Electronic Supplementary Information

A Simple and Sustainable Tetrabutylammonium Fluoride–Catalyzed Synthesis of Azaarene-Substituted 3–Hydroxy–2–oxindoles through sp^3 C–H Functionalization†

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A. General Experimental:

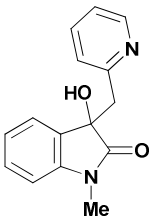
All starting materials were obtained from commercial suppliers, and were used without further purification. 2–methylpyridine, and 2–methyl quinoline were purchased from Alfa Aeser. 2,6–Lutidine, 4–methylpyridine, and TBAF·3H_2O were purchased from Sigma Aldrich, USA. 1–(Prop–2–yn–1–yl)indoline–2,3–dione, 1–allylindoline–2,3–dione, 1–benzylindoline–2,3–dione, 1–ethylindoline–2,3–dione, 5–bromoindoline–2,3–dione, 5,7–dibromoindoline–2,3–dione, and 5–nitroindoline–2,3–dione were prepared according to standard literature procedures.[1,2] Thin layer chromatography (TLC) was performed on Merck Kieselgel 60 GF_{254} plates (thickness 0.25 mm). Visualization was performed with a 254 nm UV lamp and by staining in I_2 chamber. Microwave reactions were conducted using CEM Discover BenchMate single mode microwave reactor with a sealed pressure regulation 10-mL pressurized vial with "snap-on" cap and teflon-coated magnetic stir bar using MilliQ water. The standard temperature control system consists of a non-contact calibrated infrared sensor which monitors and controls the temperature of the reaction vessel located in the instrument cavity. The ^{1}H– and ^{13}C–NMR spectra were recorded on a JEOL AL300 FTNMR spectrometer in $CDCl_3$/DMSO–d_6. Chemical shifts are expressed in parts per million (δ) using tetramethylsilane (TMS) as an internal standard. Coupling constants (J) are reported in Hertz (Hz). Splitting patterns are designated as s (singlet), br s (broad singlet), d (doublet) and m (multiplet). Single crystal X–ray data of the product were collected on an Xcalibur Oxford diffractometer.

B. General Experimental Procedure:

In a sealed pressure regulation 10-mL pressurized vial were placed α/γ–alkyl azaarene **1** (2 mmol), TBAF·3H_2O (10 mol%, 0.2 mmol, 62 mg), isatin **2** (2 mmol), H_2O (2 mL), and a teflon coated magnetic stir bar. The vial was closed with a 'snap on' cap, stirred at room temperature for 1 min and then placed into the MW cavity. Microwave irradiation of 80 W at a set temperature of 100 °C was used to conduct the reaction for 5 min. After completion of reaction (monitored through TLC), the mixture was cooled to room temperature, poured into a vessel containing distilled water and then extracted with ethyl acetate (2 x 10 mL). The combined organic phase was dried over Na_2SO_4, filtered and concentrated under rotary vacuum evaporator. The resulting crude product was purified using preparative TLC.

C. Characterization of the products:

1. 3–Hydroxy–1–methyl–3–(pyridin–2–ylmethyl)indolin–2–one (3a):



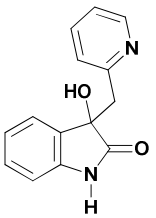
Yellow solid, m.p. 134–136 °C (lit[3]. m.p. 135–137 °C)

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.59–8.58 (m, 1H), 7.68–7.63 (m, 1H), 7.29–7.26 (m, 2H), 7.06 (d, *J* = 7.5 Hz, 2H), 6.95–6.90 (t, *J* = 7.5 Hz, 1H), 6.81–6.79 (m, 2H), 3.36 (d, *J* = 14.7 Hz, 1H), 3.18 (s, 3H), 3.10 (d, *J* = 14.7 Hz, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 157.6, 148.1, 141.5, 137.2, 131.0, 129.3, 124.6, 123.9, 122.7, 122.3, 108.2, 76.1, 42.6, 26.2 ppm

IR (KBr Pellet): 3286, 2931, 1711, 1628, 1590, 1475, 1235, 1120, 741 cm^{-1}

2. 3–Hydroxy–3–(pyridin–2–ylmethyl)indolin–2–one (3b):



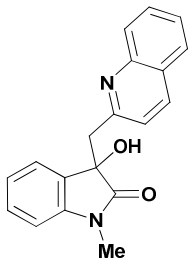
Yellow solid, m.p. 165–167 °C (lit[4]. m.p. 168–170 °C)

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.59-8.58 (m, 1H), 8.30 (br s, 1H), 7.68–7.63 (m, 1H), 7.30–7.16 (m, 3H), 7.08 (d, *J* = 7.8 Hz, 1H), 6.92–6.74 (m, 3H), 3.39 (d, *J* = 14.7 Hz, 1H), 3.13 (d, *J* = 14.7 Hz, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 179.0, 157.5, 148.3, 139.9, 137.2, 131.4, 129.3, 124.7, 124.2, 122.7, 122.4, 110.2, 61.6, 42.8 ppm

IR (KBr Pellet): 3295, 1708, 1620, 1598, 1474, 1315, 1215, 1175, 757 cm^{-1}

3. 3–Hydroxy–1–methyl–3–(quinolin–2–ylmethyl)indolin–2–one (3c):



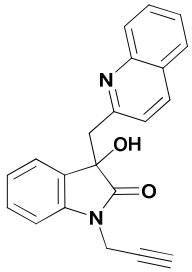
Pale yellow solid, m.p. 143–146 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.12–8.05 (m, 2H), 7.83–7.70 (m, 2H), 7.57–7.52 (m, 1H), 7.26–7.15 (m, 2H), 6.89–6.78 (m, 3H), 3.58 (d, *J* = 14.7 Hz, 1H), 3.25 (d, *J* = 14.7 Hz, 1H), 3.18 (s, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ = 176.6, 158.4, 146.4, 142.8, 137.0, 131.0, 130.0, 129.2, 128.6, 127.6, 126.9, 126.4, 123.9, 122.6, 122.6, 108.2, 76.1, 43.0, 26.0 ppm.

IR (KBr Pellet): 3110, 1714, 1635, 1586, 1485, 1326, 1276, 1188, 766 cm^{-1}

4. 3–Hydroxy–1–(prop–2–yn–1–yl)–3–(quinolin–2–ylmethyl)indolin–2–one (3d):



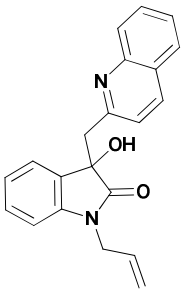
Yellow solid, m.p. 137–139 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.14–8.07 (m, 2H), 7.84–7.72 (m, 2H), 7.58–7.53 (m, 1H), 7.30–7.25 (m, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 6.94–6.86 (m, 2H), 4.63–4.57 (m, 1H), 4.37–4.31 (m, 1H), 3.57 (d, *J* = 15.3 Hz, 1H), 3.29 (d, *J* = 15.0 Hz, 1H), 2.22 (s, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 176.1, 158.7, 147.0, 141.4, 137.6, 131.4, 130.5, 129.7, 129.1, 128.1, 127.4, 127.0, 124.5, 123.5, 123.0, 109.7, 77.1, 76.7, 72.9, 43.4, 29.7 ppm

IR (KBr Pellet): 3221, 1719, 1616, 1582, 1451, 1329, 1268, 1174, 784 cm^{-1}

5. 1–Allyl–3–hydroxy–3– (quinolin–2–ylmethyl)indolin–2–one (3e):



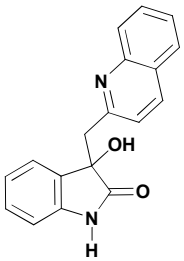
Pale yellow solid, m.p. 98–100 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.13–8.07 (m, 2H), 7.84–7.72 (m, 2H), 7.58–7.53 (m, 1H), 7.21–7.16 (m, 3H), 6.86–6.79 (m, 3H), 5.87–5.78 (m, 1H), 5.26–5.19 (m, 2H), 4.40–4.23 (m, 2H), 3.59 (d, *J* = 14.7 Hz, 1H), 3.28 (d, *J* = 14.7 Hz, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 176.3, 158.4, 146.6, 142.1, 137.1, 137.0, 131.2, 131.1, 130.1, 129.2, 128.7, 127.6, 127.0, 126.5, 124.0, 122.7, 117.6, 109.1, 76.2, 43.2, 42.3 ppm

IR (KBr Pellet): 3289, 1731, 1611, 1518, 1415, 1320, 1215, 1187, 811 cm^{-1}

6. 3–Hydroxy–3–(quinolin–2–ylmethyl)indolin–2–one (3f):



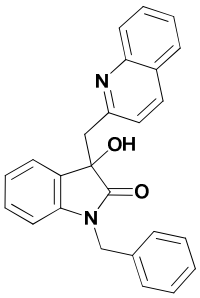
Yellow solid, m.p. 160–162 °C;

^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.19 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.68–7.63 (m, 1H), 7.53–7.48 (m, 1H), 7.37–7.34 (d, *J* = 8.4 Hz, 1H), 7.09–7.04 (m, 1H), 6.93 (d, *J* = 7.5 Hz, 1H), 6.78 (t, *J* = 7.2 Hz, 1H), 6.67 (d, *J* = 7.5 Hz, 1H), 6.38 (s, 1H), 3.49 (d, *J* = 13.5 Hz, 1H), 3.33 (d, *J* = 11.1 Hz, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$ + DMSO-d_6): δ = 178.4, 157.1, 146.5, 141.4, 135.3, 130.9, 128.8, 128.4, 128.1, 127.2, 126.2, 125.6, 124.0, 122.4, 120.9, 109.2, 75.5, 45.0 ppm

IR (KBr Pellet): 3146, 1728, 1620, 1595, 1474, 1320, 1220, 1199, 749 cm^{-1}

7. 1–Benzyl–3–hydroxy–3–(quinolin–2–ylmethyl)indolin–2–one (3g):



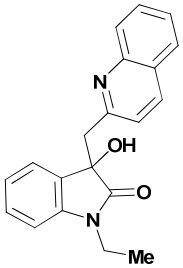
Yellow solid, m.p. 166–170 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.14–8.08 (m, 3H), 7.84–7.72 (m, 3H), 7.58–7.54 (m, 2H), 7.20–7.10 (m, 2H), 6.87 (d, *J* = 7.5 Hz, 3H), 6.70 (d, *J* = 7.5 Hz, 2H), 4.99 (d, *J* = 15.6 Hz, 1H), 4.83 (d, *J* = 15.3 Hz, 1H), 3.64 (d, *J* = 15.0 Hz, 1H), 3.33 (d, *J* = 15.0 Hz, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 176.8, 158.4, 146.6, 142.0, 137.2, 135.6, 131.1, 130.1, 129.3, 128.7, 127.7, 127.6, 127.2, 127.0, 126.6, 124.1, 122.8, 122.6, 109.3, 76.3, 43.7, 43.3 ppm

IR (KBr Pellet): 3247, 2998, 1718, 1641, 1594, 1414, 1371, 1151, 798 cm^{-1}

8. 1–Ethyl–3–hydroxy–3–(quinolin–2–ylmethyl)indolin–2–one (3h):



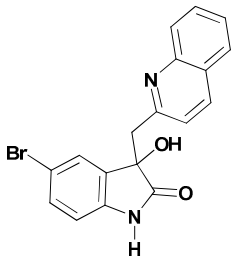
Pale yellow solid, m.p. 156-158 °C;

^{1}H NMR (300 MHz, DMSO-d_6): δ = 8.10 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.71–7.60 (m, 2H), 7.49–7.46 (m, 1H), 7.26–7.23 (m, 1H), 7.14–7.07 (m, 2H), 6.88–6.77 (m, 2H), 6.40 (s, 1H), 3.58–3.38 (m, 4H), 0.94 (t, 3H) ppm

^{13}C NMR (75 MHz, DMSO-d_6): δ = 176.4, 156.8, 146.7, 142.3, 135.4, 130.7, 129.2, 128.9, 128.3, 127.6, 126.3, 125.9, 124.2, 122.6, 121.5, 108.0, 75.3, 45.9, 33.8, 12.3 ppm

IR (KBr Pellet): 3185, 1726, 1595, 1445, 1353, 1251, 1135, 835 cm^{-1}

9. 5–Bromo–3–hydroxy–3–(quinolin–2–ylmethyl)indolin–2–one (3i):



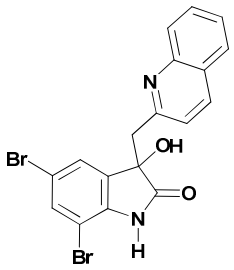
Yellow solid, m.p. 198–200 °C

^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.31 (br s, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.73-7.62 (m, 2H), 7.52 (t, *J* = 7.2 Hz 1H), 7.35 (d, *J* = 8.7 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 1H), 7.13 (s, 1H), 6.63 (d, *J* = 8.4 Hz, 1H), 6.42 (s, 1H), 3.57 (d, *J* = 13.8 Hz, 1H), 3.41 (d, *J* = 16.8 Hz, 1H) ppm

^{13}C NMR (75 MHz, DMSO-d_6): δ = 178.2, 156.7, 146.7, 141.3, 135.5, 133.8, 131.3, 129.3, 128.2, 127.6, 127.4, 126.3, 126.0, 122.6, 112.7, 75.5, 45.1 ppm

IR (KBr Pellet): 3321, 3021, 1726, 1689, 1595, 1474, 1325, 1220, 1198, 810, 789 cm^{-1}

10. 5,7–Dibromo–3–hydroxy–3–(quinolin–2–ylmethyl)indolin–2–one (3j):



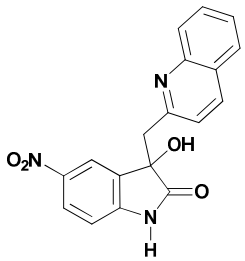
Yellow solid, m.p. 208-209 °C

^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.70 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.65 (s, 2H), 7.51–7.48 (m, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.22 (s, 1H), 6.53 (s, 1H), 3.65 (d, *J* = 14.4 Hz, 1H), 3.51 (d, *J* = 14.7 Hz, 1H) ppm

^{13}C NMR (75 MHz, DMSO-d_6): δ = 178.2, 156.6, 146.6, 141.4, 135.8, 135.7, 135.4, 133.1, 129.4, 128.0, 127.7, 126.3, 126.1, 122.3, 113.1, 102.4, 76.1, 44.7 ppm

IR (KBr Pellet): 3409, 3150, 1735, 1614, 1584, 1465, 1348, 1153, 1101, 749 cm^{-1}

11. 3–Hydroxy–5–nitro–3–(quinolin–2–ylmethyl)indolin–2–one (3k):



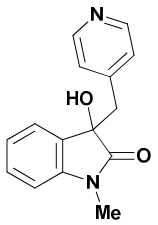
Yellow solid, m.p. 187–188 °C

^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.94 (s, 1H), 8.18–7.82 (m, 4H), 7.63 (s, 2H), 7.49–7.34 (m, 2H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.58 (s, 1H), 3.74 (d, *J* = 14.1 Hz, 1H), 3.53 (d, *J* = 14.7 Hz, 1H) ppm

^{13}C NMR (75 MHz, DMSO–d_6): δ = 179.0, 156.4, 149.0, 146.6, 141.6, 135.8, 132.6, 129.3, 128.0, 127.7, 126.3, 126.1, 122.4, 120.0, 109.4, 74.9, 44.7 ppm

IR (KBr Pellet): 3365, 3191, 1721, 1596, 1484, 1365, 1294, 1196, 841, 788 cm^{-1}

12. 3–Hydroxy–1–methyl–3–(pyridin–4–ylmethyl)indolin–2–one (3l):



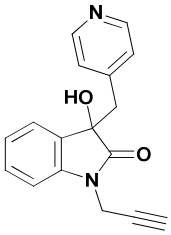
Yellow solid, m.p. 202–204 °C (lit. m.p. 201–203 °C)

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.29 (s, 2H), 7.29–7.24 (m, 1H), 7.18 (d, *J* = 6.9 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.88 (br s, 2H), 6.66 (d, *J* = 7.5 Hz, 1H), 3.32 (d, *J* = 12.9 Hz, 1H), 3.14 (d, *J* = 12.6 Hz, 1H), 2.99 (s, 3H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 177.3, 148.9, 143.5, 143.0, 130.0, 128.7, 125.4, 124.2, 123.0, 108.5, 76.6, 44.0, 26.0 ppm

IR (KBr Pellet): 3085, 1715, 1610, 1475, 1369, 1230, 1110, 821 cm^{-1}

13. 3–Hydroxy–1–(prop–2–yn–1–yl)–3–(pyridin–4–ylmethyl)indolin–2–one 9 (3m):



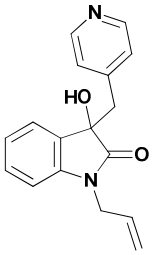
Pale yellow solid, m.p. 186–189 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.21–8.20 (m, 2H), 7.31–7.23 (m, 3H), 7.12–7.07 (m, 1H), 6.82–6.81 (m, 3H), 4.35 (d, *J* = 17.4 Hz, 1H), 4.10 (d, *J* = 17.1 Hz, 1H), 3.27 (d, *J* = 12.6 Hz, 1H), 3.13 (d, *J* = 12.6 Hz, 1H), 2.10 (s, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 176.3, 148.8, 143.3, 141.1, 129.9, 128.8, 125.4, 124.3, 123.3, 109.4, 76.7, 75.7, 72.4, 44.1, 29.0 ppm

IR (KBr Pellet): 3321, 3019, 2819, 1728, 1599, 1465, 1195, 754 cm^{-1}

14. 1–Allyl–3–hydroxy–3–(pyridin–4–ylmethyl)indolin–2–one (3n):



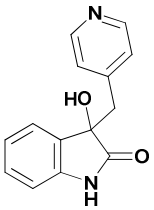
Yellow solid, m.p. 165–166 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.25 (s, 1H), 7.31–7.21 (m, 3H), 7.10–7.05 (m, 1H), 6.84 (m, 2H), 6.64 (d, *J* = 7.5 Hz, 1H), 5.51–5.41 (m, 1H), 5.00 (d, *J* = 10.2 Hz, 1H), 4.76 (d, *J* = 17.1 Hz, 1H), 4.28-4.24 (m, 1H), 3.98–3.91 (m, 1H), 3.35 (d, *J* = 12.0 Hz, 1H), 3.21 (d, *J* = 12.0 Hz, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 176.9, 149.0, 143.4, 142.3, 130.3, 129.9, 128.7, 125.5, 124.2, 123.0, 117.6, 109.4, 76.8, 44.1, 42.2 ppm

IR (KBr Pellet): 3295, 3014, 2824, 1724, 1615, 1484, 1201, 769 cm^{-1}

15. 3–Hydroxy–3–(pyridin–4–ylmethyl)indolin–2–one (3o):



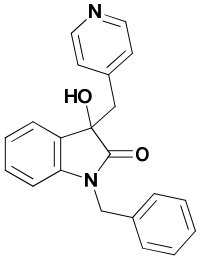
Pale yellow solid, m.p. 181–184 °C

^{1}HNMR (300 MHz, DMSO–d_6): δ = 10.15 (s, 1H), 8.30 (s, 2H), 7.13–6.93 (m, 5H), 6.64 (d, 1H, *J* = 7.8 Hz), 6.26 (s, 1H), 3.18 (d, 1H, *J* = 11.7 Hz), 3.00 (d, 1H, *J* = 12.3 Hz) ppm

^{13}C NMR (75 MHz, DMSO–d_6): δ = 178.3, 148.6, 144.4, 141.5, 130.5, 129.2, 125.6, 124.5, 121.4, 109.5, 76.0, 42.6 ppm

IR (KBr Pellet): 3312, 3029, 2825, 1722, 1621, 1604, 1473, 1205, 1121, 751 cm^{-1}

16. 1–Benzyl–3–hydroxy–3–(pyridin–4–ylmethyl)indolin–2–one (3p):



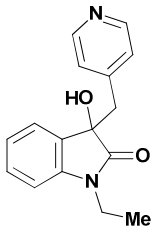
Yellow solid, m.p. 112–116 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.21 (s, 2H), 7.33–7.03 (m, 7H), 6.85–6.75 (m, 4H), 6.48 (d, *J* = 7.5 Hz, 1H), 4.89 (d, *J* = 15.6 Hz, 1H), 4.50 (d, *J* = 15.9 Hz, 1H), 3.41 (d, *J* = 12.3 Hz, 1H), 3.28 (d, *J* = 12.3 Hz, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 177.3, 148.9, 143.5, 142.4, 134.7, 130.0, 128.9, 128.7, 127.6, 126.6, 125.6, 124.2, 123.1, 109.6, 76.8, 43.9, 43.6 ppm

IR (KBr Pellet): 3324, 3025, 2801, 1715, 1619, 1510, 1236, 1154, 785 cm^{-1}

17. 1–Ethyl–3–hydroxy–3–(pyridin–4–ylmethyl)indolin–2–one (3q):



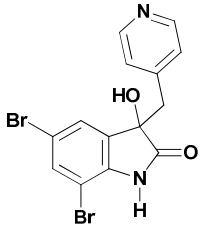
Yellow solid, m.p. 202–206 °C

^{1}H NMR (300 MHz, DMSO-d_6): δ = 8.24 (s, 2H), 7.25–7.20 (m, 2H), 7.03–6.98 (m, 1H), 6.80 (br s, 3H), 6.34 (s, 1H), 3.60–3.35 (m, 2H), 3.18 (d, *J* = 12.0 Hz, 1H), 3.07 (d, *J* = 12.0 Hz, 1H), 0.81 (t, J = 6.9 Hz, 3H) ppm

^{13}C NMR (75 MHz, DMSO-d_6): δ = 176.0, 148.8, 148.7, 143.7, 141.9, 130.0, 129.3, 125.3, 124.2, 122.0, 108.2, 75.8, 43.0, 33.6, 11.9 ppm

IR (KBr Pellet): 3278, 3041, 1728, 1631, 1549, 1241, 1164, 761 cm^{-1}

18. 5,7–Dibromo–3–hydroxy–3–(pyridin–4–ylmethyl)indolin–2–one (3r):



