

Supporting Information

Utilization of carbon disulfide as a powerful building block for the synthesis of 2-aminobenzoxazoles

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I. General Experimental Section:

^1H and ^{13}C NMR spectra were run on 300 MHz and 75 MHz JEOL AL300 FTNMR spectrometer respectively at a temperature of 300 K. NMR chemical shifts are expressed in δ values with reference to tetramethylsilane (TMS) as an internal standard.

All reagents were procured from Aldrich, USA, and were used without further purification. The solvents were purified and dried according to standard methods prior to use. All reactions were carried out under an atmosphere of air. Reactions were monitored by thin-layer chromatography (TLC) carried out on silica gel 60/KieselguhrF₂₅₄ pre-coated on aluminium sheets (thickness 0.2 mm), commercially available from Merck, using ultra-violet light as the visualizing agent and I₂ as the developing agent.

II. General Experimental Procedure:

A mixture of amine (**1**, 1.5 mmol) and CS₂ (**2**, 1.5 mmol) was taken in a 25-mL round bottomed (R.B) flask with a magnetic stir bar, and then stirred thoroughly for 60 min, which resulted in the formation of the intermediate dithiocarbamate (**DTC**). To it was added 2-aminophenol (**3**, 1 mmol), and the mixture contained in the R.B flask equipped with a condenser, was then heated at a temperature of 110 °C in an oil bath for 3 h. On completion of the reaction (TLC), the resulting mixture was subsequently partitioned between ethyl acetate (5 mL) and water (10 mL). The aqueous layer was extracted thrice with ethyl acetate (5 mL) and the collected organic phase was dried (anhyd.Na₂SO₄), concentrated under vacuum and then purified by column chromatography on silica gel using mixtures of ethyl acetate and hexane as eluting agent.

III. Physical and spectroscopic data for compounds

1. 2-(1-Piperidinyl)-benzoxazole (4a):²

Colorless amorphous solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.34–7.31 (m, 1H), 7.22–7.20 (m, 1H), 7.14–7.12 (m, 1H), 7.09–6.99 (m, 1H), 3.62 (br s, 4H), 1.64 (br s, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.1, 148.4, 143.0, 123.5, 120.0, 115.6, 108.2, 46.3, 25.0, 23.8 ppm.

2. 2-(4-Morpholinyl)-benzoxazole (4b):³

Colorless solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.38 (d, J = 9.0 Hz, 1H), 7.28 (d, J = 9.0 Hz, 1H), 7.20–7.15 (m, 1H), 7.07–7.01 (m, 1H), 3.84–3.80 (m, 4H), 3.71–3.68 (m, 4H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.1, 148.7, 142.7, 124.1, 120.9, 116.4, 108.8, 66.2, 45.7 ppm.

3. *N,N*-Diethyl-2-benzoxazolamine (4c):⁴

Colourless liquid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.36 (d, J = 9.0 Hz, 1H), 7.25 (d, J = 9.0 Hz, 1H), 7.13 (t, J = 7.5 Hz, 1H), 6.97 (t, J = 7.5 Hz, 1H), 3.61 (dd, J = 7.2 Hz, J = 6.9 Hz, 4H), 1.27 (t, J = 7.2 Hz, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.1, 148.7, 143.6, 123.7, 119.8, 115.7, 108.4, 42.8, 13.4 ppm.

4. 2-(Dimethylamino)-benzoxazole (4d):^{5, 10}

Orange solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.36 (d, J = 9.0 Hz, 1H), 7.26 (d, J = 9.0 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 6.99 (t, J = 7.5 Hz, 1H), 3.20 (s, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 163.0, 149.0, 143.4, 139.2, 123.9, 120.2, 115.9, 108.6, 37.7, 31.9, 29.7 ppm.

5. N-Benzyl-N-methylbenzoxazol-2-amine (4e):⁹

Colorless solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.39 (d, J = 7.8 Hz, 1H), 7.29–7.22 (m, 6H), 7.14 (t, J = 7.5 Hz, 1H), 6.98 (t, J = 7.5 Hz, 1H), 4.71 (s, 2H), 3.08 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.8, 148.8, 143.4, 136.2, 128.5, 127.5, 127.4, 123.8, 120.2, 115.9, 108.5, 53.6, 34.9 ppm.

6. N-Hexylbenzoxazol-2-amine (4f):⁶

Orange-red solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.34 (d, J = 7.5 Hz, 1H), 7.24 (d, J = 7.8 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 6.99 (t, J = 7.5 Hz, 1H), 6.21 (br s, 1H), 3.48–3.44 (m, 2H), 1.68–1.64 (m, 2H), 1.38–1.30 (m, 6H), 0.87 (br s, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.4, 148.3, 142.9, 123.7, 120.4, 115.8, 108.5, 43.0, 31.3, 29.7, 26.4, 22.4, 13.9 ppm.

7. N-Cyclopropylbenzoxazol-2-amine (4g):

Product formation was not observed.

8. *n*-Butyl-2-Benzoxazamine (4h):⁷

Yellow solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.35 (d, J = 7.8 Hz, 1H), 7.24 (d, J = 8.1 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 5.88 (br s, 1H), 3.50–3.45 (m, 2H), 1.69–1.61 (m, 2H), 1.46–1.39 (m, 2H), 0.97–0.92 (m, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.3, 148.4, 143.0, 123.8, 120.5, 116.0, 108.6, 42.8, 31.8, 19.9, 13.7 ppm.

9. *N,N*-Dibutylbenzoxazol-2-amine (4i):¹¹

Pale yellow liquid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.35 (d, J = 7.8 Hz, 1H), 7.23 (d, J = 7.8 Hz, 1H), 7.12 (t, J = 7.5 Hz, 1H), 6.95 (t, J = 7.5 Hz, 1H), 3.49 (t, J = 7.5 Hz, 4H), 1.70–1.60 (m, 4H), 1.44–1.32 (m, 4H), 0.98–0.93 (m, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.5, 148.6, 143.6, 123.6, 119.7, 115.7, 108.3, 48.2, 30.0, 19.9, 13.8 ppm.

10. *N*-Cyclohexylbenzoxazol-2-amine (4j):⁹

Yellow solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.35 (d, J = 7.8 Hz, 1H), 7.23 (d, J = 7.8 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 6.99 (m, 1H), 5.98 (br s, 1H), 3.74 (br s, 1H), 2.14–2.10 (m, 2H), 1.77–1.62 (m, 3H), 1.47–1.18 (m, 5H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 161.5, 148.2, 142.9, 123.7, 120.4, 115.9, 108.5, 52.0, 33.4, 25.4, 24.7 ppm.

11. *N*-(Tert-butyl)benzoxazol-2-amine (4k):⁹

Yellow solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.38 (d, *J* = 7.8 Hz, 1H), 7.26–7.23 (m, 1H), 7.19–7.12 (m, 1H), 7.04–6.99 (m, 1H), 5.48 (br s, 1H), 1.50 (s, 9H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 161.0, 148.1, 142.8, 123.7, 120.6, 116.0, 108.6, 52.1, 29.2 ppm.

12. *N*-Phenethylbenzoxazol-2-amine (4l):⁹

Light cream solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.33–7.11 (m, 8H), 7.02–6.97 (m, 1H), 5.91 (br s, 1H), 3.70 (t, *J* = 6.6 Hz, 2H), 2.96 (t, *J* = 6.9 Hz, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.0, 148.3, 142.8, 128.7, 128.5, 126.5, 123.8, 120.6, 116.0, 108.6, 44.0, 35.7 ppm.

13. *N*-Benzylbenzoxazol-2-amine (4m):^{8,9}

Yellow solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.38–7.27 (m, 5H), 7.20 (t, *J* = 7.8 Hz, 2H), 7.11 (t, *J* = 7.5 Hz, 1H), 6.99 (t, *J* = 7.5 Hz, 1H), 4.64 (s, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 162.1, 148.4, 142.7, 137.4, 128.7, 127.7, 127.5, 123.9, 120.7, 116.1, 108.7, 46.9 ppm.

14. *N,N*-Dipropylbenzoxazol-2-amine (4n):¹¹

Colorless oil;

^1H NMR (300 MHz, CDCl_3 , TMS, 300 K): δ = 7.35 (d, J = 7.5 Hz, 1H), 7.24 (d, J = 8.1 Hz, 1H), 7.12 (t, J = 7.5 Hz, 1H), 6.96 (t, J = 7.5 Hz, 1H), 3.49–3.44 (m, 4H), 1.74–1.66 (m, 4H), 0.98–0.93 (m, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 162.5, 148.6, 143.6, 123.6, 119.8, 115.6, 108.3, 50.2, 21.1, 11.1 ppm.

15. 5-Methyl-2-(piperidin-1-yl)benzoxazole (4o):¹⁰

Colorless solid;

^1H NMR (300 MHz, CDCl_3 , TMS, 300 K): δ = 7.13–7.08 (m, 2H), 6.80 (d, J = 8.1 Hz, 1H), 3.65 (br s, 4H), 2.37 (s, 3H), 1.67 (br s, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 162.6, 146.7, 143.1, 133.5, 121.0, 116.2, 110.3, 107.9, 46.5, 25.2, 24.0, 21.5 ppm.

16. *N,N*-Diethyl-5-methylbenzoxazol-2-amine (4p):⁴

Pale yellow solid;

^1H NMR (300 MHz, CDCl_3 , TMS, 300 K): δ = 7.14–7.09 (m, 2H), 6.79 (d, J = 8.1 Hz, 1H), 3.61–3.54 (m, 4H), 2.38 (s, 3H), 1.29–1.24 (m, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 161.6, 146.1, 143.5, 133.4, 120.5, 116.1, 107.8, 42.9, 21.5, 13.4 ppm.

17. *N,N*-Dibutyl-5-methylbenzoxazol-2-amine (4q):¹¹

Colorless solid;

^1H NMR (300 MHz, CDCl_3 , TMS, 300 K): δ = 7.06 (s, 1H), 7.03 (d, J = 9.0 Hz, 1H), 6.70 (d, J = 8.1 Hz, 1H), 3.41 (t, J = 7.5 Hz, 4H), 2.28 (s, 3H), 1.63–1.52 (m, 4H), 1.36–1.18 (m, 4H), 0.90–0.85 (m, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 162.8, 146.9, 143.8, 133.3, 120.4, 116.2, 107.7, 48.3, 30.1, 21.5, 20.0, 13.9 ppm.

18. 2-Morpholino-5-nitrobenzoxazole (4r):¹⁰

Bright yellow solid;

^1H NMR (300 MHz, CDCl_3 , TMS, 300 K): δ = 8.17 (s, 1H), 8.03 (d, J = 8.7 Hz, 1H), 7.33–7.27 (m, 1H), 3.86–3.83 (m, 4H), 3.75–3.72 (m, 4H) ppm.

^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 163.2, 152.6, 145.2, 143.8, 117.3, 111.9, 108.4, 66.0, 45.6, 29.7 ppm.

19. *N,N*-Diethyl-5-nitrobenzoxazol-2-amine (4s):⁴

Light yellow solid;

^1H NMR (300 MHz, CDCl_3 , TMS, 300 K): δ = 8.13 (s, 1H), 7.96–7.92 (m, 1H), 7.29 (d, J = 8.7 Hz, 1H), 3.65–3.58 (m, 4H), 1.34–1.29 (t, J = 6.9 Hz, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 163.6, 152.8, 144.9, 144.6, 116.4, 111.0, 107.9, 43.2, 13.2 ppm.

20. 5-Nitro-2-(piperidin-1-yl)benzoxazole (4t):¹⁰

Bright yellow solid;

^1H NMR (300 MHz, CDCl_3 , TMS, 300 K): δ = 8.12 (s, 1H), 7.97–7.94 (m, 1H), 7.28 (d, J = 8.7 Hz, 1H), 3.70 (br s, 4H), 1.72 (br s, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 163.7, 152.6, 145.0, 144.4, 116.7, 111.2, 108.0, 46.6, 25.1, 23.8 ppm.

21. *N,N*-Dimethyl-5-nitrobenzoxazol-2-amine (4u):³

Orange solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 8.16 (s, 1H), 7.99–7.96 (m, 1H), 7.31 (d, *J* = 9.0 Hz, 1H), 3.25 (s, 6H) ppm.

22. 2-Mercaptobenzoxazole (6):¹²

Colorless solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 10.79 (br s, 1H), 7.36–7.23 (m, 4H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 181.0, 148.9, 130.4, 125.3, 124.4, 115.2, 110.5, 110.2 ppm.

23. Piperidin-1-ium piperidine-1-carbodithioate (5):

Colorless solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 9.01 (br s, 2H), 4.38–4.35 (m, 4H), 3.34 (m, 4H), 1.91–1.84 (m, 6H), 1.63–1.59 (m, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃, TMS, 300 K): δ = 208.5, 51.8, 45.0, 26.0, 24.3, 22.6, 22.4 ppm.

24. 1,3-Diphenethylthiourea (8):¹

Pale brown solid;

¹H NMR (300 MHz, CDCl₃, TMS, 300 K): δ = 7.26–7.13 (m, 10H), 5.93 (br s, 2H), 3.59 (br s, 4H), 2.81 (t, *J* = 6.6 Hz, 4H) ppm.

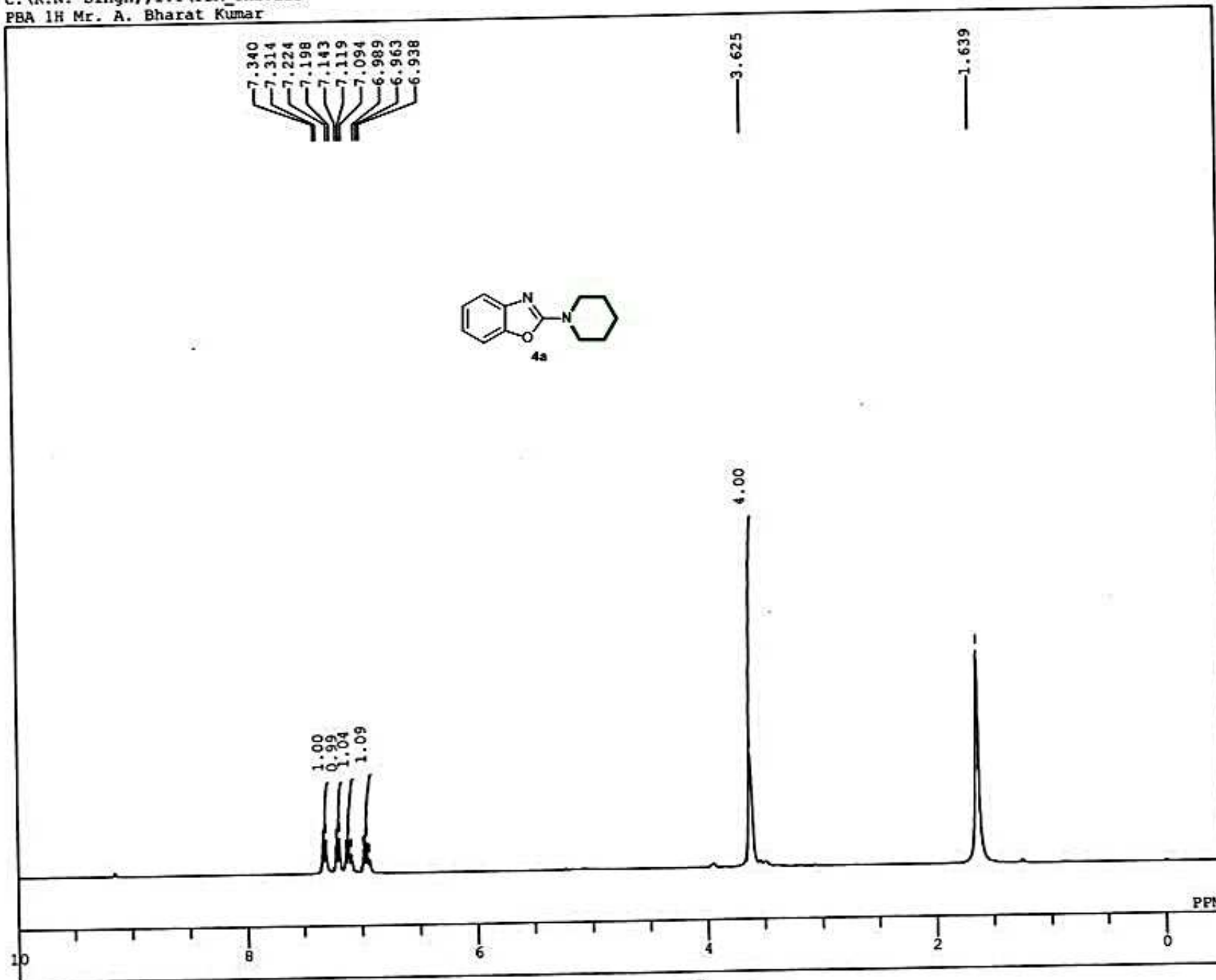
^{13}C NMR (75 MHz, CDCl_3 , TMS, 300 K): δ = 181.5, 138.2, 128.6, 128.5, 126.6, 45.3, 35.0 ppm.

IV. References:

1. M. R. Maddani and K. R. Prabhu, *J. Org. Chem.*, 2010, **75**, 2327.
2. M. Lamani and K. R. Prabhu, *J. Org. Chem.*, 2011, **76**, 7938.
3. S. H. Cho, J. Y. Kim, S. Y. Lee and S. Chang, *Angew. Chem. Int. Ed.*, 2009, **48**, 9127.
4. S. Guo, B. Qian, Y. Xie, C. Xie and H. Huang, *Org. Lett.*, 2011, **13**, 522.
5. M. Zhang, S. Zhang, M. Liu and J. Cheng, *Chem. Commun.*, 2011, **47**, 11522.
6. A. Hetzheim, G. Schlaak and C. Kerstan, *Pharmazie*, 1987, **42**, 80.
7. T. Froehr, C. P. Sindlinger, U. Kloeckner, P. Finkbeiner and B. J. Nachtsheim, *Org. Lett.*, 2011, **13**, 3754.
8. R. Yella and B. K. Patel, *J. Comb. Chem.*, 2010, **12**, 754.
9. C. L. Cioffi, J. L. Lansing and H. Yüksel, *J. Org. Chem.*, 2010, **75**, 7942.
10. S. Wertz, S. Kodama and A. Studer, *Angew. Chem. Int. Ed.*, 2011, **50**, 11511.
11. Y. Li, J. Liu, Y. Xie, R. Zhang, K. Jin, X. Wang and C. Duan, *Org. Biomol. Chem.*, 2012, **10**, 3715.
12. G. Aridoss, S. Amirthaganesan and Y. T. Jeong, *Bio. Med. Chem.*, 2010, **20**, 2242.

V. Copies of ^1H and ^{13}C Spectra of Products

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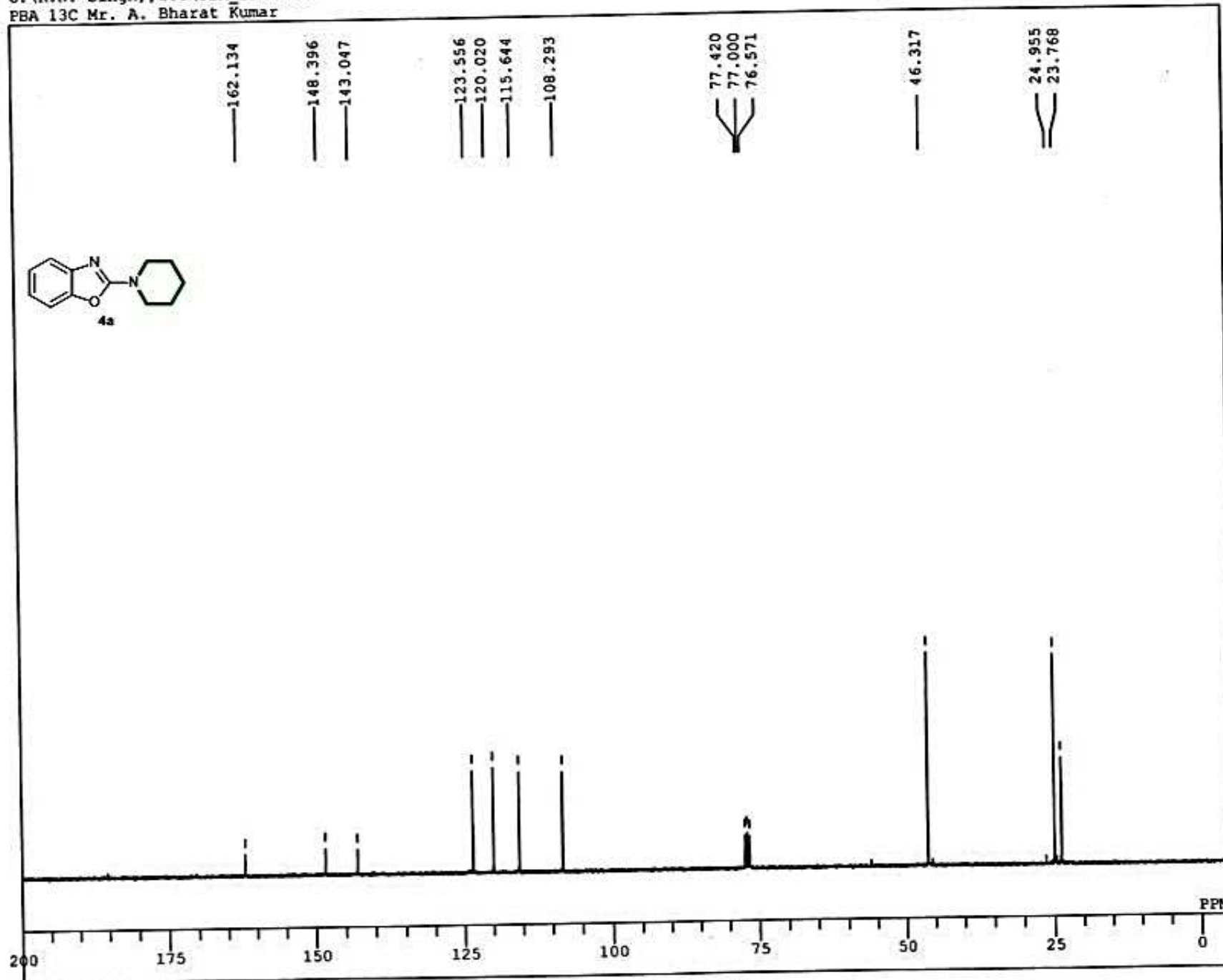
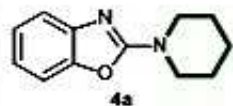


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

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Shishir Singh

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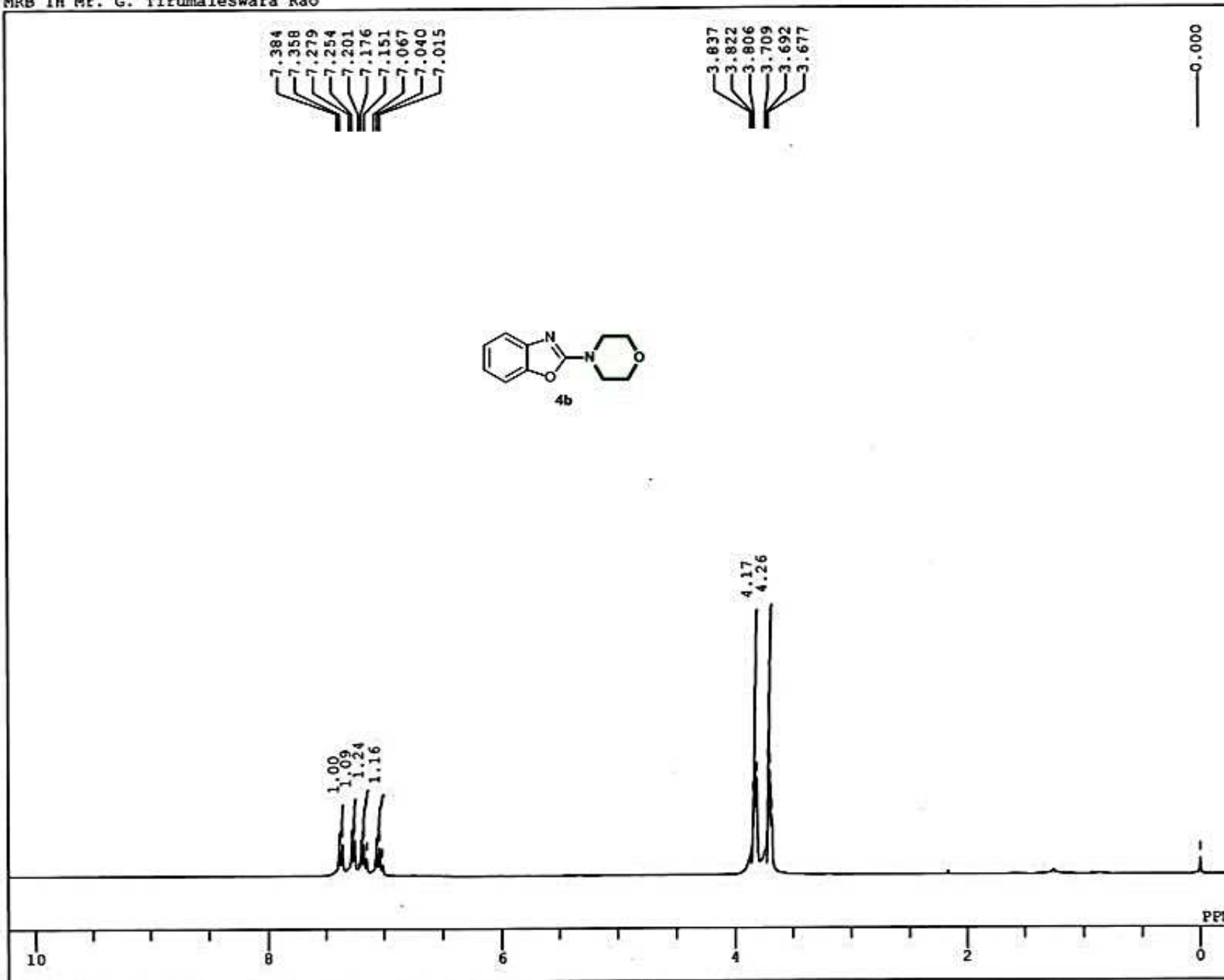


