

Supporting Information

For

## Cascade Synthesis of 2-Pyridones Using Acrylamides and Ketones

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## **1. Experimental section**

**General Considerations.** Microwave reactions were performed in a CEM Discover BenchMate single-mode microwave reactor with a new sealed pressure regulation 10-mL pressurized vial with “snap-on” cap and teflon-coated magnetic stir bar. The standard temperature control system for the Discover System consists of a non-contact calibrated infrared sensor which monitors and controls the temperature conditions of the reaction vessel located in the instrument cavity. The glassware used in the experiments was carefully cleaned and oven dried. Completion of reaction was checked by commercially available thin layer chromatography (TLC) from Merck, made up of silica gel 60/Kieselguhr F<sub>254</sub> precoated on Aluminum sheets (thickness 0.2 mm). Column chromatography was performed using Merck silica gel (100-200 mesh). Visualization of spots on TLC plate was accomplished with UV light. Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Products yield refer to either crude or isolated yield after column chromatography.

### **Synthetic procedure for Acrylamides (1-6):**

**Method A.** (Conventional): Aldehyde (20 mmol) and cyanoacetamide (20 mmol) were taken in a round bottomed flask in equimolar amount. Distilled water was added to facilitate the stirring and reaction mixture was refluxed with stirring on oil bath for specified time. Completion of reaction was confirmed by TLC. After completion of reaction, mixture was cooled at room temperature to form precipitate. Precipitate formed was filtered and dried in air.

**Method B.** (Micro Wave): In a sealed pressure regulation 10-mL pressurized vial were placed aldehyde (1 mmol), Cyanoacetamide (1 mmol), 1.0 mL distilled water and a teflon coated magnetic stir bar. The vessel was closed with a snap-on cap, stirred at room temperature for 2-5 min and then placed into the MW cavity. Microwave irradiation of 60 W at a set temperature of 120°C was used and the reaction mixture was held under these conditions for the specified time. Completion of

reaction was confirmed by TLC. After completion of reaction, mixture was cooled at room temperature to form precipitate. Precipitate formed was filtered and dried in air.

### **Physical and spectral data of products:**

#### **2-cyano-3-phenylacrylamide (1);**

Crystalline white solid; yield: 99% (MW), 98% (thermal), m.p. 102-105 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ) 3401, 3163, 2219, 1693, 1597;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  8.34 (s, 1H, Vinylic-**H**), 7.96 (d, 2H,  $J$  = 9, Ar-**H**), 7.55 (t, 3H,  $J$  = 6, Ar-**H**), 6.36 (s, 1H,  $\text{NH}_2$ ), 6.06 (s, 1H,  $\text{NH}_2$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 162.2, 153.9, 132.9, 131.5, 130.7, 129.2, 116.9, 103.1. **Chemical Formula:**  $\text{C}_{10}\text{H}_8\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 69.76; H, 4.68; N, 16.27; Found; C, 69.53; H, 4.70; N, 16.30.

#### **3-(4-chlorophenyl)-2-cyanoacrylamide (2);**

White solid; yield: 98% (MW), 92% (thermal), m.p. 183-185 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ) 3455, 3154, 2212, 1703, 1587;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  8.14 (s, 1H, Vinylic-**H**), 7.93 (d, 2H,  $J$  = 9, Ar-**H**), 7.78 (s, 2H,  $\text{NH}_2$ ), 7.64 (d, 2H,  $J$  = 9, Ar-**H**);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 162.6, 149.3, 137.0, 131.7, 130.8, 129.4, 116.3, 107.3 **Chemical Formula:**  $\text{C}_{10}\text{H}_7\text{N}_2\text{OCl}$ , **Elemental Analysis:** Calculated; C, 58.13; H, 3.41; N, 13.56; Found; C, 58.05; H, 3.50; N, 13.50.

#### **2-cyano-3-(3, 4-dimethoxyphenyl)acrylamide (3);**

Green yellow solid; yield: 98% (MW), 91% (thermal), m.p. 185-188 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ) 3394, 3165, 2214, 1694, 1584;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  8.08 (s, 1H, Vinylic-**H**), 7.77 (s, 2H,  $\text{NH}_2$ ), 7.63 (s, 1H, Ar-**H**), 7.54 (d, 1H,  $J$  = 9, Ar-**H**), 7.11 (d, 1H,  $J$  = 6, Ar-**H**), 3.83 (s, 3H,  $\text{OCH}_3$ ), 3.78 (s, 3H,  $\text{OCH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 163.1, 152.5, 150.6, 148.6, 125.6, 124.4, 117.2, 112.1, 111.7, 102.7; **Chemical Formula:**  $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_3$ , **Elemental Analysis:** Calculated; C, 62.06; H, 5.21; N, 12.06; Found; C, 62.0; H, 5.18; N, 12.10.

### **2-cyano-3-(4-methoxyphenyl)acrylamide (4):**

White solid; yield: 97% (MW), 93% (thermal), m.p. 197-199 °C; IR ( $\nu_{\max}/\text{cm}^{-1}$ ) 3447, 3176, 2208, 1698, 1583;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  8.26 (s, 1H, Vinylic-**H**), 7.97 (d, 2H,  $J = 9$ , Ar-**H**), 7.01 (d, 2H,  $J = 9$ , Ar-**H**), 6.26 (br s, 1H  $\text{NH}_2$ ), 5.65 (br s, 1H  $\text{NH}_2$ ), 3.89 (s, 3H,  $\text{OCH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 163.2, 162.4, 152.3, 132.8, 124.46, 117.3, 114.2, 100.3, 55.3; **Chemical Formula:**  $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_2$ , **Elemental Analysis:** Calculated; C, 65.34; H, 4.98; N, 13.85;. Found; C, 65.30; H, 5.00; N, 13.80.

### **2-cyano-3-(p-tolyl)acrylamide (5):**

Crystalline white solid; yield: 99% (MW), 94% (thermal), m.p. 147-149 °C; IR ( $\nu_{\max}/\text{cm}^{-1}$ ) 3416, 3116, 2224, 1704, 1605, 1379, 1350;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  8.29 (s, 1H, Vinylic-**H**), 7.87 (d, 2H,  $J = 9$ , Ar-**H**), 7.31 (d, 2H,  $J = 9$ , Ar-**H**), 6.4 (br s, 2H  $\text{NH}_2$ ), 2.43 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 162.4, 153.9, 153.8, 144.3, 130.9, 130.8, 129.9, 128.9, 117.2, 101.6, 21.8; **Chemical Formula:**  $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 70.95; H, 5.41; N, 15.04;. Found; C, 71.90; H, 5.38; N, 15.09.

### **2-cyano-3-(3-nitrophenyl)acrylamide (6):**

White solid; yield: 96% (MW), 85% (thermal), m.p. 173-175 °C; IR ( $\nu_{\max}/\text{cm}^{-1}$ ) 3416.40, 3116.34, 2224.57, 1704.25, 1605.05, 1526.42;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta_{\text{H}}$  8.74 (s, 1H, Vinylic-**H**), 8.37 (d, 1H,  $J = 7.8$ , Ar-**H**), 8.30 (d, 2H,  $J = 9$ , Ar-**H**), 7.98 (br s, 2H, N-**H**), 7.86 (m, 3H, Ar-**H**);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 162.1, 148.3, 148.0, 135.9, 133.4, 130.8, 126.2, 124.1, 115.8, 109.5; **Chemical Formula:**  $\text{C}_{10}\text{H}_7\text{N}_3\text{O}_3$ , **Elemental Analysis:** Calculated; C, 55.30; H, 3.25; N, 19.35;. Found; C, 55.28; H, 3.21; N, 19.37.

### **2-cyano-3-(2-nitrophenyl)acrylamide (7):**

White solid; yield: 92% (MW), 75% (thermal), m.p. 170-172 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ) 3393.54, 3179.31, 2234.58, 1718.96, 1613.77, 1524.39, 1387.90, 1352.98;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$  + few drop of  $\text{DMSO}_{\text{d}6}$ )  $\delta_{\text{H}}$  8.68 (s, 1H, Vinylic-**H**), 8.26 (d, 1H,  $J = 8.4$ , Ar-**H**), 7.83 (d, 2H,  $J = 3.6$ , Ar-**H**), 7.73 (m, 2H, Ar-**H**), 7.24 (s, 1H,  $\text{NH}_2$ ), 7.18 (s, 1H,  $\text{NH}_2$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 160.4, 150.0, 133.8, 131.2, 129.9, 128.1, 124.7, 120.3, 114.6; **Chemical Formula:**  $\text{C}_{10}\text{H}_7\text{N}_3\text{O}_3$ , **Elemental Analysis:** Calculated; C, 55.30; H, 3.25; N, 19.35;. Found; C, 55.29; H, 3.24; N, 19.35.

### **2-cyano-3-(4-nitrophenyl)acrylamide (8):**

Dirty white solid; yield: 95% (MW), 80% (thermal), m.p. 234-235 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ) 3441.73, 3346.68, 2244.68, 1693.36, 1602.13, 1509.82, 1344.97;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}_{\text{d}6}$ )  $\delta_{\text{H}}$  8.37 (s, 2H,  $J = 8.8$ , Ar-**H**), 8.28 (d, 1H, Vinylic-**H**), 8.16 (d, 2H,  $J = 8.8$ , Ar-**H**), 8.05 (s, 1H,  $\text{NH}_2$ ), 7.89 (s, 1H,  $\text{NH}_2$ );  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}_{\text{d}6}$ ) 162.5, 149.2, 148.7, 138.4, 131.4, 124.5, 116.1, 111.0; **Chemical Formula:**  $\text{C}_{10}\text{H}_7\text{N}_3\text{O}_3$ , **Elemental Analysis:** Calculated; C, 55.30; H, 3.25; N, 19.35;. Found; C, 55.28; H, 3.26; N, 19.36.

### **Synthetic procedure for 2-pyridones:**

Clean and freshly cut sodium metal (1.2 equivalents) was completely dissolved in dried ethanol then ketone (1.0 equivalent) was added and stirred for 30 minutes. After that acrylamide (1.0 equivalent) was added and stirring was continued for specified time. Completion of reaction was checked by TLC. After completion of the reaction water was added (to make 1:1, ethanol:water mixture) and stand at 0-5 °C for precipitate formation. Then filtered and dried in air. For isomeric mixture column chromatography was performed to isolate the isomers. Eluent ratio for separation of each isomer has been shown in table 6.

**Table 6.** Separation of isomeric mixtures by column chromatography.

Compound Name	Eluent ratio (Ethyl acetate:Hexane)
1b	80:20
1h	40:60
1d	60:40
1e	20:80
1f	25:75
1g	10:90
1i	05:95
2d	40:60
2e	20:80
2f	25:75
2g	10:90
4d	35:65
4e	20:80
5d	50:50
5e	20:80

**Physical and spectral data of products:****6-methyl-2-oxo-4-phenyl-1,2-dihydropyridine-3-carbonitrile (1a):**

Green yellow solid; yield: 85%; mp. 265-270 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2221.65, 1660.71, 1625.53;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  12.59 (br s, 1H, NH), 7.56 (m, 5H, Ar-H), 6.29 (s, 1H, Pyridone-Ring-H), 2.28 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 161.4, 160.0, 152.1, 136.0, 130.2, 128.7, 127.9, 116.6, 106.5, 97.2, 19.1; **Chemical Formula:**  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 74.27; H, 4.79; N, 13.33;. Found; C, 74.26; H, 4.78; N, 13.34.

**2-oxo-4,6-diphenyl-1,2-dihydropyridine-3-carbonitrile (1b):**

Light green yellow solid; yield: 96%; mp. 298-300 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2218.87, 1645, 1608.16;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.82 (br s, 1H NH), 7.89 (d, 2H, J = 6, Ar-H), 7.72 (d, 2H, J = 6, Ar-H), 7.55 (m, 6H, Ar-H), 6.82 (s, 1H Pyridone-Ring-H);  $^{13}\text{C}$  NMR (75 MHz, DMSO<sub>d6</sub>) 162.0, 159.8, 151.4, 136.0, 132.2, 131.1, 130.4, 128.9, 128.7, 128.5, 128.2, 127.7, 116.5, 106.1; **Chemical Formula:** C<sub>18</sub>H<sub>12</sub>N<sub>2</sub>O, **Elemental Analysis:** Calculated; C, 79.39; H, 4.44; N, 10.29;. Found; C, 79.40; H, 4.44; N, 10.28.

**6-(4-chlorophenyl)-2-oxo-4-phenyl-1,2-dihydropyridine-3-carbonitrile (1c):**

White solid; yield: 95%; mp. 270 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2222.06, 1662.48, 1613.45;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.85 (br s, 1H, NH), 7.94 (d, 2H, J = 9, Ar-H), 7.73 (dd, 2H, J = 9, Ar-H), 7.59 (m, 5H, Ar-H), 6.88 (s, 1H, Pyridone-Ring-H);  $^{13}\text{C}$  NMR (75 MHz, DMSO<sub>d6</sub>) 166.7, 162.1, 159.5, 150.5, 135.9, 131.3, 130.4, 129.6, 128.8, 128.7, 128.2, 116.3, 106.8, 98.3; **Chemical Formula:** C<sub>18</sub>H<sub>11</sub>N<sub>2</sub>OCl, **Elemental Analysis:** Calculated; C, 70.48; H, 3.61; N, 9.13;. Found; C, 70.50; H, 3.60; N, 9.10.

**5,6-dimethyl-2-oxo-4-phenyl-1,2-dihydropyridine-3-carbonitrile (1d):**

Yellow green solid; yield: 89%; mp. 270-272 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2224.60, 1648.31, 1595.18;  $^1\text{H}$  NMR (300 MHz, CDCl<sub>3</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.89 (br s, 1H, NH), 7.51 (m, 3H, Ar-H), 7.25 (d, 2H, J = 6, Ar-H), 2.40 (s, 3H, CH<sub>3</sub>), 1.81 (s, 3H, CH<sub>3</sub>);  $^{13}\text{C}$  NMR (75 MHz, CDCl<sub>3</sub>) 163.0, 162.6, 149.6, 136.0, 129.3, 128.8, 128.0, 127.6, 115.3, 106.6, 101.2, 18.7, 14.4; **Chemical Formula:** C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O, **Elemental Analysis:** Calculated; C, 74.98; H, 5.39; N, 12.49;. Found; C, 74.95; H, 5.40; N, 12.50.

**6-ethyl-2-oxo-4-phenyl-1,2-dihydropyridine-3-carbonitrile (1e):**

Yellow green solid; yield: 11%; mp. 257-260 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2224.42, 1647.95, 1605.11;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  12.57 (br s, 1H, NH), 7.60 (d, 1H,  $J$  = 2.4, Ar-H), 7.58 (d, 1H,  $J$  = 3.0, Ar-H), 7.52 (t, 3H,  $J$  = 2.7, Ar-H), 6.31 (s, 1H, Pyridone-Ring-H), 2.60 (q, 2H,  $J$  = 7.2, 7.5, 7.8 -CH<sub>2</sub>-), 1.19 (t, 3H,  $J$  = 7.5, CH<sub>3</sub>);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 161.9, 160.8, 157.7, 136.5, 130.8, 129.2, 129.1, 128.4, 117.0, 105.5, 26.3, 12.9; **Chemical Formula:** C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O, **Elemental Analysis:** Calculated; C, 74.98; H, 5.39; N, 12.49;. Found; C, 74.96; H, 5.35; N, 12.52.

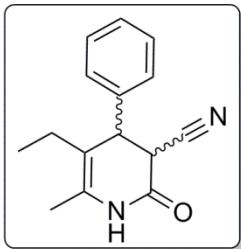
#### **5-ethyl-6-methyl-2-oxo-4-phenyl-1,2-dihydropyridine-3-carbonitrile (1f):**

White solid; yield: 27%; mp. 272-275 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2225.40, 1644.93, 1594.03;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 298 K, TMS):  $\delta_{\text{H}}$  13.82 (br s, 1H, NH), 7.50 (d, 2H,  $J$  = 5.1, Ar-H), 7.27 (m, 3H,  $J$  = 2.7, 4.8, Ar-H), 2.48 (s, 3H, CH<sub>3</sub>), 2.31 (q, 2H,  $J$  = 4.8, 7.2, -CH<sub>2</sub>-), 0.90 (t, 3H,  $J$  = 7.5, 7.2, CH<sub>3</sub>);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 163.1, 162.4, 149.5, 135.8, 129.1, 128.9, 128.7, 127.2, 120.2, 115.2, 101.5, 21.4, 17.8, 14.2; **Chemical Formula:** C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>O, **Elemental Analysis:** Calculated; C, 75.61; H, 5.92; N, 11.76;. Found; C, 75.59; H, 5.90; N, 11.78.

#### **2-oxo-4-phenyl-6-propyl-1,2-dihydropyridine-3-carbonitrile (1g):**

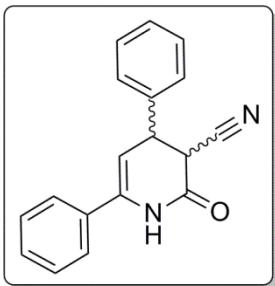
Light green yellow solid; yield: 73%; mp. 195-197 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2221.24, 1649.41, 1617.68;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 298 K, TMS):  $\delta_{\text{H}}$  13.60 (br s, 1H, NH), 7.61- 7.49 (m, 5H, Ar-H), 6.29 (s, 1H, Pyridone-Ring-H), 2.76 (t, 2H,  $J$  = 7.2, 7.5, -CH<sub>2</sub>-), 1.88 (sext, 2H,  $J$  = 7.2, 7.5, -CH<sub>2</sub>-), 1.19 (t, 3H,  $J$  = 7.5, CH<sub>3</sub>);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 161.9, 160.8, 157.7, 136.5, 130.8, 129.2, 129.1, 128.4, 117.0, 105.5, 26.3, 12.9; **Chemical Formula:** C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O, **Elemental Analysis:** Calculated; C, 74.98; H, 5.39; N, 12.49;. Found; C, 74.97; H, 5.38; N, 12.52.

#### **5-ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyridine-3-carbonitrile (1h):**



White solid; yield: 3%; mp 211-213 °C; IR ( $\nu_{\max}/\text{cm}^{-1}$ ): 3219.66, 3107.79, 2253.32, 1698.85, 1677.36;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 298 K, TMS):  $\delta_{\text{H}}$  8.51 (br s, 1H, NH), 7.33 – 7.15 (m, 5H, Ar-H), 4.09 (d, 0.81 x 1H,  $J$  = 6.9), 3.81 (d, 0.18 x 1H,  $J$  = 2.1), 3.68 (d, 0.82 x 1H,  $J$  = 6.9), 3.59 (d, 0.18 x 1H,  $J$  = 2.7), 2.28 – 2.12 (m, 2H, - $\text{CH}_2$ -), 1.90 (s, 3H,  $\text{CH}_3$ ), 0.91 (t, 3H,  $J$  = 7.2, 7.5,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 162.2, 135.8, 129.1, 128.9, 128.3, 128.2, 12.4, 116.8, 114.9, 44.5, 41.8, 23.6, 15.3, 134; **Chemical Formula:**  $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 74.97; H, 6.71; N, 11.66;. Found; C, 74.95; H, 6.70; N, 11.68.

### **2-oxo-4,6-diphenyl-1,2,3,4-tetrahydropyridine-3-carbonitrile (1i):**



White solid; yield: 92%; mp 218-220 °C; IR ( $\nu_{\max}/\text{cm}^{-1}$ ): 3475.32, 3373.49, 3351.02, 2258.57, 1698.36, 1595.78;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  8.88 (s, 1H, NH), 7.57 – 7.33 (m, 10H, Ar-H), 5.30 (s, 1H, = $\text{CH}$ -), 4.94 (d, 1H,  $J$  = 12.9), 4.39 (d, 1H,  $J$  = 12.9);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 163.7, 162.9, 135.1, 134.5, 129.1, 128.6, 128.2, 127.8, 116.7, 115.3, 60.4, 46.4; **Chemical Formula:**  $\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 78.81; H, 5.14; N, 10.21;. Found; C, 78.80; H, 5.12; N, 10.24.

### **4-(4-chlorophenyl)-6-methyl-2-oxo-1,2-dihydropyridine-3-carbonitrile (2a):**

Chartreuse yellow solid; yield: 83%; mp (d) > 300 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2220.95, 1661.29, 1626.27;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.64 (br s, 1H, NH), 7.63 (m, 4H, Ar-H), 6.32 (s, 1H Pyridone-Ring-H), 2.29 (s, 3H, CH<sub>3</sub>);  $^{13}\text{C}$  NMR (75 MHz, DMSO<sub>d6</sub>) 161.2, 158.8, 152.4, 135.1, 134.8, 129.8, 128.8, 116.4, 106.3, 97.3, 19.1; **Chemical Formula:** C<sub>13</sub>H<sub>9</sub>N<sub>2</sub>OCl, **Elemental Analysis:** Calculated; C, 63.81; H, 3.71; N, 11.45;. Found; C, 63.79; H, 3.75; N, 11.41.

#### **4-(4-chlorophenyl)-2-oxo-6-phenyl-1,2-dihydropyridine-3-carbonitrile (2b):**

White solid; yield: 94%; mp (d) > 290 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2219.11, 1642.89, 1607.59;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  7.90 (d, 2H, J = 9, Ar-H), 7.76 (d, 2H, J = 9, Ar-H), 7.64 (d, 2H, J = 9, Ar-H), 7.53 (d, 3H, J = 6, Ar-H), 6.82 (s, 1H, Pyridone-Ring-H);  $^{13}\text{C}$  NMR (75 MHz, DMSO<sub>d6</sub>) 162.5, 158.3, 152.1, 135.2, 135.0, 132.7, 131.1, 130.2, 12., 128.8, 127.7, 116.6, 105.9; **Chemical Formula:** C<sub>18</sub>H<sub>11</sub>N<sub>2</sub>OCl, **Elemental Analysis:** Calculated; C, 70.48; H, 3.61; N, 9.13;. Found; C, 70.52; H, 3.65; N, 9.05.

#### **4,6-bis(4-chlorophenyl)-2-oxo-1,2-dihydropyridine-3-carbonitrile (2c):**

Light yellow solid; yield: 97%; mp (d) 240 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2201.47, 1657.94, 1595.73;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  7.99 (d, 2H, J = 9, Ar-H), 7.64 (d, 2H, J = 9, Ar-H), 7.56 (d, 2H, J = 9, Ar-H), 7.48 (d, 2H, J = 9, Ar-H), 6.66 (s, 1H, Pyridone-Ring-H);  $^{13}\text{C}$  NMR (75 MHz, DMSO<sub>d6</sub>) 155.5, 154.9, 136.8, 134.1, 133.8, 1331, 132.9, 130.0, 128.9, 128.5, 128.3, 119.5, 103.3; **Chemical Formula:** C<sub>18</sub>H<sub>10</sub>N<sub>2</sub>OCl<sub>2</sub>, **Elemental Analysis:** Calculated; C, 63.36; H, 2.95; N, 8.21;. Found; C, 63.30; H, 3.00; N, 8.20.

#### **4-(4-chlorophenyl)-5,6-dimethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile (2d):**

Light green yellow solid; yield: 91%; mp (d) 270 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2223.25, 1645.16, 1606.48;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.61 (br s, 1H, NH), 7.58 (d, 2H, J = 8.4, Ar-H), 7.33

(d, 2H,  $J = 8.4$ , Ar-H), 2.30 (s, 3H, CH<sub>3</sub>), 1.68 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 160.5, 159.9, 150.7, 135.2, 135.1, 134.9, 133.8, 129.9, 129.6, 128.8, 116.3, 116.2, 111.2, 99.7, 1.0, 13.9;

**Chemical Formula:** C<sub>14</sub>H<sub>11</sub>N<sub>2</sub>OCl, **Elemental Analysis:** Calculated; C, 65.00; H, 4.29; N, 10.83;. Found; C, 65.02; H, 4.30; N, 10.85.

**4-(4-chlorophenyl)-6-ethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile (2e):**

Yellow green solid; yield: 9%: mp 257-260 °C ; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2219.88, 1645.77, 1613.96; <sup>1</sup>H NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.56 (br s, 1H, NH), 7.56 (d, 2H,  $J = 9$ , Ar-H), 7.52 (d, 2H,  $J = 8.7$ , Ar-H), 6.25 (s, 1H, Pyridone-Ring-H), 2.50 (q, 2H,  $J = 7.5$ , -CH<sub>2</sub>-), 1.11 (t, 3H,  $J = 7.5$ , CH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 161.4, 159.1, 157.5, 135.2, 134.9, 128.9, 116.4, 105.1, 105.0, 104.9, 97.7, 26.1, 12.7; **Chemical Formula:** C<sub>14</sub>H<sub>11</sub>N<sub>2</sub>OCl, **Elemental Analysis:** Calculated; C, 65.00; H, 4.29; N, 10.83;. Found; C, 65.07; H, 4.31; N, 10.80.

**4-(4-chlorophenyl)-5-ethyl-6-methyl-2-oxo-1,2-dihydropyridine-3-carbonitrile (2f):**

Green yellow solid; yield: 30%: mp 270 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2226.47, 1650.69, 1599.76; <sup>1</sup>H NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.61 (br s, 1H, NH), 7.58 (d, 2H,  $J = 8.1$ , Ar-H), 7.35 (d, 2H,  $J = 8.4$ , Ar-H), 2.34 (s, 3H, CH<sub>3</sub>), 2.11 (q, 2H,  $J = 6.9, 7.5, 6.9$ , -CH<sub>2</sub>-), 0.77 (t, 3H,  $J = 7.5, 7.2$ , CH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 160.8, 159.7, 150.5, 135.0, 133.7, 129.4, 128.7, 117.5, 116.0, 100.3, 20.4, 17.2, 13.9; **Chemical Formula:** C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>OCl, **Elemental Analysis:** Calculated; C, 66.06; H, 4.80; N, 10.27;. Found; C, 66.03; H, 4.82; N, 10.30.

**4-(4-chlorophenyl)-2-oxo-6-propyl-1,2-dihydropyridine-3-carbonitrile (2g):**

Green yellow solid; yield: 70%: mp 225-228 °C ; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2221.03, 1649.66, 1614.20; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, 298 K, TMS):  $\delta_{\text{H}}$  13.52 (br s, 1H, NH), 7.54 (d, 2H,  $J = 8.4$ , Ar-H), 7.47 (d, 2H,  $J = 8.1$ , Ar-H), 6.25 (s, 1H, Pyridone-Ring-H), 2.72 (t, 2H,  $J = 7.2, 7.5$ , -CH<sub>2</sub>-), 1.81 (sext,

2H, J = 7.5, -CH<sub>2</sub>-), 1.04 (t, 3H, J = 7.5, 7.2, CH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 164.0, 159.9, 155.7, 136.9, 134.2, 129.4, 129.2, 115.4, 107.2, 98.6, 35.5, 21.8, 13.5; **Chemical Formula:** C<sub>15</sub>H<sub>13</sub>N<sub>2</sub>OCl, **Elemental Analysis:** Calculated; C, 66.06; H, 4.80; N, 10.27; Found; C, 66.02; H, 4.79; N, 10.27

**4-(3,4-dimethoxyphenyl)-6-methyl-2-oxo-1,2-dihdropyridine-3-carbonitrile (3a):**

White solid; yield: 81%; mp (d) > 280 °C ; IR ( $\nu_{\text{max}}$ /cm<sup>-1</sup>): 2214.76, 1667.34, 1627.43, 160.34; <sup>1</sup>H NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS): δ<sub>H</sub> 7.22 (d, 2H, J = 9, Ar-H), 7.10 (d, 1H, J = 9, Ar-H), 6.36 (s, 1H, Pyridone-Ring-H); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 161.7, 159.7, 151.6, 150.6, 148.5, 128.0, 121.2, 117.1, 111.5, 106.4, 96.5, 55.6, 19.2; **Chemical Formula:** C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub>, **Elemental Analysis:** Calculated; C, 66.66; H, 5.22; N, 10.36; Found; C, 66.64; H, 5.25; N, 10.33.

**4-(3,4-dimethoxyphenyl)-2-oxo-6-phenyl-1,2-dihdropyridine-3-carbonitrile (3b):**

White solid; yield: 91%; mp (d) 248 °C; IR ( $\nu_{\text{max}}$ /cm<sup>-1</sup>): 2202.27, 1666.14, 1606.06; <sup>1</sup>H NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS): δ<sub>H</sub> 7.98 (d, 2H, J = 9, Ar-H), 7.40 (m, 4H, Ar-H), 7.18 (d, 2H, J = 9, Ar-H), 7.05 (s, 1H, Ar-H), 6.61 (s, 1H Pyridone-Ring-H) 3.81 (s, 3H, OCH<sub>3</sub>) 3.80 (s, 3H, OCH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 157.9, 155.1, 149.2, 148.3, 139.3, 136.5, 133.1, 131.0, 128.8, 128.2, 127.0, 120.6, 111.5, 102.8, 91.9, 55.5; **Chemical Formula:** C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>, **Elemental Analysis:** Calculated; C, 72.28; H, 4.85; N, 8.43; Found; C, 72.20; H, 4.87; N, 8.40.

**6-(4-chlorophenyl)-4-(3,4-dimethoxyphenyl)-2-oxo-1,2-dihdropyridine-3-carbonitrile (3c):**

White solid; yield: 94%; mp (d) 280 °C; IR ( $\nu_{\text{max}}$ /cm<sup>-1</sup>): 2203.79, 1680.65, 1595.41; <sup>1</sup>H NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS): δ<sub>H</sub> 8.26 (s, 1H, NH), 8.02 (d, 2H, J = 9, Ar-H), 7.44 (d, 2H, J = 9, Ar-H), 7.16 (d, 2H, J = 9, Ar-H), 7.04 (s, 1H, Ar-H), 6.63 (s, 1H, Pyridone-Ring-H), 3.80 (s, 6H, OCH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 157.3, 155.0, 149.3, 148.4, 138.7, 133.5, 131.2, 128.8, 128.3,

121.2, 120.7, 111.9, 91.9, 55.7, 55.6; **Chemical Formula:** C<sub>20</sub>H<sub>15</sub>N<sub>2</sub>O<sub>3</sub>Cl, **Elemental Analysis:** Calculated; C, 65.49; H, 4.12; N, 7.64;. Found; C, 65.5; H, 4.15; N, 7.61.

**4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2-dihydropyridine-3-carbonitrile (4a):**

White solid; yield: 78%; mp (d) 242 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2219.10, 1661.89, 1608.48; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ<sub>H</sub> 7.60 (d, 2H, J = 9, Ar-H), 7.01 (d, 2H, J = 9, Ar-H), 6.26 (s, 1H, Pyridone-Ring-H), 3.86 (s, 3H, OCH<sub>3</sub>), 2.29 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 164.3, 161.6, 160.7, 150.5, 129.7, 127.9, 116.1, 114.3, 108.1, 97.7, 55.4, 19.7; **Chemical Formula:** C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>, **Elemental Analysis:** Calculated; C, 69.99; H, 5.03; N, 11.66;. Found; C, 69.95; H, 5.11; N, 11.71.

**4-(4-methoxyphenyl)-2-oxo-6-phenyl-1,2-dihydropyridine-3-carbonitrile (4b):**

White solid; yield: 85%; mp (d) 198-200 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2208.92, 1662.33, 1608.16; <sup>1</sup>H NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS): δ<sub>H</sub> 7.99 (d, 2H, J = 6, Ar-H), 7.59 (d, 2H, J = 9, Ar-H), 7.39 (d, 2H, J = 6, Ar-H), 7.05 (d, 2H, J = 9, Ar-H), 6.66 (s, 1H, Pyridone-Ring-H), 3.81 (s, 3H, OCH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 159.8, 157.7, 155.1, 138.8, 136.5, 131.7, 130.5, 129.4, 128.2, 17.1, 120.3, 113.8, 112.4, 103.7, 55.2; **Chemical Formula:** C<sub>19</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>, **Elemental Analysis:** Calculated; C, 75.48; H, 4.67; N, 9.27;. Found; C, 75.45; H, 4.65; N, 9.30.

**6-(4-chlorophenyl)-4-(4-methoxyphenyl)-2-oxo-1,2-dihydropyridine-3-carbonitrile (4c):**

White solid; yield: 91%; mp (d) 190-195 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2208.92, 1667.69, 1610.39; <sup>1</sup>H NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS): δ<sub>H</sub> 8.00 (d, 2H, J = 9, Ar-H), 7.58 (d, 2H, J = 6, Ar-H), 7.43 (d, 2H, J = 9, Ar-H), 7.05 (d, 2H, J = 9, Ar-H), 6.69 (s, 1H, Pyridone-Ring-H), 3.80 (s, 3H, OCH<sub>3</sub>); <sup>13</sup>C NMR (75 MHz, DMSO<sub>d6</sub>) 159.9, 156.3, 155.4, 137.5, 133.8, 130.3, 129.5, 129.1, 128.9, 128.7, 128.5, 128.3, 120.1, 113.9, 55.2; **Chemical Formula:** C<sub>19</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub>Cl, **Elemental Analysis:** Calculated; C, 67.76; H, 3.89; N, 8.32;. Found; C, 67.75; H, 3.90; N, 8.30.

**5-ethyl-4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2-dihdropyridine-3-carbonitrile (4d):**

Light green yellow solid; yield: 29%; mp 280-282 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2223.20, 1651.52, 1606.64;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 298 K, TMS):  $\delta_{\text{H}}$  13.75 (br s, 1H, NH), 7.19 (d, 2H,  $J = 8.4$ , Ar-H), 7.01(d, 2H,  $J = 8.7$ , Ar-H), 3.86 (s, 1H,  $\text{OCH}_3$ ), 2.51 (s, 3H,  $\text{CH}_3$ ), 2.31 (quint, 2H,  $J = 7.2$ , - $\text{CH}_2$ -) 0.88 (t, 3H,  $J = 7.2$ , 7.5,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 163.1, 162.5, 160.3, 149.0, 128.8, 128.1, 120.5, 115.4, 114.3, 55.2, 21.0, 17.9, 14.2; **Chemical Formula:**  $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2$ , **Elemental Analysis:** Calculated; C, 71.62; H, 6.01; N, 10.44;. Found; C, 71.60; H, 6.00; N, 10.45.

**4-(4-methoxyphenyl)-2-oxo-6-propyl-1,2-dihdropyridine-3-carbonitrile (4e):**

Green yellow solid; yield: 71%; mp 180-182 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2222.77, 1654.40, 1604.79;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 298 K, TMS):  $\delta_{\text{H}}$  7.60 (d, 2H,  $J = 7.8$ , Ar-H), 7.01(d, 2H,  $J = 8.1$ , Ar-H), 6.26 (s, 1H, Pyridone-Ring-H), 5.99 (br s, 1H, NH), 3.87 (s, 1H,  $\text{OCH}_3$ ), 2.69 (t, 2H, - $\text{CH}_2$ -), 1.80 (sext, 2H,  $J = 4.8$ , 7.5, 7.2, - $\text{CH}_2$ -) 1.03 (t, 3H,  $J = 6.6$ , 7.2,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 164.4, 161.6, 160.7, 154.8, 129.7, 128.0, 116.1, 114.3, 107.2, 97.8, 55.4, 35.5, 21.5, 13.4; **Chemical Formula:**  $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2$ , **Elemental Analysis:** Calculated; C, 71.62; H, 6.01; N, 10.44;. Found; C, 71.63; H, 6.05; N, 10.40.

**6-methyl-2-oxo-4-(p-tolyl)-1,2-dihdropyridine-3-carbonitrile (5a):**

White solid; yield: 80%; mp 220-222 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2216.91, 1651.27, 1614.82;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 298 K, TMS):  $\delta_{\text{H}}$  7.50 (d, 2H,  $J = 9$ , Ar-H), 7.29 (d, 2H,  $J = 9$ , Ar-H), 6.28 (s, 1H Pyridone-Ring-H), 5.70 (br s, 1H, NH), 2.50 (s, 3H,  $\text{CH}_3$ ), 2.41 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 164.2, 161.2, 150.9, 141.1, 132.8, 129.5, 127.9, 115.9, 108.3, 108.2, 98.0, 21.3, 19.7; **Chemical Formula:**  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 74.98; H, 5.39; N, 12.49;. Found; C, 75.03; H, 5.40; N, 12.45.

**2-oxo-6-phenyl-4-(p-tolyl)-1,2-dihdropyridine-3-carbonitrile (5b):**

White solid; yield: 90%; mp 215-216 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2210.42, 1672.80, 1613.78;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  8.01 (d, 2H,  $J = 6$ , Ar-H), 7.50 (d, 2H,  $J = 9$ , Ar-H), 7.38 (m, 3H, Ar-H), 7.29 (d, 2H,  $J = 6$ , Ar-H), 6.68 (s, 1H, Pyridone-Ring-H), 2.36 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 158.6, 155.0, 139.5, 138.1, 135.7, 128.9, 128.8, 128.1, 127.9, 127.6, 127.0, 126.4, 103.8, 91.4, 68.8, 20.8; **Chemical Formula:**  $\text{C}_{19}\text{H}_{14}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 79.70; H, 4.93; N, 9.78;. Found; C, 79.72; H, 4.90; N, 9.80.

**6-(4-chlorophenyl)-2-oxo-4-(p-tolyl)-1,2-dihdropyridine-3-carbonitrile (5c):**

White solid; yield: 88%; mp 223-224 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2209.89, 1659.07, 1609.22;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  8.02 (d, 2H,  $J = 9$ , Ar-H), 7.50 (d, 2H,  $J = 6$ , Ar-H), 7.43 (d, 2H,  $J = 9$ , Ar-H), 7.29 (d, 2H,  $J = 6$ , Ar-H), 6.68 (s, 1H, Pyridone-Ring-H), 2.35 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 171.1, 156.5, 155.6, 138.4, 137.6, 135.4, 133.8, 129.0, 128.2, 128.0, 120.1, 103.7, 92.5, 20.8; **Chemical Formula:**  $\text{C}_{19}\text{H}_{13}\text{N}_2\text{OCl}$ , **Elemental Analysis:** Calculated; C, 71.14; H, 4.08; N, 8.73;. Found; C, 71.10; H, 4.10; N, 8.75.

**5,6-dimethyl-2-oxo-4-(p-tolyl)-1,2-dihdropyridine-3-carbonitrile (5d):**

Green yellow solid; yield: 90%; mp(d) > 290 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2225.72, 1647.27, 1599.70;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  12.53 (br s, 1H, NH), 7.31 (d, 2H,  $J = 7.2$ , Ar-H), 7.17(d, 2H,  $J = 7.2$ , Ar-H), 2.36 (s, 3H,  $\text{CH}_3$ ), 2.29 (s, 3H,  $\text{CH}_3$ ), 1.69 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 161.9, 160.0, 150.2, 138.5, 133.3, 129.1, 127.5, 116.4, 111.3, 99.7, 20.8, 17.9, 13.9; **Chemical Formula:**  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 75.61; H, 5.92; N, 11.76;. Found; C, 75.60; H, 5.90; N, 11.78.

**6-ethyl-2-oxo-4-(p-tolyl)-1,2-dihydropyridine-3-carbonitrile (5e):**

Green yellow solid; yield: 10%; mp 230 °C ; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2217.95, 1644.75, 169.86;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ , 298 K, TMS):  $\delta_{\text{H}}$  13.51 (br s, 1H, NH), 7.51 (d, 2H,  $J = 7.5$ , Ar-H), 7.29 (d, 2H,  $J = 7.5$ , Ar-H), 6.28 (s, 1H, Pyridone-Ring-H), 2.79 (q, 2H, - $\text{CH}_2-$ ), 2.42 (s, 3H,  $\text{CH}_3$ ), 1.37 (t, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 164.3, 161.4, 156.4, 141.0, 1331, 129.5, 127.9, 115.9, 106.5, 98.3, 26.9, 21.3, 12.3; **Chemical Formula:**  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}$ , **Elemental Analysis:** Calculated; C, 75.61; H, 5.92; N, 11.76;. Found; C, 75.64; H, 5.95; N, 11.72.