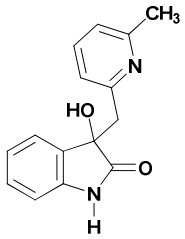
Yellow solid, m.p. 248–250 °C

^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.67 (s, 1H), 8.35 (d, *J* = 4.5 Hz, 2H), 7.60 (d, *J* = 1.5 Hz, 1H), 7.23 (s, 1H), 6.97 (d, *J* = 5.1 Hz, 2H), 6.53 (s, 1H), 3.23 (d, *J* = 12.6 Hz, 1H), 3.03 (d, *J* = 12.6 Hz, 1H) ppm

^{13}C NMR (75 MHz, DMSO-d_6): δ = 177.8, 148.9, 143.4, 140.4, 134.2, 133.6, 126.6, 125.5, 113.6, 102.7, 76.8, 42.0 ppm

IR (KBr Pellet): 3411, 3225, 3014, 1734, 1641, 1571, 1190, 1164, 761 cm^{-1}

19. 3–Hydroxy–3–(6–methylpyridin–2–yl)indolin–2–one (3s):



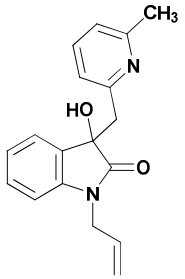
Pale yellow solid, m.p. 177–180 °C (lit[4]. 178–180 °C)

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.57–7.47 (m, 2H), 7.25–7.12 (m, 3H), 6.92–6.74 (m, 4H), 3.32 (d, *J* = 14.7 Hz, 1H), 3.05 (d, *J* = 14.7 Hz, 1H), 2.61 (s, 3H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 179.0, 157.3, 156.7, 139.9, 137.5, 131.7, 129.2, 124.2, 122.7, 122.0, 121.6, 110.1, 79.9, 42.4, 24.2 ppm

IR (KBr Pellet): 3268, 2981, 1717, 1622, 1599, 1475, 1176, 1111, 737 cm^{-1}

20. 1–Allyl–3–hydroxy–3–(6–methylpyridin–2–yl)indolin–2–one (3t):



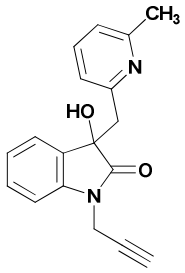
Viscous liquid

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.57-7.52 (m, 1H), 7.27–7.11 (m, 2H), 6.93–6.78 (m, 4H), 5.86–5.75 (m, 1H), 5.24–5.18 (m, 2H), 4.37–4.21 (m, 2H), 3.34 (d, *J* = 14.7 Hz, 1H), 3.05 (d, *J* = 14.7 Hz, 1H), 2.58 (s, 3H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 176.4, 157.0, 156.5, 141.9, 137.4, 131.0, 130.9, 129.0, 123.8, 122.5, 121.9, 121.5, 117.4, 109.0, 76.0, 42.4, 42.1, 24.0 ppm

IR (KBr Pellet): 3254, 3069, 1724, 1649, 1576, 1169, 1125, 768 cm^{-1}

21.3–Hydroxy–3–((6–methylpyridin–2–yl)methyl)–1–(prop–2–yn–1–yl)indolin–2–one (3u):



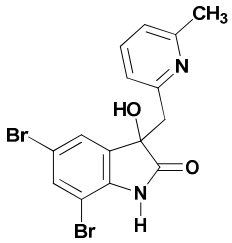
Brown viscous liquid

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.54–7.49 (m, 1H), 7.29–7.24 (m, 1H), 7.11–6.82 (m, 6H), 4.59 (d, *J* = 14.7 Hz, 1H), 4.35 (d, *J* = 14.7 Hz, 1H), 3.29 (d, *J* = 14.7 Hz, 1H), 3.07 (d, *J* = 14.4 Hz, 1H), 2.57 (s, 3H), 2.21 (s, 1H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 175.9, 157.2, 156.7, 141.1, 137.3, 131.2, 129.2, 124.0, 122.9, 121.8, 121.5, 109.2, 76.1, 72.4, 72.2, 42.5, 29.3, 24.1 ppm

IR (KBr Pellet): 3269, 3052, 1718, 1645, 1589, 1225, 1124, 814 cm^{-1}

22. 5,7–Dibromo–3–hydroxy–3–((6–methylpyridin–2–yl)methyl)indolin–2–one (3v):



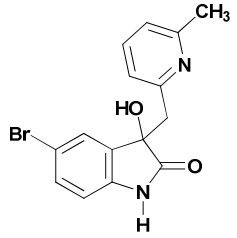
Yellow solid, m.p. 177–178 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.21 (br s, 1H), 7.60–7.49 (m, 2H), 7.16 (d, *J* = 7.8 Hz, 1H), 6.89 (d, *J* = 7.5 Hz, 2H), 6.82 (s, 1H), 3.25 (d, *J* = 14.7 Hz, 1H), 3.00 (d, *J* = 14.7 Hz, 1H), 2.60 (s, 3H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 177.2, 157.3, 155.8, 138.6, 137.6, 134.3, 133.9, 126.4, 122.3, 121.6, 115.4, 103.7, 77.7, 42.0, 24.1 ppm

IR (KBr Pellet): 3448, 3072, 1738, 1613, 1580, 1451, 1189, 1156, 830 cm^{-1}

23. 5–Bromo–3–hydroxy–3–((6–methylpyridin–2–yl)methyl)indolin–2–one (3w):



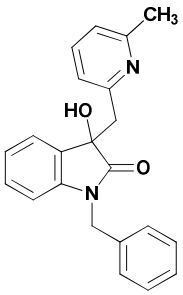
Pale yellow solid, m.p. 178–180 °C

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.58 (br s, 1H), 7.60–7.55 (m, 1H), 7.32–7.26 (m, 1H), 7.17 (d, *J* = 7.8 Hz, 1H), 6.89–6.83 (m, 2H), 6.75 (d, *J* = 8.1 Hz, 1H), 3.32 (d, *J* = 14.7 Hz, 1H), 3.02 (d, *J* = 14.7 Hz, 1H), 2.60 (s, 3H) ppm

^{13}C NMR (75 MHz, $CDCl_3$): δ = 178.7, 157.3, 156.1, 139.0, 137.7, 133.5, 132.1, 127.5, 122.3, 121.7, 115.2, 111.8, 75.0, 42.1, 24.1 ppm

IR (KBr Pellet): 3286, 3068, 1720, 1611, 1588, 1465, 1170, 849 cm^{-1}

24. 1–Benzyl–5–bromo–3–hydroxy–3–((6–methylpyridin–2–yl)methyl)indolin–2–one (3x):



Yellow solid, m.p. 175–177 °C (lit[3]. m.p. 176–178 °C)

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.10 (br, s, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.33–7.29 (m, 5H), 7.15-7.11 (m, 2 H), 6.91-6.78 (m, 3H), 6.70 (d, *J* = 7.8 Hz, 1H), 4.97 (d, *J* = 15.6 Hz, 1H), 4.84 (d, *J* = 15.6 Hz, 1H), 3..37 (d, *J* = 14.7 Hz, 2H), 3.08 (d, *J* = 14.7 Hz, 2H), 2.61 (s, 3H) ppm

^{13}C NMR (75 MHz, DMSO-d_6): δ = 176.9, 156.4, 155.0, 142.9, 142.3, 136.2, 130.5, 128.7, 128.4, 126.9, 124.2, 121.7, 121.1, 120.8, 108.5, 75.4, 45.0, 42.5, 23.8 ppm

IR (KBr Pellet): 3287, 2924, 1728, 1618, 1469, 1386, 1189, 1095, 785 cm^{-1}

D. References:

1. M. S. Shmidt, I. A. Perillo, M. González and M. M. Blanco, *Tetrahedron Lett.*, 2012, **53,** 2514–2517.

2. M. Presset, K. Mohanan, M. Hamann, Y. Coquerel and J. Rodriguez, *Org. Lett.*, 2011, **13,** 4124–4127.

3. R. Niu, J. Xiao, T. Liang and X. Li, *Org. Lett.*, 2012, **14**, 676−679.

4. H. M. Meshram, N. Nageswara Rao, L. Chandrasekhara Rao and N. Satish Kumar, *Tetrahedron Lett.*, 2012, **53**, 3963−3966.

E. Copies of ^{1}H- & ^{13}C- Spectra of Products

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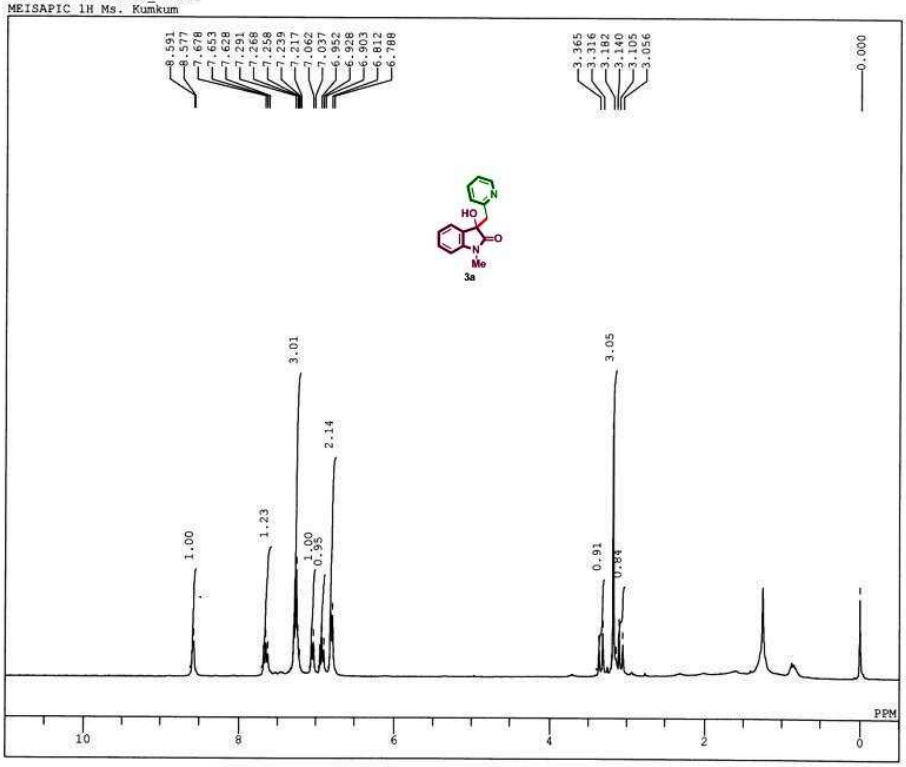

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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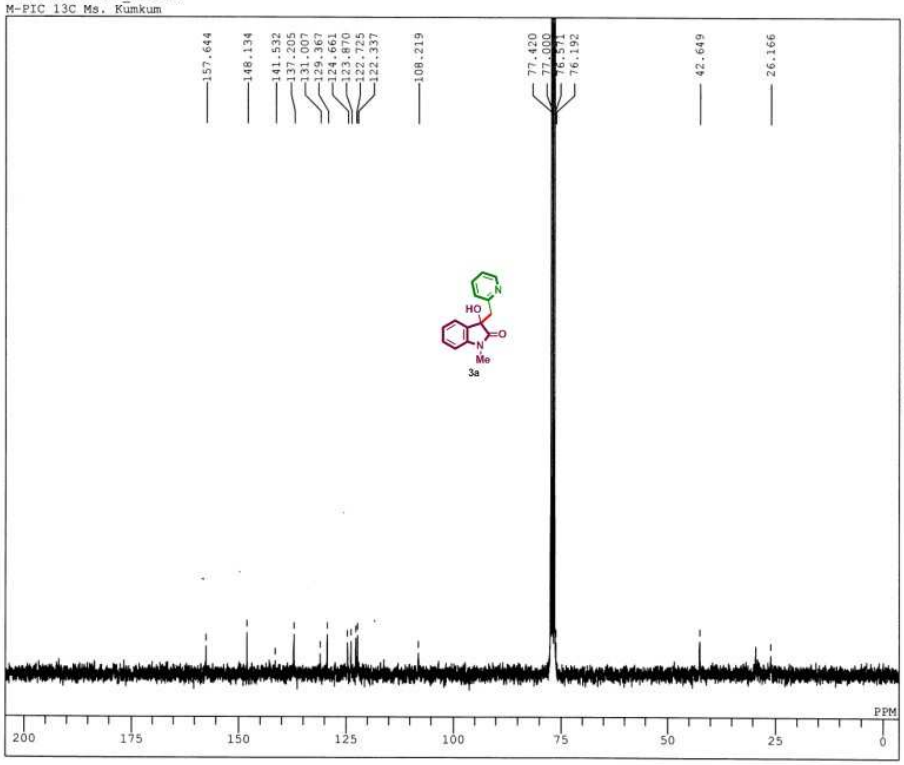

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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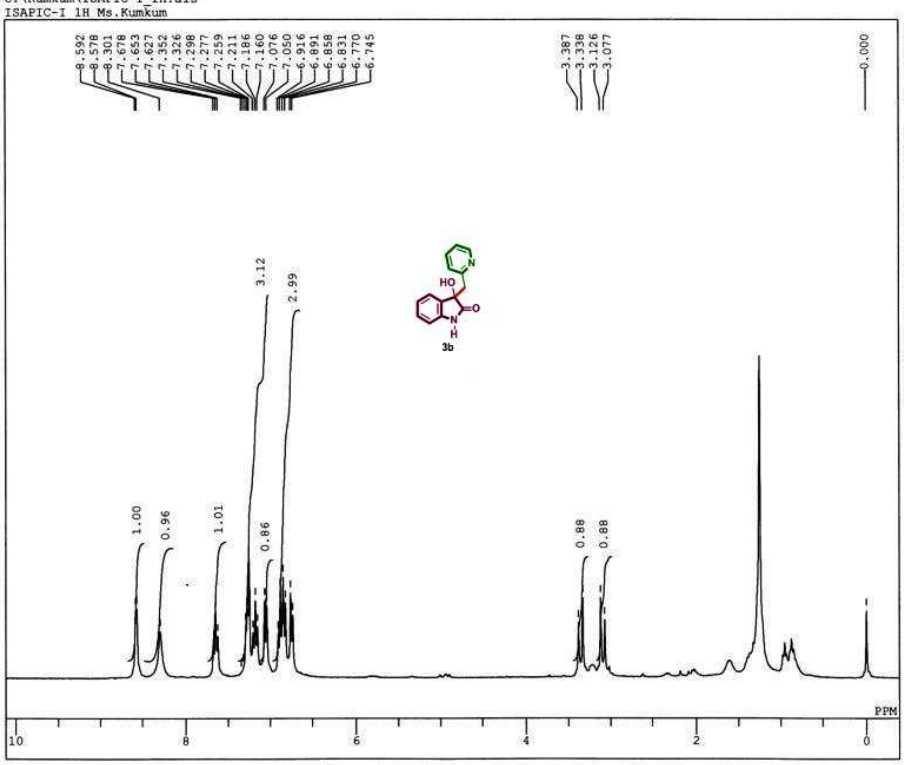

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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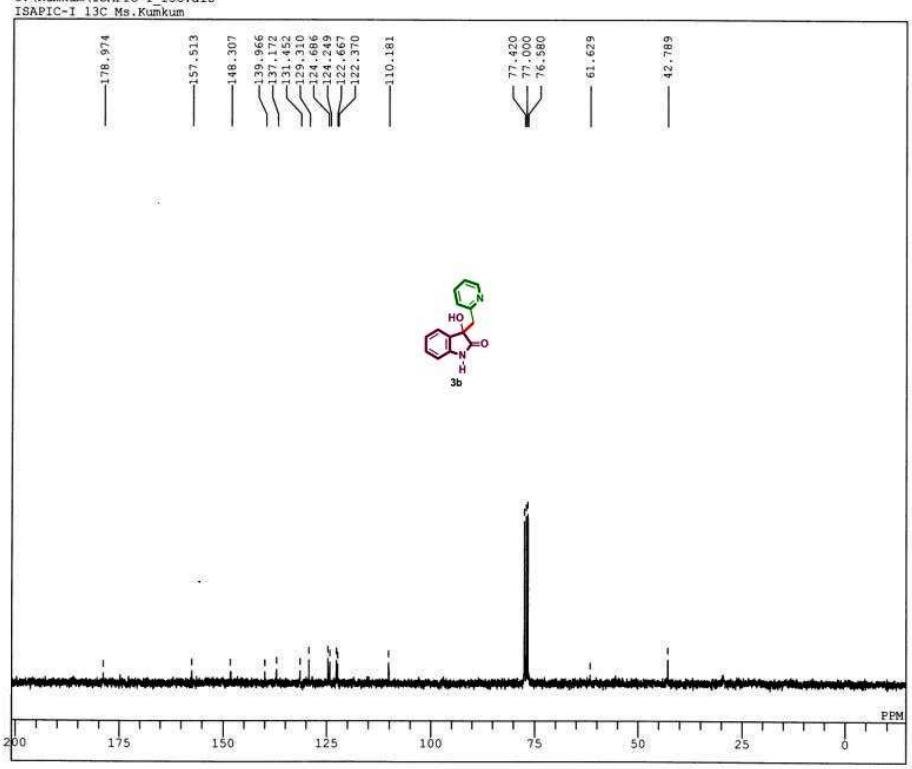

