

Supporting Information

An unprecedented deoxygenation protocol of benzylic alcohols using *bis*(1-benzotriazolyl)methanethione

Dhananjay Kumar,[§] Anoop S. Singh and Vinod K. Tiwari*

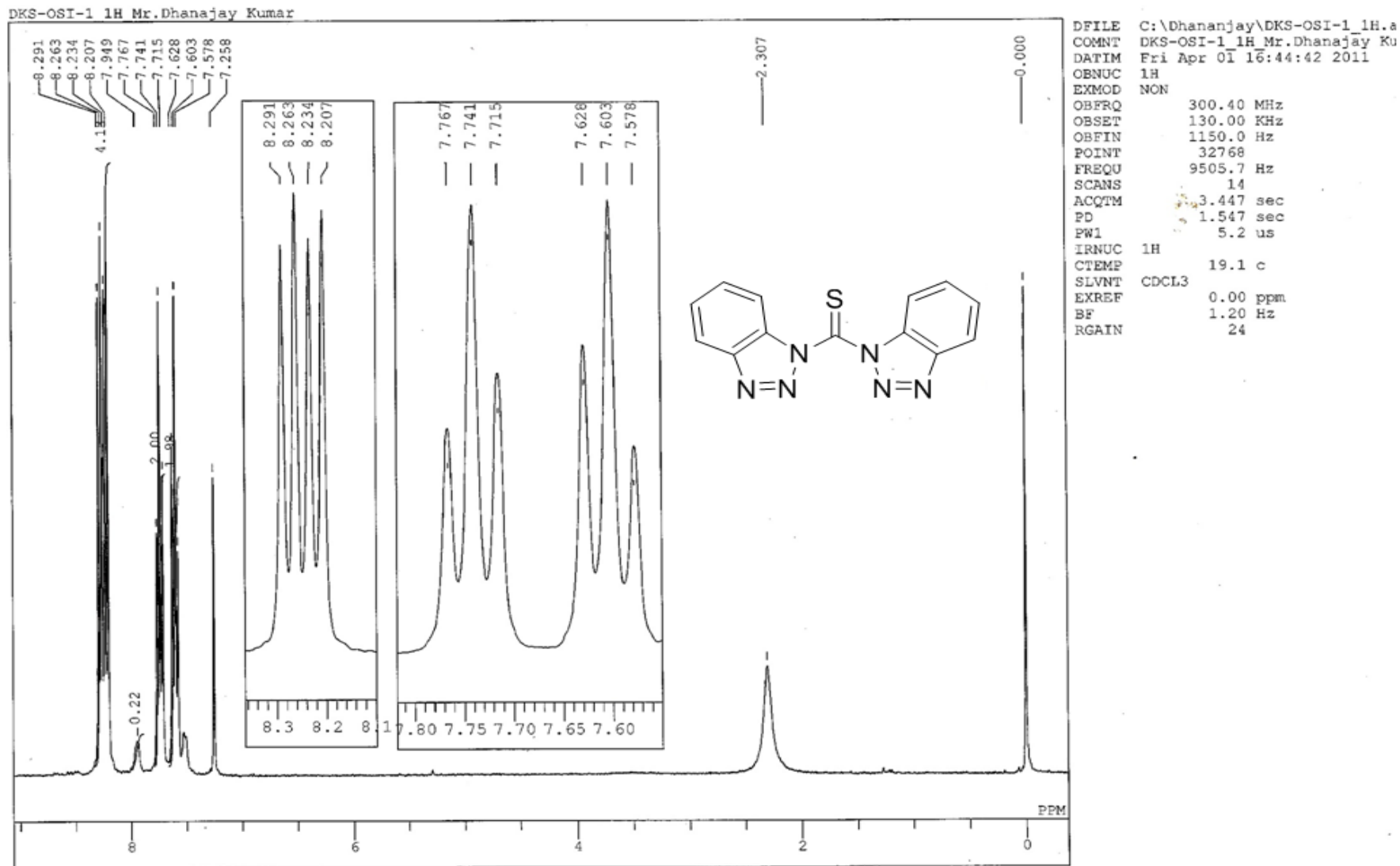
Department of Chemistry, Faculty of Science, Banaras Hindu University, Varanasi 221 005, India.

[§]*Present address:* Department of Chemistry, Indian Institute of Technology Delhi, New Delhi, Delhi 110 016, India.

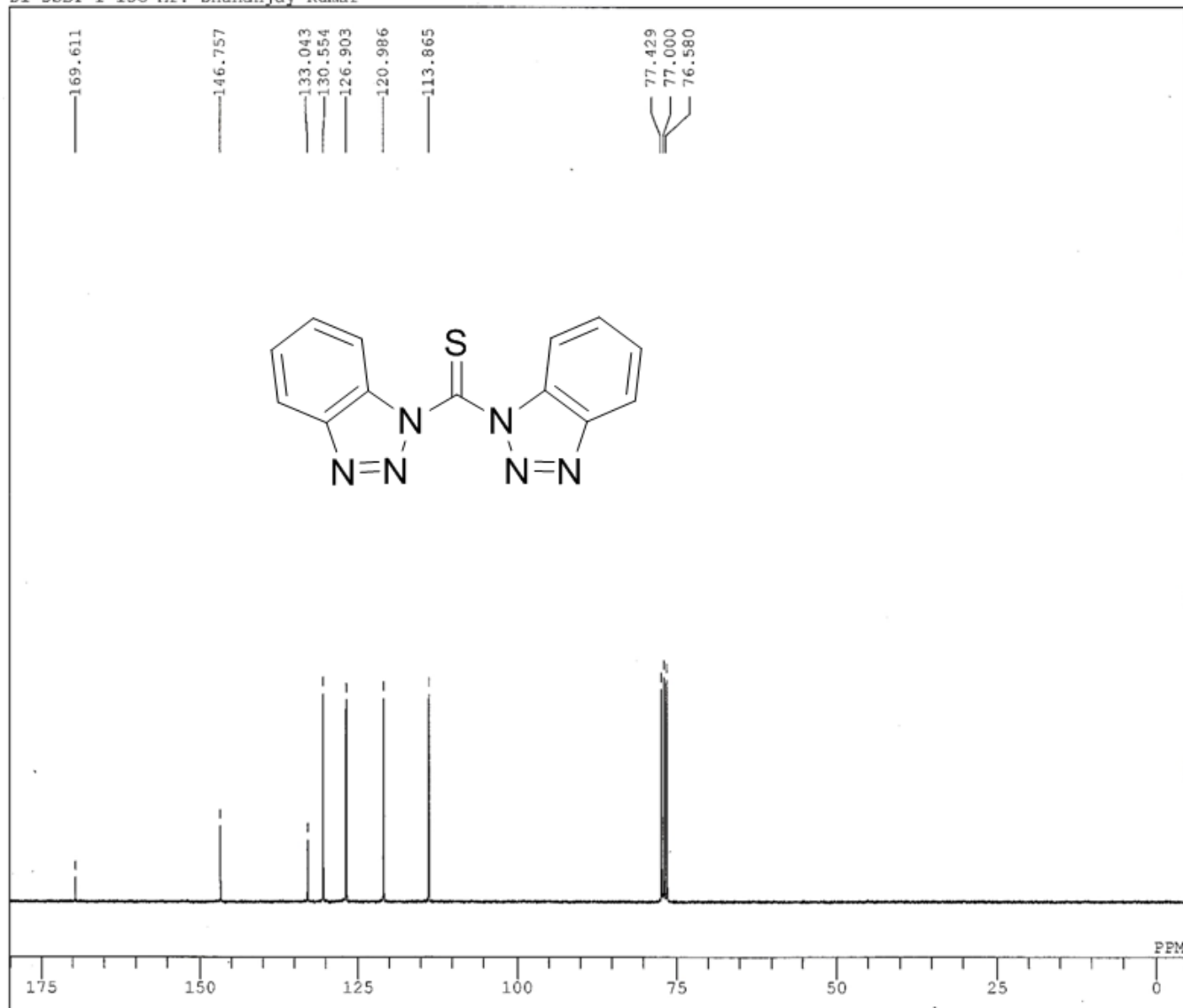
**Corresponding author: E-mail: tiwari_chem@yahoo.co.in, Tel.: +91-542-6702466; fax: +91-542-236817*

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Spectrum 1: 300 MHz ¹H NMR of compound 2

D1-DSBT-1 13C Mr. Dhananjay Kumar

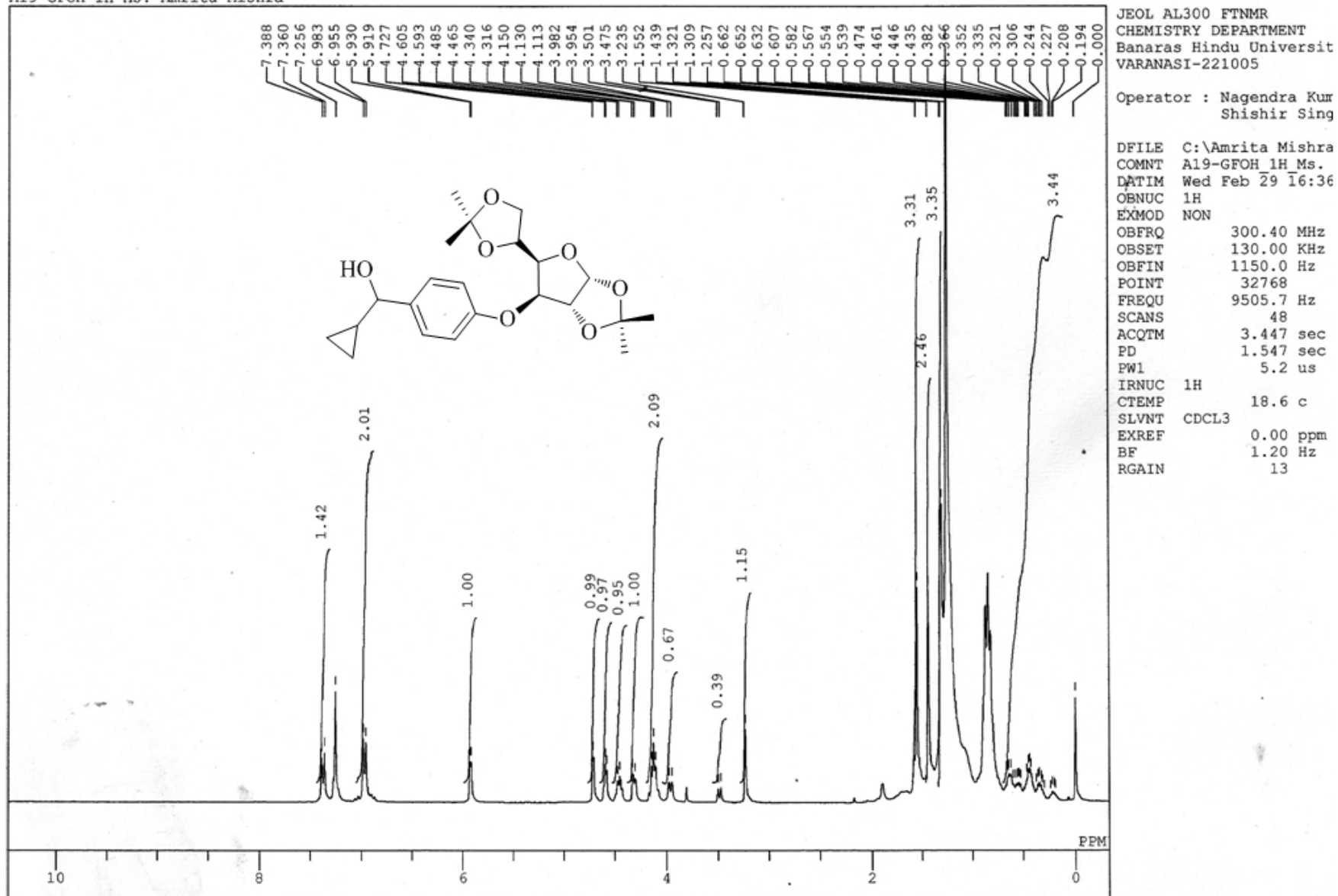
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005Operator : Nagendra Kumar
Shishir Singh

D1-DSBT-1 13C Mr. Dhananjay Kumar

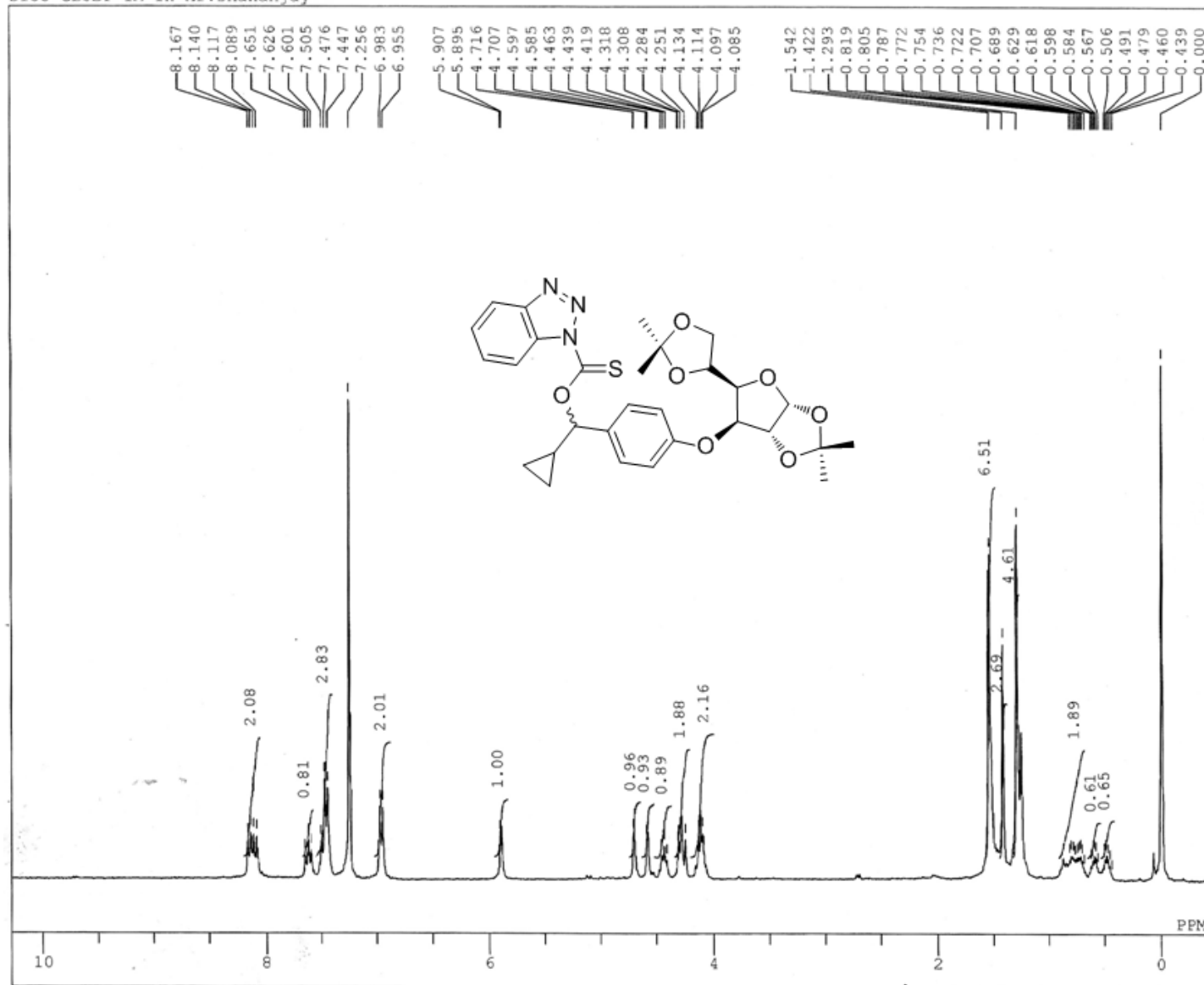
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POINT 32768
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PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 27

Spectrum 2: 75 MHz ¹³C NMR of compound 2

A19-GFOH 1H Ms. Amrita Mishra

Spectrum 3: 300 MHz ^1H NMR of compound 10

D153-GLUBT-1A 1H Mr.Dhananjay



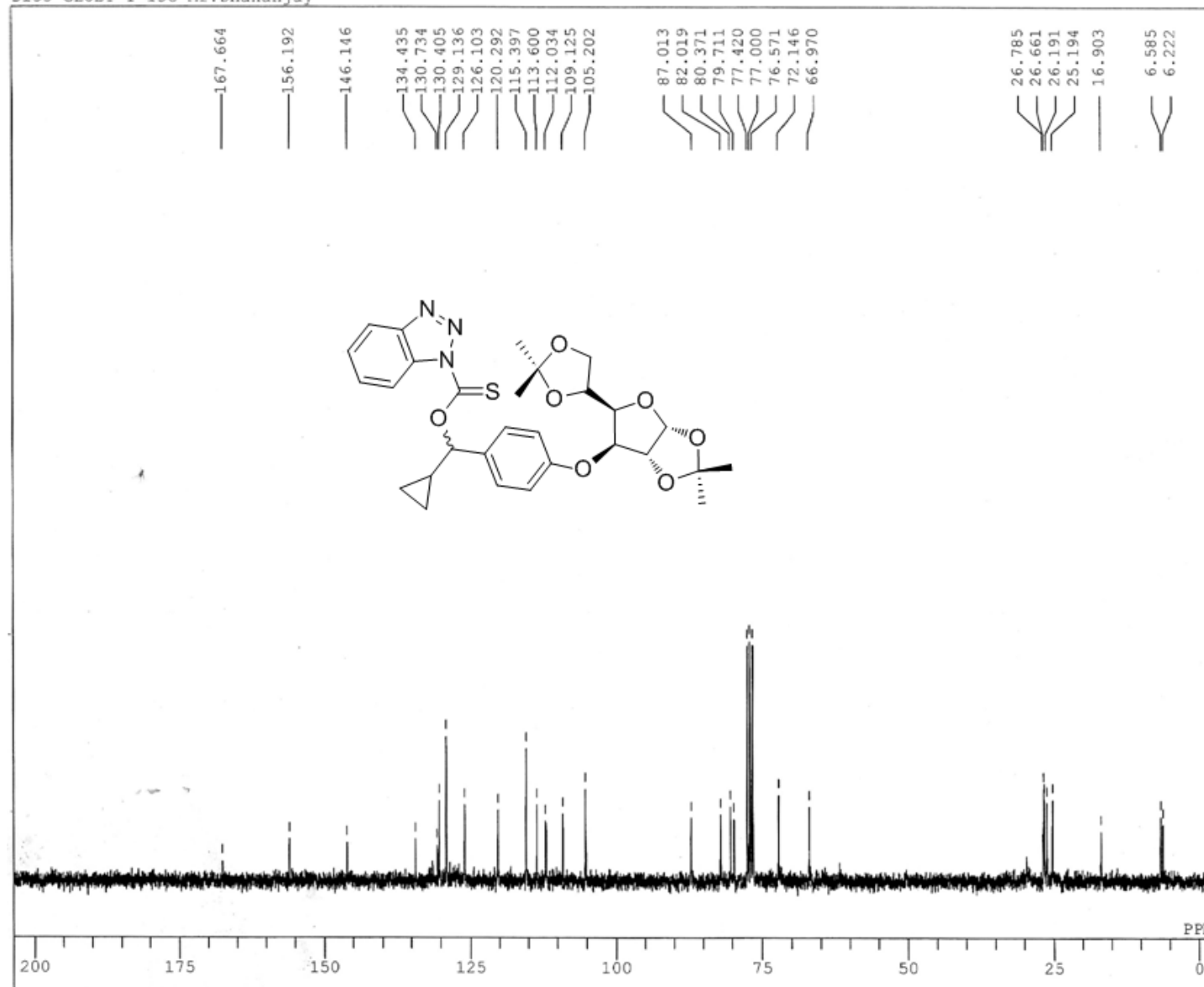
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 POINT 32768
 FREQU 9505.7 Hz
 SCANS 26
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 PW1 5.2 us
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 CTEMP 21.3 c
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 BF 1.20 Hz
 RGAIN 22

Spectrum 4: 300 MHz ¹H NMR of compound 11

D153-GLUBT-1 13C Mr.Dhananjay



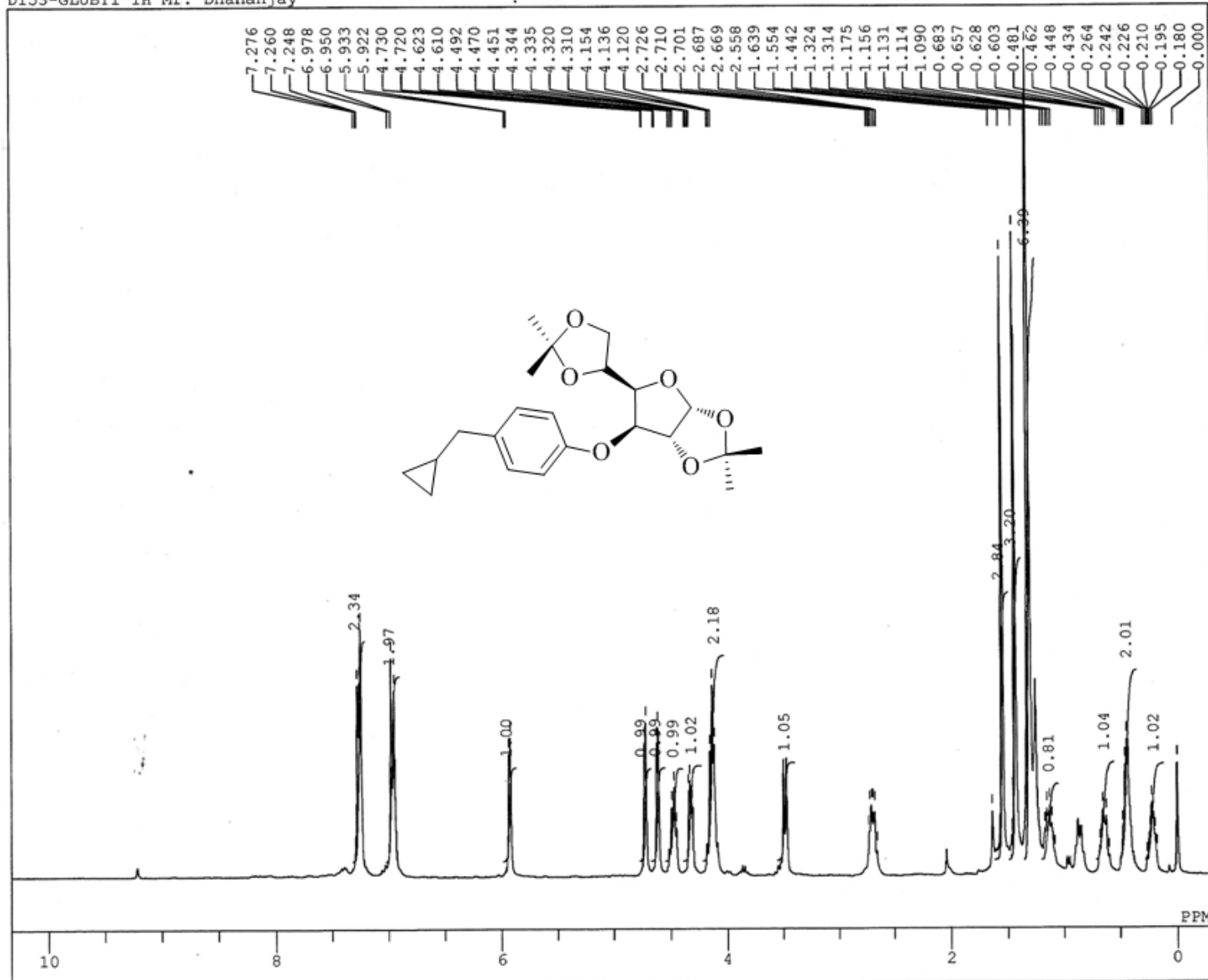
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 RGAIN 24

