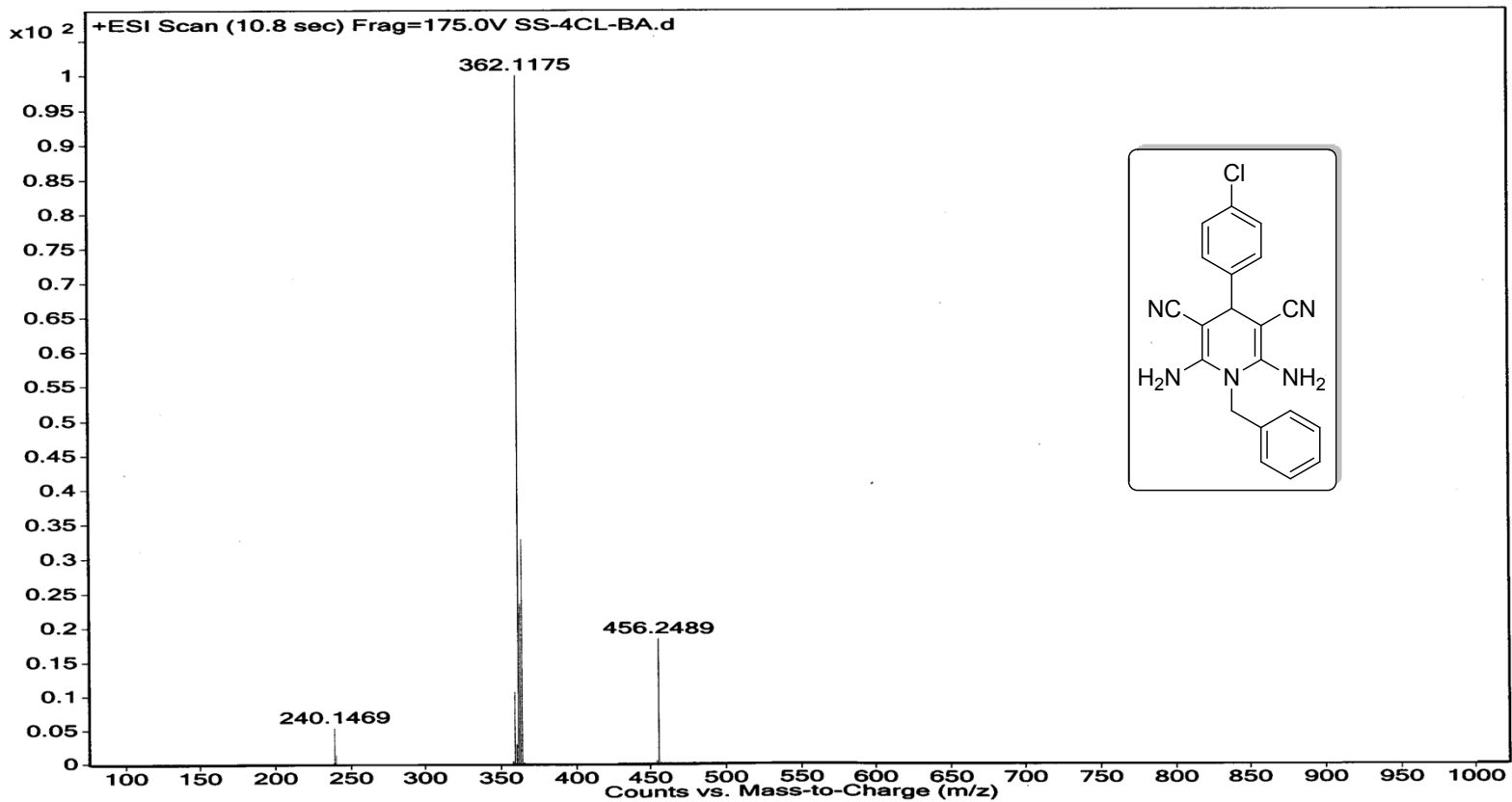


¹³C-NMR spectra of compound **6d**

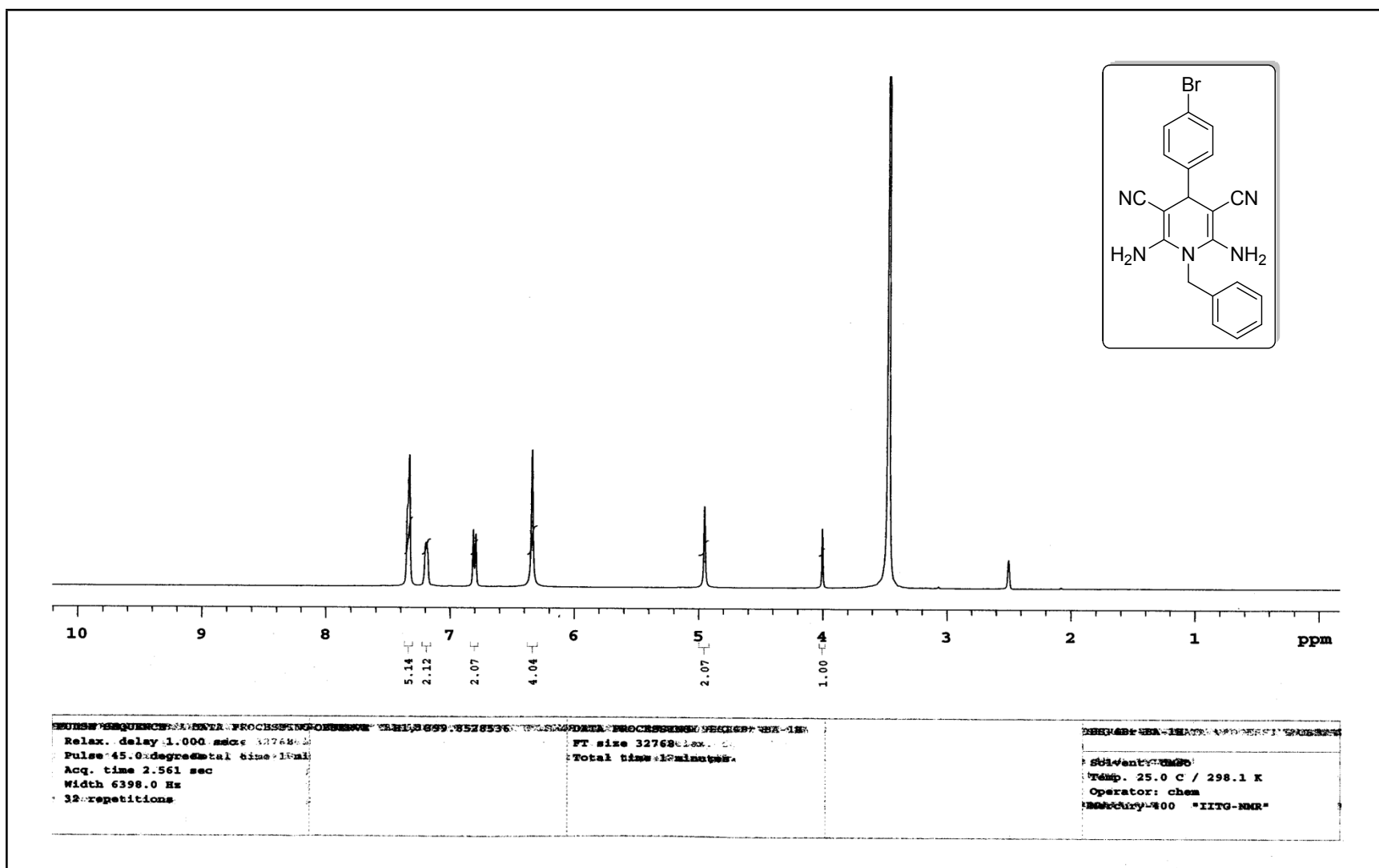


HRMS-spectra of compound **6d**

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	SS-4CL-BA.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H-spectra of compound 6e



