

Supporting Information

Hypervalent Iodine Catalyzed Transamidation of Carboxamides with Amines

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I. General Experimental Section:

All the reagents were purchased from commercial suppliers and were used as such. The solvents used in the reactions were distilled and dried prior to use. All the reactions conducted under conventional heating were performed under air atmosphere in a Schlenk flask. Microwave reactions were performed using an Anton Paar Monowave 300 mono-mode microwave reactor with a sealed 10-mL vial containing teflon-coated magnetic stir bar. The microwave system contains a single magnetron that delivers up to 850 W installed microwave power in unpulsed mode over the full power range. The sophisticated software prevents thermal overshoots and the design of the microwave applicator provides utmost field density, which allows efficient heating, even of low-absorbing solvents at any scale. A precisely adjusted IR sensor reflects the internal reaction temperature up to 300 °C. Pressure control up to 30 bar is provided by a non-invasive hydraulic piston embedded in the swiveling cover. For cooling, the cavity is flushed with compressed air automatically after the programmed experiment has been processed. Column chromatography was performed using Merck silica gel (100–200 mesh). Thin layer chromatography (TLC) was performed using silica gel 60/KieselguhrF₂₅₄ pre-coated on aluminum sheets (thickness 0.2 mm), commercially available from Merck. Visualization of spots on TLC plate was accomplished with UV light and by staining in I₂ chamber.

All the melting points were determined in open capillary tubes and are uncorrected. ¹H and ¹³C NMR spectra were recorded 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 internal standard. Product yields refer to isolated yields after column chromatography.

II. Experimental procedures:

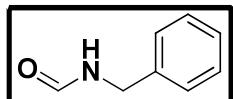
- a) General conventional experimental procedure:** Diacetoxyiodobenzene (DIB) (0.15 mmol, 48.3 mg) was added to a Schlenk flask, equipped with a rubber septum and teflon-coated stir bar, containing carboxamide (3 mmol) and amine (3 mmol). The resulting mixture was vigorously stirred at the appropriate temperature for a specified time. The progress of the reaction was monitored through TLC. After completion of the reaction, mixture was cooled to room temperature; distilled water (10 mL) was added and then extracted with ethyl acetate (3×10 mL). The combined organic phase was dried over Na_2SO_4 , and then concentrated using rotary vacuum evaporator. The crude product was purified by column chromatography using a mixture of ethyl acetate/n-hexane as an eluent.
- b) General MW experimental procedure:** An oven-dried 10-mL microwave reaction vial containing a teflon-coated magnetic stir bar was charged with carboxamide (3 mmol), amine (3 mmol), and diacetoxyiodobenzene (DIB) (0.15 mmol, 48.3 mg). The vessel was sealed with a plastic microwave septum, stirred at room temperature for 5 min and then placed into the MW cavity for a specified temperature and time. After completion of reaction (TLC), the mixture was cooled to room temperature and worked-up as given in conventional method.

III. Complete Optimization Table:

Entry	Accelerator	mol (%)	Solvent	Conventional heating			MW heating		
				T (°C)	t (h)	Yield (%)	T (°C)	t (min.)	Yield (%)
1.	–	–	–	120	24	n.r	120	20	n.r
2.	<i>p</i> -TSA	10	–	120	24	60	120	20	62
3.	TFA	10	–	120	24	40	120	20	41
4.	BF ₃ ·Et ₂ O	10	–	120	24	57	120	20	57
5.	I ₂	10	–	120	24	51	120	20	52
6.	Zn(OAc) ₂ ·2H ₂ O	10	–	120	24	20	120	20	23
7.	CdI ₂	10	–	120	24	33	120	20	39
8.	FeCl ₃	10	–	120	24	41	120	20	42
9.	NiCl ₂ ·6H ₂ O	10	–	120	24	30	120	20	30
10.	ZrOCl ₂	10	–	120	24	40	120	20	41
11.	KOH	10	–	120	24	n.r	120	20	n.r
12.	DBU	10	–	120	24	n.r	120	20	n.r
13.	TBAB	10	–	120	24	trace	120	20	trace
14.	[BmIm]BF ₄	10	–	120	24	50	120	20	55
15.	DIB	10	–	120	24	81	120	20	83
16.	DIB	5	–	120	24	81	120	20	83
17.	DIB	5	–	120	17	72	120	10	77
18.	DIB	3	–	120	24	67	120	20	69
19.	DIB	5	Toluene	120	24	18	120	20	27
20.	DIB	5	Xylene	120	24	29	120	20	30
21.	DIB	5	Chlorobenzene	120	24	20	120	20	25
22.	DIB	5	DMSO	120	24	19	120	20	21
23.	DIB	5	DMF	120	24	24	120	20	27
24.	DIB	5	H ₂ O	100	24	17	120	20	23
25.	DIB	5	n-C ₅ H ₁₁ OH	120	24	n.r	120	20	n.r

IV. Characterization of Products:

1. N-Benzylformamide (3a)¹:

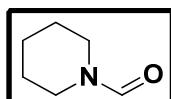


Colorless solid; m.p.: 59–60 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.28 (s, 0.8H), 8.23 (d, *J* = 12.0 Hz, 0.2H), 7.37–7.29 (m, 5H), 5.75 (br s, 1H, NH), 4.51 (d, *J* = 6 Hz, 1.8H), 4.44 (d, *J* = 6.3 Hz, 0.2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 164.7, 161.3, 137.5, 128.6, 128.4, 127.7, 127.6, 127.4, 127.2, 45.4, 41.8.

2. Piperidine-1-carbaldehyde (3b)²:

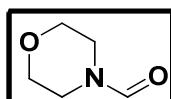


Colorless oil.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.99 (s, 1H), 3.47 (t, *J* = 5.4 Hz, 2H), 3.32 (t, *J* = 5.4 Hz, 2H), 1.69–1.54 (m, 6H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 160.4, 46.4, 40.2, 26.2, 24.7, 24.3.

3. N-Formylmorpholine (3c)³:

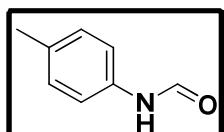


Colorless oil.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.06 (s, 1H), 3.72–3.56 (m, 6H), 3.42–3.39 (m, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 160.8, 67.1, 66.3, 45.7, 40.5.

4. N-4-Tolylformamide(3d)⁴:

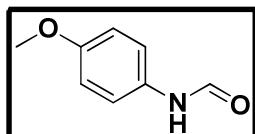


Colorless solid; m.p.: 53–54 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 9.05 (br s, 1H), 8.63 (d, *J* = 11.1 Hz, 1H), 8.39 (s, 1H), 8.27 (s, 1H), 7.43 (d, *J* = 7.5 Hz, 2H), 7.12–6.96 (m, 6H), 2.30/2.28 (each s, 6H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 163.1, 159.5, 134.8, 134.4, 134.2, 134.1, 130.0, 129.3, 120.1, 118.9, 20.7, 20.6.

5. N-(4-Methoxyphenyl)formamide (3e)⁵:



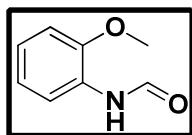
Light brownish solid; m.p.: 80–83 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 9.01 (br s, 1H, NH), 8.53 (d, *J* = 11.1 Hz, 1H), 8.46 (br s, 1H, NH), 8.24 (s, 1H), 7.45 (d, 2H), 7.03 (d, 2H), 6.87–6.79 (m, 4H), 3.77/3.75 (s, 6H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 163.3, 159.4, 157.3, 156.4, 130.0, 129.6, 121.8, 121.2, 114.7, 114.0, 55.3, 55.2.

IR (KBr Disc, $\bar{\nu}$ /Cm⁻¹): 3246, 3192, 3129, 3050, 3001, 2969, 2937, 2895, 1678, 1656, 1604, 1551, 1510, 1462, 1396, 1308, 1235, 1182, 1109, 1029, 835, 808, 783, 696.

6. N-(2-Methoxyphenyl)formamide (3f)⁶:



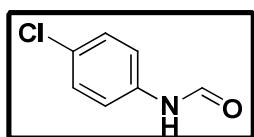
Brown solid; m.p.: 84–85 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.74 (d, *J* = 11.4 Hz, 1H), 8.44 (s, 1H), 8.37 (d, *J* = 6.9 Hz, 1H), 7.87 (s, 1H), 7.20–6.87 (m, 8H), 3.87 (s, 6H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 161.4, 158.7, 148.7, 147.7, 126.7, 126.1, 125.1, 124.2, 121.0, 120.4, 116.6, 111.2, 110.0, 55.6.

IR (KBr Disc, $\bar{\nu}/\text{Cm}^{-1}$): 3254, 3008, 2922, 2937, 2835, 1694, 1659, 1597, 1535, 1460, 1396, 1287, 1227, 1182, 1109, 1029, 865, 813, 745.

7. N-(4-Chlorophenyl)formamide (3g)⁷:

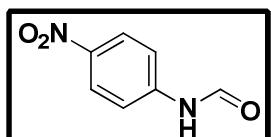


Grey solid; m.p.: 99–100 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.88 (br s, 1H), 8.67 (d, $J = 11.4$ Hz, 1H), 8.34 (s, 1H), 7.99 (br s, 1H), 7.51 (d, $J = 8.7$ Hz, 2H), 7.33 (m, 4H), 7.05 (d, $J = 8.4$ Hz, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 162.7, 159.3, 135.4, 135.3, 130.6, 129.7, 129.0, 121.2, 119.9.

8. N-(4-Nitrophenyl)formamide (3h)⁵:



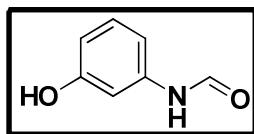
Yellow solid; m.p.: 197–199 °C.

¹H NMR (300 MHz, DMSO-d₆, TMS) δ/ppm: 10.77 (s, 1H), 9.03 (br s, 1H), 8.38 (s, 1H), 8.20 (d, $J = 6.2$ Hz, 2H), 7.80 (d, $J = 7.8$ Hz, 2H), 7.40 (br s, 1H).

¹³C NMR (75 MHz, DMSO-d₆, TMS) δ/ppm: 162.7, 160.5, 144.2, 142.5, 125.4, 125.0, 119.0, 116.5.

IR (KBr Disc, $\bar{\nu}/\text{Cm}^{-1}$): 3259, 3214, 3152, 3090, 3060, 3050, 2925, 2885, 2629, 1689, 1620, 1596, 1563, 1493, 1411, 1382, 1331, 1302, 1270, 1177, 1155, 1111, 853, 829, 752, 688.

9. N-(3-Hydroxyphenyl)formamide (3i)⁸:

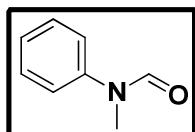


Brown solid; m.p.: 117–118 °C.

¹H NMR (300 MHz, DMSO-d₆, TMS) δ/ppm: 10.02 (br s, 1H), 9.53 (s, 1H, OH), 9.42 (s, 1H), 8.72 (d, *J* = 11.1 Hz, 1H), 8.21 (s, 1H), 7.17–6.45 (m, 4H).

¹³C NMR (75 MHz, DMSO-d₆, TMS) δ/ppm: 162.5, 159.6, 158.3, 157.7, 139.5, 139.3, 130.3, 129.6, 110.9, 110.0, 108.1, 106.5, 104.8.

10. N-Methyl-N-phenylformamide (3j)⁹:

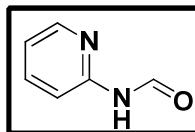


Colorless oil.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.46 (s, 1H), 7.43–7.15 (m, 5H), 3.31 (s, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 161.4, 161.3, 141.4, 128.8, 128.1, 125.4, 125.1, 122.5, 121.3, 30.9.

11. N-(Pyridin-2-yl)formamide (3k)¹⁰:

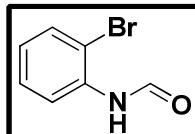


Yellow solid; m.p.: 70–71 °C

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 10.68 (br s, 1H), 10.54 (br s, 1H), 9.36 (d, *J* = 9.9 Hz, 1H), 8.56 (s, 1H), 8.35–8.26 (m, 3H), 7.76–7.64 (m, 2H), 7.11–6.95 (m, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 163.2, 159.7, 151.0, 148.2, 147.1, 138.7, 138.5, 119.9, 119.6, 115.0, 110.4.

12. N-(2-Bromophenyl)formamide (3l)⁸:

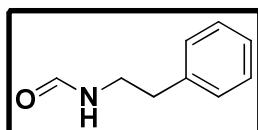


Colorless solid; m.p.: 91 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.72 (d, 1H), 8.49 (s, 1H), 8.40 (d, *J* = 8.1 Hz, 1H), 7.67 (br s, 1H), 7.61–7.01 (m, 8H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 161.6, 158.9, 134.7, 133.4, 132.3, 128.6, 128.4, 126.3, 125.6, 122.1, 118.9, 113.0.

13. N-Phenethylformamide (3m)¹¹:

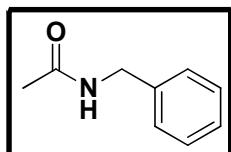


Colorless oil.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.08 (s, 1H), 7.89 (d, *J* = 11.7 Hz, 1H), 7.33–7.15 (m, 5H), 5.85 (br s, 1H, NH), 3.59–3.49 (m, 2H), 3.44 (t, *J* = 6.6 Hz, 2H), 2.85–2.78 (m, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 164.4, 161.2, 138.4, 128.7, 128.7, 128.6, 126.8, 126.5, 43.1, 39.1, 37.6, 35.4.

14. N-Benzylacetamide (3o)¹²:



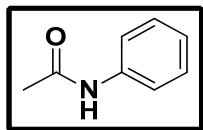
Brown solid; m.p.: 60–61 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.29–7.21 (m, 5H), 6.61 (br s, 1H), 4.34 (d, *J* = 3.9 Hz, 2H), 1.93 (s, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 170.1, 138.2, 128.4, 127.6, 127.2, 43.4, 22.9.

IR (KBr Disc, $\bar{\nu}$ /cm⁻¹): 3295, 3063, 3033, 2928, 1647, 1548, 1499, 1454, 1374, 1357, 1221, 1162, 1097, 1033, 907, 741, 696.

15. N-Phenylacetamide (3p)¹³:

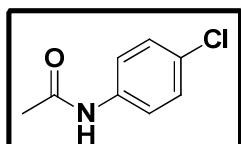


Colorless solid; m.p.: 113–114 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.50 (br s, 1H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.28–7.23 (m, 2H), 7.08–7.06 (m, 1H), 2.11 (s, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 169.2, 138.0, 128.7, 124.1, 120.2, 24.1.

16. **N-(4-Chlorophenyl)acetamide (3q)¹⁴:**

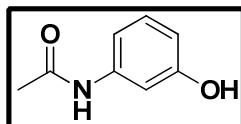


Yellow solid; m.p.: 177–178 °C.

¹H NMR (300 MHz, DMSO-d₆, TMS) δ/ppm: 10.03 (s, 1H), 7.60 (d, *J* = 6.3 Hz, 2H), 7.31 (d, *J* = 6.3 Hz, 2H), 2.03 (s, 3H).

¹³C NMR (75 MHz, DMSO-d₆, TMS) δ/ppm: 168.5, 138.3, 128.5, 126.6, 120.5, 24.0.

17. **N-(3-Hydroxyphenyl)acetamide (3r)¹⁵:**

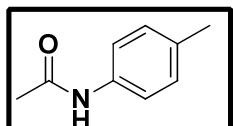


Colorless solid; m.p.: 148–149 °C.

¹H NMR (300 MHz, DMSO-d₆, TMS) δ/ppm: 9.77 (br s, 1H), 9.34 (s, 1H), 7.17 (s, 1H), 7.03 (t, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 6.42 (d, *J* = 6.9 Hz, 1H), 1.99 (s, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.3, 157.6, 140.4, 129.3, 110.2, 109.9, 106.3, 24.1.

18. **N-(4-Tolyl)acetamide (3s)¹⁶:**

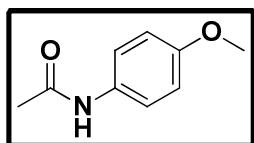


Colorless solid; m.p.: 149–150 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.83 (br s, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.1 Hz, 2H), 2.29 (s, 3H), 2.12 (s, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.6, 135.4, 133.8, 129.3, 120.1, 24.3, 20.8.

19. **N-(4-Methoxyphenyl)acetamide (3t)¹⁷:**

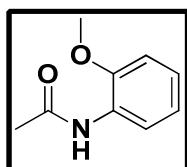


Colorless solid; m.p.: 126–128 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.04 (s, 1H), 7.39 (d, *J* = 8.7 Hz, 2H), 6.81 (d, *J* = 8.7 Hz, 2H), 3.76 (s, 3H), 2.10 (s, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.7, 156.3, 131.1, 122.0, 113.9, 55.3, 24.1.

20. **N-(2-Methoxyphenyl)acetamide (3u)¹⁸:**

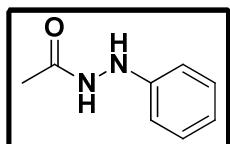


Colorless solid; m.p.: 87–88 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 8.35 (d, *J* = 7.8 Hz, 1H), 7.77 (br s, NH), 7.04–6.84 (m, 4H), 3.86 (s, 3H), 2.19 (s, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.1, 147.6, 127.6, 123.5, 120.9, 119.7, 109.8, 55.5, 24.8.

21. **N'-Phenylacetohydrazide (3v)¹⁹:**



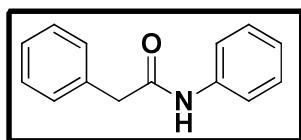
Pale brown solid; m.p.: 129–130 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.72 (br s, 1H, NH), 7.26–7.18 (m, 5H), 6.93–6.71 (m, 6H), 6.20 (br s, 1H, NH), 5.85 (br s, 1H, NH), 2.08/2.01 (s, 6H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 177.0, 170.3, 147.8, 147.0, 129.4, 129.1, 121.2, 121.1, 113.4, 112.4, 20.8, 19.1.

IR (KBr Disc, $\bar{\nu}/\text{Cm}^{-1}$): 3287, 3234, 3031, 2928, 1665, 1643, 1597.

22. N,2-Diphenylacetamide (3x)²⁰:



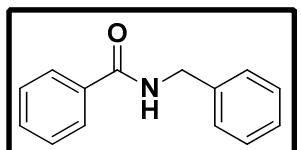
Colorless solid: m.p.: 115–116 °C.

¹H NMR (CDCl₃, 300 MHz, TMS) δ/ppm: 7.75 (br s, 1H), 7.43 (d, *J* = 7.8 Hz, 2H), 7.32–7.02 (m, 8H), 3.64 (s, 2H).

¹³C NMR (CDCl₃, 75 MHz, TMS) δ/ppm: 169.4, 137.7, 134.5, 129.3, 128.9, 128.8, 127.4, 124.3, 119.9, 44.5.

IR (KBr Disc, $\bar{\nu}/\text{Cm}^{-1}$): 3285, 3256, 3060, 1657, 1601, 1556, 1496, 1442, 1167, 755, 724, 691.

23. N-Benzylbenzamide (3y)²¹:



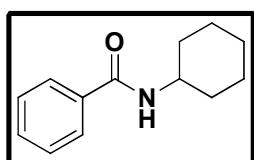
Colorless solid; m.p.: 101–102 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.80 (d, *J* = 6.9 Hz, 2H), 7.50–7.25 (m, 8H), 6.37 (br s, 1H), 4.67 (d, *J* = 5.4 Hz, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 167.3, 138.2, 134.3, 131.4, 128.7, 128.5, 127.8, 127.5, 126.9, 44.0.

IR (KBr Disc, $\bar{\nu}/\text{Cm}^{-1}$): 3291, 3061, 3030, 2926, 2853, 1638, 1602, 1550, 1452, 1417, 1362, 1260, 1151, 1056, 1027, 928, 726, 695.

24. N-Cyclohexylbenzamide (**3z**)²²:



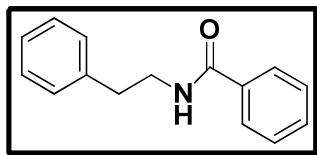
Colorless solid; m.p.: 156–157 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.76–7.74 (m, 2H), 7.47–7.38 (m, 3H), 6.09 (br s, 1H, NH), 4.03–3.91 (m, 1H, NHCH), 2.04–1.17 (m, 10H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 166.6, 135.0, 131.1, 128.4, 126.8, 48.6, 33.1, 25.5, 24.9.

IR (KBr Disc, ȏ/Cm⁻¹): 3239, 3078, 2928, 2851, 1639, 1626, 1564, 1488, 1453, 1330, 1295, 1262, 1241, 1152, 1083, 1025, 1001, 970, 891, 849, 804, 700, 670.

25. N-Phenethylbenzamide (**3aa**)²²:

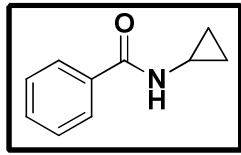


Colorless solid; m.p.: 117–118 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.66 (d, *J* = 7.2 Hz, 2H), 7.47–7.19 (m, 8H), 6.11 (br s, 1H, NH), 3.72–3.66 (m, 2H), 2.90 (t, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 167.5, 138.8, 134.5, 131.3, 128.7, 128.5, 128.4, 126.7, 41.1, 35.6.

26. N-Cyclopropylbenzamide (**3ab**)²³:



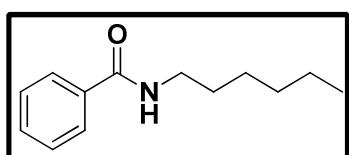
Colorless solid; m.p.: 94–95 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.74 (d, *J* = 6.9 Hz, 2H), 7.50–7.38 (m, 3H), 6.34 (br s, 1H, NH), 2.91–2.88 (m, 1H), 0.87 (br s, 2H), 0.62 (br s, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ ppm: 168.9, 134.4, 131.4, 128.6, 128.5, 127.2, 126.8, 125.8, 31.9, 23.1, 6.7.

IR (KBr Disc, $\bar{\nu}/\text{Cm}^{-1}$): 3303, 2924, 2852, 1641, 1531, 1488, 1310, 1050, 1027, 862, 799, 693, 667.

27. **N-Hexylbenzamide (3ac)²⁴:**



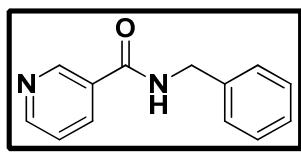
Colorless liquid.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ ppm: 7.78 (d, $J = 7.2$ Hz, 2H), 7.49–7.36 (m, 3H), 6.47 (br s, 1H, NH), 3.45–3.38 (m, 2H), 1.61–1.54 (m, 2H), 1.31 (br s, 6H), 0.88 (t, $J = 6.3$ Hz, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ ppm: 167.5, 134.8, 131.1, 128.4, 126.8, 40.0, 31.4, 29.5, 26.6, 22.5, 13.9.

IR (KBr Disc, $\bar{\nu}/\text{Cm}^{-1}$): 3321, 2929, 2857, 1632, 1578, 1541, 1491, 1310, 695.

28. **N-Benzylnicotinamide (3ad)²⁵:**

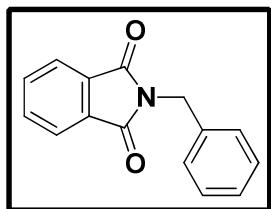


Pale yellow solid; m.p.: 72–73 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ ppm: 8.93 (br s, 1H), 8.61 (br s, 1H), 8.12 (br s, 1H), 7.32–7.31 (br s, 6H), 4.61 (s, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ ppm: 165.5, 151.9, 147.8, 137.7, 135.3, 130.0, 128.7, 127.8, 127.6, 123.5, 44.0.

29. **2-Benzylisoindoline-1,3-dione (3ae)²⁶:**



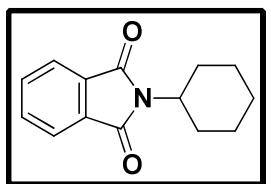
Colorless crystals; m.p.: 116–117 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.85–7.81 (m, 2H), 7.71–7.67 (m, 2H), 7.44–7.41 (m, 2H), 7.33–7.23 (m, 3H), 4.84 (s, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.0, 136.3, 133.9, 132.1, 128.6, 128.5, 127.7, 123.3, 41.5.

IR (KBr Disc, $\bar{\nu}/\text{cm}^{-1}$): 3459, 3086, 3060, 3035, 2947, 2852, 1775, 1765, 1715, 1611, 1603, 1583, 1491, 1466, 1391, 1331, 1298, 1276, 1184, 1101, 792, 763.

30. 2-Cyclohexylisoindoline-1,3-dione (3af)²⁷:

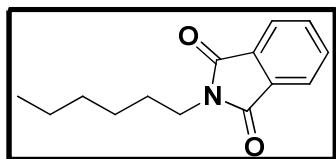


Colorless solid; m.p.: 169–171 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.82–7.79 (dd, *J* = 3.3 Hz, *J* = 3 Hz, 2H), 7.70–7.67 (dd, *J* = 3 Hz, *J* = 3.3 Hz, 2H), 4.15–4.06 (m, 1H), 2.26–2.14 (m, 2H), 1.89–1.71 (m, 5H), 1.44–1.25 (m, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.4, 133.6, 132.0, 122.9, 50.8, 29.8, 26.0, 25.1.

31. 2-Hexylisoindoline-1,3-dione (3ag)²⁸:

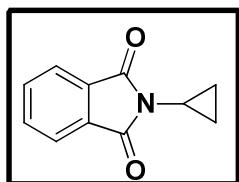


Colorless liquid.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.84–7.81 (m, 2H), 7.72–7.69 (m, 2H), 3.67 (t, J = 7.5 Hz, 2H), 1.69–1.65 (m, 2H), 1.31 (br s, 6H), 0.89–0.85 (m, 3H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.1, 133.6, 132.0, 122.9, 37.8, 31.2, 28.3, 26.3, 22.3, 13.8.

32. **2-Cyclopropylisoindoline-1,3-dione (3ah)²⁹:**



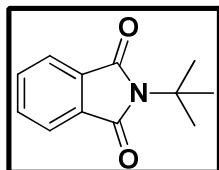
White solid; m.p.: 134–136 °C.

¹H NMR (CDCl₃, 300 MHz, TMS) δ/ppm: 7.83–7.80 (m, 2H), 7.72–7.69 (m, 2H), 2.75–2.68 (m, 1H), 1.04–1.01 (m, 4H).

¹³C NMR (CDCl₃, 75 MHz, TMS) δ/ppm: 168.8, 133.9, 131.7, 123.0, 20.8, 5.1.

IR (KBr Disc, $\bar{\nu}$ /Cm⁻¹): 3026, 1767, 1713, 1699, 1610, 1463, 1402, 1140, 946, 699.

33. **N-tert-Butylphthalimide (3ai)³⁰:**

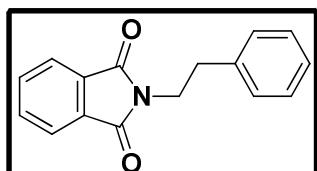


White solid; m.p.: 204–205 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.76 (br s, 2H), 7.68 (br s, 2H), 1.70/1.64 (s, 9H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 169.5, 133.6, 132.1, 122.5, 57.8, 29.1.

34. **2-(Phenethyl)isoindole-1,3-dione (3aj)³¹:**



Colorless solid; m.p.: 130 °C.

¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 7.84–7.81 (m, 2H), 7.71–7.68 (m, 2H), 7.26 (br s, 5H), 3.92 (t, J = 7.8 Hz, 2H), 2.99 (t, J = 7.2 Hz, 2H).

¹³C NMR (75 MHz, CDCl₃, TMS) δ/ppm: 168.1, 138.0, 133.9, 132.0, 128.8, 128.5, 126.6, 123.2, 39.2, 34.6.

IR (KBr Disc, $\bar{\nu}/\text{cm}^{-1}$): 3020, 1770, 1710, 1614, 1496, 1429, 1396, 1359, 1083, 989, 869, 755, 633.

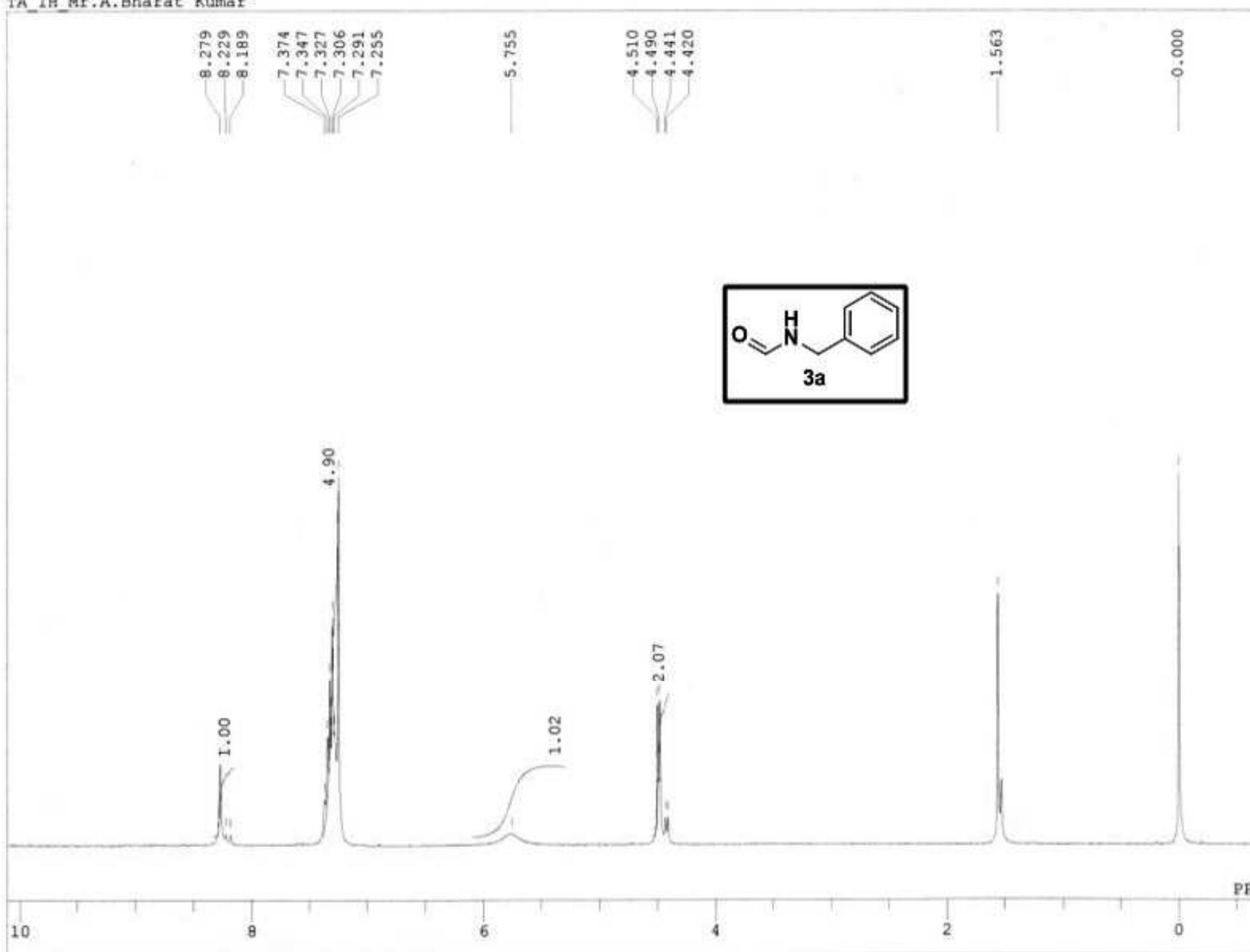
V. References:

1. M. Suchý, A. A. H. Elmehriki and R. H. E. Hudson, *Org. Lett.*, 2011, **13**, 3952.
2. G.-L. Li, K. K.-Y. Kung and M.-K. Wong, *Chem. Commun.*, 2012, **48**, 4112.
3. T. B. Nguyen, J. Sorres, M. Q. Tran, L. Ermolenko and A. Al-Mourabit, *Org. Lett.*, 2012, **14**, 3202.
4. G. B. Villeneuve and T. H. Chan, *Tetrahedron Lett.*, 1997, **38**, 6489.
5. L. Di Nunno and A. Scilimati, *Tetrahedron*, 1986, **42**, 3913.
6. A. Ghorbani-Choghamarani and Z. Akbaripanah, *Chinese Chem. Lett.*, 2012, **23**, 450.
7. H. Tumma, Nagaraju N and K. V. Reddy, *J. Mol. Cat. A: Chem.*, 2009, **310**, 121.
8. M. Hosseini-Sarvari and H. Sharghi, *J. Org. Chem.*, 2006, **71**, 6652.
9. J.-G. Kim and D.-O. Jang, *Synlett*, 2010, **8**, 1231.
10. S. Ko, H. Han and S. Chang, *Org. Lett.*, 2003, **5**, 2687.
11. M. C. Elliott and E. Williams, *Org. Biomol. Chem.*, 2003, **1**, 3038.
12. J. E. Taylor, M. D. Jones, J. M. J. Williams and S. D. Bull, *J. Org. Chem.*, 2012, **77**, 2808.
13. (a) D. R. Stuart, M. Bertrand-Laperle, K. M. N. Burgess and K. Fagnou, *J. Am. Chem. Soc.*, 2008, **130**, 16474; (b) M. Li, L. Hu, X. Cao, H. Hong, J. Lu and H. Gu, *Chem. -Eur. J.*, 2001, **17**, 2763.
14. B. T. Gowda, K. M. Usha and K. L. Z. Jayalakshmi, *Naturforsch., A: Phys. Sci.*, 2003, **58**, 801.
15. S. R. Narahari, B. R. Reguri and K. Mukkanti, *Tetrahedron Lett.*, 2011, **52**, 4888.

16. A. R. Katritzky, C. Cai and S. K. Singh, *J. Org. Chem.*, 2006, **71**, 3375.
17. (a) C. J. Bennett, S. T. Caldwell, D. B. McPhail, P. C. Morrice, G. G. Duthie and R. C. Hartley, *Bioorg. Med. Chem.*, 2004, **12**, 2079; (b) B. P. Fors, P. Krattiger, E. Strieter and S. L. Buchwald, *Org. Lett.*, 2008, **10**, 3505.
18. B. S. Kim, C. Jang, D. J. Lee and S. W. Youn, *Chem. -Asian. J.*, 2010, **5**, 2336.
19. (a) S. Xun, G. LeClair, J. D. Zhang, X. Chen, J. P. Gao and Z. Y. Wang, *Org. Lett.*, 2006, **8**, 1697; (b) K. Hisler, A. G. J. Commeureuc, S.-Z. Zhou and J. A. Murphy, *Tetrahedron Lett.*, 2009, **50**, 3290.
20. L. U. Nordstrom, H. Vogt and R. Madsen, *J. Am. Chem. Soc.*, 2008, **130**, 17672.
21. J. Pan, N. O. Devarie-Baez and M. Xian, *Org. Lett.*, 2011, **13**, 1092.
22. S. Das, B. Join, K. Junge and M. Beller, *Chem. Commun.*, 2012, **48**, 2683.
23. N. D. Kokare, R. R. Nagawade, V. P. Rane and D. B. Shinde, *Synthesis*, 2007, 766.
24. T. Ohshima, T. Iwasaki, Y. Maegawa, A. Yoshiyama and K. Mashima, *J. Am. Chem. Soc.*, 2008, **130**, 2944.
25. T. H. Graham, W. Liu and D.-M. Shen, *Org. Lett.*, 2011, **13**, 6232.
26. H. Cao and H. Alper, *Org. Lett.*, 2010, **12**, 4126.
27. D. N. Sawant, Y. S. Wagh, K. D. Bhatte and B. M. Bhanage, *Eur. J. Org. Chem.*, 2011, 6719.
28. M.-L. Wang and W.-H. Chen, *React. Kinet. Catal. Lett.*, 2006, **89**, 377.
29. S. Bénard, L. Neuville and J. Zhu, *J. Org. Chem.*, 2008, **73**, 6441.
30. D. Marosvölgyi-Haskó, A. Petz, A. Takács and L. Kollér, *Tetrahedron*, 2011, **67**, 9122.
31. Y.-P. Li, F.-X. Ning, M.-B. Yang, Y.-C. Li, M.-H. Nie, T.-M. Ou, J.-H. Tan, S.-L. Huang, D. Li, L.-Q. Gu and Z.-S. Huang, *Eur. J. Med. Chem.*, 2011, **46**, 1572.