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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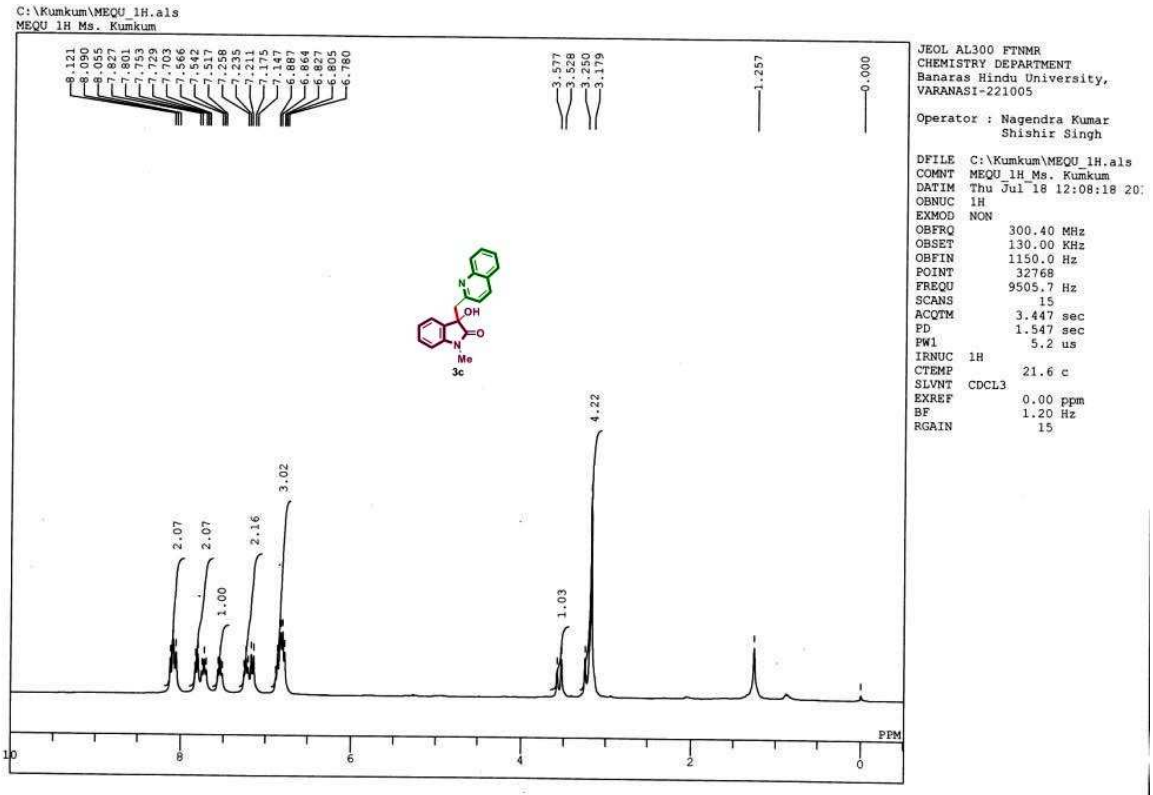
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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
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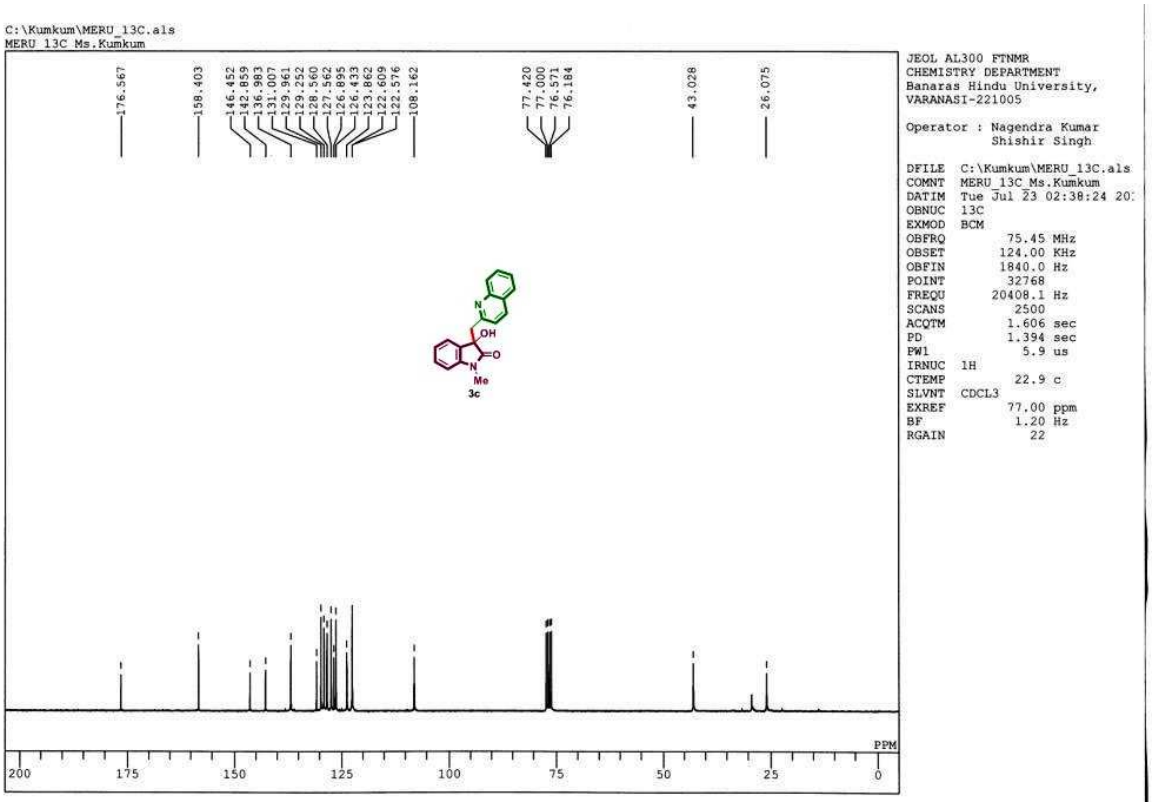
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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
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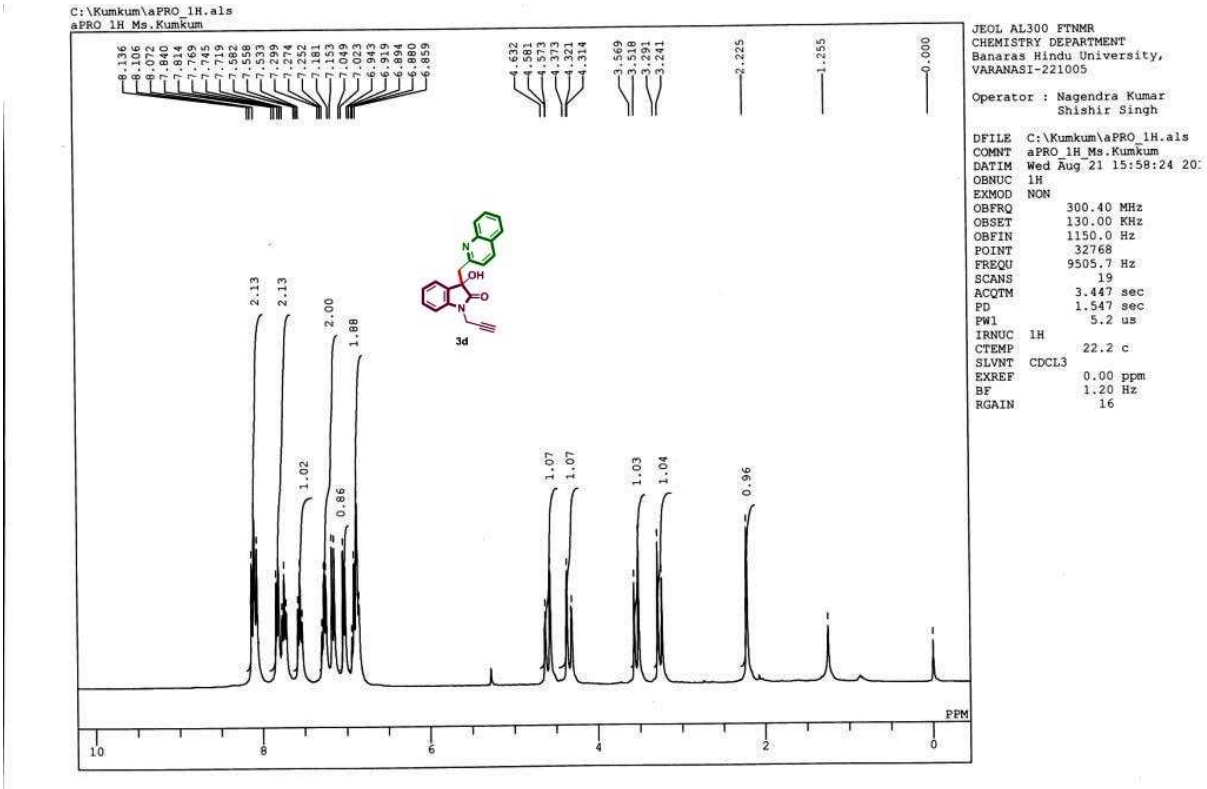
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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
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Shishir Singh
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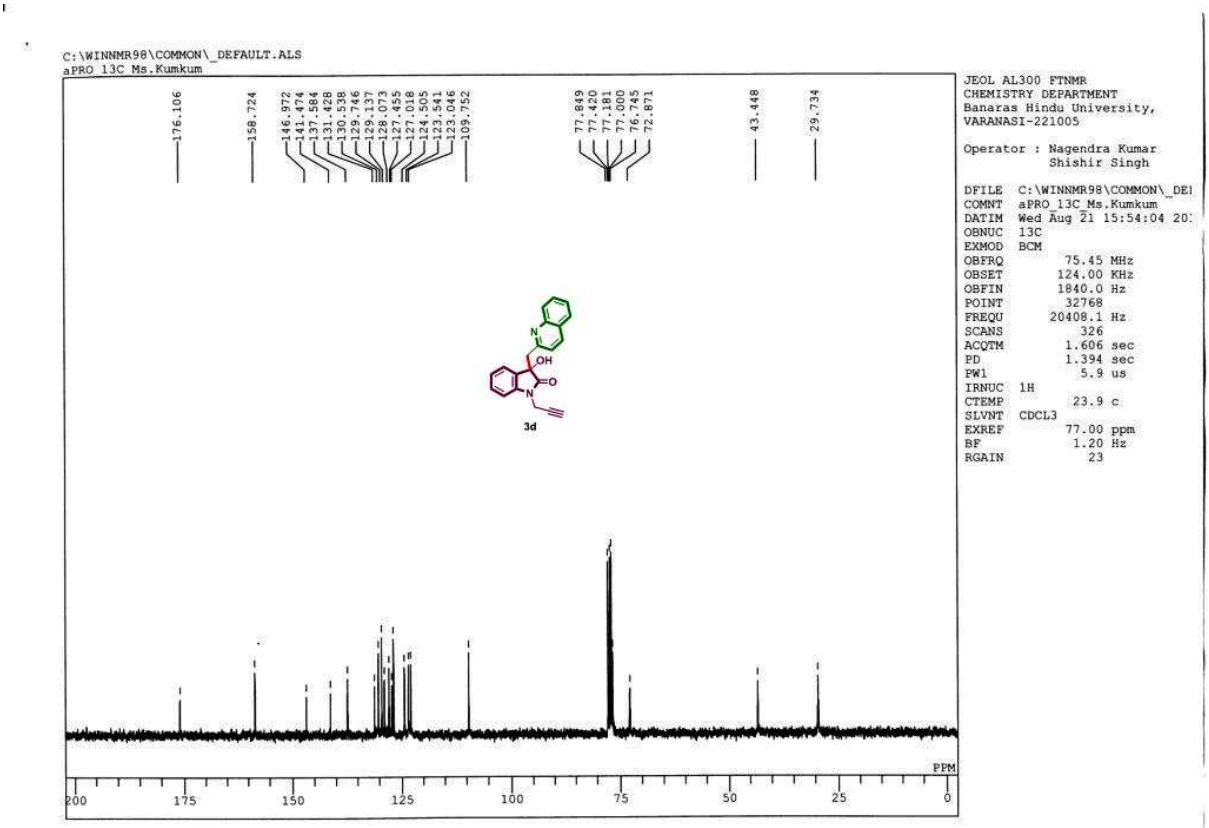
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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
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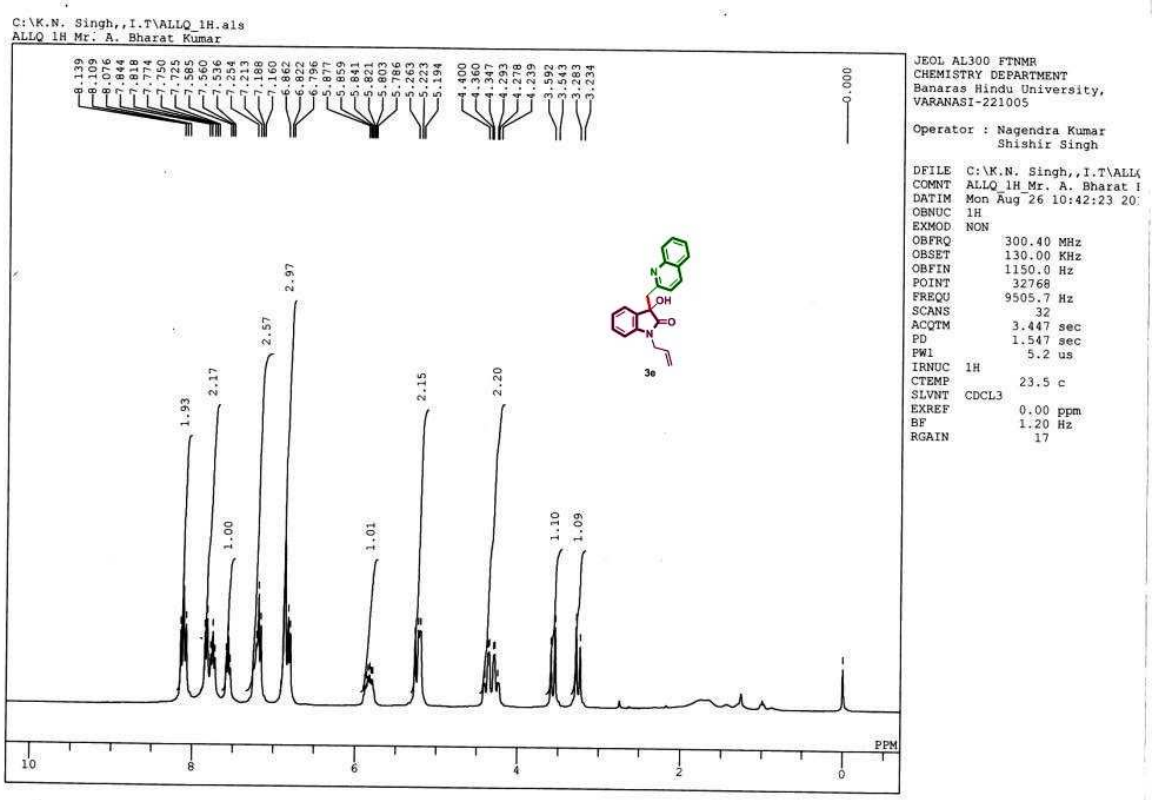
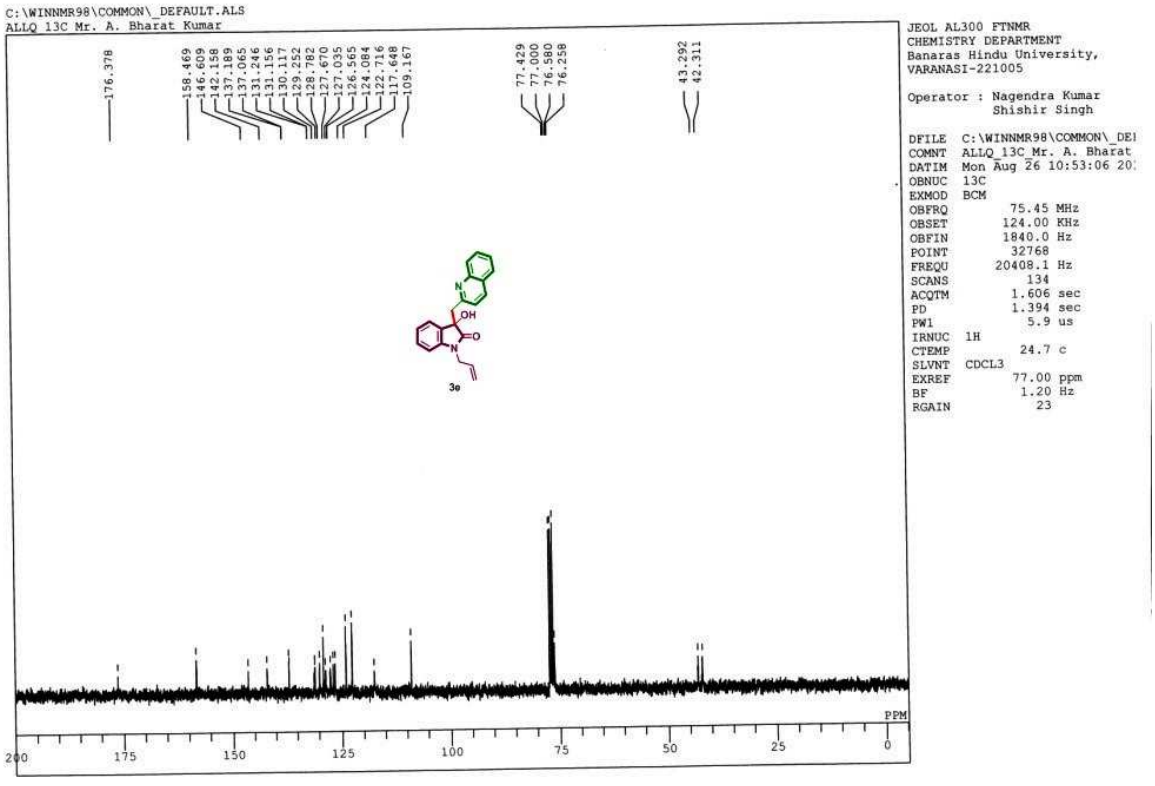
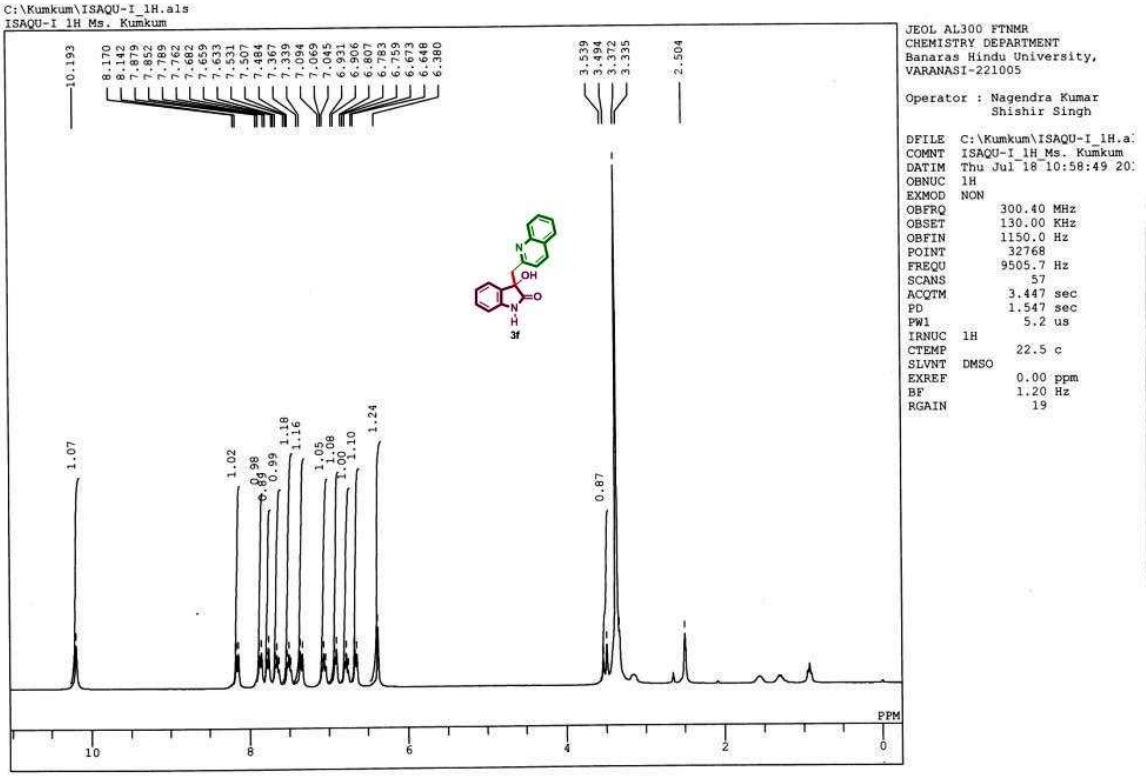
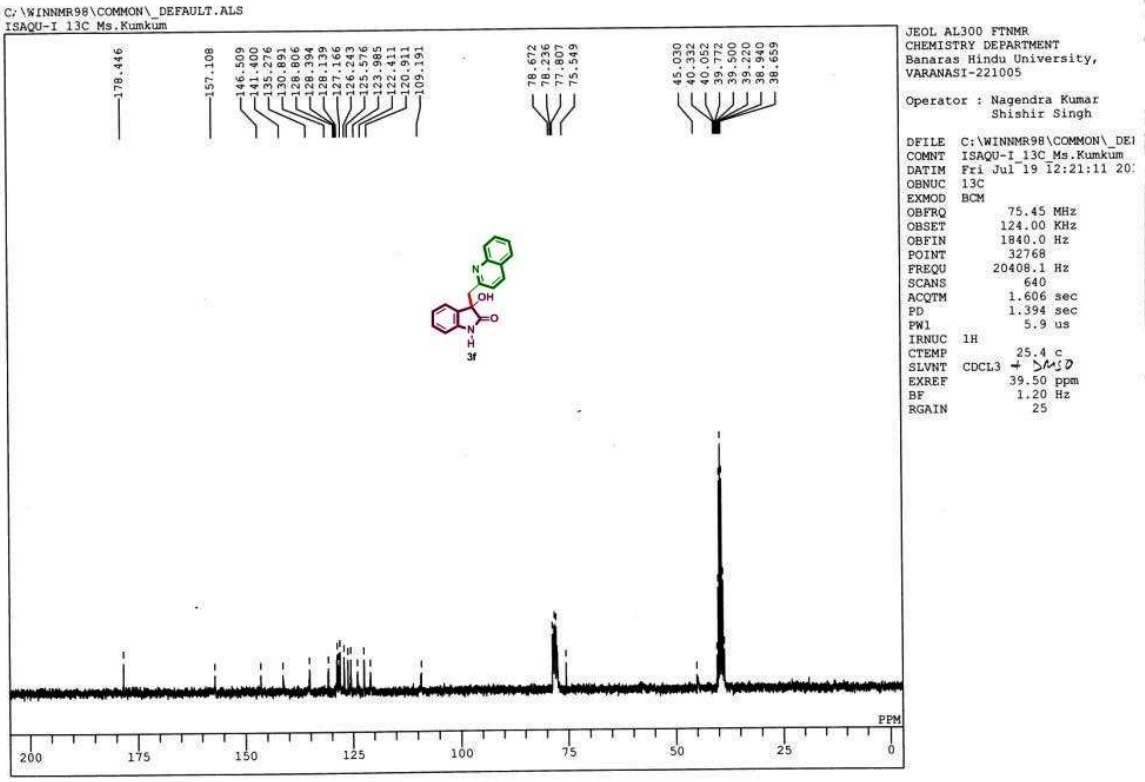
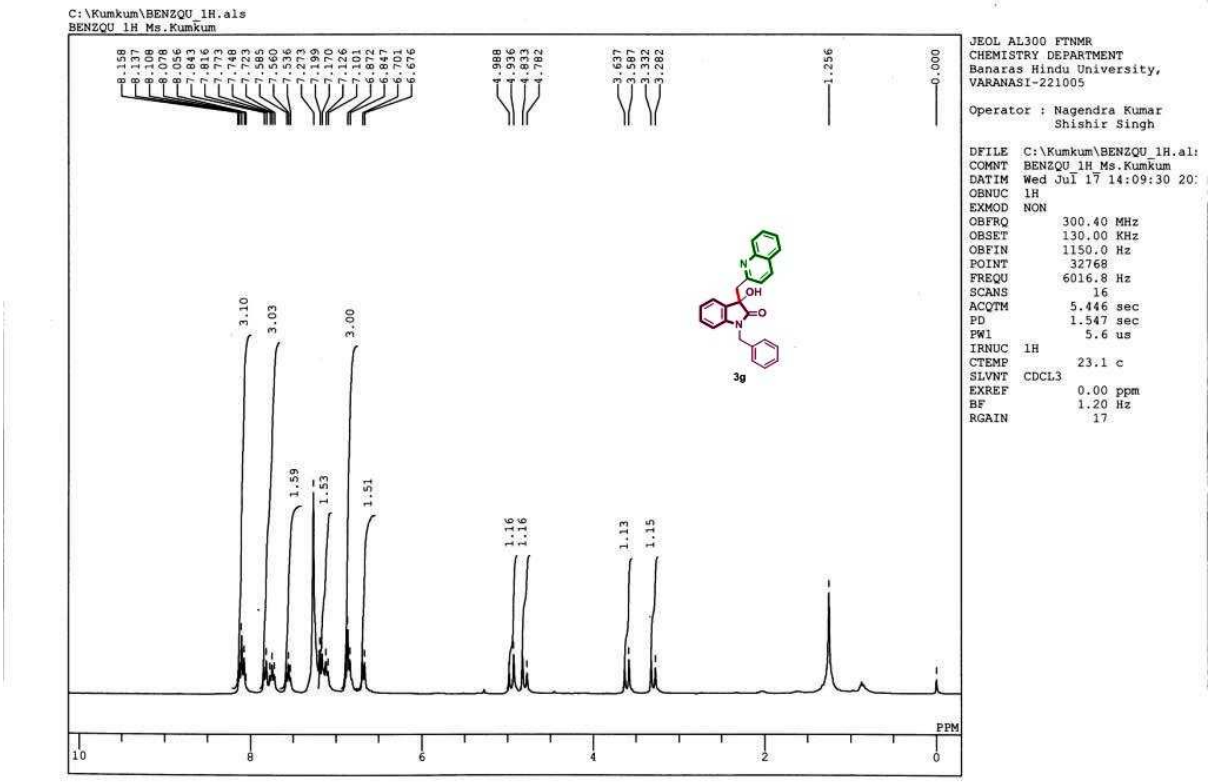
PW1 5.9 us
IRNUC 1H
CTEMP 23.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