¹³C-spectra of compound 6e

3S-4Br-BA-13C



Current Data Parameters
NAME SS-4Br-BA-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140529
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 226
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 299.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

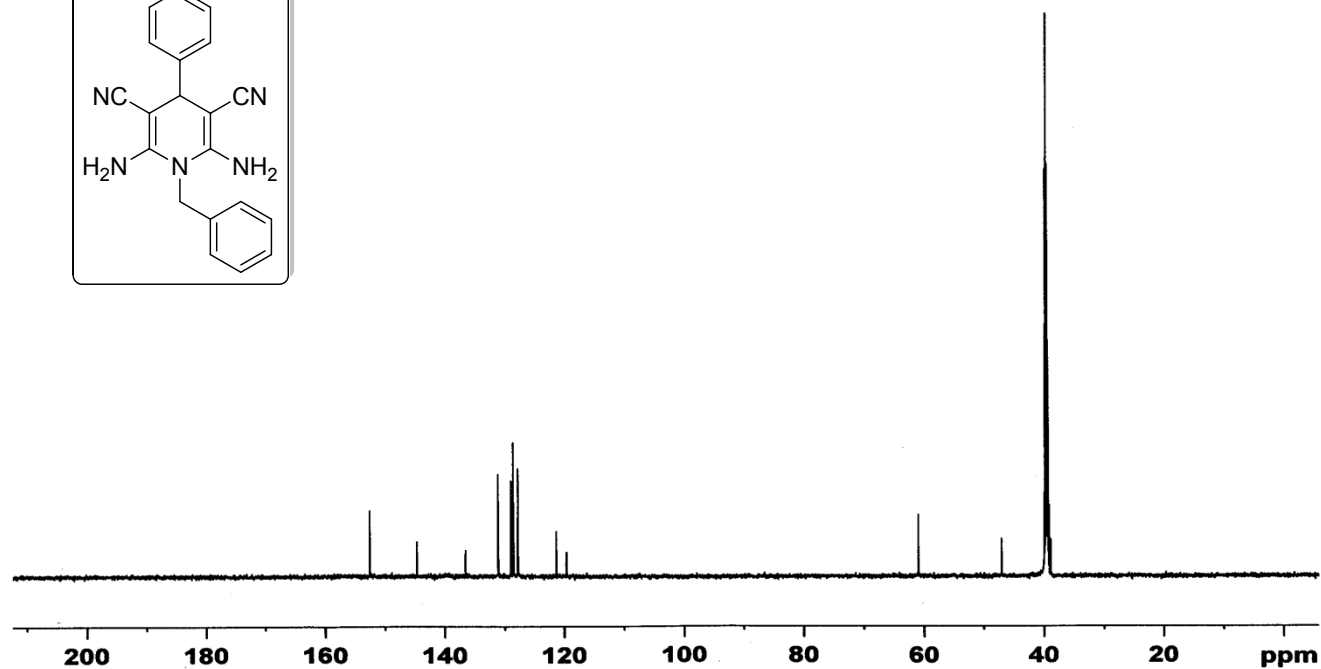
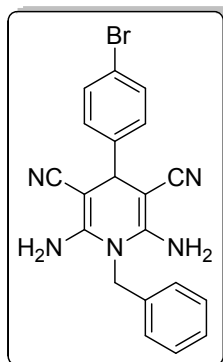
===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.0000000 W

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 21.0000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9129254 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

152.61
144.70
136.58
131.13
128.97
128.59
127.86
127.79
121.36
119.68

60.95
46.99
39.91
39.78
39.63
39.50
39.36
39.22
39.08
38.84



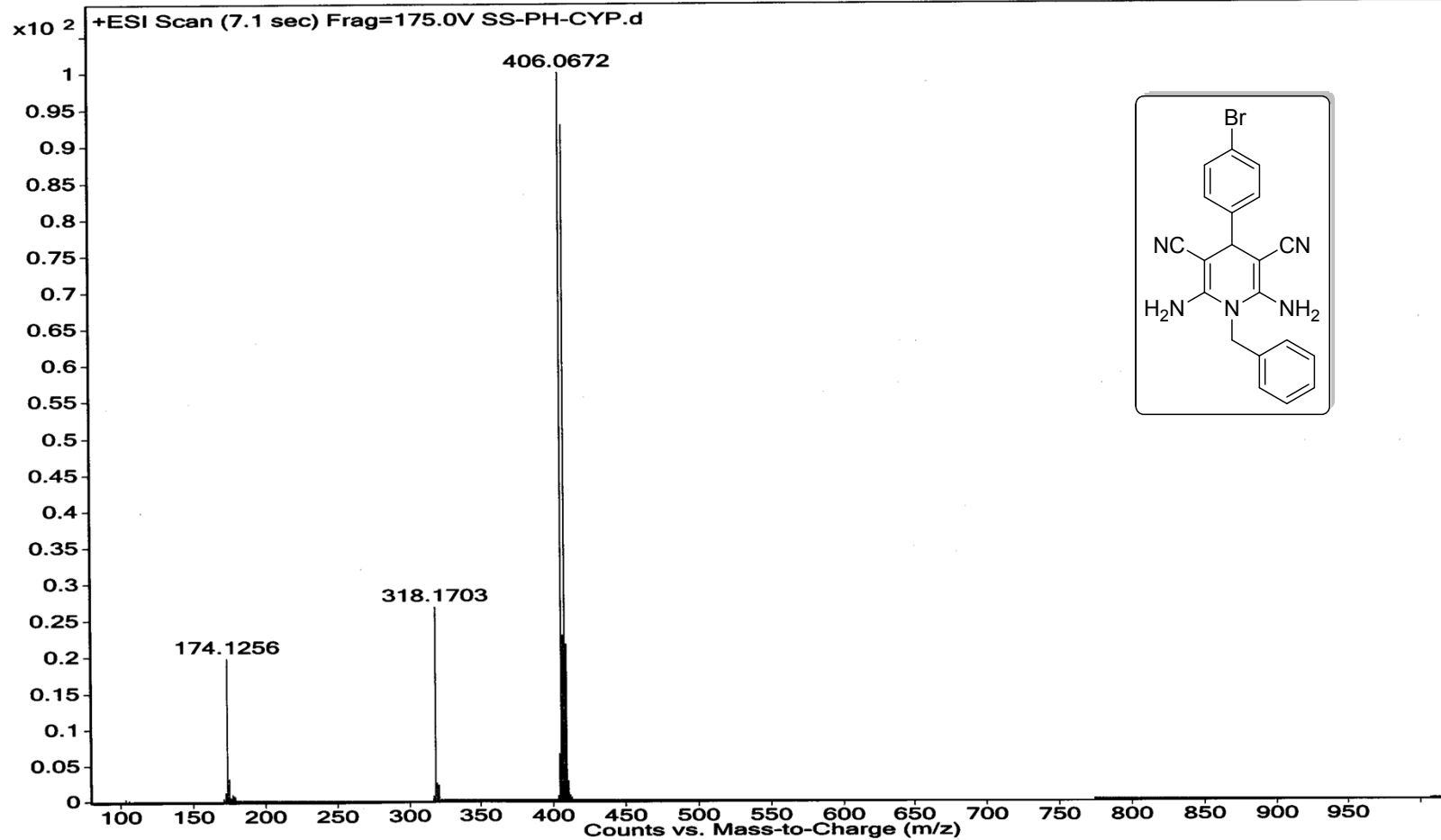
HRMS-spectra of compound 6e

Sample Name
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

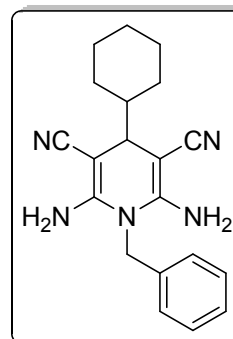
Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