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

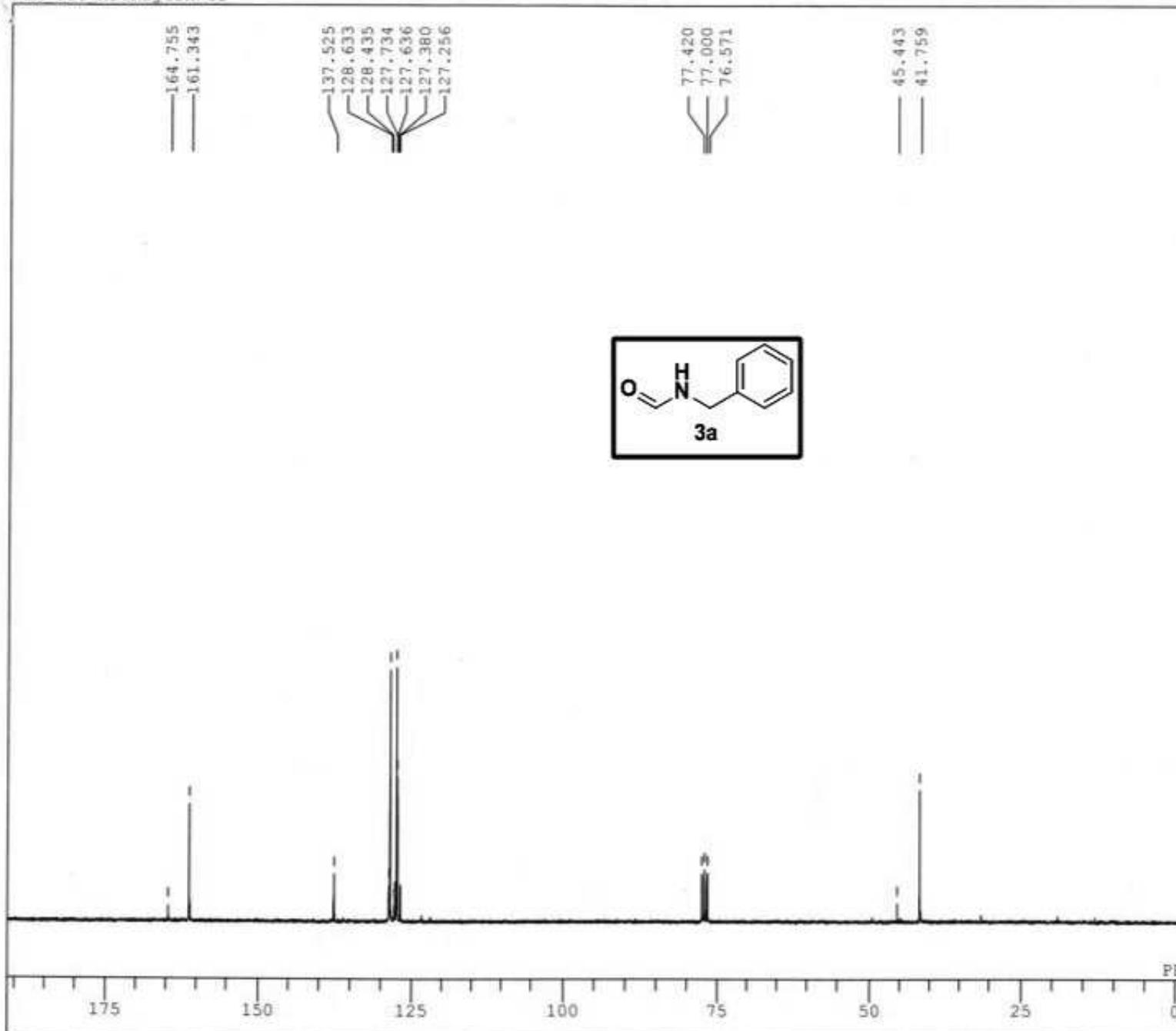
C:\K.N. Singh,, I.T\TA_1H.als
TA_1H Mr.A.Bharat Kumar



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

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COMNT TA_1H Mr.A.Bharat
DATIM Tue Jun 12 13:00:
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OBFIN 1150.0 Hz
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BF 1.20 Hz
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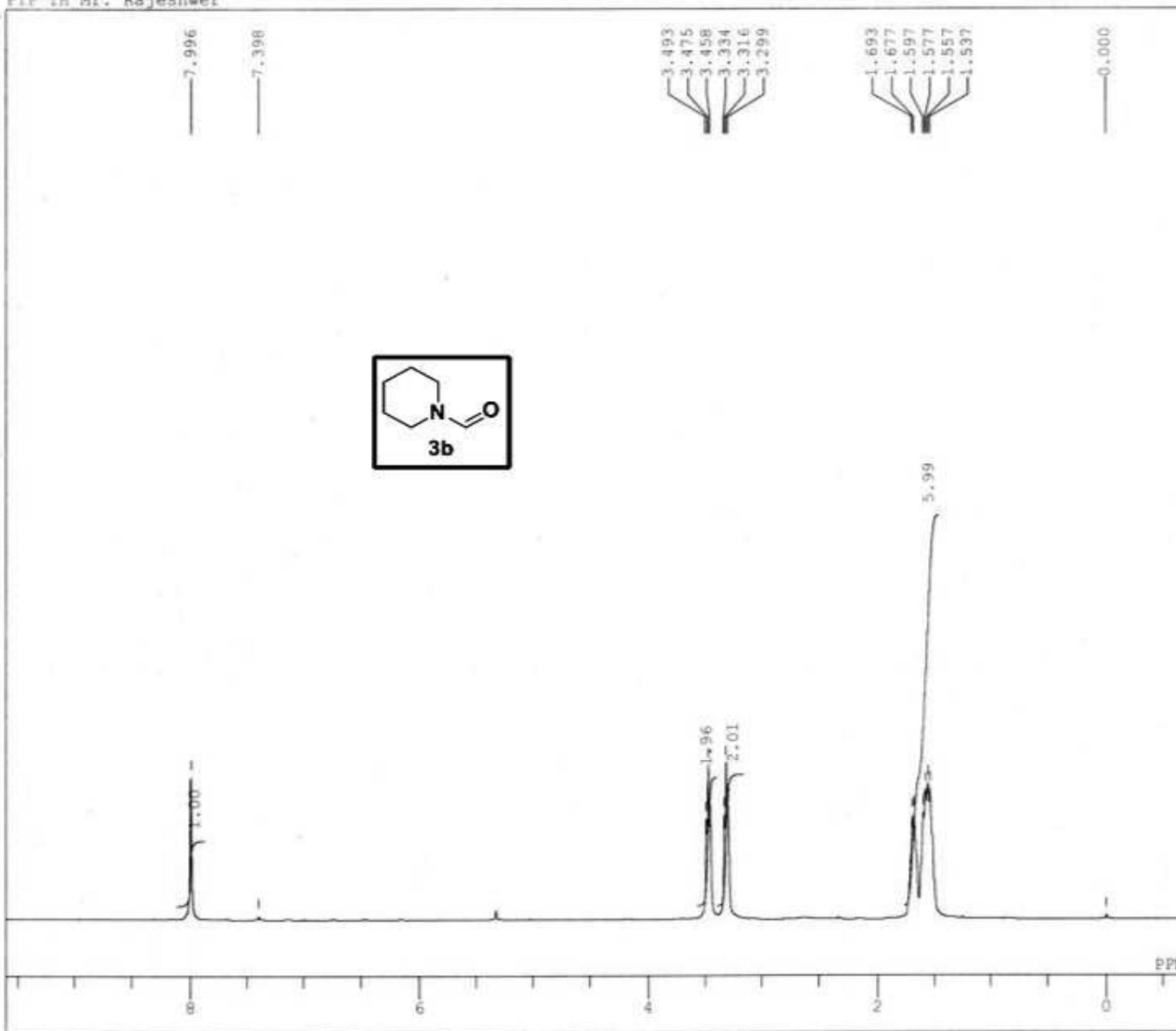


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\NBA_13C.e
COMNT NBA_13C Mr.Rajeshwer
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OBSET 127.30 KHz
OBFIN 44.7 Hz
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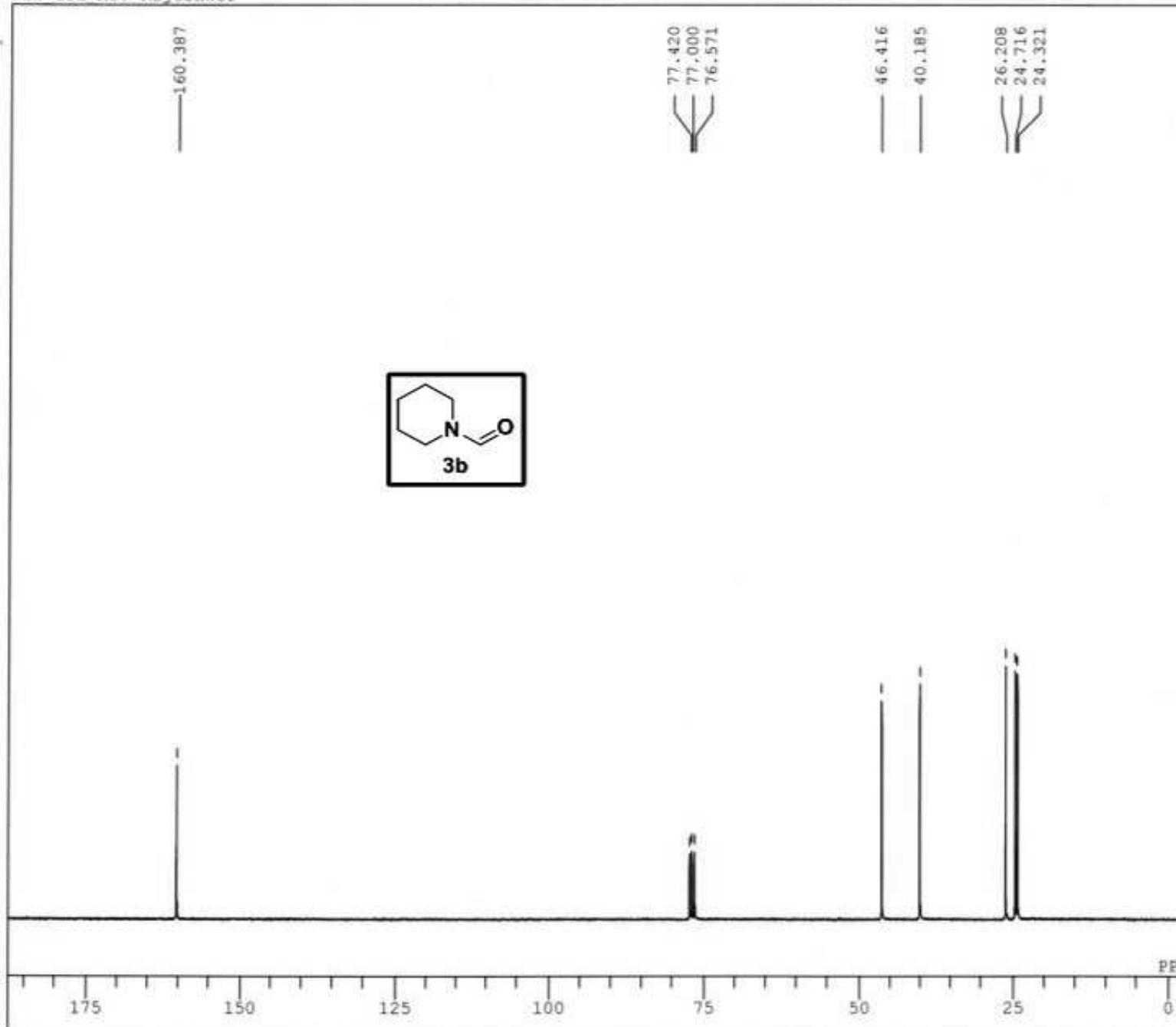
PIP_1H Mr. Rajeshwer



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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\PIP_1H.al
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DATIM Tue Jul 03 12:19:52 2012
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EXMOD NON
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OBSET 130.00 KHz
OBFIN 1150.0 Hz
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RGAIN 8

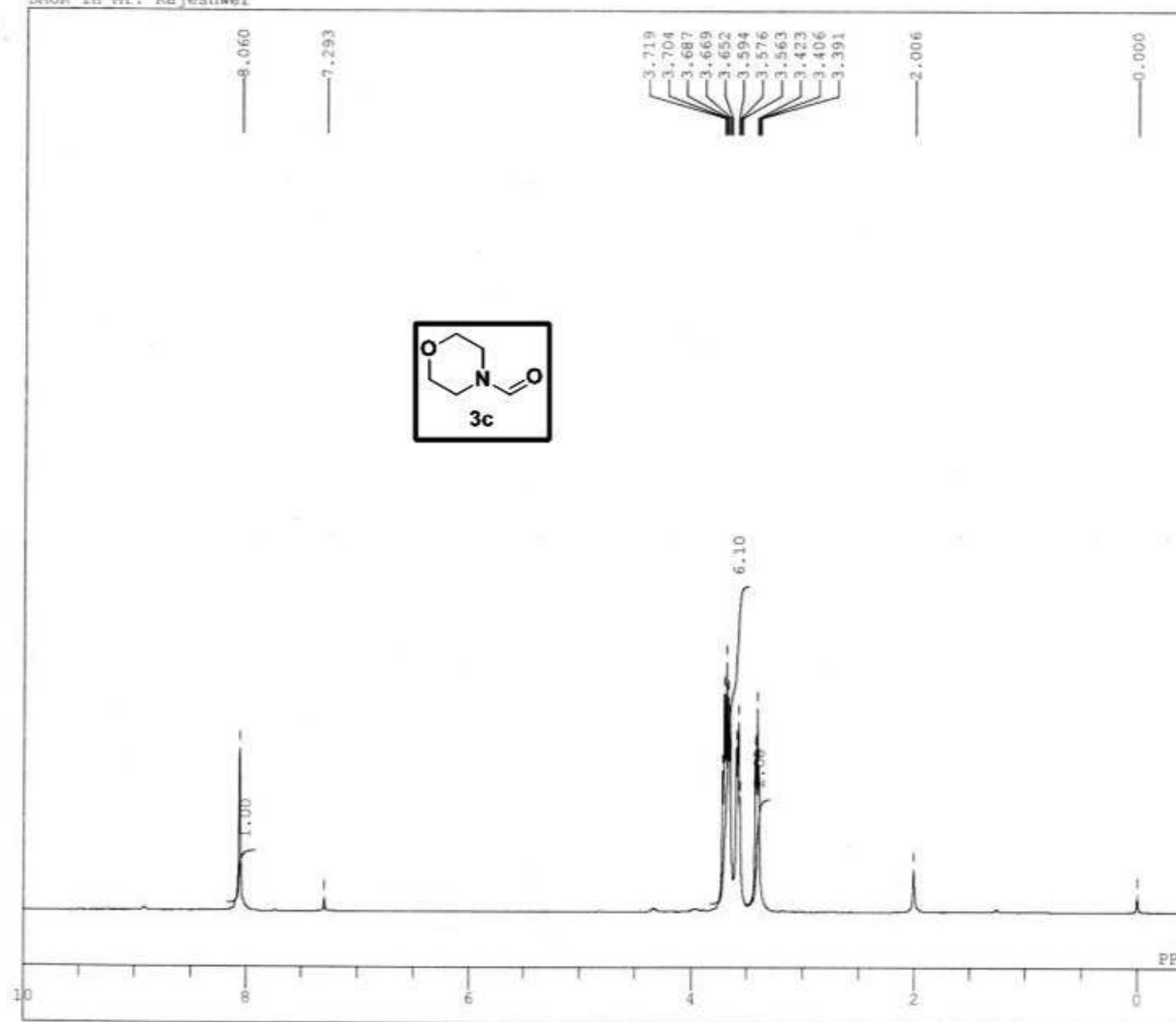


J₂₄

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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
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DATIM Wed Jul 04 16:13:39 2012
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EXMOD BCM
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OBSET 127.30 KHz
OBFIN 44.7 Hz
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BF 1.20 Hz
RGAIN 24

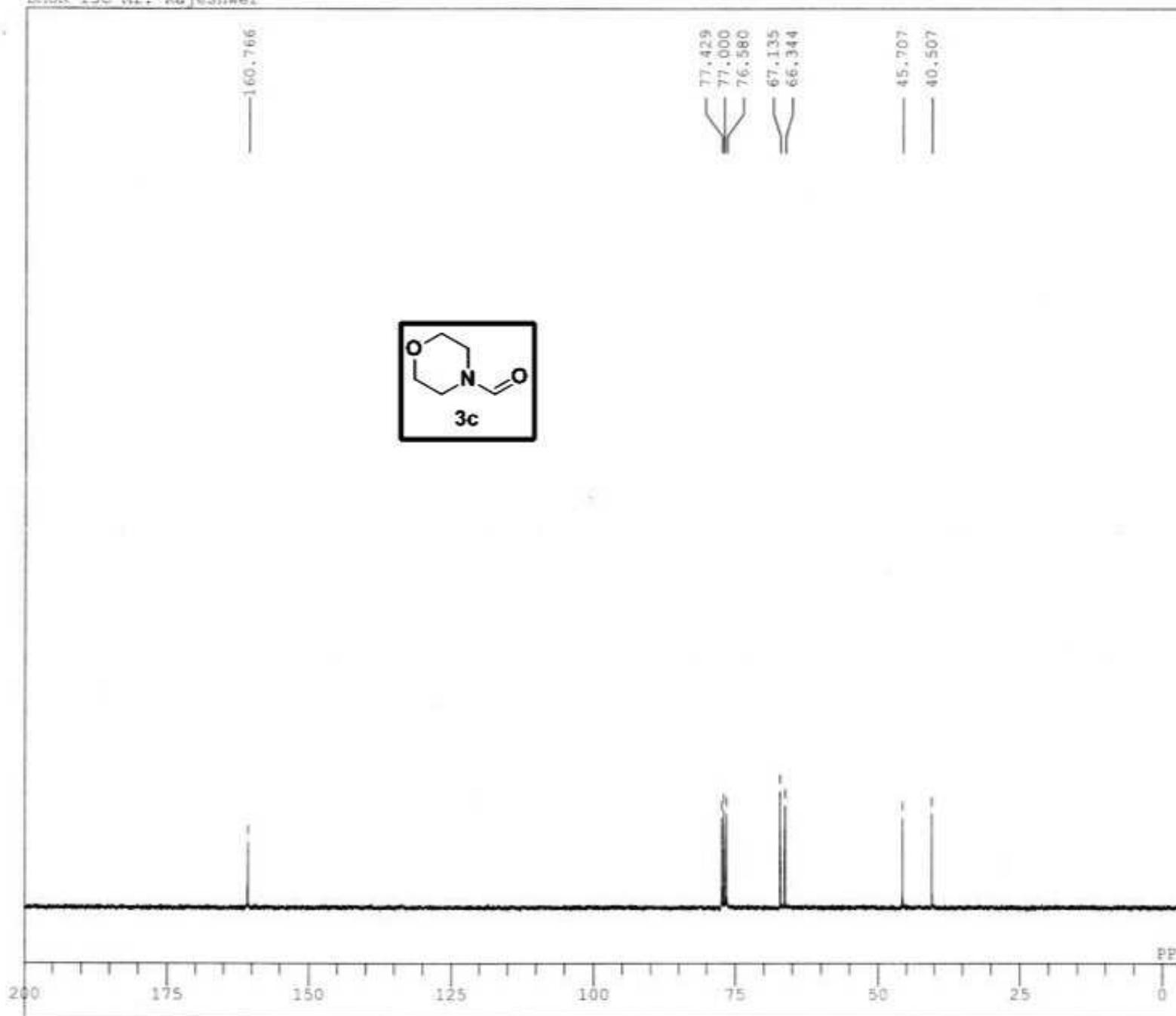


J₂₅

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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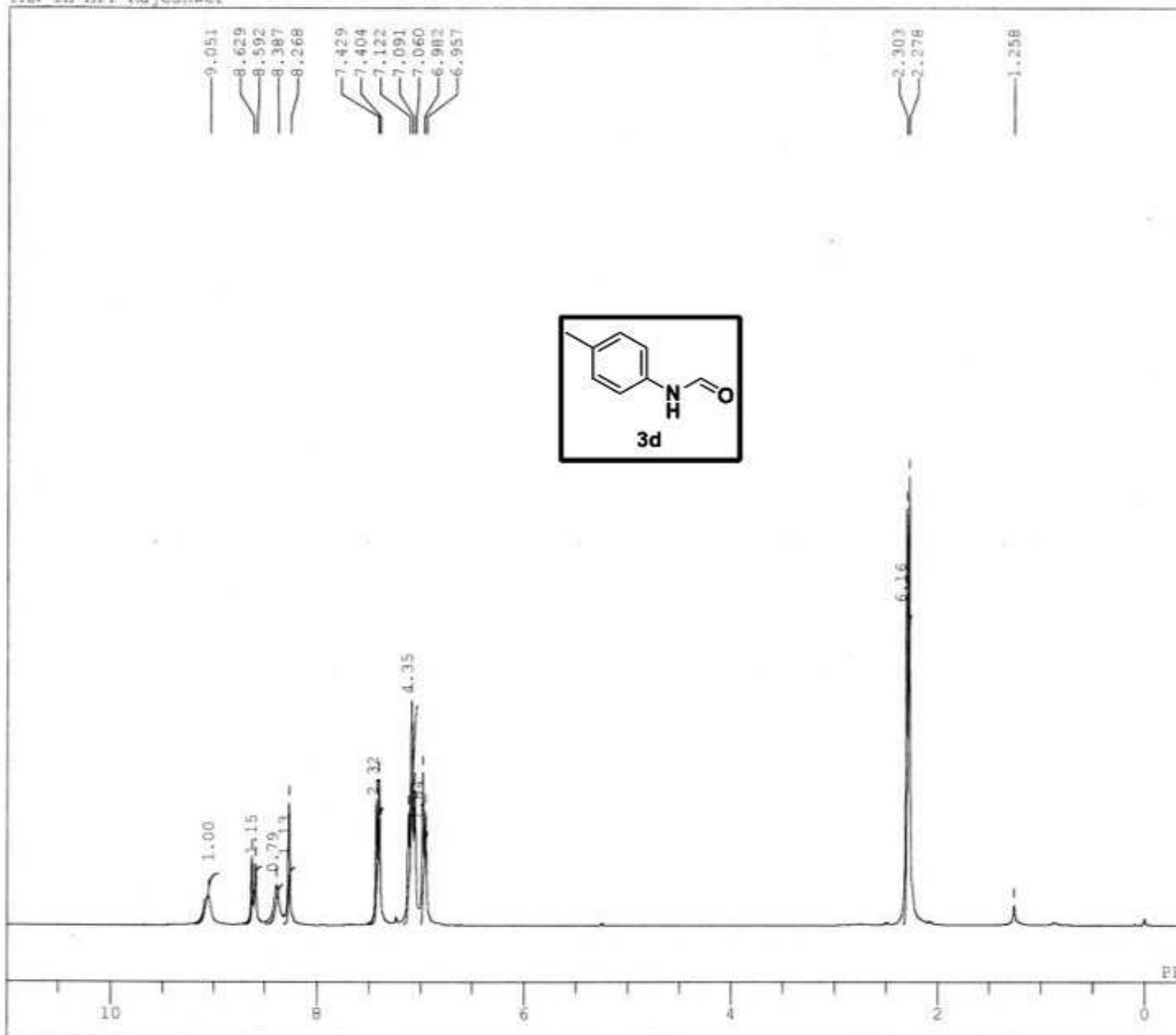


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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OBFIN 44.7 Hz
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RGAIN 25

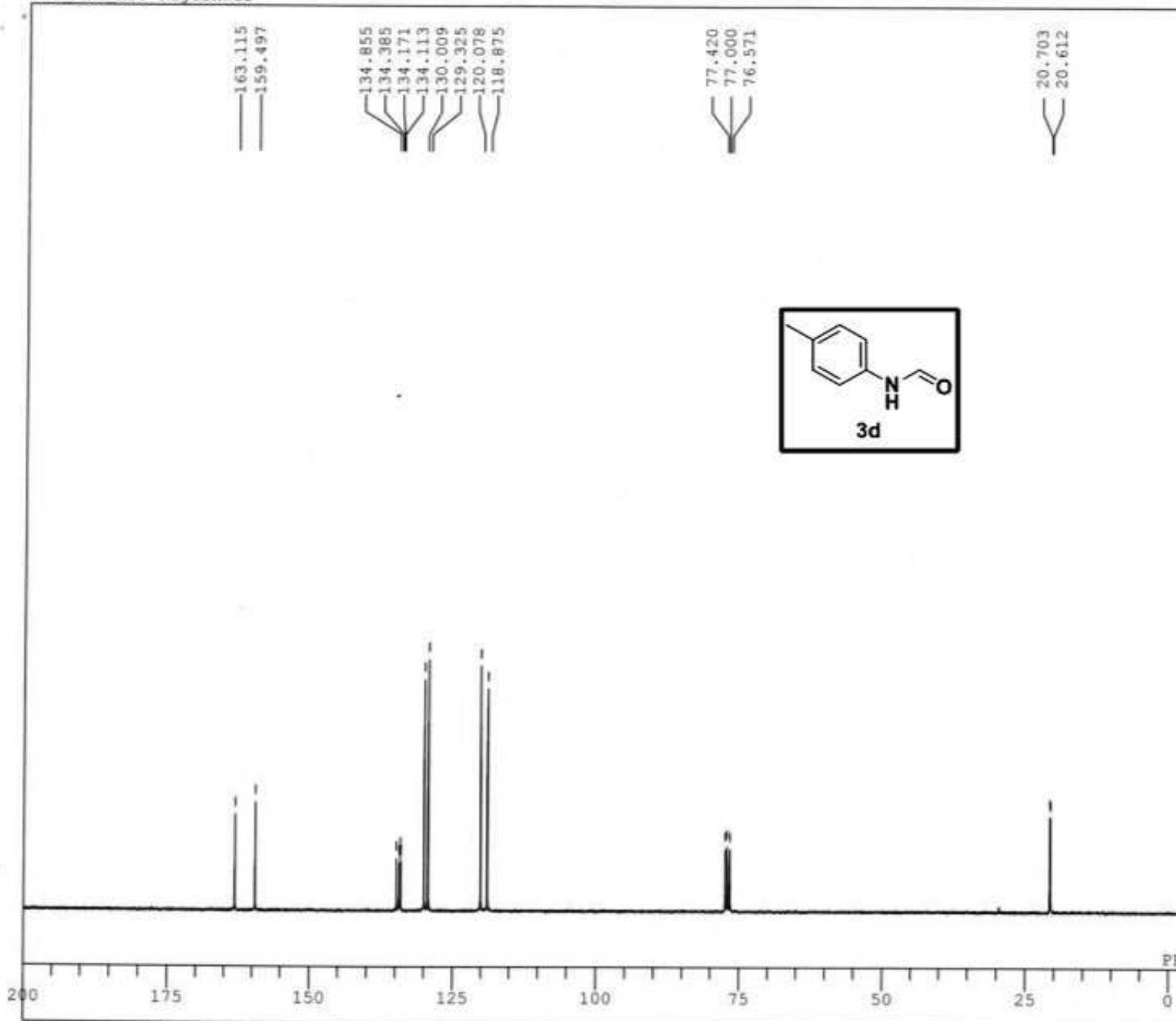
PAN_1H Mr. Rajeshwer



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

Operator : Nagendra Kumar
Shishir Singh

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DATIM Tue Jul 03 12:06:32 2012
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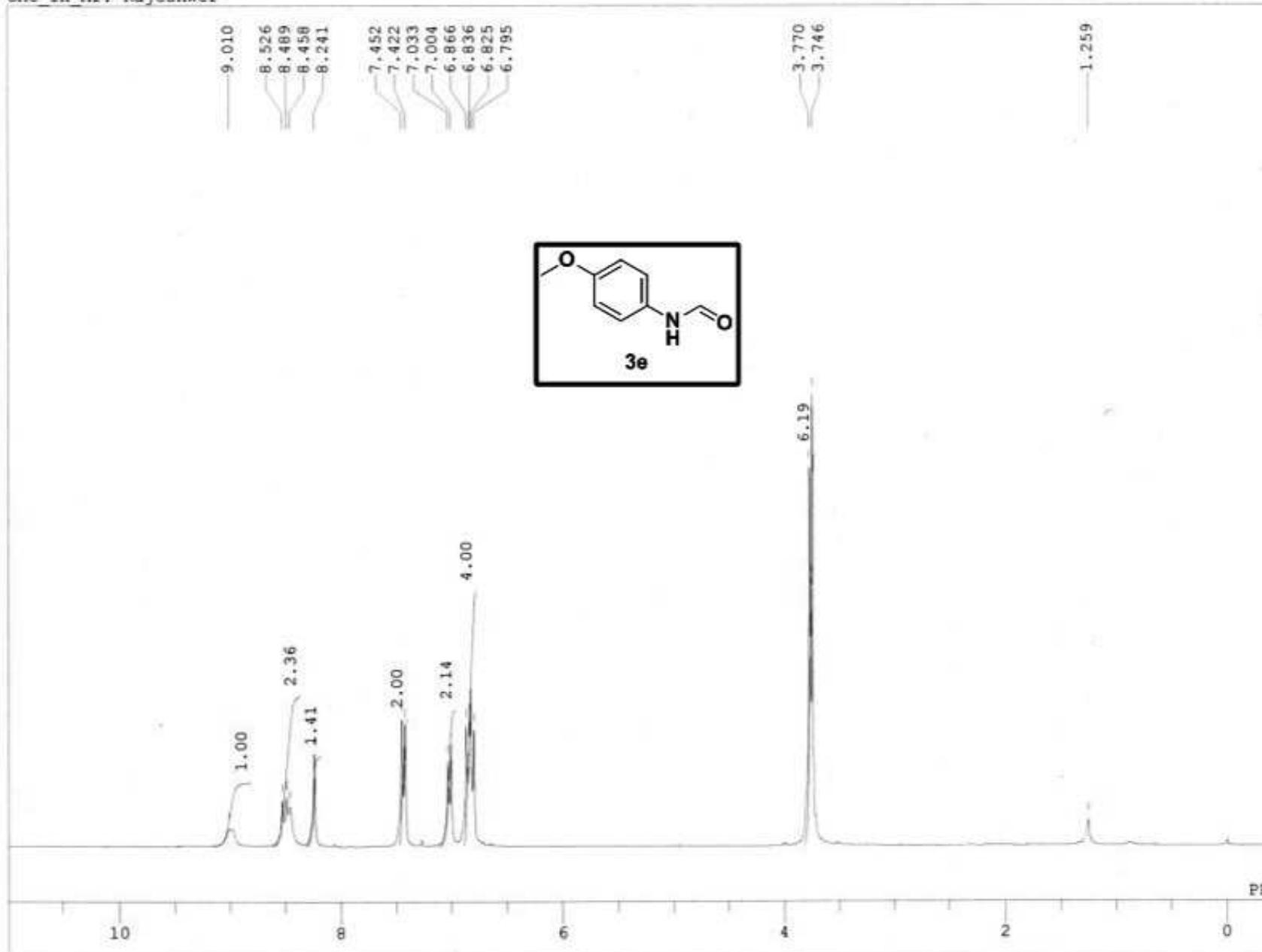


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT PAN 13C Mr. Rajeshwer
DATIM Tue Jul 03 11:59:58 2012
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OBSET 127.30 KHz
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PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,,I.T\OMe_1H.als
OMe_1H Mr. Rajeshwar

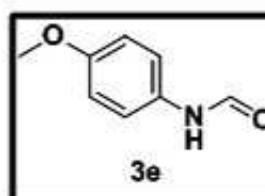
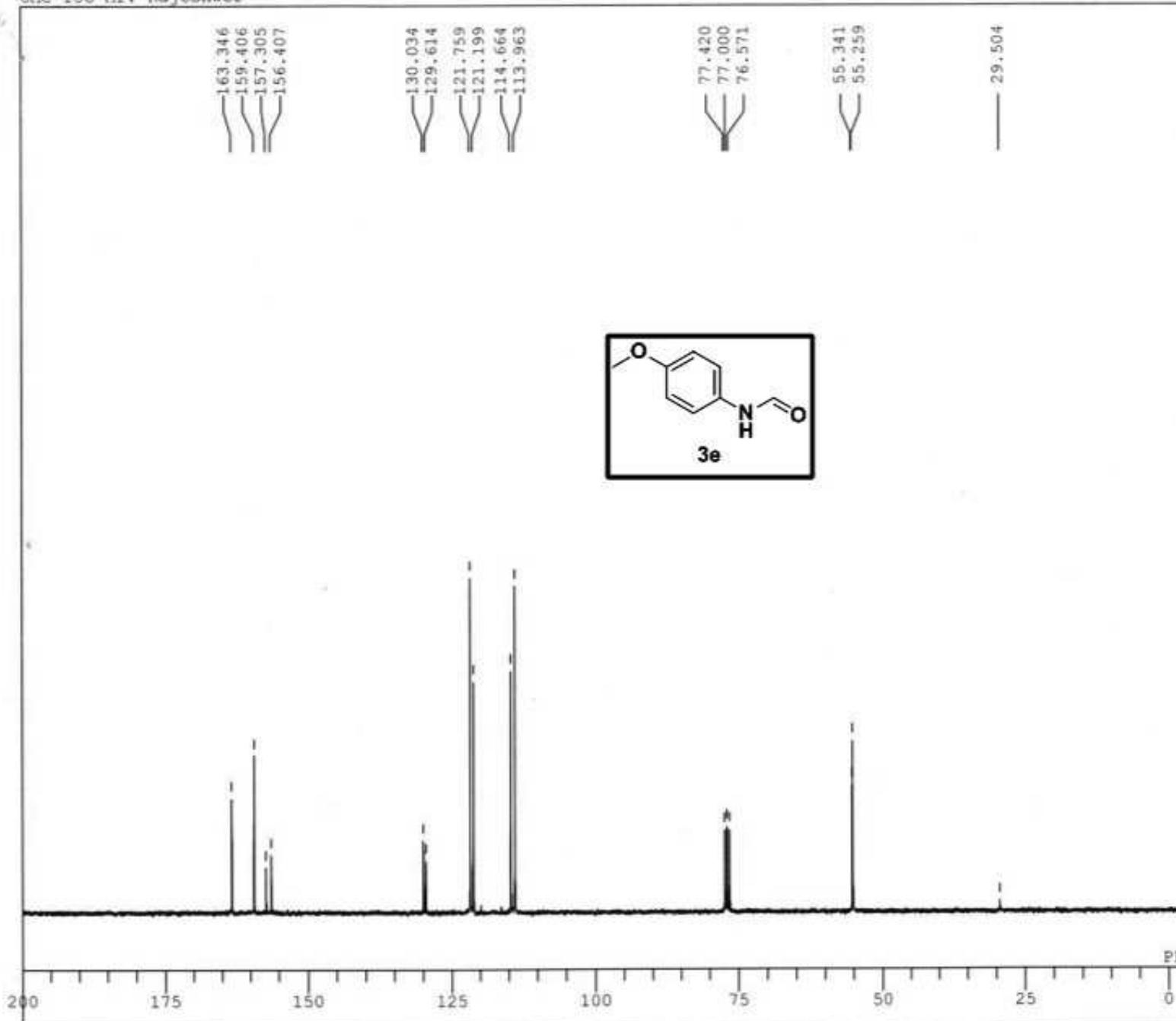


J₂₉

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT OMe_1H Mr. Rajesh
DATIM Mon Jul 16 12:15:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 kHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 25
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 10

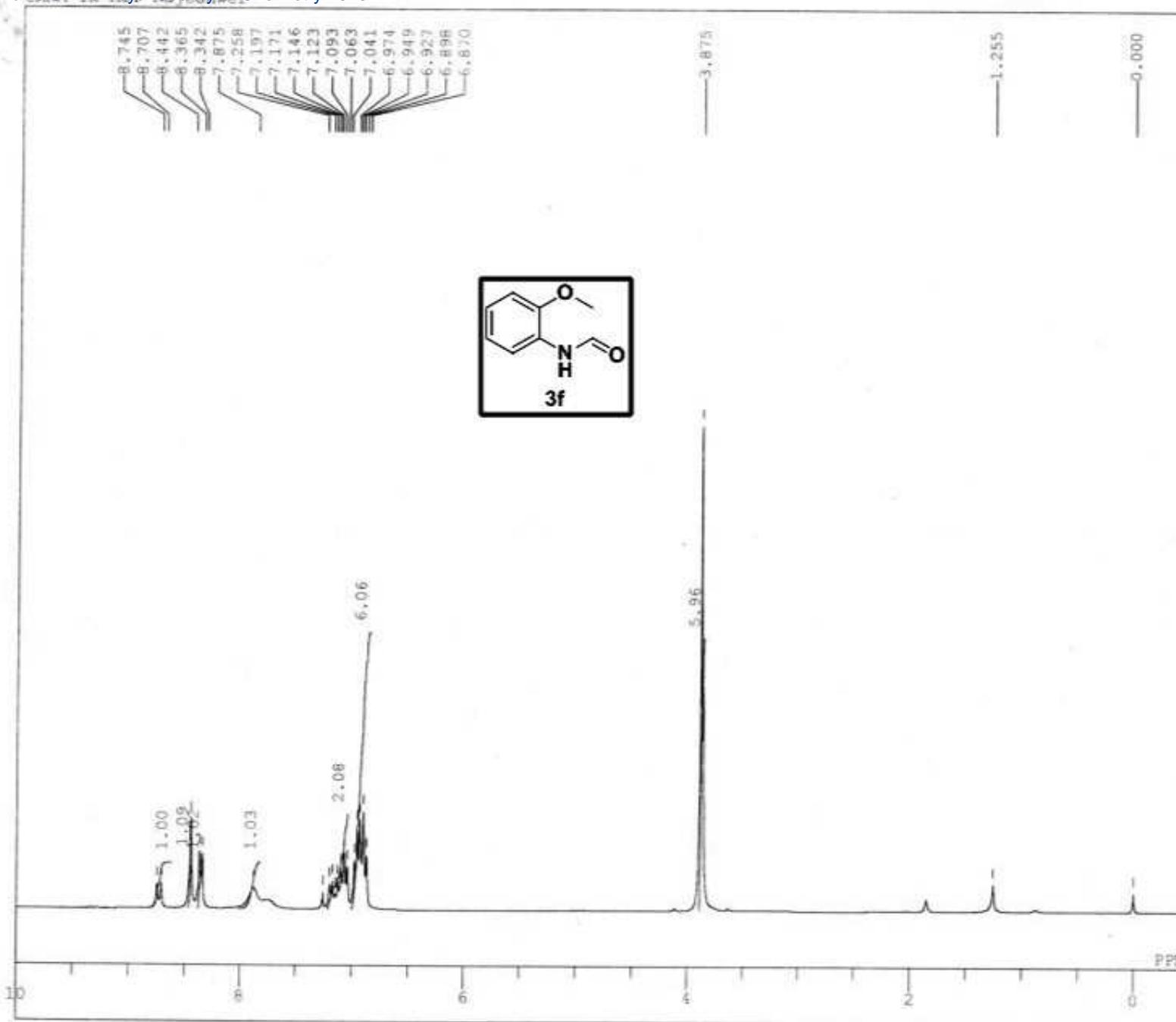


J₃₀

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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT OMe_13C_Mr. Rajeshwer
DATIM Mon Jul 16 15:52:34 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 229
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 24.7 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