JEOL AL300 FTNMR
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Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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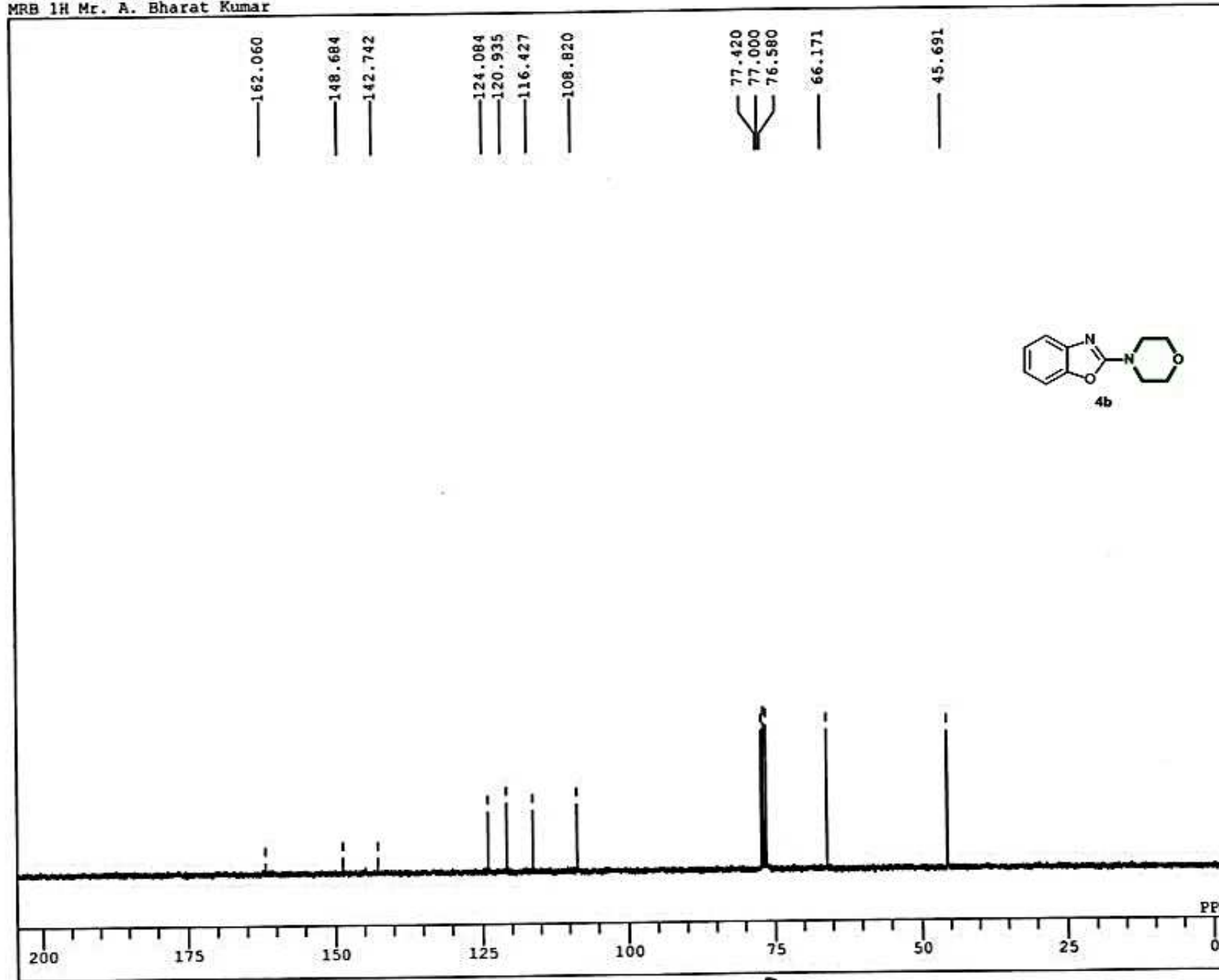


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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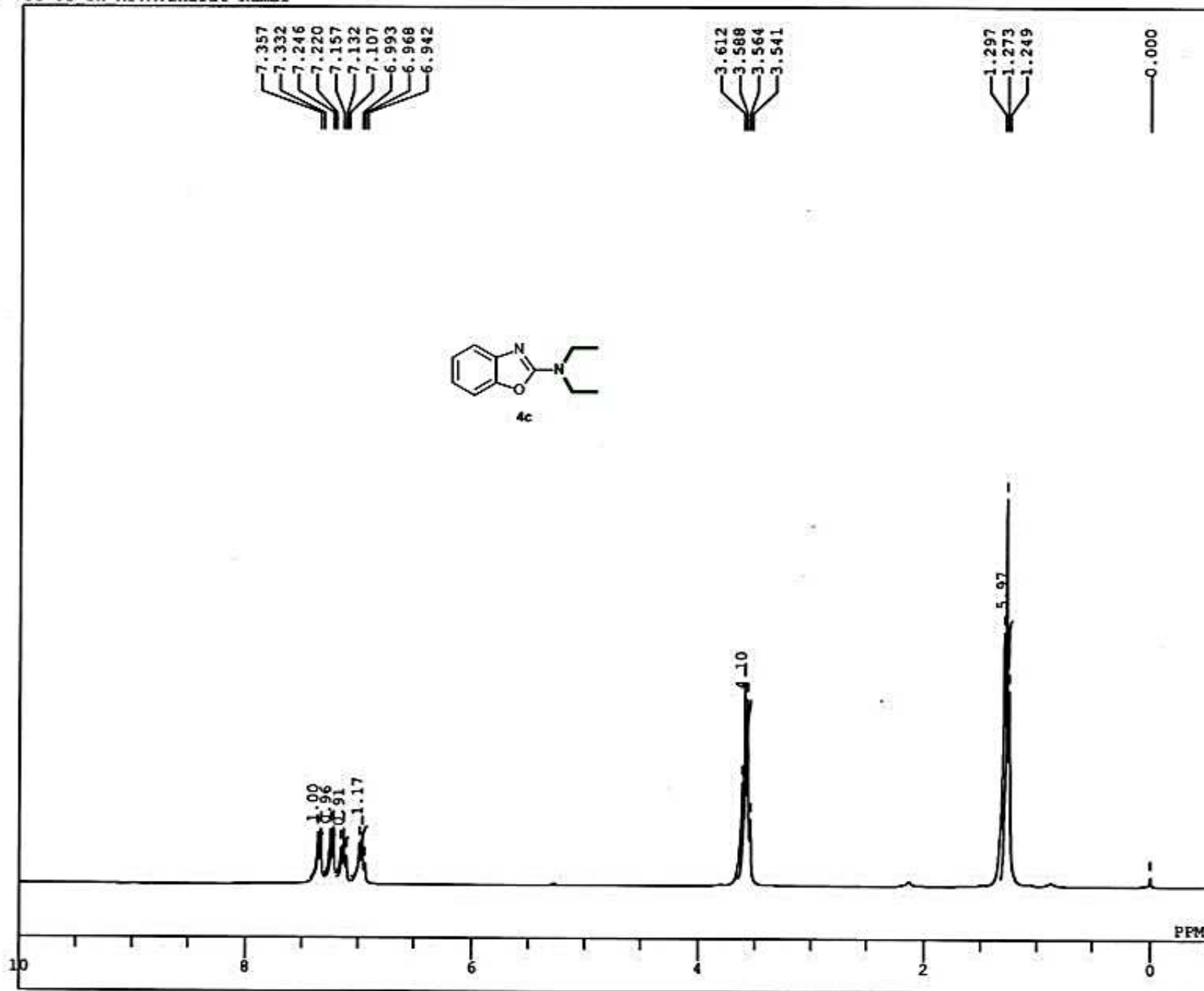


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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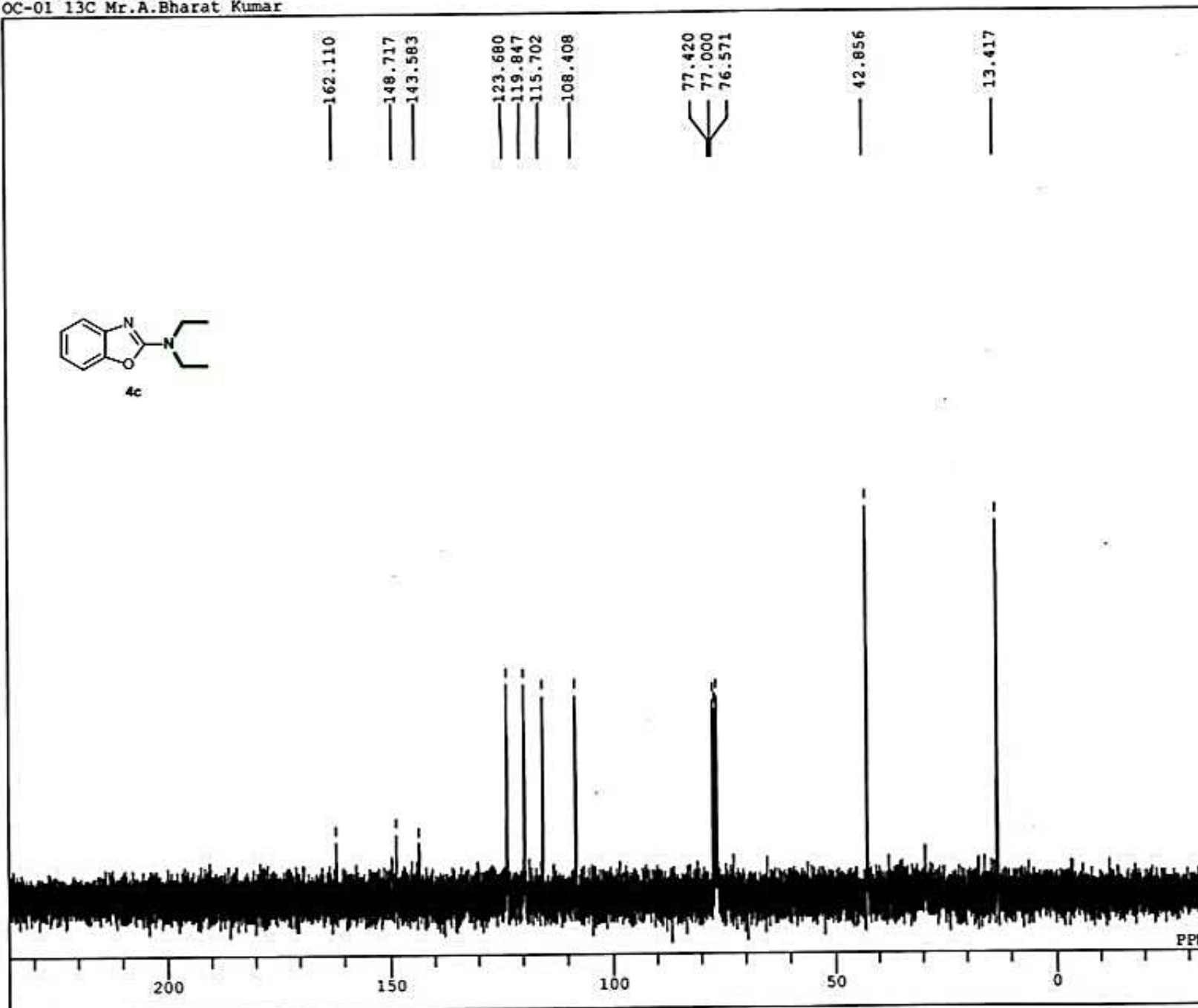
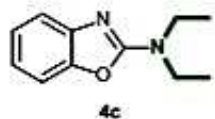


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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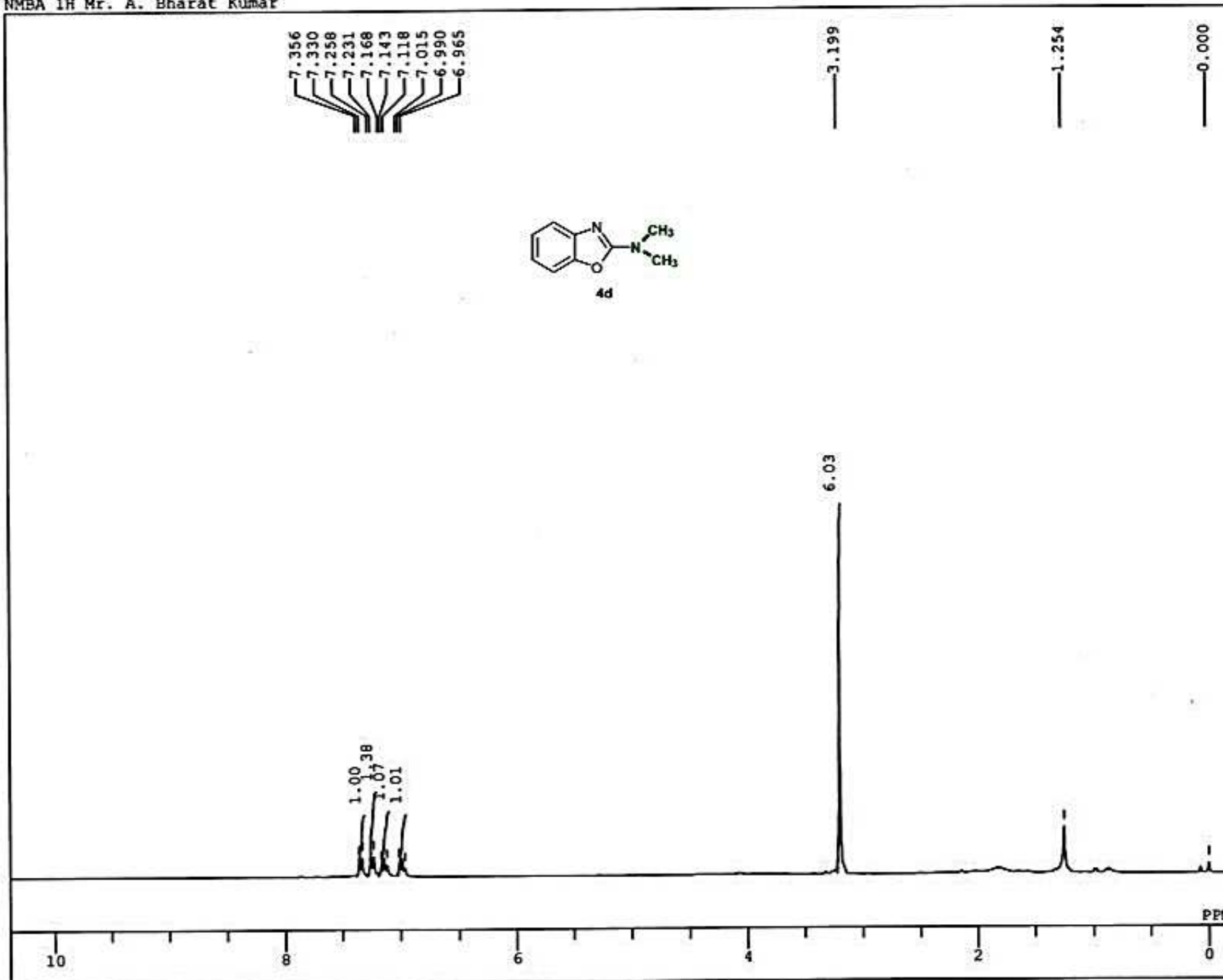


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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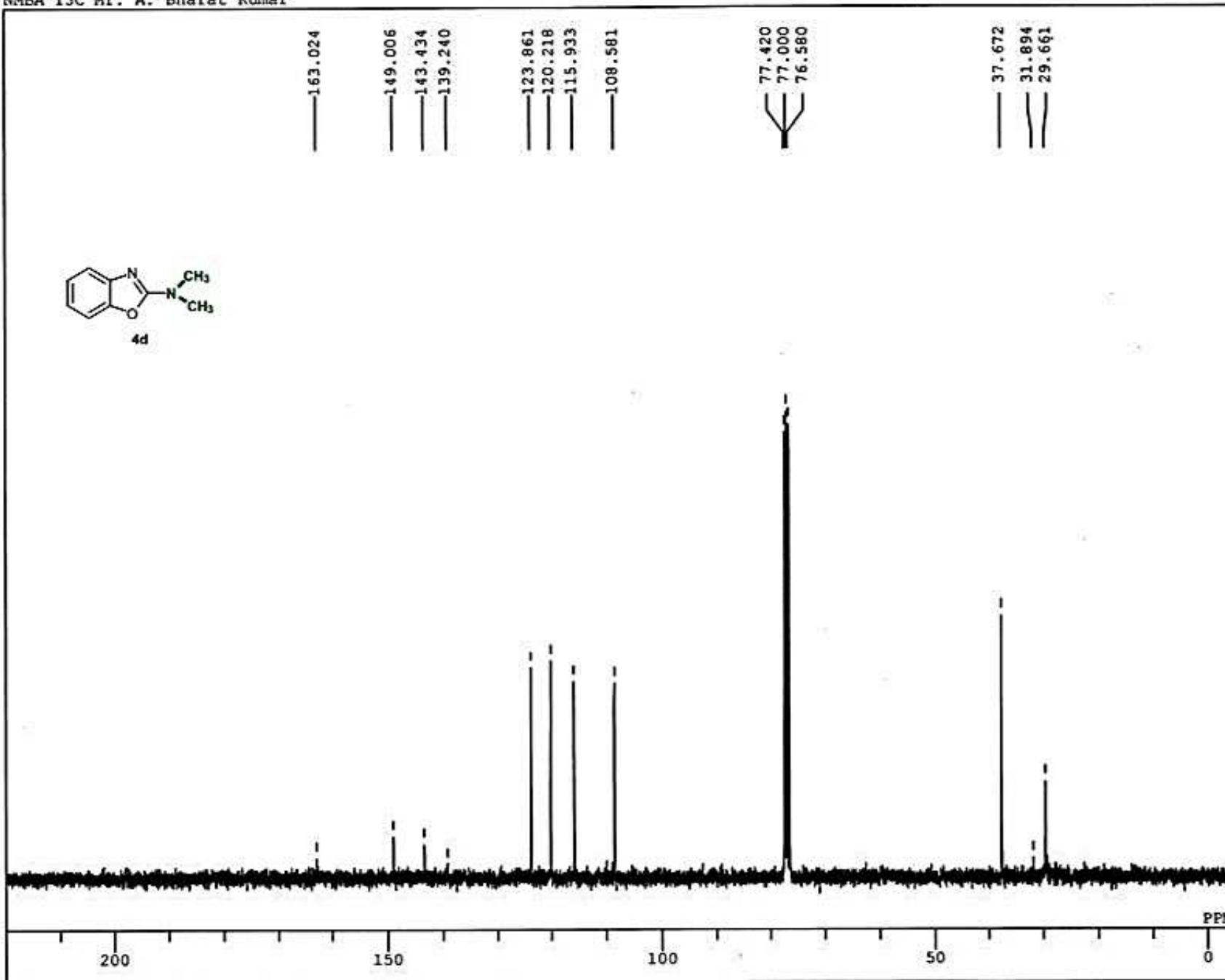


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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DATIM Fri Aug 03 13:24:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PWI 5.2 us
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 16

C:\K.N. Singh,,I.T\NMBA 13C.als
NMBA 13C Mr. A. Bharat Kumar

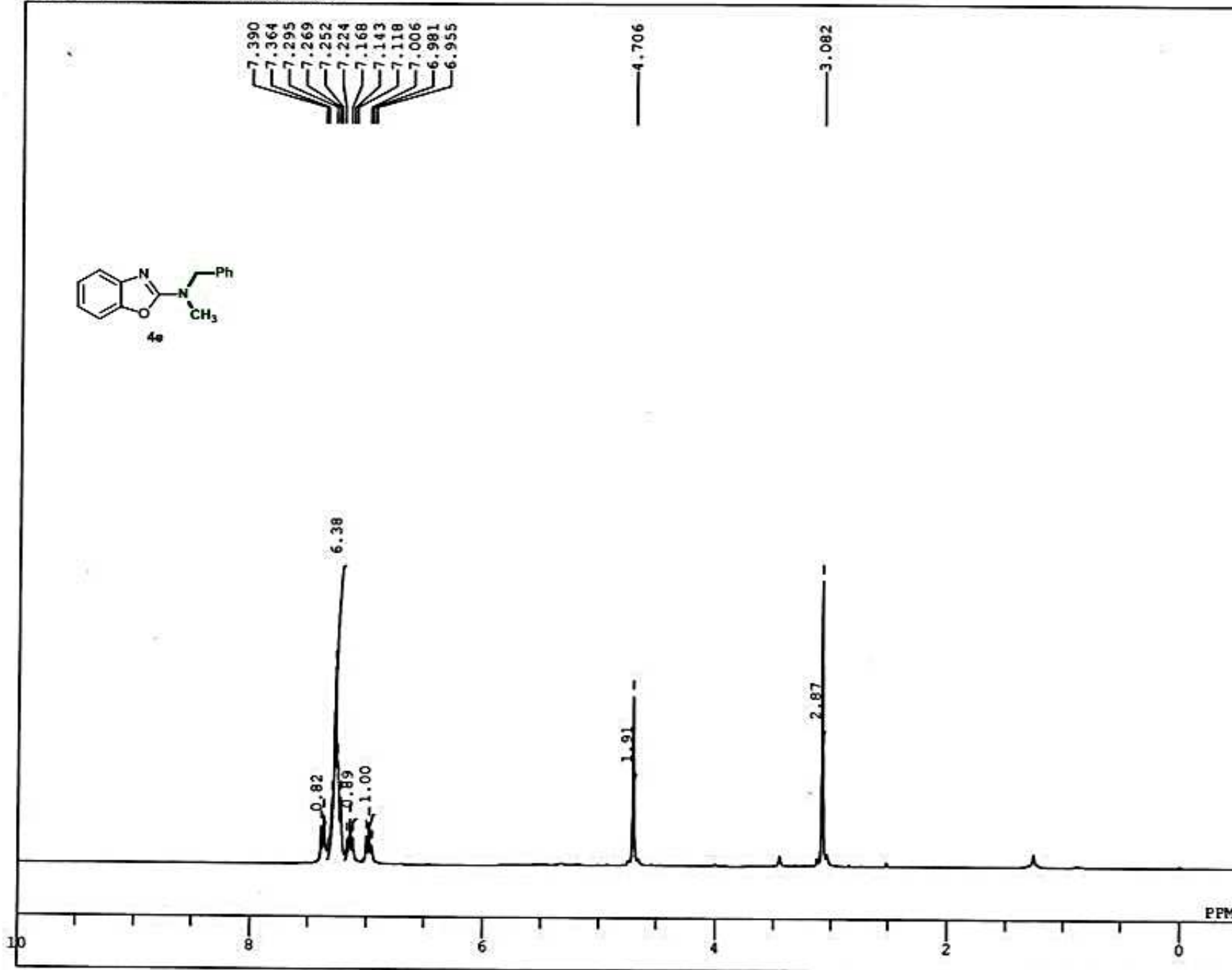
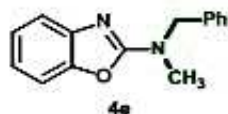