¹H-spectra of compound 6f

SS-CY-BA_1H

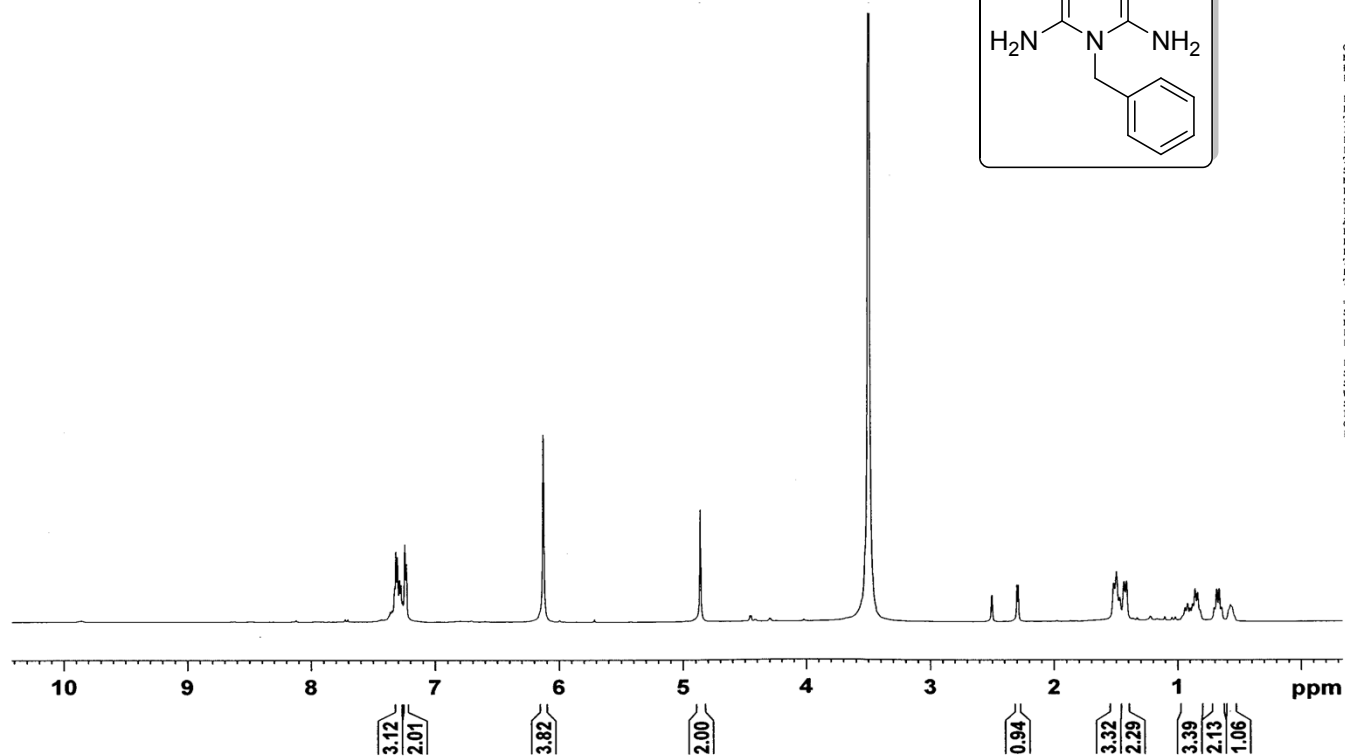


```
Current Data Parameters
NAME      SS-CY-BA_1H
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20140919
Time     11.12
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  DMSO
NS       16
DS       2
SWH      12019.230 Hz
FIDRES   0.366796 Hz
AQ       1.3631488 sec
RG       15.83
DW       41.600 usec
DE       6.50 usec
TE       298.7 K
D1       1.0000000 sec
TDO      1

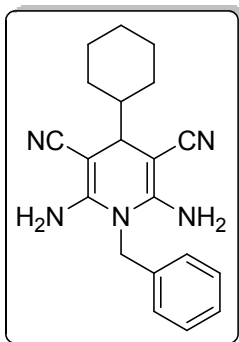
===== CHANNEL f1 =====
SFO1     600.1737063 MHz
NUC1     1H
P1       12.00 usec
PLW1     21.00000000 W

F2 - Processing parameters
SI       16384
SF       600.1700051 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
```



¹³C-spectra of compound 6f

SS-CY-BA_13C



153.14

136.71

128.40

128.38

127.84

122.55

60.04

47.47

46.55

40.12

39.92

39.78

39.64

39.50

39.36

39.22

39.08

29.27

26.11

25.73



Current Data Parameters
NAME SS-CY-BA_13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140919
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 291
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 298.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.0000000 W

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.0000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9129176 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

¹H-spectra of compound 6g

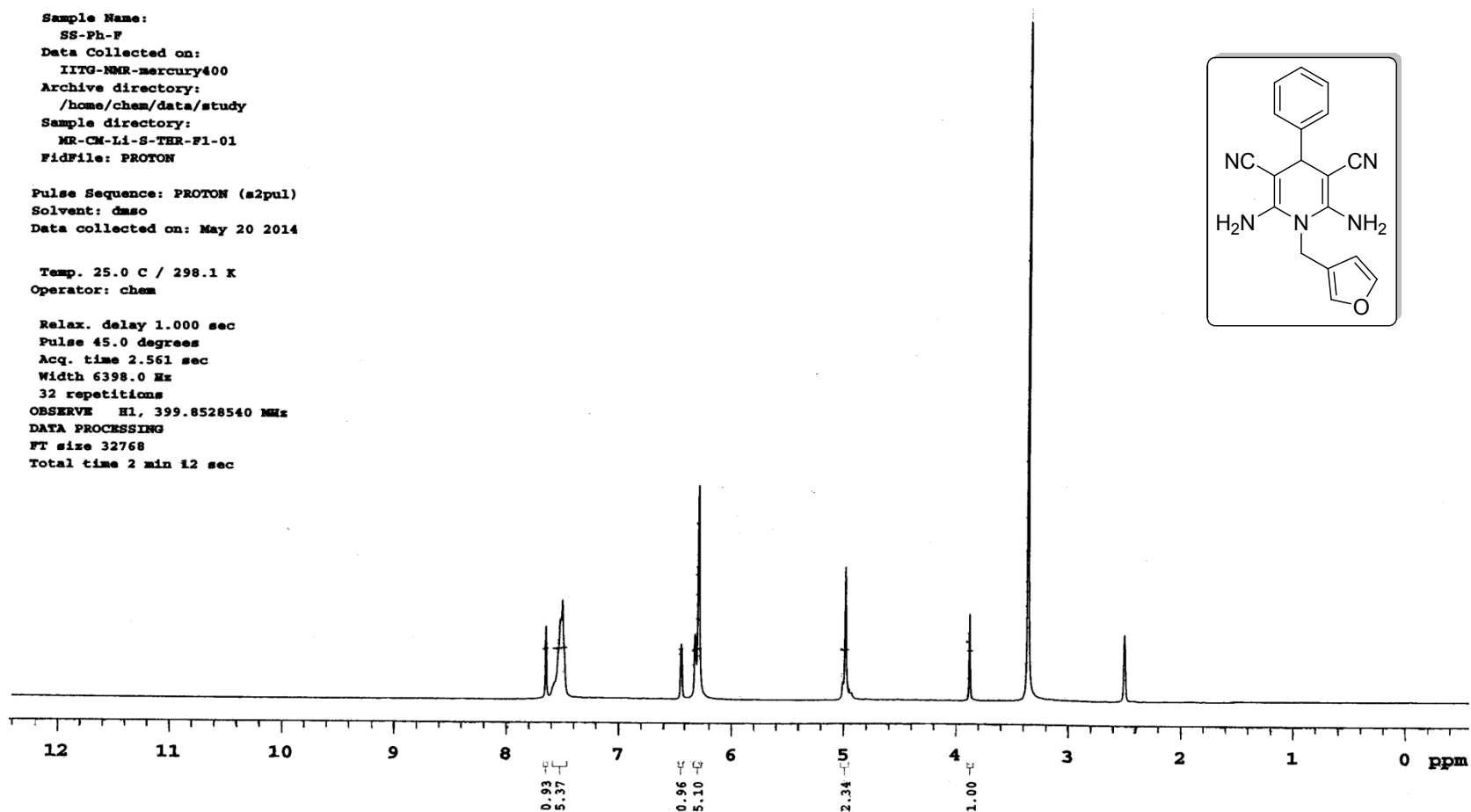
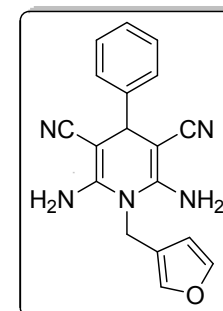
SS-Ph-F