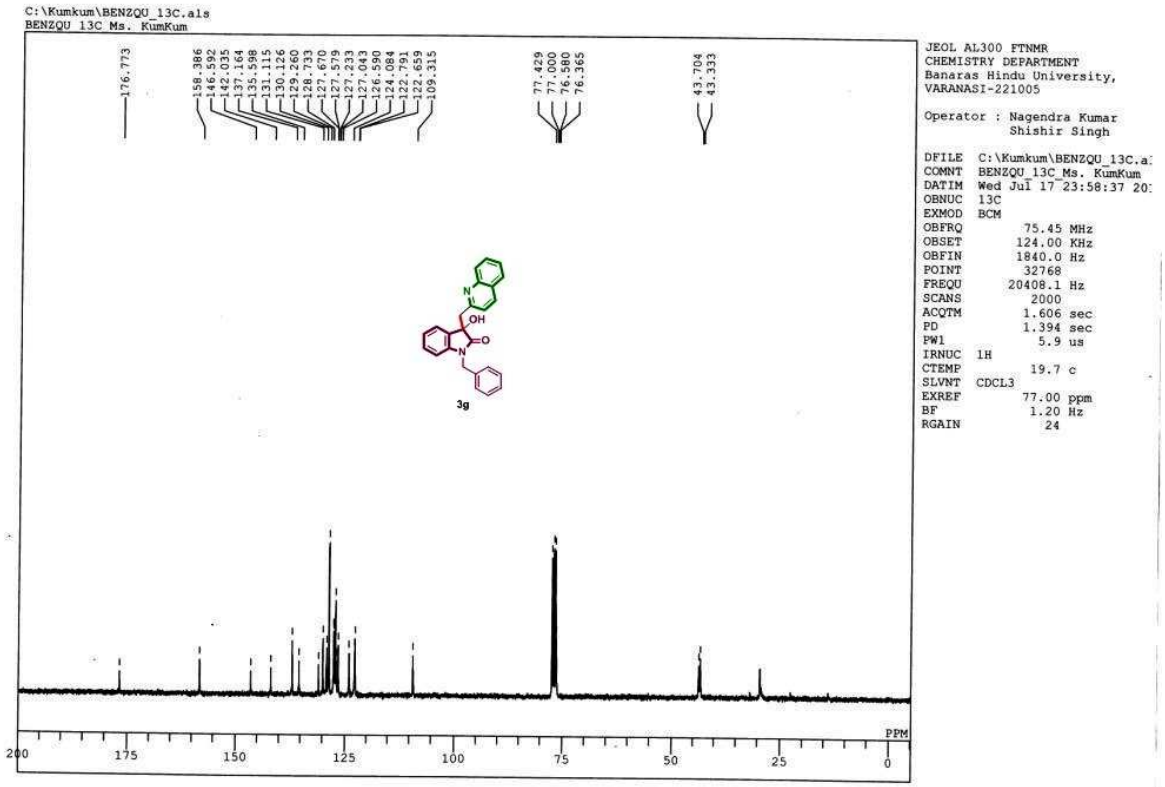

C:\K.N. Singh,,I.T\ALLQ_1H.als
ALLQ 1H Mr. A. Bharat Kumar
8.139
8.109
8.076
7.844
7.818
7.774
7.750
7.725
7.585
7.560
7.536
7.254
7.213
7.188
7.160
6.862
6.822
6.796
5.877
5.859
5.841
5.821
5.803
5.786
5.263
5.223
5.194
4.400
4.360
4.347
4.293
4.278
4.239
3.592
3.543
3.283
3.234
0.000
1.93
2.17
1.00
2.57
2.97
1.01
2.15
2.20
1.10
1.09
3e
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\K.N. Singh,,I.T\ALL(
COMNT ALLQ 1H Mr. A. Bharat I
DATIM Mon Aug 26 10:42:23 20
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 23.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17


C:\WINNMR98\COMMON_DEFAULT.ALS
ALLQ 13C Mr. A. Bharat Kumar
176.378
158.469
146.609
142.158
137.189
137.065
131.246
131.116
130.252
129.782
127.672
127.035
126.565
124.084
122.716
117.648
109.167
77.429
77.000
76.580
76.258
43.292
42.311
3e
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\WINNMR98\COMMON_DE
COMNT ALLQ 13C Mr. A. Bharat
DATIM Mon Aug 26 10:53:06 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 134
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 24.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

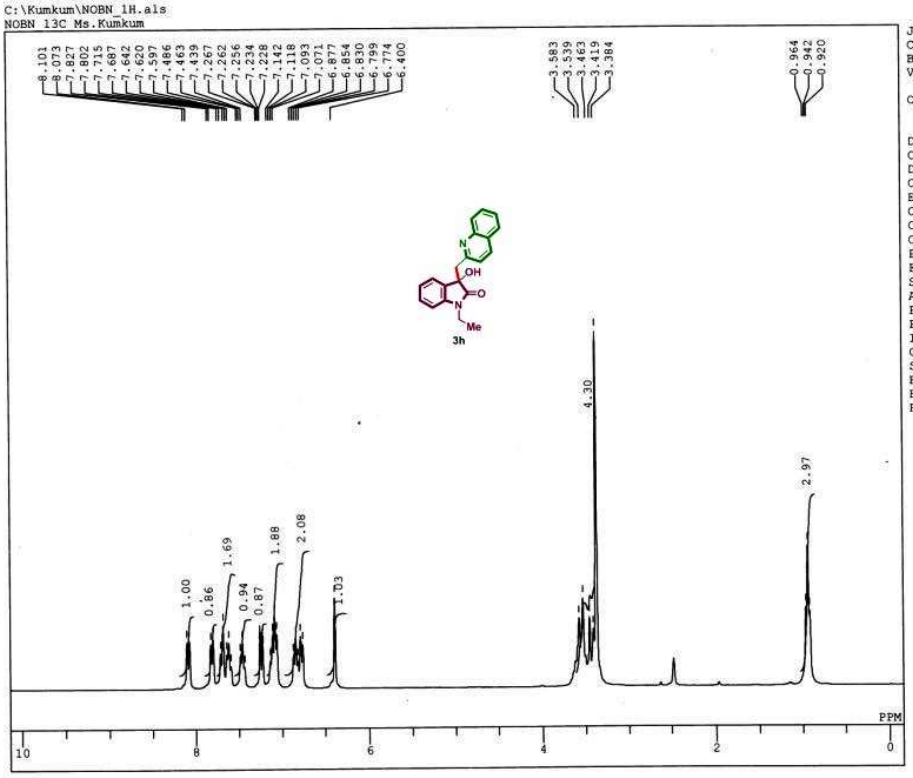

C:\Kumkum\ISAQU-I_1H.als
ISAQU-I 1H Ms. Kumkum
10.193
8.170
8.142
7.879
7.852
7.789
7.762
7.682
7.659
7.633
7.531
7.507
7.484
7.367
7.339
7.094
7.069
7.045
6.931
6.906
6.807
6.783
6.759
6.673
6.648
6.380
3.539
3.494
3.372
3.335
2.504
1.07
1.02
0.98
0.89
0.99
1.18
1.16
1.05
1.08
1.00
1.10
1.24
0.87
3f
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\ISAQU-I_1H.a
COMNT ISAQU-I_1H_Ms. Kumkum
DATIM Thu Jul 18 10:58:49 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 57
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.5 c
SLVNT DMSO
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 19


C:\WINNMR98\COMMON_DEFAULT.ALS
ISAQU-I 13C Ms.Kumkum
178.446
157.108
146.509
141.400
135.276
130.891
128.806
128.394
128.139
127.166
126.243
125.576
123.985
122.411
120.911
109.191
78.672
78.236
77.807
75.549
45.030
40.332
40.052
39.772
39.500
39.220
38.940
38.659
3f
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\WINNMR98\COMMON_DE
COMNT ISAQU-I_13C_Ms.Kumkum
DATIM Fri Jul 19 12:21:11 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 640
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 25.4 c
SLVNT CDCL3 + DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 25


C:\Kumkum\BENZQU_1H.als
BENZQU_1H_Ms.KumKum
8.158
8.137
8.108
8.078
8.056
7.843
7.816
7.773
7.748
7.723
7.585
7.560
7.536
7.273
7.199
7.170
7.126
7.101
6.872
6.847
6.701
6.676
4.988
4.936
4.833
4.782
3.637
3.587
3.332
3.282
1.256
0.000
3.10
3.03
3.00
1.59
1.53
1.51
1.16
1.16
1.13
1.15
OH
O
N
3g
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\BENZQU_1H.al
COMNT BENZQU_1H_Ms.KumKum
DATIM Wed Jul 17 14:09:30 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 16
ACQTM 5.446 sec
PD 1.547 sec
PW1 5.6 us
IRNUC 1H
CTEMP 23.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17


C:\Kumkum\BENZQU_13C.als
BENZQU_13C_Ms._KumKum
176.773
158.386
146.592
142.035
137.164
135.598
131.115
130.126
129.260
128.733
127.670
127.539
127.233
127.041
126.590
124.084
122.791
122.659
109.315
77.429
77.000
76.580
76.365
43.704
43.333
OH
O
N
3g
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\BENZQU_13C.a
COMNT BENZQU_13C_Ms._KumKum
DATIM Wed Jul 17 23:58:37 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 2000
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

C:\Kumkum\NOBN_1H.als
NOBN_13C_Ms.Kumkum

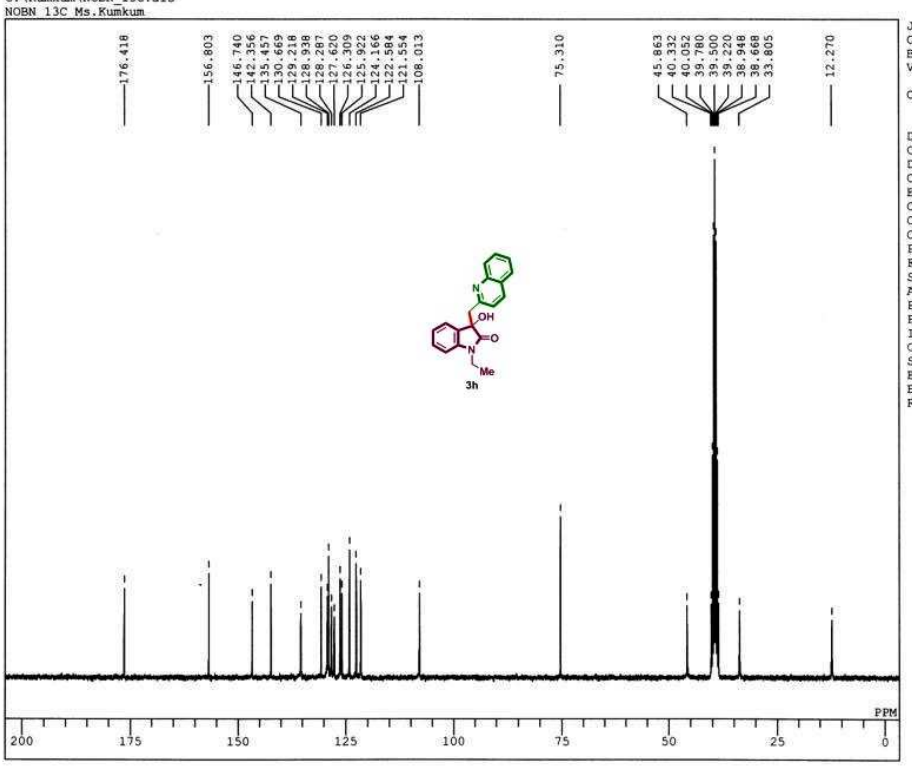


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\Kumkum\NOBN_1H.als
COMNT	NOBN_13C_Ms.Kumkum
DATIM	Fri Aug 23 04:13:13 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	5.6 us
IRNUC	1H
CTEMP	19.8 c
SLVNT	DMSO
EXREF	2.49 ppm
BF	1.20 Hz
RGAIN	13

C:\Kumkum\NOBN_13C.als
NOBN_13C_Ms.Kumkum

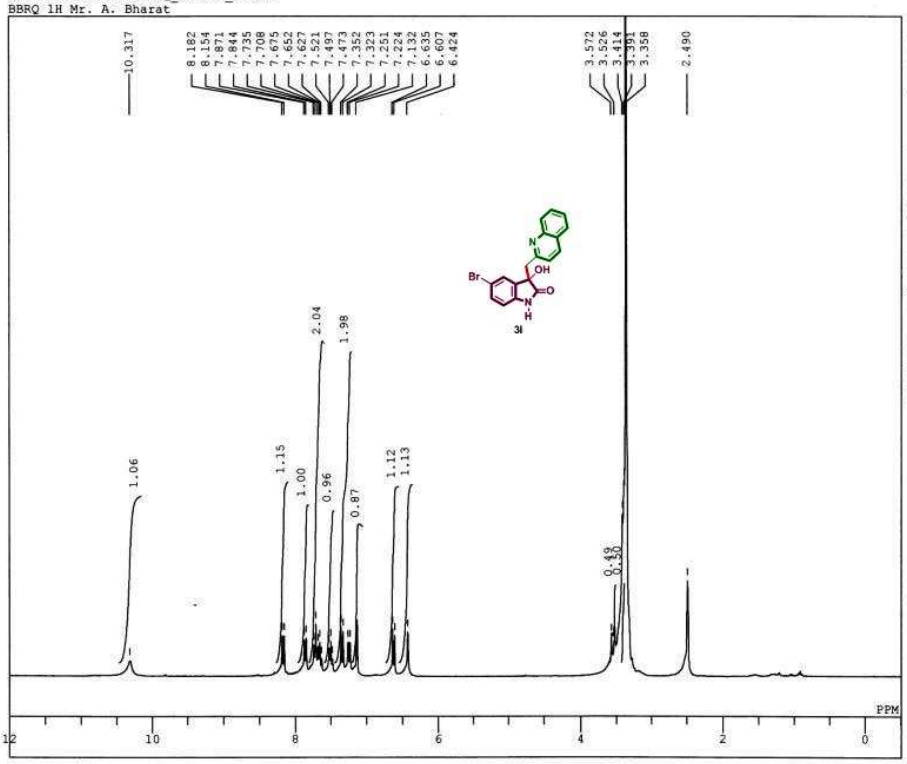


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\Kumkum\NOBN_13C.als
COMNT	NOBN_13C_Ms.Kumkum
DATIM	Fri Aug 23 04:08:58 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	1500
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	21.9 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	23

C:\WINNMR98\Data\BBRQ_1H1NON_E5.als
BBRQ 1H Mr. A. Bharat

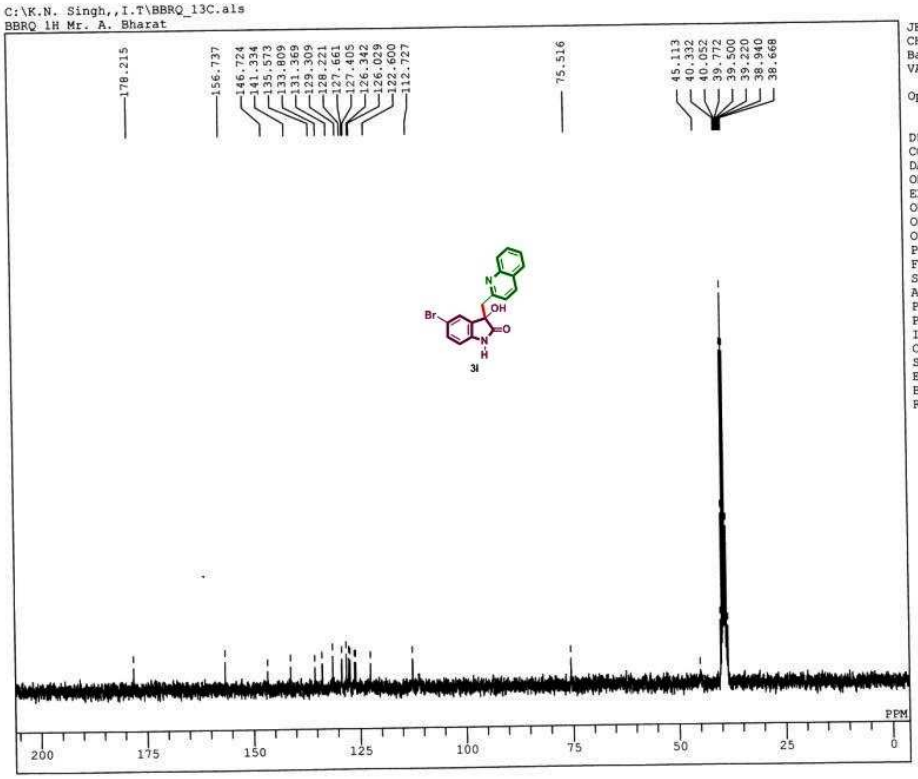


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\WINNMR98\Data\BBRQ_
COMNT	BBRQ_1H_Mr. A. Bharat
DATIM	Tue Oct 15 14:53:03 20
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	6016.8 Hz
SCANS	16
ACQTM	5.446 sec
PD	1.547 sec
PW1	5.6 us
IRNUC	1H
CTEMP	22.3 c
SLVNT	DMSO
EXREF	2.49 ppm
BF	1.20 Hz
RGAIN	18

C:\K.N. Singh,,I.T\BBRQ_13C.als
BBRQ 1H Mr. A. Bharat

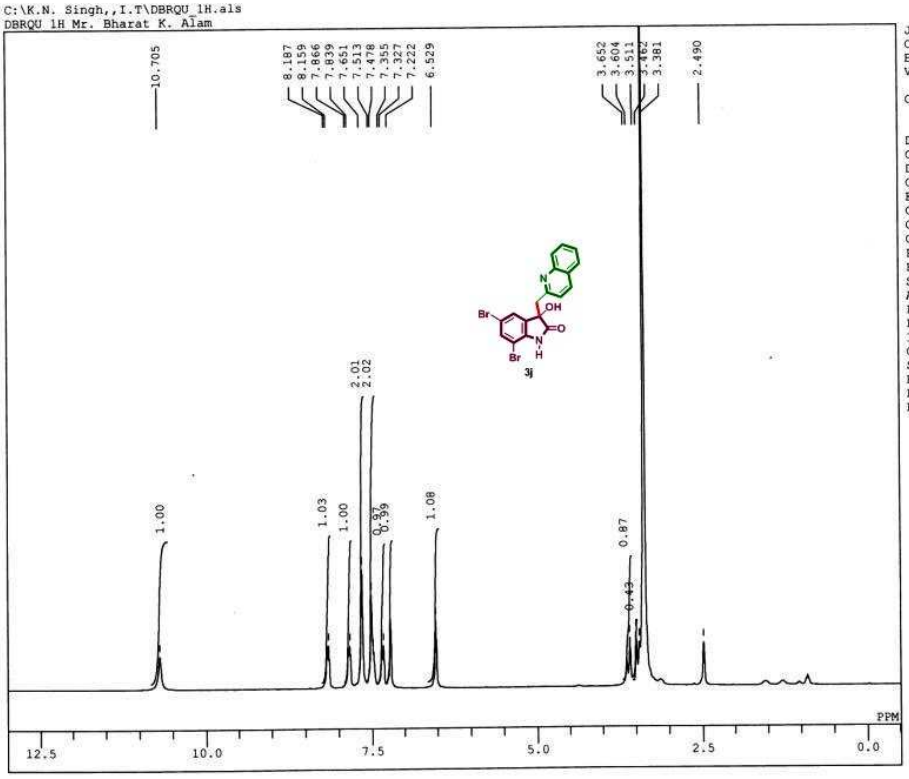


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\K.N. Singh,,I.T\BBR(
COMNT	BBRQ_1H_Mr. A. Bharat
DATIM	Tue Oct 15 15:01:26 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	161
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	24.3 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	22

C:\K.N. Singh,,I.T\DBRQU_1H.als
DBRQU 1H Mr. Bharat K. Alam

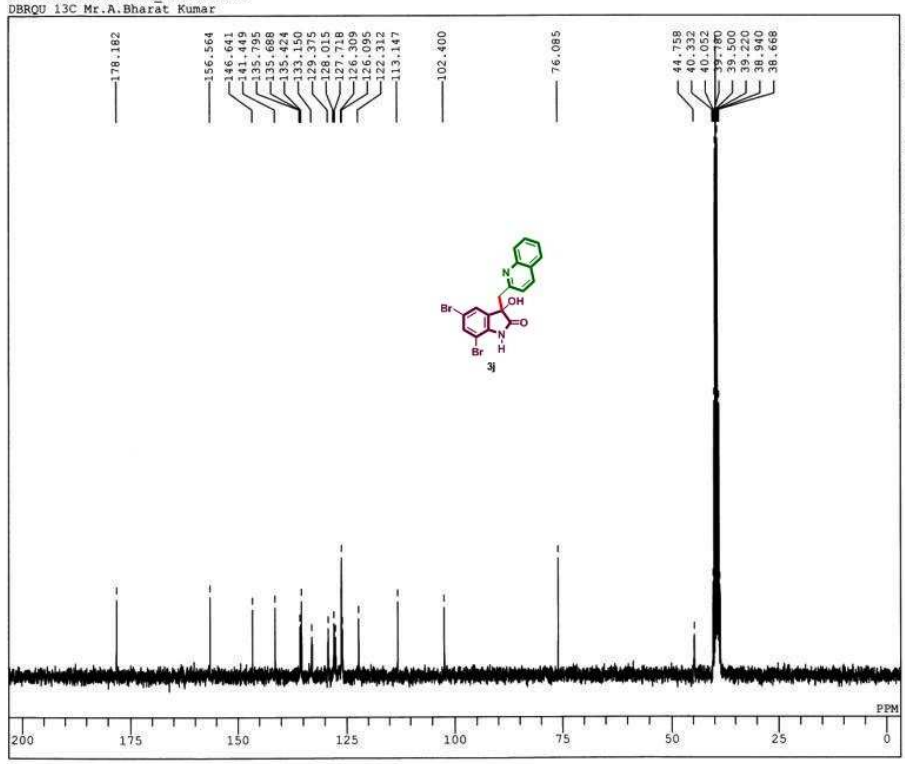


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\K.N. Singh,,I.T\DBR(
COMNT	DBRQU_1H Mr. Bharat K.
DATIM	Tue Aug 13 11:47:02 20
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	23.9 c
SLVNT	DMSO
EXREF	2.49 ppm
BF	1.20 Hz
RGAIN	17

