

Studies on Isoniazid Derivatives through a Medicinal Chemistry Approach for the Identification of New Inhibitors of Urease and Inflammatory Markers

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Key Words:

Isoniazid, Urease Inhibitors, Anti-Inflammatory agents

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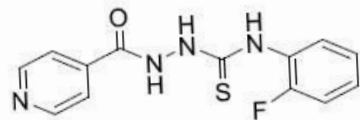
M. Iqbal Choudhary

hej@cyber.net.pk

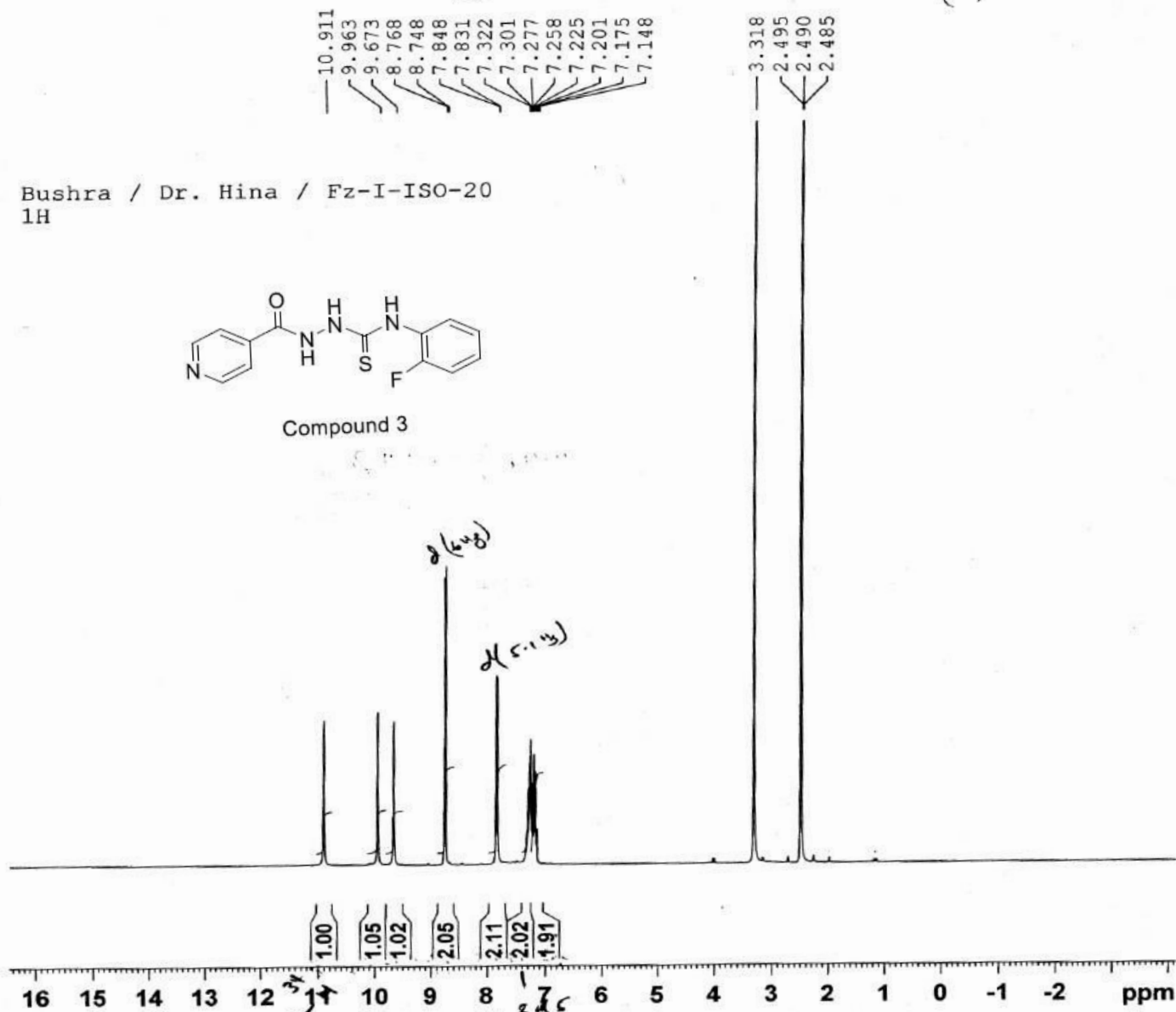
Hina Siddiqui

hinahej@gmail.com

Bushra / Dr. Hina / Fz-I-ISO-20
1H



Compound 3

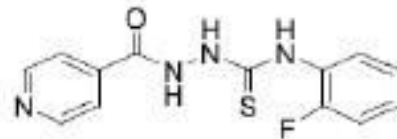


AVANCE AV - III
300 MHz, LAB # 116

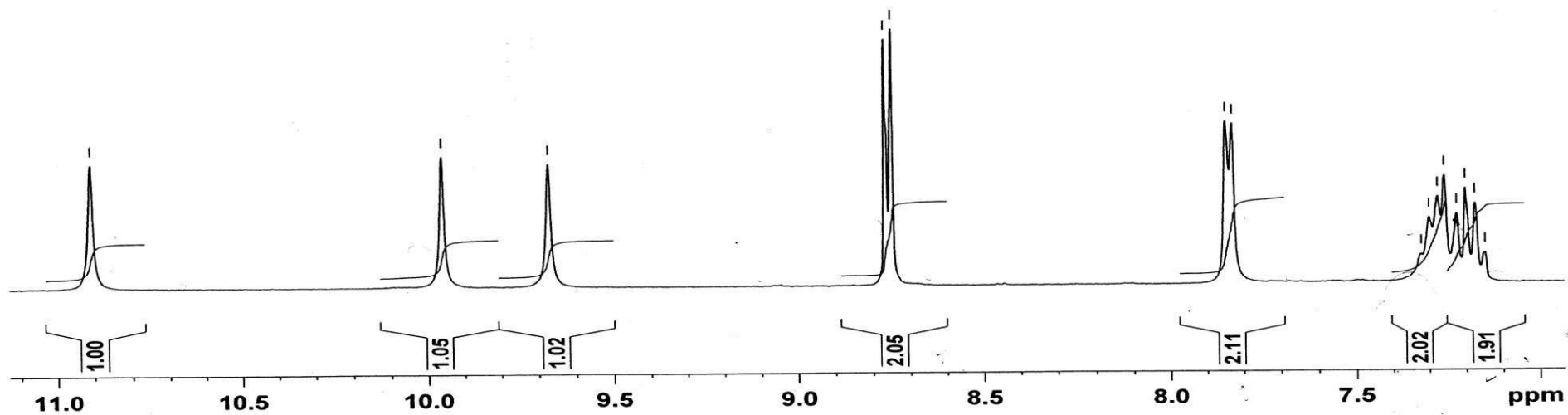
NAME	Oct04-16
EXPNO	3
PROCNO	1
Date_	20161004
Time_	10.36
INSTRUM	Spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	6188.119 Hz
FIDRES	0.188846 Hz
AQ	2.6477044 sec
RG	203
DW	80.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TDO	1

===== CHANNEL f1 =====	
NUC1	1H
P1	12.50 usec
PL1	0.00 dB
PL1W	13.16228485 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300040 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Bushra / Dr. Hina / Fz-I-ISO-20
1H



Compound 3



10.911

9.963

9.673

8.768
8.748

7.848
7.831

7.322
7.301
7.277
7.258
7.225
7.201
7.175
7.148

File: FZ-I-ISO20
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-05-2016 (Time Run: 09:59:13)

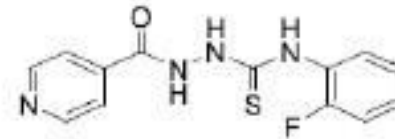
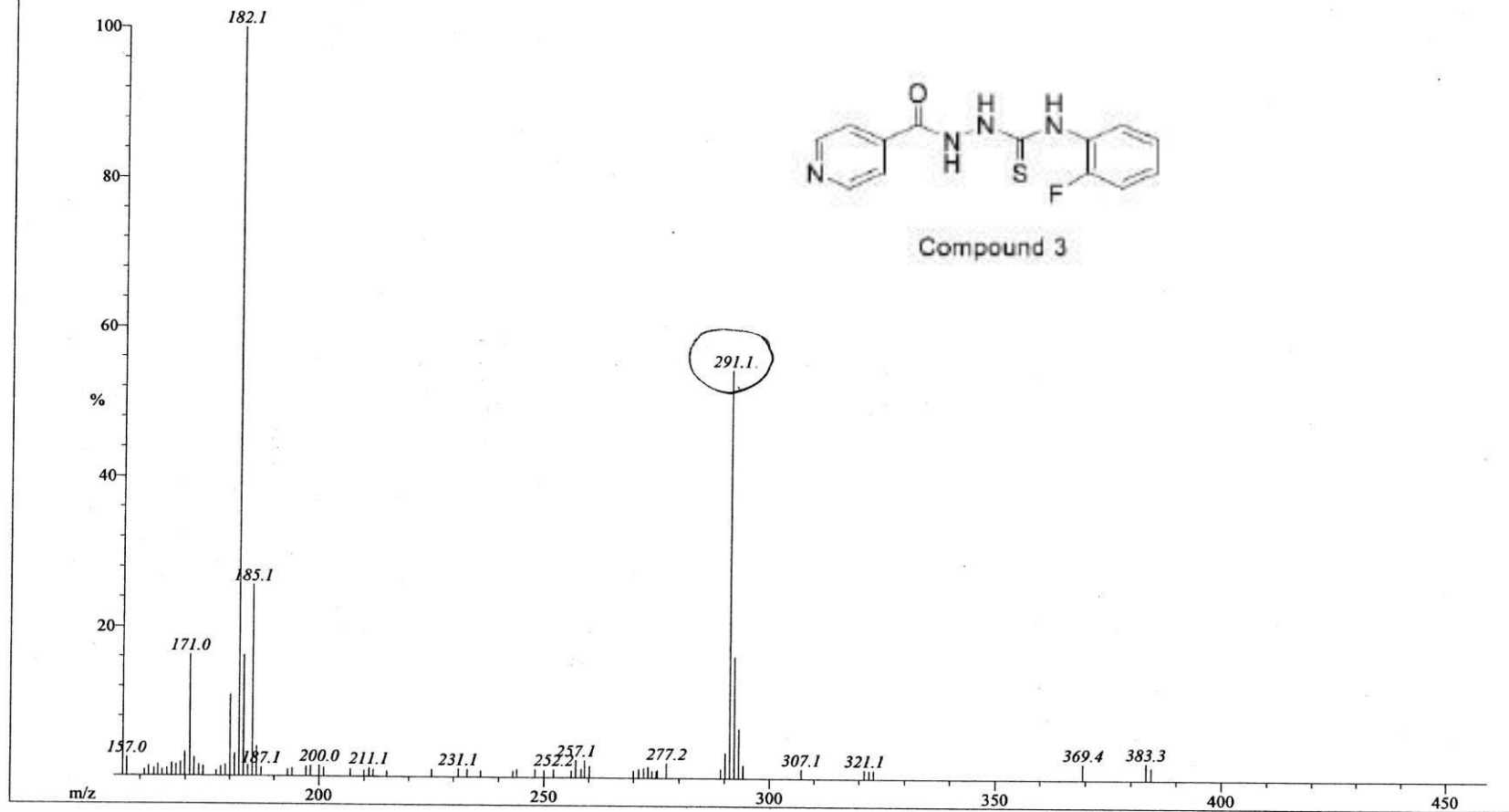
Ionization mode: FAB+

Scan: 3

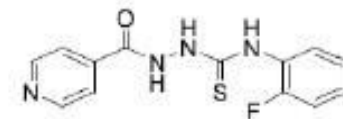
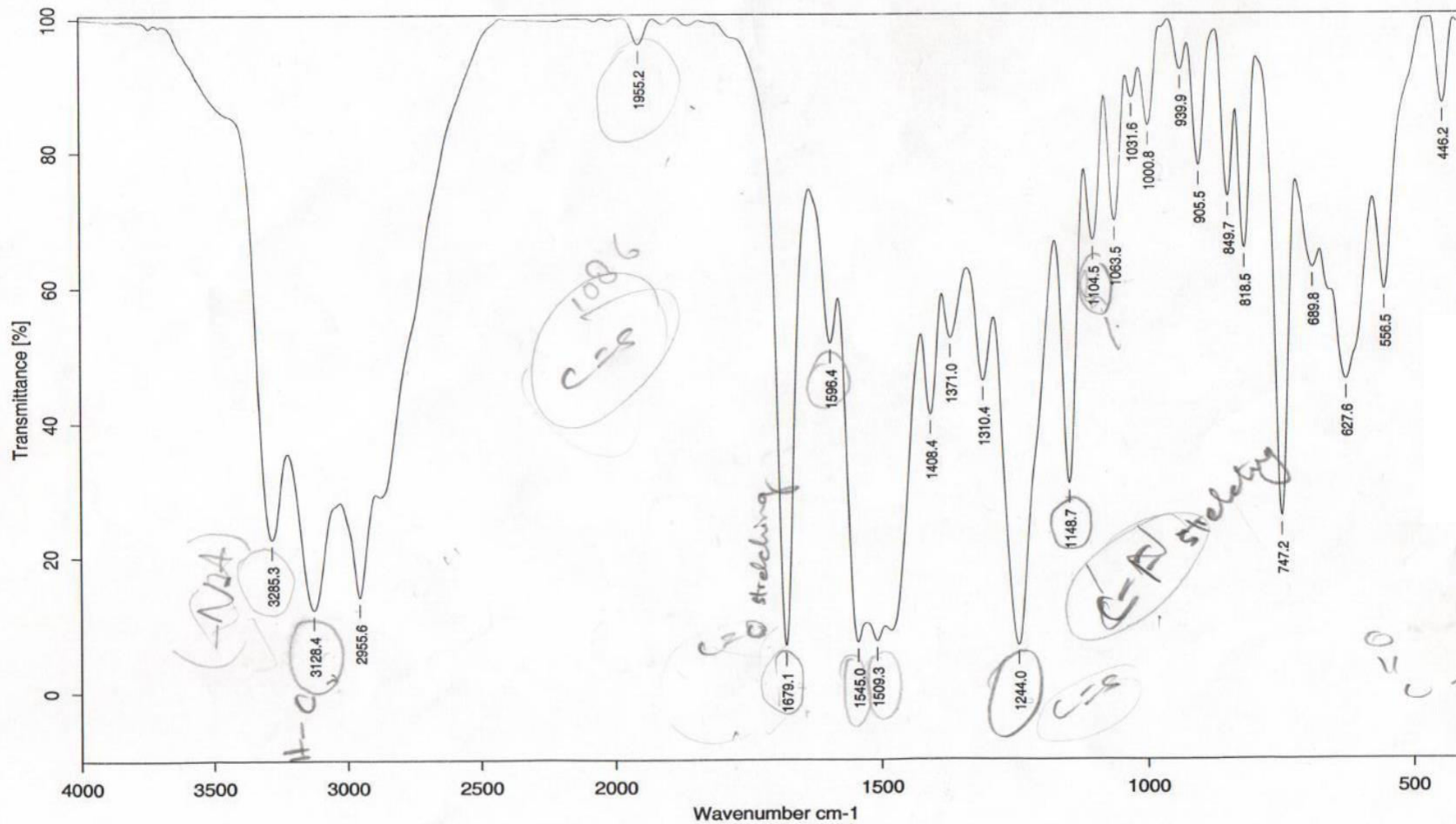
R.T.: .18

Base: m/z 182; 20.7%FS TIC: 986634

#Ions: 99



Compound 3



Compound 3

Sample : Fz-I-Iso20/Fazila Rizvi/Dr. Hina

Spectrum : Fz-I-Iso20.0 (in D:\IRSTUDENT)

Measured : 29/12/2016 on VECTOR22

Technic : Solid

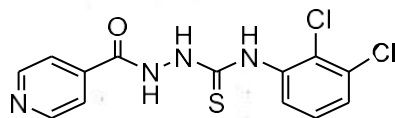
Resolution : 4 cm-1 (10 scans)

Analyst : M. Asif

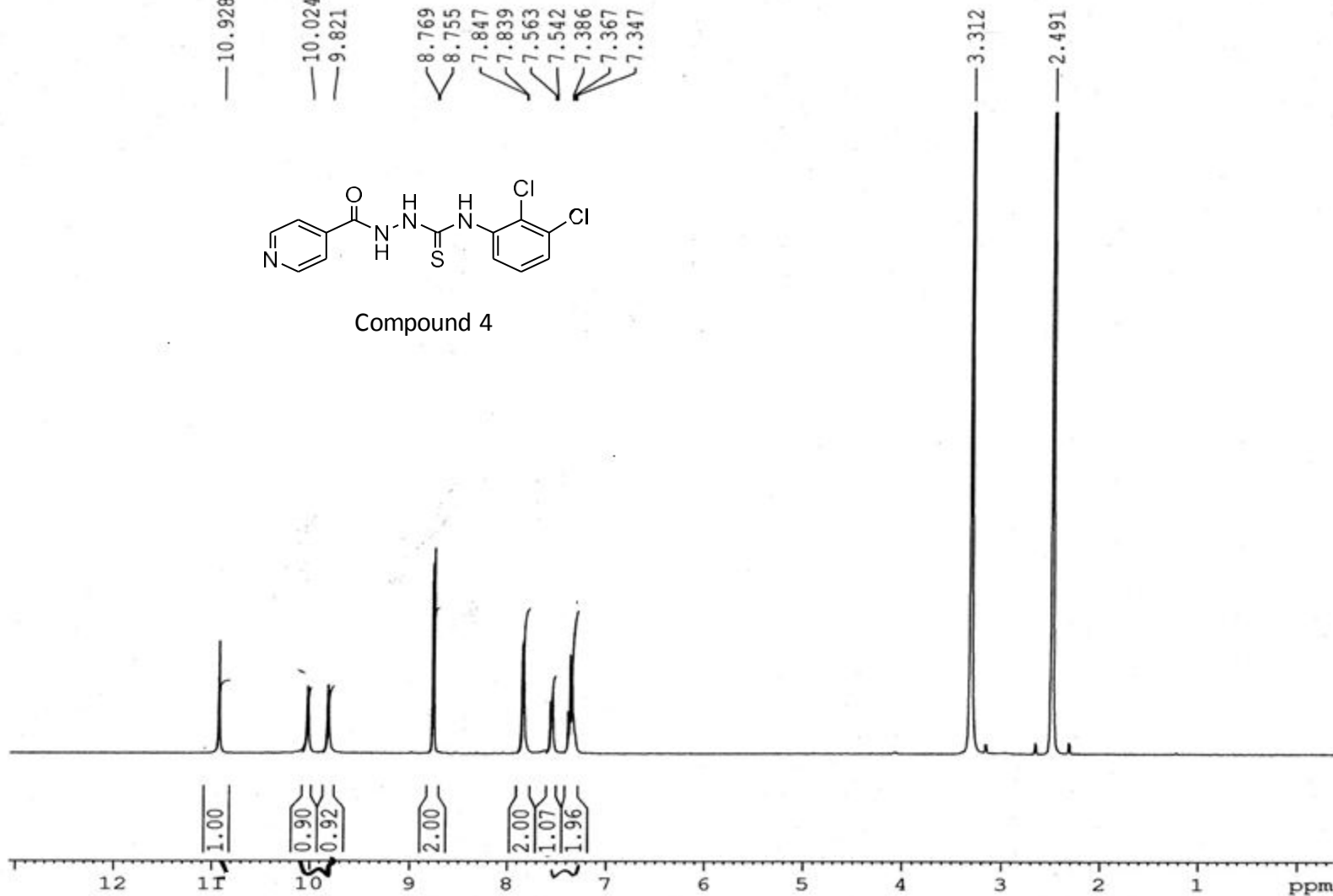
BUSHRA/DR, HINA/FZ-I-ISO-26/
ICCBS, U.O.K/

AVANCE 400
LAB NO 117

— 10.928
— 10.024
— 9.821
8.769
8.755
7.847
7.839
7.563
7.542
7.386
7.367
7.347



Compound 4



NAME nov01-16
EXPNO 3
PROCNO 1
Date_ 20161101
Time_ 11.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 512
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 8.40 usec
PL1 0.00 dB
SFO1 400.1332010 MHz
SI 16384
SF 400.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

File: FZ-I-ISO26-FABP
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

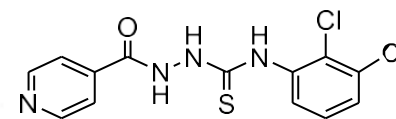
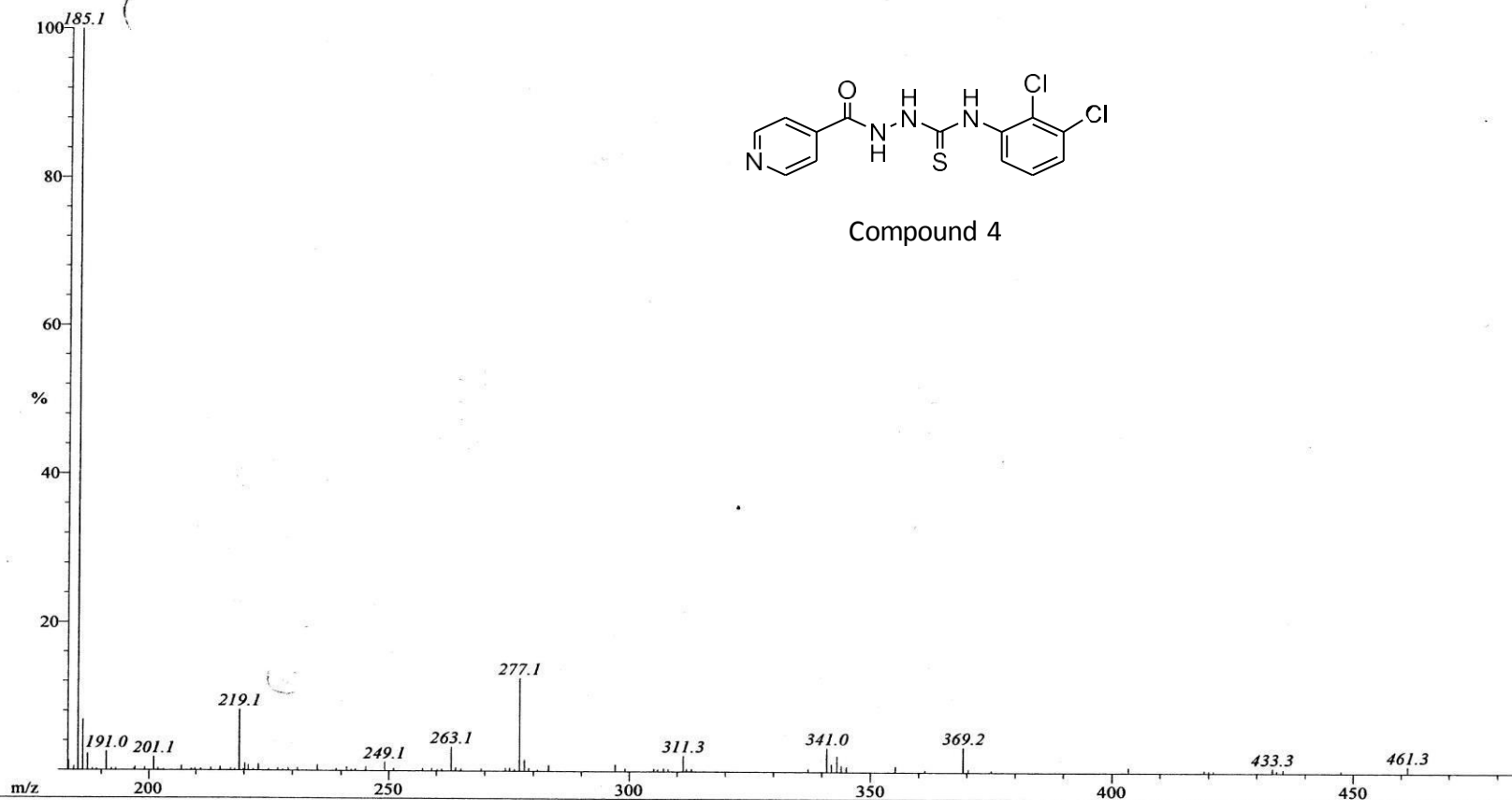
Date Run: 10-18-2016 (Time Run: 15:43:04)

Ionization mode: FAB+

Scan: 11
Base: m/z 185; 84.7%FS TIC: 2250680

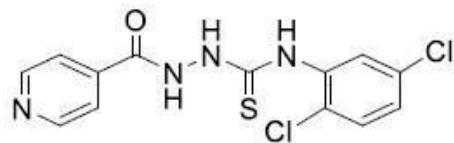
R.T.: .88

#Ions: 124

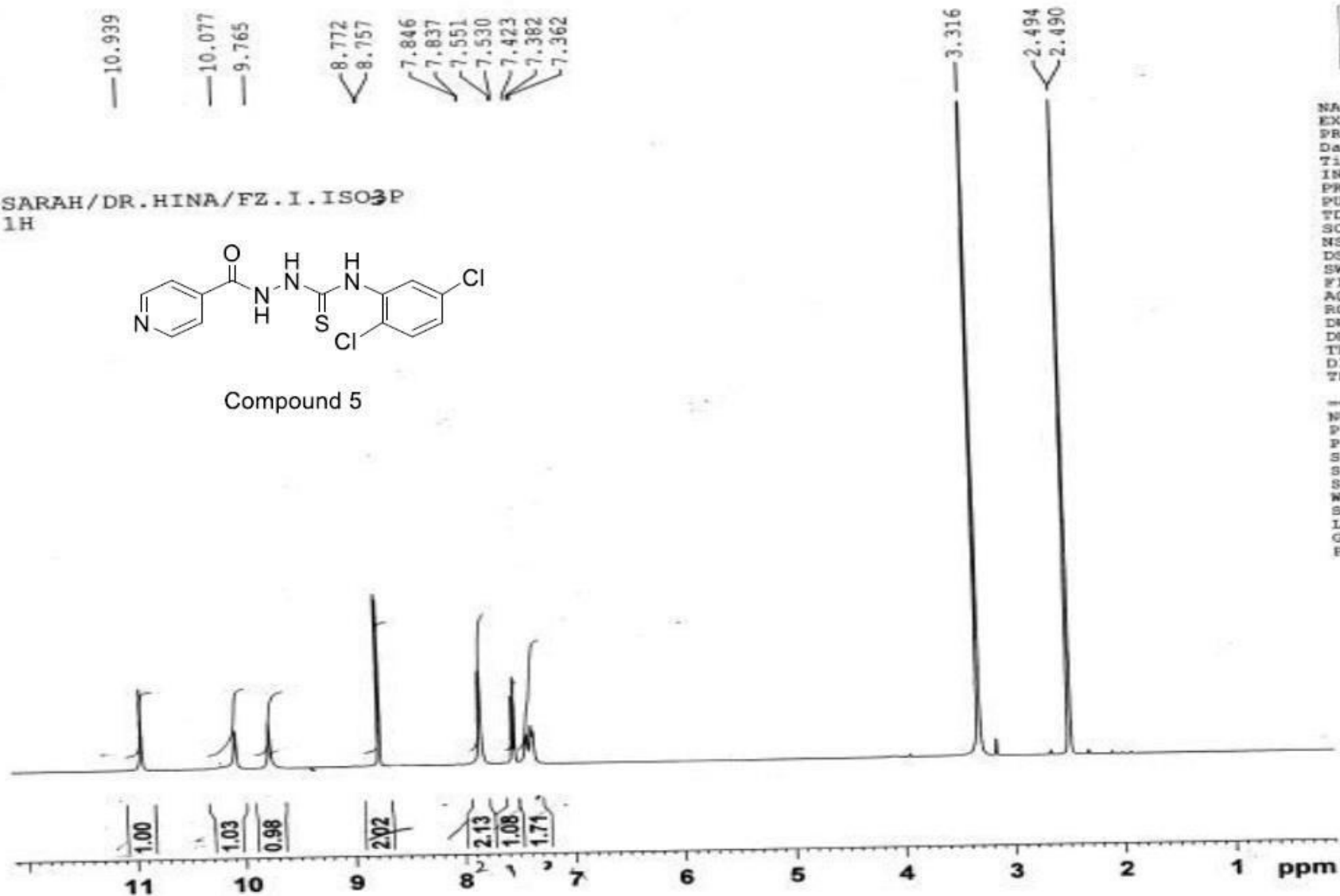


Compound 4

SARAH/DR.HINA/FZ.I.ISO3P
1H



Compound 5



AVANCE AV-400 MHz
Lab # 115

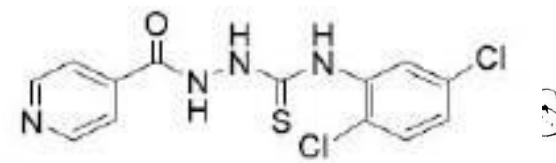
```

NAME      feb10-16
EXPNO     15
PROCNO    1
Date_     20160210
Time      16.21
INSTRUM   spect
PROBHD    5 mm SEI 1H-13
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         128
DS         0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         256
DM         62.400 usec
DE         6.50 usec
TE         300.0 K
D1         1.50000000 sec
TDS        1
  