Sample Name:
SS-Ph-F
Data Collected on:
IITG-NMR-mercury400
Archive directory:
/home/chem/data/study
Sample directory:
MR-CM-Li-S-THR-F1-01
FidFile: PROTON

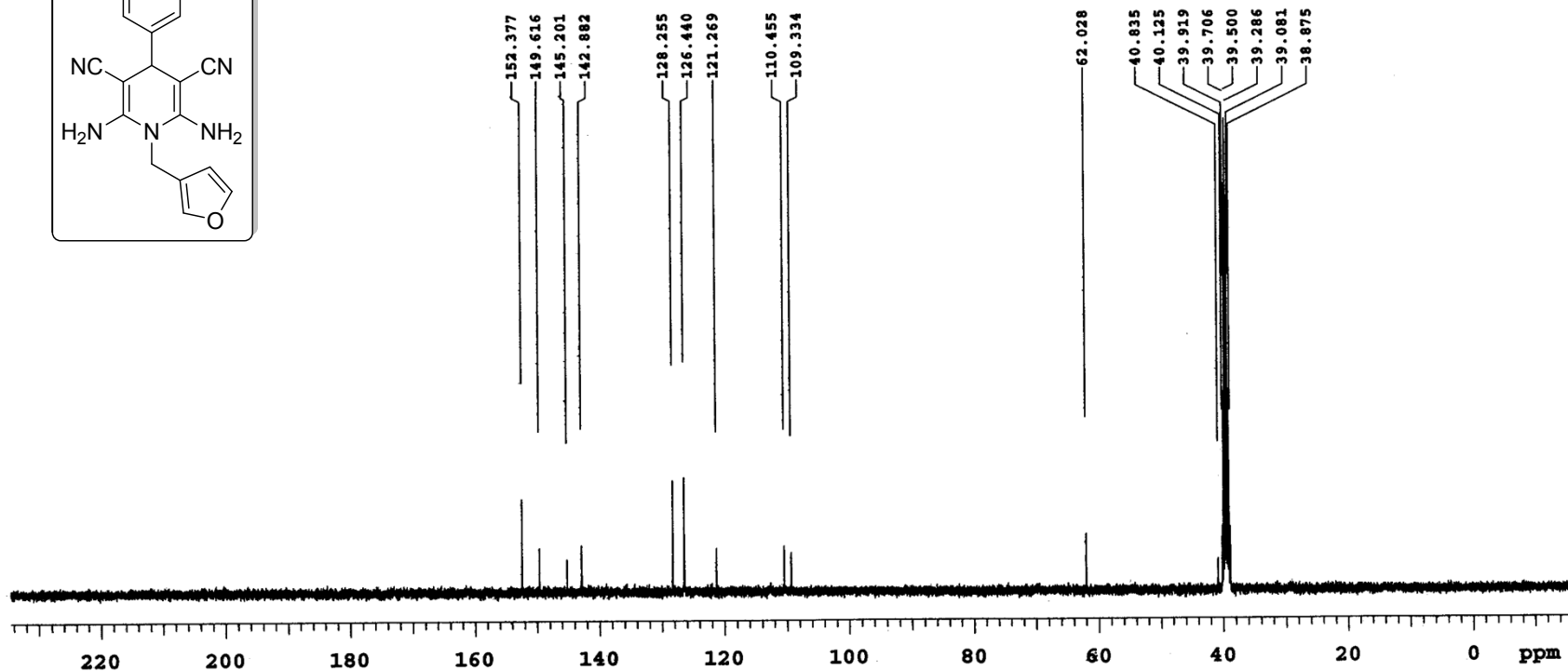
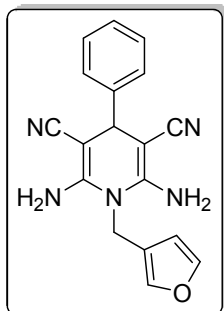
Pulse Sequence: PROTON (s2pul)
Solvent: dms
Data collected on: May 20 2014

Temp. 25.0 C / 298.1 K
Operator: chem

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions
OBSERVE H1, 399.8528540 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 12 sec