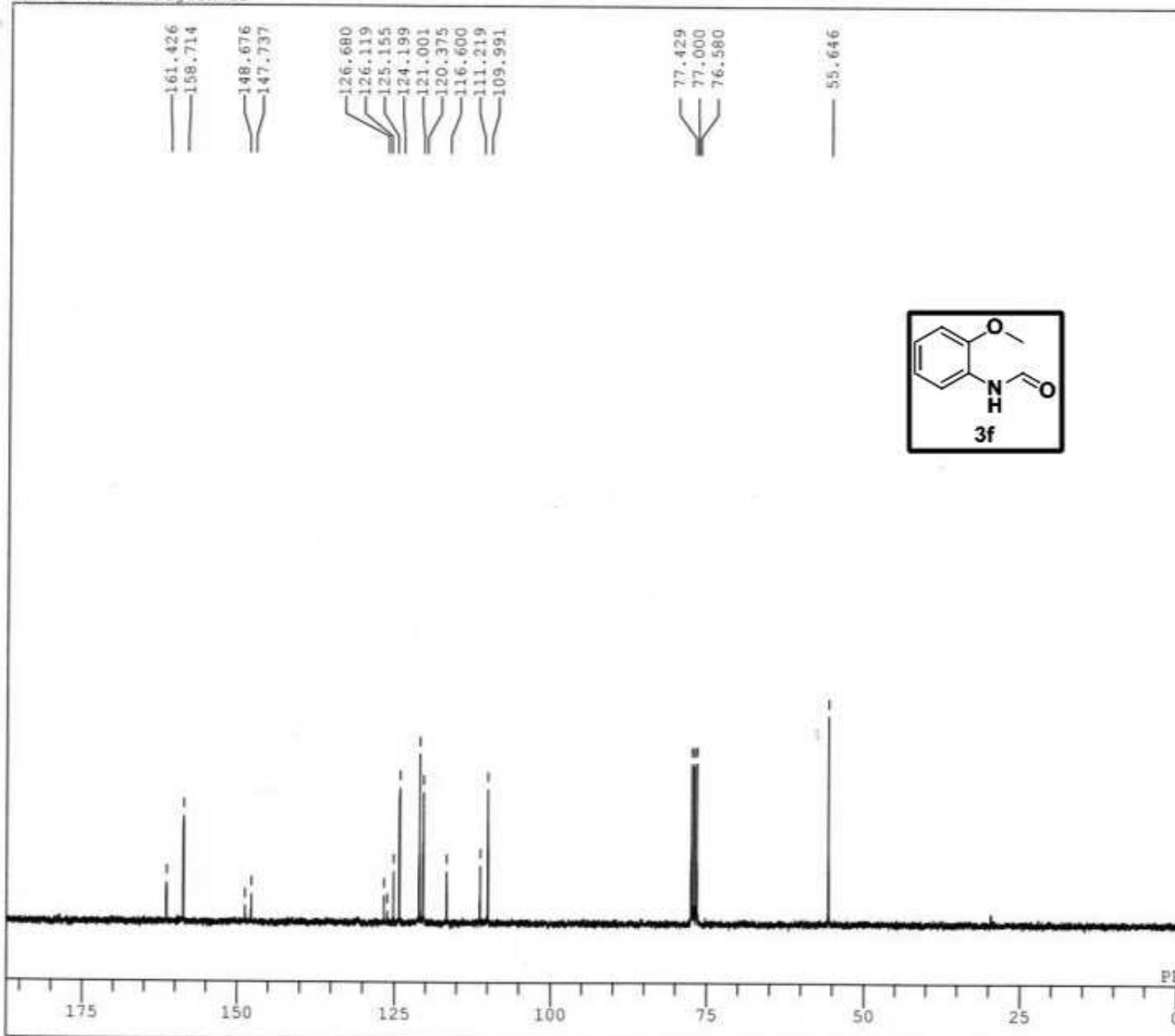


J₃₁

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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\OANA_1H.e
COMNT OANA 1H Mr. Rajeshwer
DATIM Thu Jul 19 17:19:16 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 54
ACQTM 3.447 sec
PD 1.547 sec
PWI 5.2 us
IRNUC 1H
CTEMP 21.5 c
SLVNT CDCl₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 13

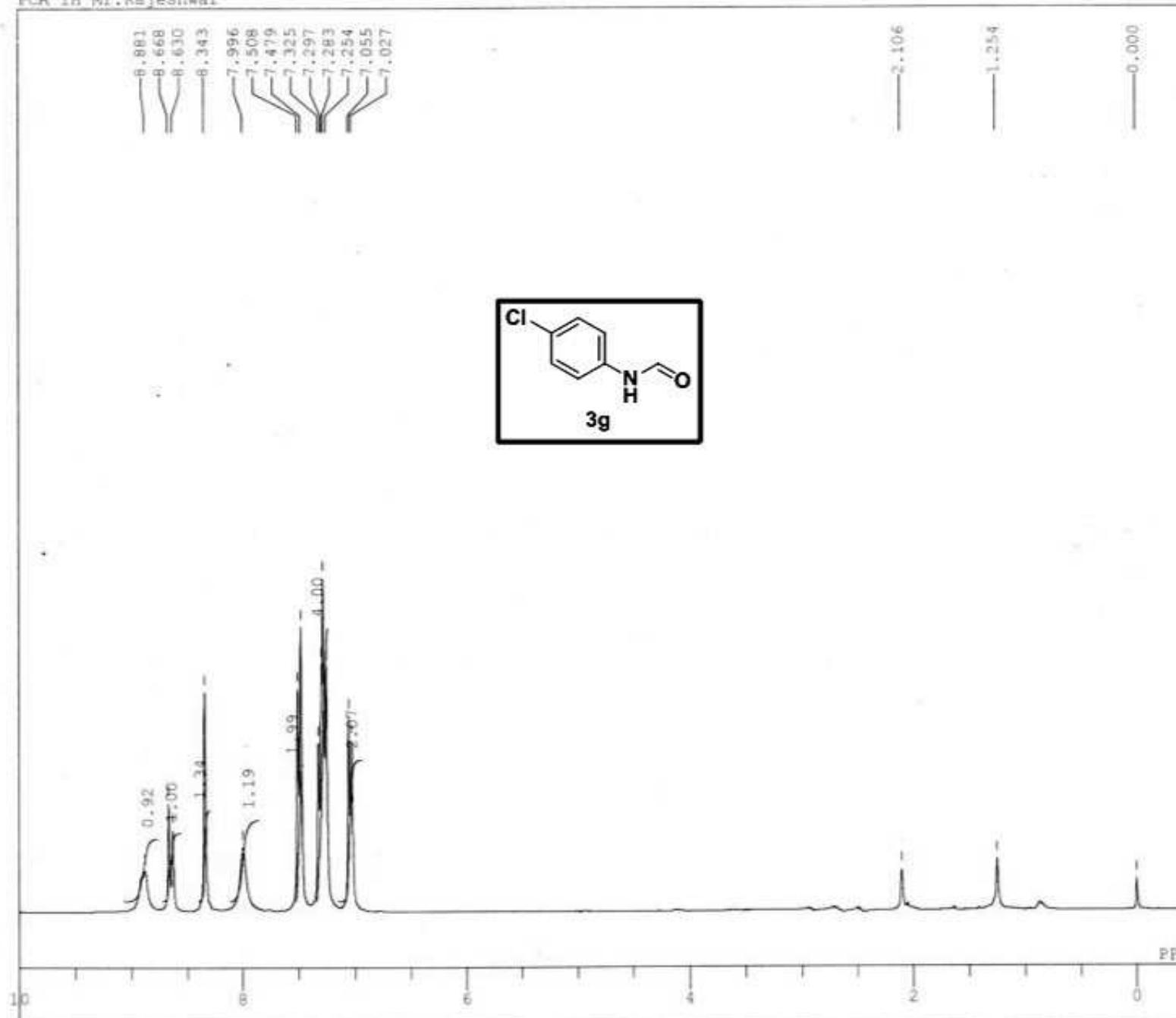


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT OANA_13C Mr. Rajeshwer
DATIM Thu Jul 19 17:37:30 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 283
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 24.1 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

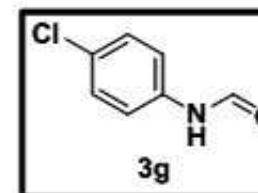
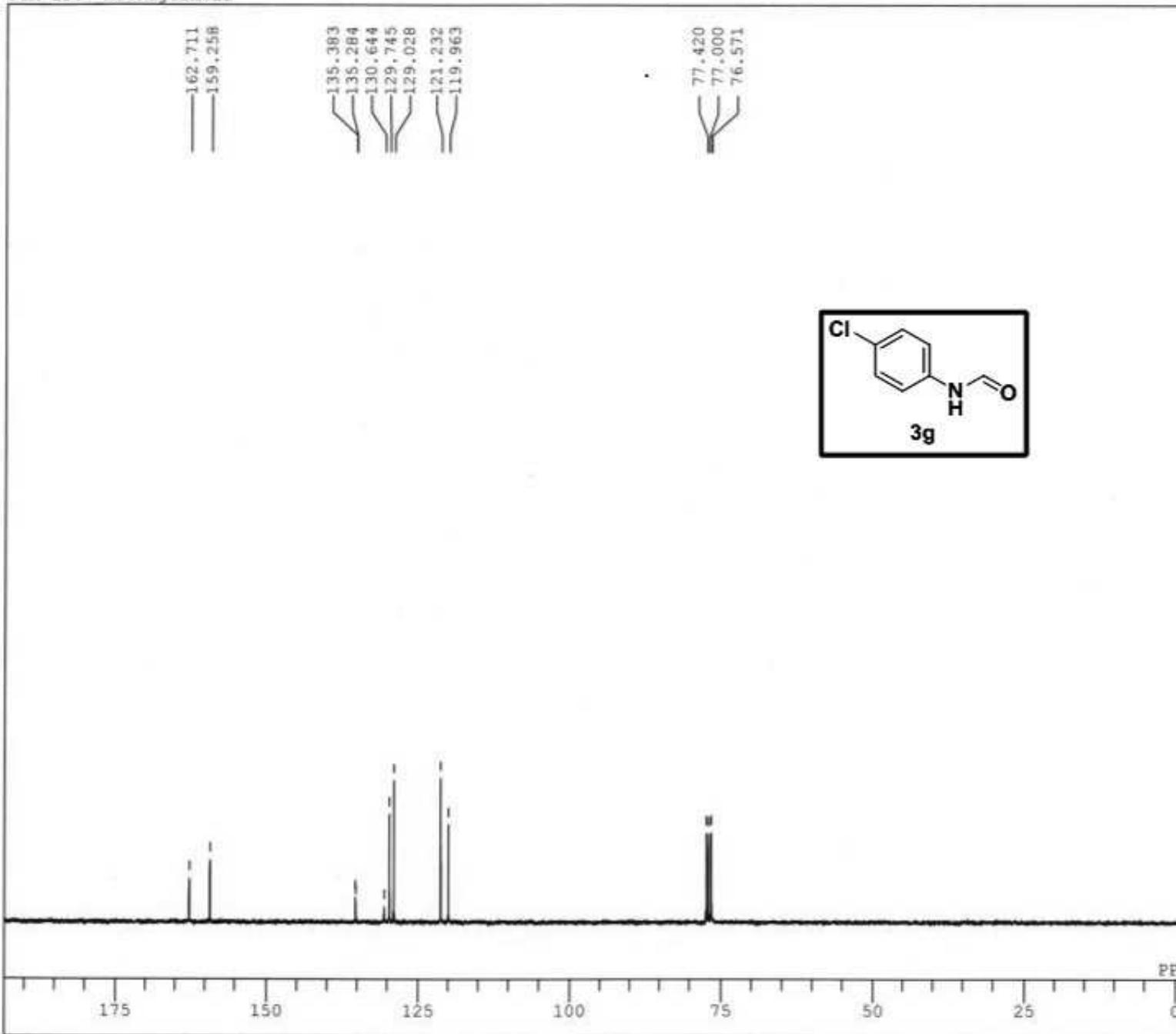
PCA_1H Mr.Rajeshwar



JEOL AL300G FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\PCA_1H.al
COMNT PCA_1H Mr.Rajeshwar
DATIM Tue Jul 10 13:13:47 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 36
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 19.1 c
SLVNT CDCL₃
EXREF 0.00 ppm
BF 1.120 Hz
RGAIN 14

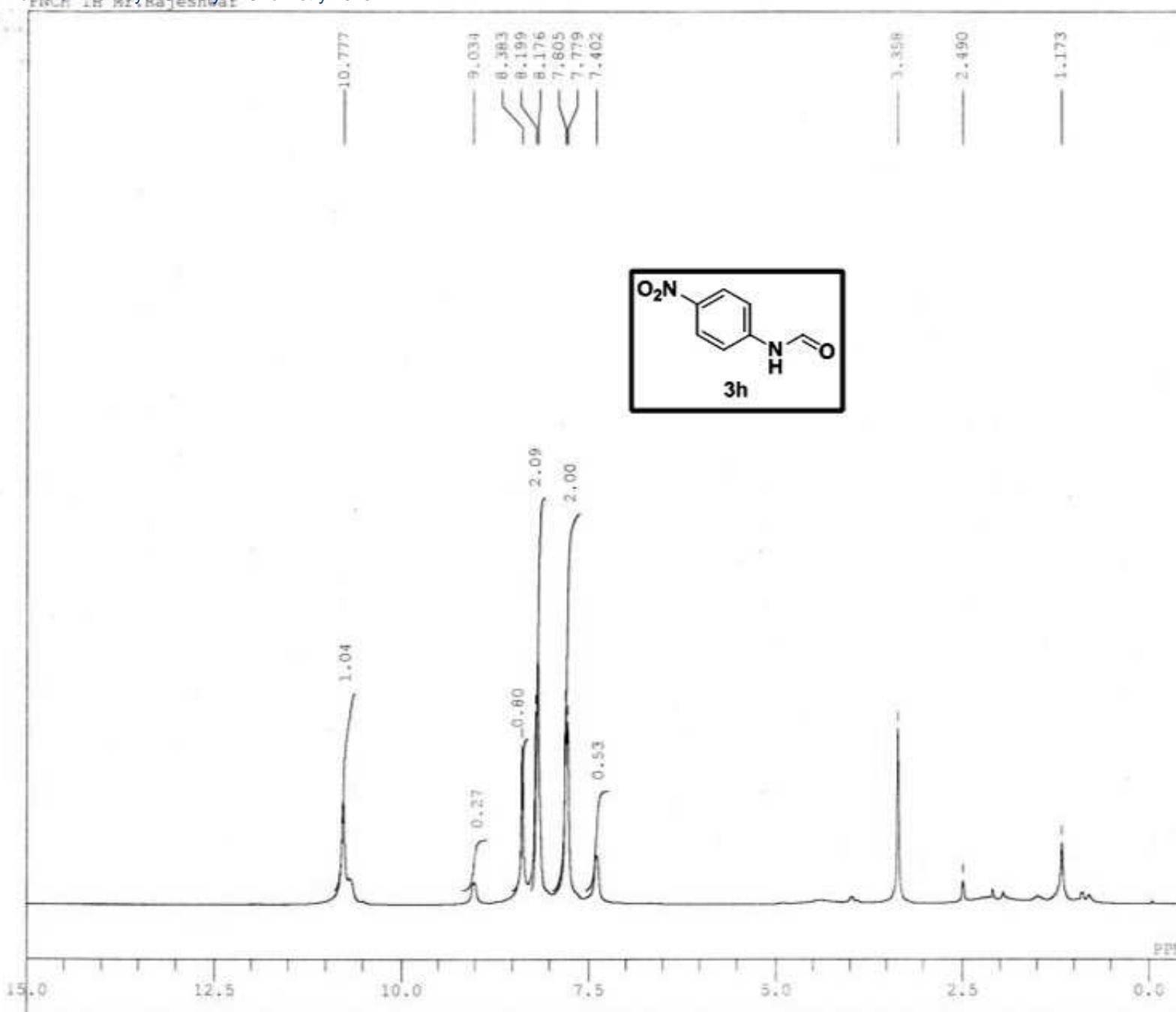


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JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

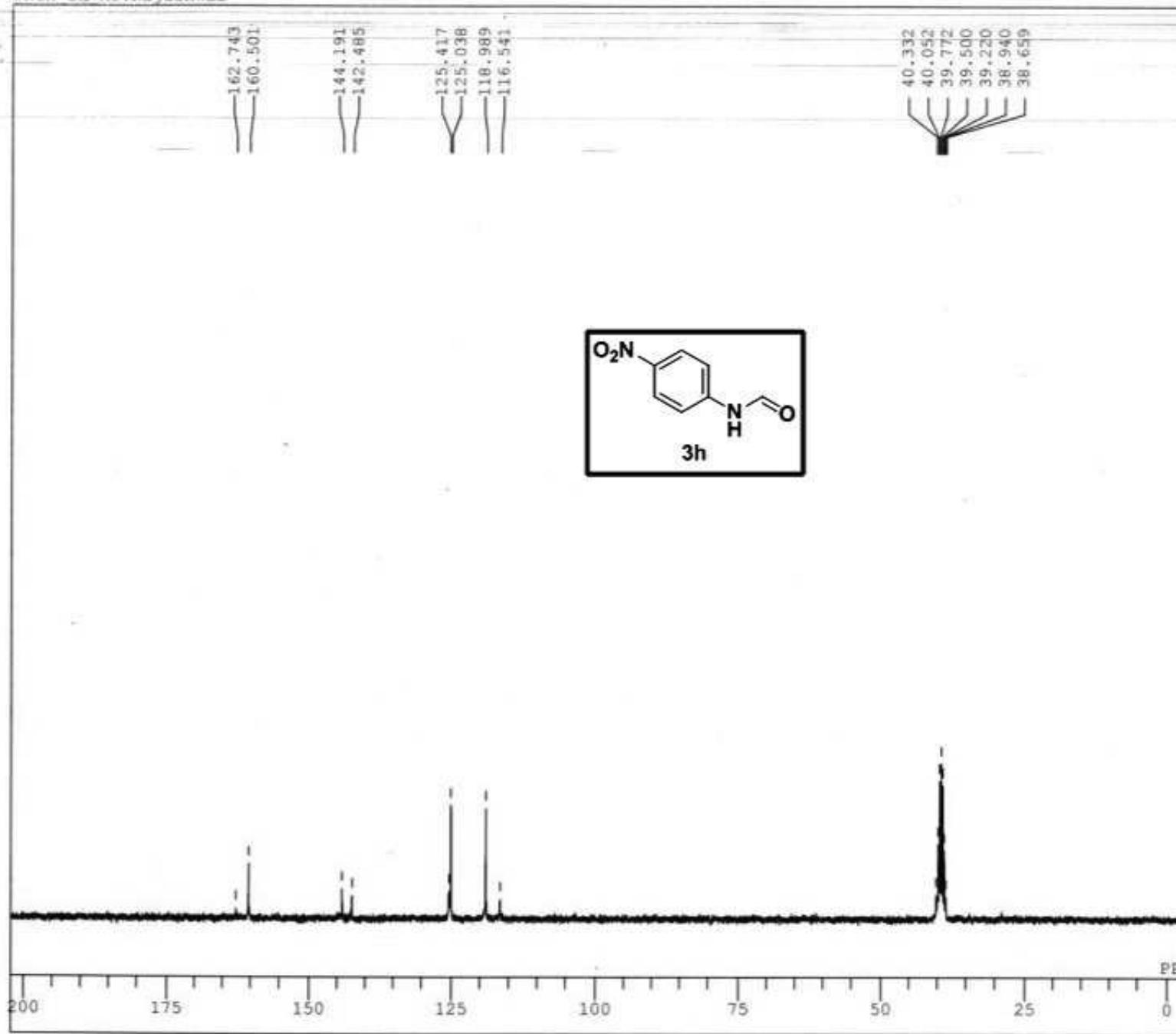
DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT PCA 13C Mr.Rajeshwar
DATIM Tue Jul 10 13:34:38 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 160
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23



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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\PNCH_1H.e
COMNT PNCH 1H Mr.Rajeshwar
DATIM Wed Aug 22 12:06:45 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 32
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 21.1 c
SLVNT DMSO
EXREF 2.49 ppm
BF 1.20 Hz
RGAIN 13

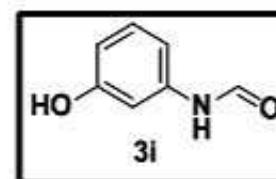
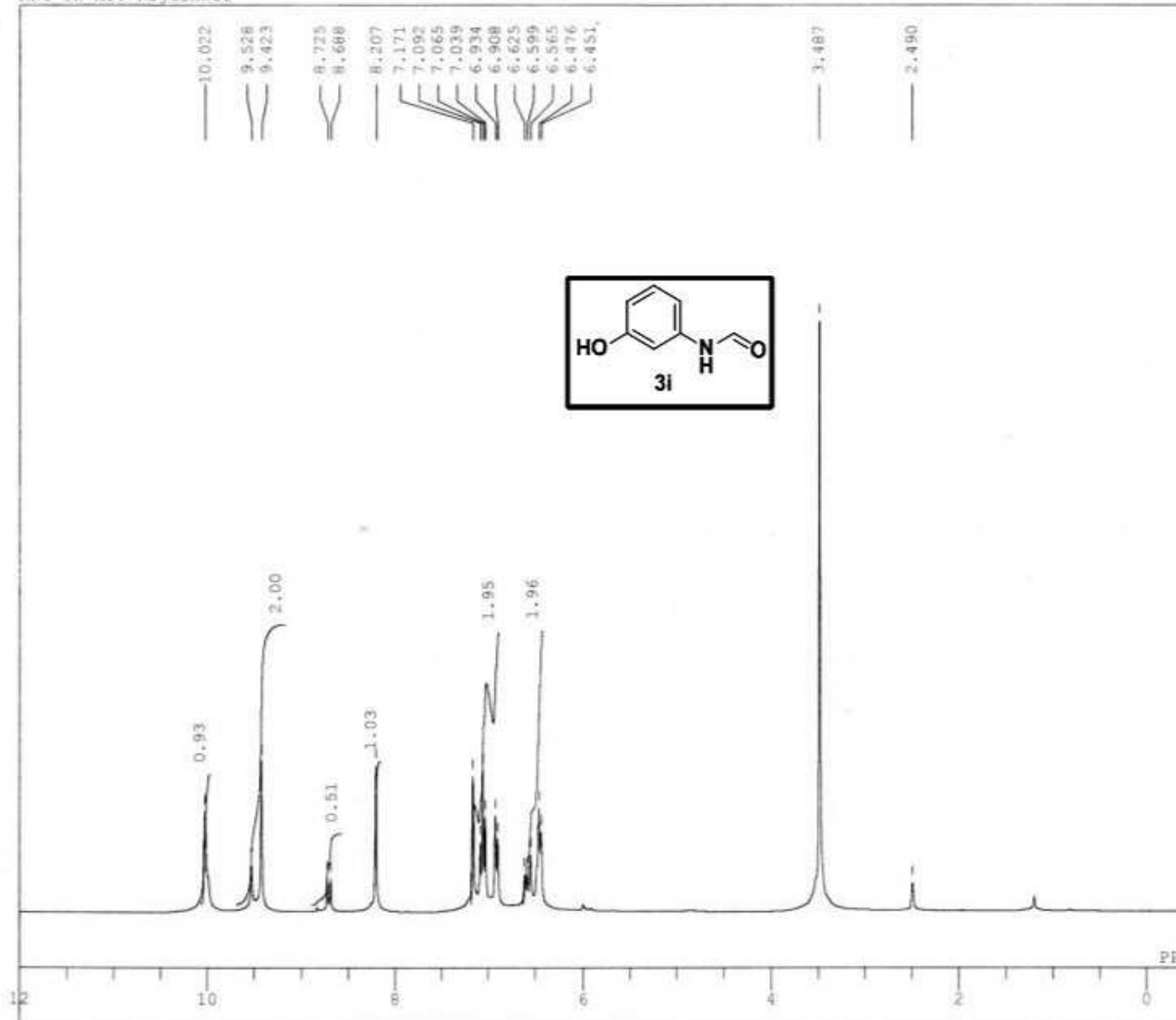


PNCH 1H Mr.Rajeshwar
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON\ DEFAULT.
COMNT PNCH 1H Mr.Rajeshwar
DATIM Wed Aug 22 12:14:59 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 100
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 24.8 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 24