Spectrum 5: 75 MHz ^{13}C NMR of compound 11

D153-GLUBTI 1H Mr. Dhananjay



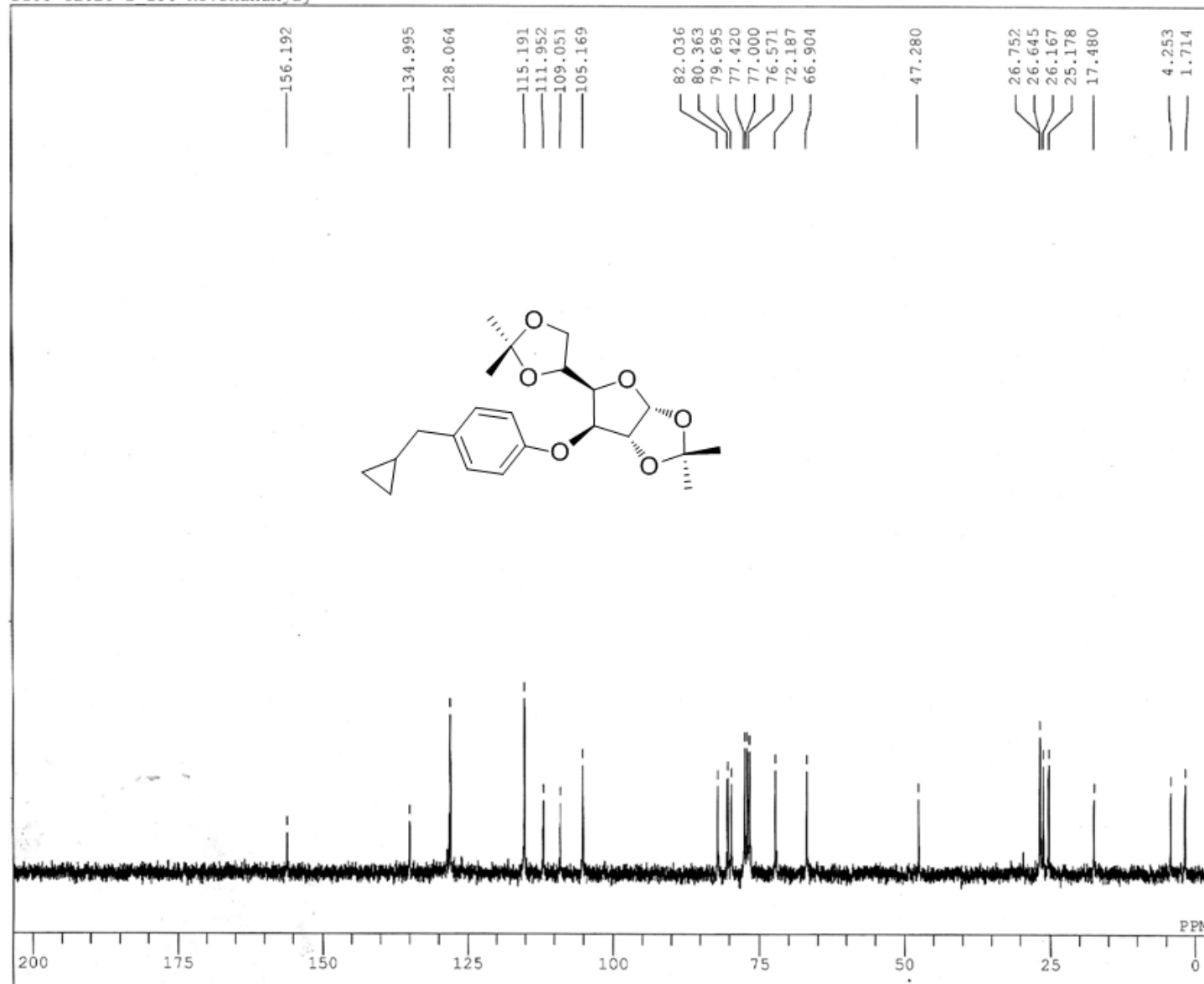
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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Fri Mar 16 16:49
1H
NON
300.40 MHz
130.00 KHz
1150.0 Hz
32768
9505.7 Hz
16
3.447 sec
1.547 sec
5.2 us
1H
20.9 c
CDCL3
0.00 ppm
1.20 Hz
14

Spectrum 6: 300 MHz ¹H NMR of compound 12

D153-GLUBT-2 13C Mr.Dhananjay



JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

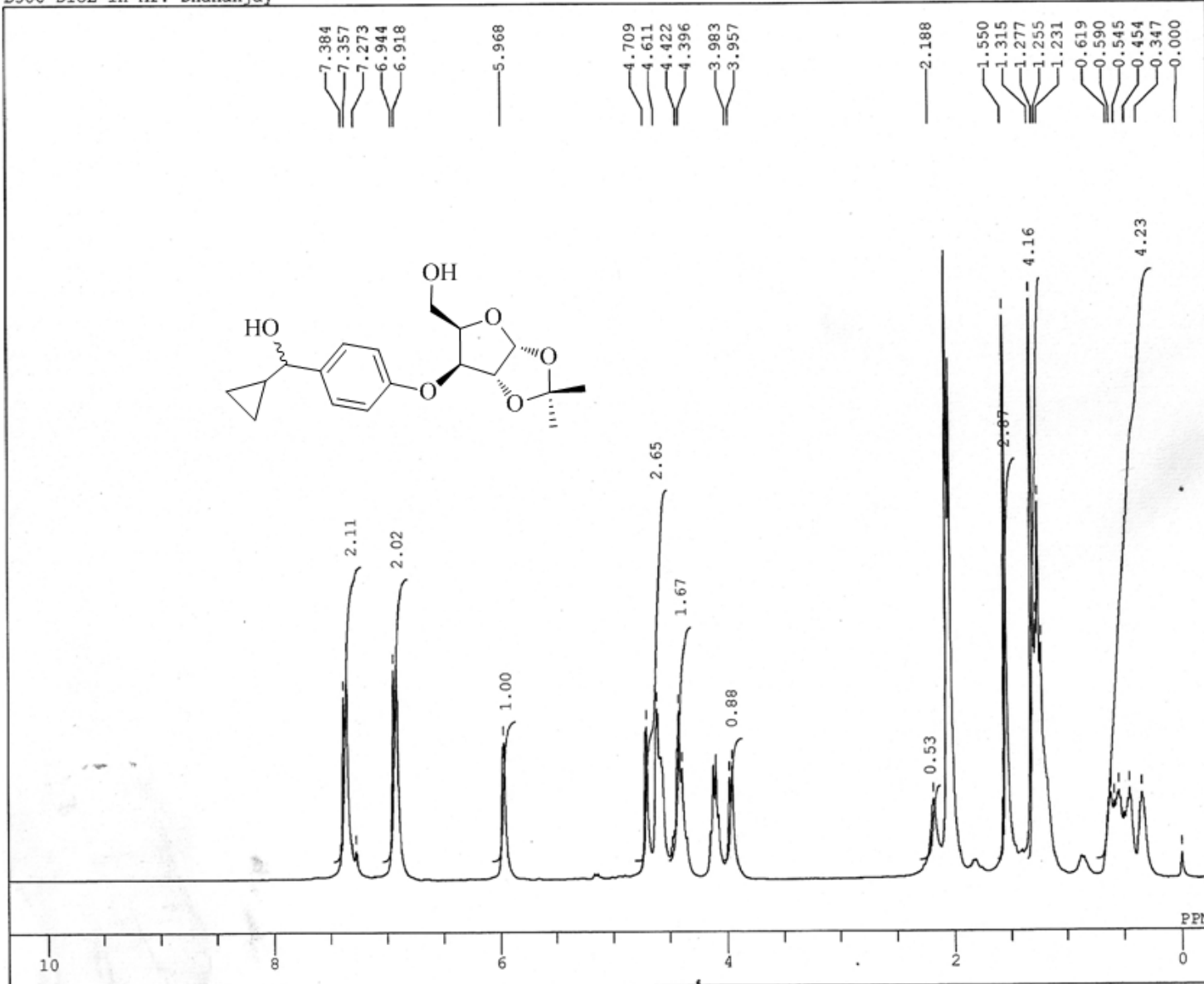
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 Shishir Singh

D153-GLUBT-2 13C Mr.Dhananjay

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 PW1 6.0 us
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 CTEMP 21.0 c
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 RGAIN 25

Spectrum 7: 75 MHz ^{13}C NMR of compound 12

D380-DIOL 1H Mr. Dhananjay



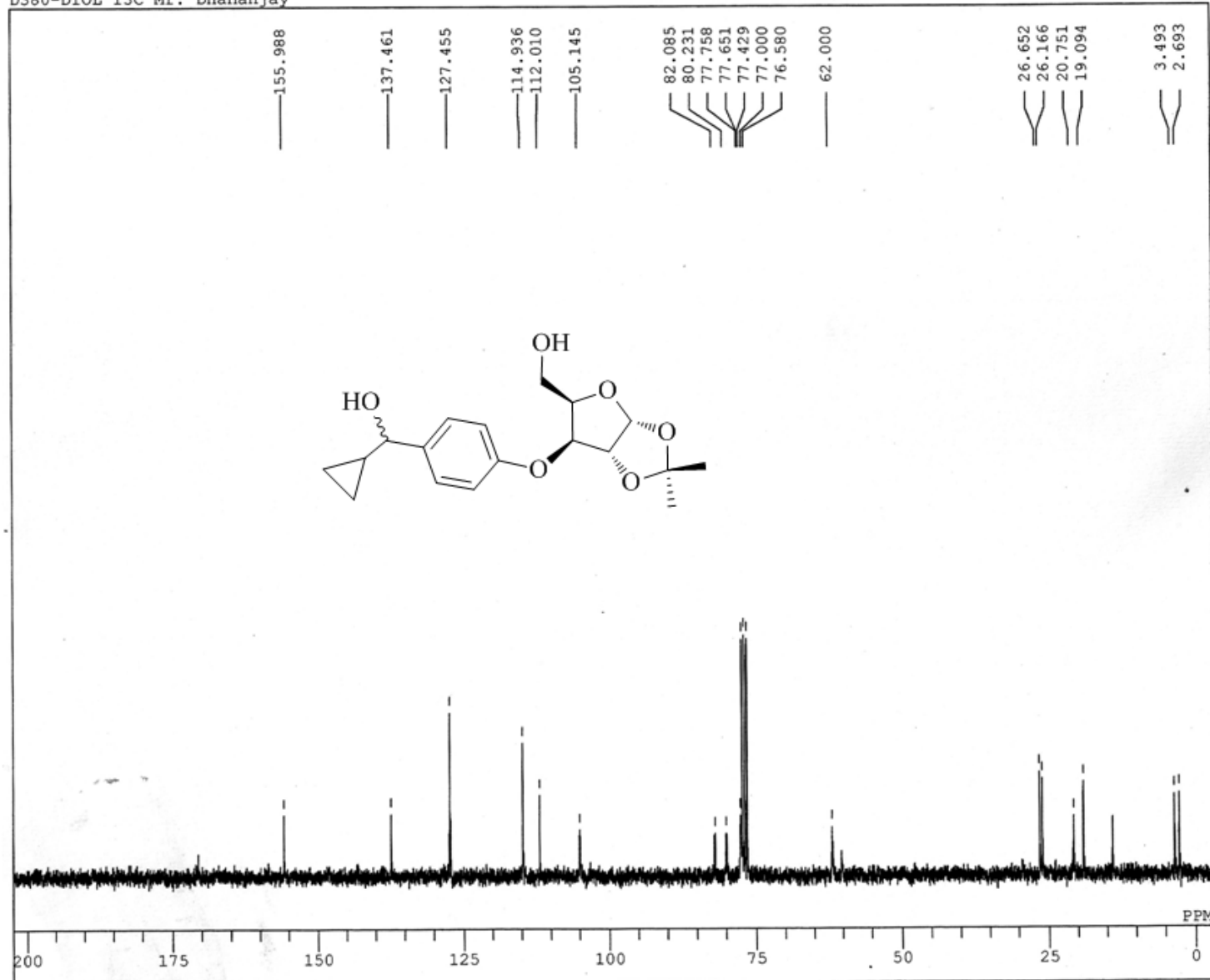
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu Universit
 VARANASI-221005

Operator : Nagendra Kum
 Shishir Sing

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 CTEMP 24.3 c
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 RGAIN 13

Spectrum 8: 300 MHz ¹H NMR of compound 16

D380-DIOL 13C Mr. Dhananjay



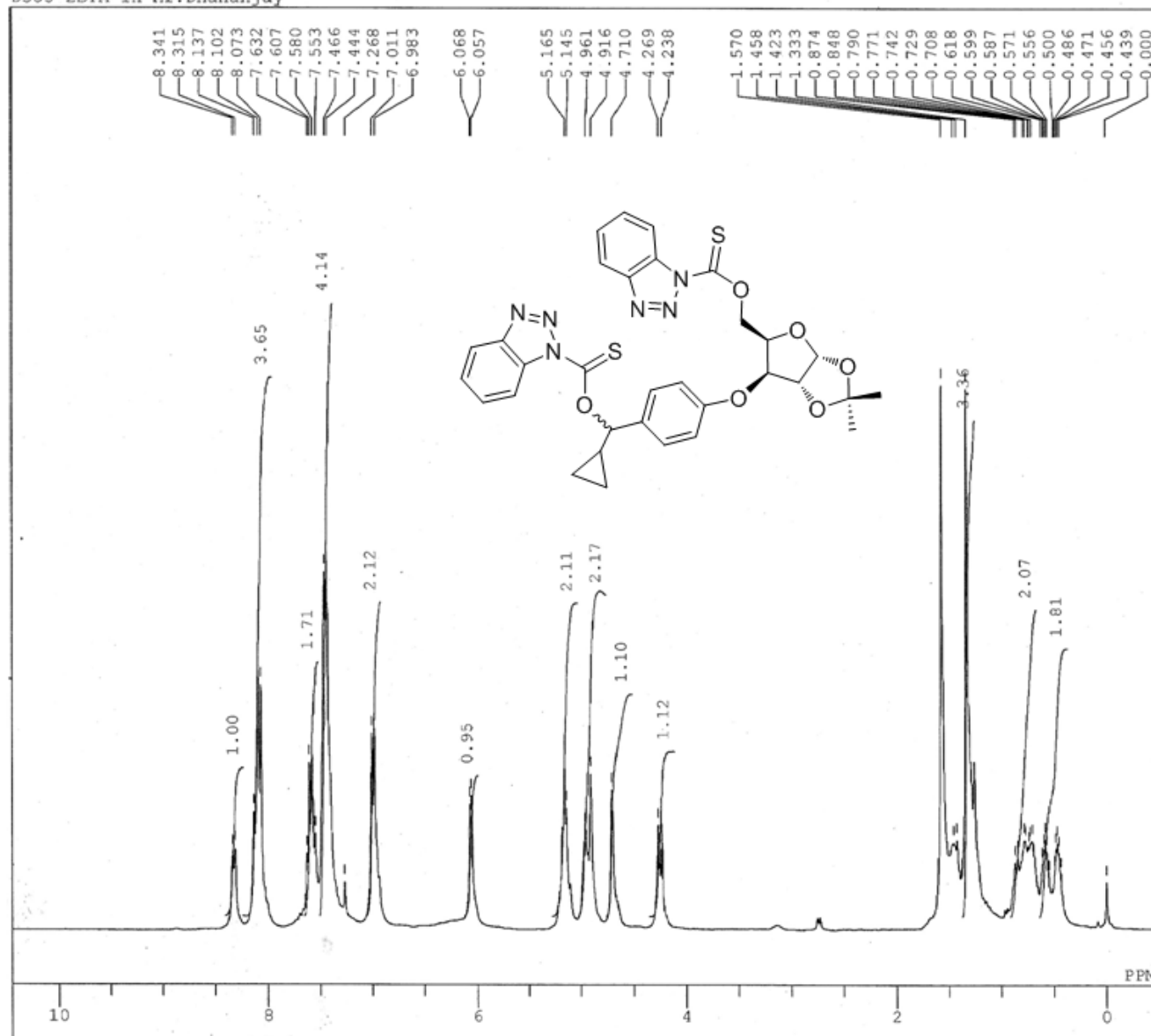
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu Universit
 VARANASI-221005

Operator : Nagendra Kum
 Shishir Sing

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 POINT 32768
 FREQU 20408.1 Hz
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 PW1 5.9 us
 IRNUC 1H
 CTEMP 25.8 c
 SLVNT CDCL3
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 BF 1.20 Hz
 RGAIN 23

Spectrum 9: 75 MHz ^{13}C NMR of compound 16

D385-2BTA 1H Mr.Dhananjay



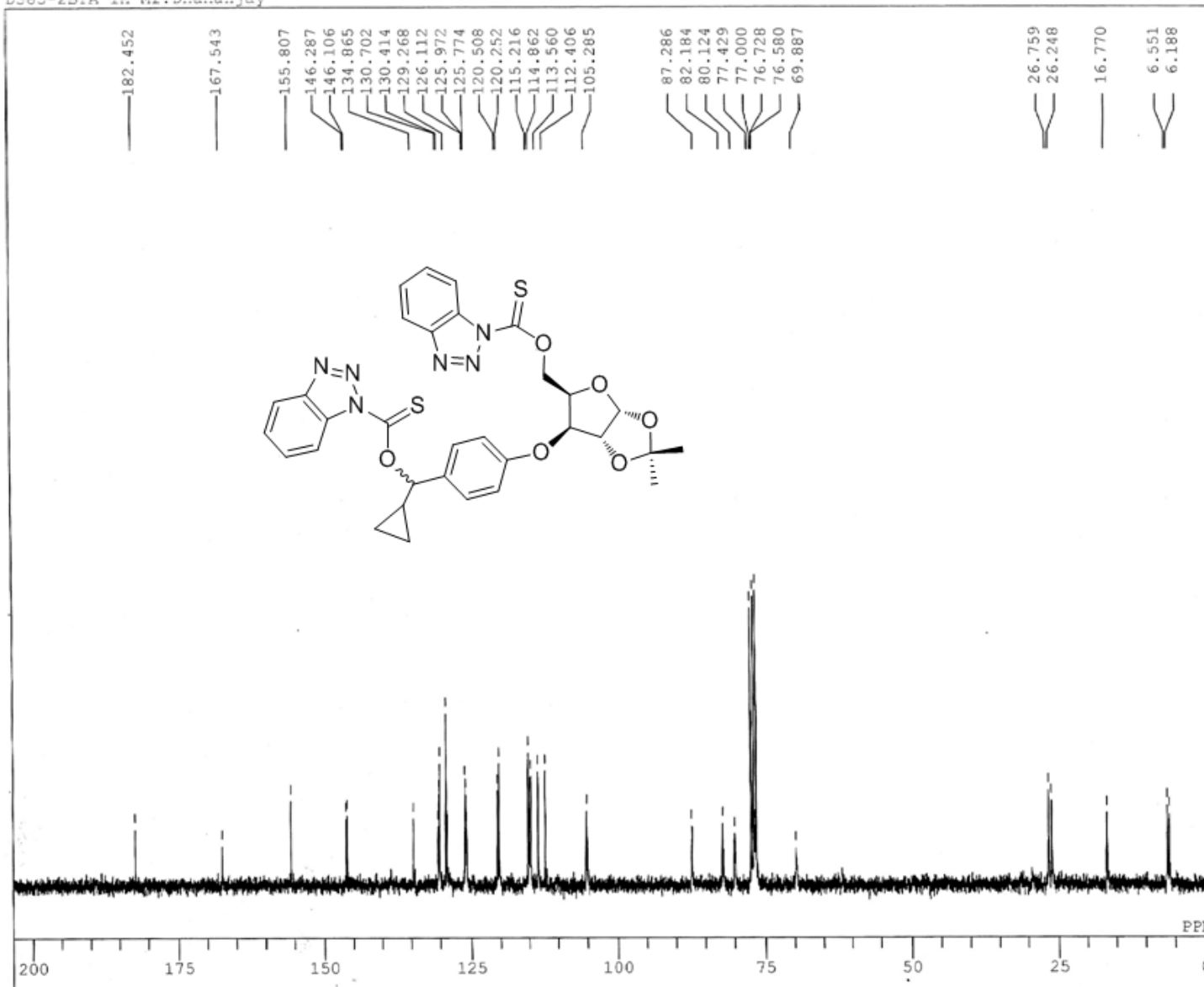
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBSET 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
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 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 22.1 c
 SLVNT CDCL3
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 BF 1.20 Hz
 RGAIN 13

Spectrum 10: 300 MHz ¹H NMR of compound 17

D385-2BTA 1H Mr.Dhananjay



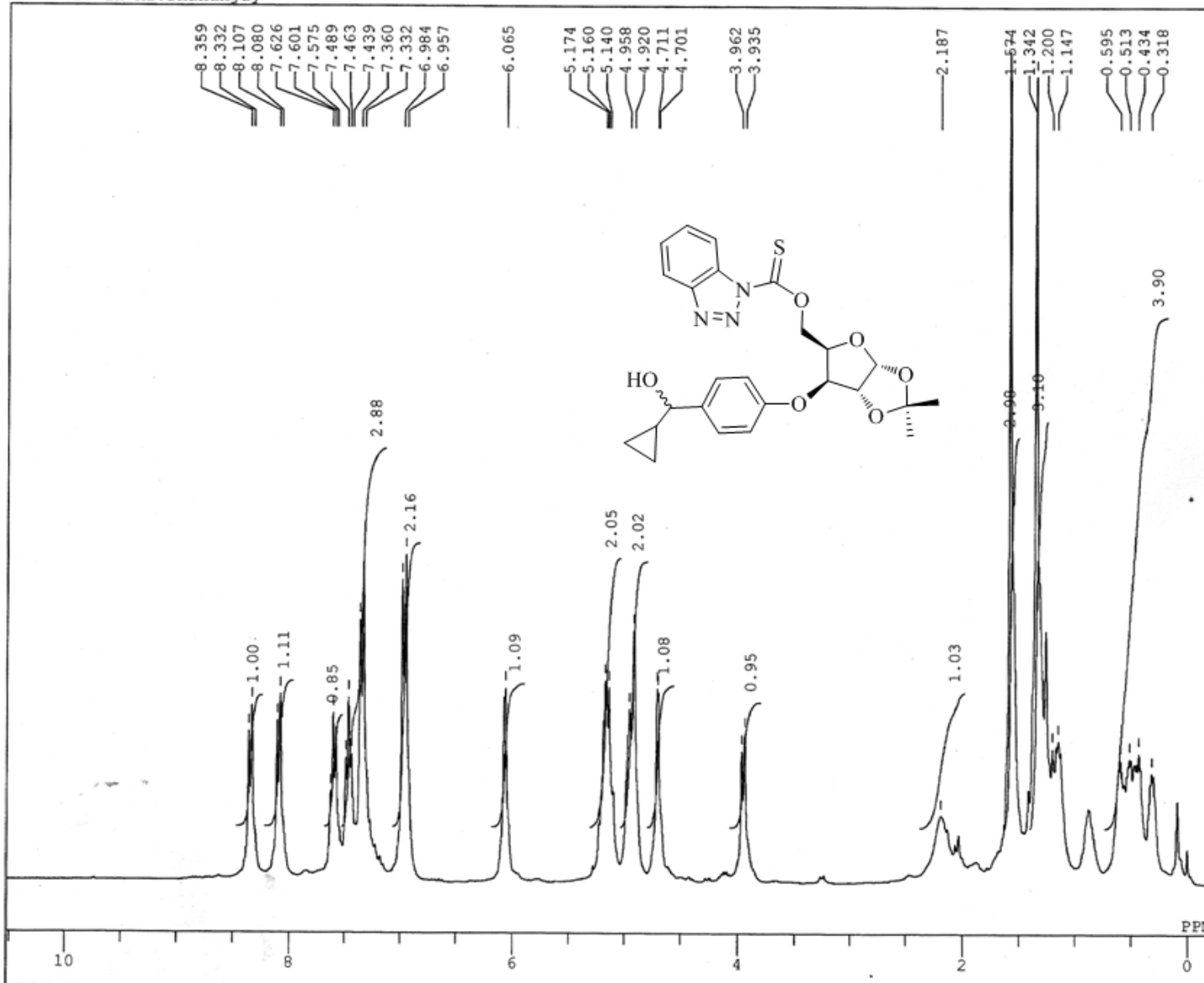
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Tue Jul 30 16:39:31
 OBNUC ¹³C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 320
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 28.2 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 22

Spectrum 11: 75 MHz ¹³C NMR of compound 17

D385-1BT 1H Mr.Dhananjay



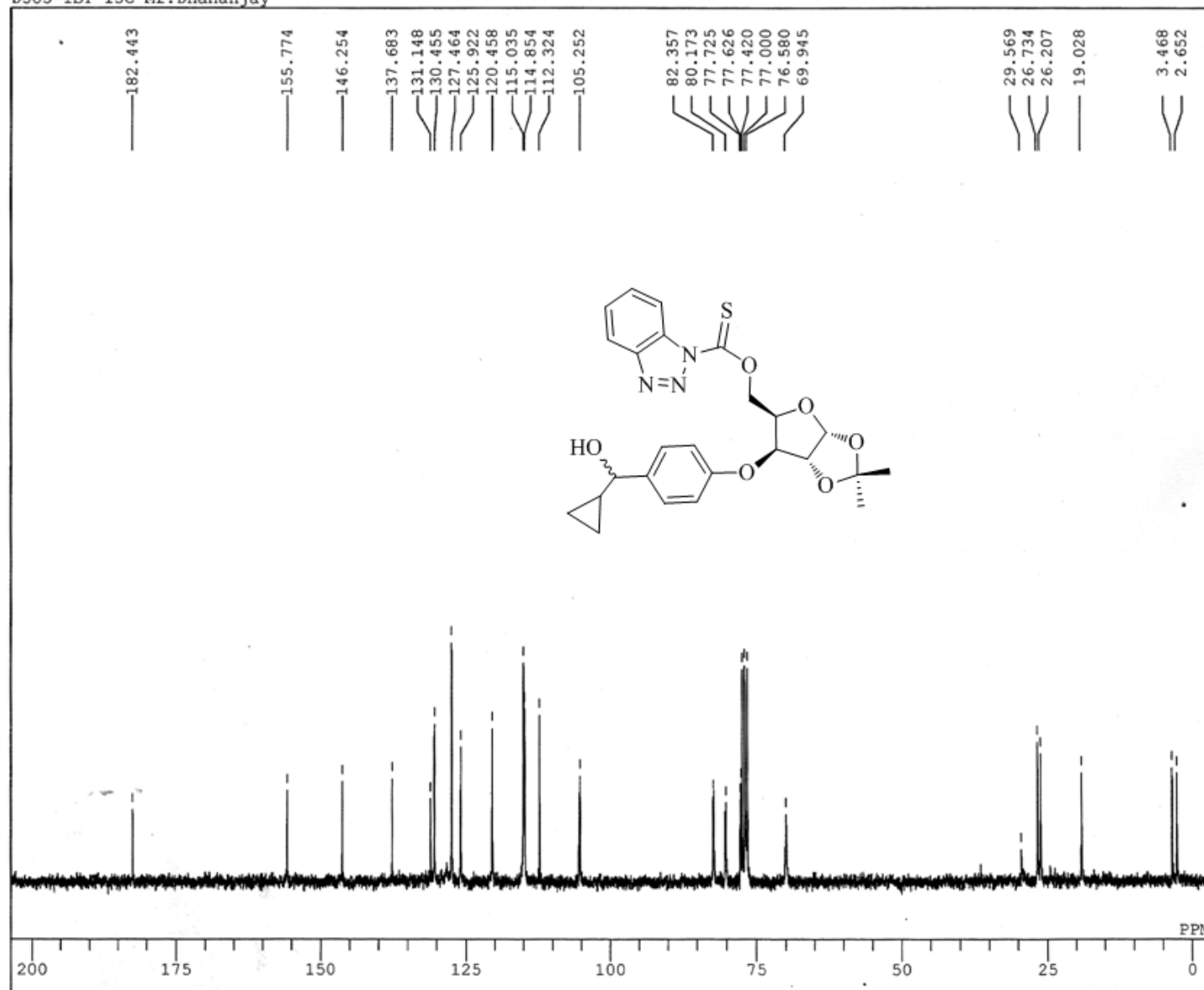
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University
 VARANASI-221005