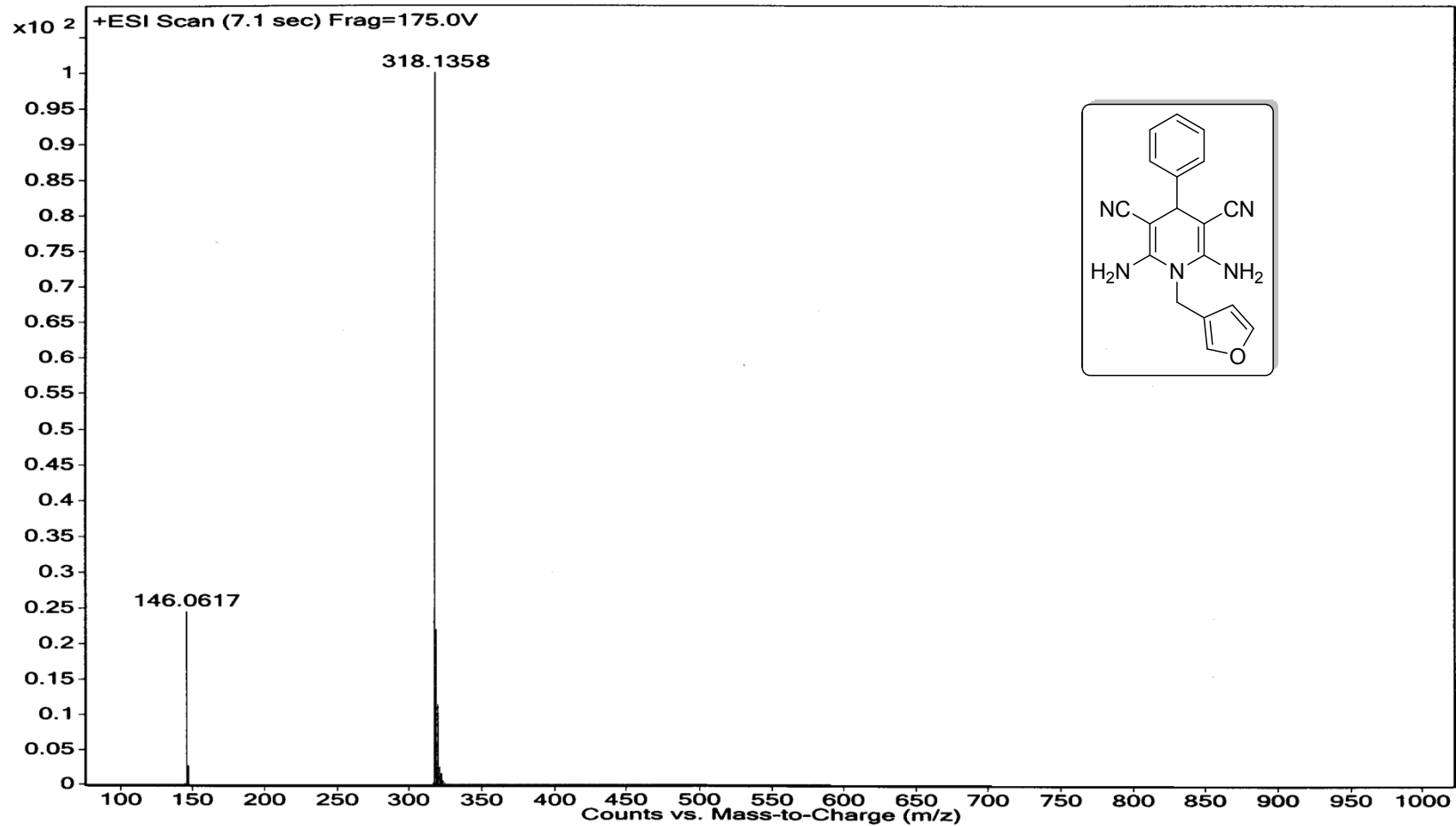
¹³C-spectra of compound 6g



SEQUENCE DATA PROCESSING Ref: 65536 Delay 1.000 sec Pulse 45.0 degree Acq. time 1.304 sec Width 25125.6 Hz 322 repetitions "IITG-NMR"	OBSERVE-FILE 130.5431293 DECOUPLE H1, 399.8548987 Power: 20 dB continuously on WALTZ-16 modulated	DATA PROCESSING VIEW: F Line broadening 0.5 Hz FT size 65536 Total time 38 minutes	SS-Ph-File PROCESSING OBSERVE Solvent: dms 65536 Temp. 25.0 C / 298.15 K Operator: chem File: SS-Ph-F-13C Mercury-400 "IITG-NMR"
---	--	--	---

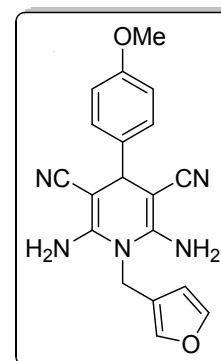
HRMS-spectra of compound 6g

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename		ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H-NMR spectra of compound 6h

SS-4OMe-fur-1H

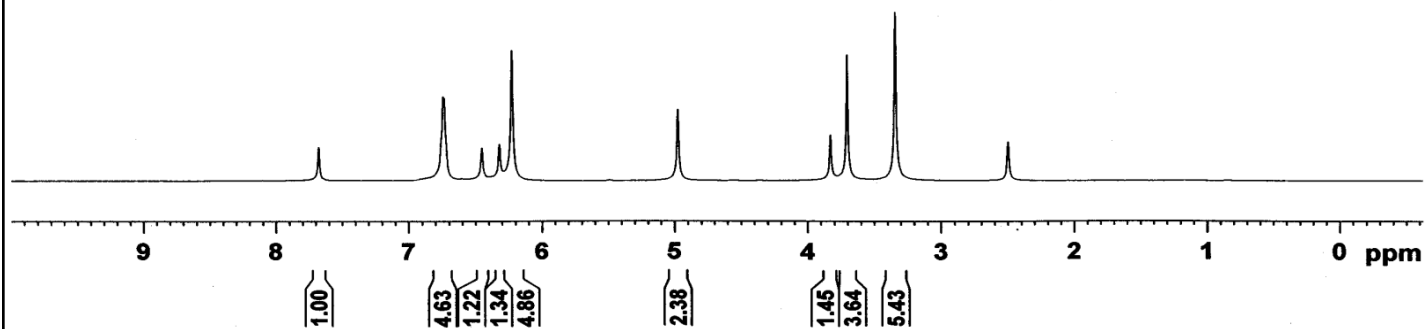


Current Data Parameters
NAME SS-4OMe-fur-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131125
Time 9.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 54.94
DW 41.600 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 600.1737063 MHz
NUC1 1H
P1 12.00 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 16384
SF 600.1700048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00



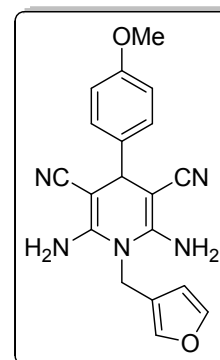
¹³C-NMR spectra of compound 6h

SS-4OMe-Fur-13C



157.93
152.20
149.66
142.97
137.43
127.52
121.35
113.66
110.50
109.31

62.45
55.03
40.87
39.93
39.79
39.66
39.52
39.38
39.24
39.10
38.94



Current Data Parameters
NAME SS-4OMe-Fur-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131125
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 135
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 297.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.0000000 W