**6-methyl-4-(3-nitrophenyl)-2-oxo-1,2-dihydropyridine-3-carbonitrile (6a):**

White solid; yield: 88%; mp (d) > 300 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2221.75, 1663.75, 1624.77;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  12.74 (br s, 1H, NH), 8.39(d, 2H,  $J = 9$ , Ar-H), 8.07 (d, 1H,  $J = 6$ , Ar-H), 7.86 (t, 1H,  $J = 9, 6$ , Ar-H), 6.44 (s, 1H, Pyridone-Ring-H), 2.32 (s, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 161.1, 157.6, 152.9, 147.7, 137.4, 134.5, 130.5, 124.9, 122.7, 16.2, 1064, 97.8, 19.2; **Chemical Formula:**  $\text{C}_{13}\text{H}_9\text{N}_3\text{O}_3$ , **Elemental Analysis:** Calculated; C, 61.18; H, 3.55; N, 16.46; Found; C, 61.15; H, 3.52; N, 16.50.

**4-(3-nitrophenyl)-2-oxo-6-phenyl-1,2-dihydropyridine-3-carbonitrile (6b):**

White solid; yield: 88%; mp (d) > 300 °C ; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2222.55, 1651.66, 1604.35;  $^1\text{H}$  NMR (300 MHz,  $\text{DMSO}_{\text{d}6}$ , 298 K, TMS):  $\delta_{\text{H}}$  12.95 (br s, 1H, NH), 8.55(s, 1H, Ar-H), 8.41 (d, 1H,  $J = 6$ , Ar-H), 8.20 (d, 1H,  $J = 9$ , Ar-H), 7.92 (m, 3H, Ar-H), 7.56 (t, 3H,  $J = 4.5, 6.9$ , Ar-H) 6.98 (s, 1H, Pyridone-Ring-H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO}_{\text{d}6}$ ) 161.8, 157.4, 151.3, 147.8, 139.3, 138.3, 137.4, 134.9, 131.3, 130.4, 128.9, 127.8, 124.9, 123.2, 116.1, 106.0; **Chemical Formula:**  $\text{C}_{18}\text{H}_{11}\text{N}_3\text{O}_3$ , **Elemental Analysis:** Calculated; C, 68.14; H, 3.49; N, 13.24; Found; C, 68.12; H, 3.50; N, 13.24.

**6-(4-chlorophenyl)-4-(3-nitrophenyl)-2-oxo-1,2-dihydropyridine-3-carbonitrile (6c):**

White solid; yield: 88%; mp (d) > 300 °C; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2226.48, 1632.65, 1603.72;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.97 (br s, 1H, NH), 8.54(s, 1H, Ar-H), 8.41 (d, 1H, J = 9, Ar-H), 8.19 (d, 1H, J = 9, Ar-H), 7.96 (d, 2H, J = 6, Ar-H), 7.88 (t, 1H, J = 7.8, 8.1, Ar-H) 7.60 (d, 2H, J = 7.8, Ar-H), 7.05 (s, 1H, Pyridone-Ring-H);  $^{13}\text{C}$  NMR (75 MHz, DMSO<sub>d6</sub>) 161.0, 157.1, 147.8, 137.3, 136.1, 134.9, 133.6, 132.7, 130.4, 129.6, 128.9, 124.9, 123.2, 115.9, 105.7; **Chemical Formula:** C<sub>18</sub>H<sub>10</sub>ClN<sub>3</sub>O<sub>3</sub>, **Elemental Analysis:** Calculated; C, 61.46; H, 2.87; N, 11.95; Found; C, 61.48; H, 2.88; N, 11.92.

#### **4-(2-nitrophenyl)-2-oxo-6-phenyl-1,2-dihydropyridine-3-carbonitrile (7a):**

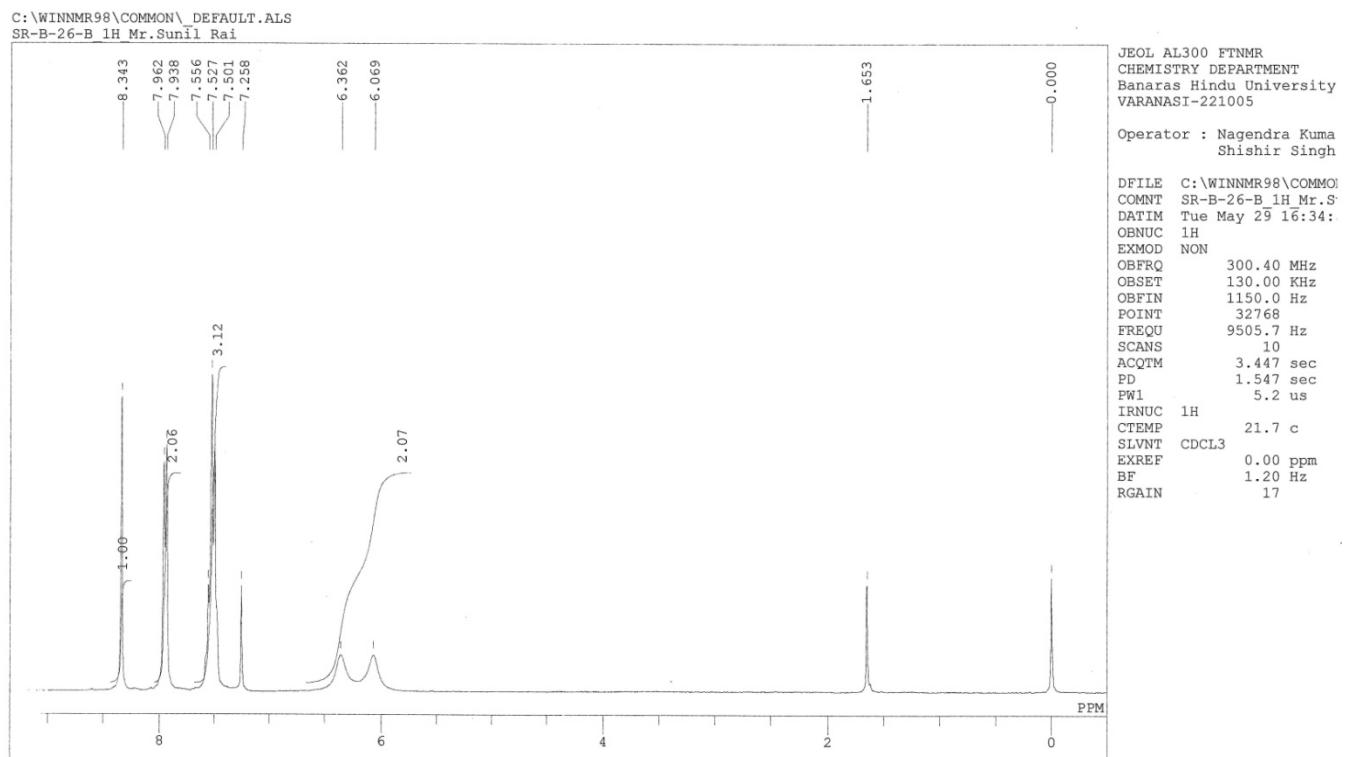
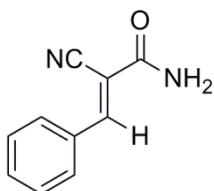
Yellow crystalline solid; yield: 60%; mp 275-277 °C ; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2218.22, 1651.03, 1528.05, 1502.88, 1353.39;  $^1\text{H}$  NMR (400 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  8.29(d, 1H, J = 1.0, Ar-H), 7.97-7.87 (m, 1H, Ar-H), 7.85 (t, 3H, J = 7.0, Ar-H), 7.73-7.70 (m, 1H, Ar-H), 7.57-7.50 (m, 3H, Ar-H) 6.90 (s, 1H, Pyridone-Ring-H);  $^{13}\text{C}$  NMR (100 MHz, DMSO<sub>d6</sub>) 161.8, 158.8, 152.5, 146.9, 135.0, 132.4, 131.9, 131.7, 131.7, 131.4, 129.5, 128.1, 125.6, 115.9, 106.3; **Chemical Formula:** C<sub>18</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>, **Elemental Analysis:** Calculated; C, 68.14; H, 3.49; N, 13.24; Found; C, 68.13; H, 3.49; N, 13.23.

#### **4-(4-nitrophenyl)-2-oxo-6-phenyl-1,2-dihydropyridine-3-carbonitrile (8a):**

Green solid; yield: 87%; mp (d) > 300 °C ; IR ( $\nu_{\text{max}}/\text{cm}^{-1}$ ): 2219.64, 1658.52, 1607.07, 1515.58, 1352.46;  $^1\text{H}$  NMR (300 MHz, DMSO<sub>d6</sub>, 298 K, TMS):  $\delta_{\text{H}}$  12.97 (br s, 1H, NH), 8.38(d, 2H, J = 8.1, Ar-H), 8.01-7.89 (m, 4H, Ar-H), 7.56-7.53 (m, 3H, Ar-H), 6.92 (s, 1H, Pyridone-Ring-H);  $^{13}\text{C}$  NMR (75 MHz, DMSO<sub>d6</sub>) 148.3, 142.2, 131.3, 129.8, 128.9, 127.8, 123.7, 115.9; **Chemical Formula:** C<sub>18</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>, **Elemental Analysis:** Calculated; C, 68.14; H, 3.49; N, 13.24; Found; C, 68.15; H, 3.48; N, 13.22.

## 2. Copies of $^1\text{H}$ and $^{13}\text{C}$ NMR spectra:

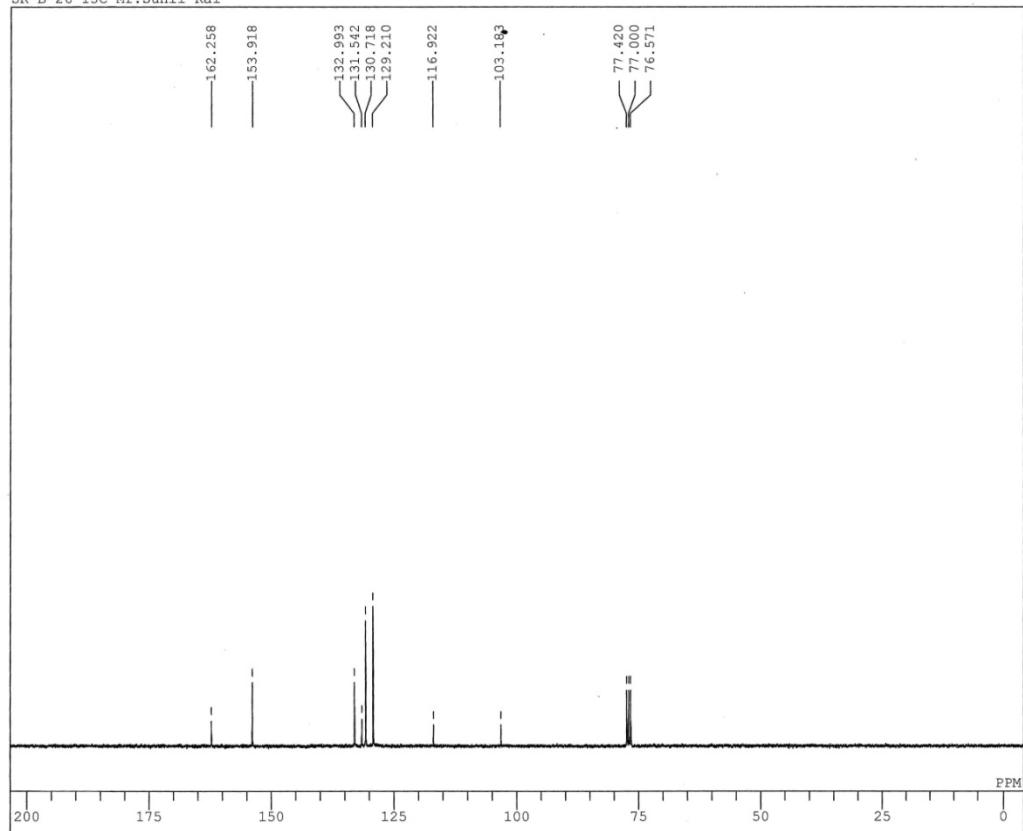
Compound (1):  $^1\text{H}$  NMR



Compound (1):  $^{13}\text{C}$  NMR



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SR-B-26 13C Mr.Sunil Rai

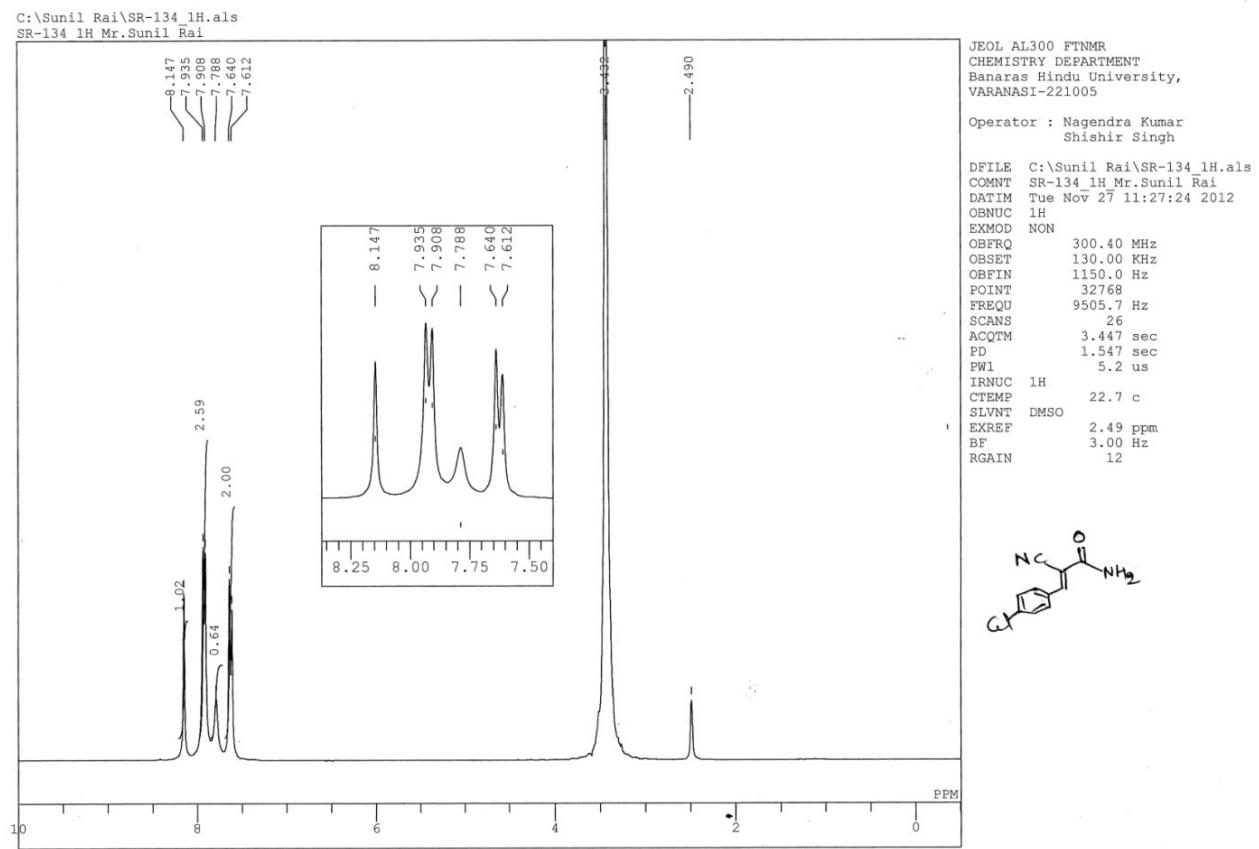


JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

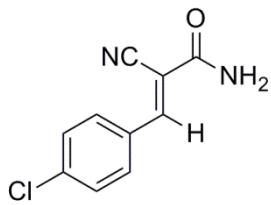
Operator : Nagendra Kumar  
Shishir Singh

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RGAIN 24

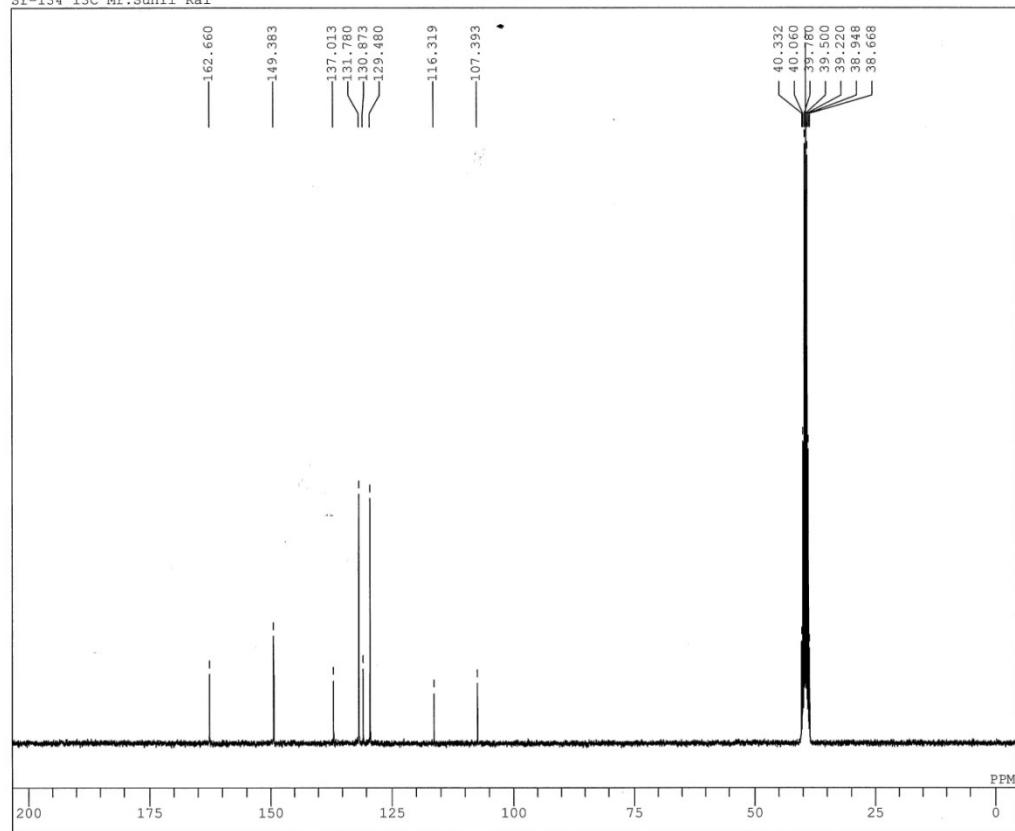
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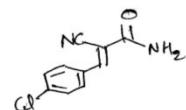
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Sr-134 13C Mr.Sunil Rai



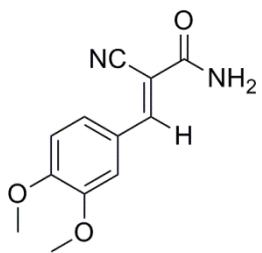
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CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

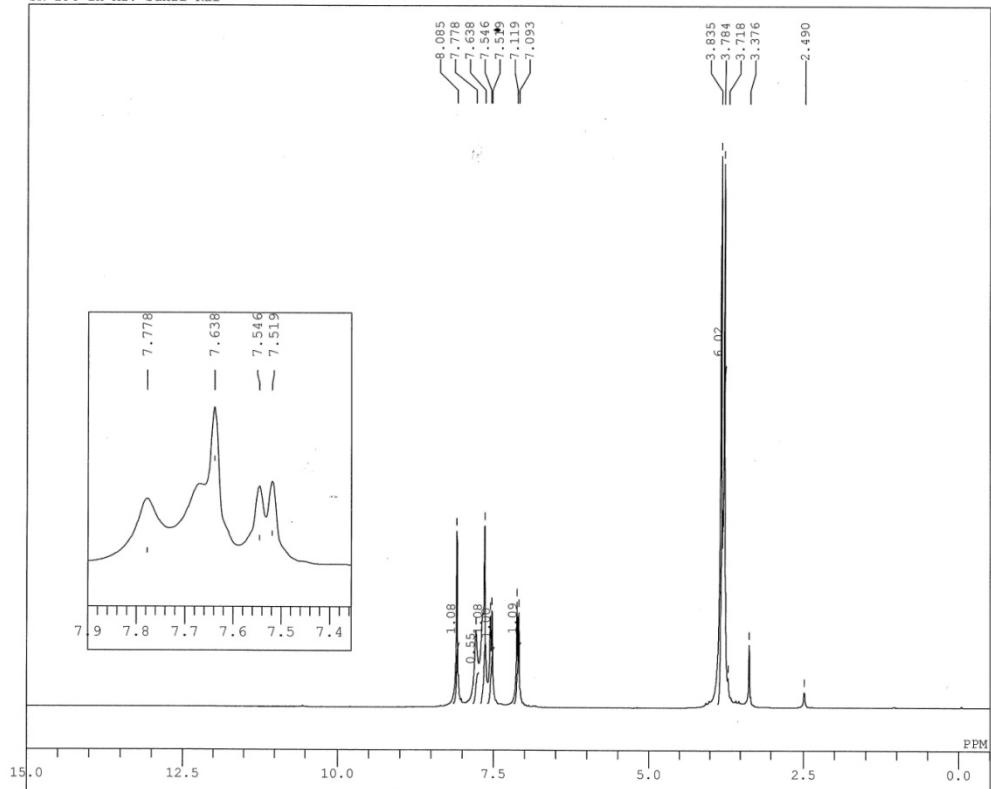
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PD 1.394 sec  
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RGAIN 25



Compound (3):  $^1\text{H}$  NMR



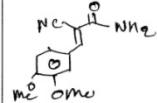
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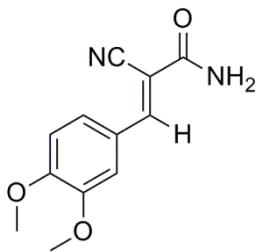
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CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
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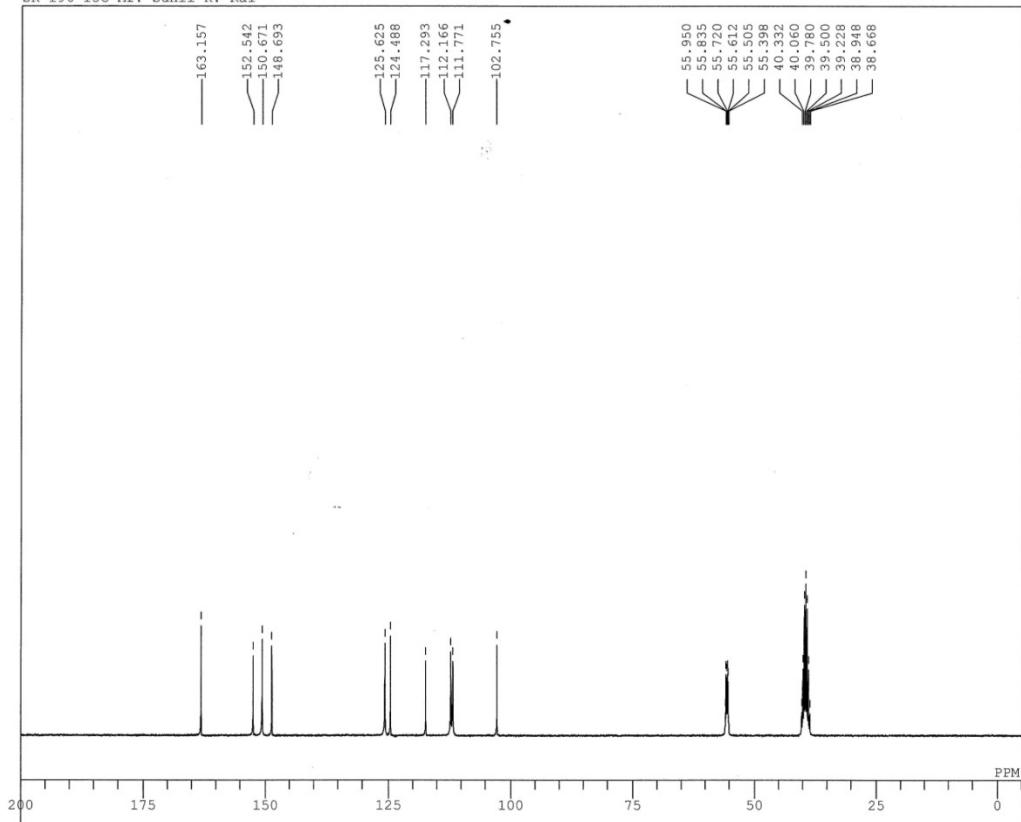
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Compound (3):  $^{13}\text{C}$  NMR



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SR-196 13C Mr. Sunil K. Rai



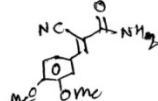
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CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

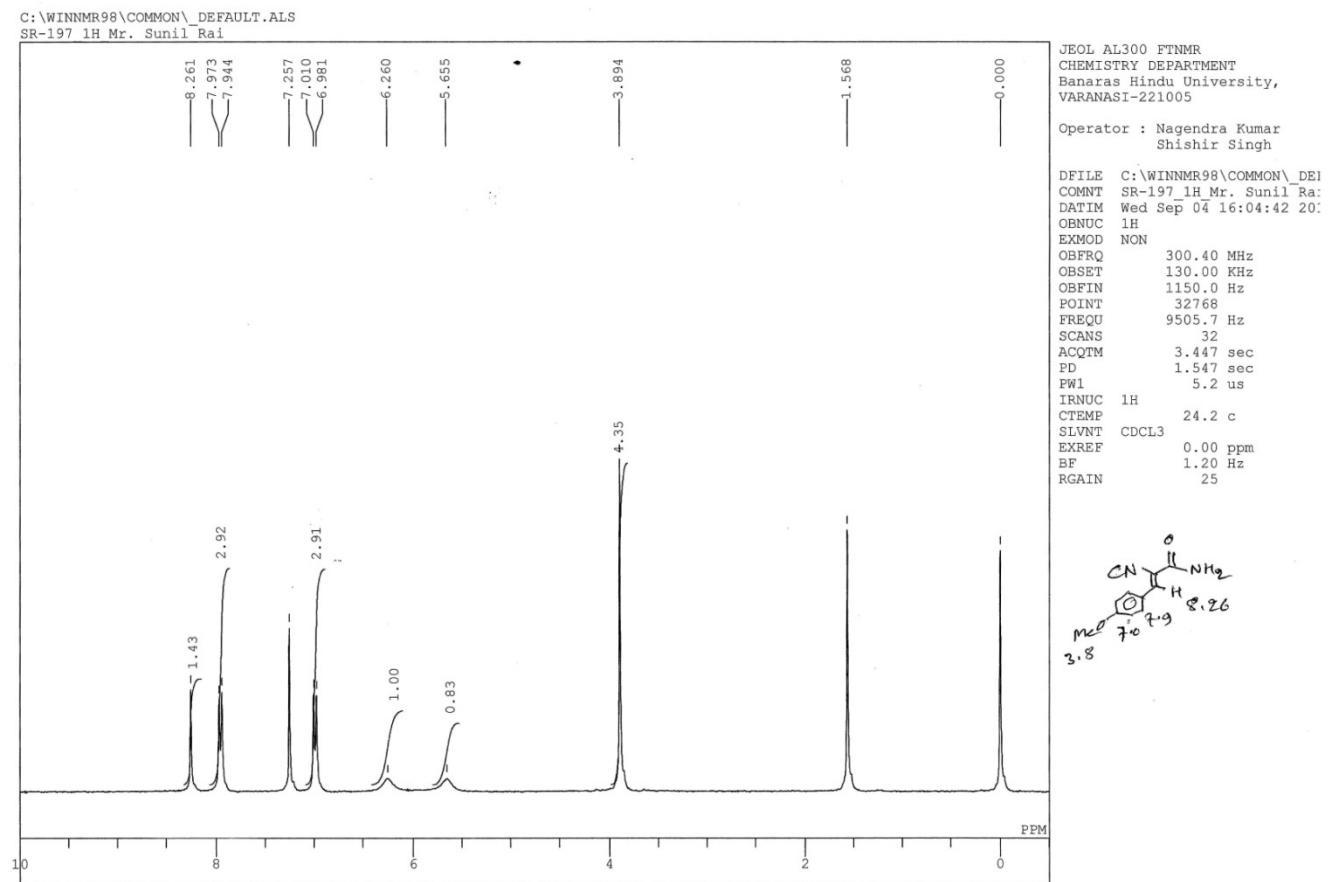
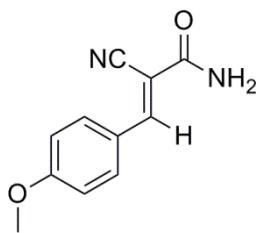
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RGAIN 21

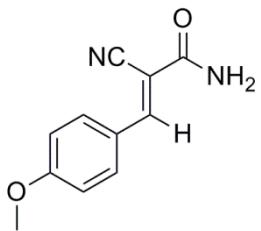
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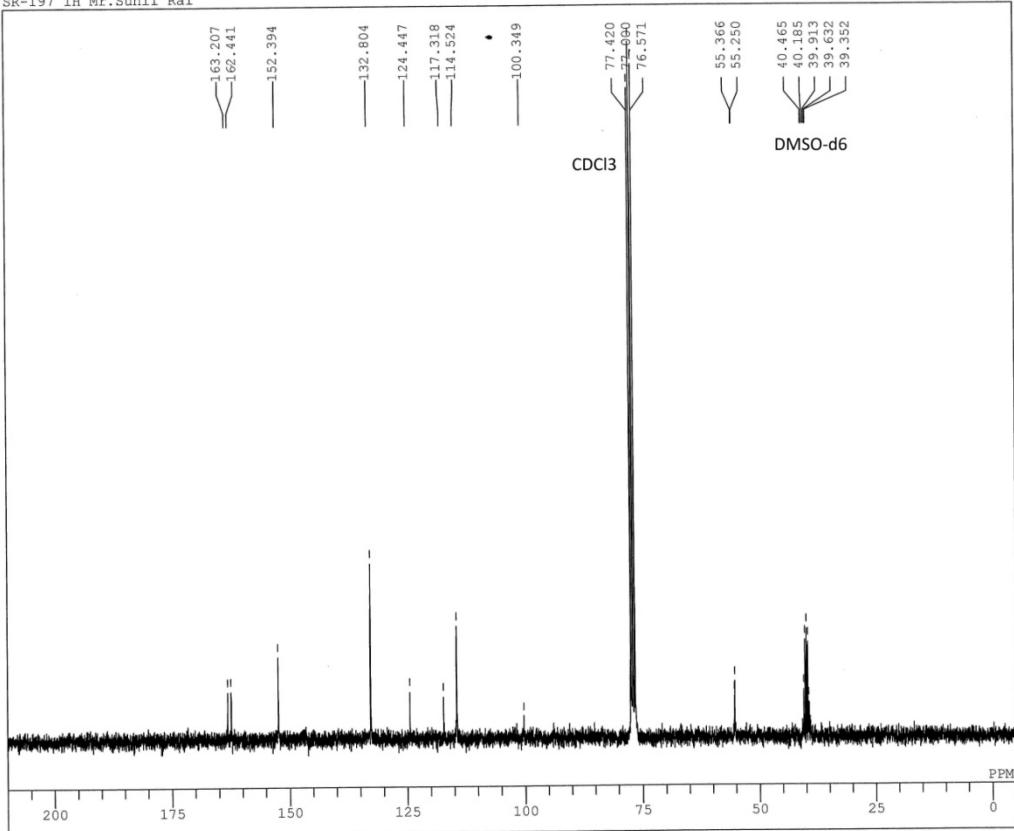
Compound (4):  $^1\text{H}$  NMR



Compound (4):  $^{13}\text{C}$  NMR



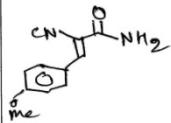
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SR-197 1H Mr.Sunil Rai



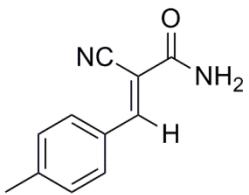
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

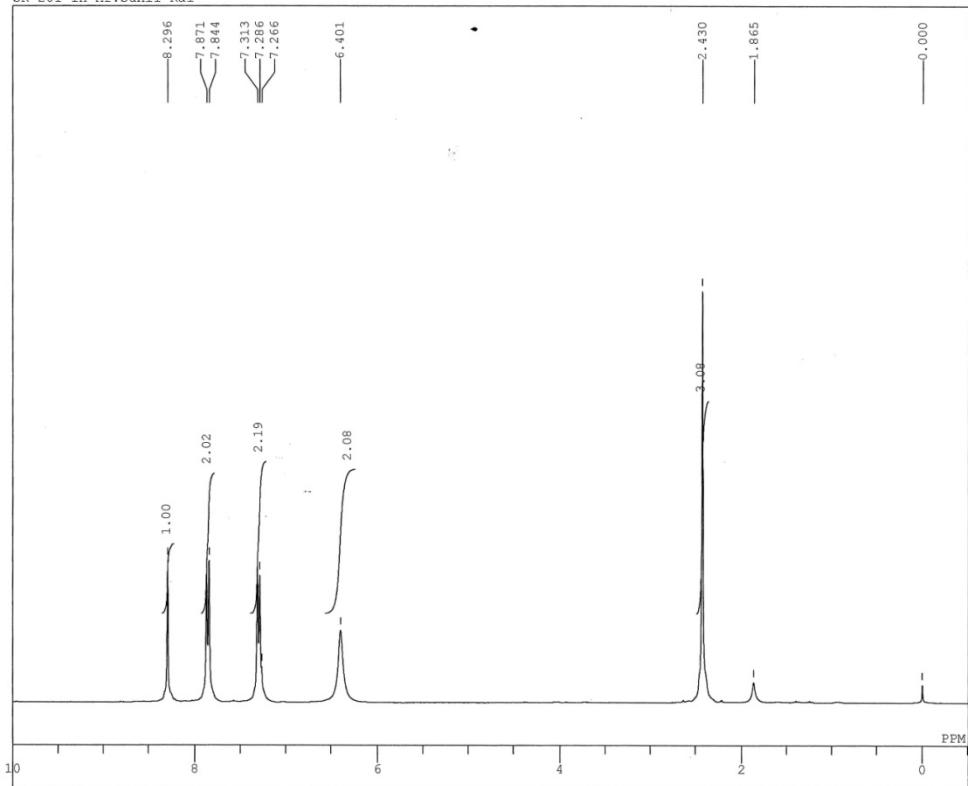
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RGAIN 23



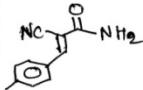
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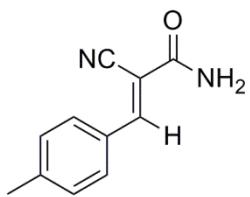
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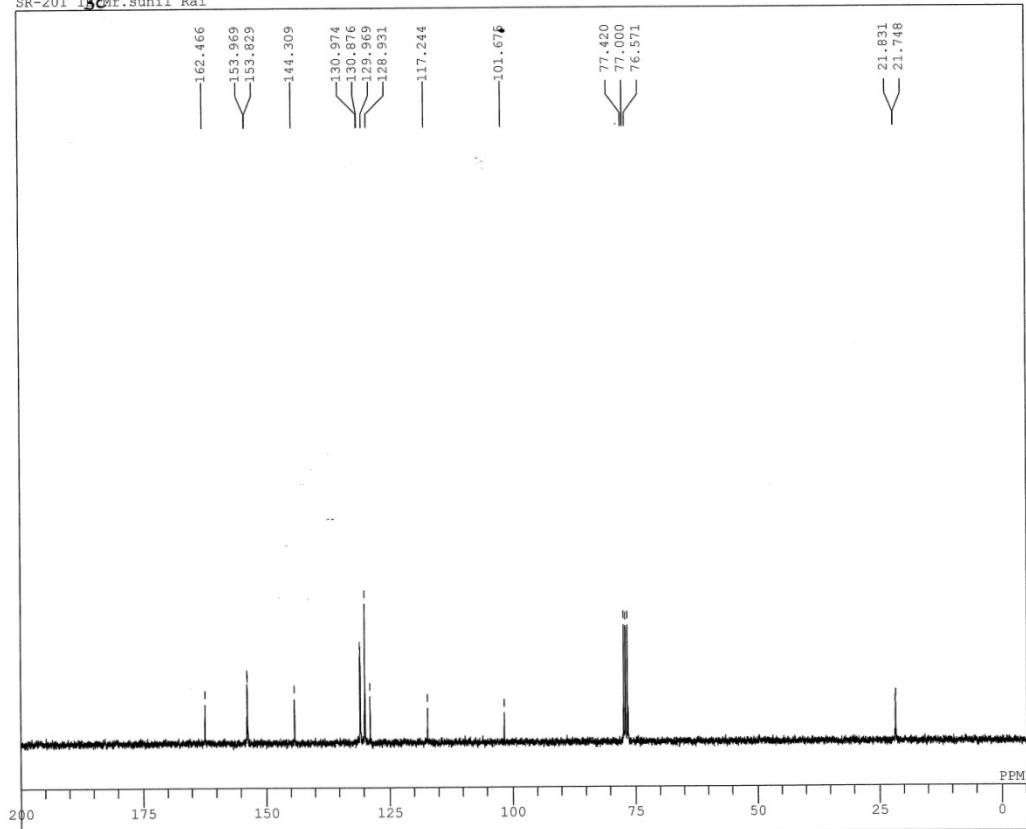
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005  
Operator : Nagendra Kumar  
Shishir Singh  
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RGAIN 16



Compound (5):  $^{13}\text{C}$  NMR



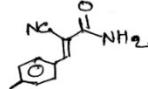
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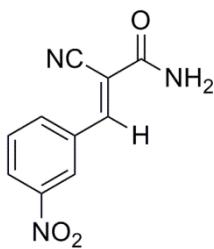
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CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

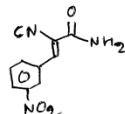
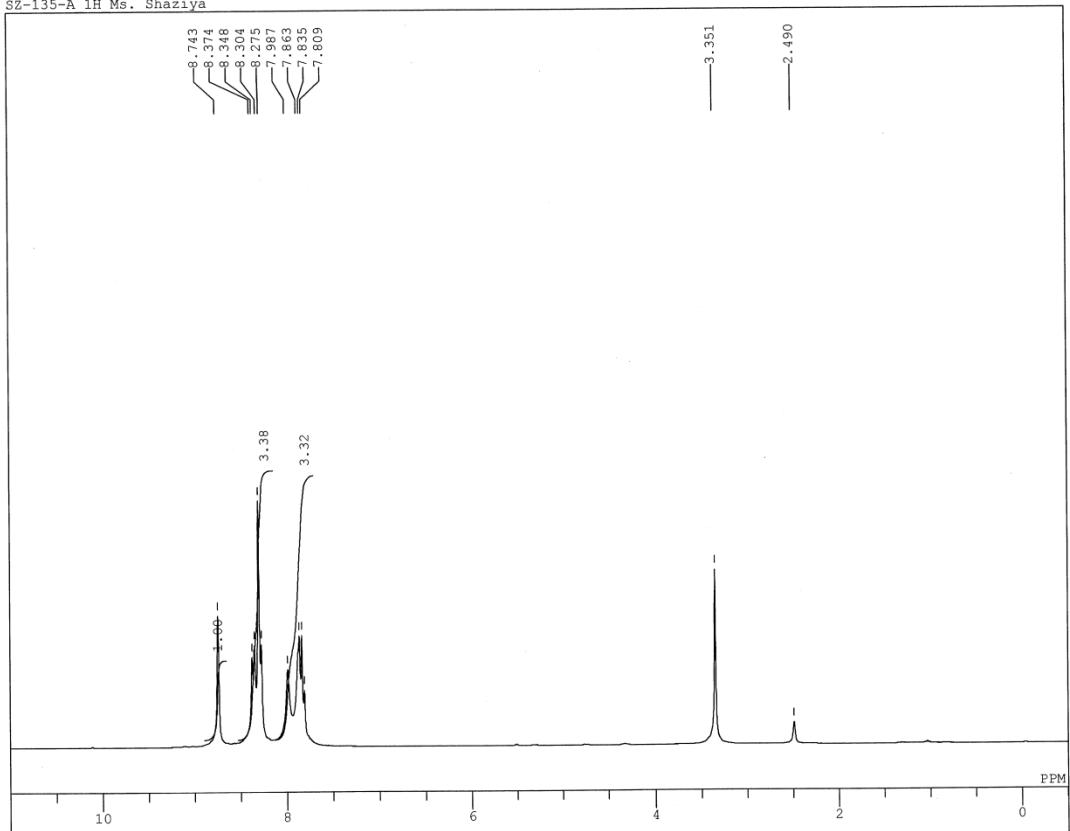
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RGAIN 24