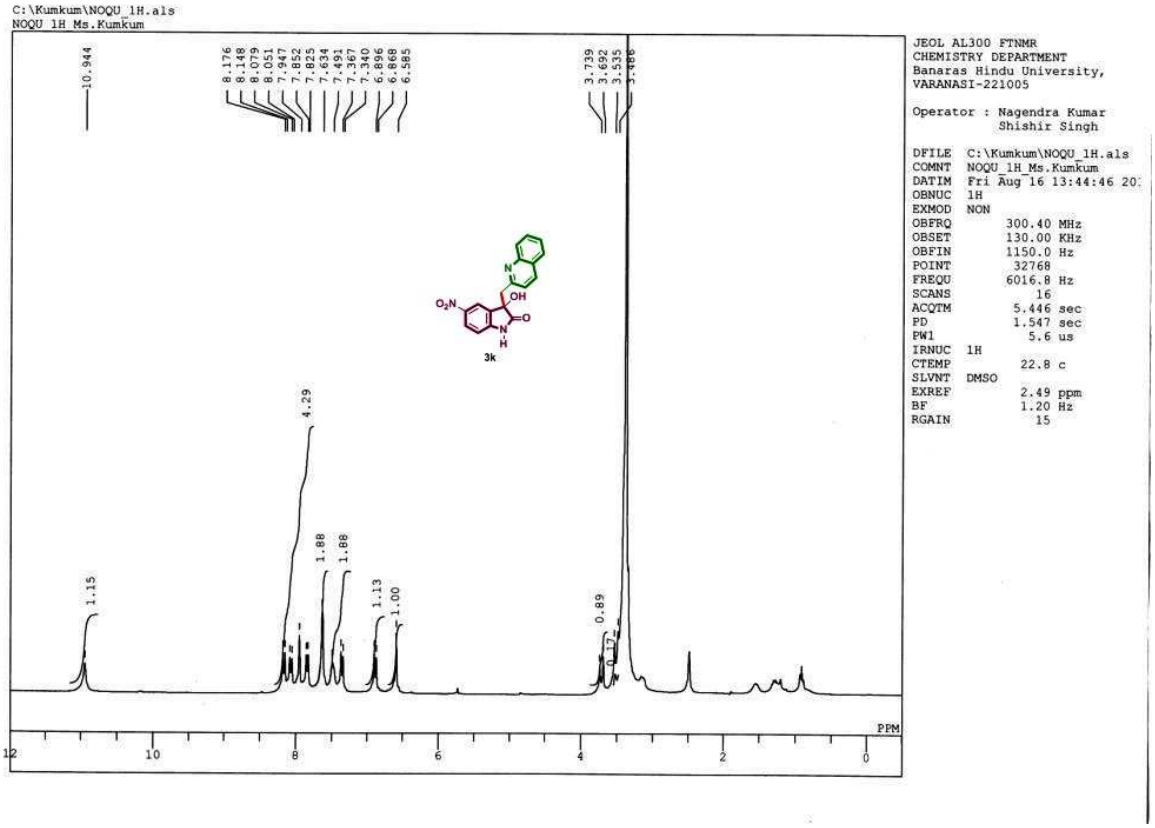
C:\WINNMR98\COMMON_DEFAULT.ALS
DBRQU 13C Mr.A.Bharat Kumar

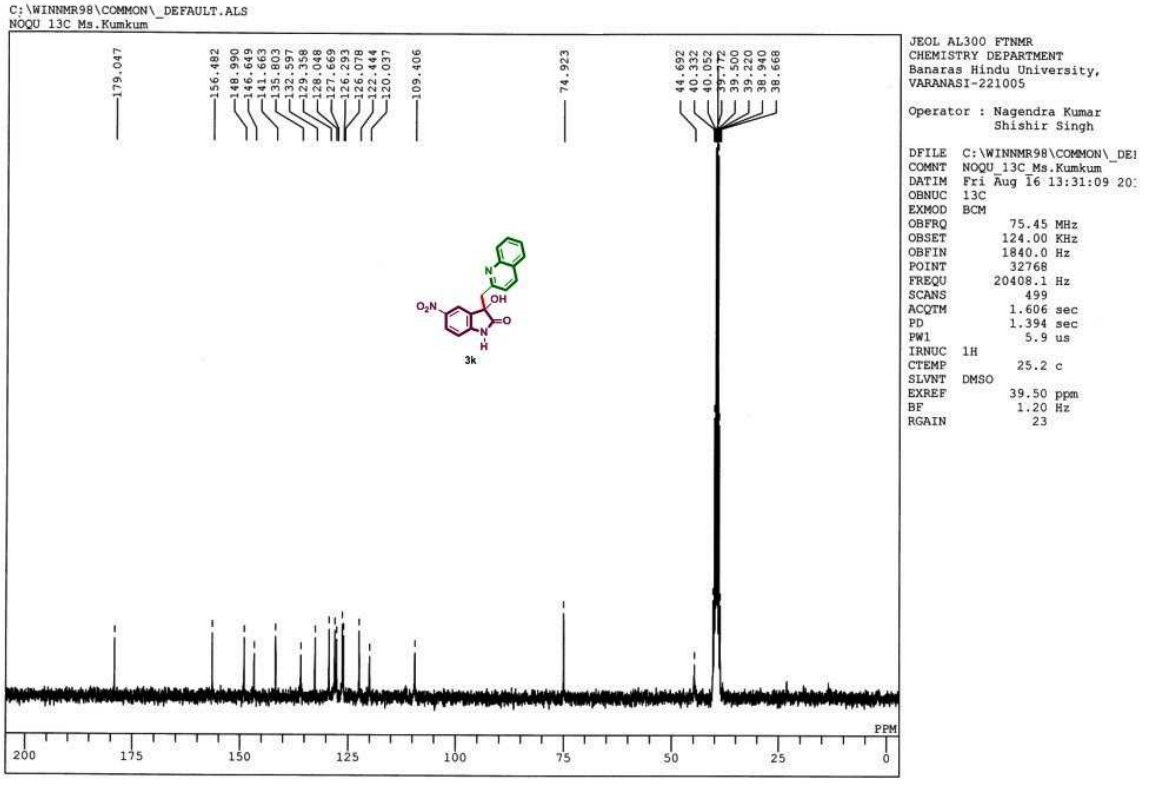


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

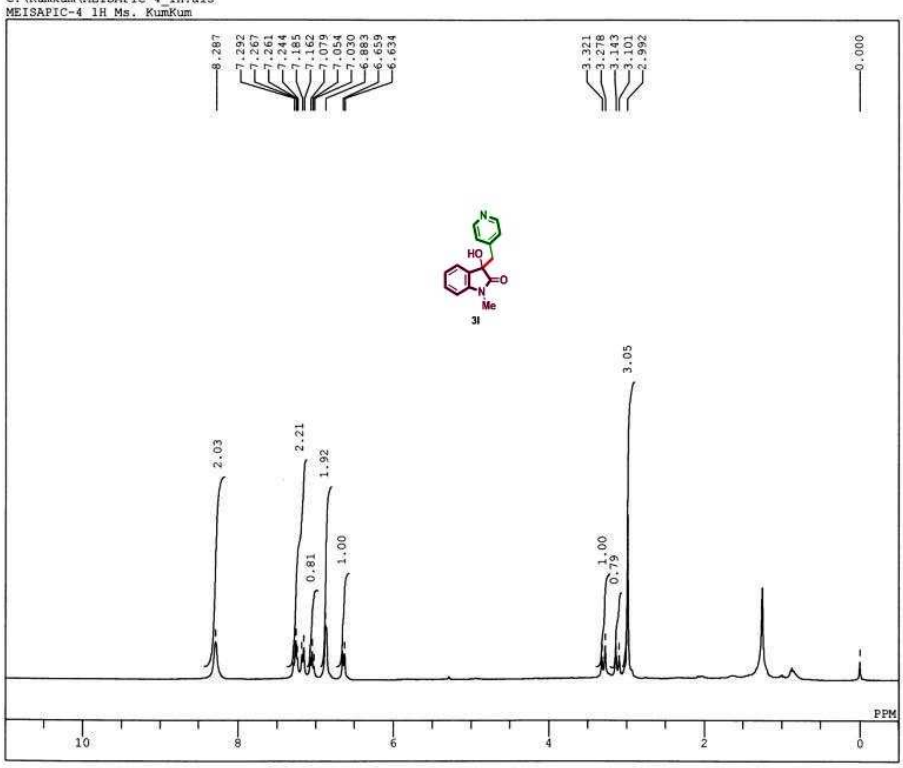
Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\WINNMR98\COMMON_DEI
COMNT	DBRQU_13C Mr.A.Bharat I
DATIM	Tue Aug 13 12:40:30 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	206
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	27.9 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	23


C:\Kumkum\NOQU_1H.als
NOQU_1H_Ms.Kumkum
10.944
8.176
8.148
8.079
8.051
7.947
7.852
7.825
7.634
7.491
7.367
7.340
6.896
6.868
6.585
3.739
3.692
3.535
3.466
4.29
1.88
1.88
1.15
1.13
1.00
0.89
0.17
3k
PPM
12
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\NOQU_1H.als
COMNT NOQU_1H_Ms.Kumkum
DATIM Fri Aug 16 13:44:46 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 16
ACQTM 5.446 sec
PD 1.547 sec
PW1 5.6 us
IRNUC 1H
CTEMP 22.8 c
SLVNT DMSO
EXREF 2.49 ppm
BF 1.20 Hz
RGAIN 15


C:\WINNMR98\COMMON_DEFAULT.ALS
NOQU_13C_Ms.Kumkum
179.047
156.482
148.990
146.649
141.663
135.803
132.597
129.358
128.048
127.669
126.293
126.078
122.444
120.037
109.406
74.923
44.692
40.332
40.052
39.772
39.500
39.220
38.940
38.668
3k
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\WINNMR98\COMMON_DE
COMNT NOQU_13C_Ms.Kumkum
DATIM Fri Aug 16 13:31:09 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 499
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 25.2 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 23

C:\Kumkum\MEISAPIC-4_1H.als
MEISAPIC-4_1H Ms. KumKum

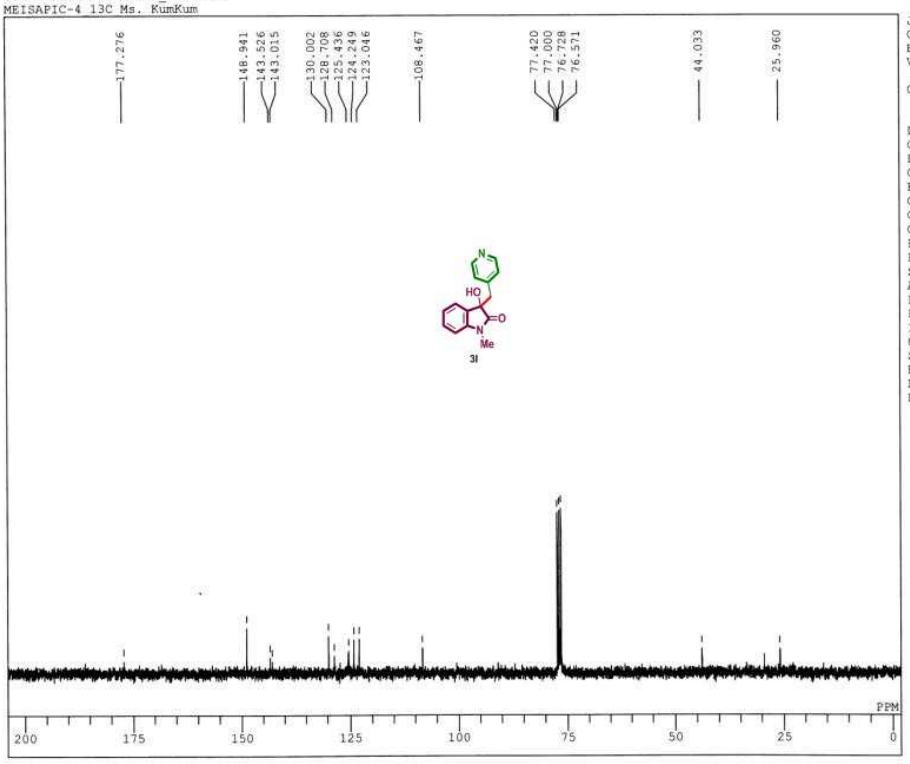


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\Kumkum\MEISAPIC-4_1I
COMNT	MEISAPIC-4_1H_Ms. KumKu
DATIM	Fri Jul 05 18:07:18 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	24.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	19

C:\Kumkum\MEISAPIC-4_13C.als
MEISAPIC-4_13C Ms. KumKum

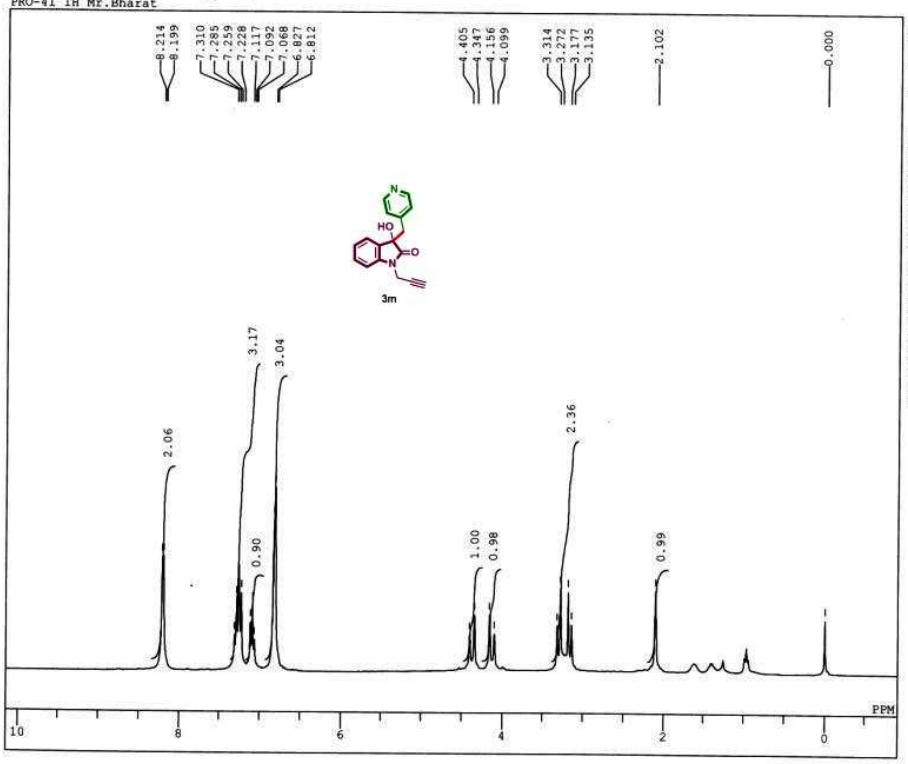


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\Kumkum\MEISAPIC-4_1
COMNT	MEISAPIC-4_13C_Ms. Kum
DATIM	Fri Jul 05 18:04:09 20:
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	178
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	25.5 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	23

C:\K.N. Singh,,I.T\PRO-41_1H.als
PRO-41_1H Mr.Bharat

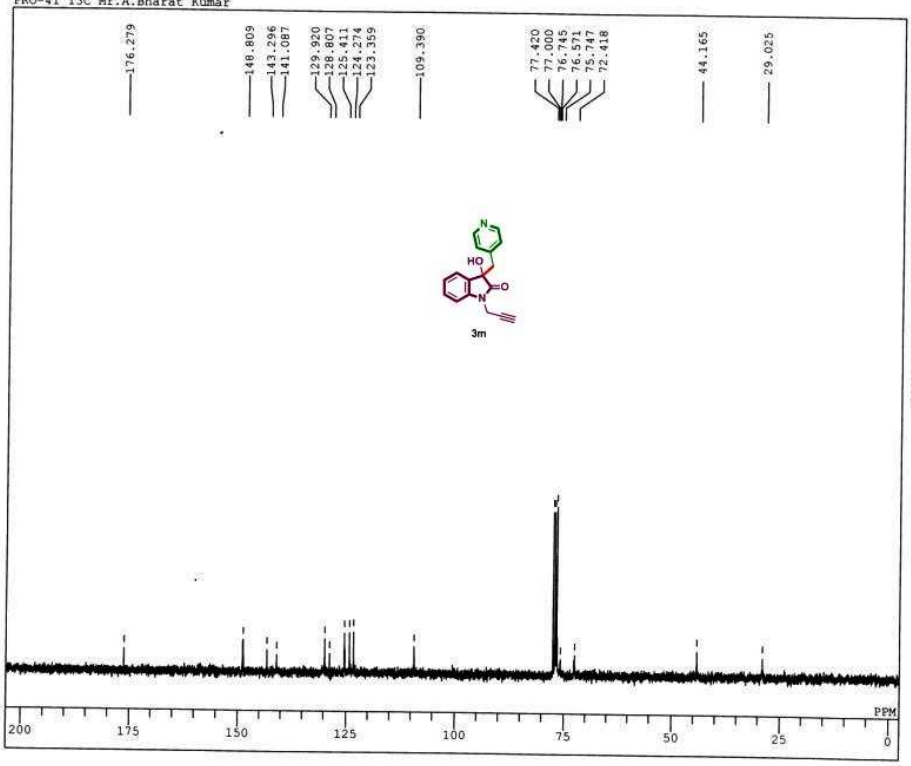


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\K.N. Singh,,I.T\PRO-
COMNT	PRO-41_1H Mr.Bharat
DATIM	Wed Aug 07 17:32:16 20
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	9505.7 Hz
SCANS	27
ACQTM	3.447 sec
PD	1.547 sec
PW1	5.2 us
IRNUC	1H
CTEMP	26.2 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	19

C:\K.N. Singh,,I.T\PRO-41_13C.als
PRO-41_13C Mr.A.Bharat Kumar

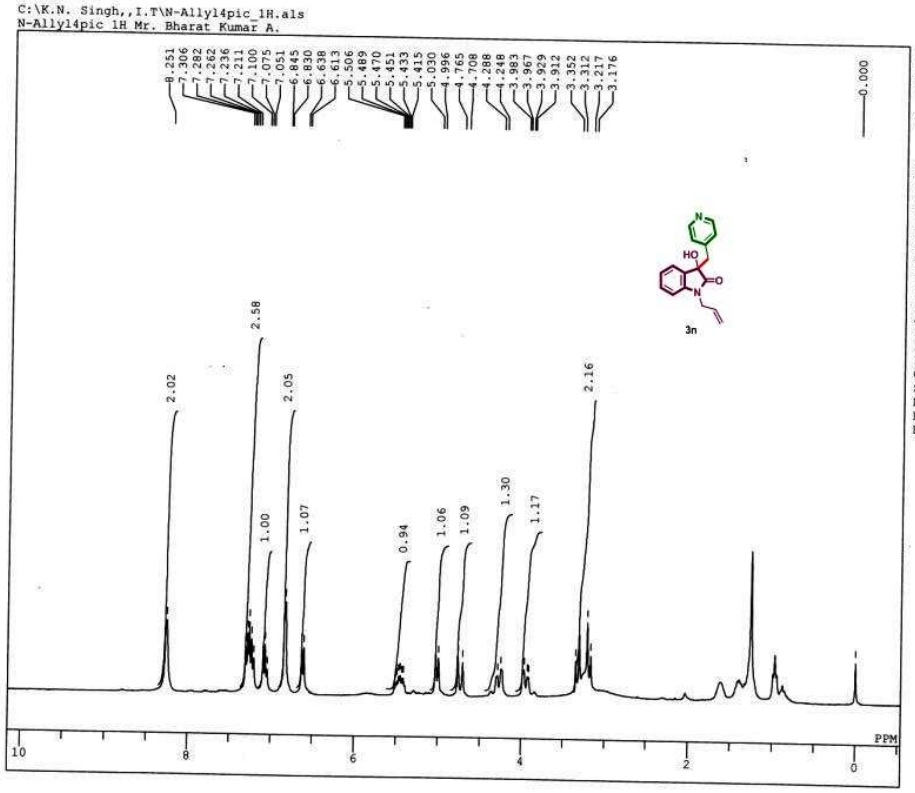


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\K.N. Singh,,I.T\PRO-
COMNT	PRO-41_13C Mr.A.Bharat
DATIM	Wed Aug 07 17:14:11 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	259
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	25.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	24

C:\K.N. Singh,,I.T\N-Allyl4pic_1H.als
N-Allyl4pic 1H Mr. Bharat Kumar A.