Operator : Nagendra Kum
 Shishir Sing

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 OBNUC 1H
 EXMOD NON
 OBFRQ 300.40 MHz
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 FREQU 9505.7 Hz
 SCANS 16
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 23.7 c
 SLVNT CDCL3
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 BF 1.20 Hz
 RGAIN 12

Spectrum 12: 300 MHz ¹H NMR of compound 18

D385-1BT 13C Mr.Dhananjay



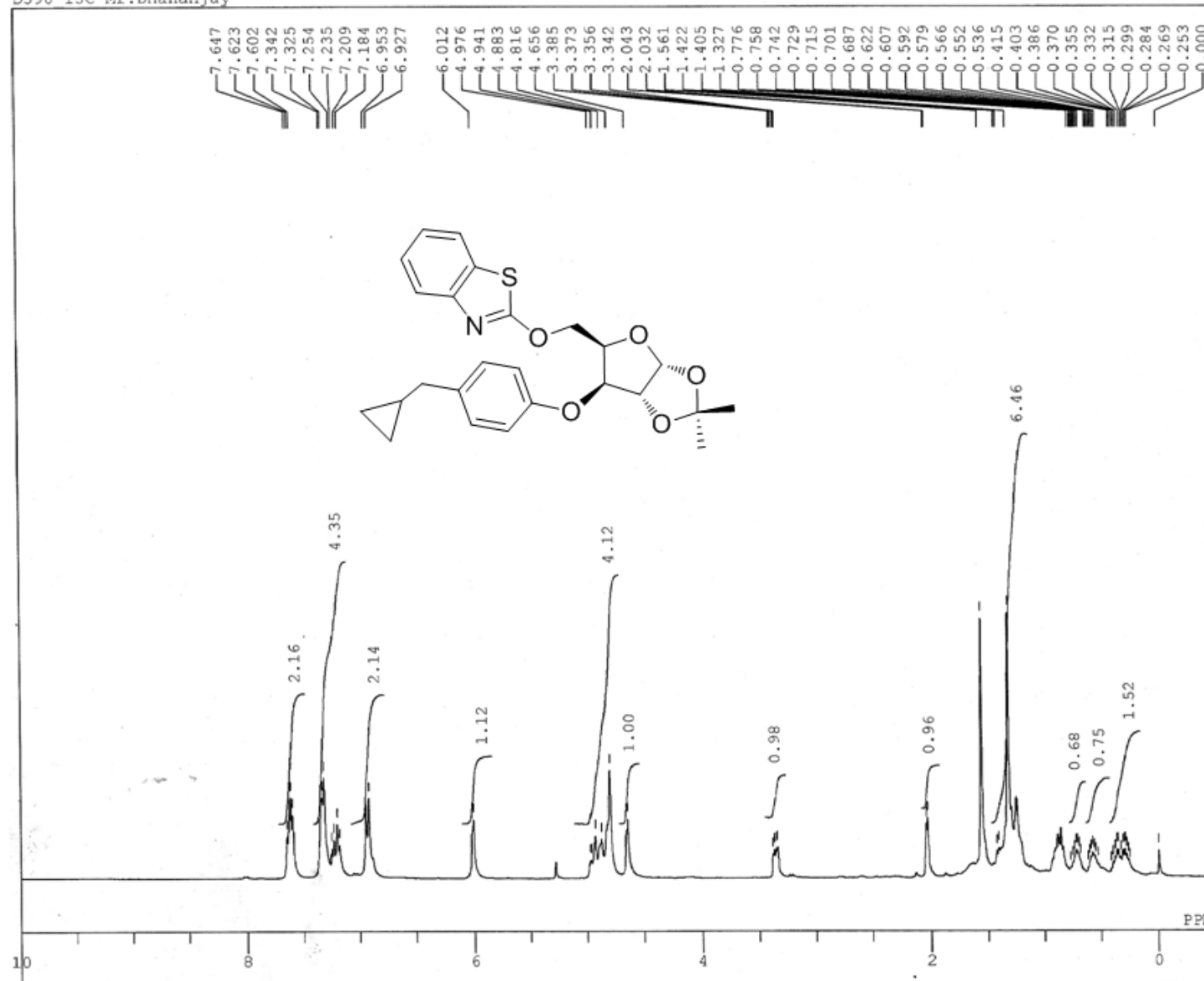
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu Universit
 VARANASI-221005

Operator : Nagendra Kum
 Shishir Sing

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 DATIM Thu Jul 25 17:25
 OBNUC 13C
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 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
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 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 28.5 c
 SLVNT CDCL3
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 BF 1.20 Hz
 RGAIN 22

Spectrum 13: 75 MHz ^{13}C NMR of compound 18

D398 13C Mr.Dhananjay



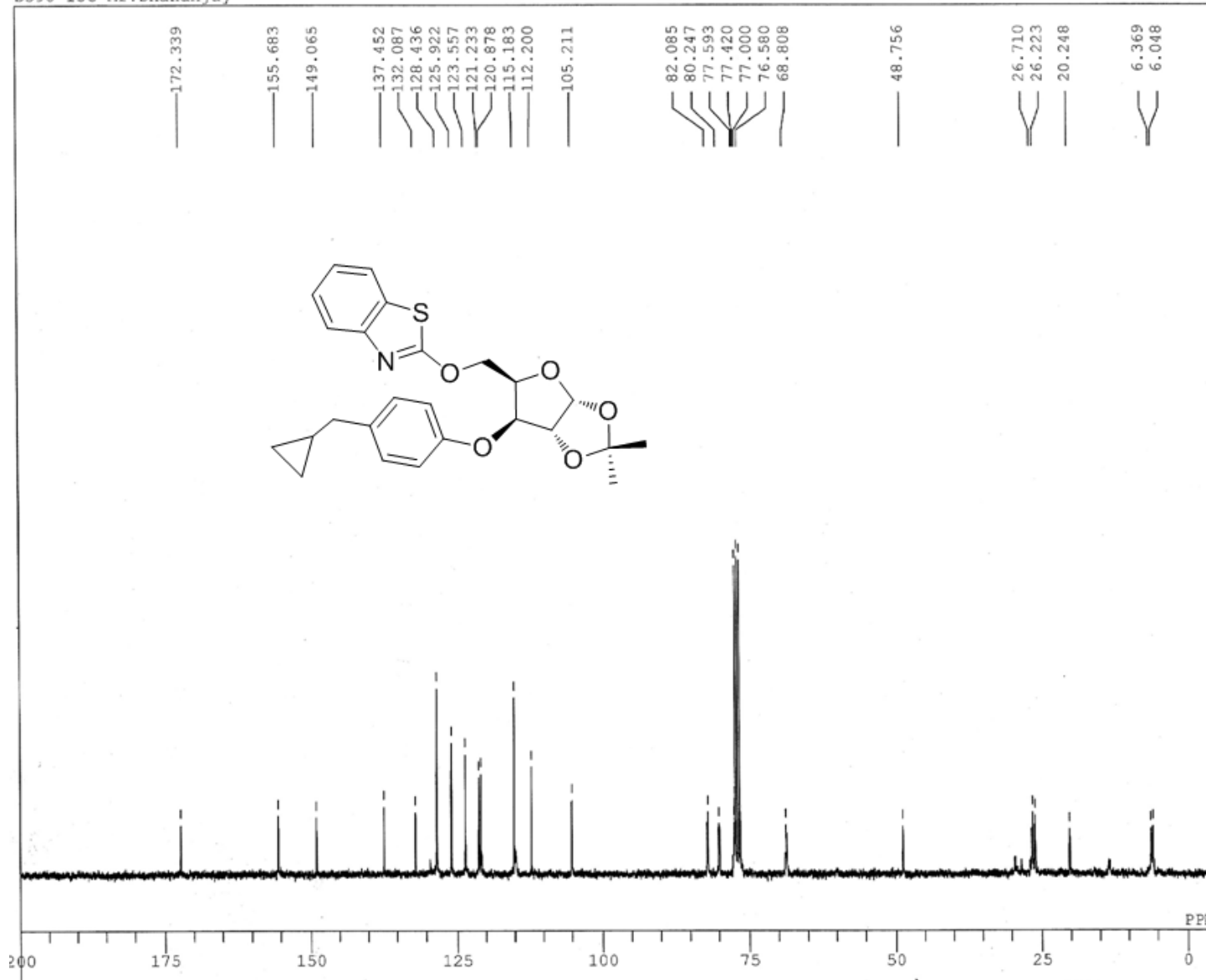
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 6016.8 Hz
 SCANS 32
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 PD 1.547 sec
 PW1 5.6 us
 IRNUC 1H
 CTEMP 22.0 c
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 BF 1.20 Hz
 RGAIN 17

Spectrum 14: 300 MHz ¹H NMR of compound 19

D398 13C Mr.Dhananjay



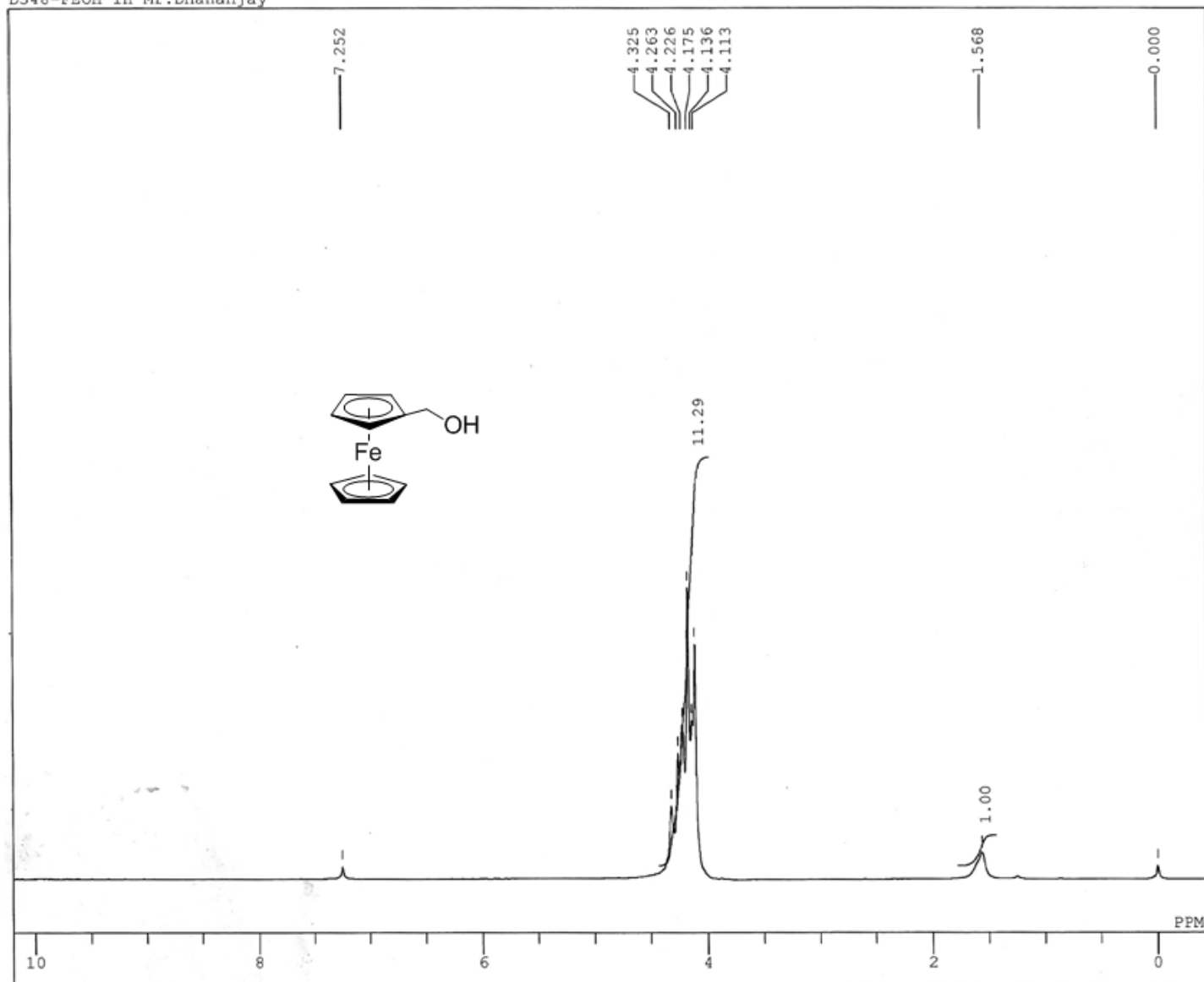
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 1500
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 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 23.9 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 25

Spectrum 15: 75 MHz ^{13}C NMR of compound 19

D348-FEOH 1H Mr.Dhananjay



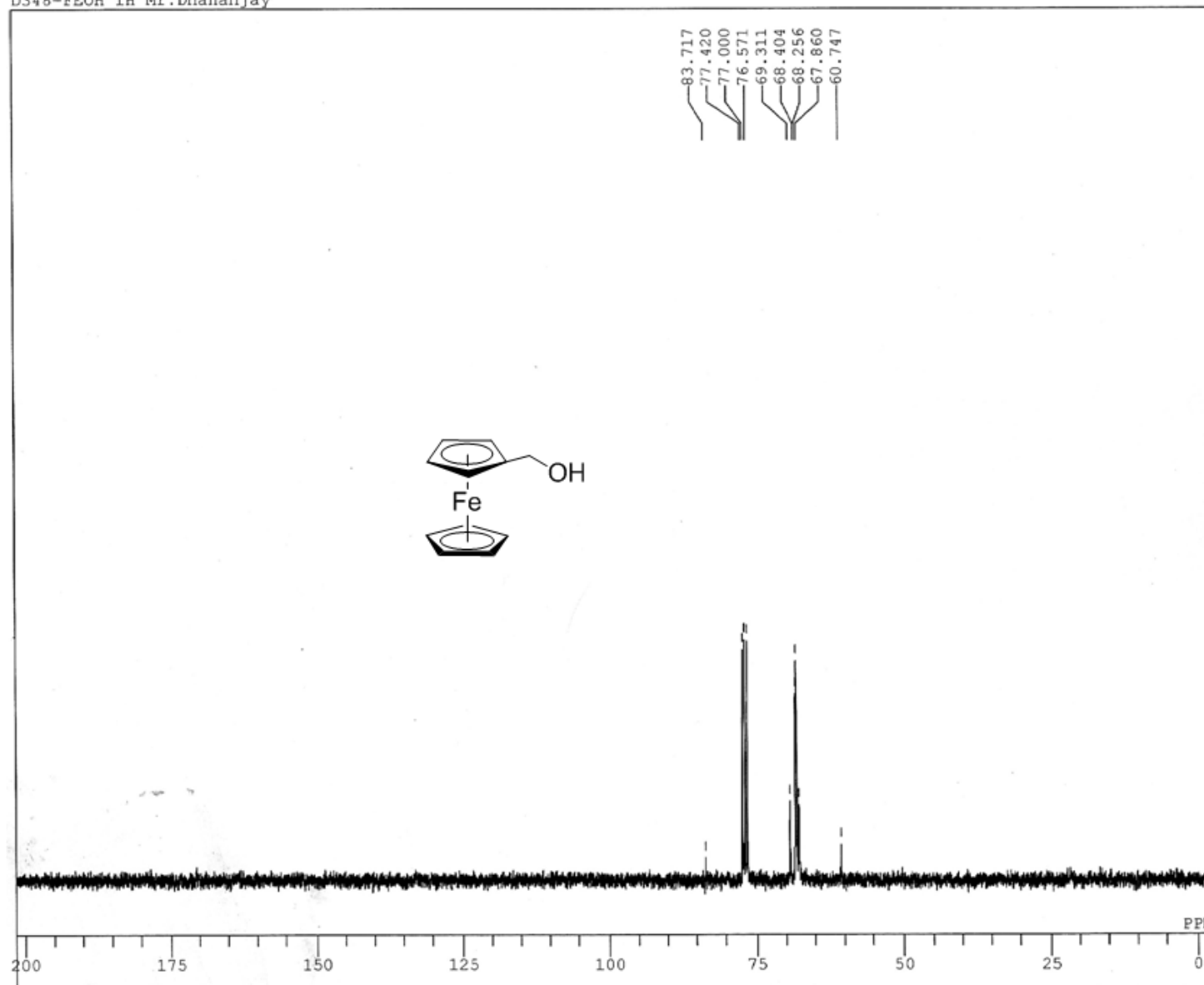
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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DATIM Thu Jul 04 15:02:11 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
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ACQTM 5.446 sec
PD 1.547 sec
PW1 5.6 us
IRNUC 1H
CTEMP 21.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.22 Hz
RGAIN 16

Spectrum 16: 300 MHz ^1H NMR of compound 21

D348-FEOH 1H Mr.Dhananjay



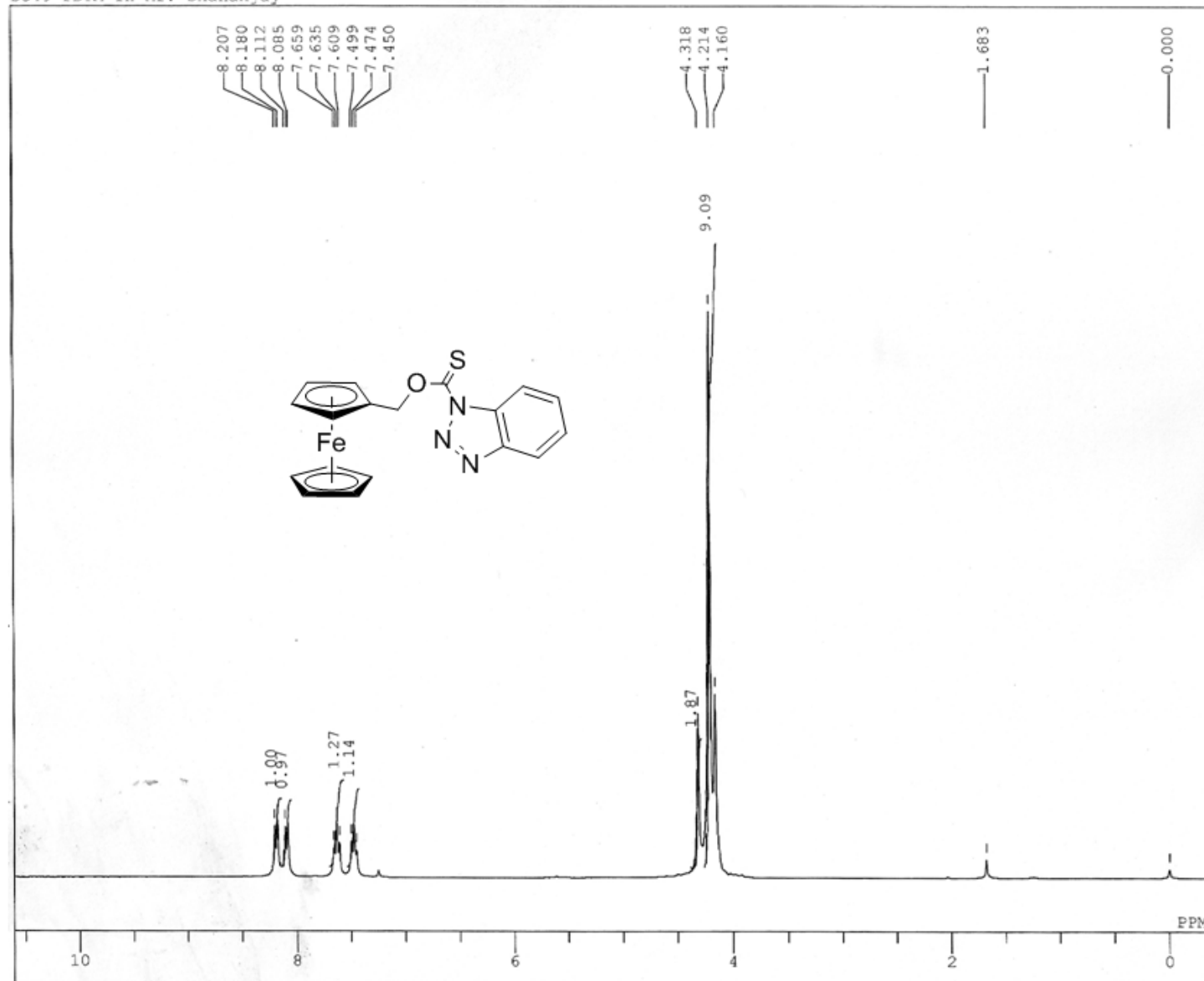
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 24.3 c
SLVNT CDCL3
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BF 1.22 Hz
RGAIN 24

Spectrum 17: 75 MHz ^{13}C NMR of compound 21

D349-FBTA 1H Mr. Dhananjay



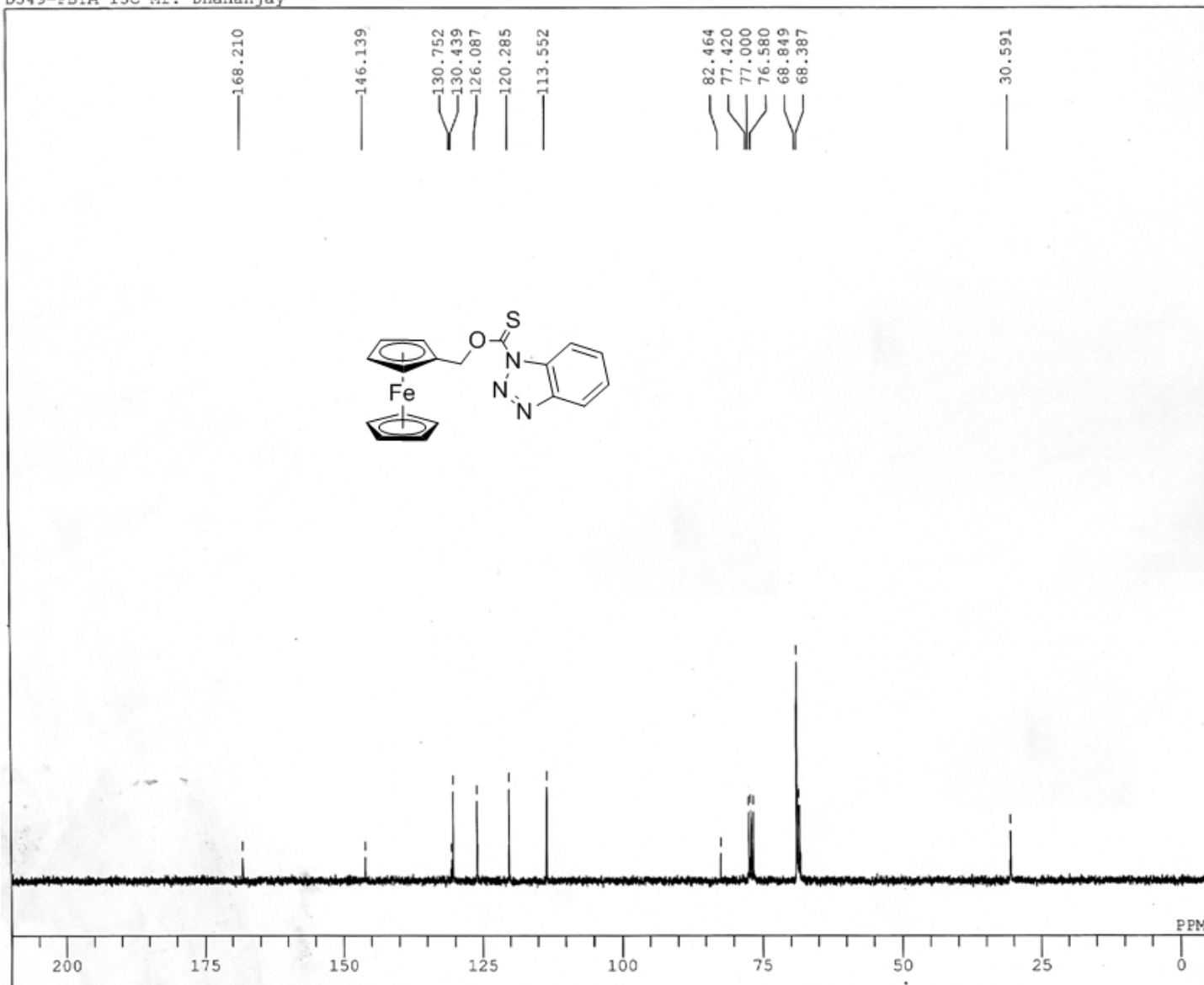
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBFIN 1150.0 Hz
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 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 21.8 c
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 RGAIN 12