ANS © The Royal Society of
Medicine, Bayswater



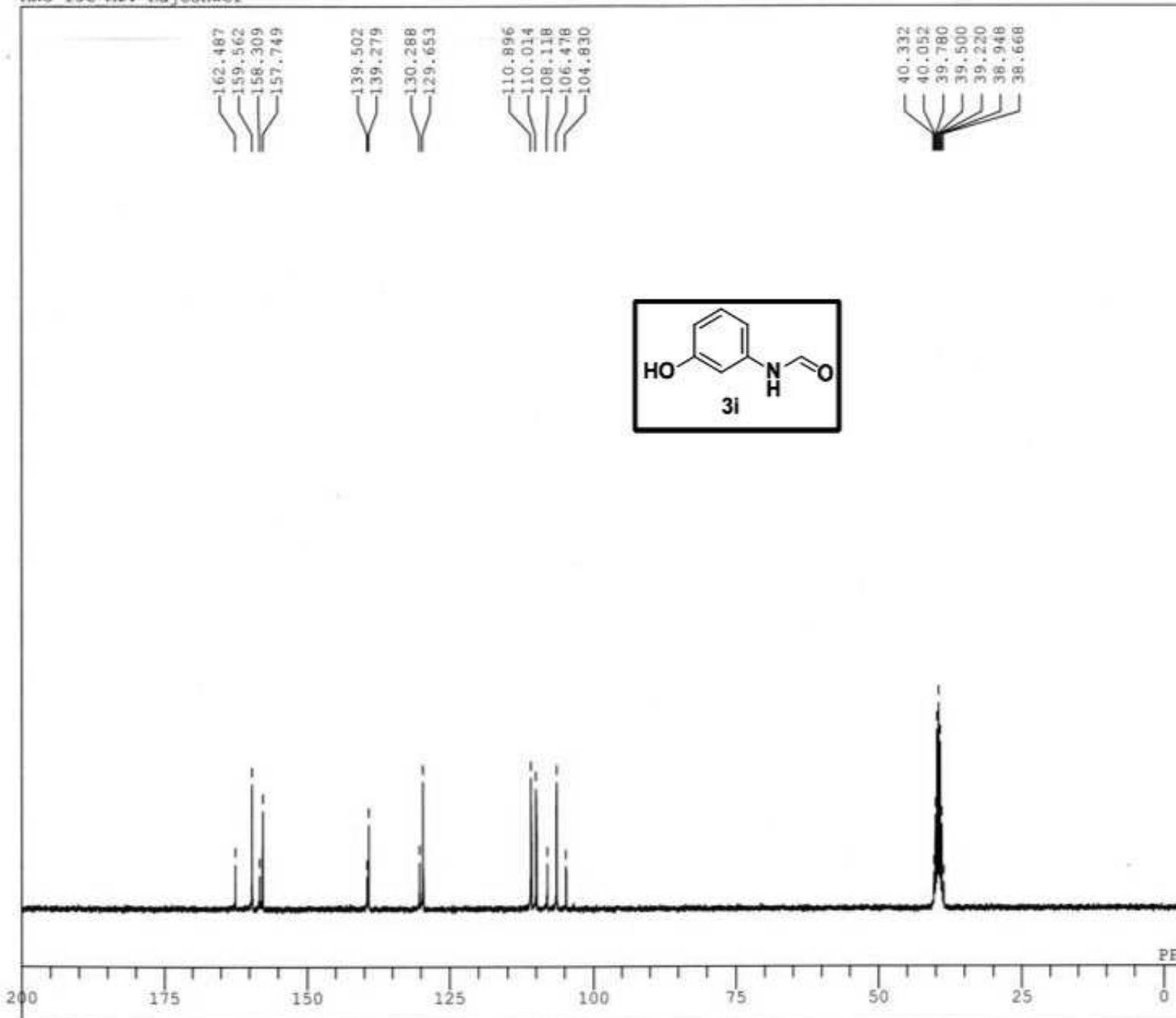
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

```

DFILE C:\K.N. Singh,,I.T\MNO_1H.al
COMNT MNO_1H Mr. Rajeshwer
DATIM Sat Jul 28 11:16:01 2012
OBNUC 1H
EXMOD NON
OBFRQ      300.40 MHz
OBSET      130.00 KHz
OBFIN      1150.0 Hz
POINT      32768
FREQU      9505.7 Hz
SCANS       64
ACQTM      3.447 sec
PD         1.547 sec
PW1        5.2 us
IRNUC     1H
CTEMP      21.7 c
SLVNT     DMSO
EXREF      2.49 ppm
BF         1.20 Hz
RGAIN      11

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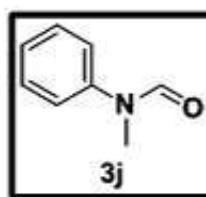
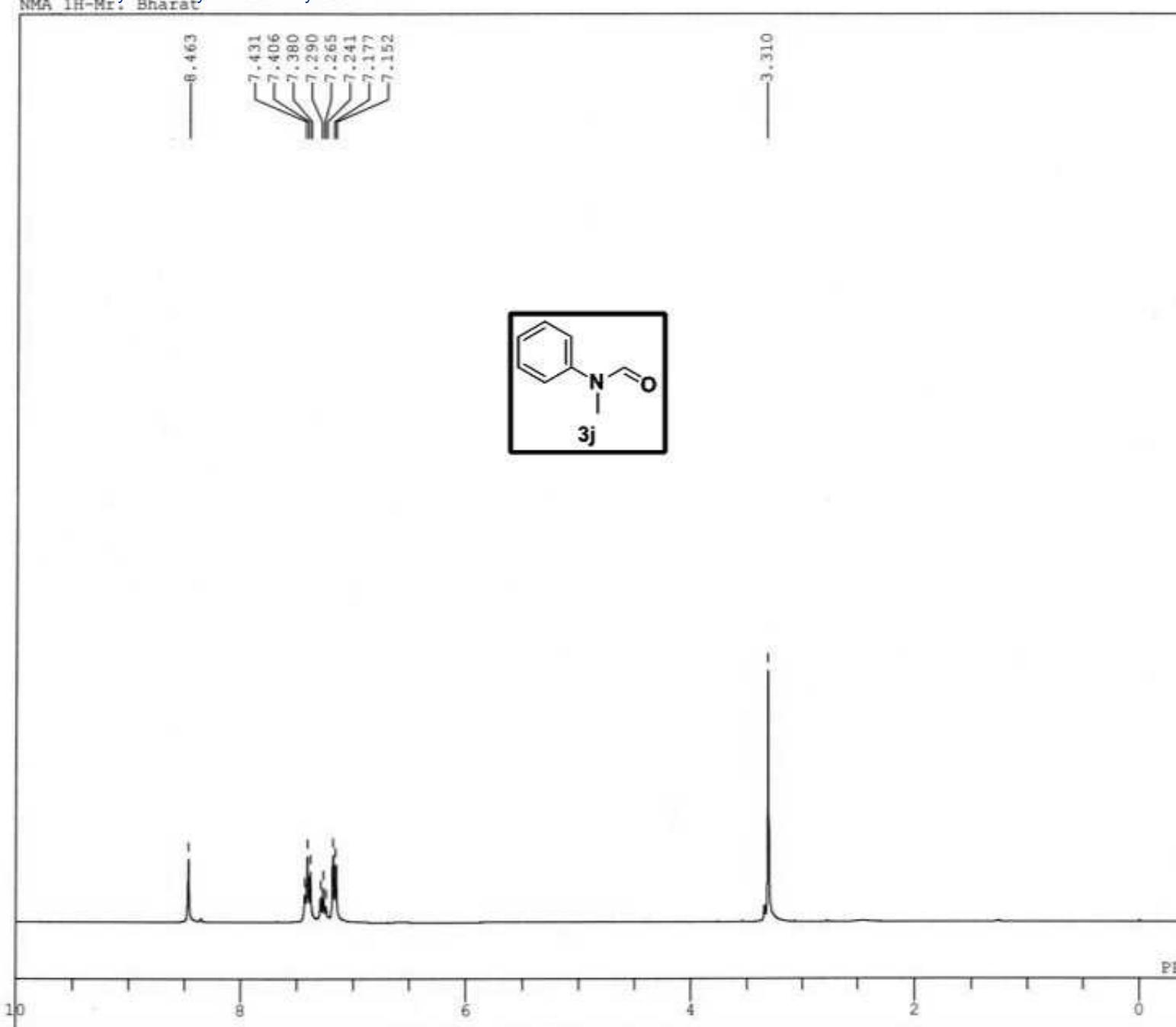


J₃₈

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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT MNO_13C Mr. Rajeshwer
DATIM Sat Jul 28 11:30:01 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 202
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 21.6 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 24

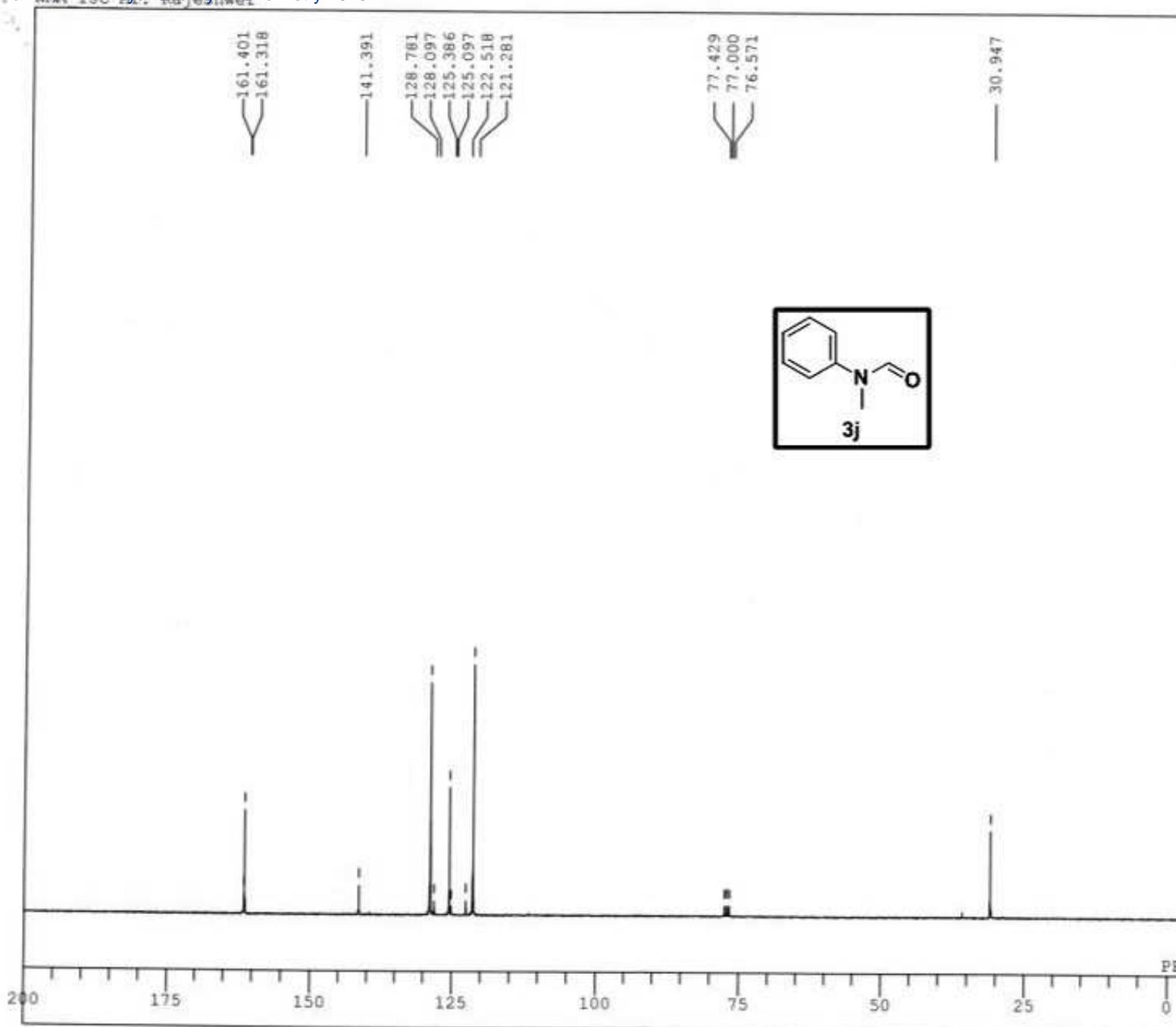


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\NMA_1HINC
COMNT NMA 1H-Mr. Bharat
DATIM Sat Dec 01 13:55:16 2012
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 19.3 c
SLVNT CDCL₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 10

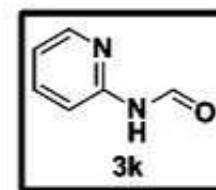
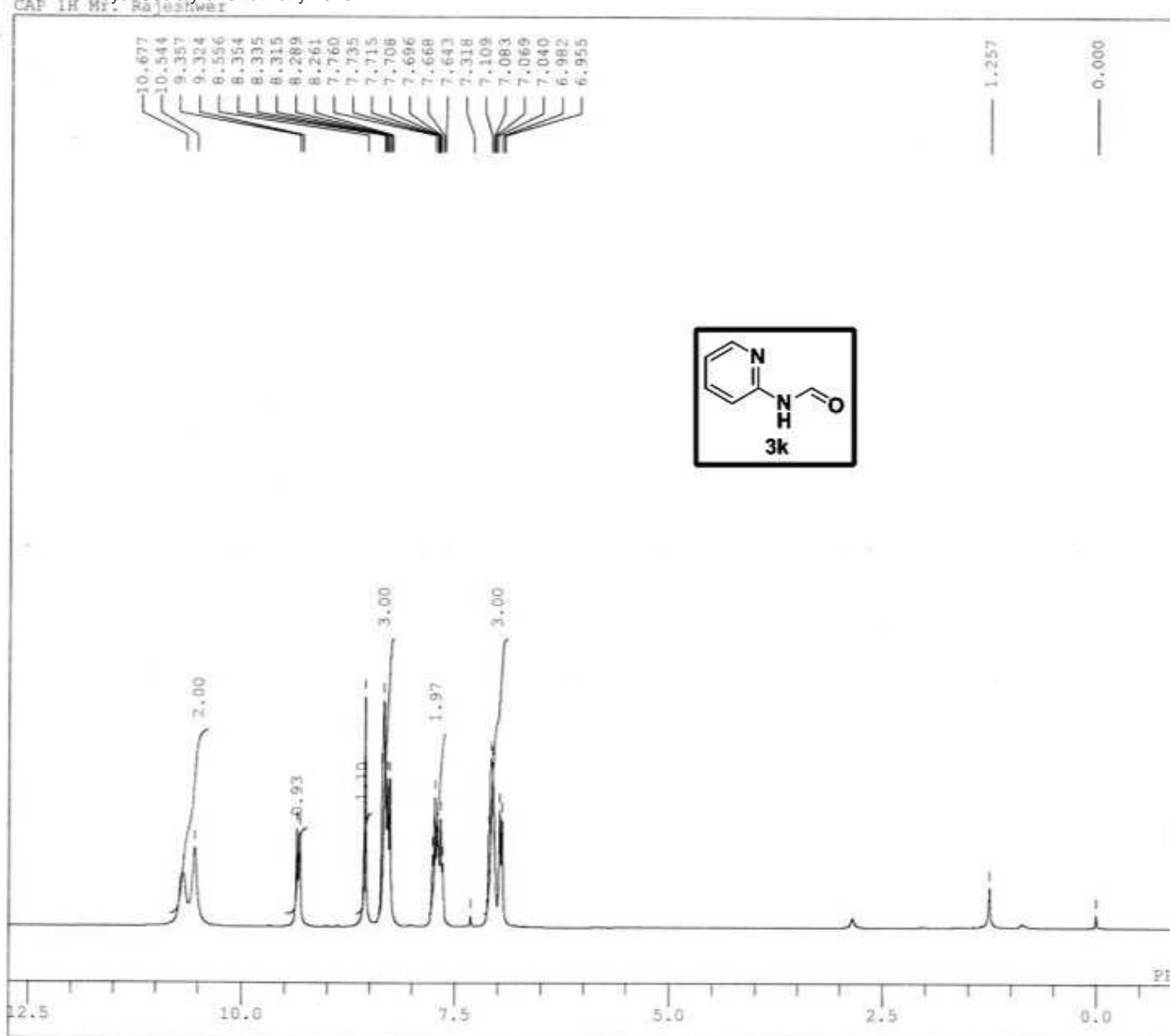
J₃₉



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

Operator : Nagendra Kumar
Shishir Singh

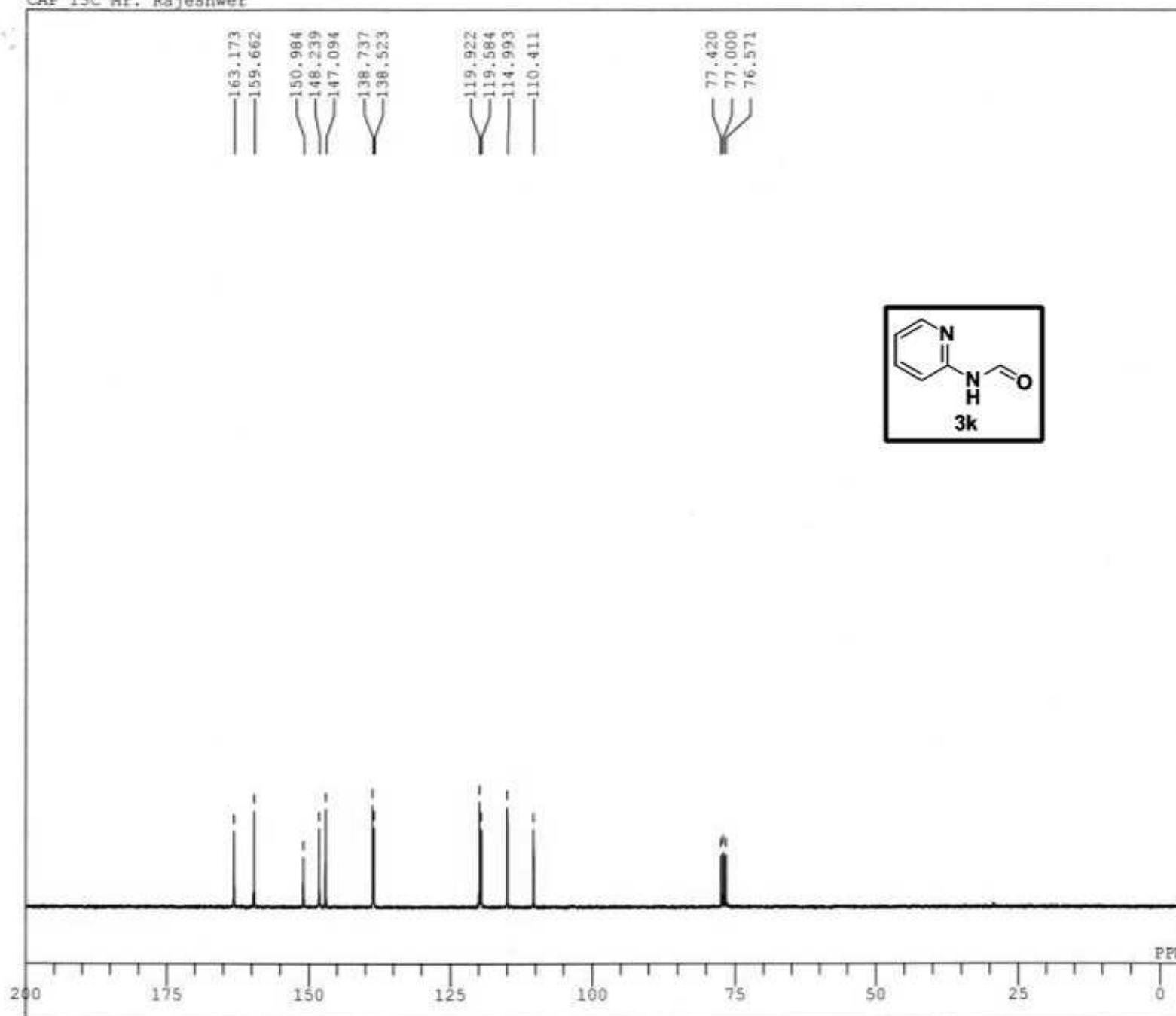
DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT NMA_13C_Mr. Rajeshwer
DATIM Wed Jul 04 13:24:38 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 160
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 22



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

Operator : Nagendra Kumar
Shishir Singh

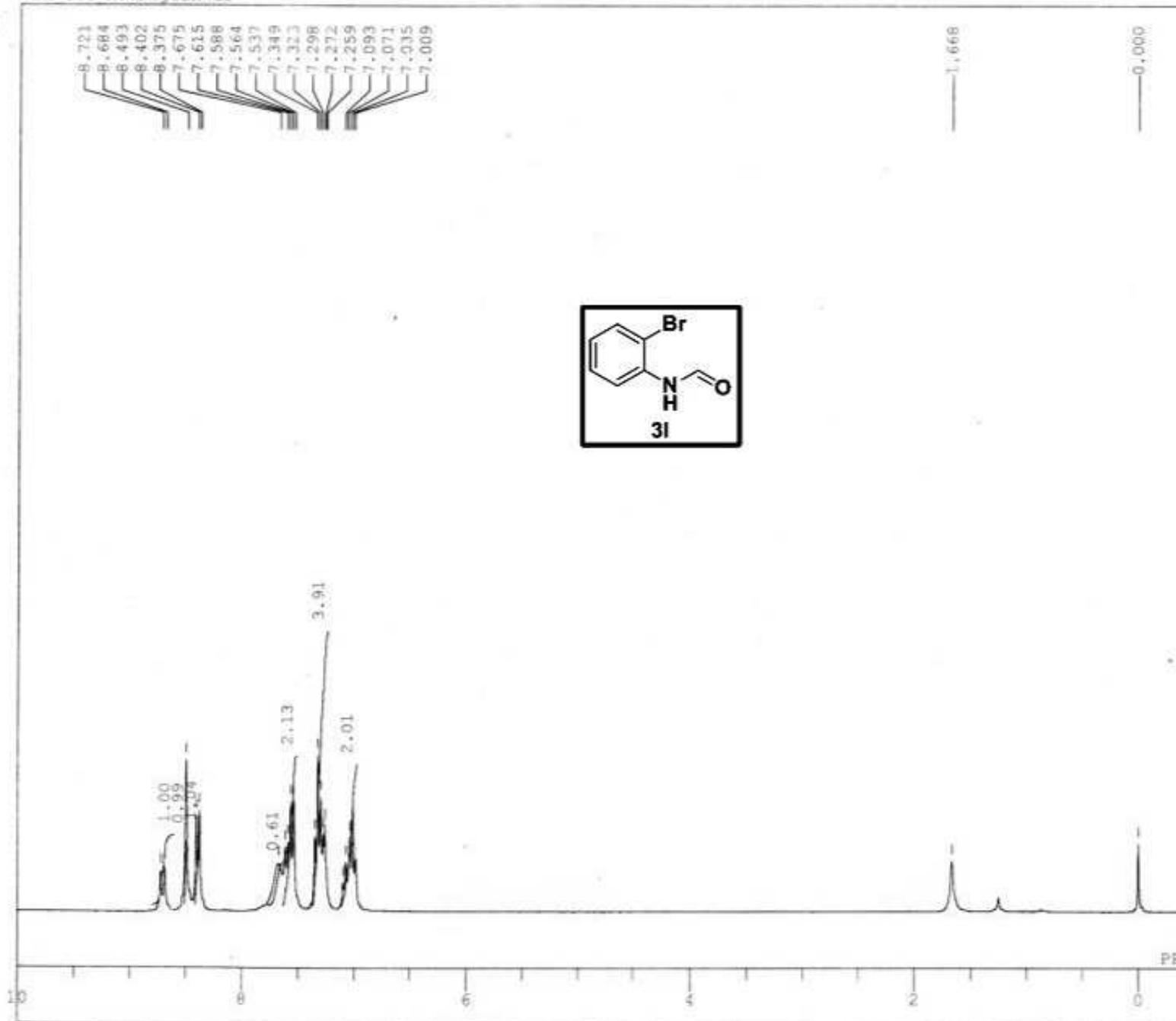
DFILE C:\K.N. Singh,,I.T\CAP_1H.al
COMNT CAP_1H Mr. Rajeshwer
DATIM Mon Jul 02 12:12:26 2012
IRNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 98
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCl₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 10



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

Operator : Nagendra Kumar
Shishir Singh

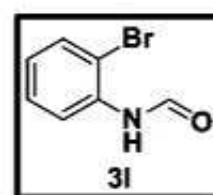
DFILE C:\WINNMR98\COMMON_DEFAULT.
COMT CAP_13C_Mr. Rajeshwer
DATIM Mon Jul 02 12:33:01 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 135
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

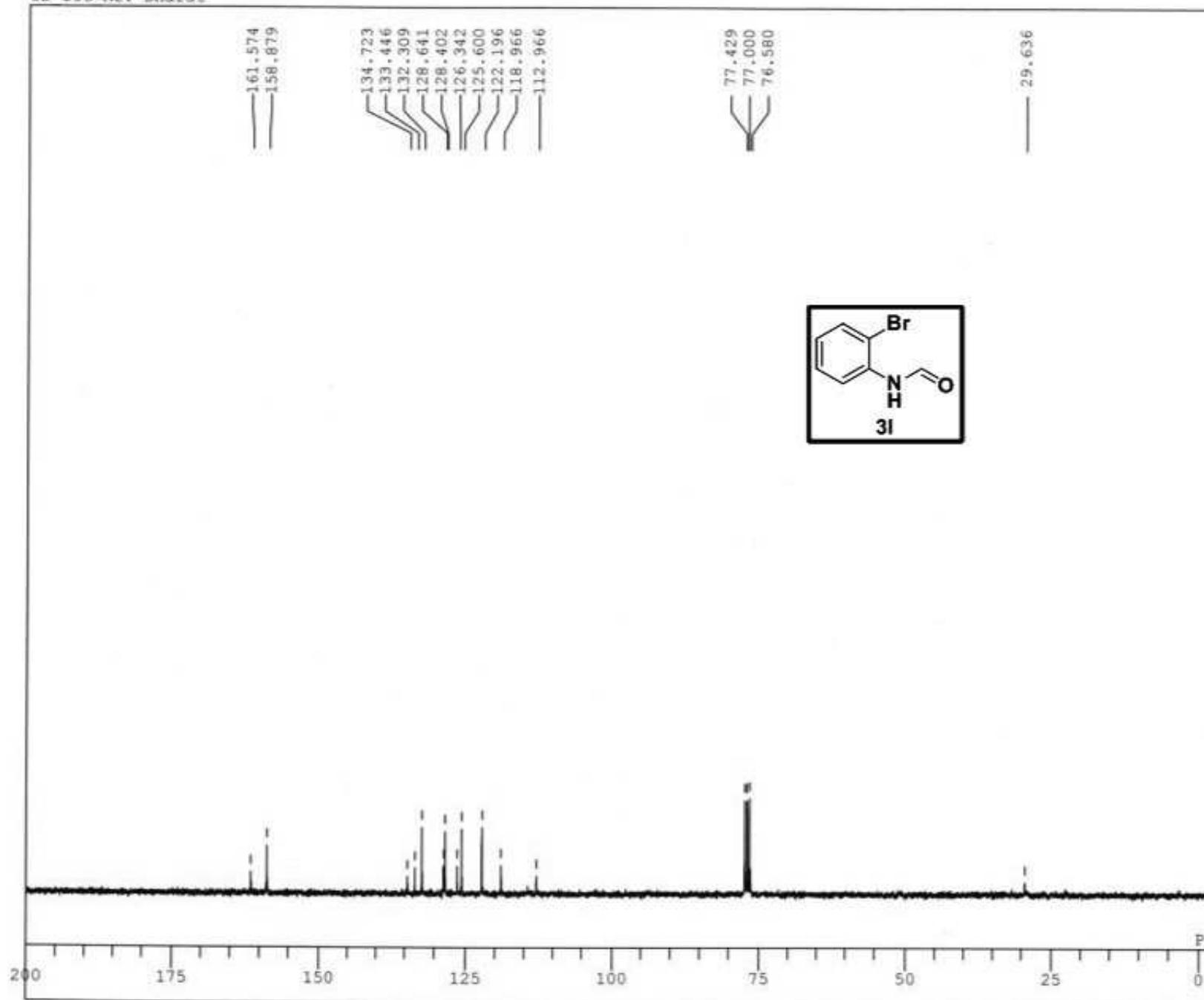


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\W.N. Singh,,I.T\OBA_1H.dat
COMNT OBA_13C_Mr.Rajeshwar
DATIM Mon Sep 10 12:04:51 2012
OBNUC 1H
EXMOD N0N
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 20.5 c
SLVNT CDCl₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 18



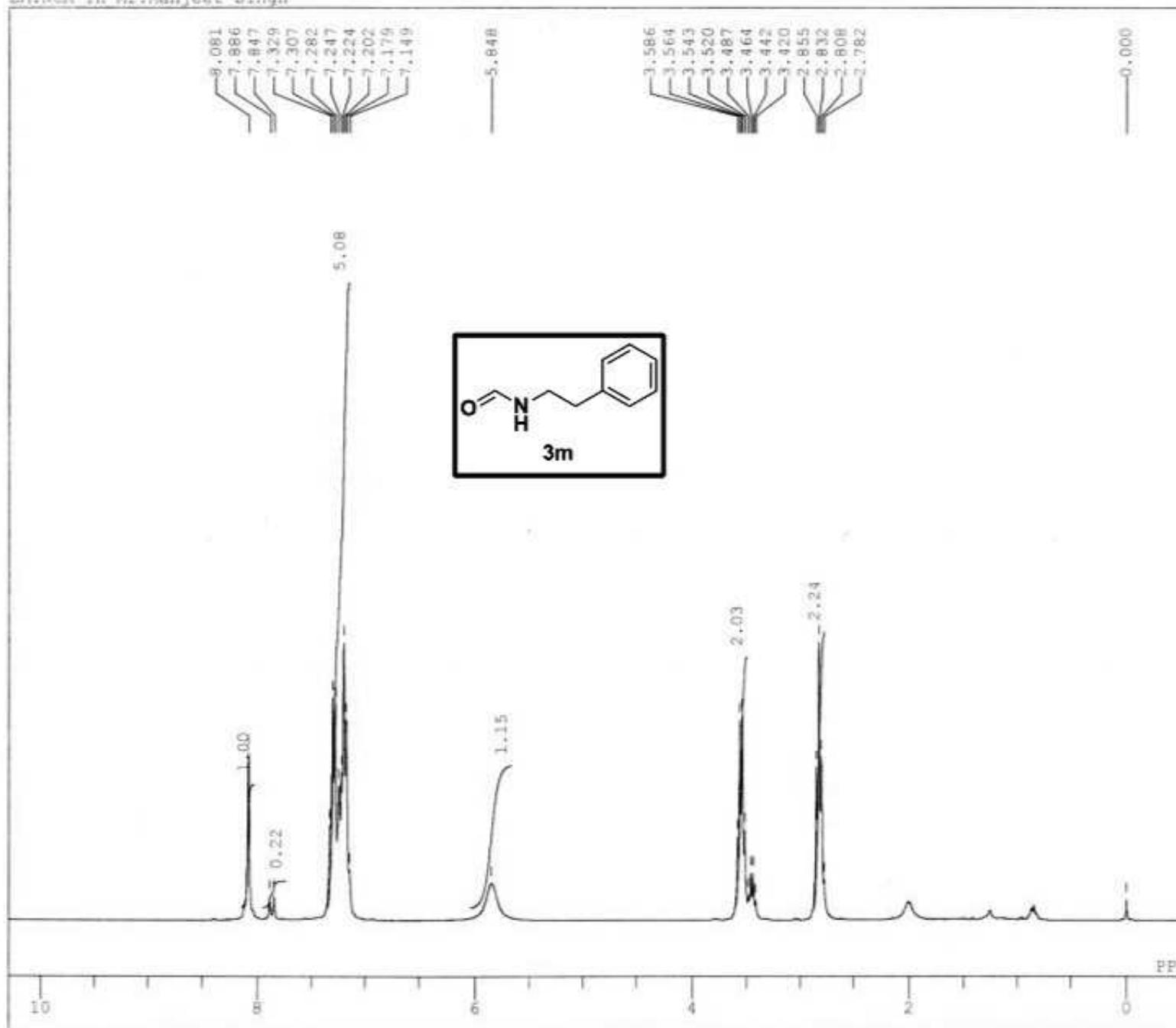


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEI
COMNT OB_13C Mr. Bharat
DATIM Sat Dec 01 15:40:14 20:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 171
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 25

EA.NCA 1H Mr.Manjeet Singh

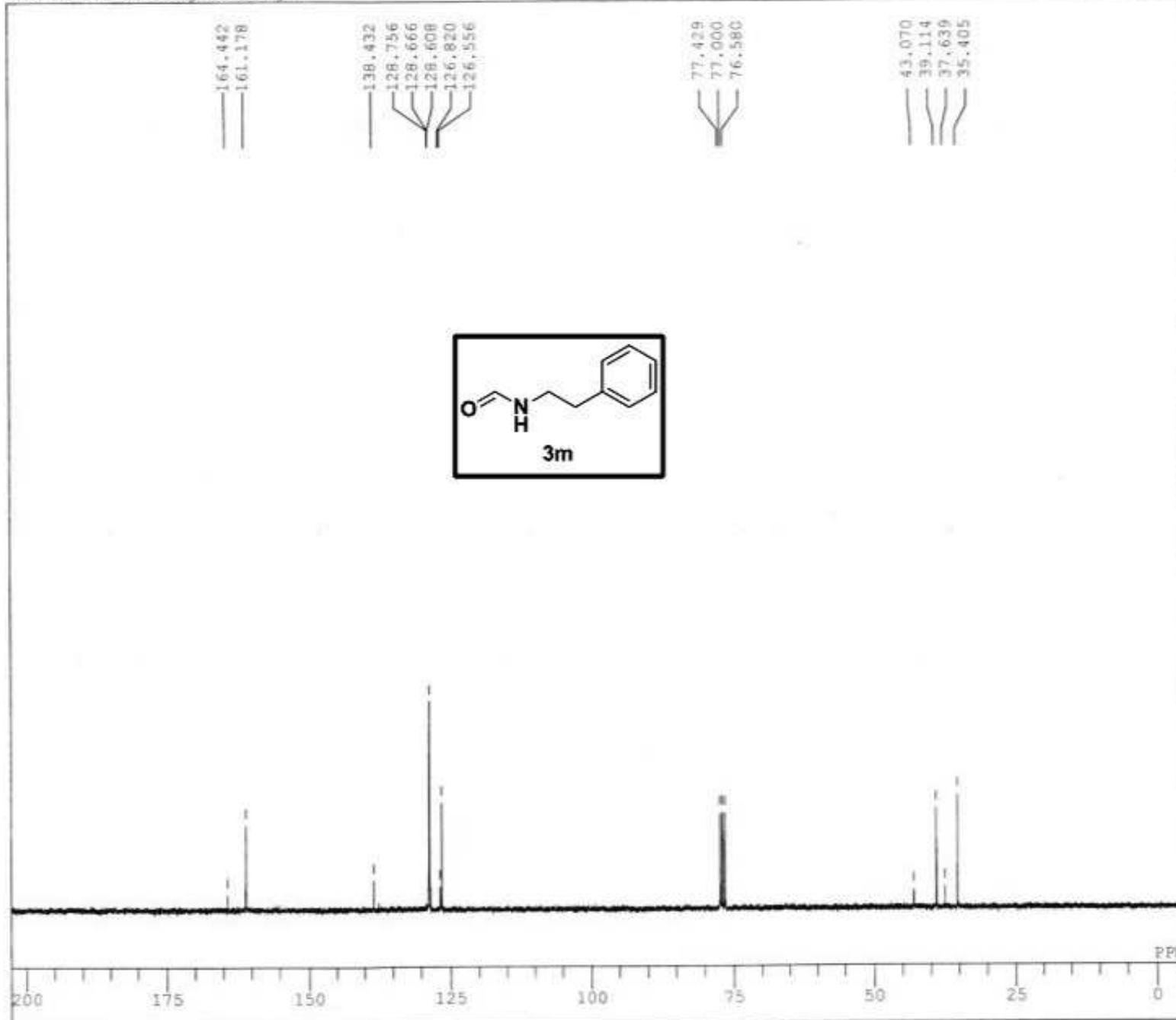


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\R.N. Rai\EA.NCA 1H.als
COMNT EA.NCA 1H Mr.Manjeet Singh
DATIM Wed Sep 12 13:04:21 2012
CBNUC 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 22.5 °C
SLVNT CDCL₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 12

EA.NCA 13C Mr. Manjeet Singh

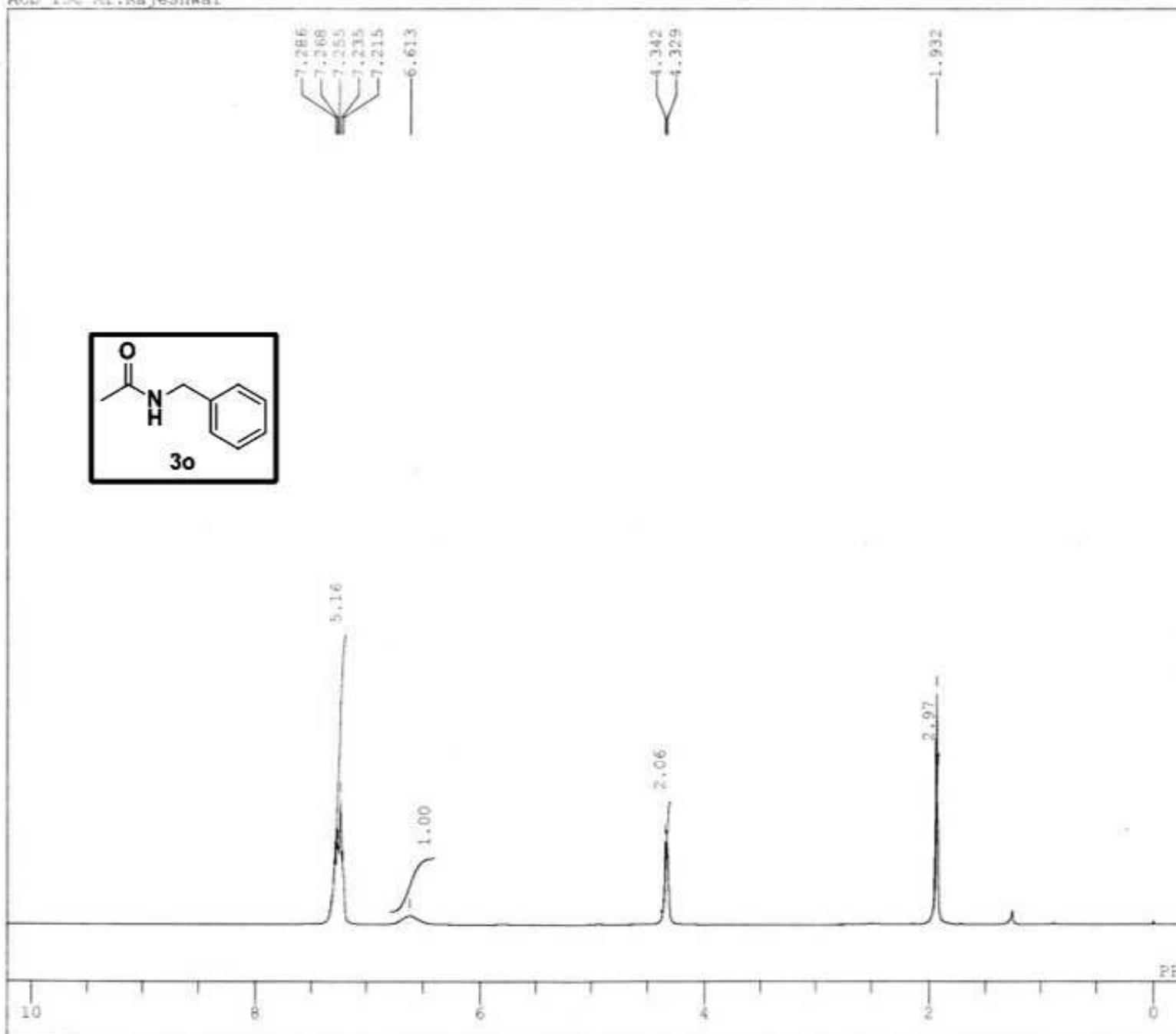


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT EA.NCA_13C Mr. Manjeet Singh
DATIM Wed Sep 12 12:59:21 2012
ORNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20400.1 Hz
SCANS 162
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

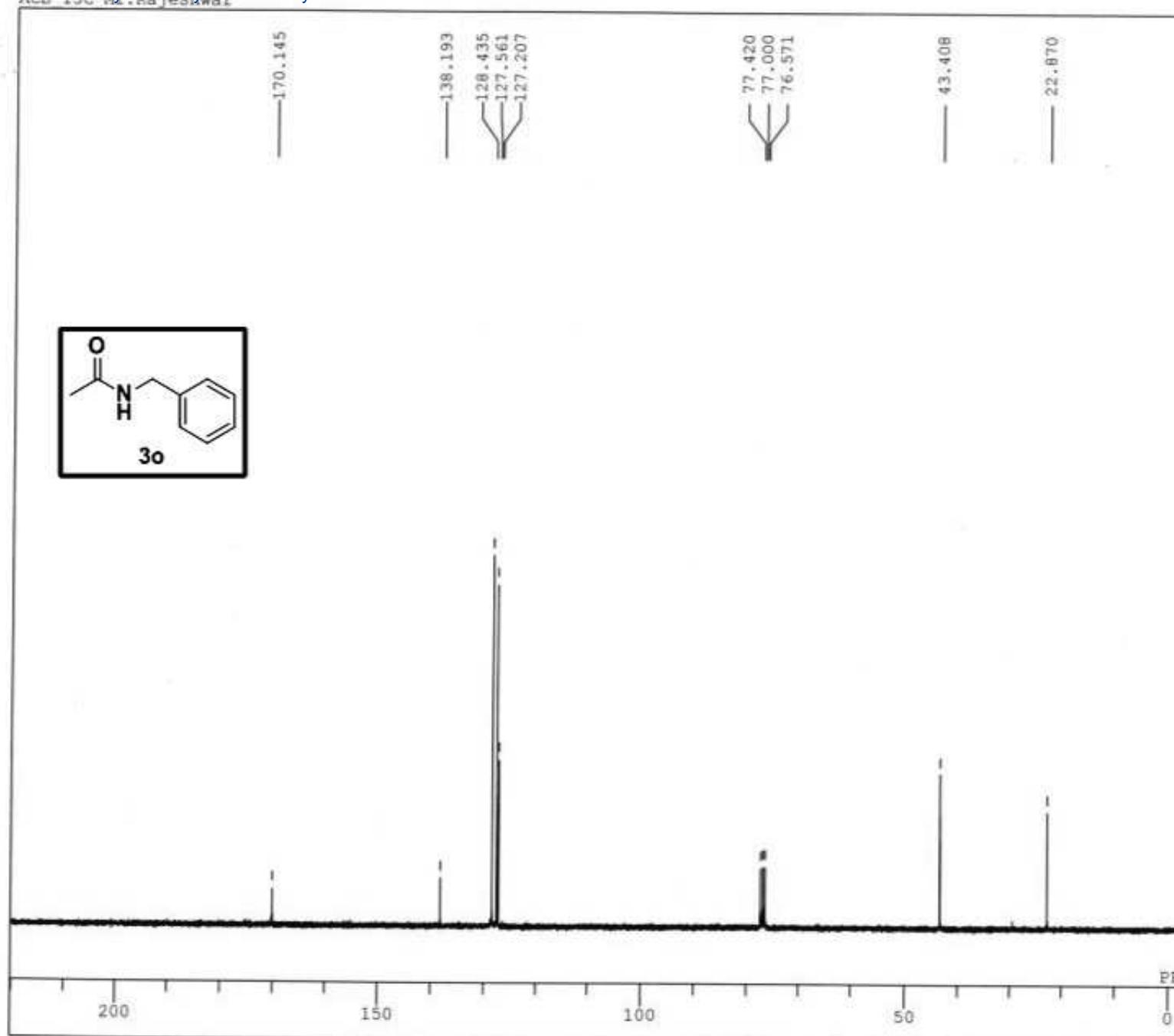
ACB_13C_Mr.Rajeshwar