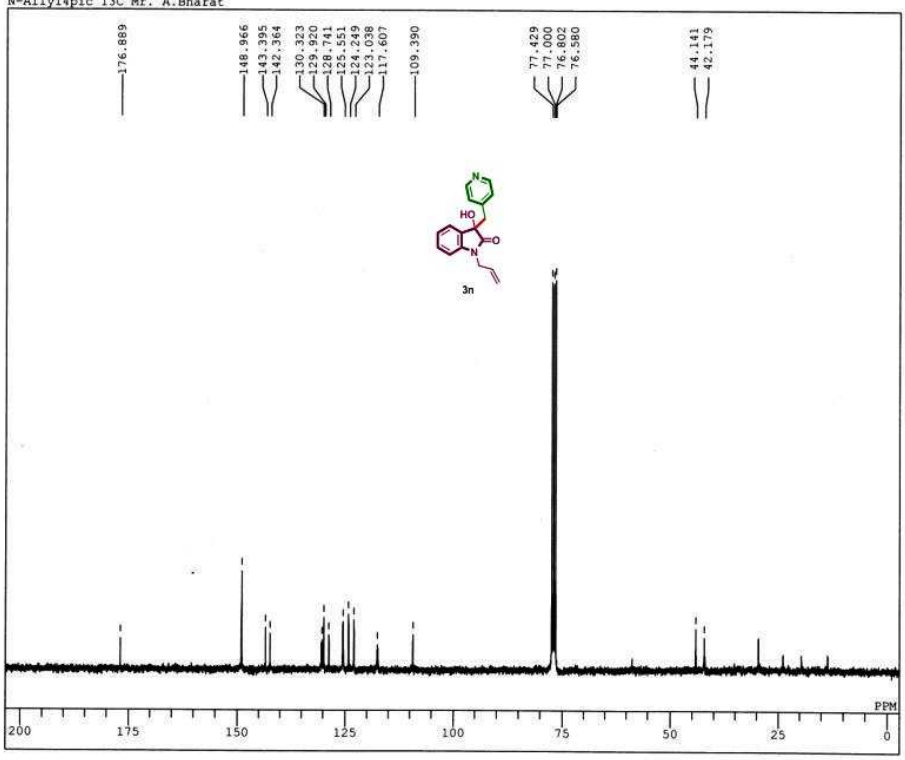


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\K.N. Singh,,I.T\N-A
COMNT	N-Allyl4pic_1H_Mr. Bha
DATIM	Mon Jul 15 16:22:35 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	22.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	18

C:\K.N. Singh,,I.T\N-Allyl4pic_13C.als
N-Allyl4pic 13C Mr. A.Bharat

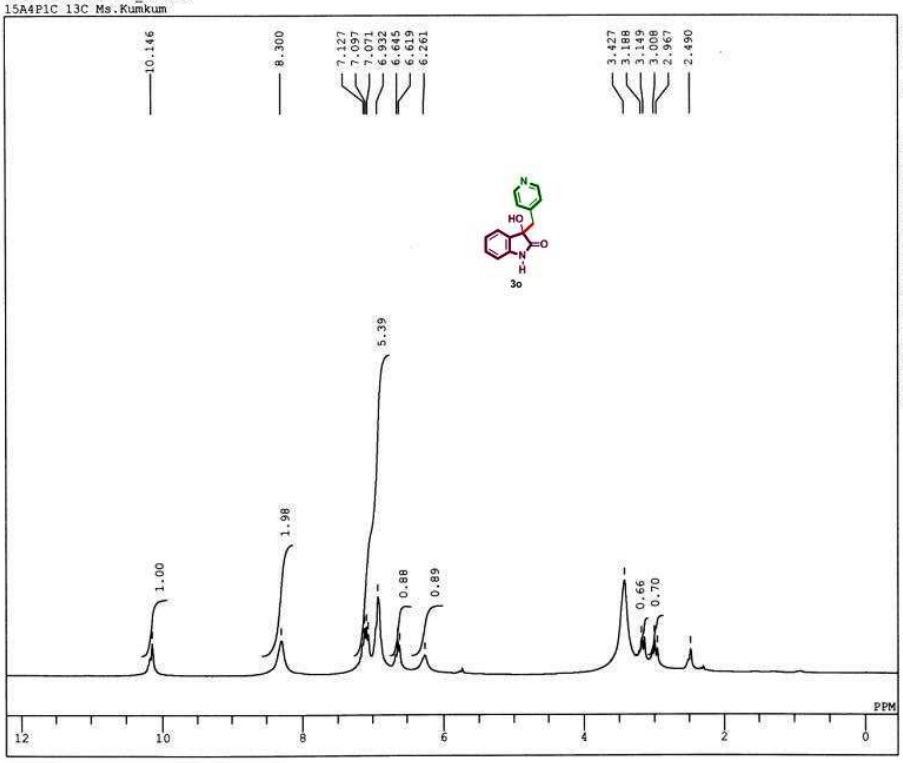


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\K.N. Singh,,I.T\N-A
COMNT	N-Allyl4pic_13C_Mr. A.I
DATIM	Tue Jul 16 03:53:14 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	2000
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	22.5 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	24

C:\Kumkum\15A4P1C_1H.als
15A4P1C 13C Ms.Kumkum

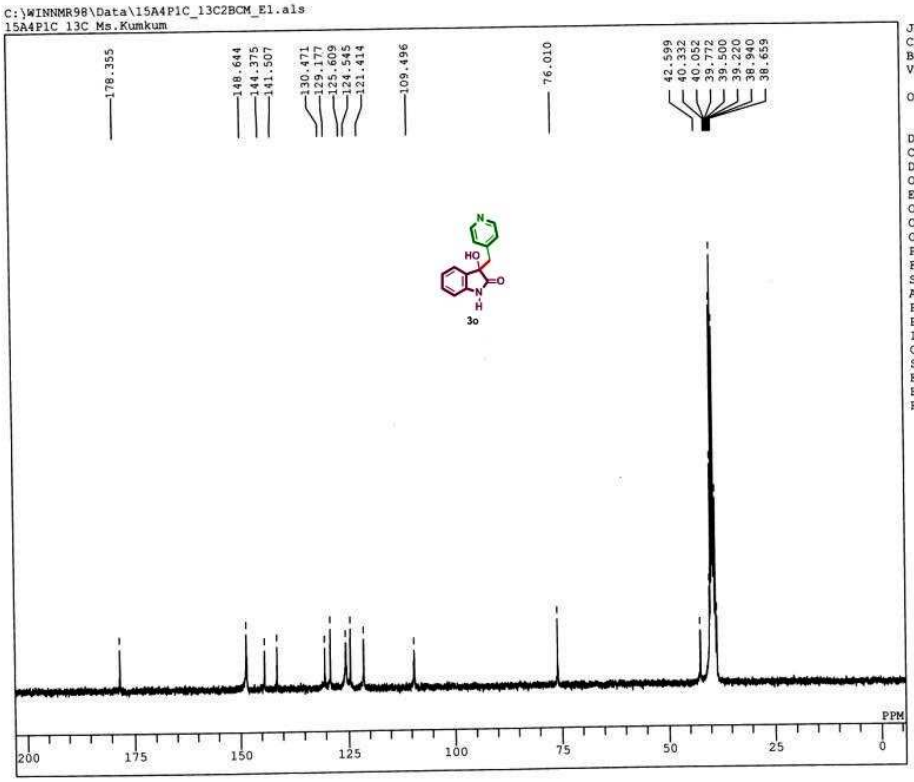


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\Kumkum\15A4P1C_1H.a
COMNT	15A4P1C_13C_Ms.Kumkum
DATIM	Thu Jul 11 18:27:43 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	5.6 us
IRNUC	1H
CTEMP	21.9 c
SLVNT	DMSO
EXREF	2.49 ppm
BF	1.20 Hz
RGAIN	17

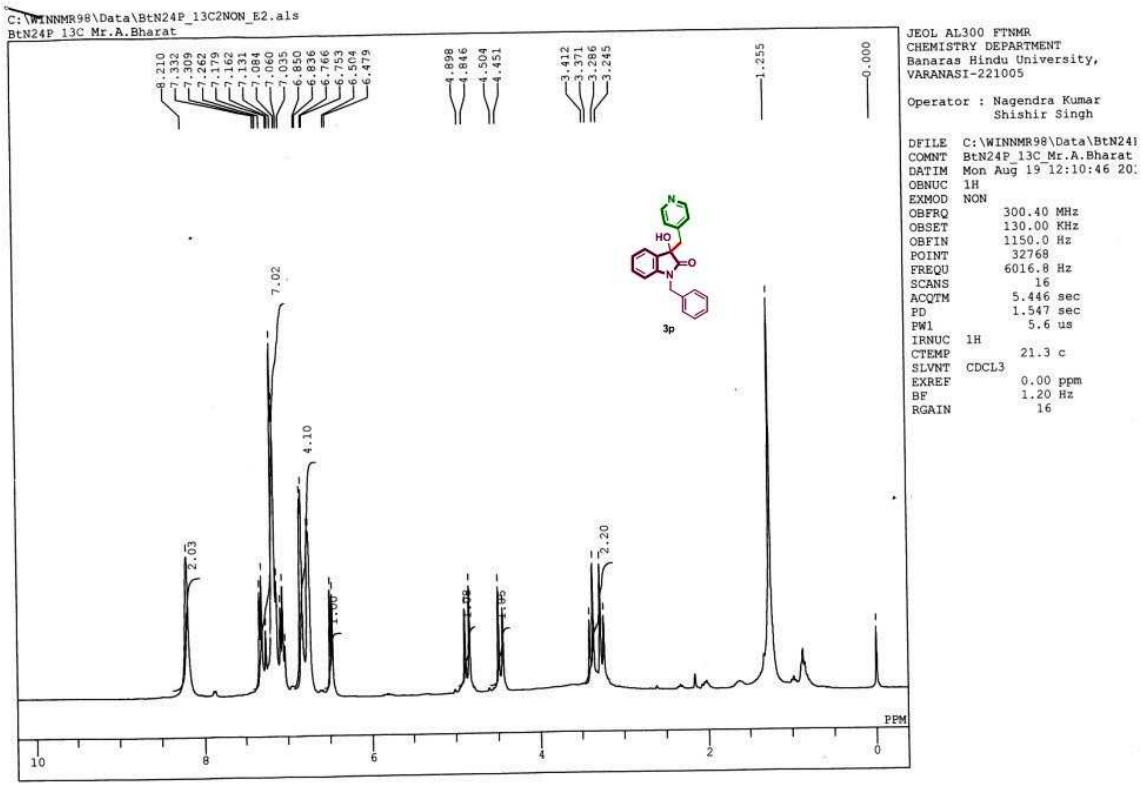
C:\WINNMR98\Data\15A4P1C_13C2BCM_E1.als
15A4P1C 13C Ms.Kumkum

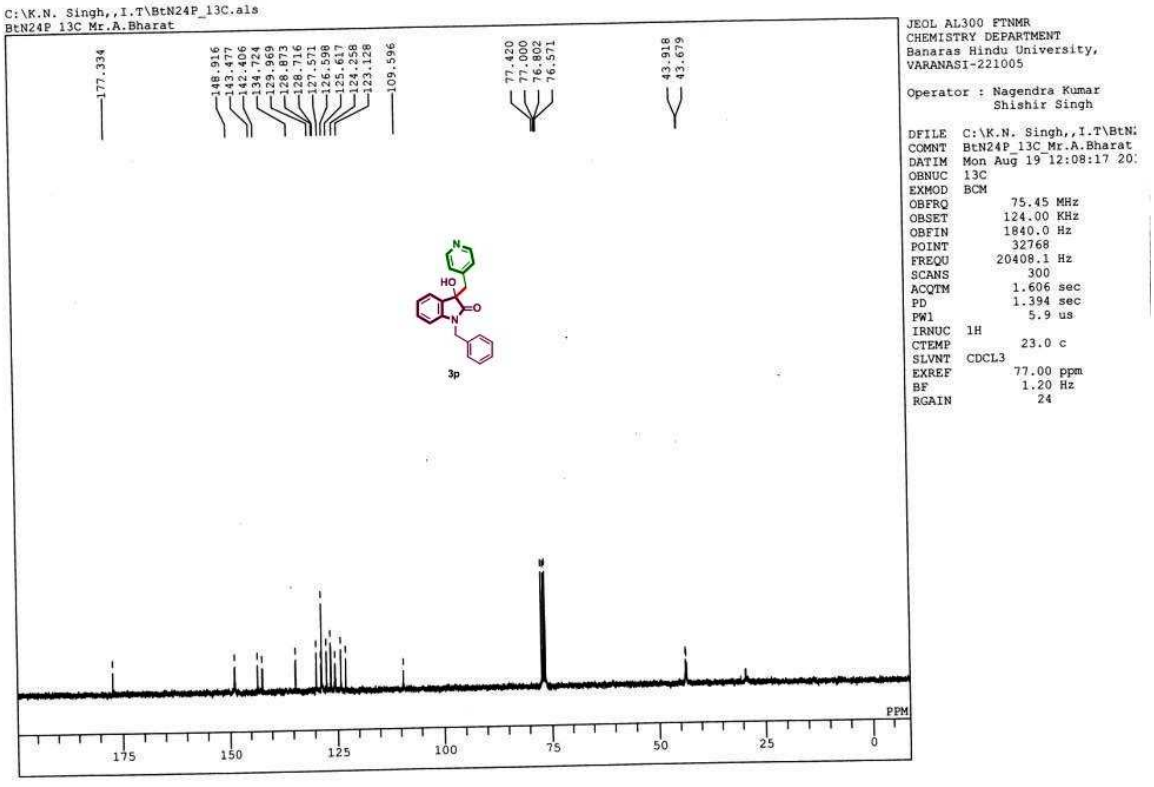


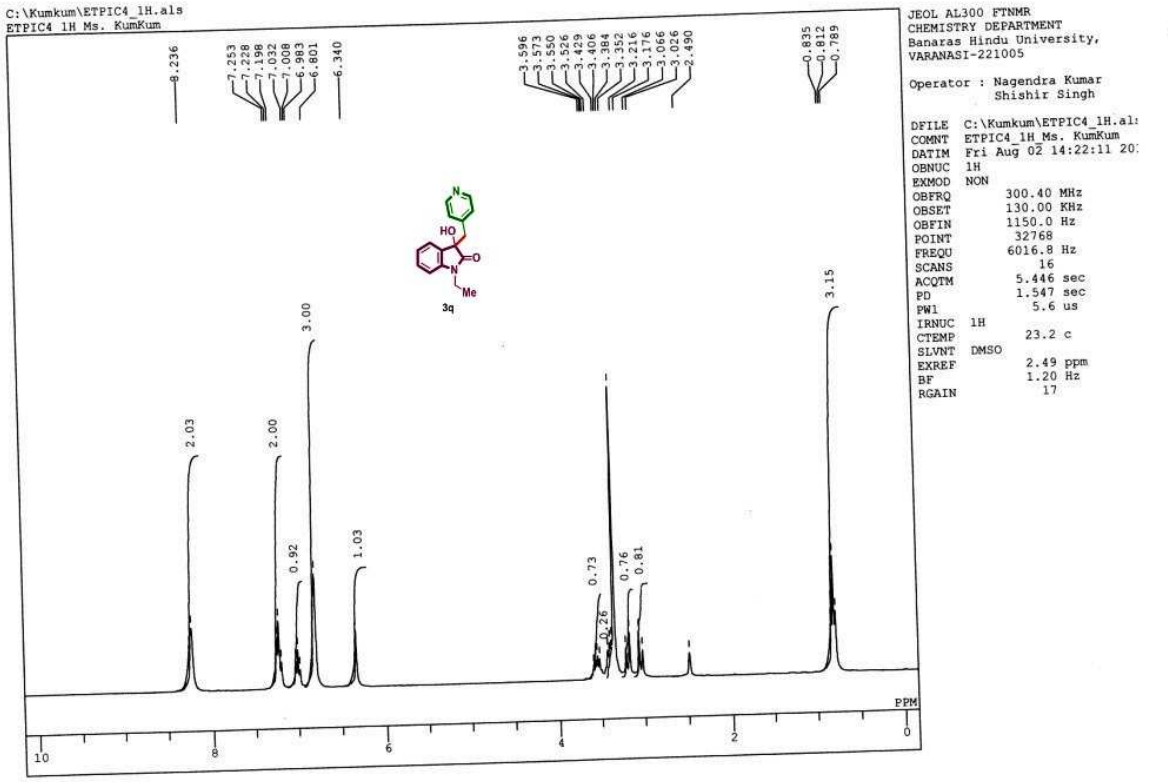
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

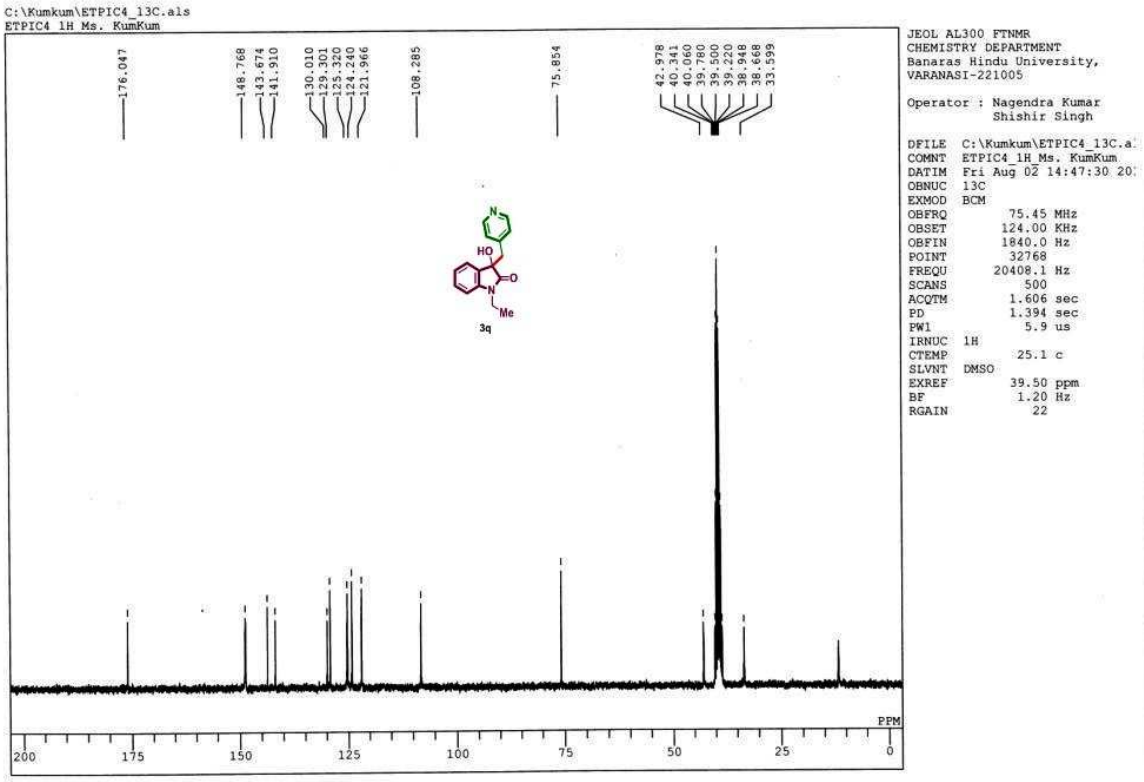
Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\WINNMR98\Data\15A4P1
COMNT	15A4P1C_13C_Ms.Kumkum
DATIM	Thu Jul 11 20:08:05 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	2000
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	19.3 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	23

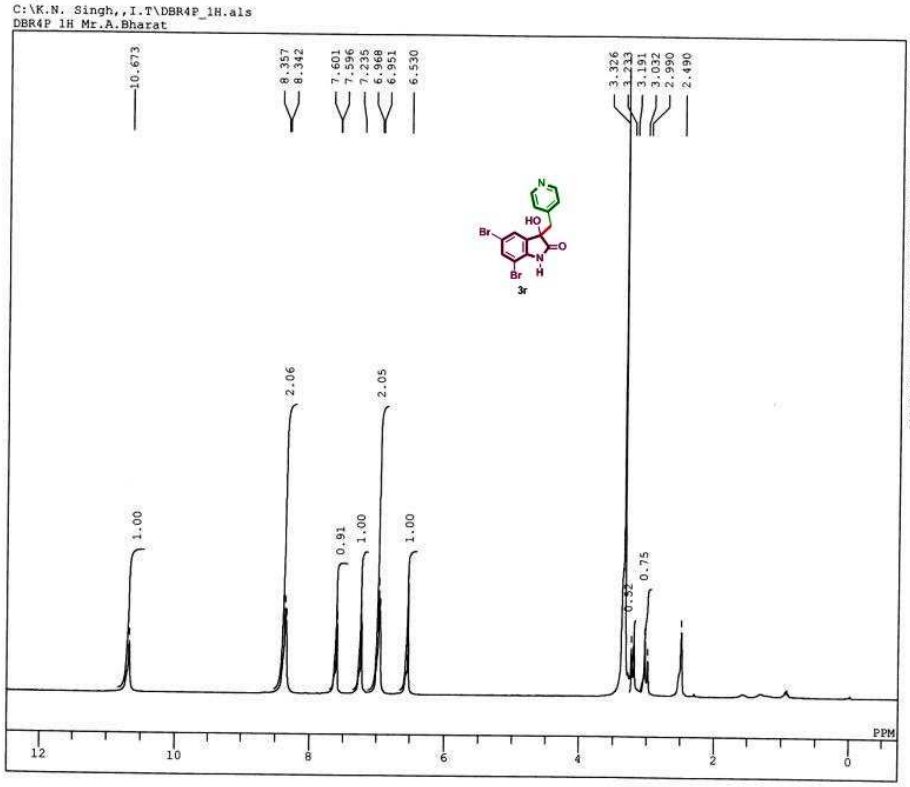

C:\WINNMR98\Data\BtN24P_13C2NON_E2.als
BtN24P_13C Mr.A.Bharat
8.210
7.332
7.309
7.262
7.179
7.162
7.131
7.084
7.060
7.035
6.850
6.836
6.766
6.753
6.504
6.479
4.898
4.846
4.504
4.451
3.412
3.371
3.286
3.245
1.255
0.000
7.02
4.10
2.03
2.20
3p
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\WINNMR98\Data\BtN24
COMNT BtN24P_13C_Mr.A.Bharat
DATIM Mon Aug 19 12:10:46 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 16
ACQTM 5.446 sec
PD 1.547 sec
PW1 5.6 us
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 16


C:\K.N. Singh,,I.T\BtN24P_13C.als
BtN24P_13C Mr.A.Bharat
177.334
148.916
143.477
142.406
134.724
129.969
128.873
128.716
127.571
126.598
125.617
124.258
123.128
109.596
77.420
77.000
76.802
76.571
43.918
43.679
3p
PPM
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\K.N. Singh,,I.T\BtN
COMNT BtN24P_13C_Mr.A.Bharat
DATIM Mon Aug 19 12:08:17 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 300
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24


C:\Kumkum\ETPIC4_1H.als
ETPIC4 1H Ms. KumKum
8.236
7.253
7.228
7.198
7.032
7.008
6.983
6.801
6.340
3.596
3.573
3.550
3.526
3.429
3.406
3.384
3.352
3.216
3.176
3.066
3.026
2.490
0.835
0.812
0.789
HO
N
O
Me
3q
2.03
2.00
3.00
0.92
1.03
0.73
0.26
0.76
0.81
3.15
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\ETPIC4_1H.al
COMNT ETPIC4_1H_Ms. KumKum
DATIM Fri Aug 02 14:22:11 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 16
ACQTM 5.446 sec
PD 1.547 sec
PW1 5.6 us
IRNUC 1H
CTEMP 23.2 c
SLVNT DMSO
EXREF 2.49 ppm
BF 1.20 Hz
RGAIN 17