```

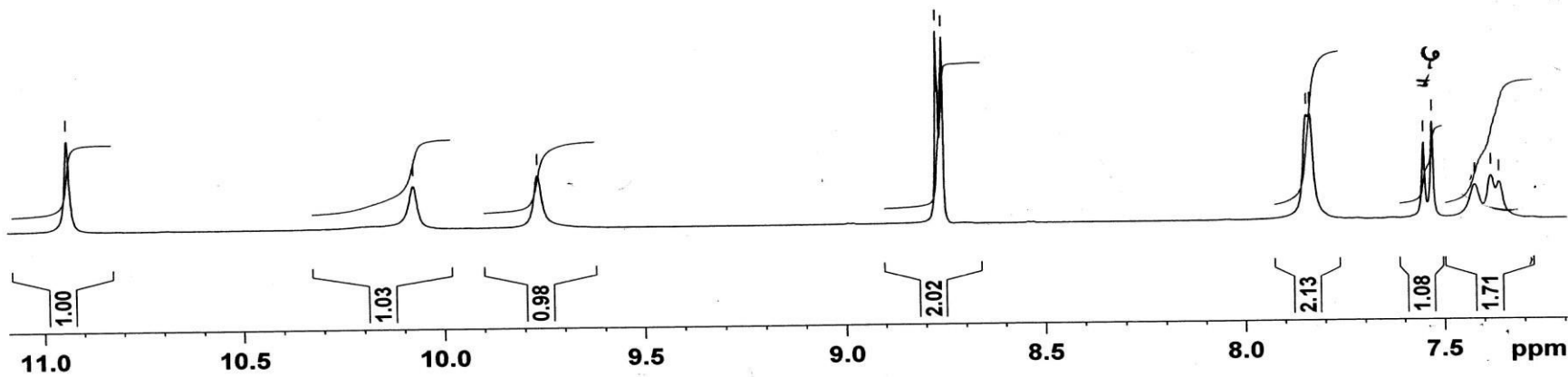
```

----- CHANNEL f1 -----
NUC1      1H
P1        10.80 usec
PL1       3.00 dB
SFO1     400.0332002 MHz
SI        32768
SF        400.0300041 MHz
WDM       EM
SBB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

SARAH/DR.HINA/FZ.I.ISO.P
1H



Compound 5



File: FZ-I-ISO3(P)-FABN-1
Sample: FAZILA /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 04-06-2016 (Time Run: 10:03:56)

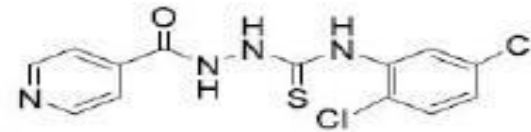
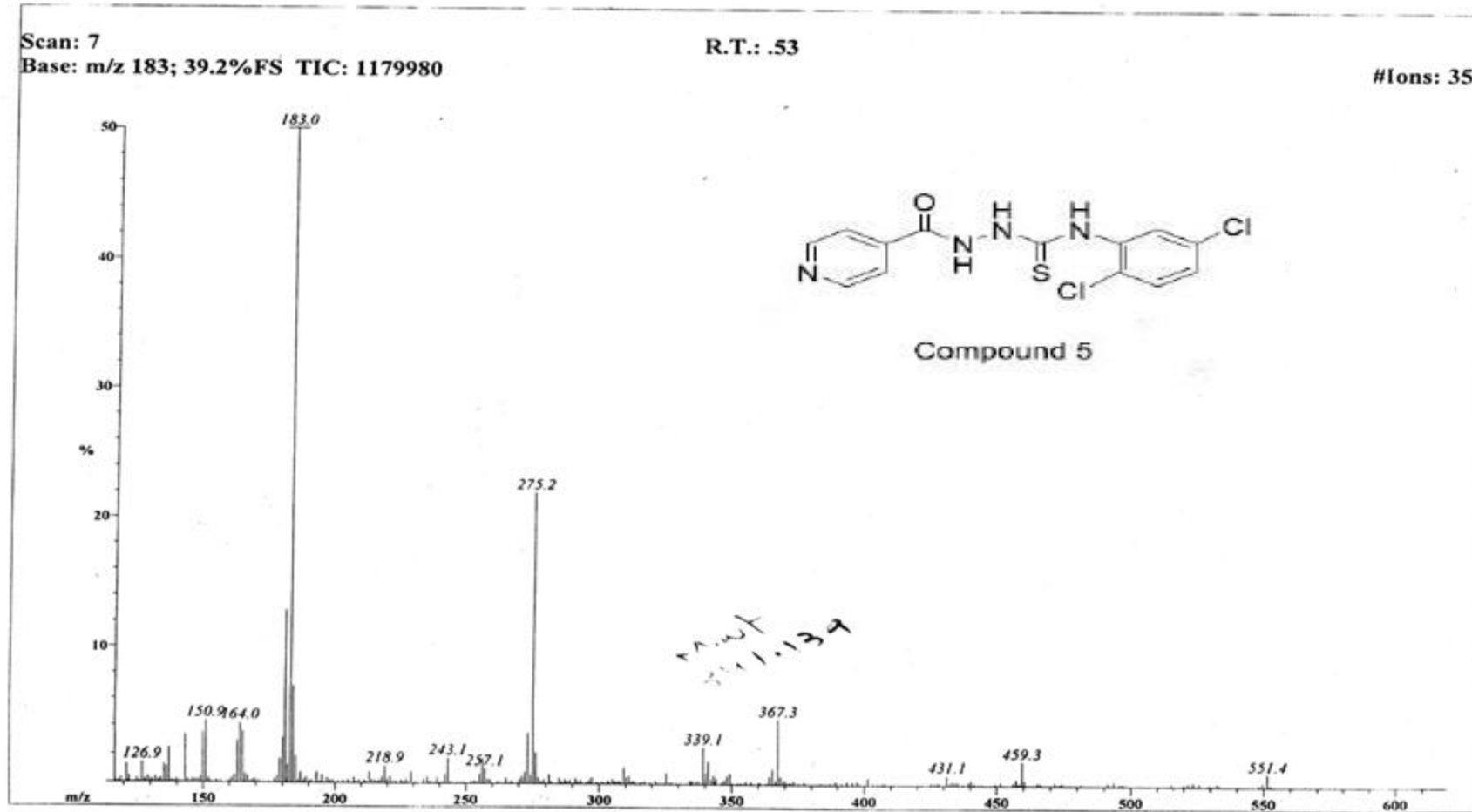
Ionization mode: FAB-

Scan: 7

R.T.: .53

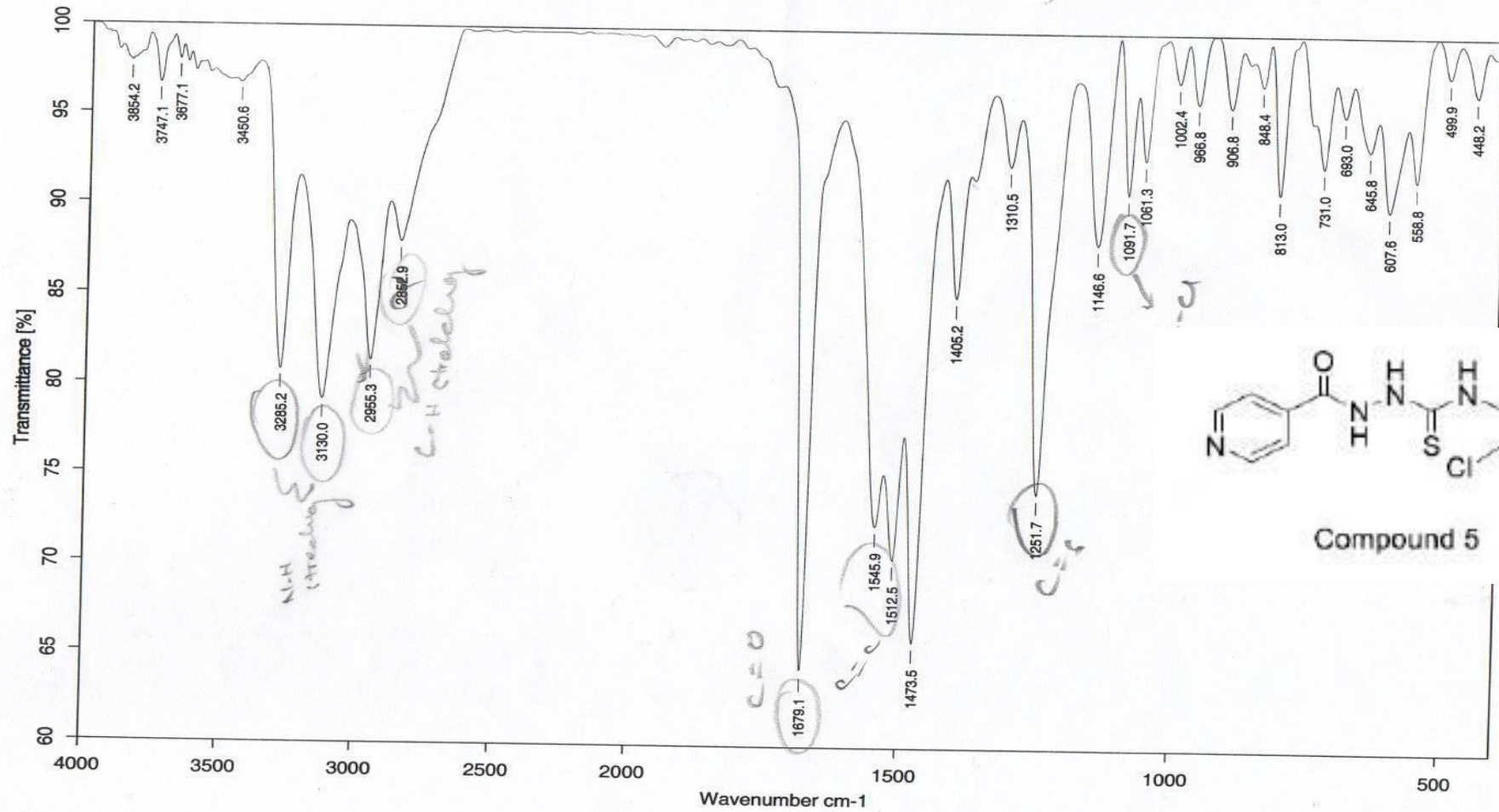
Base: m/z 183; 39.2%FS TIC: 1179980

#Ions: 354



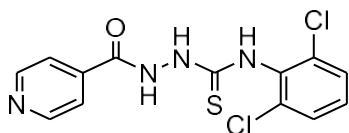
Compound 5

Handwritten note:
m.w.t
211.139

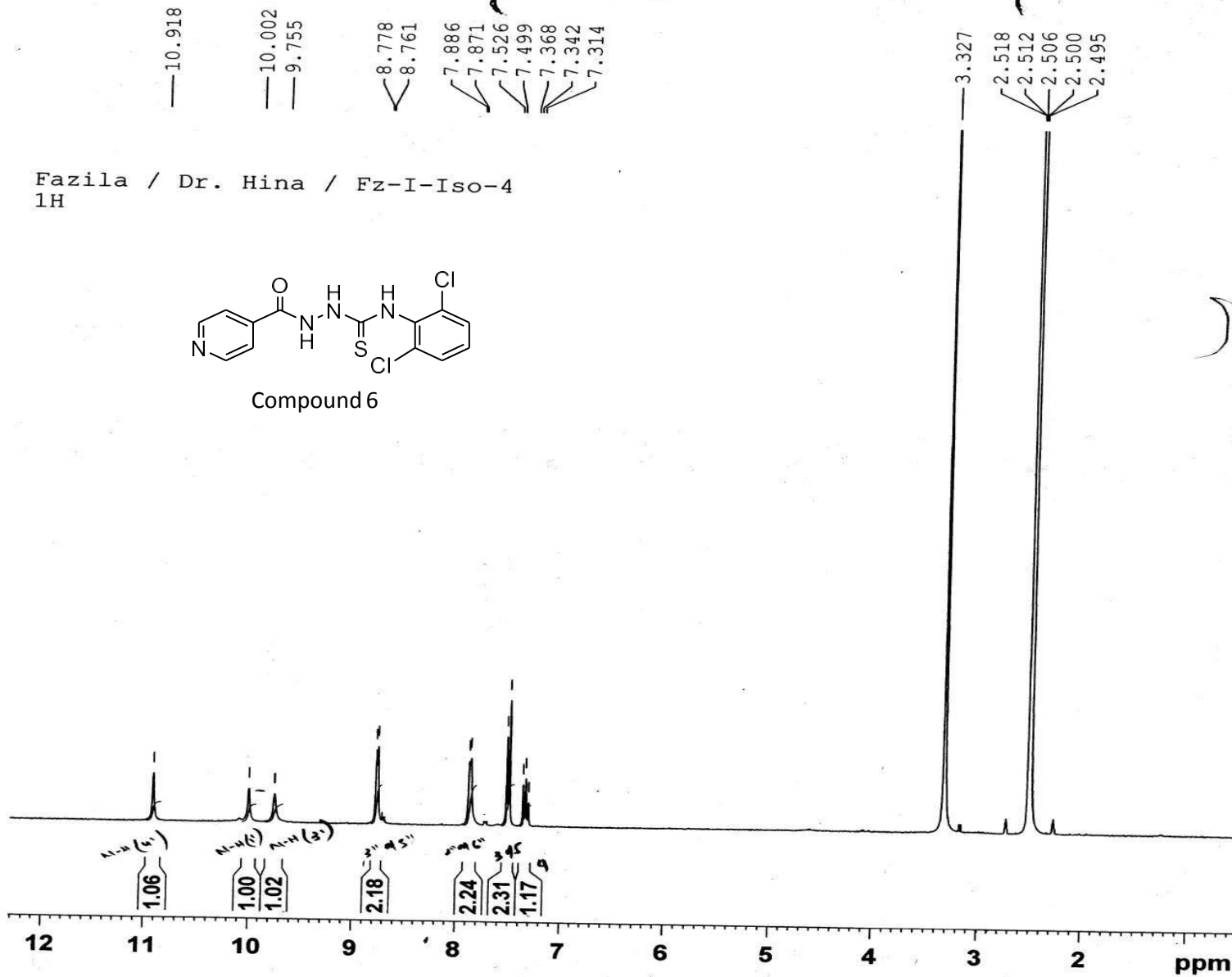


Sample : FZI-ISO3/Fazila Rizvi	Spectrum : FZ-I-ISO3.0 (in D:VRSTUDENT)
Measured : 19/04/2017 on VECTOR22	Technic : Solid
Resolution : 4 cm ⁻¹ (10 scans)	Analyst : MA/ZA/JS

Fazila / Dr. Hina / Fz-I-Iso-4
1H



Compound 6

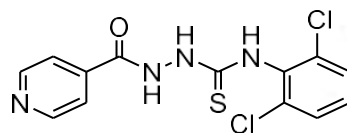


AVANCE AV - III
300 MHz, LAB # 116

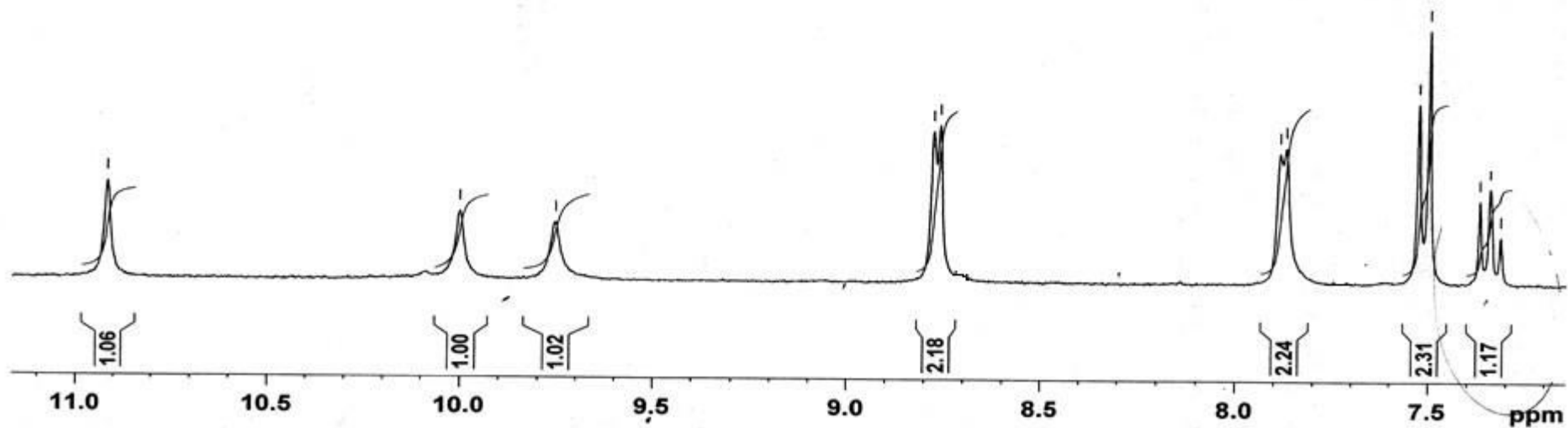
NAME mar22-16
EXPNO 1
PROCNO 1
Date_ 20160322
Time_ 13.13
INSTRUM Spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 128
DS 0
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 0.00 dB
PL1W 13.16228485 W
SF01 300.1318534 MHz
SI 32768
SF 300.1299992 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fazila / Dr. Hina / Fz-I-Iso-4
1H



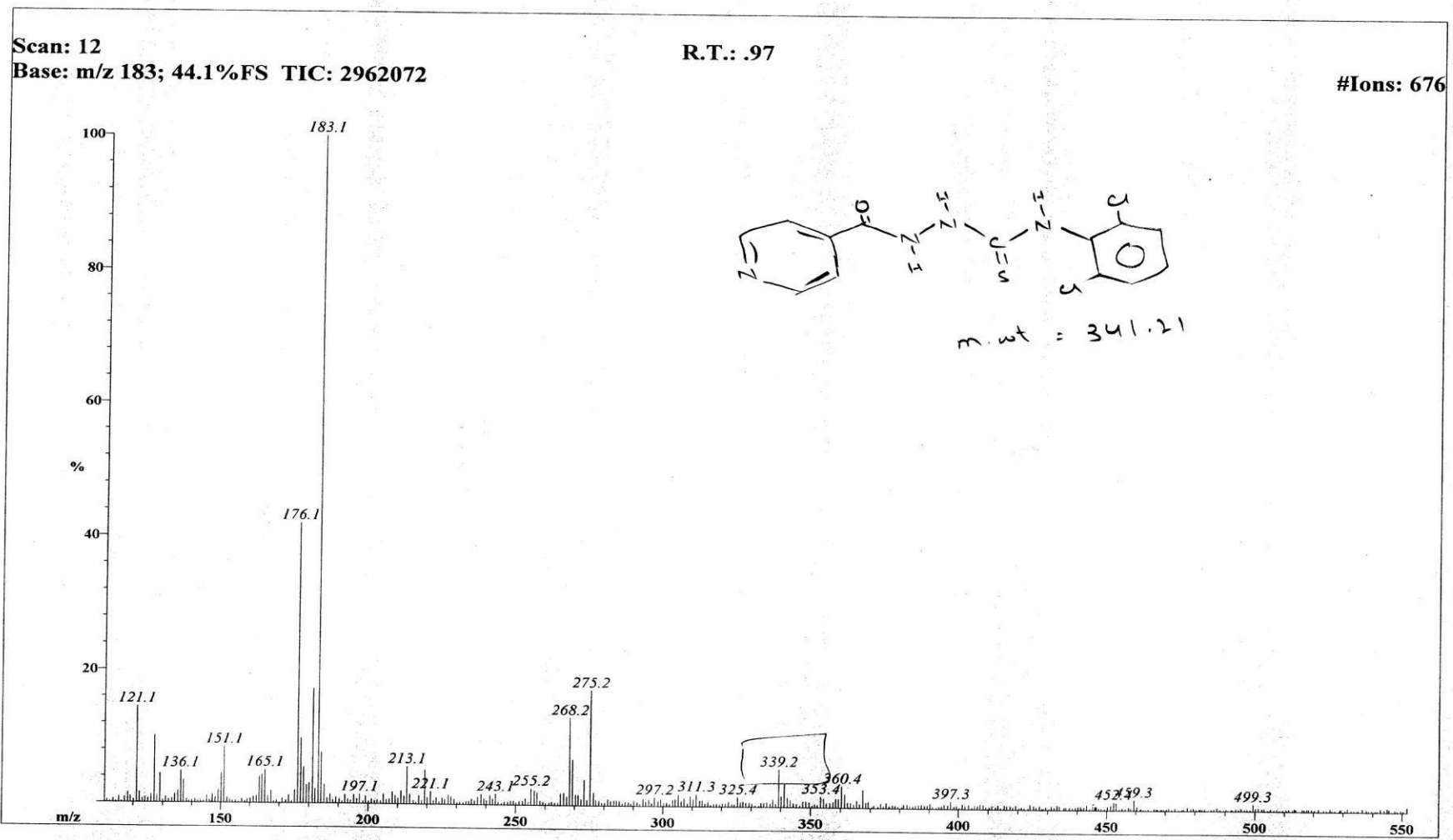
Compound 6

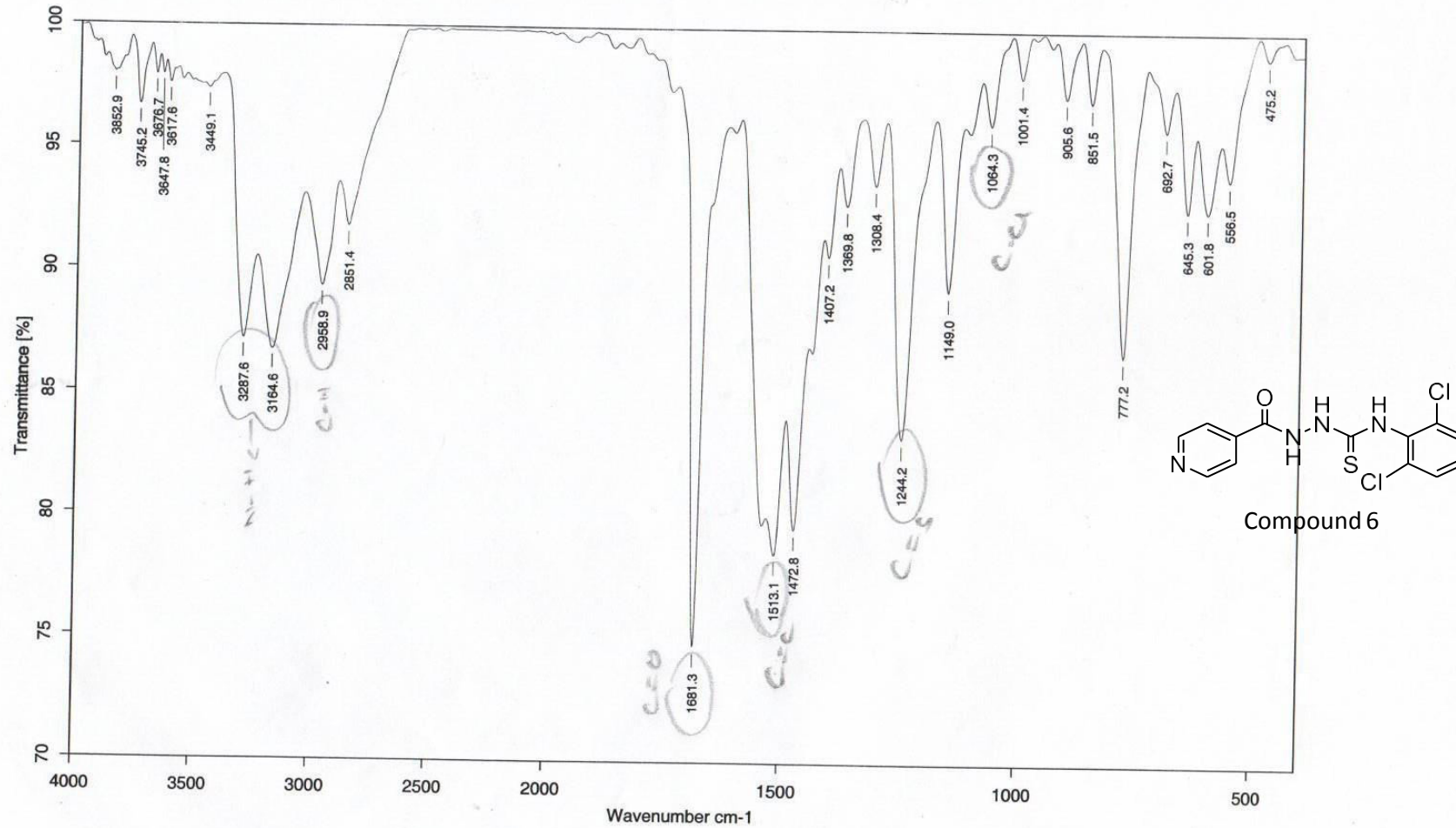


File: FZ-I-ISO4(P)-FABN
Sample: FAZILA /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 03-03-2016 (Time Run: 13:21:15)

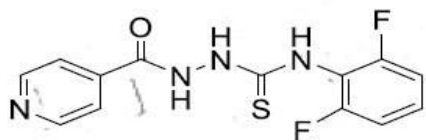
Ionization mode: FAB-



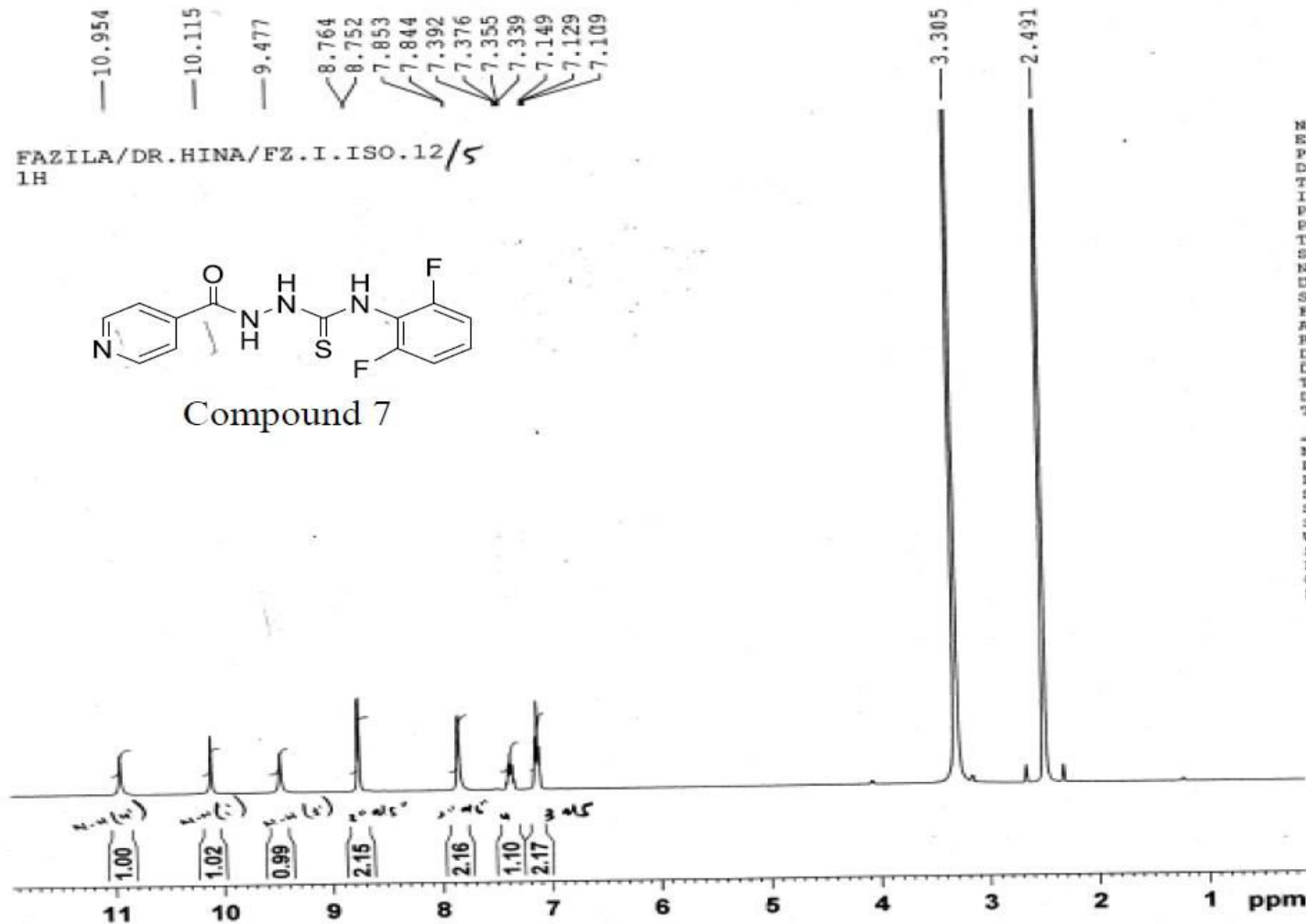


Sample : FZI-ISO4/Fazila Rizvi	Spectrum : FZ-I-ISO4.0 (in D:IRSTUDENT)
Measured : 19/04/2017 on VECTOR22	Technic : Solid
Resolution : 4 cm-1 (10 scans)	Analyst : MA/ZA/JS

FAZILA/DR.HINA/FZ.I.ISO.12/5
1H



Compound 7



AVANCE AV-400 MHz
Lab # 115

NAME	AUG15-16
EXPNO	5
PROCNO	1
Date_	20160815
Time	12.59
INSTRUM	spcct
PROBHD	5 mm SRI 1H-13
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	128
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	256
DW	62.400 usec
DE	6.50 usec
TE	300.0 K
DE	1.50000000 sec
TD0	1

----- CHANNEL f1 -----		
NUC1	1H	
P1	10.80	usec
PL1	3.00	dB
SFO1	400.0332002	MHz
SI	32768	
SF	400.0300041	MHz
WDM	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	0.20	

—10.954

—10.115

—9.477

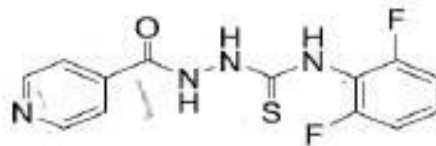
<8.764
<8.752

<7.853
<7.844

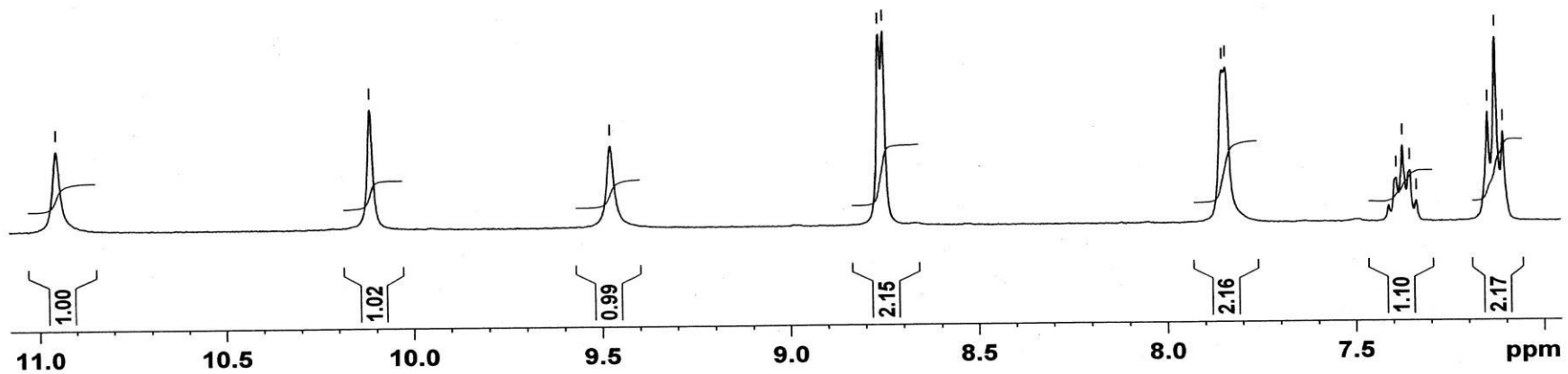
<7.392
<7.376
<7.355
<7.339

<7.149
<7.129
<7.109

FAZILA/DR.HINA/FZ.I.ISO.12
1H



Compound 7



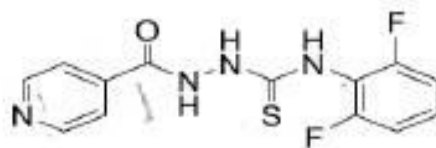
8.764
8.752

7.853
7.844

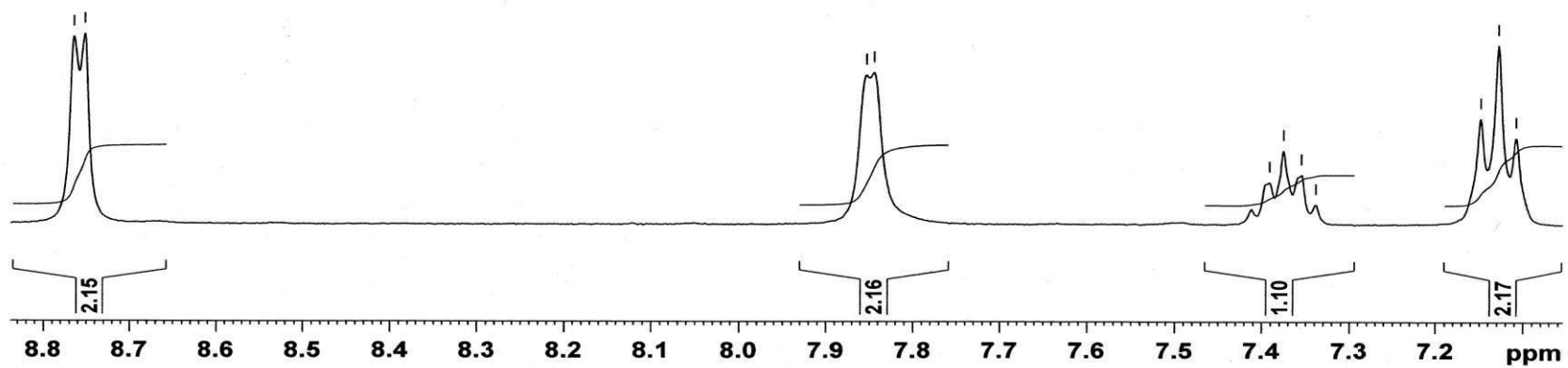
7.392
7.376
7.355
7.339

7.149
7.129
7.109

FAZILA/DR.HINA/FZ.I.ISO.12
1H



Compound 7



File: FZ-I-ISO-12
Sample: FAZILA RIZVI /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

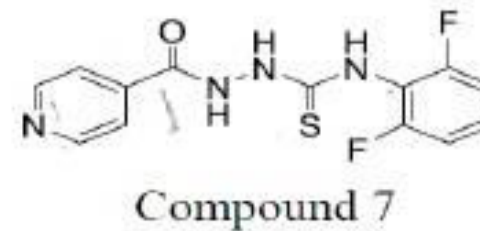
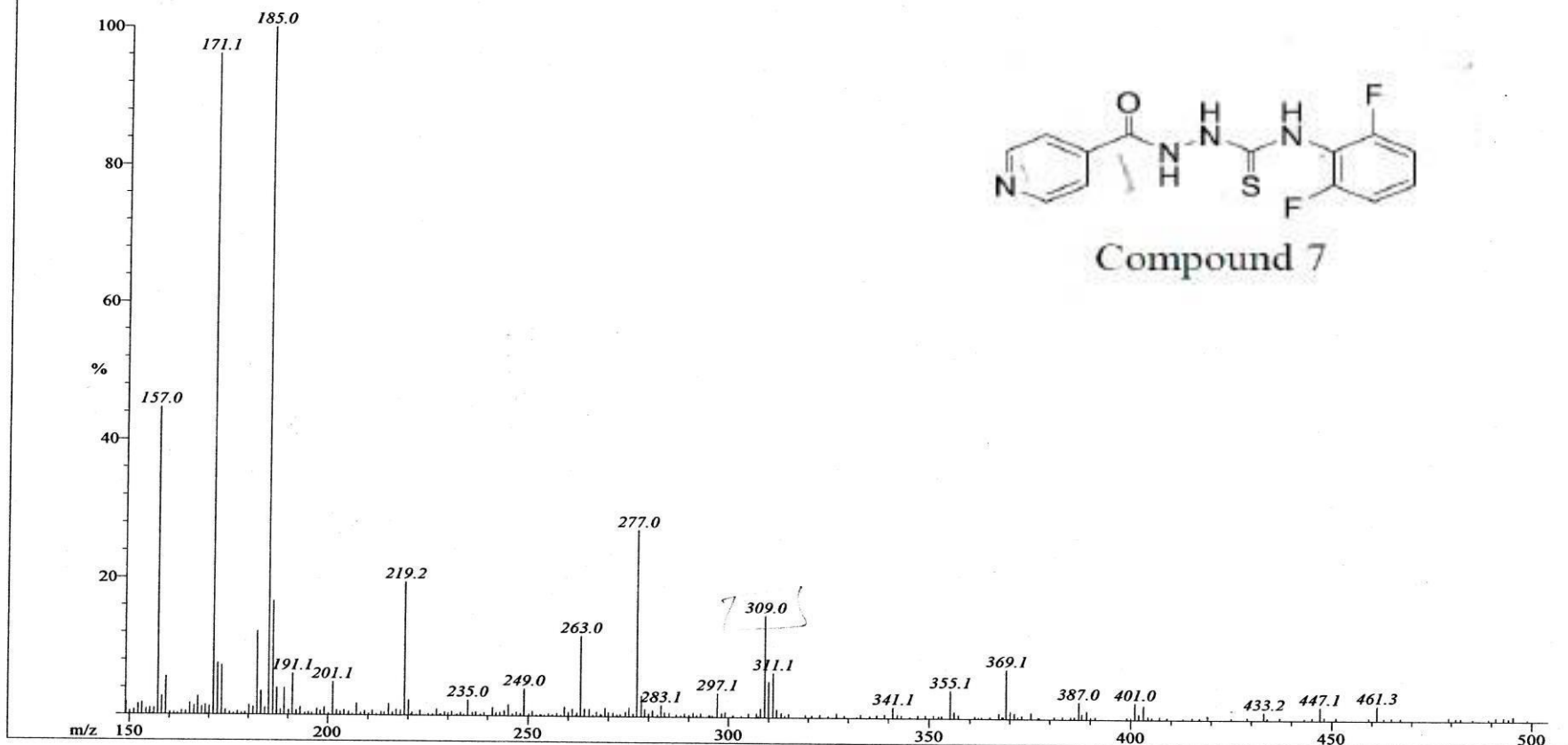
Date Run: 08-15-2016 (Time Run: 16:05:45)

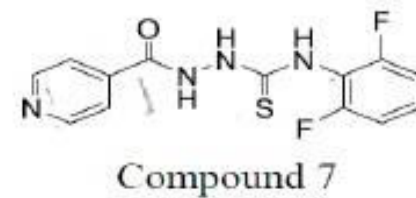
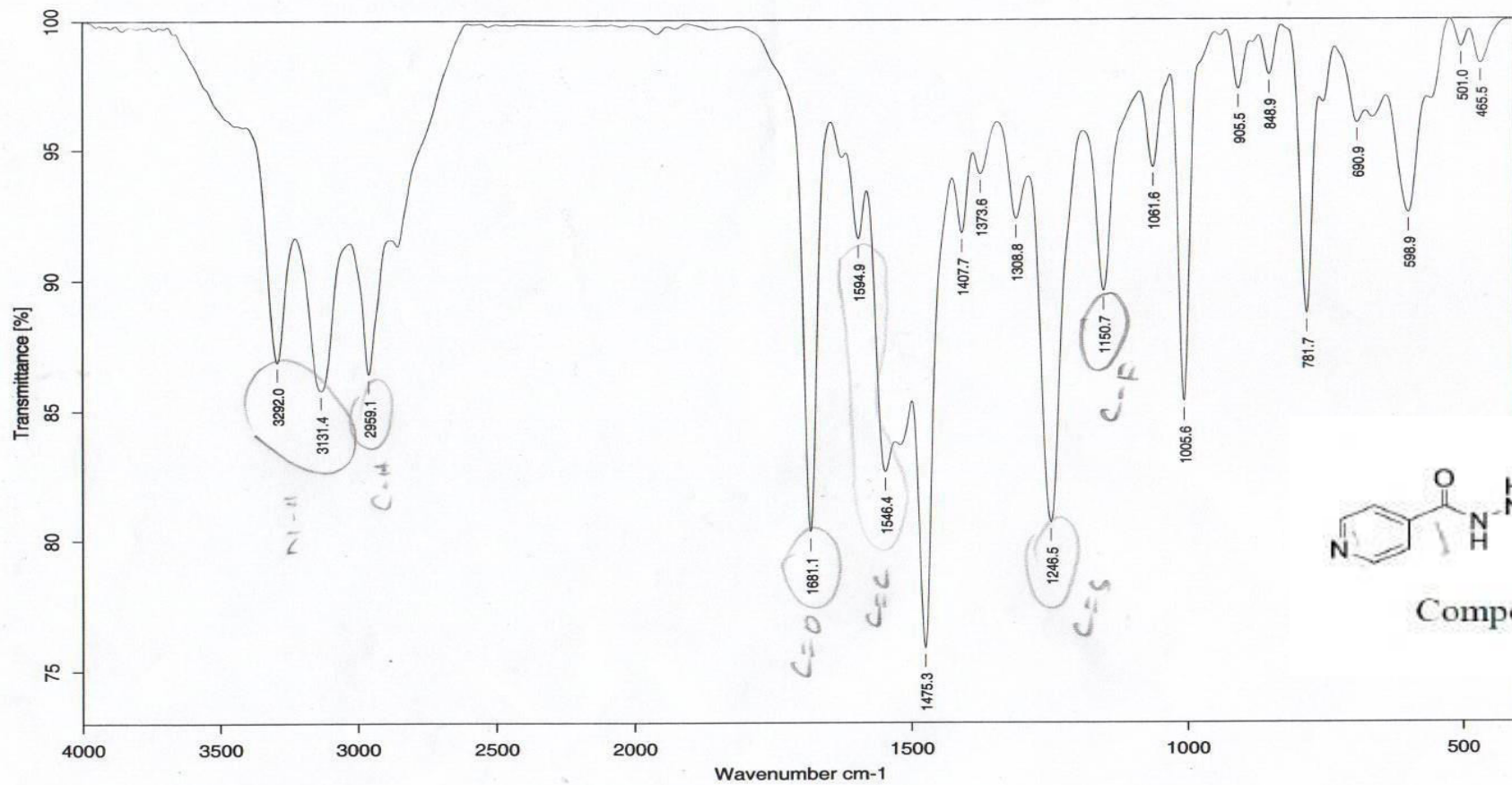
Ionization mode: FAB+

Scan: 4
Base: m/z 185; 100%FS TIC: 6513332

R.T.: .27

#Ions: 302





Sample : FZI-ISO12/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

Resolution : 4 cm-1 (10 scans)

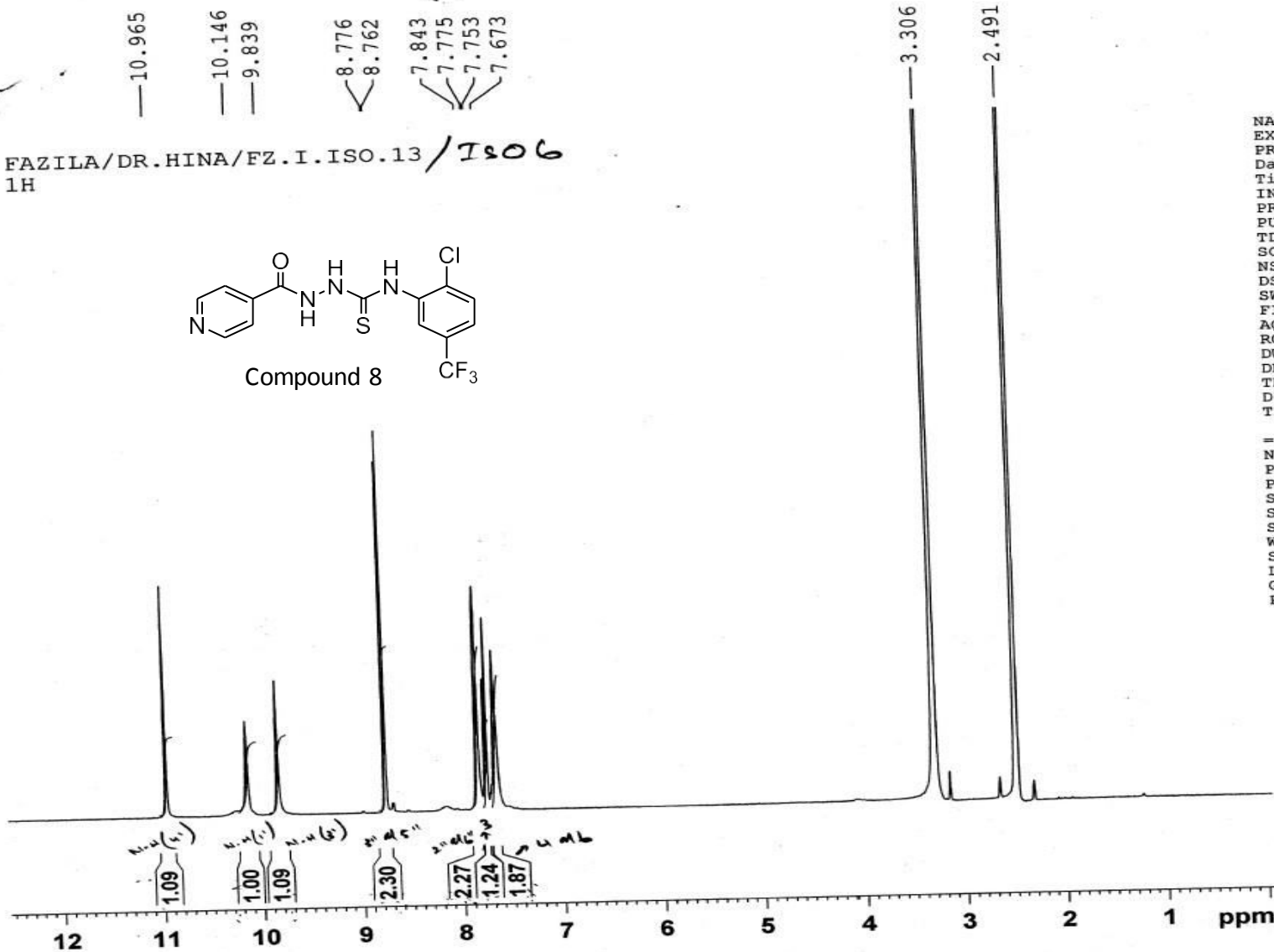
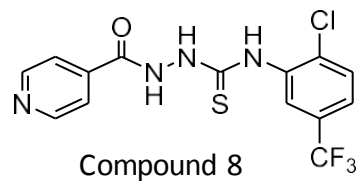
Spectrum : FZ-I-ISO12.0 (in D:\IRSTUDENT)

Technic : Solid

Analyst : MA/ZA/JS

AVANCE AV-400 MHz
Lab # 115

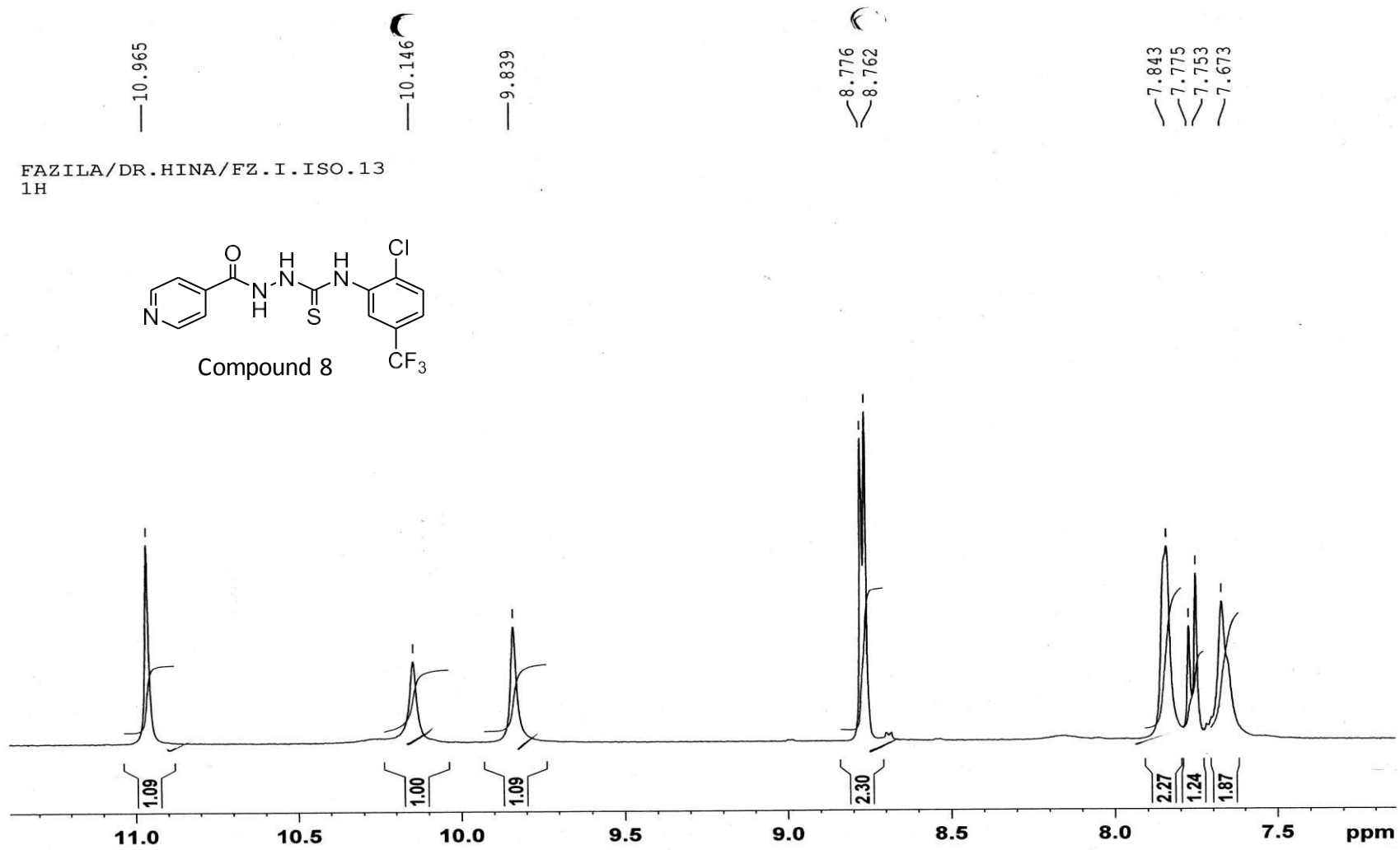
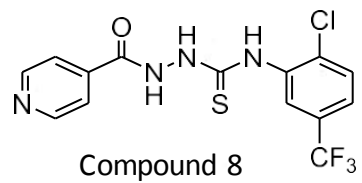
FAZILA/DR.HINA/FZ.I.ISO.13/1206
1H



NAME AUG23-16
 EXPNO 9
 PROCNO 1
 Date 20160823
 Time 16.21
 INSTRUM spect
 PROBHD 5 mm SEI 1H-13
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 362
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 3.00 dB
 SFO1 400.0332002 MHz
 SI 32768
 SF 400.0300041 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.20

FAZILA/DR.HINA/FZ.I.ISO.13
1H



File: FZ-I-ISO6(Me)-FABN
Sample: FAZILA /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 04-06-2016 (Time Run: 10:12:59)

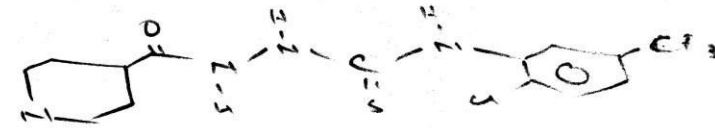
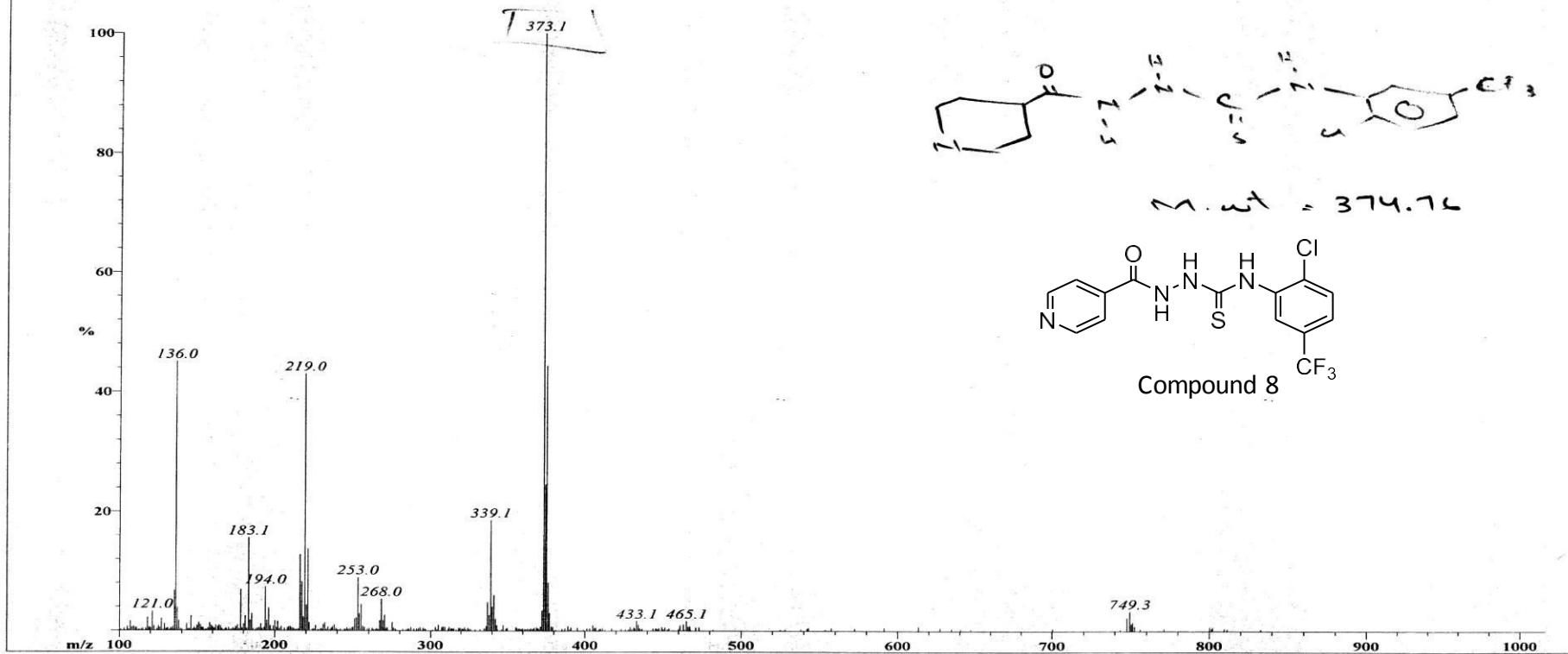
Ionization mode: FAB-

Scan: 2

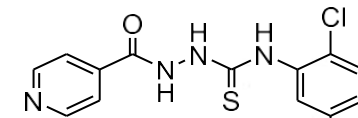
R.T.: .1

Base: m/z 373; 17.1%FS TIC: 1081342

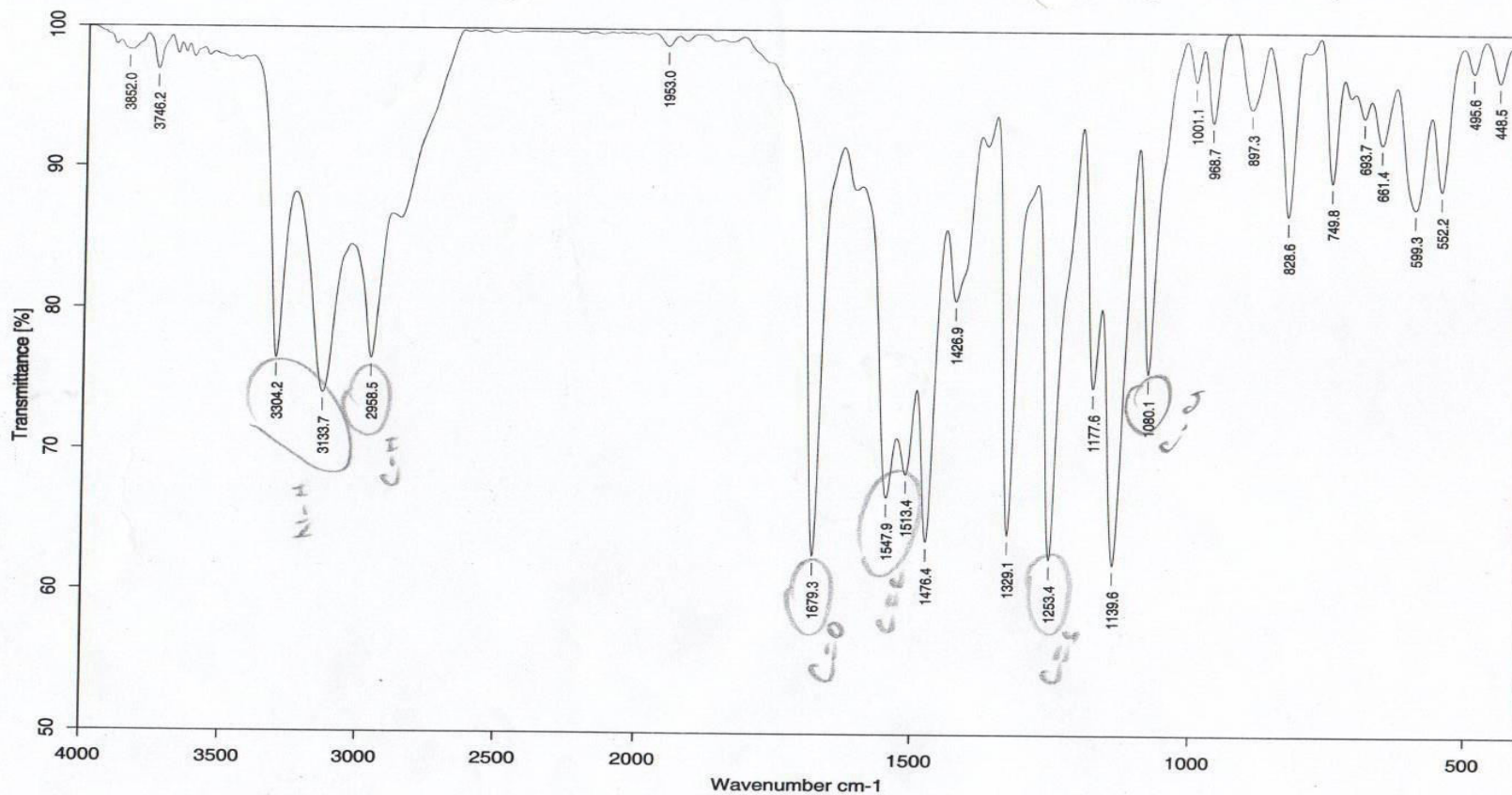
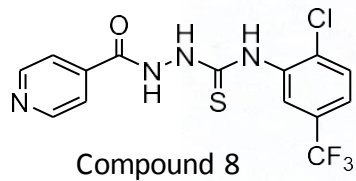
#Ions: 353



M.Wt = 374.76



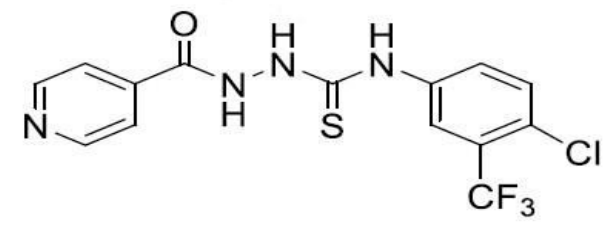
Compound 8



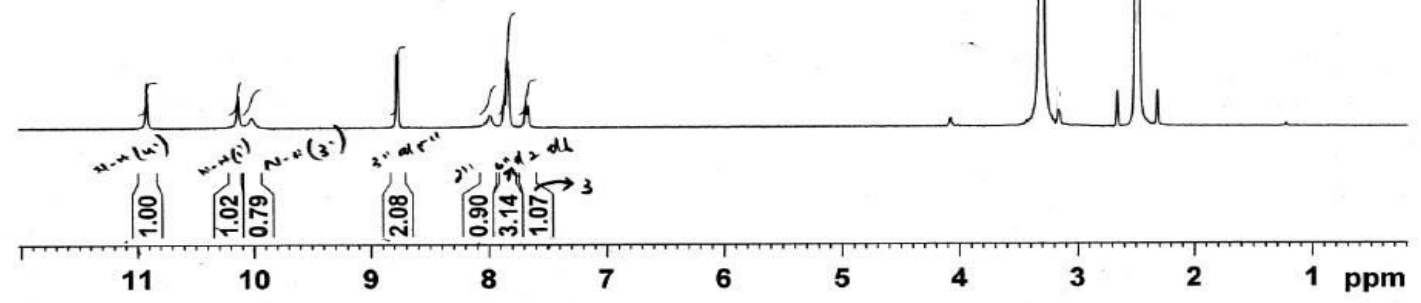
Sample : FZI-ISO6/Fazila Rizvi	Spectrum : FZ-I-ISO6.0 (in D:\IRSTUDENT)
Measured : 19/04/2017 on VECTOR22	Technic : Solid
Resolution : 4 cm-1 (10 scans)	Analyst : MA/ZA/JS

10.923
 10.142
 10.022
 8.785
 8.771
 7.995
 7.871
 7.847
 7.689
 7.668

FAZILA/DR.HINA/FZ.I.ISO.14 / 2000 / 18016
 ICCBS, U.O.K/1H/.



Compound 9



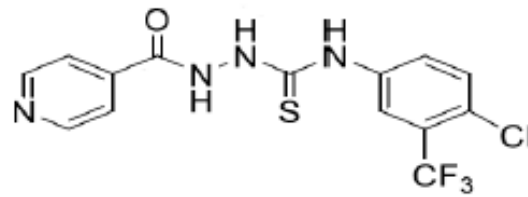
AVANCE AV-400 MHz
 Lab # 115

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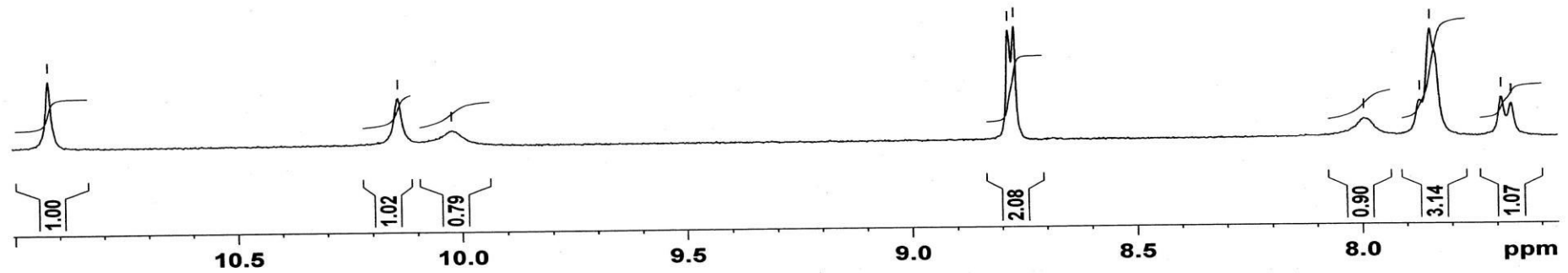
NAME          sep07-16
EXPNO         1
PROCNO        1
Date_         20160907
Time          12.09
INSTRUM       spect
PROBHD        5 mm SEI 1H-13
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            128
DS            0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            322.5
DW            62.400 usec
DE            6.50 usec
TE            300.0 K
D1            1.50000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            10.80 usec
PL1           3.00 dB
SFO1          400.0332002 MHz
SI            32768
SF            400.0300042 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            0.20
  
```

—10.5.
—10.142
—10.022
FAZILA/DR.HINA/FZ.I.ISO.14
ICCBS,U.O.K/1H/.



Compound 9



—10.5.
—10.142
—10.022
8.785
8.771
7.995
7.871
7.847
7.689
7.668

File: FZ-I-ISO-14
Sample: FAZILA RIZVI /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 09-07-2016 (Time Run: 15:27:11)

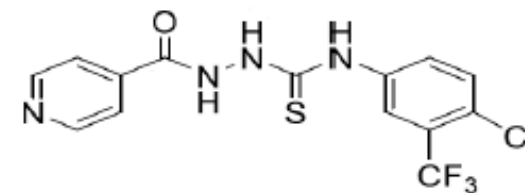
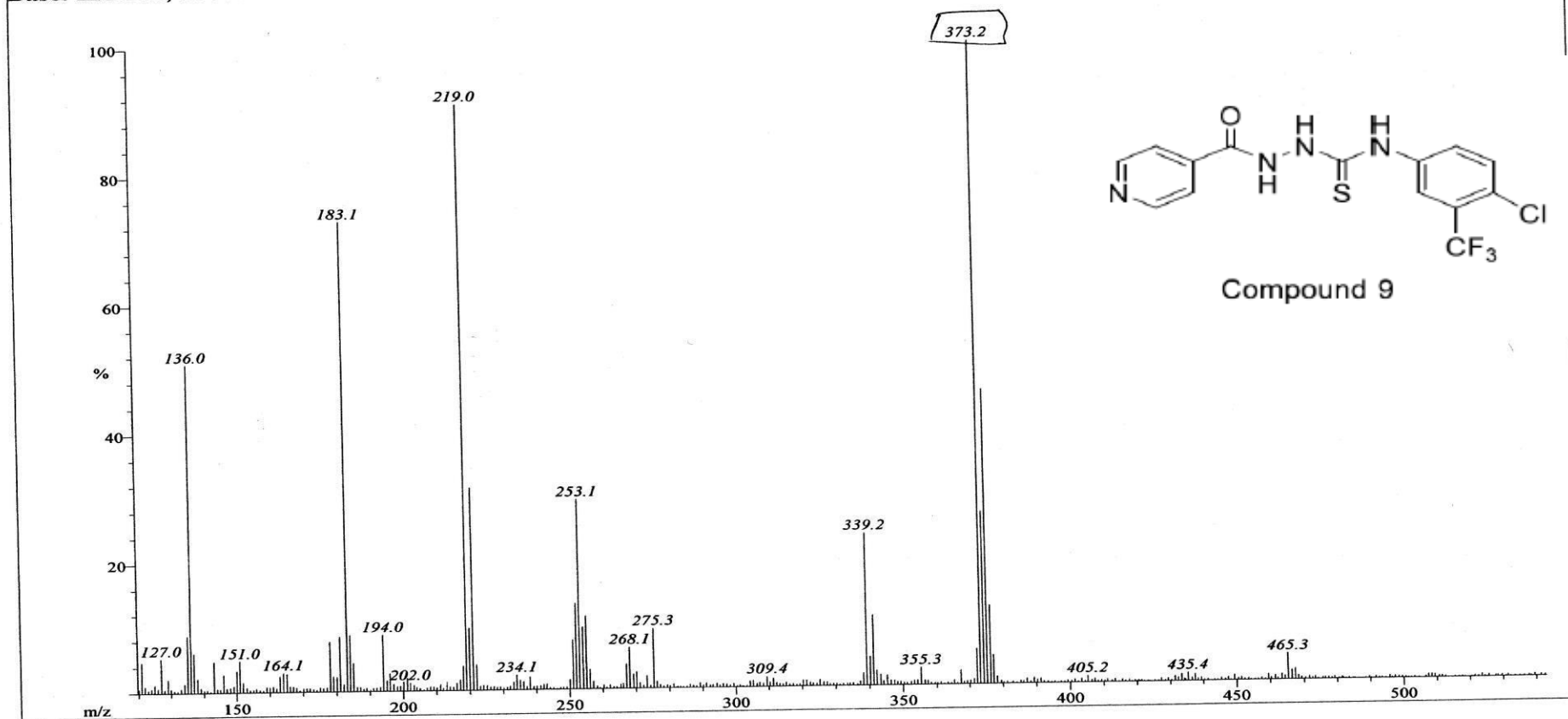
Ionization mode: FAB-

Scan: 3

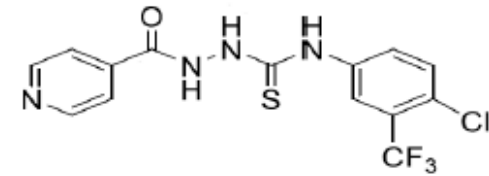
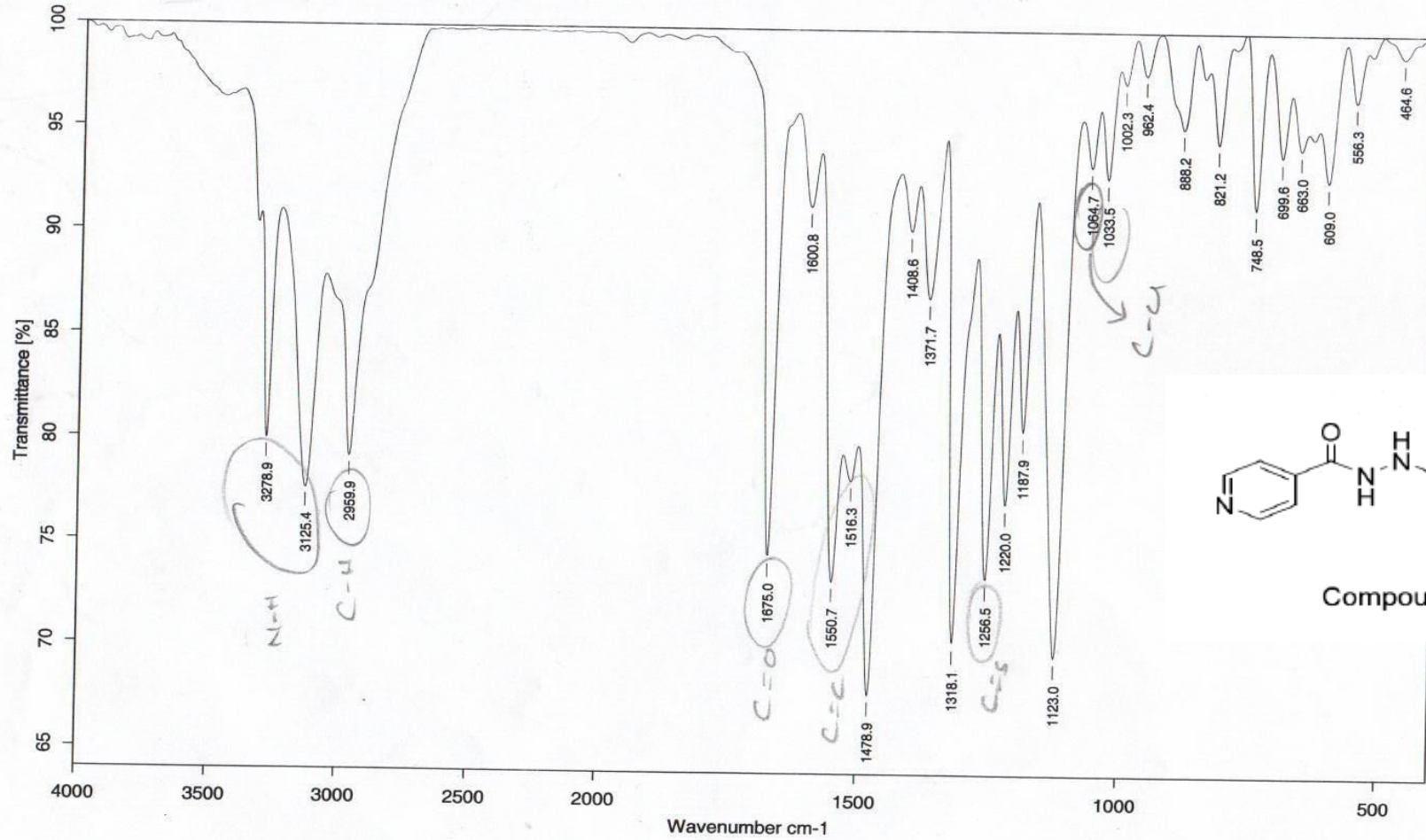
R.T.: .18

#Ions: 954

Base: m/z 373; 100%FS TIC: 10685212



Compound 9



Compound 9

Sample : FZI-ISO14/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

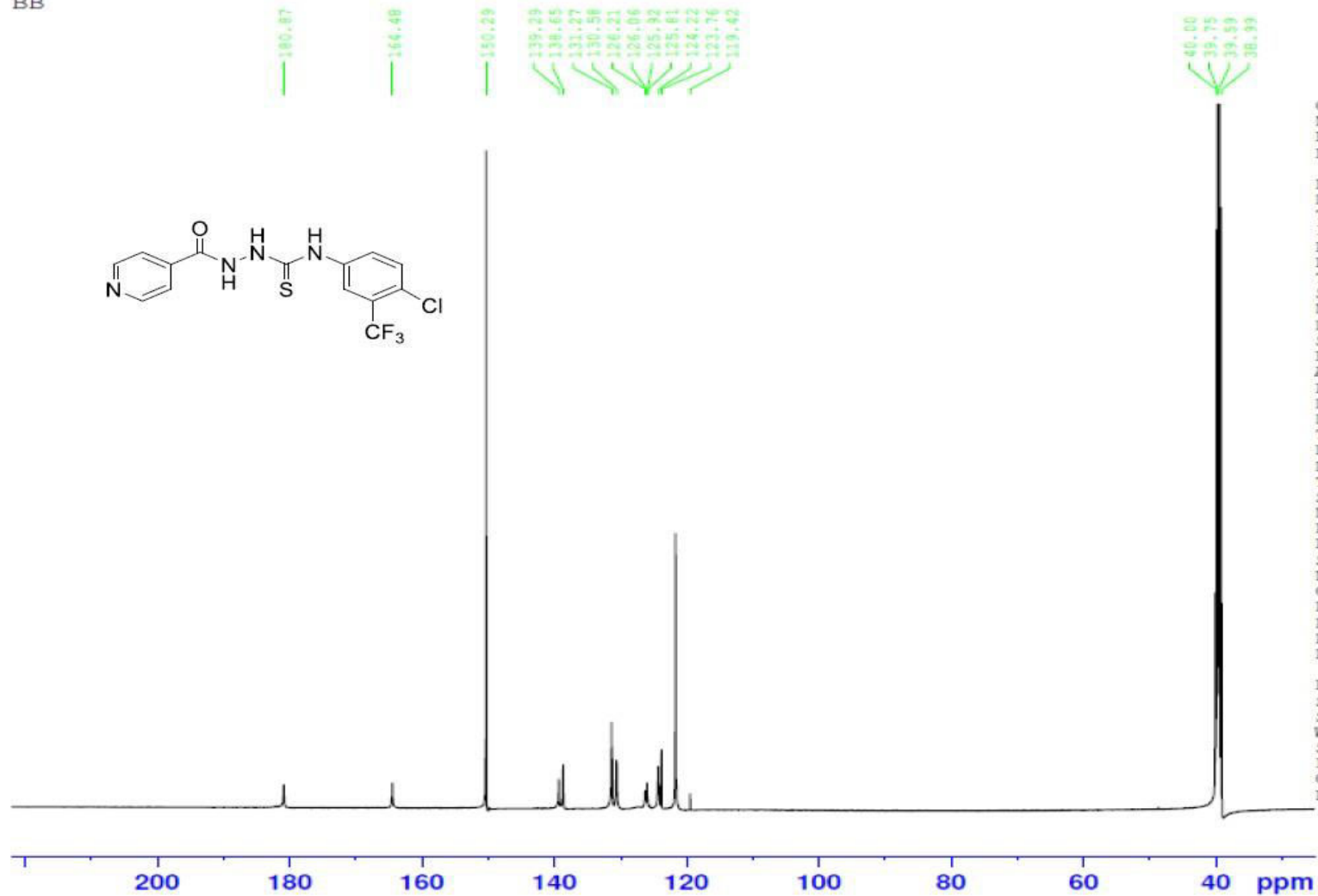
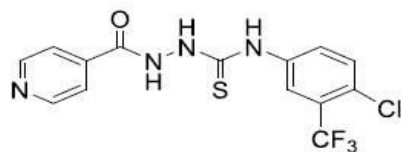
Resolution : 4 cm⁻¹ (10 scans)

Spectrum : FZI-ISO14.0 (in D:IRSTUDENT)

Technic : Solid

Analyst : MA/ZA/JS

FAZILA/DR.HINA/FZ-I-1SO14/DMSO
BB

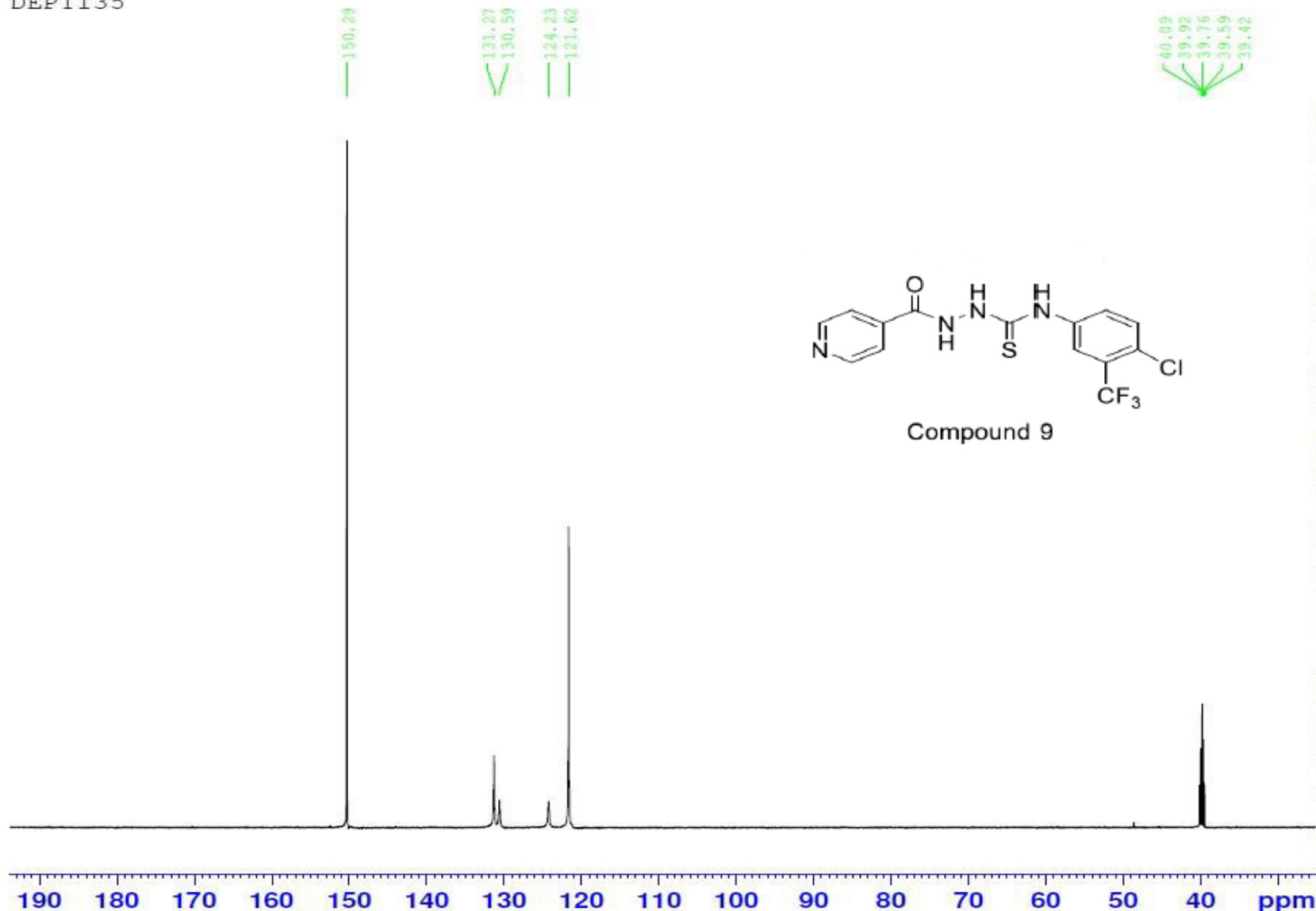


Current Data Parameters
NAME ISO 14 NMR
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190205
Time 3.55 h
INSTRUM Avance Neo 500
PROBHD Z44862_0021 (C
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 16384
DS 8
SWH 30120.482 Hz
FIDRES 1.838408 Hz
AQ 0.5439488 sec
RG 101
DW 16.600 usec
DE 20.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 16
SFO1 125.8227986 MHz
NUC1 13C
P1 10.00 usec
PLW1 26.46199989 W
SFO2 500.3320013 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 9.74149990 W
PLW12 0.34246999 W
PLW13 0.17199001 W

F2 - Processing parameters
SI 16384
SF 125.8081399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

FAZILA/DR.HINA/FZ-I-1SO14/DMSO
DEPT135



Current Data Parameters
NAME ISO 14 NMR
EXPNO 6
PROCNO 1

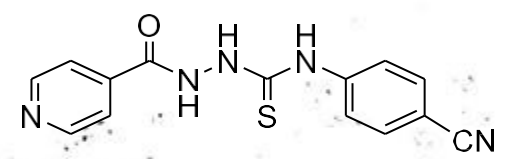
F2 - Acquisition Parameters

Date_ 20190205
Time 8.56 h
INSTRUM Avance Neo 500
PROBHD Z44862_0021 (C
PULPROG deptsp135
TD 32768
SOLVENT DMSO
NS 8192
DS 8
SWH 25000.000 Hz
FIDRES 1.525879 Hz
AQ 0.6553600 sec
RG 101
DW 20.000 usec
DE 20.00 usec
TE 298.0 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 8
SFO1 125.8200303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 26.46199989 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 4.04309988 W
SFO2 500.3320013 MHz
NUC2 1H
CPDPRG[2] waltz65
P3 15.00 usec
P4 30.00 usec
PCPD2 80.00 usec
PLW2 9.74149990 W
PLW12 0.34246999 W

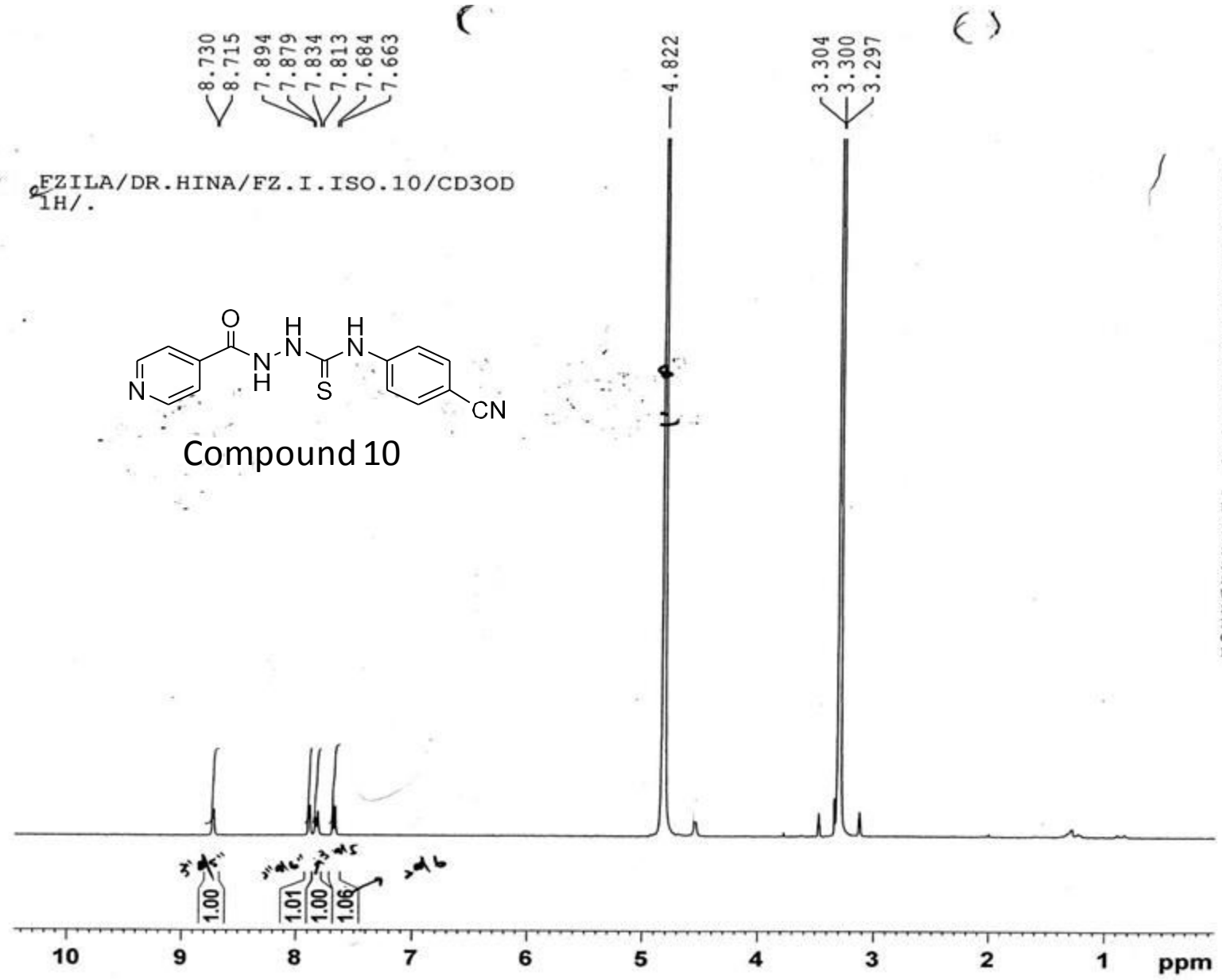
F2 - Processing parameters

SI 16384
SF 125.8081395 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

FZILA/DR.HINA/FZ.I.ISO.10/CD3OD
1H/.