Spectrum 18: 300 MHz ¹H NMR of compound 22

D349-FBTA 13C Mr. Dhananjay



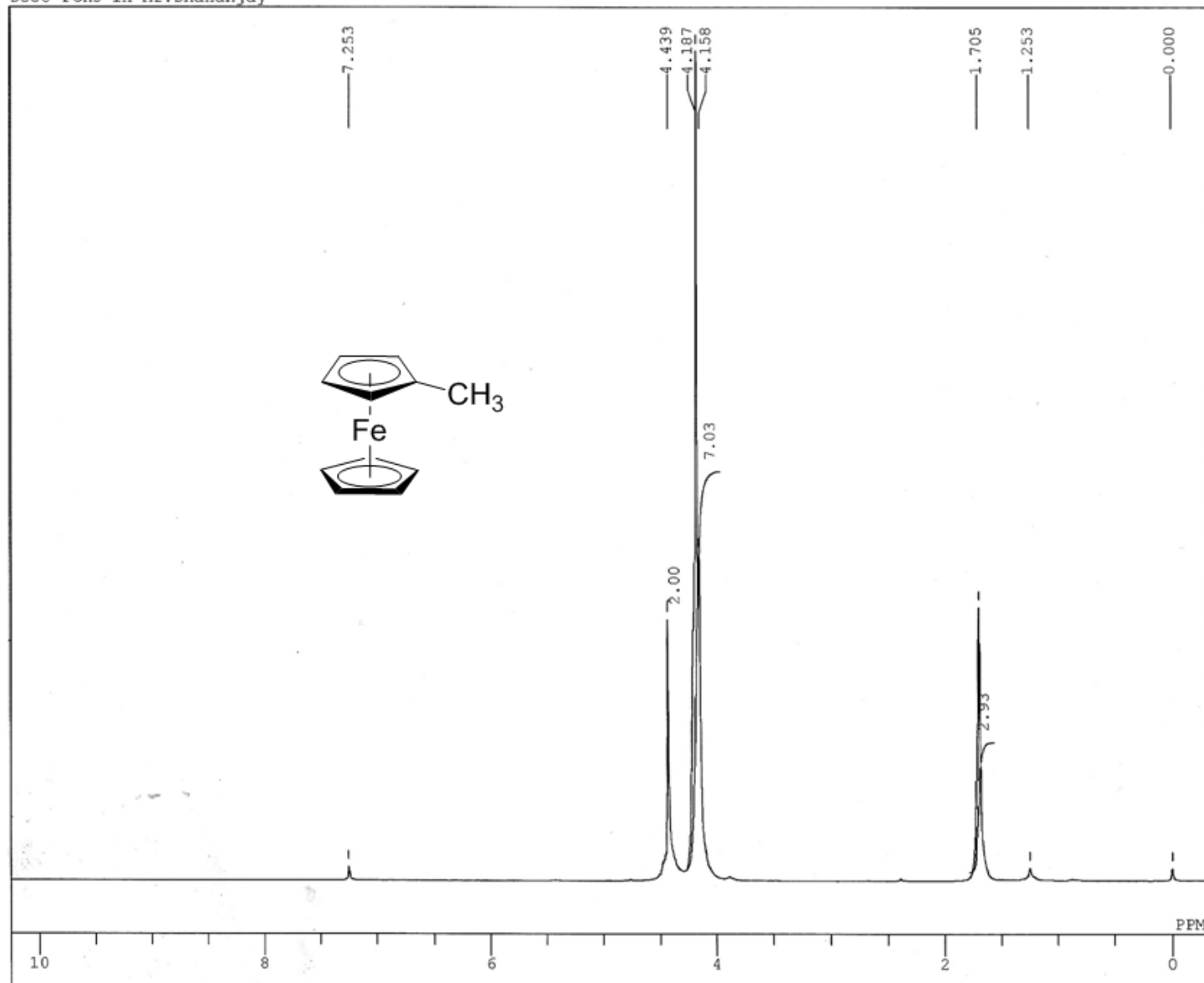
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 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 27.5 c
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 BF 1.22 Hz
 RGAIN 22

Spectrum 19: 75 MHz ^{13}C NMR of compound 22

D358-FCH3 1H Mr.Dhananjay



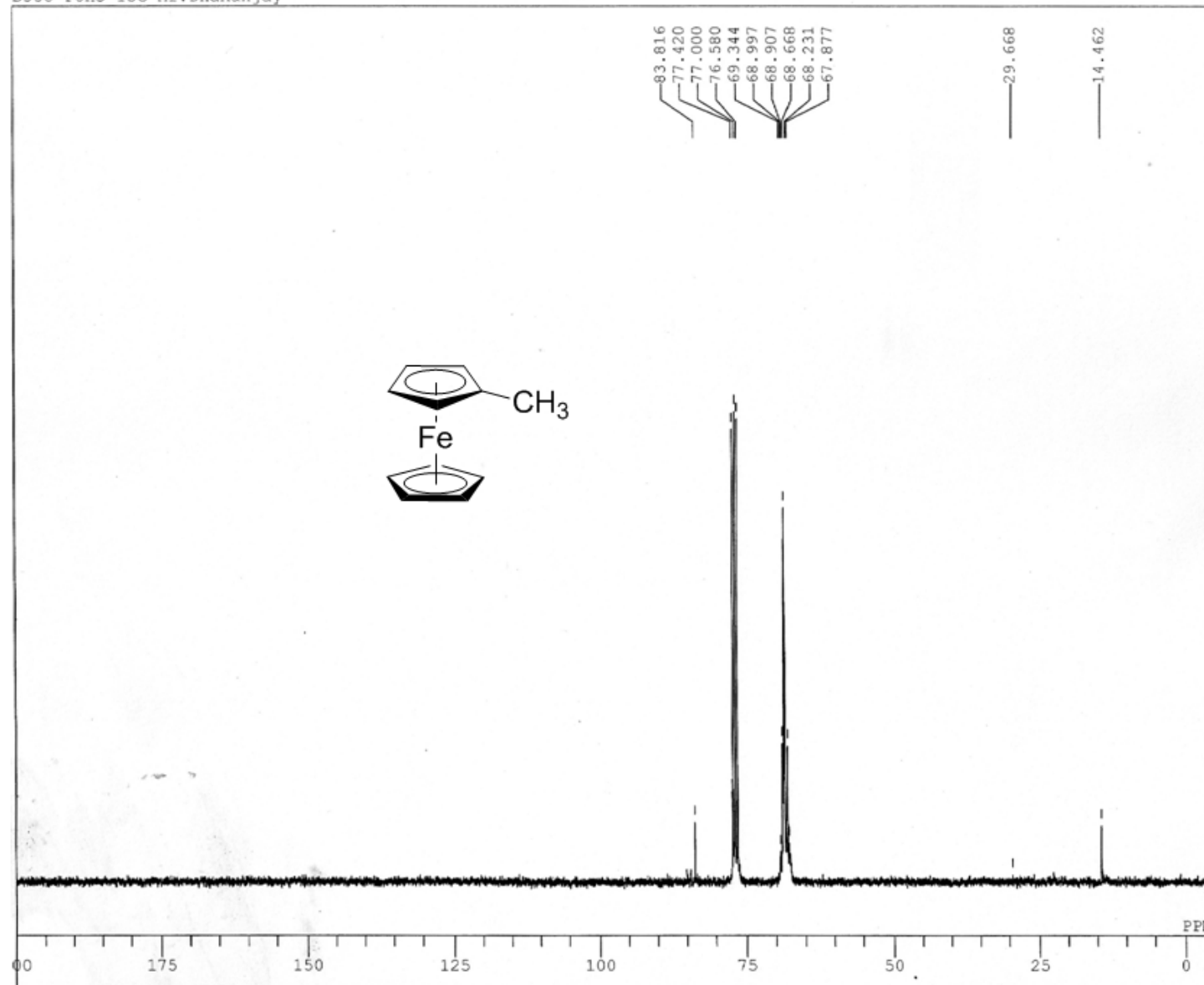
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

D358-FCH3 1H Mr.Dha
Fri Jul 05 13:50:05
1H
NON
300.40 MHz
130.00 KHz
1150.0 Hz
32768
6016.8 Hz
16
5.446 sec
1.547 sec
5.6 us
1H
22.2 c
CDCL3
0.00 ppm
1.20 Hz
13

Spectrum 20: 300 MHz ^1H NMR of compound 23

D358-FUH3 13C Mr.Dhananjay



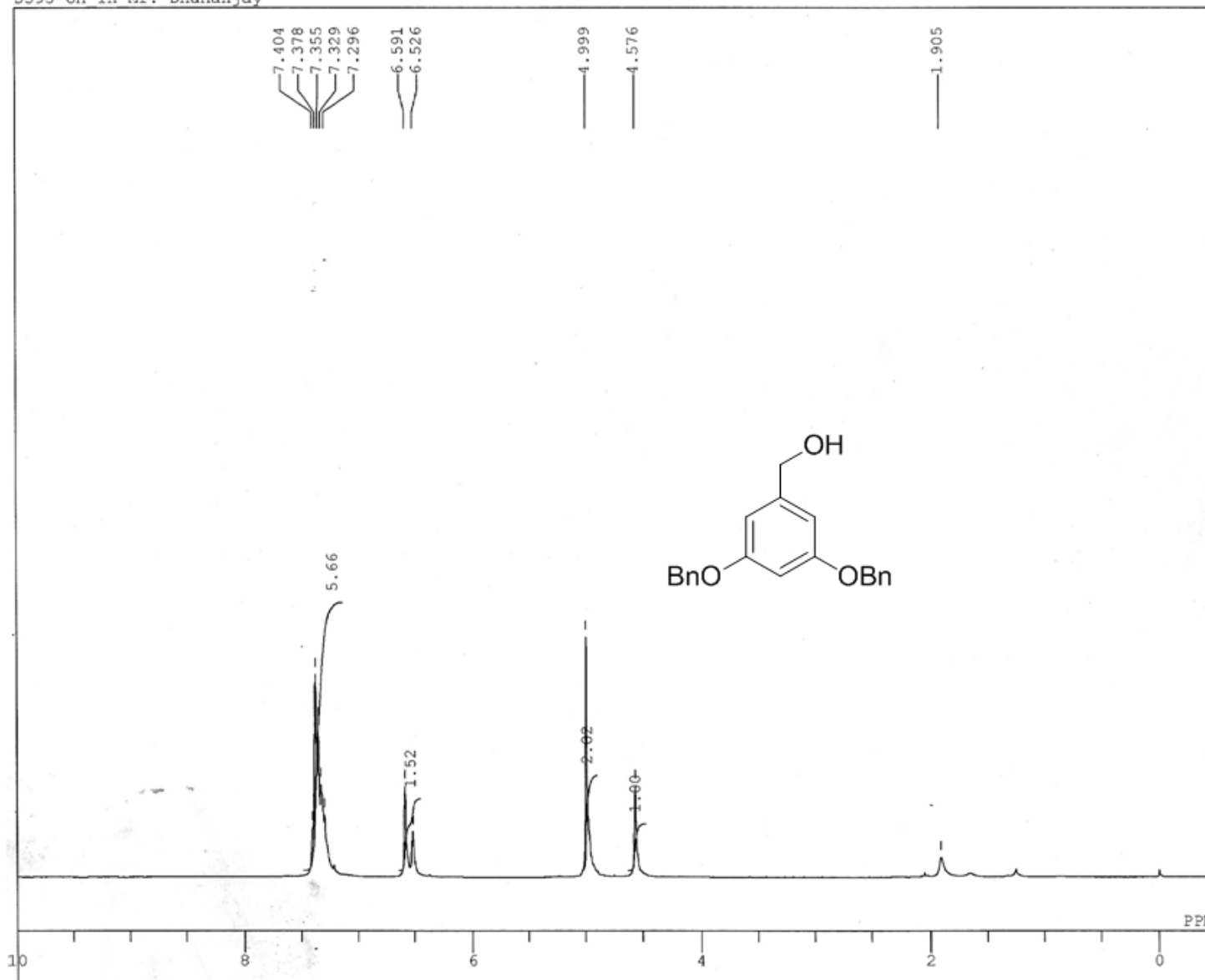
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 20.1 c
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 RGAIN 24

Spectrum 21: 75 MHz ^{13}C NMR of compound 23

D395-OH 1H Mr. Dhananjay



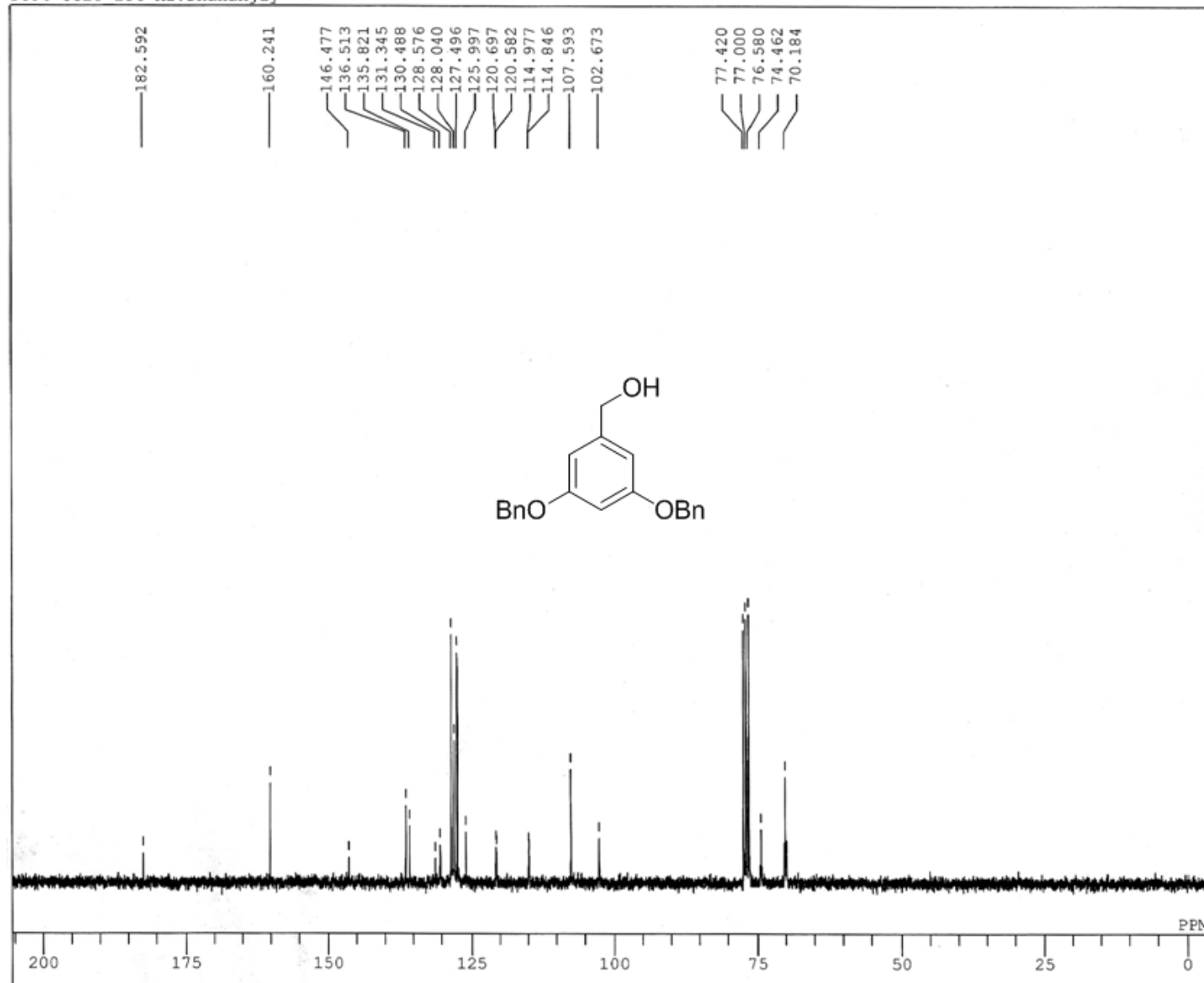
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBFIN 1150.0 Hz
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 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 25.5 c
 SLVNT CDCL3
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 BF 1.20 Hz
 RGAIN 13

Spectrum 22: 300 MHz ¹H NMR of compound 24a

D396-35BT 13C Mr.Dhananjay

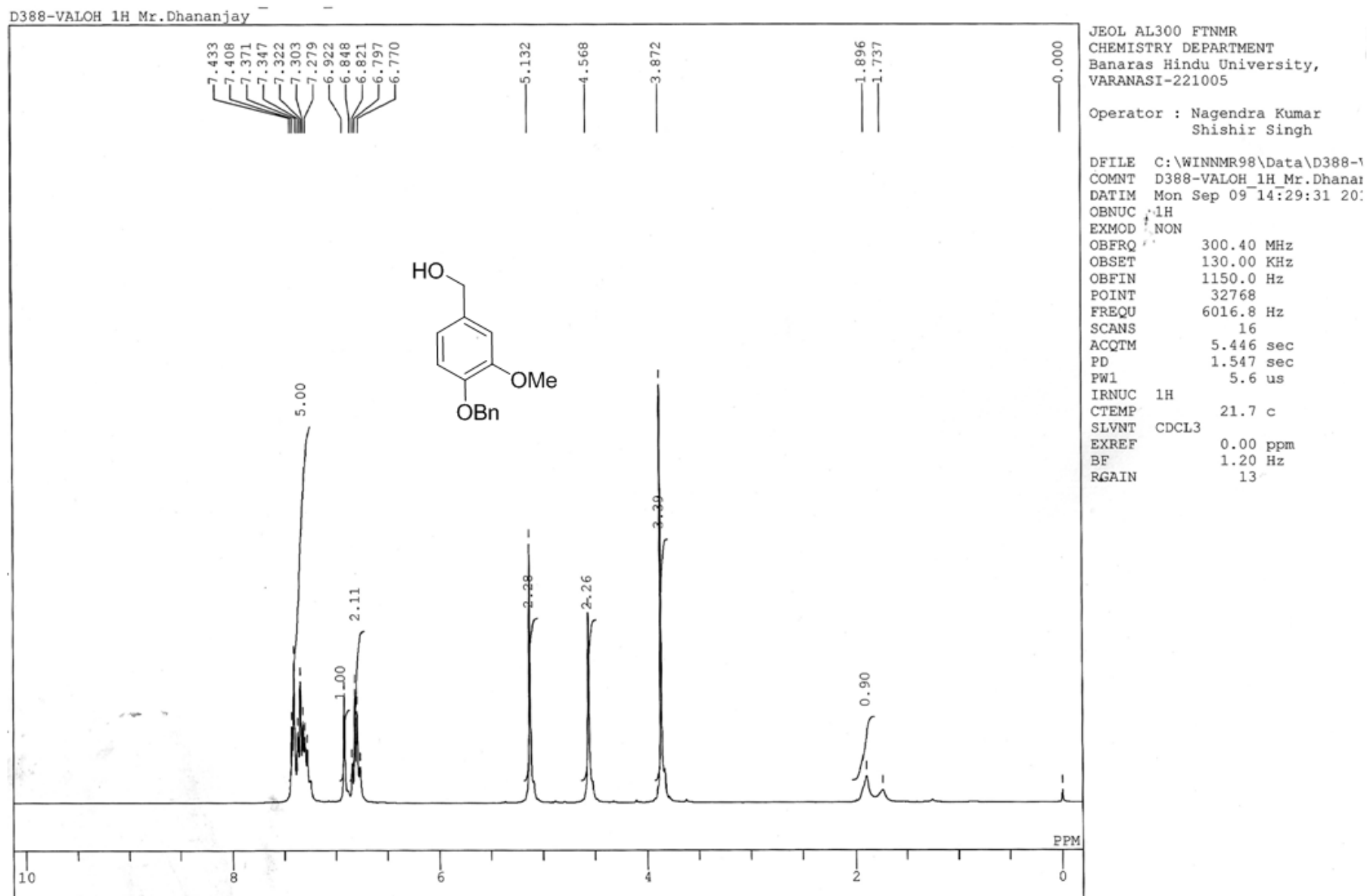


JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

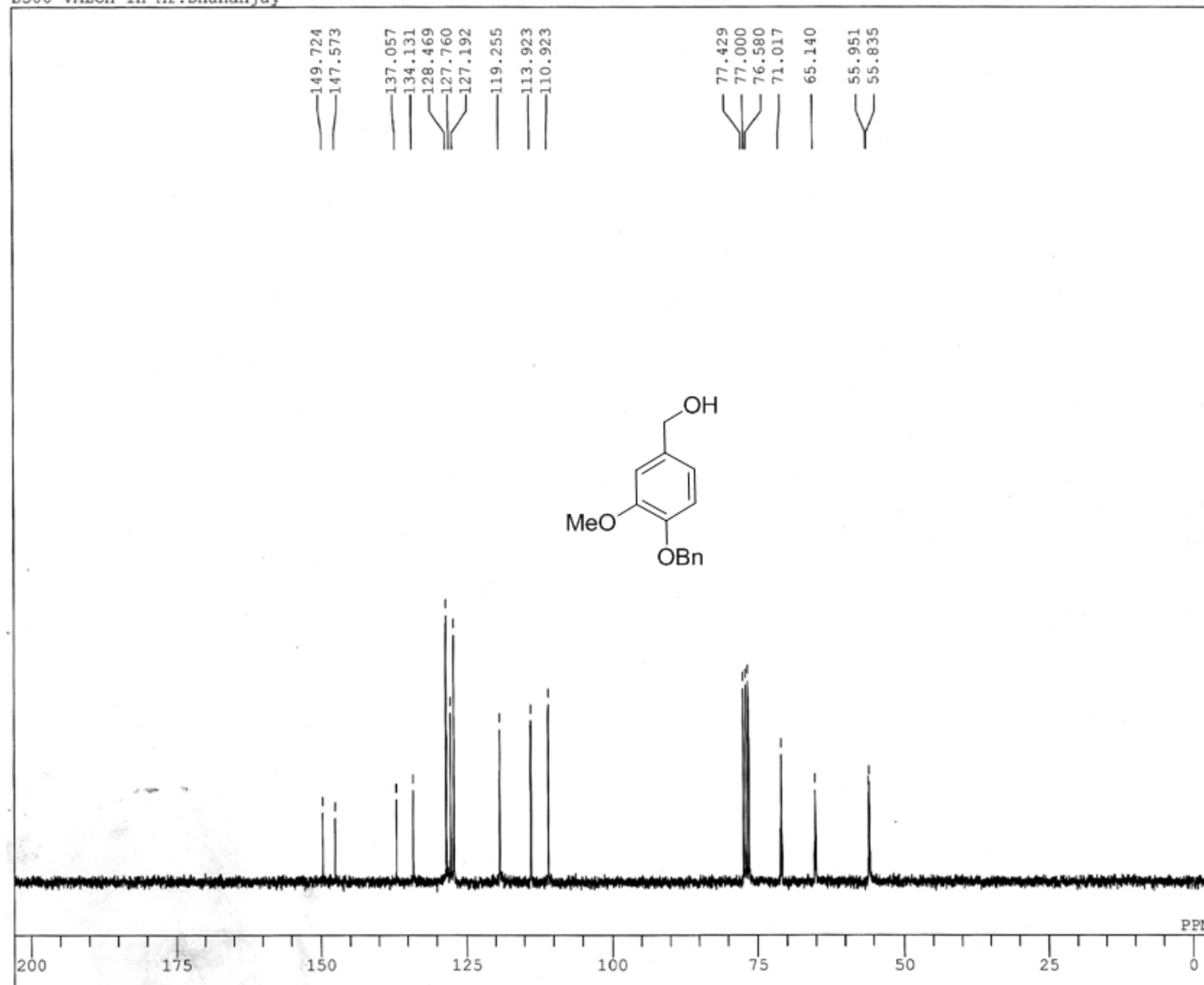
Operator : Nagendra Kumar
 Shishir Singh

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 IRNUC 1H
 CTEMP 24.8 c
 SLVNT CDCL3
 EXREF 77.00 ppm
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 RGAIN 23

Spectrum 23: 75 MHz ^{13}C NMR of compound 24a

Spectrum 24: 300 MHz ¹H NMR of compound 24b

D388-VALOH 1H Mr.Dhananjay



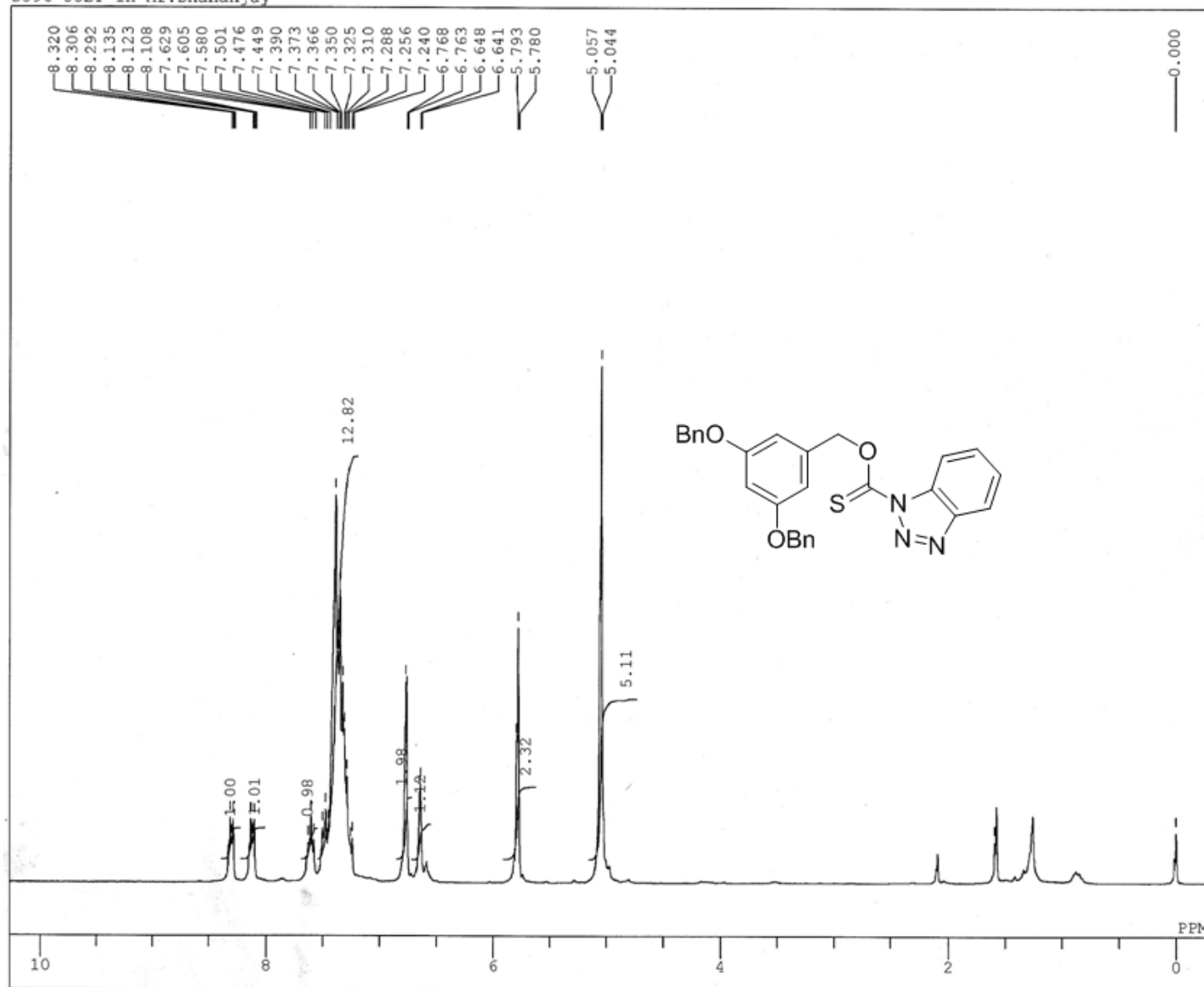
JEOL AL300 FTNMR
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 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 23.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 22