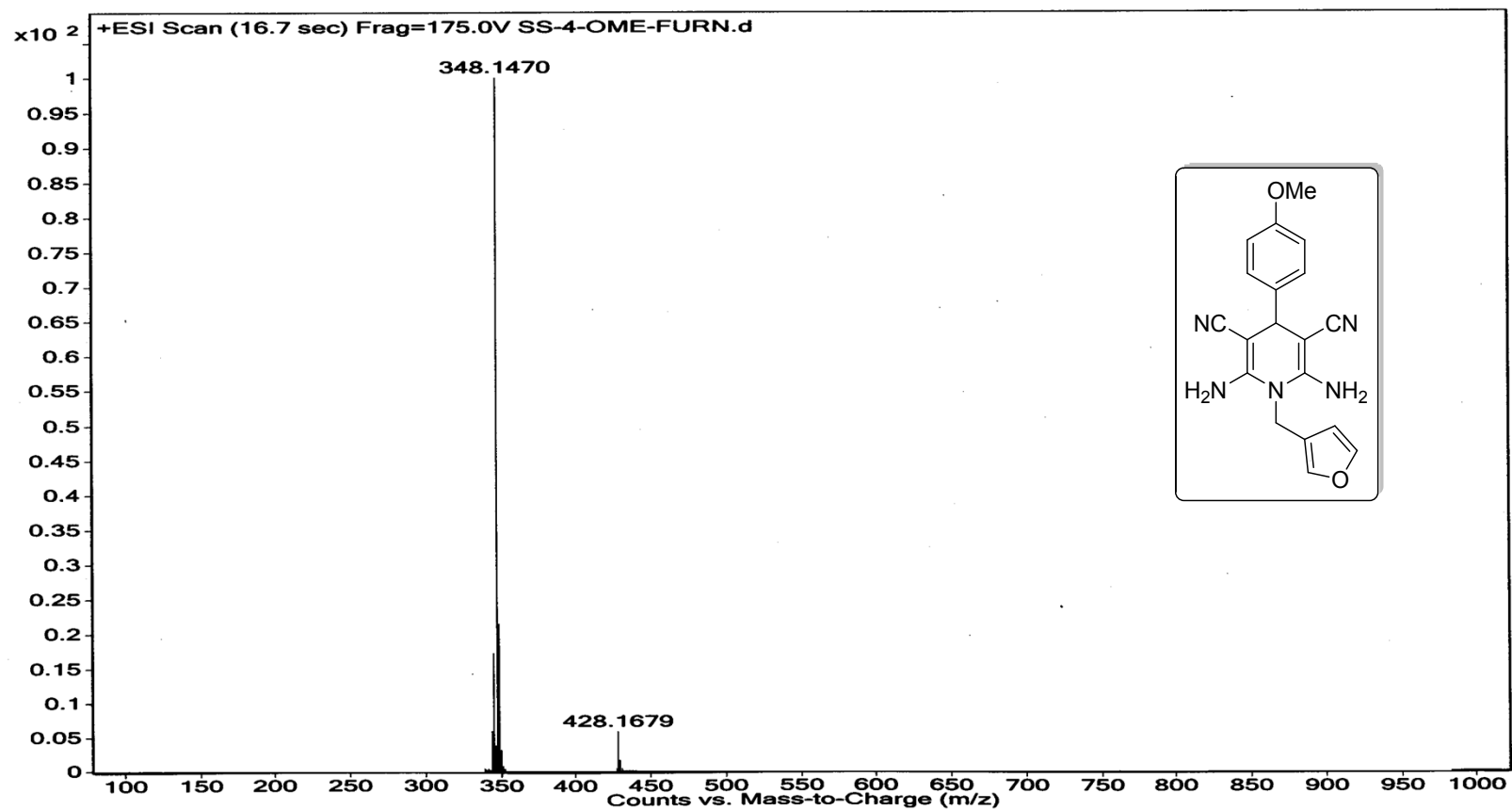
===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 21.0000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

F2 - Processing parameters
SI 16384
SF 150.9129365 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

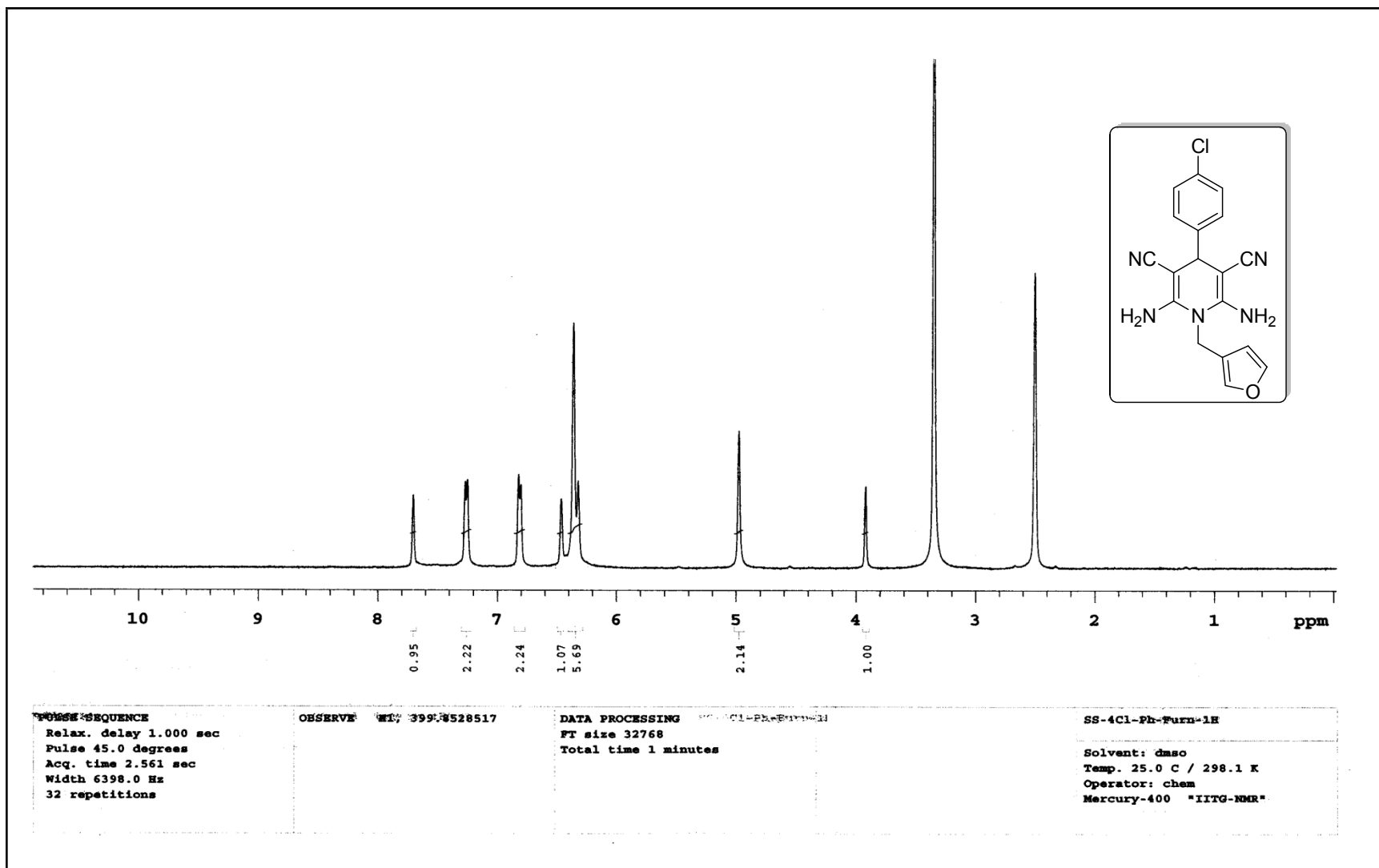
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