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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\ACB_13C.r1e
COMNT ACB_13C_Mr.Rajeshwar
DATIM Fri Jul 06 16:13:43 2012
OBNUC 1H
EXMOD NON
QBFRQ 300.40 MHz
OBSET 130.00 KHz
QBFIN 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 20.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 10

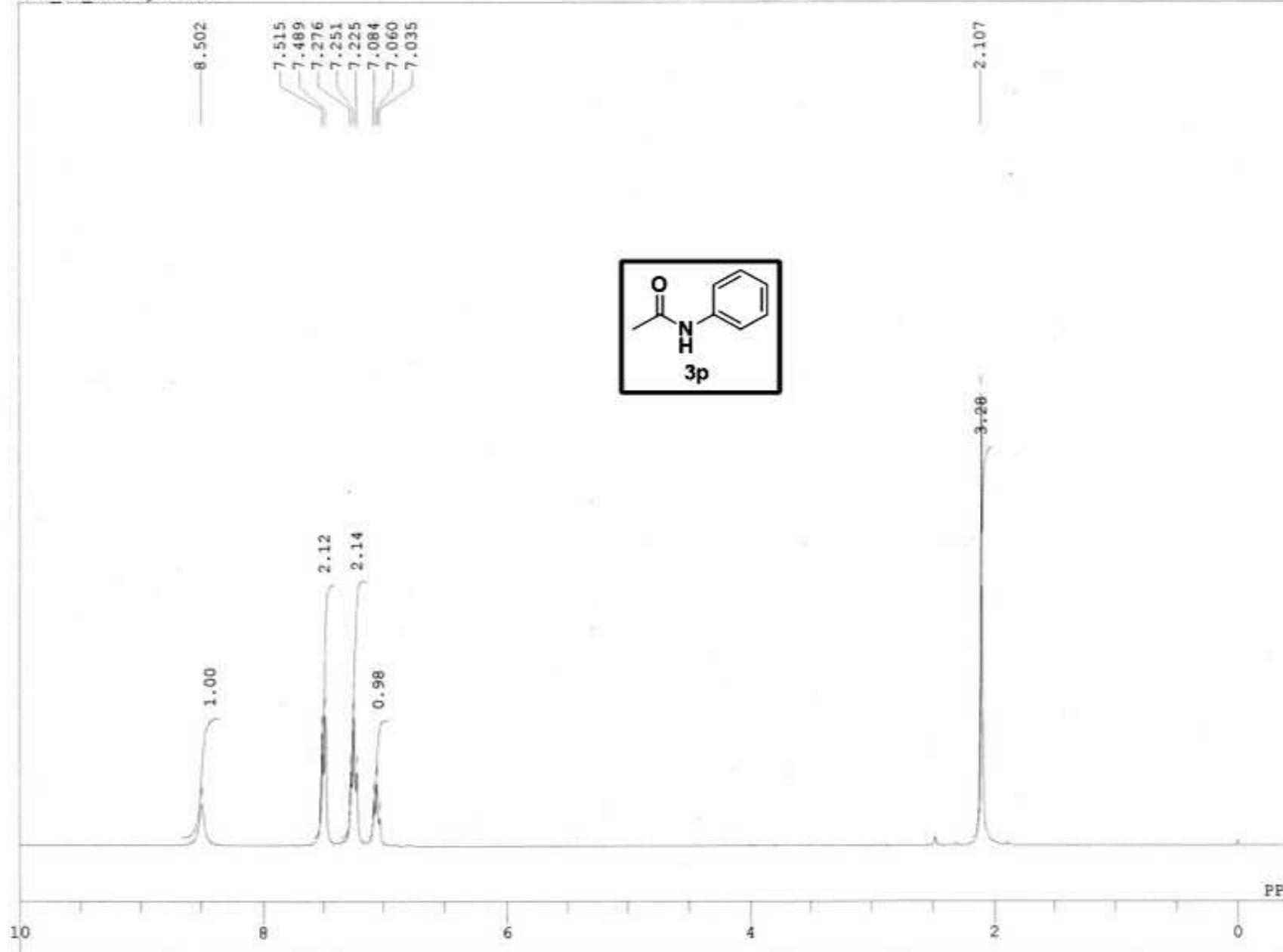


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\Data\ACB_13C2BCM
COMNT ACB_13C_Mr.Rajeshwar
DATIM Fri Jul 06 16:39:05 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 500
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 0.12 Hz
RGAIN 25

C:\K.N. Singh,,I.T\CAC_1H.als
CAC_1H Mr.Rajeshwar



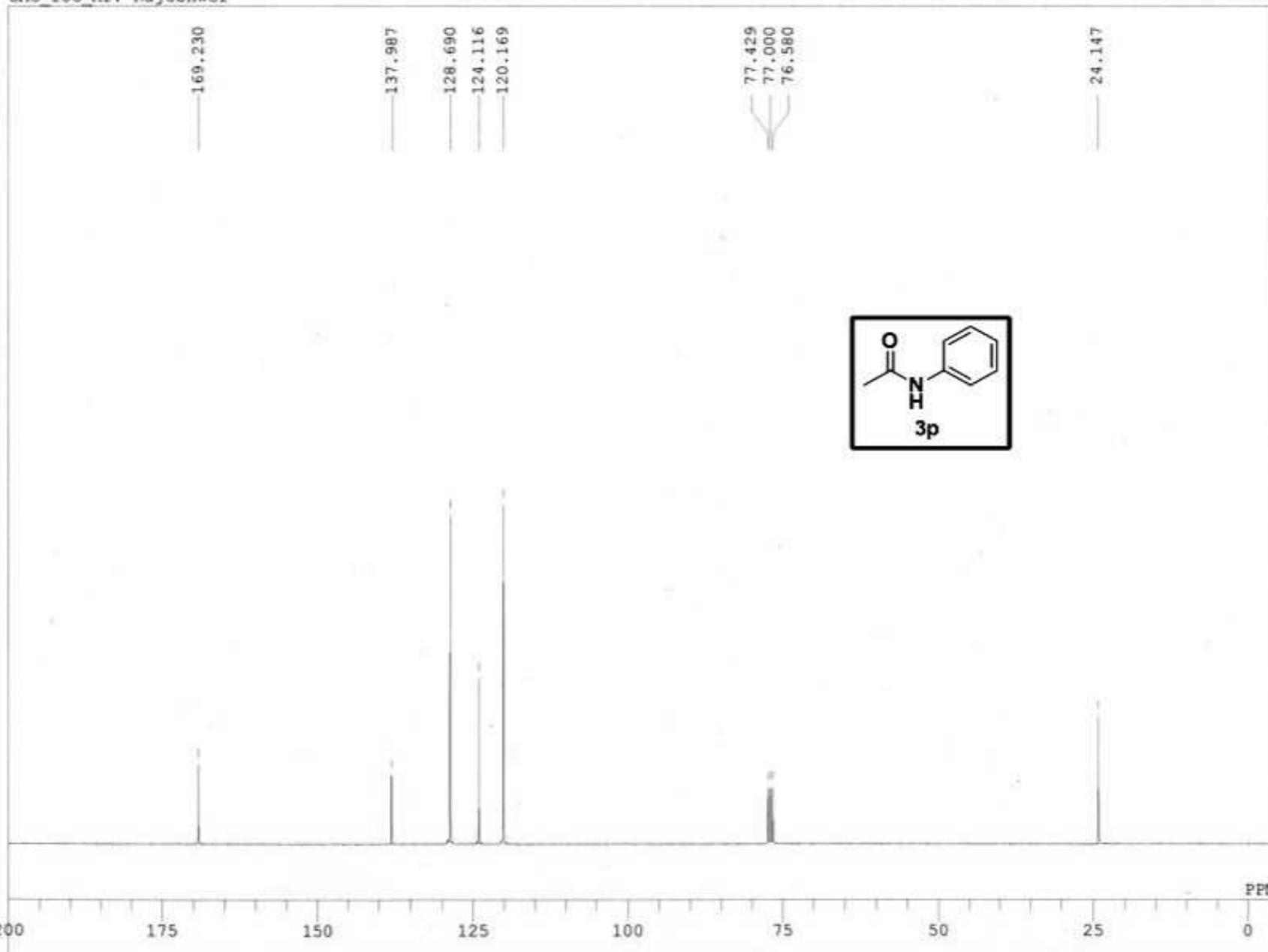
J₄₉

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT CAC_1H Mr.Rajeshw.
DATIM Tue Jun 26 16:15:
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 21.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 10

C:\K.N. Singh,,I.T\CAC_13C.als
CAC_13C Mr. Rajeshwer



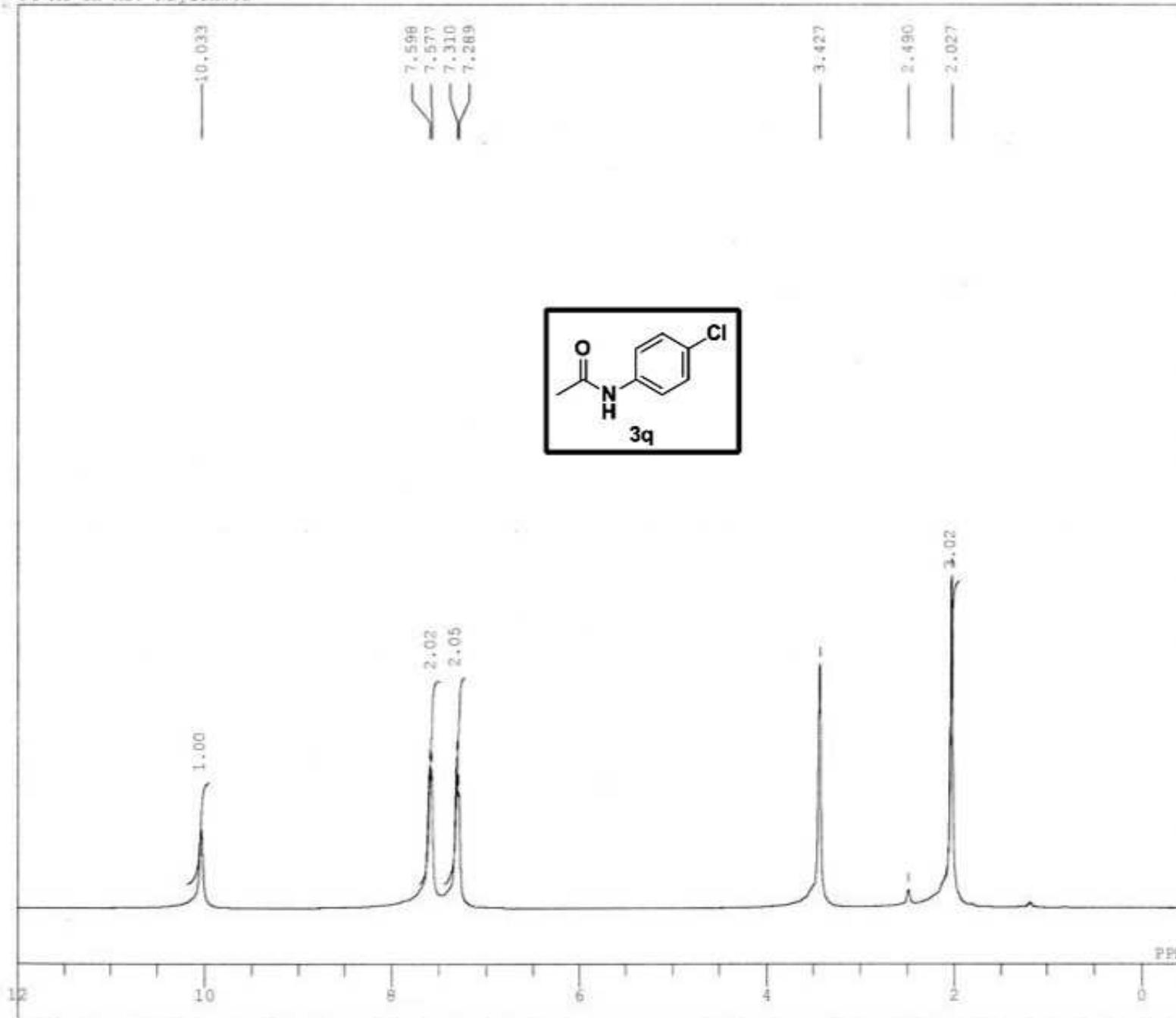
JEOL AL300 FWNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT CAC_13C_Mr. Rajes
DATIM Fri Jun 29 00:13:
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 3500
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

J₅₀

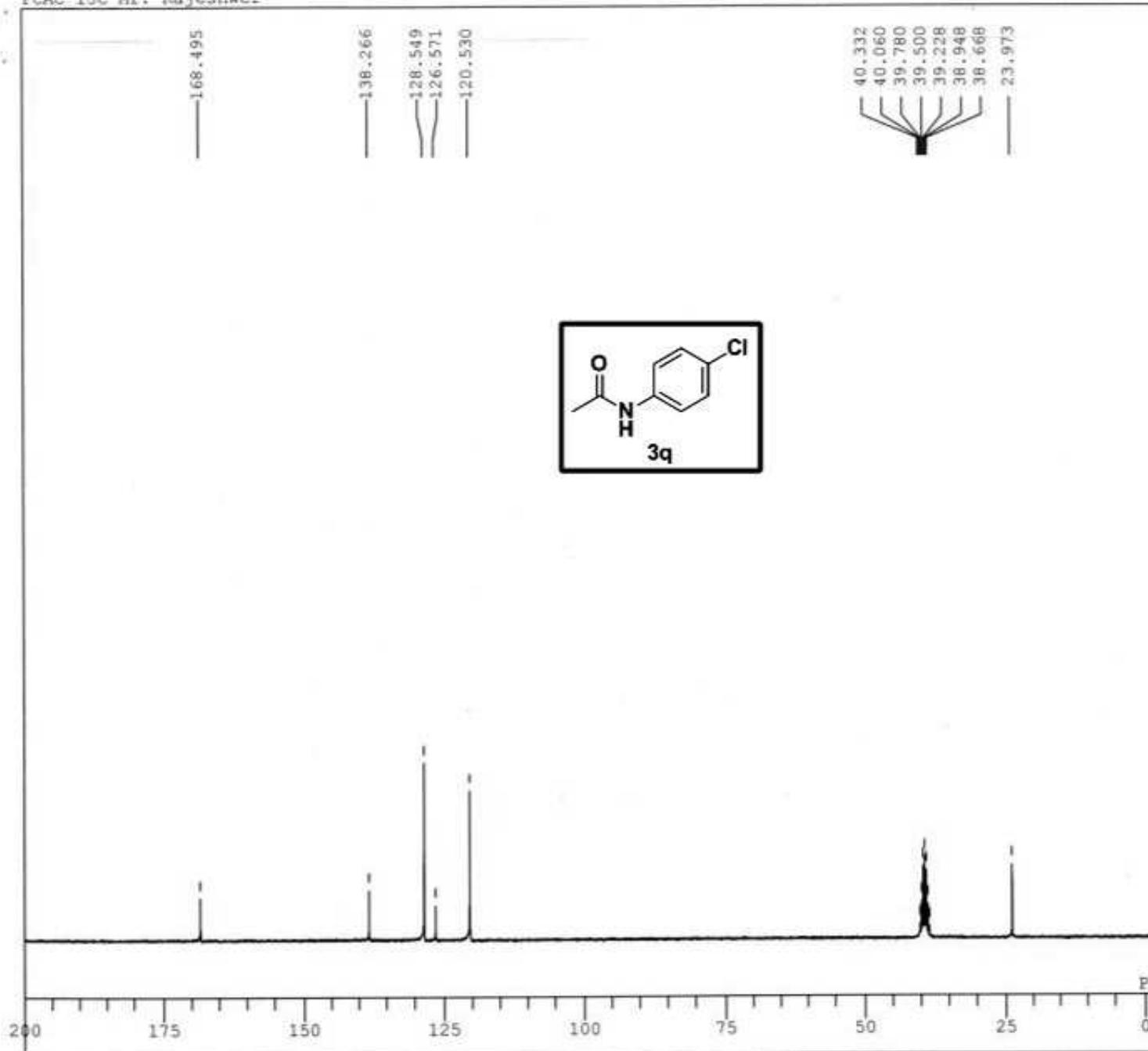
PC-AC 1H Mr. Rajeshwer



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

Operator : Nagendra Kumar
Shishir Singh

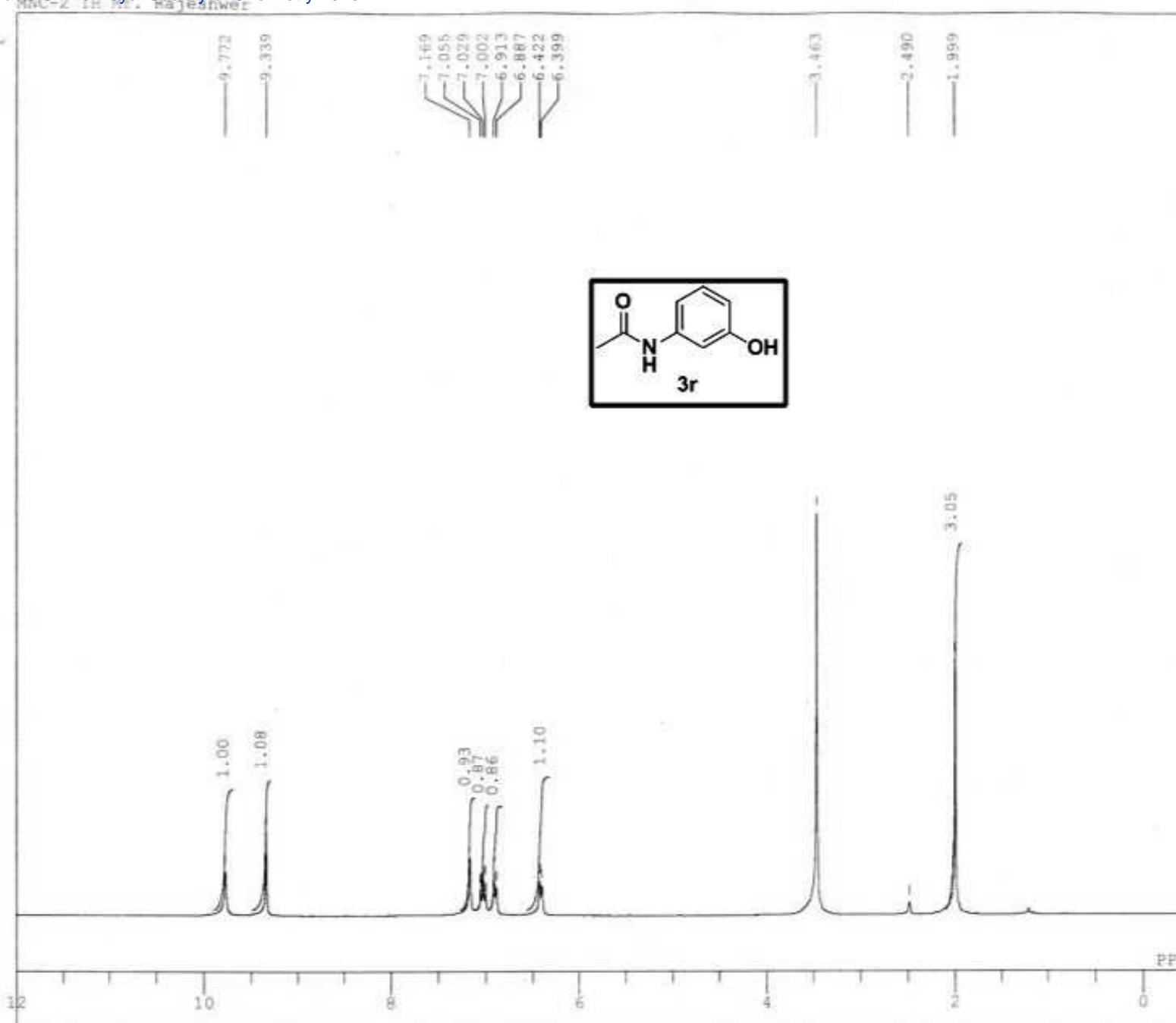
DFILE C:\K.N. Singh,, I.T\PC-AC_1H.
COMNT PC-AC 1H Mr. Rajeshwer
DATIM Sat Jul 28 10:58:39 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.5 c
SLVNT DMSO
EXREF 2.49 ppm
BF 1.20 Hz
RGAIN 11



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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.ALS
COMNT PCAC 13C Mr. Rajeshwer
DATIM Sat Jul 28 11:45:18 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 274
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 21.9 °C
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 23

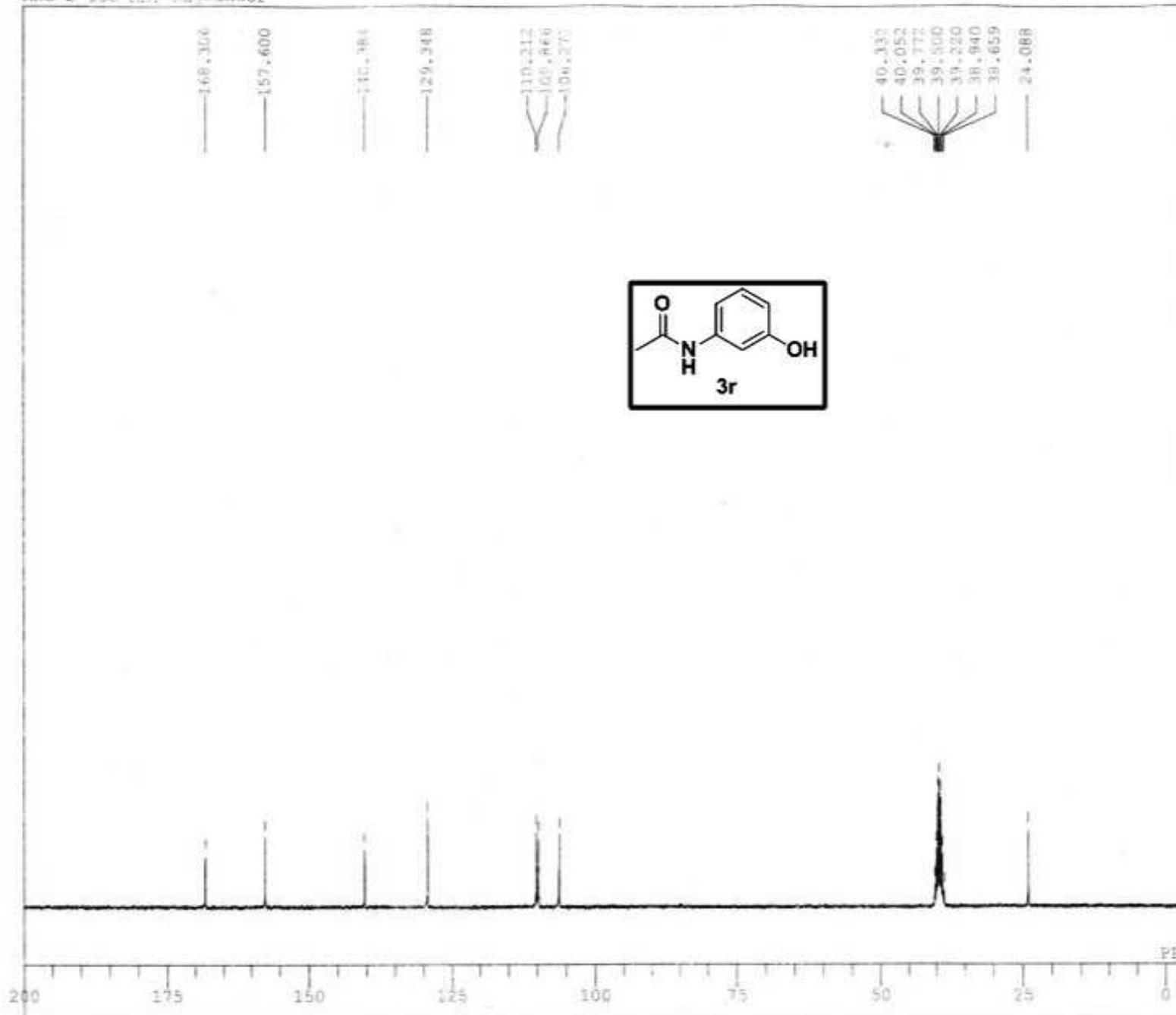


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\MNC-2_1H.
COMNT MNC-2_1H Mr. Rajeshwer
DATIM Tue Jul 31 12:56:40 2012
GBNUC 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 20.6 c
SLVNT DMSO
EXREF 2.49 ppm
BF 1.20 Hz
RGAIN 11

MNC-2_13C MR. Rajeshwar



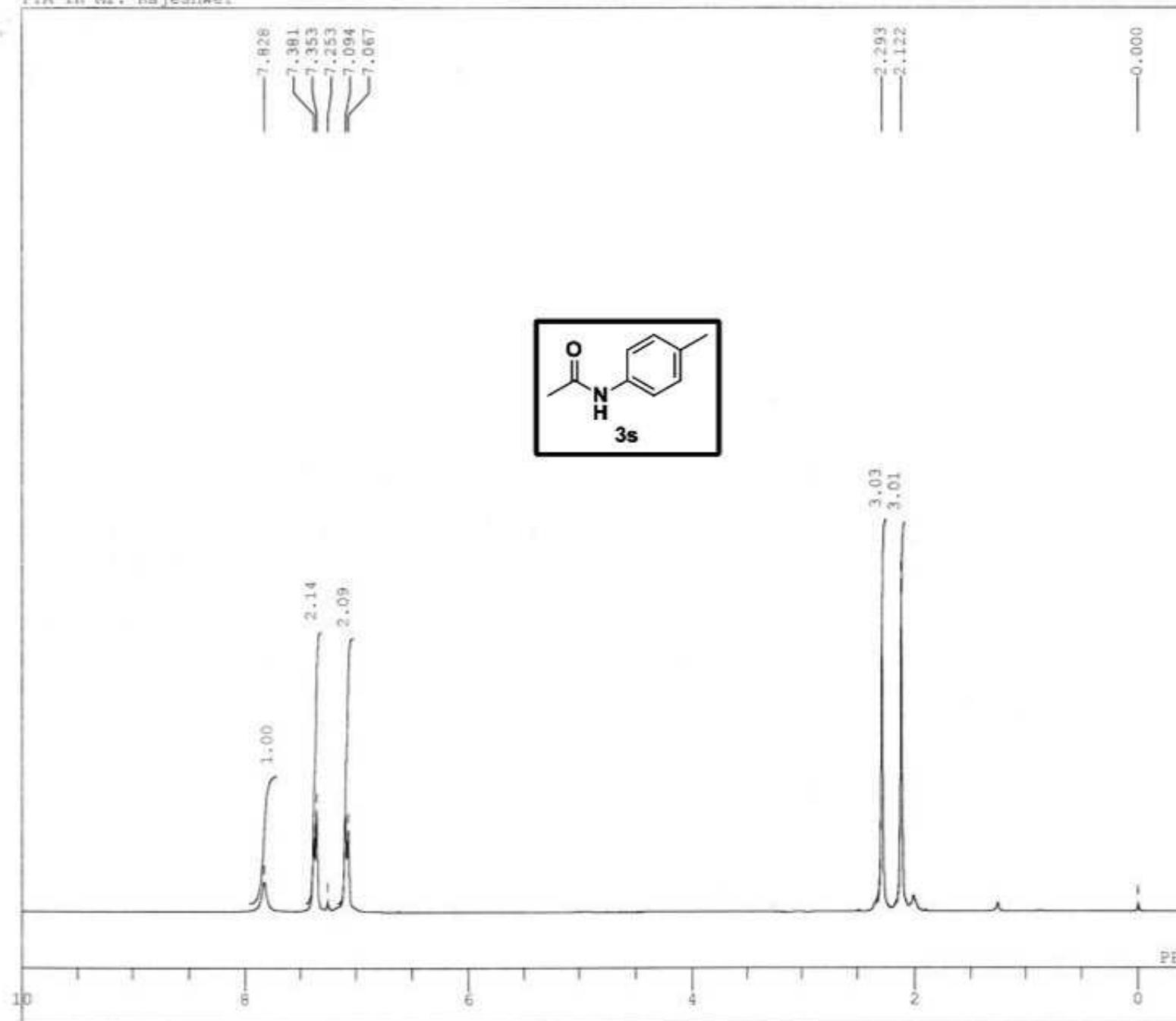
J₅₄

JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh\I.T\ME
COMNT MNC-2_13C MR. Rajeshwar
DATIM Tue Jul 31 13:25:43 2012
OBNUC ¹³C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 277
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 23.5 °C
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 22

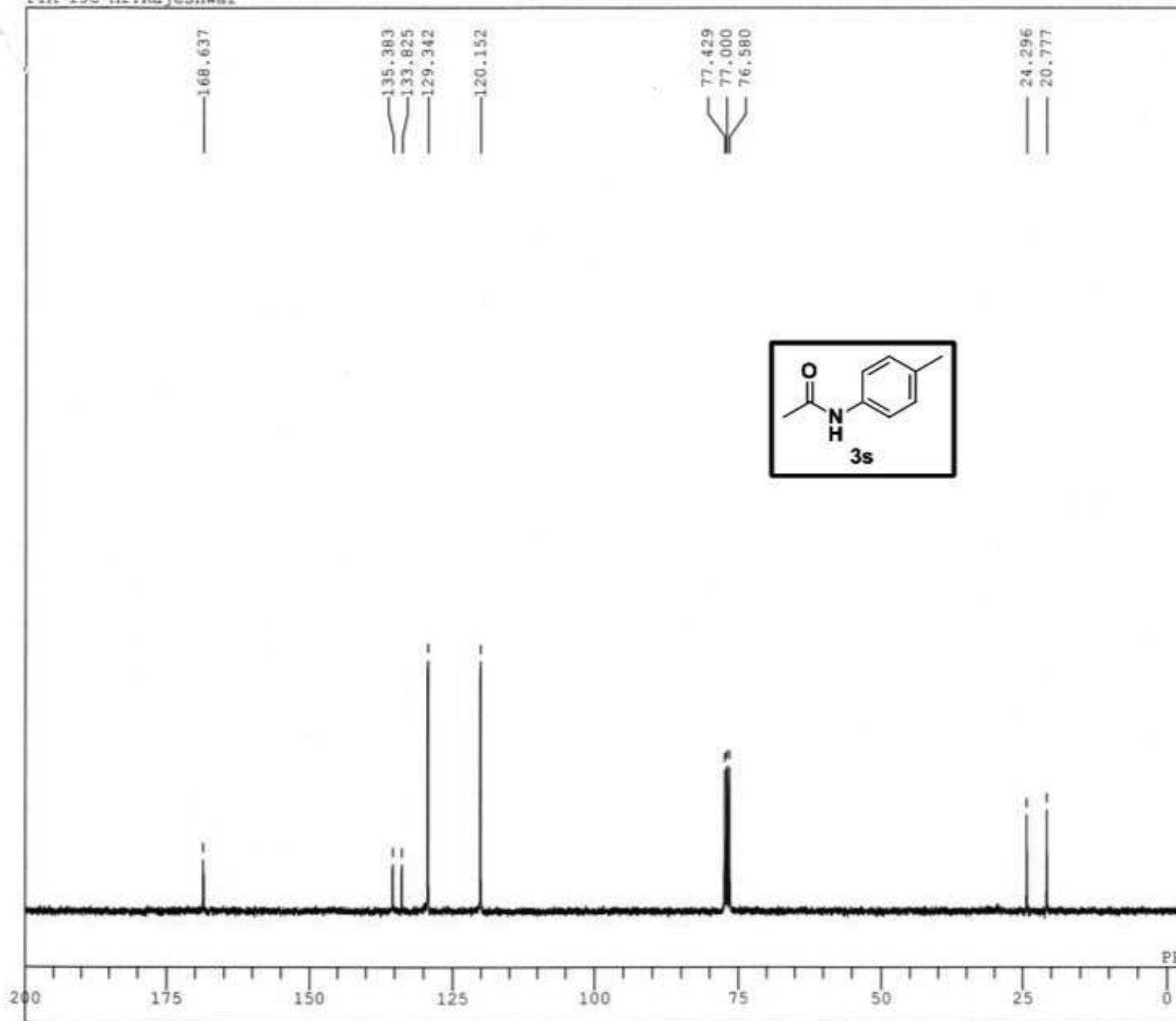
PTA_1H Mr. Rajeshwer



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

Operator : Nagendra Kumar
Shishir Singh

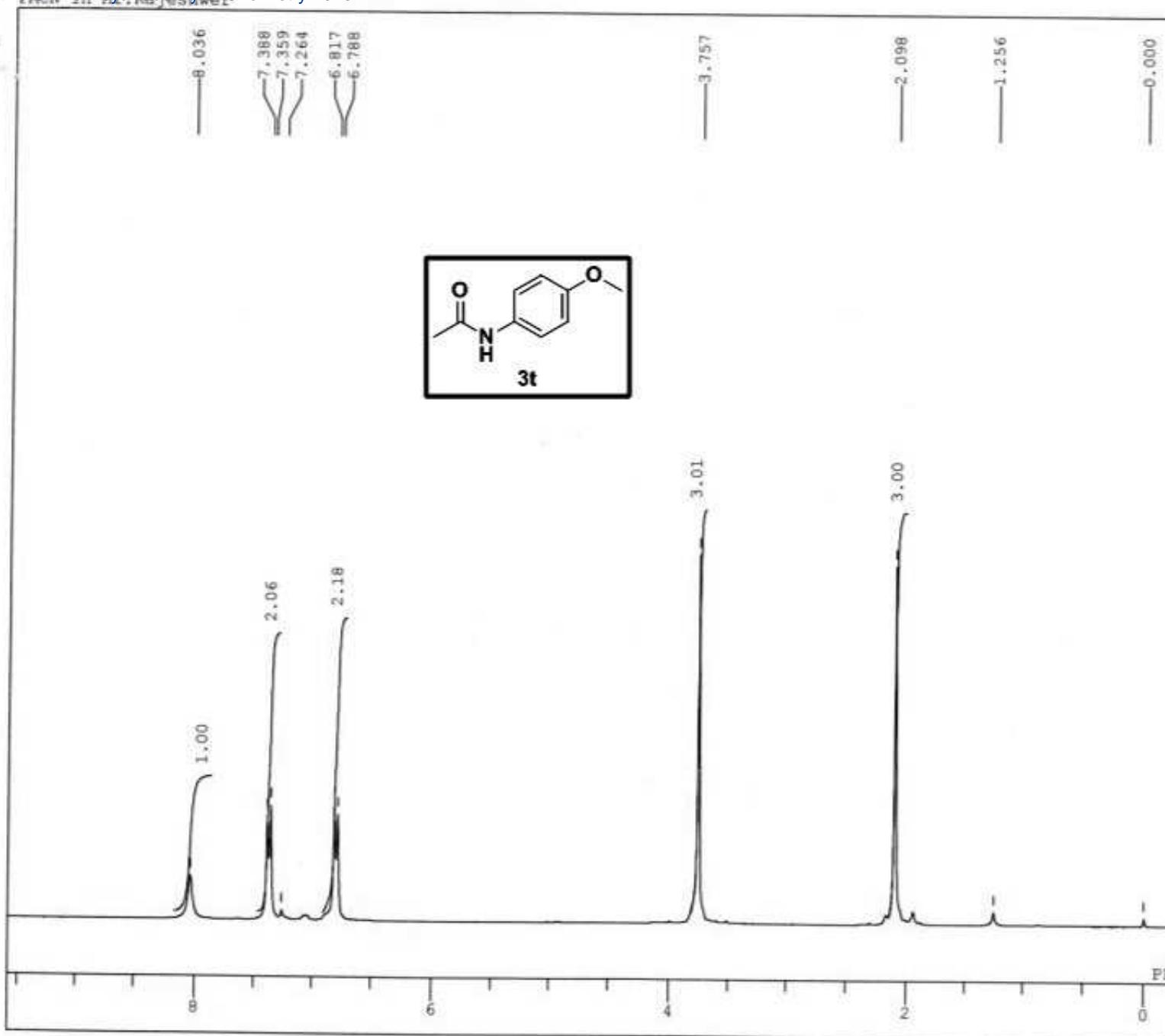
DFILE C:\K.N. Singh,,I.T\PTA_1H.al
COMNT PTA_1H Mr. Rajeshwer
DATIM Tue Jul 17 12:02:15 2012
QBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 67
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 18.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN -12



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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

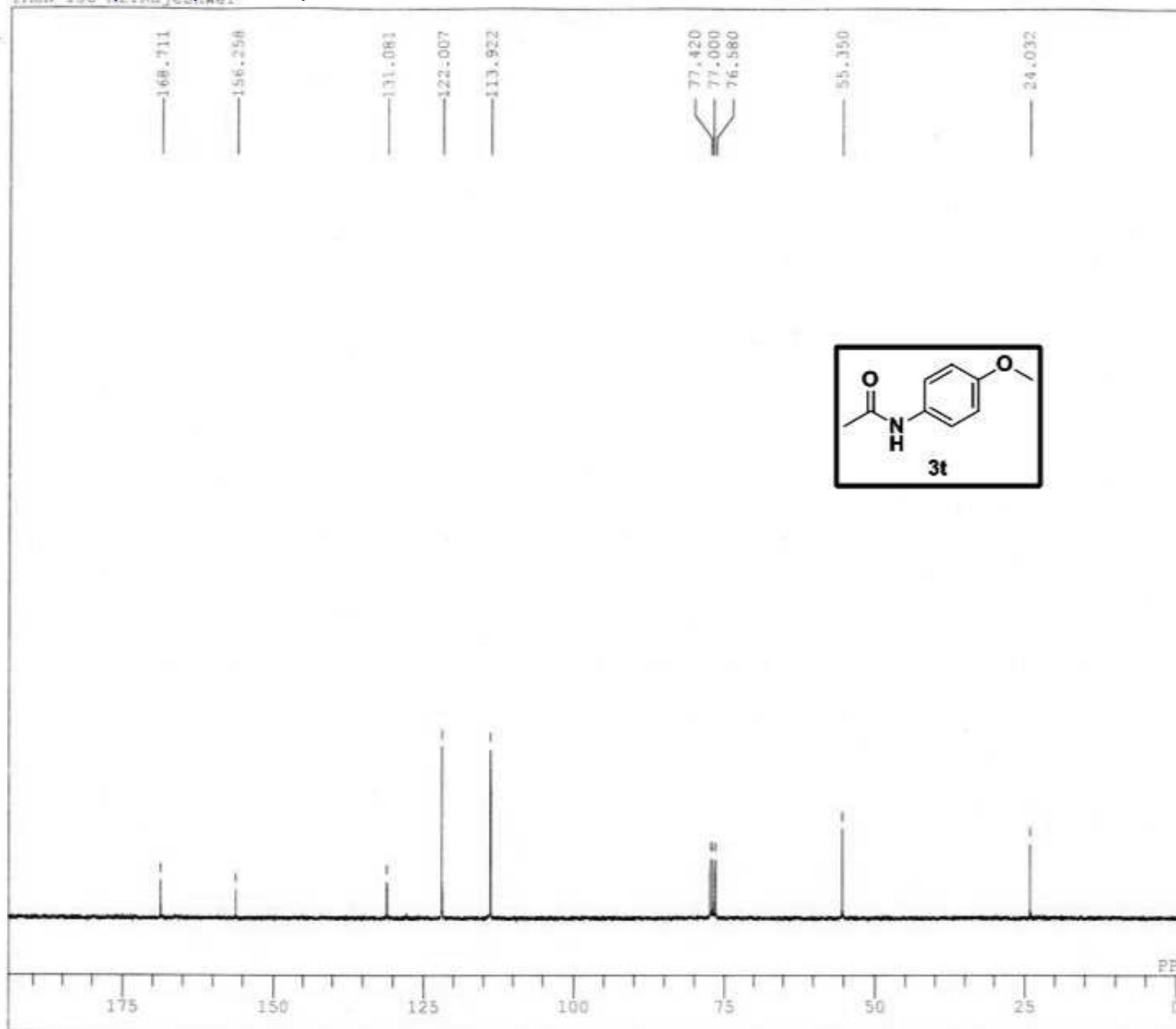
DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT PTA_13C Mr.Rajeshwar
DATIM Wed Jul 18 17:13:07 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 539
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 25.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25



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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT PACN 1H Mr.Rajeshwer
DATIM Wed Jul 18 12:23:09 2012
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 23.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 13



JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\PACN_13C.
COMNT PACN_13C Mr.Rajeshwer
DATIM Wed Jul 18 12:18:40 2012
CBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 98
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.0 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

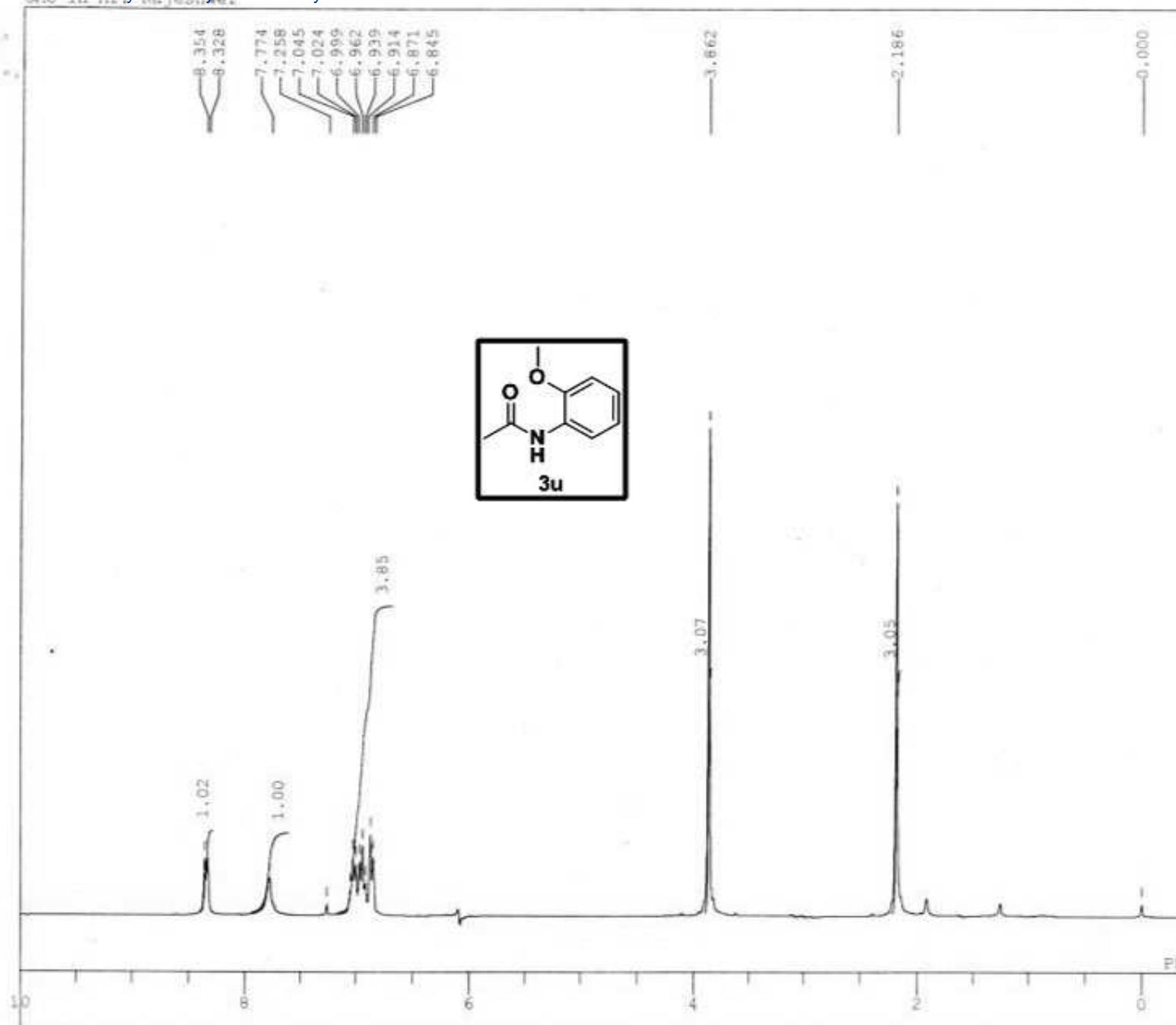
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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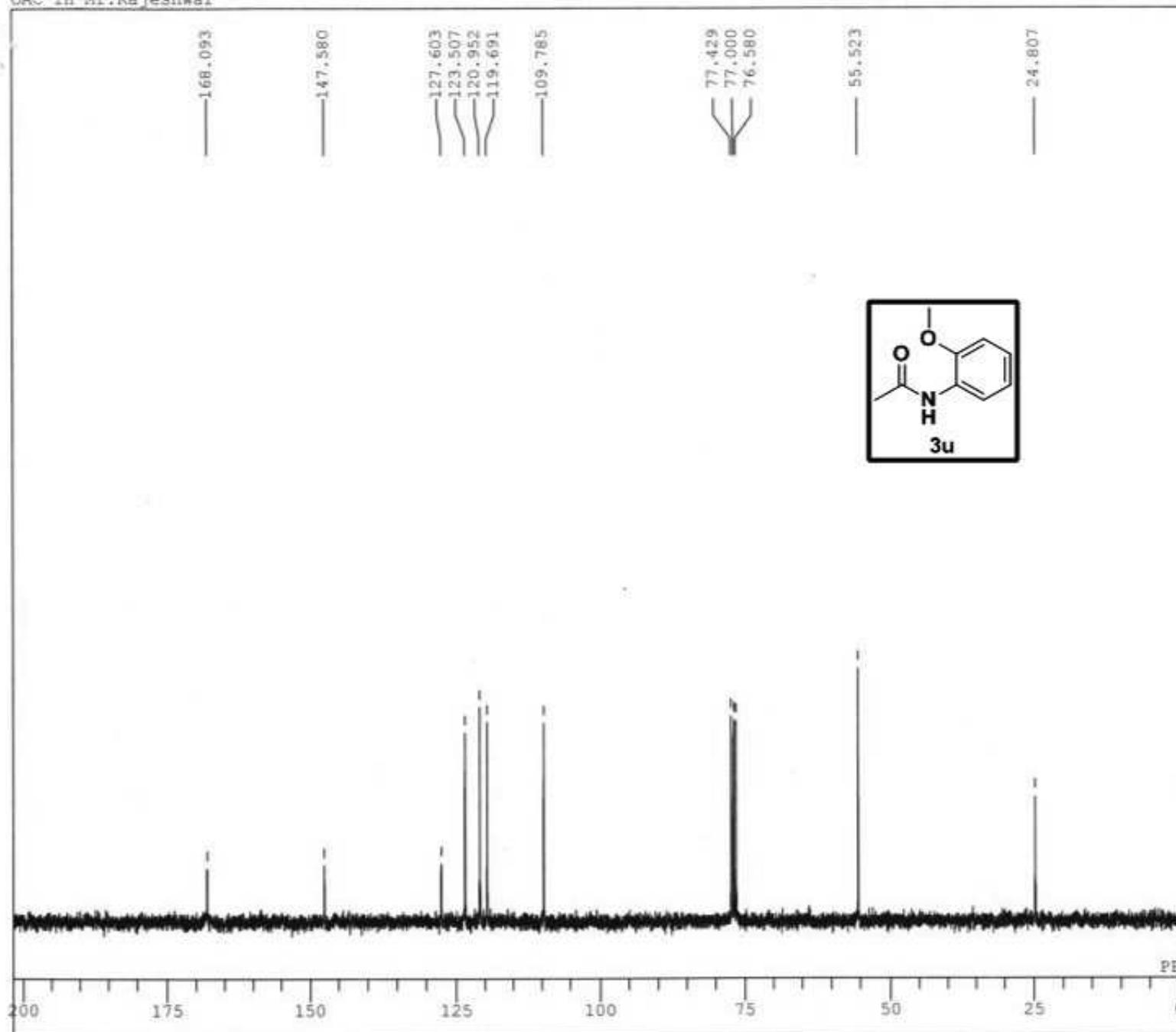
DFILE C:\K.N. Singh\I.T\OAC_1H.al
COMNT OAC_1H Mr. Rajeshwer
DATIM Mon Jul 23 16:08:29 2012
OBNUC 1H
EXMOD NON
OBFRQ      300.40 MHz
OBSET      130.00 KHz
OBFIN      1150.0 Hz
POINT      32768
FREQU      9505.7 Hz
SCANS       43
ACQTM       3.447 sec
PD          1.547 sec
PW1         5.2 us
IRNUC      1H
CTEMP       21.3 c
SLVNT      CDCL3
EXREF       0.00 ppm
BF          1.20 Hz
RGAIN      13

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OAC 1H Mr.Rajeshwar

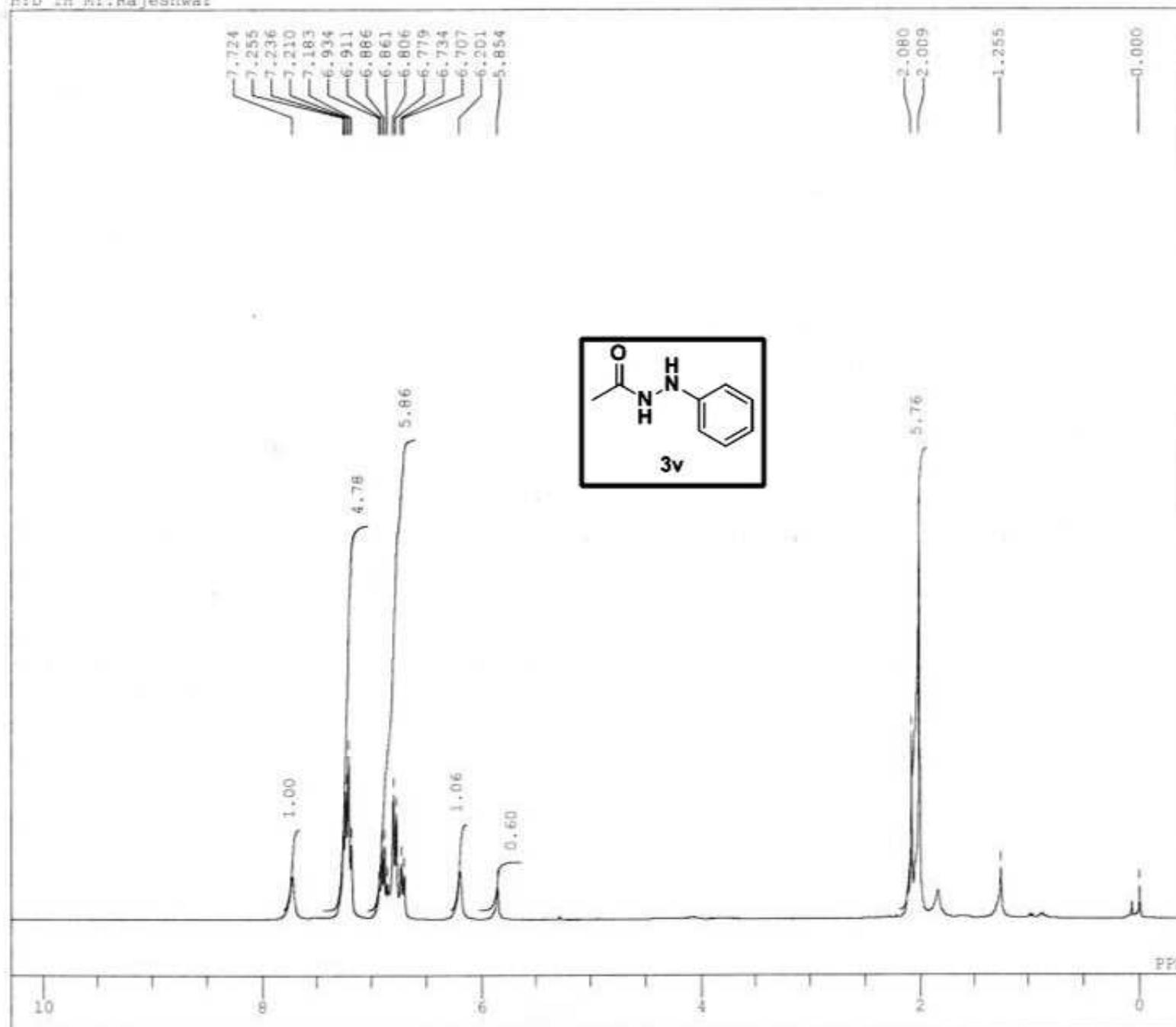


JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\OAC_13C.e
COMNT OAC_1H Mr.Rajeshwar
DATIM Wed Jul 25 15:52:54 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 100
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

HYD 1H Mr.Rajeshwar

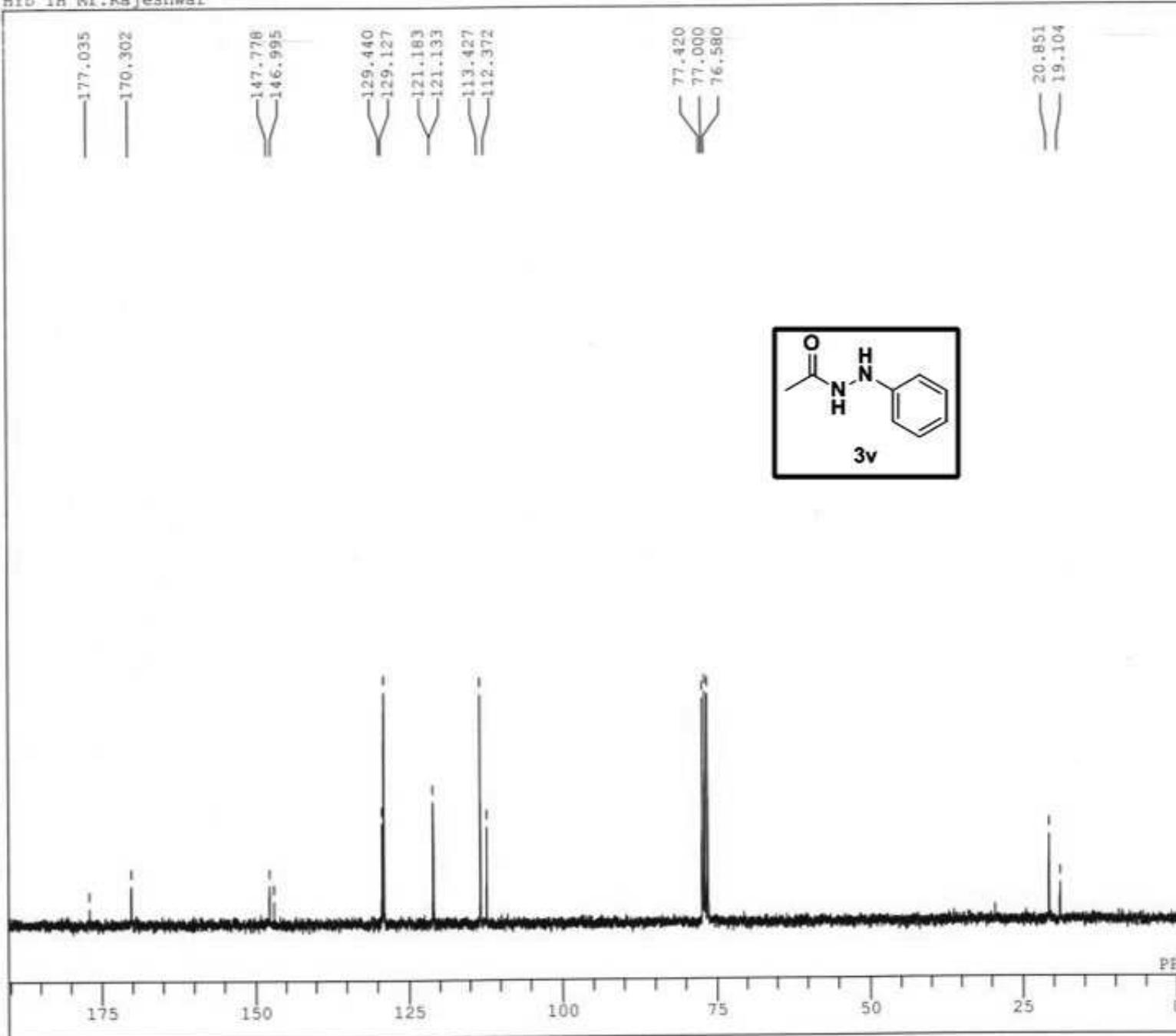


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\HYD_1H.al
COMNT HYD 1H Mr.Rajeshwar
DATIM Fri Jul 27 14:17:18 2012
QBNUC 1H
EXMOD NON
QBFRQ 300.40 MHz
QBSET 130.00 kHz
QBFIN 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 20.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BP 1.20 Hz
RGAIN 14

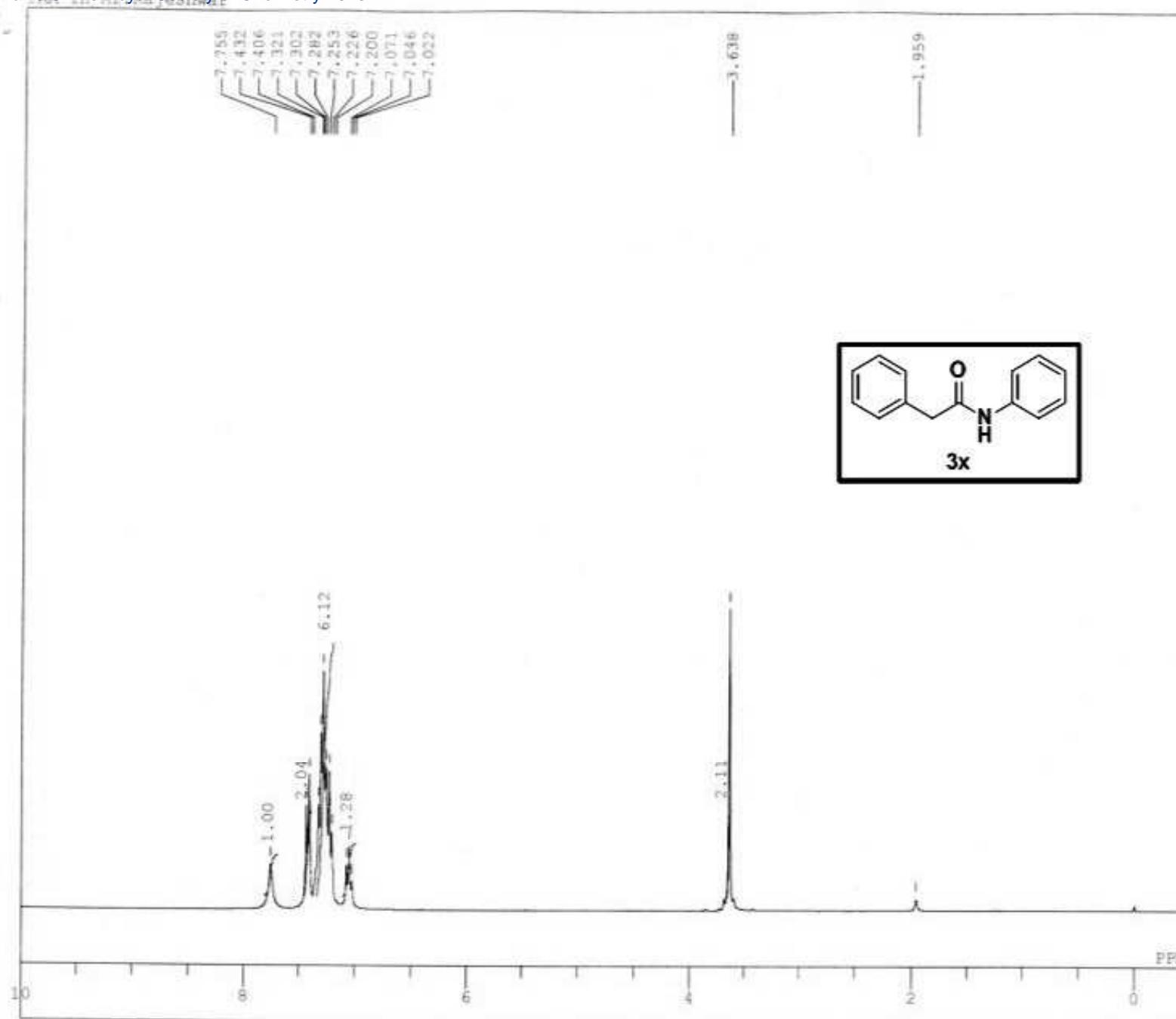
HYD 1H Mr.Rajeshwar



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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

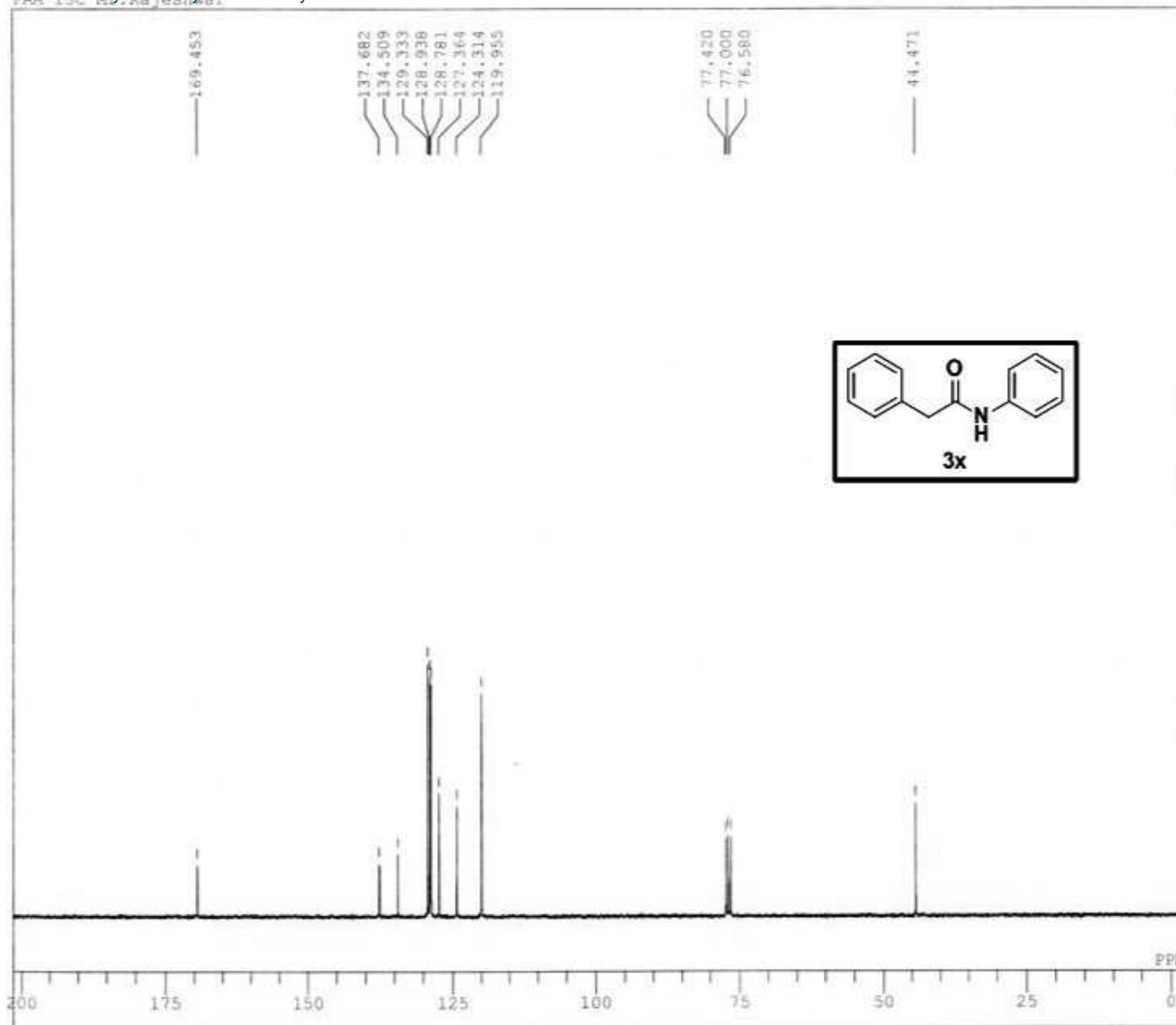
DFILE C:\WINNMR98\Data\HYD_1H_2BCM
COMNT HYD 1H Mr.Rajeshwar
DATIM Fri Jul 27 14:32:40 2012
QBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 300
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25



JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\PAA_1H.al
COMNT PAA_1H_Mr.Rajeshwar
DATIM Fri Sep 07 12:36:16 2012
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 20.7 c
SLVNT CDCL₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 10

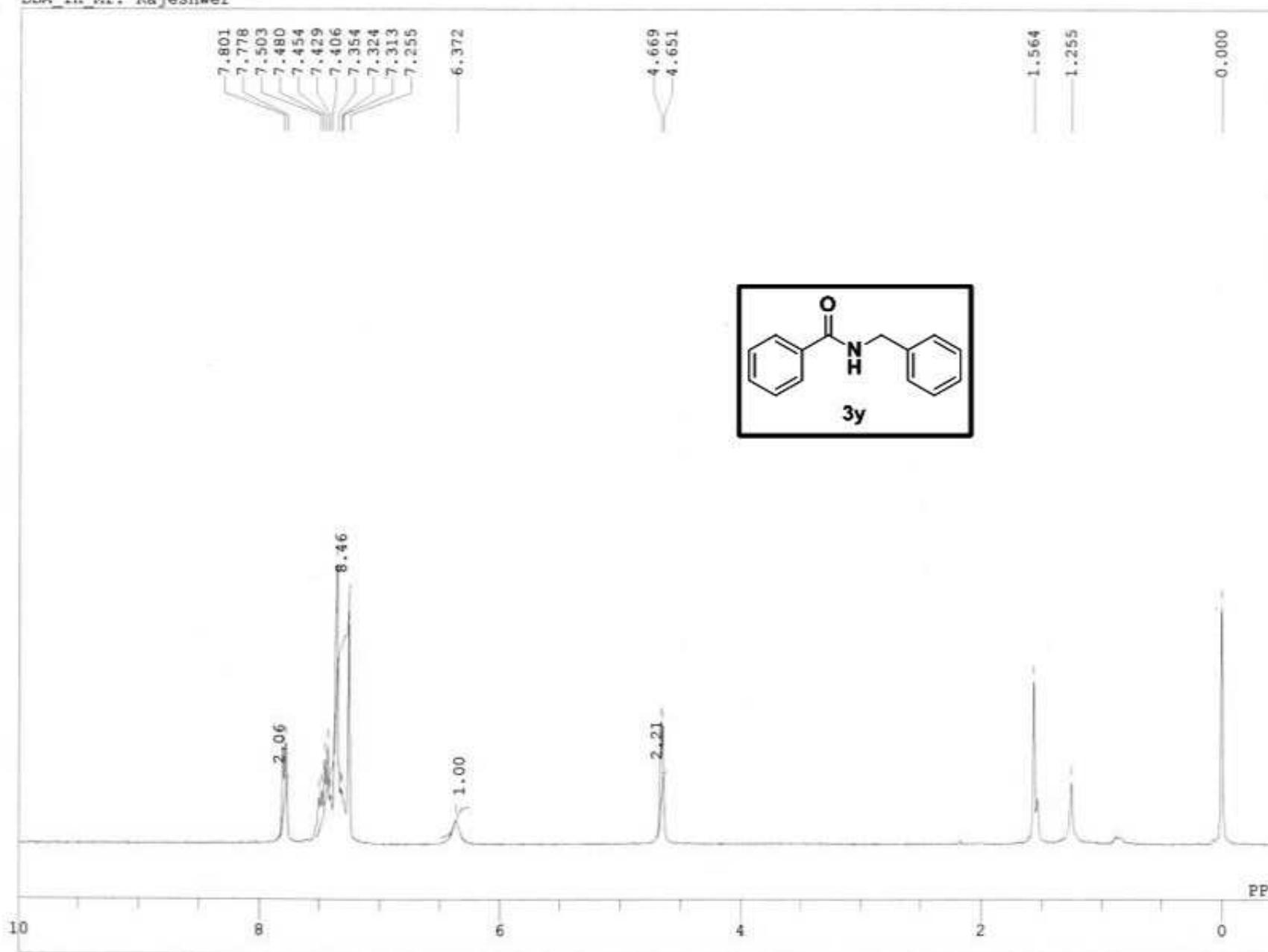


JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT PAA_13C_Mr.Rajeshwar
DATIM Fri Sep 07 12:31:48 2012
QBNUC 13C
EXMOD BCM
QBFRQ 75.45 MHz
QBSET 127.30 KHz
QBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 161
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,,I.T\BBA_1H.als
BBA_1H Mr. Rajeshwer

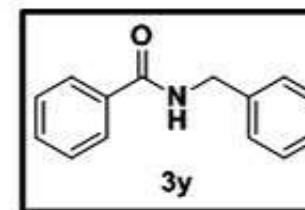
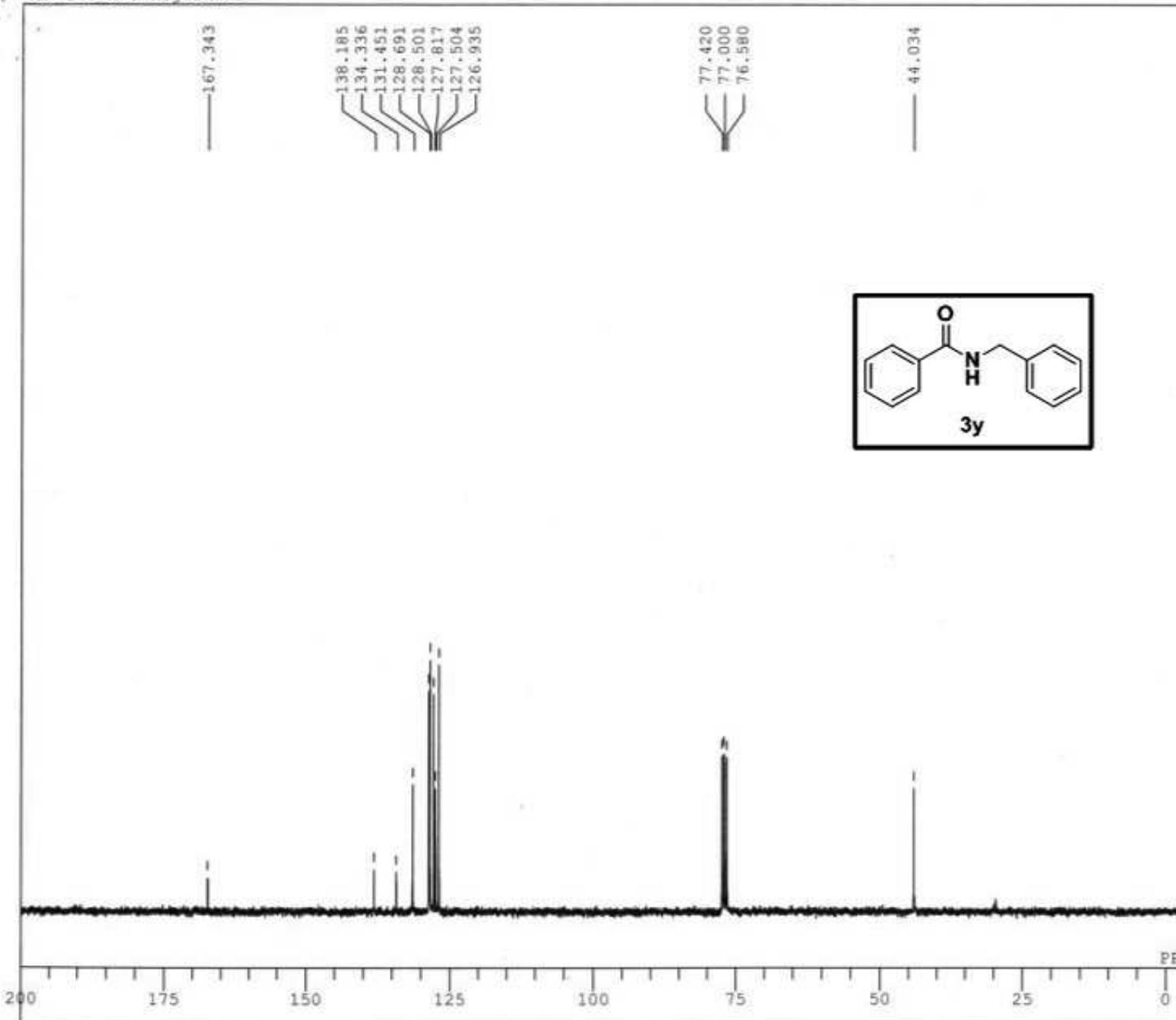


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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT BBA_1H Mr. Rajesh
DATIM Tue Apr 24 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 21
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 23.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 23

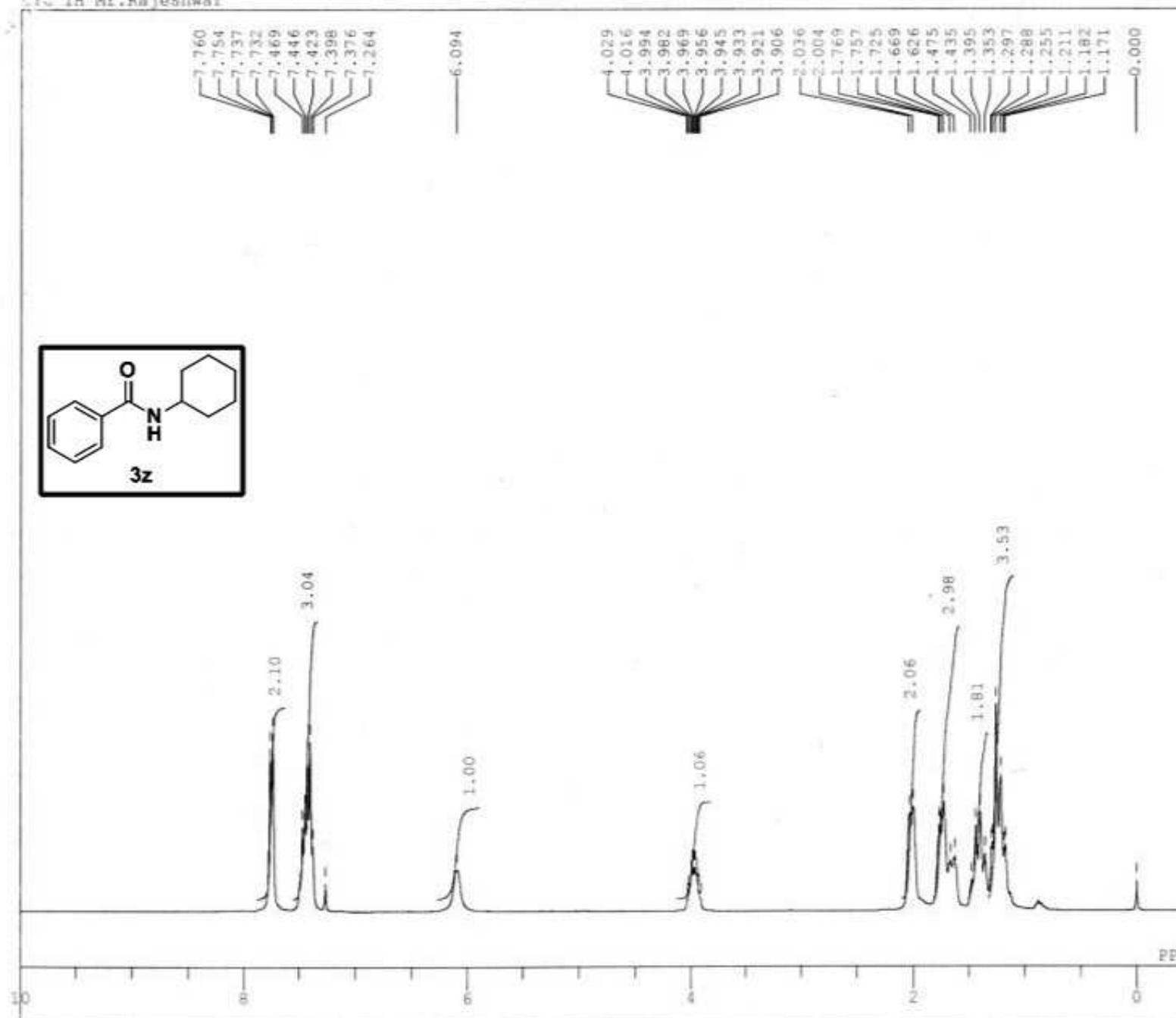


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\ACN_13C.e
COMNT ACN_13C_Mr. Rajeshwer
DATIM Fri Jun 29 17:00:51 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 236
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 23.3 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

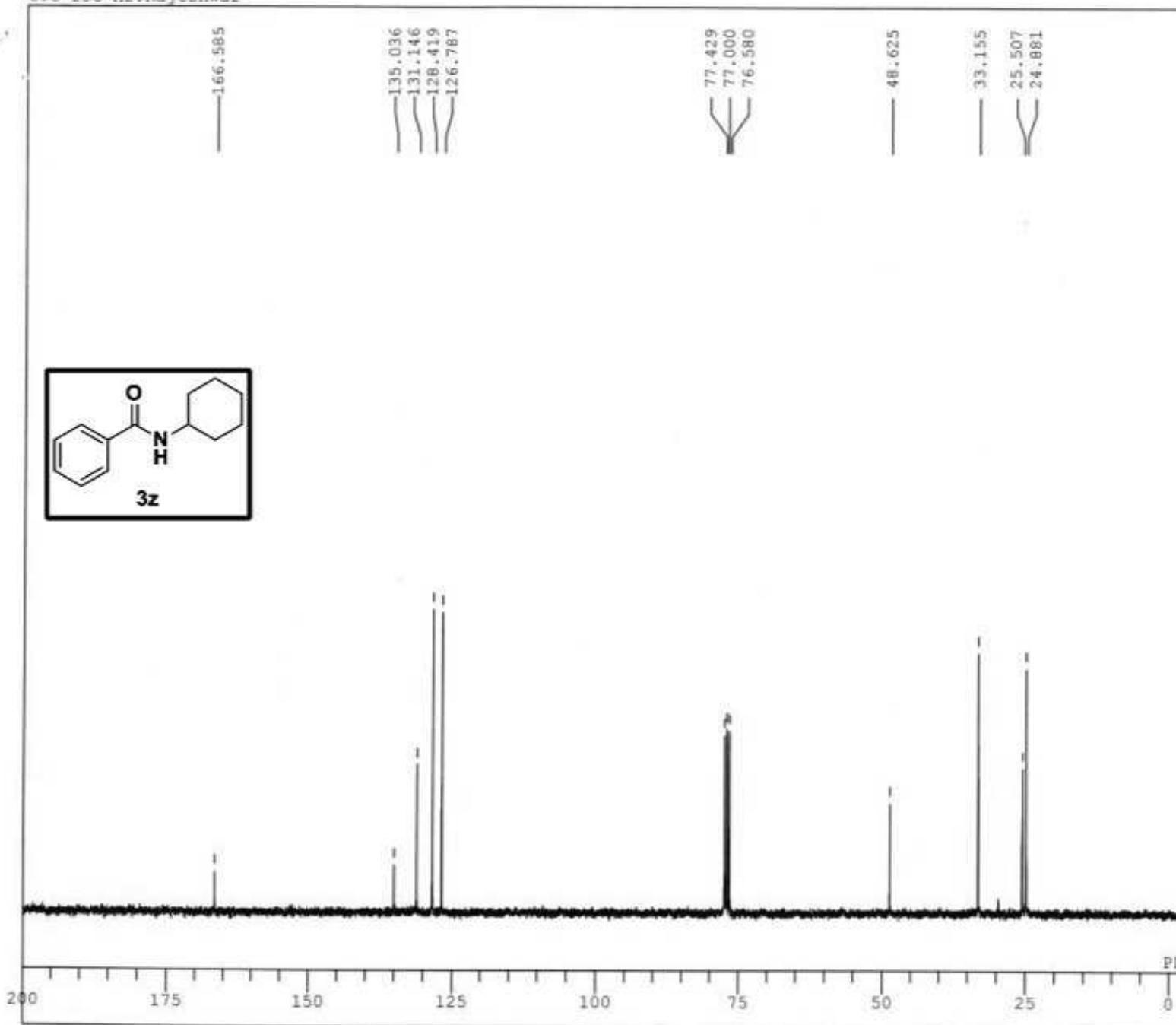
CYC 1H Mr.Rajeshwar



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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\CYC_1H.al
COMNT CYC_1H Mr.Rajeshwar
DATIM Mon Jul 09 13:18:58 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 kHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 32
ACQTM 3.447 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