Spectrum 25: 75 MHz ^{13}C NMR of compound 24b

D396-35BT 1H Mr.Dhananjay



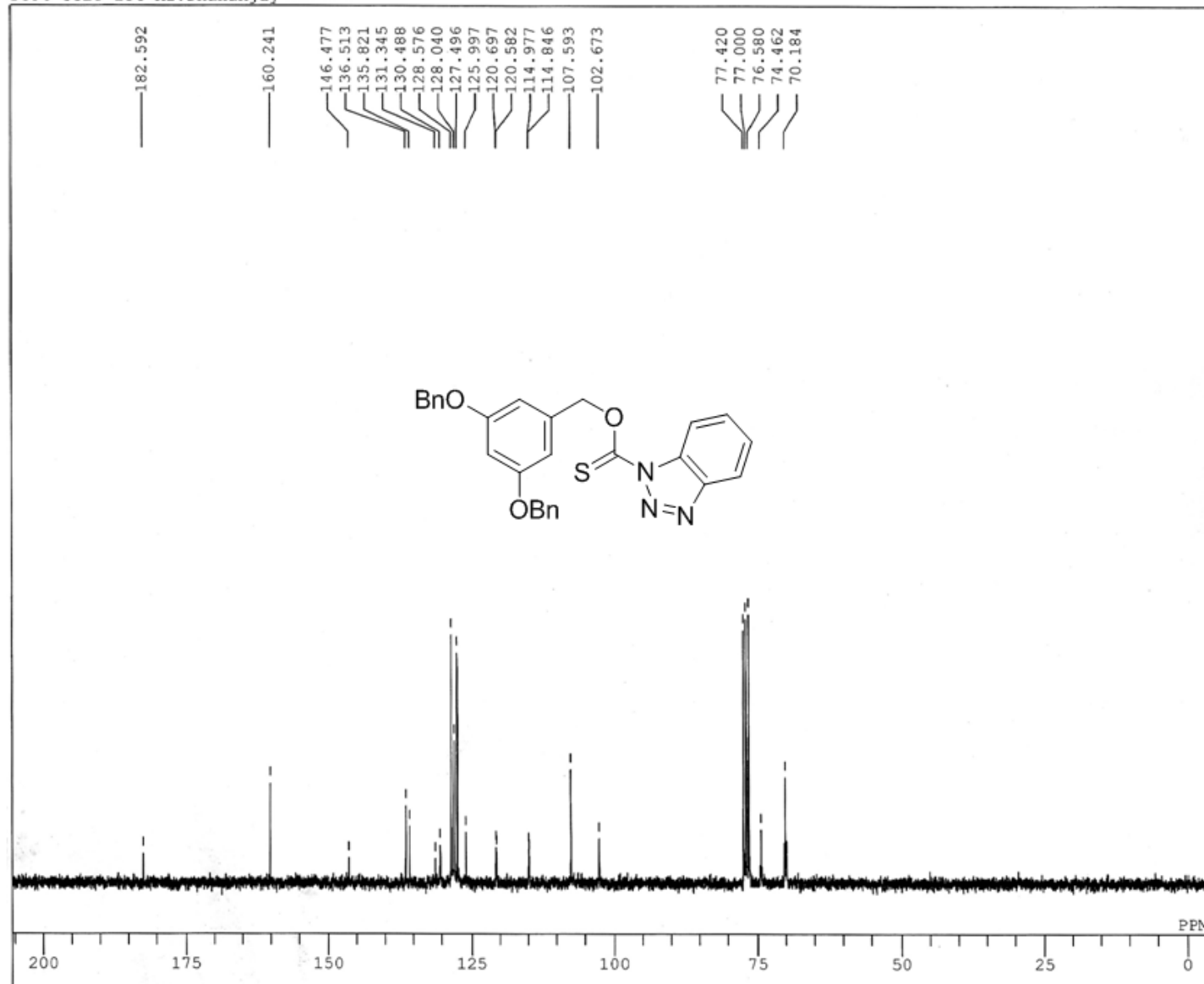
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 EXMOD NON
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 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 9
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 25.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 16

Spectrum 26: 300 MHz ¹H NMR of compound **25a**

D396-35BT 13C Mr.Dhananjay



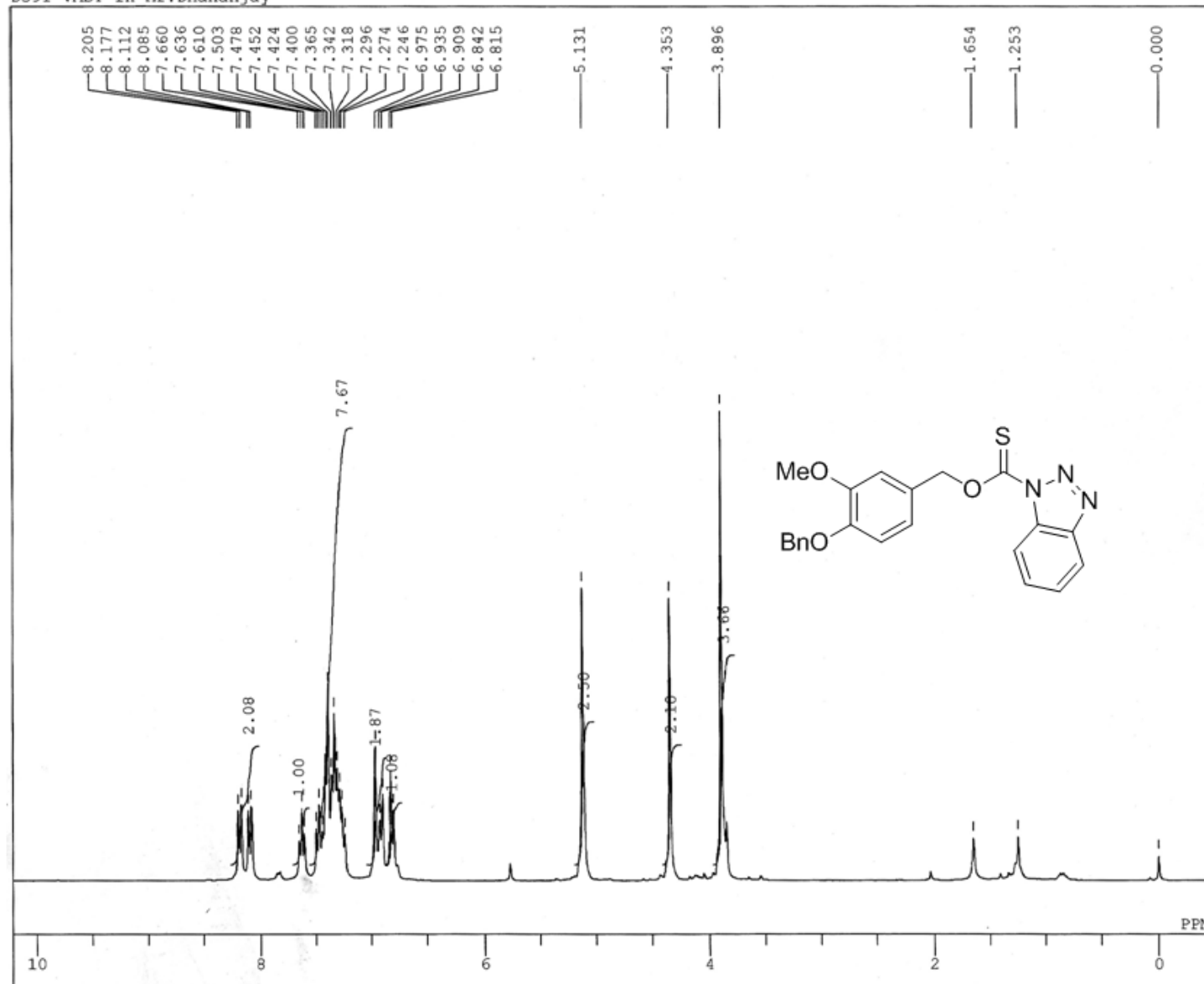
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 315
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 24.8 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 23

Spectrum 27: 75 MHz ¹³C NMR of compound 25a

D391-VABT 1H Mr.Dhananjay



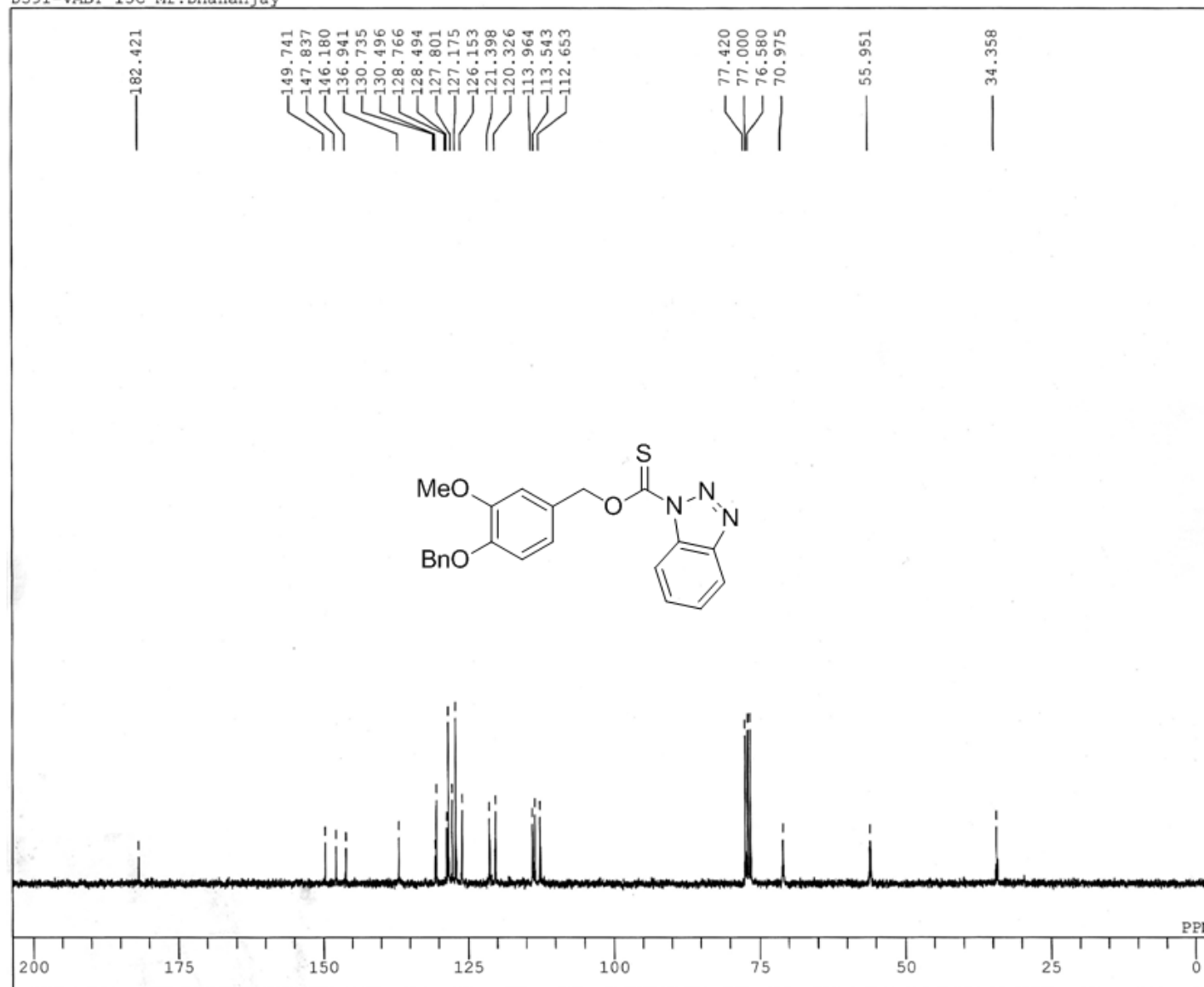
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBSET 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 8
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 22.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 14

Spectrum 28: 300 MHz ¹H NMR of compound 25b

D391-VABT 13C Mr.Dhananjay



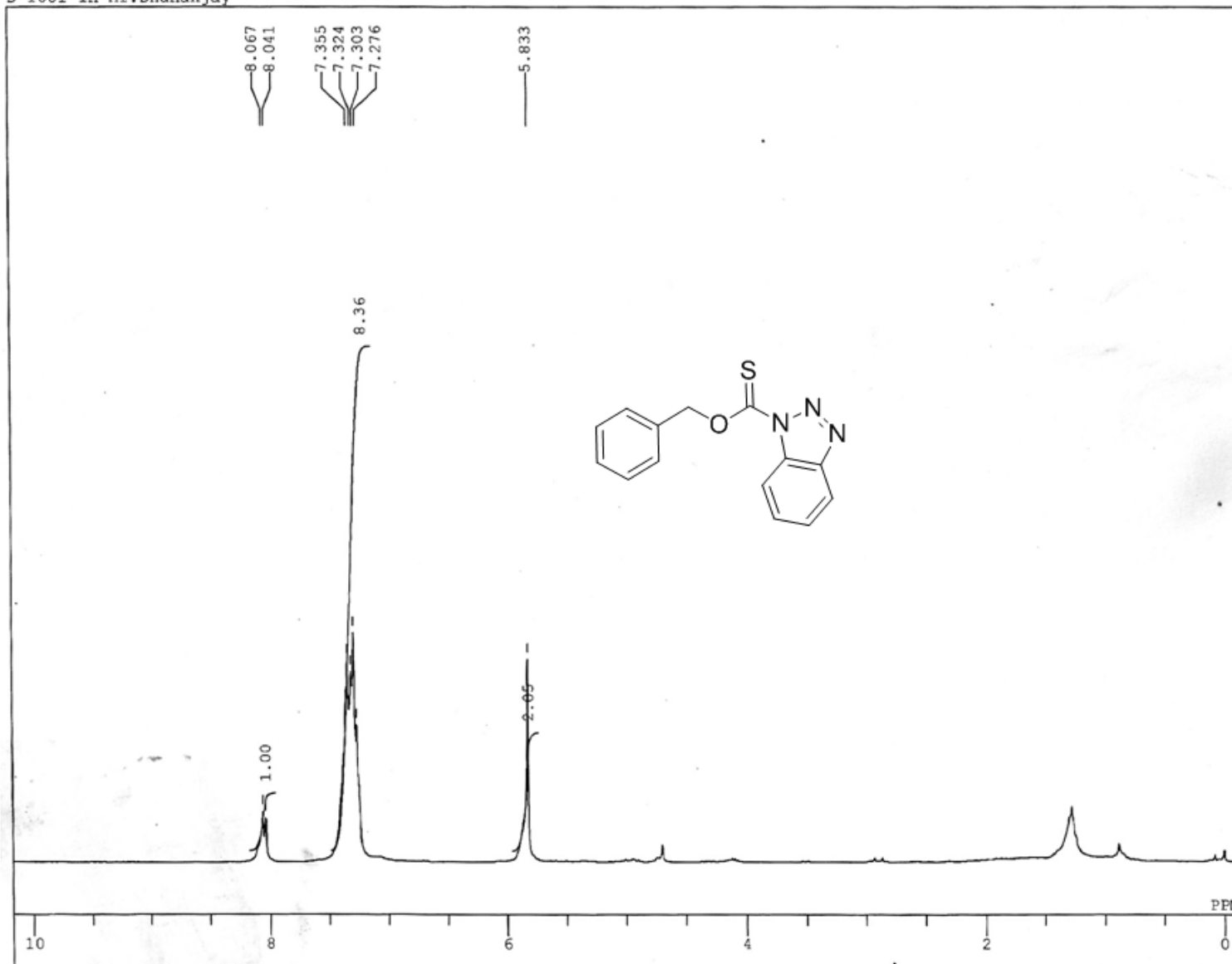
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 287
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 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 24.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 24

Spectrum 29: 75 MHz ^{13}C NMR of compound 25b

D-1001 1H Mr.Dhananjay



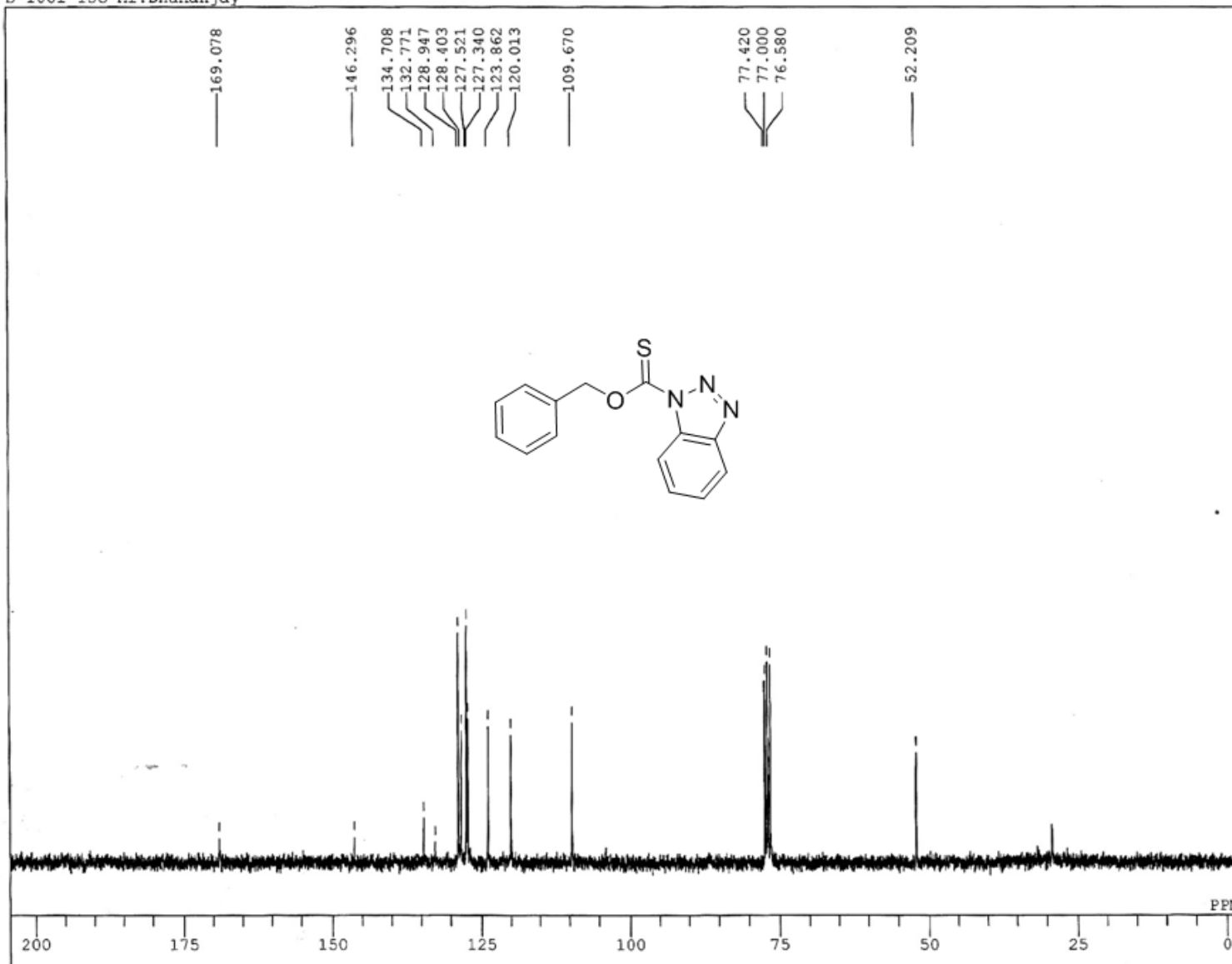
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CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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DATIM Thu May 08 14:50:
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EXMOD NON
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OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 8
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 26.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 15

Spectrum 30: 300 MHz ¹H NMR of compound 25c

D-1001 13C Mr.Dhananjay



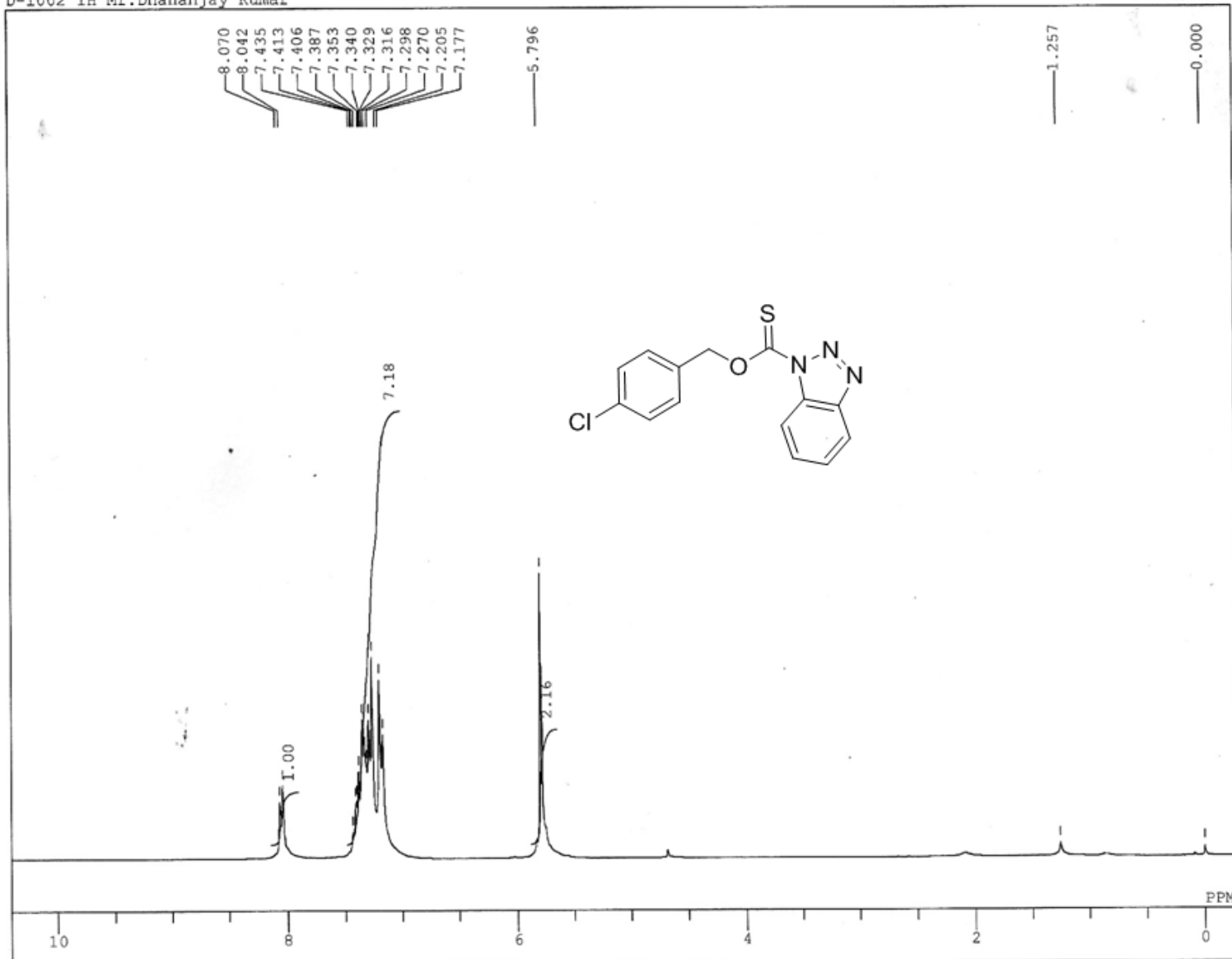
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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DATIM Thu May 08 14:45:
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EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 288
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 25.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