Compound 10



AVANCE AV-400 MHz
Lab # 115

NAME june08-16
EXPNO 1
PROCNO 1
Date_ 20160608
Time_ 13.12
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 128
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 574.7
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 400.0332002 MHz
SI 32768
SF 400.0300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.20

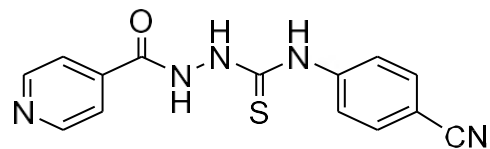
8.730
8.715

7.894
7.879

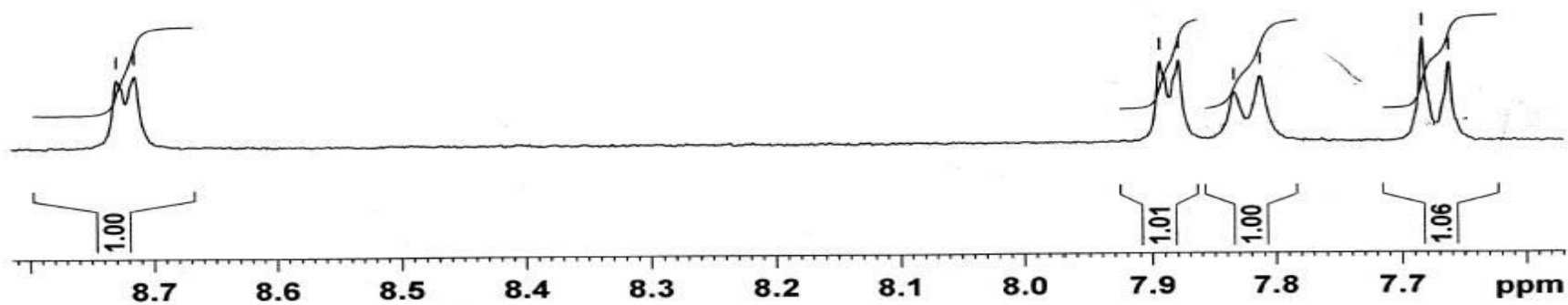
7.834
7.813

7.684
7.663

FZILA/DR.HINA/FZ.I.ISO.10/CD3OD
1H/.



Compound 10



File: FZ-I-ISO10-FABP
Sample: FAZILA /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

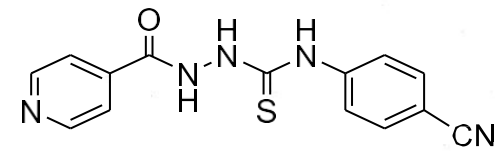
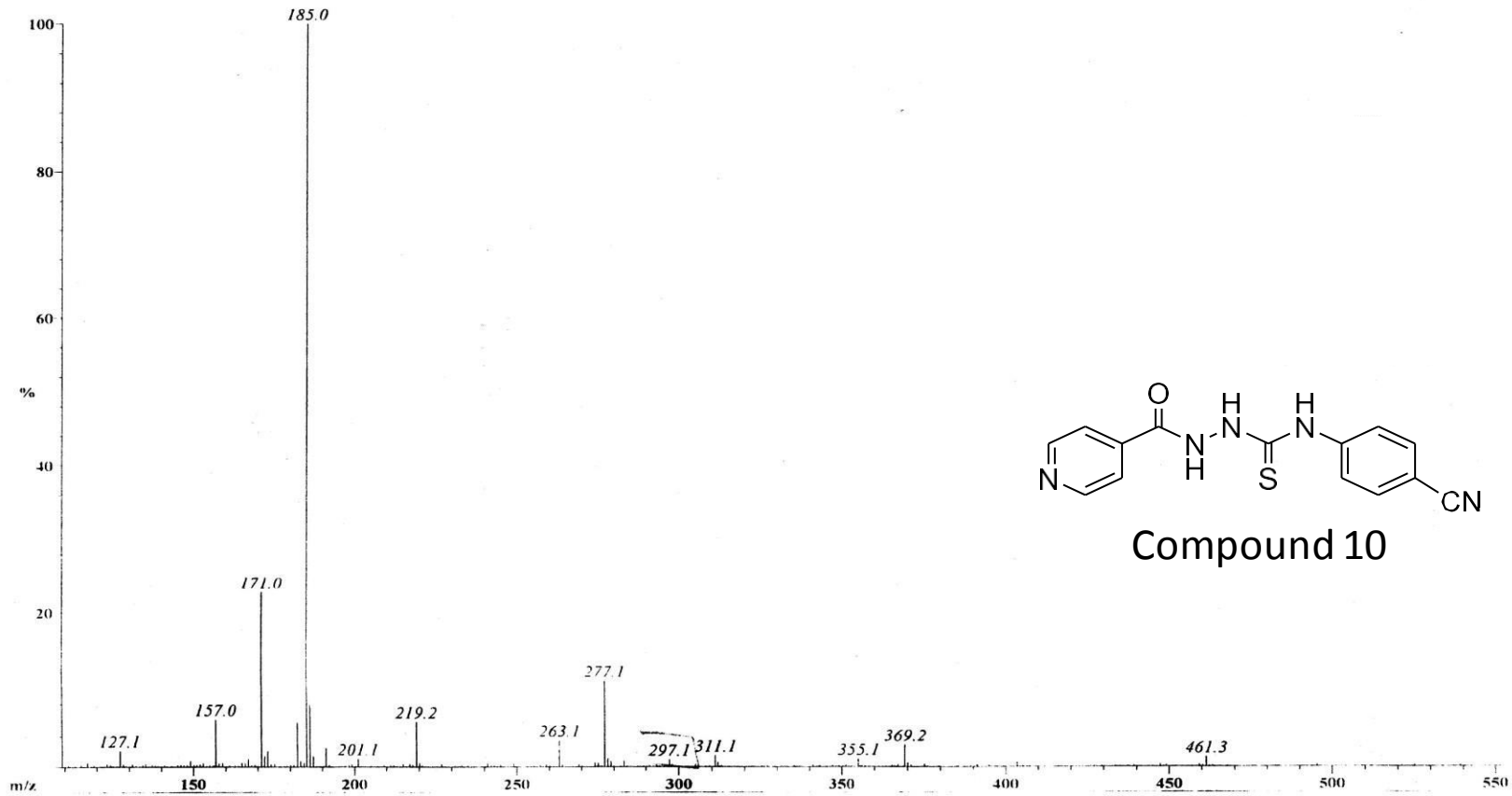
Date Run: 06-09-2016 (Time Run: 12:40:22)

Ionization mode: FAB+

Scan: 11
Base: m/z 185; 36.5%FS TIC: 1004100

R.T.: .88

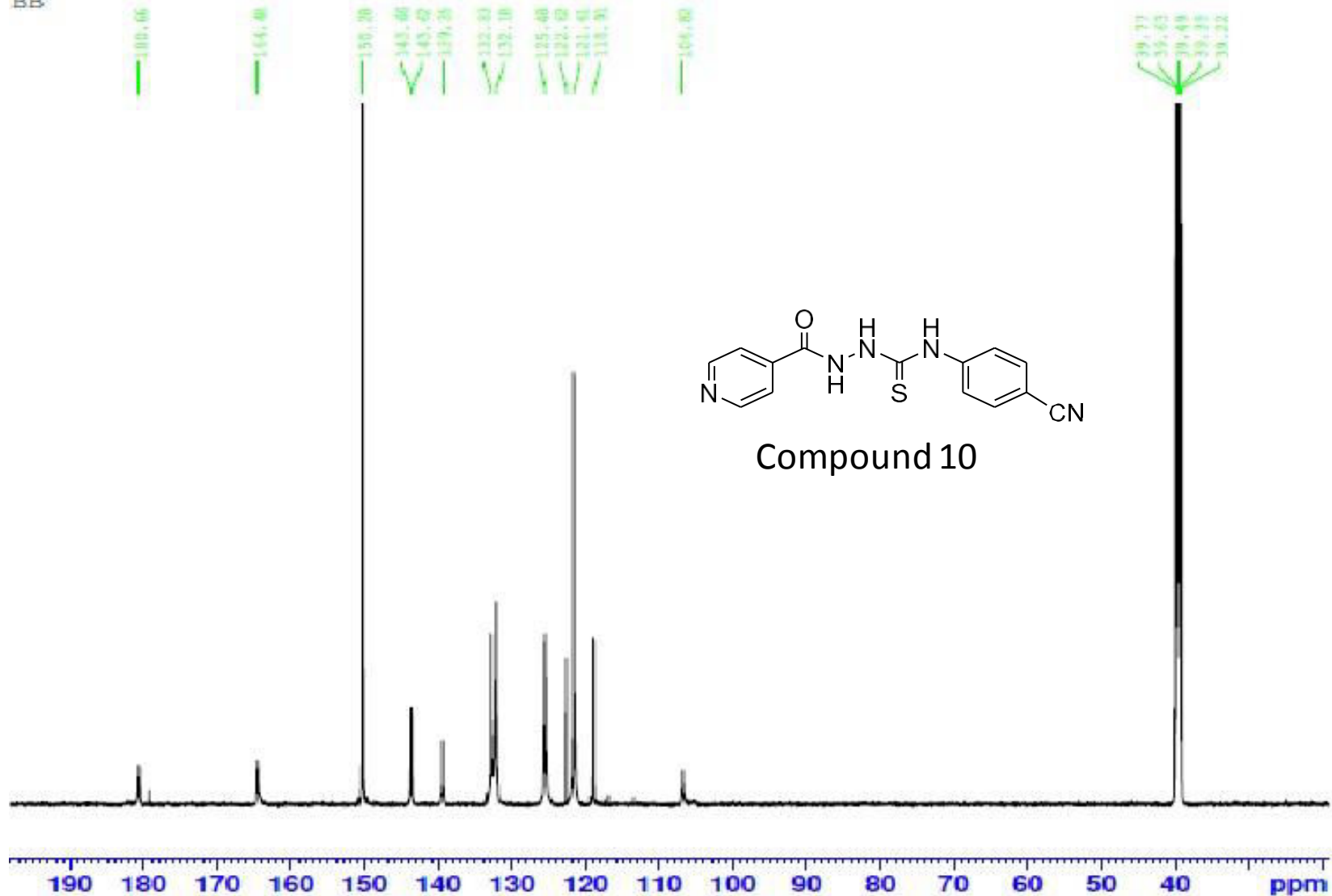
#Ions: 542



Compound 10

cal

Fazila / Dr. Hina / FZ-I-ISO-10 / DMSO
BB

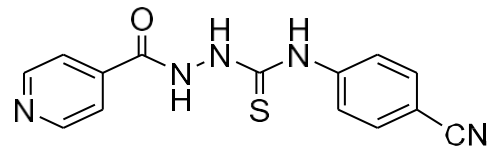


Current Data Parameters
NAME ISO 10
EXPNO 4
PROCNO 1

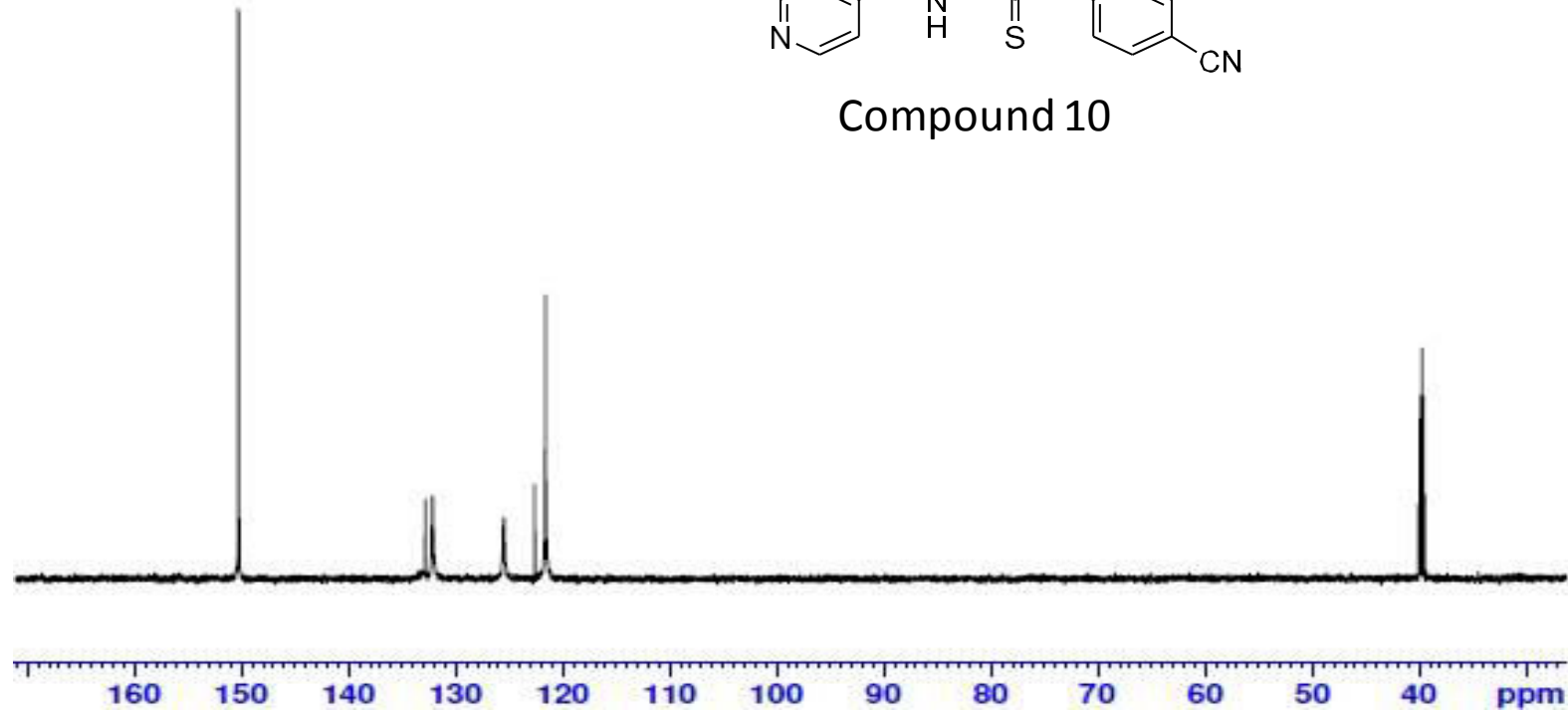
F2 - Acquisition Parameters
Date_ 20190207
Time 14.14 h
INSTRUM AVNeo_600
PROBHD Z117768_0039 (1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 6606
DS 4
SWH 35714.285 Hz
FIDRES 2.179827 Hz
AQ 0.4587520 sec
RG 101
DW 14.000 usec
DE 18.00 usec
TE 298.0 K
D1 1.50000000 sec
D11 0.03000000 sec
ID0 8
SFO1 150.9553694 MHz
NUC1 13C
P1 12.00 usec
PLW1 107.76000214 W
SFO2 600.2724011 MHz
NUC2 1H
CPDPRG[2] waltz45
PCPD2 70.00 usec
PLW2 9.53950024 W
PLW12 0.12460000 W
PLW13 0.06267200 W

F2 - Processing parameters
SI 16384
SF 150.9380853 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fazila / Dr. Hina / FZ-I-ISO-10 / DMSO
DEPT135



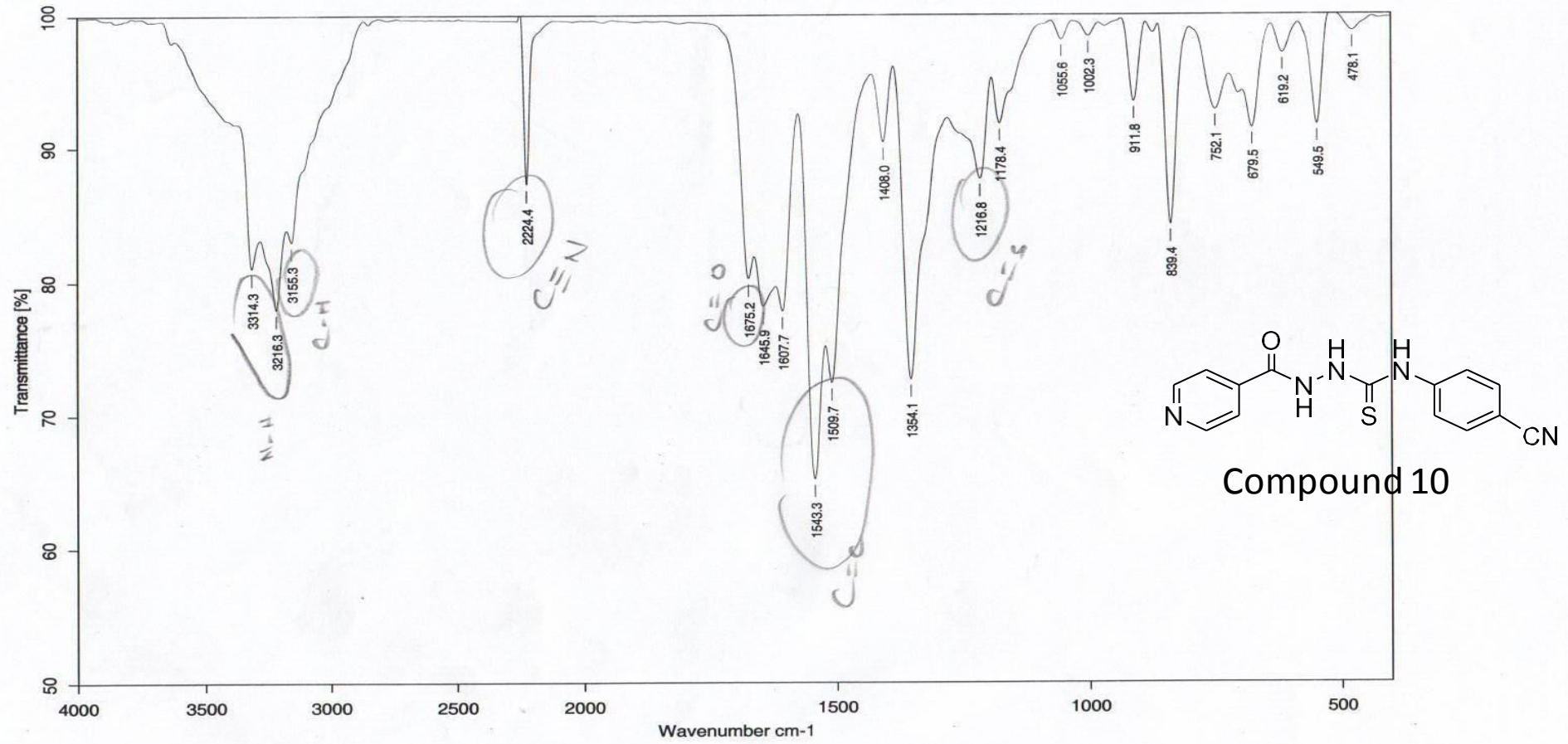
Compound 10



```
NAME          ISO 10
EXPNO          5
PROCNO         1

F2 - Acquisition Parameters
Date_          20190207
Time           15.26 h
INSTRUM       AVNeo_600
PROBHD        Z117768_0039 (
PULPROG       deptspl35
ID            32768
SOLVENT       DMSO
NS            2058
DS            8
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.5439488 sec
RG            101
DW            16.600 usec
DE            18.00 usec
TE            298.0 K
CNST2         145.0000000
D1            1.50000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0           4
SFO1          150.9523507 MHz
NUC1           13C
P1            12.00 usec
P13           2000.00 usec
PLW0          0 W
PLW1          107.76000214 W
SPNAM[5]      Crp60comp.4
SFOALS        0.500
SPOFFS5       0 Hz
SPW5          23.70800018 W
SFO2          600.2724011 MHz
NUC2           1H
CPDPRG[2]     waltz65
P3            8.00 usec
P4            16.00 usec
PCPD2         70.00 usec
PLW2          9.53950024 W
PLW12         0.12460000 W

F2 - Processing parameters
SI            16384
SF            150.9380853 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

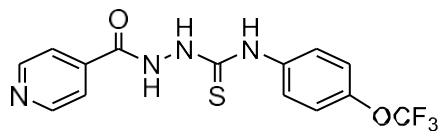


Sample : FZI-ISO10/Fazila Rizvi
Measured : 19/04/2017 on VECTOR22
Resolution : 4 cm⁻¹ (10 scans)

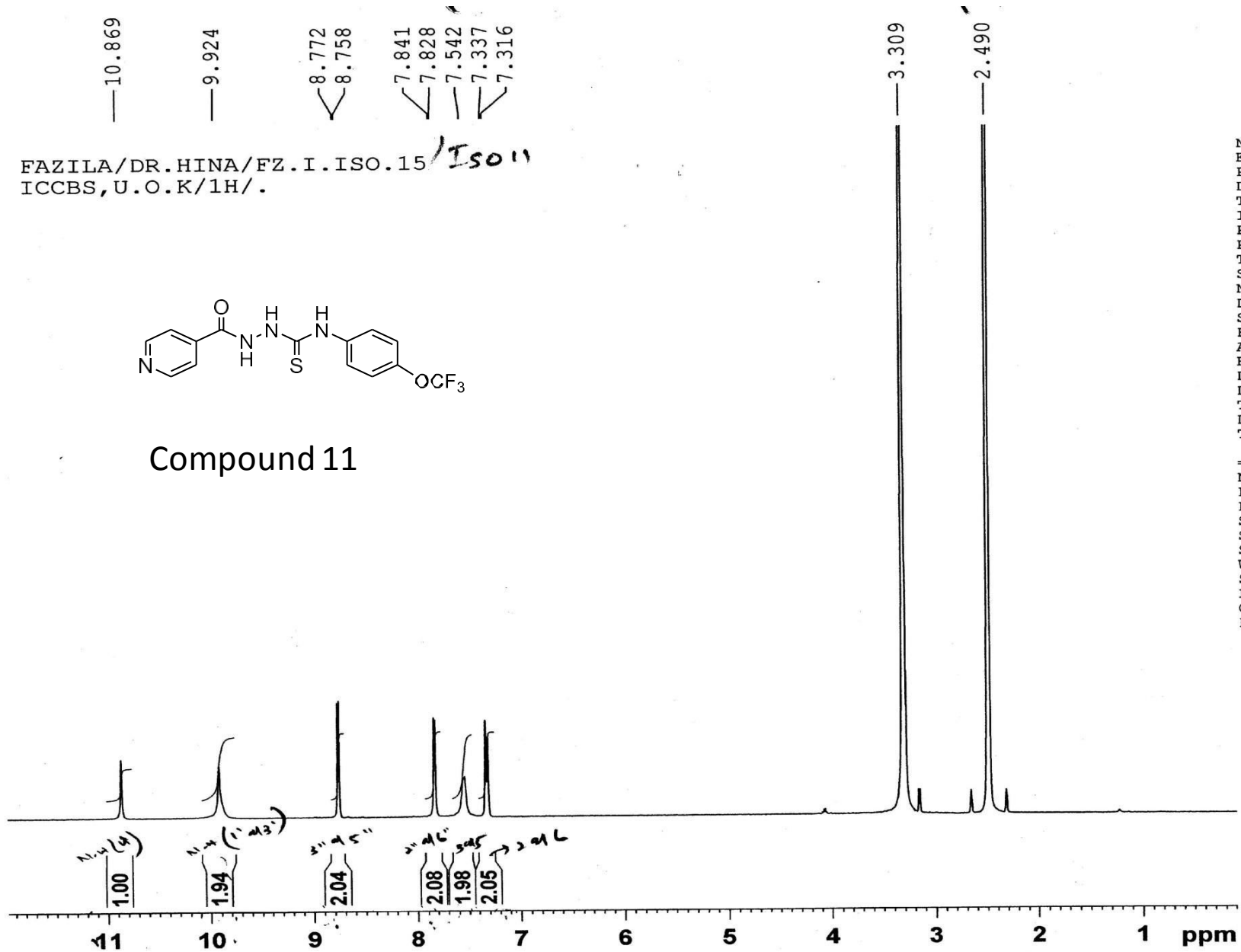
Spectrum : FZ-I-ISO10.0 (in D:\MRSTUDENT)
Technic : Solid
Analyst : MA/ZA/JS

AVANCE AV-400 MHz
Lab # 115

FAZILA/DR.HINA/FZ.I.ISO.15 / *ISO 11*
ICCBS, U.O.K/1H/.



Compound 11



```

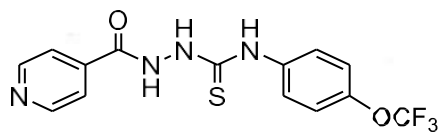
NAME          sep07-16
EXPNO         3
PROCNO        1
Date_         20160907
Time_         12.46
INSTRUM       spect
PROBHD        5 mm SEI 1H-13
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            128
DS            0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            322.5
DW            62.400 usec
DE            6.50 usec
TE            300.0 K
D1            1.50000000 sec
TD0           1
  
```

```

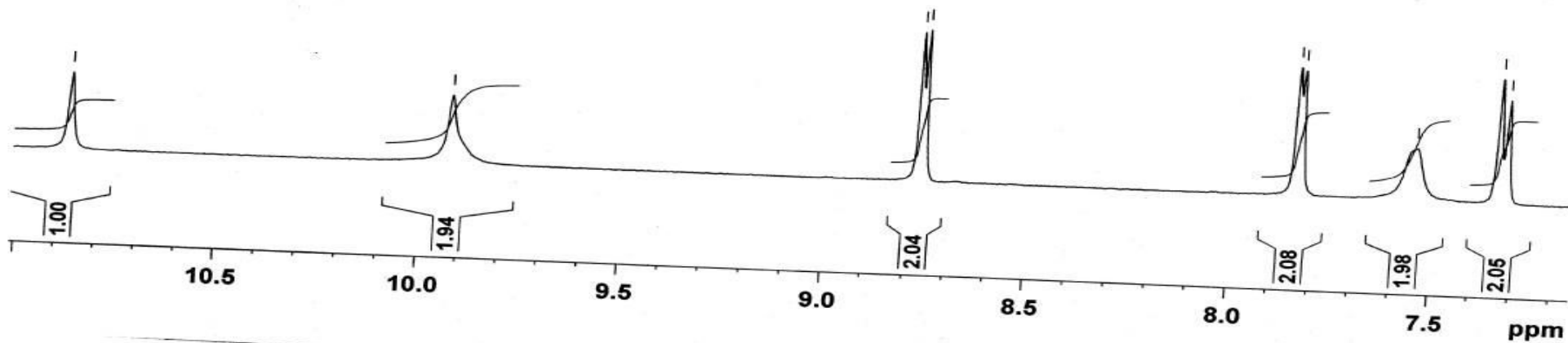
===== CHANNEL f1 =====
NUC1          1H
P1            10.80 usec
PL1           3.00 dB
SFO1          400.0332002 MHz
SI            32768
SF            400.0300042 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            0.20
  
```

—10.869
—9.924

FAZILA/DR.HINA/FZ.I.ISO.15
ICCBS,U.O.K/1H/.



Compound 11



File: FZ-I-ISO15/~~1011~~
Sample: FAZILA RIZVI /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

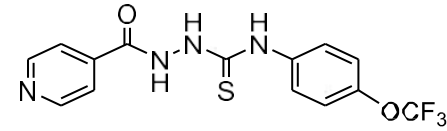
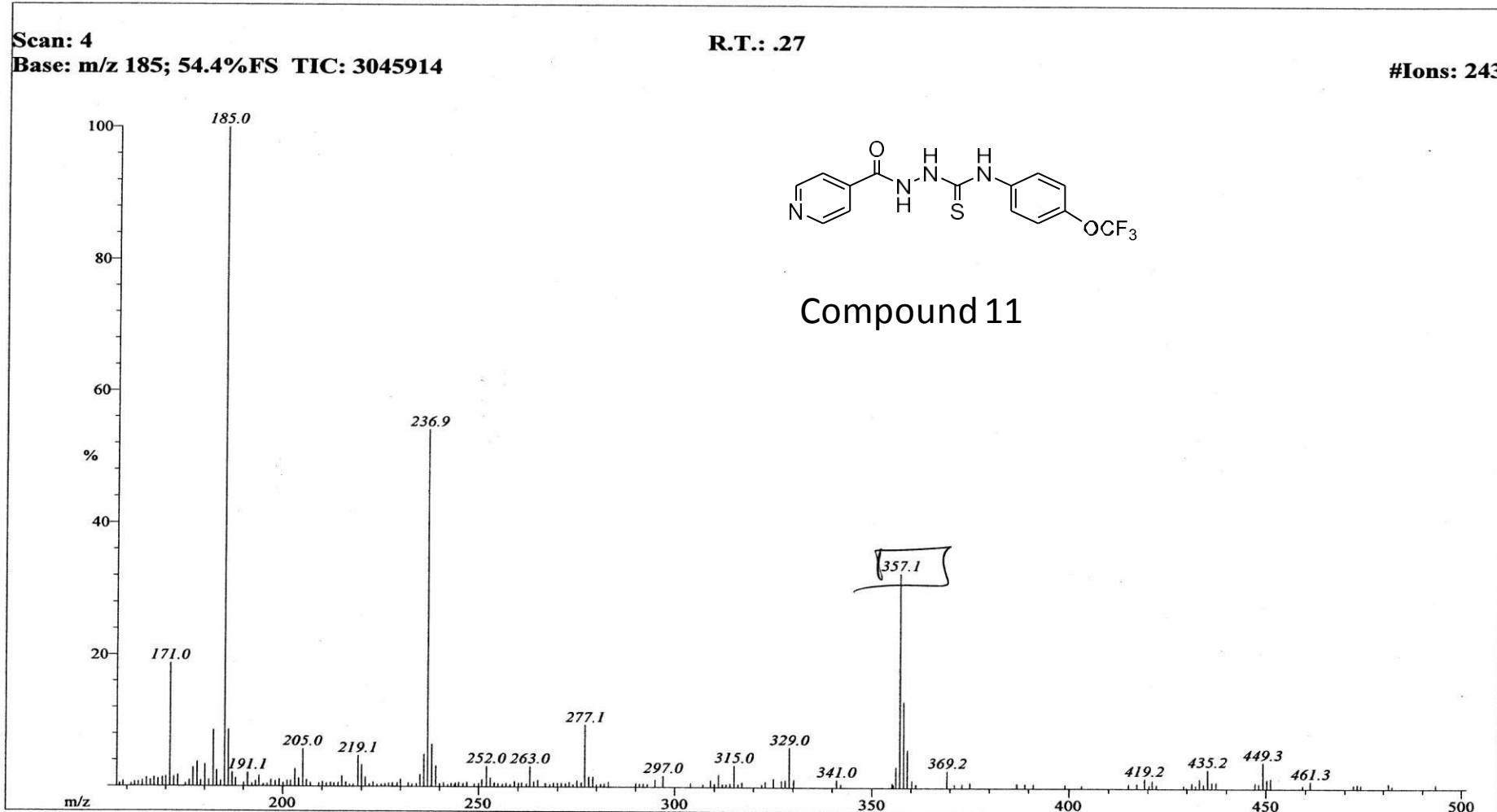
Date Run: 09-07-2016 (Time Run: 14:52:37)

Ionization mode: FAB+

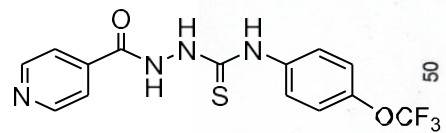
Scan: 4
Base: m/z 185; 54.4%FS TIC: 3045914

R.T.: .27

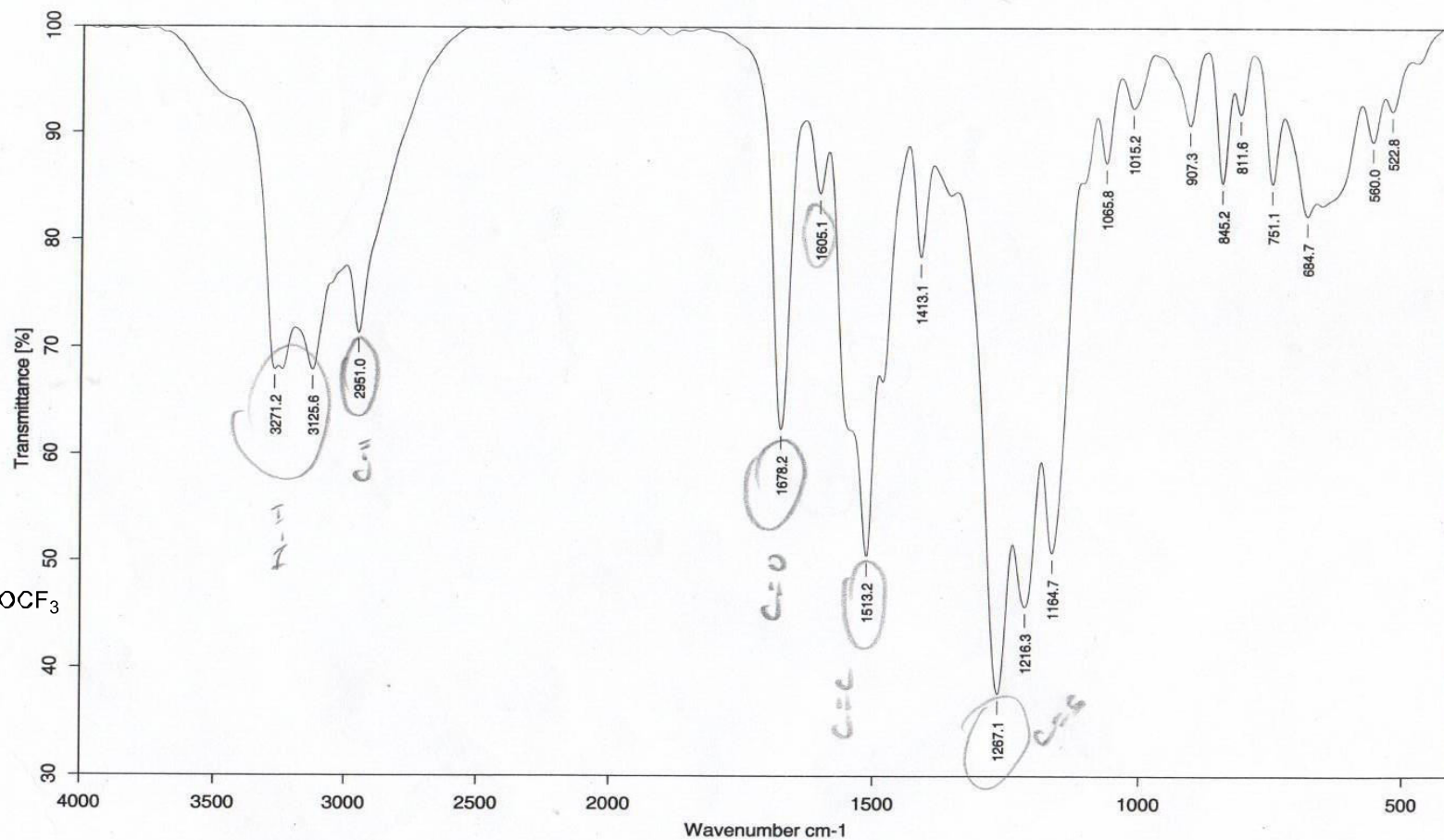
#Ions: 243



Compound 11



Compound 11



Sample : FZI-ISO11/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

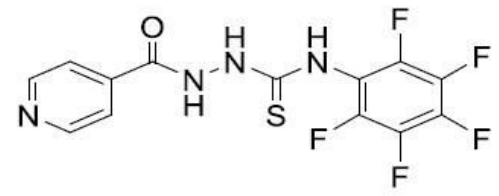
Resolution : 4 cm⁻¹ (10 scans)

Spectrum : FZ-I-ISO11.0 (in D:\IRSTUDENT)

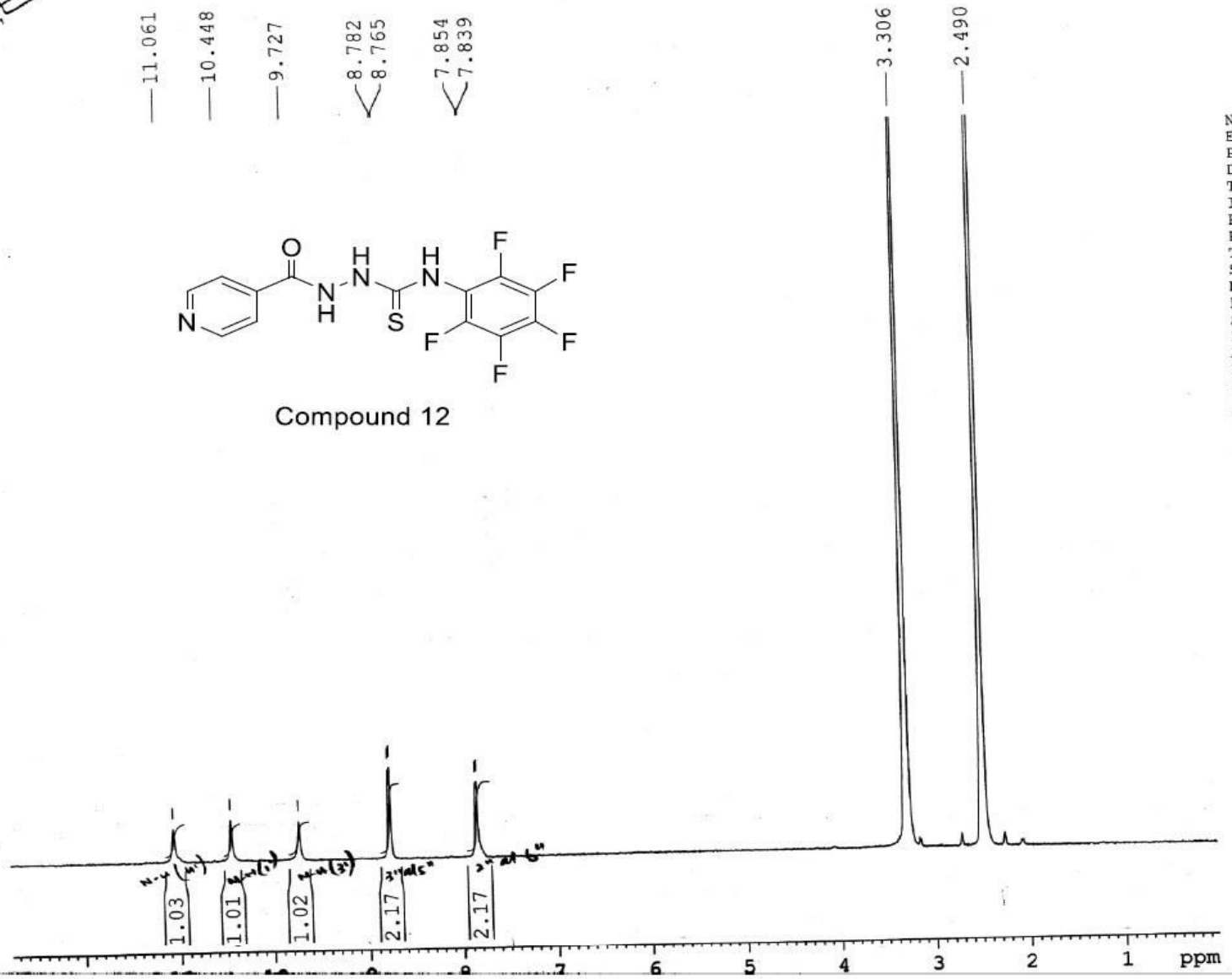
Technic : Solid

Analyst : MA/ZA/JS

— 11.061
— 10.448
— 9.727
∨ 8.782
∨ 8.765
∨ 7.854
∨ 7.839



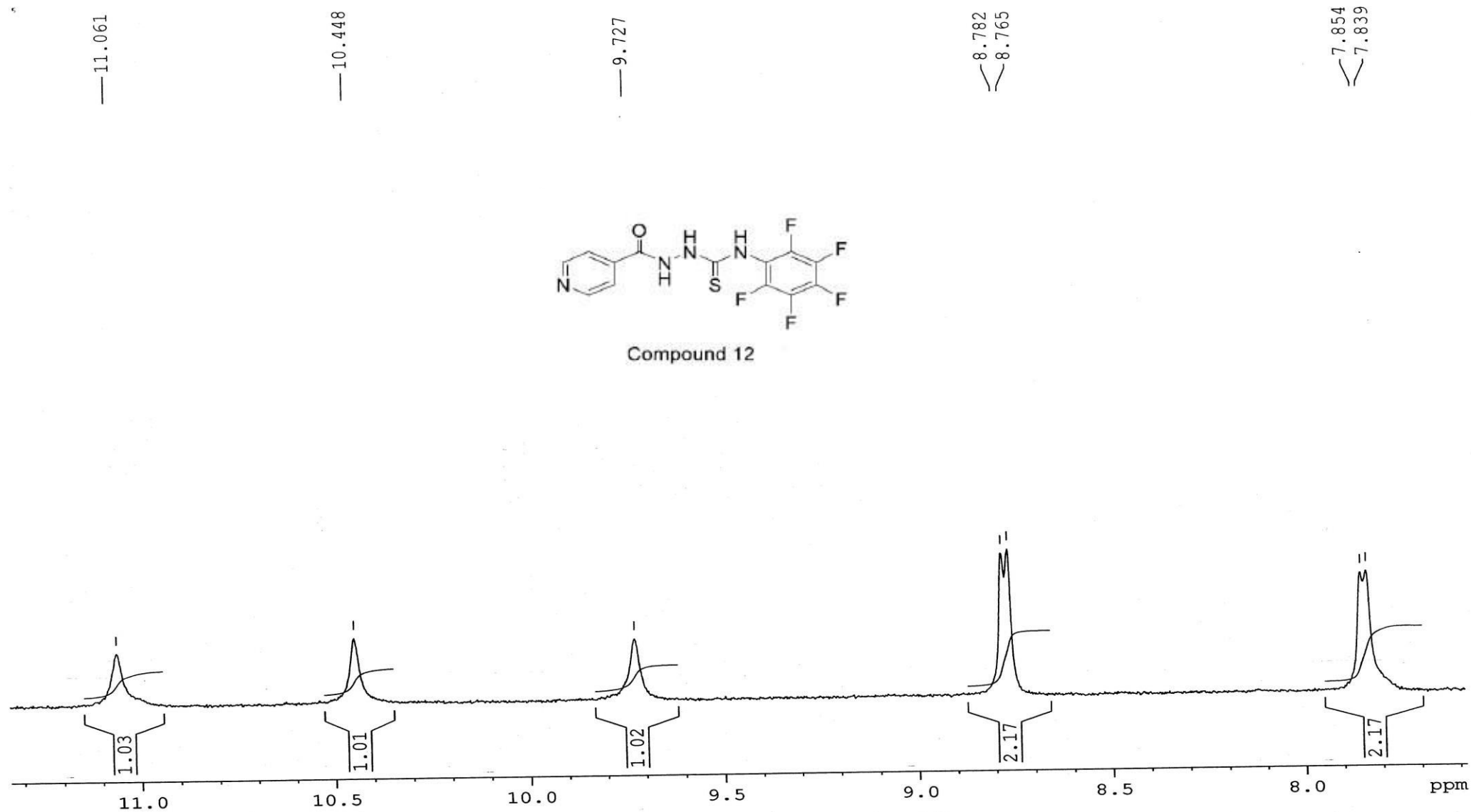
Compound 12



AVANCE AV-300
LAB NO: 108

NAME Sep26-16
EXPNO 1
PROCNO 1
Date 20160926
Time 9.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 574.7
DW 83.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.50000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.30 usec
PL1 4.00 dB
SFO1 300.1321009 MHz
SI 16384
SF 300.1300039 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.60



File: FZ-I-ISO-17
Sample: FAZILA RIZVI /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-04-2016 (Time Run: 15:38:00)

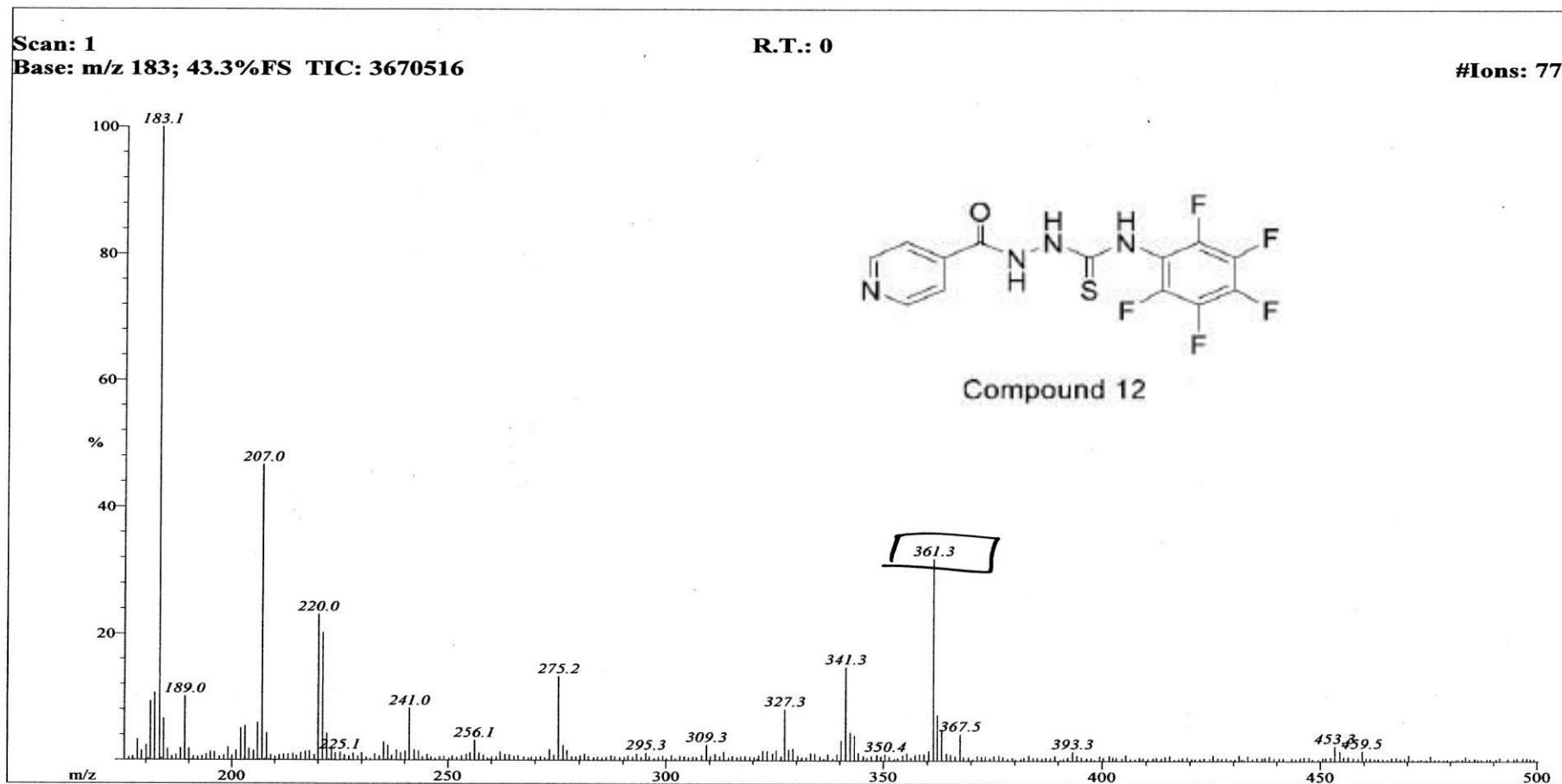
Ionization mode: FAB-

Scan: 1

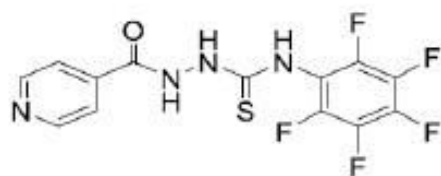
R.T.: 0

Base: m/z 183; 43.3%FS TIC: 3670516

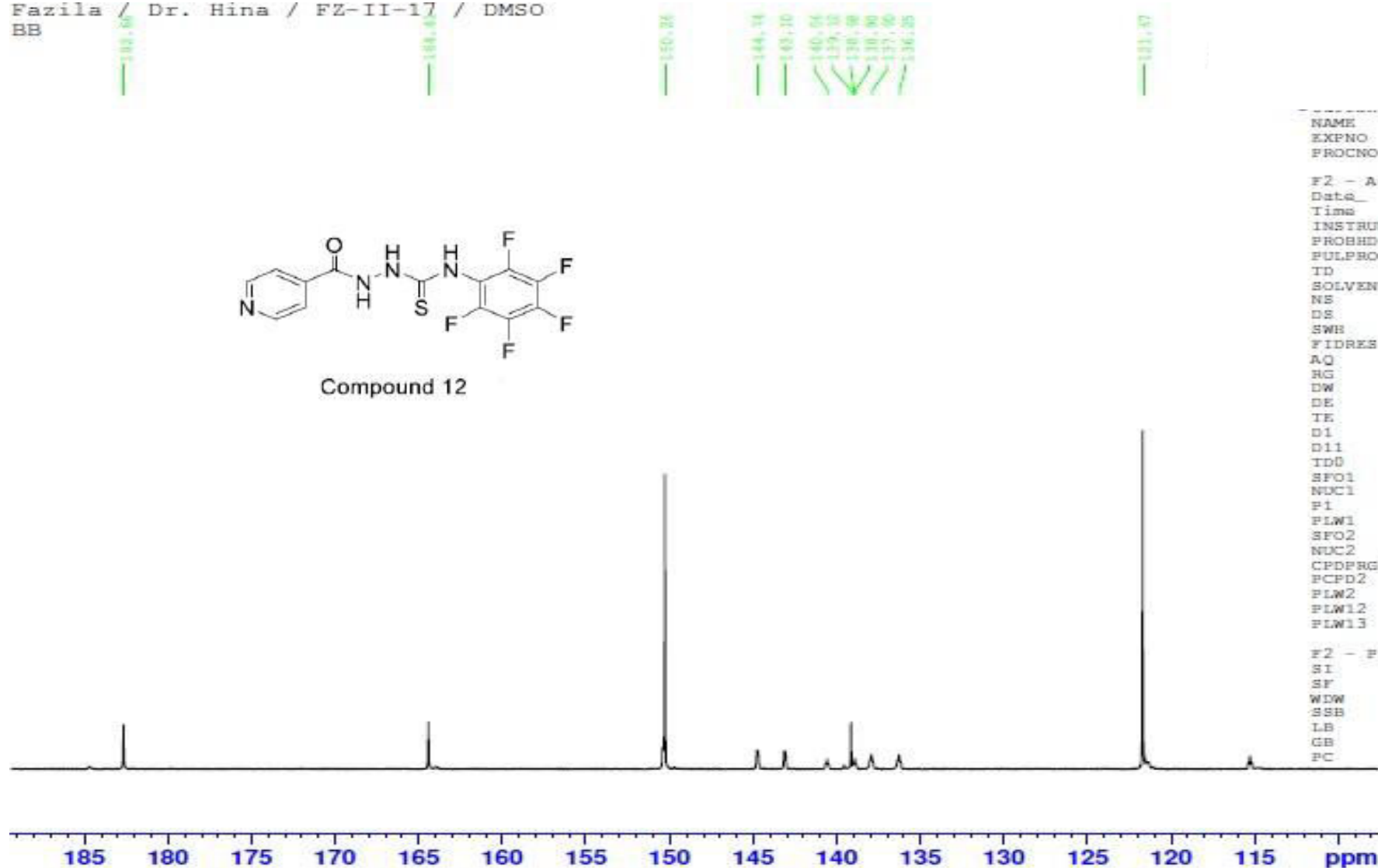
#Ions: 774



Fazila / Dr. Hina / FZ-II-17 / DMSO
BB



Compound 12

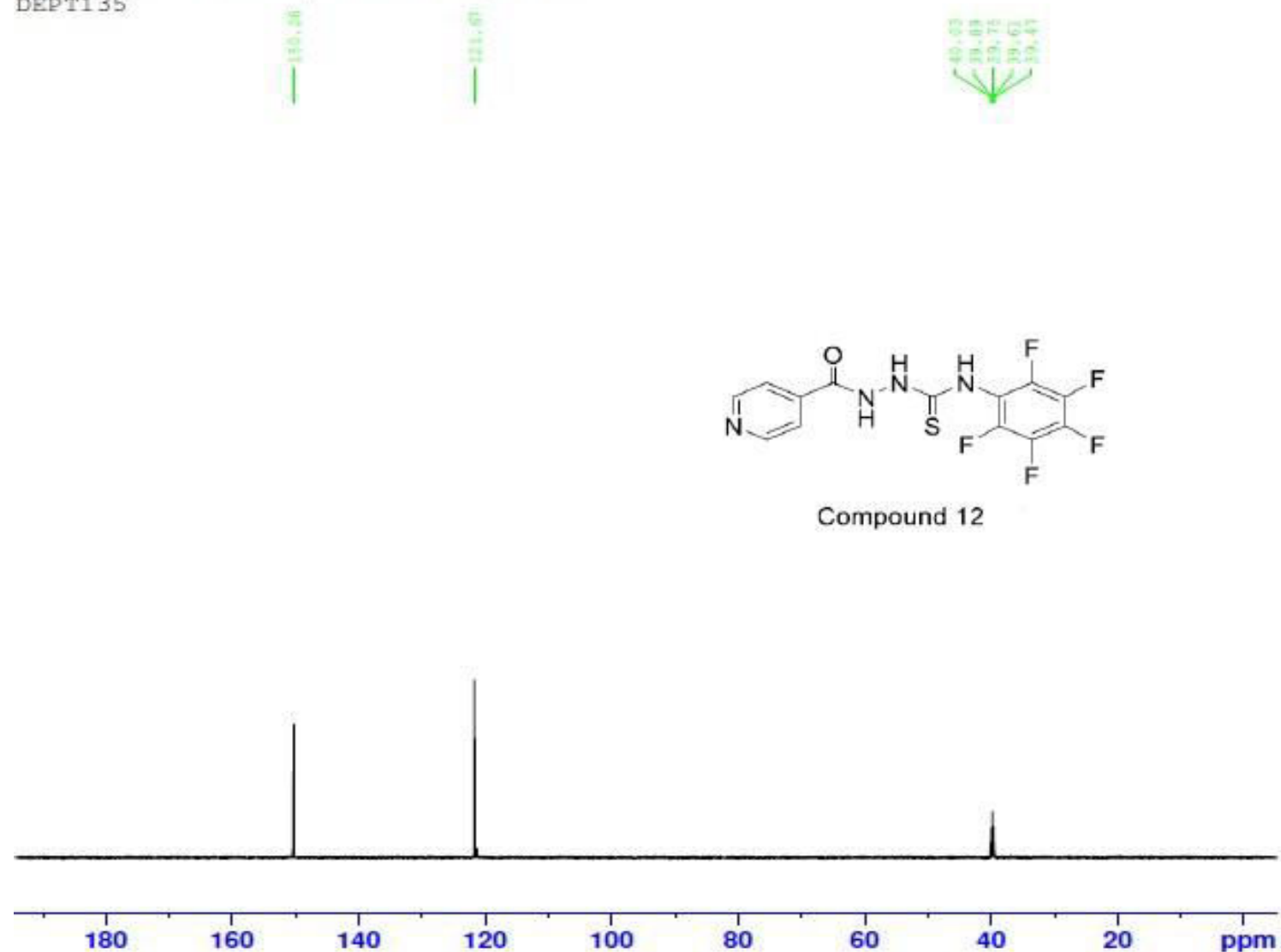