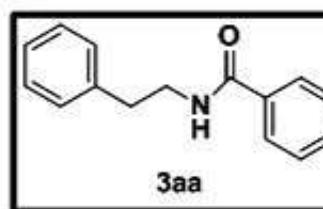
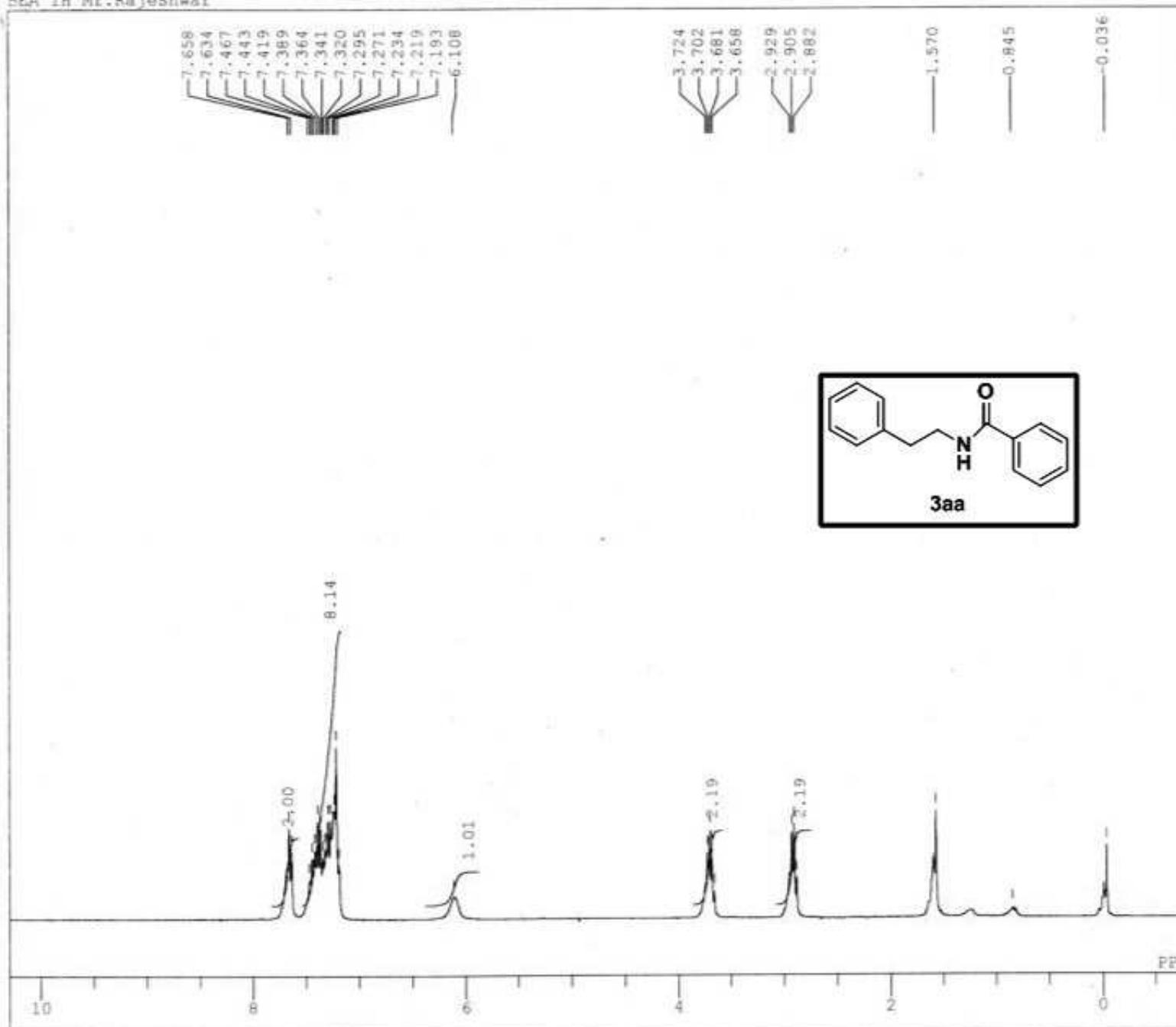


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT CYC_13C_Mr.Rajeshwar
DATIM Mon Jul 09 13:33:54 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 200
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.8 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

BEA_1H Mr.Rajeshwar

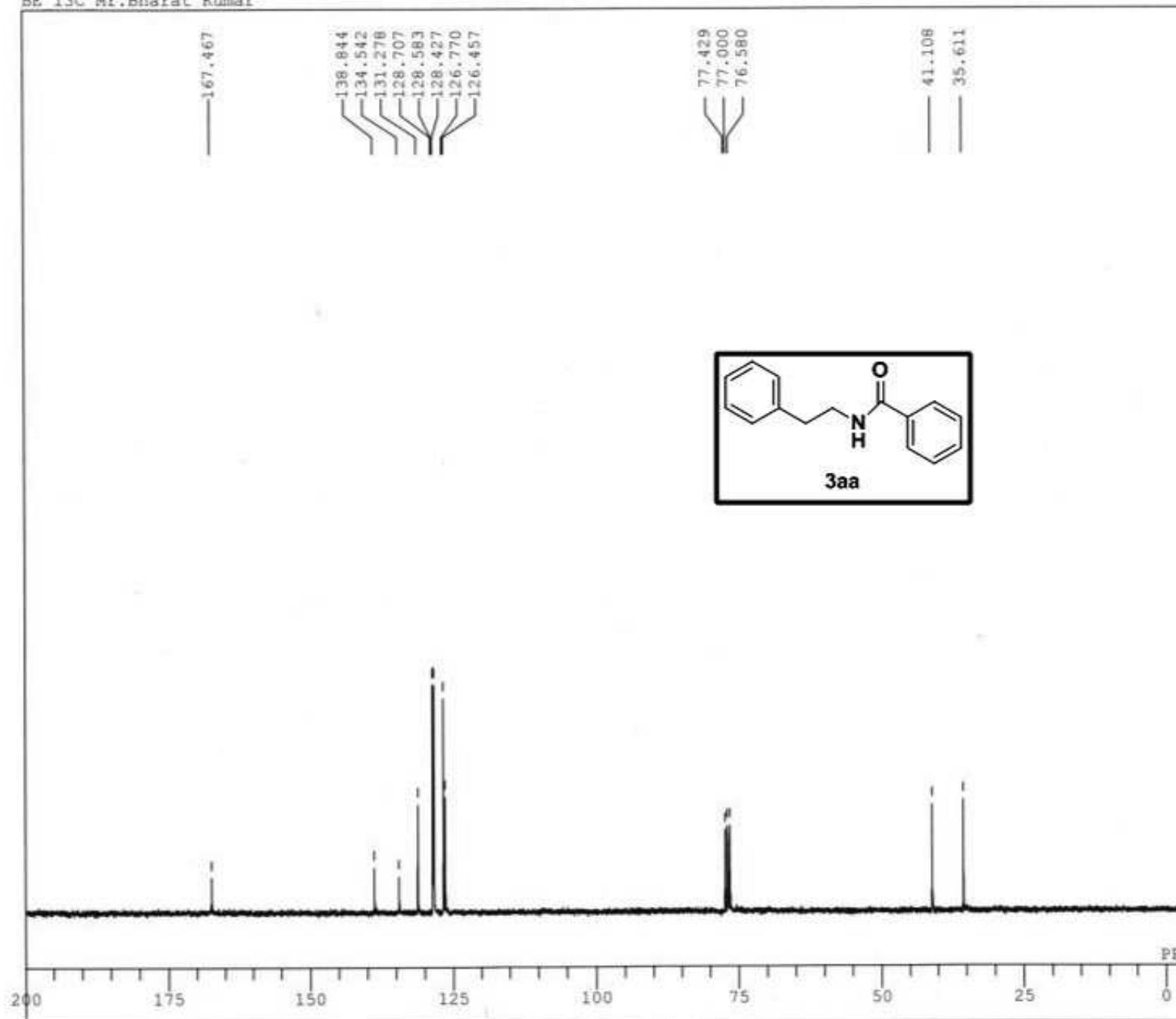


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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

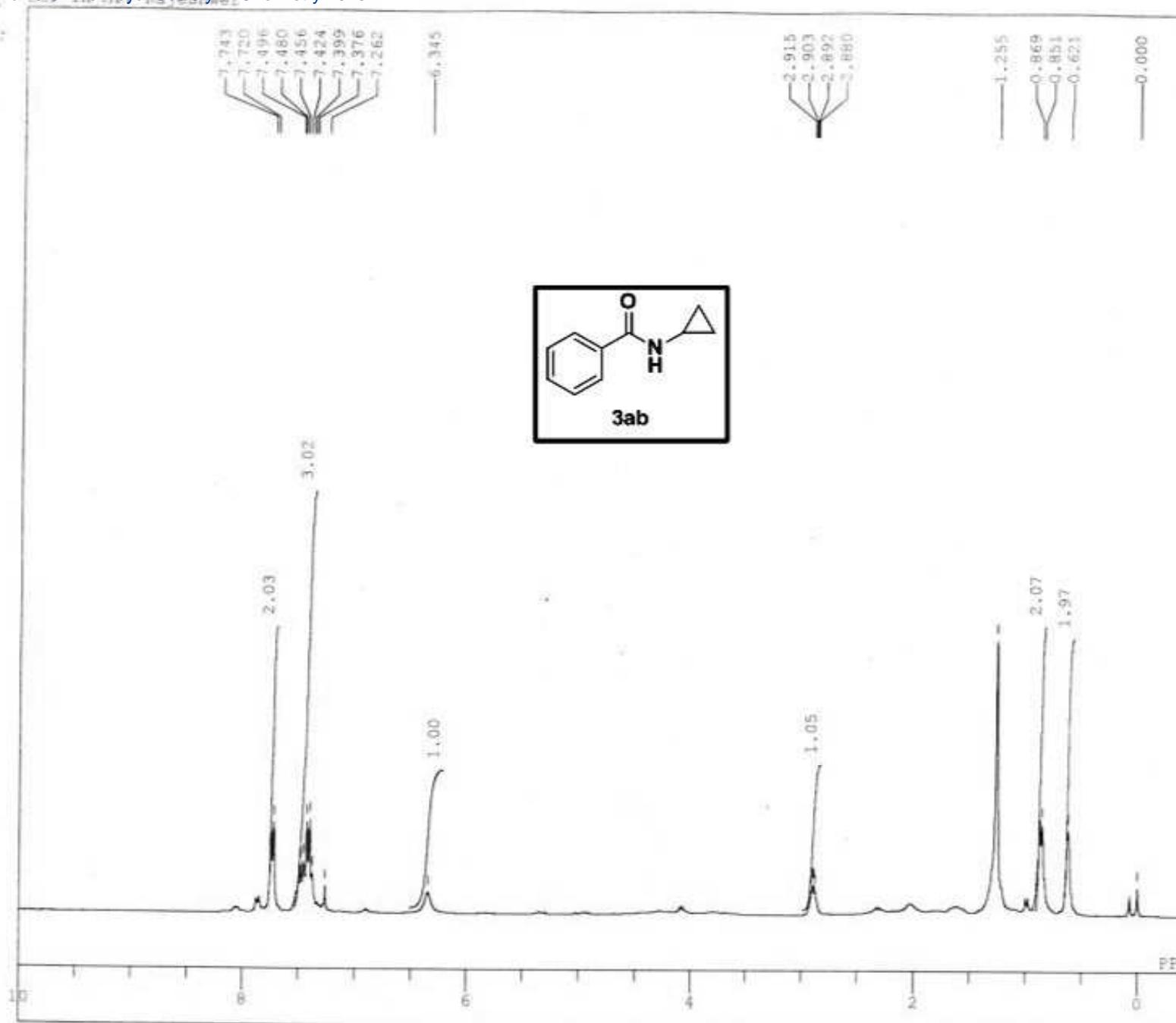
DFILE C:\K.N. Singh,,I.T\BEA_1H.al
COMNT BEA_1H_Mr.Rajeshwar
DATIM Thu Sep 13 11:17:49 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 18.4 c
SLVNT CDCL₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 21



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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT BE_13C_Mr.Bharat_Kumar
DATIM Thu Nov 29 11:08:58 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 133
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



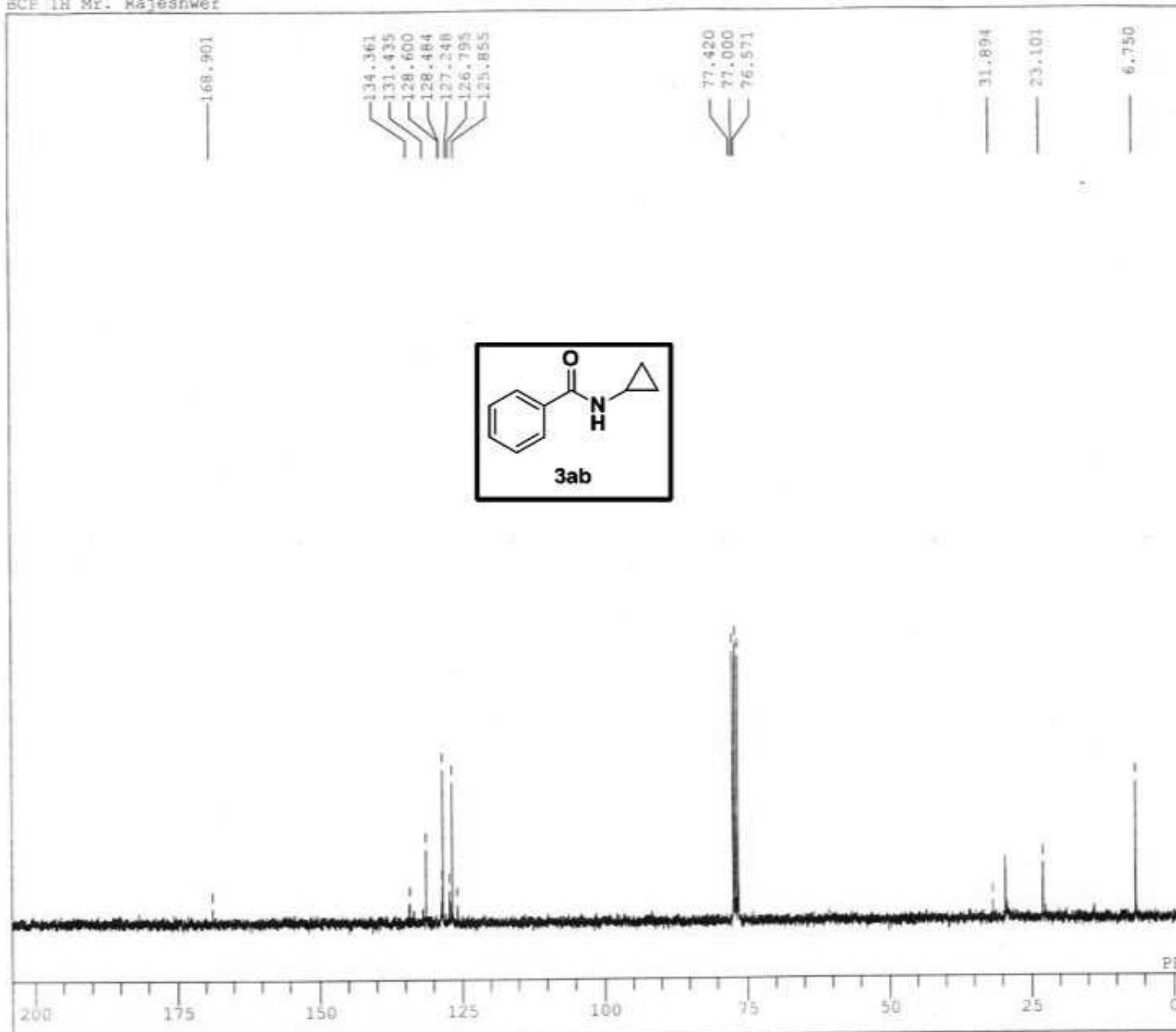
J₇₁

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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\BCP_1H.al
COMNT BCP_1H_Mr. Rajeshwer
DATIM Thu Sep 06 16:15:17 2012
QBNUC 1H
EXMOD NON
QBFRQ 300.40 MHz
QBSET 130.00 kHz
QBFIN 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 20.1 c
SLVNT CDCl₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 14

BCE 1H Mr. Rajeshwer

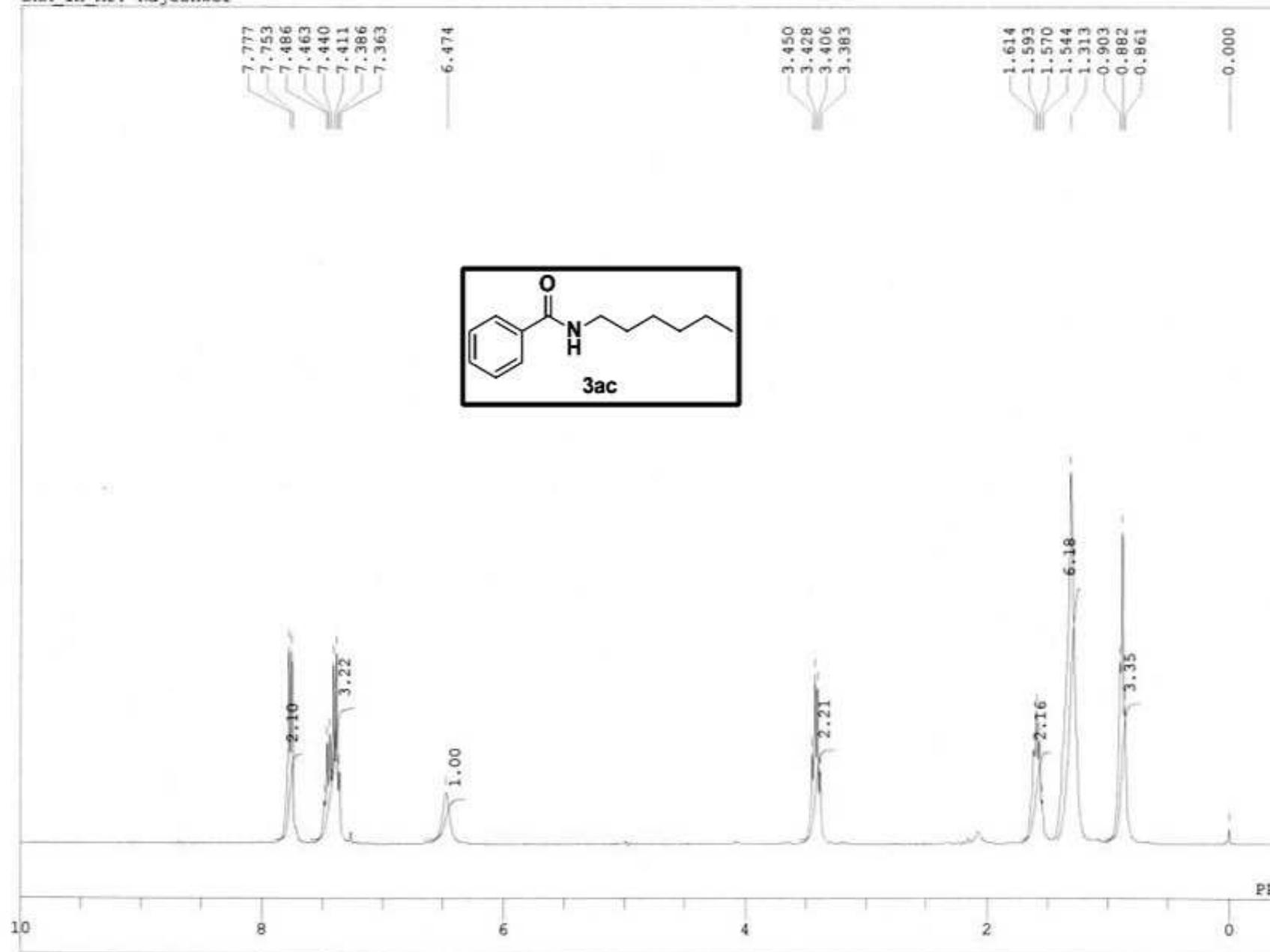


JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\BCP_13C.e
COMNT BCP_1H Mr. Rajeshwer
DATIM Thu Sep 06 16:28:09 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 250
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

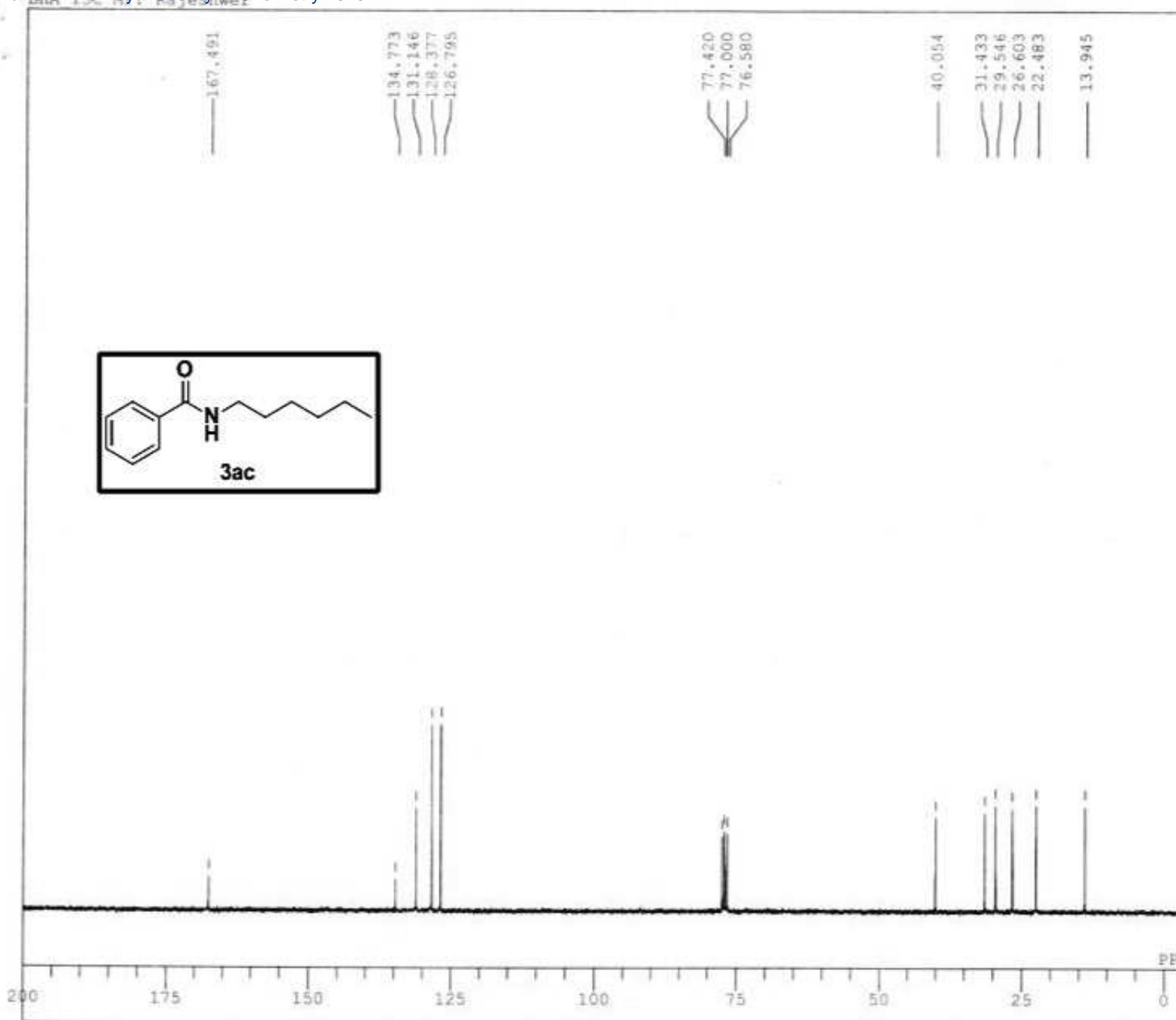
C:\K.N. Singh,,I.T\BHA_1H.als
BHA_1H Mr. Rajeshwer



JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT BHA_1H_Mr. Rajesh
DATIM Thu Sep 13 12:13:
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 18.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 12

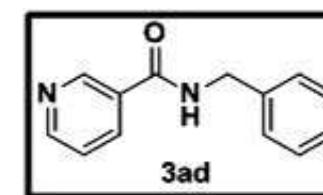
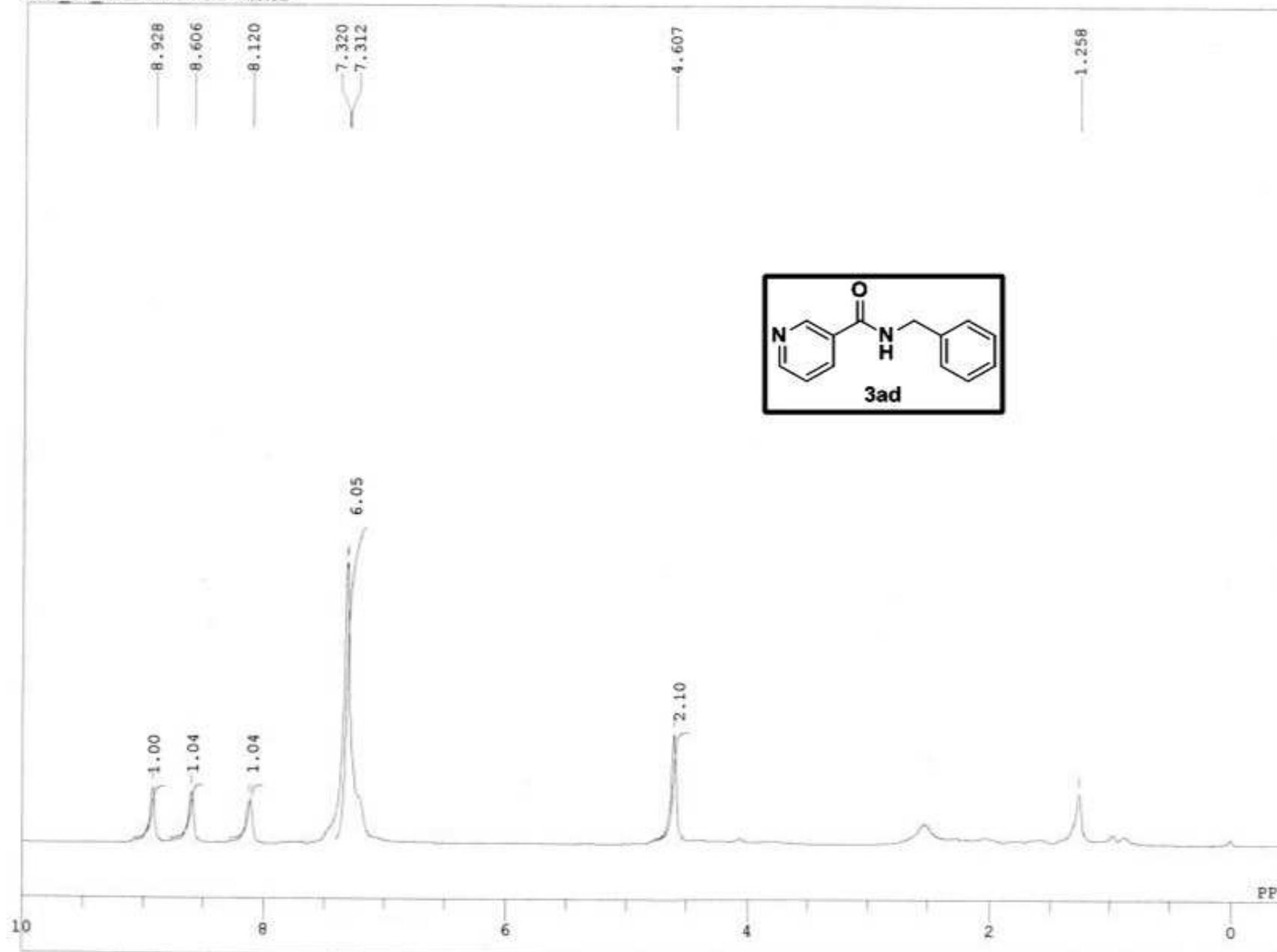


JEOL AL300 FTNMR
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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT BHA_13C Mr. Rajeshwer
DATIM Thu Sep 13 12:23:53 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 120
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCl₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

C:\R.N. Rai\NCA_1H.als
NCA_1H Mr.A. Bharat Kumar

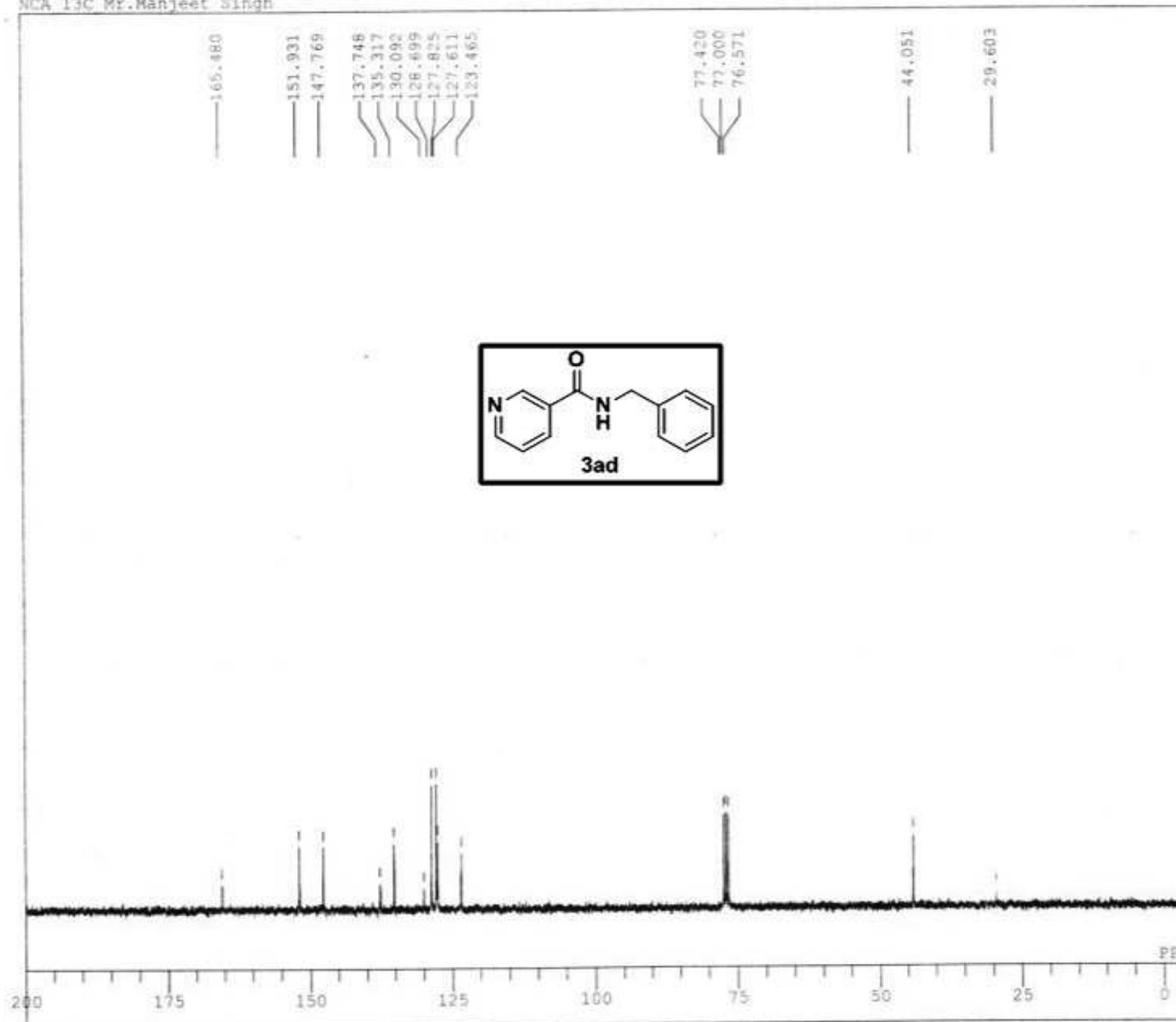


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\R.N. Rai\NCA_1
COMNT NCA_1H Mr.A. Bhar.
DATIM Tue Sep 11 17:03:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 kHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 19
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 14

NCA_13C Mr. Manjeet Singh

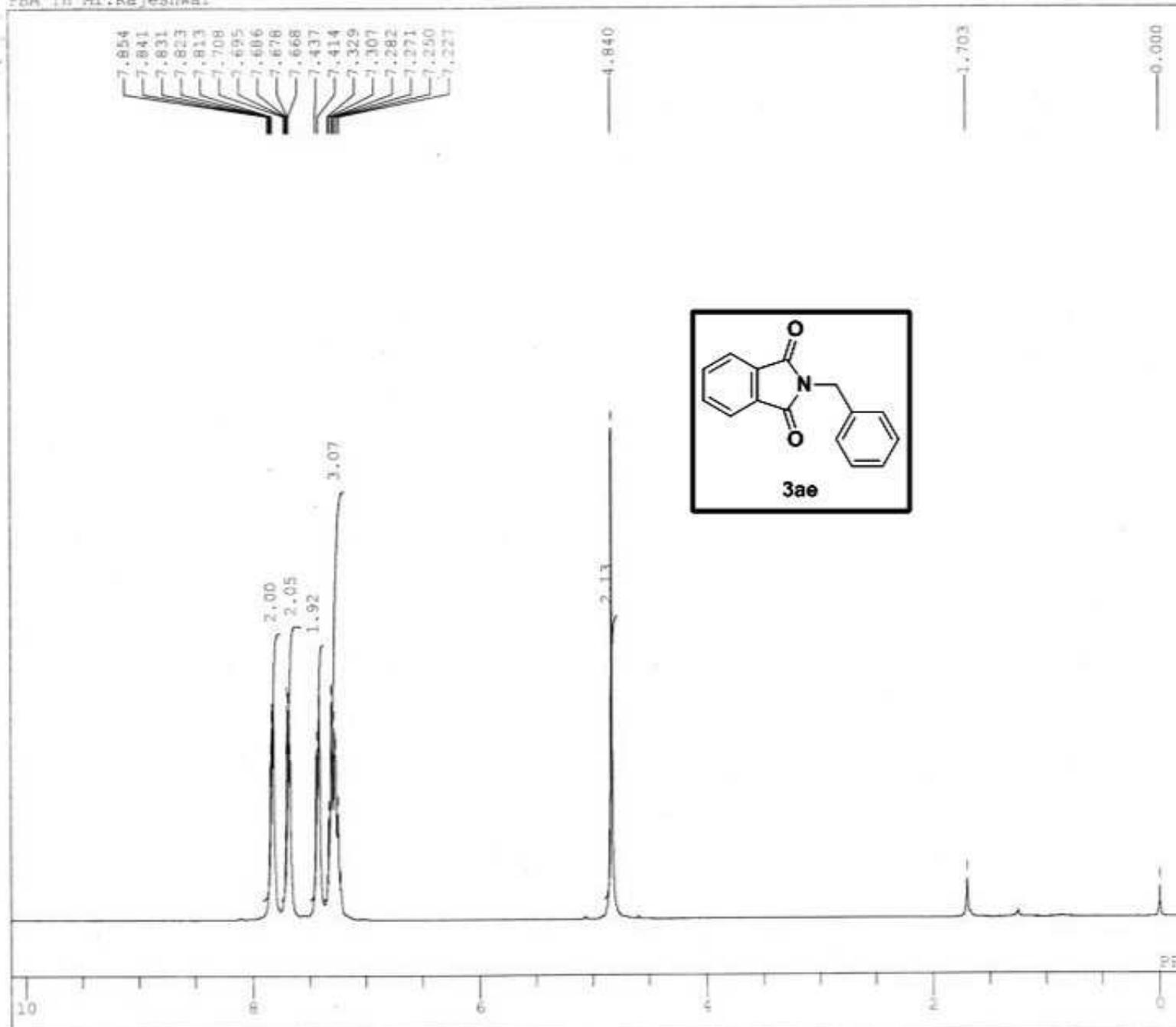


JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT NCA_13C Mr. Manjeet Singh
DATIM Tue Sep 11 17:12:31 2012
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 22.8 °C
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

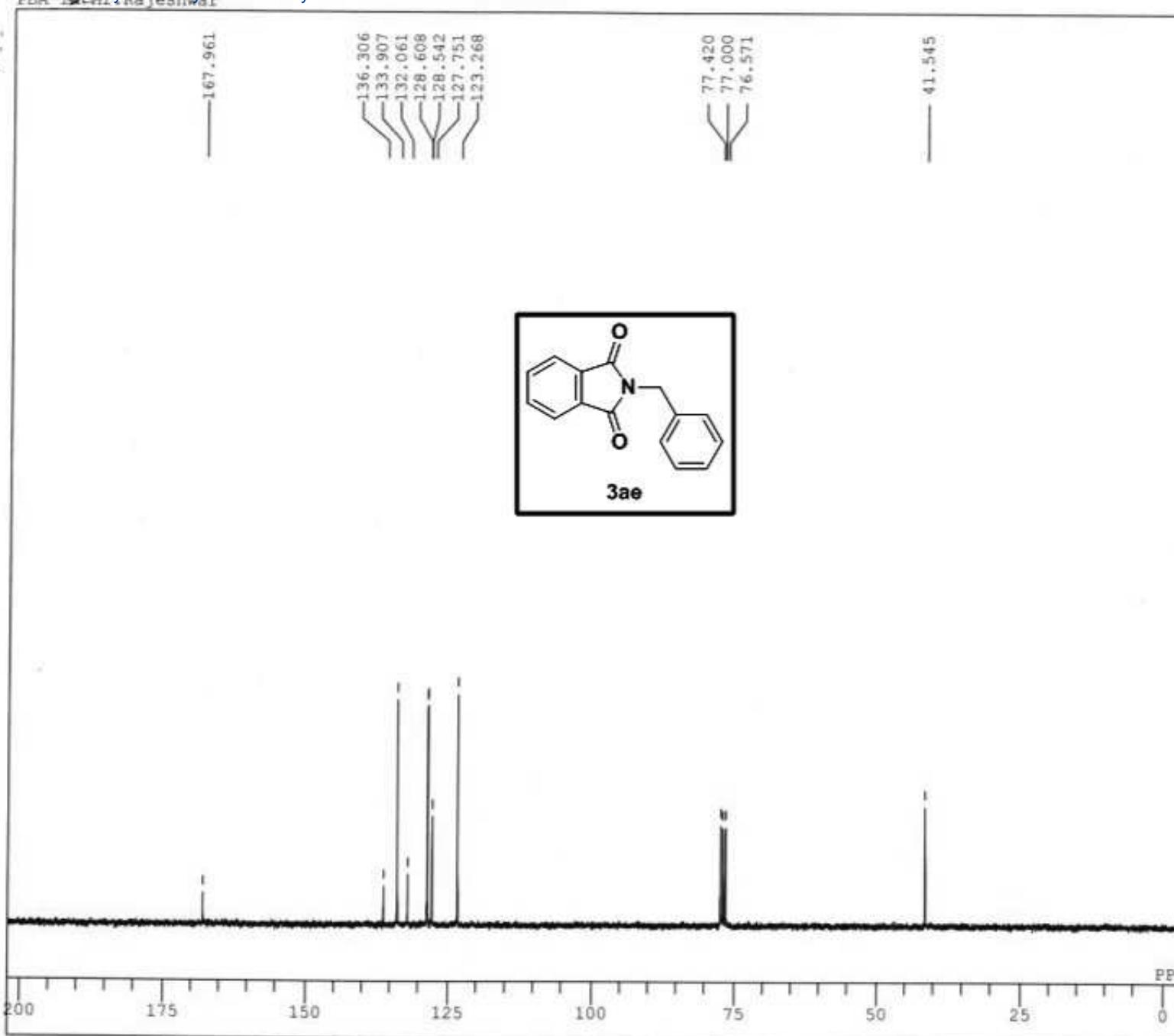
PBA_1H Mr.Rajeshwar



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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\PBA_1H.al
COMNT PBA_1H Mr.Rajeshwar
DATIM Thu Jul 05 14:40:30 2012
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 21.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 14

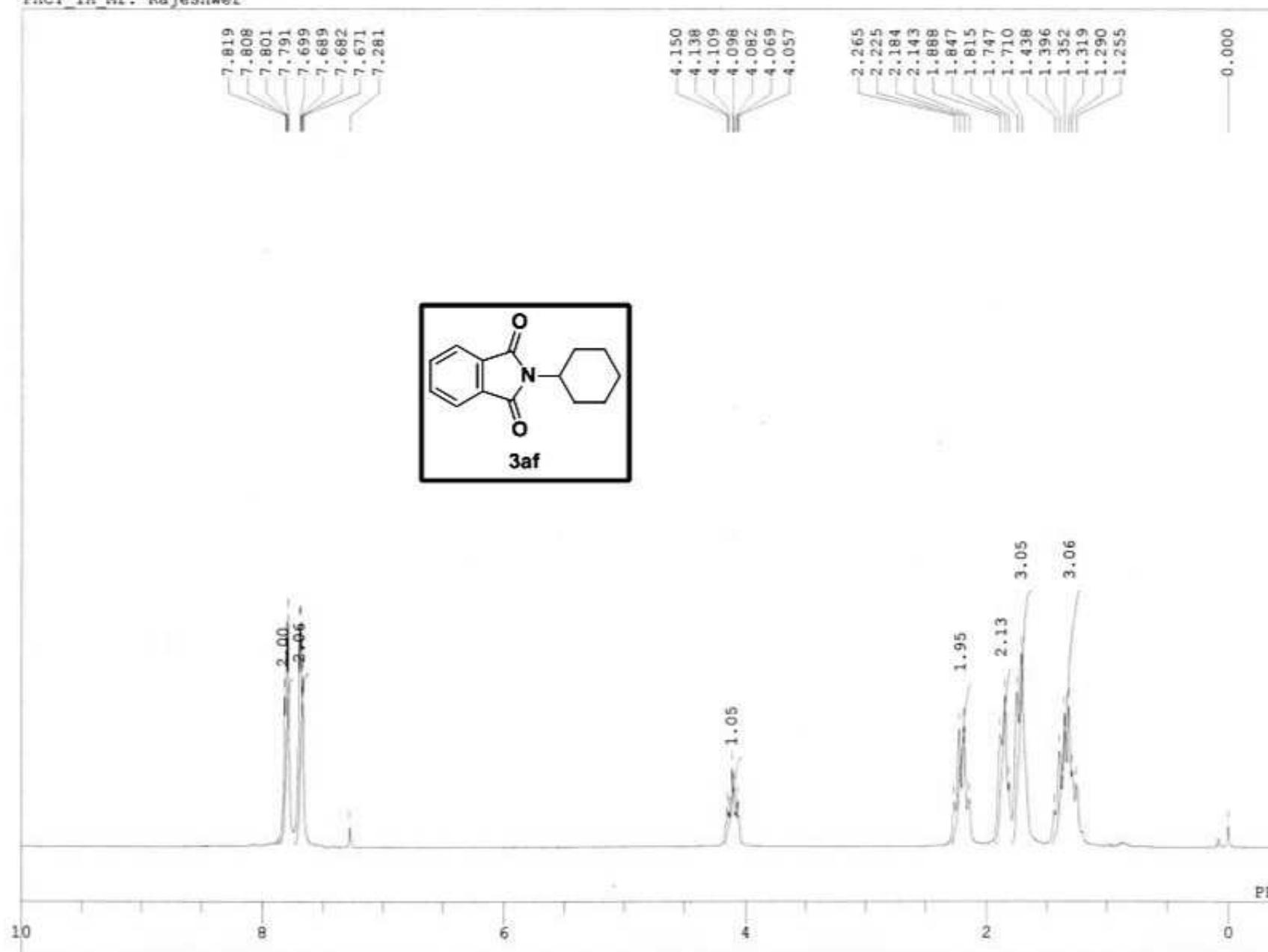


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\Data\PBA_1H2BCM.
COMNT PBA_1H Mr.Rajeshwar
DATIM Thu Jul 05 14:48:20 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 150
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