Spectrum 31: 75 MHz ¹³C NMR of compound 25c

D-1002 1H Mr.Dhananjay Kumar



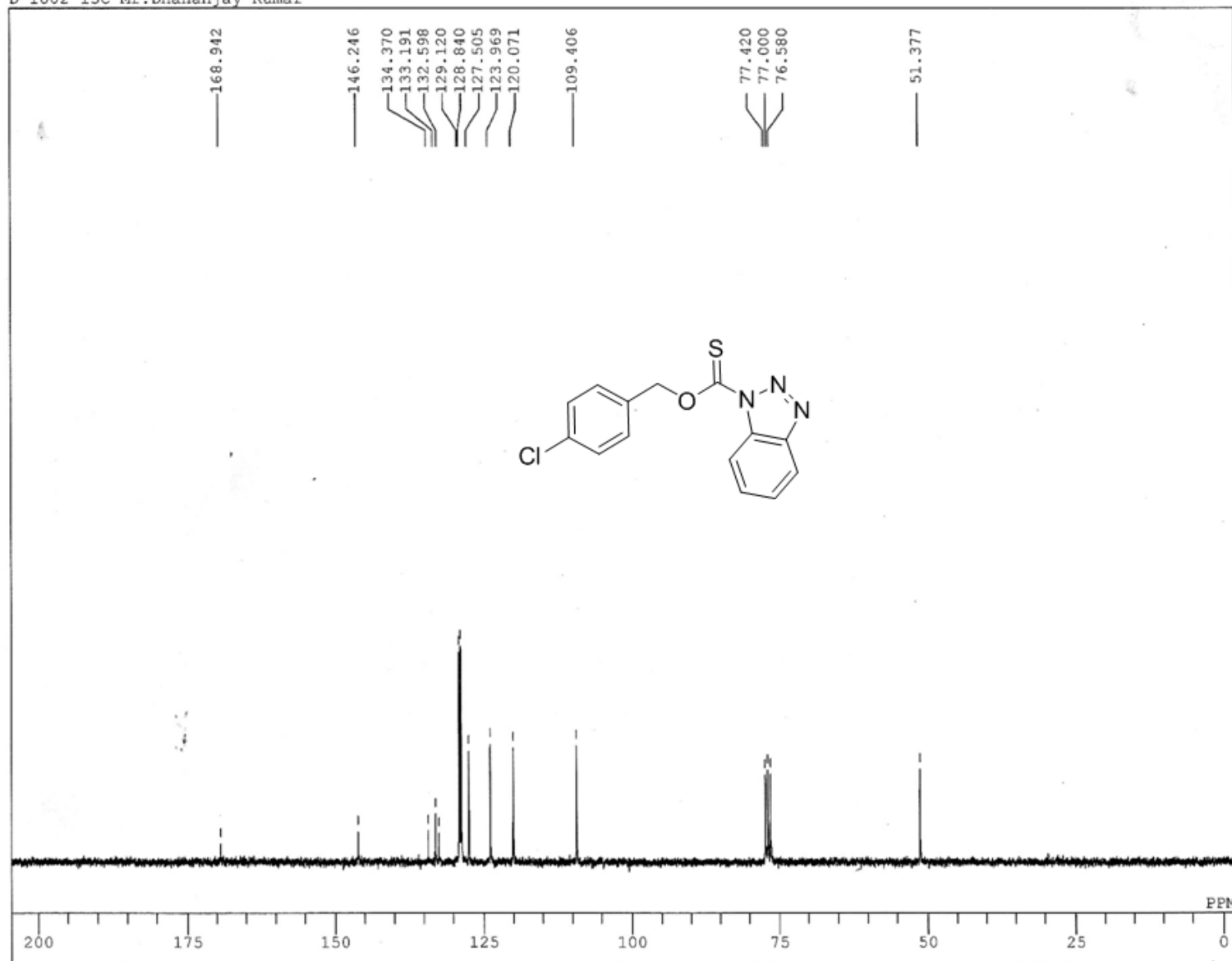
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Tue May 20 22:55:
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 EXMOD NON
 OBFRQ 300.40 MHz
 OBSET 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 61
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 23.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 15

Spectrum 32: 300 MHz ^1H NMR of compound 25d

D-1002 13C Mr.Dhananjay Kumar



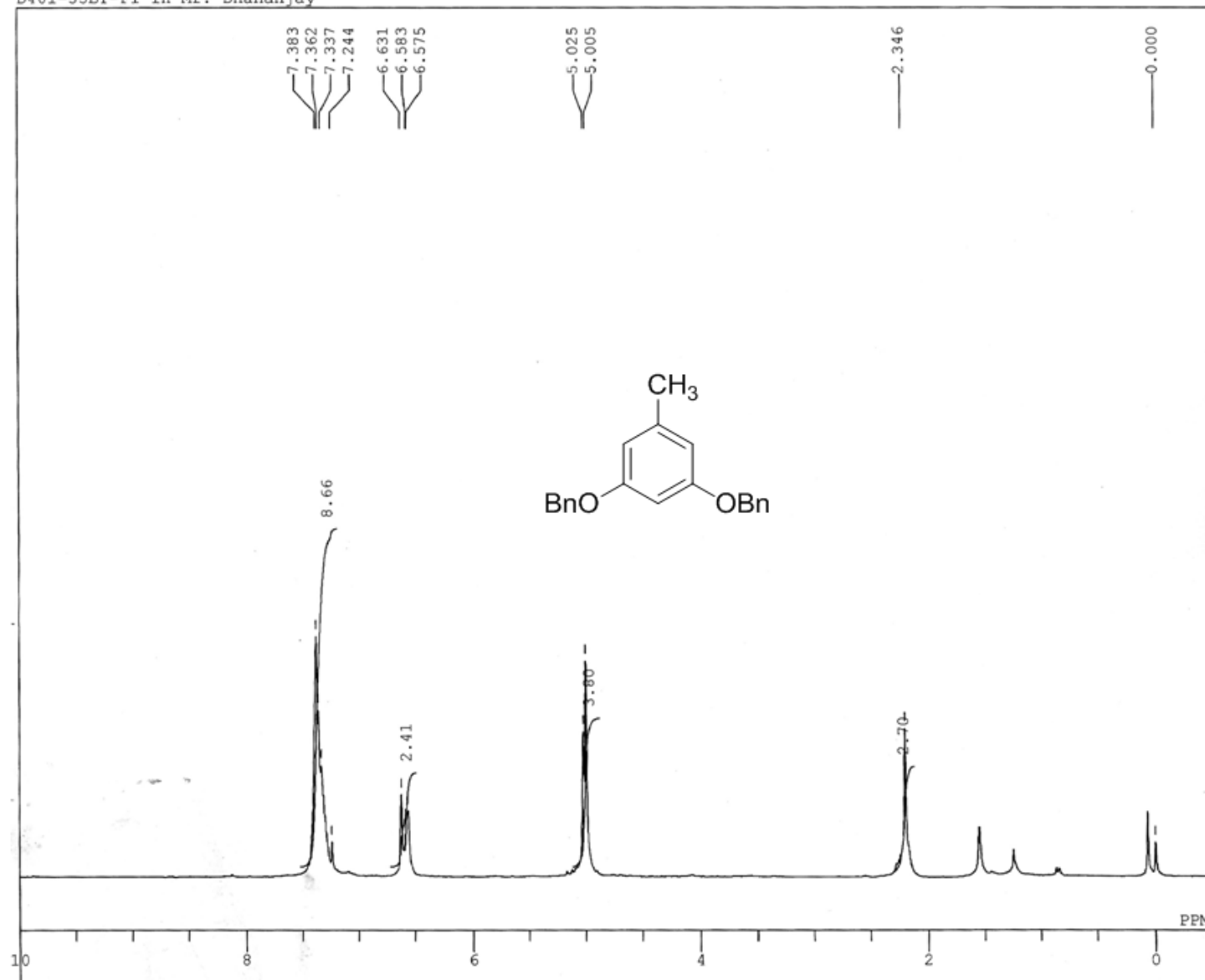
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University
 VARANASI-221005

Operator : Nagendra Kuma
 Shishir Singh

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 DATIM Tue May 20 22:36:
 OBNUC 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 190
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 6.0 us
 IRNUC 1H
 CTEMP 25.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 24

Spectrum 33: 75 MHz ^{13}C NMR of compound 25d

D401-35BT-F1 1H Mr. Dhananjay



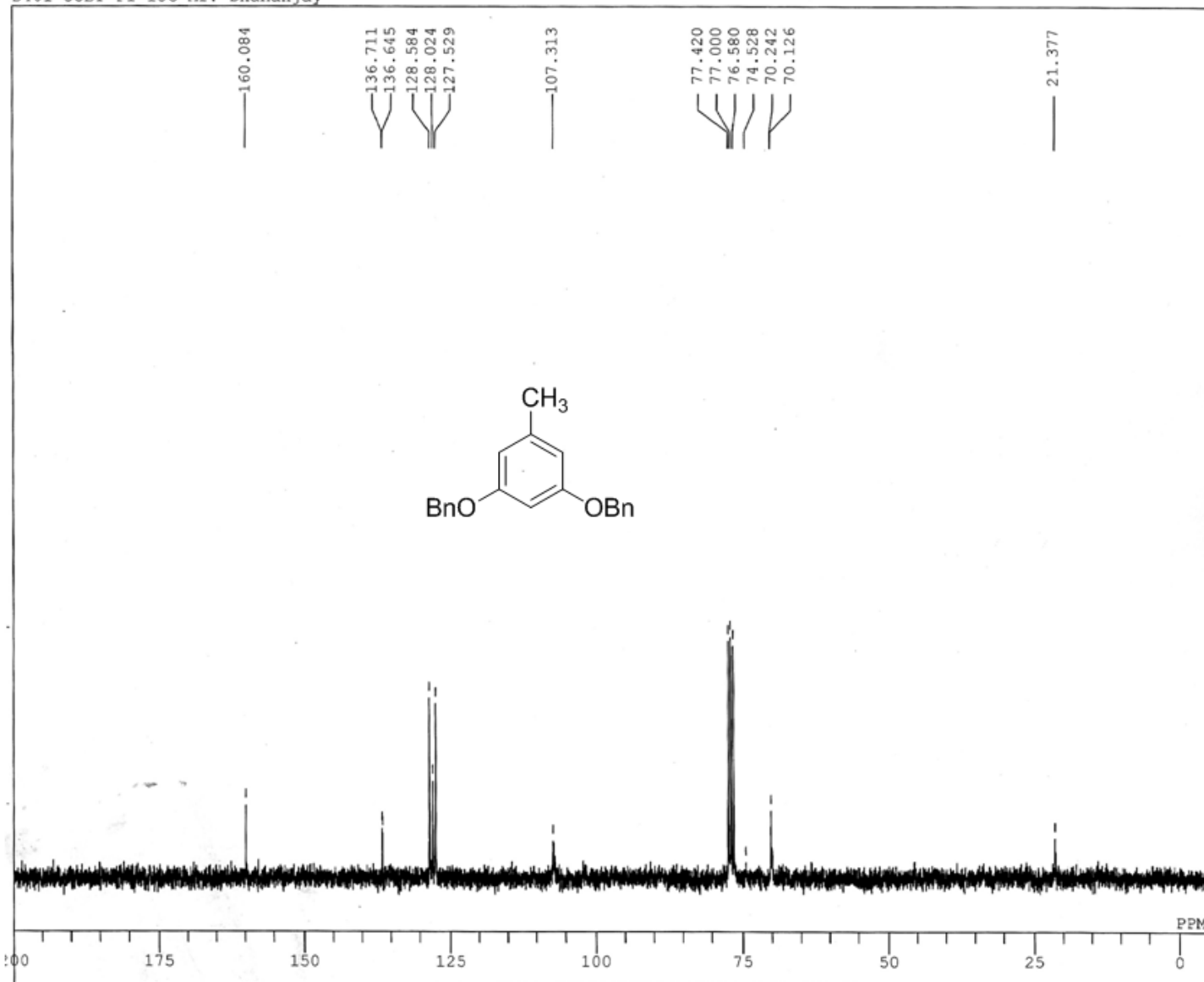
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Thu Sep 05 15:43:52 20
 OBNUC 1H
 EXMOD NON
 OBFRQ 300.40 MHz
 OBSET 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 20
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 24.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 19

Spectrum 34: 300 MHz ¹H NMR of compound 26a

D401-35BT-F1 13C Mr. Dhananjay



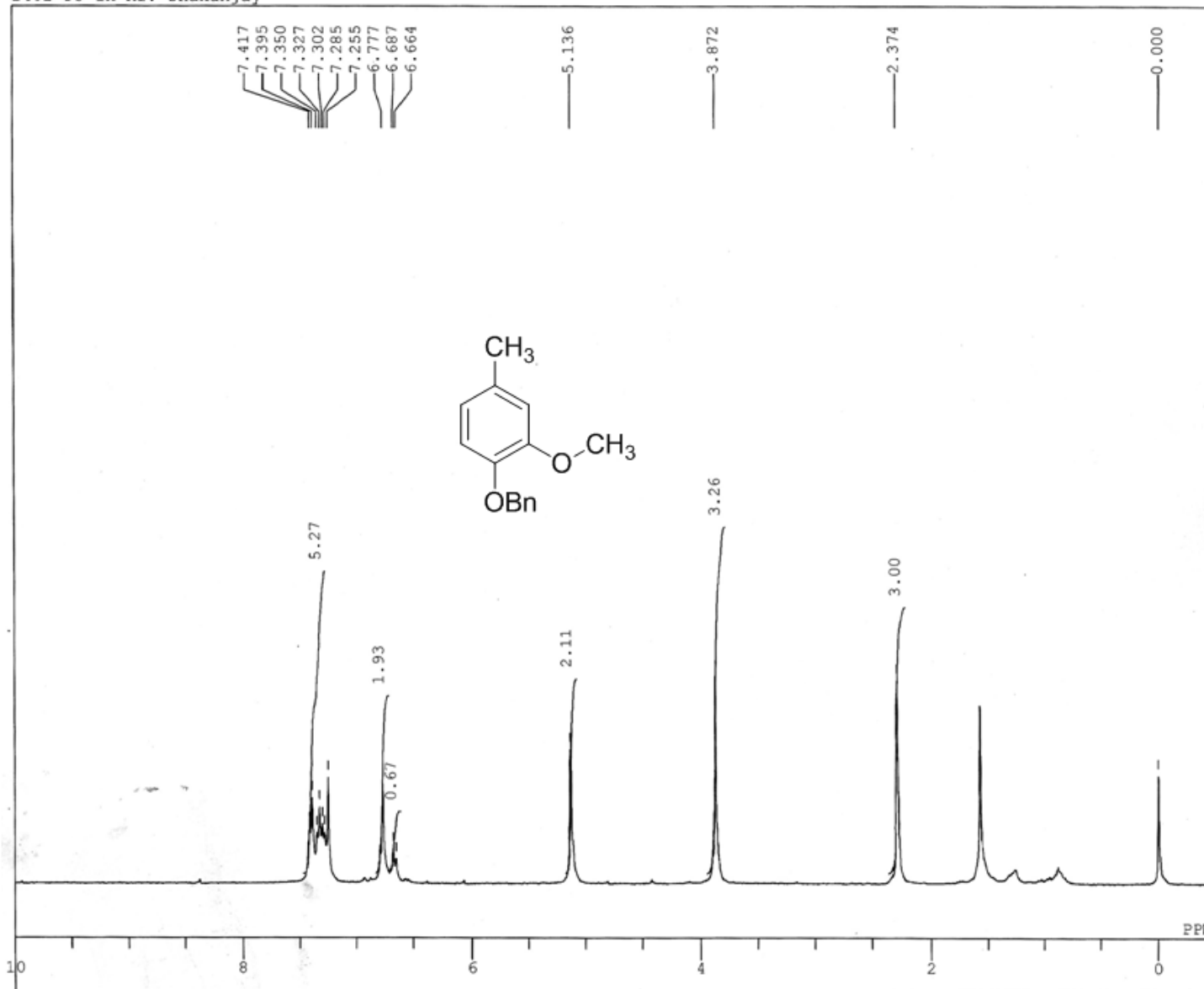
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Thu Sep 05 15:37:06 20:
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 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 157
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 24.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 25

Spectrum 35: 75 MHz ¹³C NMR of compound 26a

D402-F3 1H Mr. Dhananjay



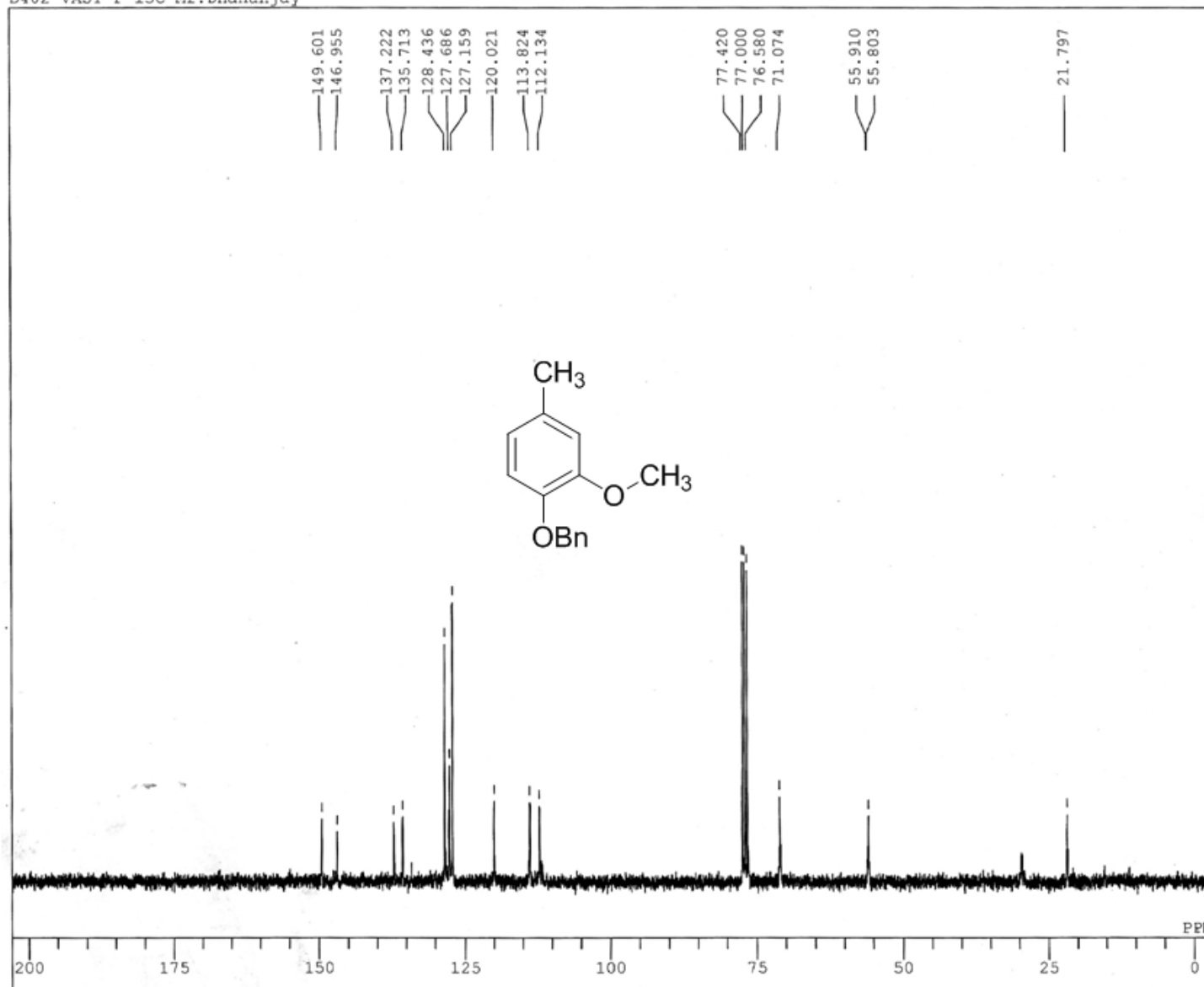
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Thu Sep 05 15:12:12 20
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 EXMOD NON
 OBFRQ 300.40 MHz
 OBSET 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 20
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 25.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 23

Spectrum 36: 300 MHz ¹H NMR of compound 26b

D402-VAST-F 13C Mr.Dhananjay

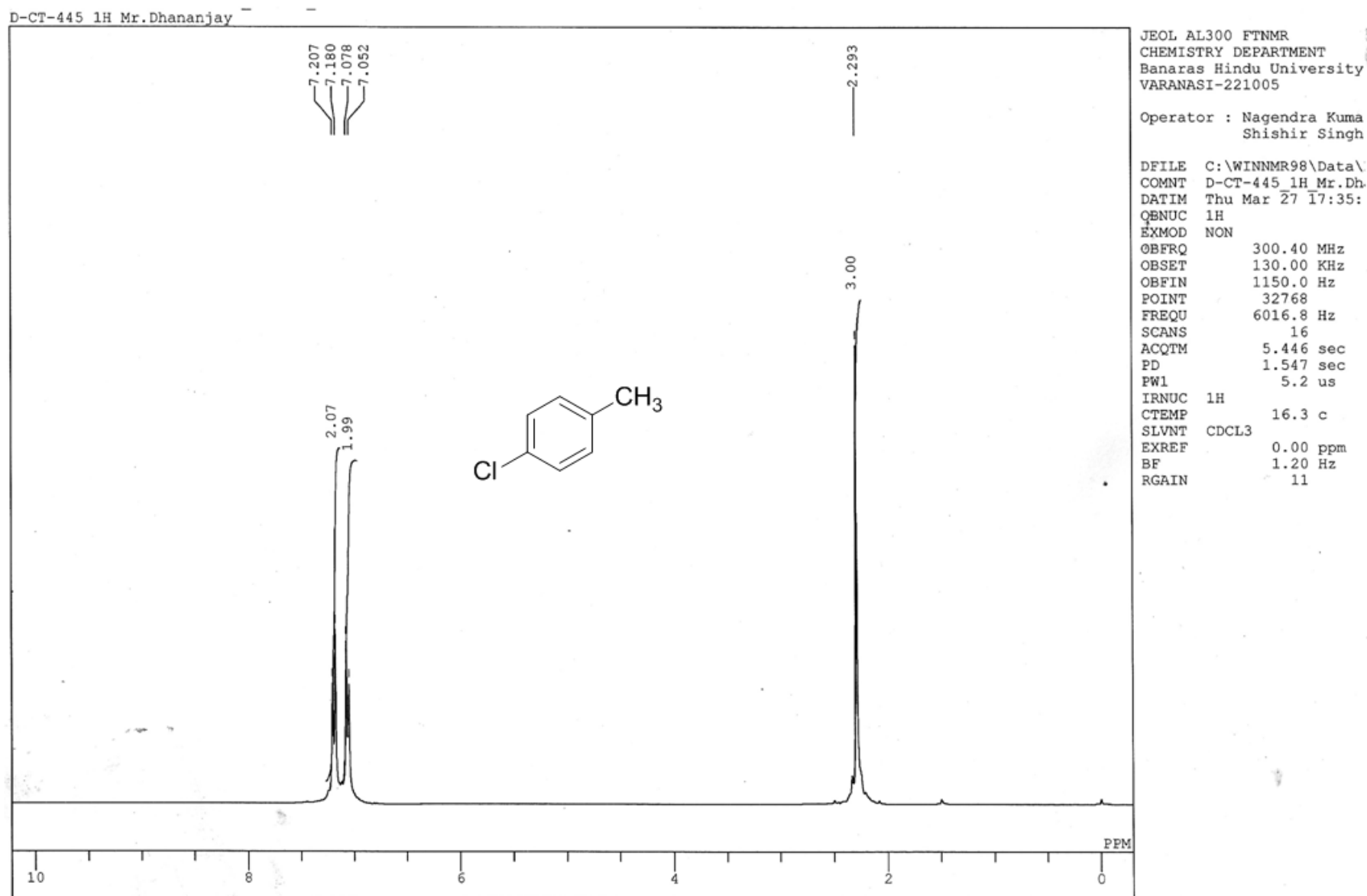


JEOL AL300 FTNMR
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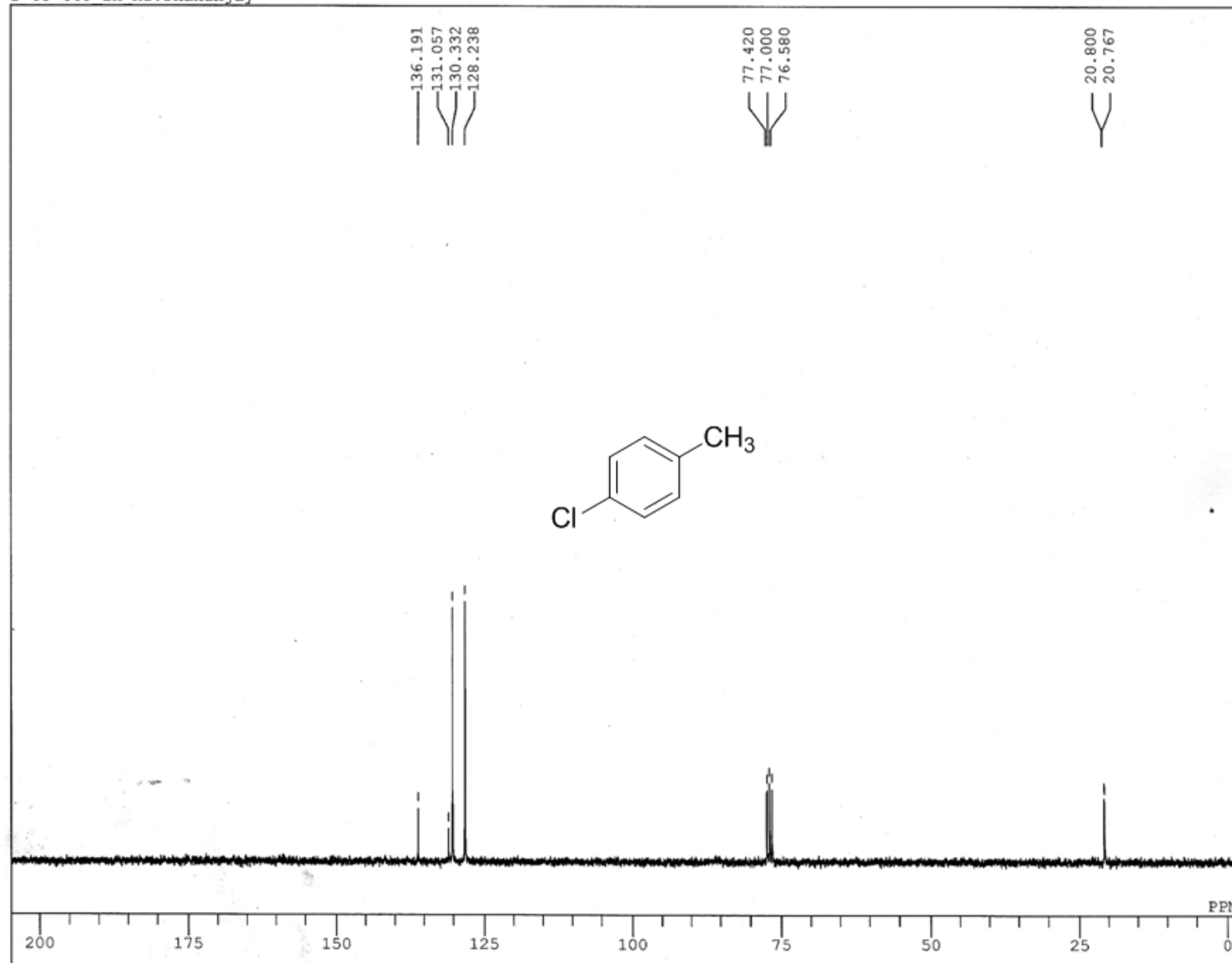
Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Wed Aug 28 15:10:07 20
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 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 305
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 22.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 24