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT NMBA 13C Mr. A. B
DATIM Mon Aug 06 16:58:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 481
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,,I.T\NBEA_1H.als
NBEA 1H Mr. G. Tirumaleswar Rao

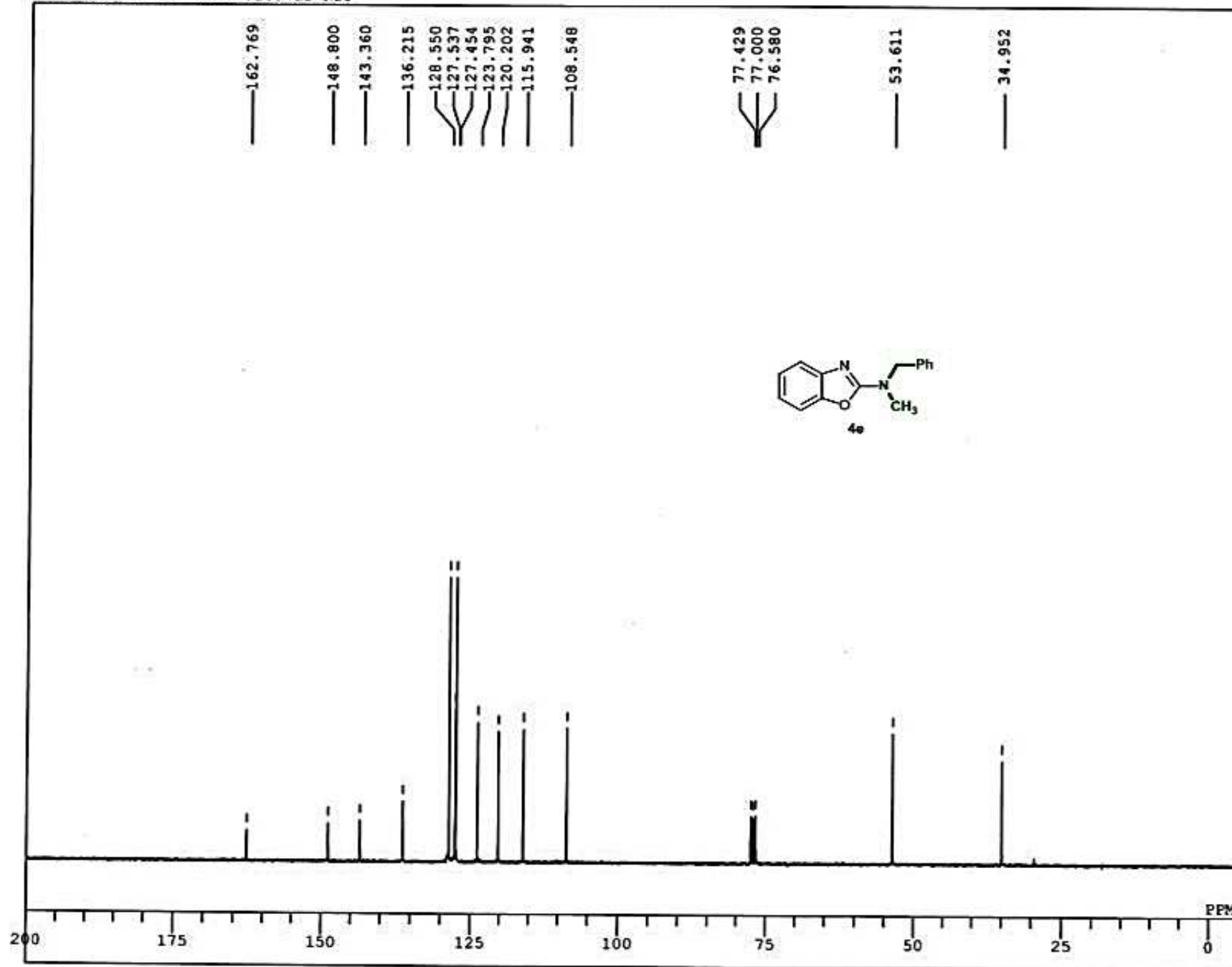


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT NBEA_1H Mr. G. Ti
DATIM Mon Oct 08 12:49:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 50
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 8

C:\K.N. Singh,,I.T\NBEA_13C.als
NBEA 13C Mr. G. Tirumaleswar Rao

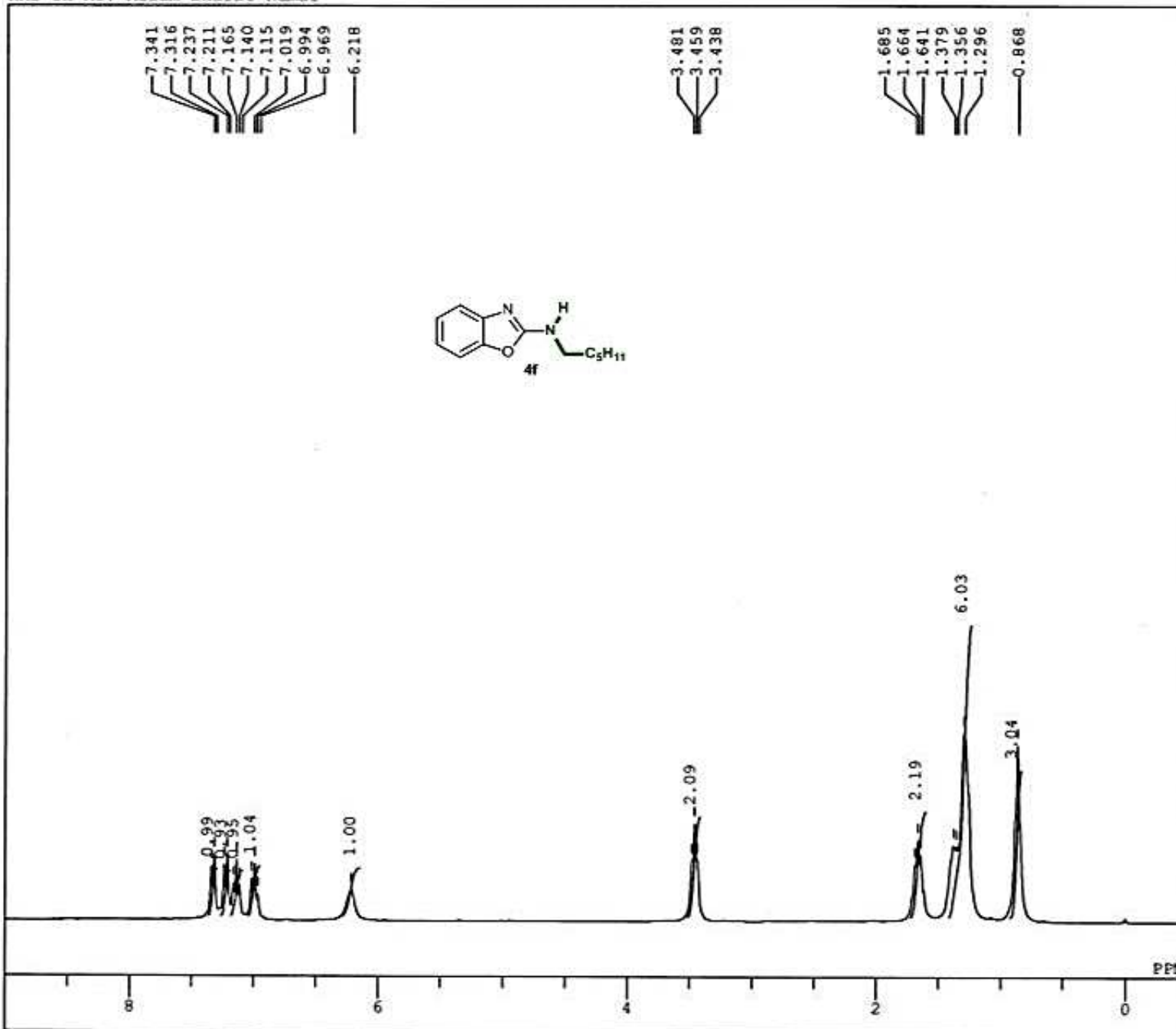


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT NBEA 13C Mr. G. T
DATIM Mon Oct 08 12:58:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 117
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 23.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh,,I.T\HXB_1H.als
HXB 1H Mr. Allam Bharat Kumar

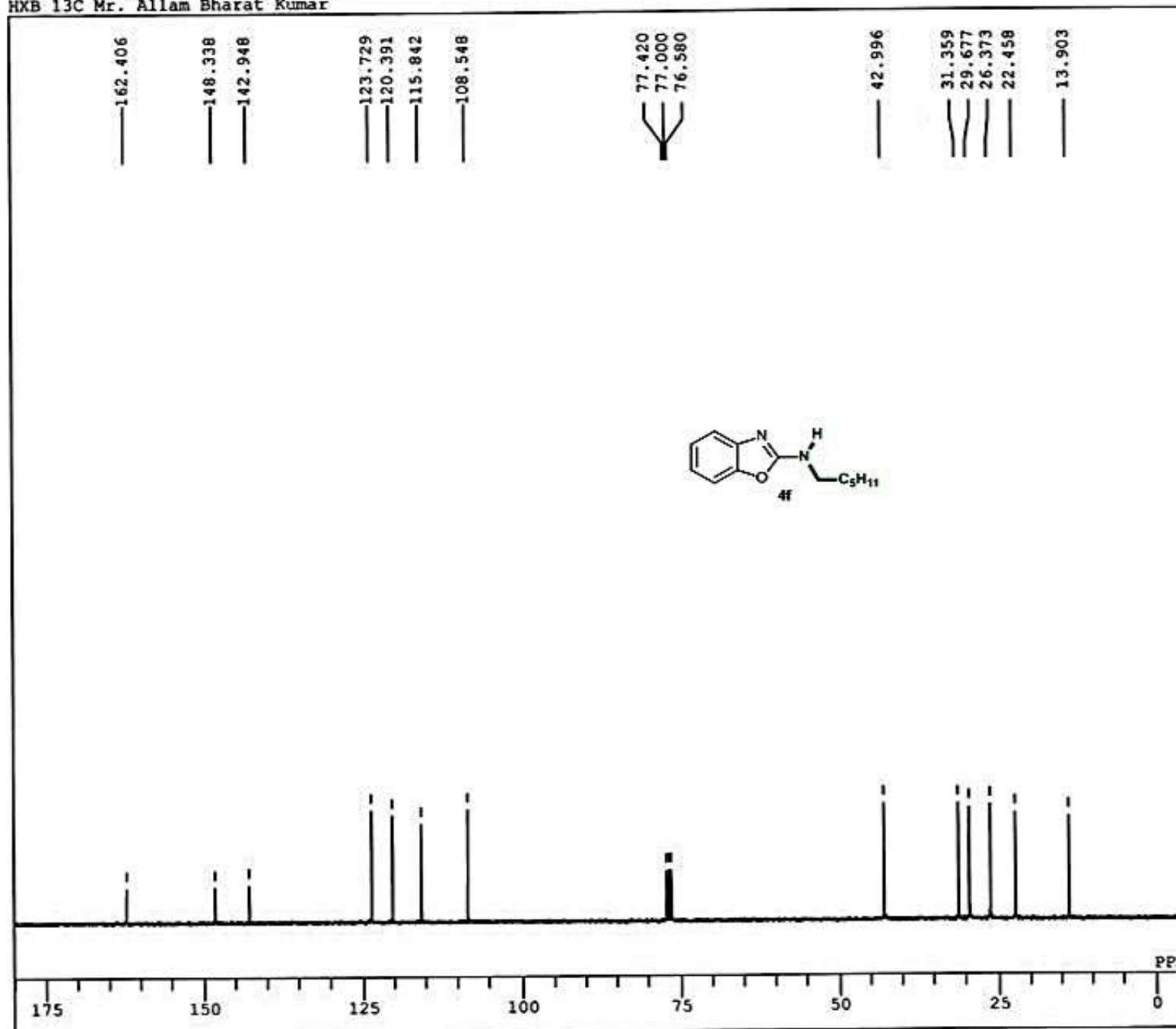


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\HXB_1H.als
COMNT HXB_1H_Mr. Allam Bharat Kumar
DATIM Wed Sep 26 12:51:56 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 33
ACQTM 3.447 sec
PD 1.547 sec
PWL 5.2 us
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.22 Hz
RGAIN 8

C:\WINNMR98\COMMON\DEFAULT.ALS
HXB 13C Mr. Allam Bharat Kumar

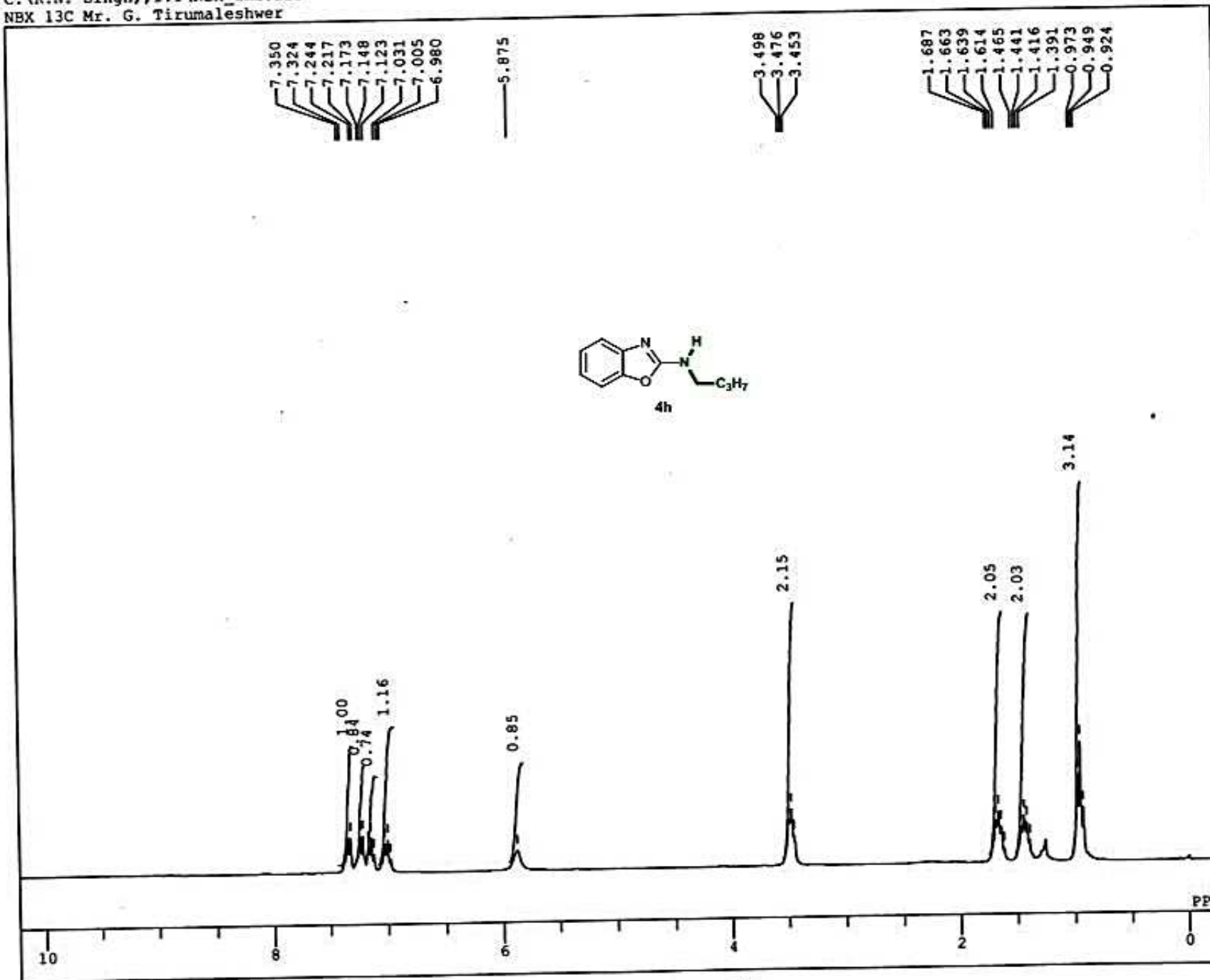


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON\DEFAULT.
COMNT HXB 13C Mr. Allam Bharat Kum
DATIM Wed Sep 26 13:04:20 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 111
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.22 Hz
RGAIN 25

C:\K.N. Singh,, I.T\NBX_1H2.als
NBX 13C Mr. G. Tirumaleshwer

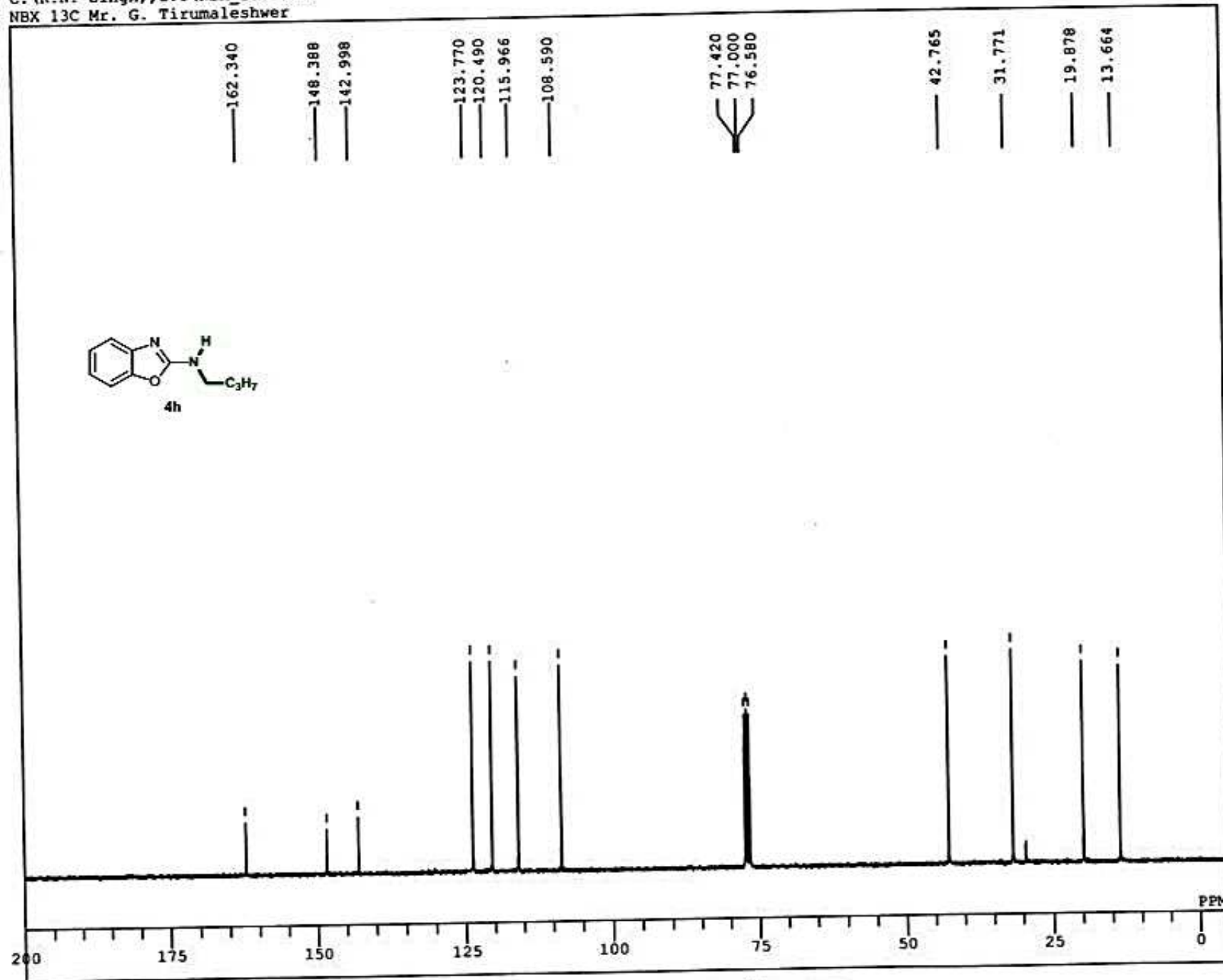


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,, I.
COMNT NBX_13C Mr. G. Ti
DATIM Tue Sep 18 20:27:
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 5.2 us
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 12

C:\K.N. Singh,,I.T\NBX_13C.als
NBX 13C Mr. G. Tirumaleshwer

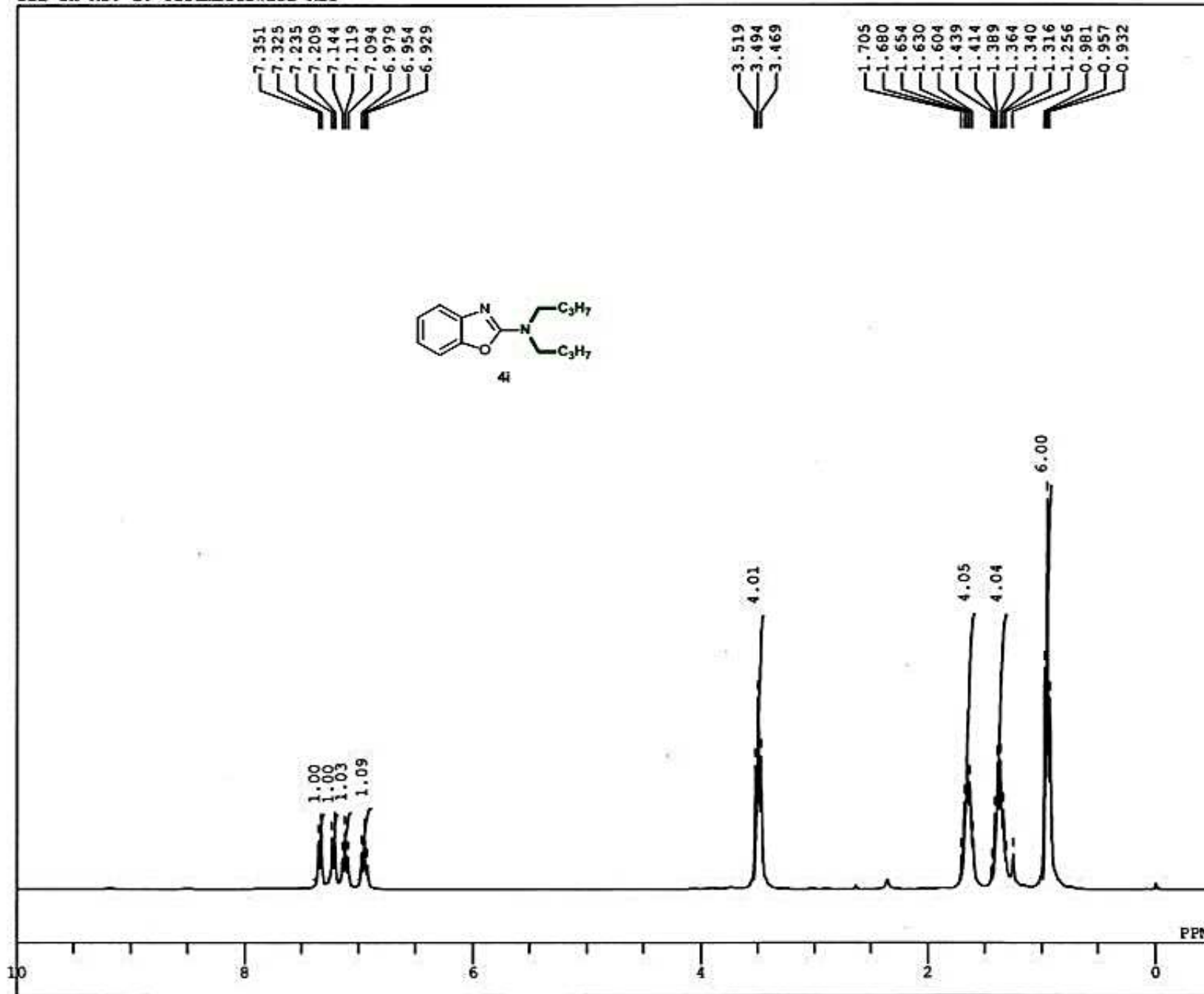


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT NBX_13C_Mr. G. Ti
DATIM Tue Sep 18 20:23:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 1500
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,,I.T\DBB_1H.als
DBB 1H Mr. G. Tirumaleswara Rao