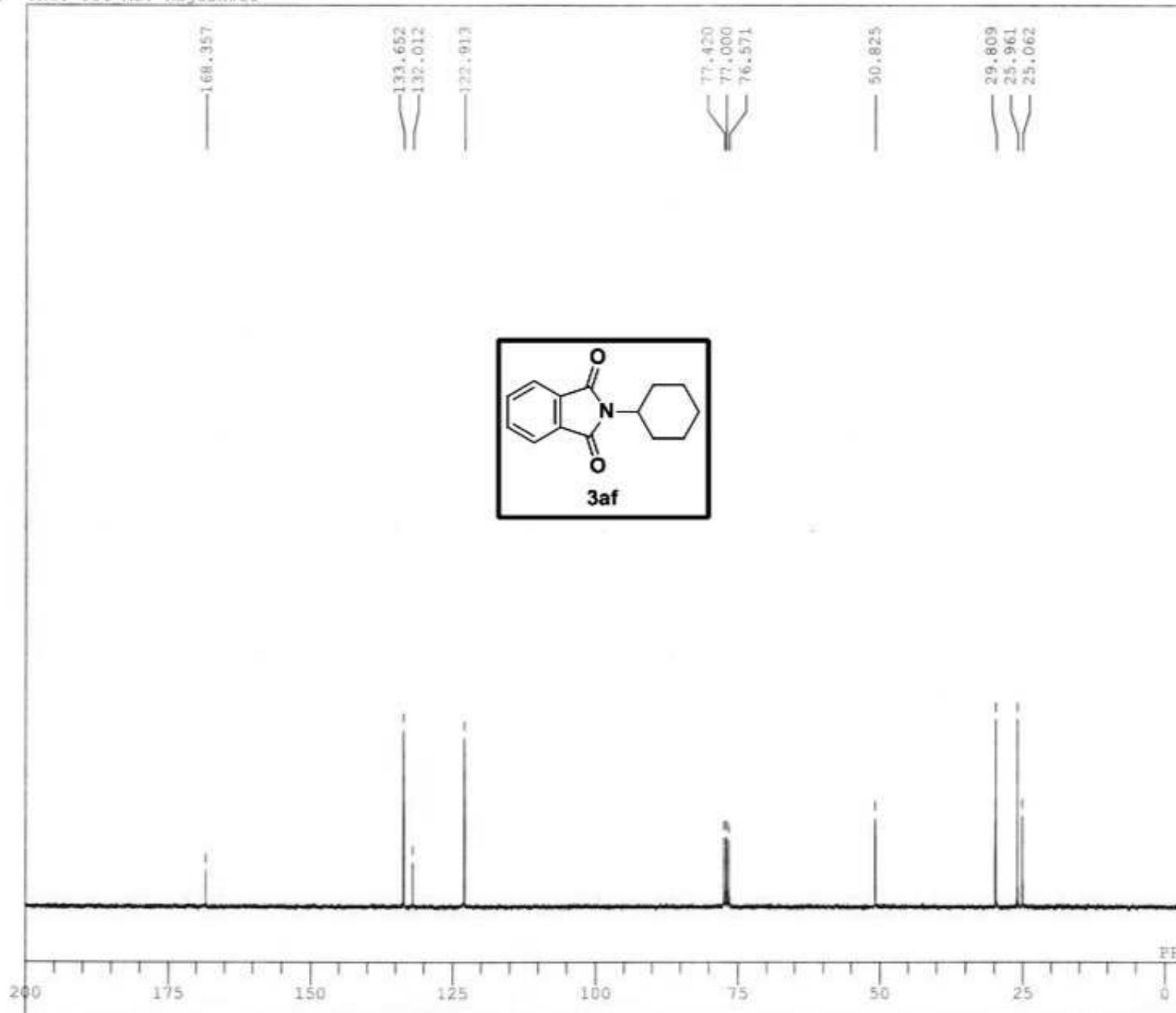
C:\K.N. Singh,,I.T\PhCY_1H.als
PhCY_1H Mr. Rajeshwer



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Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

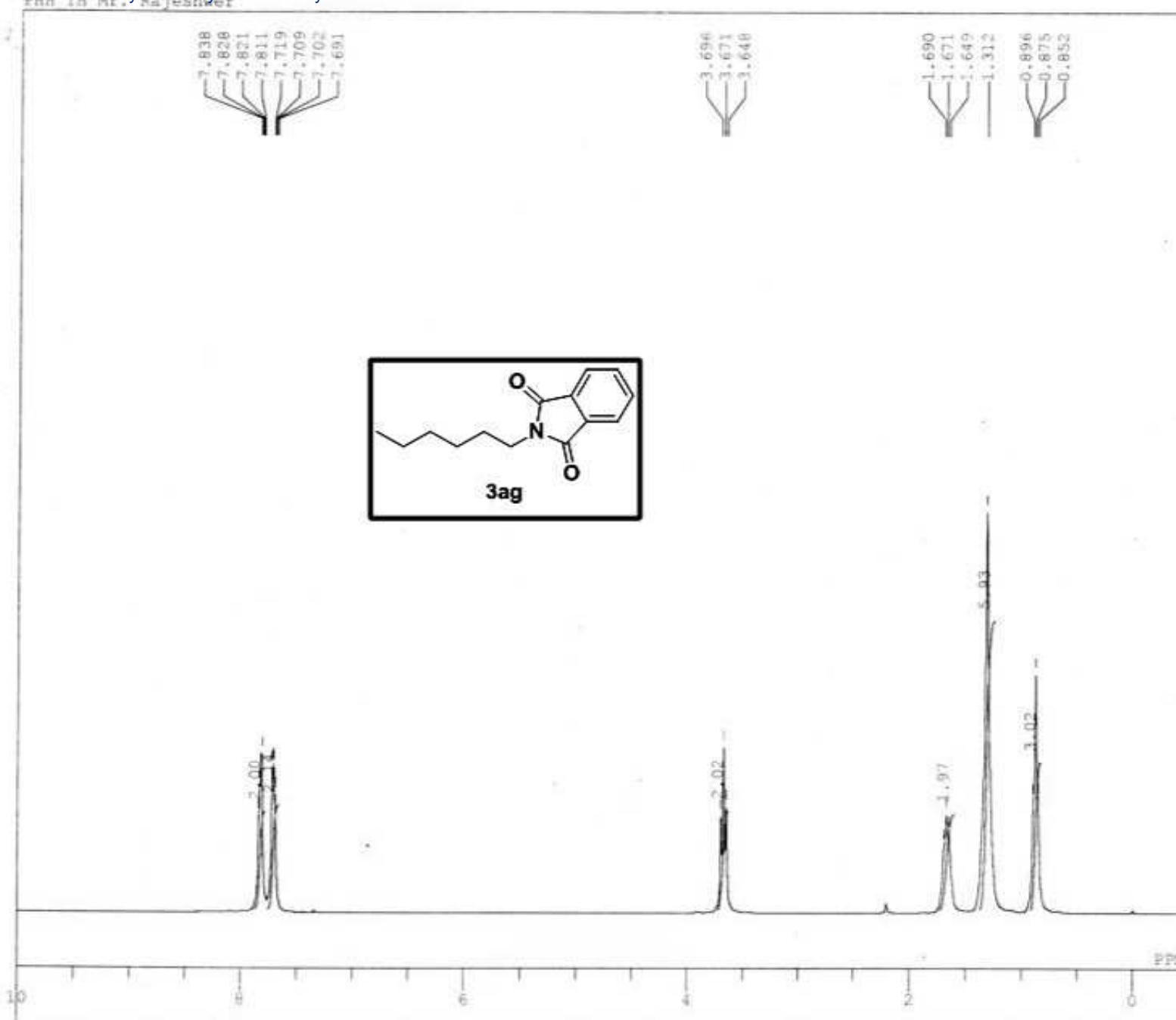
DFILE C:\K.N. Singh,,I.
COMNT PhCY_1H Mr. Rajes
DATIM Mon Jul 30 15:34:
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 kHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 11



JEOL AL300 FTNMR
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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\PhCY_13C.
COMNT PhCY_13C Mr. Rajeshwer
DATIM Mon Jul 30 16:09:30 2012
OBNUC 13C
EXMOD BCM
QBFRQ 75.45 MHz
QBSET 127.30 KHz
QBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 100
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

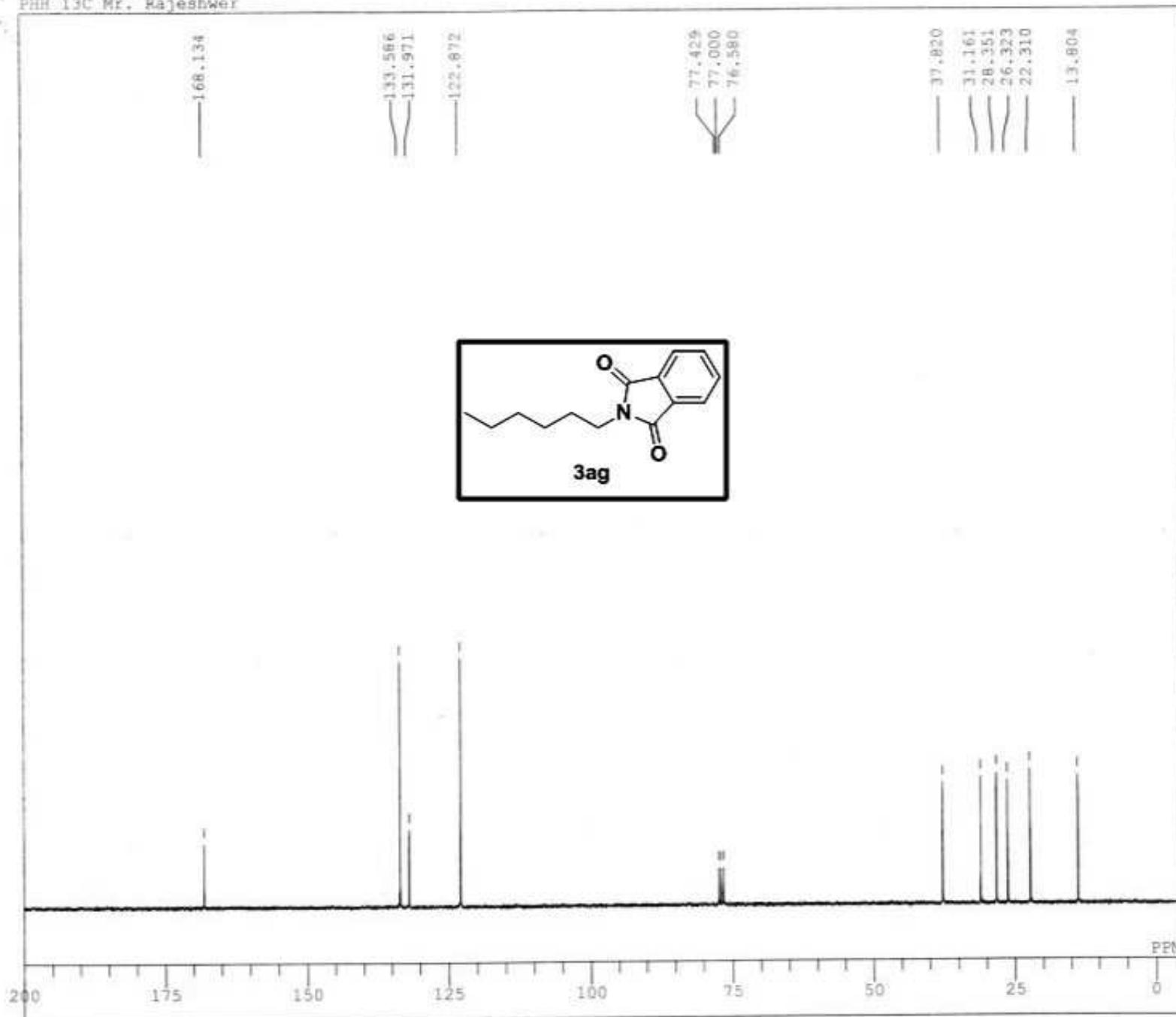


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JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

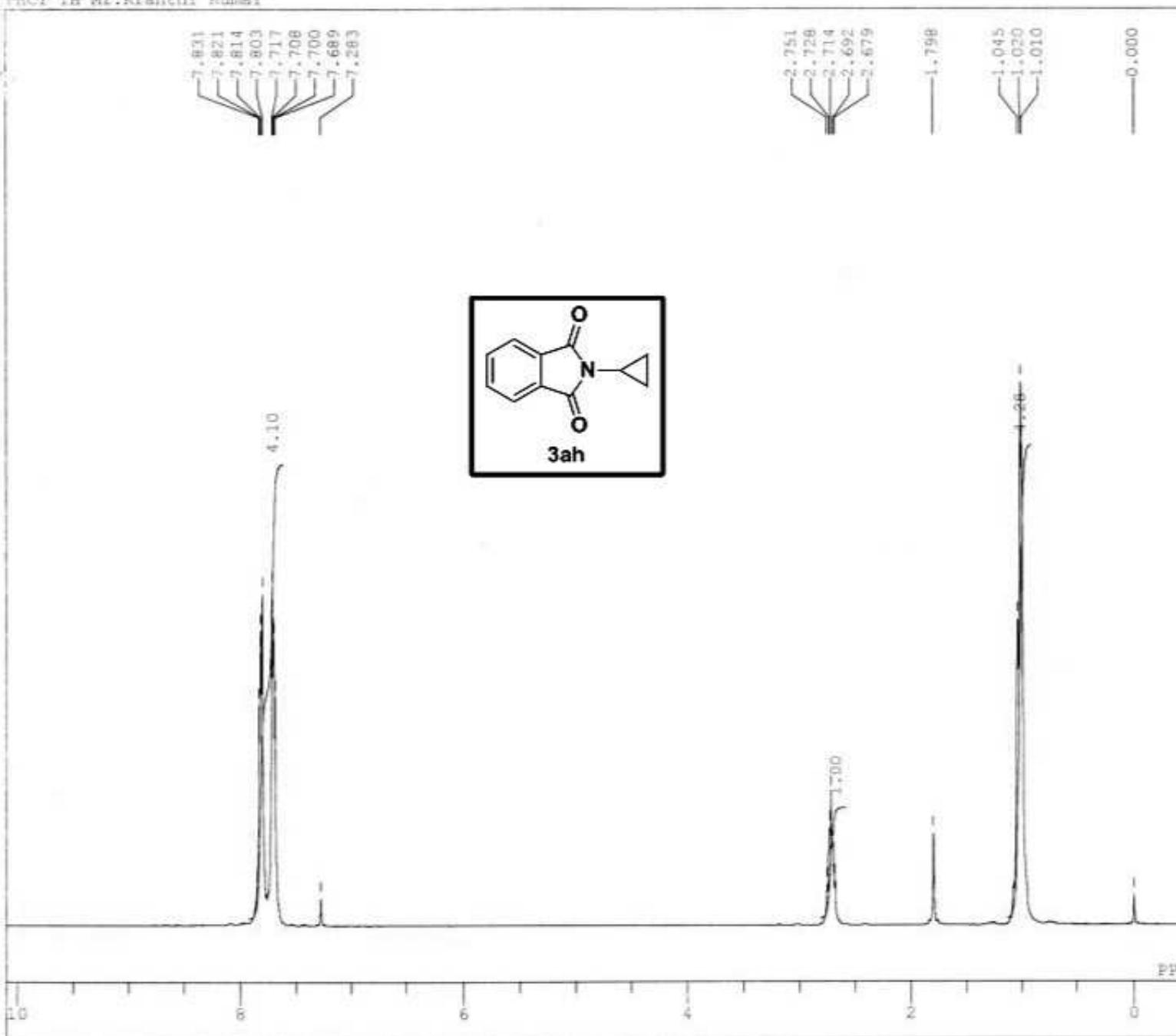
DFILE C:\K.N. Singh,,I.T\PHH_1H.s1
COMNT PHH_1H Mr. Rajeshwer
DATIM Tue Sep 11 13:11:23 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 kHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCl₃
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 7



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

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON\ DEFAULT.
COMNT PHH 13C Mr. Rajeshwer
DATIM Tue Sep 11 13:16:24 2012
QBNUC 13C
EXMOD BCM
QBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 32
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 1.20 Hz
RGAIN 23

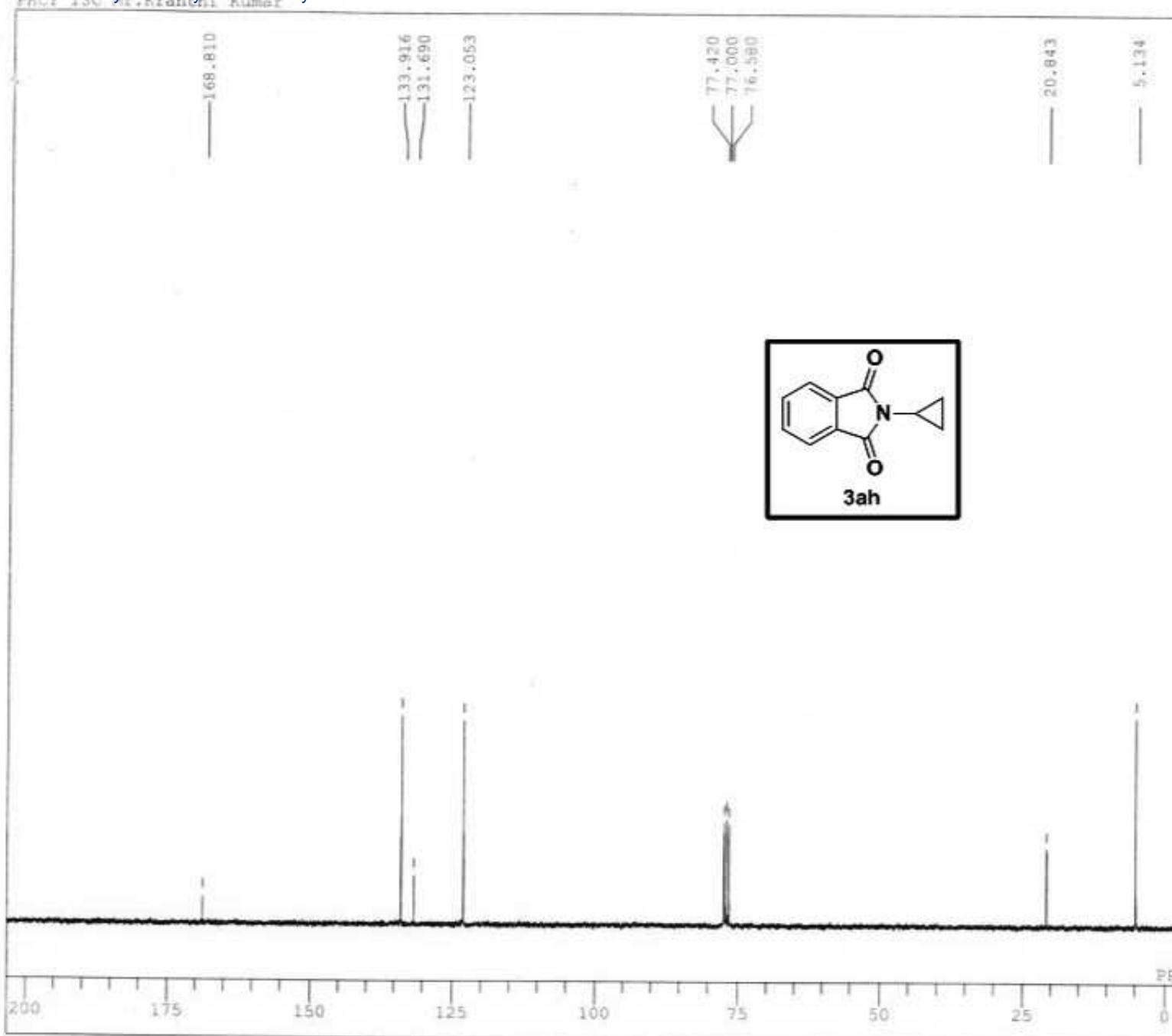


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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON_DEFAULT.
COMNT PHCY 1H Mr.Kranthi Kumar
DATIM Fri Sep 07 12:13:46 2012
QBNUC 1H
EXMOD NON
QBFRQ 300.40 MHz
QBSET 130.00 KHz
QBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 12
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 19.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 14

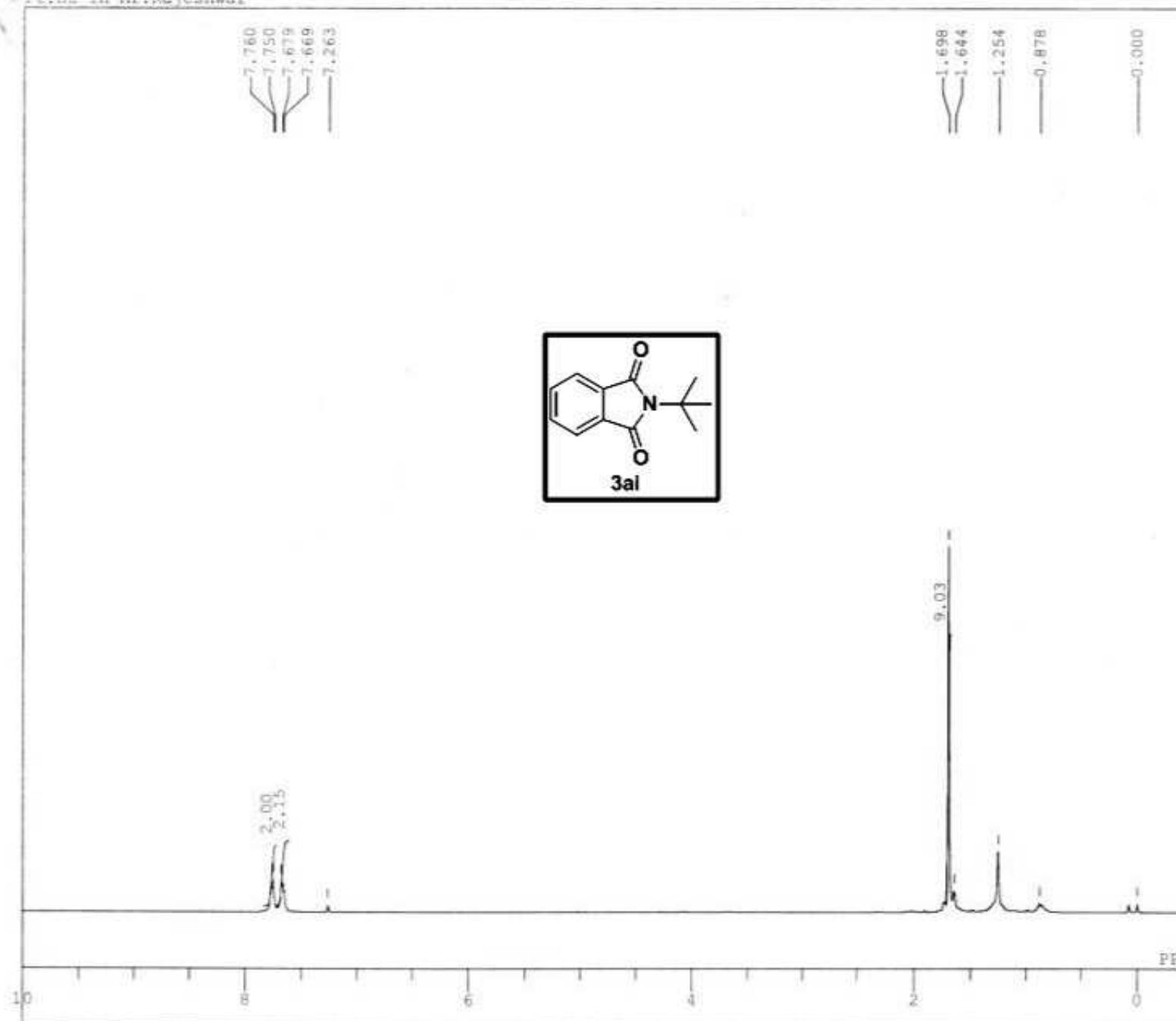


JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\Krantaz K. Tunagala\PHCY_13C Mr.Kranthi Kumar
COMNT PHCY 13C
DATIM Fri Sep 07 12:22:13 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 102
ACQTM 1.606 sec
FD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

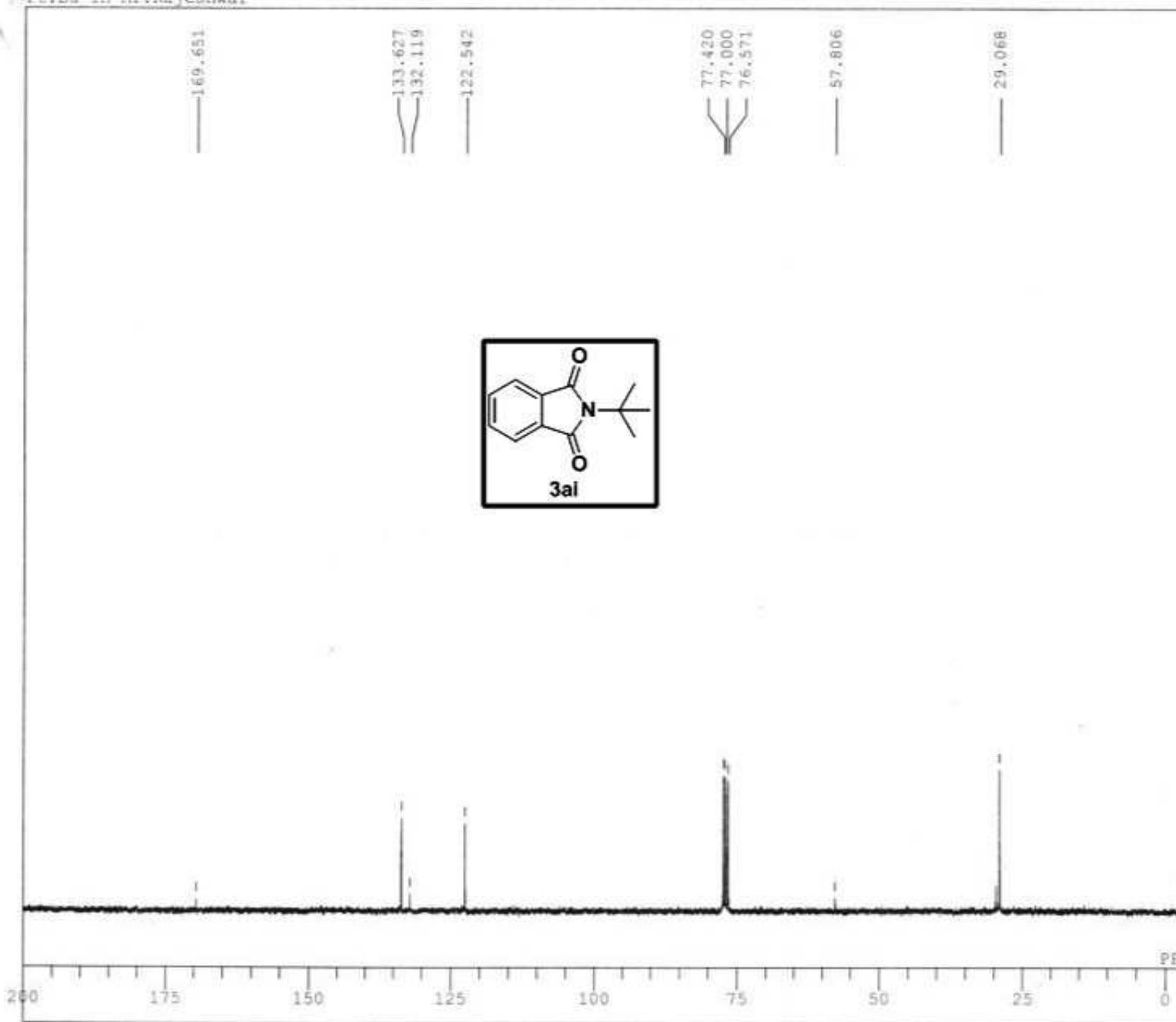
Pt.Bu_1H Mr.Rajeshwar



JEOL AL300 FTNMR
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Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\Pt.Bu_1H.
COMNT Pt.Bu_1H Mr.Rajeshwar
DATIM Fri Sep 14 12:13:43 2012
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 19.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 15

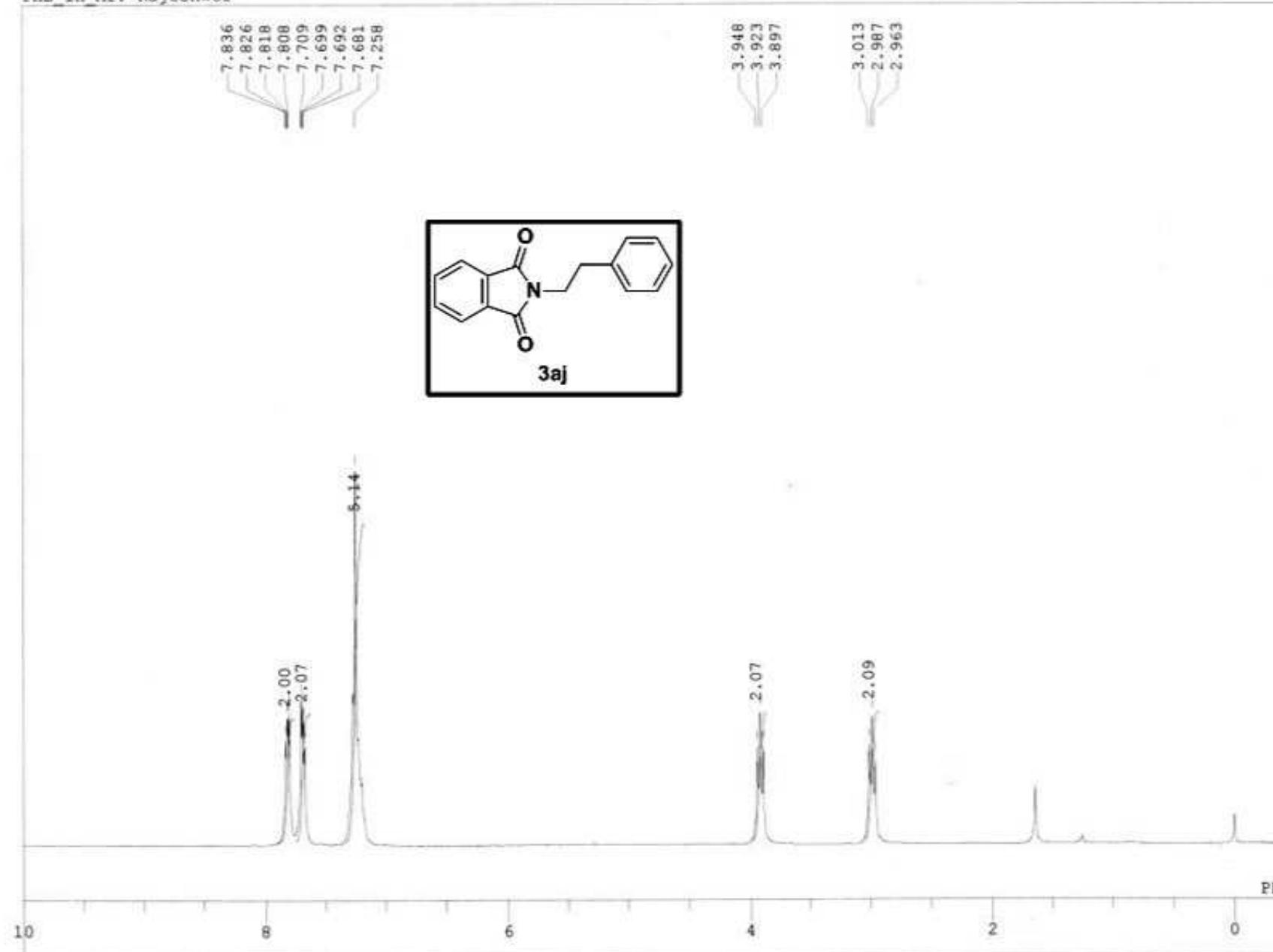


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,, I.T\Pt.Bu_13C
COMNT Pt.Bu_1H Mr.Rajeshwar
DATIM Fri Sep 14 12:06:26 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 230
ACQTM 1.606 sec
PD 1.394 sec
FW1 6.0 us
IRNUC 1H
CTEMP 18.1 c
SLVNT CDCL₃
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh,,I.T\PHE_1H.als
PHE_1H Mr. Rajeshwer

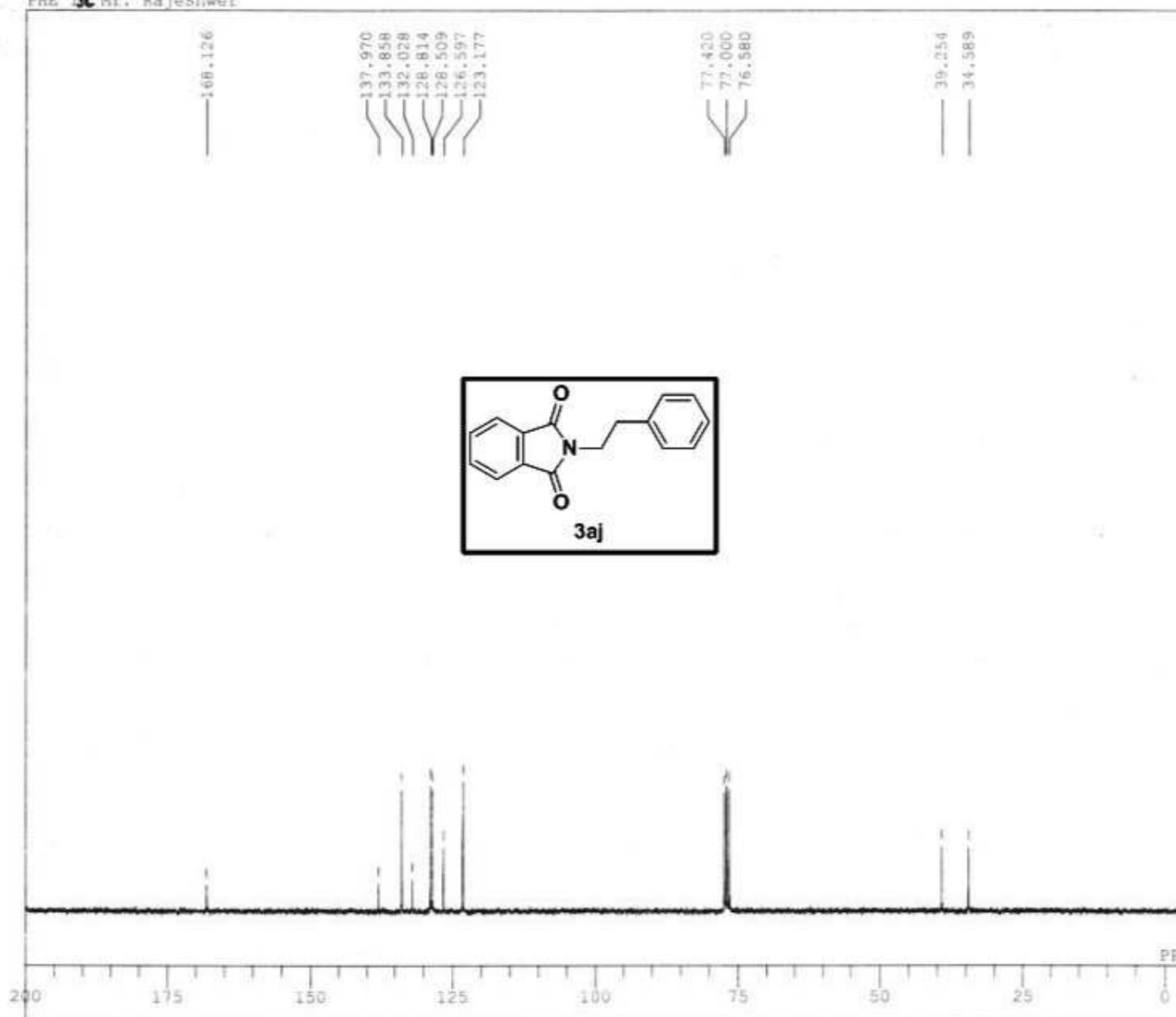


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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University
VARANASI-221005

Operator : Nagendra Kuma
Shishir Singh

DFILE C:\K.N. Singh,,I.
COMNT PHE_1H Mr. Rajesh
DATIM Mon Sep 10 15:04:
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 20.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 14



JEOL AL300 FTNMR
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Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\Data\PHE_1H2BCM
COMNT PHE 1H Mr. Rajeshwer
DATIM Mon Sep 10 15:19:25 2012
GBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 250
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 24