```
-----meters
NAME          fz-ii-17
EXPNO         5
PROCNO        1

F2 - Acquisition Parameters
Date_         20190206
Time          15.00 h
INSTRUM       AVNao_600
PROBHD        Z117768_0039 (
PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            5038
DS            4
SWH           35714.285 Hz
FIDRES        2.179827 Hz
AQ            0.4587520 sec
RG            101
DW            14.000 usec
DE            18.00 usec
TE            298.0 K
D1            1.5000000 sec
D11           0.03000000 sec
TD0           8
SFO1          150.9553694 MHz
NUC1          13C
F1            12.00 usec
PLW1          107.76000214 W
SFO2          600.2724011 MHz
NUC2          1H
CPDPRG[2]    waltz65
PCPD2         70.00 usec
PLW2          9.53950024 W
PLW12         0.12460000 W
PLW13         0.06267200 W

F2 - Processing parameters
SI            16384
SF            150.9380853 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

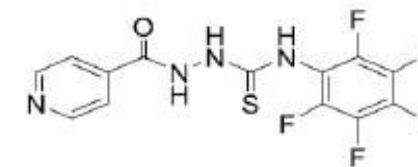
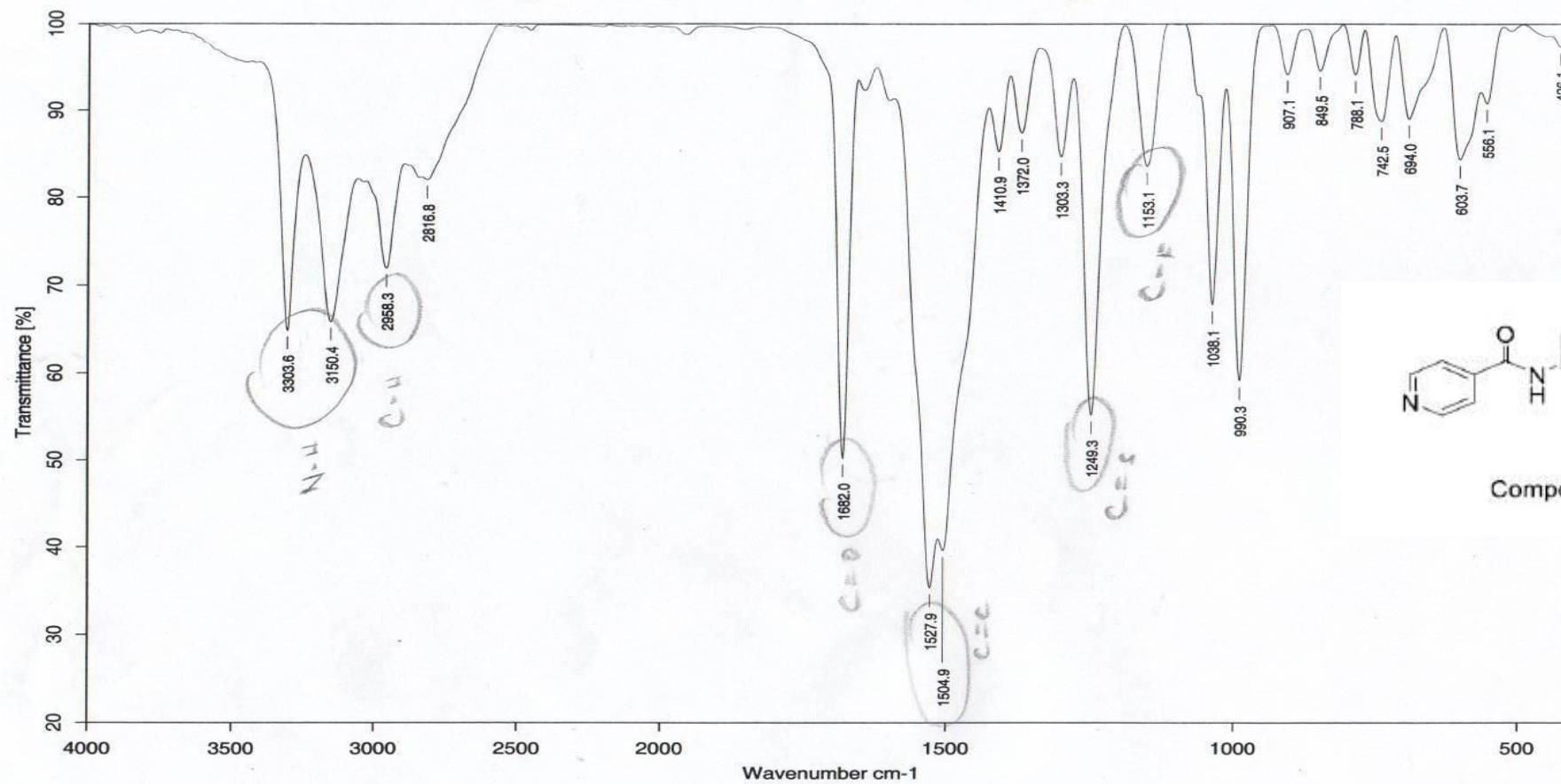
Fazila / Dr. Hina / FZ-II-17 / DMSO
DEPT135



```
NAME          0
PROCNO        1

F2 - Acquisition Parameters
Date_         20190206
Time          15.33 h
INSTRUM       AVNac_600
PROBHD        Z117768_0039 (
PULPROG       deptsp135
ID            32768
SOLVENT       DMSO
NS            925
DS            8
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.5439488 sec
RG            101
DW            16.600 usec
DE            18.00 usec
TE            298.0 K
CNST1         145.0000000
D1            1.500000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0           4
SFO1          150.9523507 MHz
NUC1          13C
P1            12.00 usec
P13           2000.00 usec
PLW0          0 W
PLW1          107.76000214 W
SPNAM[5]      Crp60ccomp.4
SFOALS        0.500
SFOFFS5       0 Hz
SPW5          23.70800018 W
SFO2          600.2724011 MHz
NUC2          1H
CPDPRG12      waltz65
P3            8.00 usec
P4            16.00 usec
PCPD2         70.00 usec
PLW2          9.53950024 W
PLW12         0.12460000 W

F2 - Processing parameters
SI            16384
SF            150.9380853 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



Compound 12

Sample : FZI-ISO17/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

Resolution : 4 cm⁻¹ (10 scans)

Spectrum : FZ-I-ISO17.0 (in D:\IRSTUDENT)

Technic : Solid

Analyst : MA/ZA/JS

Dr. Hina / Fz-I-ISO18 / DMSO
1H

10.544

9.264

8.752

8.736

7.813

7.794

4.114

3.311

2.490

1.779

1.690

1.586

1.550

1.275

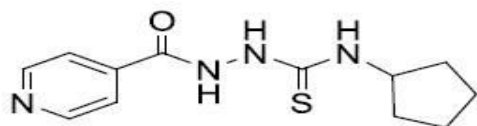
1.242

1.206

1.094

1.065

1.035

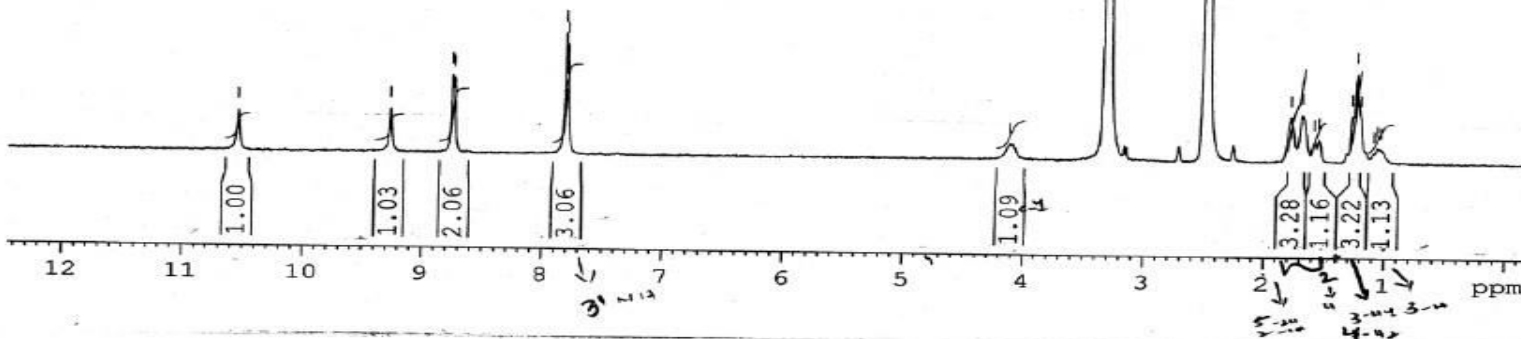


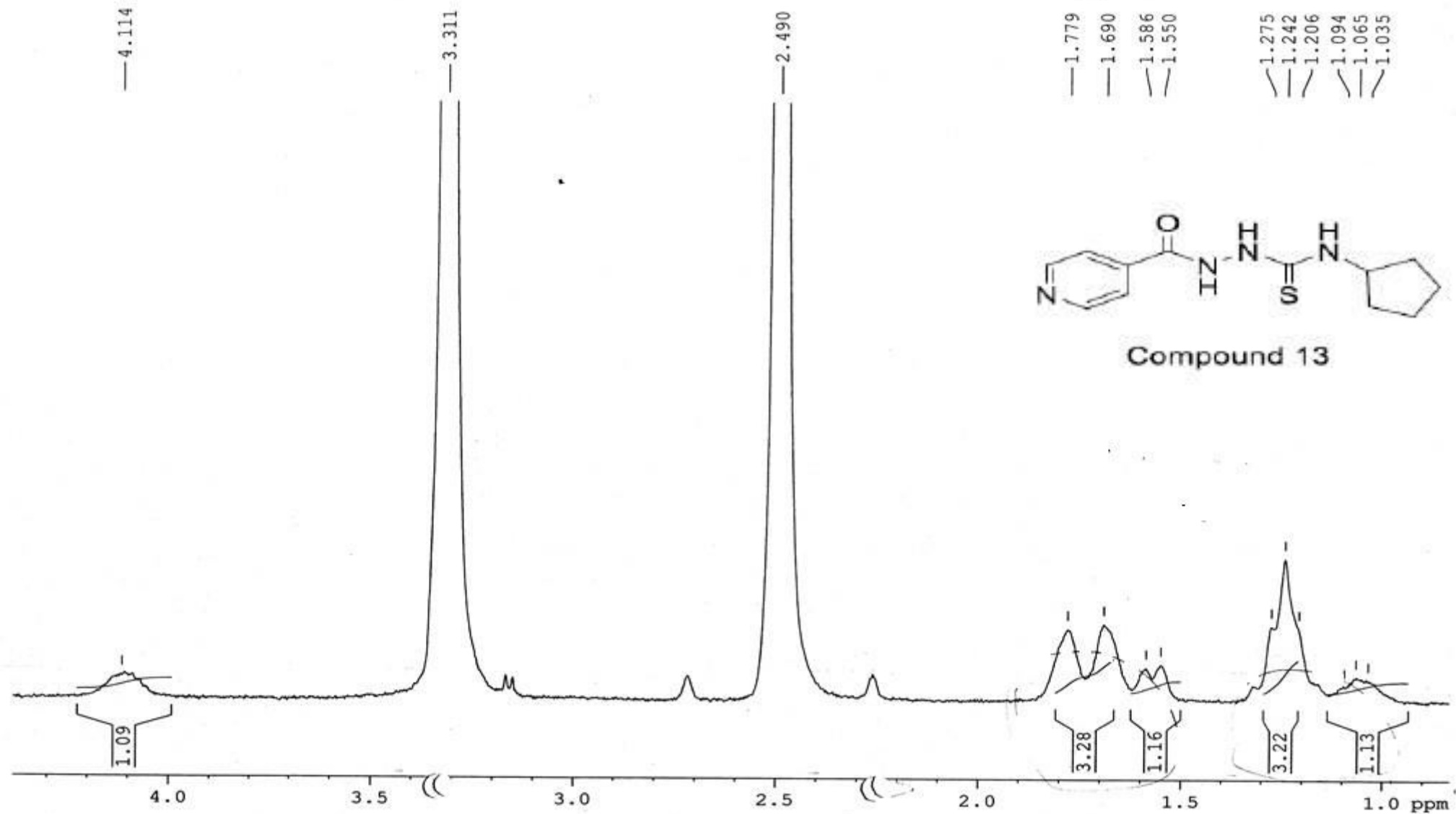
Compound 13

AVANCE AV-300
LAB NO: 108

NAME Sep26-16
EXPNO 7
PROCNO 1
Date 20160926
Time 10.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 574.7
DW 83.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.50000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.30 usec
PL1 4.00 dB
SFO1 300.1321009 MHz
SI 16384
SF 300.1300039 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.60





File: FZ-I-ISO-18
Sample: FAZILA RIZVI /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

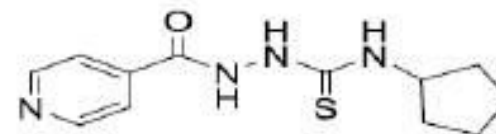
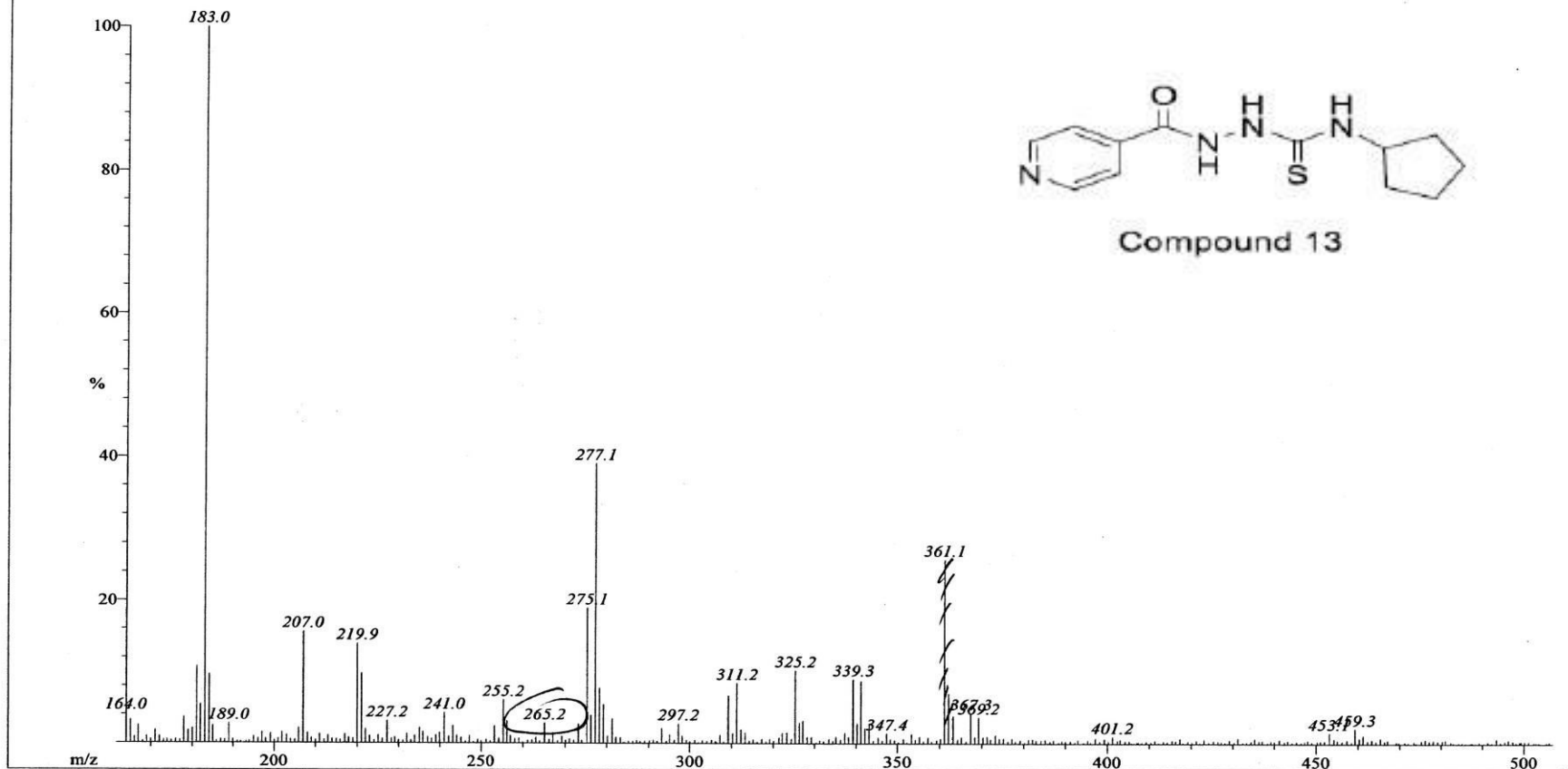
Date Run: 10-04-2016 (Time Run: 15:42:59)

Ionization mode: FAB-

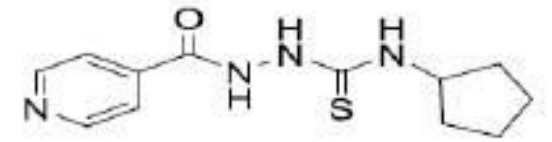
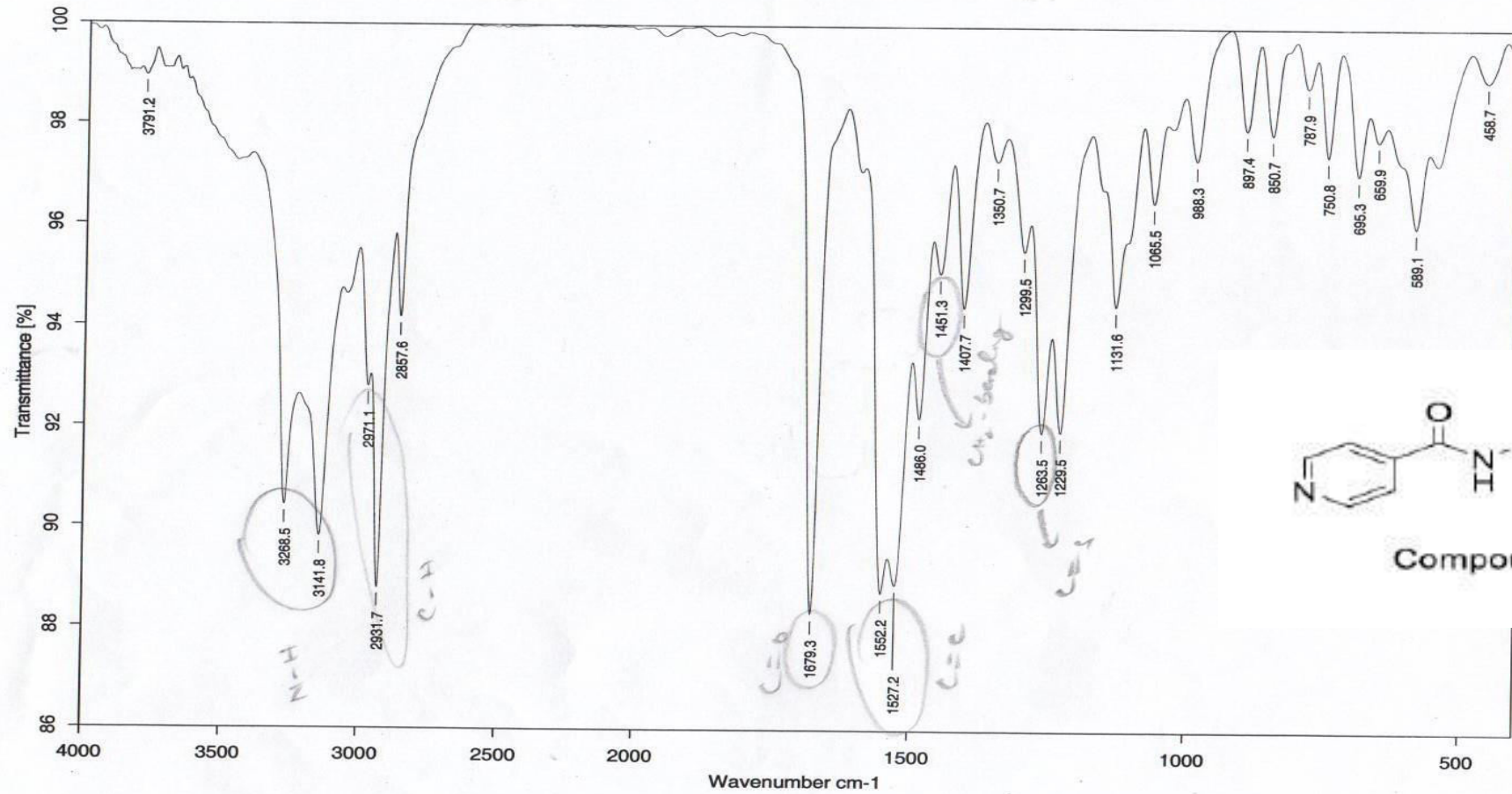
Scan: 2
Base: m/z 183; 100%FS TIC: 8366892

R.T.: .1

#Ions: 954



Compound 13



Compound 13

Sample : FZI-ISO18/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

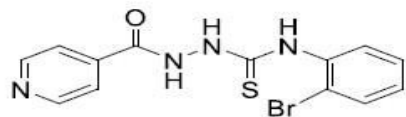
Resolution : 4 cm^{-1} (10 scans)

Spectrum : FZ-I-ISO18.0 (in D:\IRSTUDENT)

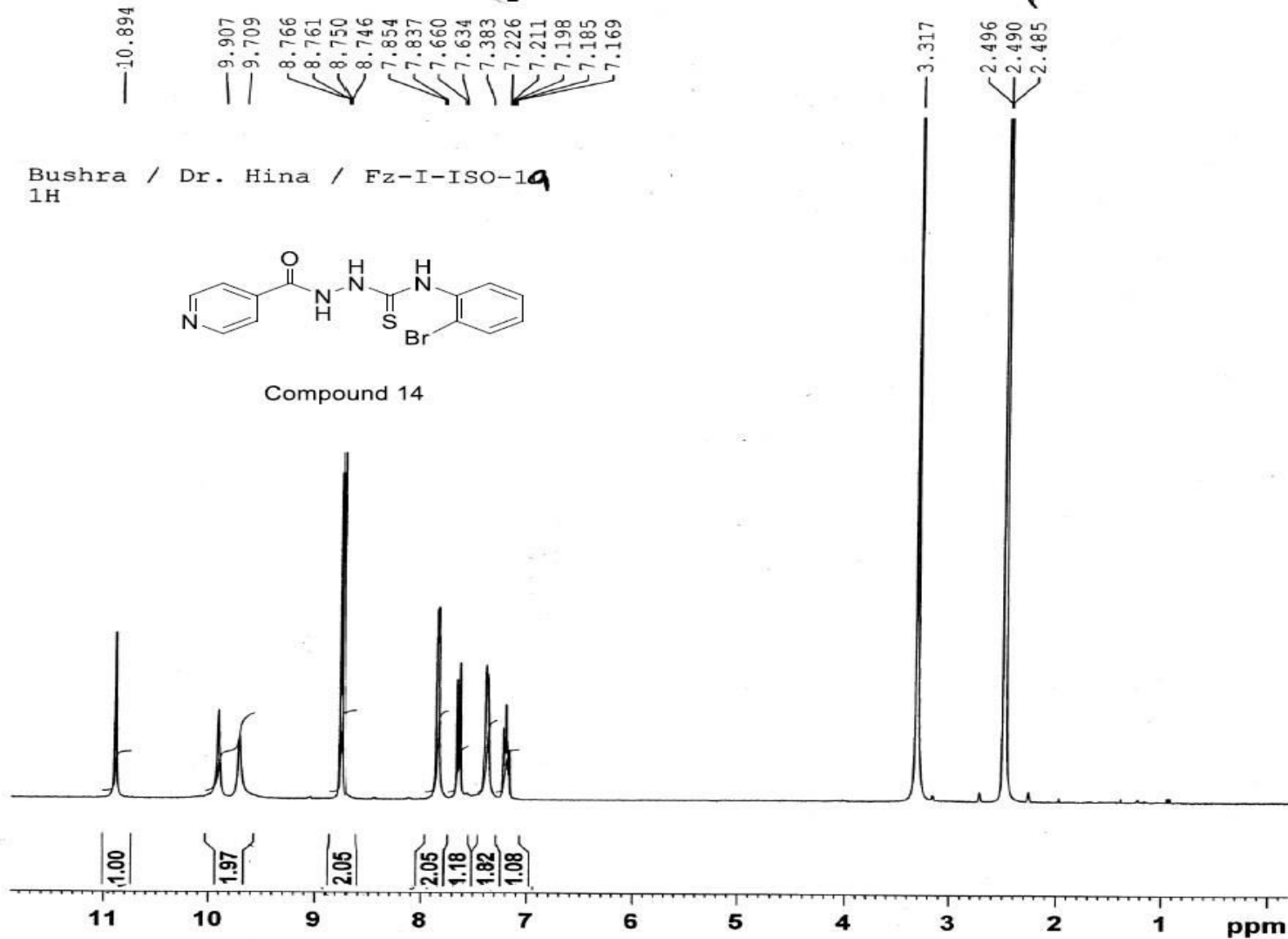
Technic : Solid

Analyst : MA/ZA/JS

Bushra / Dr. Hina / Fz-I-ISO-19
1H



Compound 14



AVANCE AV - III
300 MHz, LAB # 116

NAME	Oct04-16
EXPNO	4
PROCNO	1
Date_	20161004
Time	10.47
INSTRUM	Spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	6188.119 Hz
FIDRES	0.188846 Hz
AQ	2.6477044 sec
RG	203
DW	80.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1

===== CHANNEL f1 =====		
NUC1	1H	
P1	12.50 usec	
PL1	0.00 dB	
PL1W	13.16228485 W	
SFO1	300.1318534 MHz	
SI	32768	
SF	300.1300040 MHz	
WDW	EM	
SSB	0	
LB	0.30 Hz	
GB	0	
PC	1.00	

—10.894

—9.907 ²

—9.709

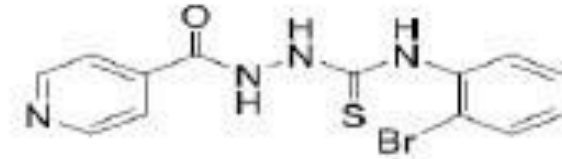
8.766
8.761
8.750
8.746

7.854
7.837

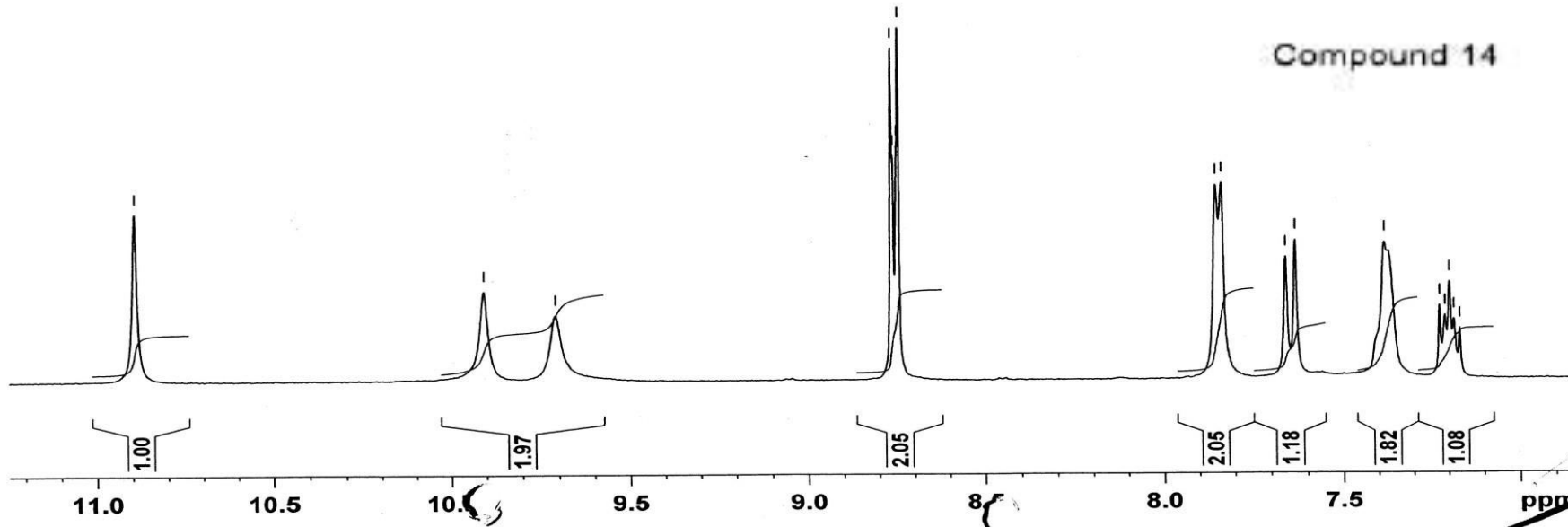
7.660
7.634

7.383
7.226
7.211
7.198
7.185
7.169

Bushra / Dr. Hina / Fz-I-ISO-10
1H



Compound 14



File: FZ-I-ISO19
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-05-2016 (Time Run: 10:05:14)

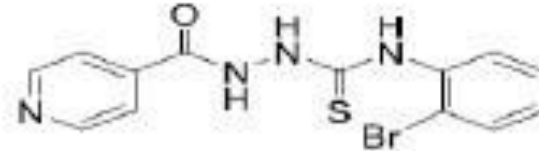
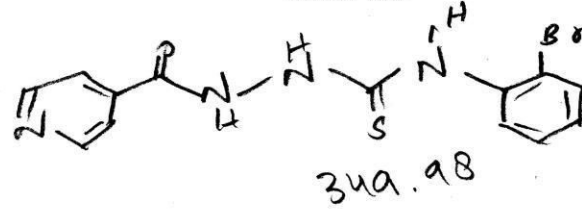
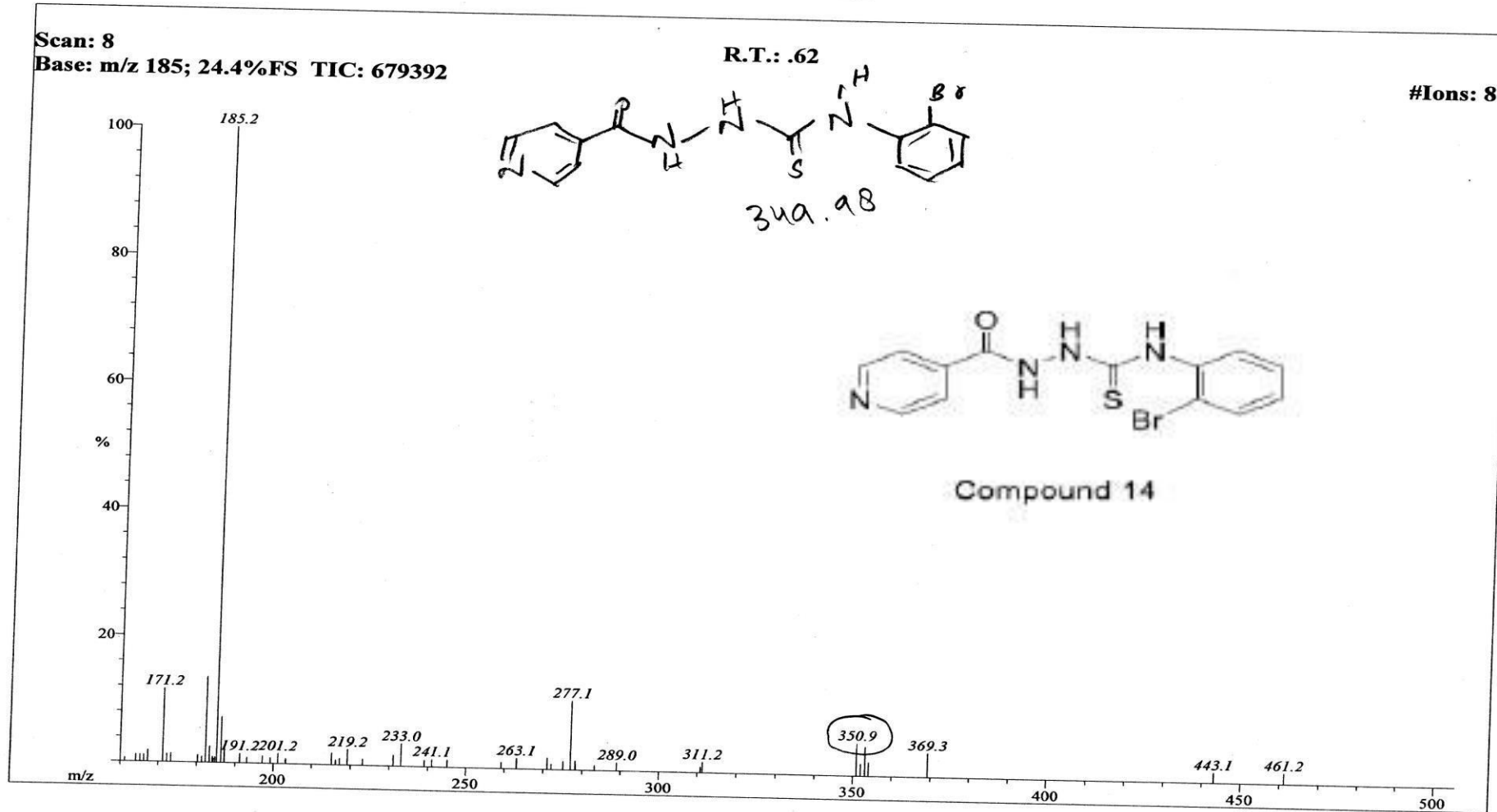
Ionization mode: FAB+

Scan: 8

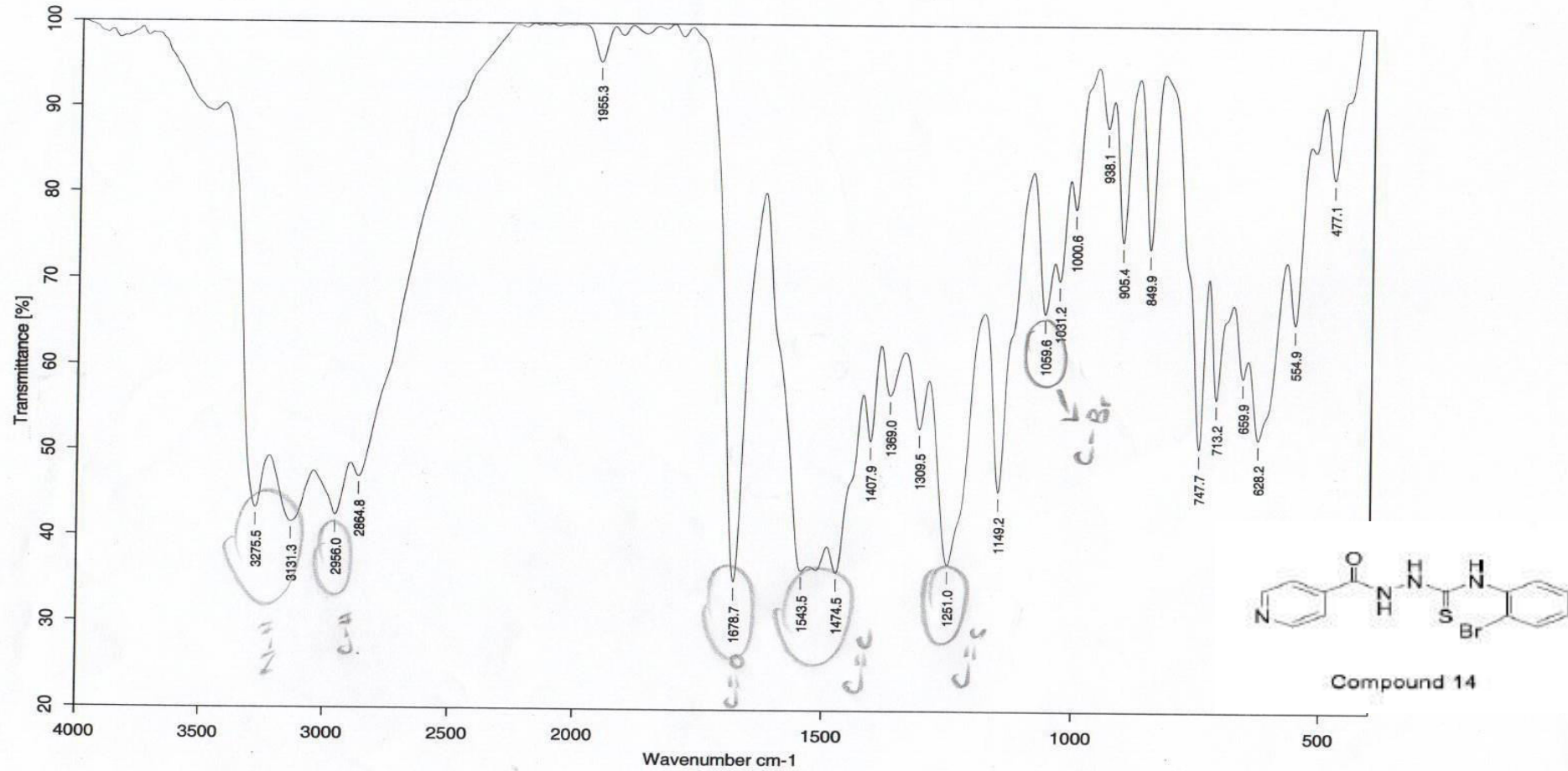
Base: m/z 185; 24.4%FS TIC: 679392

R.T.: .62

#Ions: 80



Compound 14

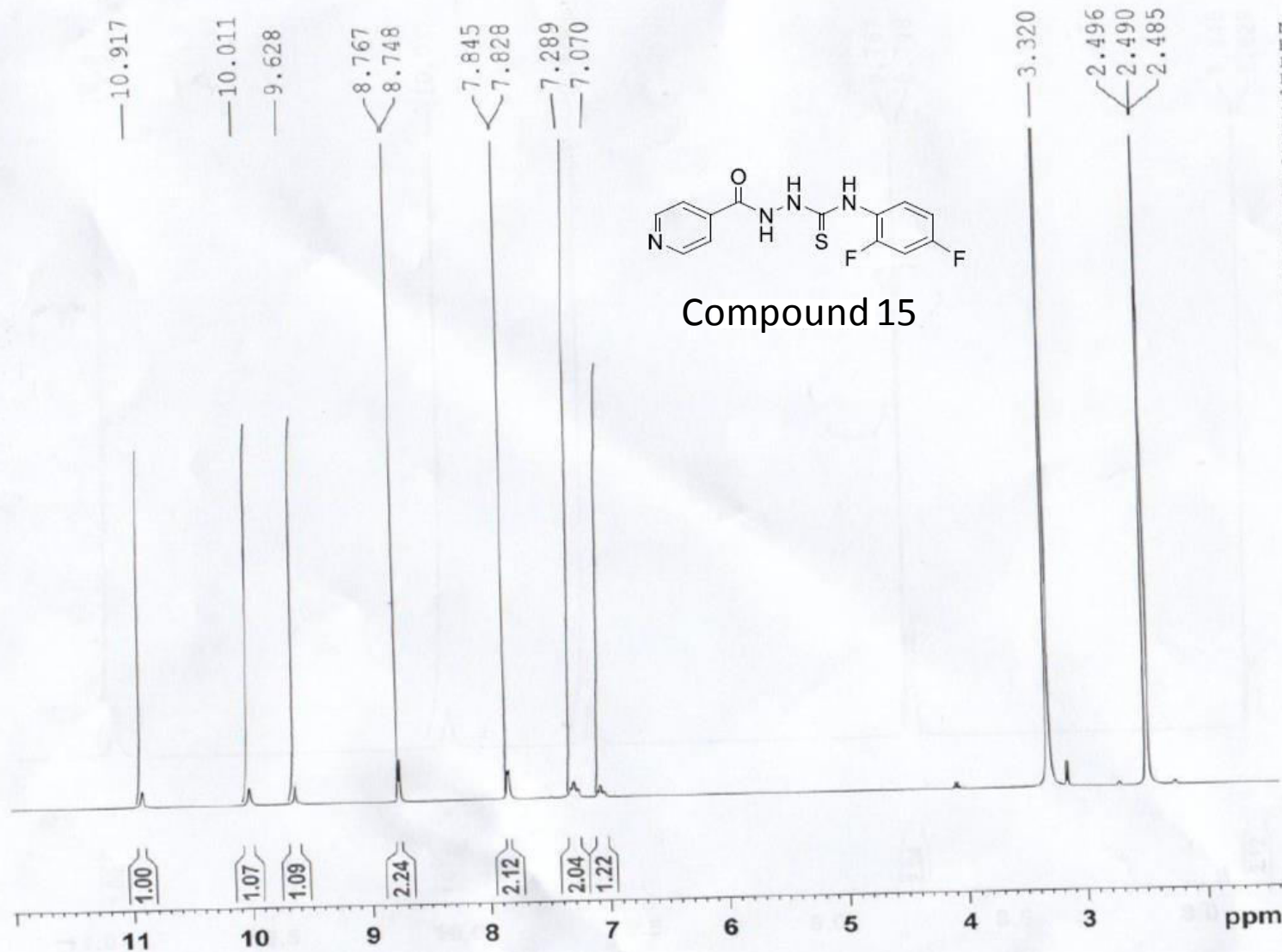


Sample : FZI-ISO19/Fazila Rizvi
 Measured : 19/04/2017 on VECTOR22
 Resolution : 4 cm-1 (10 scans)

Spectrum : FZ-I-ISO19.0 (in D:\IRSTUDENT)
 Technic : Solid
 Analyst : MA/ZA/JS

FAZILA/DR, HINA/FZ-I-IS01/
ICCBS.U.O.K/

AVANCE AV - III
300 MHz, LAB # 116

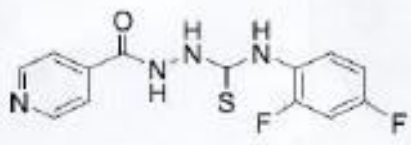


NAME jan03-19
EXPNO 8
PROCNO 1
Date_ 20190103
Time_ 11.59
INSTRUM Spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 128
DS 0
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 406
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1

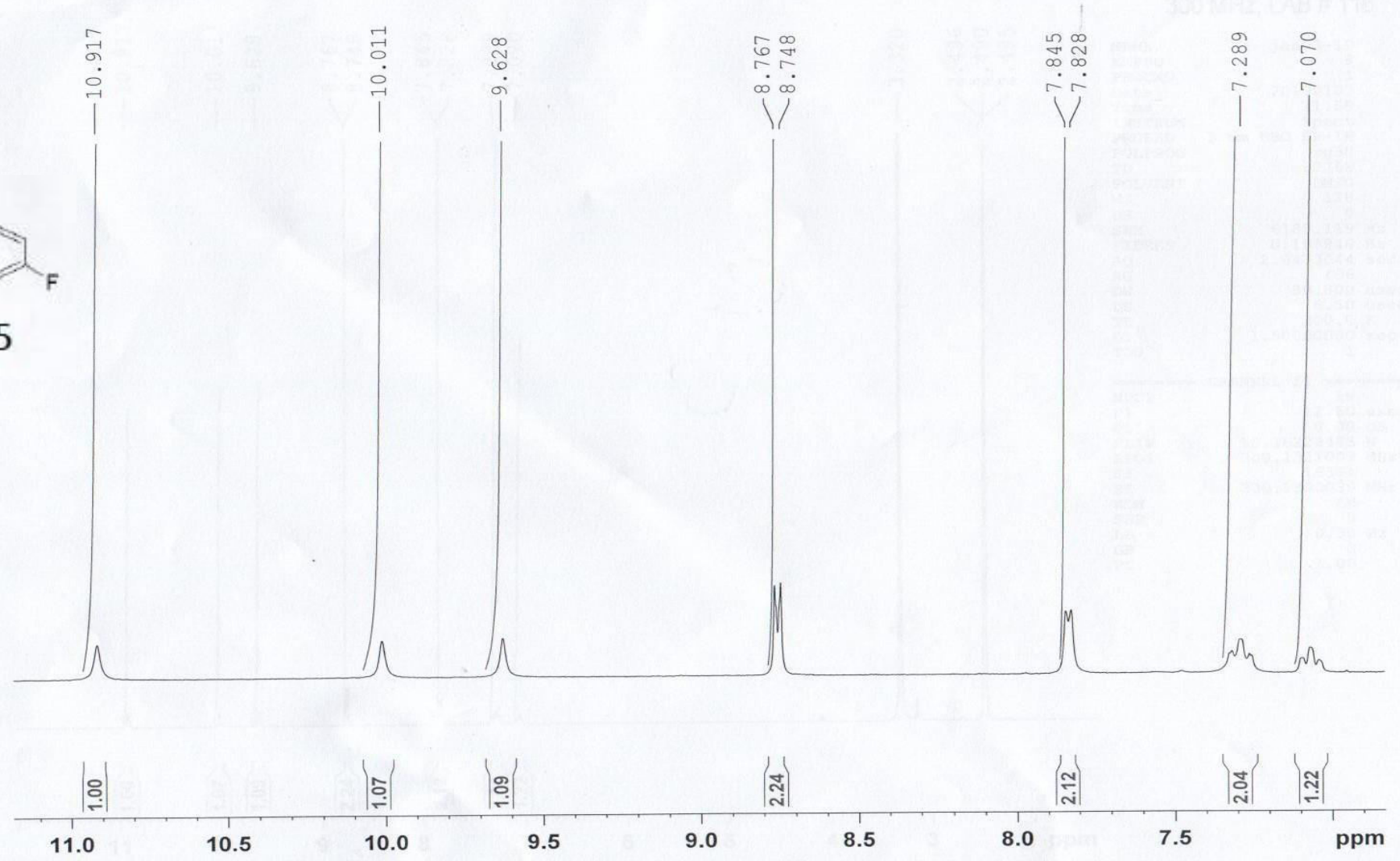
----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 0.00 dB
PL1W 13.16228485 W
SFO1 300.1321009 MHz
SI 16384
SF 300.1300039 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

FAZILA/DR, HINA/FZ-I-ISO1/
ICCBS.U.O.K/

AVANCE AV - III
300 MHz, LAB # 118



Compound 15



HEJ MASS SECTION
1/22/2016 11:23:32 AM

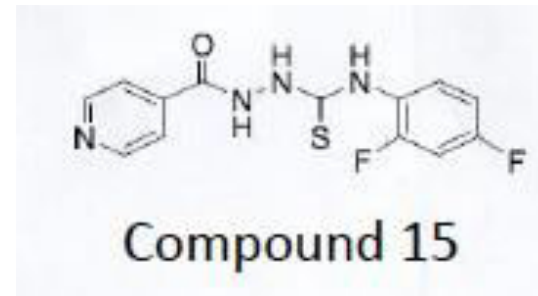
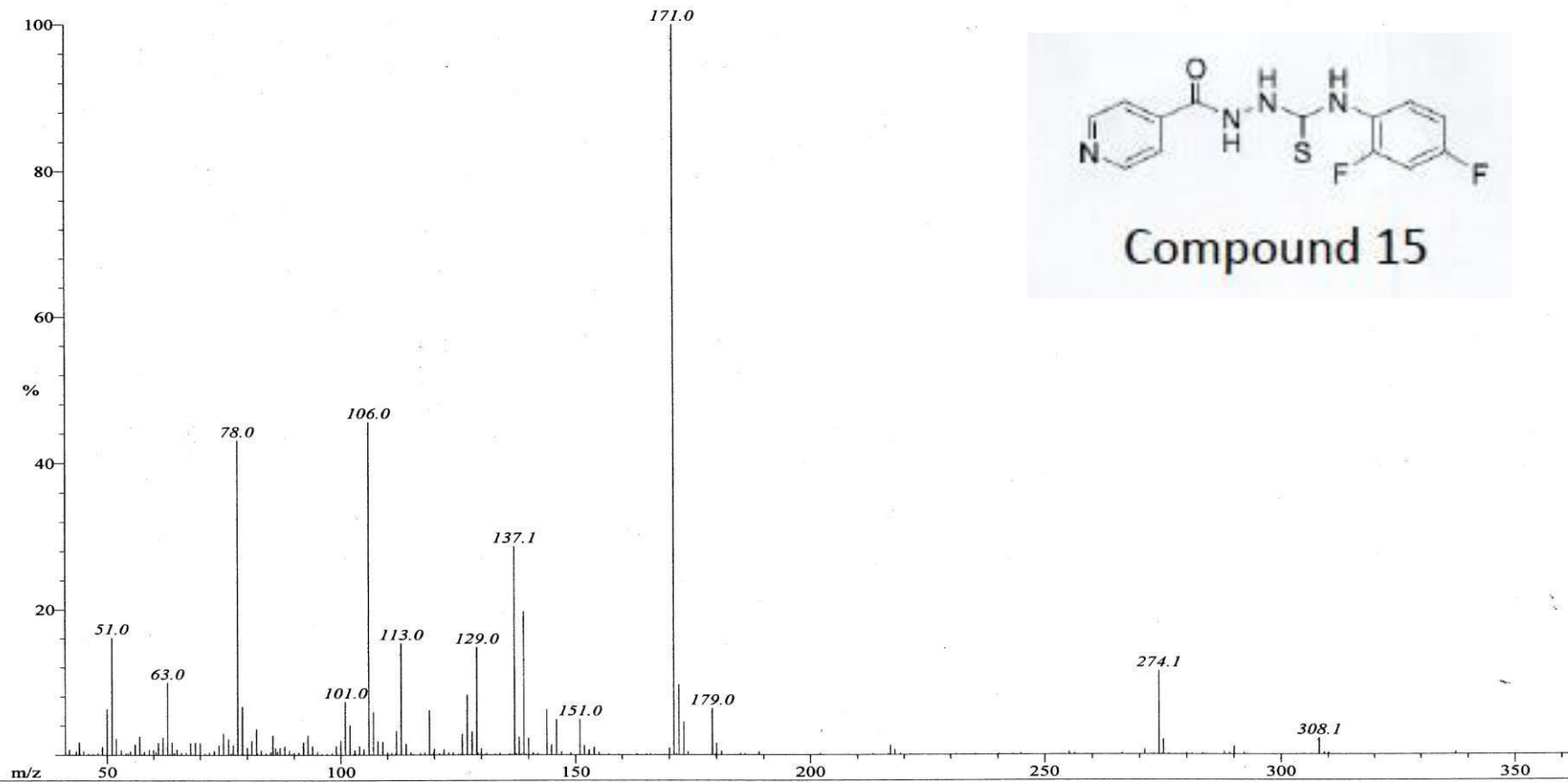
File: FZ-I-IS01
Sample: FAZILA RIZVI / DR. HINA
Instrument: JEOL MS 600H-1

Date Run: 01-22-2016 (Time Run: 11:17:36)

Ionization mode: EI+

Scan: 22
Base: m/z 171; 22.7%FS TIC: 1213396

R.T.: 1.87



HEJ MASS SECTION
1/22/2016 11:23:57 AM

File: FZ-I-IS01
Sample: FAZILA RIZVI / DR. HINA
Instrument: JEOL MS 600H-1

Date Run: 01-22-2016 (Time Run: 11:17:36)

Ionization mode: EI+

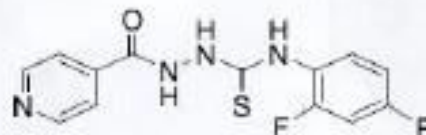
Scan: 22
Base: m/z 171; 22.7%FS TIC: 1213396

R.T.: 1.87

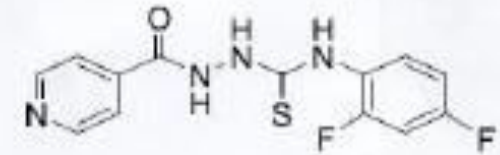
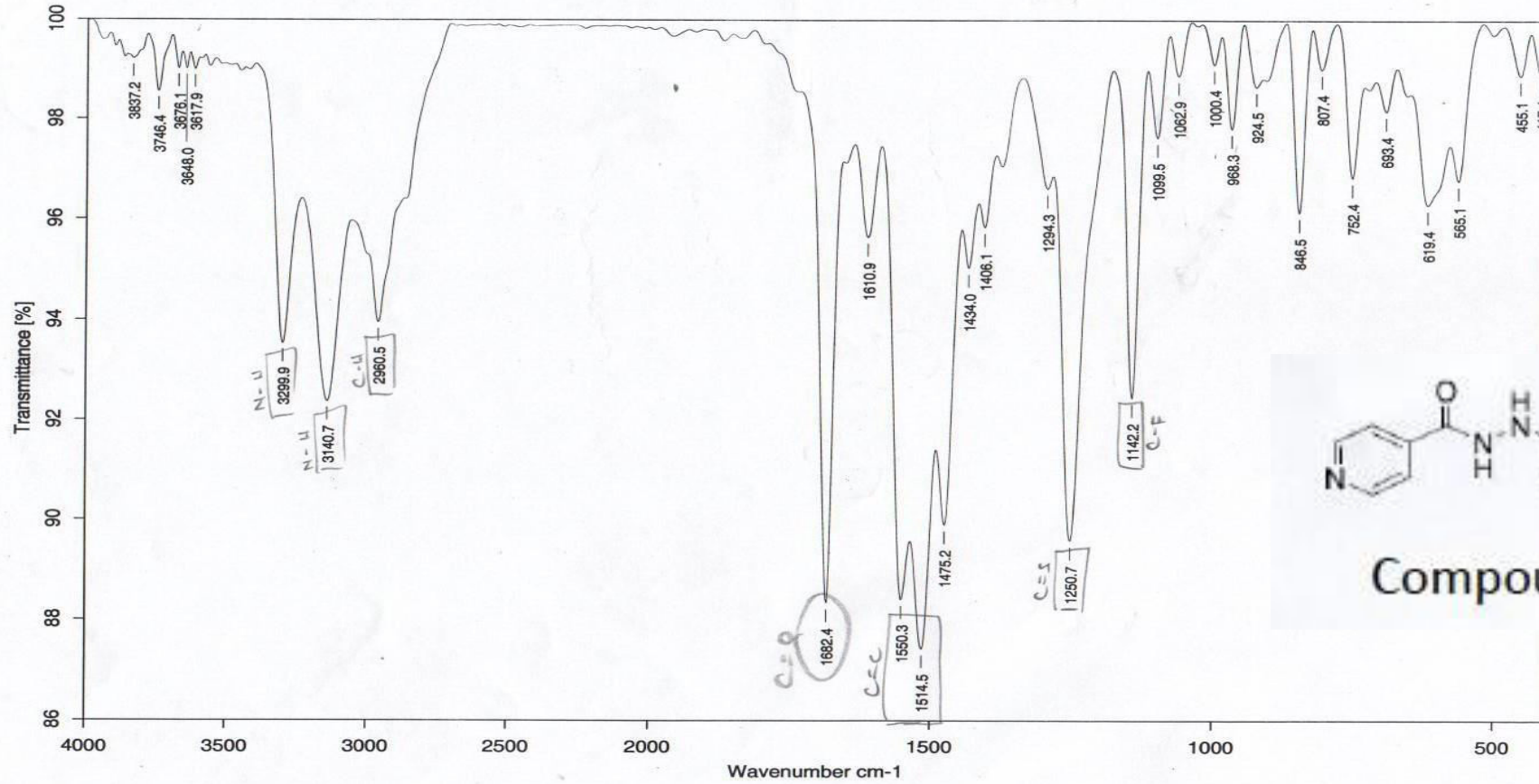
Threshold: .2% of Base

Displayed TIC: 1213396

Mass	%Base	Mass	%Base	Mass	%Base	Mass	%Base	Mass	%Base	Mass	%Base	Mass	%Base	Mass	%Base
41.9	.8	59.0	.8	76.5	.2	93.0	2.7	114.0	1.5	136.1	.2	170.0	1.0	271.1	.7
43.3	.5	60.0	.7	77.0	1.4	94.0	1.2	115.1	.4	137.1	28.7	171.0	100.0	273.0	.2
44.0	1.8	60.5	.5	78.0	43.1	95.0	.5	117.0	.3	137.4	.2	171.5	.2	274.1	11.5
44.1	.3	61.0	1.7	79.0	6.7	97.1	.2	118.0	.3	138.1	2.5	172.0	9.6	275.1	2.1
44.9	.6	62.0	2.4	80.0	1.0	98.1	.3	119.0	6.1	139.0	19.8	173.0	4.5	279.9	.2
45.9	.2	63.0	9.9	81.0	2.0	99.0	1.2	119.9	.4	140.0	2.3	174.0	.5	288.0	.4
46.9	.2	64.0	1.8	82.0	3.6	100.0	2.0	120.0	.9	141.0	.3	179.0	6.4	289.1	.2
48.0	.3	64.5	.3	82.2	.2	101.0	7.3	121.0	.2	142.0	.3	180.0	1.6	290.1	1.1
49.0	1.1	65.0	.8	83.0	.7	102.0	4.1	121.1	.2	144.0	6.3	181.1	.6	292.1	.3
50.0	6.3	66.0	.3	83.9	.2	103.0	.7	122.0	.8	144.9	1.4	185.1	.3	308.1	2.2
51.0	16.2	67.0	.4	84.9	.4	104.0	1.2	123.1	.3	146.0	4.8	186.0	.2	309.1	.3
52.0	2.2	68.0	1.7	85.5	2.7	105.0	.8	124.0	.4	147.0	.5	189.0	.5	310.0	.2
53.0	.7	69.0	1.7	86.0	.9	106.0	45.6	126.0	2.9	149.0	.3	202.1	.2	310.2	.2
54.0	.2	70.0	1.7	86.5	.5	107.0	5.9	127.0	8.2	151.0	4.9	217.0	1.3	337.4	.4
54.5	.3	71.0	.2	87.0	1.0	108.0	1.9	128.0	3.2	152.0	1.3	218.0	.8		
55.0	.5	72.0	.4	88.0	1.2	109.0	1.8	129.0	14.8	153.0	.7	219.2	.2		
56.0	1.5	73.0	.6	89.0	.7	110.0	.4	129.3	.3	154.0	1.1	245.0	.2		
57.0	2.6	74.0	1.3	90.0	.3	111.0	.3	130.0	.9	155.0	.4	255.2	.4		
57.9	.2	75.0	2.9	91.0	.4	112.0	3.3	131.0	.3	163.1	.2	256.3	.2		
58.0	.5	76.0	2.2	92.0	1.8	113.0	15.4	134.0	.3	166.0	.2	266.3	.2		



Compound 15



Compound 15

Sample : FZI-ISO1/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

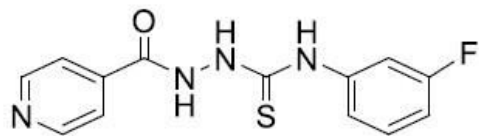
Resolution : 4 cm⁻¹ (10 scans)

Spectrum : FZ-I-ISO1.0 (in D:\IRSTUDENT)

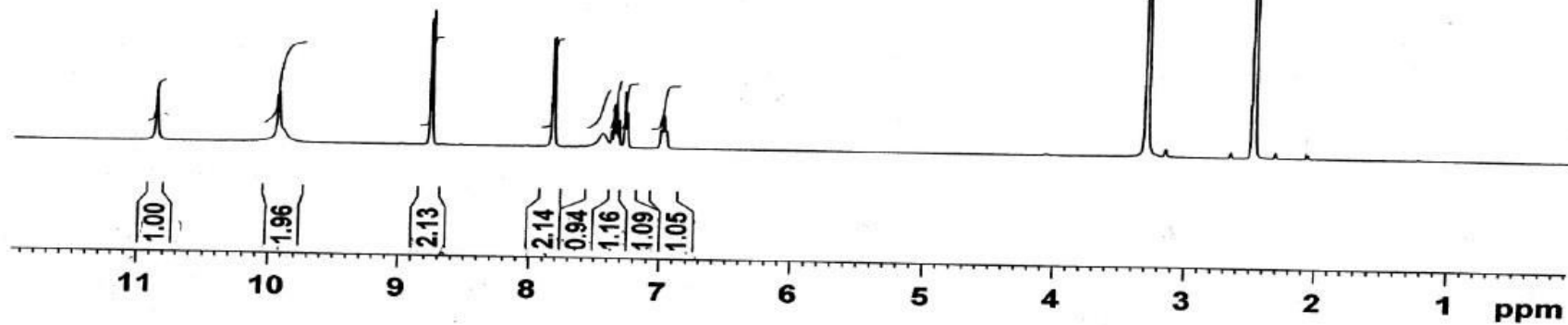
Technic : Solid

Analyst : MA/ZA/JS

BUSHRA/DR.HINA/FZ.I.ISO.21
1H



Compound 16



AVANCE AV-400 MHz
Lab # 115