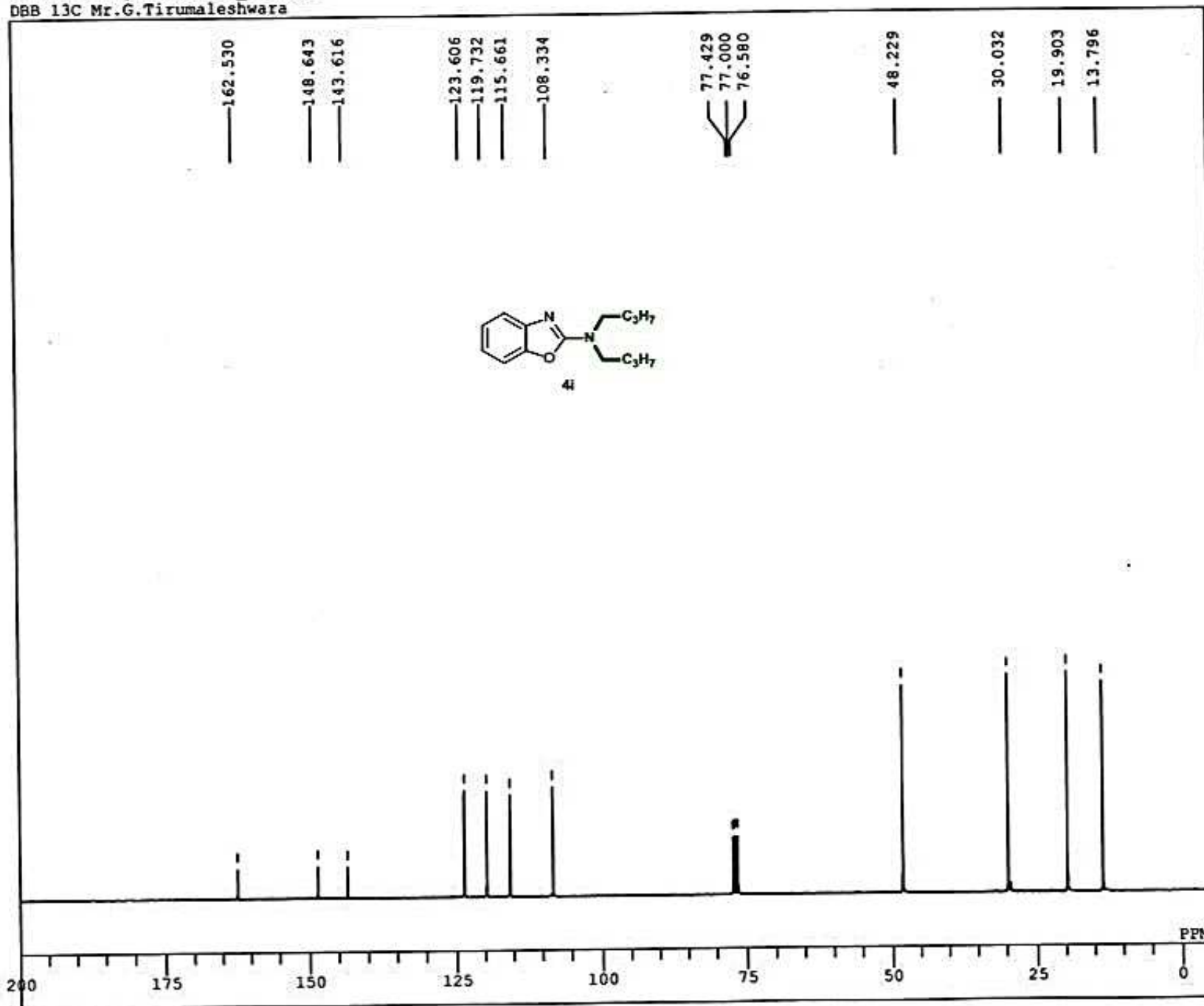


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\DBB_1H.Mr. G. Tirumale:
COMNT DBB_1H_Mr. G. Tirumale:
DATIM Mon Sep 24 14:52:27 20:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 45
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 19.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 8

C:\K.N. Singh,,I.T\DBB 13C.als
DBB 13C Mr.G.Tirumaleshwara

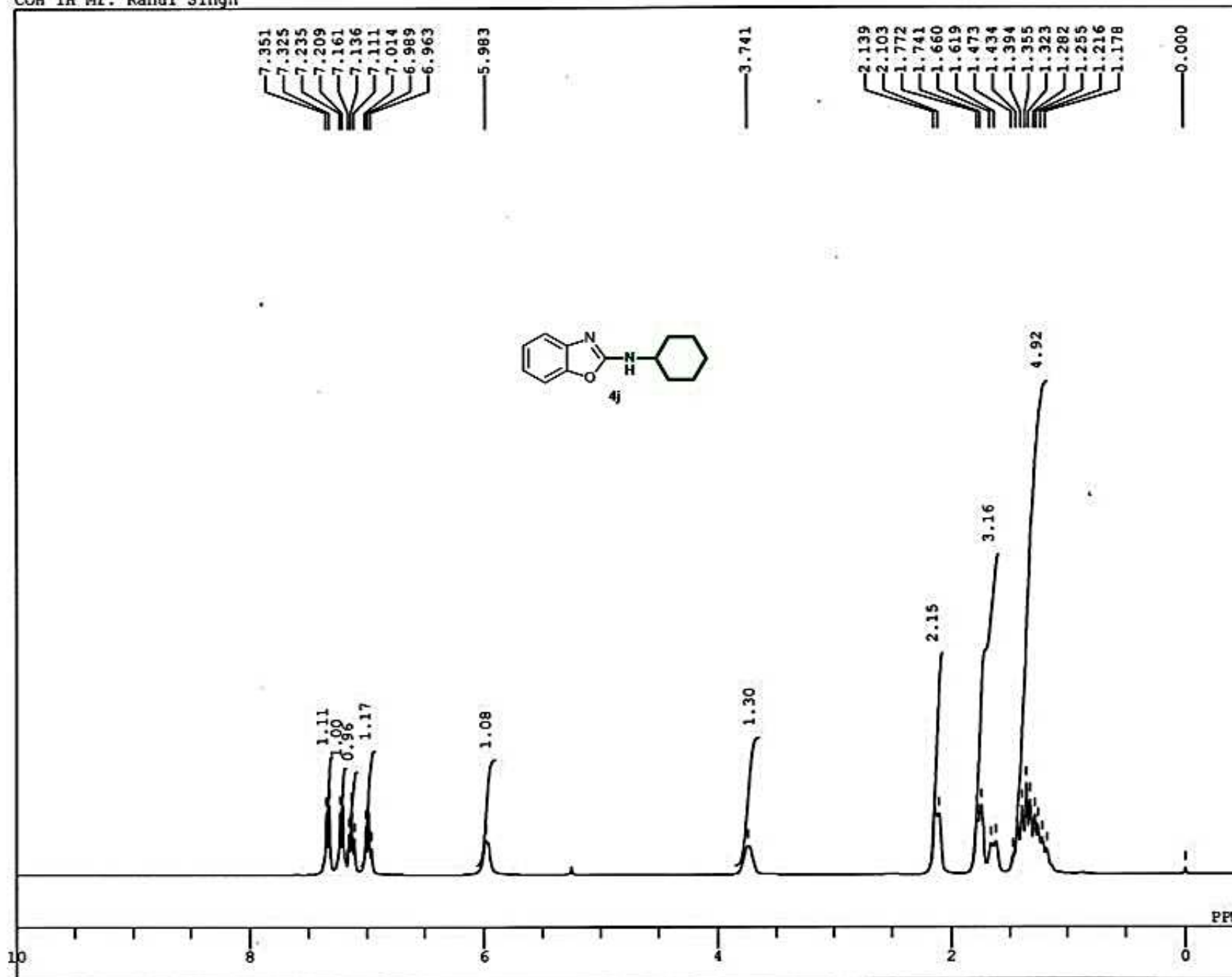


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\DBB
COMNT DBB_13C_Mr.G.Tirumalesh
DATIM Wed Sep 26 08:49:38 201
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 2000
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 18.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.22 Hz
RGAIN 23

C:\Rahul singh\COH_1H.als
COH_1H Mr. Rahul Singh

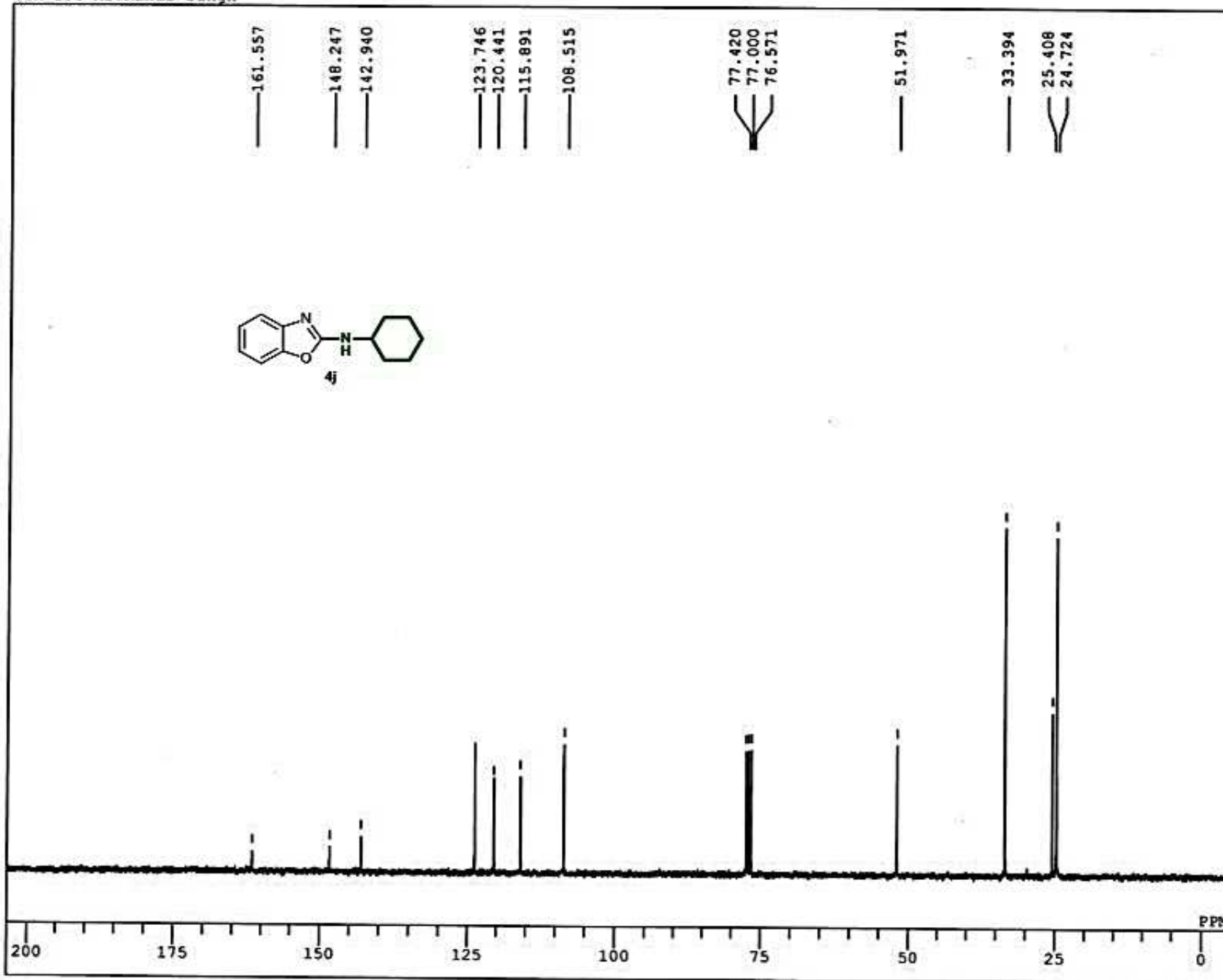


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\Rahul singh\CO
COMNT COH_1H Mr. Rahul
DATIM Thu Jun 28 14:56:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 11

C:\Rahul singh\COH_13C.als
COH 13C Mr.Rahul Singh



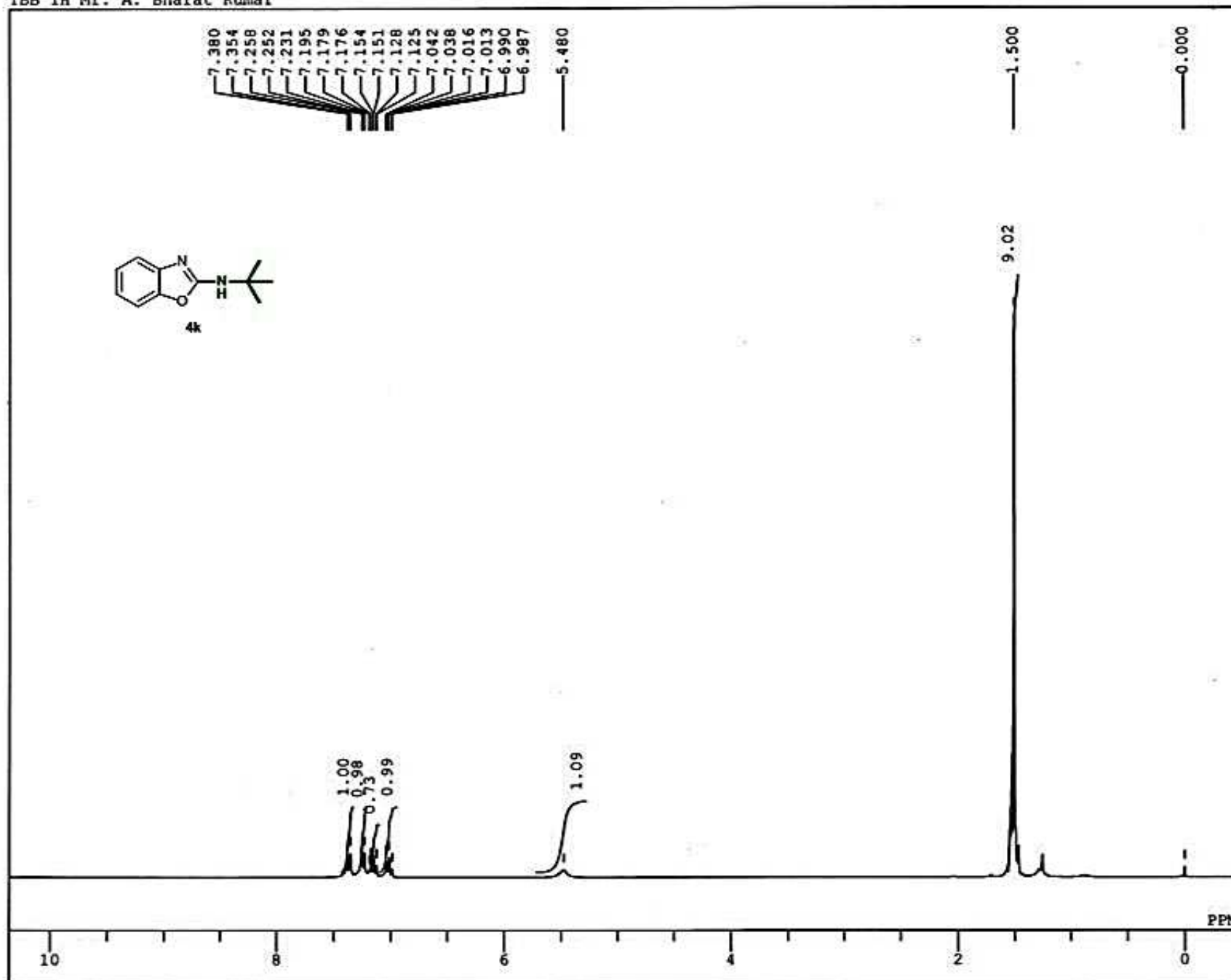
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\Rahul singh\CO
COMNT COH_13C_Mr.Rahul
DATIM Wed Jul 04 15:22:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 173
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

B₃₀

C:\K.N. Singh,,I.T\TBB_1H.als
TBB 1H Mr. A. Bharat Kumar

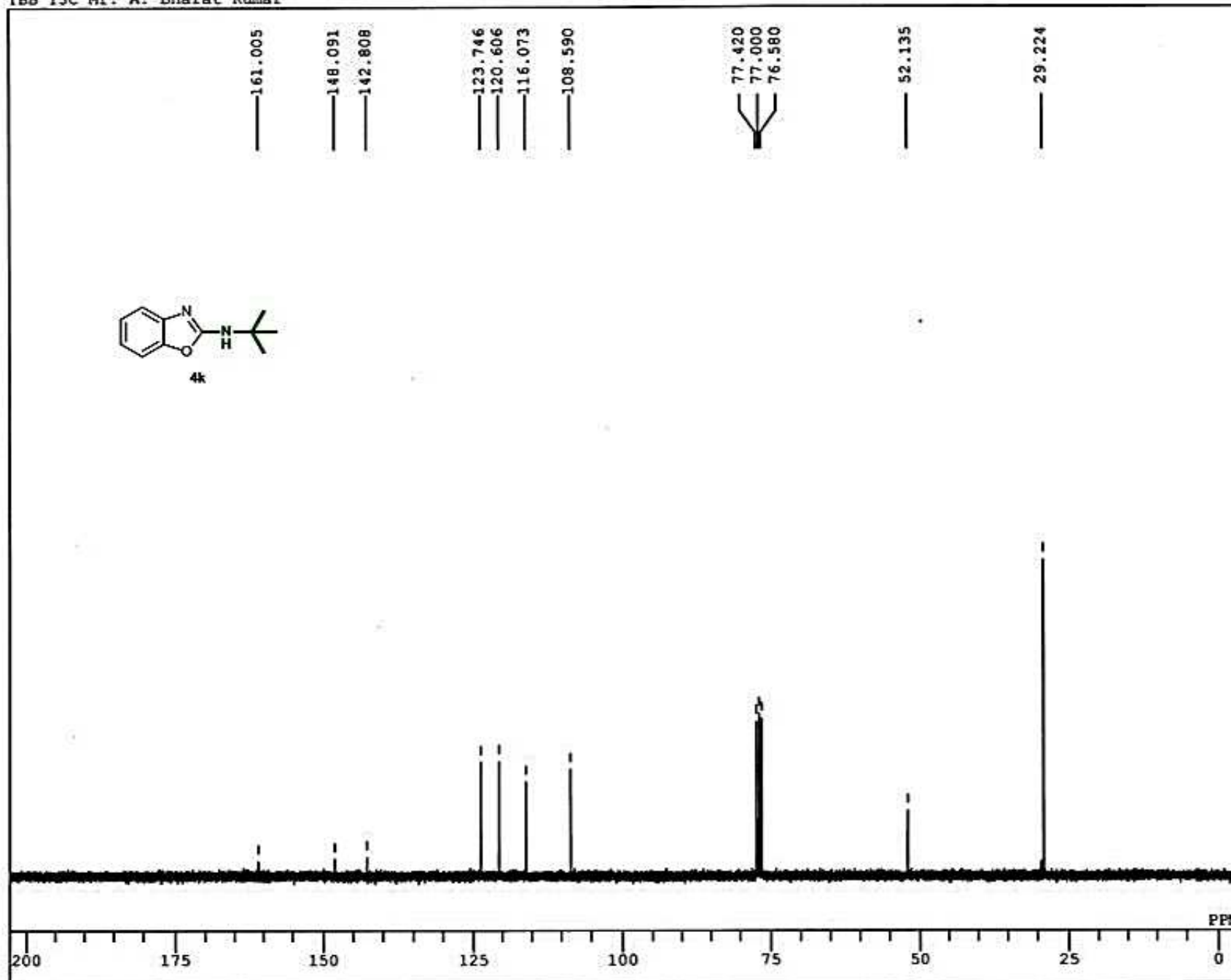
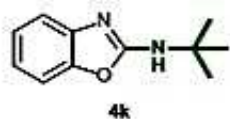


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT TBB_1H Mr. A. Bha
DATIM Wed Sep 26 15:54:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13

C:\K.N. Singh,, I.T\TBB_13C.als
TBB_13C Mr. A. Bharat Kumar



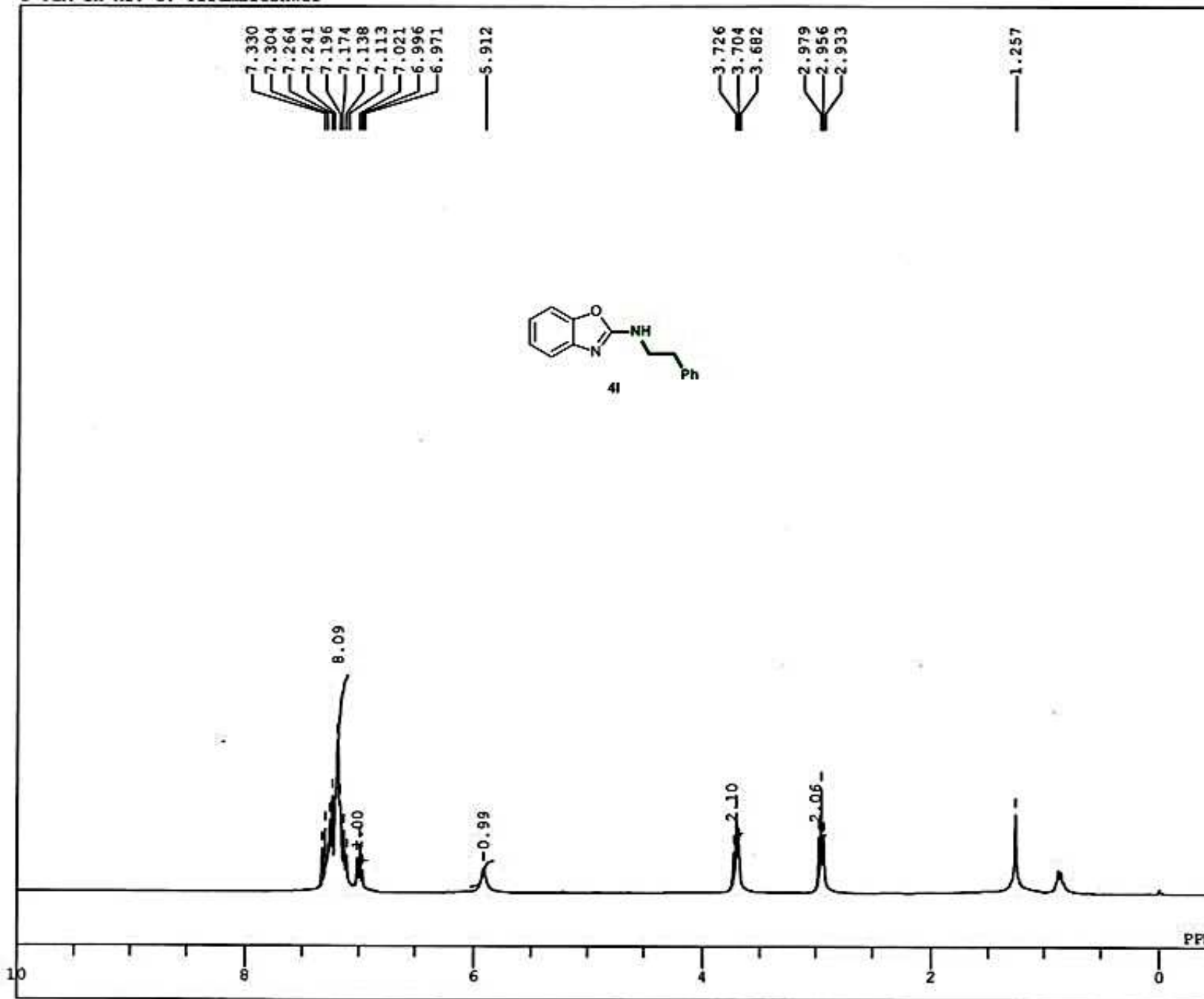
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,, I.
COMNT TBB_13C Mr. A. Bh.
DATIM Wed Sep 26 16:21:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 467
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 23.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 25