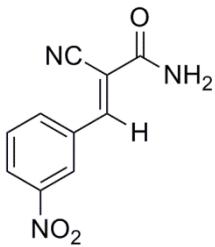
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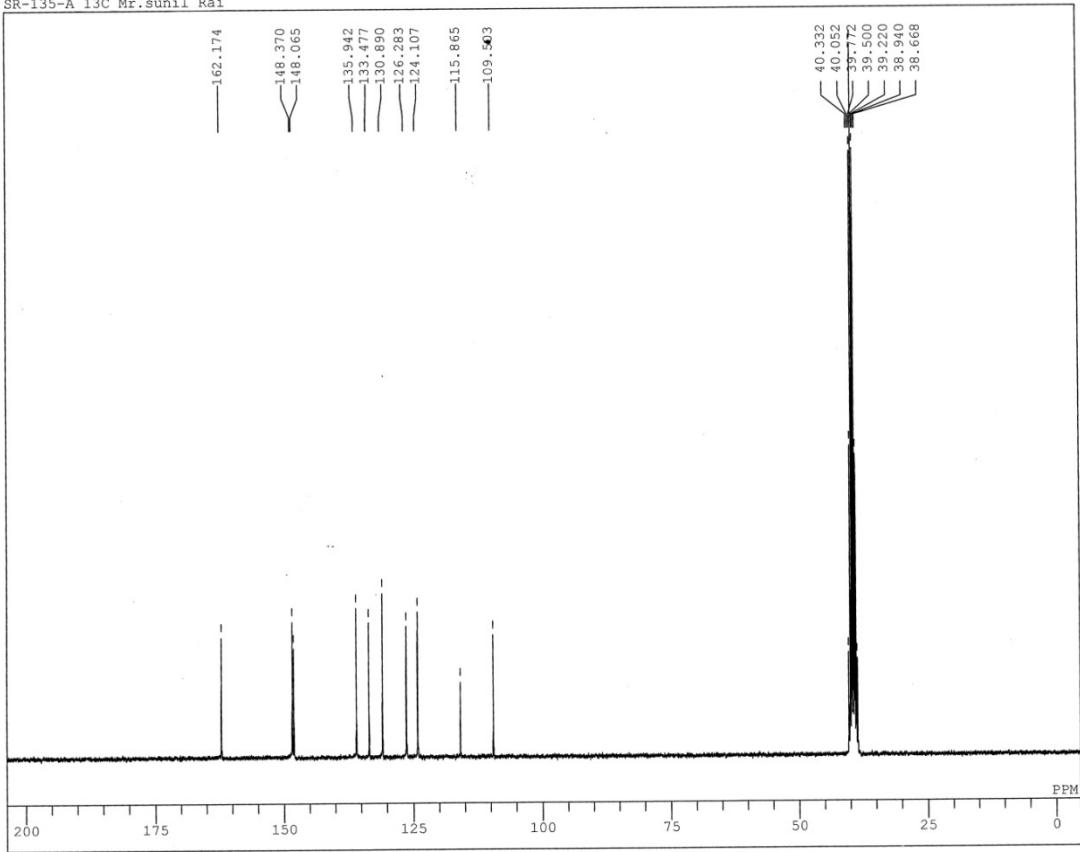
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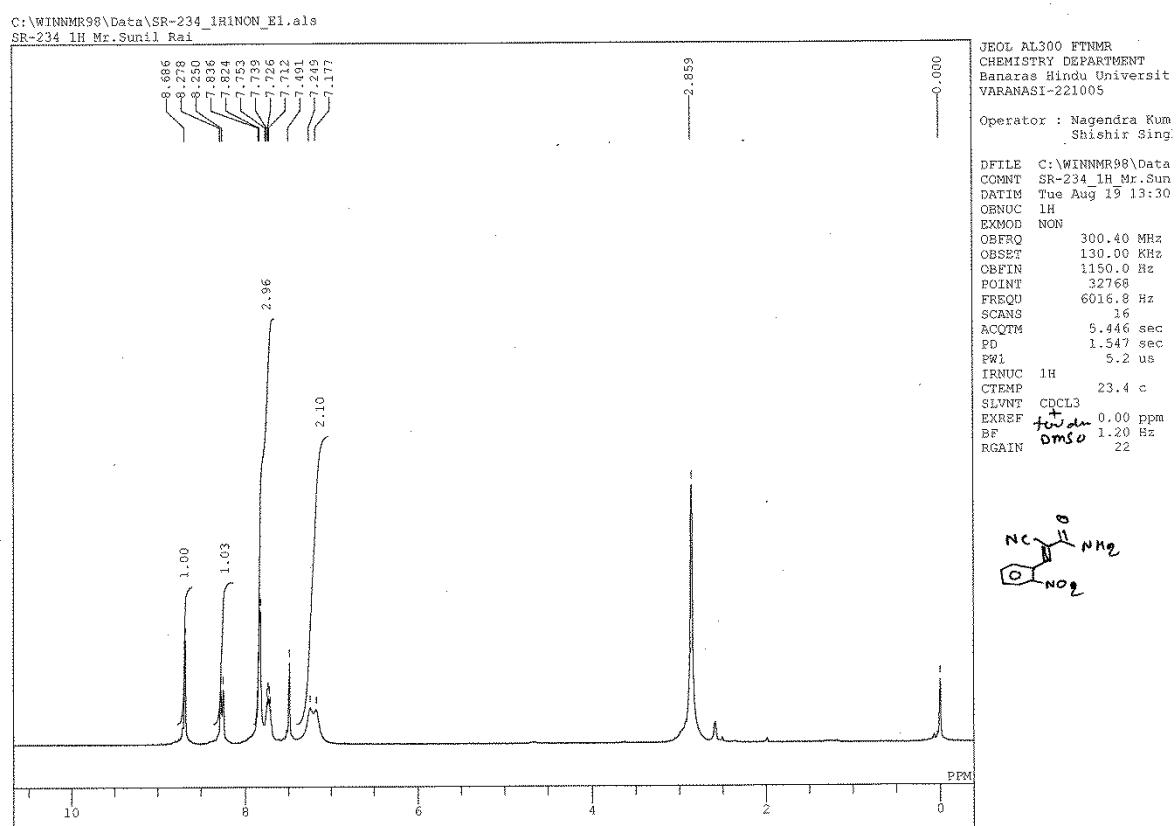
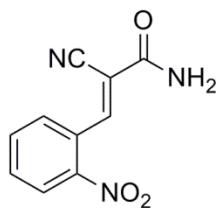
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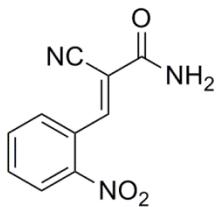
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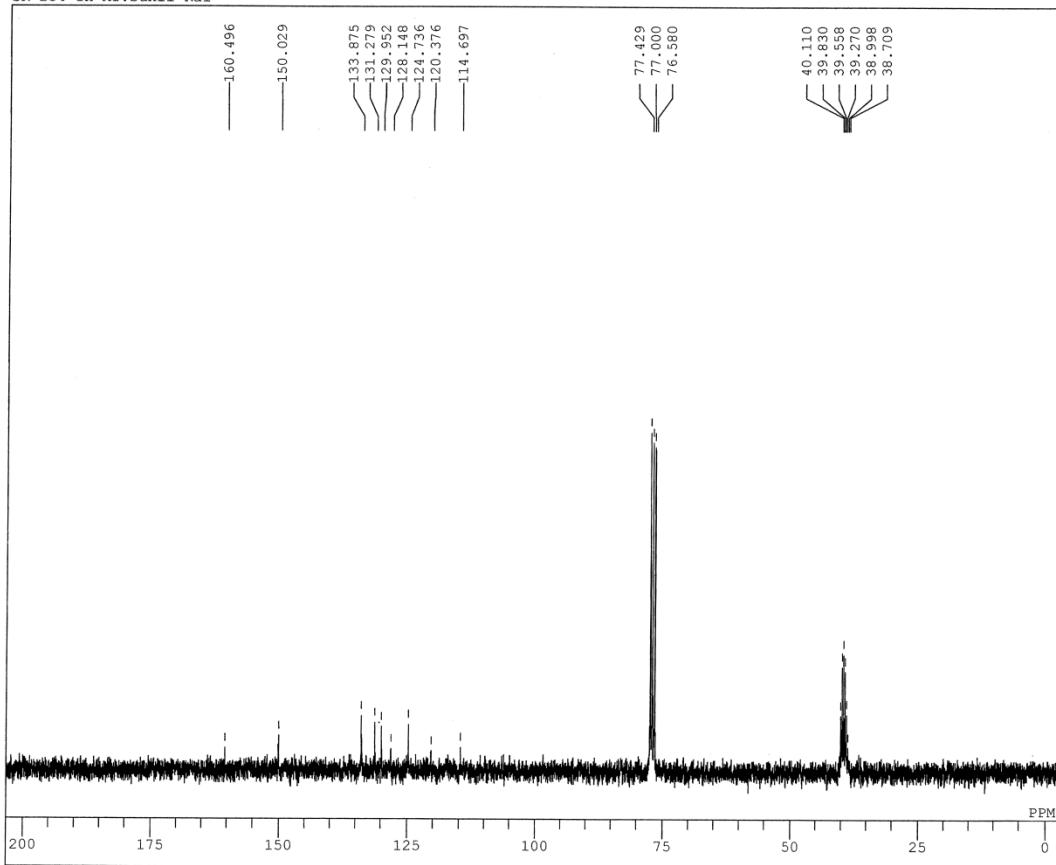
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Compound (7):  $^{13}\text{C}$  NMR



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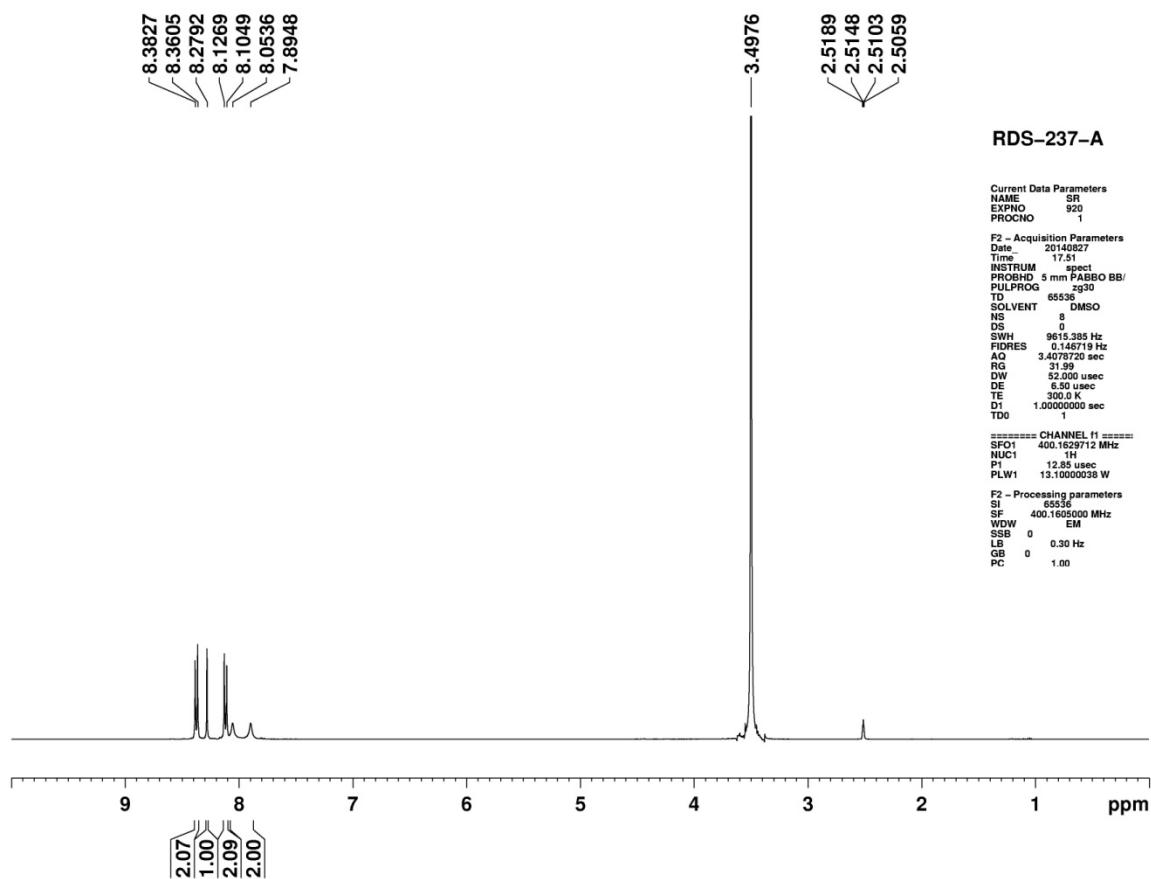
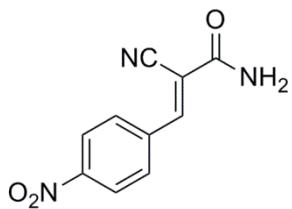


JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu Universit  
VARANASI-221005

Operator : Nagendra Kum  
Shishir Sing

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RGAIN 23

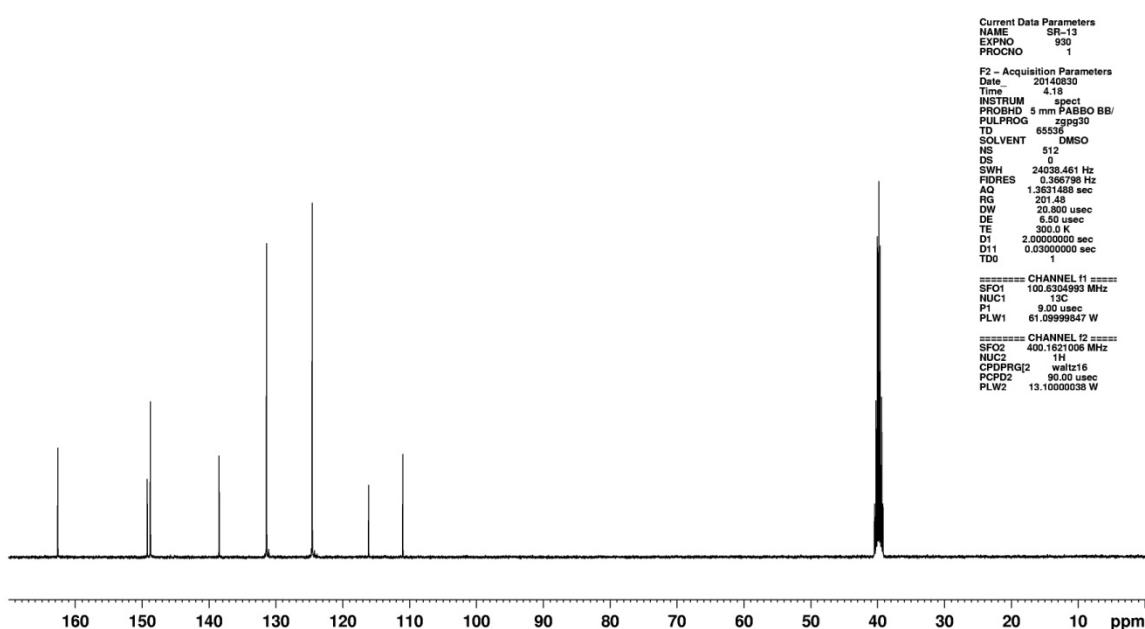
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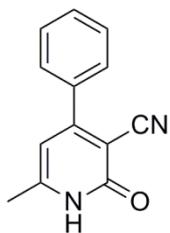
Compound (8):  $^{13}\text{C}$  NMR



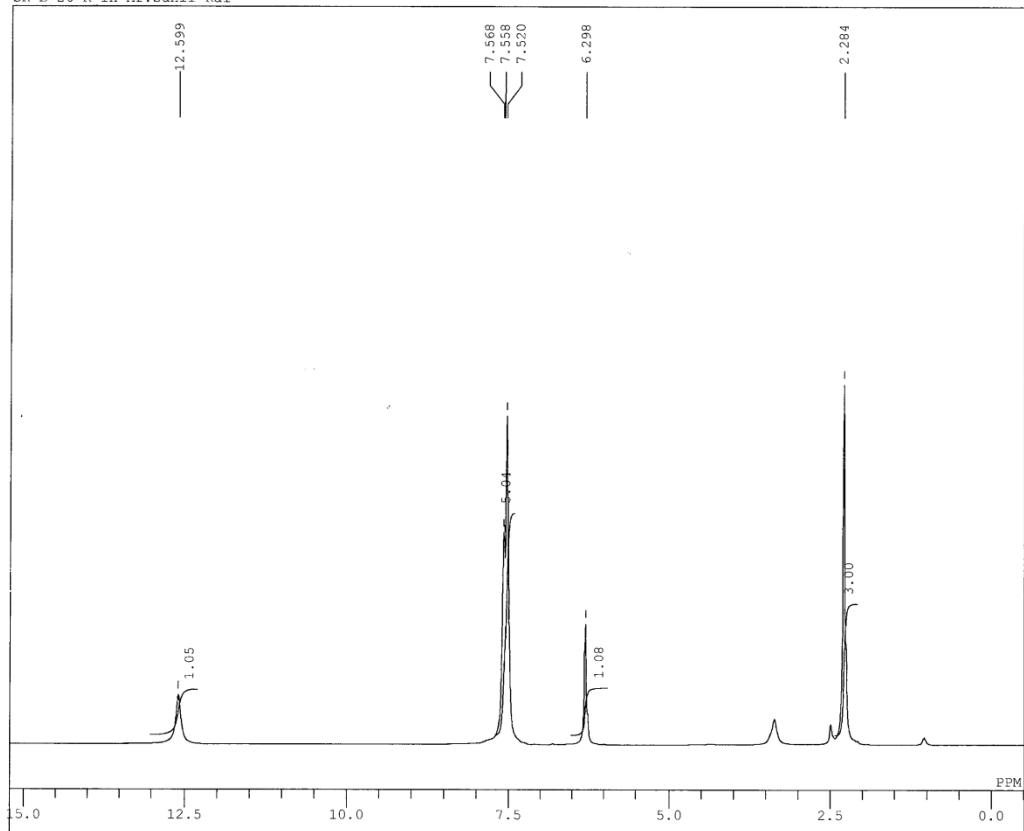
RDS-237-A



Compound (1a):  $^1\text{H}$  NMR



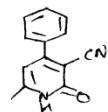
C:\Sunil Rai\SR-B-26-R\_1H.als  
SR-B-26-R\_1H Mr.Sunil Rai



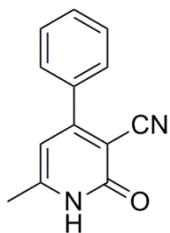
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

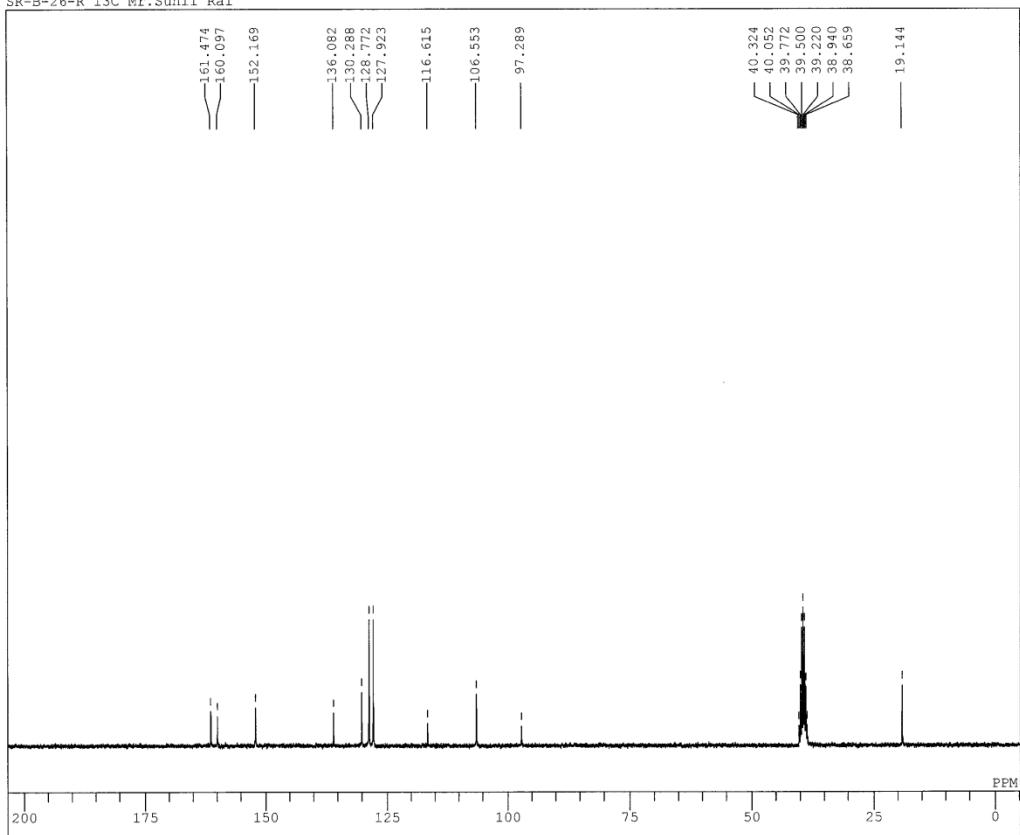
DFILE C:\Sunil Rai\SR-B-26-R  
COMNT SR-B-26-R\_1H Mr.Sunil  
DATIM Wed Nov 07 12:50:29 20  
OBNUC 1H  
EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 9505.7 Hz  
SCANS 44  
ACQTM 3.447 sec  
PD 1.547 sec  
PW1 5.2 us  
IRNUC 1H  
CTEMP 18.3 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 1.20 Hz  
RGAIN 13



Compound (1a):  $^{13}\text{C}$  NMR



C:\WINNNMR98\COMMON\ DEFAULT.ALS  
SR-B-26-R 13C Mr.Sunil Rai



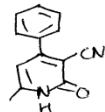
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

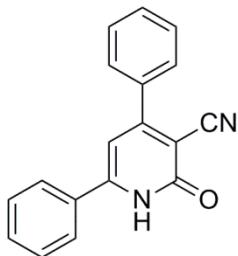
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DATIM Wed Nov 07 12:34:04 20:
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EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 205
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.6 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 23

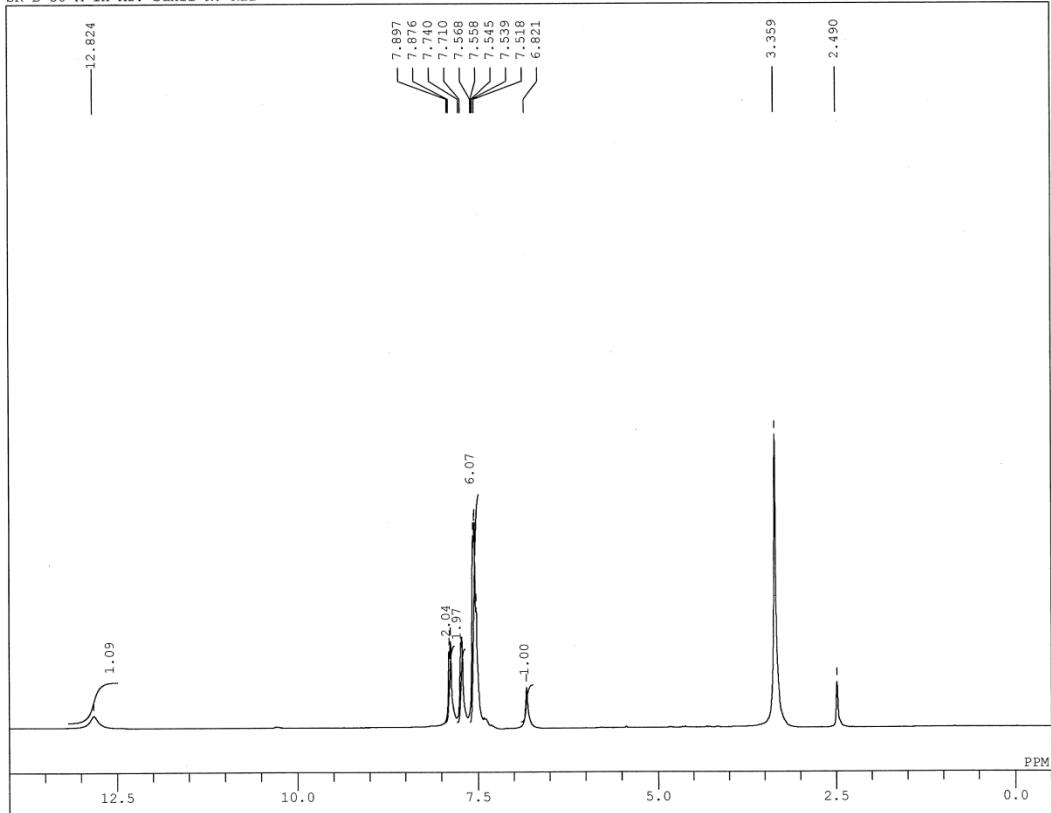
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Compound (1b):  $^1\text{H}$  NMR



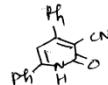
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SR-B-30-A 1H Mr. Sunil K. Rai



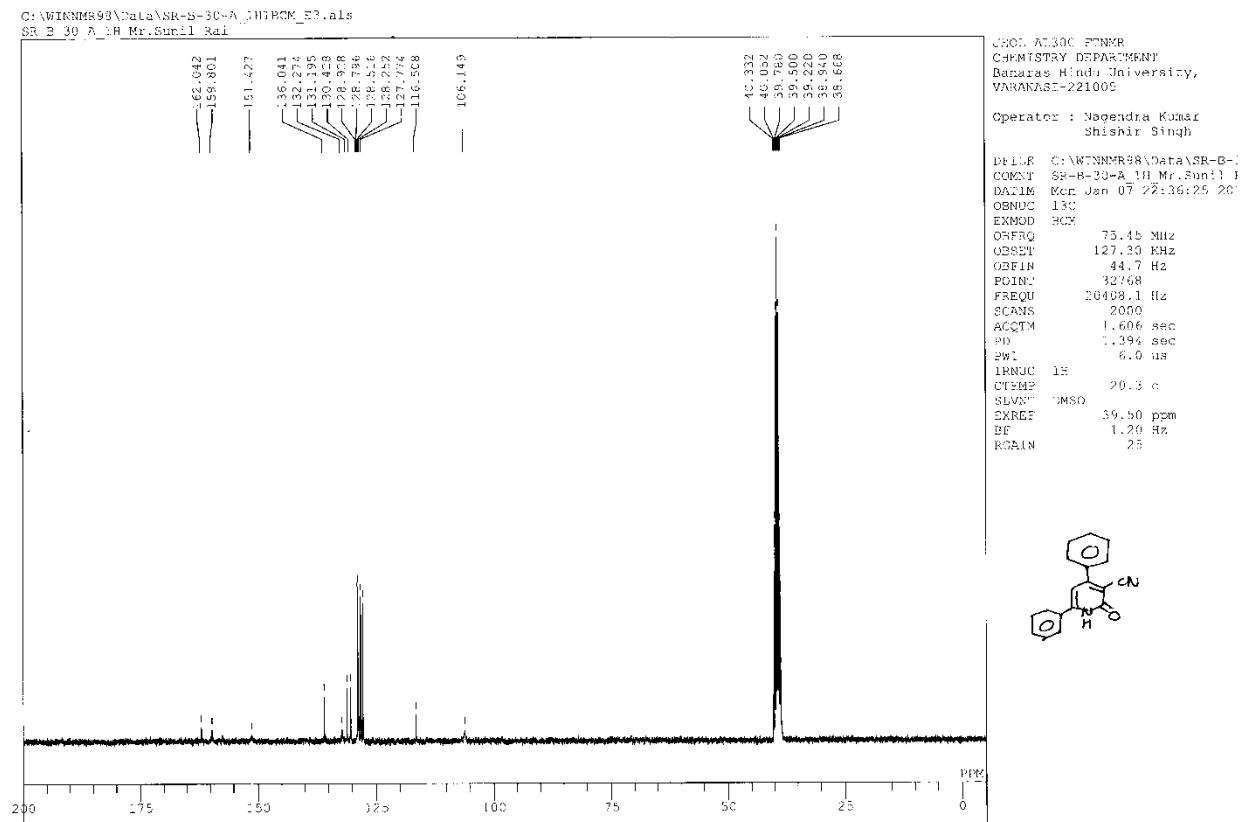
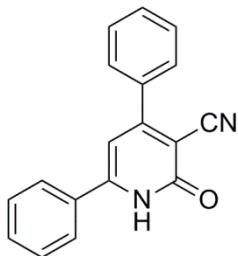
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University  
VARANASI-221005

Operator : Nagendra Kuma  
Shishir Singh

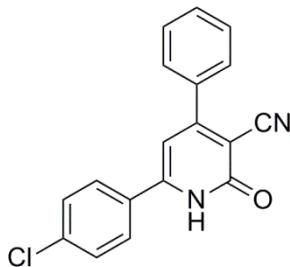
DFILE C:\Sunil Rai\SR-B  
COMNT SR-B-30-A\_1H Mr.  
DATIM Mon Jan 07 15:18:  
OBNUC 1H  
EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 KHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 6016.8 Hz  
SCANS 32  
ACQTM 5.446 sec  
PD 1.547 sec  
PW1 5.2 us  
IRNUC 1H  
CTEMP 18.4 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 1.20 Hz  
RGAIN 17



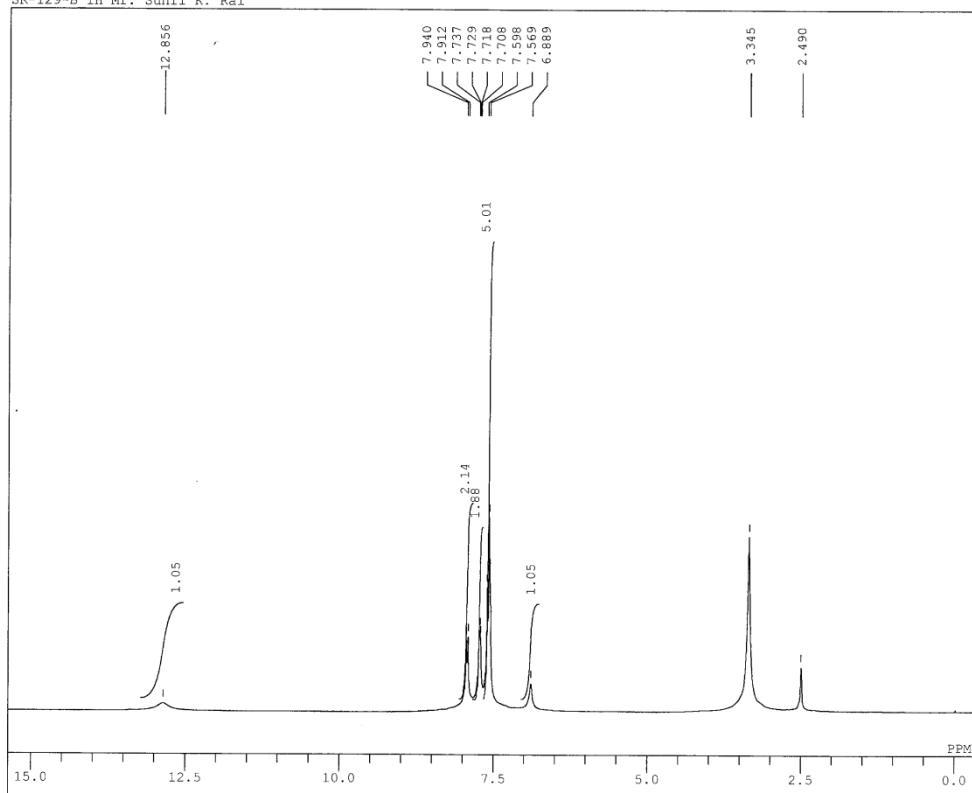
Compound (1b):  $^{13}\text{NMR}$



Compound (1c):  $^1\text{H}$  NMR



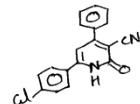
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SR-129-B 1H Mr. Sunil K. Rai



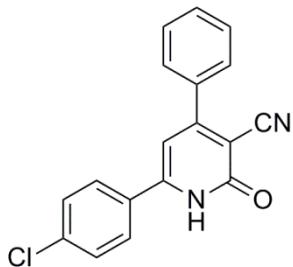
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

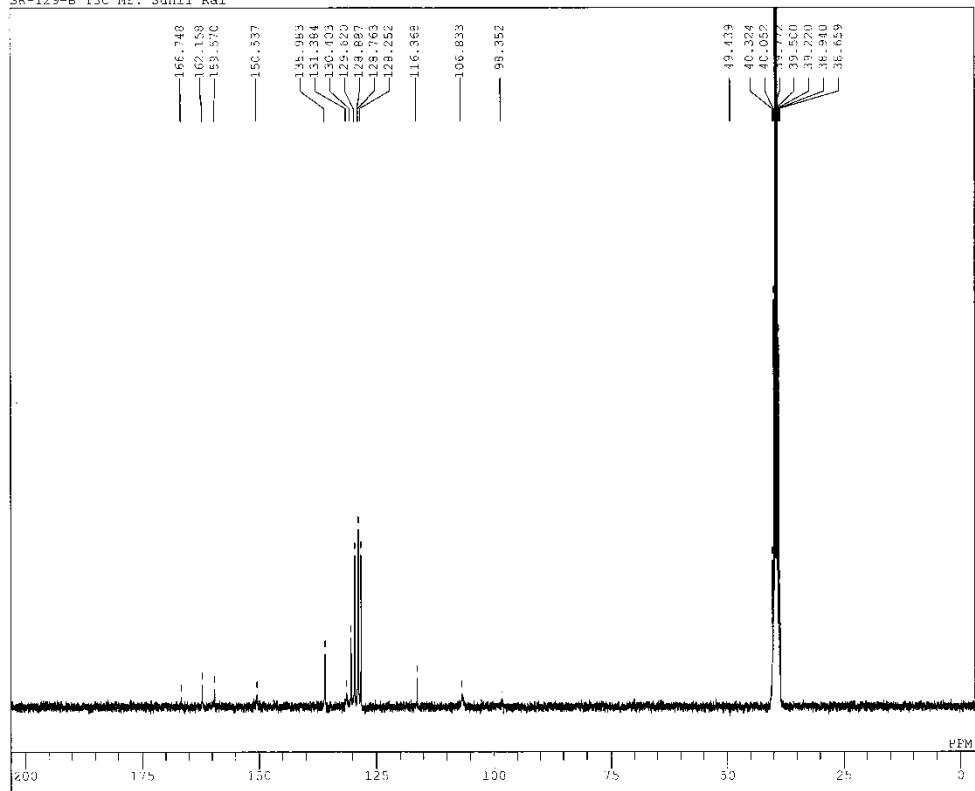
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EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 9505.7 Hz  
SCANS 20  
ACQTM 3.447 sec  
PD 1.547 sec  
PW1 5.2 us  
IRNUC 1H  
CTEMP 21.3 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 1.20 Hz  
RGAIN 17



Compound (1c):  $^{13}\text{C}$  NMR



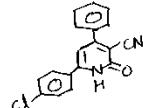
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SR-129-B 13C Mr. Sunil Rai



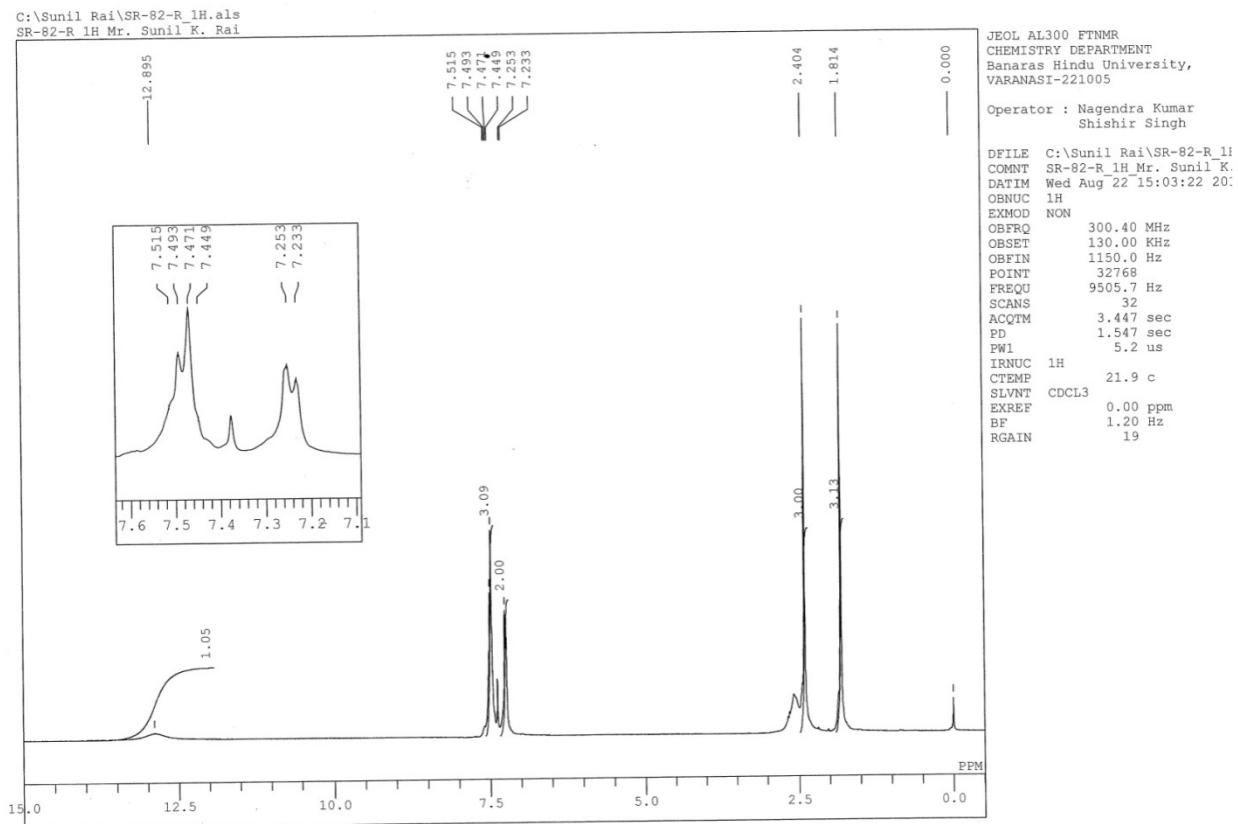
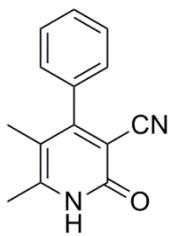
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

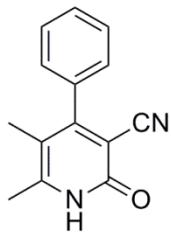
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CCM11 SR-129-B 13C Mr. Sunil  
DATIM Tue Jan 22 01:02:59 20:  
OSNUC 13C  
EXMOD BCM  
OSF3Q 75.45 MHz  
OSF3T 127.30 kHz  
OSFIN 44.7 Hz  
PCINT 32768  
FREQJ 20408.1 Hz  
SCANS 2000  
ACQTM 1.606 sec  
PD 1.294 sec  
PWL 6.0 us  
LRNOC 1B  
CTFMP 22.7 c  
SI1VN2 DMSO  
EXREF 39.50 ppm  
BF 1.20 Hz  
RGATN 23