```
NAME      oct06-16
EXPNO     7
PROCNO    1
Date_     20161006
Time      15.32
INSTRUM   spect
PROBHD    5 mm SEI 1H-13
PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS        128
DS        0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        362
DW        62.400 usec
DE        6.50 usec
TE        300.0 K
D1        1.50000000 sec
TDO       1
```

```
----- CHANNEL f1 -----
NUC1      1H
P1        10.80 usec
PL1       3.00 dB
SFO1     400.0332002 MHz
SI        32768
SF        400.0300041 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        0.20
```

File: FZ-I-ISO21-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-19-2016 (Time Run: 15:44:52)

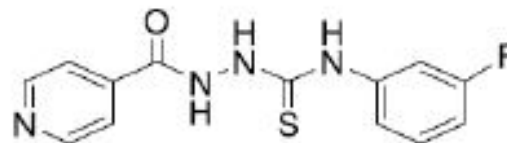
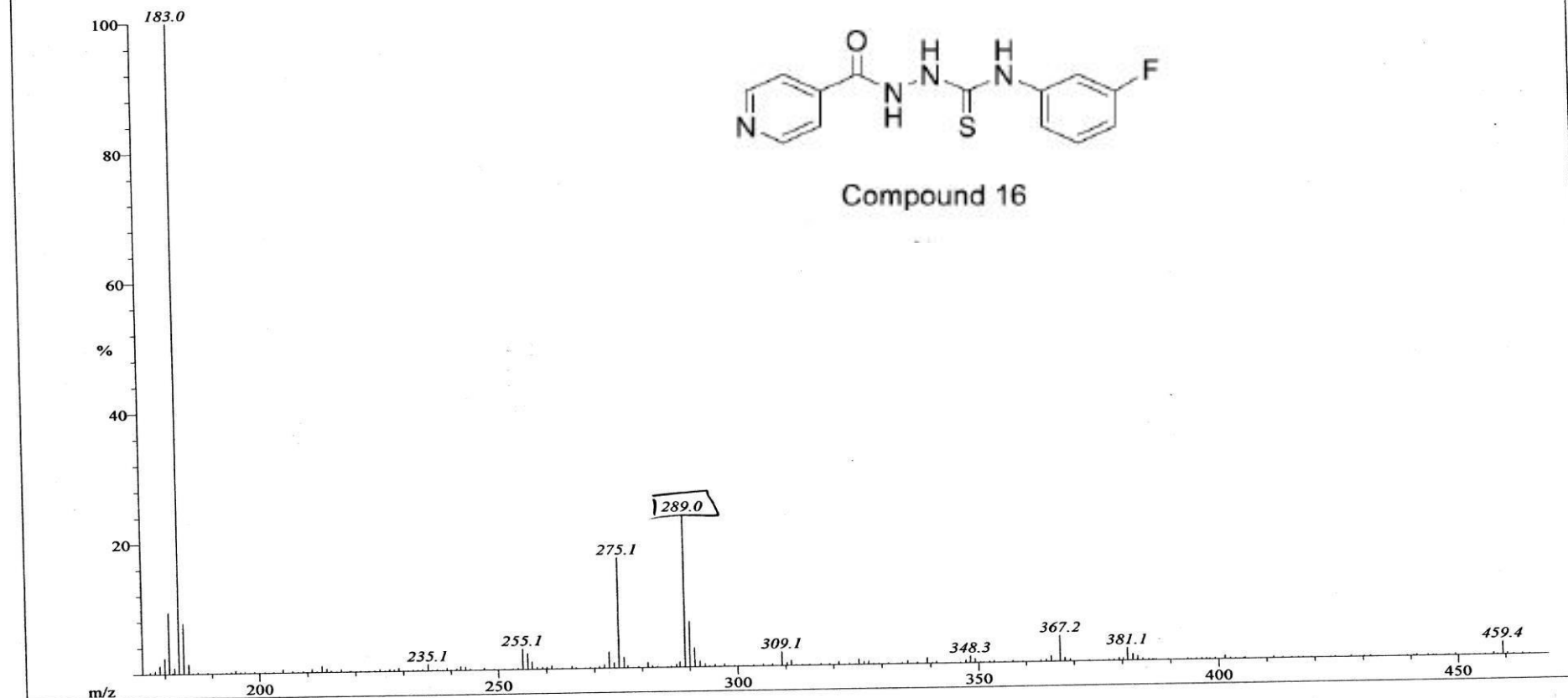
Ionization mode: FAB-

Scan: 10

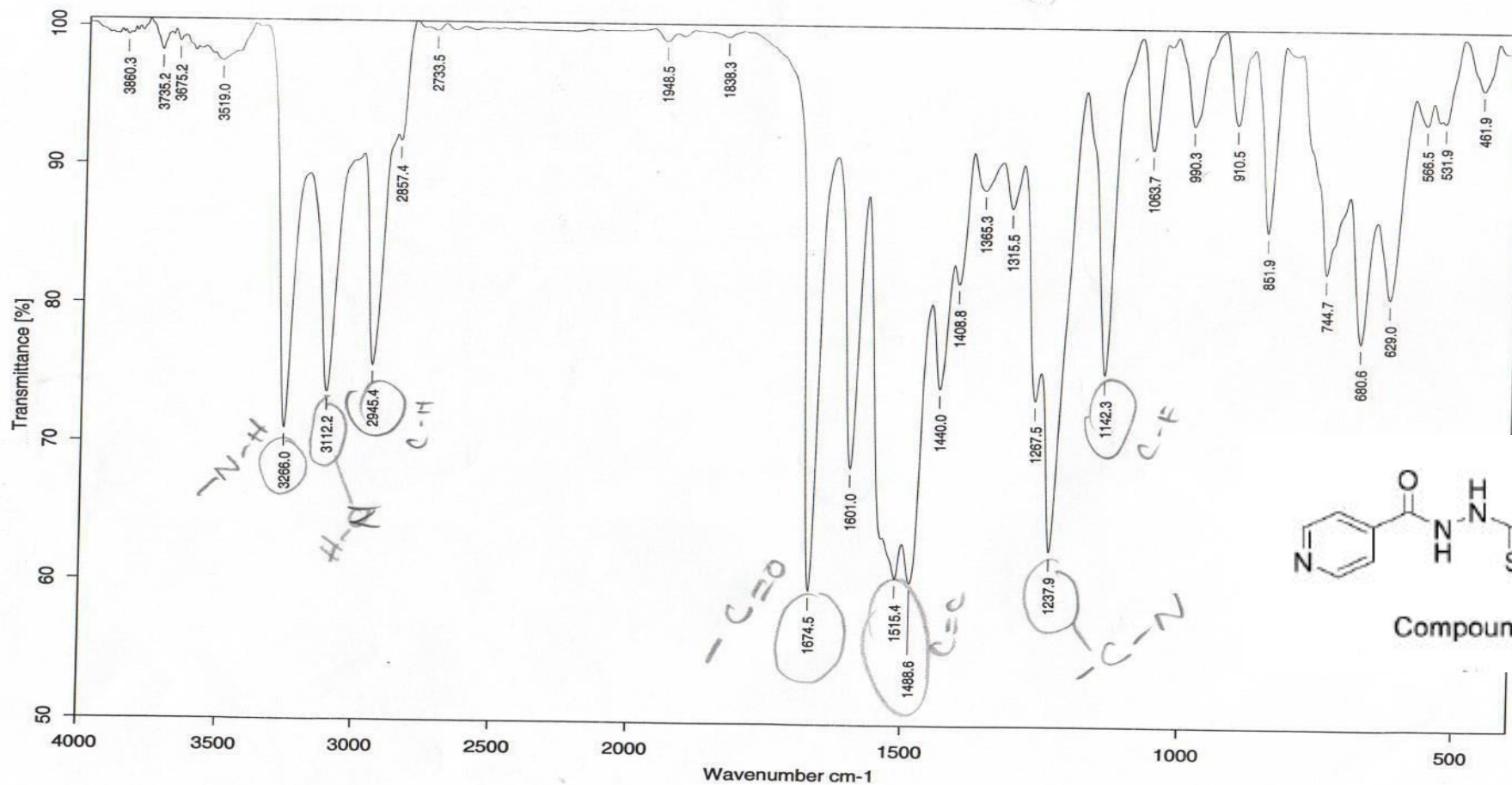
R.T.: .8

#Ions: 427

Base: m/z 183; 59.2%FS TIC: 2167114



Compound 16



Sample : Fz-I-Iso21/Fazila Rizvi/Dr. Hina

Measured : 29/12/2016 on VECTOR22

Resolution : 4 cm^{-1} (10 scans)

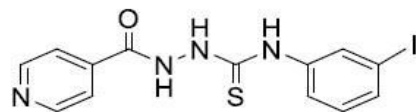
Spectrum : Fz-I-Iso21.0 (in D:\IRSTUDENT)

Technic : Solid

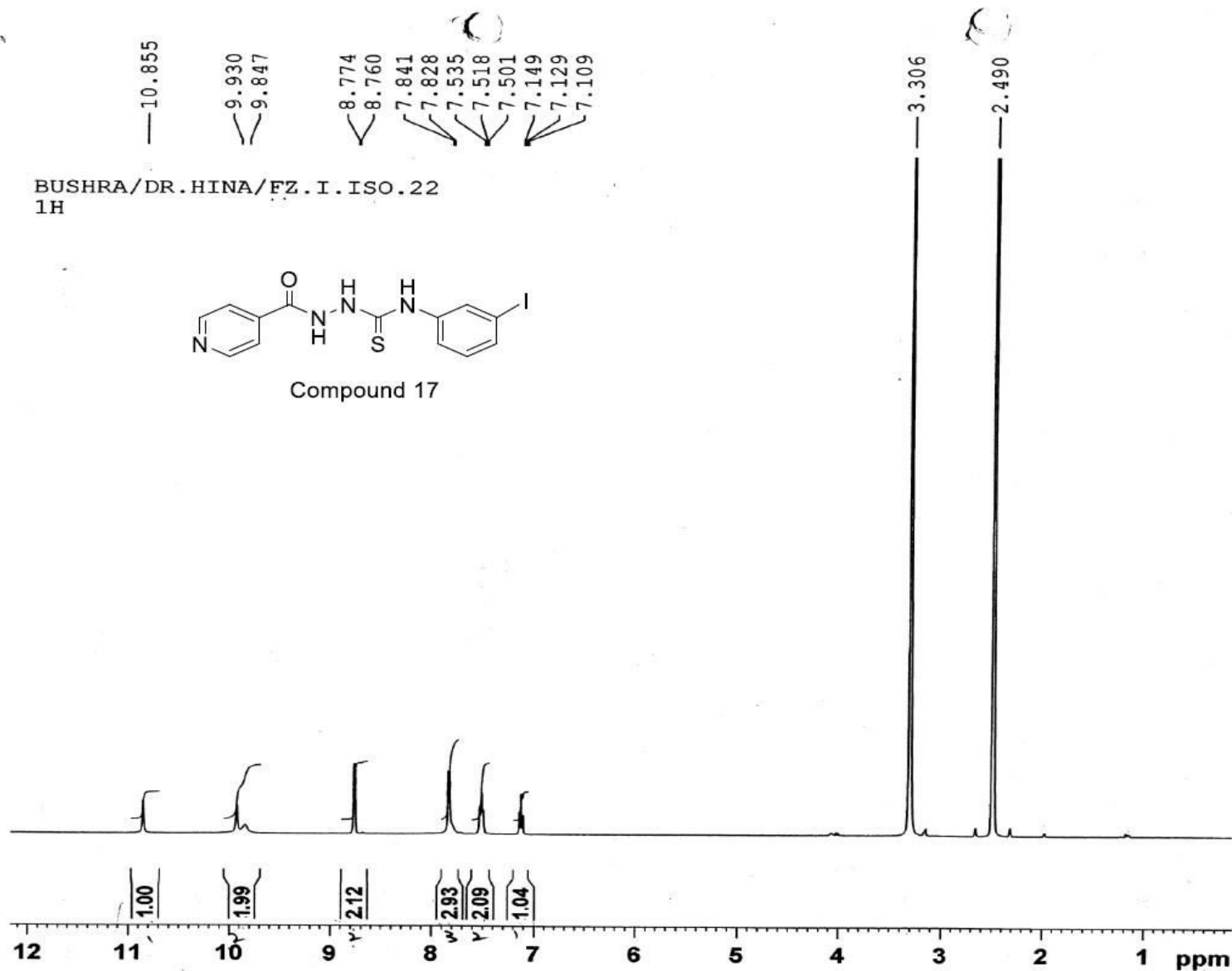
Analyst : M. Asif

AVANCE AV-400 MHz
Lab # 115

BUSHRA/DR.HINA/FZ.I.ISO.22
1H



Compound 17