B₃₂

C:\K.N. Singh,,I.T\2-PEA_1H.als
2-PEA 1H Mr. G. Tirumaleshwer

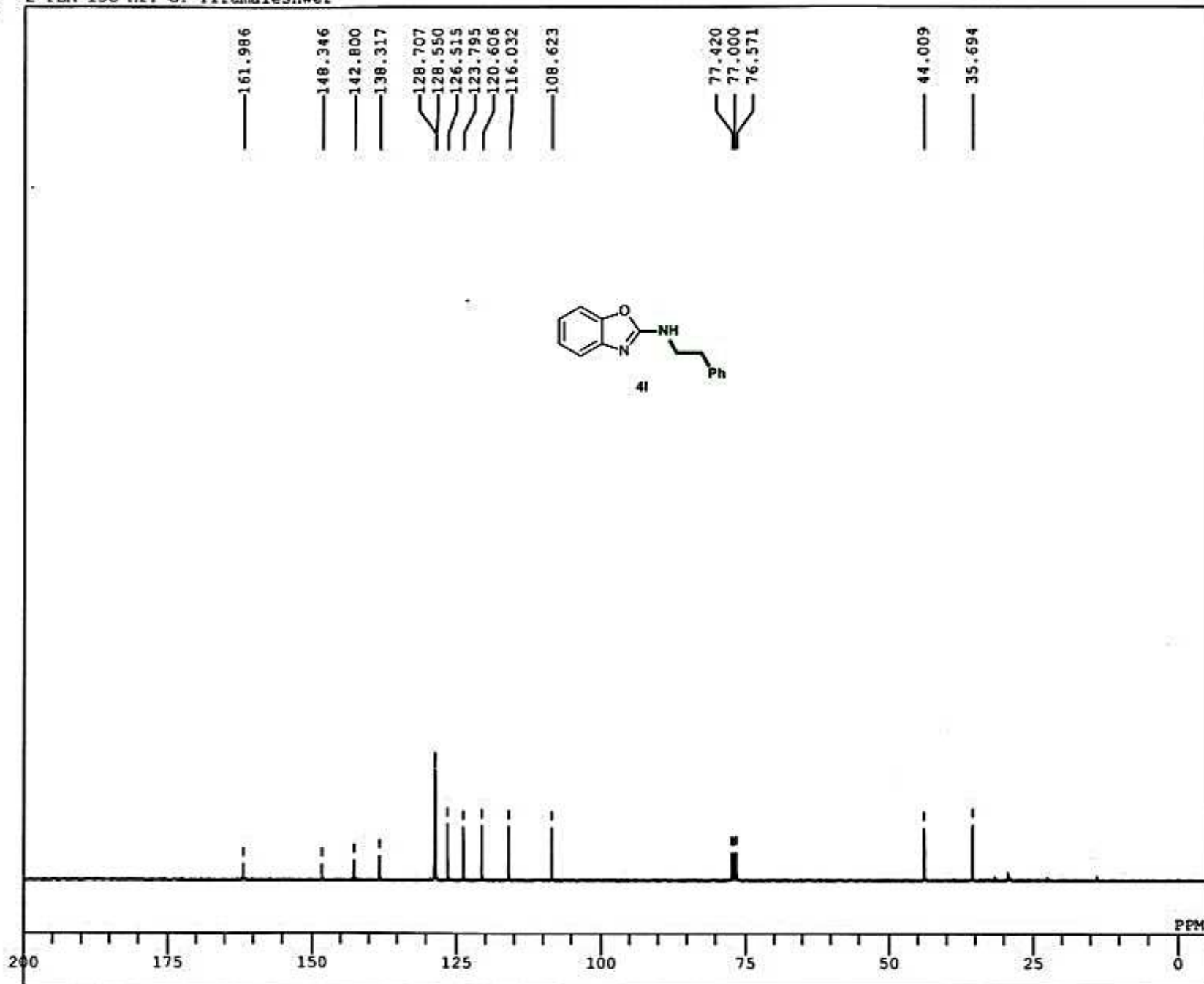


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\2-PEA_1H.als
COMNT 2-PEA_1H Mr. G. Tirumaleshwer
DATIM Sat Dec 01 15:12:22 2013
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
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 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 11

C:\K.N. Singh,,I.T\2-PEA_13C.als
2-PEA 13C Mr. G. Tirumaleshwer

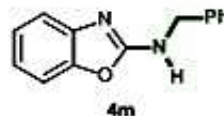
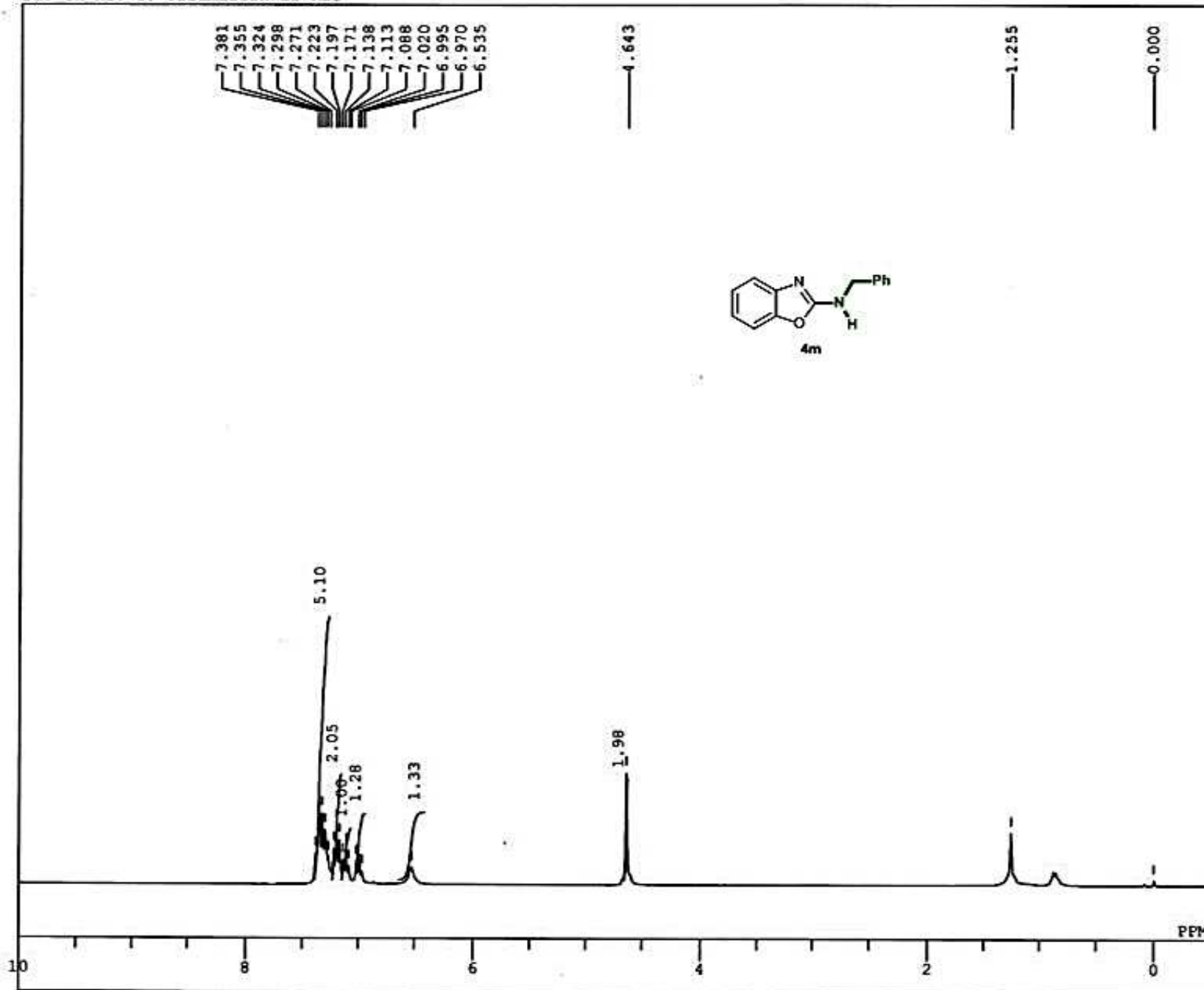


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\2-PEA_13C.als
COMNT 2-PEA 13C Mr. G. Tirumaleshwer
DATIM Sat Dec 01 15:07:55 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 81
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,,I.T\BEP_1H.als
BEP_1H Mr. G. Tirumaleshwar Rao

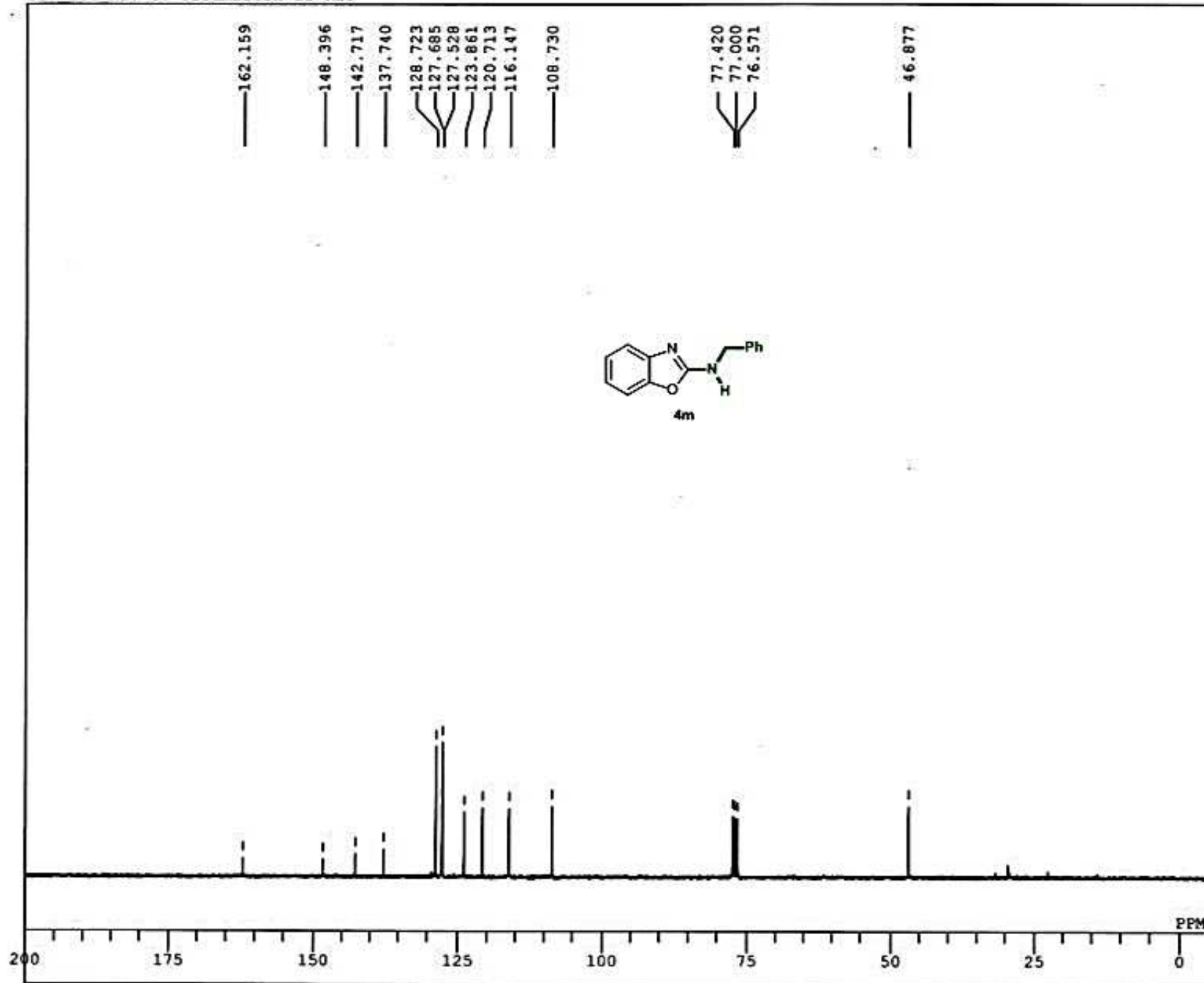


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\BEP_1H
COMT BEP_1H_Mr. G. Tirumale:
DATIM Fri Nov 16 16:14:56 20:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
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 18.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 13

C:\K.N. Singh,,I.T\BEP_13C_als
BEP 13C Mr. G. Tirumaleswar Rao

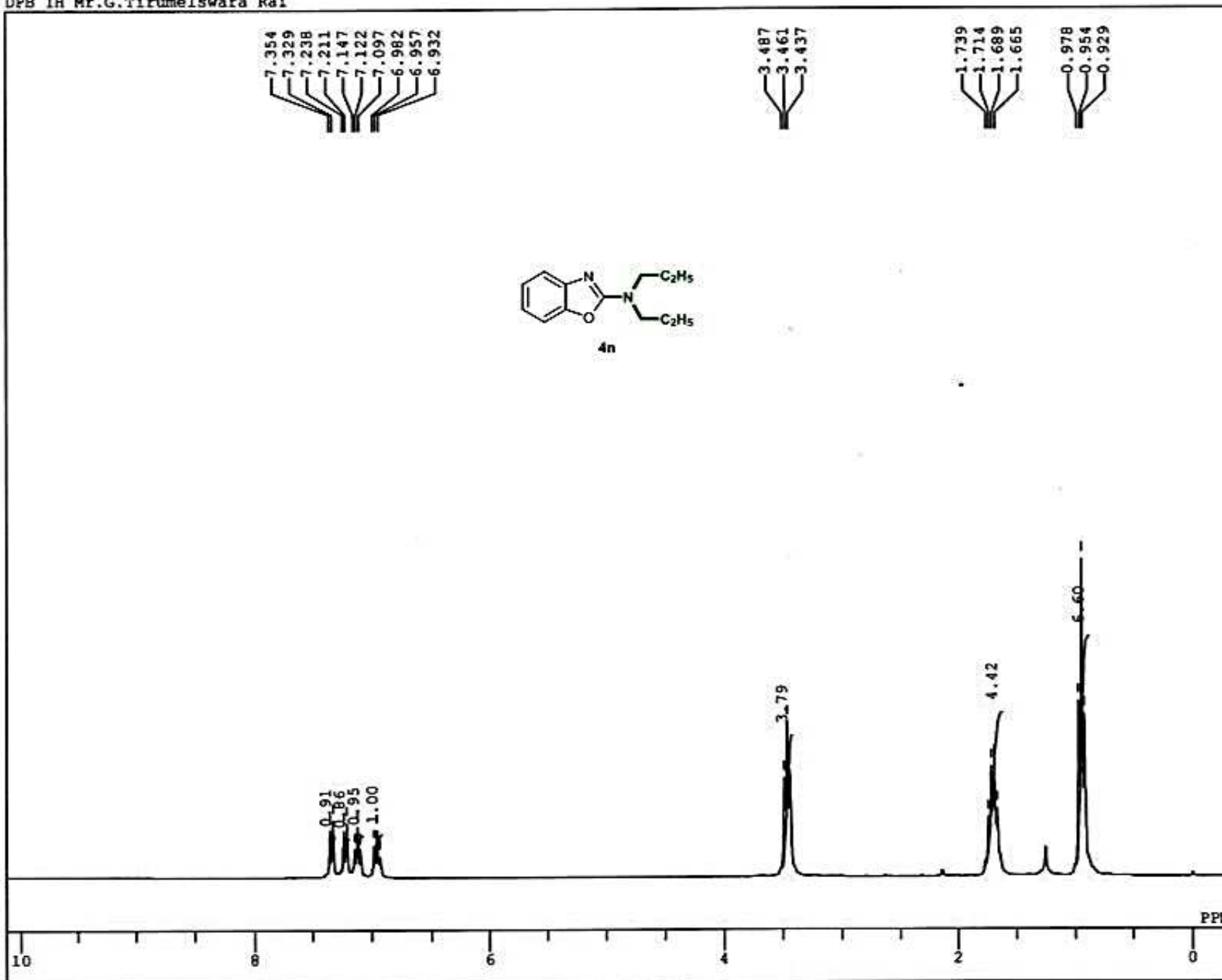


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\BEP_13C_als
COMNT BEP_13C Mr. G. Tirumaleswar Rao
DATIM Fri Nov 16 16:24:18 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 119
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh,,I.T\DPB_1H.als
DPB 1H Mr.G.Tirumelswara Rai

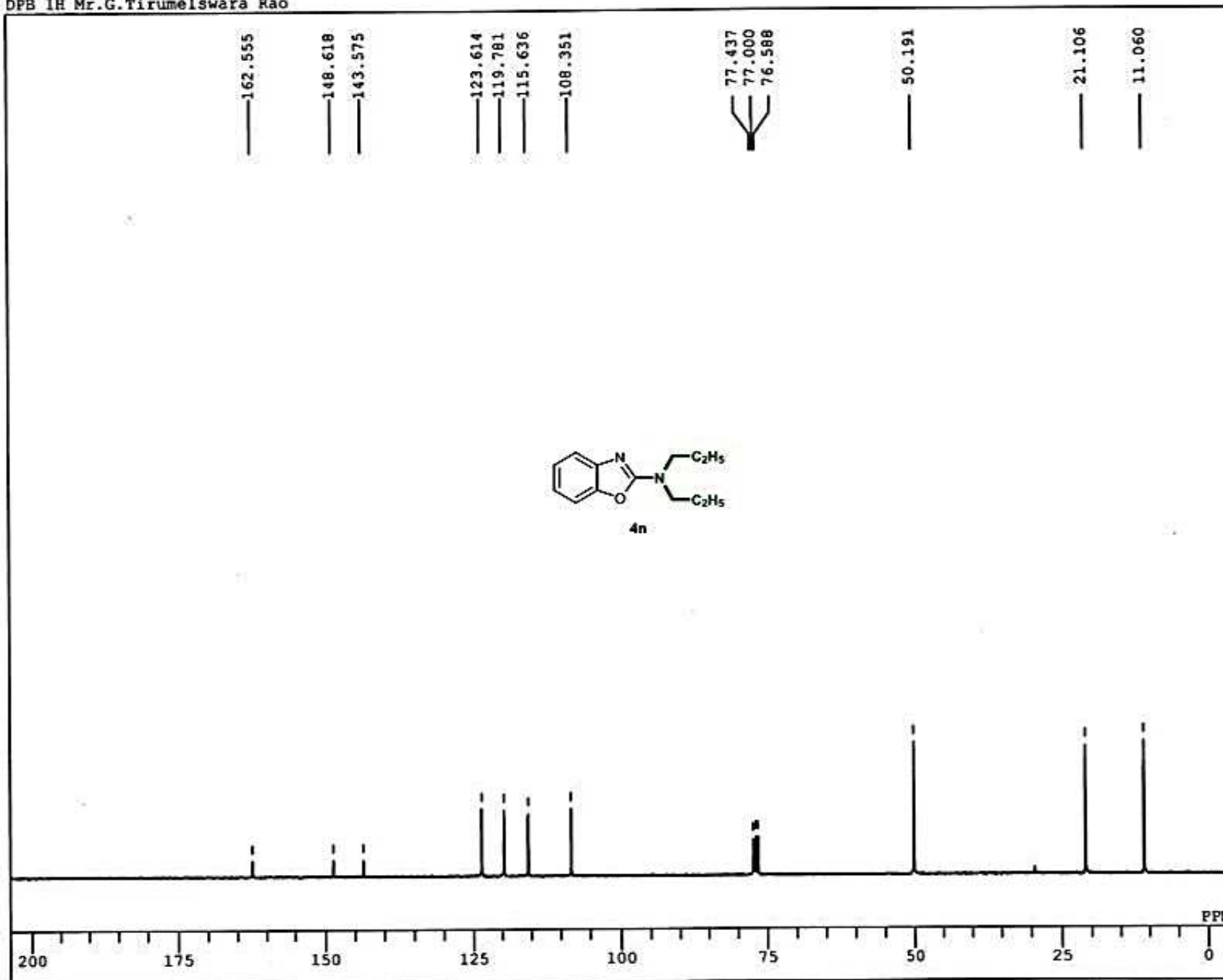


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.'
COMNT DPB_1H Mr.G.Tirum
DATIM Thu Sep 06 17:45:
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 5.2 us
IRNUC 1H
CTEMP 19.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 9

C:\K.N. Singh,,I.T\DPB_13C.als
DPB 1H Mr.G.Tirumelswara Rao

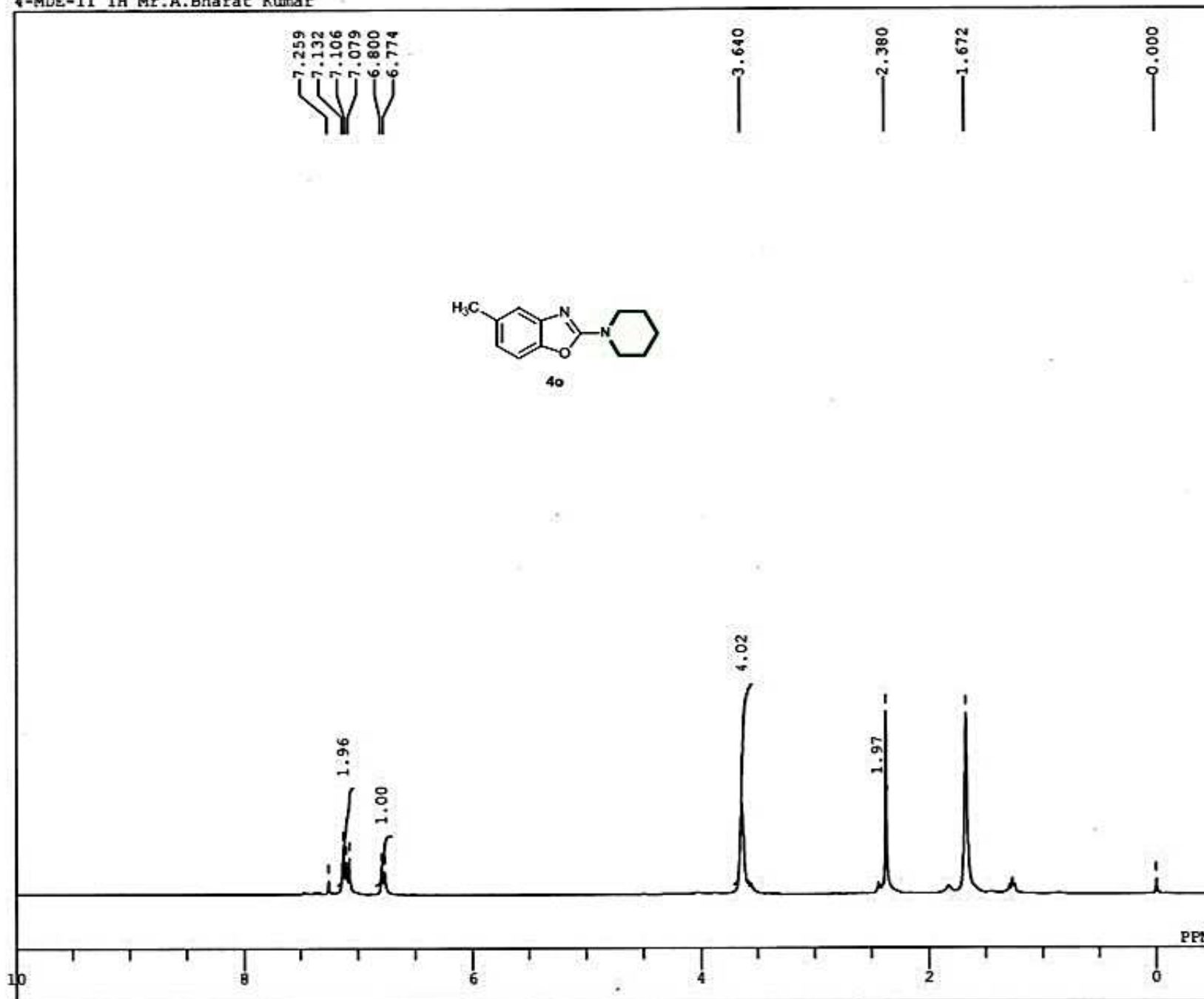


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT DPB_1H Mr.G.Tirum
DATIM Thu Sep 06 18:36:
OBNUC 13C
EXMOD BCM
OBFREQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 1000
ACQTM 1.606 sec
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 23