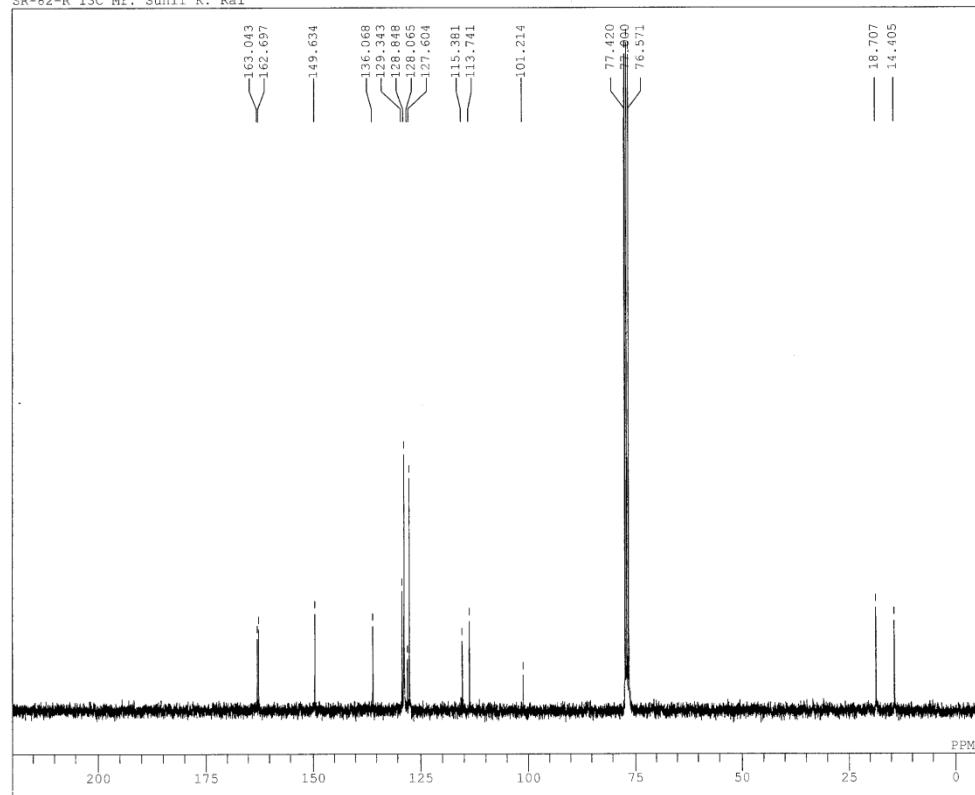
Compound (1d):  $^1\text{H}$  NMR



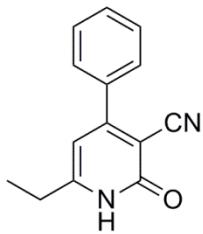
Compound (1d):  $^{13}\text{C}$  NMR



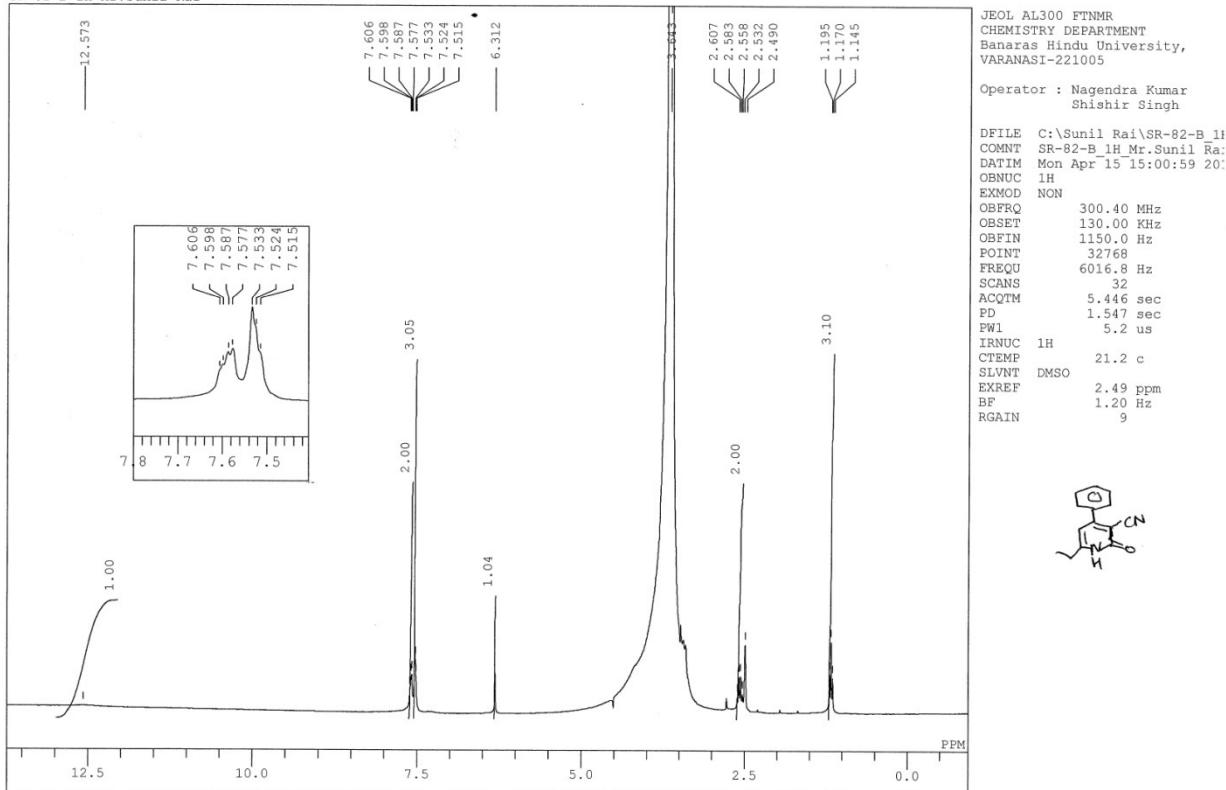
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SR-82-R 13C Mr. Sunil K. Rai



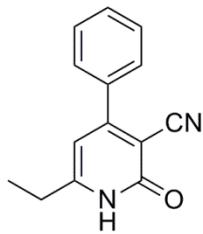
Compound (1e):  $^1\text{H}$  NMR



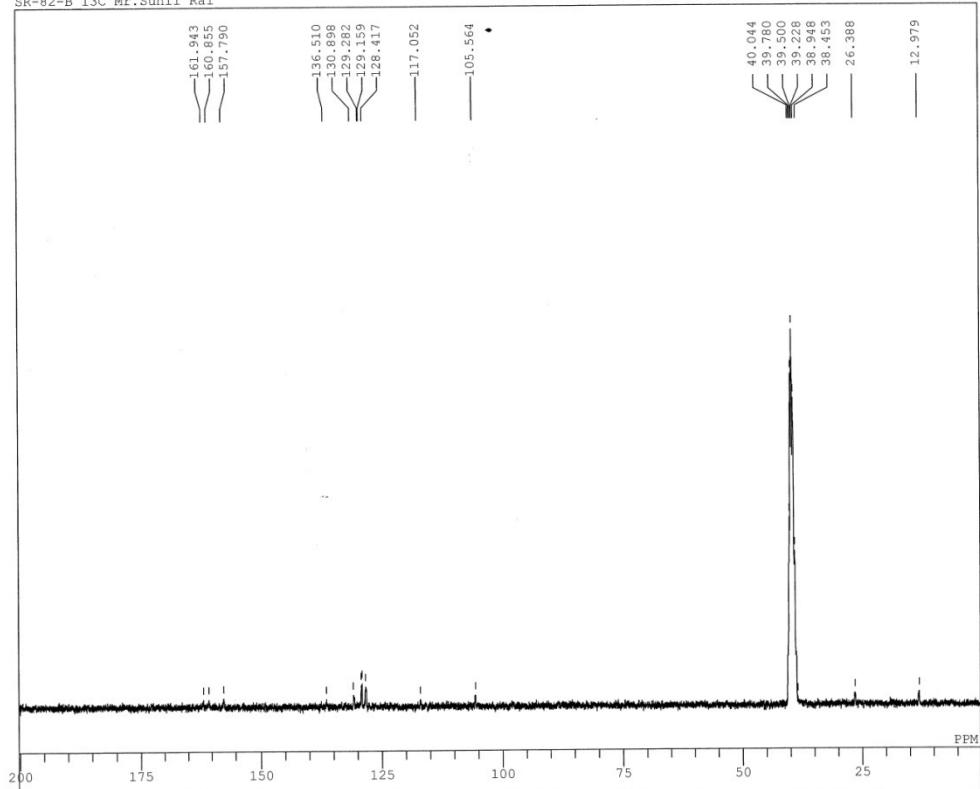
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SR-82-B\_1H Mr.Sunil Rai



Compound (1e):  $^{13}\text{C}$  NMR



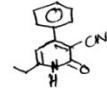
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SR-82-B\_13C Mr.Sunil Rai



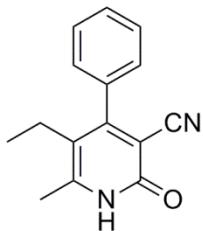
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

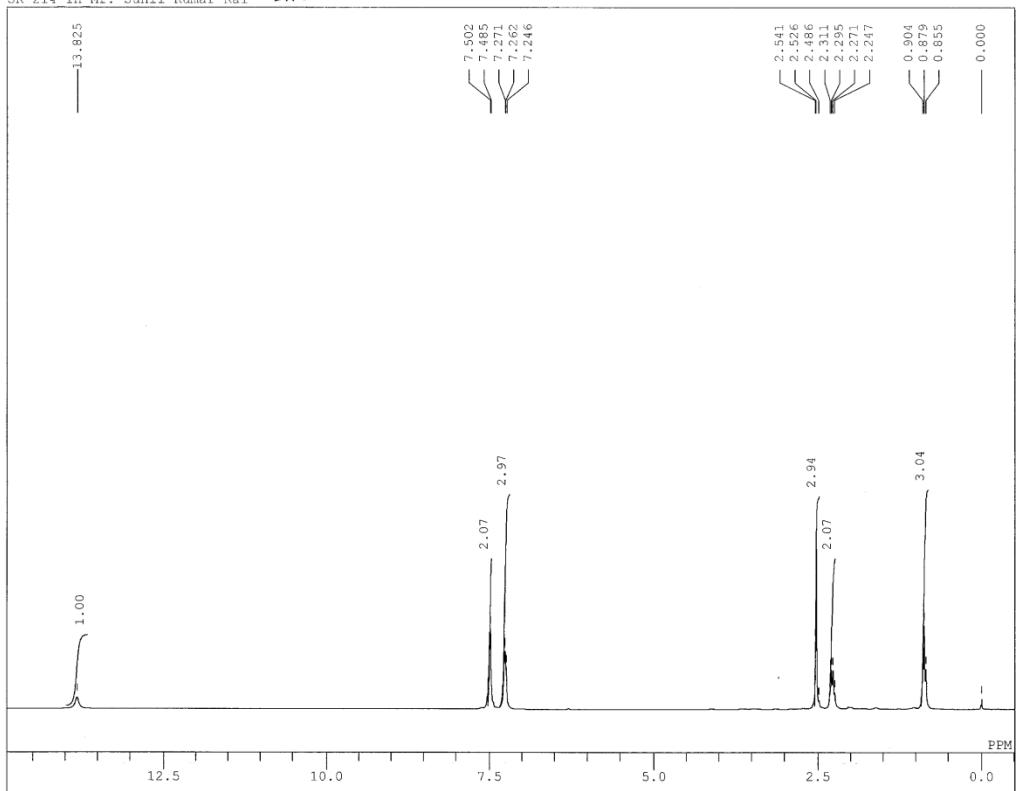
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DATIM Mon Apr 15 20:15:09 20:  
OBNUC 13C  
EXMOD BCM  
OBFRQ 75.45 MHz  
OBSET 127.30 KHz  
OBFIN 44.7 Hz  
POINT 32768  
FREQU 20408.1 Hz  
SCANS 2500  
ACQTM 1.606 sec  
PD 1.394 sec  
PW1 6.0 us  
IRNUC 1H  
CTEMP 21.9 c  
SLVNT DMSO  
EXREF 39.50 ppm  
BF 1.20 Hz  
RGAIN 23



Compound (1f):  $^1\text{H}$  NMR



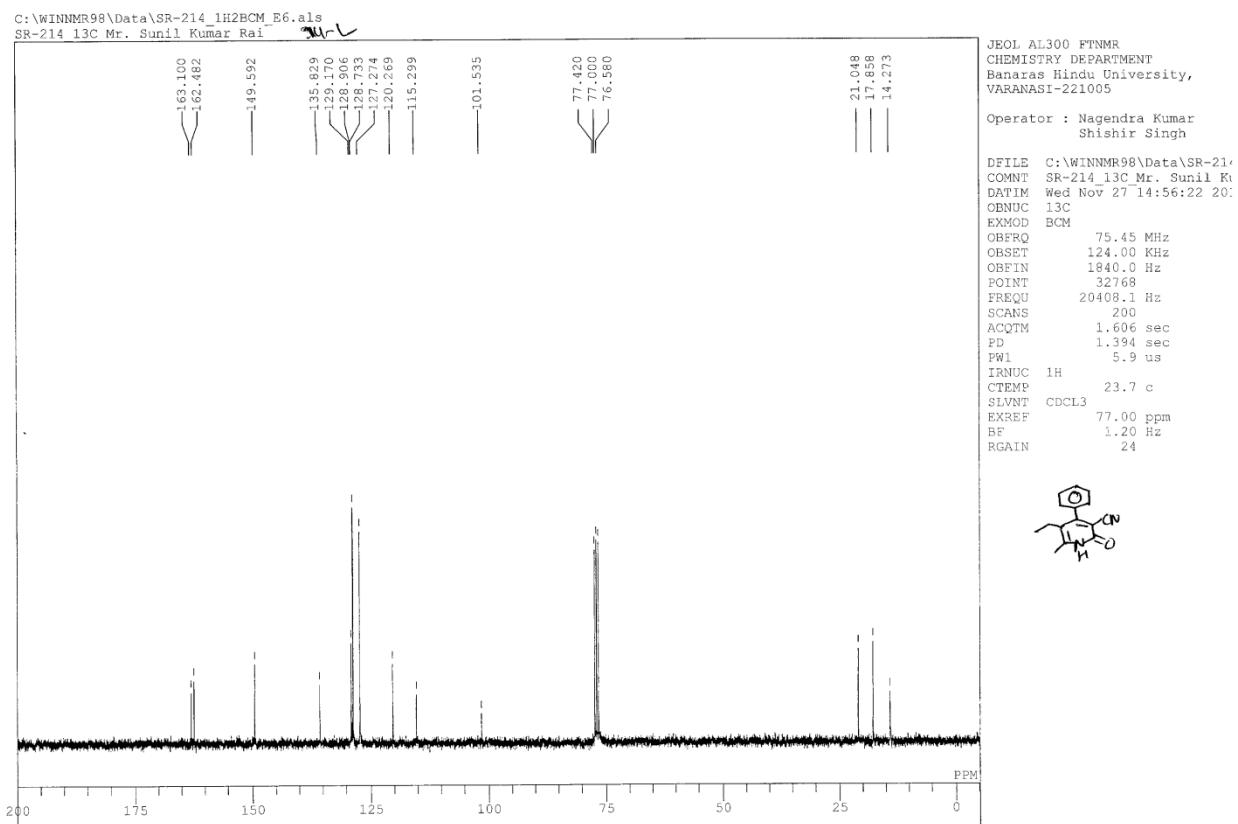
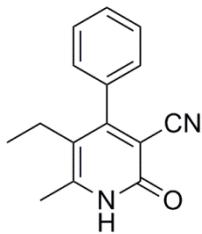
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SR-214\_1H Mr. Sunil Kumar Rai SR-214-L



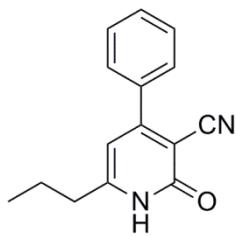
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University  
VARANASI-221005  
Operator : Nagendra Kuma  
Shishir Singh  
DFILE C:\Sunil Rai\SR-2  
COMNT SR-214\_1H Mr. Sun  
DATIM Wed Nov 27 14:46:  
OBNUC 1H  
EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 KHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 6016.8 Hz  
SCANS 16  
ACQTM 5.446 sec  
PD 1.547 sec  
PW1 5.6 us  
IIRNUC 1H  
CTEMP 22.0 c  
SLVNT CDCL3  
EXREF 0.00 ppm  
RF 1.20 Hz  
RGAIN 16



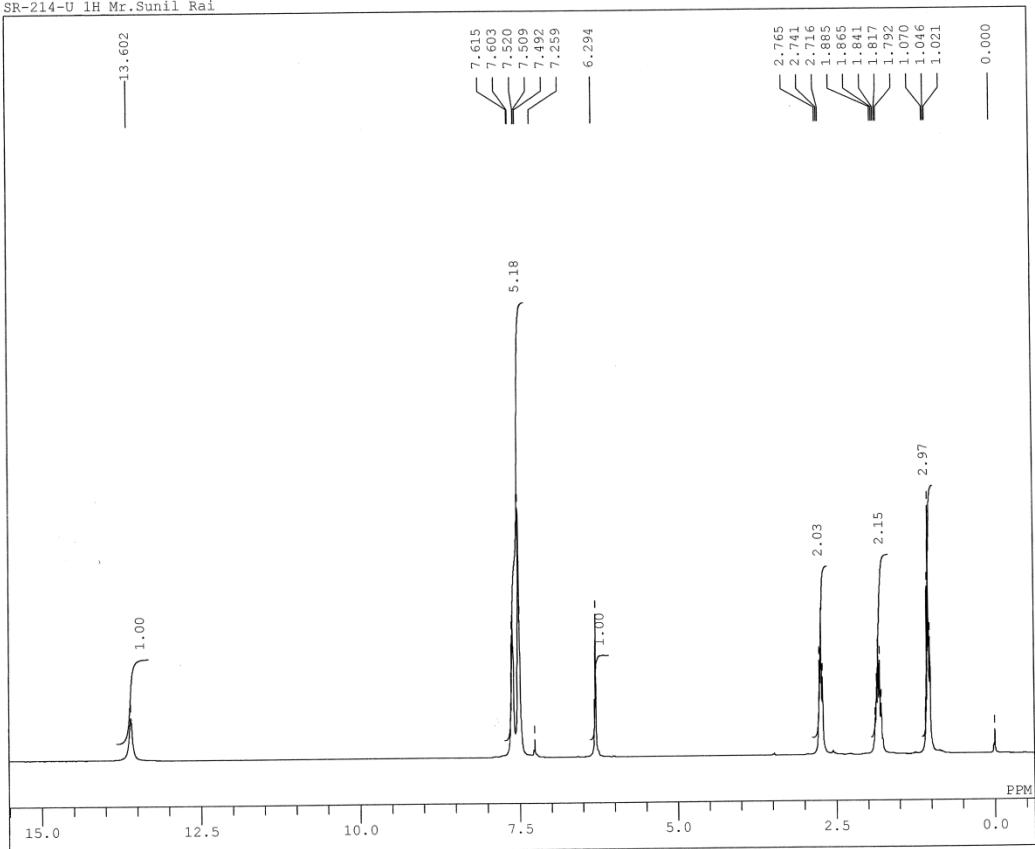
Compound (1f):  $^{13}\text{C}$  NMR



Compound (1g):  $^1\text{H}$  NMR



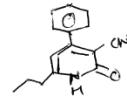
C:\Sunil Rai\SR-214-U 1H.als  
SR-214-U 1H Mr.Sunil Rai



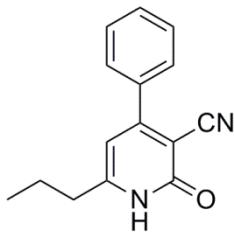
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

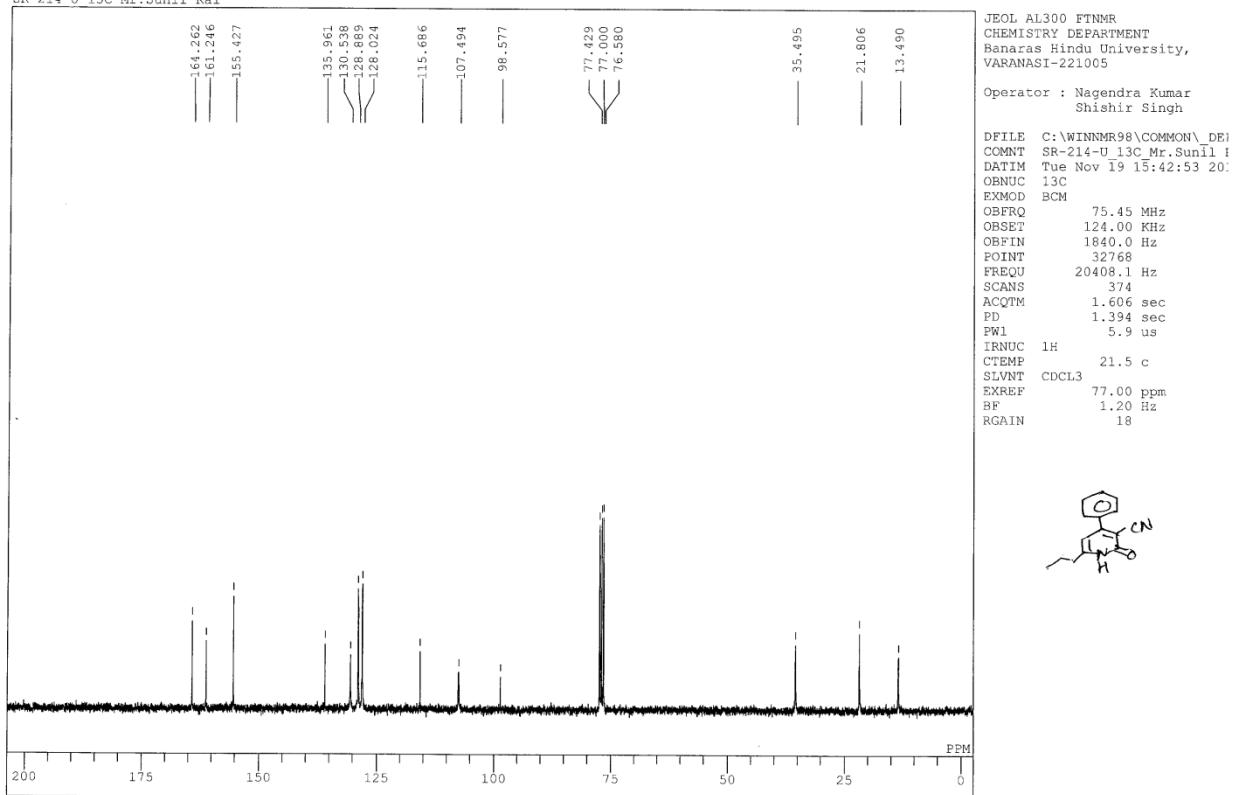
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EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 9505.7 Hz  
SCANS 54  
ACQTM 3.447 sec  
PD 1.547 sec  
PWI 5.2 us  
IRNUC 1H  
CTEMP 19.0 c  
SLVNT CDCL<sub>3</sub>  
EXREF 0.00 ppm  
BF 1.20 Hz  
RGAIN 16



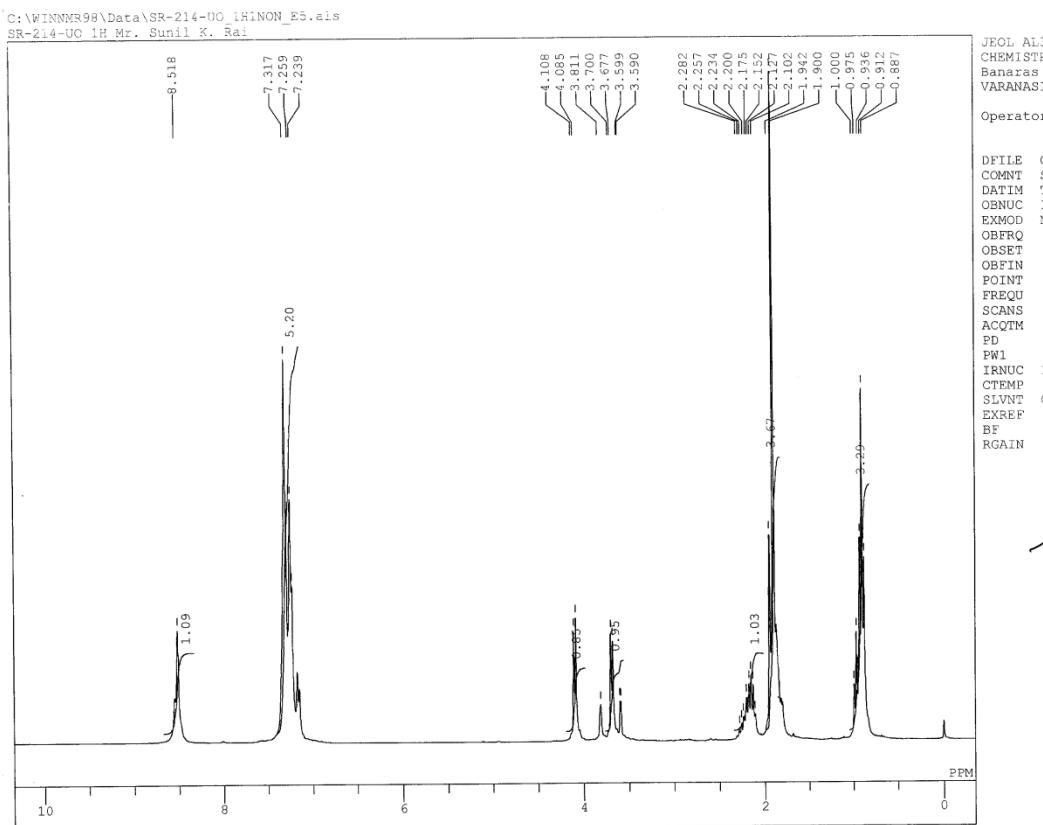
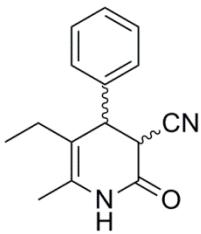
Compound (1g):  $^{13}\text{C}$  NMR



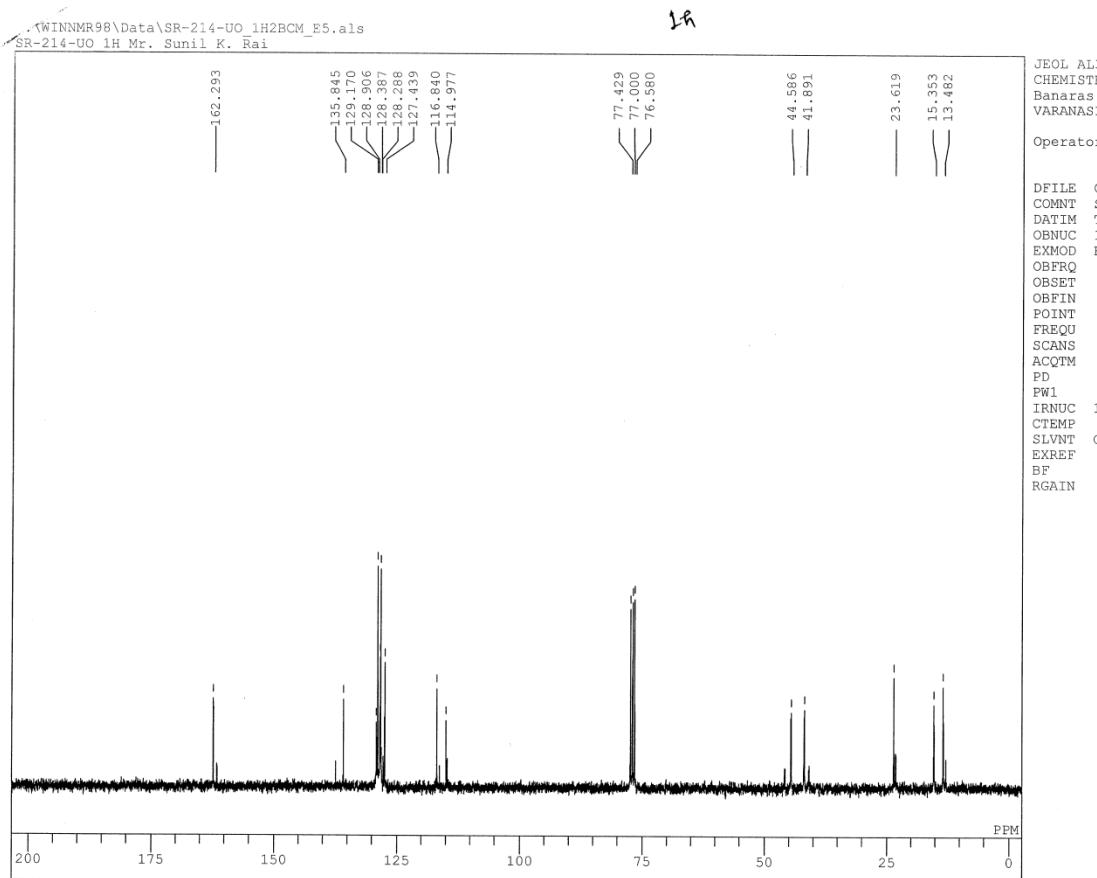
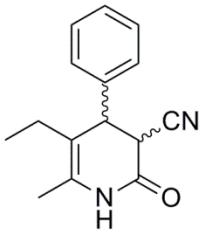
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SR-214-U 13C Mr. Sunil Rai



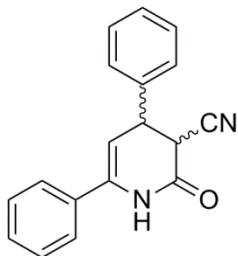
Compound (1h):  $^1\text{H}$  NMR



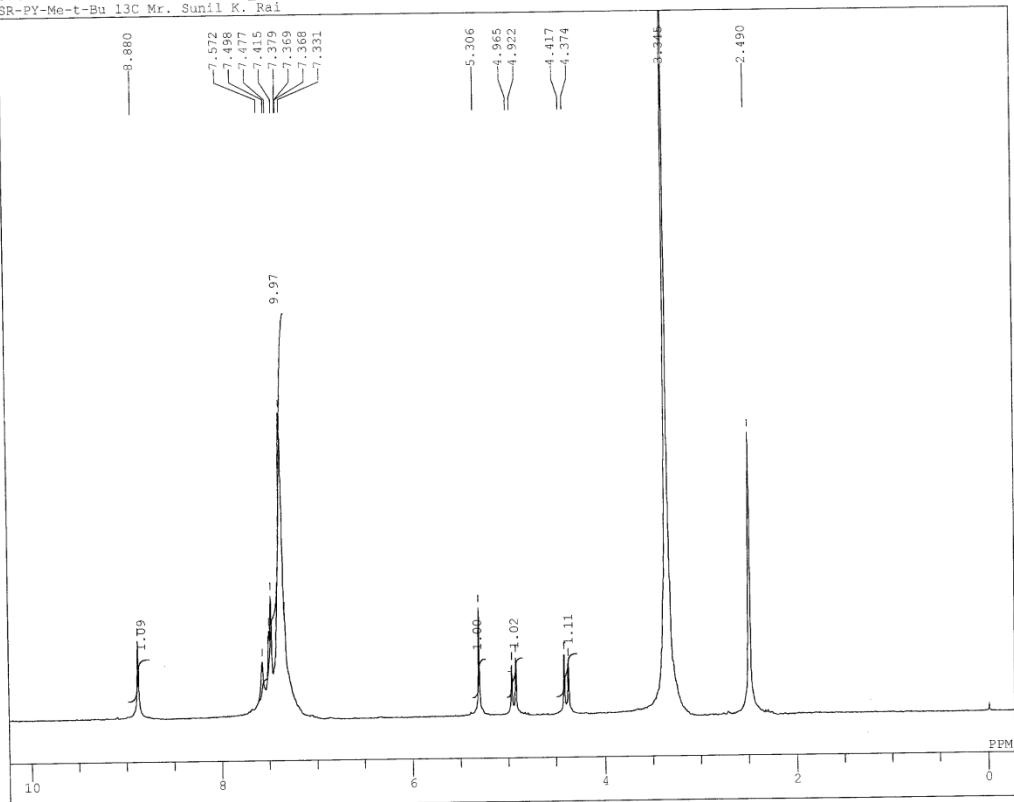
Compound (1h):  $^{13}\text{C}$  NMR



Compound (1i):  $^1\text{H}$  NMR



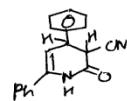
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SR-PY-Me-t-Bu\_13C Mr. Sunil K. Rai



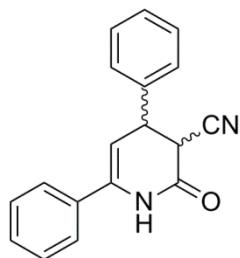
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University  
VARANASI-221005

Operator : Nagendra Kuma  
Shashir Singh

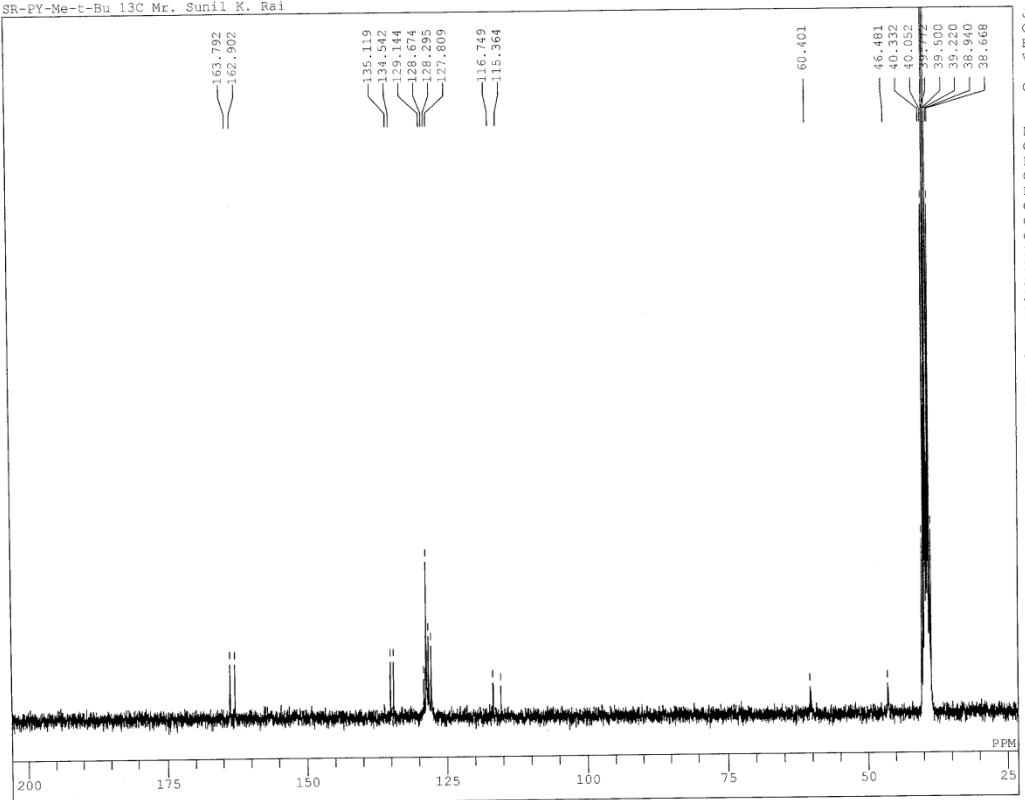
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OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 6016.8 Hz  
SCANS 16  
ACQTM 5.446 sec  
PD 1.547 sec  
PW1 5.6 us  
IENUC 1H  
CTEMP 19.3 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 1.20 Hz  
RGAIN 18



Compound (1i):  $^{13}\text{C}$  NMR



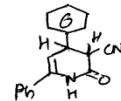
C:\WINNMR98\Data\SR-PY-Me-t-Bu\_13C1BCM\_E8.als  
SR-PY-Me-t-Bu 13C Mr. Sunil K. Rai



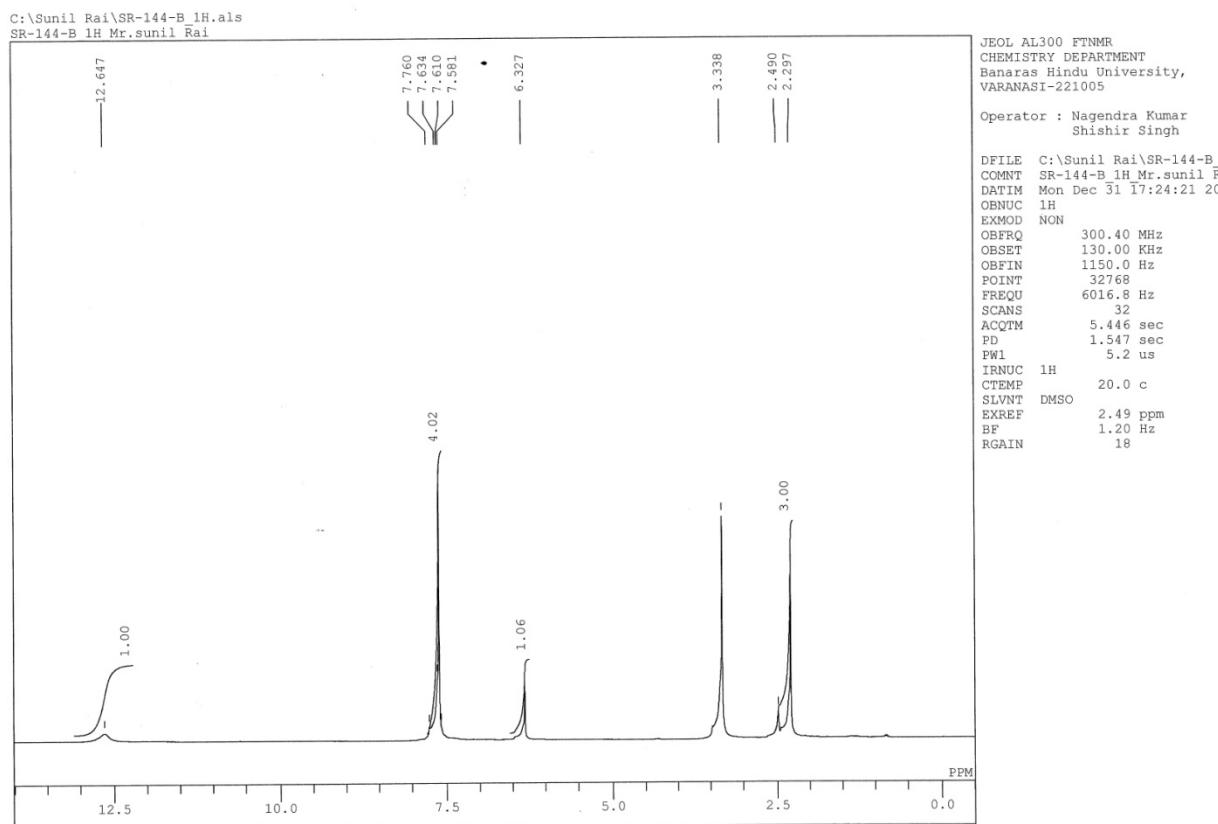
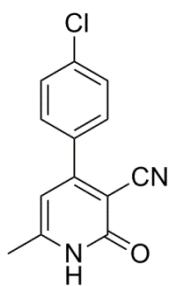
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