Spectrum 37: 75 MHz ^{13}C NMR of compound 26b

Spectrum 38: 300 MHz ¹H NMR of compound 26d

D-CT-445 1H Mr.Dhananjay



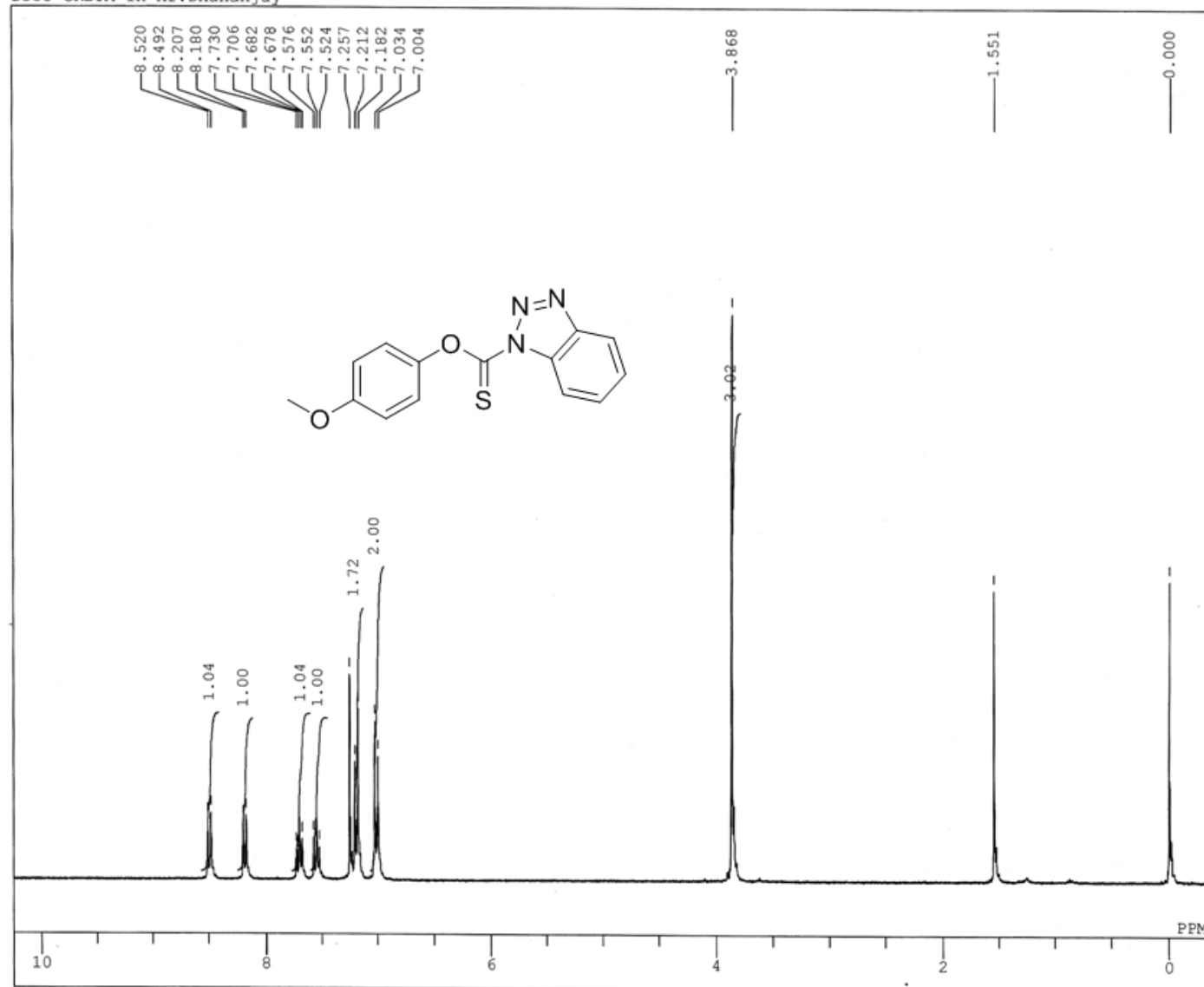
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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COMNT D-CT-445 1H Mr.Dh.
DATIM Thu Mar 27 17:40:
QBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 100
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 17.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

Spectrum 39: 75 MHz ^{13}C NMR of compound 26d

D355-GRBTA 1H Mr.Dhananjay



JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

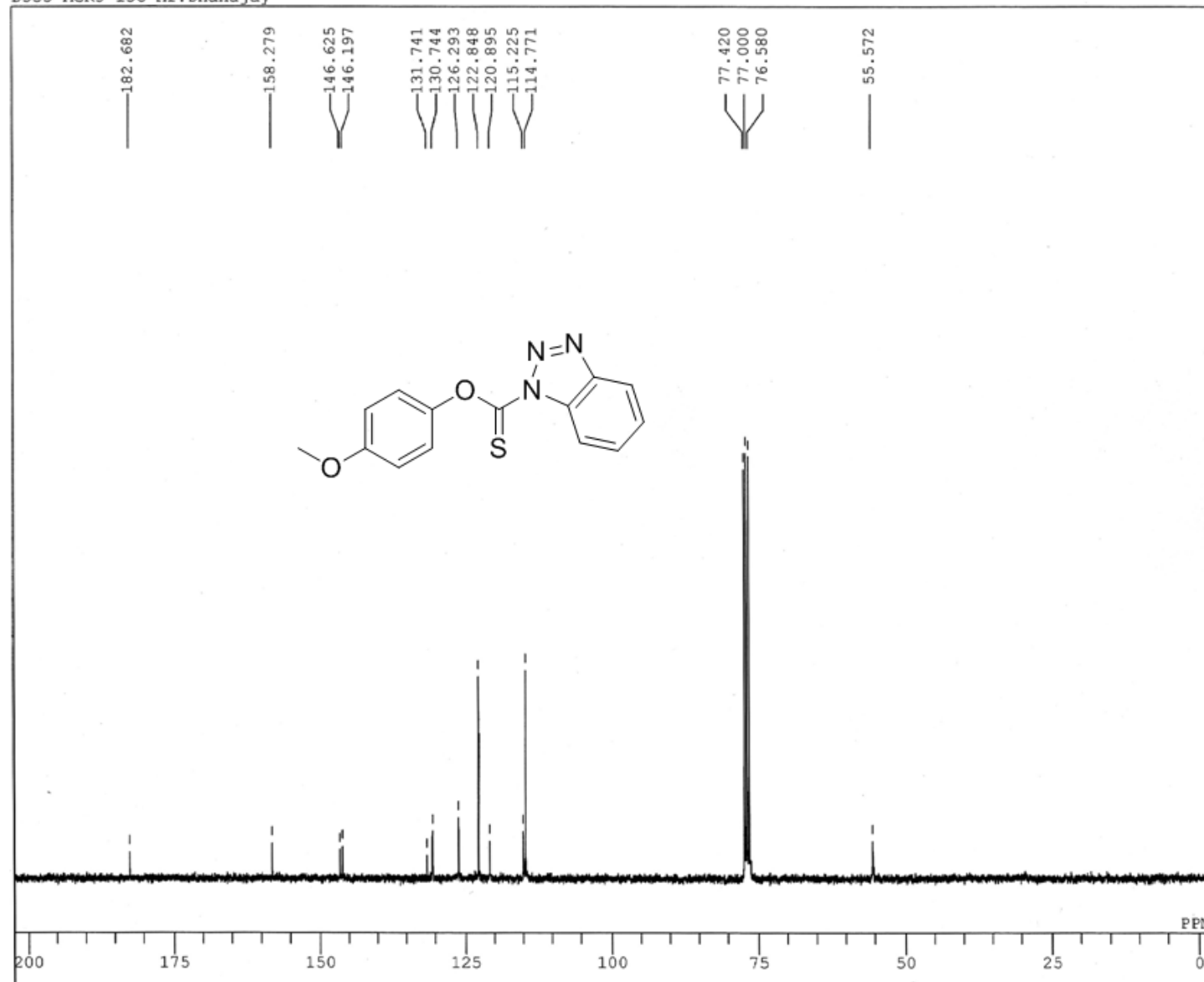
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 Shishir Singh

D355-GRBTA 1H Mr.Dhananjay

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 OBNUC 1H
 EXMOD NON
 OBFRQ 300.40 MHz
 OBSET 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 6016.8 Hz
 SCANS 16
 ACQTM 5.446 sec
 PD 1.547 sec
 PW1 5.6 us
 IRNUC 1H
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 24

Spectrum 40: 300 MHz ¹H NMR of compound 28

D355-AGR3 13C Mr.Dhanajay



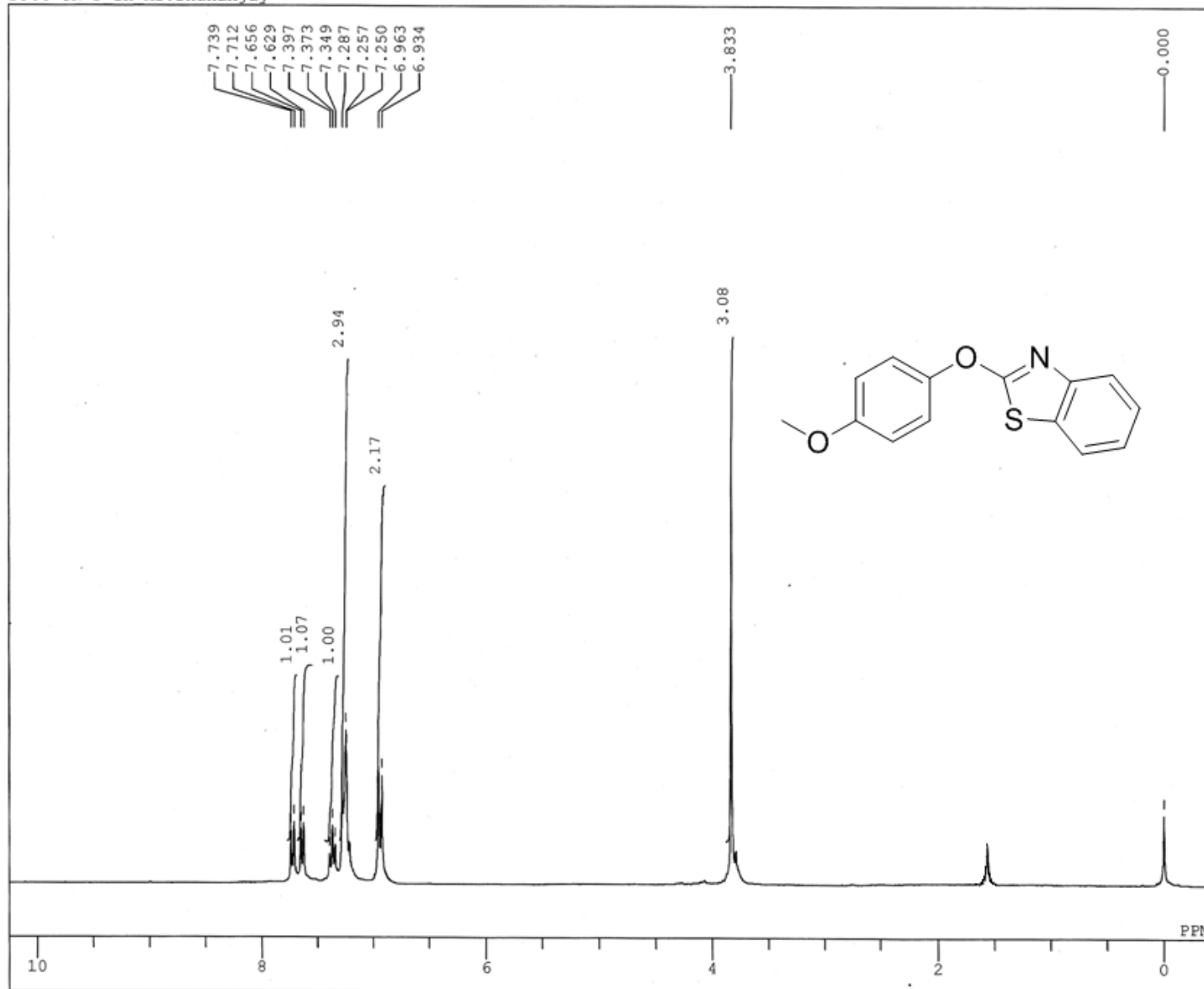
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Thu Jun 06 20:50:31 20
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 EXMOD BCM
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 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 2000
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 21.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 24

Spectrum 41: 75 MHz ¹³C NMR of compound 28

D364-GR-F 1H Mr.Dhananjay



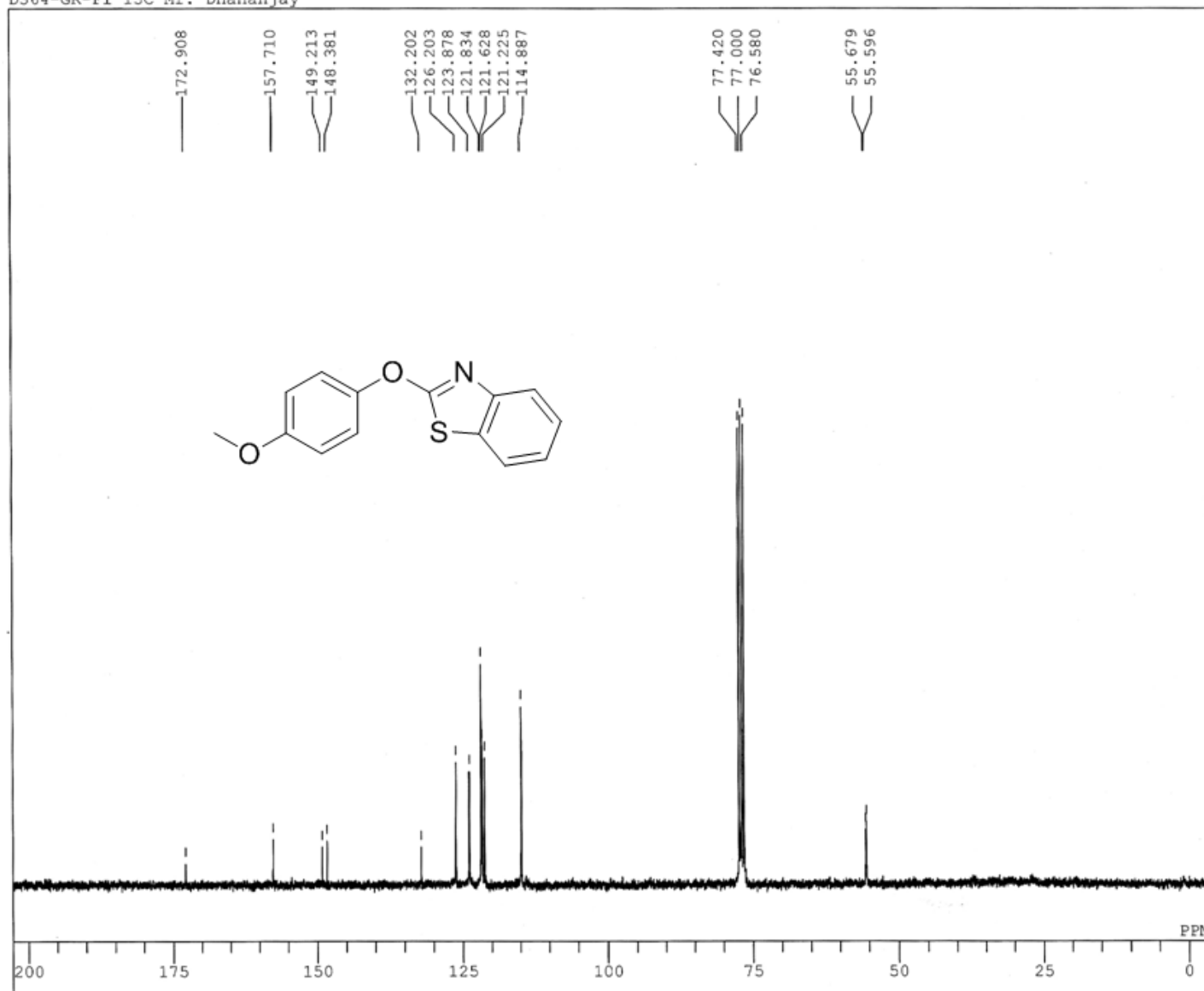
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 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Thu Jun 13 16:53:45 20
 OBNUC 1H
 EXMOD NON
 OBFRQ 300.40 MHz
 OBSET 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 10
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 23.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.22 Hz
 RGAIN 16

Spectrum 42: 300 MHz ^1H NMR of compound **29**

D364-GR-F1 13C Mr. Dhananjay



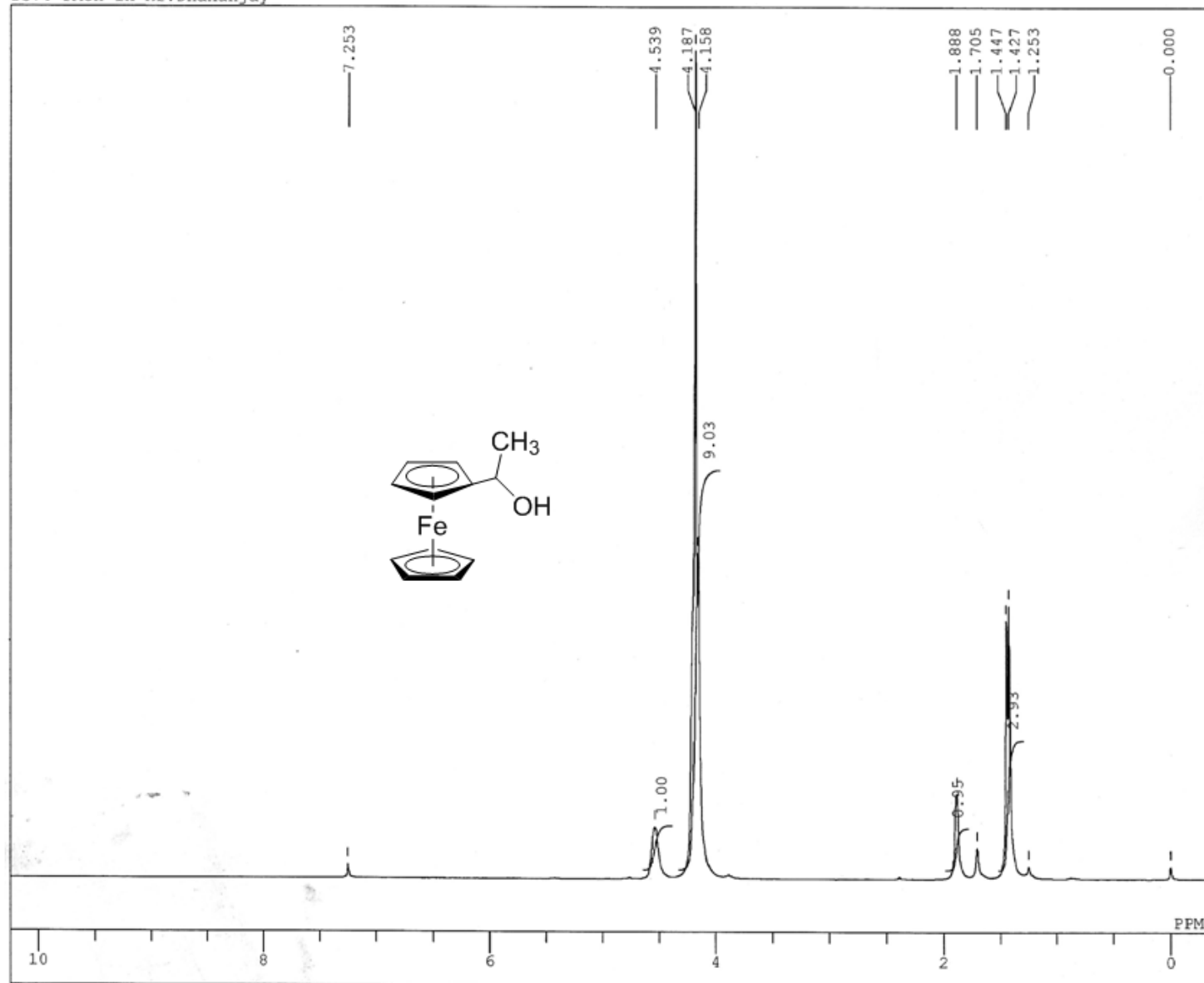
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 DATIM Wed Jul 10 09:51:16 20
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 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 2500
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 22.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 24

Spectrum 43: 75 MHz ^{13}C NMR of compound 29

D374-FAOH 1H Mr.Dhananjay



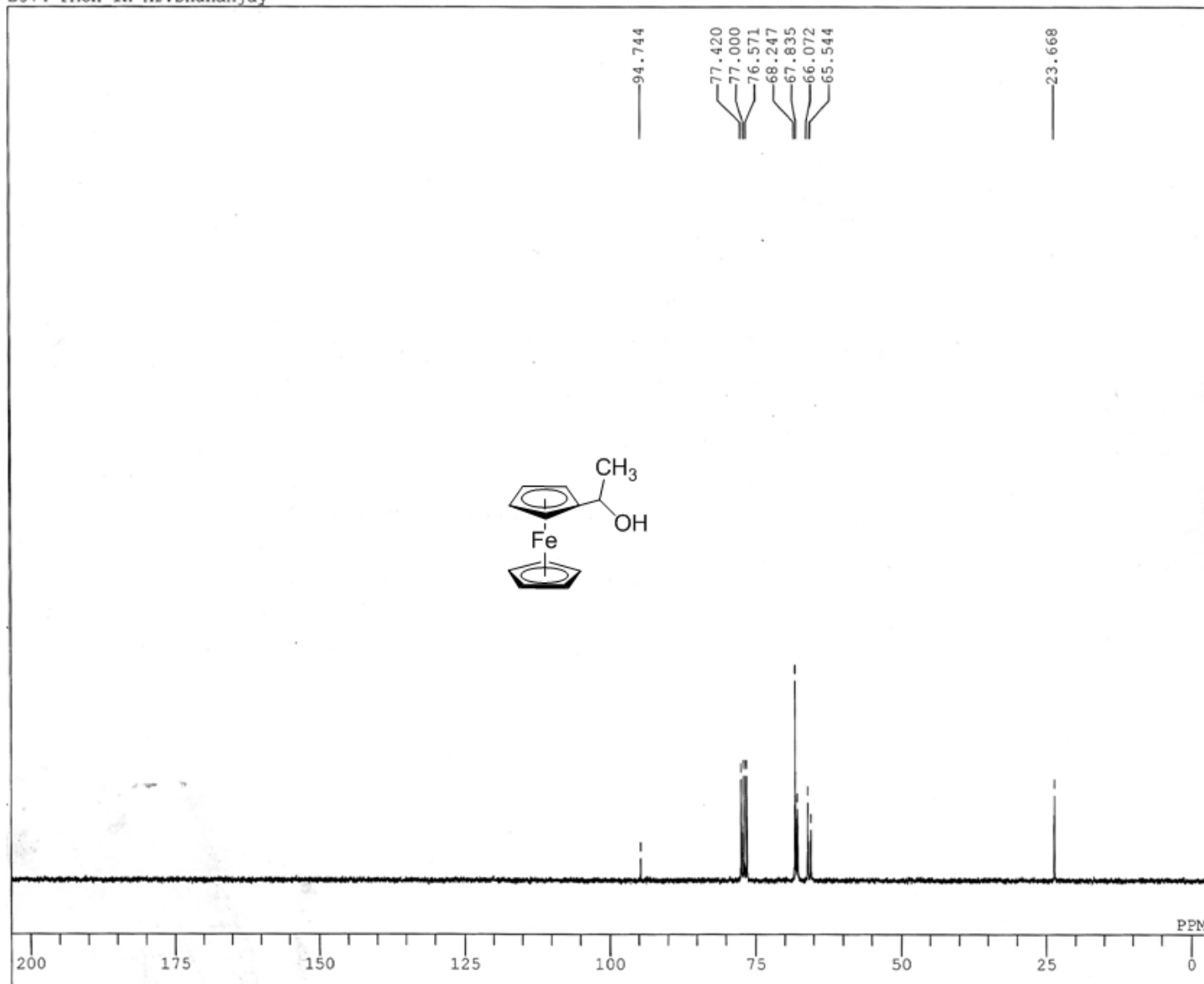
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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DATIM Fri Jul 05 13:50:05 20:
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EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 16
ACQTM 5.446 sec
PD 1.547 sec
PWL 5.6 us
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 13