```

NAME          oct06-16
EXPNO         6
PROCNO        1
Date_         20161006
Time_         15.15
INSTRUM       spect
PROBHD        5 mm SEI 1H-13
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            128
DS            0
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894966 sec
RG            574.7
DW            62.400 usec
DE            6.50 usec
TE            300.0 K
D1            1.5000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            10.80 usec
PL1           3.00 dB
SF01          400.0332002 MHz
SI            32768
SF            400.0300041 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            0.20
  
```


File: FZ-I-ISO22-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-19-2016 (Time Run: 15:28:48)

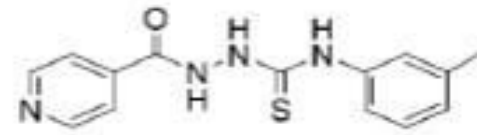
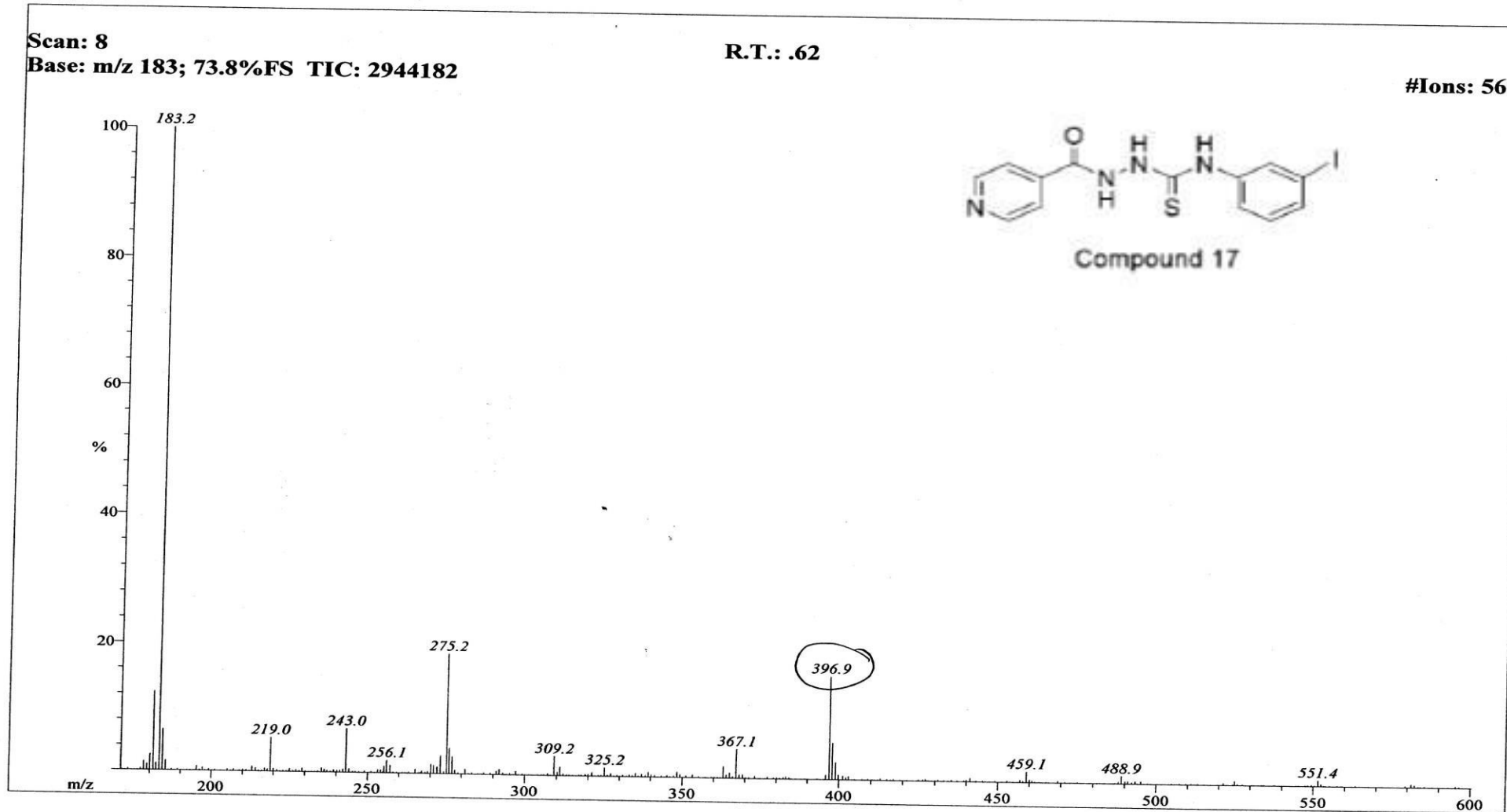
Ionization mode: FAB-

Scan: 8

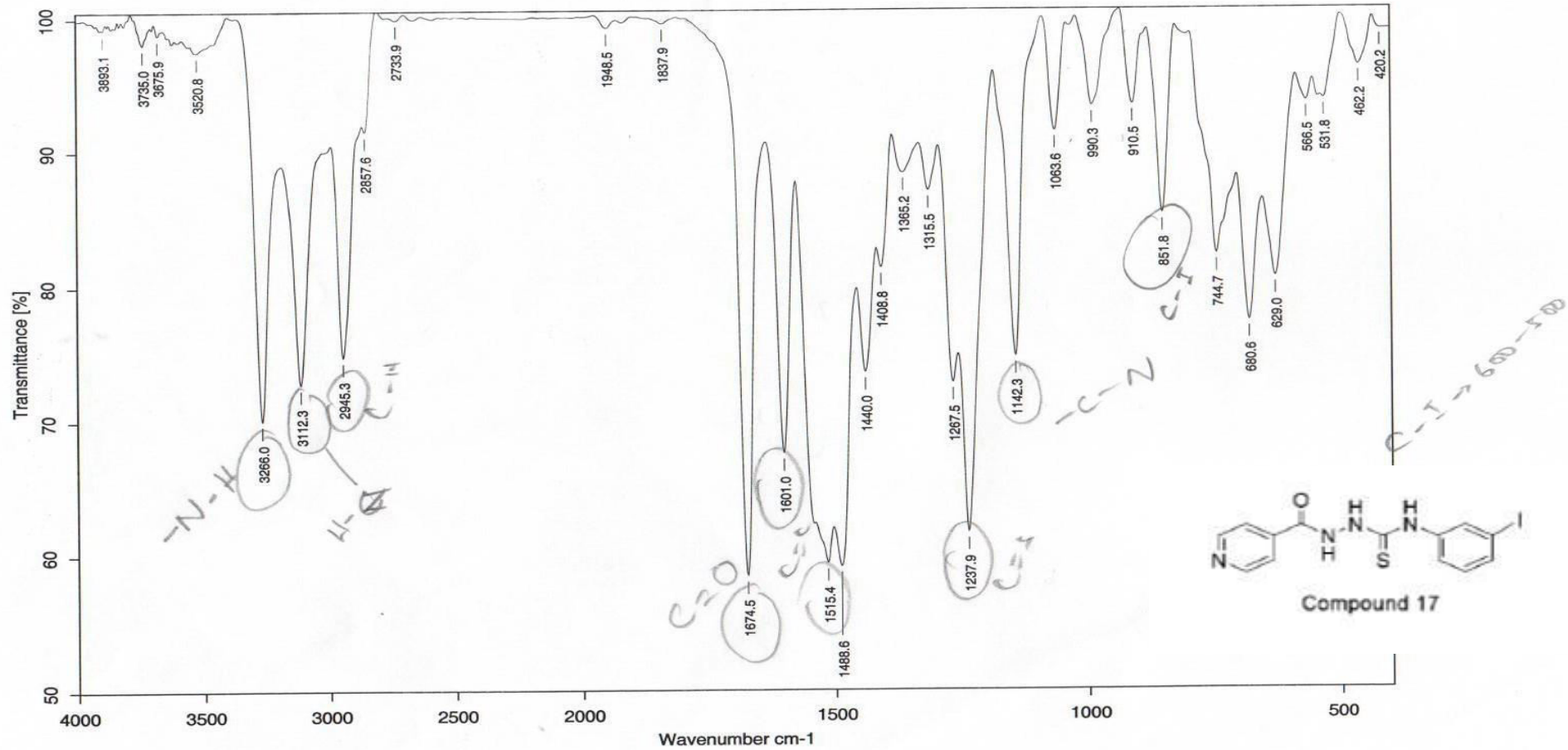
Base: m/z 183; 73.8%FS TIC: 2944182

R.T.: .62

#Ions: 565



Compound 17



Sample : Fz-I-Iso22/Fazila Rizvi/Dr. Hina

Measured : 29/12/2016 on VECTOR22

Resolution : 4 cm⁻¹ (10 scans)

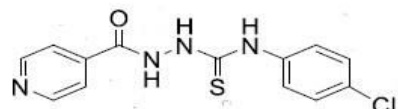
Spectrum : Fz-I-Iso22.0 (in D:\IRSTUDENT)

Technic : Solid

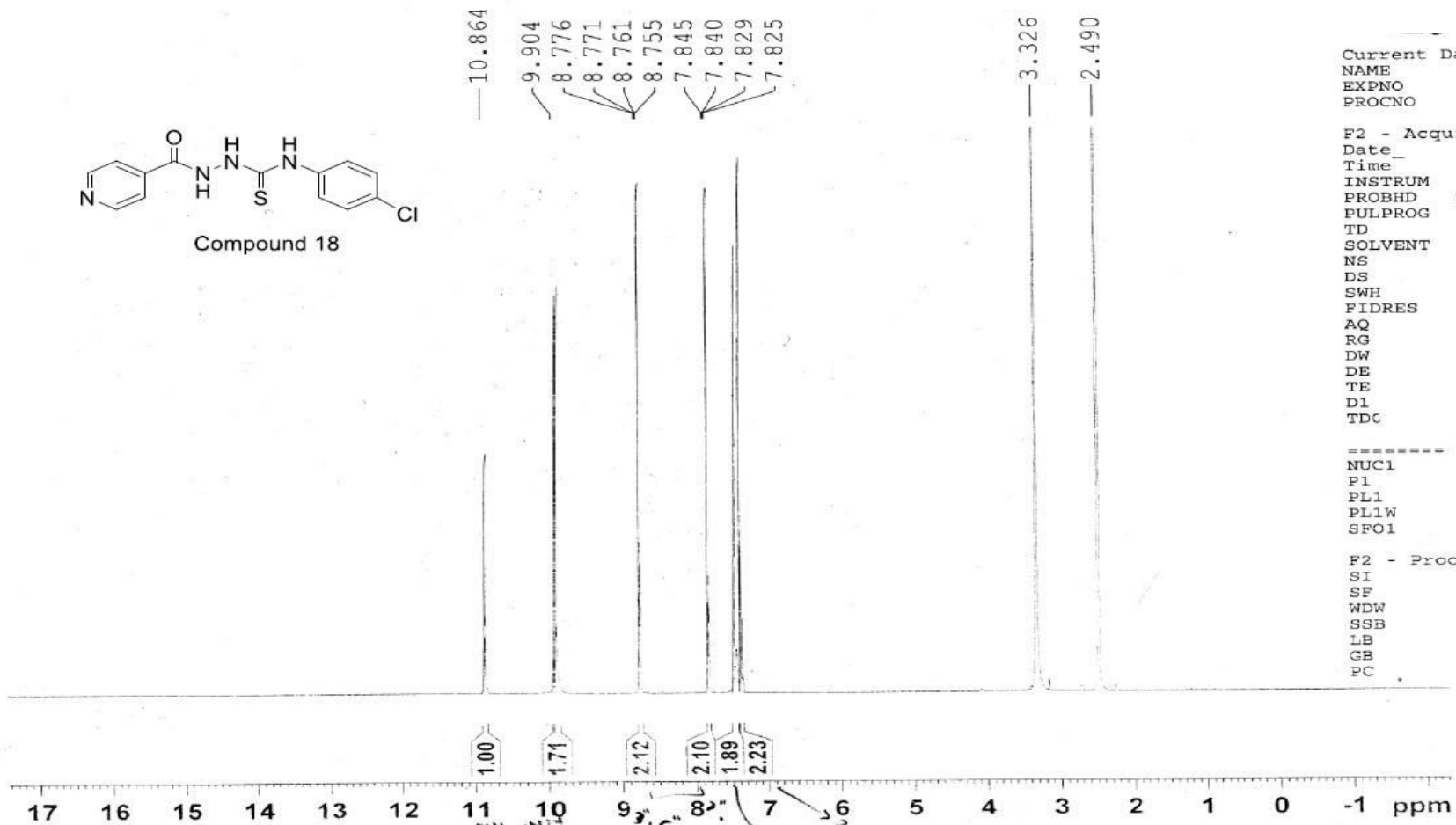
Analyst : M. Asif

fazila rizvi/Dr.Hina/Fz-I-iso23

¹H



Compound 18



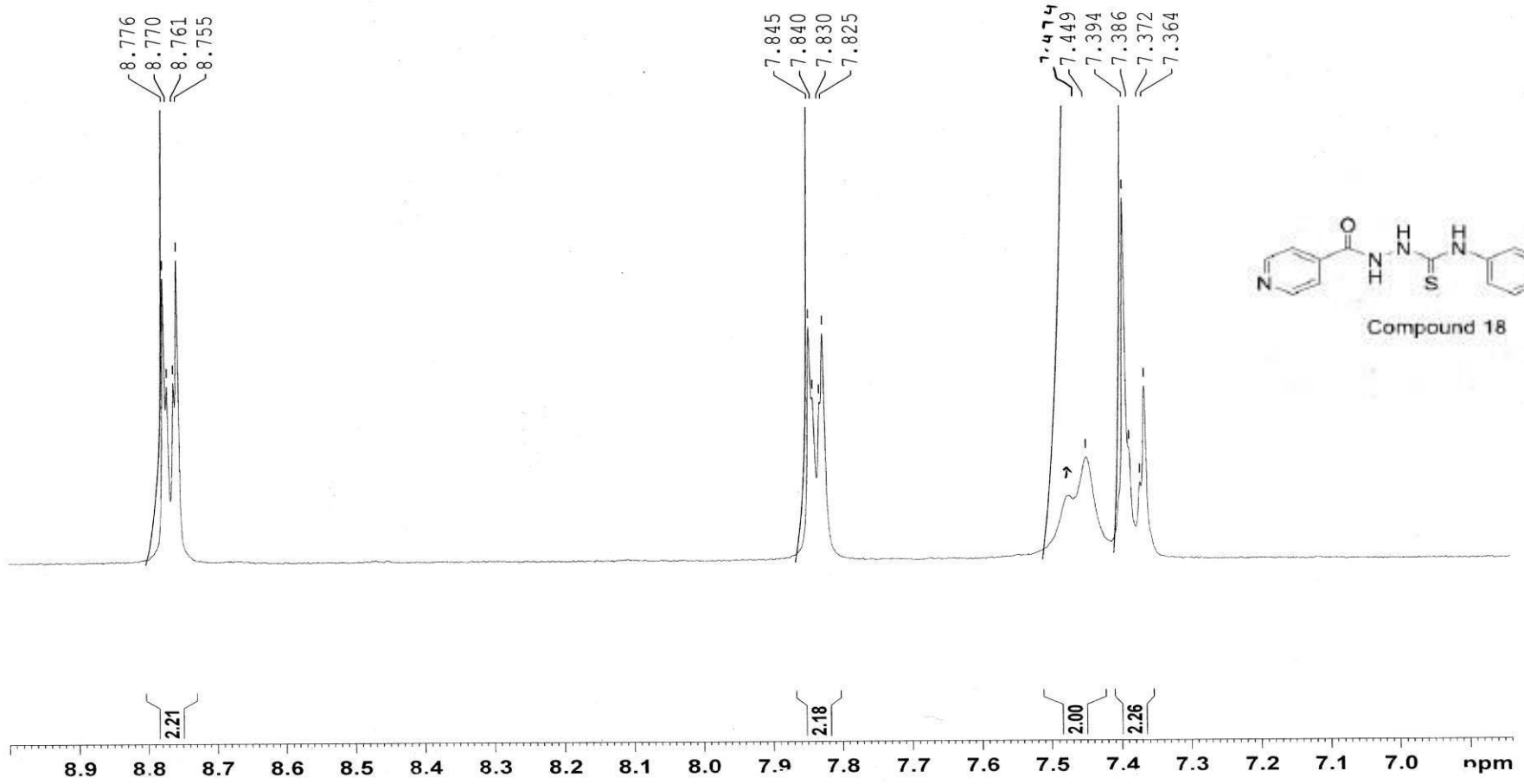
Current Data Parameters
NAME iso23
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date 20161117
Time 11.36
INSTRUM Spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TDC 1

===== CHANNEL f1 =====
NUC1 ¹H
P1 12.50 usec
PL1 0 dB
PL1W 13.16228485 W
SFO1 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300040 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

fazila rizvi/Dr.Hina/Fz-I-iso23
'¹H



File: FZ-I-SO23-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

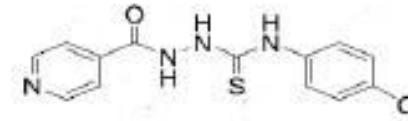
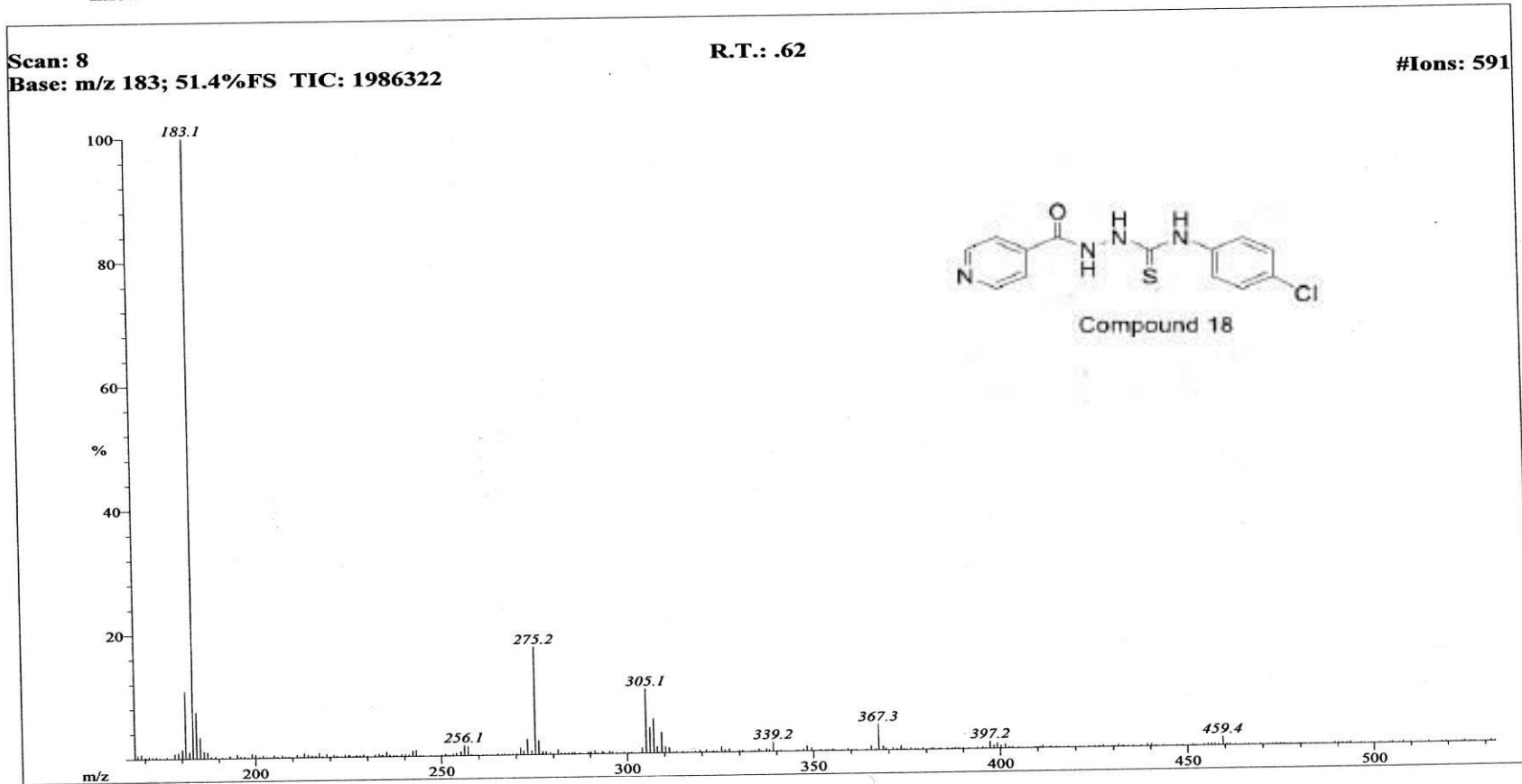
Date Run: 10-19-2016 (Time Run: 15:52:27)

Ionization mode: FAB-

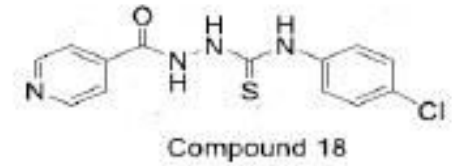
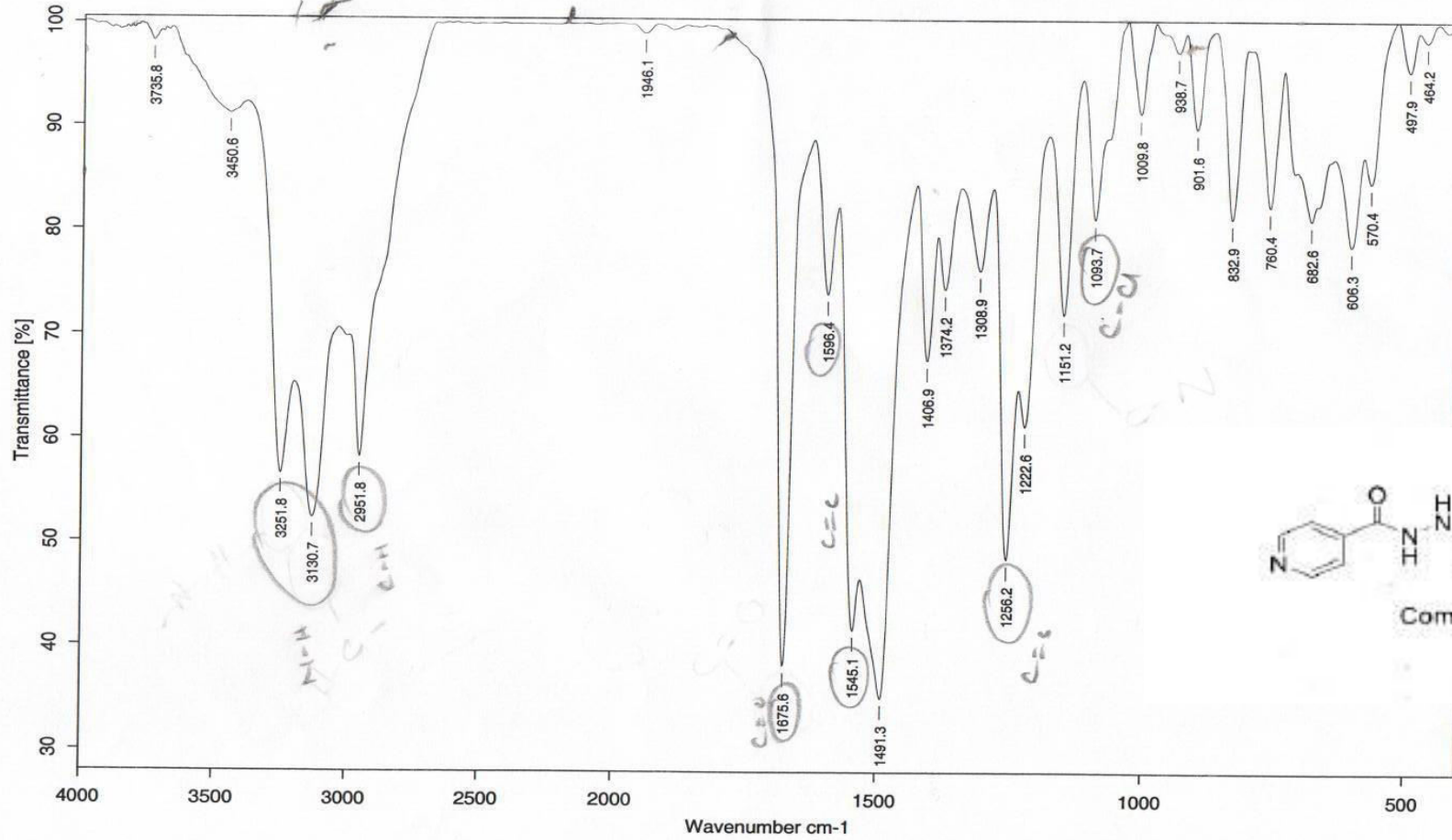
Scan: 8
Base: m/z 183; 51.4%FS TIC: 1986322

R.T.: .62

#Ions: 591



Compound 18

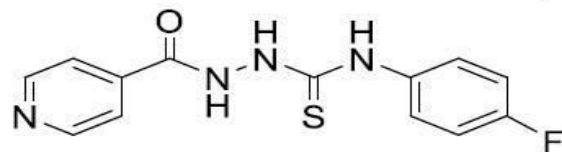


Sample : Fz-I-Iso23/Fazila Rizvi/Dr. Hina
 Measured : 29/12/2016 on VECTOR22
 Resolution : 4 cm⁻¹ (10 scans)
 Spectrum : Fz-I-Iso23.0 (in D:\IRSTUDENT)
 Technic : Solid
 Analyst : M. Asif

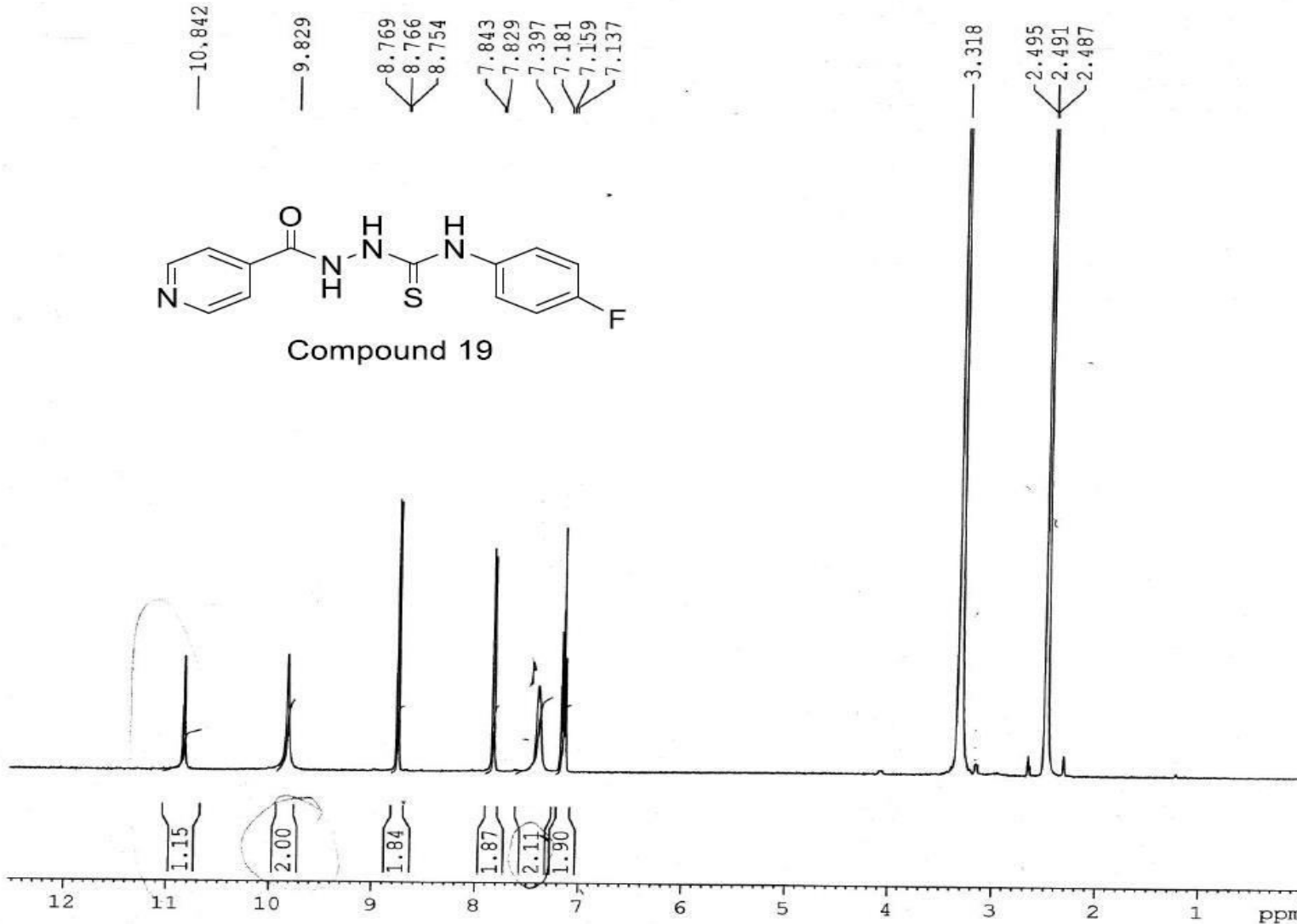
BUSHRA/DR, HINA/FZ-I-ISO-24
 ICCBS, U.O.K/

AVANCE 400
 LAB NO 117

—10.842
 —9.829
 {8.769
 {8.766
 {8.754
 {7.843
 {7.829
 {7.397
 {7.181
 {7.159
 {7.137



Compound 19



NAME Oct10-16
 EXPNO 4
 PROCNO 1
 Date 20161010
 Time 11.03
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 512
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.40 usec
 PL1 0.00 dB
 SFO1 400.1332010 MHz
 SI 16384
 SF 400.1300064 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

File: FZ-I-ISO24-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-19-2016 (Time Run: 15:36:52)

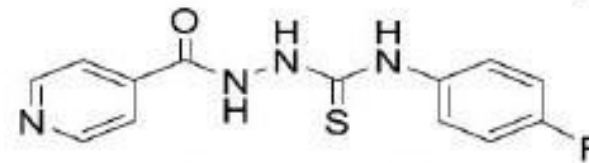
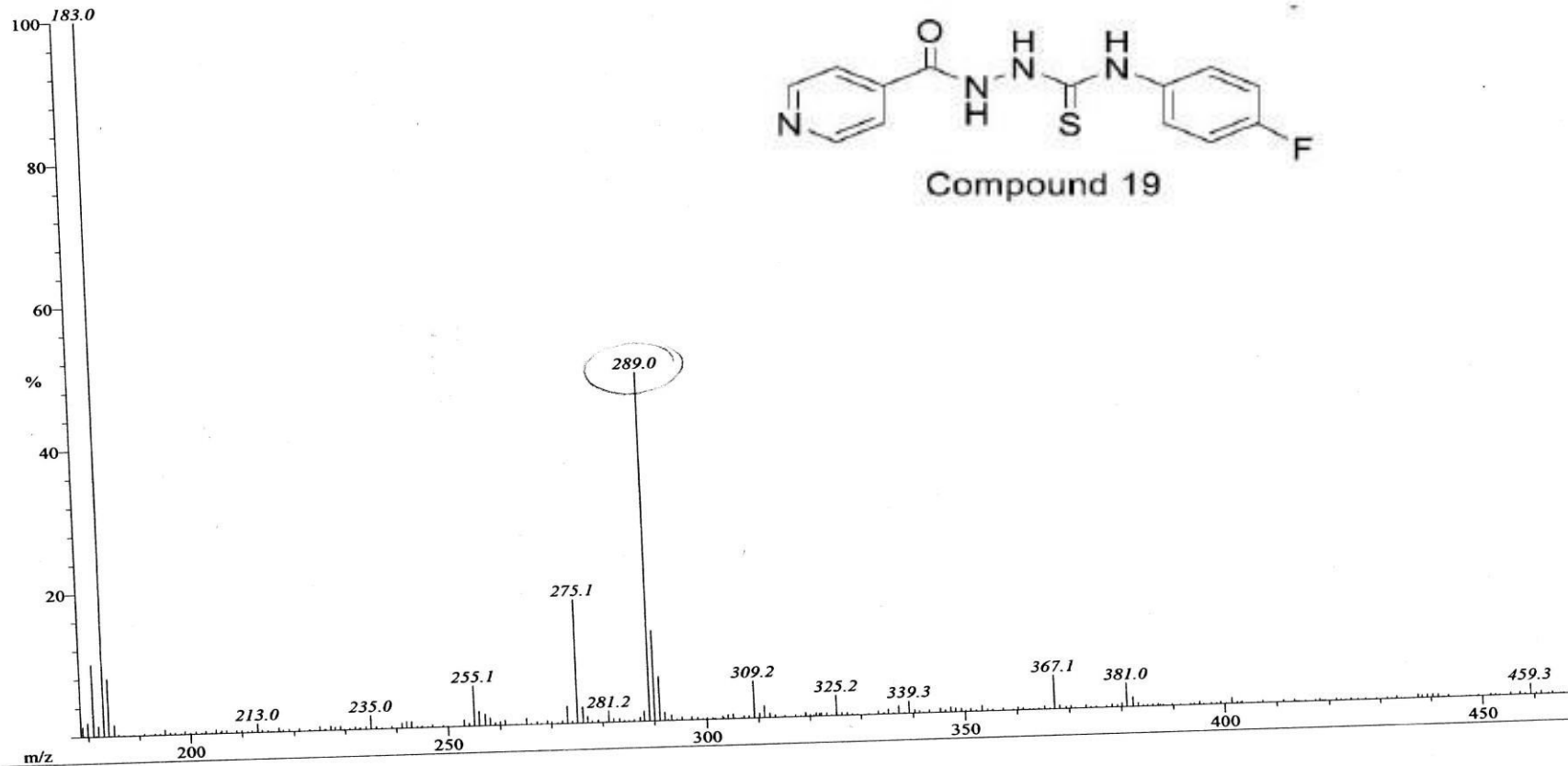
Ionization mode: FAB-

Scan: 7

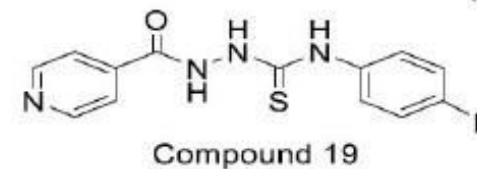
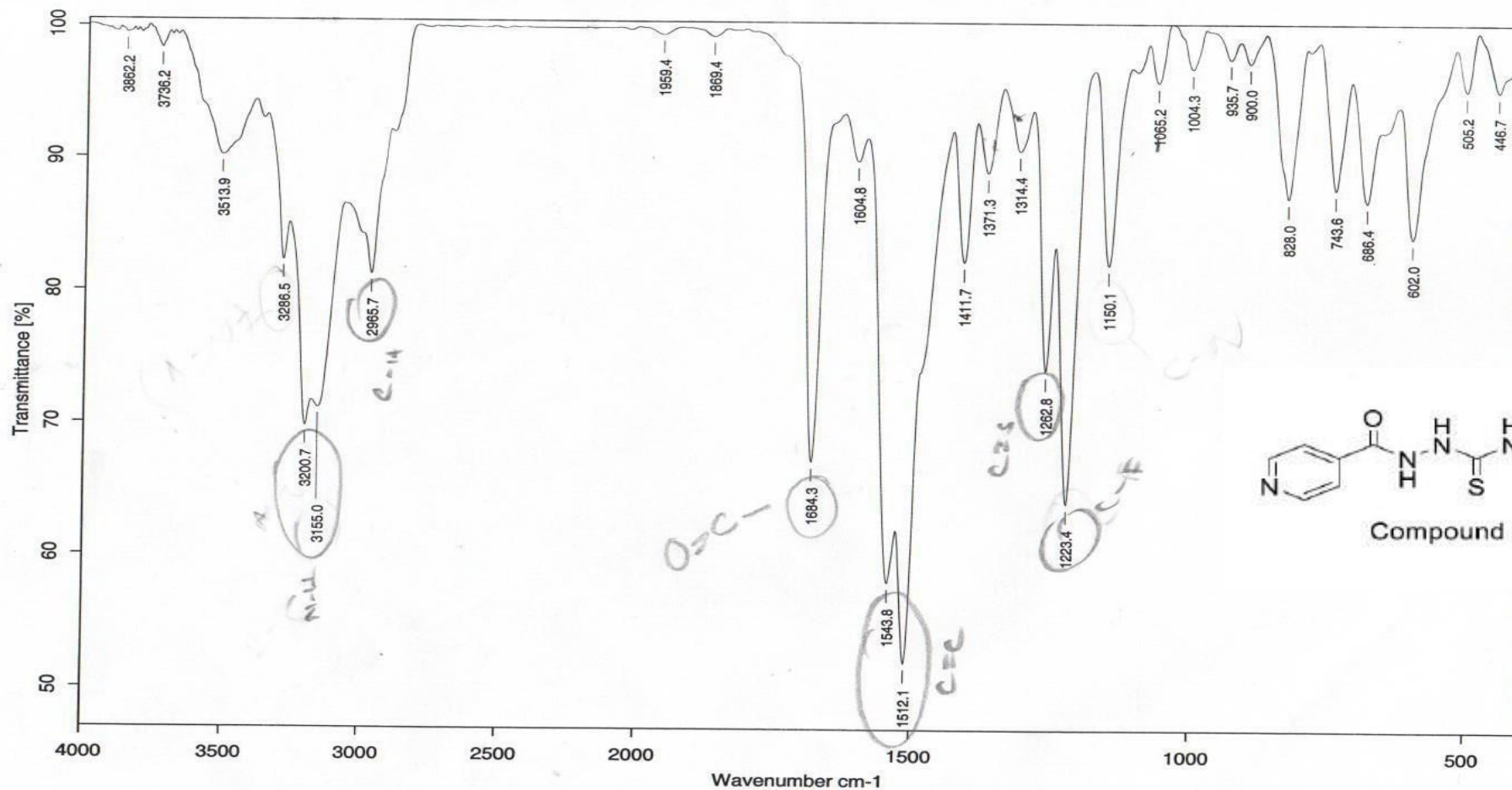
R.T.: .53

#Ions: 564

Base: m/z 183; 45.7%FS TIC: 2412440



Compound 19



Sample : Fz-I-Iso24/Fazila Rizvi/Dr. Hina

Measured : 29/12/2016 on VECTOR22

Resolution : 4 cm^{-1} (10 scans)

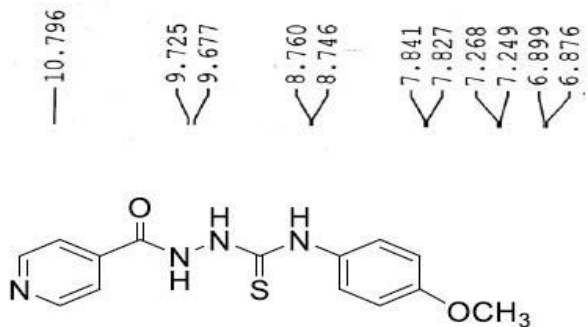
Spectrum : Fz-I-Iso24.0 (in D:\IRSTUDENT)

Technic : Solid

Analyst : M. Asif

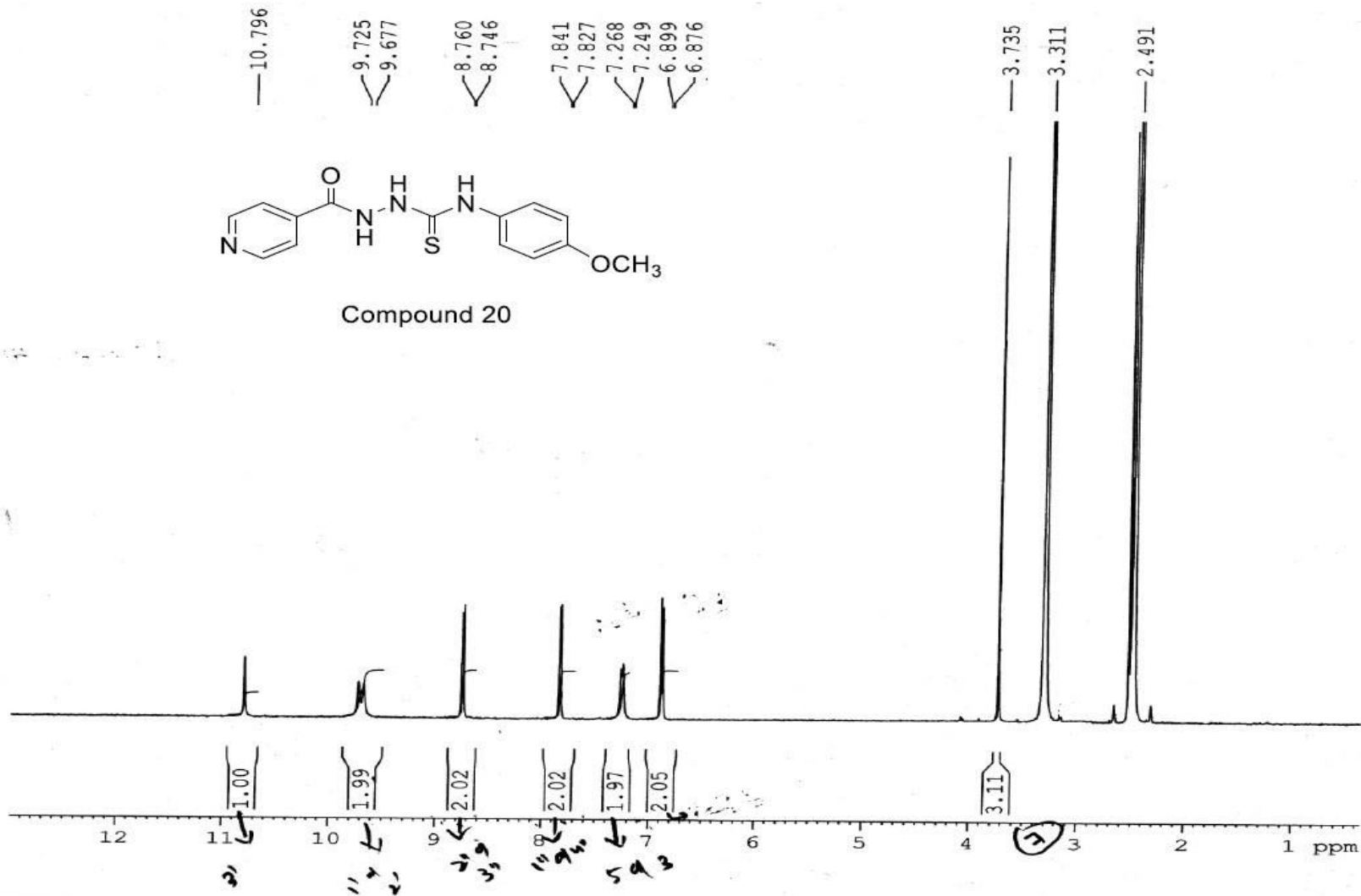
BUSHRA/DR, HINA/FZ-I-ISO-25/
 ICCBS, U.O.K/

AVANCE 400
 LAB NO 117



NAME nov01-16
 EXPNO 2
 PROCNO 1
 Date_ 20161101
 Time_ 11.07
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 512
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.40 usec
 PL1 0.00 dB
 SFO1 400.1332010 MHz
 SI 16384
 SF 400.1300064 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BUSHRA/DR, HINA/FZ-I-ISO-25/
ICCBS, U.O.K/

10.796

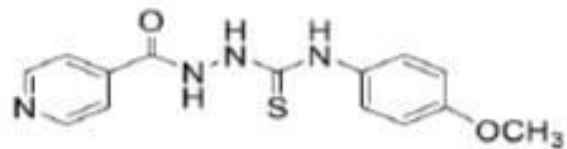
9.725
9.677

8.760
8.746

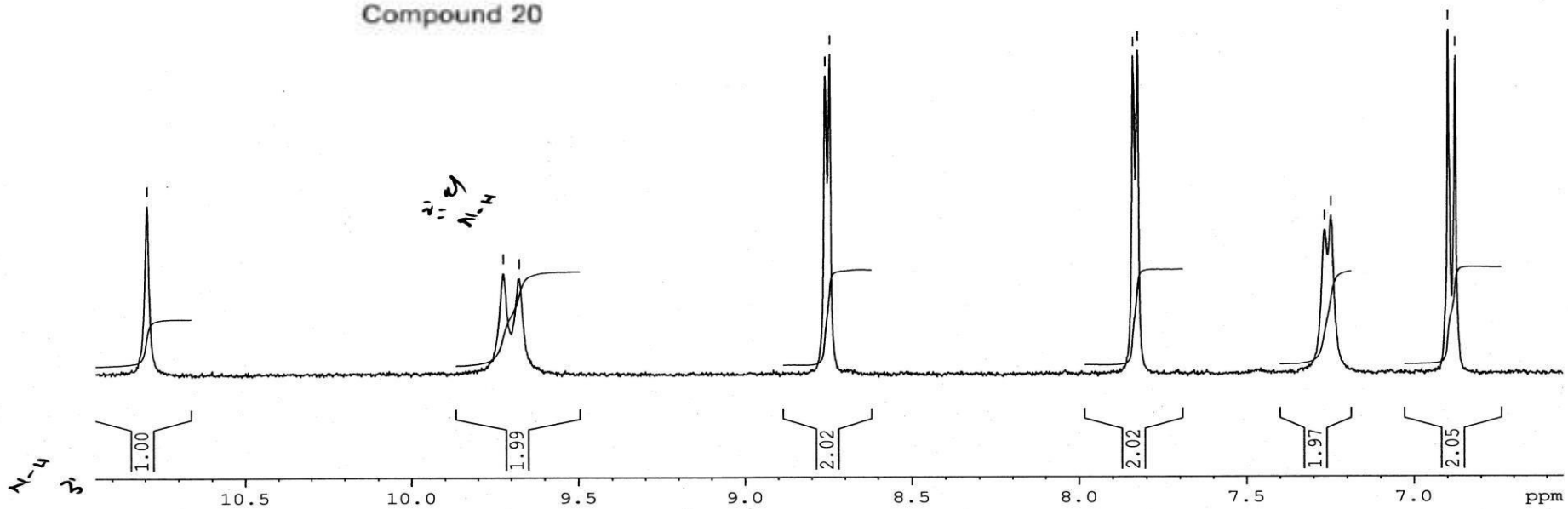
7.841
7.827

7.268
7.249

6.899
6.876



Compound 20



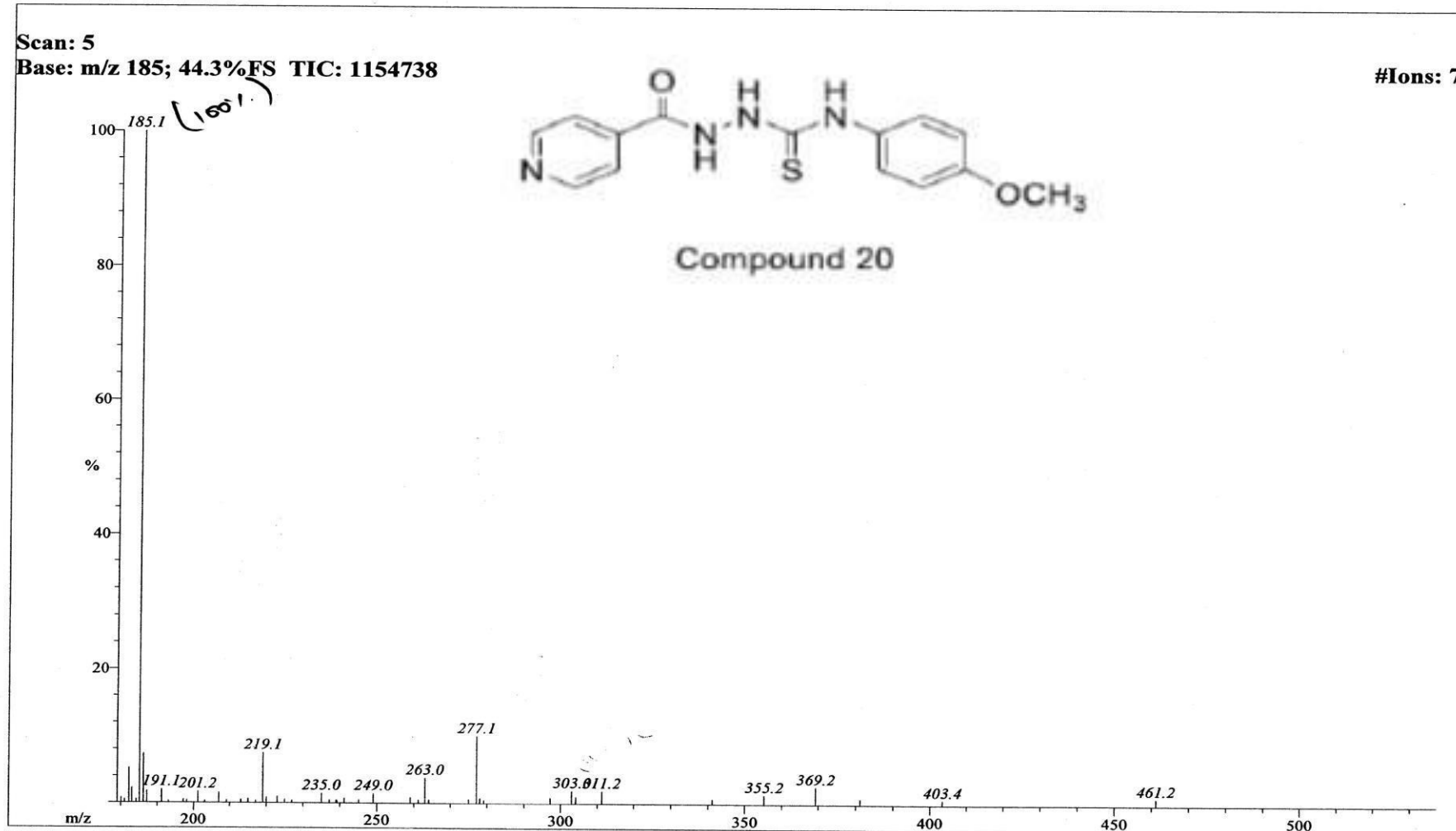
File: FZ-I-ISO25-FABP
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

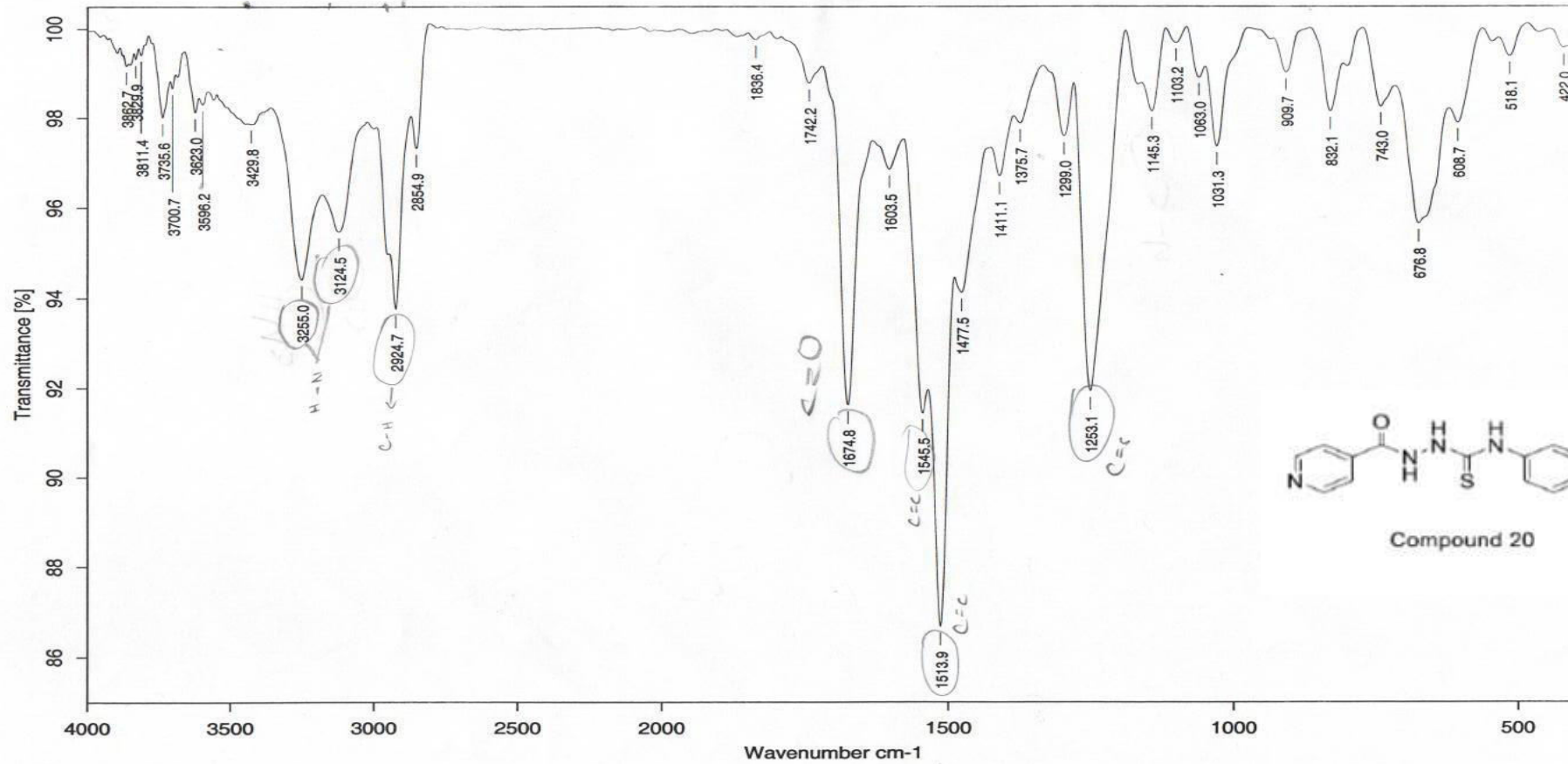
Date Run: 10-18-2016 (Time Run: 15:16:35)

Ionization mode: FAB+

Scan: 5
Base: m/z 185; 44.3%FS TIC: 1154738

#Ions: 71





Sample : Fz-I-Iso25/Fazila Rizvi/Dr. Hina	Spectrum : Fz-I-Iso25.0 (in D:\IRSTUDENT)
Measured : 29/12/2016 on VECTOR22	Technic : Solid
Resolution : 4 cm^{-1} (10 scans)	Analyst : M. Asif

FAZILA/DR, HINA/FZ-I-ISO2/
ICCBS.U.O.K/

—10.958

—10.157

—9.807

8.777

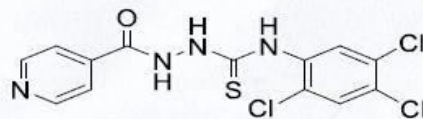
8.757

7.932

7.847

7.833

7.608



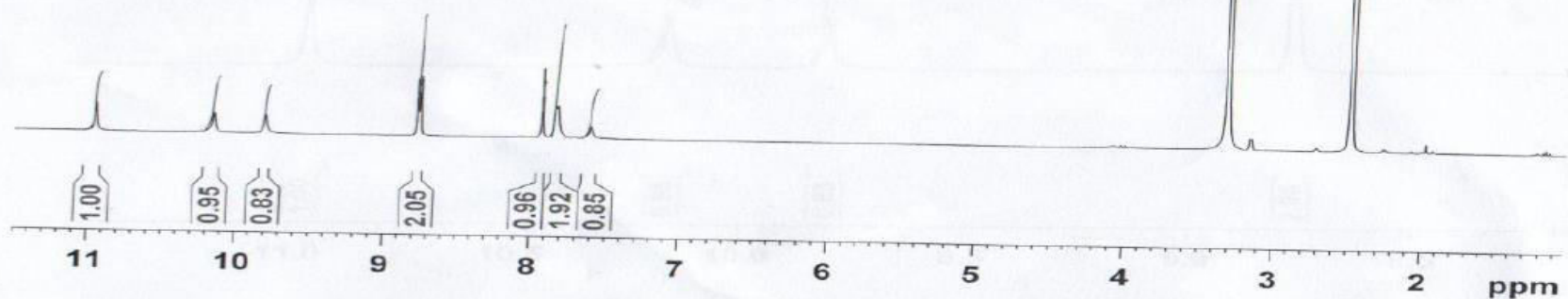
Compound 21

3.319

2.496

2.490

2.485



AVANCE AV - III
300 MHz, LAB # 116

NAME	jan03-19
EXPNO	9
PROCNO	1
Date_	20190103
Time_	12.13
INSTRUM	Spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	128
DS	0
SWH	6188.119 Hz
FIDRES	0.188846 Hz
AQ	2.6477044 sec
RG	406
DW	80.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.50000000 sec
TDO	1

=====	CHANNEL f1	=====
NUC1	1H	
P1	12.50	usec
PL1	0.00	dB
PL1W	13.16228485	W
SFO1	300.1321009	MHz
SI	16384	
SF	300.1300039	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

FAZILA/DR, HINA/FZ-I-ISO2/
ICCBS.U.O.K/

—10.958

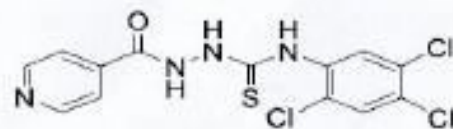
—10.157

—9.807

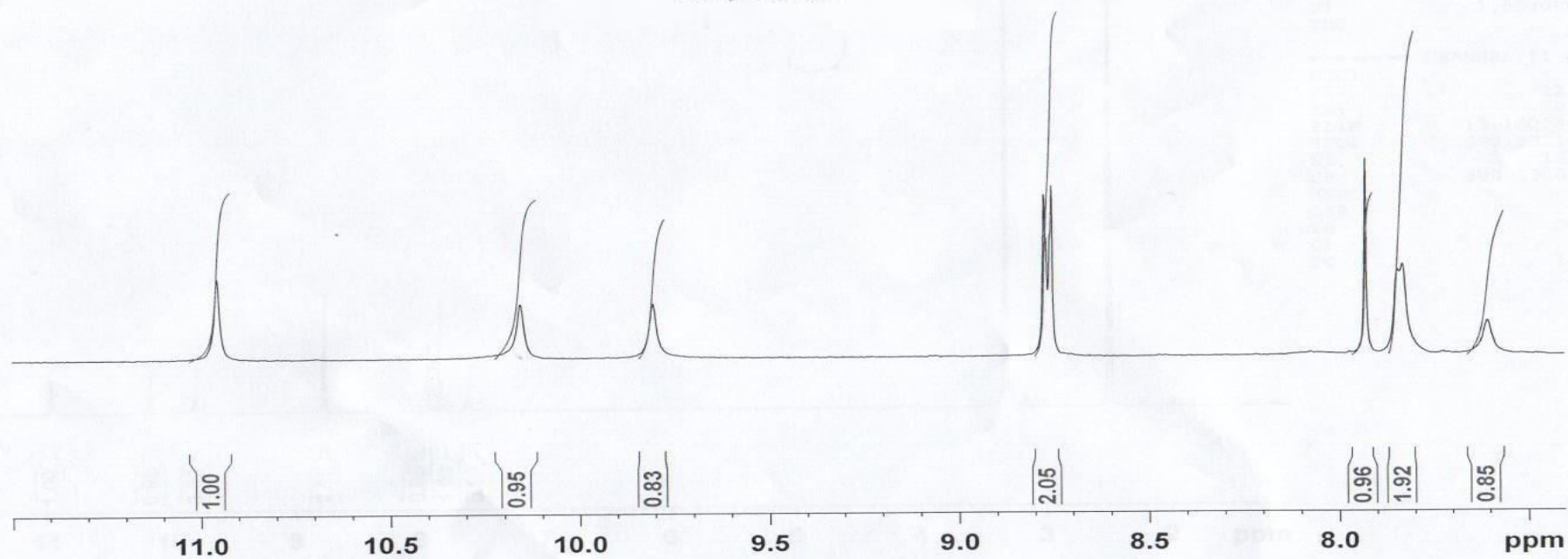
<8.777
<8.757

<7.932
<7.847
<7.833

—7.608



Compound 21



File: FZ-I-ISO2(F)-FABN
Sample: FAZILA /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

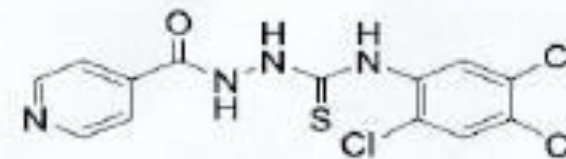
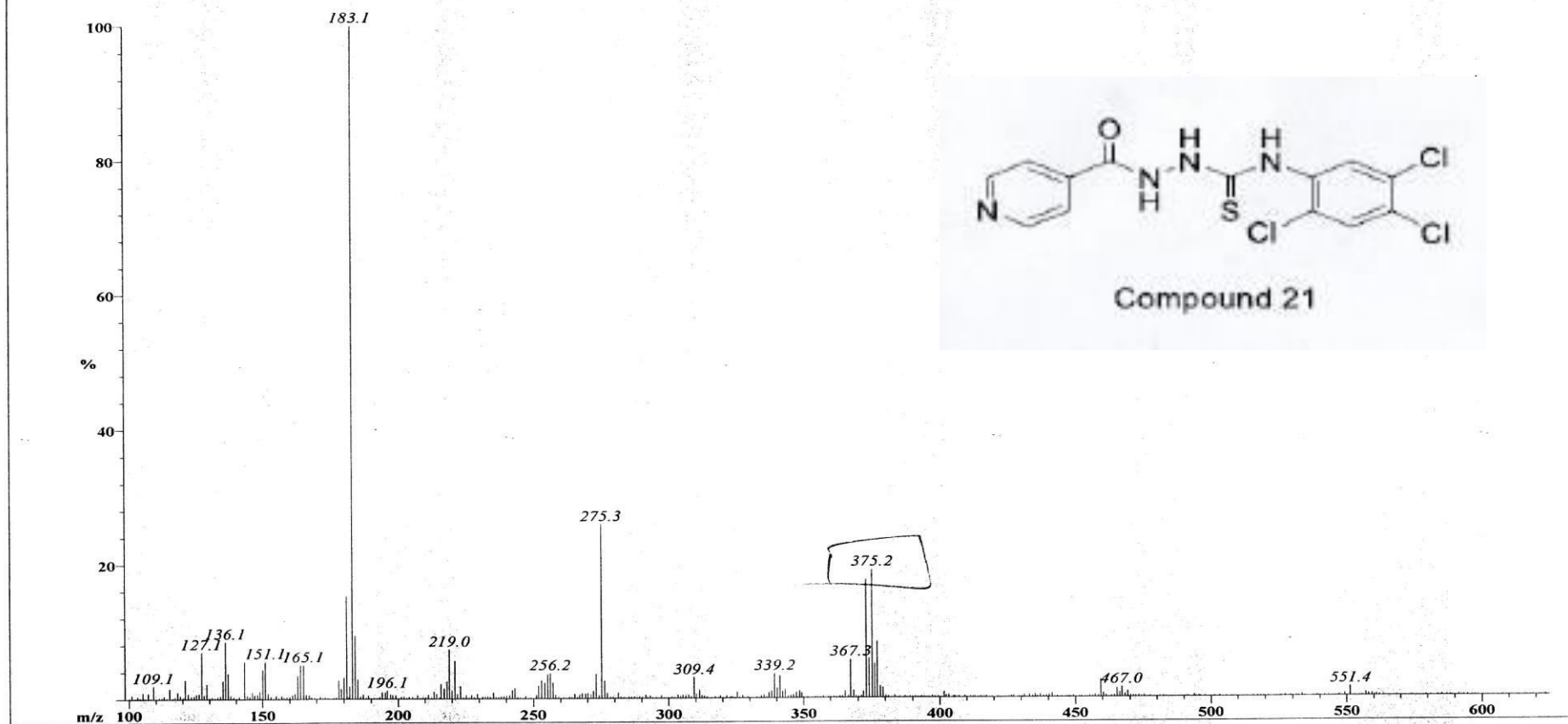
Date Run: 04-09-2016 (Time Run: 13:50:04)

Ionization mode: FAB-

Scan: 9
Base: m/z 183; 100%FS TIC: 5396524

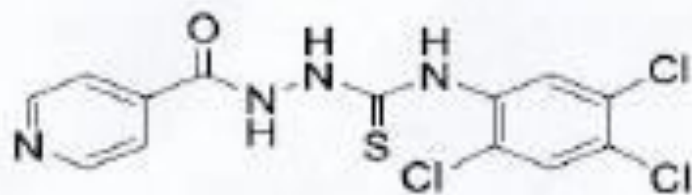
R.T.: .72

#Ions: 834

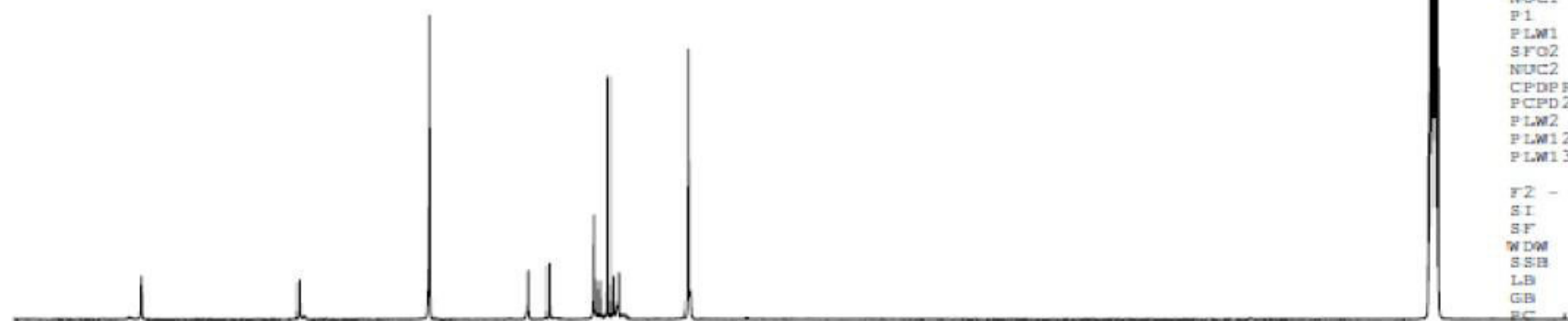


Compound 21

Fazila / D. Hina / FZ-I-ISO2
BB



Compound 21



```
Cu
NAME          fz-I-Iso2
EXPNO         1
PROCNO       1

F2 - Acquisition Parameters
Date_         20190204
Time          3.45 h
INSTRUM       Avance Neo 500
PROBHD        z44862_0021 (C)
PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            16384
DS            8
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.5439488 sec
RG            101
DW            16.600 usec
DE            20.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0           16
SFO1          125.8227986 MHz
NUC1          13C
P1            10.00 usec
PLW1          26.46199989 W
SFO2          500.3320013 MHz
NUC2          1H
CPDPRG[2]     waltz65
PCPD2         80.00 usec
PLW2          9.74149990 W
PLW12         0.34246999 W
PLW13         0.17199001 W

F2 - Processing parameters
SI            16384
SF            125.8081399 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

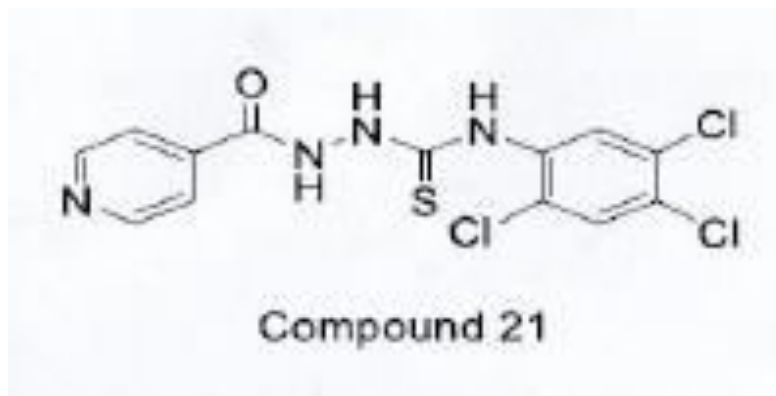
Fazila / D. Hina / FZ-I-ISO2
DEPT135

150.20

132.00
130.48

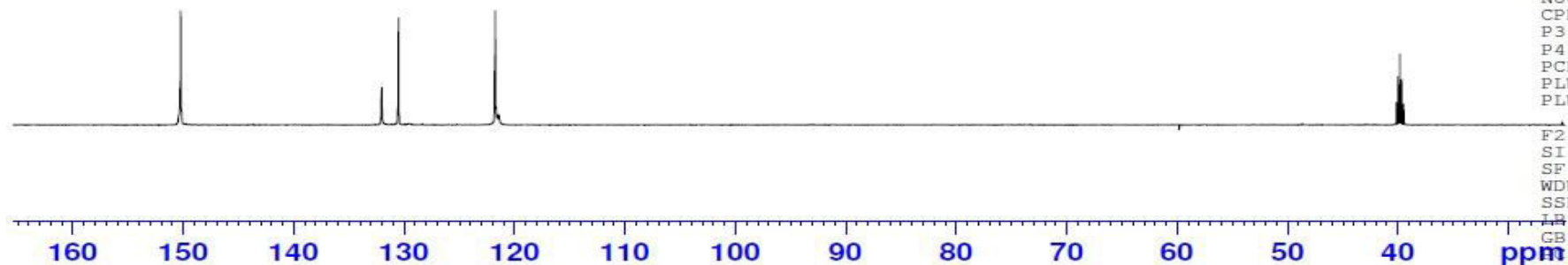
121.73

40.10
39.93
39.76
39.59
39.43

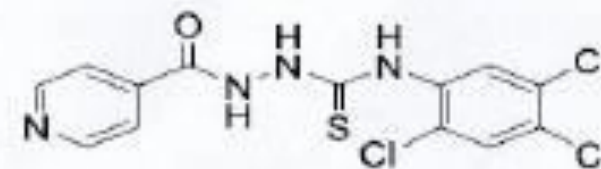
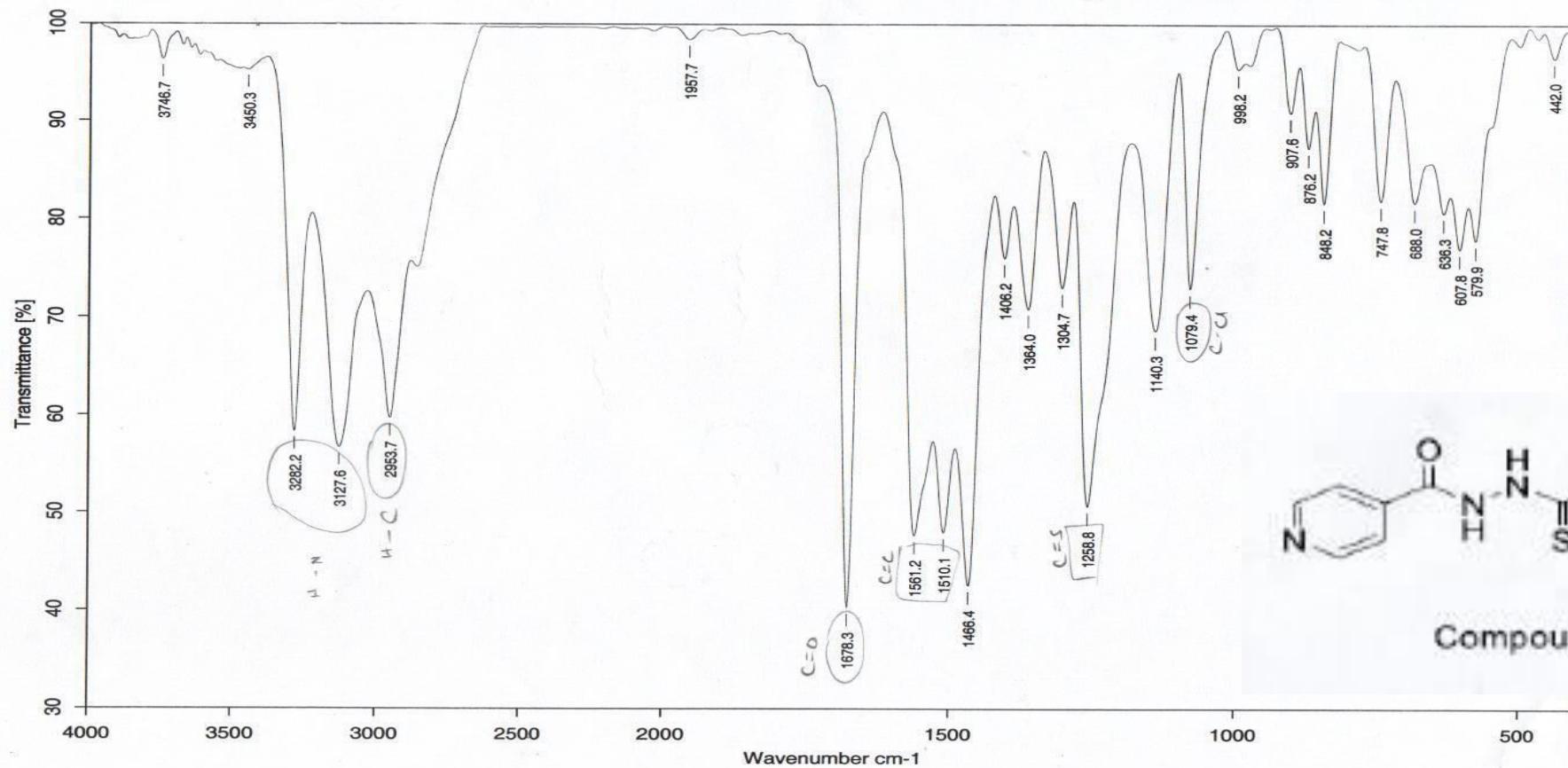


Current Data Parameters
NAME fz-I-Iso2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190204
Time_ 8.47 h
INSTRUM Avance Neo 500
PROBHD Z44862_0021 (C
PULPROG deptsp135
TD 32768
SOLVENT DMSO
NS 8233
DS 8
SWH 25000.000 Hz
FIDRES 1.525879 Hz
AQ 0.6553600 sec
RG 101
DW 20.000 usec
DE 20.00 usec
TE 298.0 K
CNST2 145.000000
D1 1.5000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 10
SFO1 125.8200303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 26.46199989 W
SPNAM[5] Crp60comp.4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 4.04309988 W
SFO2 500.3320013 MHz
NUC2 1H
CPDPRG[2] waltz65
P3 15.00 usec
P4 30.00 usec
PCPD2 80.00 usec
PLW2 9.74149990 W
PLW12 0.34246999 W



F2 - Processing parameters
SI 16384
SF 125.8081395 MHz
WDW EM
SSB 0
LR 1.00 Hz
GB 0
1.40



Compound 21

Sample : FZI-ISO2/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

Resolution : 4 cm^{-1} (10 scans)

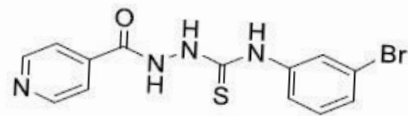
Spectrum : FZ-I-ISO2.0 (in D:\IRSTUDENT)

Technic : Solid

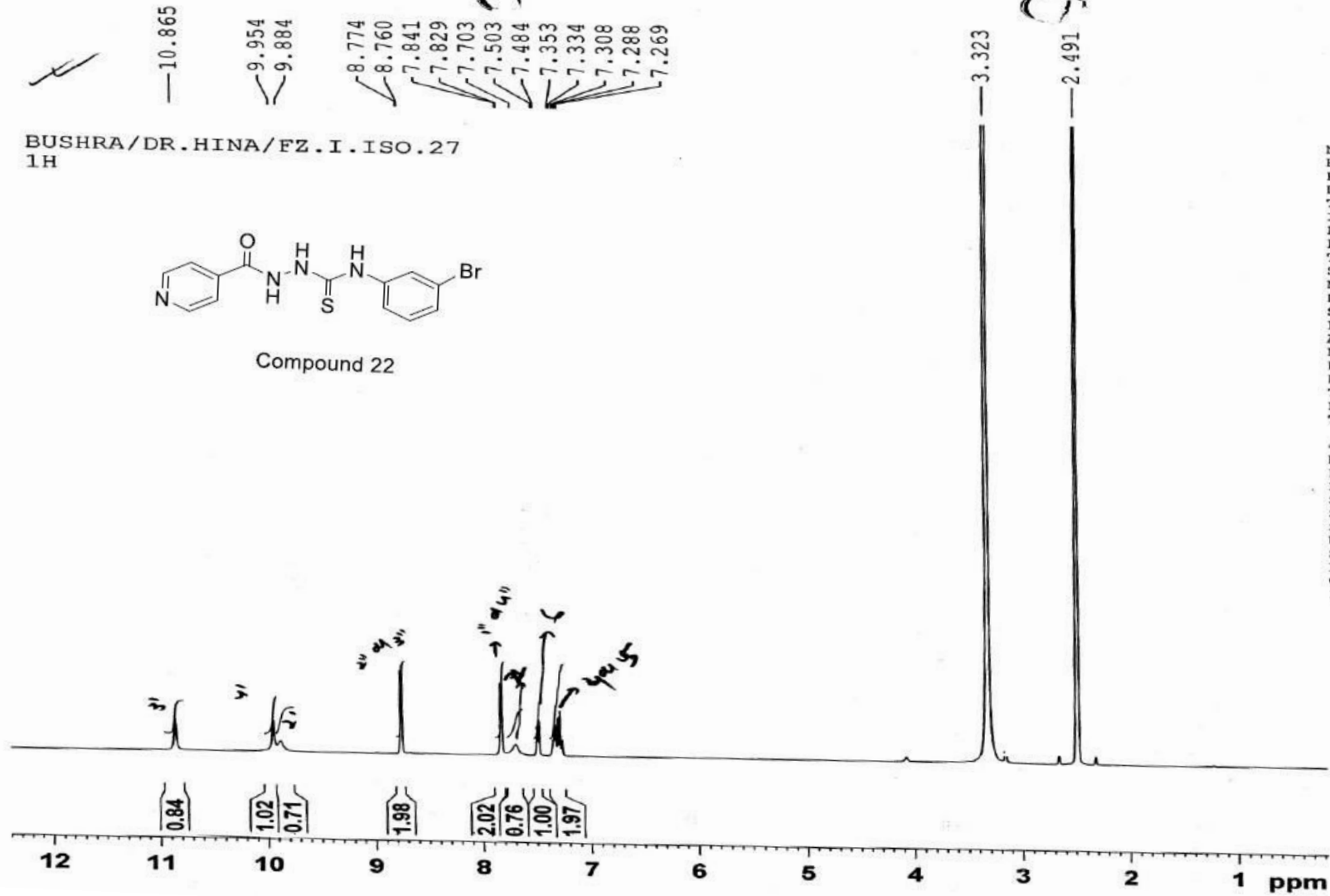
Analyst : MA/ZA/JS

AVANCE AV-400 MHz
Lab # 115

BUSHRA/DR.HINA/FZ.I.ISO.27
1H



Compound 22



```

NAME      oct017-16
EXPNO     4
PROCNO    1
Date_     20161017
Time      12.32
INSTRUM   spect
PROBHD    5 mm SEI 1H-13
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         128
DS         0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG         322.5
DW        62.400 usec
DE         6.50 usec
TE        300.0 K
D1        1.50000000 sec
TDO       1

----- CHANNEL f1 -----
NUC1      1H
P1        10.80 usec
PL1       3.00 dB
SFO1     400.0332002 MHz
SI        32768
SF        400.0300041 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        0.20

```

8.774
8.760

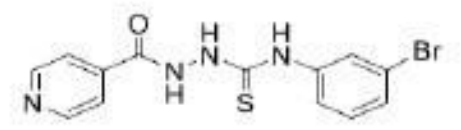
7.841
7.829

7.703

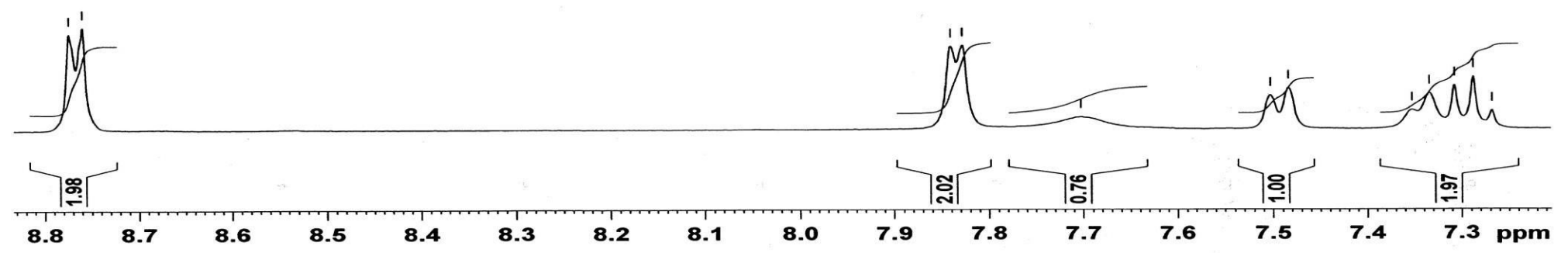
7.503
7.484

7.353
7.334
7.308
7.288
7.269

BUSHRA/DR.HINA/FZ.I.ISO.27
1H



Compound 22



File: FZ-I-ISO27-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-19-2016 (Time Run: 16:13:01)