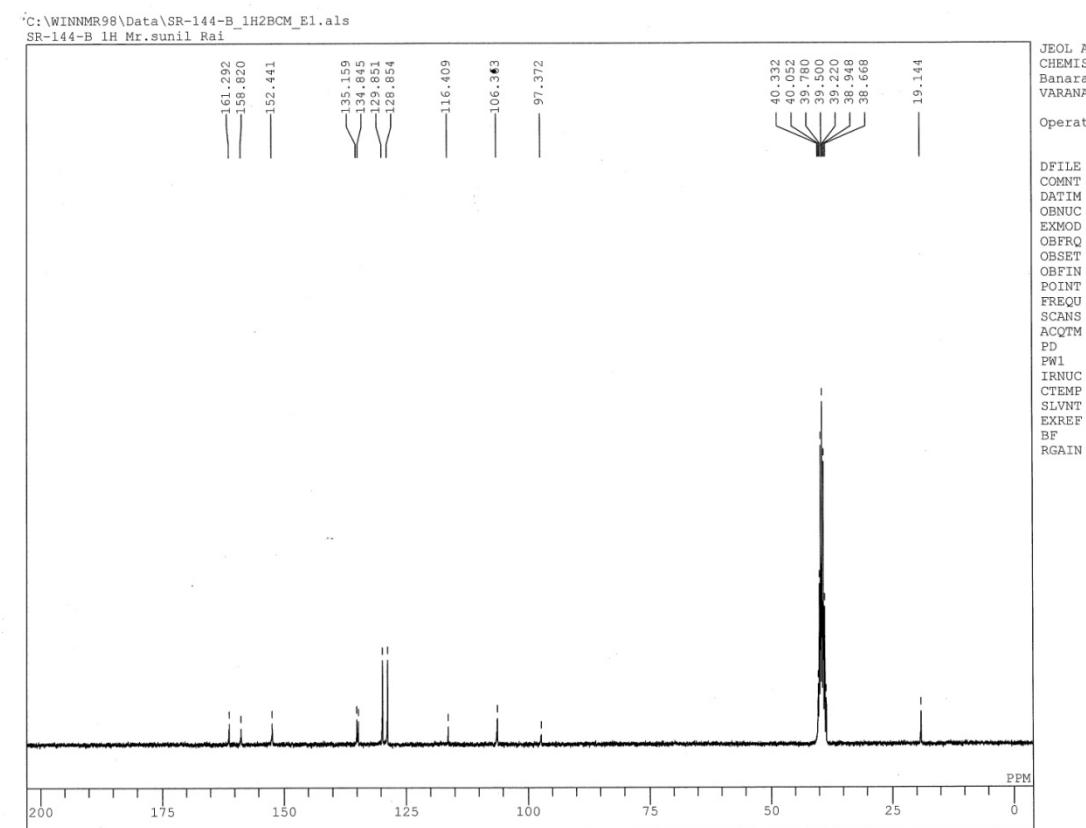
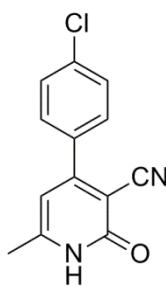
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EXMOD BCM  
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OBSET 124.00 KHz  
OBFIN 1840.0 Hz  
POINT 32768  
FREQU 20408.1 Hz  
SCANS 2000  
ACQTM 1.606 sec  
PD 1.394 sec  
PWI 5.9 us  
IRNUC 1H  
CTEMP 21.1 c  
SLVNT DMSO  
EXREF 39.50 ppm  
BF 1.20 Hz  
RGAIN 24
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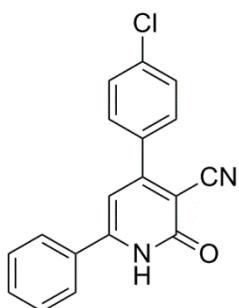
Compound (2a):  $^1\text{H}$  NMR



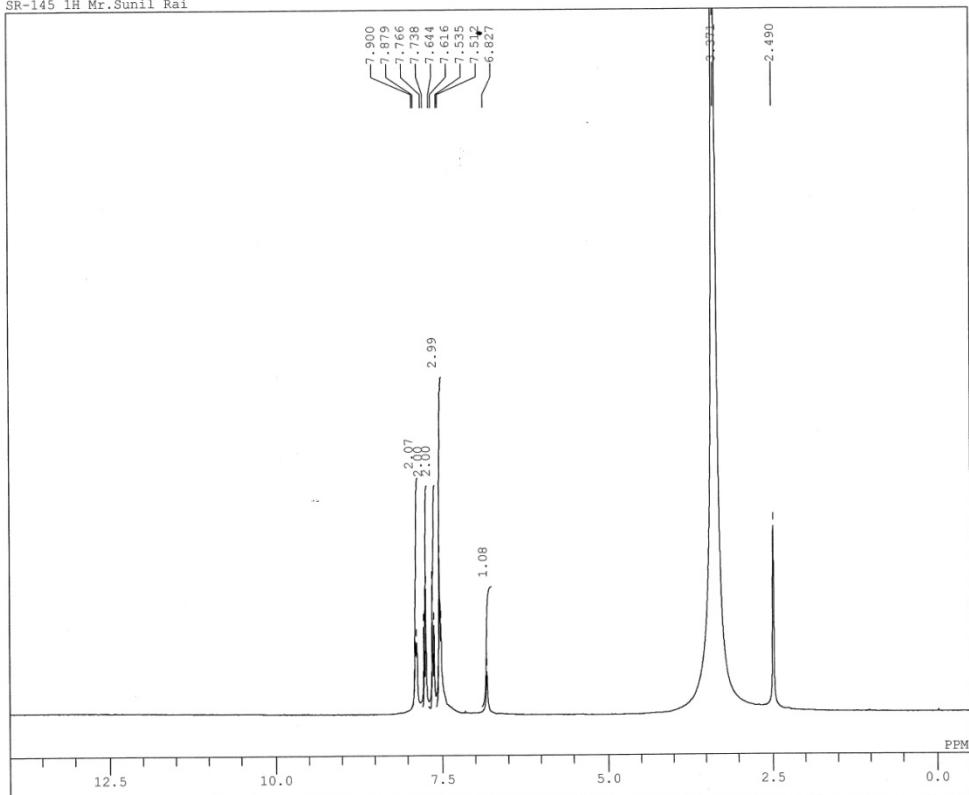
Compound (2a):  $^{13}\text{C}$  NMR



Compound (2b):  $^1\text{H}$  NMR



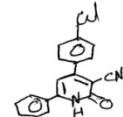
C:\Sunil Rai\SR-145\_1H.als  
SR-145\_1H Mr.Sunil Rai



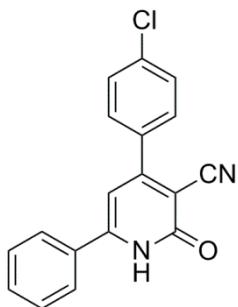
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

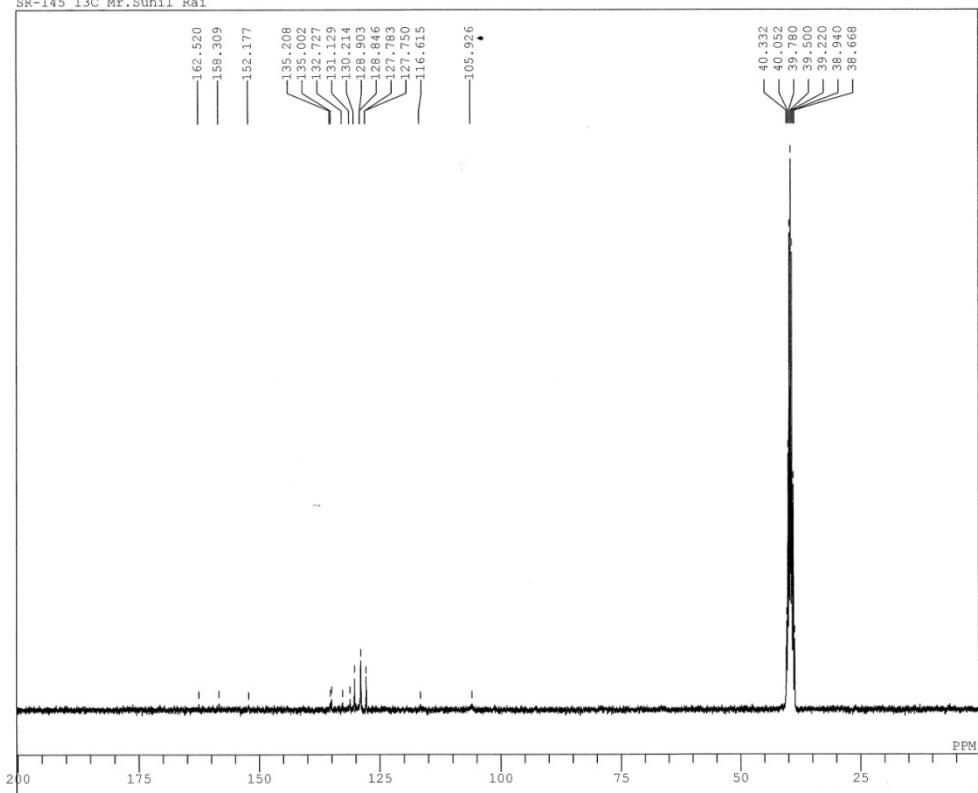
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DATIM Tue Dec 11 15:34:53 20:  
OBNUC 1H  
EXMOD NON  
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OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 6016.8 Hz  
SCANS 32  
ACQTM 5.446 sec  
PD 1.547 sec  
PW1 5.2 us  
IRNUC 1H  
CTEMP 19.6 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 1.20 Hz  
RGAIN 16



Compound (2b):  $^{13}\text{C}$  NMR



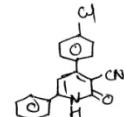
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SR-145 13C Mr.Sunil Rai



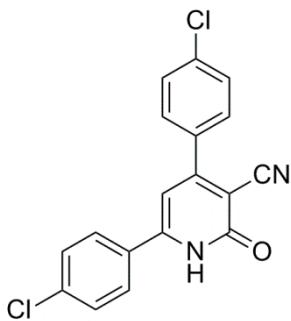
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

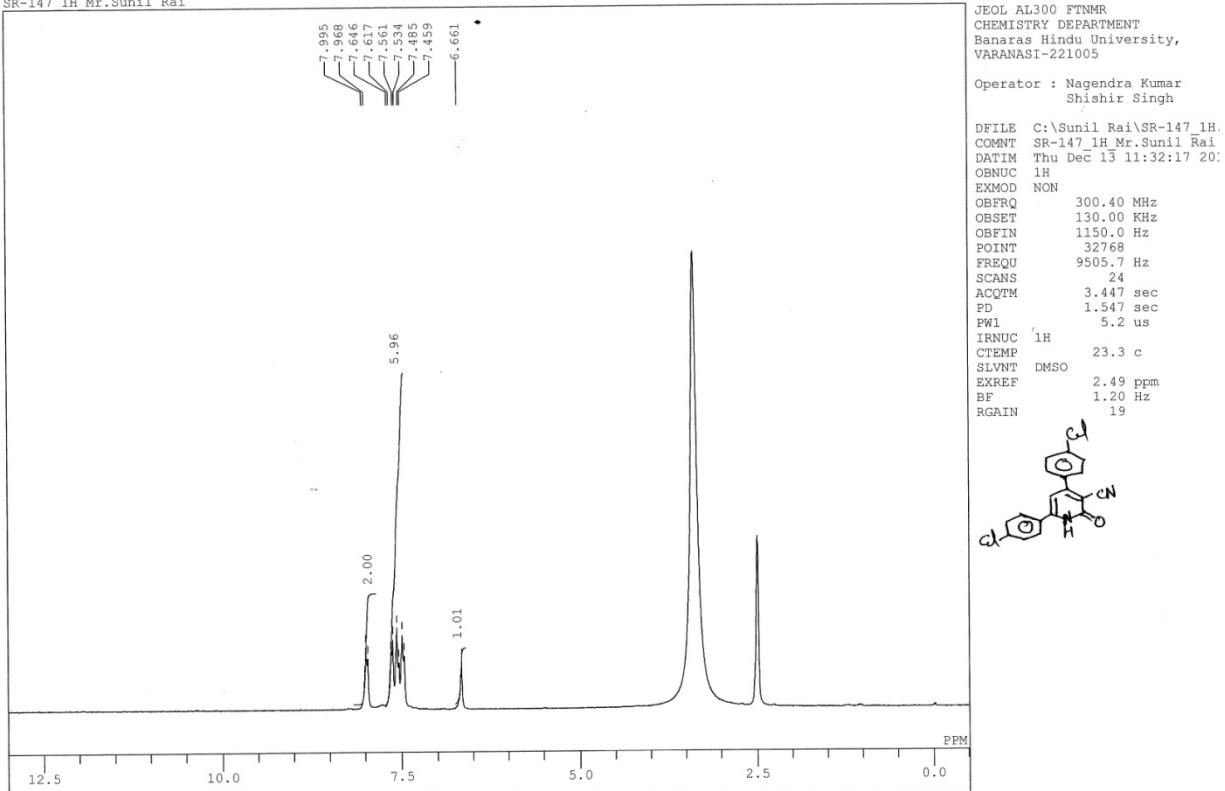
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COMMENT SR-145\_13C Mr.Sunil Rai  
DATIM Wed Dec 12 10:25:02 20:  
OBNUC 13C  
EXMOD BCM  
OBFRQ 75.45 MHz  
OBSET 127.30 kHz  
OBFIN 44.7 Hz  
POINT 32768  
FREQU 20408.1 Hz  
SCANS 2000  
ACQTM 1.606 sec  
PD 1.394 sec  
PW1 6.0 us  
IRNUC 1H  
CTEMP 21.5 c  
SLVNT DMSO  
EXREF 39.50 ppm  
BF 1.20 Hz  
RGAIN 25



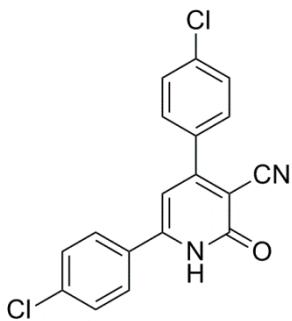
Compound (2c):  $^1\text{H}$  NMR



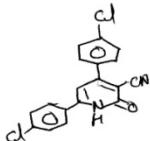
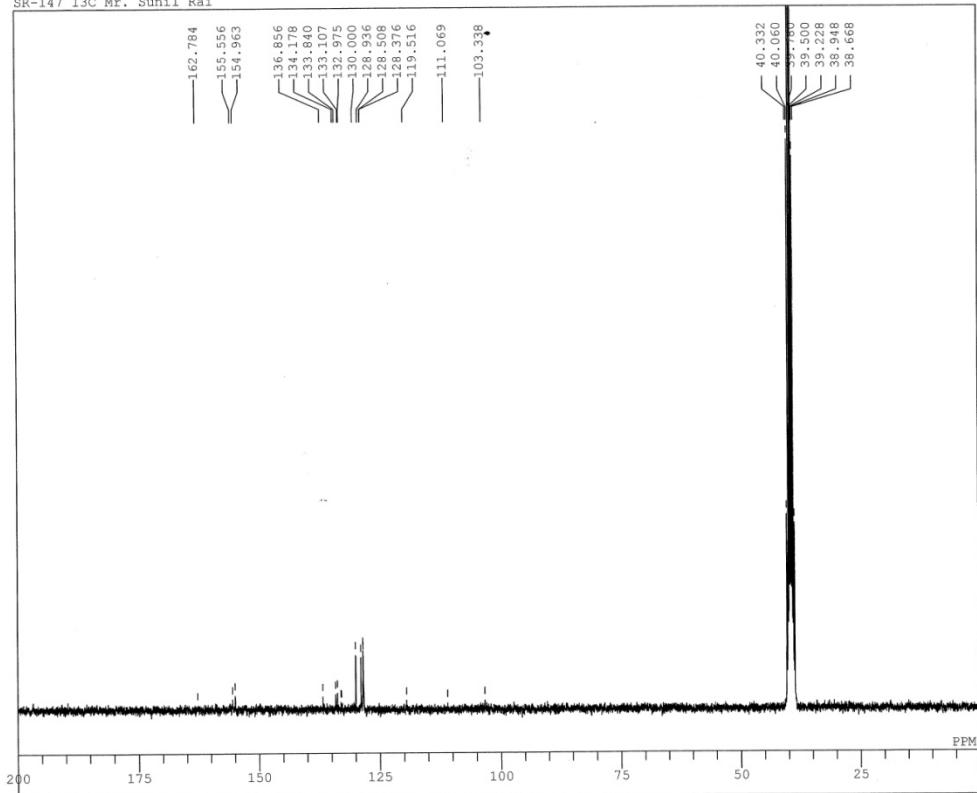
C:\Sunil Rai\SR-147\_1H.als  
SR-147\_1H Mr.Sunil Rai



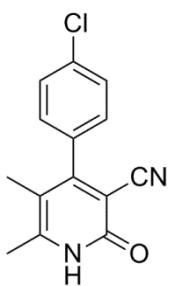
Compound (2c):  $^{13}\text{C}$  NMR



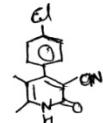
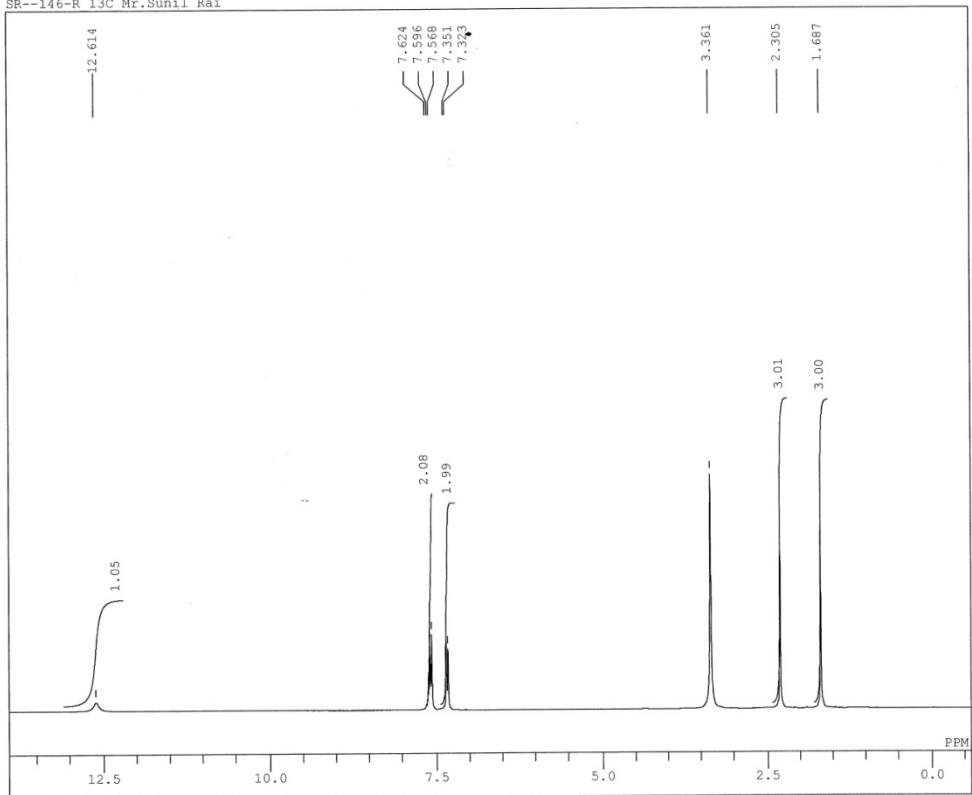
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SR-147.13C Mr. Sunil Rai



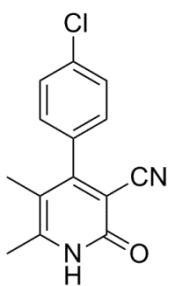
Compound (2d):  $^1\text{H}$  NMR



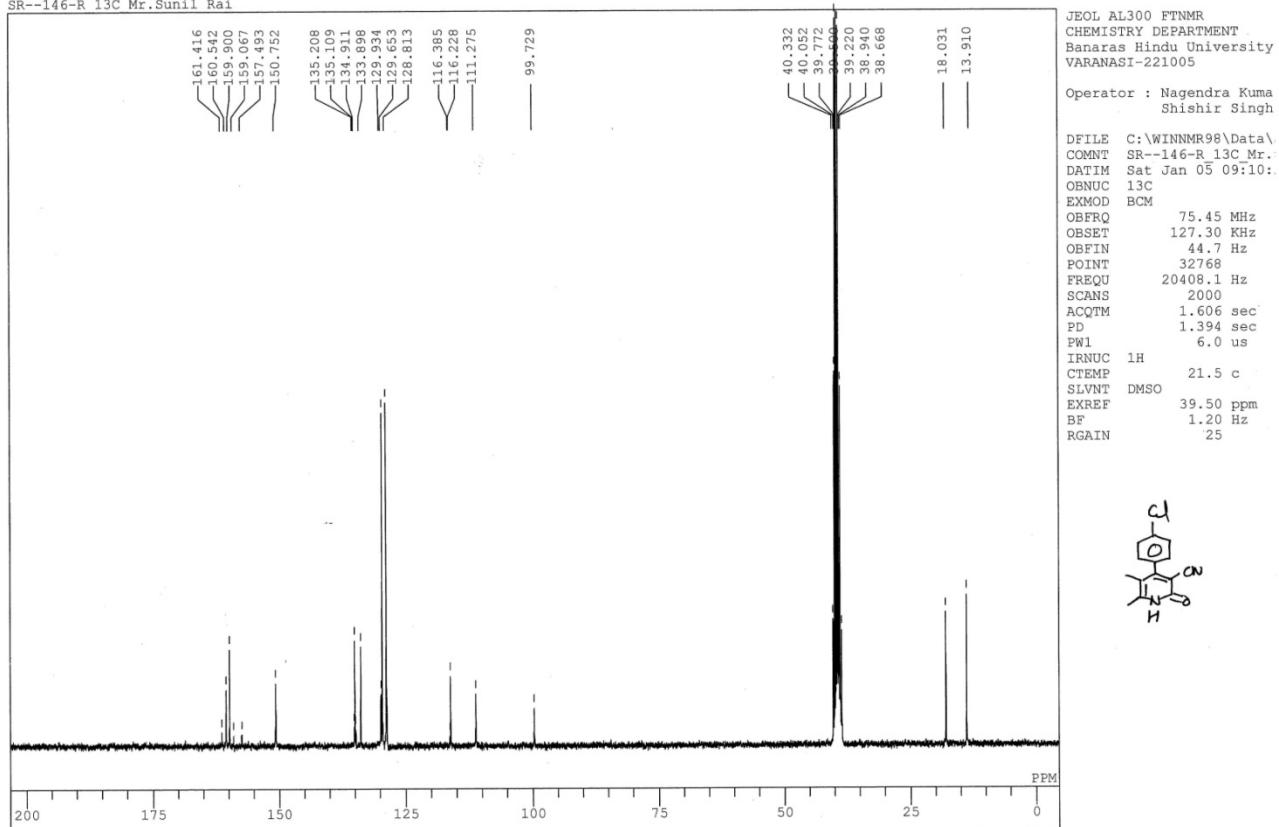
C:\Sunil Rai\SR--146-R\_1H.als  
SR--146-R 13C Mr.Sunil Rai



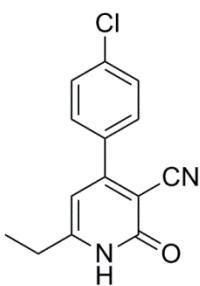
Compound (2d):  $^{13}\text{C}$  NMR



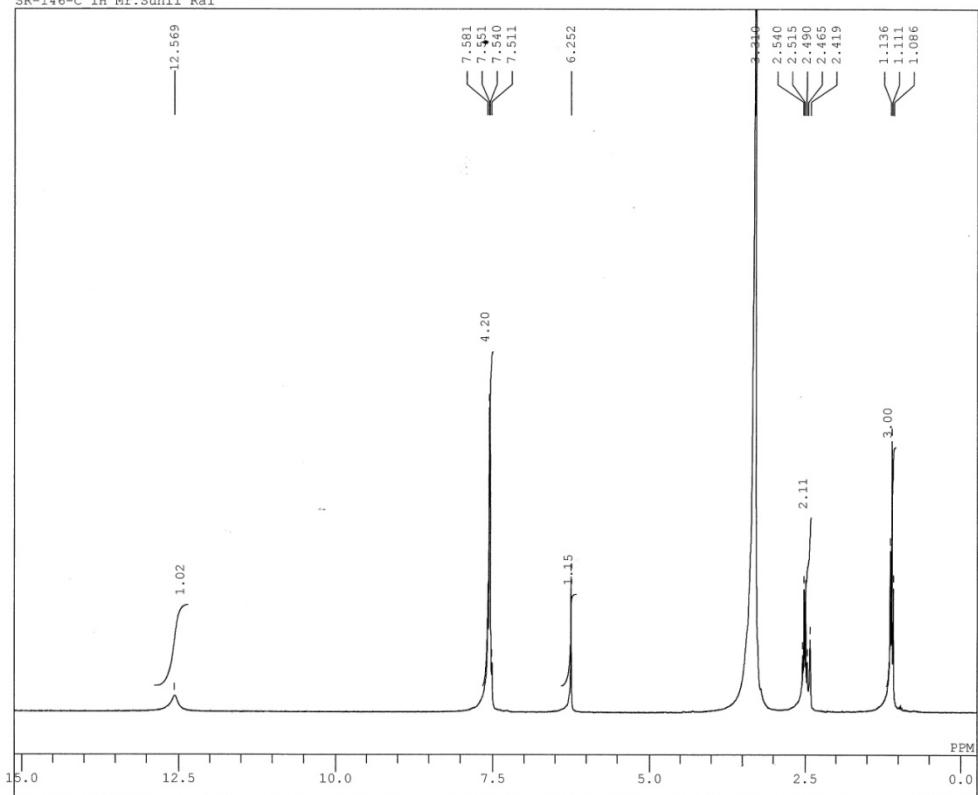
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 SR--146-R 13C Mr.Sunil Rai



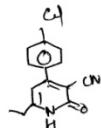
Compound (2e):  $^1\text{H}$  NMR



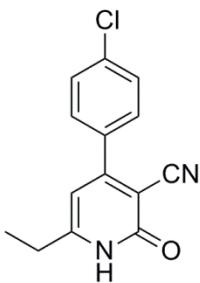
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SR-146-C 1H Mr.Sunil Rai



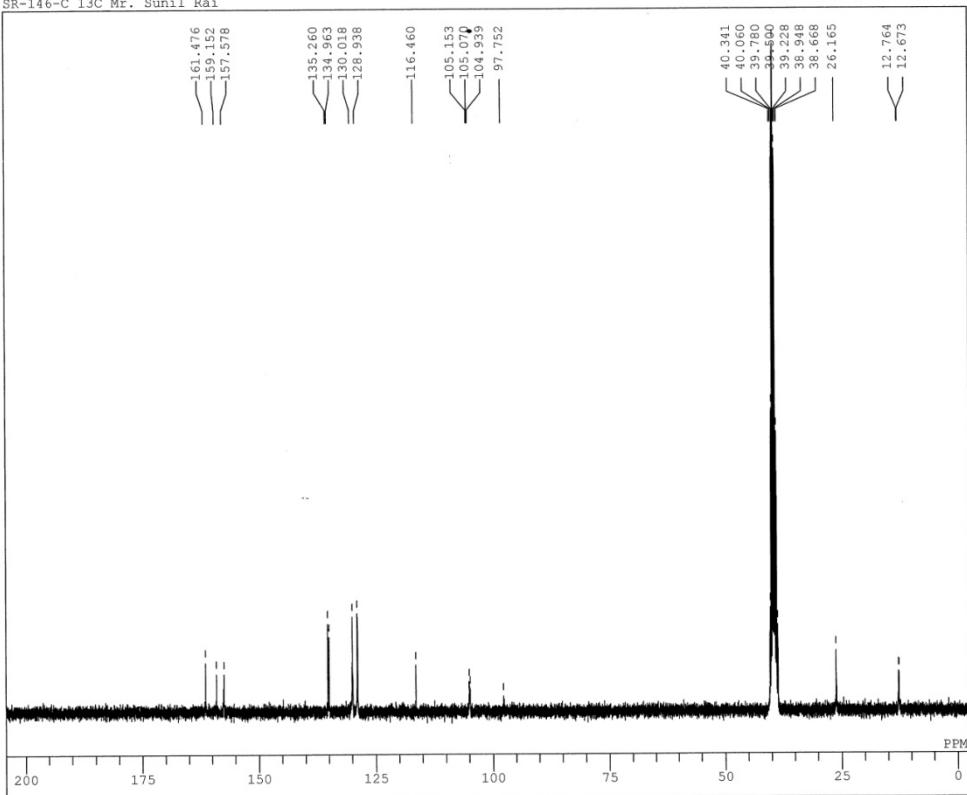
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005  
Operator : Nagendra Kumar  
Shishir Singh  
DFILE C:\WINNNMR98\COMMON\DEI  
COMNT SR-146-C 1H Mr.Sunil Rai  
DATIM Tue Jun 11 16:10:15 20:  
OBNUC 1H  
EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 9505.7 Hz  
SCANS 32  
ACQTM 3.447 sec  
PD 1.547 sec  
PW1 5.2 us  
IRNUC 1H  
CTEMP 22.8 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 0.12 Hz  
RGAIN 14



Compound (2e):  $^{13}\text{C}$  NMR



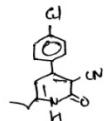
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SR-146-C 13C Mr. Sunil Rai



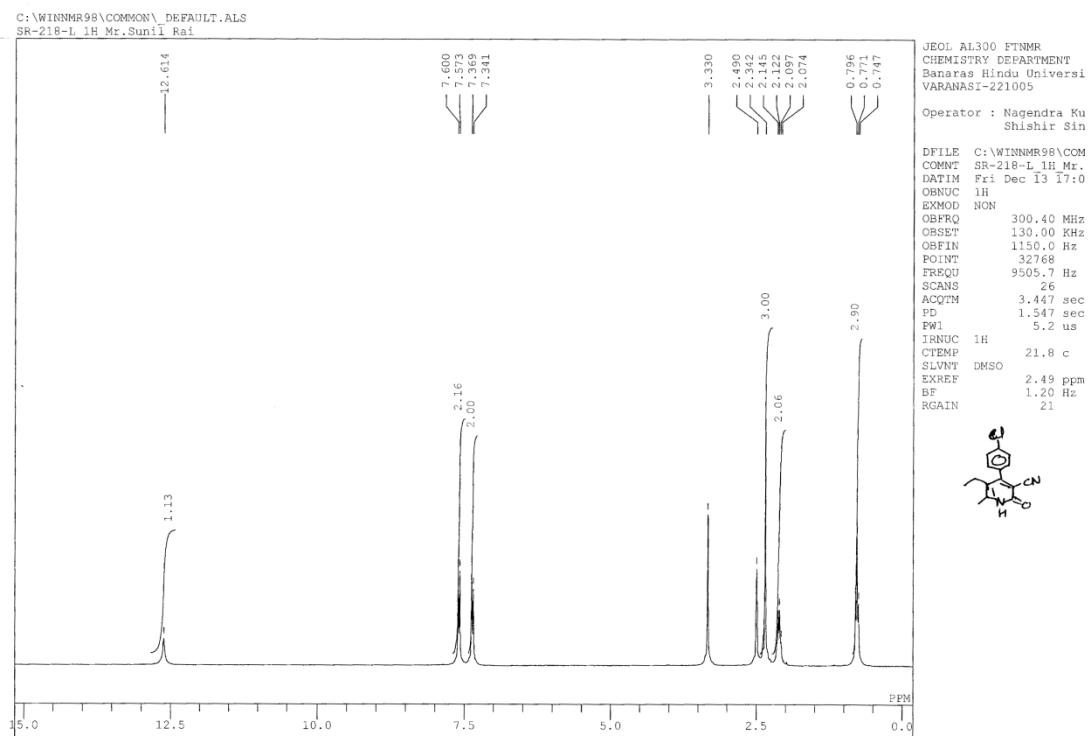
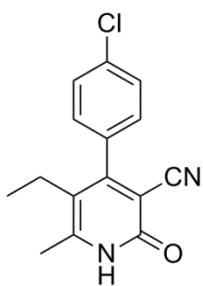
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

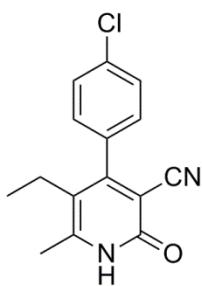
DFILE C:\WINNMR98\Data\SR-146-C\_13C Mr. Sunil  
COMNT SR-146-C 13C Mr. Sunil  
DATIM Wed Jun 12 00:43:36 20:  
OBNUC 13C  
EXMOD BCM  
OBFRQ 75.45 MHz  
OBSET 124.00 KHz  
OBFIN 1840.0 Hz  
POINT 32768  
FREQU 20408.1 Hz  
SCANS 2500  
ACQTM 1.606 sec  
PD 1.394 sec  
PW1 5.9 us  
IRNUC 1H  
CTEMP 20.1 c  
SLVNT DMSO  
EXREF 39.50 ppm  
BF 0.12 Hz  
RGAIN 22



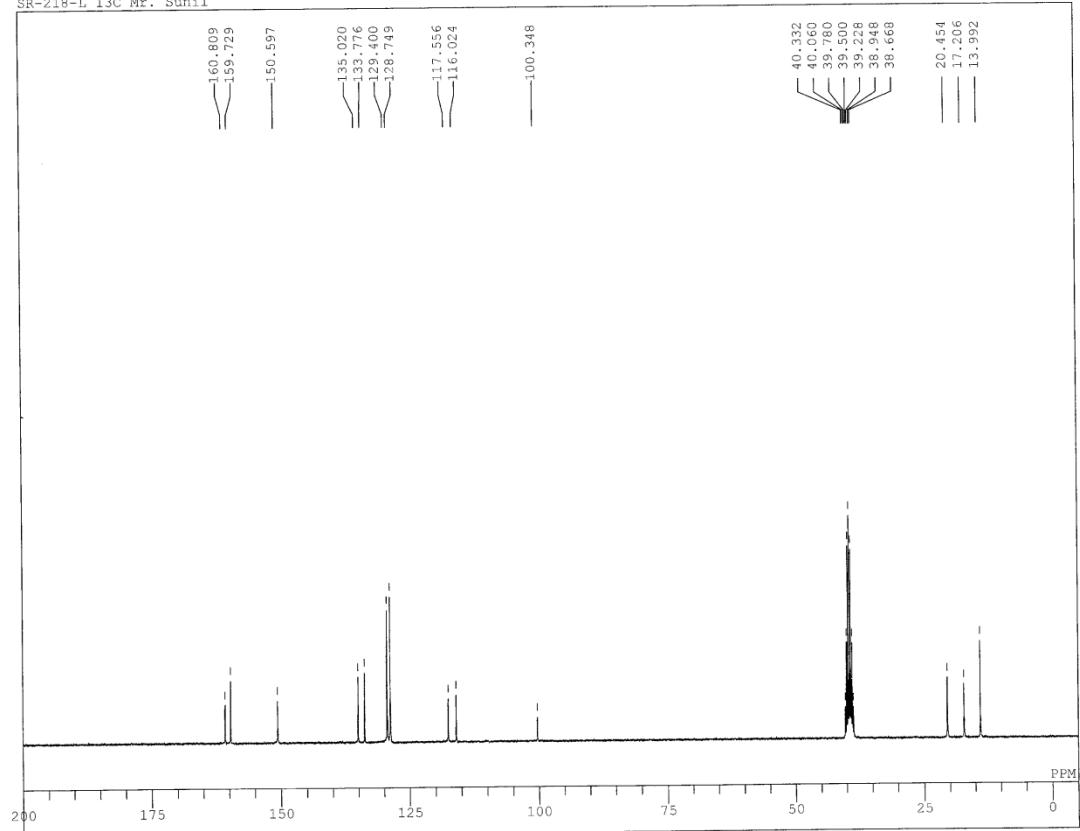
Compound (2f): 1H NMR



Compound (2f):  $^{13}\text{C}$  NMR



C:\WINNMR98\Data\SR-218-L\_13C1BCM\_E5.als  
SR-218-L 13C Mr. Sunil

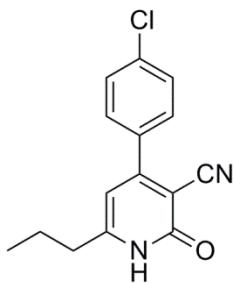


JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu Universit  
VARANASI-221005

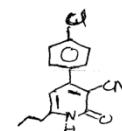
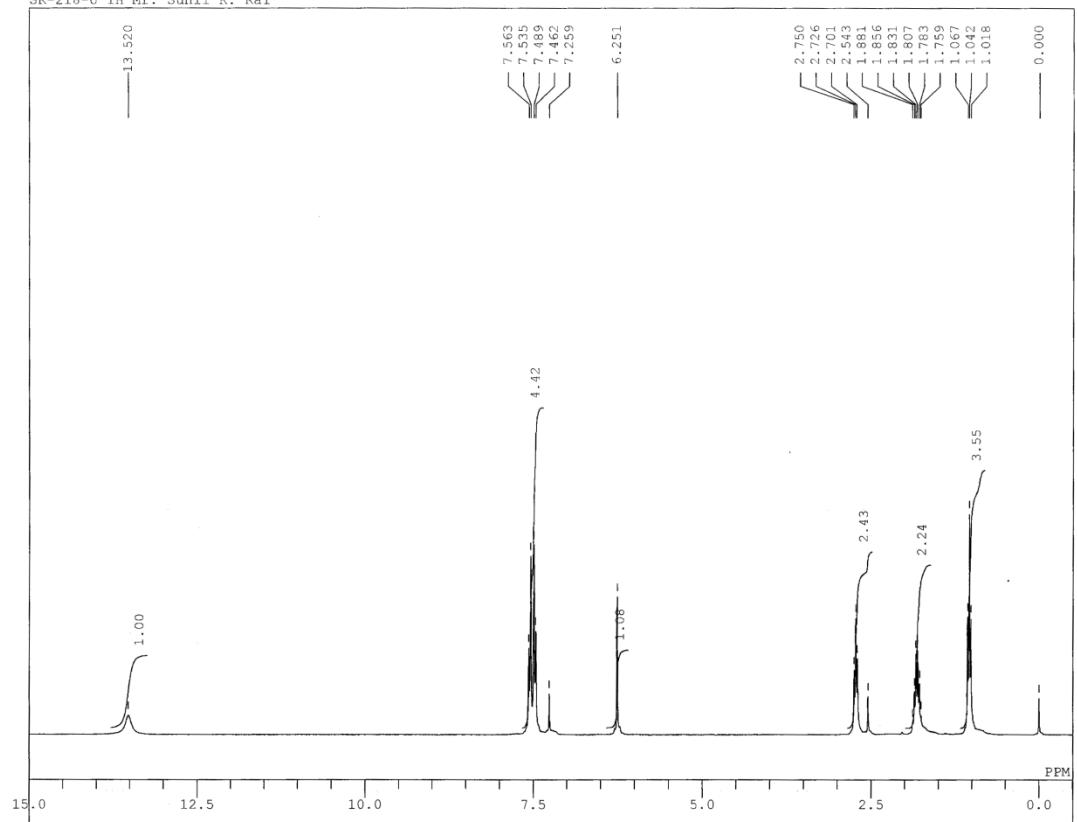
Operator : Nagendra Kun  
Shishir Sing

DFILE C:\WINNMR98\Date  
COMNT SR-218-L\_13C\_Mr.  
DATIM Tue Dec 17 00:32  
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 24.3 c  
SLVNT DMSO  
EXREF 39.50 ppm  
BF 1.20 Hz  
RGAIN 22

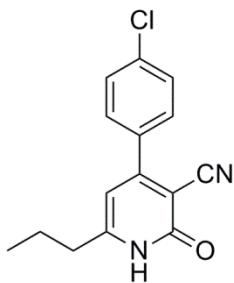
Compound (2g):  $^1\text{H}$  NMR



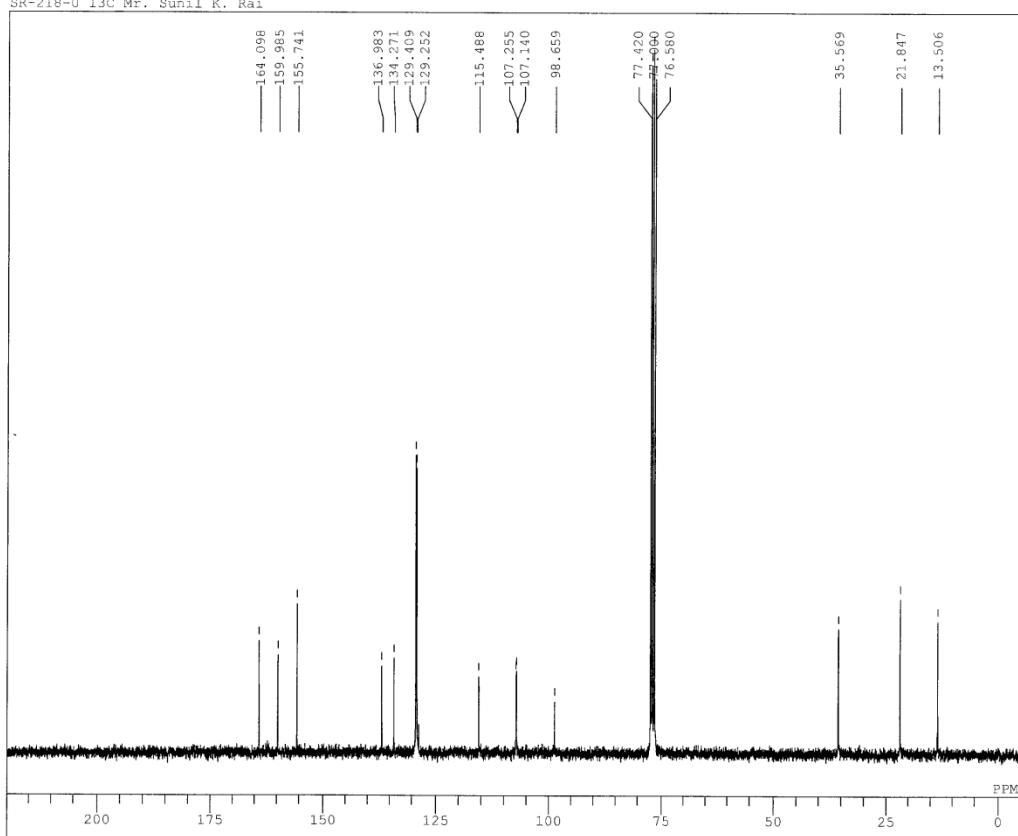
C:\Sunil Rai\SR-218-U\_1H.als  
 SR-218-U\_1H Mr. Sunil K. Rai