HRMS-spectra of compound 6h

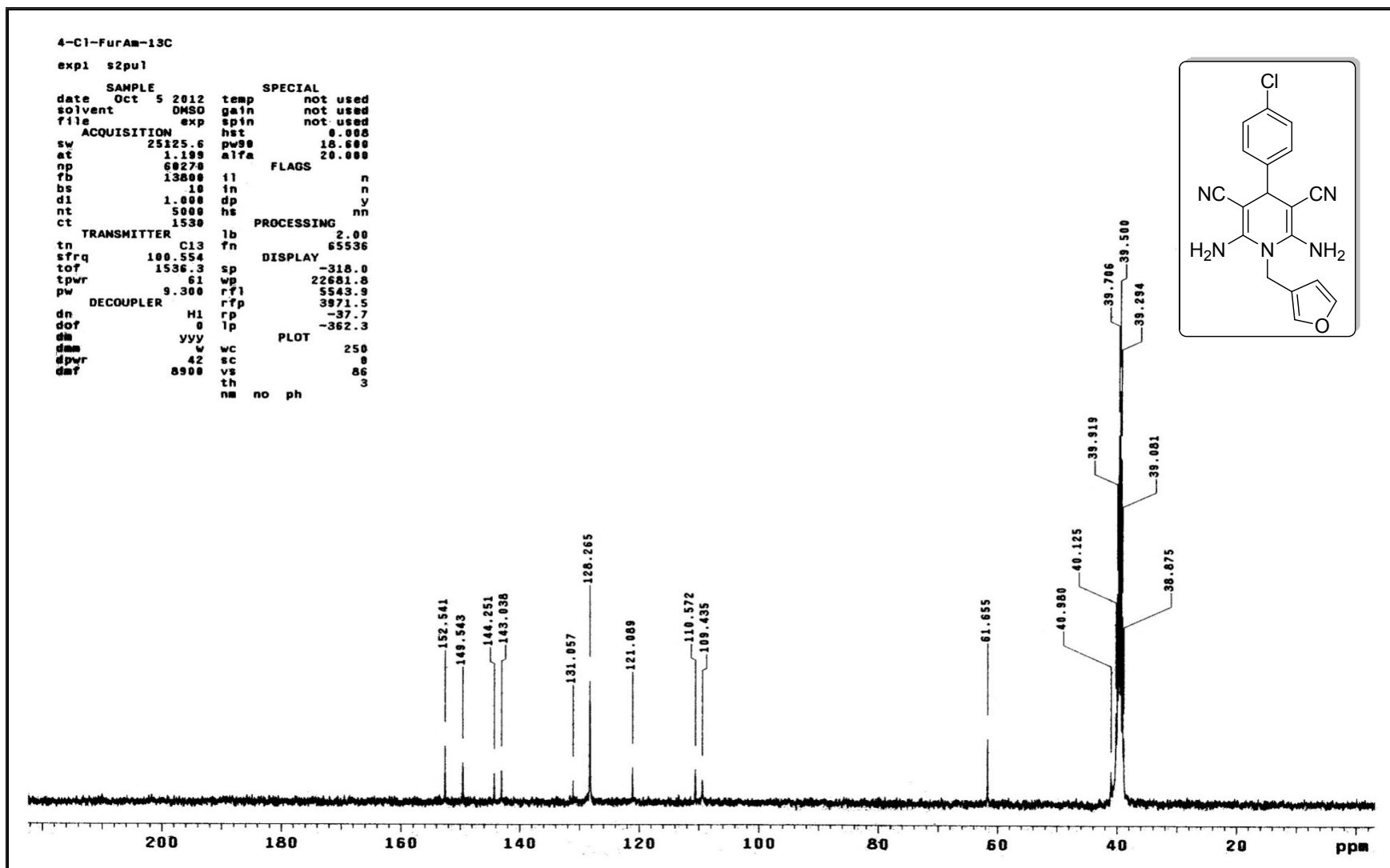
Sample Name	SS-4-OME-FURN	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SS-4-OME-FURN.d	ACQ Method		Comment		Acquired Time	4/10/2014 11:36:21 AM



¹H-NMR spectra of compound **6i**

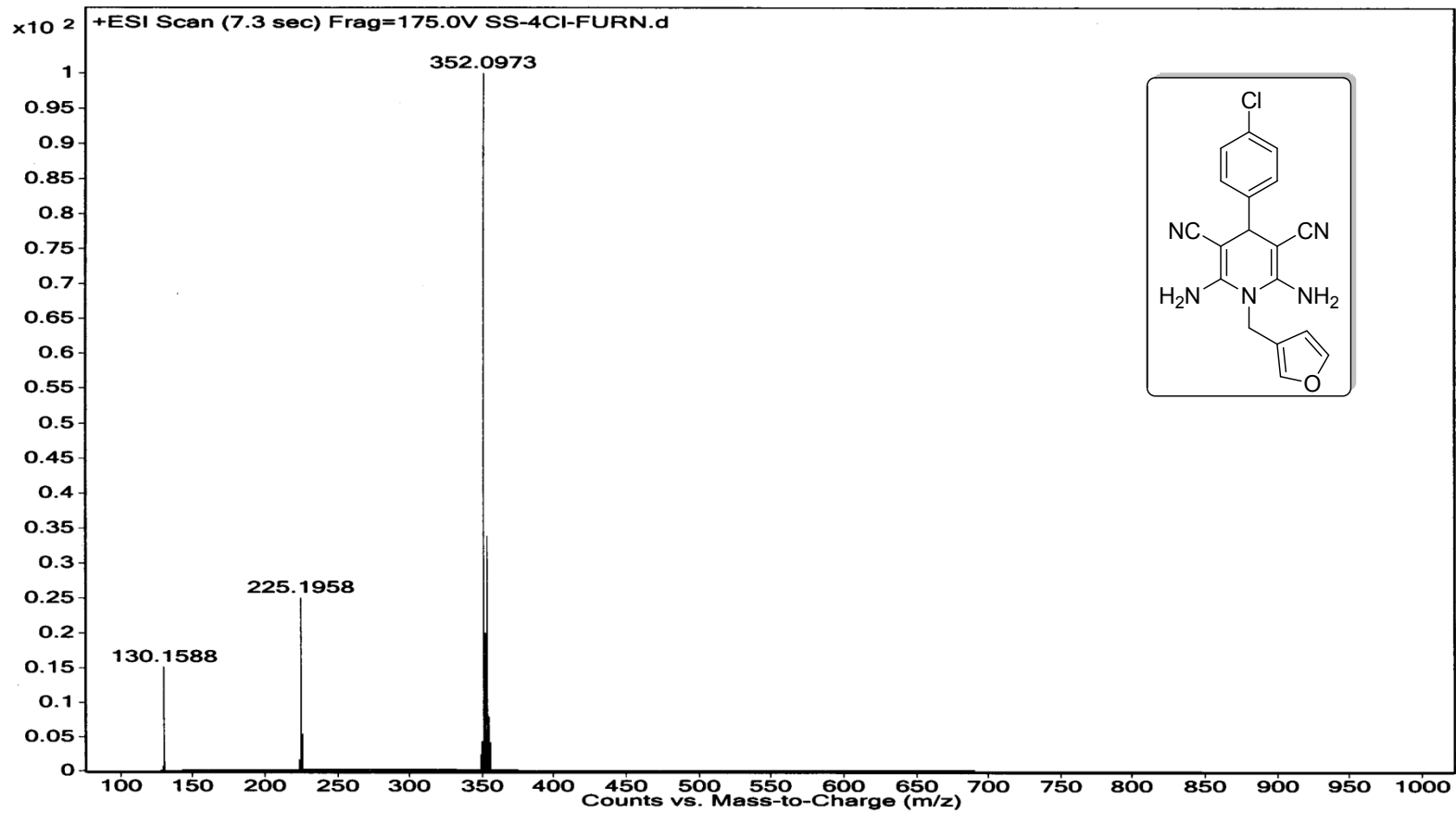


¹³C-NMR spectra of compound 6i



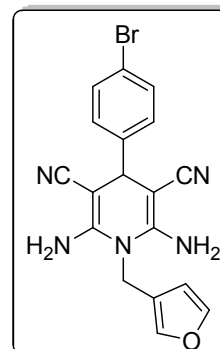
HRMS-spectra of compound 6i

Sample Name	SS-4Cl-FURN	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SS-4Cl-FURN.d	ACQ Method		Comment		Acquired Time	3/24/2014 12:05:16 PM