C:\Kumkum\ETPIC4_13C.als
ETPIC4 1H Ms. KumKum
176.047
148.768
143.674
141.910
130.010
129.301
125.320
124.240
121.966
108.285
75.854
42.978
40.341
40.060
39.780
39.500
39.220
38.948
38.668
33.599
HO
N
O
Me
3q
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\ETPIC4_13C.a
COMNT ETPIC4_1H_Ms. KumKum
DATIM Fri Aug 02 14:47:30 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 500
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 25.1 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 22

C:\K.N. Singh,,I.T\DBR4P_1H.als
DBR4P 1H Mr.A.Bharat

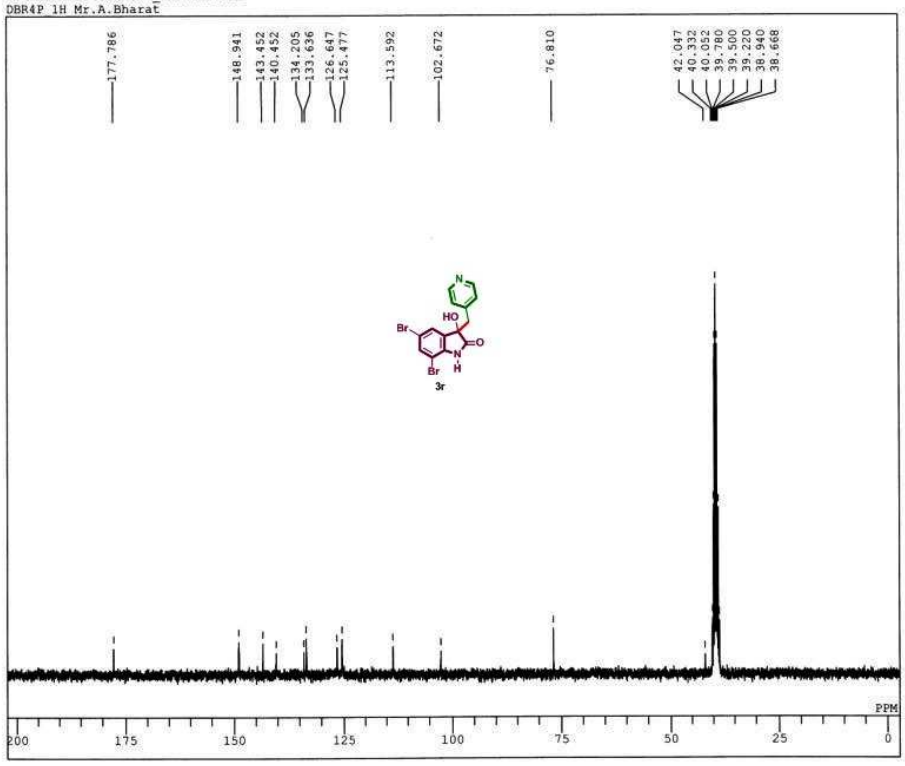


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\K.N. Singh,,I.T\DBR
COMNT	DBR4P_1H Mr.A.Bharat
DATIM	Thu Aug 22 16:41:10 20
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	6016.8 Hz
SCANS	16
ACQTM	5.446 sec
PD	1.547 sec
PW1	5.6 us
IRNUC	1H
CTEMP	23.1 c
SLVNT	DMSO
EXREF	2.49 ppm
BF	1.20 Hz
RGAIN	19

C:\WINNMR98\COMMON_DEFAULT.ALS
DBR4P 1H Mr.A.Bharat

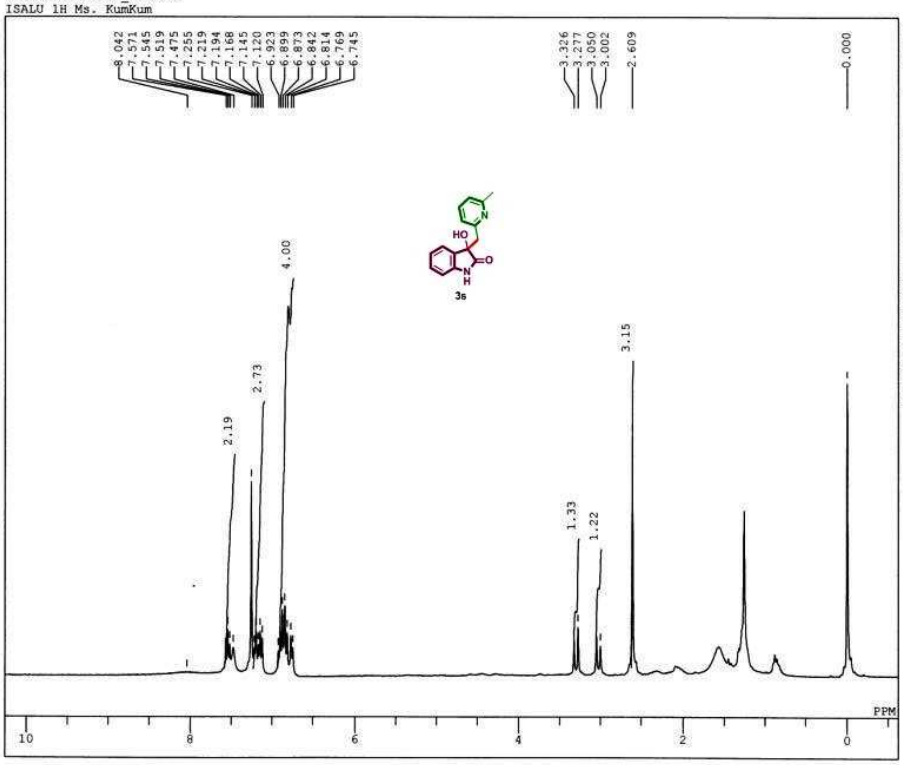


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\WINNMR98\COMMON_DEI
COMNT	DBR4P_1H Mr.A.Bharat
DATIM	Thu Aug 22 16:57:23 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	300
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	28.3 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	21

C:\Kumkum\ISALU_1H2.als
ISALU_1H Ms. KumKum

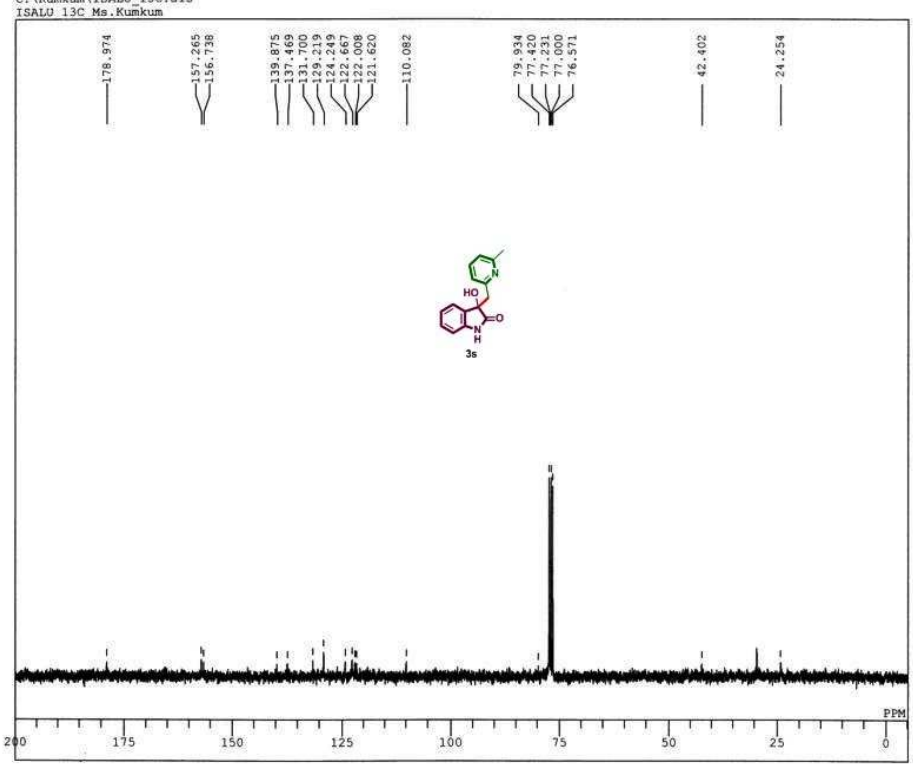


JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE	C:\Kumkum\ISALU_1H2.als
COMNT	ISALU_1H Ms. KumKum
DATIM	Tue Sep 24 14:46:12 20
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	23.7 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	23

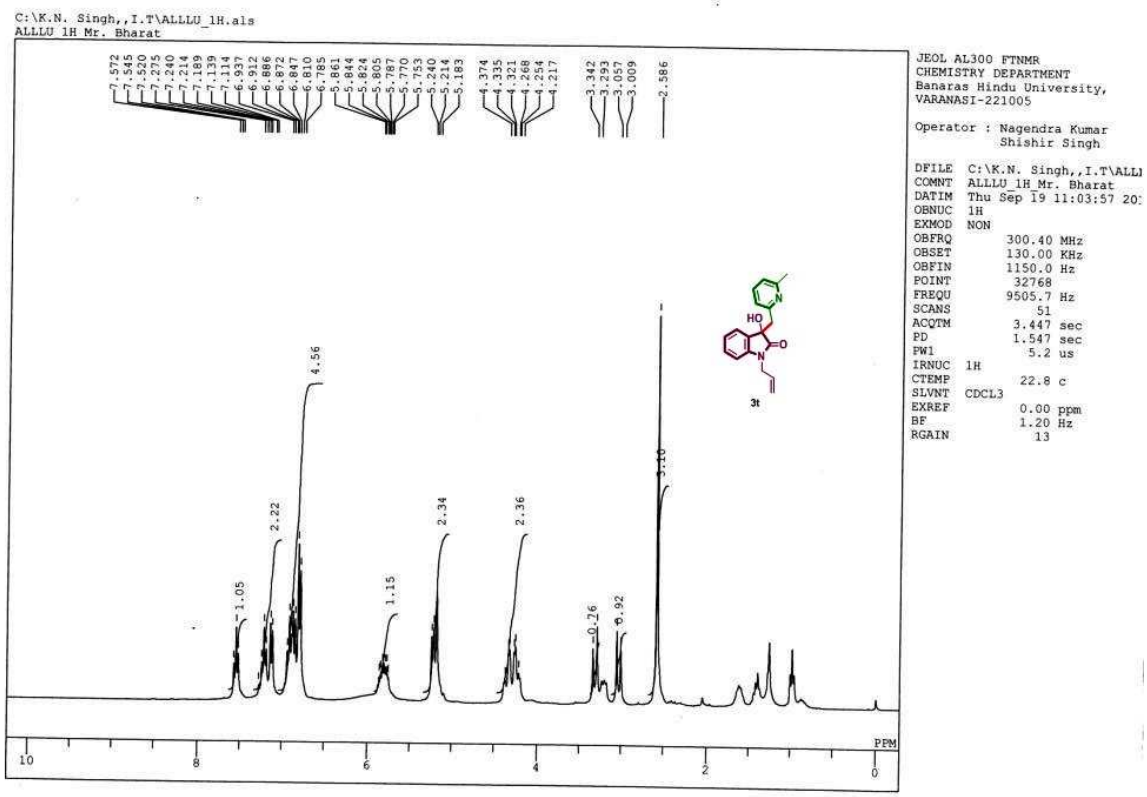
C:\Kumkum\ISALU_13C.als
ISALU_13C Ms.Kumkum

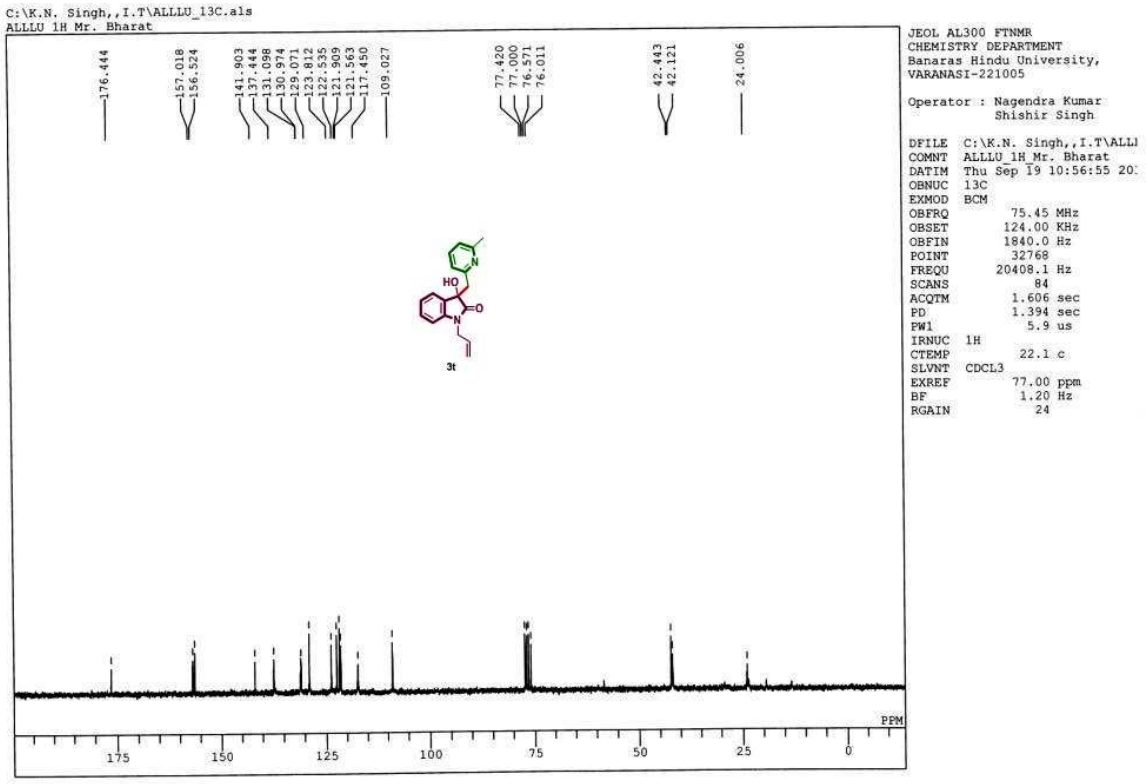


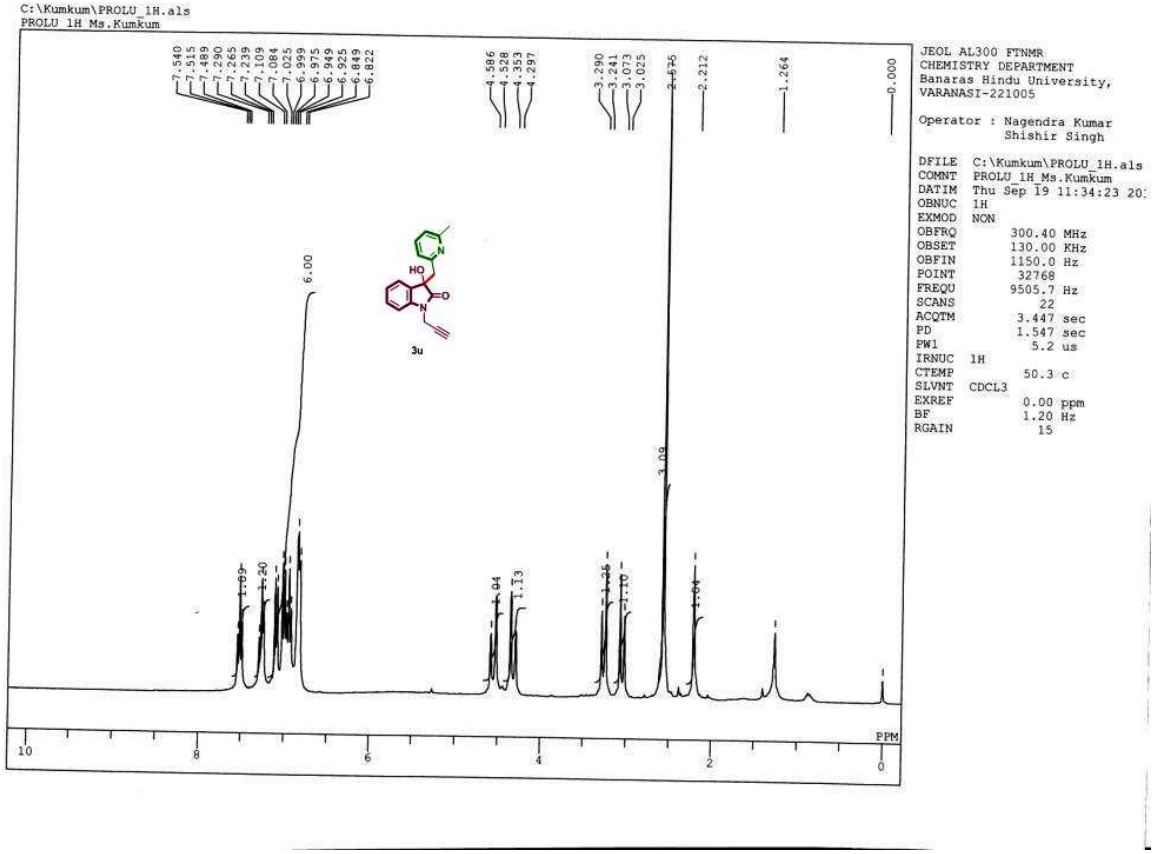
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

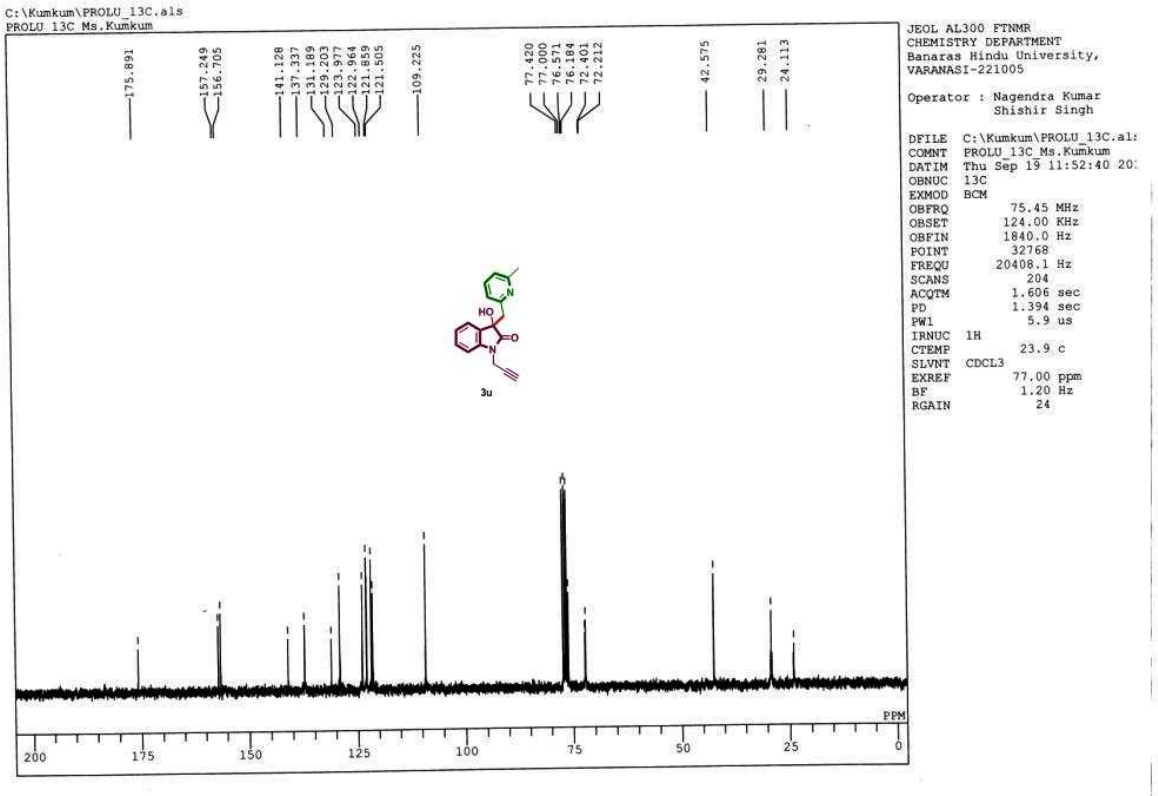
Operator : Nagendra Kumar
Shishir Singh

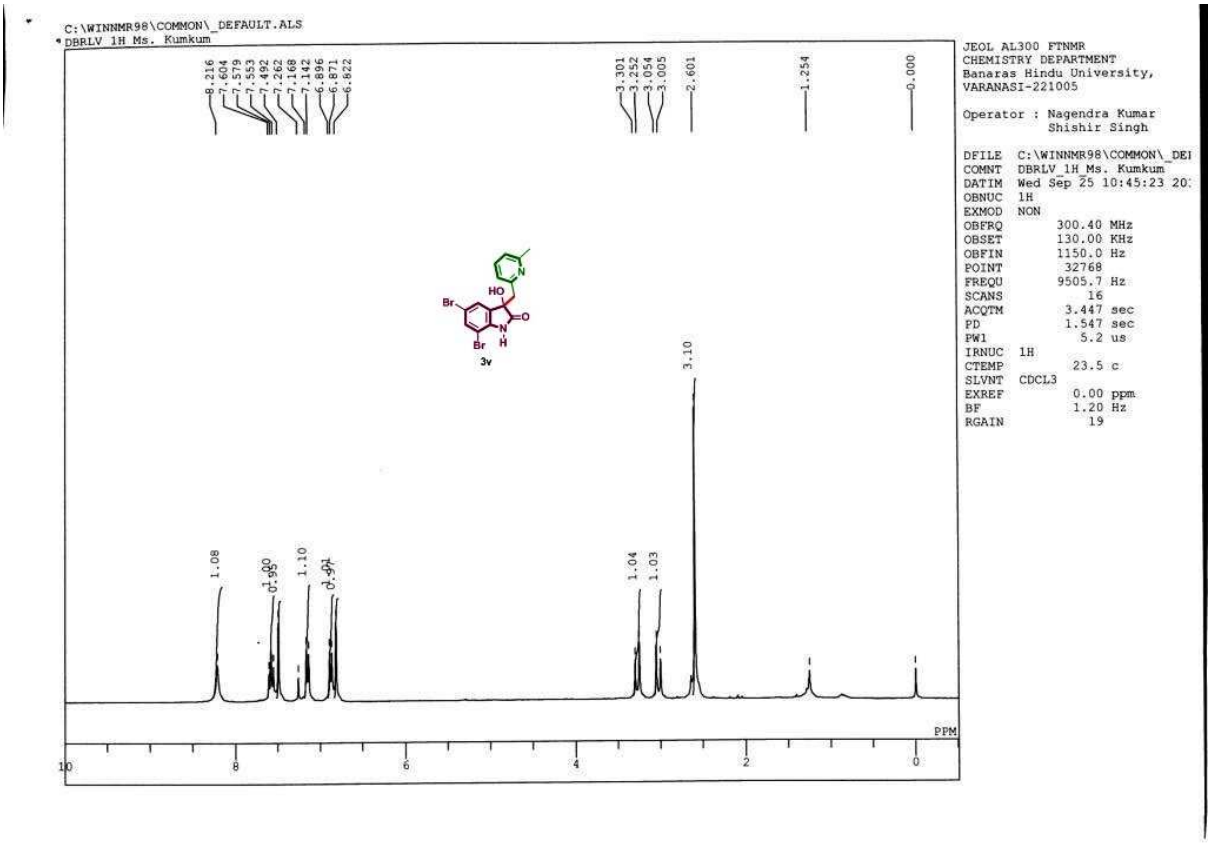
DFILE	C:\Kumkum\ISALU_13C.als
COMNT	ISALU_13C Ms.Kumkum
DATIM	Mon Sep 02 14:54:28 20
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	218
ACQTM	1.606 sec
PD	1.394 sec
PW1	5.9 us
IRNUC	1H
CTEMP	24.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	24