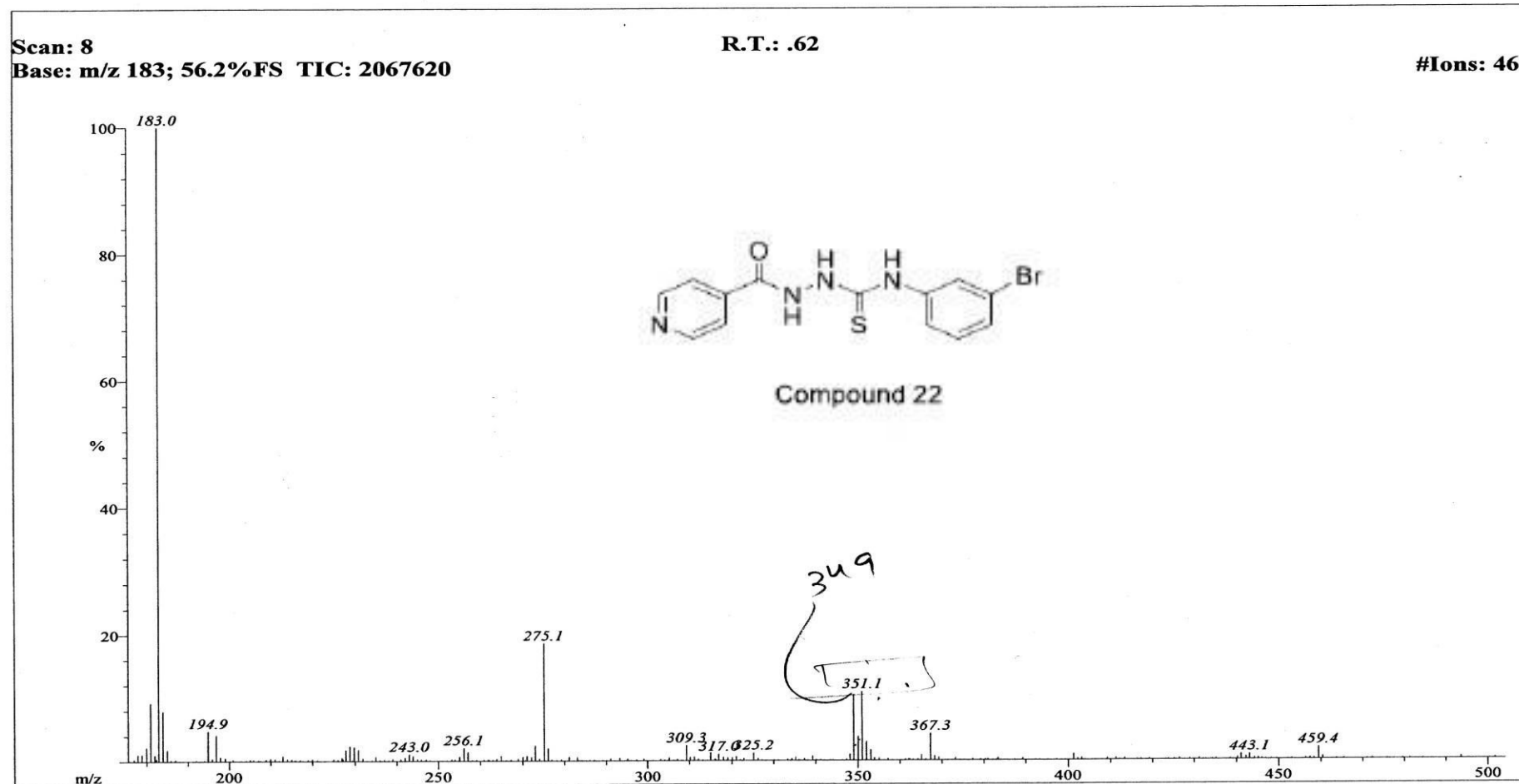
Ionization mode: FAB-

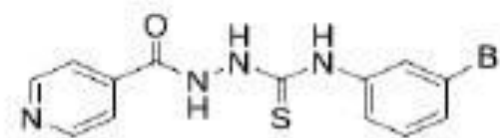
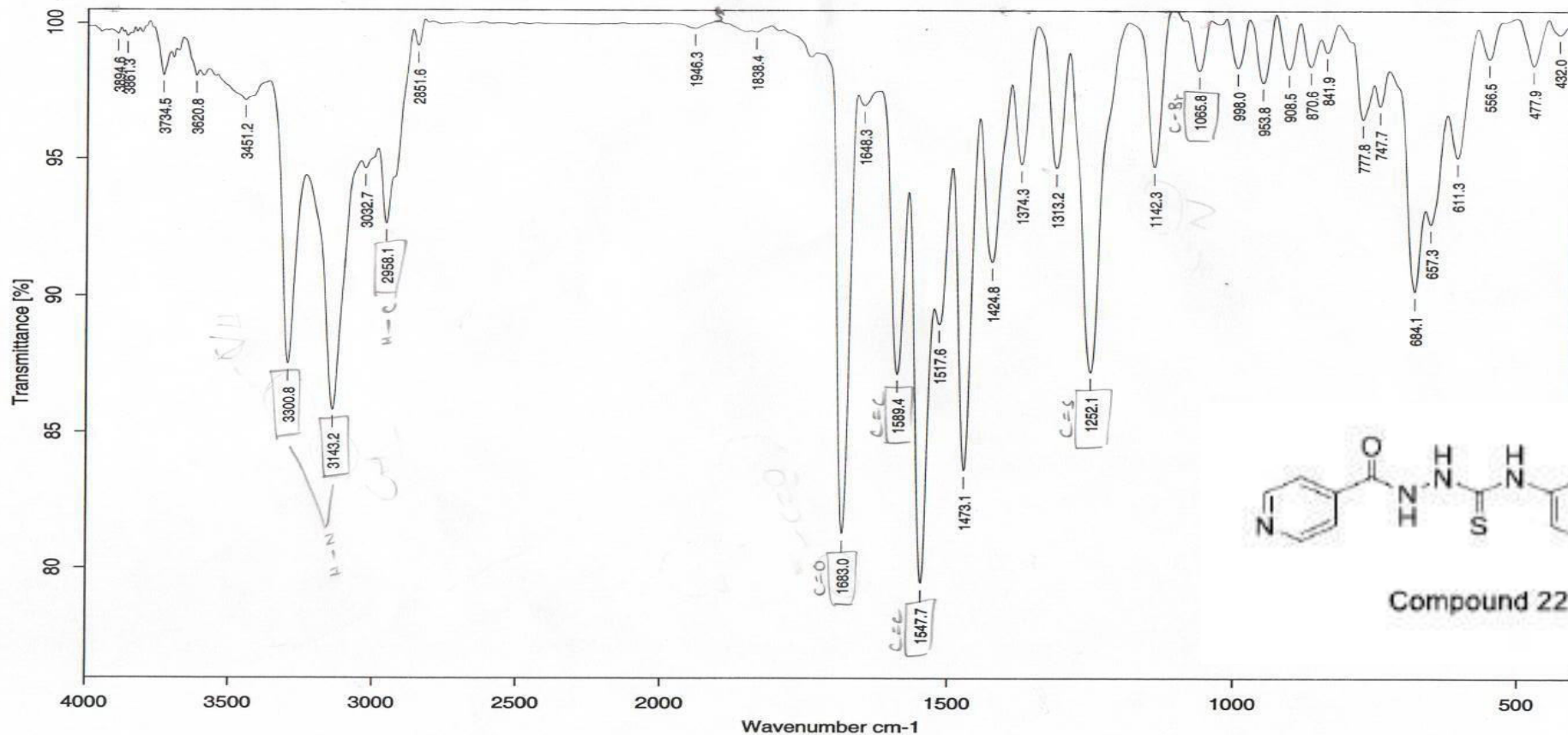
Scan: 8

R.T.: .62

#Ions: 462

Base: m/z 183; 56.2%FS TIC: 2067620

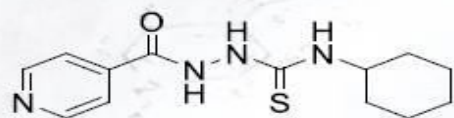




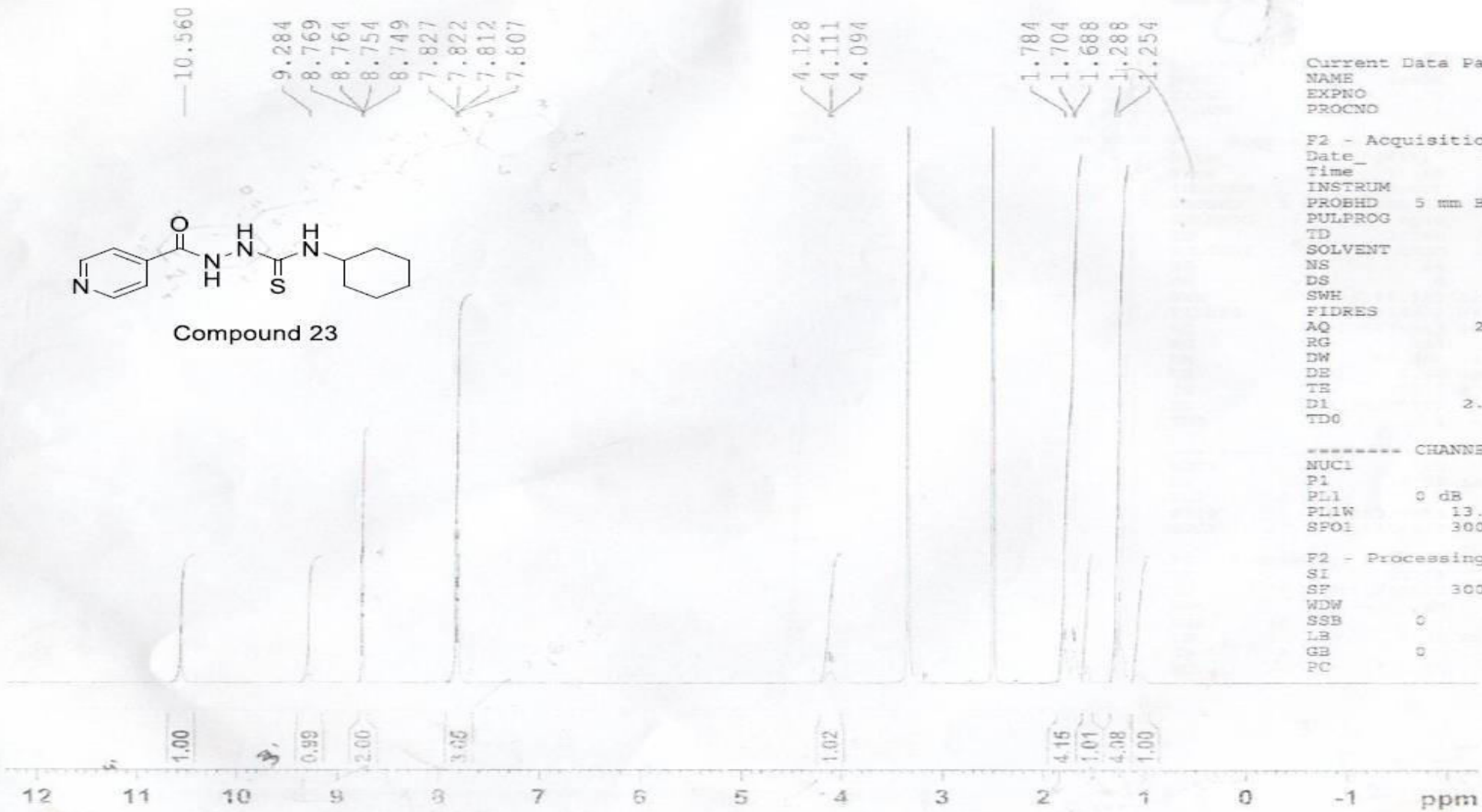
Compound 22

Sample : Fz-I-Iso27/Fazila Rizvi/Dr. Hina	Spectrum : Fz-I-Iso27.0 (in D:\IRSTUDENT)
Measured : 29/12/2016 on VECTOR22	Technic : Solid
Resolution : 4 cm ⁻¹ (10 scans)	Analyst : M. Asif

fazila_rizvi/Dr.Hina/Fz-1-isc28
1H



Compound 23



Current Data Parameters
NAME iso28
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161117
Time_ 11.46
INSTRUM Spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

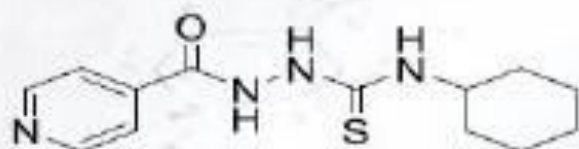
----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 0 dB
PL1W 13.16228485 W
SFO1 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1360000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

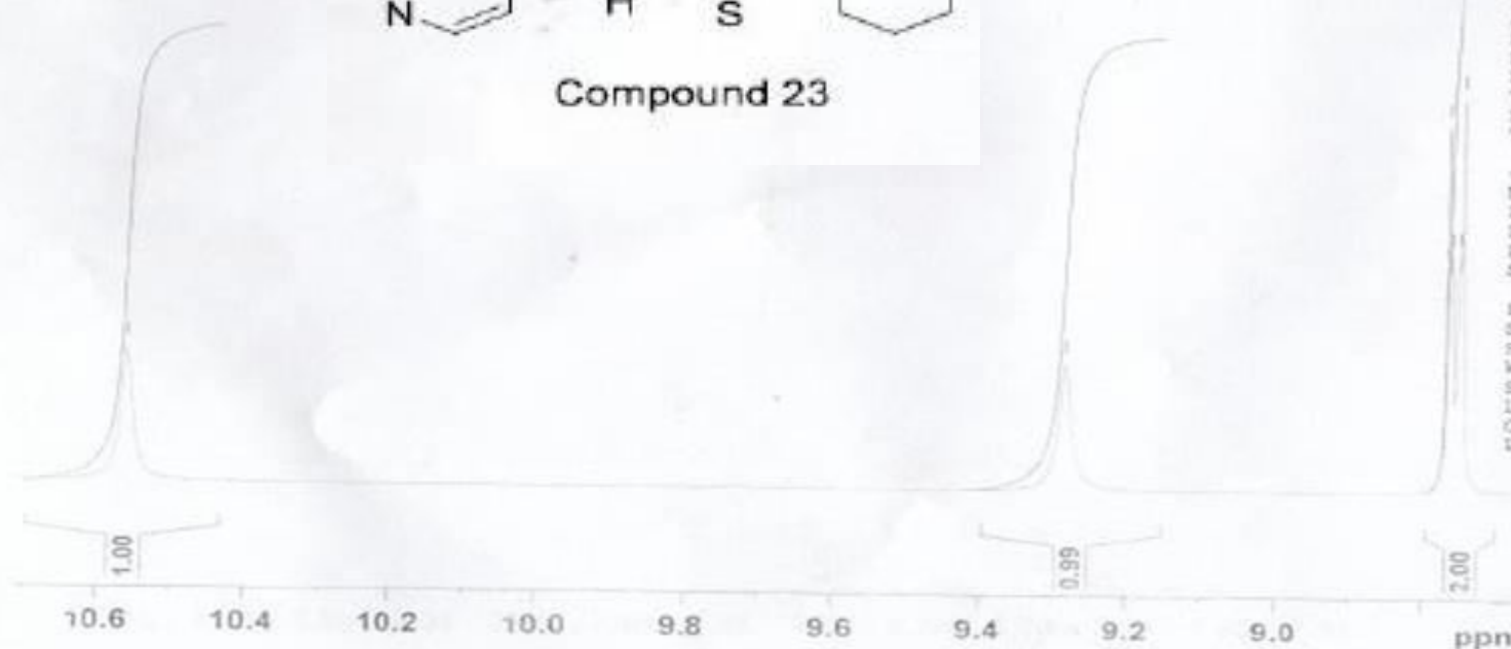
azila rizvi/Dr.Hina/Fz-I-iso28
1H

10.560

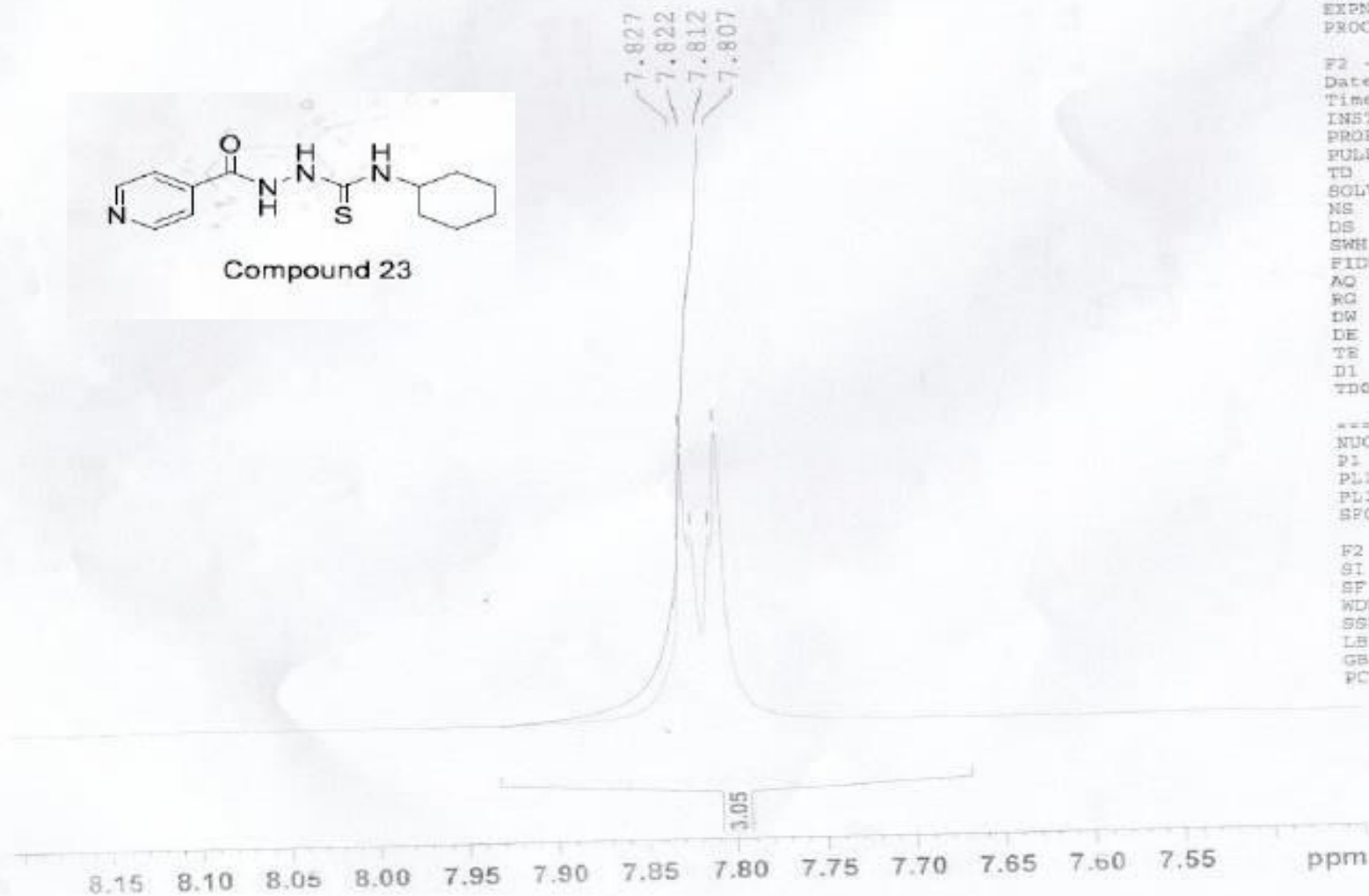
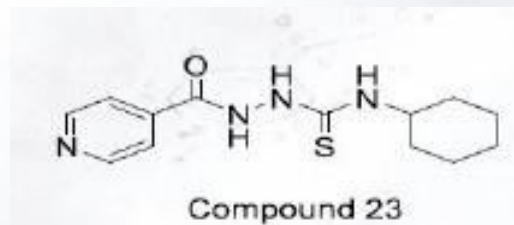
9.284



Compound 23



```
Current Data Parameters
NAME          iso28
EXPNO         3
PROCNO        1
-----
F2 - Acquisition Parameters
Date_         20161117
Time          11.48
INSTRUM       Spect
PROBHD        5 mm BBO BB-1H
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            64
DS            0
SWH           6188.119 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            203
DM            80.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TDO           1
-----
***** CHANNEL f1 *****
NUC1          1H
P1            12.50 usec
PL1           0 dB
PL1W          13.16228485 W
SFO1          300.1324010 MHz
-----
F2 - Processing parameters
SI            32768
SF            300.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
DC            1.00
```



Current Data Parameters
NAME iso28
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161117
Time 11.48
INSTRUM Spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TDC 1

----- CHANNEL F1 -----
NUC1 1H
P1 12.50 usec
PL1 0 dB
PL1W 13.16228485 W
SFO1 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1324010 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

File: FZ-I-ISO28-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-19-2016 (Time Run: 16:20:39)

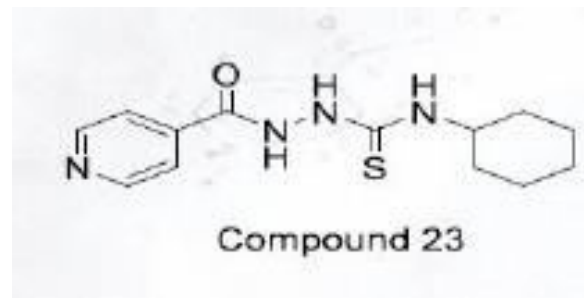
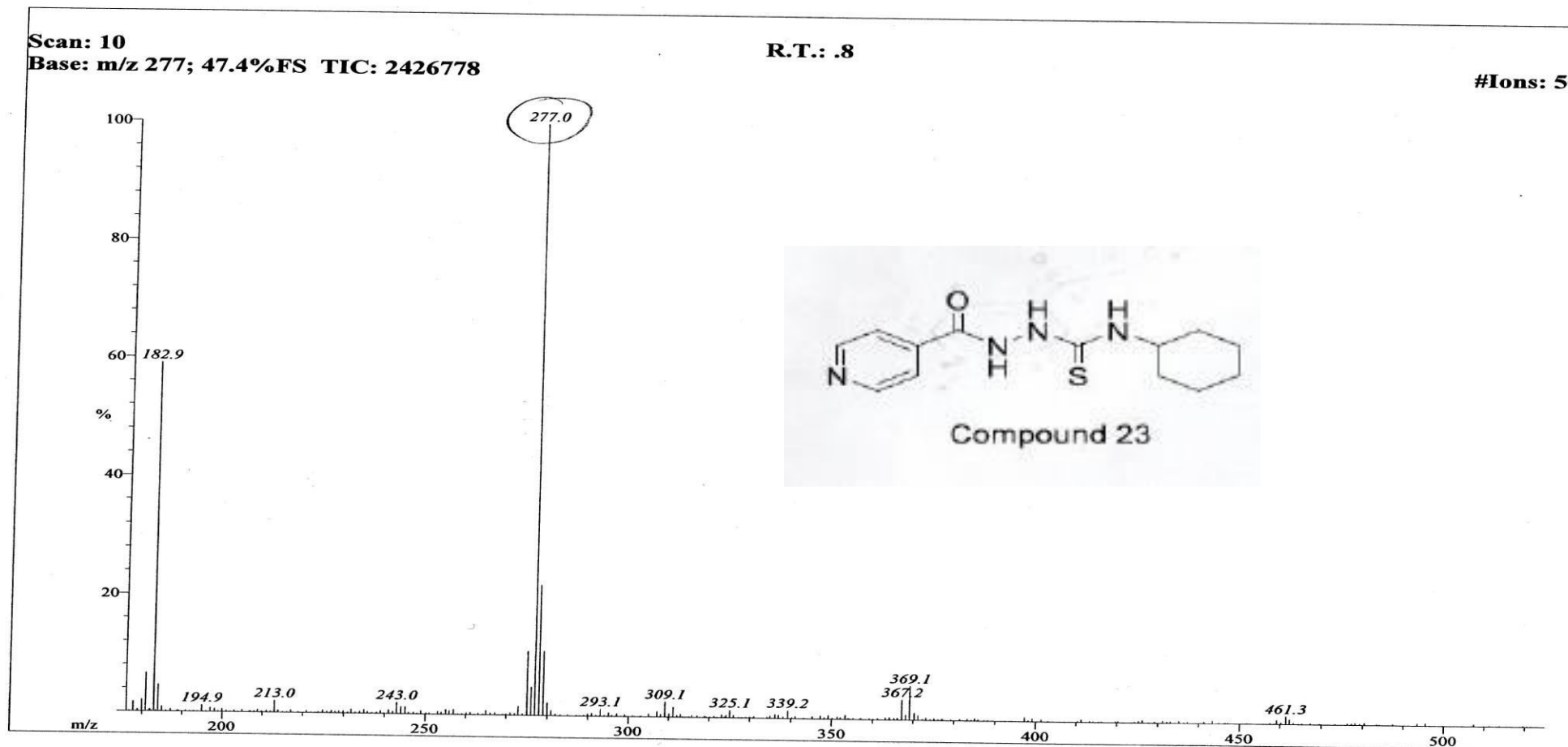
Ionization mode: FAB-

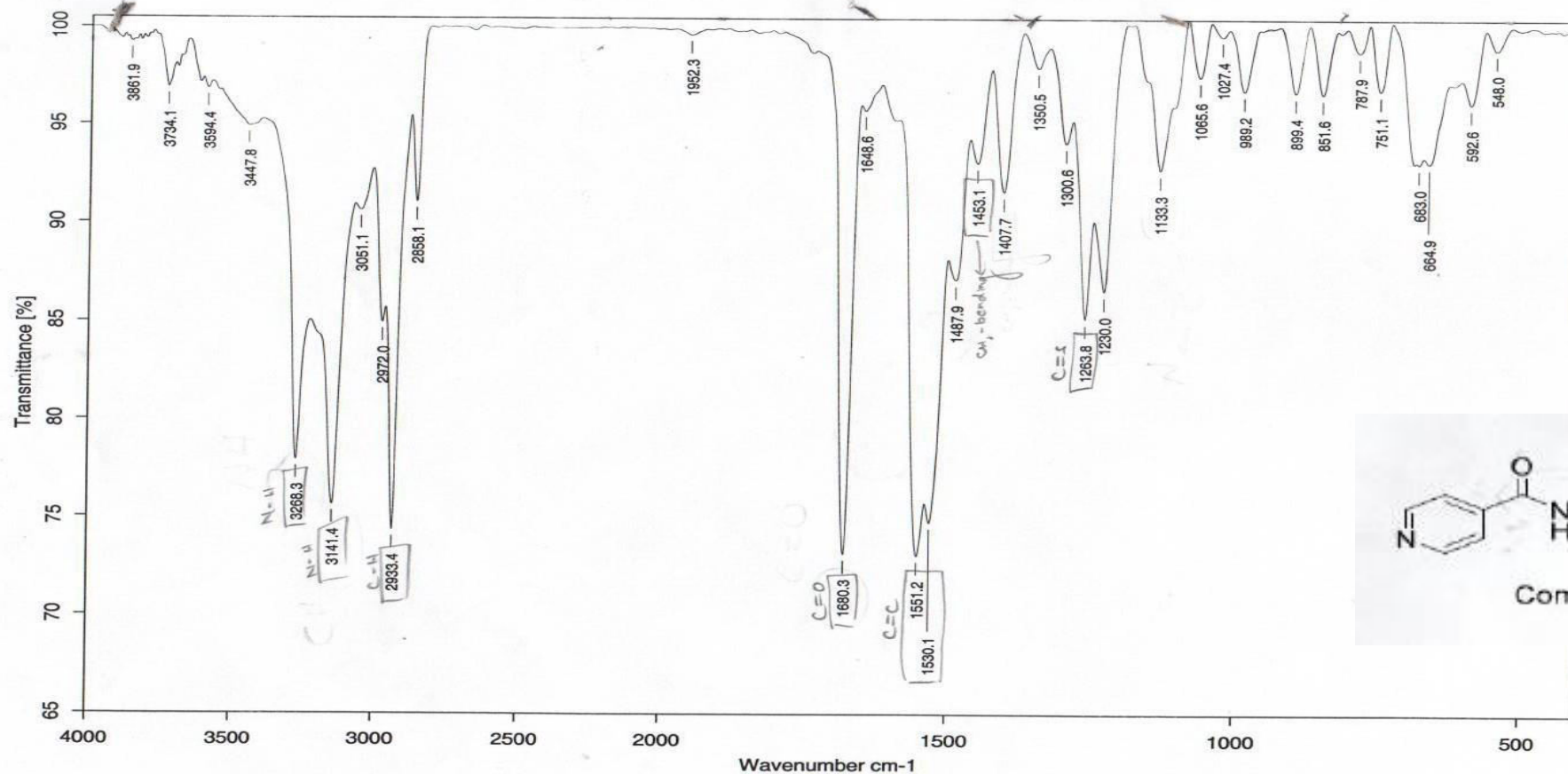
Scan: 10

R.T.: .8

Base: m/z 277; 47.4%FS TIC: 2426778

#Ions: 507





Sample : Fz-I-Iso28/Fazila Rizvi/Dr. Hina

Measured : 29/12/2016 on VECTOR22

Resolution : 4 cm^{-1} (10 scans)

Spectrum : Fz-I-Iso28.0 (in D:\IRSTUDENT)

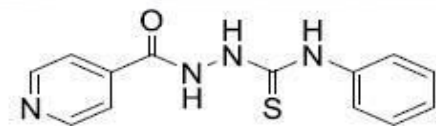
Technic : Solid

Analyst : M. Asif

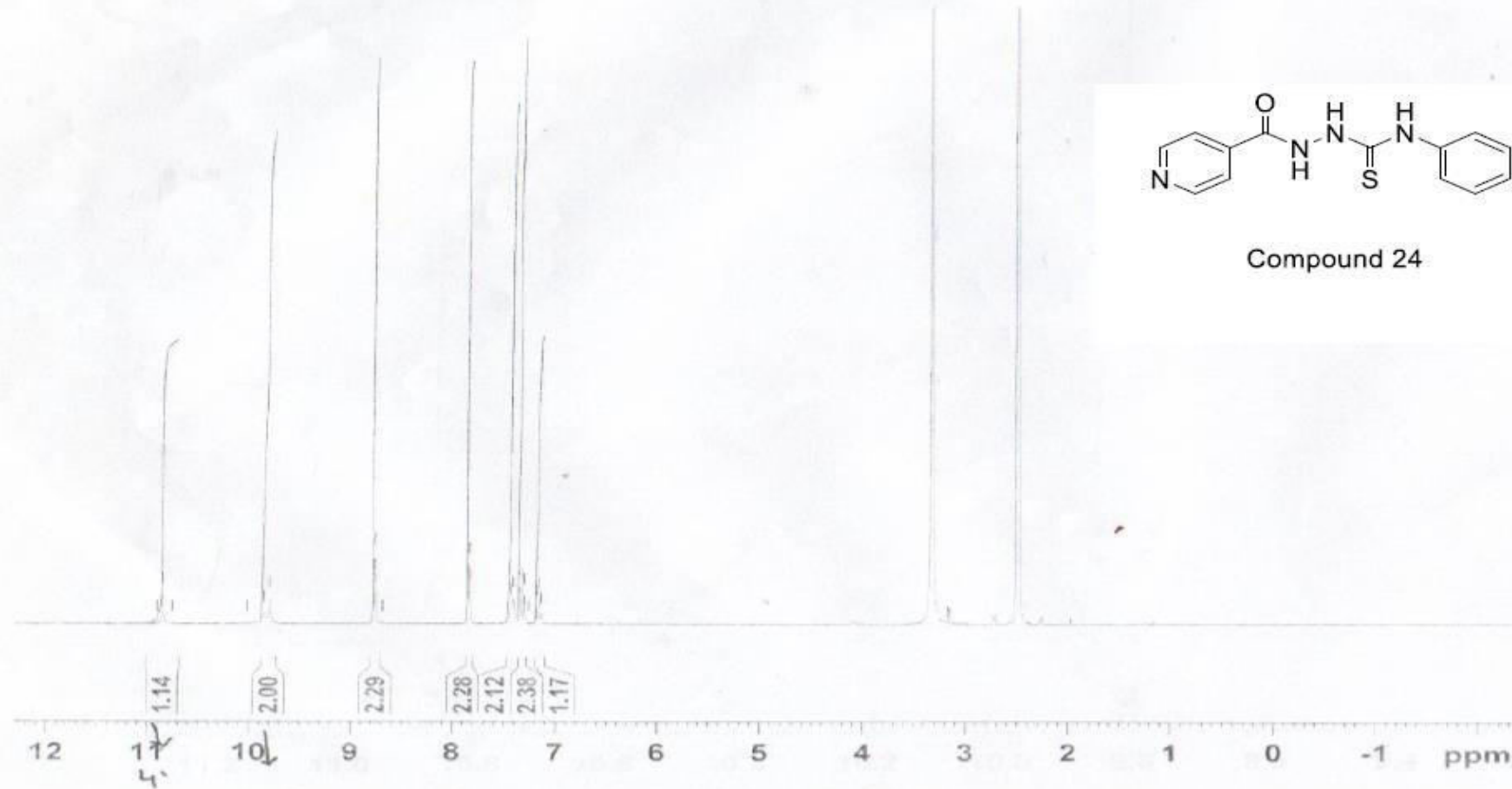
600 mg

Fazila rizvi/Dr.Hina/Fz-I-iso29
1H

10.899
10.840
10.752
10.013
9.848
9.789
8.769
8.765
8.754
8.749
8.681
7.847
7.827
7.429
7.405
7.351
7.299
7.254
7.180
7.156
7.132



Compound 24



EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161117
Time 11.58
INSTRUM Spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 0 dB
PL1W 13.16228485 W
SFO1 300.1324010 MHz

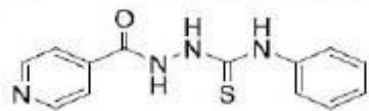
F2 - Processing parameters
SI 32768
SF 300.1300040 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

5.6 H₃
4 - a = 0
3 - 3 = 3
0 - 1 = 0

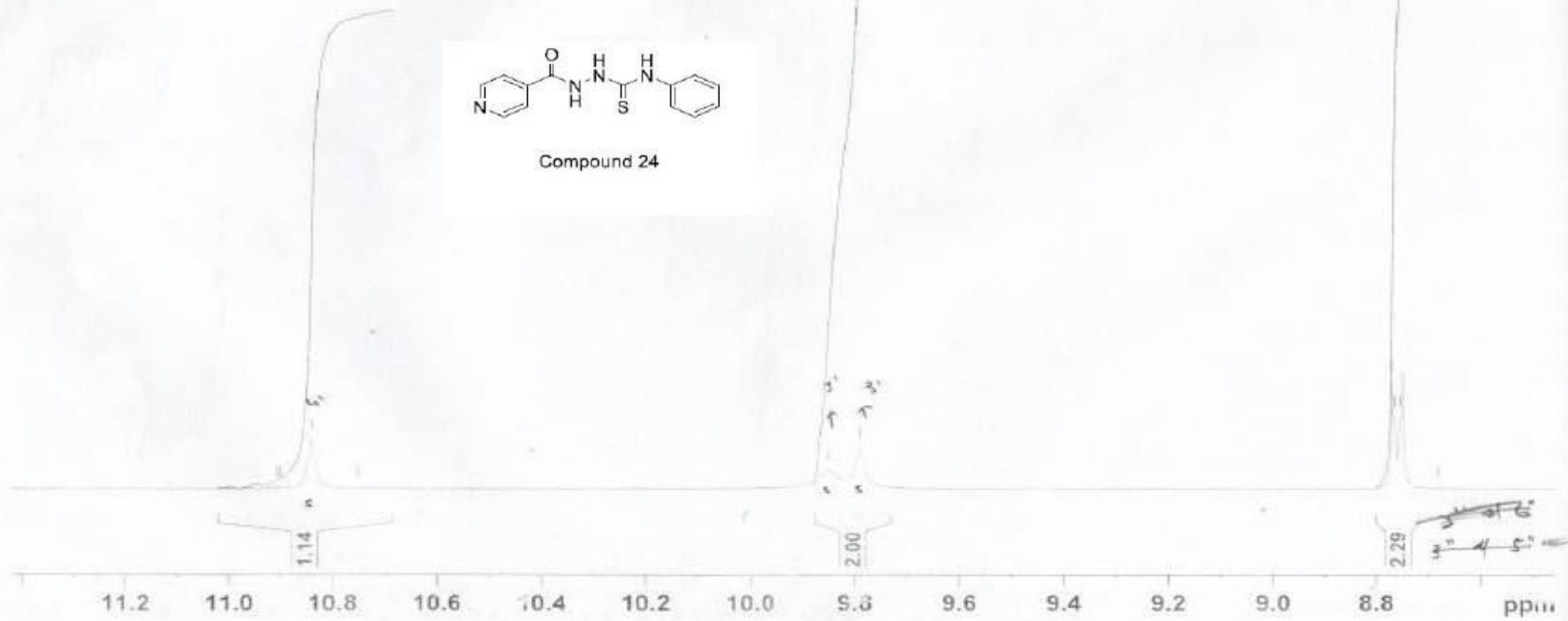
10.905
10.899
10.840
10.752

9.818
9.789

8.769
8.765
8.754
8.681



Compound 24



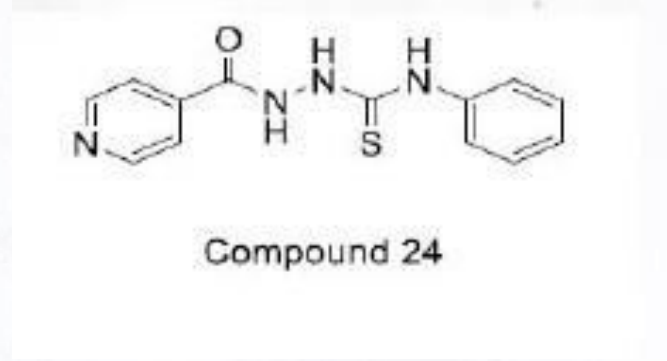
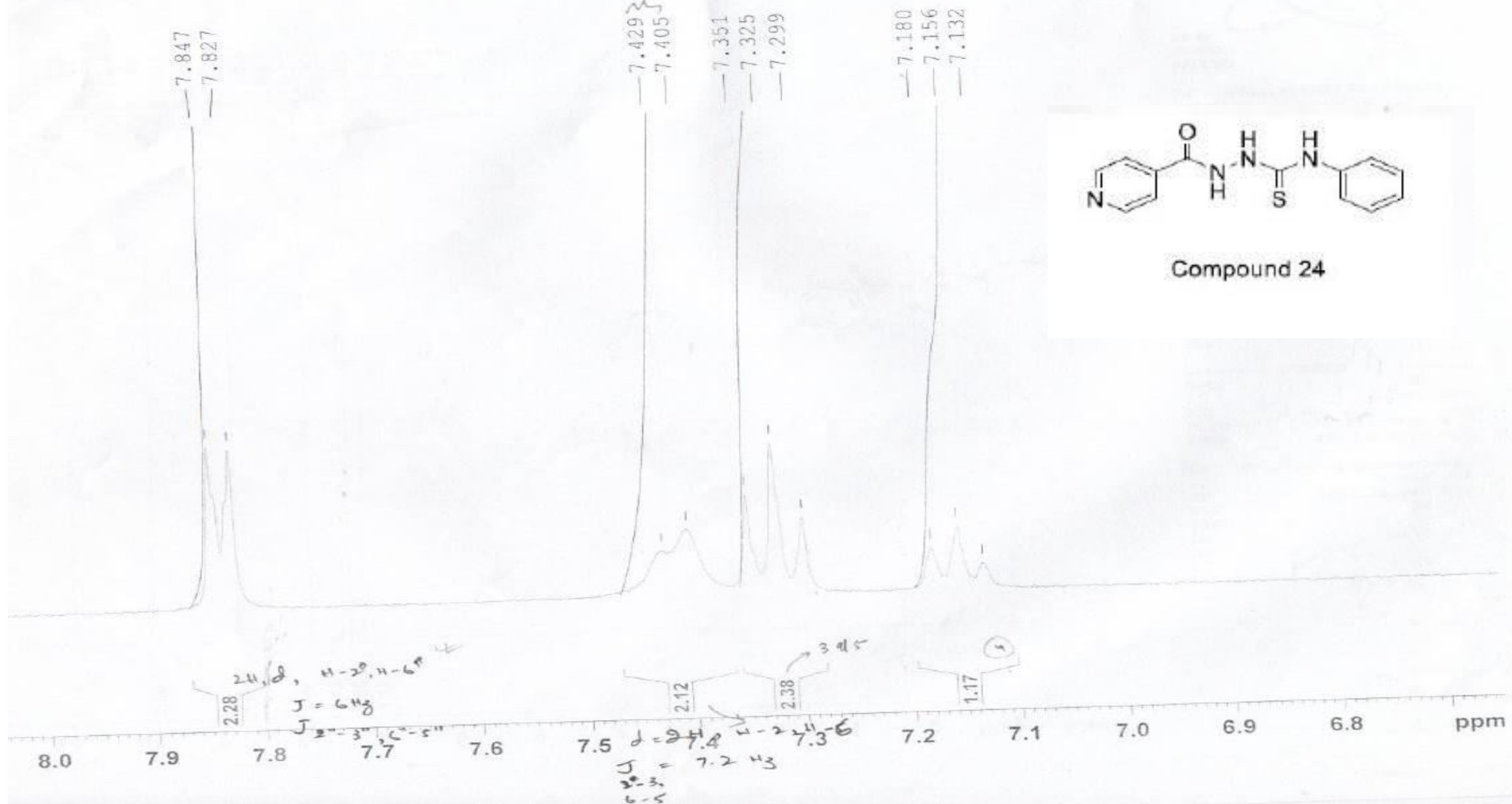
1.14

2.00

2.29

ppm

a rizvi/Dr.Hina/F2-I-iso29



File: FZ-I-ISO29-FABP
Sample: bushra qamar /dr. hina
Instrument: JEOL-600H-2
Inlet: Direct Probe

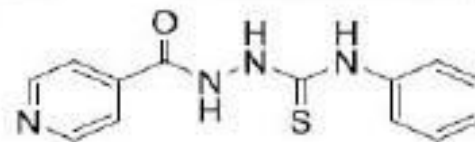
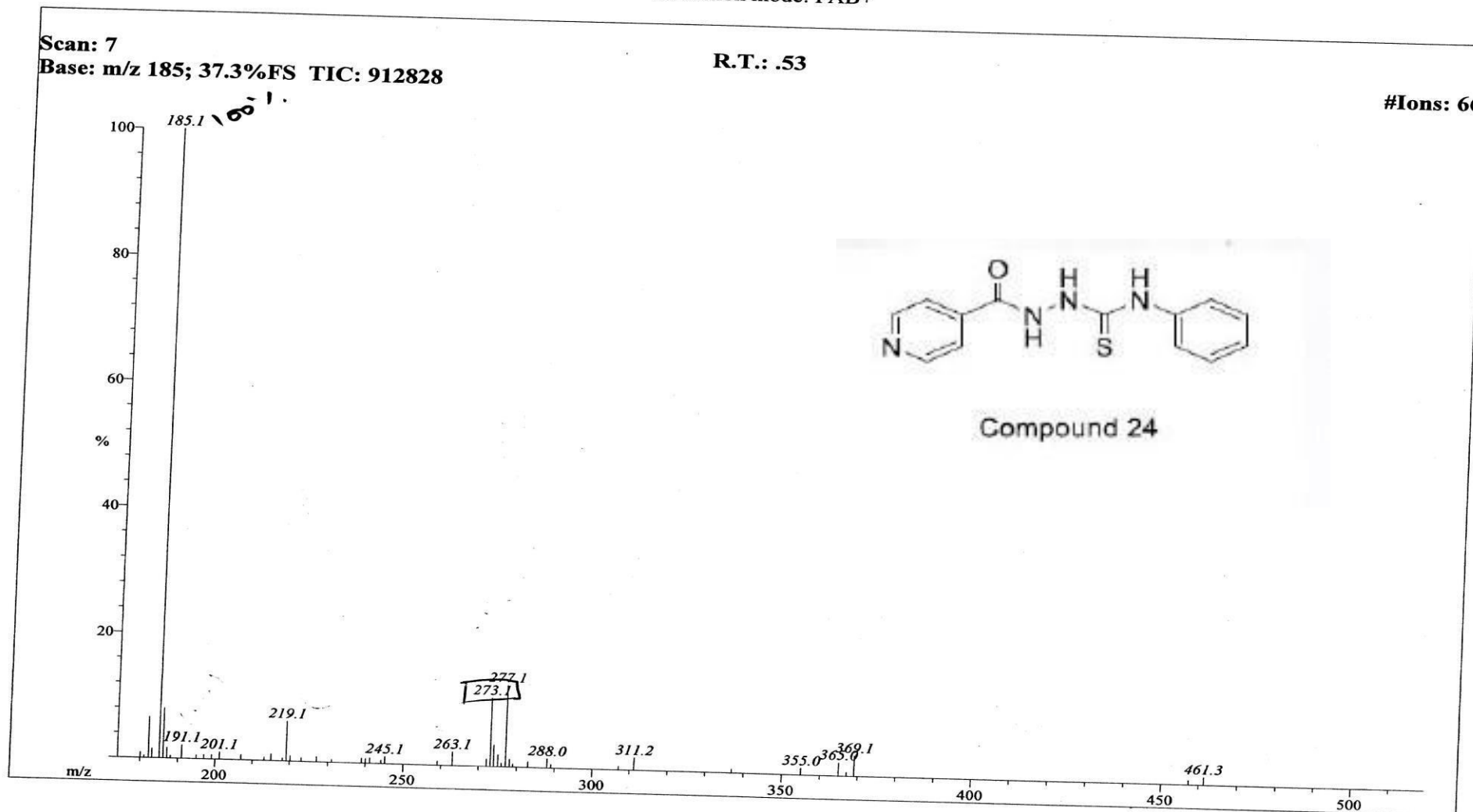
Date Run: 10-21-2016 (Time Run: 10:35:30)

Ionization mode: FAB+

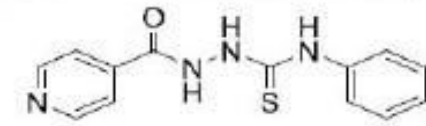
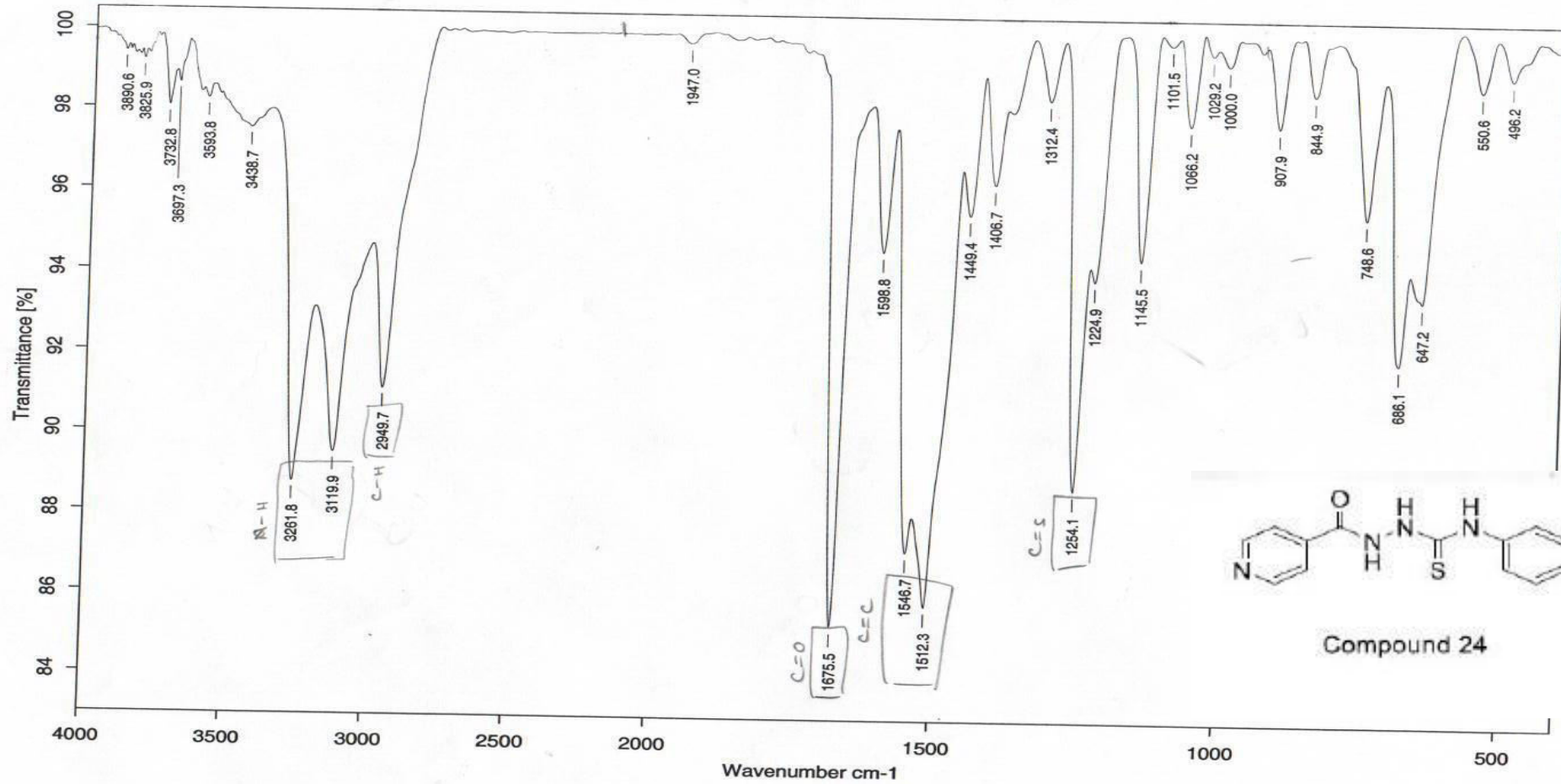
Scan: 7
Base: m/z 185; 37.3%FS TIC: 912828

R.T.: .53

#Ions: 66



Compound 24



Compound 24

Sample : Fz-I-Iso29/Fazila Rizvi/Dr. Hina

Measured : 29/12/2016 on VECTOR22

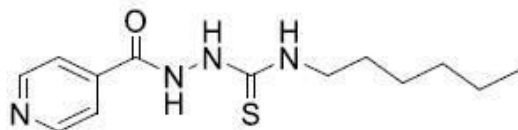
Resolution : 4 cm^{-1} (10 scans)

Spectrum : Fz-I-Iso29.0 (in D:\IRSTUDENT)