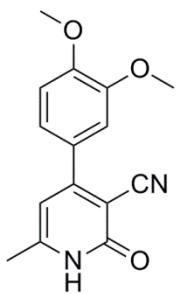
Compound (2g):  $^{13}\text{C}$  NMR



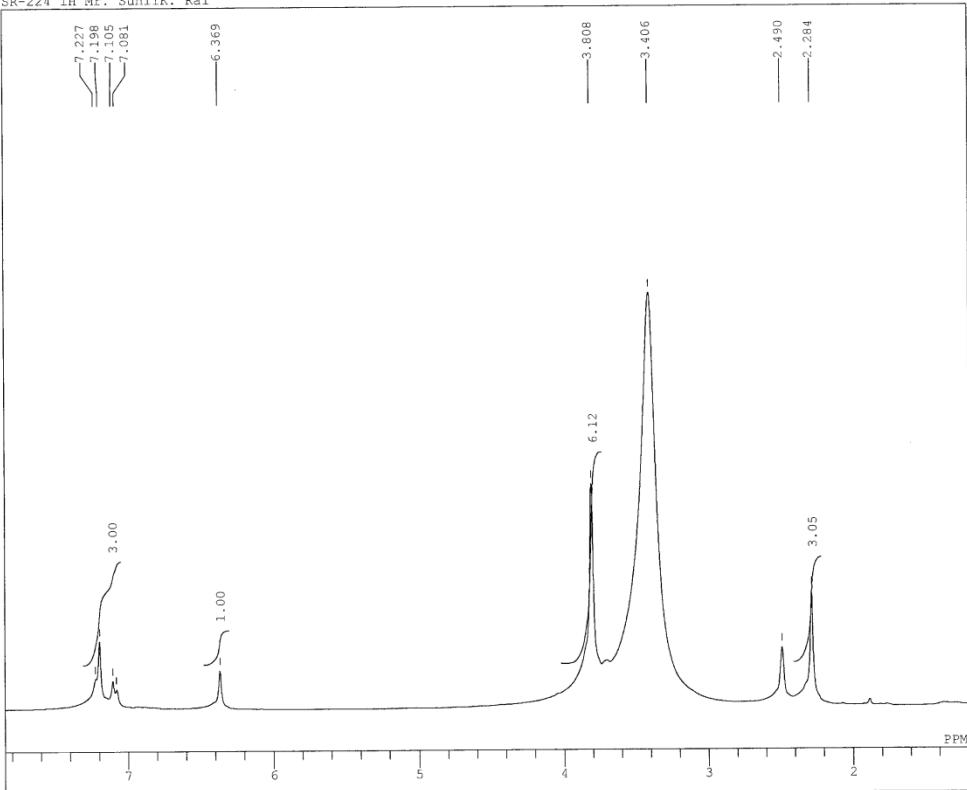
C:\WINNMR98\Data\SR-218-U\_13C1BCM\_E7.als  
 SR-218-U\_13C Mr. Sunil K. Rai



Compound (3a):  $^1\text{H}$  NMR



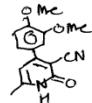
C:\Sunil Rai\SR-224\_1H.als  
 SR-224\_1H Mr. SunilK. Rai



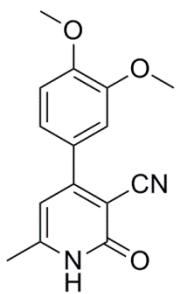
JEOL AL300 FTNMR  
 CHEMISTRY DEPARTMENT  
 Banaras Hindu University,  
 VARANASI-221005

Operator : Nagendra Kumar  
 Shishir Singh

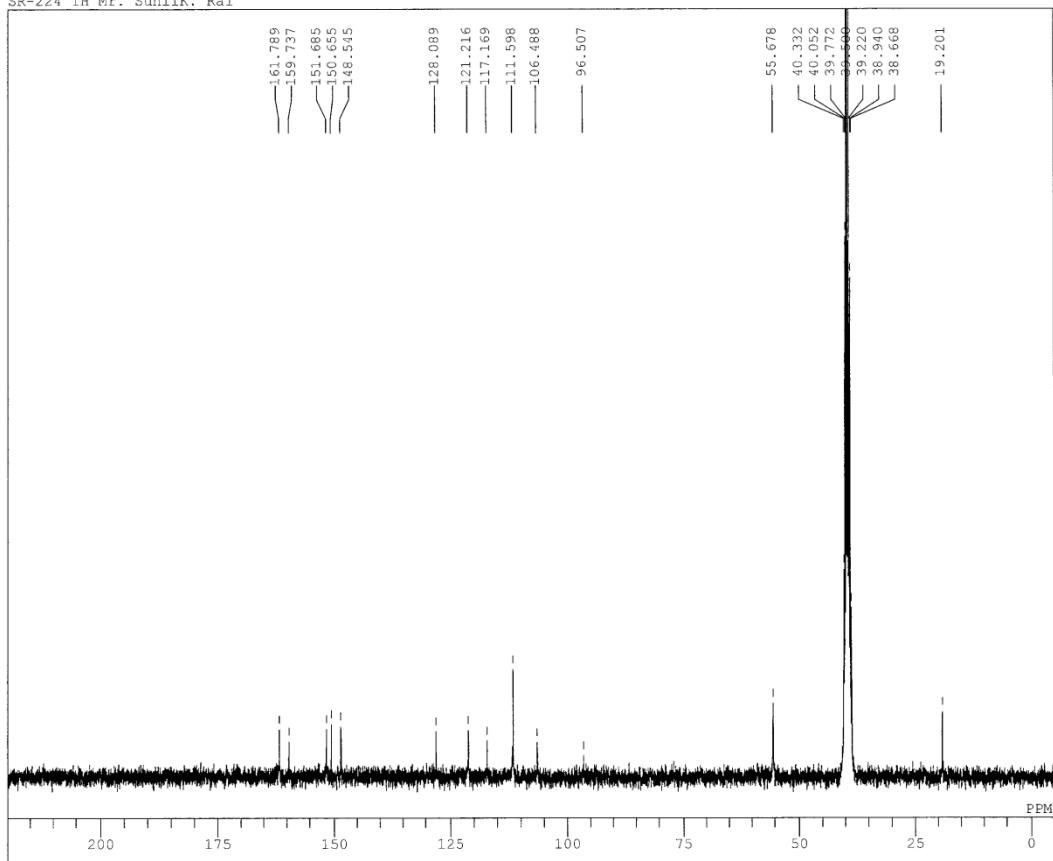
DFILE C:\Sunil Rai\SR-224\_1H.  
 COMNT SR-224\_1H Mr. SunilK. I  
 DATIM Fri Nov 29 13:23:51 20:  
 ORNUC 1H  
 EXMOD NON  
 OEMRQ 300.40 MHz  
 OBSET 130.00 kHz  
 OBFIN 1150.0 Hz  
 POINT 32768  
 FREQU 6016.8 Hz  
 SCANS 32  
 ACQTM 5.446 sec  
 PD 1.547 sec  
 PW1 5.6 us  
 IRNUC 1H  
 CTEMP 18.4 c  
 SLVNT DMSO  
 EXREF 2.49 ppm  
 BF 1.20 Hz  
 RGAIN 14



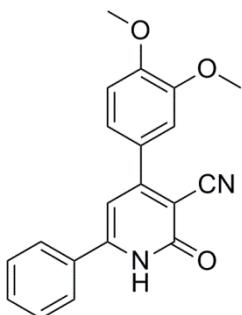
Compound (3a):  $^{13}\text{C}$  NMR



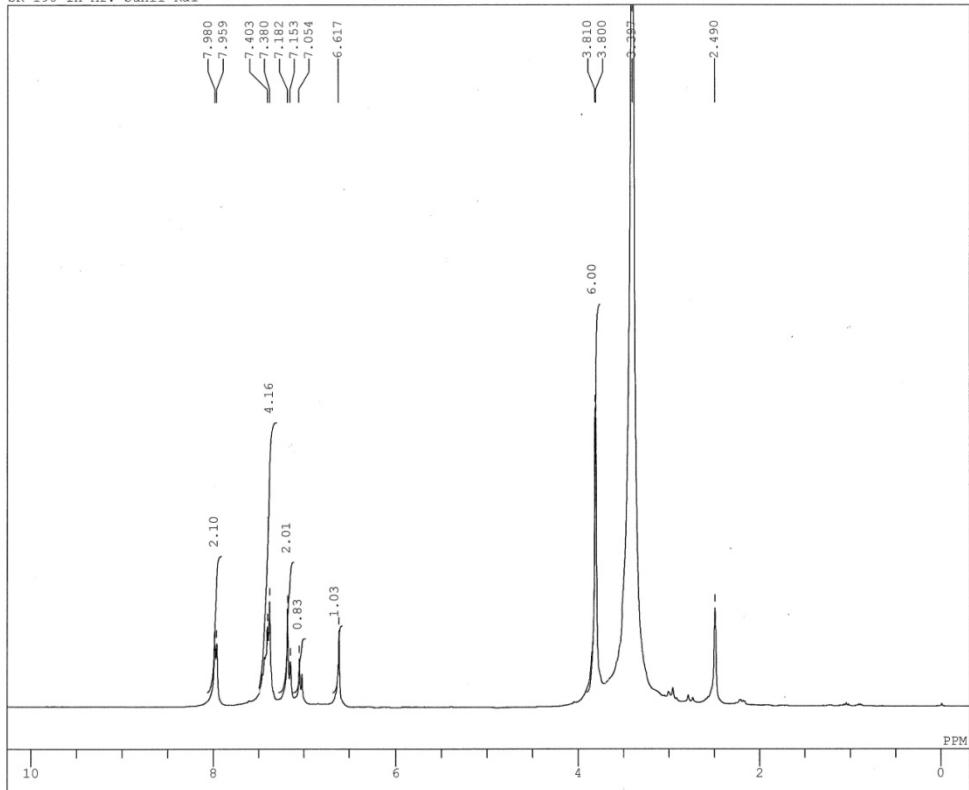
C:\WINNMR98\Data\SR-224\_1H2BCM\_E3.als  
SR-224\_1H Mr. SunilK. Rai



Compound (3b):  $^1\text{H}$  NMR



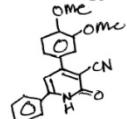
C:\Sunil Rai\SR-198\_1H.als  
SR-198\_1H Mr. Sunil Rai



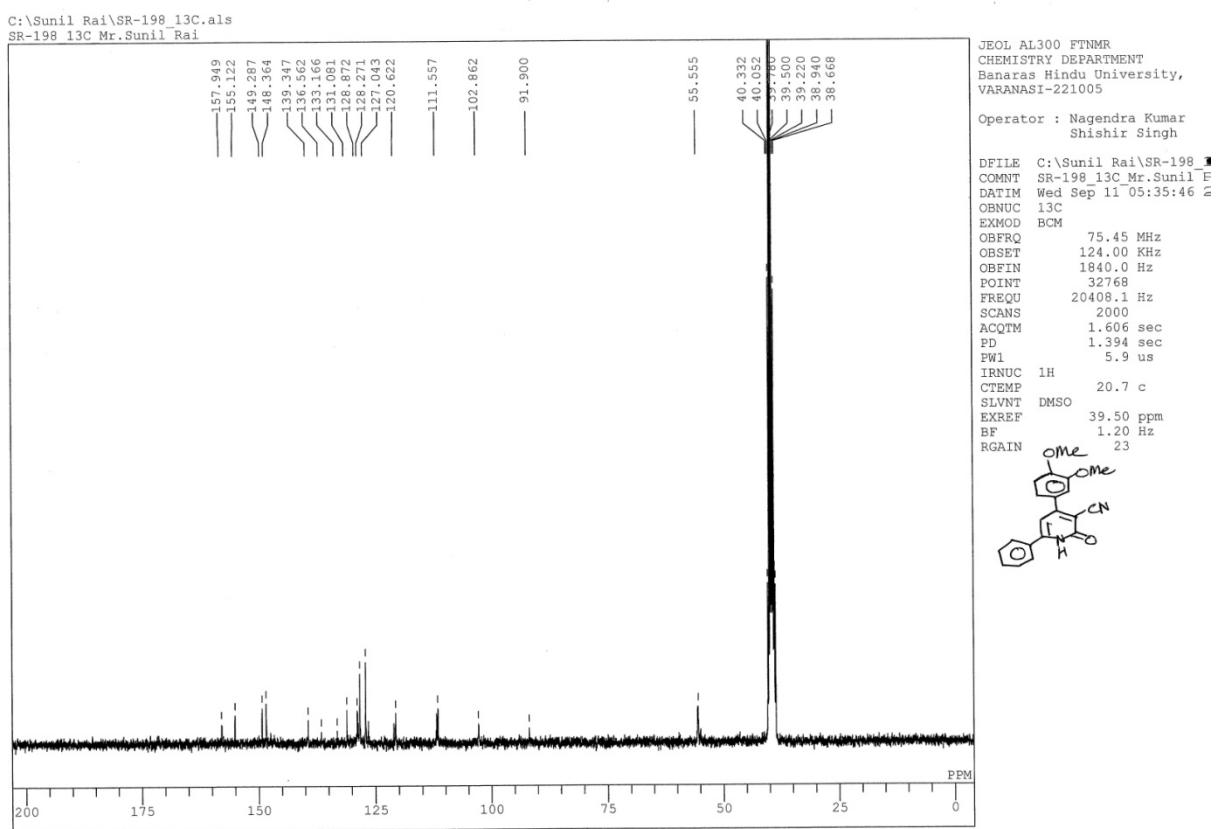
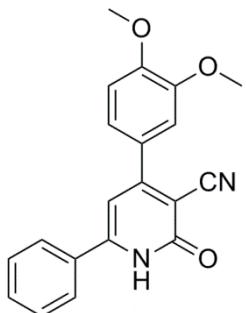
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

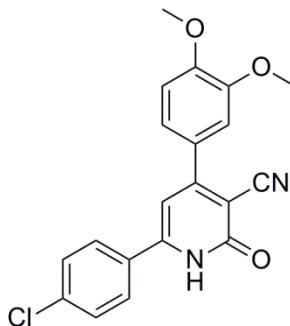
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COMNT SR-198\_1H Mr. Sunil Rai:  
DATIM Tue Sep 10 12:25:23 20:  
OBNUC 1H  
EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 9505.7 Hz  
SCANS 65  
ACQTM 3.447 sec  
PD 1.547 sec  
PW1 5.2 us  
IRNUC 1H  
CTEMP 20.8 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 1.20 Hz  
RGAIN 16



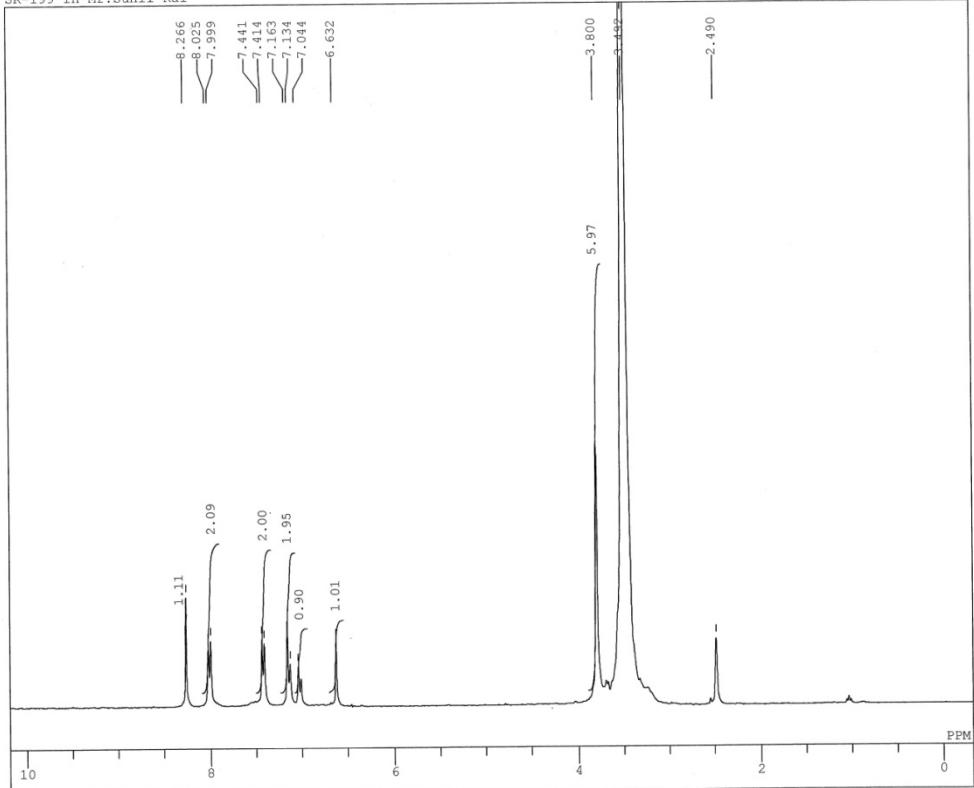
### Compound (3b): $^{13}\text{C}$ NMR



Compound (3c):  $^1\text{H}$  NMR

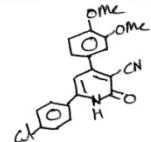


C:\Sunil Rai\SR-199 1H.als  
SR-199 1H Mr.Sunil Rai

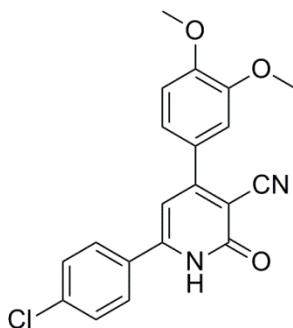


JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005  
Operator : Nagendra Kumar  
Shishir Singh

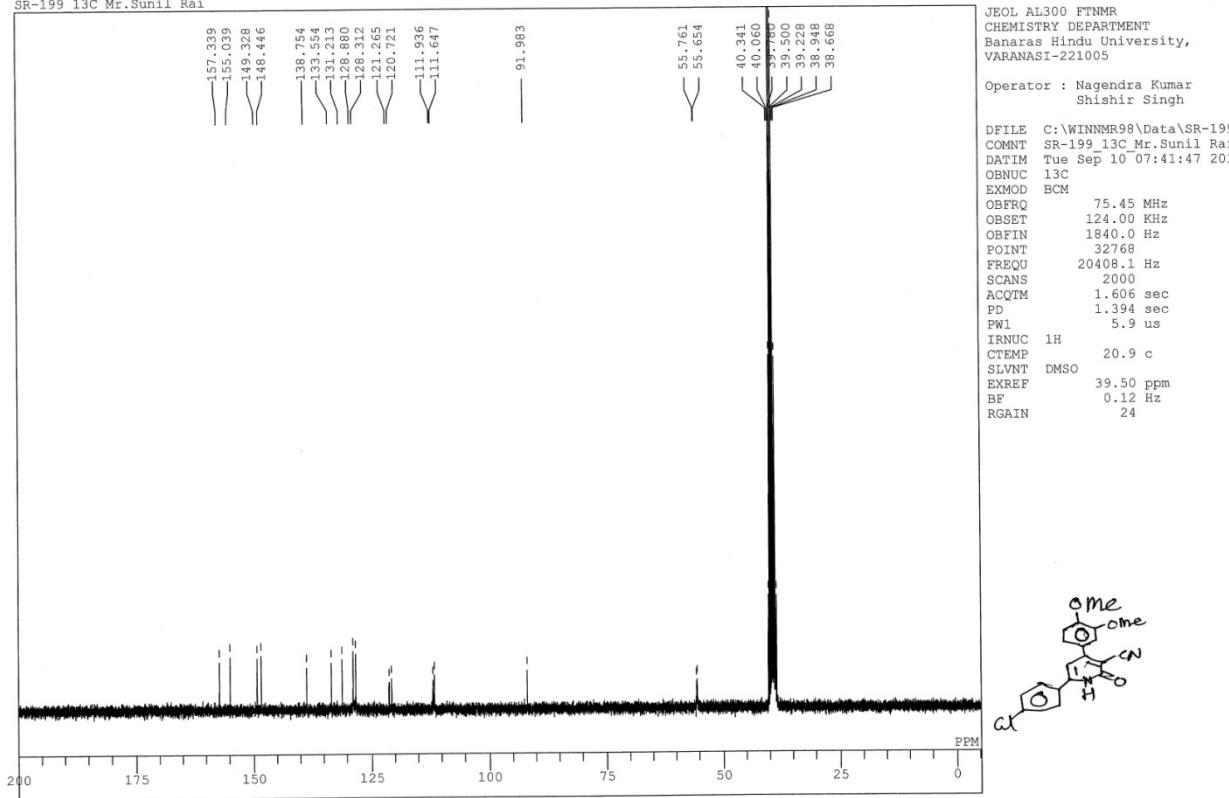
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COMNT SR-199\_1H Mr.Sunil Rai  
DATIM Wed Sep 11 14:33:04 20:  
OBNUC 1H  
EXMOD NON  
OBFRQ 300.40 MHz  
OBSET 130.00 kHz  
OBFIN 1150.0 Hz  
POINT 32768  
FREQU 9505.7 Hz  
SCANS 20  
ACQTM 3.447 sec  
PD 1.547 sec  
PW1 5.2 us  
IRNUC 1H  
CTEMP 22.6 c  
SLVNT DMSO  
EXREF 2.49 ppm  
BF 1.20 Hz  
RGAIN 11



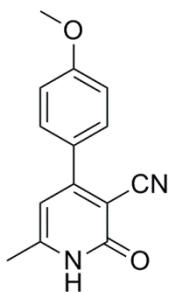
Compound (3c):  $^{13}\text{C}$  NMR



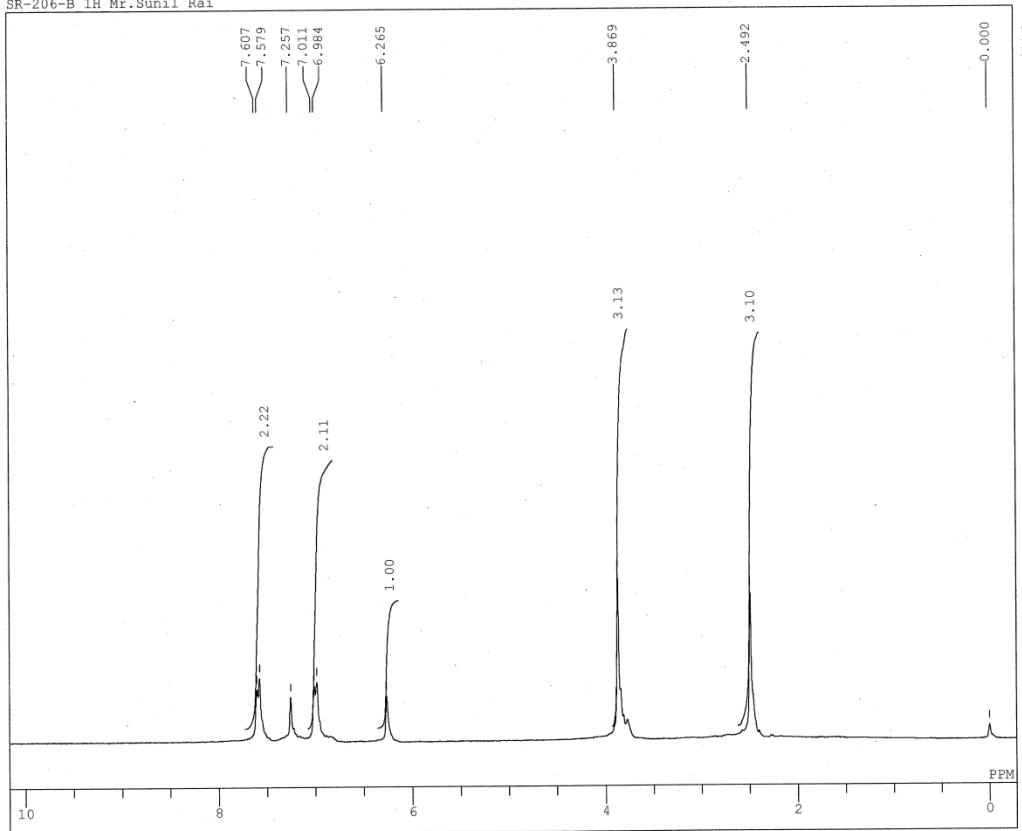
C:\WINNMR98\Data\SR-199\_1H2BCM\_E7.als  
SR-199  $^{13}\text{C}$  Mr.Sunil Rai



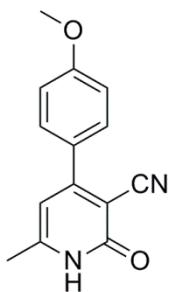
Compound (4a):  $^1\text{H}$  NMR



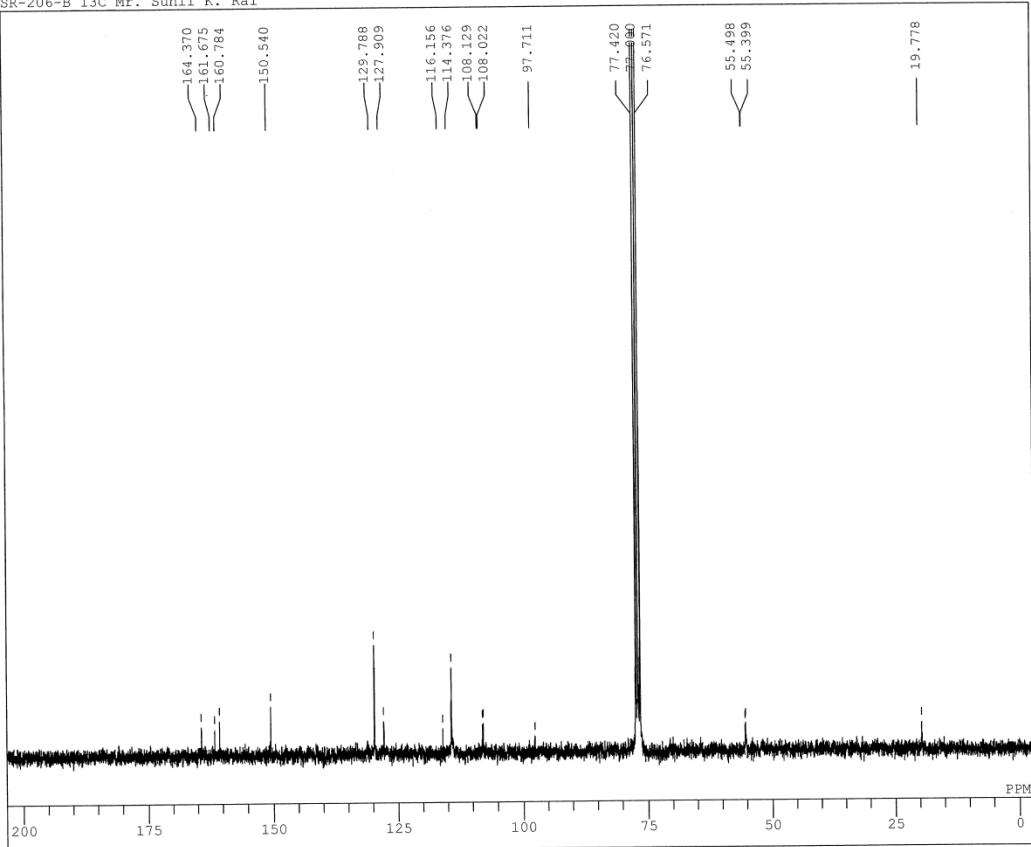
C:\Sunil Rai\SR-206-B\_1H.als  
SR-206-B\_1H Mr.Sunil Rai



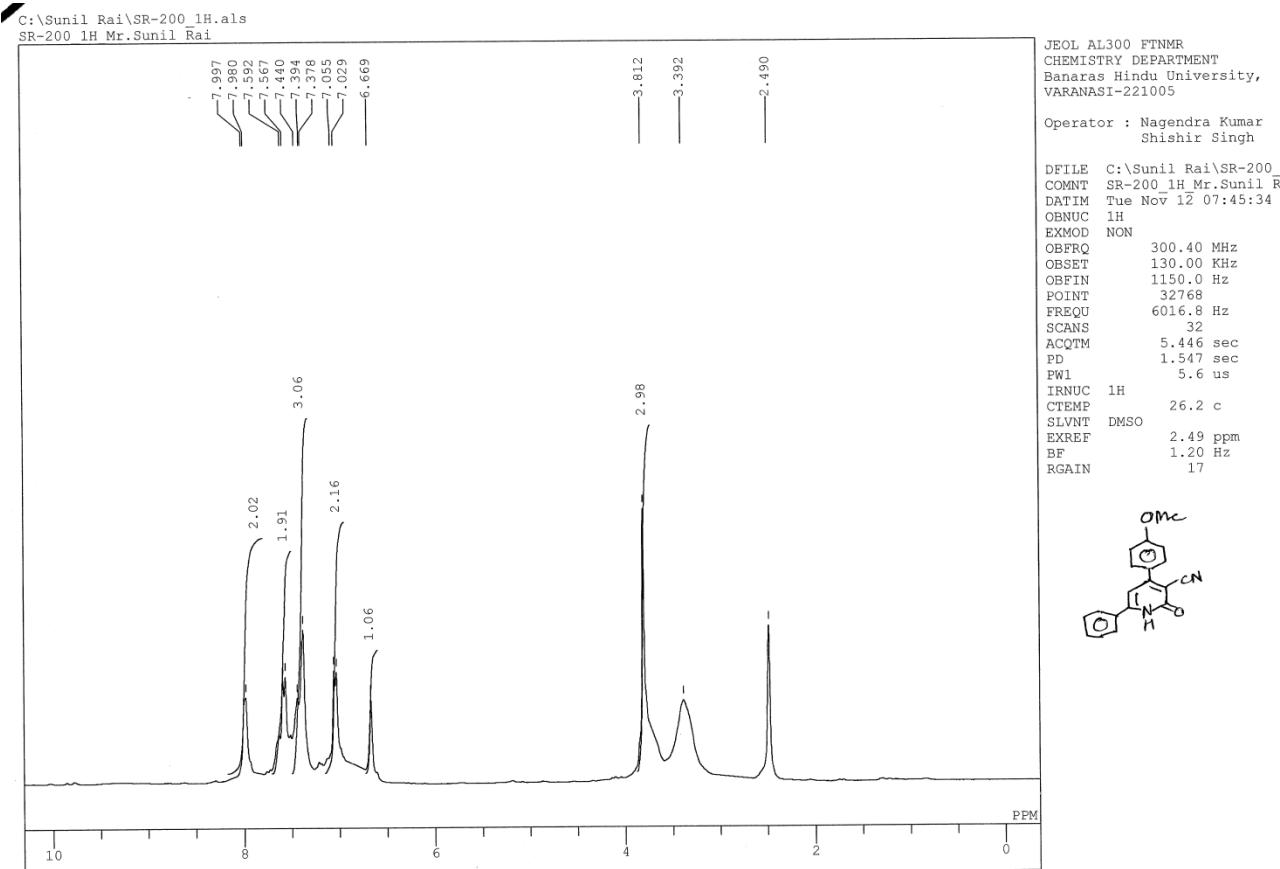
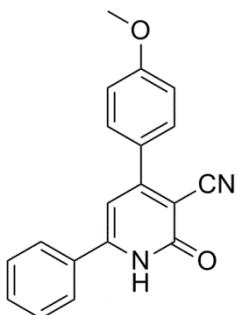
Compound (4a):  $^{13}\text{C}$  NMR



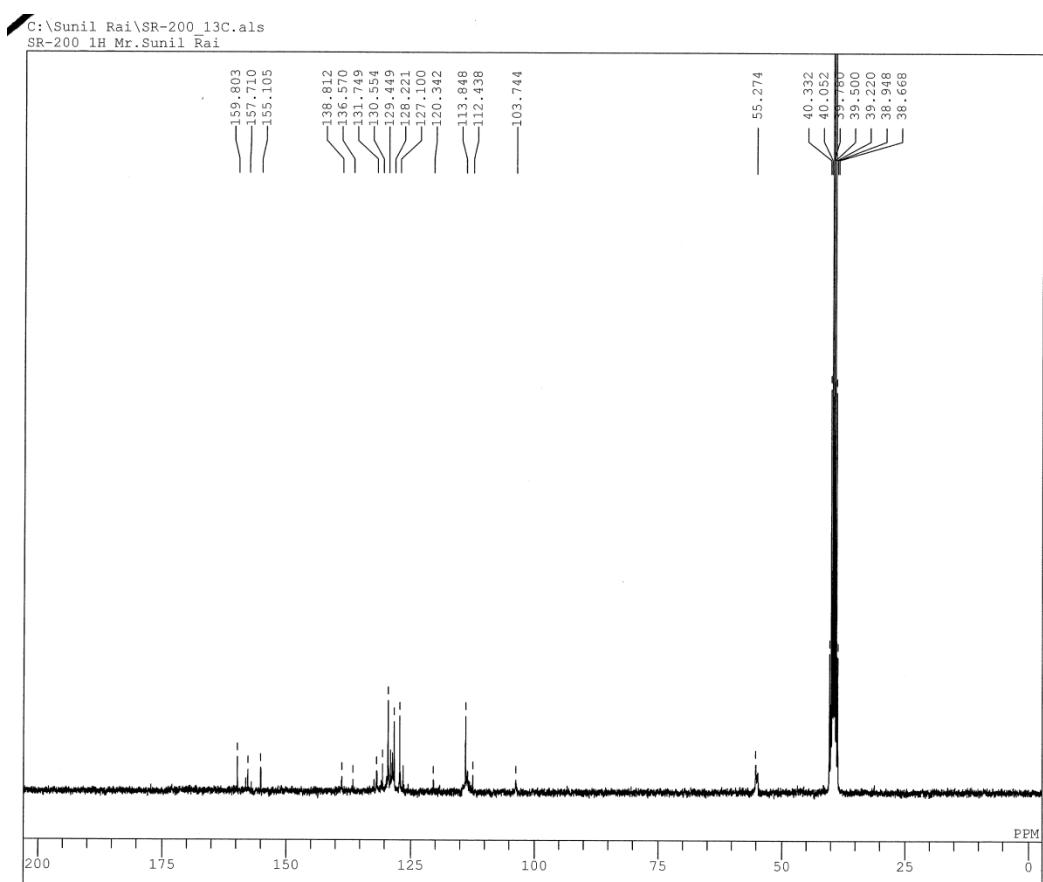
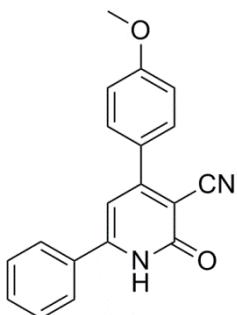
C:\WINNNMR98\Data\SR-206-B\_13C1BCM\_E3.als  
 SR-206-B 13C Mr. Sunil K. Rai



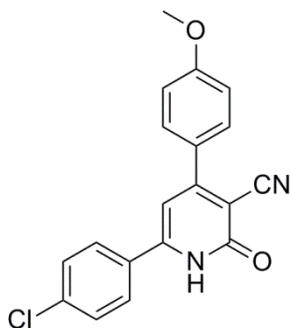
Compound (4b):  $^1\text{H}$  NMR



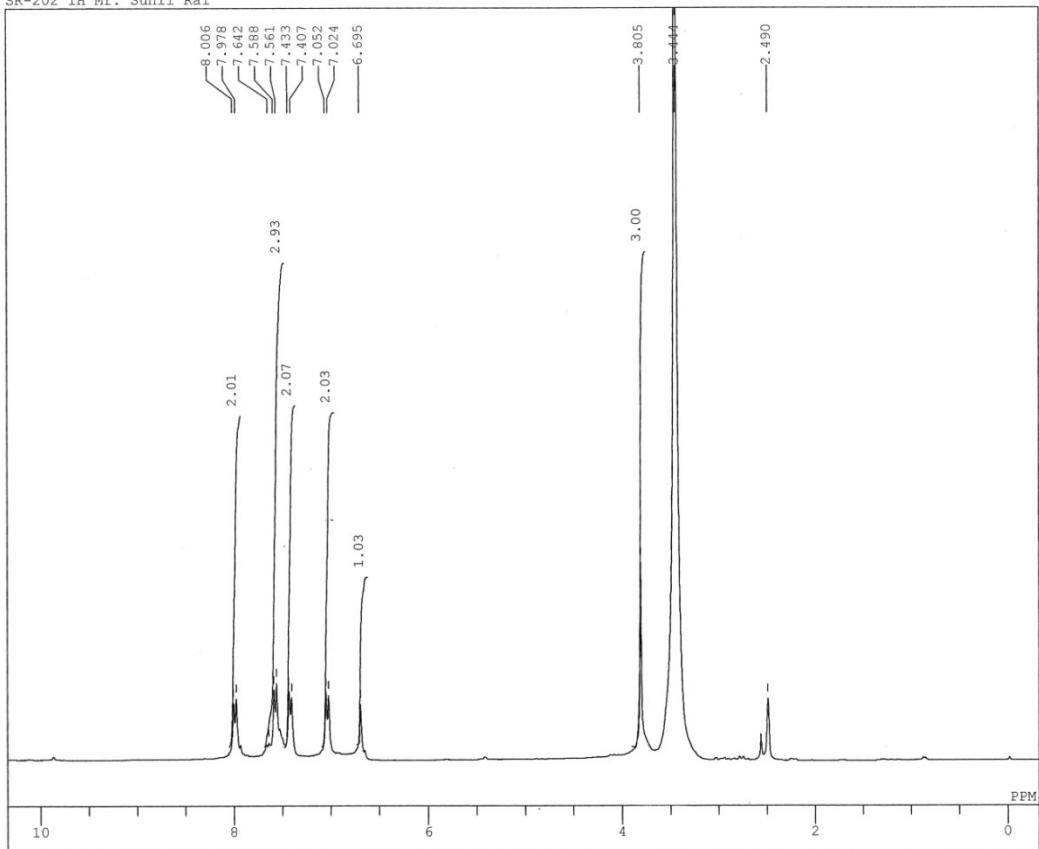
Compound (4b):  $^{13}\text{C}$  NMR



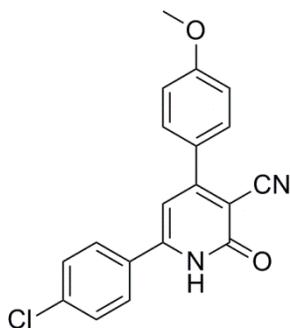
Compound (4c):  $^1\text{H}$  NMR



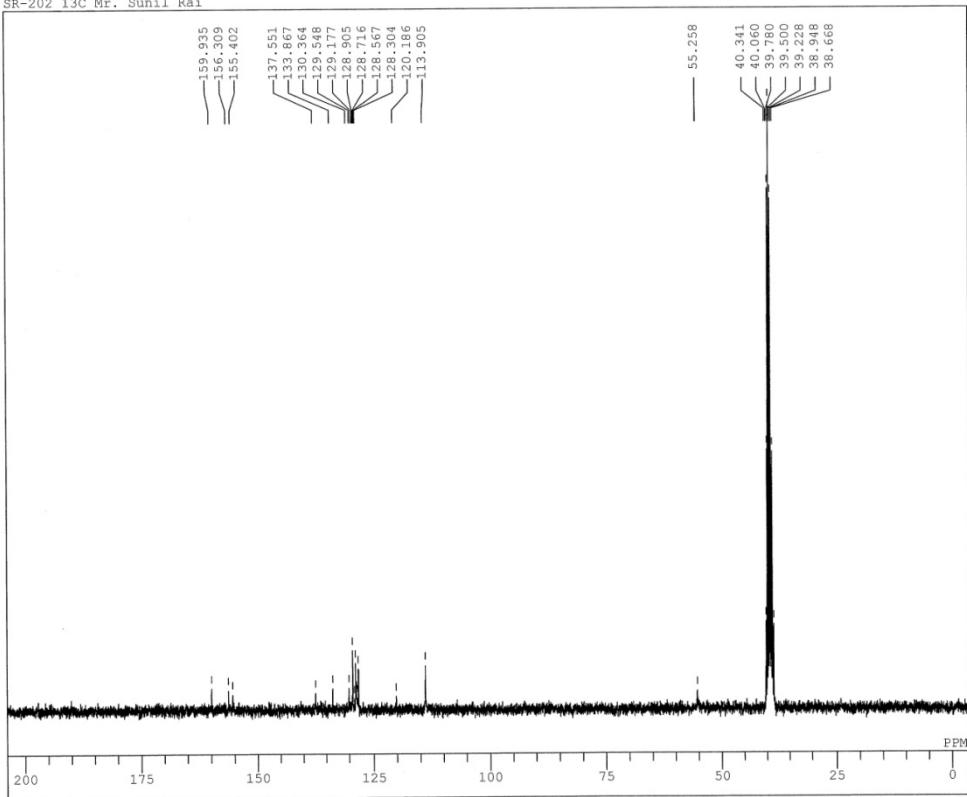
C:\Sunil Rai\SR-202\_1H.als  
SR-202 1H Mr. Sunil Rai