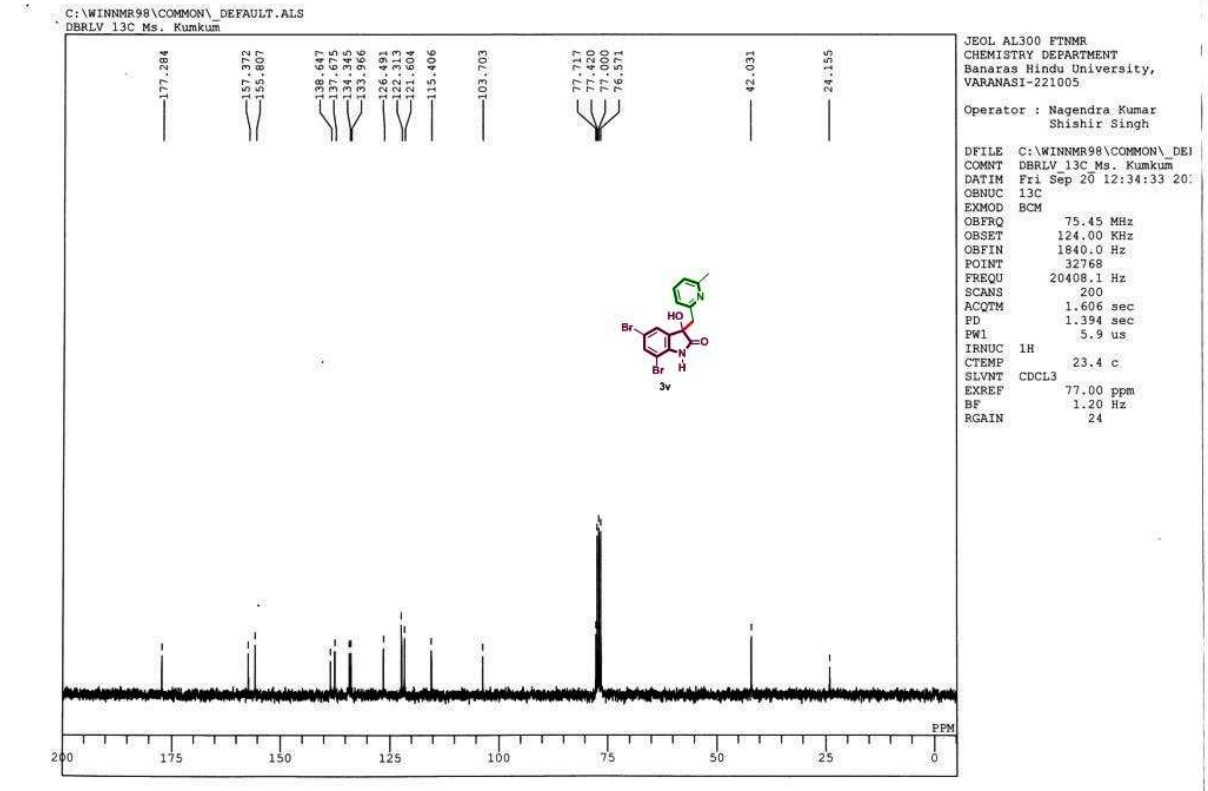

C:\K.N. Singh,,I.T\ALLLU_1H.als
ALLLU 1H Mr. Bharat
7.572
7.545
7.520
7.275
7.240
7.214
7.189
7.139
7.114
6.937
6.912
6.886
6.872
6.847
6.810
6.785
5.861
5.844
5.824
5.805
5.787
5.770
5.753
5.240
5.214
5.183
4.374
4.335
4.321
4.268
4.254
4.217
3.342
3.293
3.057
3.009
2.586
4.56
2.22
1.05
1.15
2.34
2.36
0.26
0.92
3.10
3t
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\K.N. Singh,,I.T\ALL
COMNT ALLLU_1H Mr. Bharat
DATIM Thu Sep 19 11:03:57 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 51
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 13

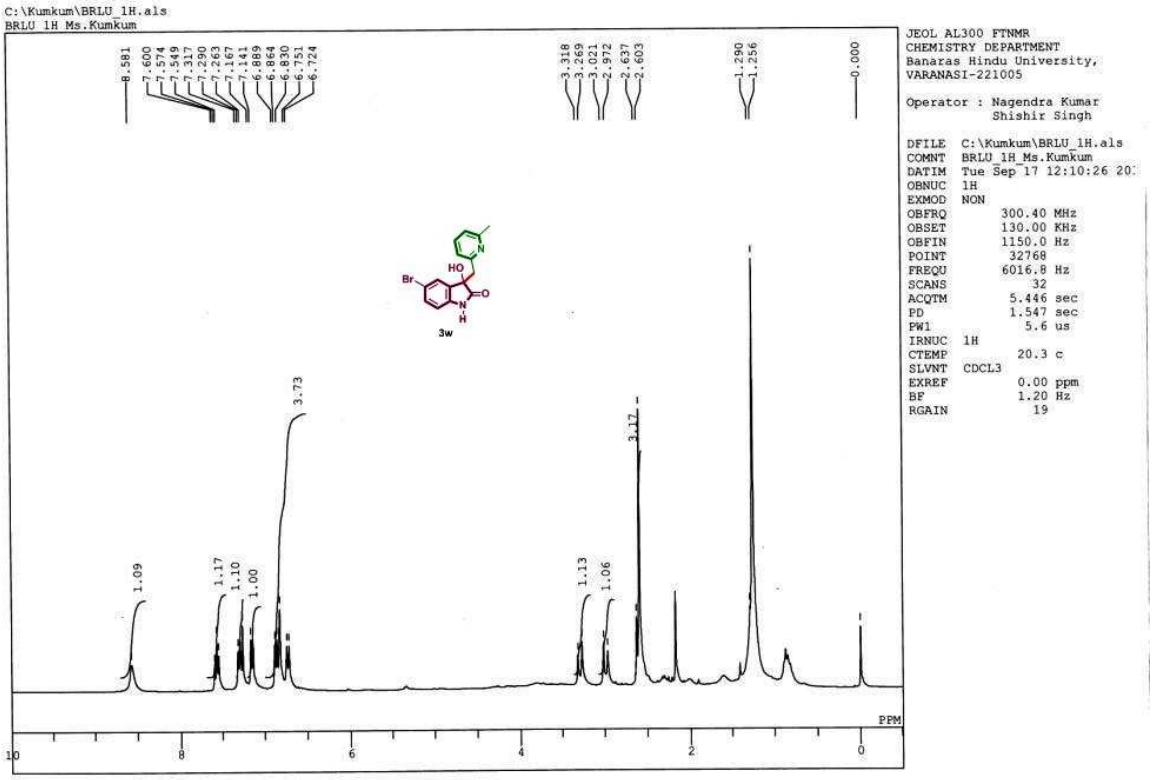

C:\K.N. Singh,,I.T\ALLLU_13C.als
ALLLU 1H Mr. Bharat
176.444
157.018
156.524
141.903
137.444
131.098
130.974
129.071
123.812
122.535
121.909
121.563
117.450
109.027
77.420
77.000
76.571
76.011
42.443
42.121
24.006
3t
PPM
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\K.N. Singh,,I.T\ALL
COMNT ALLLU_1H Mr. Bharat
DATIM Thu Sep 19 10:56:55 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 84
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

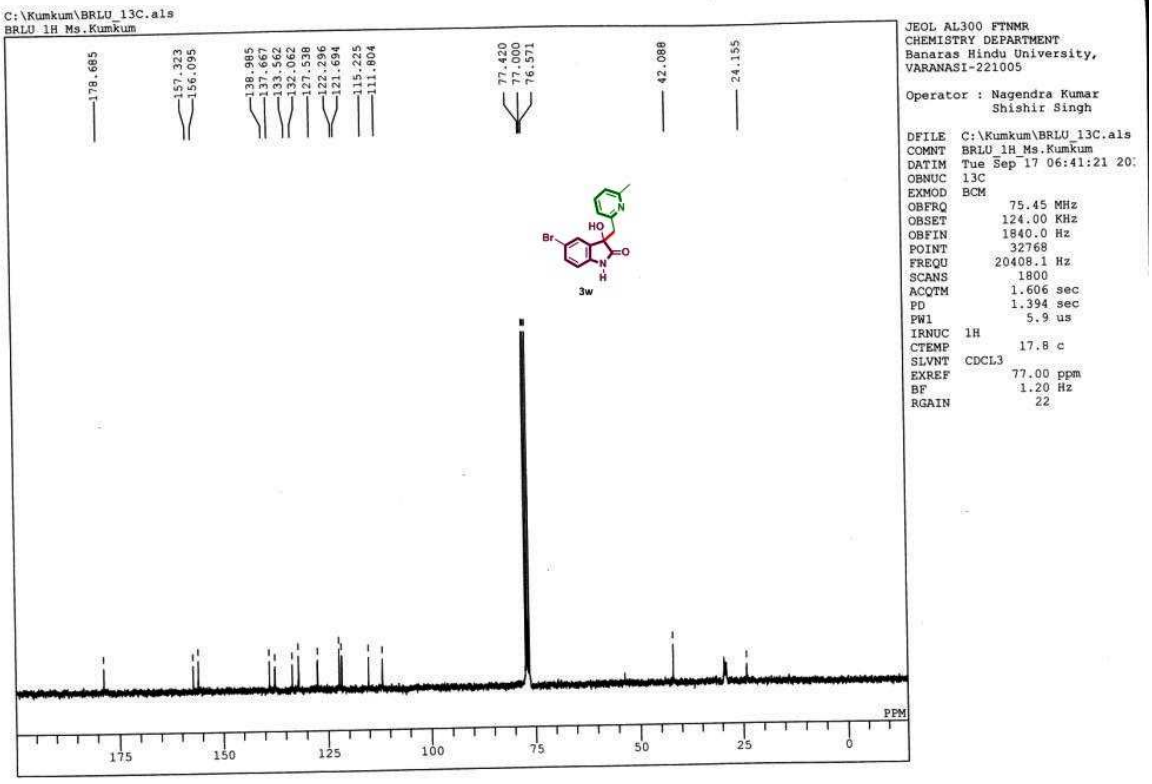

C:\Kumkum\PROLU_1H.als
PROLU_1H_Ms.Kumkum
7.540
7.515
7.489
7.290
7.265
7.239
7.109
7.084
7.025
6.999
6.975
6.949
6.925
6.849
6.822
4.586
4.528
4.353
4.297
3.290
3.241
3.073
3.025
2.675
2.212
1.264
0.000
6.00
1.89
1.20
1.04
1.13
1.26
1.10
3.09
1.04
3u
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\PROLU_1H.als
COMNT PROLU_1H_Ms.Kumkum
DATIM Thu Sep 19 11:34:23 20
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 22
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 50.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 15

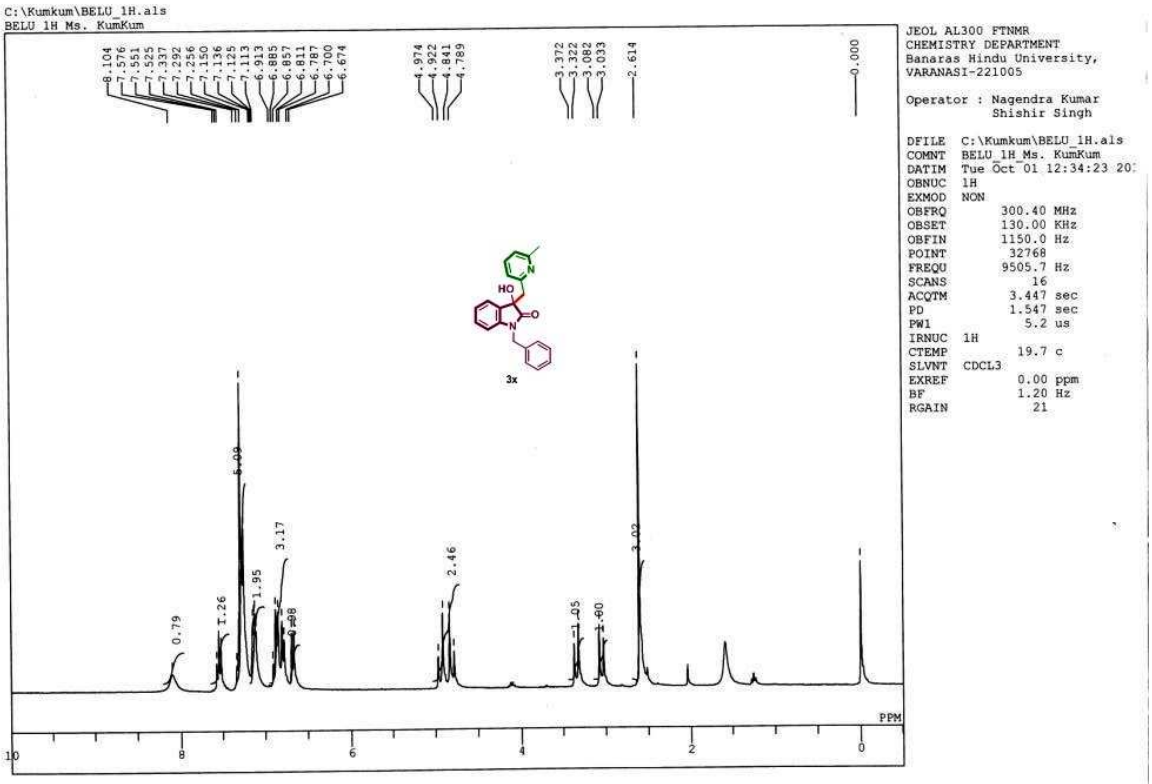

C:\Kumkum\PROLU_13C.als
PROLU_13C_Ms.Kumkum
175.891
157.249
156.705
141.128
137.337
131.189
129.203
123.977
122.964
121.859
121.505
109.225
77.420
77.000
76.571
76.184
72.401
72.212
42.575
29.281
24.113
3u
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\PROLU_13C.al
COMNT PROLU_13C_Ms.Kumkum
DATIM Thu Sep 19 11:52:40 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 204
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 23.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

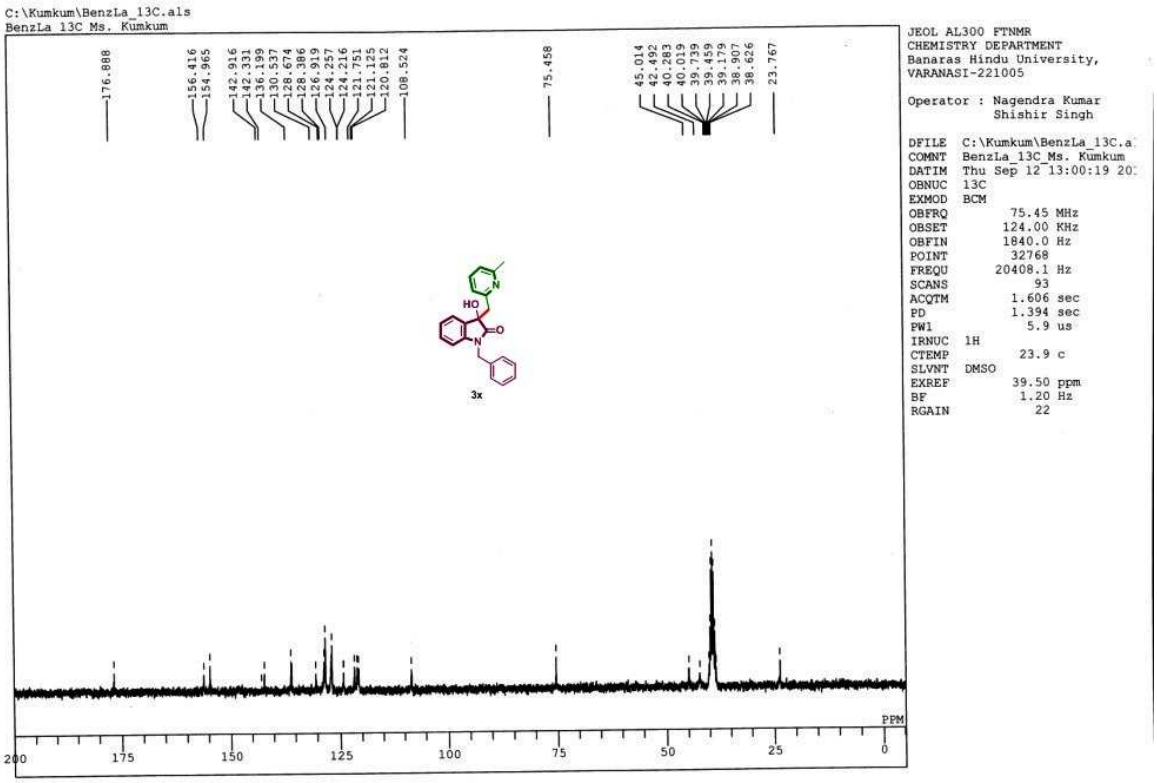

C:\WINNMR98\COMMON_DEFAULT.ALS
DBRLV_1H Ms. Kumkum
8.216
7.604
7.579
7.553
7.492
7.262
7.168
7.142
6.896
6.871
6.622
3.301
3.252
3.054
3.005
2.601
1.254
0.000
1.08
1.00
0.99
1.10
0.94
0.91
1.04
1.03
3.10
3v
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\WINNMR98\COMMON_DEI
COMNT DBRLV_1H Ms. Kumkum
DATIM Wed Sep 25 10:45:23 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 23.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 19


C:\WINNMR98\COMMON_DEFAULT.ALS
DBRLV_13C Ms. Kumkum
177.284
157.372
155.807
138.647
137.675
134.345
133.966
126.491
122.313
121.604
115.406
103.703
77.717
77.420
77.000
76.571
42.031
24.155
3v
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\WINNMR98\COMMON_DEI
COMNT DBRLV_13C Ms. Kumkum
DATIM Fri Sep 20 12:34:33 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 200
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24


C:\Kumkum\BRLU_1H.als
BRLU_1H_Ms.Kumkum
8.581
7.600
7.574
7.549
7.317
7.290
7.263
7.167
7.141
6.889
6.864
6.830
6.751
6.724
3.318
3.269
3.021
2.972
2.637
2.603
1.290
1.256
0.000
3w
3.73
3.17
1.09
1.17
1.10
1.00
1.13
1.06
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\BRLU_1H.als
COMNT BRLU_1H_Ms.Kumkum
DATIM Tue Sep 17 12:10:26 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 5.6 us
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 19


C:\Kumkum\BRLU_13C.als
BRLU_1H_Ms.Kumkum
178.685
157.323
156.095
138.985
137.667
133.562
132.062
127.538
122.296
121.694
115.225
111.804
77.420
77.000
76.571
42.088
24.155
3w
PPM
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\BRLU_13C.als
COMNT BRLU_1H_Ms.Kumkum
DATIM Tue Sep 17 06:41:21 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 1800
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 17.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 22


C:\Kumkum\BELU_1H.als
BELU 1H Ms. KumKum
8.104
7.576
7.551
7.525
7.337
7.292
7.256
7.150
7.136
7.125
7.113
6.913
6.885
6.857
6.811
6.787
6.700
6.674
4.974
4.922
4.841
4.789
3.372
3.322
3.082
3.033
2.614
0.000
HO
O
N
3x
6.09
3.17
1.95
2.46
3.02
1.05
1.00
0.79
1.26
PPM
10
8
6
4
2
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\BELU_1H.als
COMNT BELU_1H_Ms. KumKum
DATIM Tue Oct 01 12:34:23 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 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 21


C:\Kumkum\BenzLa_13C.als
BenzLa 13C Ms. Kumkum
176.888
156.416
154.965
142.916
142.331
136.199
130.537
128.674
128.386
126.919
124.257
124.216
121.751
121.125
120.812
108.524
75.458
45.014
42.492
40.283
40.019
39.739
39.459
39.179
38.907
38.626
23.767
HO
O
N
3x
PPM
200
175
150
125
100
75
50
25
0
JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Kumkum\BenzLa_13C.a
COMNT BenzLa_13C_Ms. Kumkum
DATIM Thu Sep 12 13:00:19 20
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 93
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.9 us
IRNUC 1H
CTEMP 23.9 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 22