C:\WINNMR98\Data\4-MDE-II_1H1NON_E4.als
4-MDE-II 1H Mr.A.Bharat Kumar

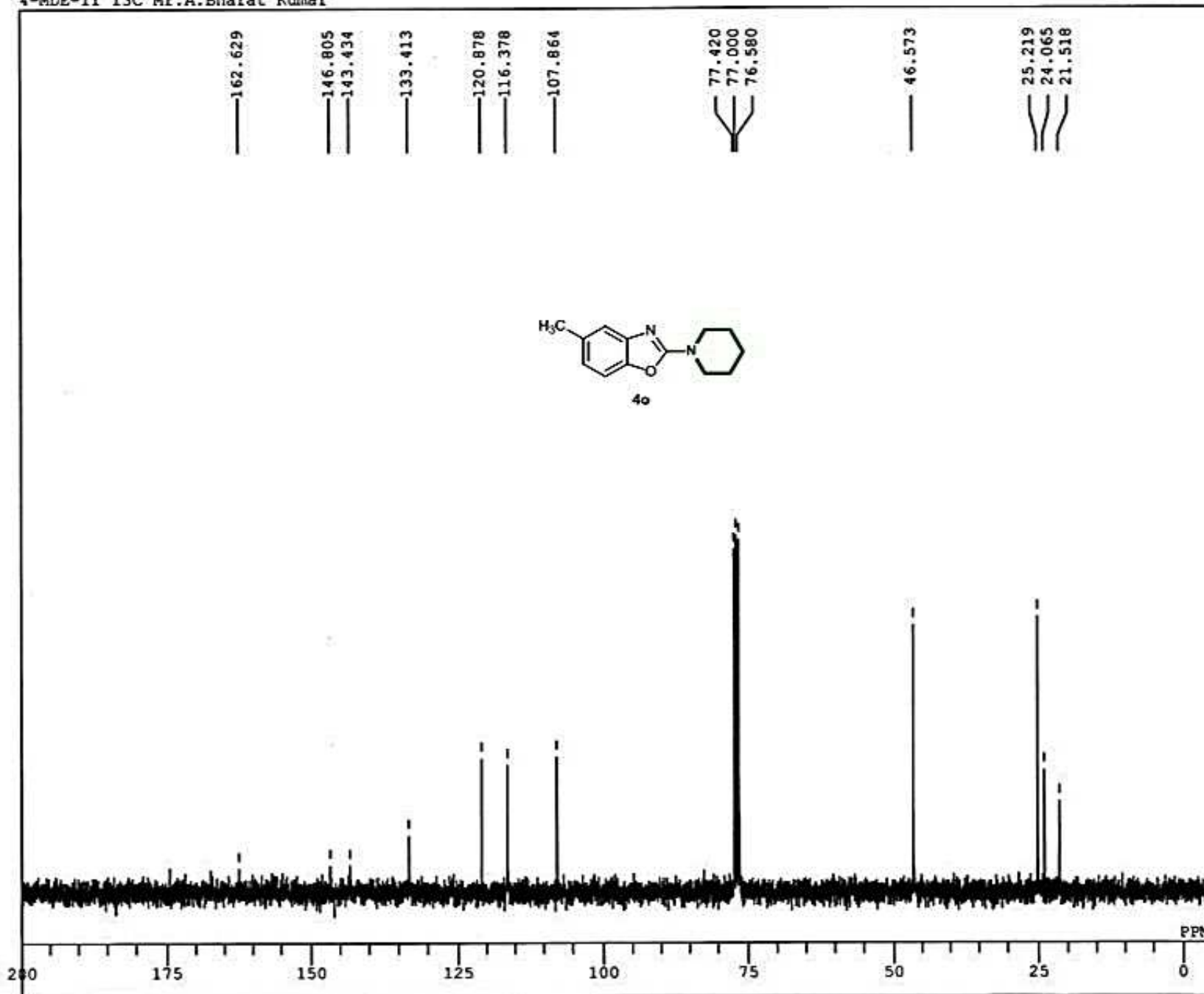


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\Data\4-MDE-
COMNT 4-MDE-II_1H Mr.A.Bharat
DATIM Fri Jan 04 13:00:49 20
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 5.2 us
IRNUC 1H
CTEMP 19.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17

C:\K.N. Singh,,I.T\4-MDE-II_13C.als
4-MDE-II 13C Mr.A.Bharat Kumar



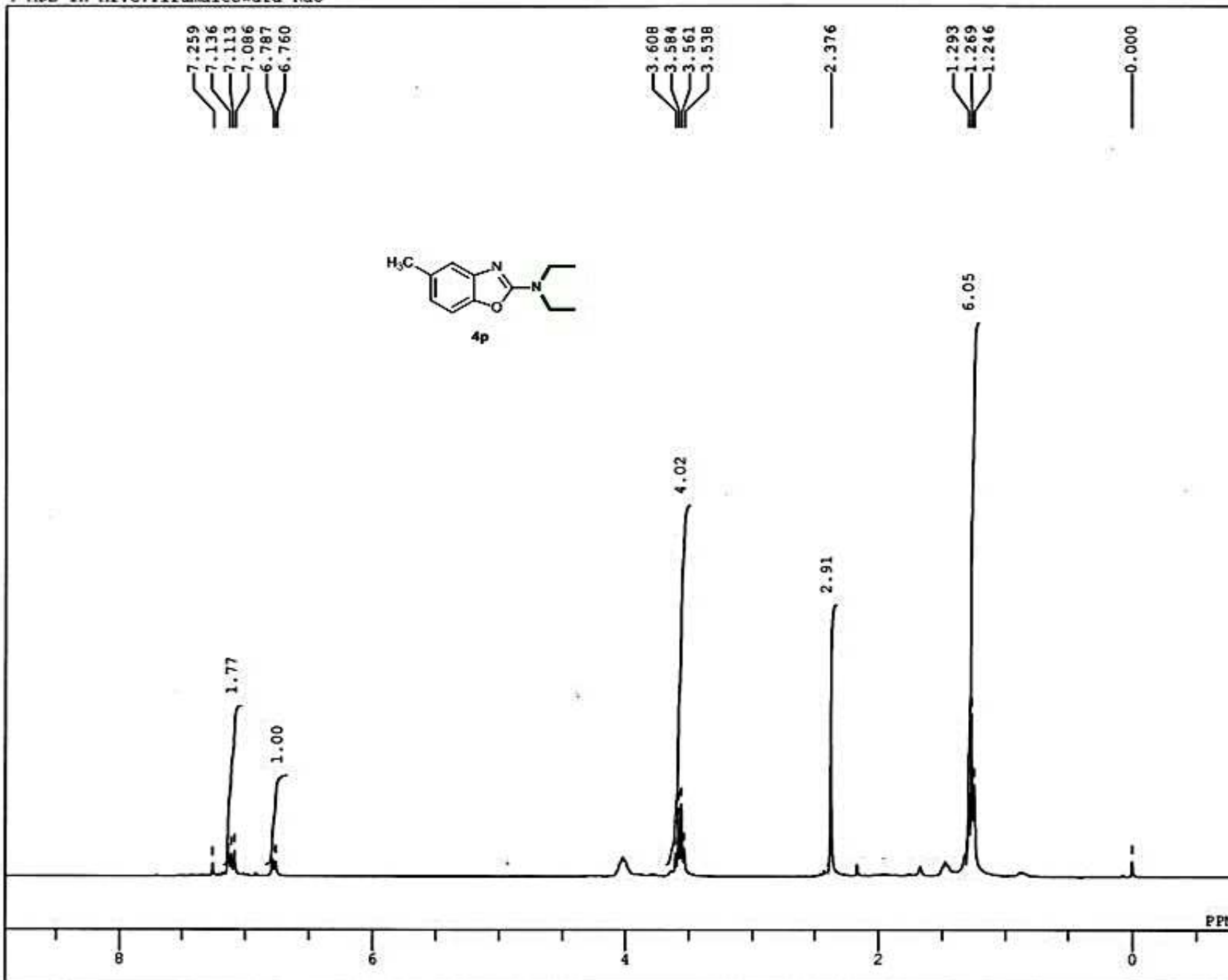
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\4-MI
COMNT 4-MDE-II_13C Mr.A.Bharat
DATIM Fri Jan 04 13:25:37 2013
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 117
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

B₄₀

C:\K.N. Singh,,I.T\4-MDE_1H.als
4-MDE 1H Mr.G.Tirumaleswara Rao

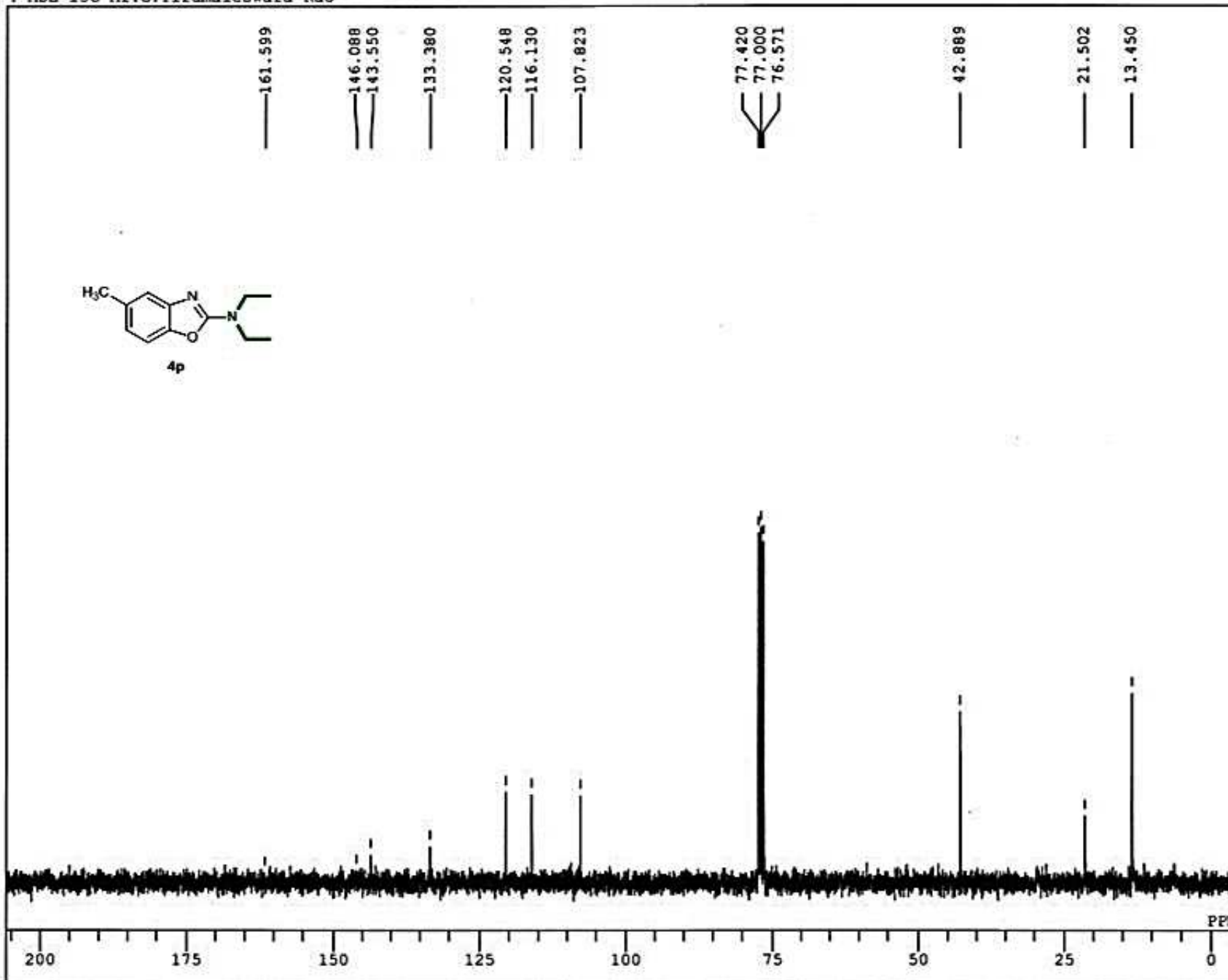


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.'
COMNT 4-MDE_1H Mr.G.Tir
DATIM Mon Dec 17 12:17:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
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 21.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17

C:\K.N. Singh,,I.T\4-MDE_13C_.als
4-MDE 13C Mr.G.Tirumaleswara Rao

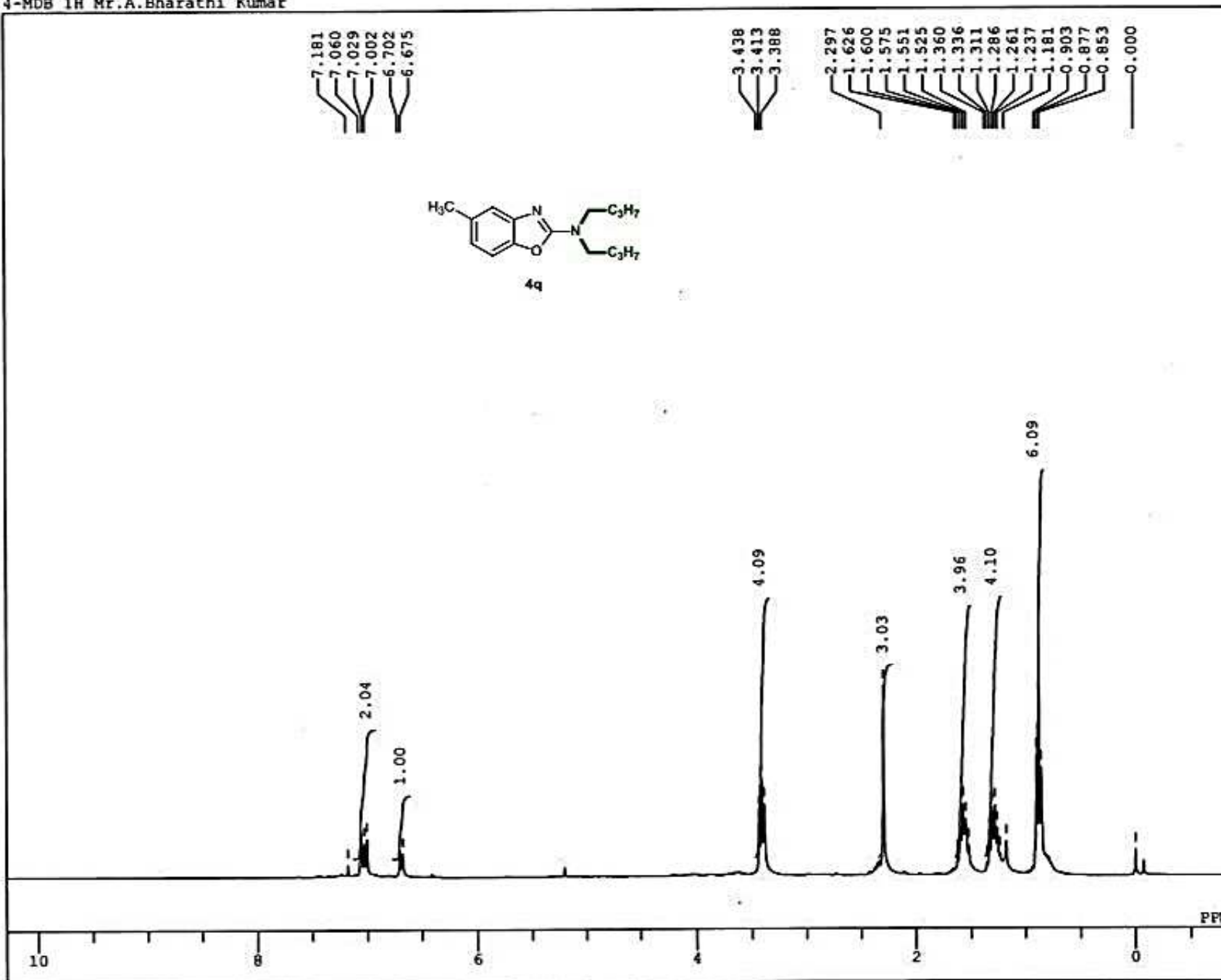


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT 4-MDE_13C Mr.G.Ti
DATIM Mon Dec 17 12:25:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 104
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 25.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

C:\K.N. Singh,,I.T\4-MDB_1H.als
4-MDB 1H Mr.A.Bharathi Kumar



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

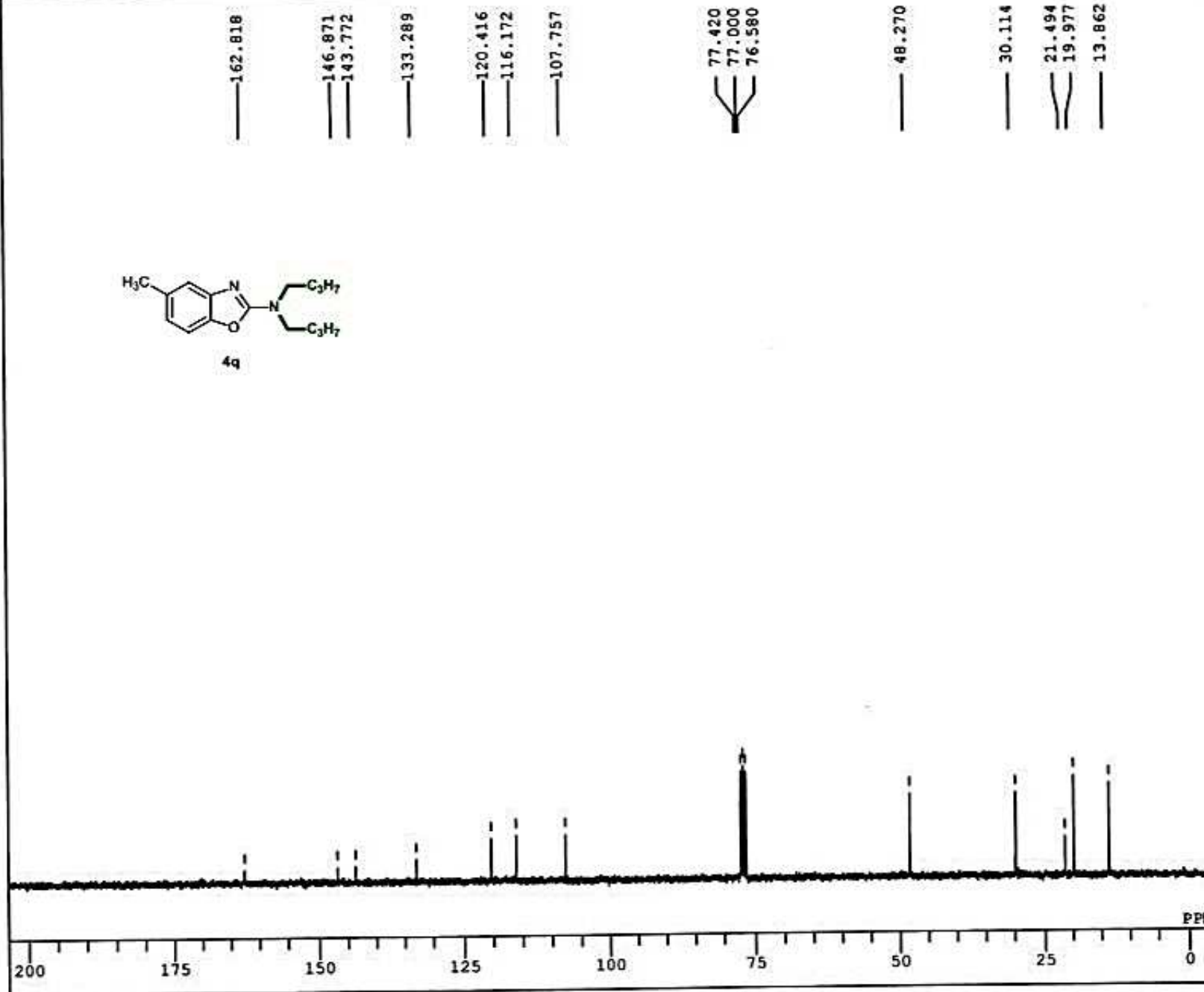
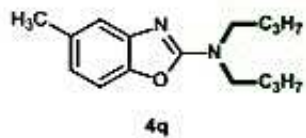
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COMNT 4-MDB 1H Mr.A.Bha
DATIM Wed Dec 05 15:26:
OBNUC 1H
EXMOD NON
OBFREQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 30
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 13

C:\WINNMR98\COMMON\DEFAULT.ALS
4-MDB 13C Mr.A.Bharathi Kumar

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

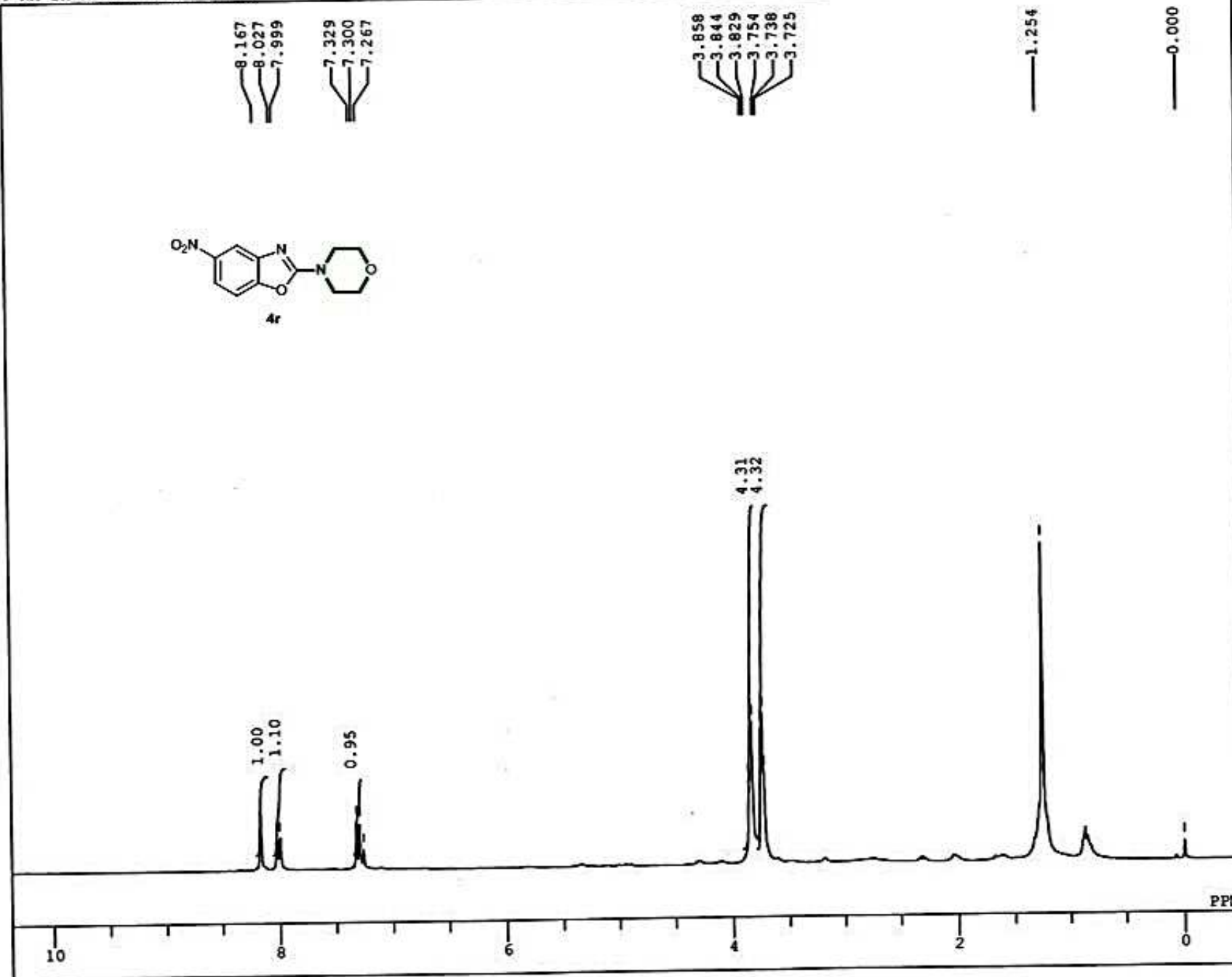
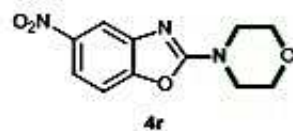
Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON\DEI
COMNT 4-MDB_13C Mr.A.Bharath:
DATIM Wed Dec 05 15:21:14 20:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 117
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 23.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24



B₄₄

C:\K.N. Singh,,I.T\4-NM 1H.als
4-NM 1H Mr.A.Bharat Kumar



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT 4-NM 1H Mr.A.Bhar.
DATIM Wed Oct 03 12:55:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 17
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 15