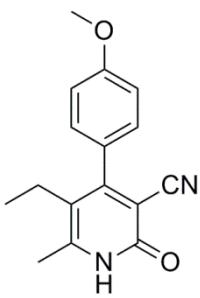
Compound (4c):  $^{13}\text{C}$  NMR



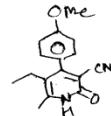
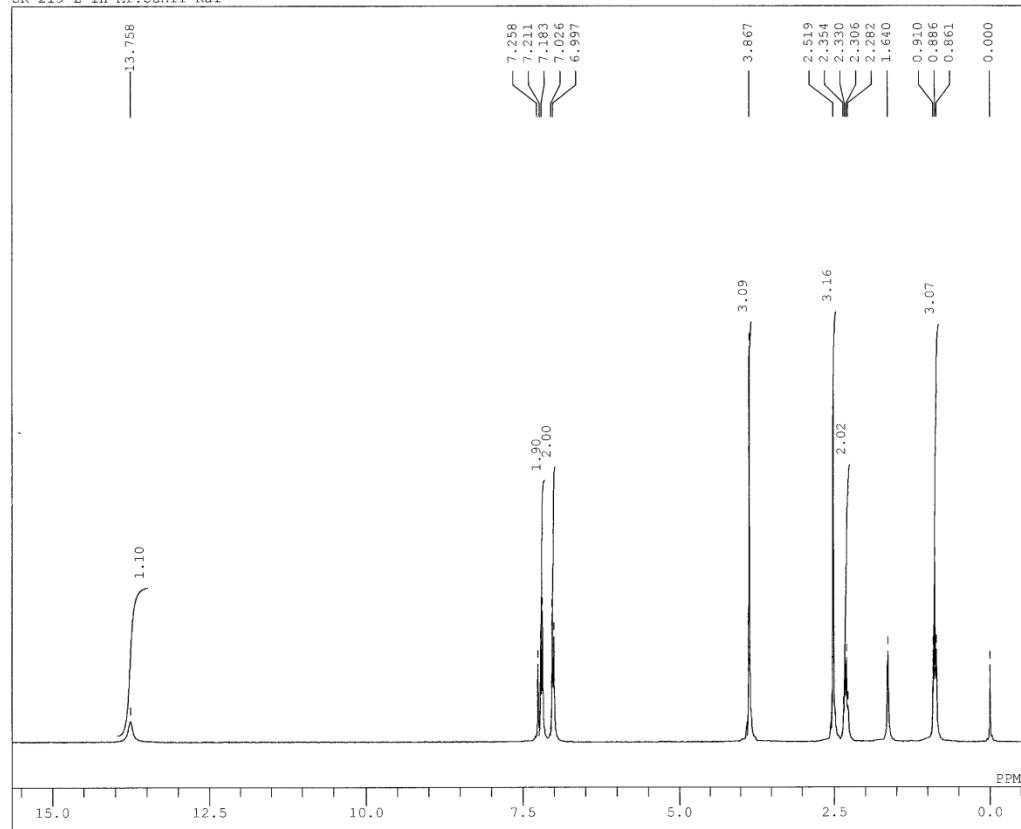
C:\Sunil Rai\SR-202\_13C.als  
SR-202\_13C Mr. Sunil Rai



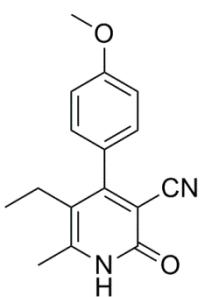
Compound (4d):  $^1\text{H}$  NMR



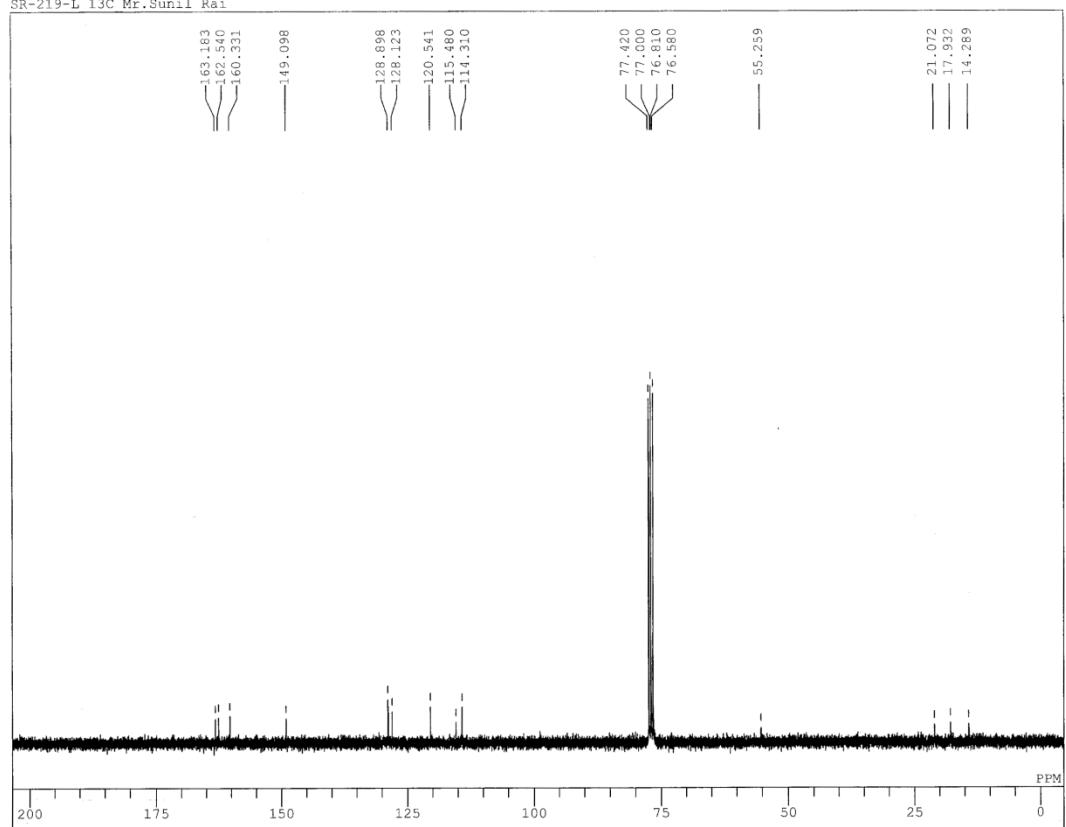
C:\WINNNMR98\COMMON\ DEFAULT.ALS  
SR-219-L 1H Mr. Sunil Rai



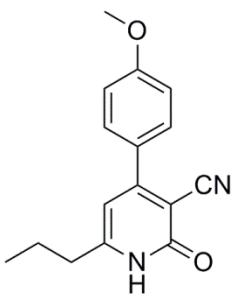
Compound (4d):  $^{13}\text{C}$  NMR



C:\Sunil Rai\SR-219-L 13C.als  
SR-219-L 13C Mr.Sunil Rai

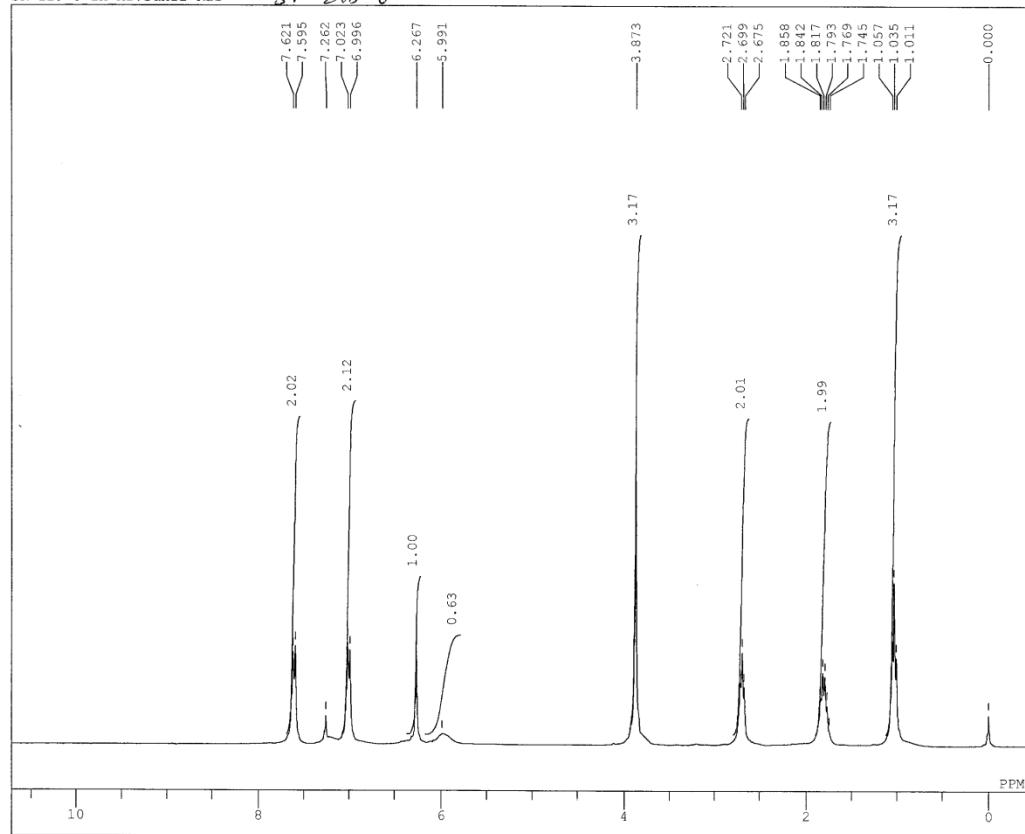


Compound (4e):  $^1\text{H}$  NMR



C:\Sunil Rai\SR-129\_U\_1H.als  
 SR-129\_U\_1H\_Mr.sunil Rai

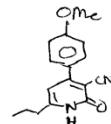
**SR-129-U**



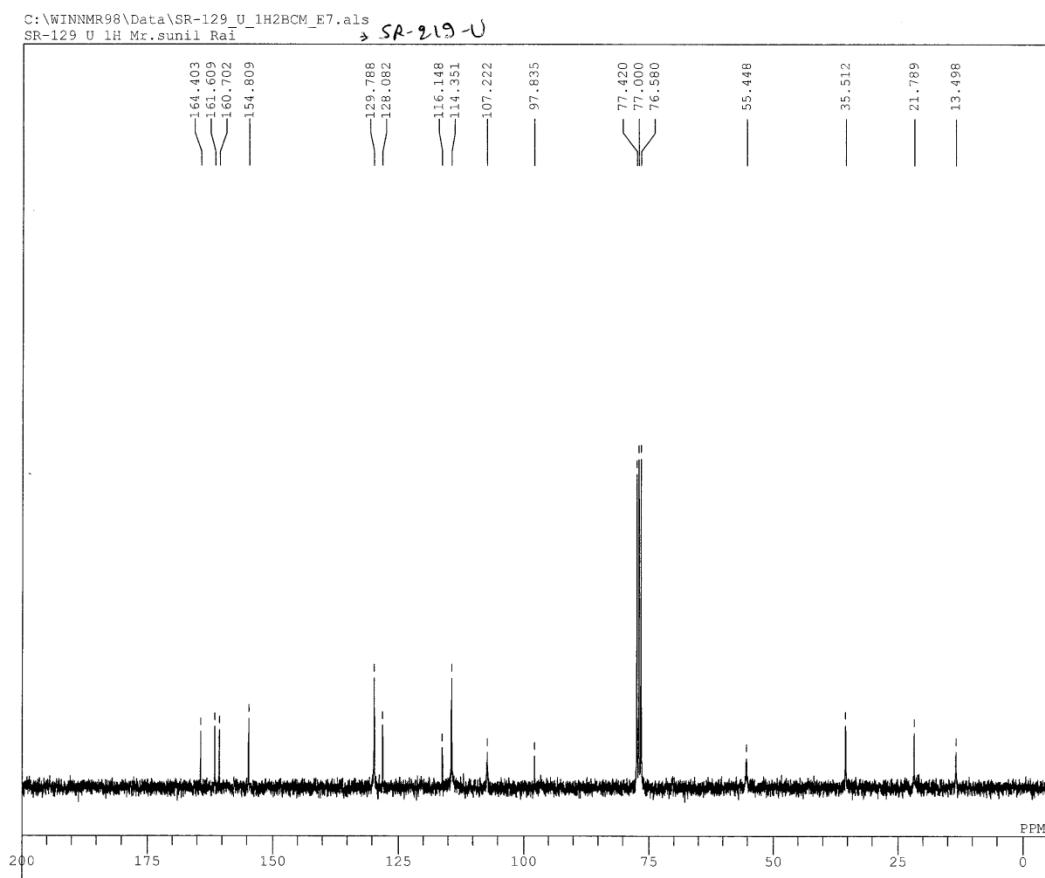
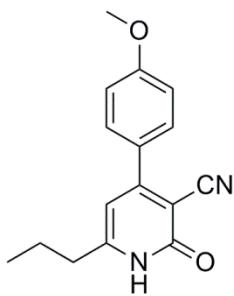
JEOL AL300 FTNMR  
 CHEMISTRY DEPARTMENT  
 Banaras Hindu University,  
 VARANASI-221005

Operator : Nagendra Kumar  
 Shishir Singh

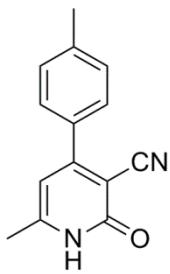
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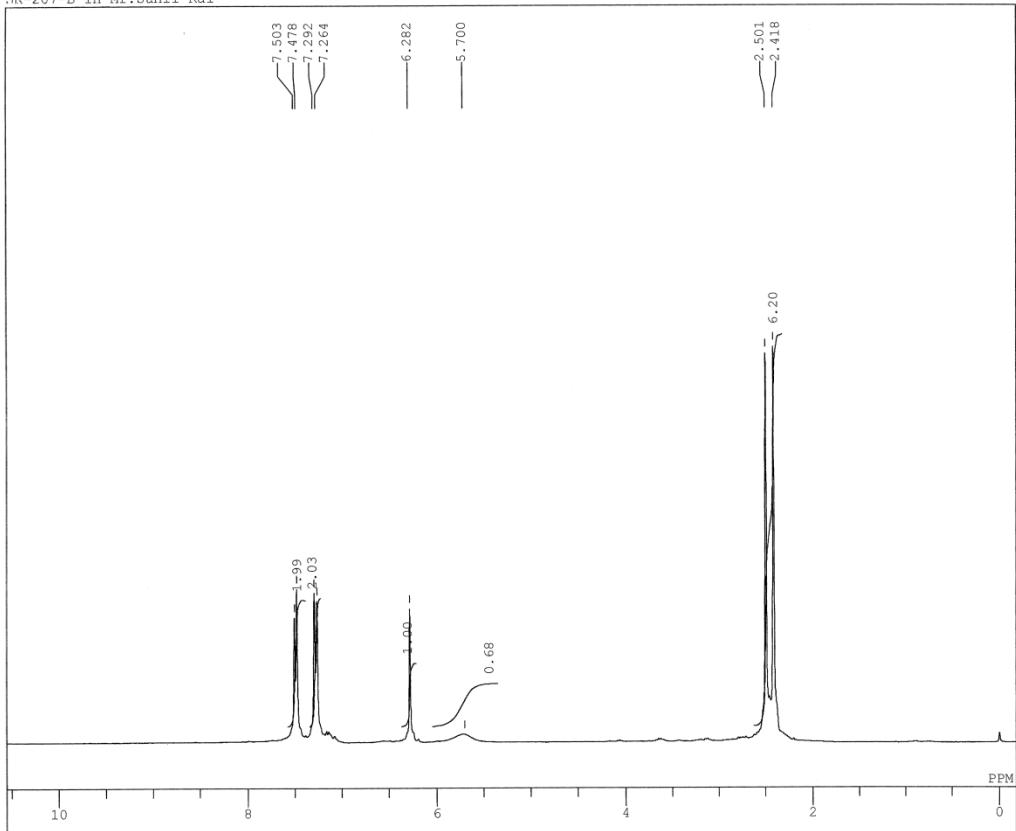
Compound (4e):  $^{13}\text{C}$  NMR



Compound (5a):  $^1\text{H}$  NMR



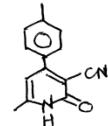
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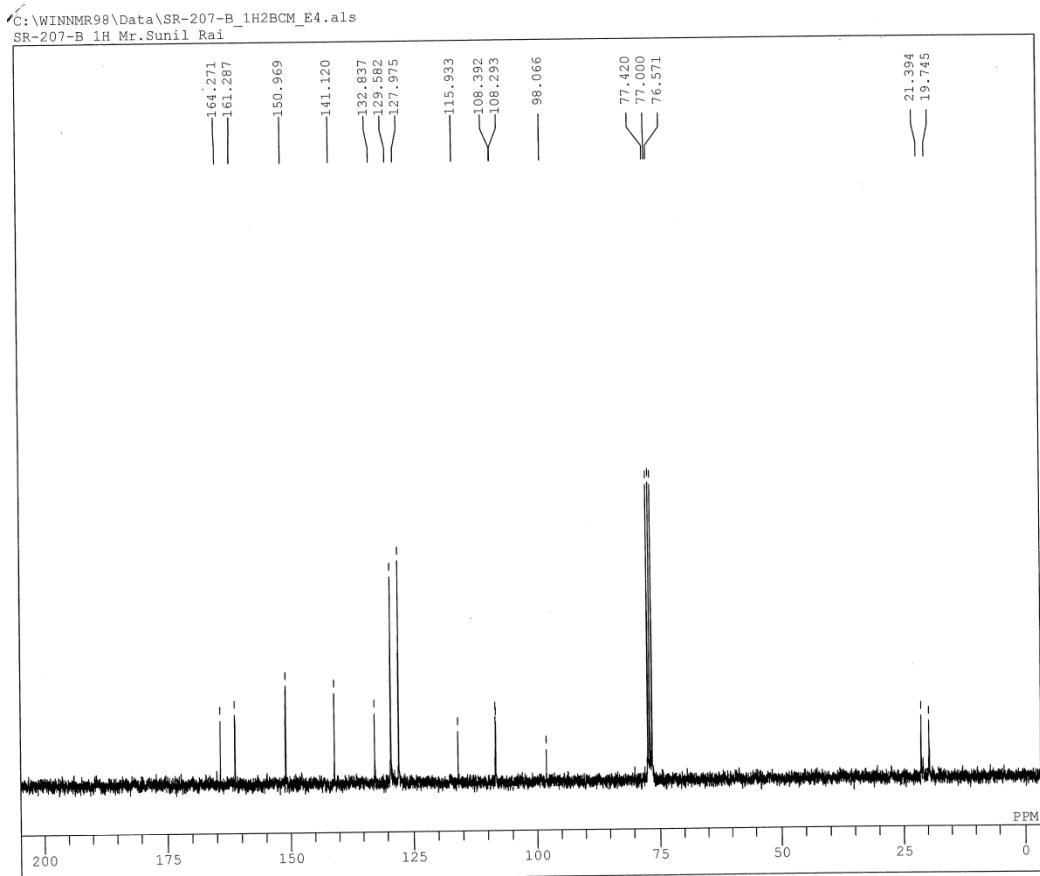
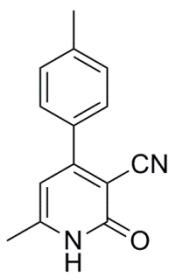
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

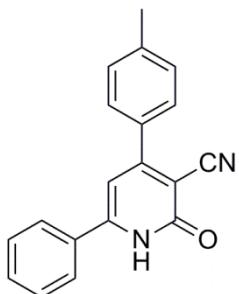
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RGAIN 19



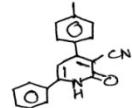
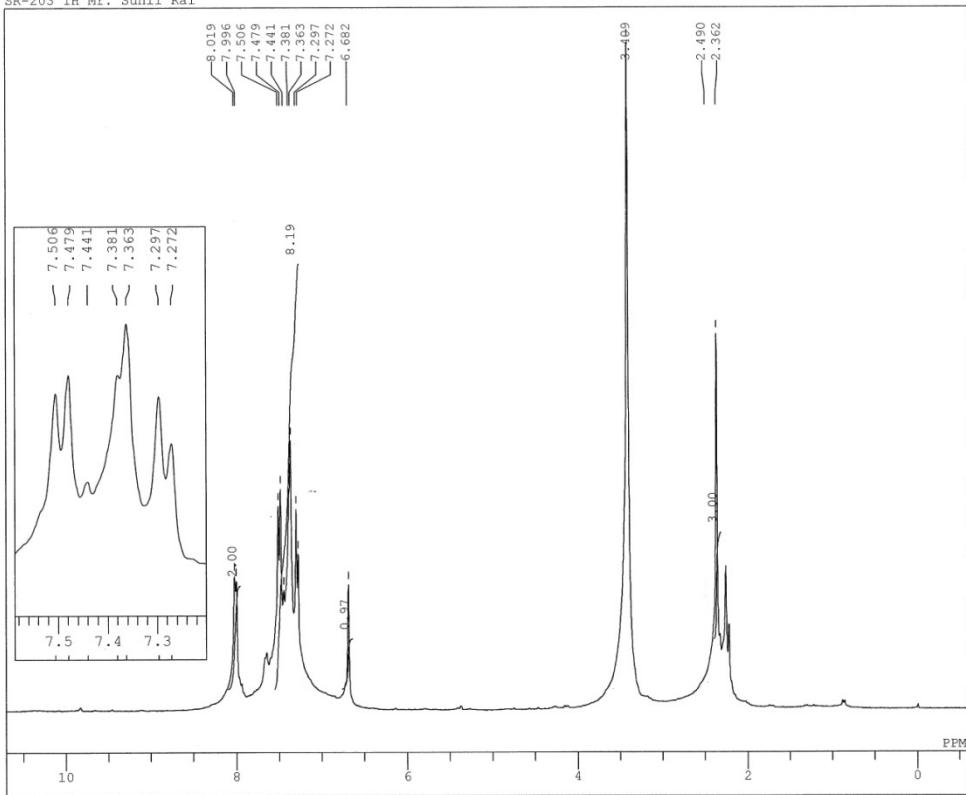
Compound (5a):  $^{13}\text{C}$  NMR



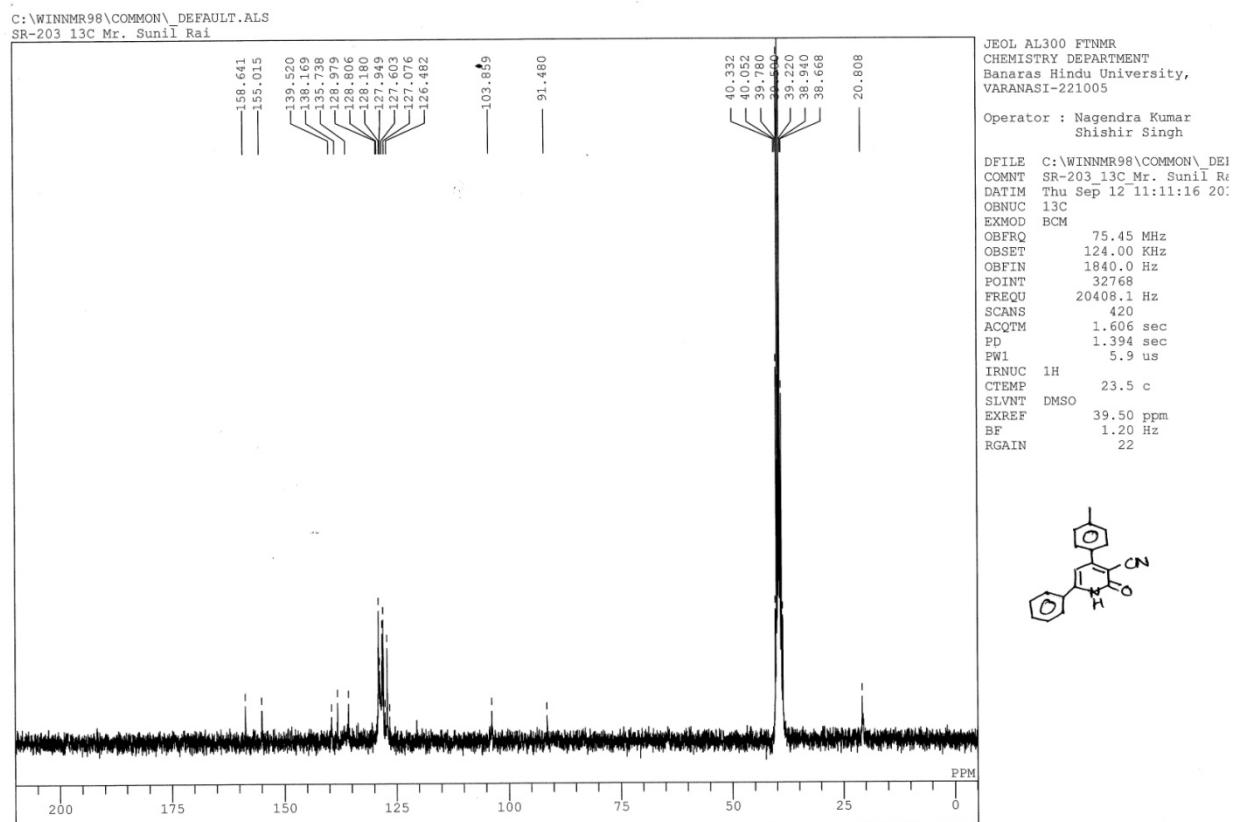
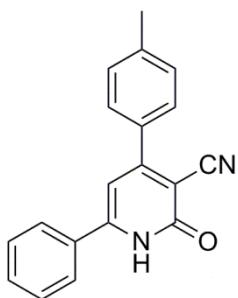
Compound (5b):  $^1\text{H}$  NMR



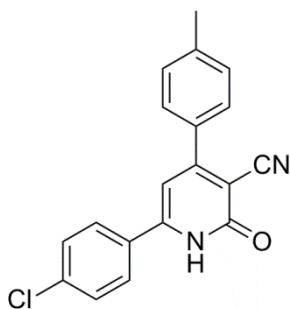
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SR-203 1H Mr. Sunil Rai



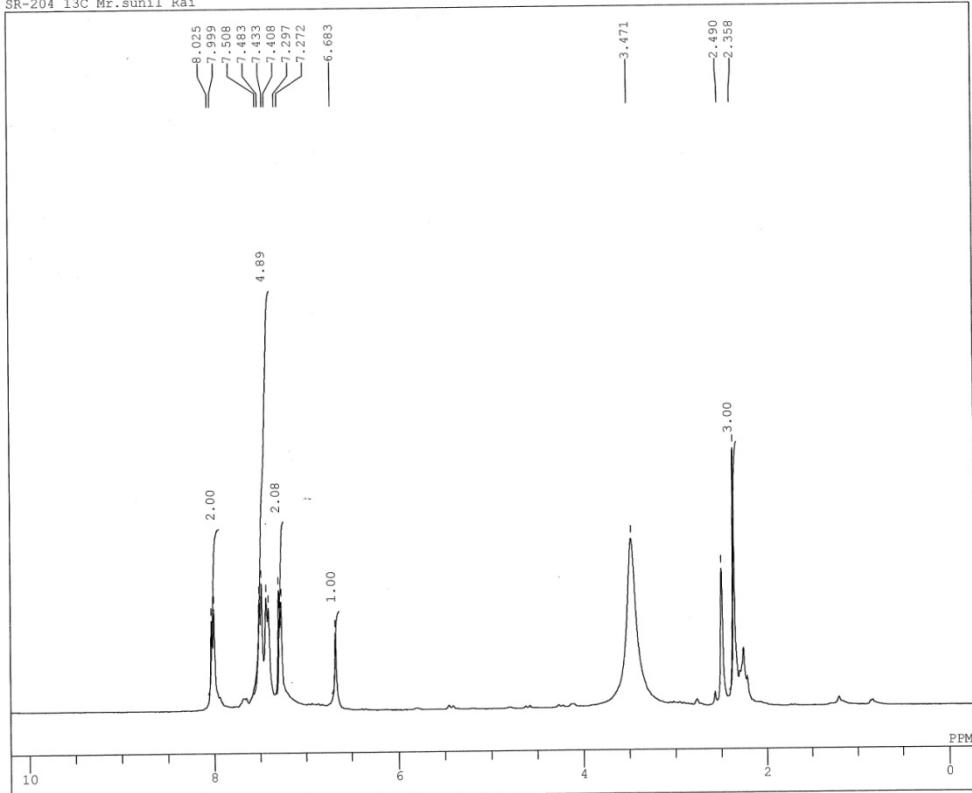
Compound (5b):  $^{13}\text{C}$  NMR



Compound (5c):  $^1\text{H}$  NMR



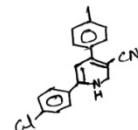
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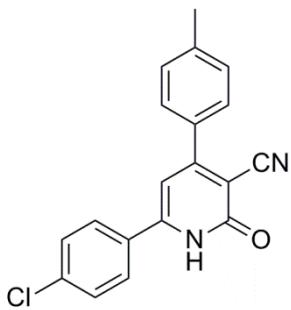
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

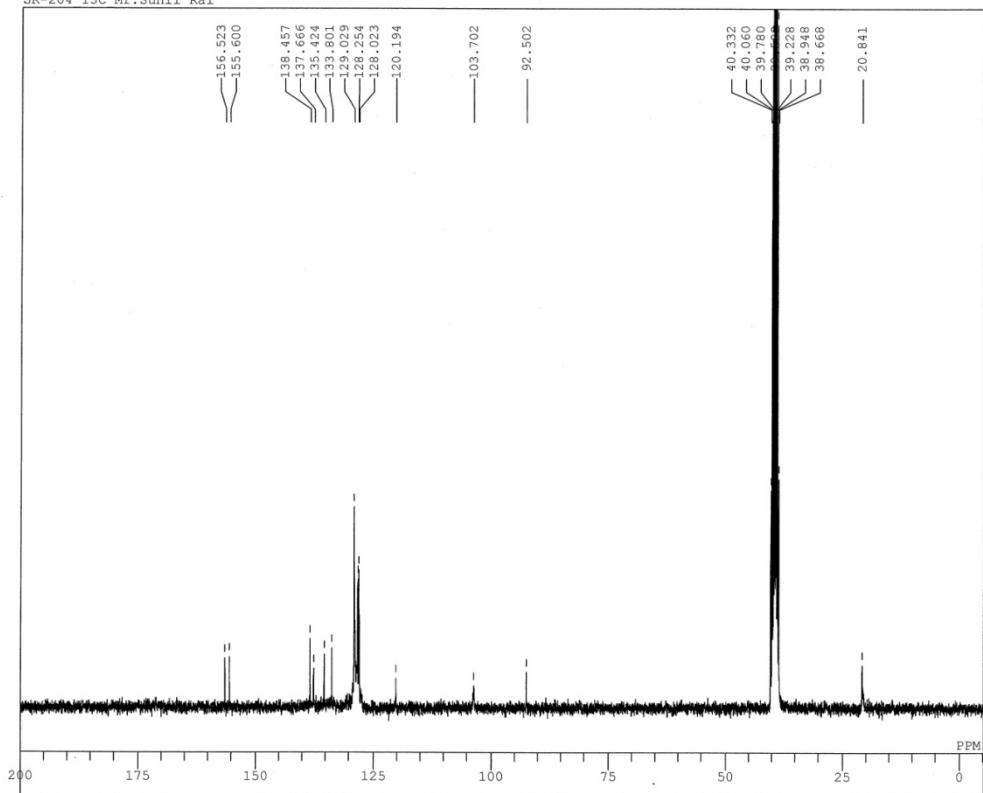
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SLVNT DMSO  
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BF 1.20 Hz  
RGAIN 17



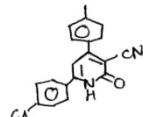
Compound (5c).<sup>13</sup>C NMR



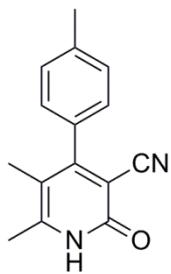
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SR-204 13C Mr.Sunil Rai



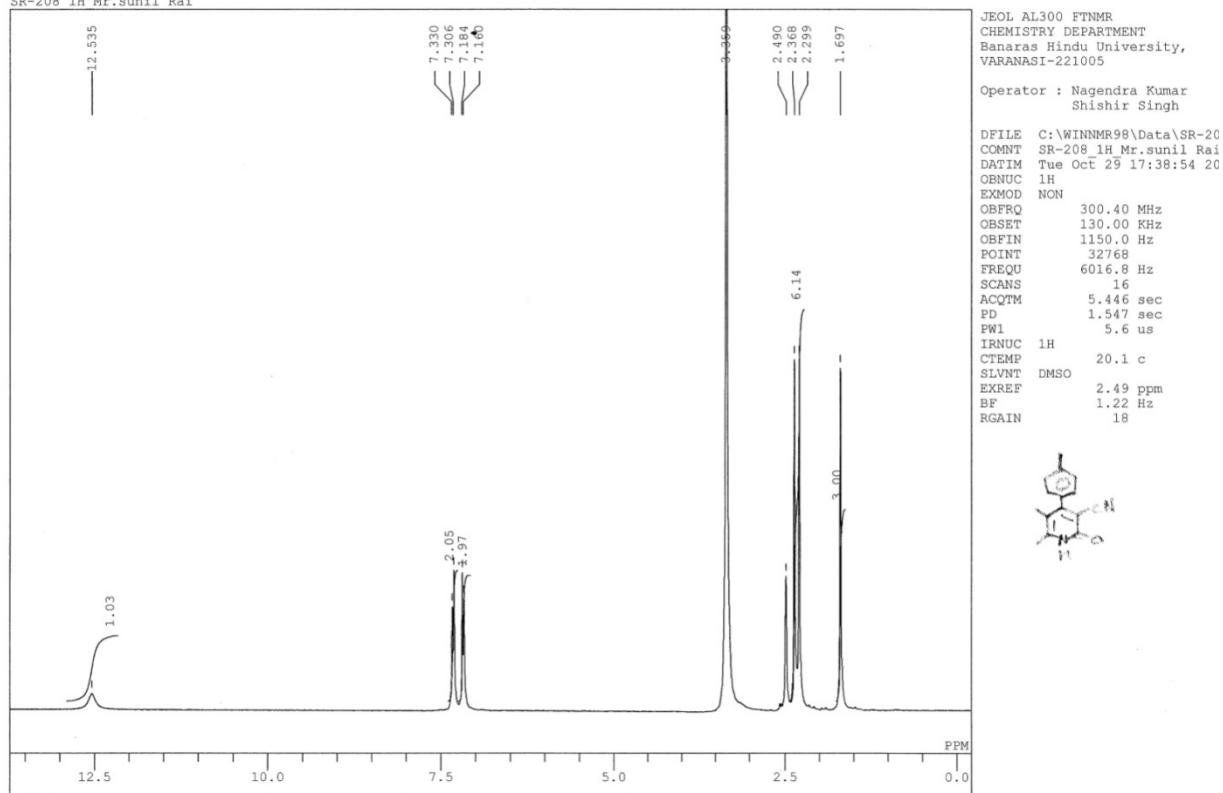
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005  
Operator : Nagendra Kumar  
Shishir Singh  
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PD 1.394 sec  
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SLVNT DMSO  
EXREF 39.50 ppm  
BF 1.20 Hz  
RGAIN 21



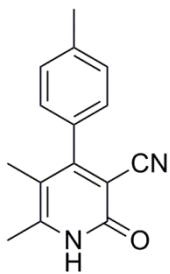
Compound (5d):  $^1\text{H}$  NMR



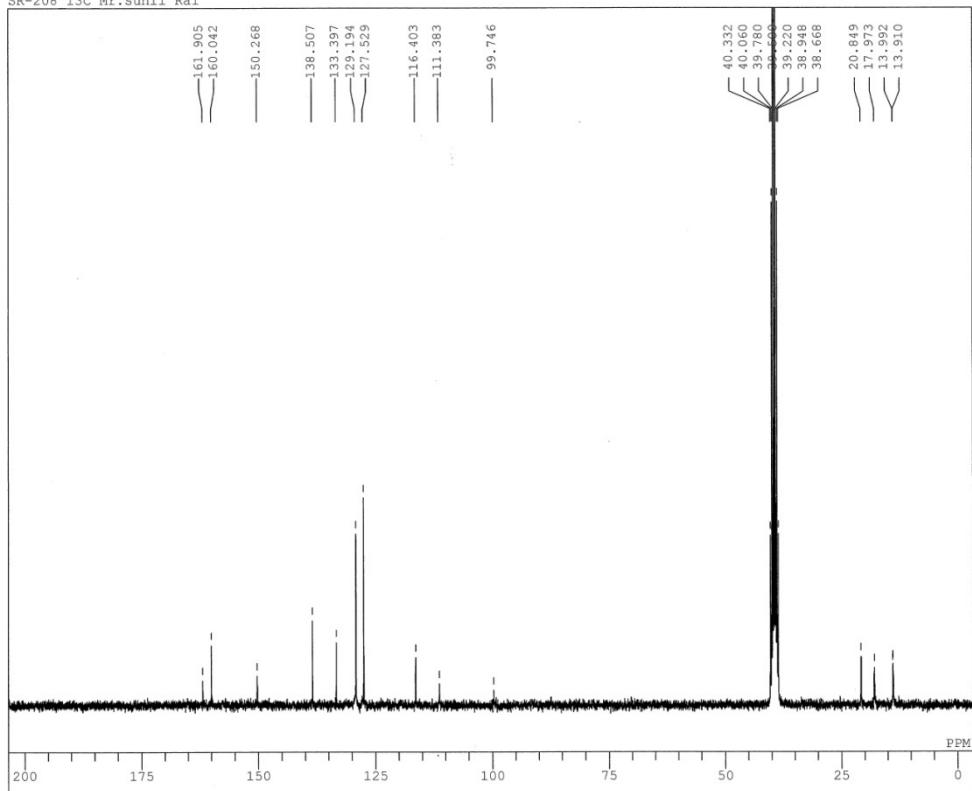
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SR-208 1H Mr.sunil Rai