¹H-NMR spectra of compound **6j**

SS-4Br-FUR-NH2-1H

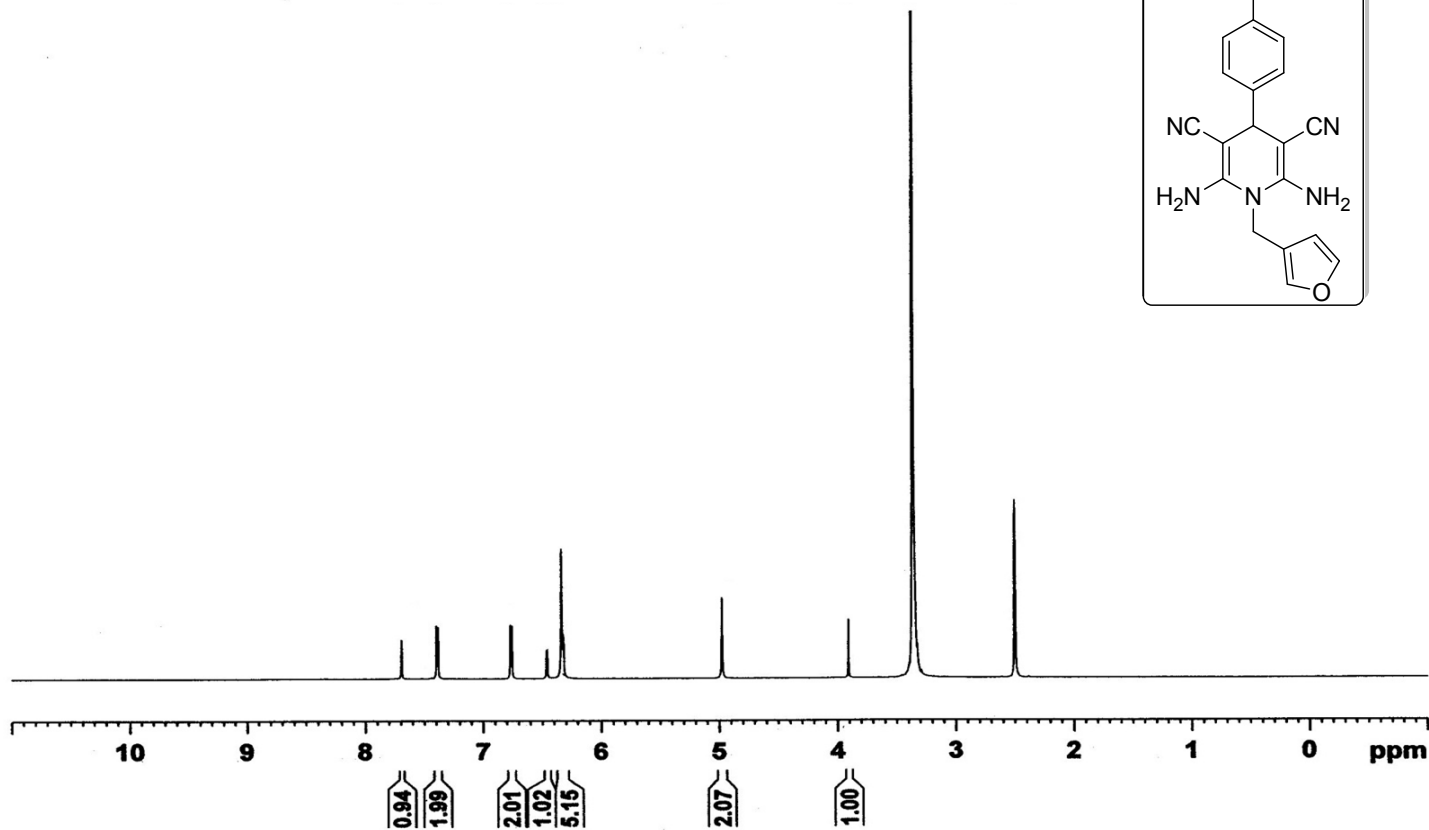


Current Data Parameters
NAME SS-4Br-FUR-NH2-1H
EXPNO 1
PROCNO 1

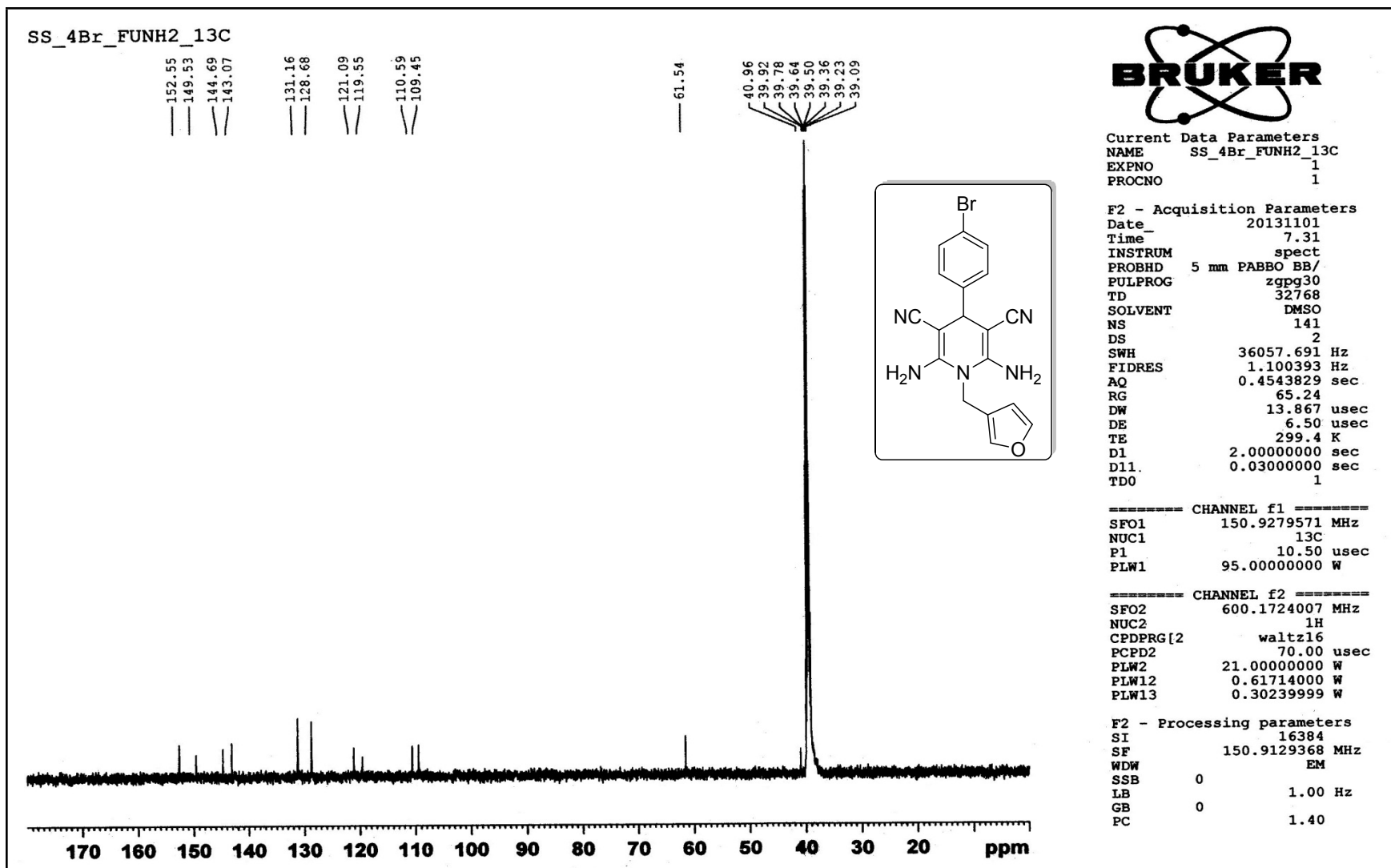
F2 - Acquisition Parameters
Date 20131031
Time 11.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 113
DW 41.600 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
SF01 600.1737063 MHz
NUC1 1H
P1 12.00 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 16384
SF 600.1700051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C-NMR spectra of compound 6j



HRMS-spectra of compound 6j

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	SS-4BR-FURN.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable