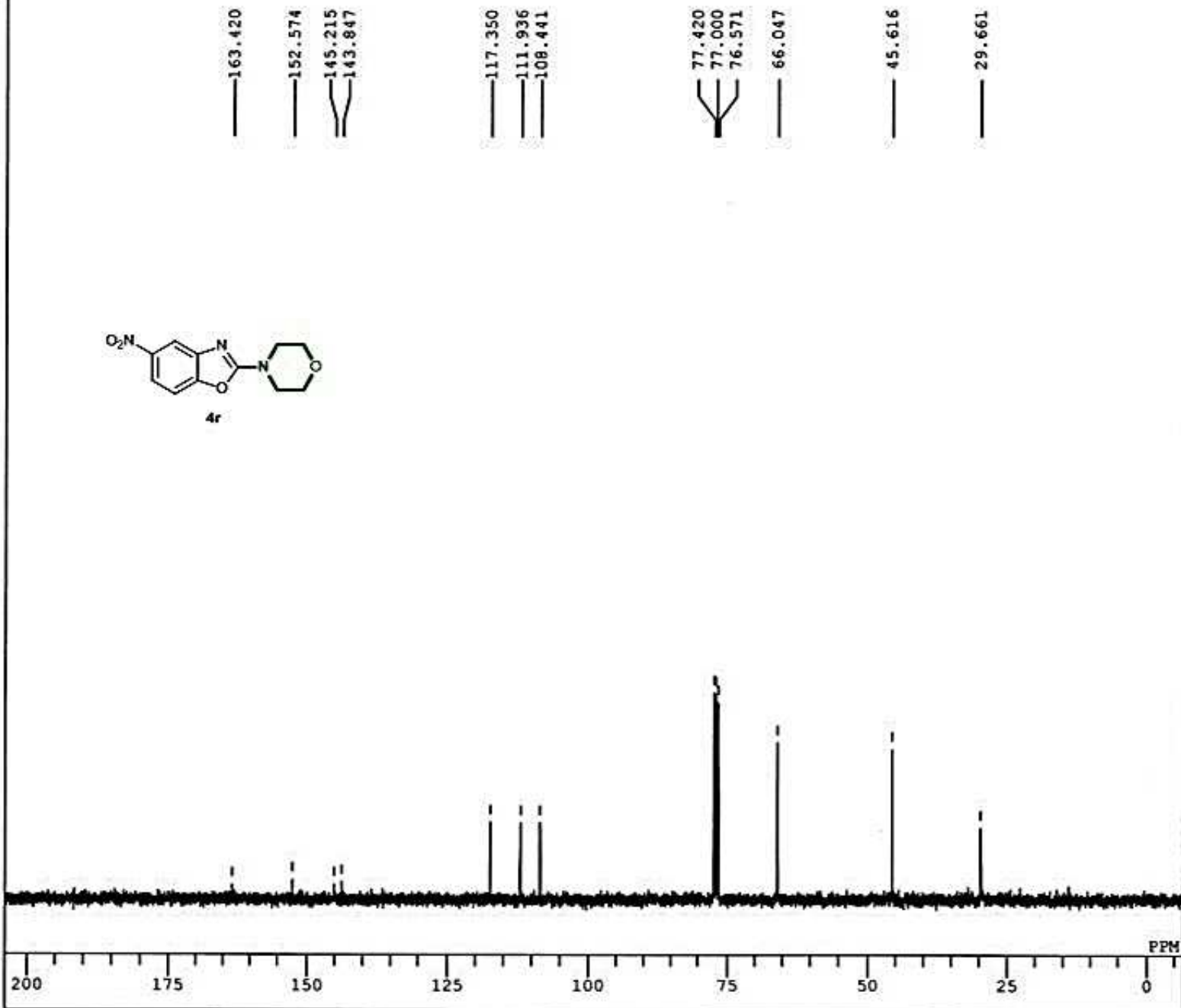
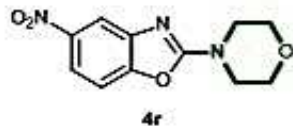
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C:\WINNMR98\COMMON_DEFAULT.ALS
4-NM ~~Dr~~ Mr.A.Bharat Kumar

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

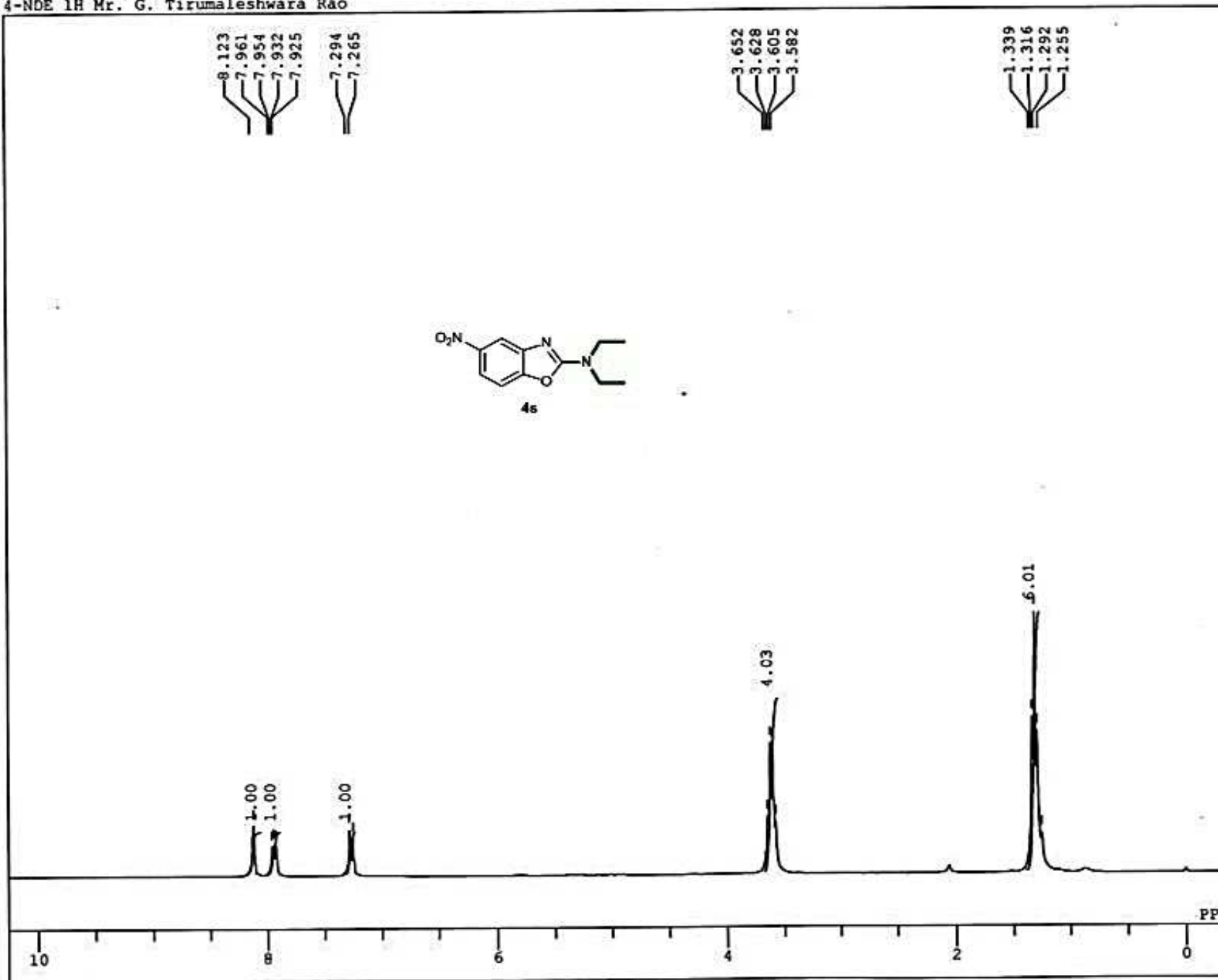
Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT 4-NM_1H_Mr.A.Bharat_Kumar
DATIM Wed Oct 03 12:51:05 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 110
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 20.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25



B₄₆

C:\K.N. Singh,,I.T\4-NDE 1H.als
4-NDE 1H Mr. G. Tirumaleshwara Rao



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

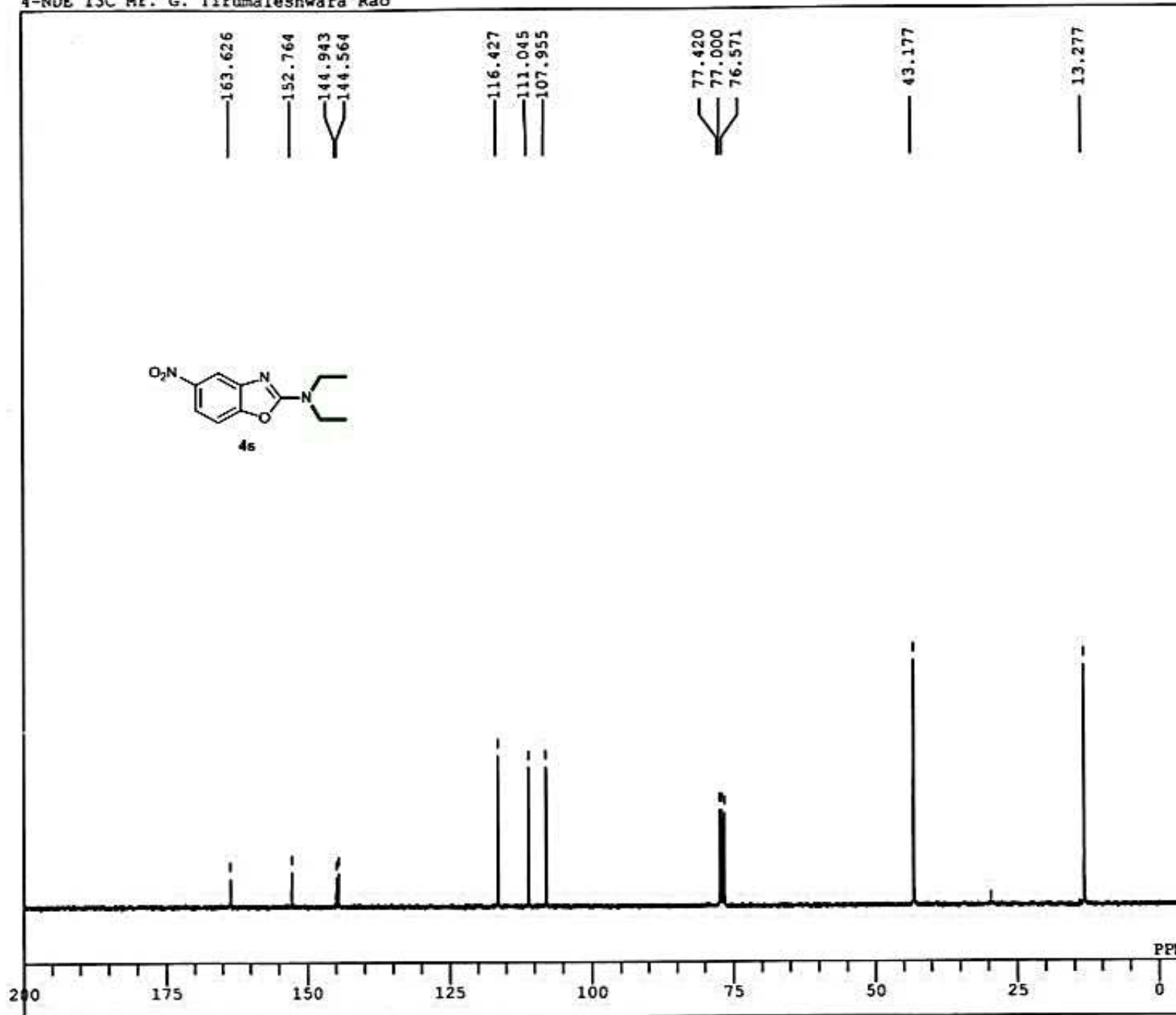
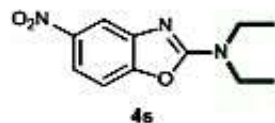
DFILE C:\K.N. Singh,,I.'
COMNT 4-NDE 1H Mr. G. T
DATIM Tue Nov 06 11:58:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 10

C:\WINNMR98\COMMON_DEFAULT.ALS
4-NDE 13C Mr. G. Tirumaleshvara Rao

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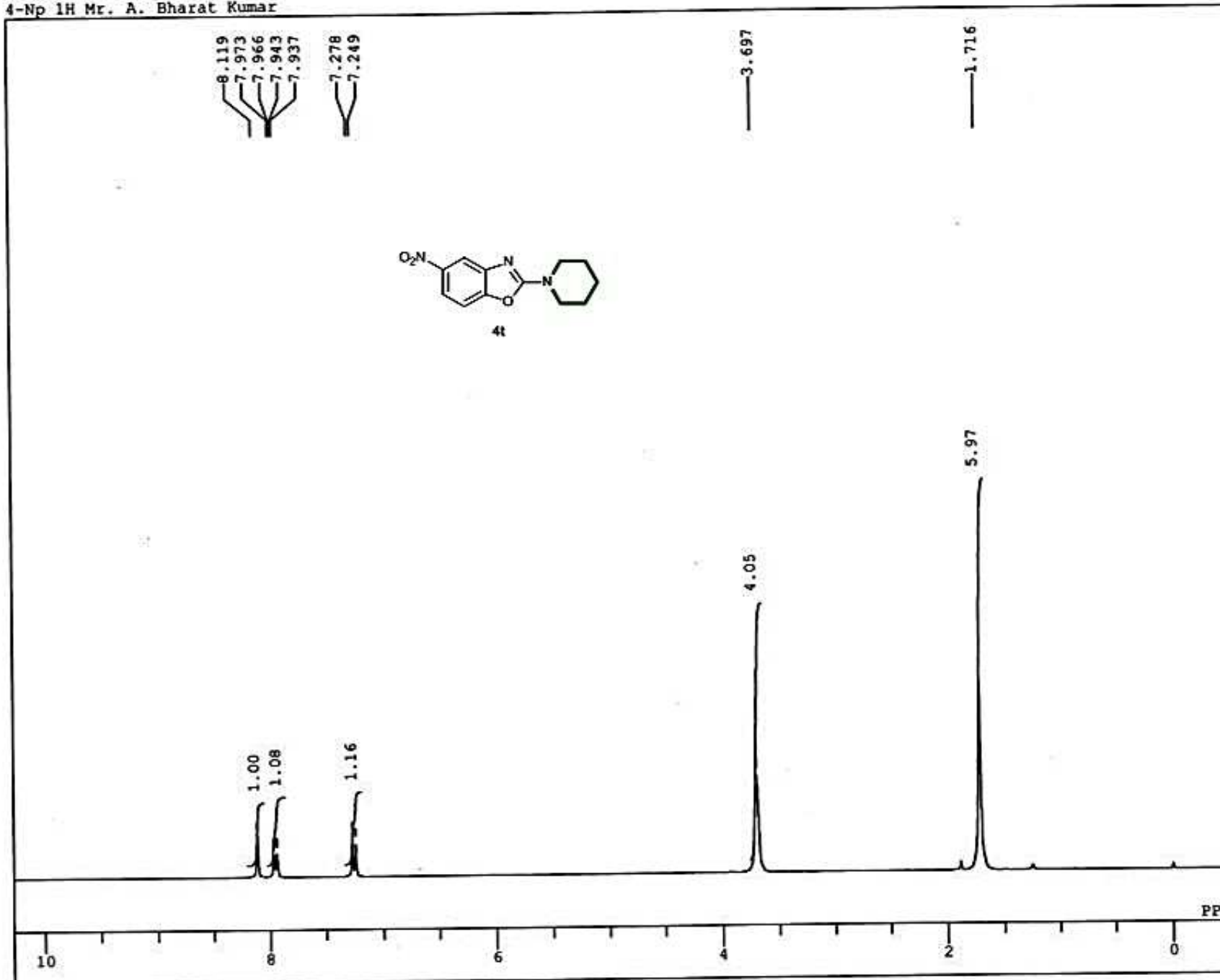
Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT 4-NDE_13C Mr. G. Tirumaleshw
DATIM Tue Nov 06 12:19:54 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 335
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 24.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25



B₄₈

C:\K.N. Singh,,I.T\4-Np_1H.als
4-Np 1H Mr. A. Bharat Kumar



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

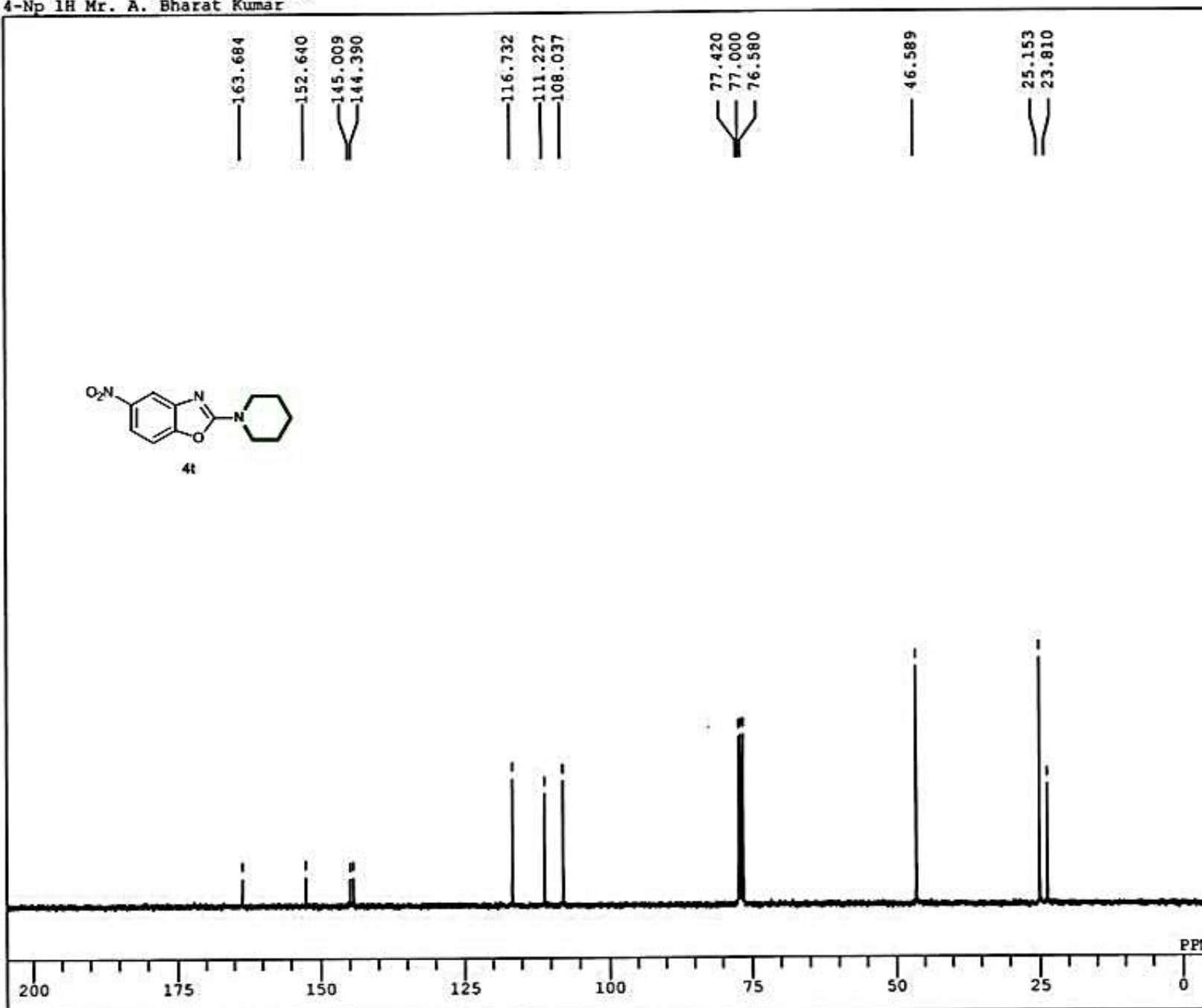
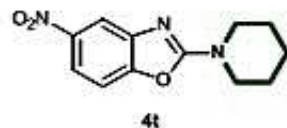
DFILE C:\K.N. Singh,,I.
COMNT 4-Np_1H_Mr. A. Bh.
DATIM Mon Oct 08 14:28:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 32
ACQTM 5.446 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 19.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 12

C:\WINNMR98\Data\4-Np_1H2BCM_E1.als
 4-Np 1H Mr. A. Bharat Kumar

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 VARANASI-221005

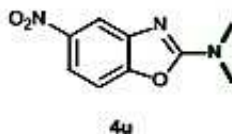
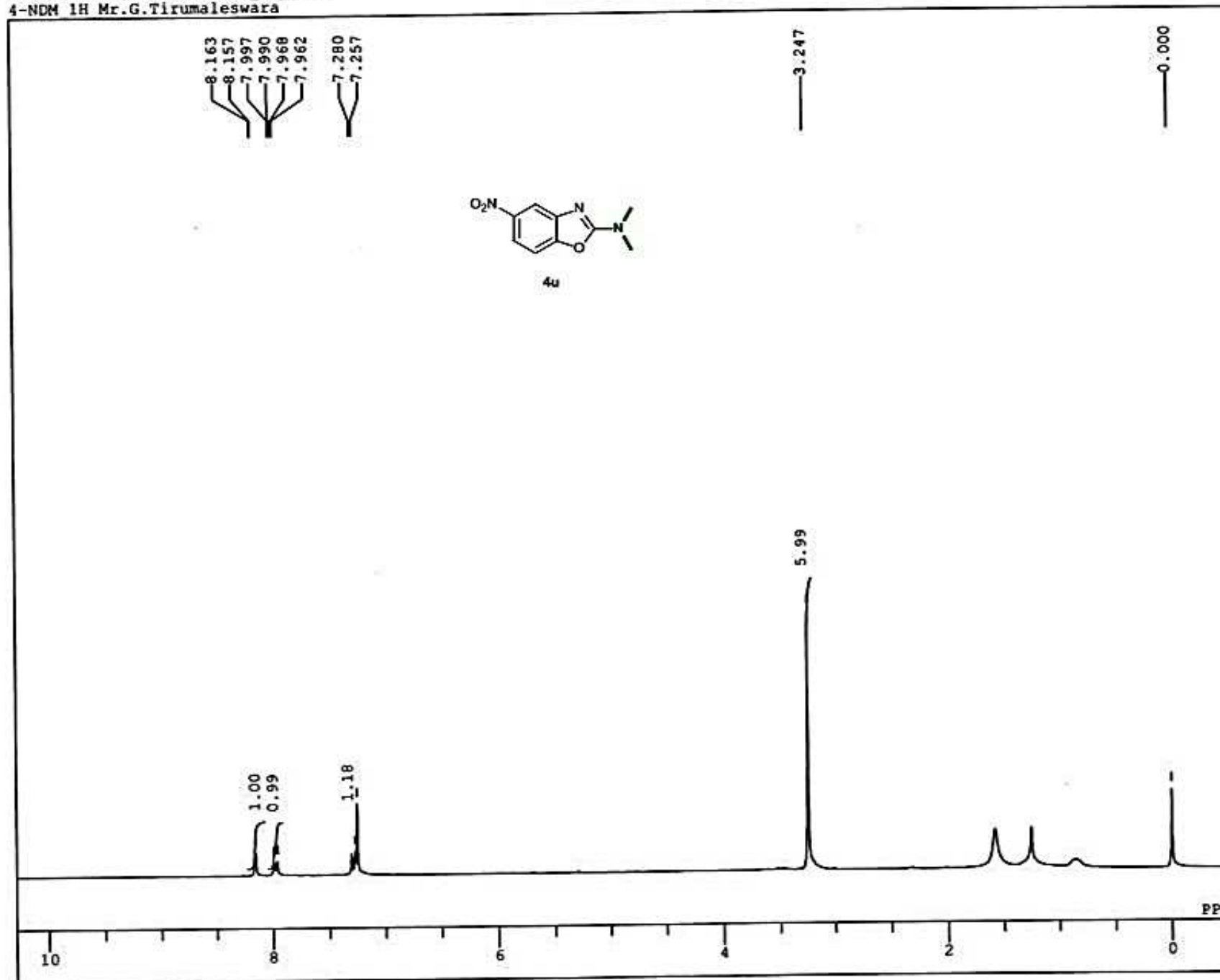
Operator : Nagendra Kumar
 Shishir Singh

DFILE C:\WINNMR98\Data\4-Np_
 COMNT 4-Np_1H Mr. A. Bharat i
 DATIM Mon Oct 08 14:54:15 20:
 OBNUC 13C
 EXMOD BCM
 OBFRQ 75.45 MHz
 OBSET 127.30 KHz
 OBFIN 44.7 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 500
 ACQTM 1.606 sec
 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 23