Spectrum 44: 300 MHz ^1H NMR of compound 30

D374-FAOH 1H Mr.Dhananjay



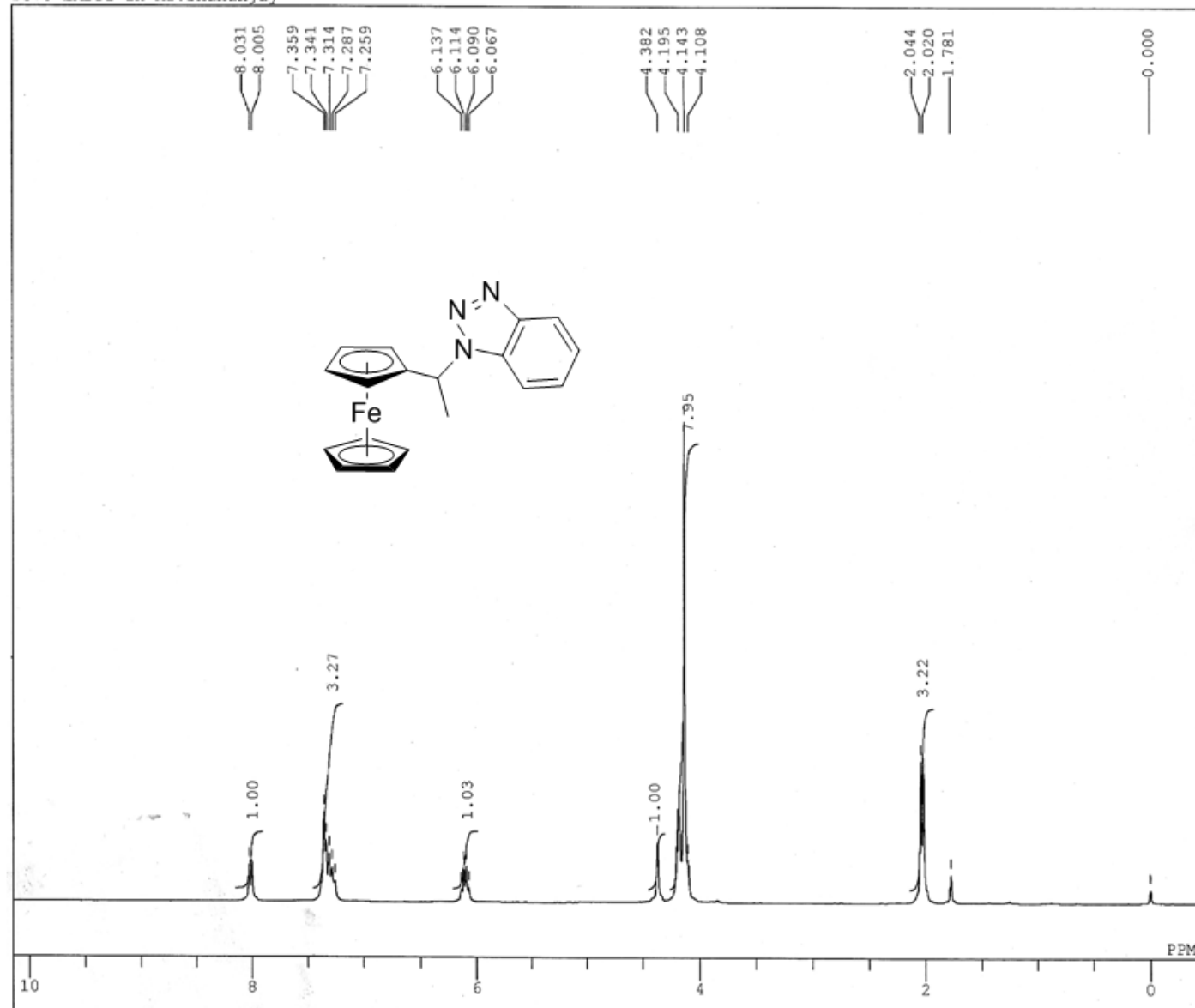
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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DATIM Fri Jul 05 14:07:57 20:
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EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 350
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 24.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

Spectrum 45: 75 MHz ^{13}C NMR of compound 30

D375-EABT1 1H Mr.Dhananjay



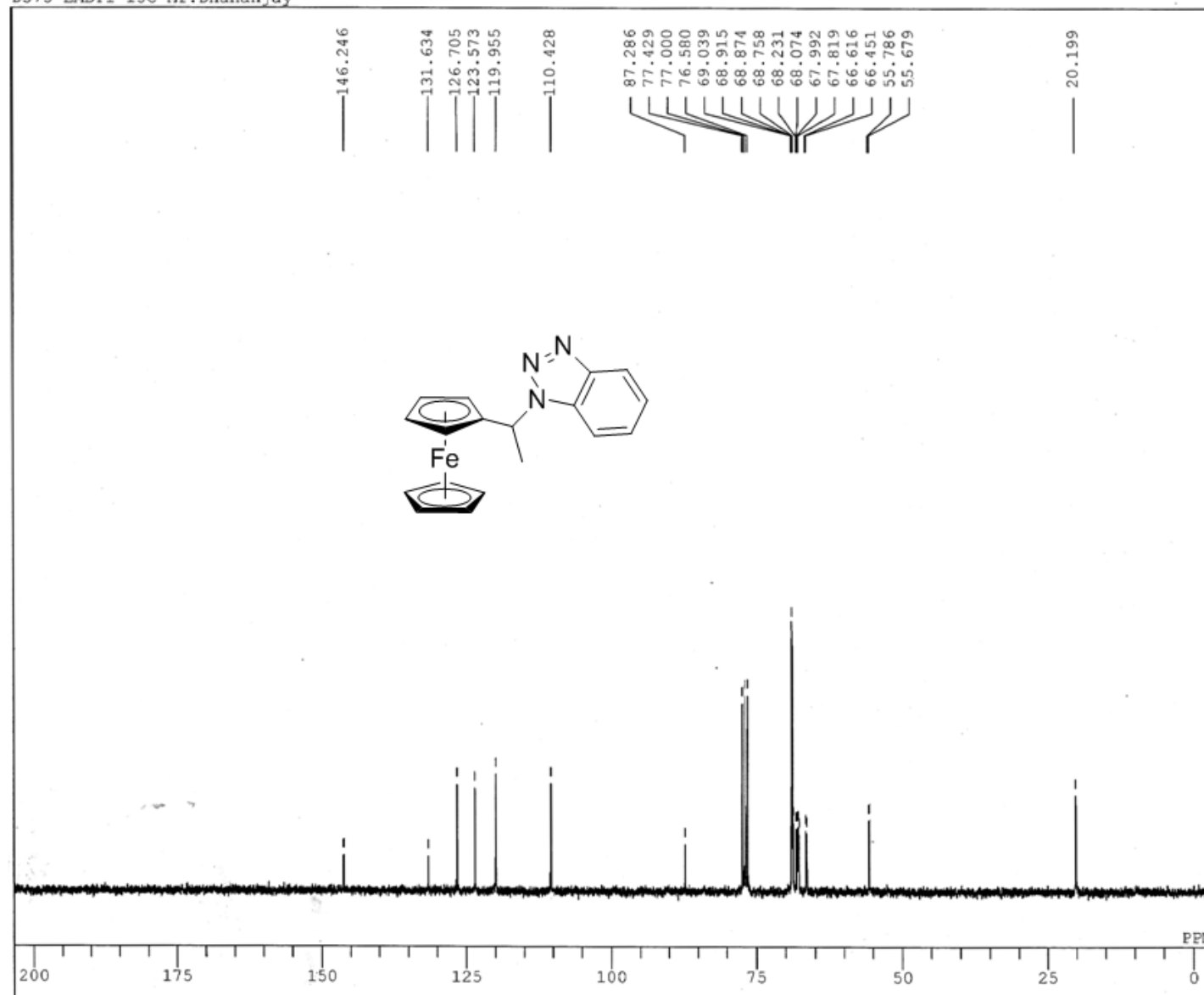
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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DATIM Tue Jul 23 13:01:20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 10
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 25.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.22 Hz
RGAIN 15

Spectrum 46: 300 MHz ^1H NMR of compound 31

D375-EABT1 13C Mr.Dhananjay



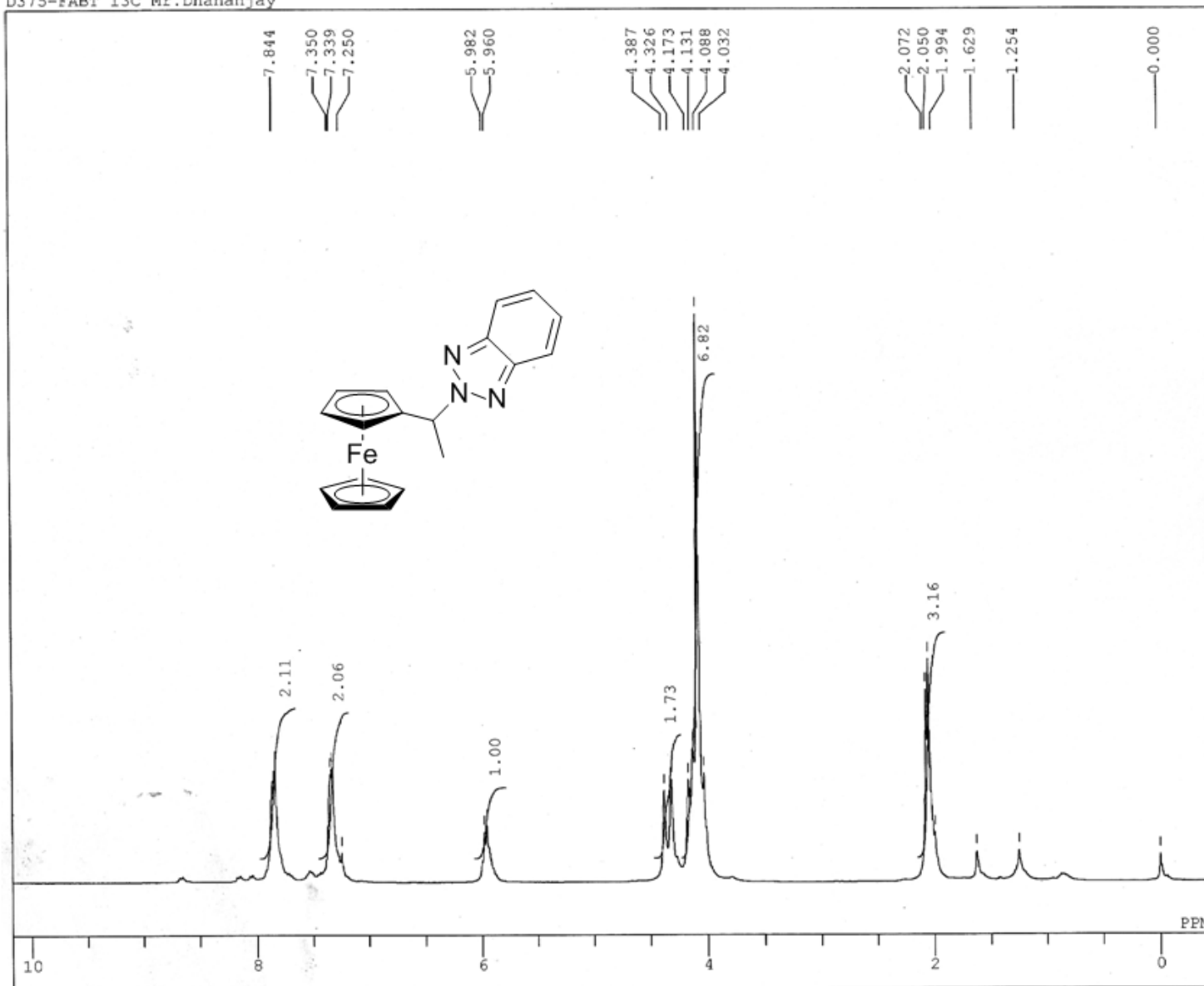
JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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 COMNT D375-EABT1_13C Mr.
 DATIM Tue Jul 23 12:57:2
 OBNUC 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 354
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 25.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.22 Hz
 RGAIN 24

Spectrum 47: 75 MHz ^{13}C NMR of compound 31

D375-FABT 13C Mr.Dhananjay



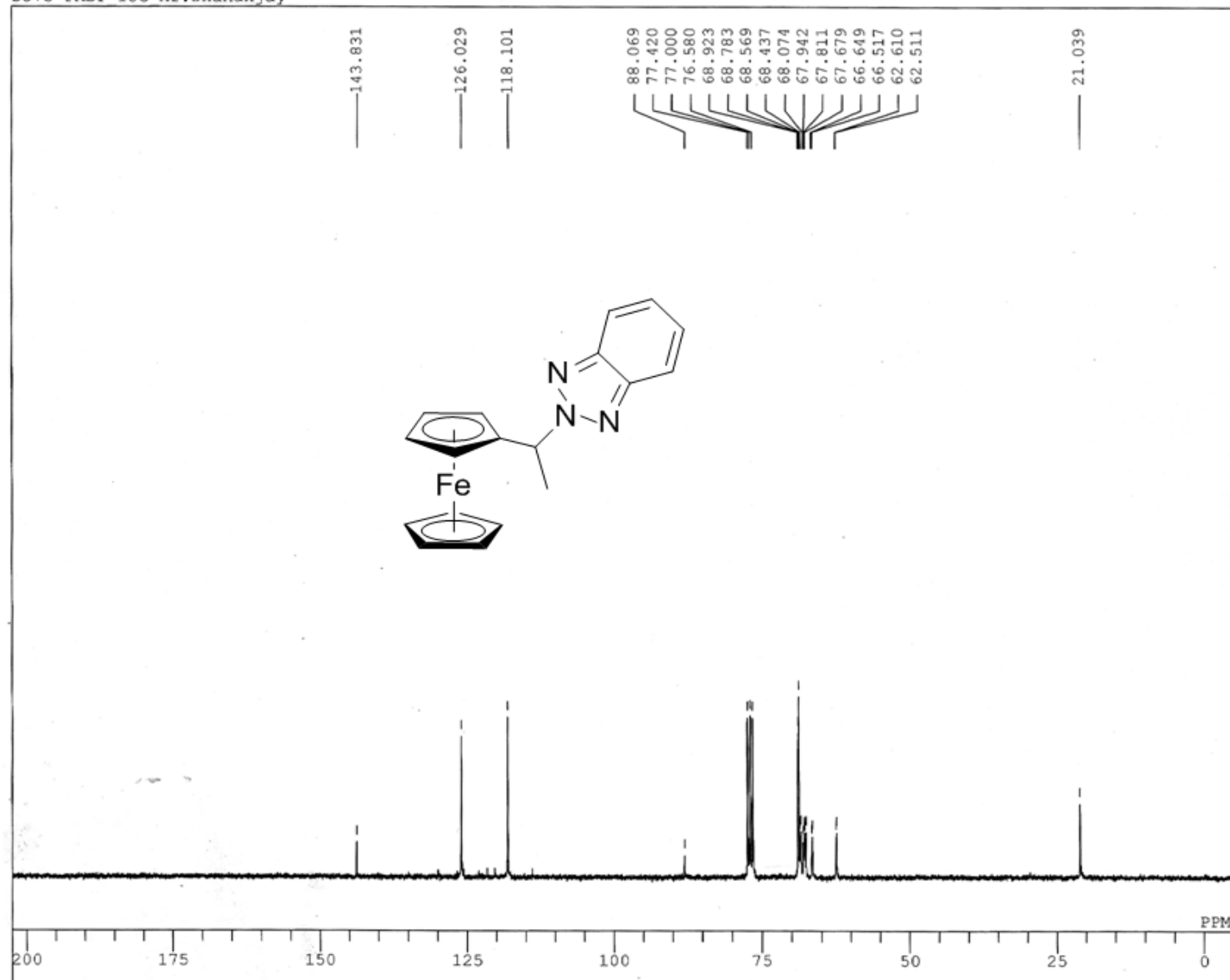
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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DATIM Tue Jul 16 18:23:1
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 32
ACQTM 5.446 sec
PD 1.547 sec
PW1 5.6 us
IRNUC 1H
CTEMP 24.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17

Spectrum 48: 300 MHz ^1H NMR of compound 32

D375-FABT 13C Mr.Dhananjay



JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

DFILE C:\WINNMR98\Data\D3
 COMNT D375-FABT 13C_Mr.Dh.
 DATIM Tue Jul 16 20:03:38
 OBNUC 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 2000
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.9 us
 IRNUC 1H
 CTEMP 21.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 23

Spectrum 49: 75 MHz ^{13}C NMR of compound 32

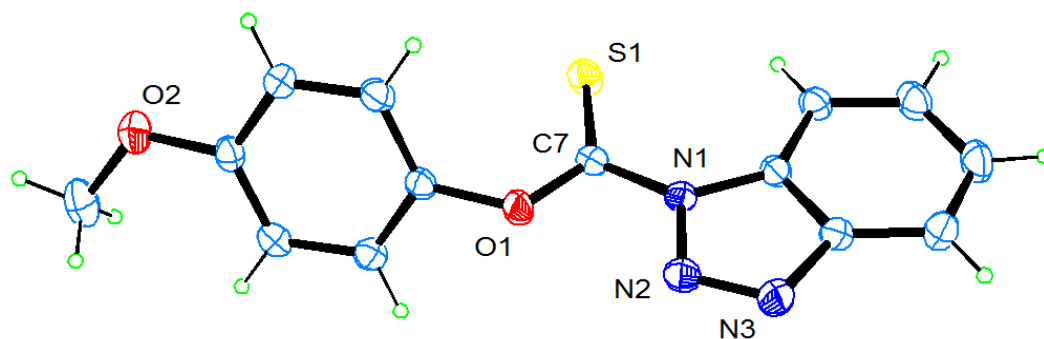
2. Single Crystal X-Ray Experimental details, refinement data and visualized molecular structure of compounds 28, 31 & 32

Data Collection and Refinement

Single-crystal X-ray data of compounds were collected on Xcalibur Eos (Oxford) CCD-Diffractometer using graphite monochromated MoK α radiation ($\lambda = 0.71073$ Å). The data integration and reduction were processed with CrysAlis Pro software. The structures were solved by the direct method and then refined on F^2 by the full matrix least-squares technique with the SHELX-97 set of software using the WinGX (version 1.80.05) program package. All non-hydrogen atoms were refined anisotropically and hydrogen atoms were treated as riding atoms using SHELX default parameters. Molecular structures have drawn using ORTEP software given in [Figures S1-3](#). Further information on the crystal structure determination (excluding structure factors) has been given as [Table S1-3](#) and also deposited in the Cambridge Crystallographic Data Centre as supplementary publications nos. **978009**, **978010** and **978011** for compounds **28**, **31** and **32** respectively. Copies of the data can be obtained free of charge upon application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033. e-mail: deposit@ccdc.cam.ac.uk) or via internet.

Procedure for crystallization of compound 28, 31 & 32

For crystallization a 40:60 mixture of ethyl acetate and hexane has been used and kept in dark place at temperature 25 °C. The single crystal was isolated in its initial state of growth.

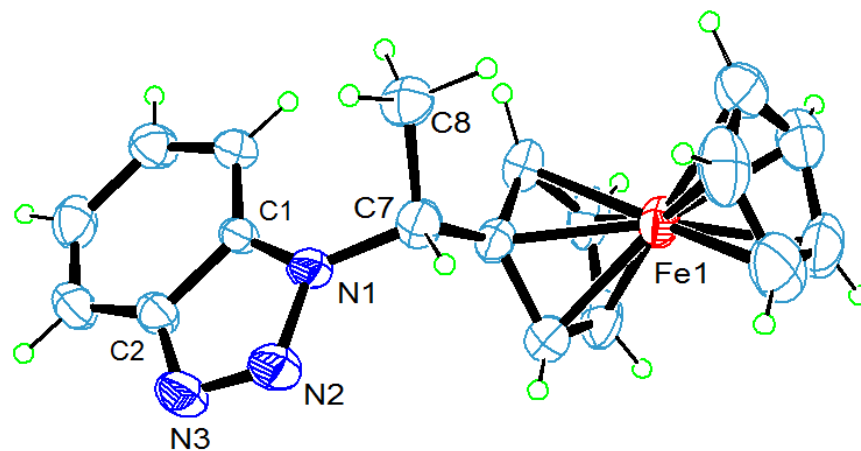


Selected bond length (Å): S1-C7 1.622, O1-C7 1.333, O1-C8 1.414, N1-N2 1.406, N1-C7 1.386, N1-C1 1.383, N2-N3 1.281, O2-C11 1.373, O2-C14 1.417; **Selected bond angles:** C7-O1-C8 120.2, N2-N1-C7 119.8, N2-N1-C1 109.0, C7-N1-C1 131.2, N1-N2-N3 108.4, S1-C7-O1 127.4, S1-C7-N1 123.9, O1-C7-N1 108.7, O1-C8-C13 117.1, O1-C8-C9 120.6, N1-C1-C6 134.6, N1-C1-C2 104.3, C1-C2-N3 108.8.

Figure S1. Molecular structure of compound **28**. Thermal ellipsoids of carbon, nitrogen, sulfur and oxygen are set at 40 % probability.

Table S1. Crystallographic refinement data for compound **28**

Compound 28	
Empirical Formula	C₁₄ H₁₁ N₃ O₂ S
Formula Weight	285.33
Crystal System	Triclinic
Space group	P -1
<i>a</i> (Å)	4.2311(7)
<i>b</i> (Å)	8.0019(16)
<i>c</i> (Å)	20.415(3)
β (°)	92.671(13)
<i>V</i> (Å ³)	676.2(2)
<i>Z</i>	2
Density (calc)	1.401
F(000)	280
μ (mm ⁻¹)	0.234
Crystal Size [mm]	0.16 x 0.17 x 0.24
Temperature (K)	293
Radiation	MoK α 0.71073
θ Min-Max [°]	3.31, 28.87
<i>h, k, l</i>	-5:5; -8:10; -26:22
Tot.,UniqData, R(int)	5013, 3051, 0.0264
Obs. data [<i>I</i> > 2.0 σ (<i>I</i>)]	1550
Nref, Npar	3580, 181
R1, wR2, S	0.0590, 0.1104, 1.019
Min. - Max. resd. dens. [e/ Å ³]	-0.205, 0.167
CCDC	978009

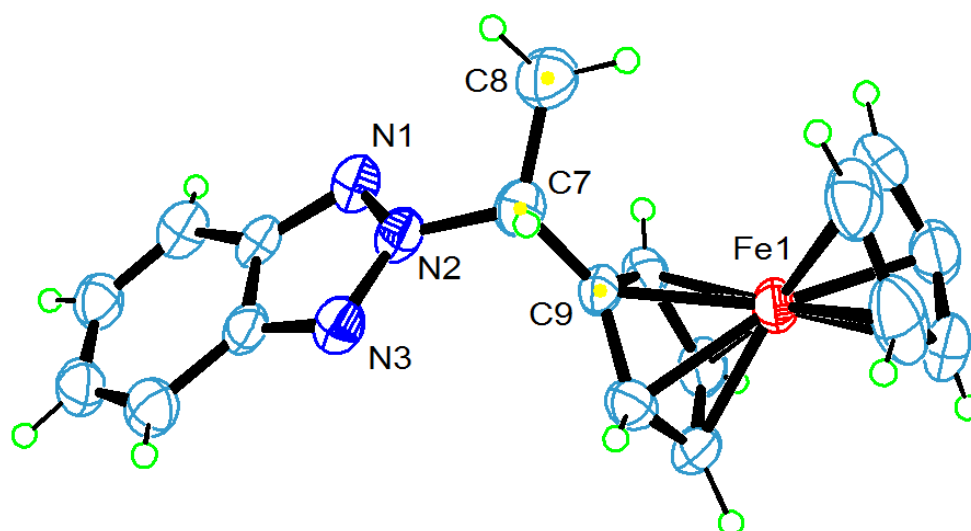


Selected bond length (Å): N1-N2 1.356, N1-C1 1.359, N1-C7 1.476, N2-N3 1.299, N3-C6 1.373; **Selected bond angles (°):** N2-N1-C1 109.9, N2-N1-C7 118.5, C1-N1-C7 131.4, N1-N2-N3 108.9, N2-N3-C6 109.0, N1-C1-C2 134.6, N1-C1-C6 104.6, N3-C6-C1 107.6.

Figure S2. Molecular structure of compound **31**. Thermal ellipsoids of carbon, nitrogen and iron are set at 40 % probability.

Table S2. Crystallographic refinement data for compound **31**

Compound 31 (N1)	
Empirical Formula	C₁₈ H₁₇ Fe N₃
Formula Weight	331.20
Crystal System	Monoclinic
Space group	P 1 21/n 1
<i>a</i> (Å)	6.6888(7)
<i>b</i> (Å)	28.847(2)
<i>c</i> (Å)	8.3300(10)
β (°)	104.396(11)
<i>V</i> (Å ³)	1556.8(3)
<i>Z</i>	4
Density (calc)	1.413
F(000)	688.0
μ (mm ⁻¹)	0.968
Crystal Size [mm]	0.13 x 0.15 x 0.23
Temperature (K)	293
Radiation	MoK α 0.71073
θ Min-Max [°]	3.22, 29.13
<i>h, k, l</i>	-8:8; -18:39; -5:11
Tot.,UniqData, R(int)	6934, 3558, 0.0425
Obs. data [<i>I</i> > 2.0 σ (<i>I</i>)]	2076
Nref, Npar	4193, 259
R1, wR2, S	0.0694, 0.1545, 1.097
Min. - Max. resd. dens. [e/ Å ³]	-0.288, 0.370
CCDC	978010



Selected bond length (Å): N2-N3 1.33, N2-N1 1.32, N2-C7 1.48, N3-C6 1.36, N1-C1 1.35; **Selected bond angles (°):** N3-N2-N1 117.6, N3-N2-C7 120.1, N1-N2-C7 121.8, N2-N3-C6 102.7, N2-N1-C1 102.4, N1-C1-C2 130.0, N1-C1-C6 109.2, N3-C6-C5 129, N2-C7-C9 104.8, N2-C7-C8 111.3, N2-C7-H7 101, N3-C6-C5 131.1, N3-C6-C1 108.1.

Figure S3. Molecular structure of compound **32**. Thermal ellipsoids of carbon, nitrogen and iron are set at 40 % probability.

Table S3. Crystallographic refinement data for compound **32**

Compound 32 (N2)	
Empirical Formula	C₁₈ H₁₇ Fe N₃
Formula Weight	331.20
Crystal System	Monoclinic
Space group	P 1 21 1
<i>a</i> (Å)	6.1853(6)
<i>b</i> (Å)	30.023(3)
<i>c</i> (Å)	8.4797(9)
β (°)	104.478(10)
<i>V</i> (Å ³)	1524.7(3)
<i>Z</i>	4
Density (calc)	1.443
F(000)	688
μ (mm ⁻¹)	0.988
Crystal Size [mm]	0.12 x 0.18 x 0.20
Temperature (K)	293
Radiation	MoK α 0.71073
θ Min-Max [°]	3.40, 29.08
<i>h, k, l</i>	-8:7; -38:39; -9:11
Tot.,UniqData, R(int)	6476, 4835, 0.0328
Obs. data [<i>I</i> > 2.0 σ (<i>I</i>)]	3163
Nref, Npar	4835, 433
R1, wR2, S	0.0611, 0.1212, 1.046
Min. - Max. resd. dens. [e/ Å ³]	-0.349, 0.416
CCDC	978011