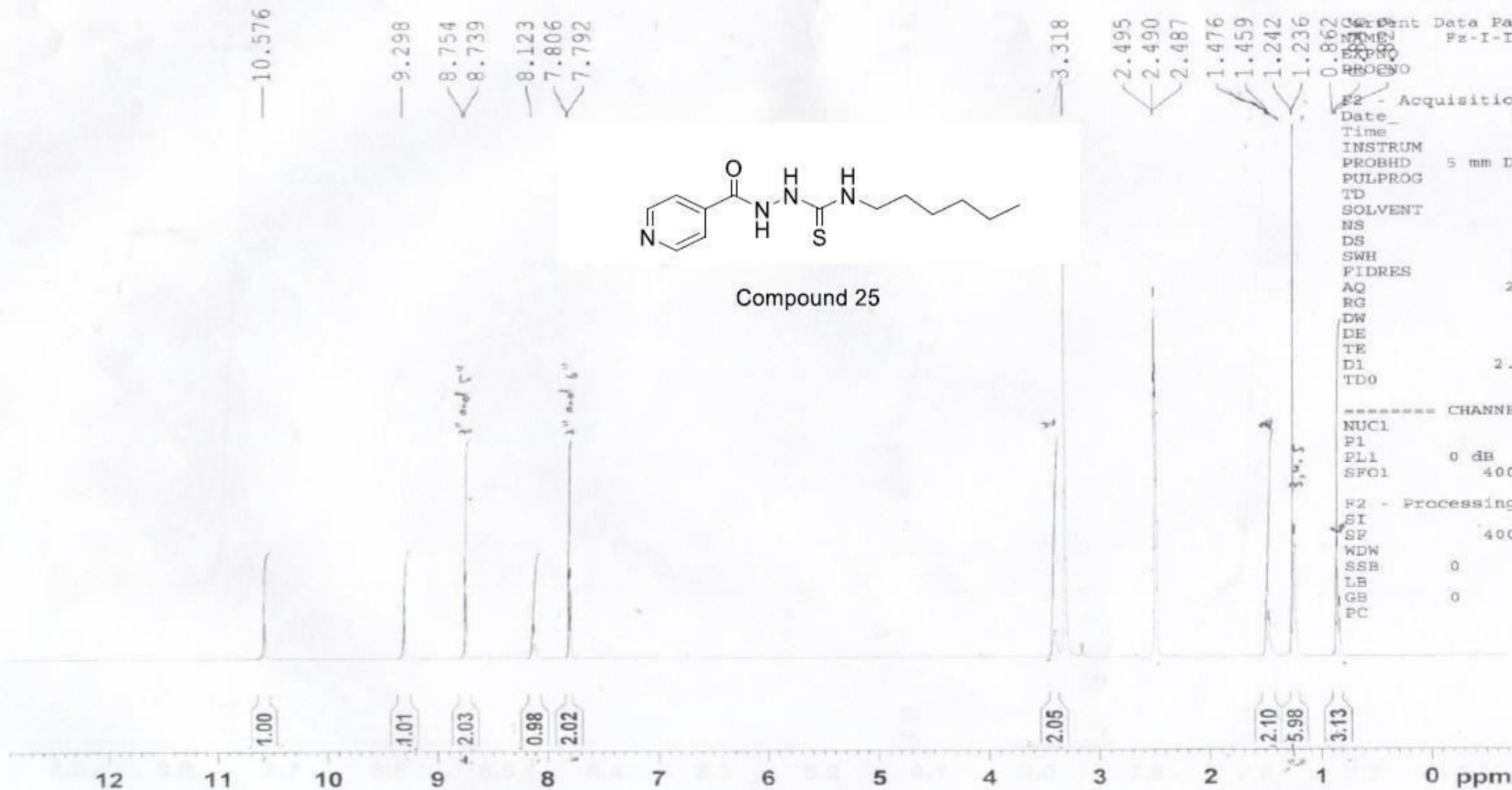
Technic : Solid

Analyst : M. Asif

Fazila/DR.Hina/Fz-I-ISO30
 ICCBS, U.O.K/1H



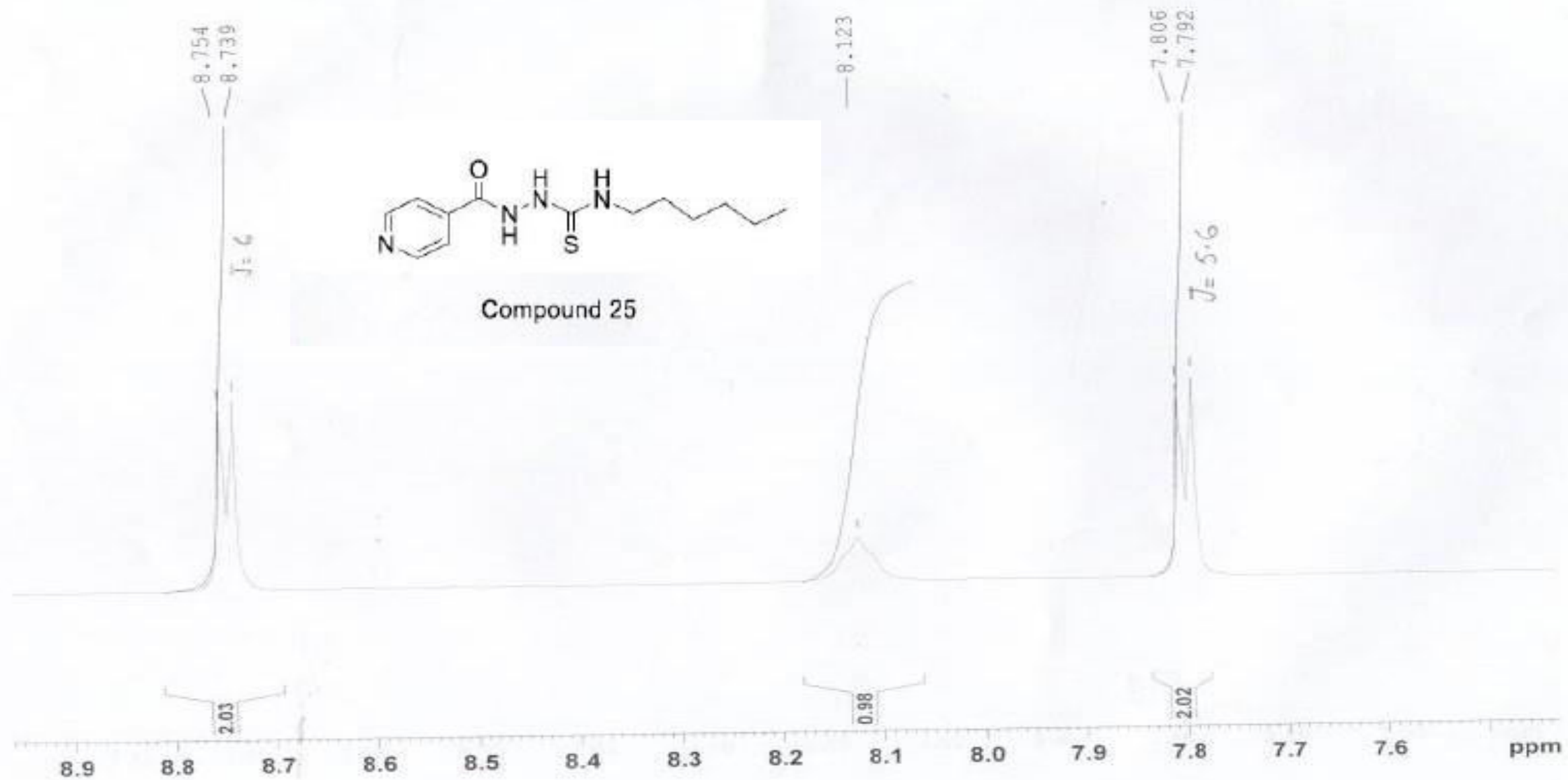
Compound 25



===== Channel f1 =====
 NUC1 1H
 P1 8.40 usec
 PL1 0 dB
 SFO1 400.1332010 MHz

F2 - Acquisition Parameters
 Date 20170418
 Time 15.32
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 322.5
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TDO 1

F2 - Processing parameters
 SI 16384
 SF 400.1300065 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



File: FZ-I-ISO30-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-20-2016 (Time Run: 12:51:42)

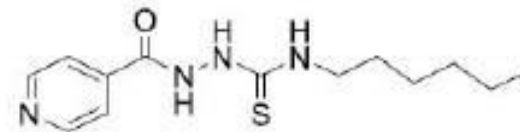
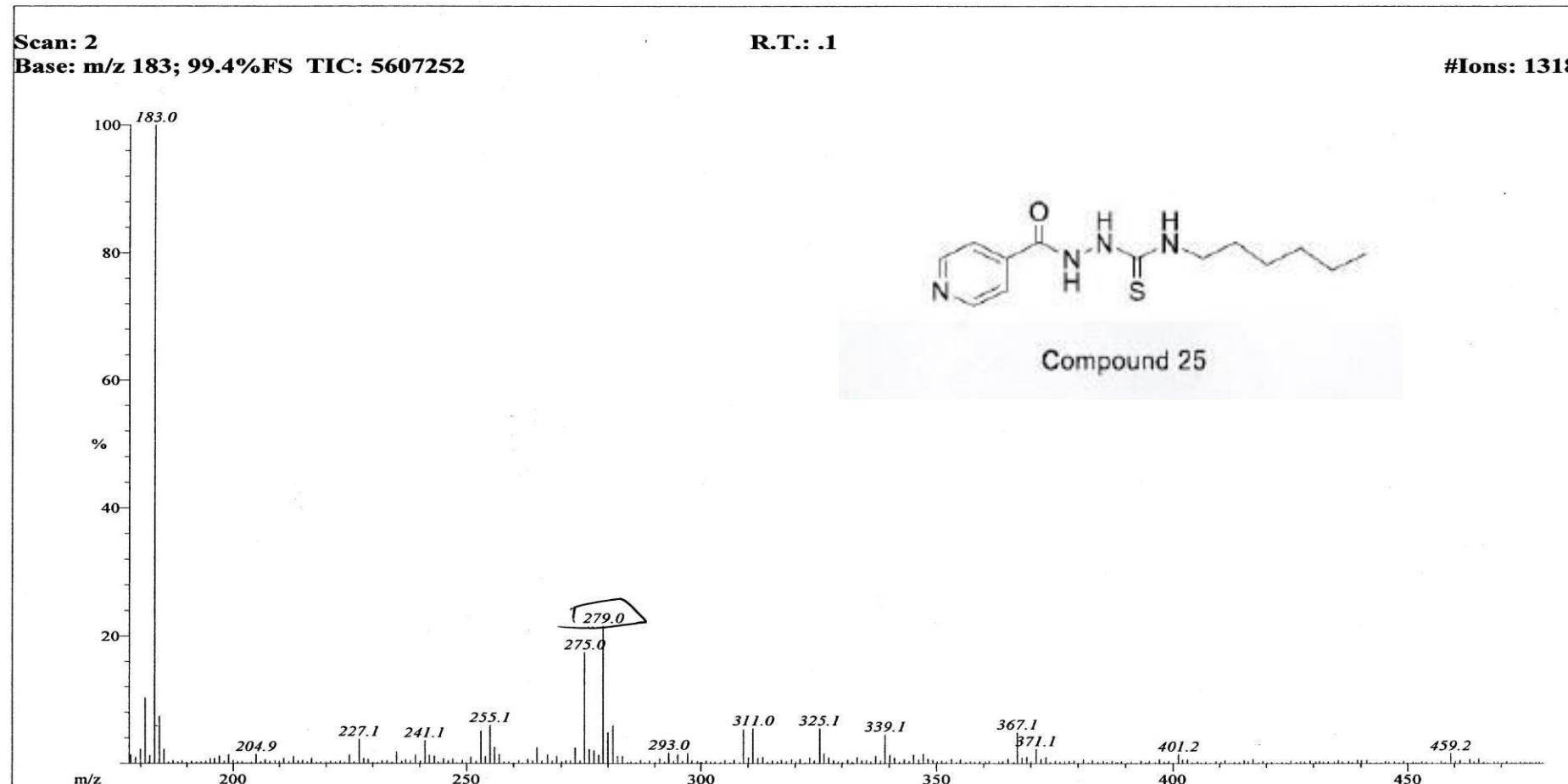
Ionization mode: FAB-

Scan: 2

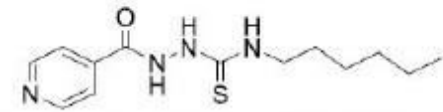
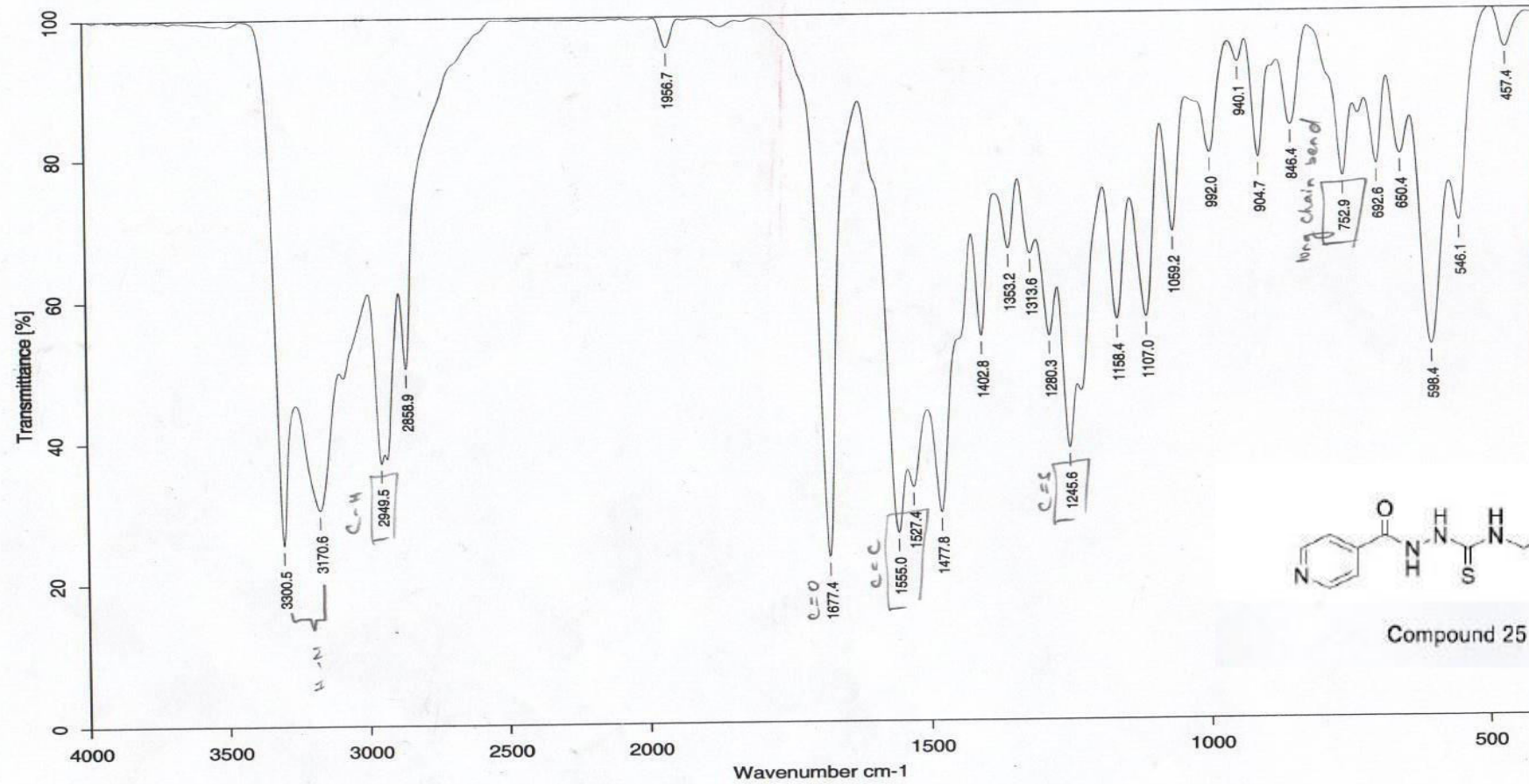
R.T.: .1

Base: m/z 183; 99.4%FS TIC: 5607252

#Ions: 1318



Compound 25



Compound 25

Sample : FZI-ISO30/Fazila Rizvi

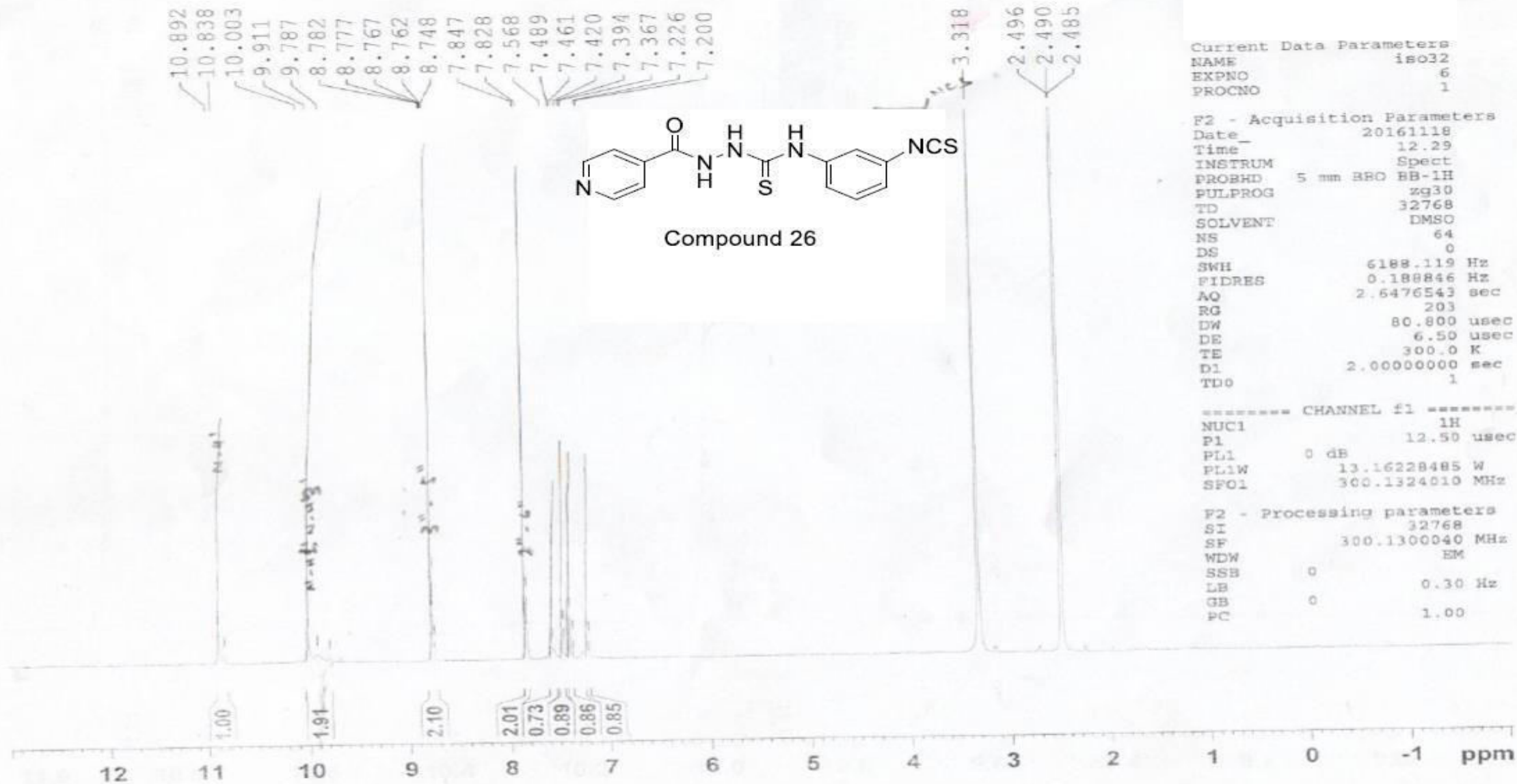
Measured : 19/04/2017 on VECTOR22

Resolution : 4 cm^{-1} (10 scans)

Spectrum : FZ-I-ISO30.0 (in D:\IRSTUDENT)

Technic : Solid

Analyst : MA/ZA/JS



Current Data Parameters

NAME	iso32
EXPNO	6
PROCNO	1

F2 - Acquisition Parameters

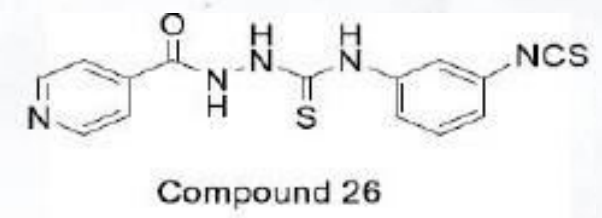
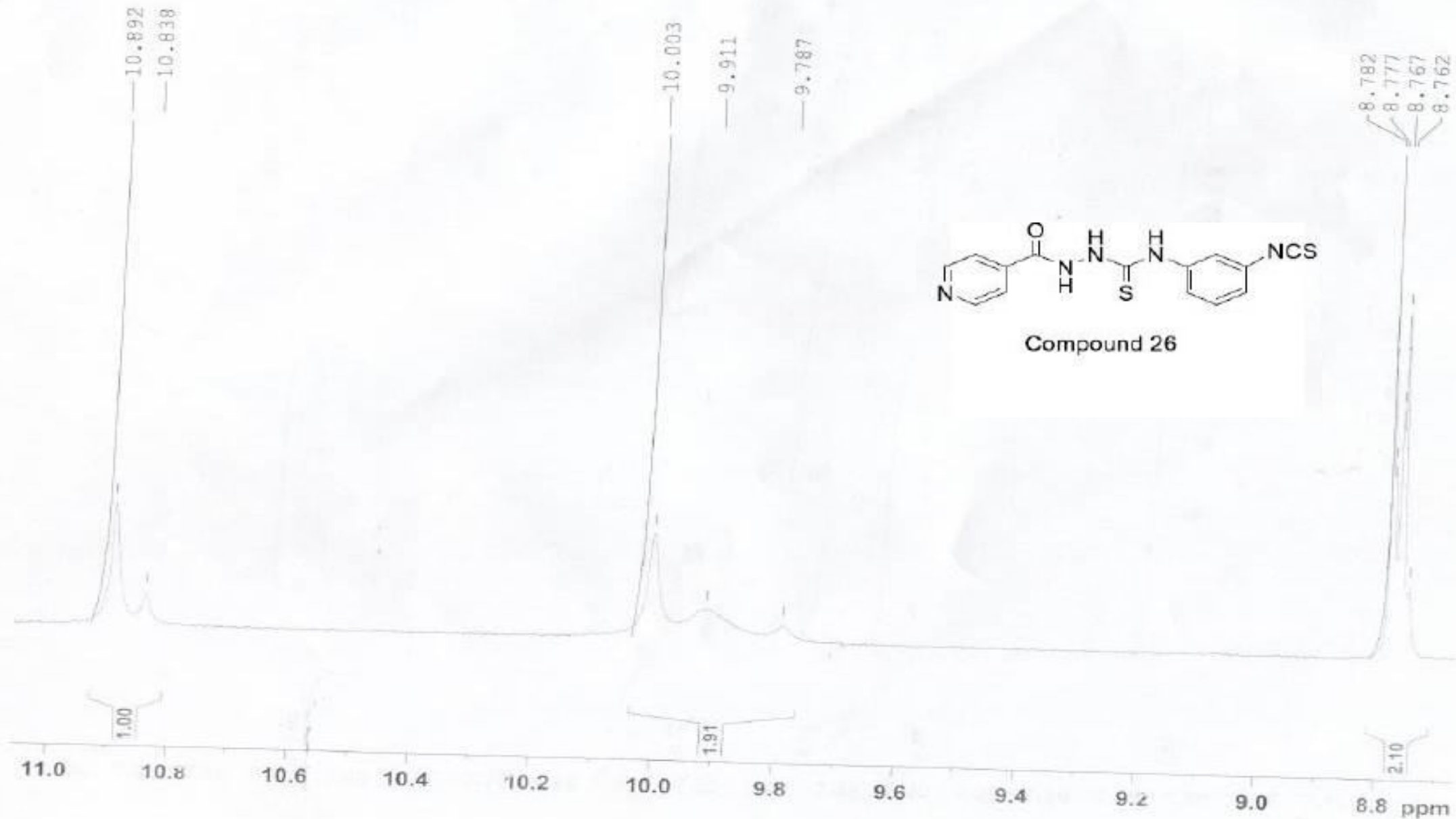
Date_	20161118
Time	12.29
INSTRUM	Spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	6188.119 Hz
FIDRES	0.188846 Hz
AQ	2.6476543 sec
RG	203
DW	80.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1

===== CHANNEL f1 =====

NUC1	1H
P1	12.50 usec
PL1	0 dB
PL1W	13.16228485 W
SFO1	300.1324010 MHz

F2 - Processing parameters

SI	32768
SF	300.1300040 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



File: FZ-I-ISO32-FABN
Sample: BUSHRA QAMAR /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 10-27-2016 (Time Run: 12:13:20)

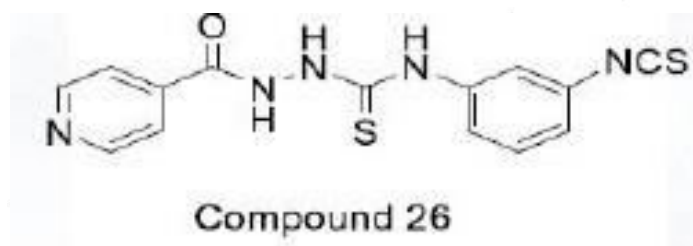
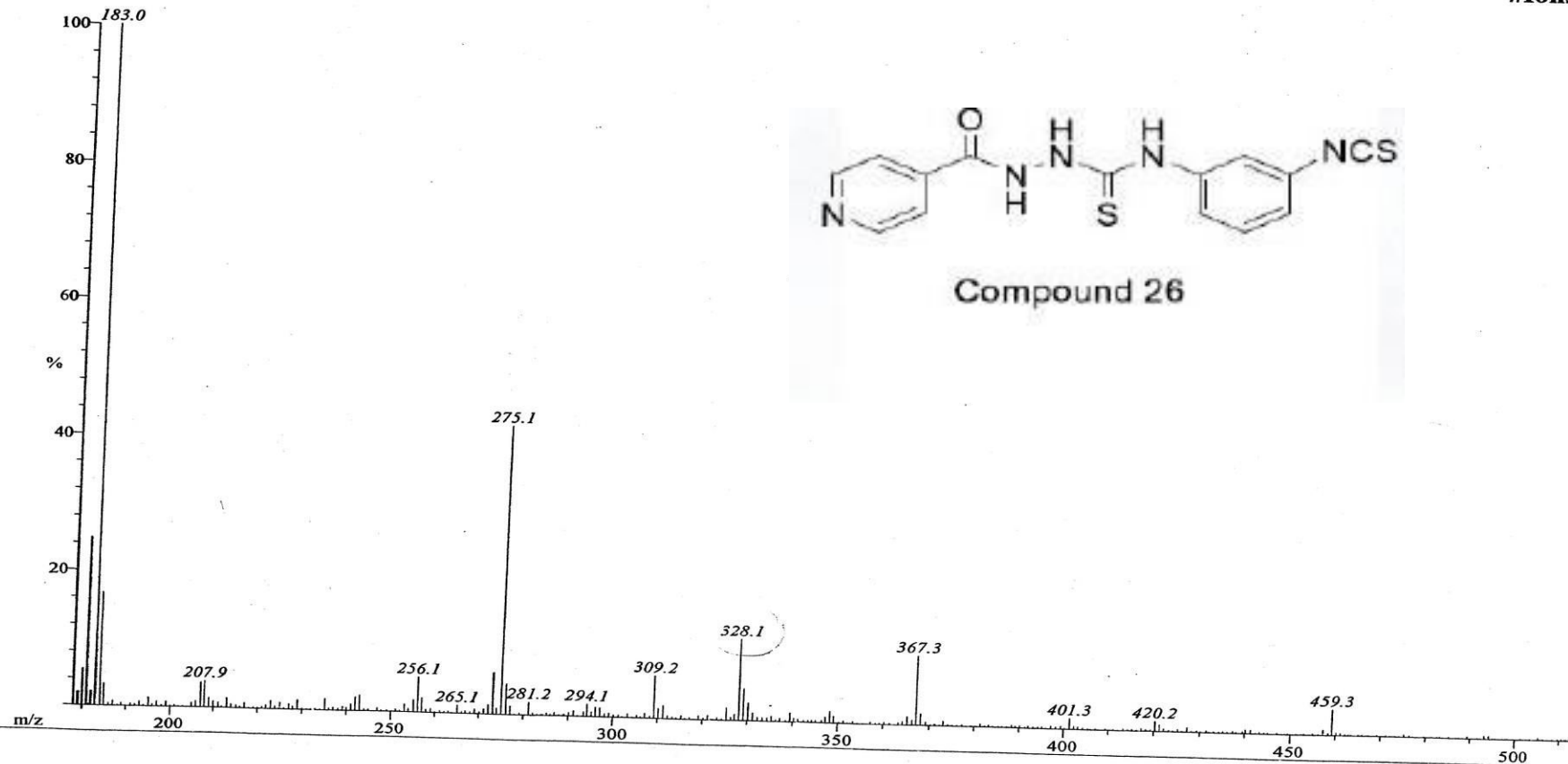
Ionization mode: FAB-

Scan: 5

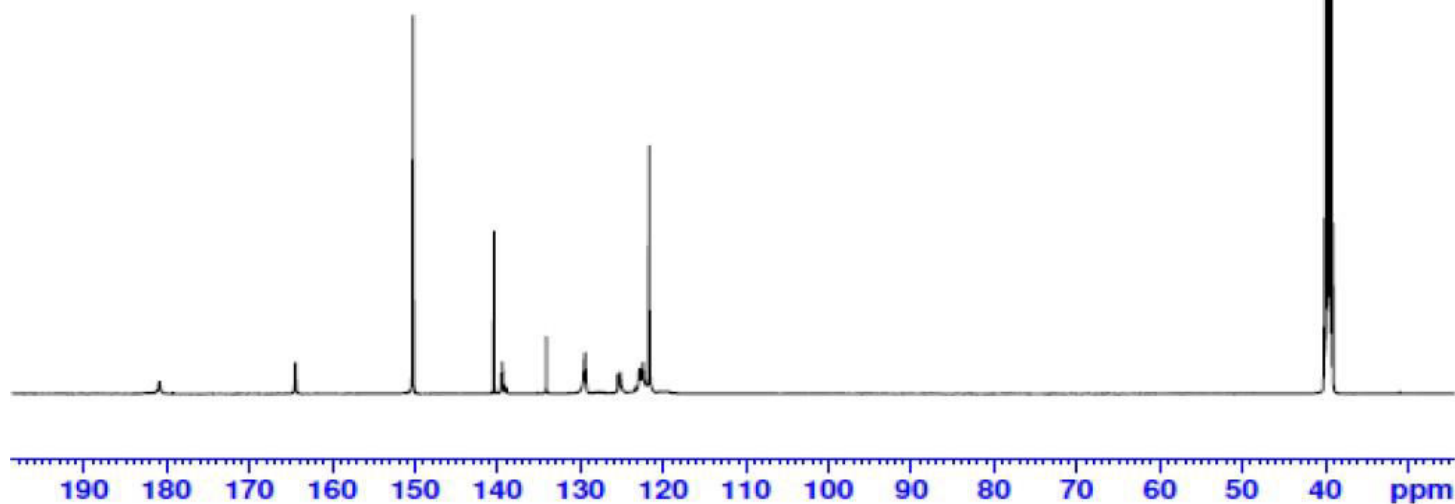
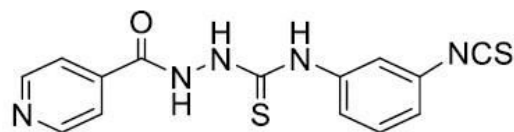
Base: m/z 183; 100%FS TIC: 5774642

R.T.: .37

#Ions: 1271



Fazila / D. Hina / FZ-I-ISO32
BB



```
parameters
NAME          ISO32 NMR
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Data_         20190205
Time          23.45 h
INSTRUM      Avance Neo 500
PROBHD       Z44862_0021 (C
PULPROG      zgpg
TD            32768
SOLVENT      DMSO
NS            16384
DS            8
SWH           30120.482 Hz
FIDRES        1.838408 Hz
AQ            0.5439488 sec
RG            101
DW            16.600 usec
DE            20.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.03000000 sec
TD0           16
SFO1          125.8227986 MHz
NUC1          13C
P1            10.00 usec
PLW1          26.46199989 W
SFO2          500.3320013 MHz
NUC2          1H
CPDPRG[2]    waltz65
PCPD2         80.00 usec
PLW2          9.74149990 W
PLW12         0.34246999 W
PLW13         0.17199001 W

F2 - Processing parameters
SI            16384
SF            125.8081399 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

Fazila / D. Hina / FZ-I-ISO32
DEPT135

150.24

129.43

125.50

125.21

122.81

122.43

121.64

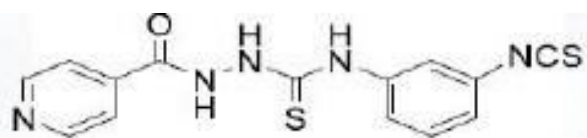
40.10

39.93

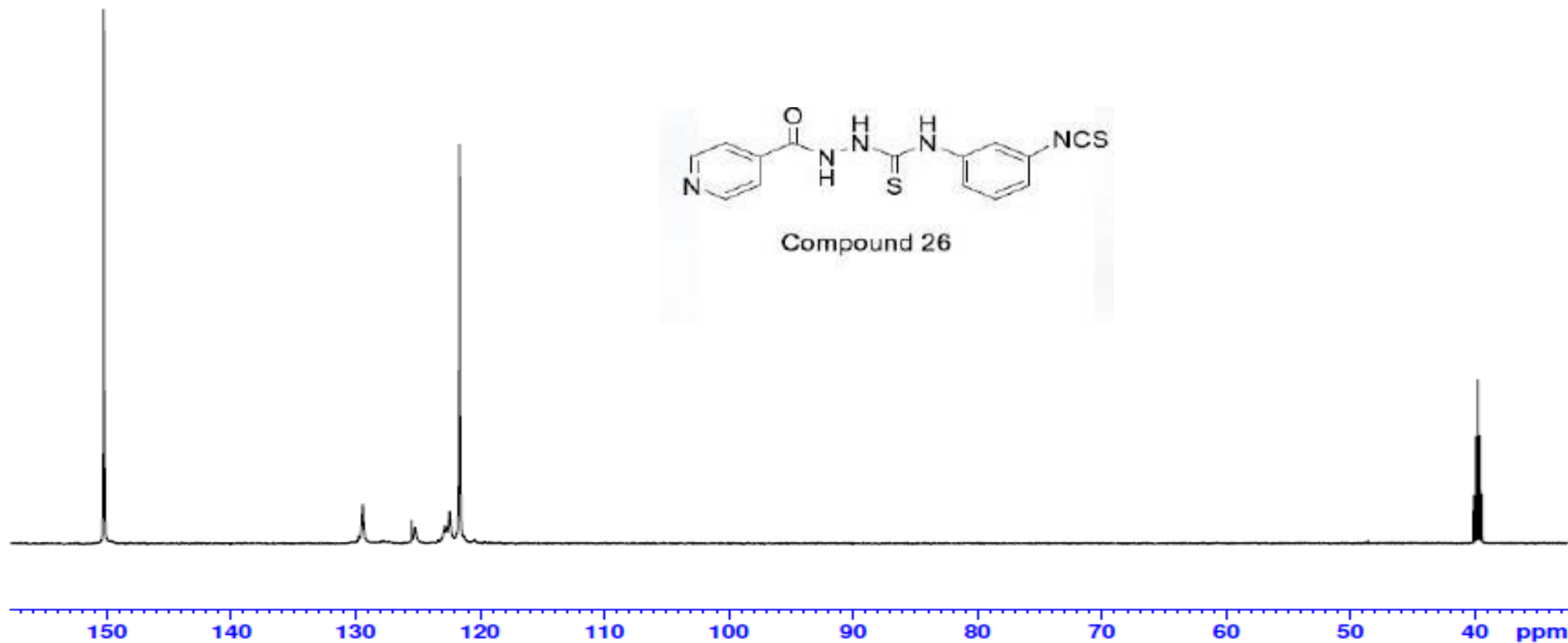
39.76

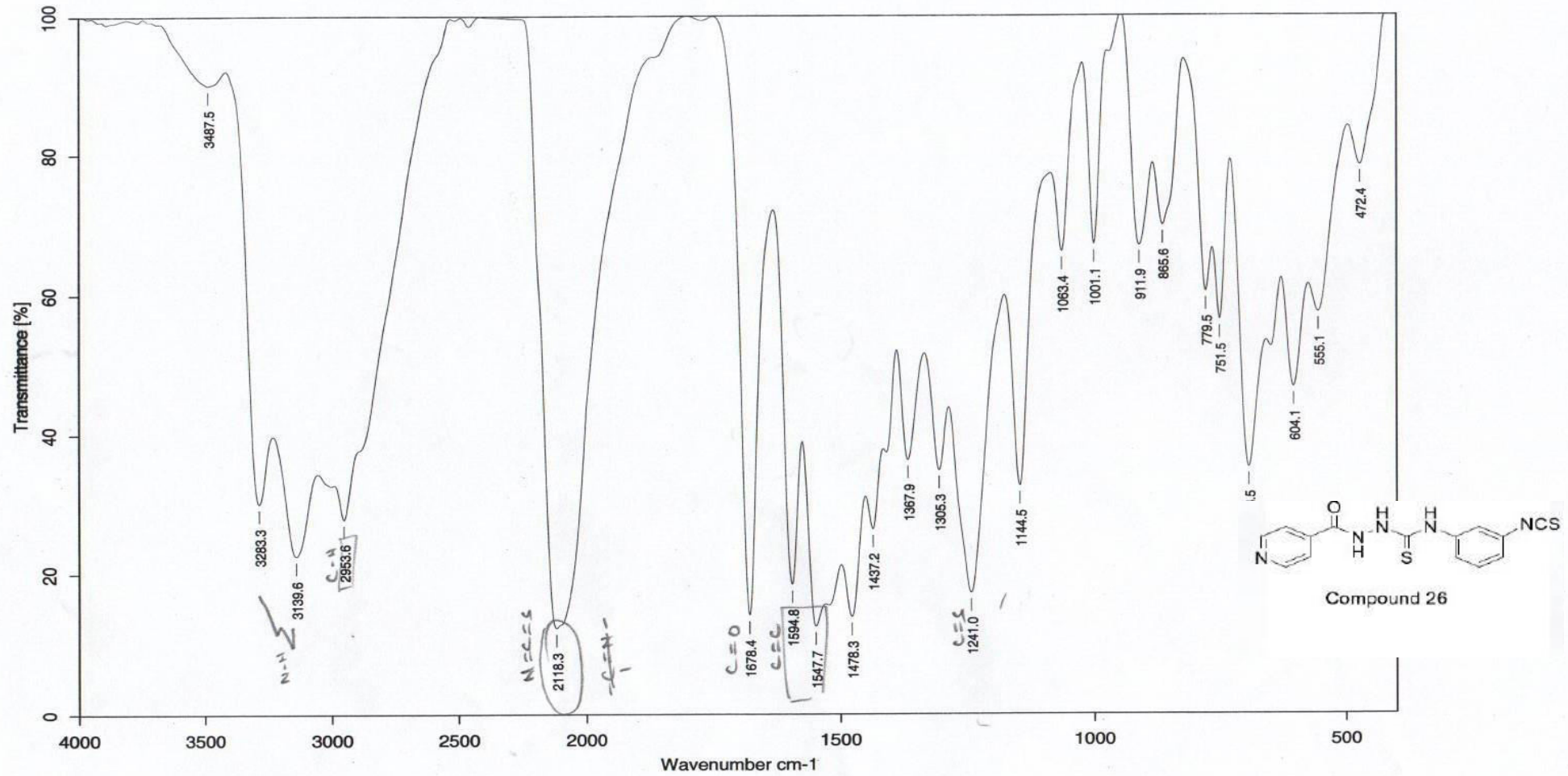
39.59

39.43



Compound 26





Sample : FZI-ISO32/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

Resolution : 4 cm⁻¹ (10 scans)

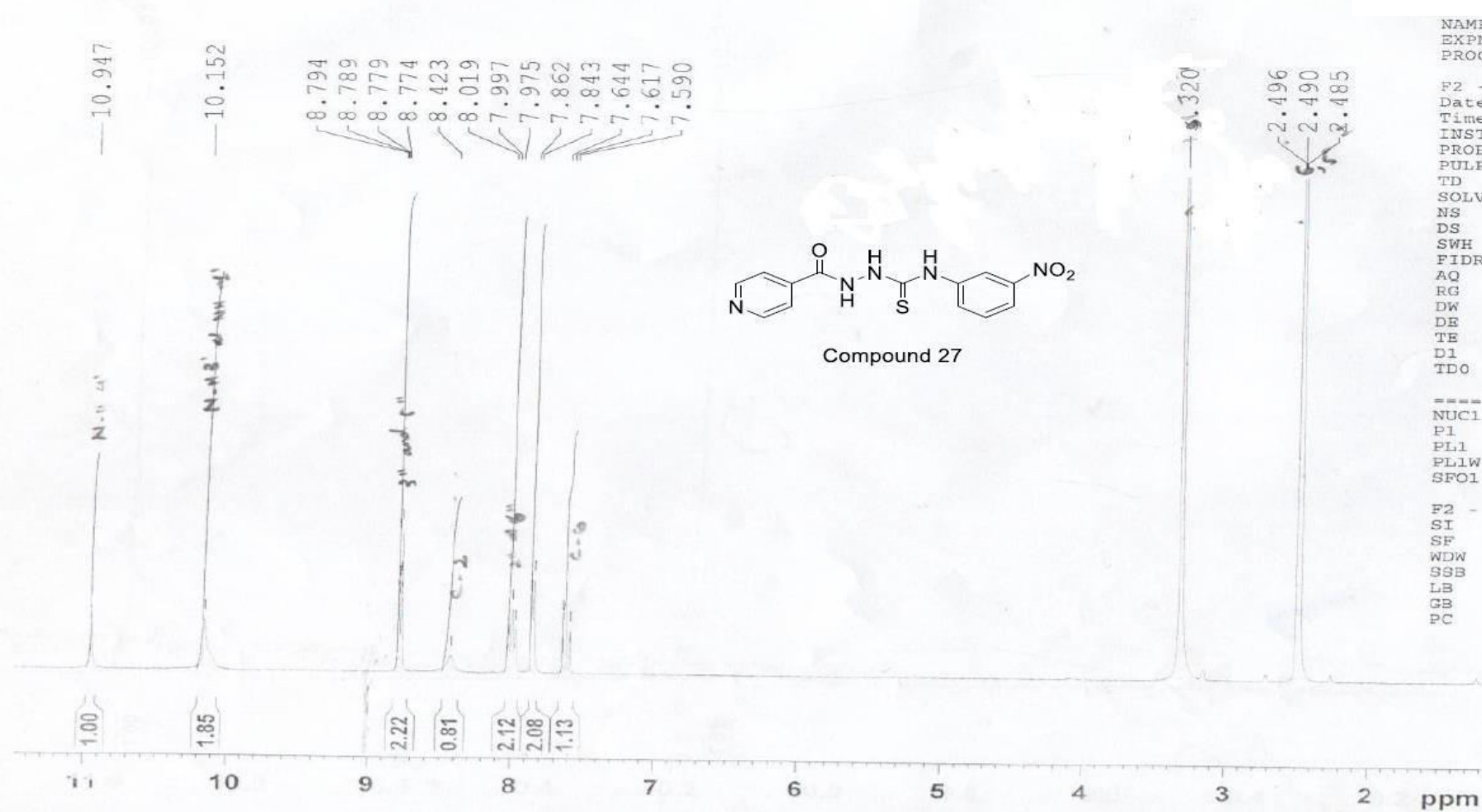
Spectrum : FZ-I-ISO32.0 (in D:\IRSTUDENT)

Technic : Solid

Analyst : MA/ZA/JS

fazila rizvi/Dr.Hina/Fz-I-iso33

14



NAME
EXPNO
PROCNO

eters
iso33
7
1

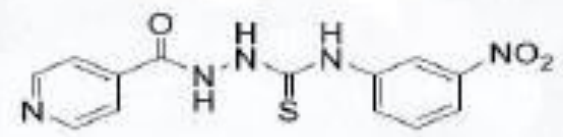
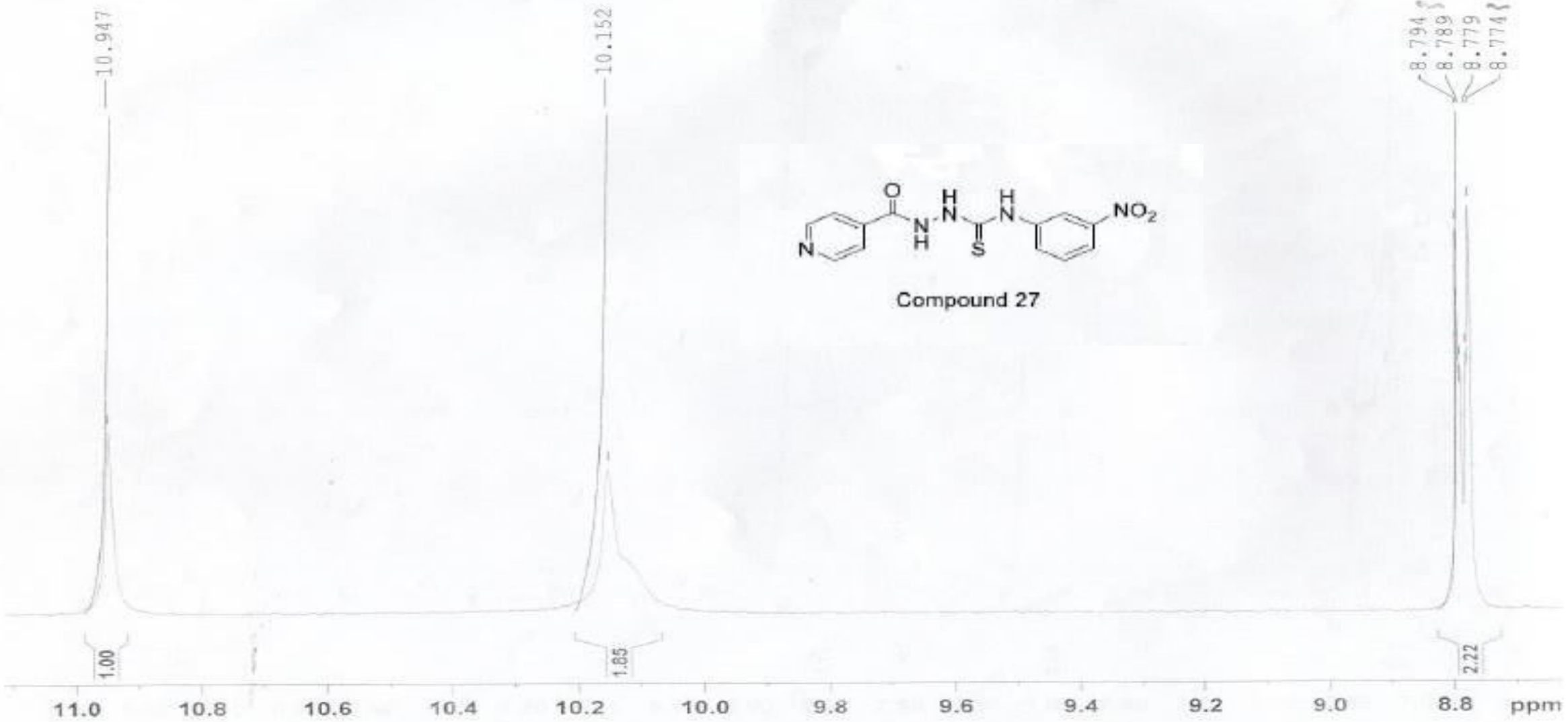
F2 - Acquisition Parameters

Date_ 20161118
Time_ 12.39
INSTRUM Spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 0 dB
PL1W 13.16228485 W
SF01 300.1324010 MHz

F2 - Processing parameters

SI 32768
SF 300.1300040 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Compound 27

File: FZ-I-ISO33-FABN
Sample: FAZILA /DR. HINA
Instrument: JEOL-600H-2
Inlet: Direct Probe

Date Run: 12-01-2016 (Time Run: 13:41:56)

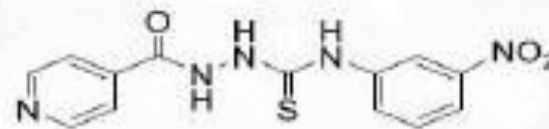
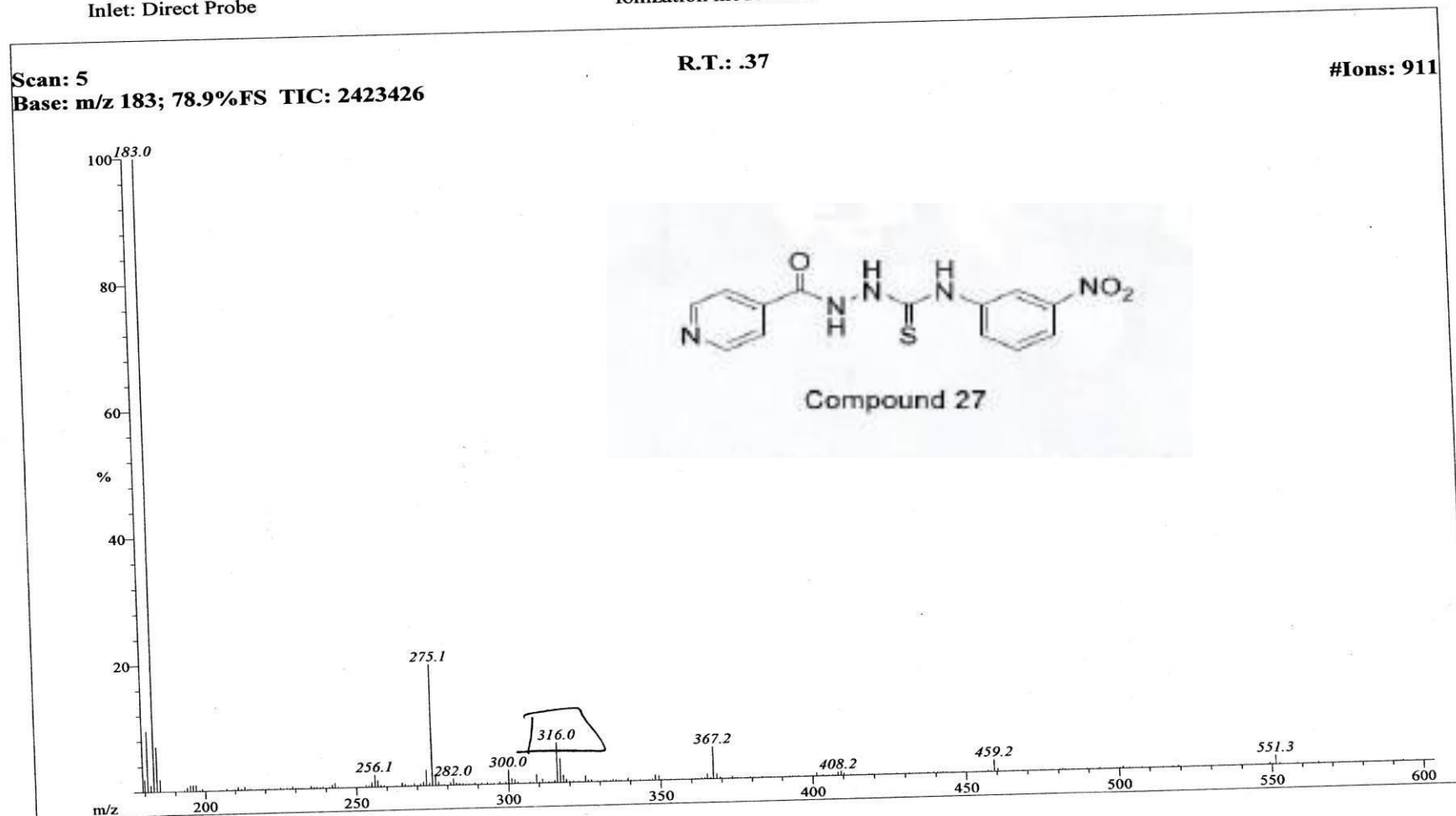
Ionization mode: FAB-

Scan: 5

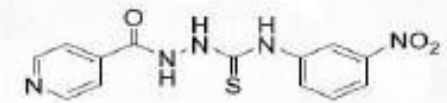
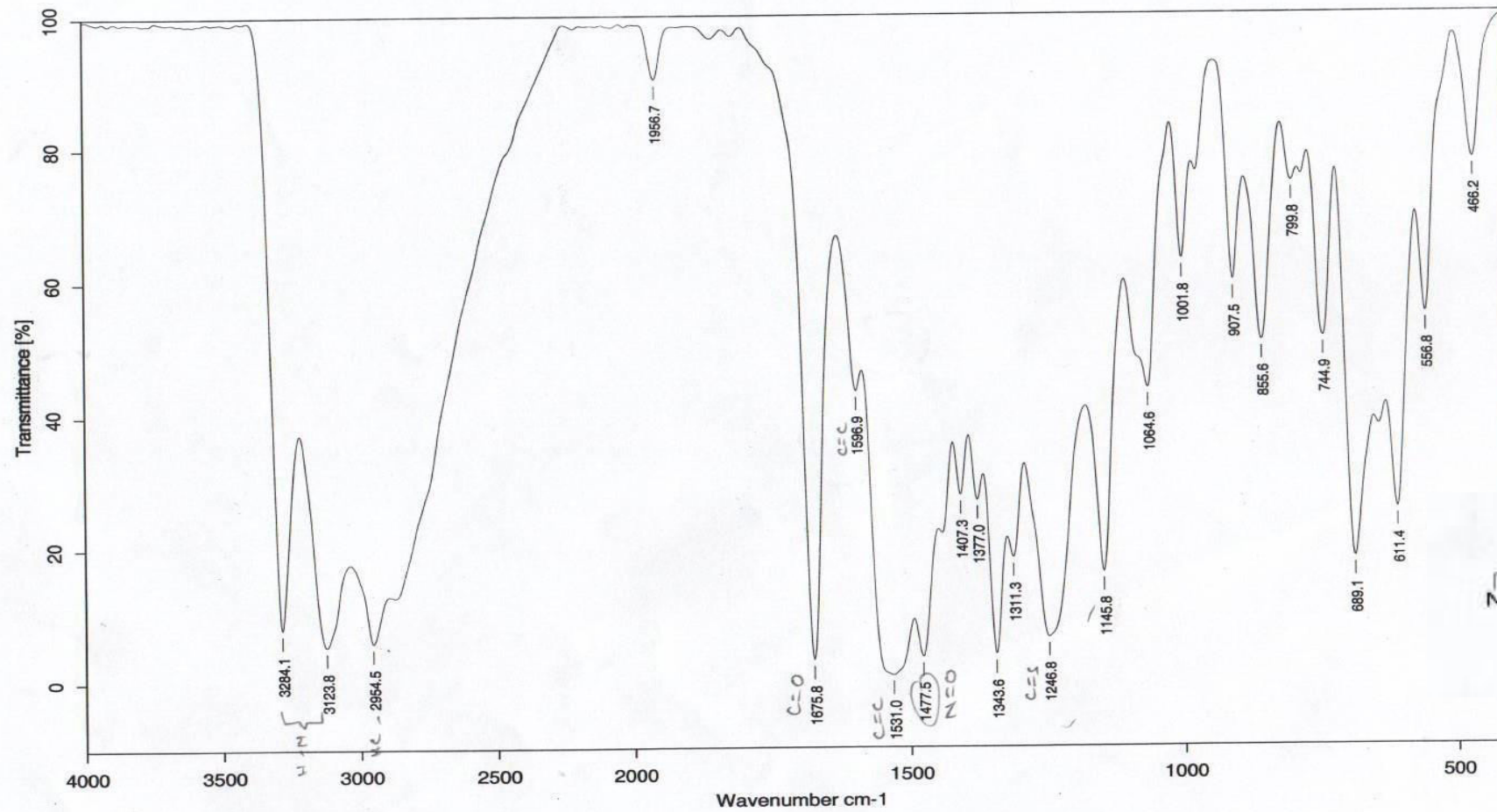
R.T.: .37

#Ions: 911

Base: m/z 183; 78.9%FS TIC: 2423426



Compound 27



Compound 27

Sample : FZI-ISO33/Fazila Rizvi

Measured : 19/04/2017 on VECTOR22

Resolution : 4 cm^{-1} (10 scans)

Spectrum : FZ-I-ISO33.0 (in D:\IRSTUDENT)

Technic : Solid

Analyst : MA/ZA/JS