B₅₀

C:\K.N. Singh,,I.T\4-NDM_1H_.als
4-NDM 1H Mr.G.Tirumaleswara

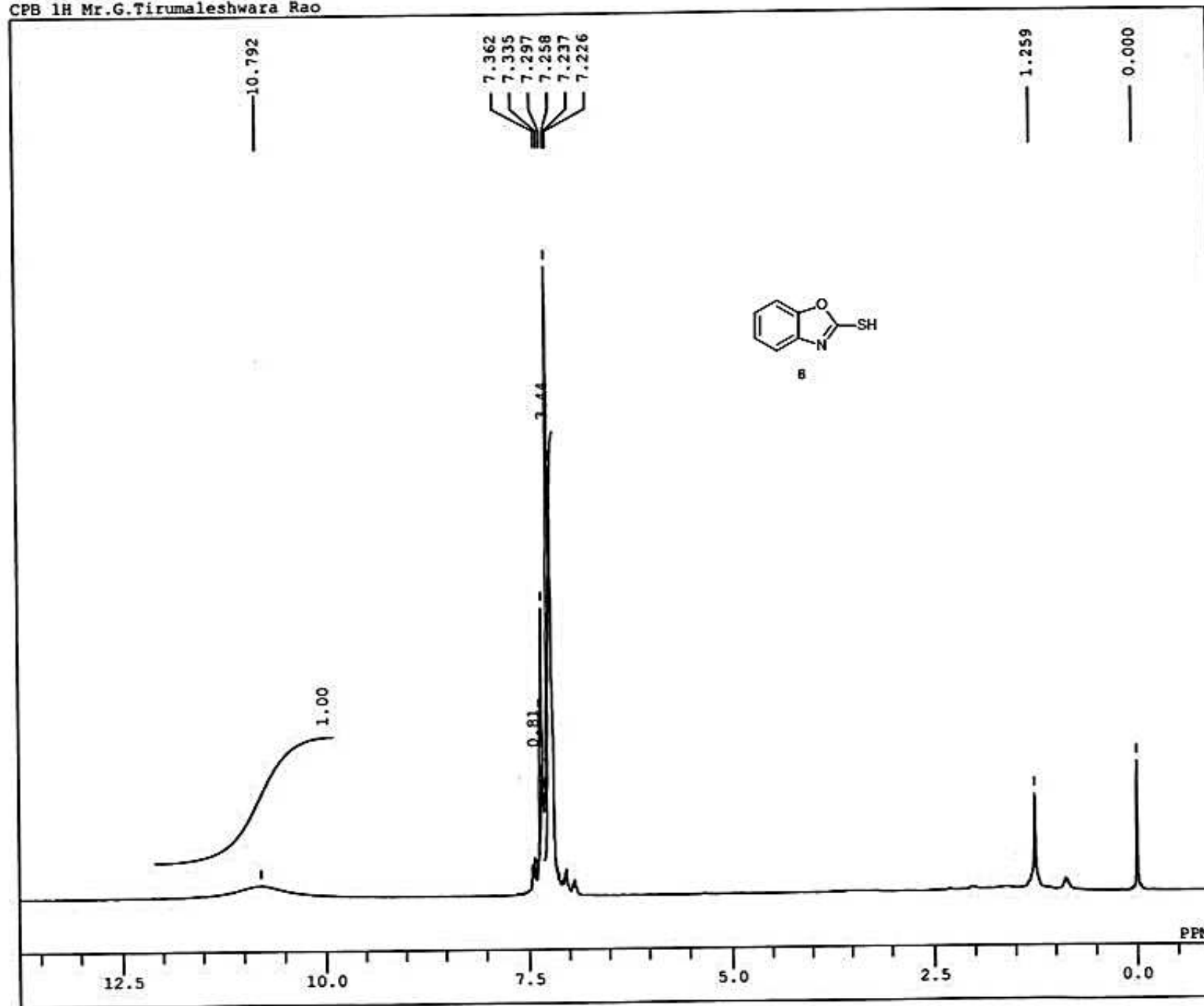


JEOL AL300 FTNMR
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VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT 4-NDM_1H Mr.G.Tir
DATIM Mon Dec 03 15:30:
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 20.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh,,I.T\CPB_1H.als
CPB 1H Mr.G.Tirumaleshwara Rao

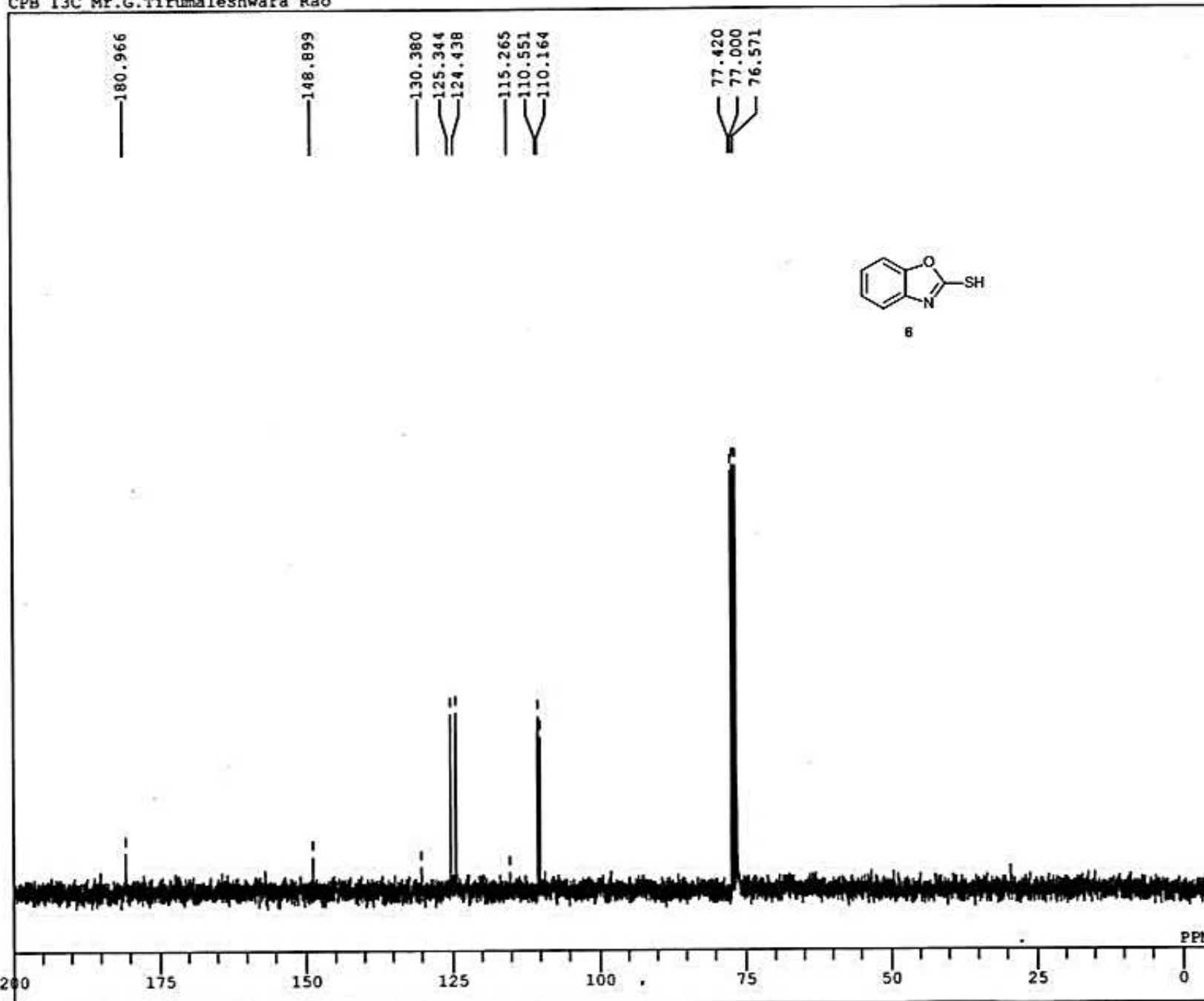


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\CPB_1H.als
COMNT CPB_1H_Mr.G.Tirumaleshwara Rao
DATIM Mon Oct 01 12:58:16 2013
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 44
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 31.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 19

C:\K.N. Singh,,I.T\CPB_13C.als
CPB 13C Mr.G.Tirumaleshwara Rao

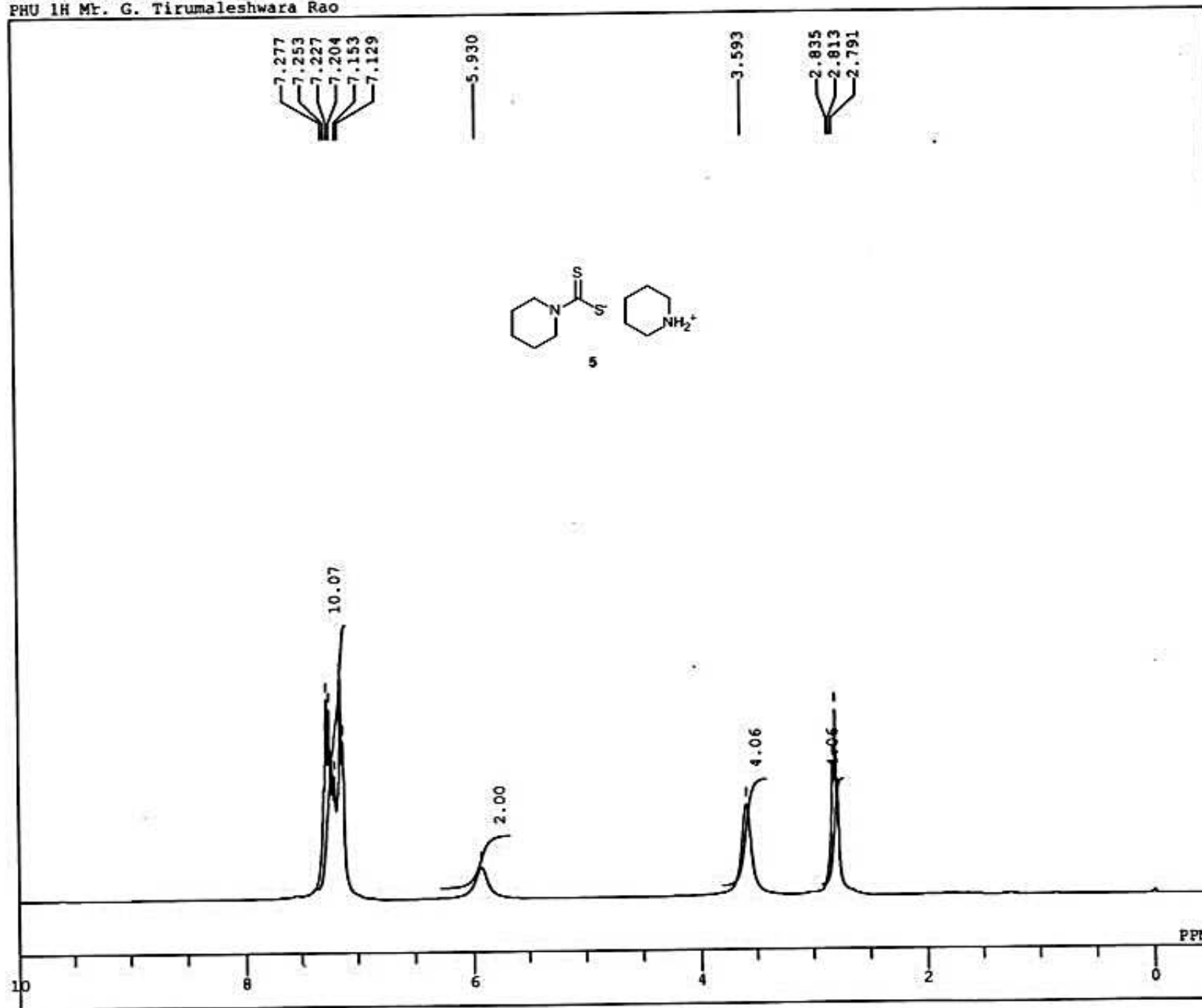


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\CPB_13C.als
COMNT CPB_13C_Mr.G.Tirumaleshwara Rao
DATIM Mon Oct 01 12:49:56 2013
OBNUC 13C
EXMOD BCM
OBFREQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 214
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 40.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh,,I.T\PHU_1H.als
PHU_1H Mr. G. Tirumaleshwara Rao

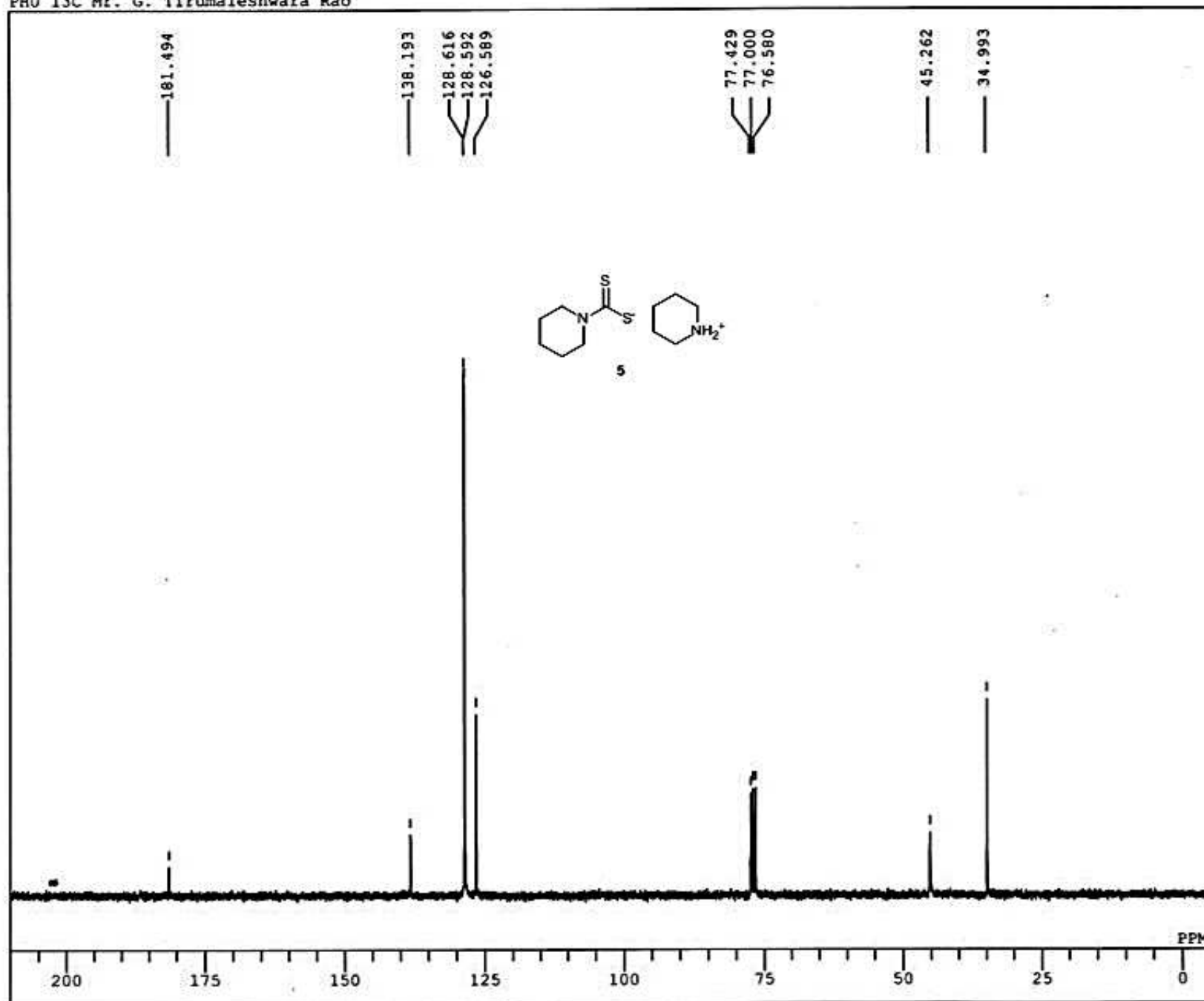


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\PHU_1H
COMNT PHU_1H Mr. G. Tirumale:
DATIM Mon Dec 31 11:38:10 20:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 11

C:\WINNMR98\COMMON_DEFAULT.ALS
PHU 13C Mr. G. Tirumaleshwara Rao



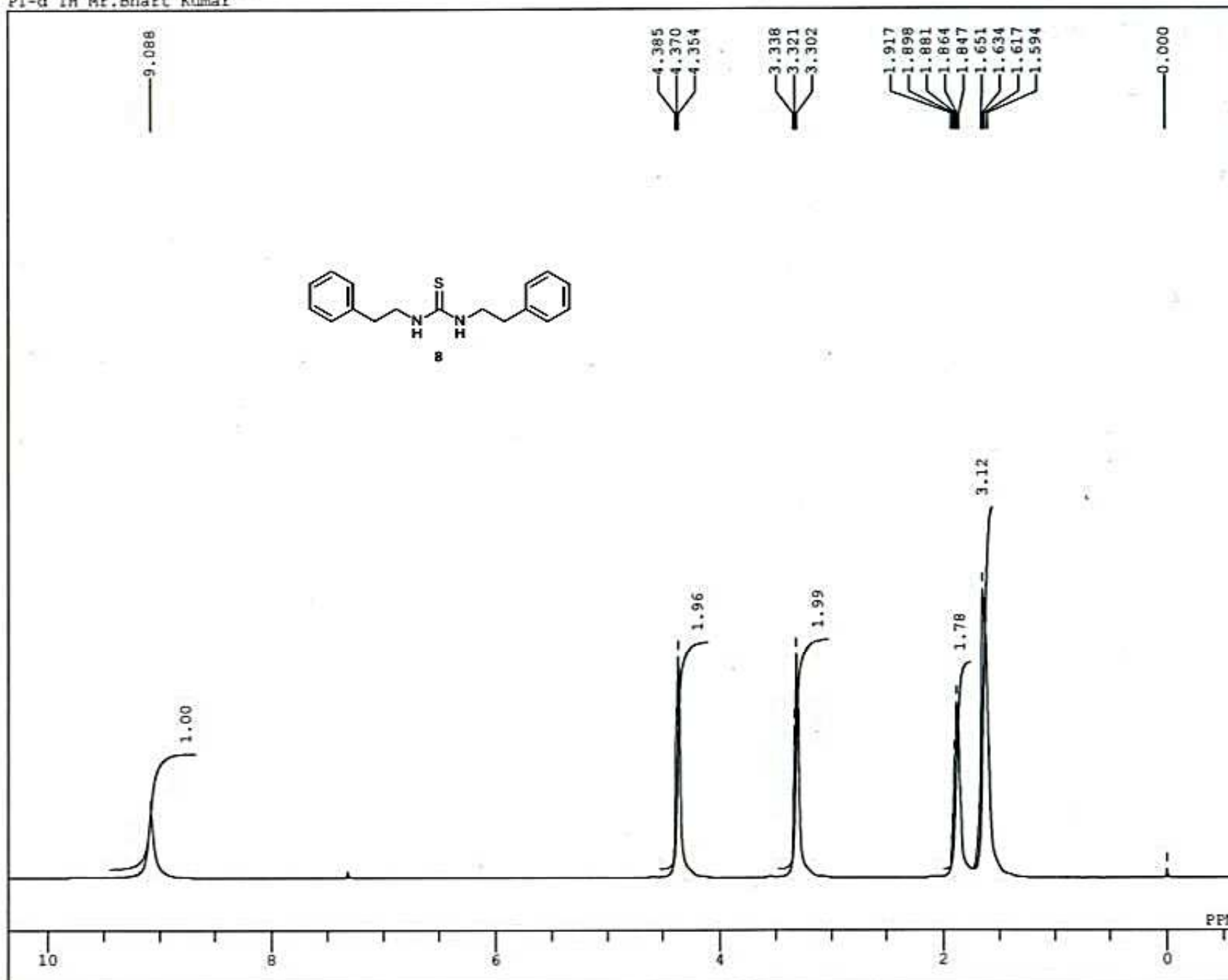
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEI
COMNT PHU_13C Mr. G. Tirumal:
DATIM Mon Dec 31 11:34:17 20:
OBNUC 13C
EXMOD BCM
OBFREQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 92
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

B₅₅

C:\K.N. Singh,,I.T\PI-d_1H.als
PI-d 1H Mr.Bhart Kumar

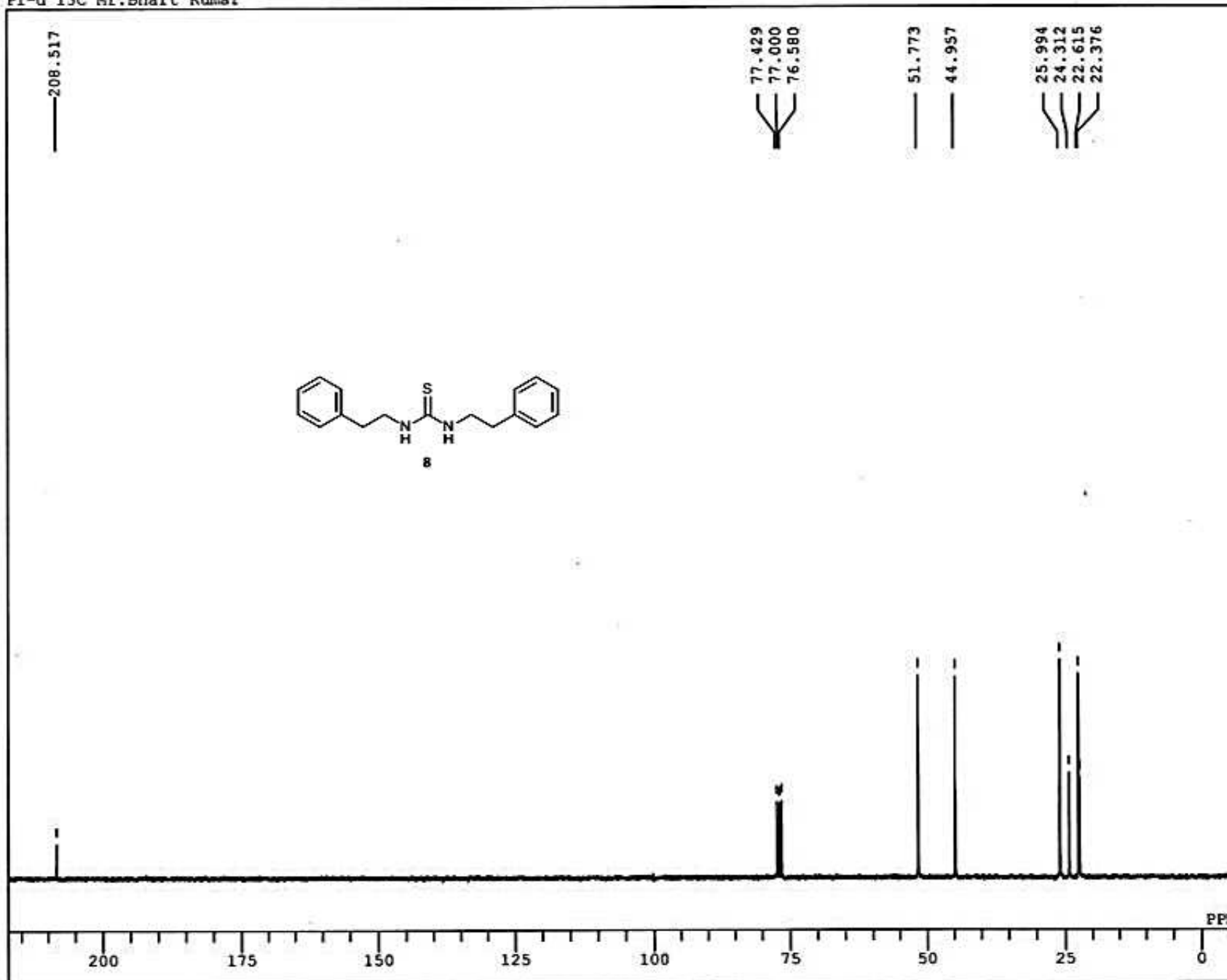


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT PI-d 1H Mr.Bhart
DATIM Wed Jan 02 11:27:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 50
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 10

C:\WINNMR98\COMMON_DEFAULT.ALS
PI-d 13C Mr.Bhart Kumar



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Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\WINNMR98\COMMON
COMNT PI-d 13C Mr.Bhart
DATIM Wed Jan 02 11:15:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 159
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 24.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25