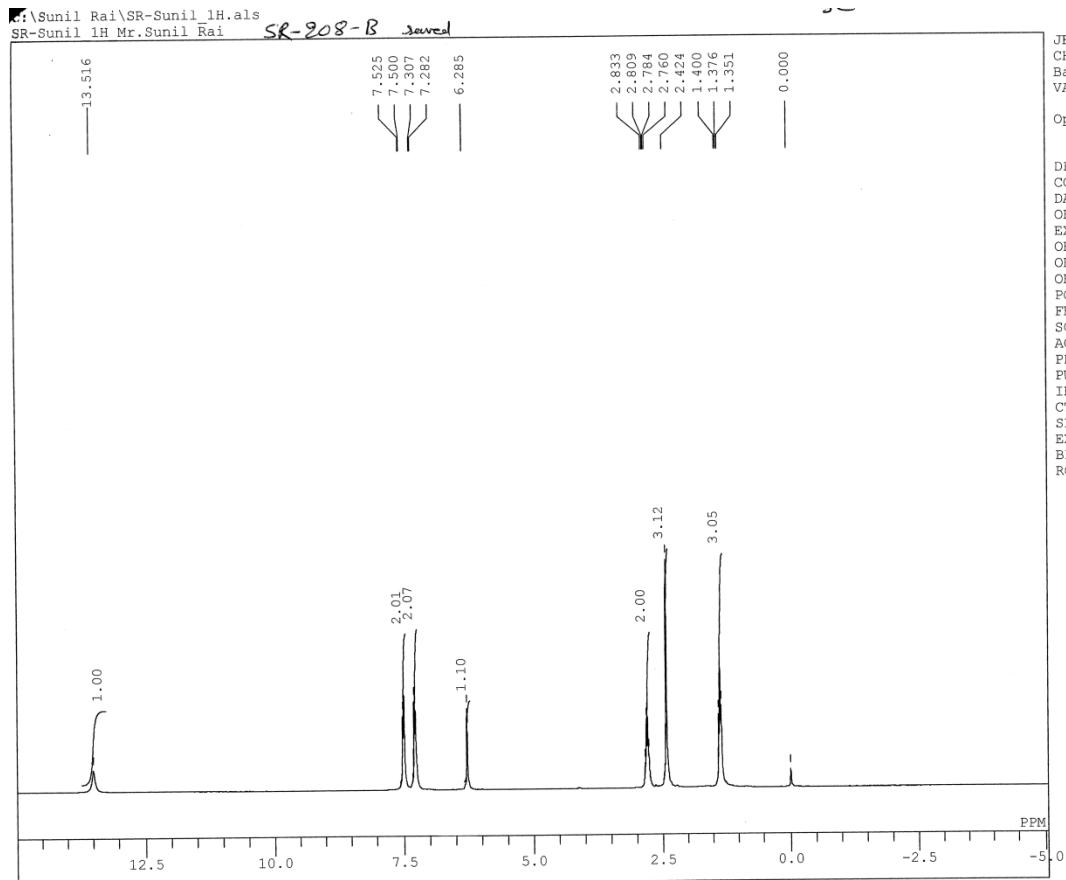
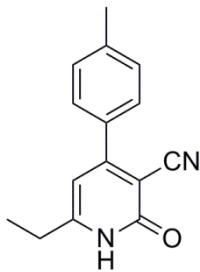
Compound (5d):  $^{13}\text{C}$  NMR



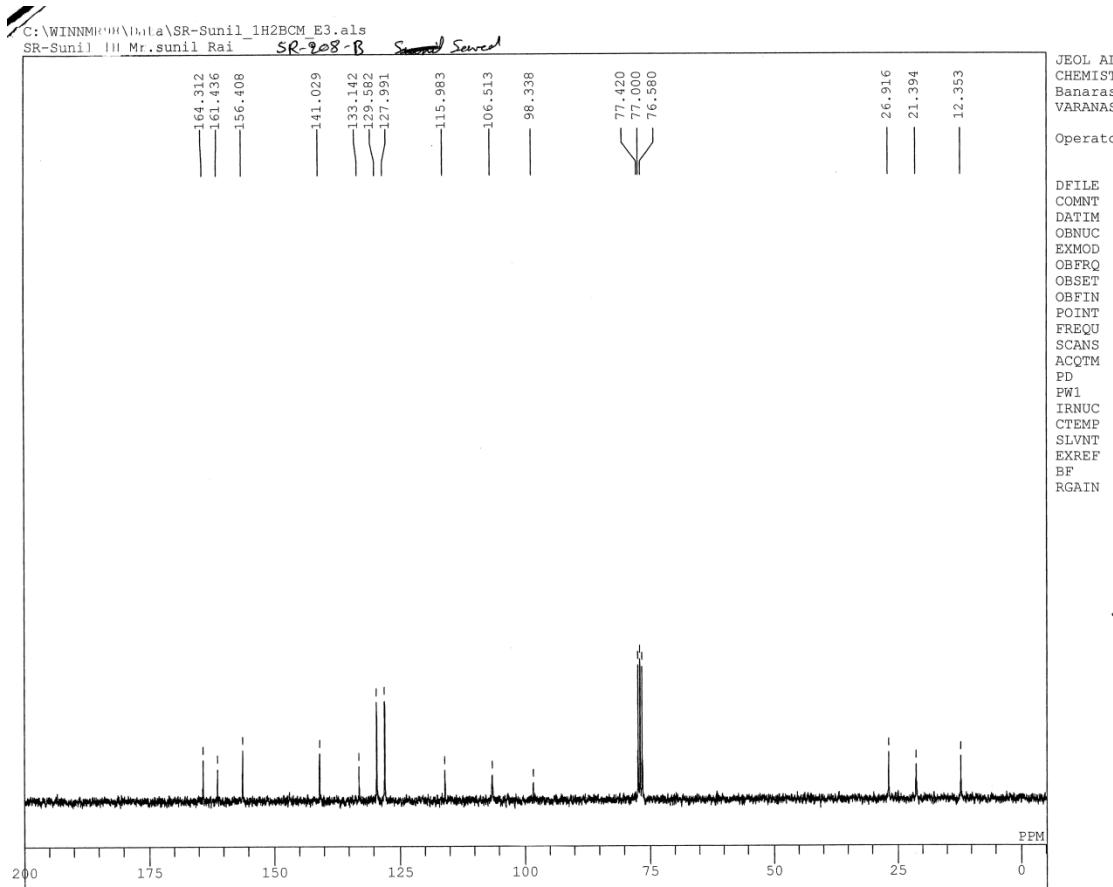
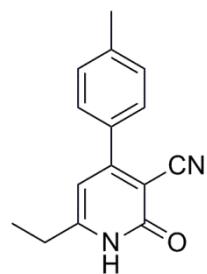
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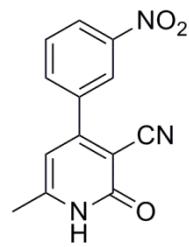
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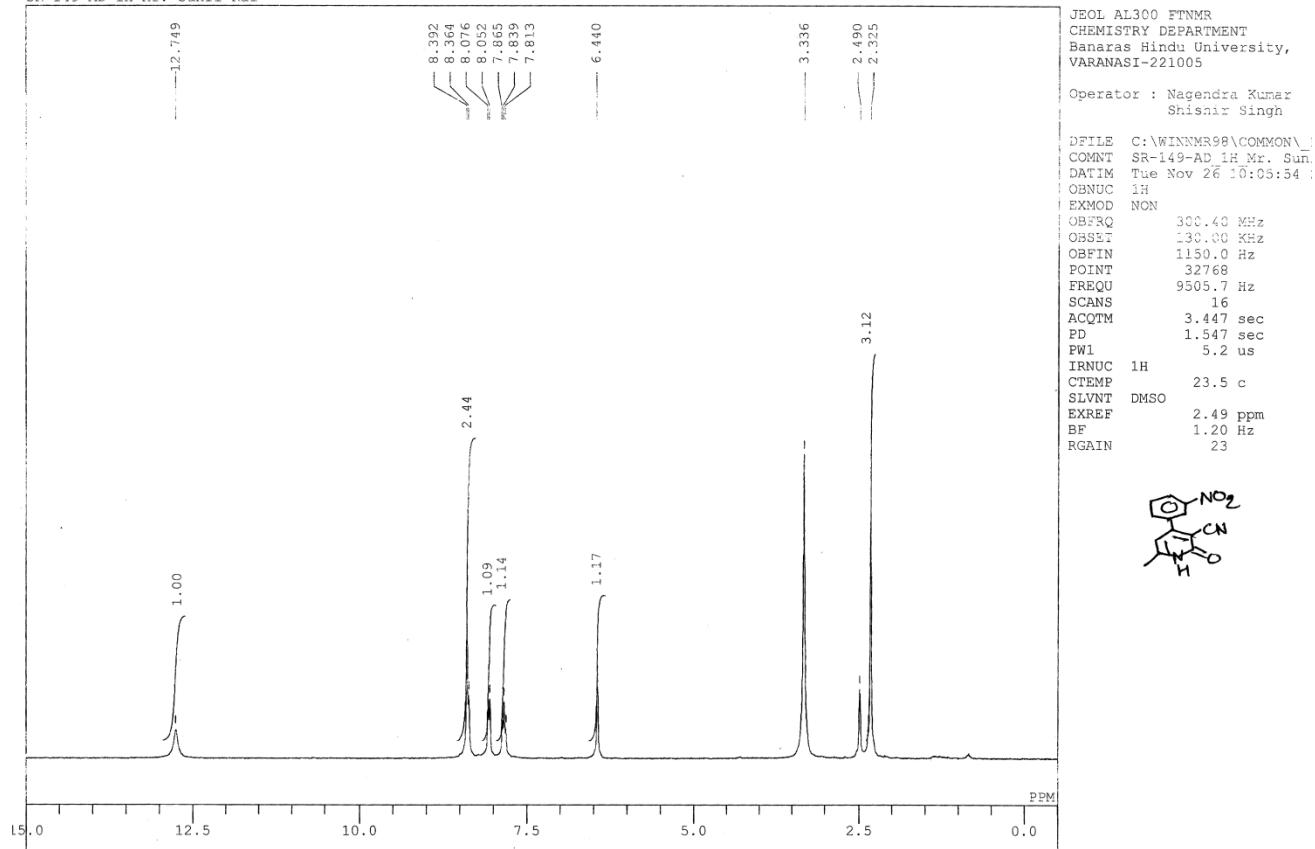
Compound (5e):  $^{13}\text{C}$  NMR



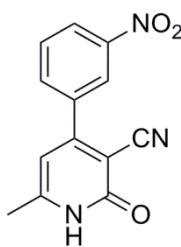
Compound (6a):  $^1\text{H}$  NMR



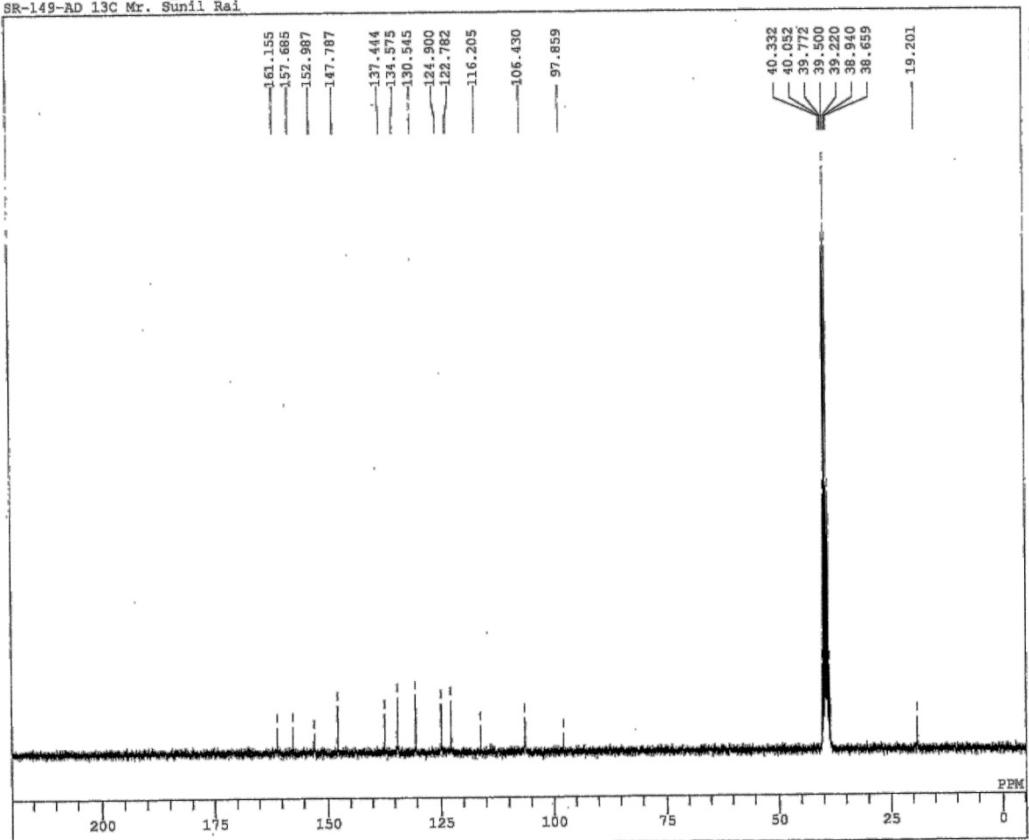
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Compound (6a):  $^{13}\text{C}$  NMR



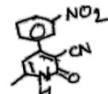
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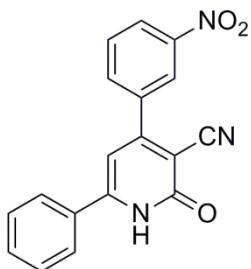
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

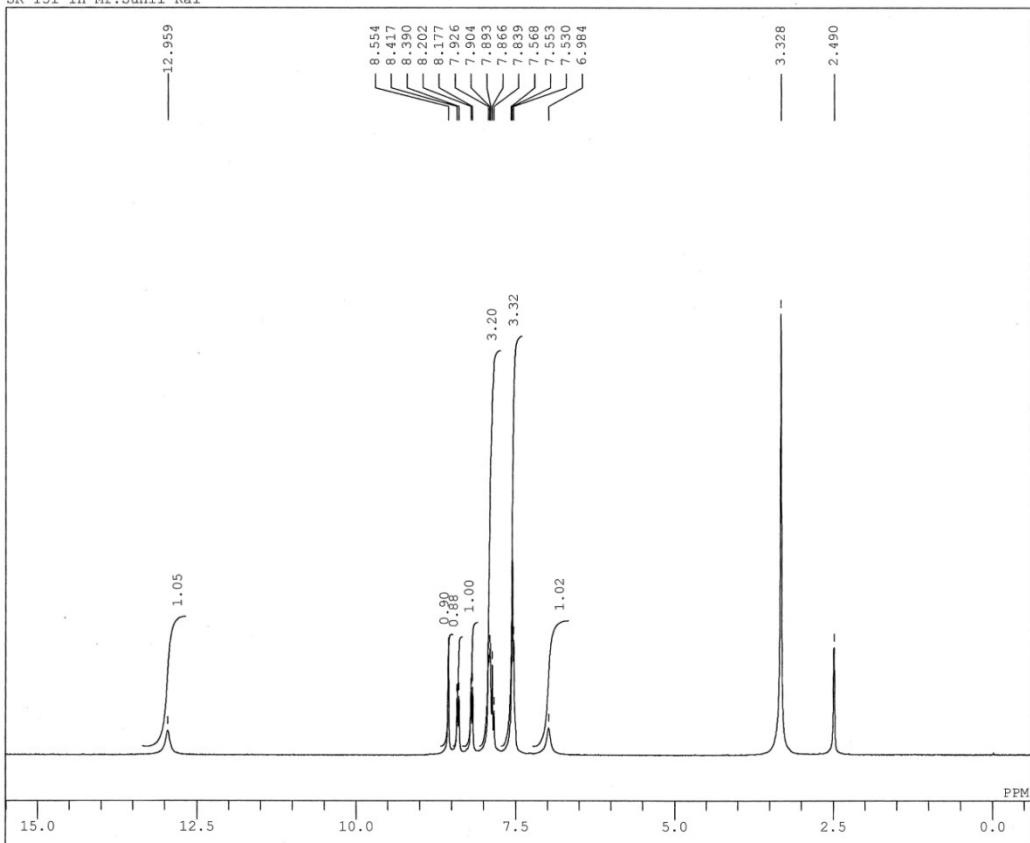
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FREQU 20408.1 Hz  
SCANS 317  
ACQTM 1.606 sec  
PD 1.394 sec  
PW1 5.9 us  
IRNUC 1H  
CTEMP 22.1 c  
SLVNT DMSO  
EKREF 39.50 ppm  
BF 1.20 Hz  
RGAIN 23



Compound (6b):  $^1\text{H}$  NMR



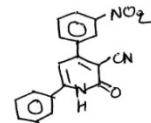
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SR-151\_1H Mr.Sunil Rai



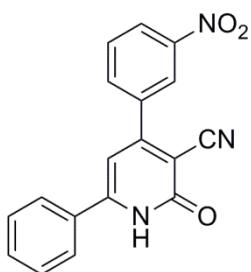
JEOL AL300 FTNMR  
CHEMISTRY DEPARTMENT  
Banaras Hindu University,  
VARANASI-221005

Operator : Nagendra Kumar  
Shishir Singh

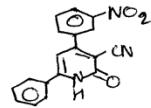
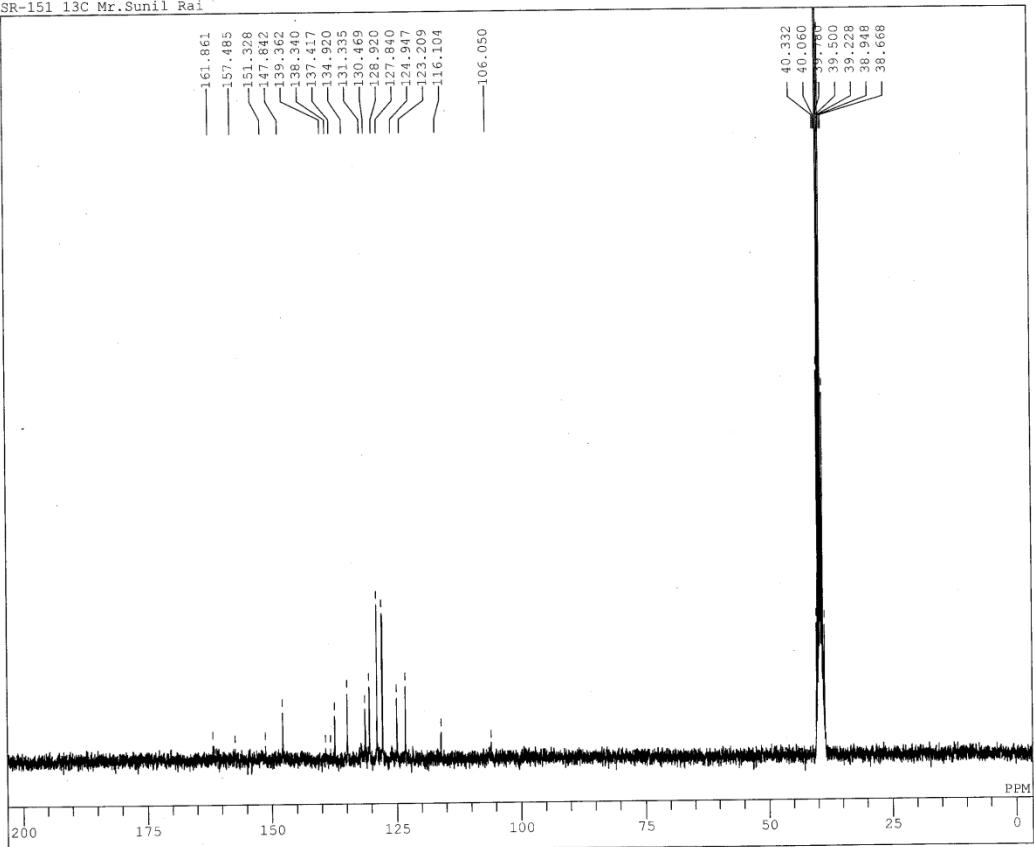
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SCANS 8  
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EXREF 2.49 ppm  
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RGAIN 19



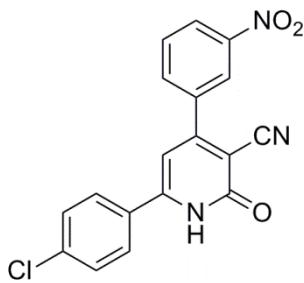
Compound (6b):  $^{13}\text{C}$  NMR



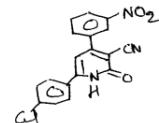
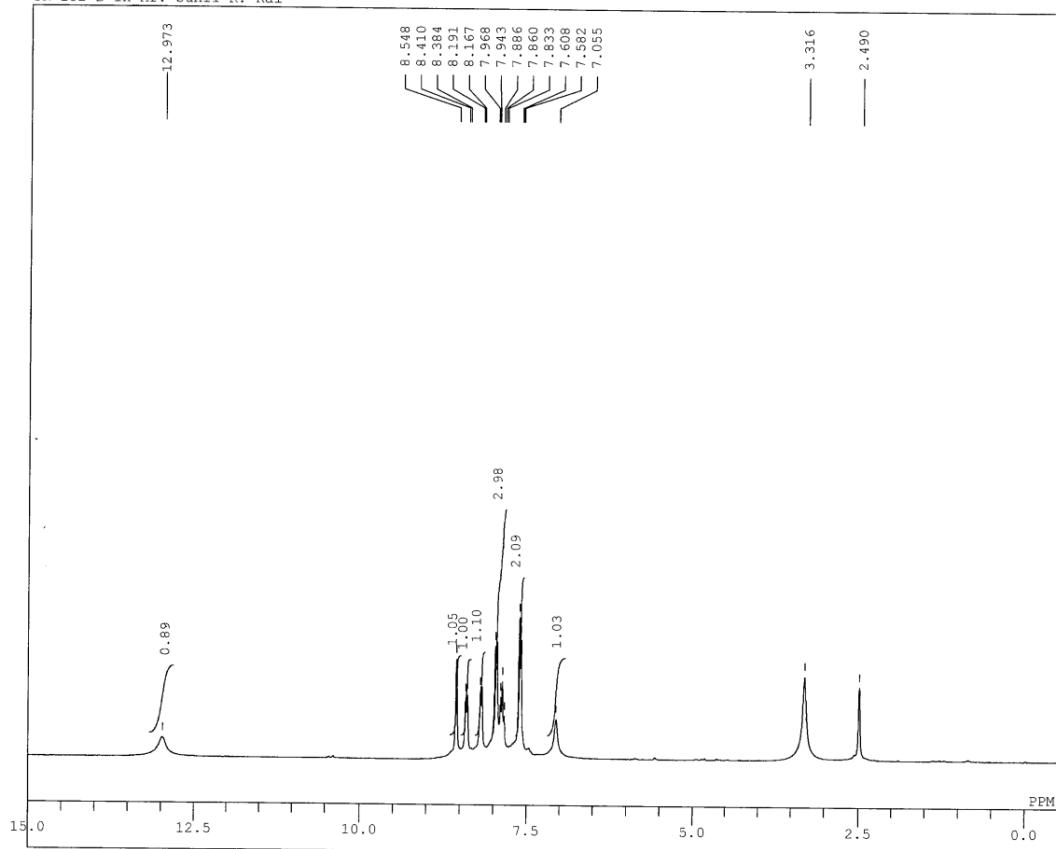
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SR-151 13C Mr.Sunil Rai



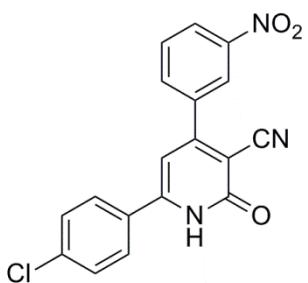
Compound (6c):  $^1\text{H}$  NMR



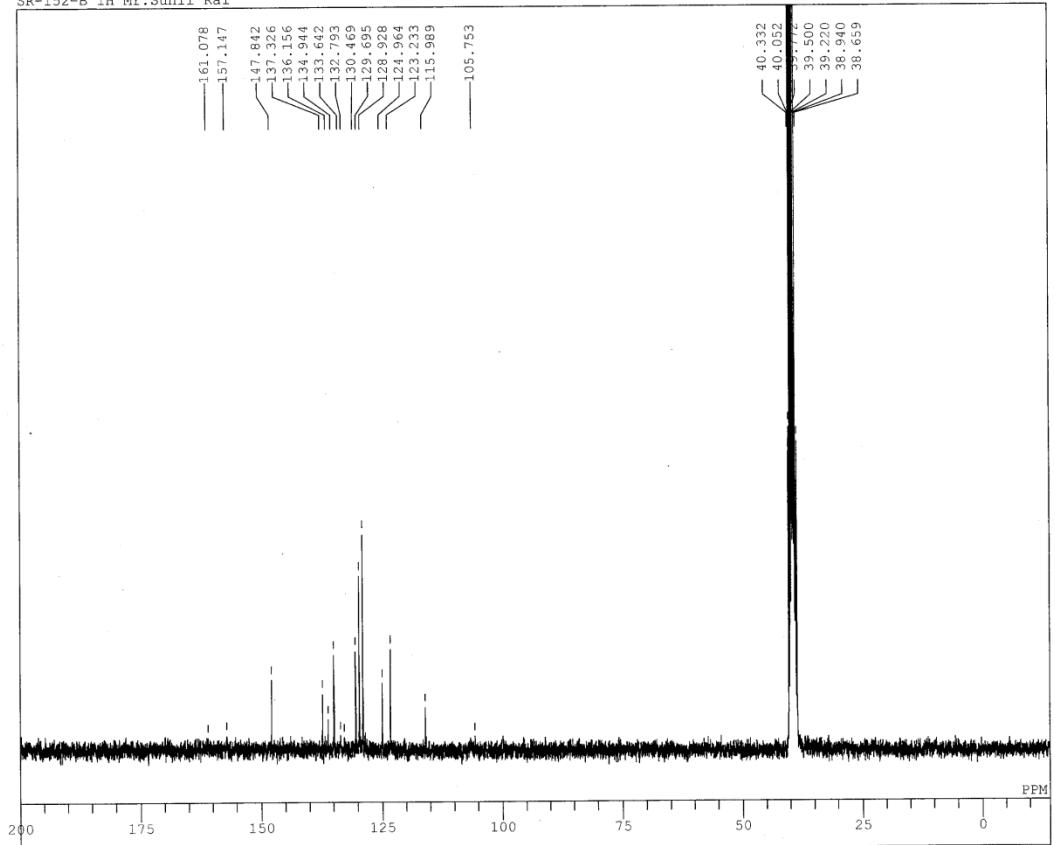
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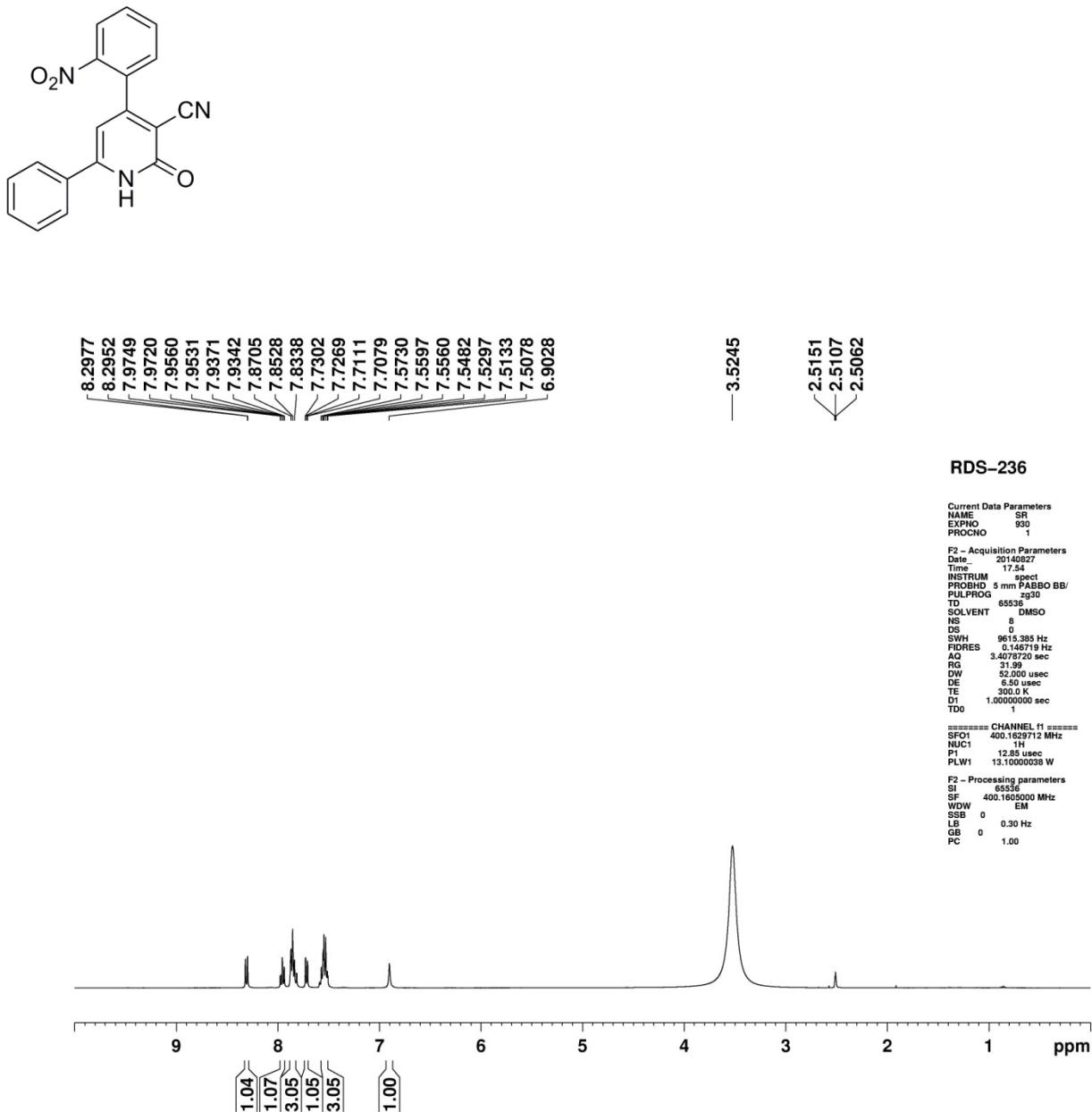
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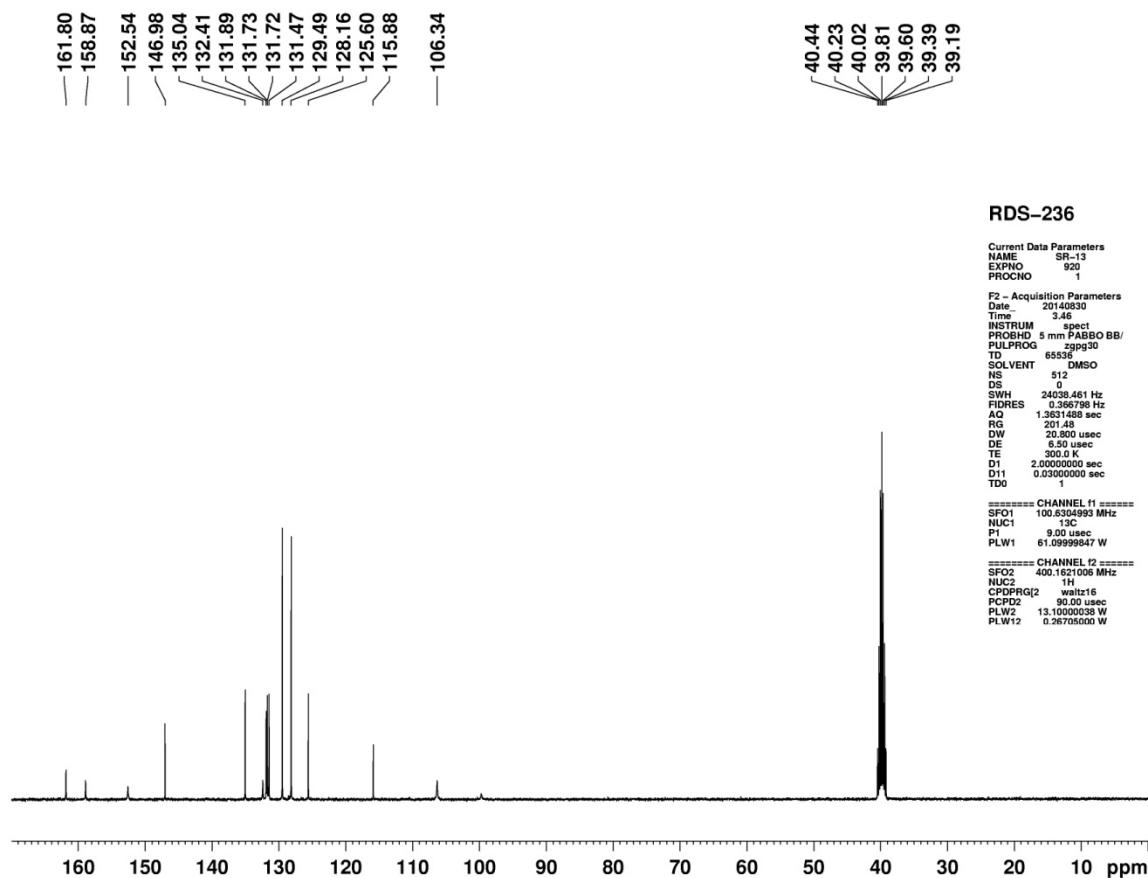
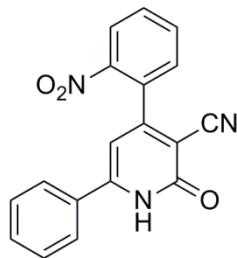
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SR-152-B\_1H Mr.Sunil Rai



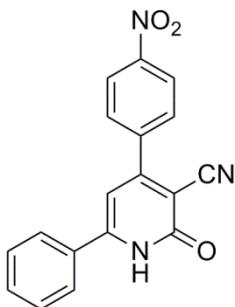
Compound (7a):  $^1\text{H}$  NMR



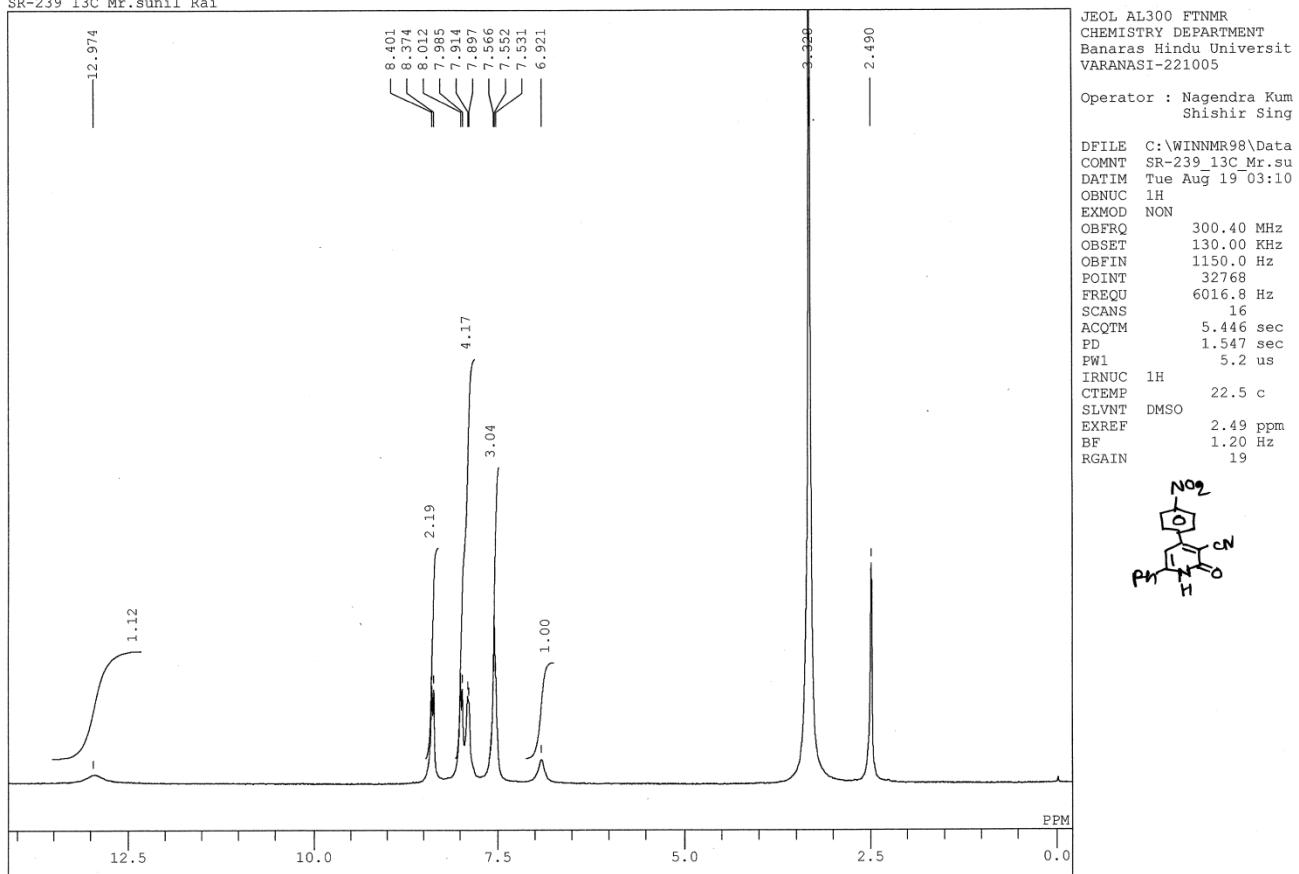
Compound (7a):  $^{13}\text{C}$  NMR



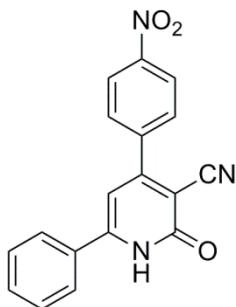
Compound (8a):  $^1\text{H}$  NMR



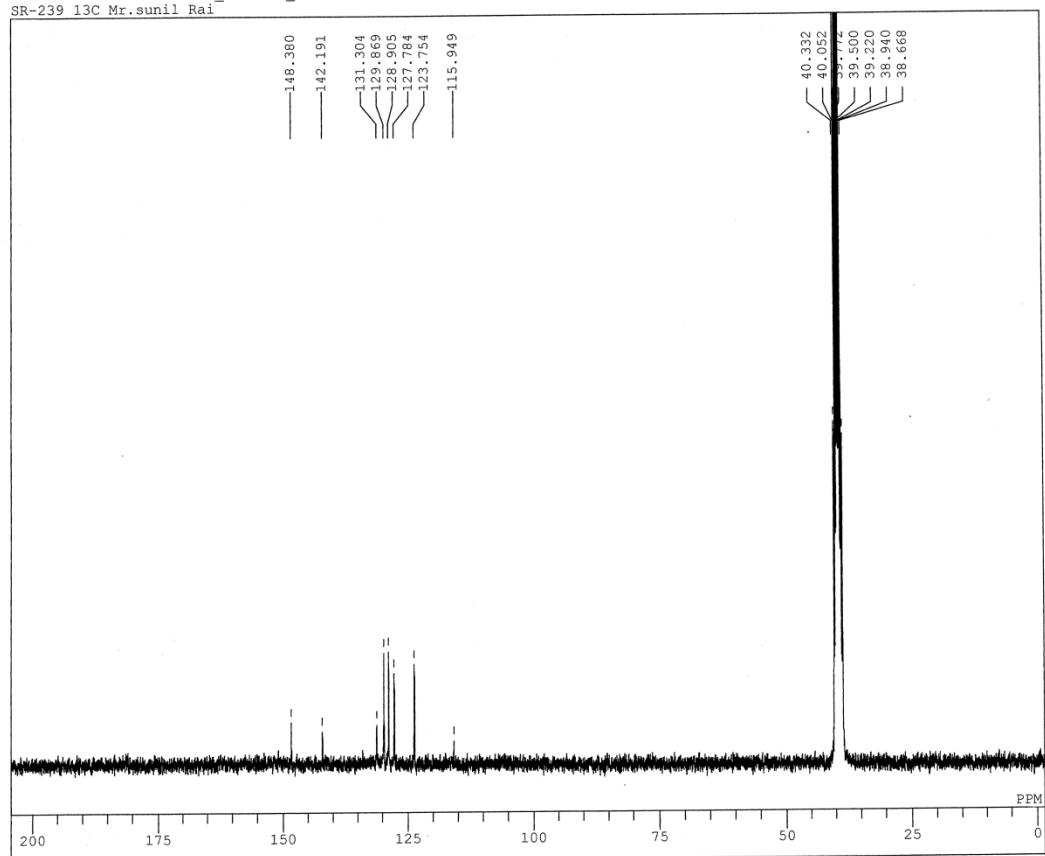
C:\WINNMR98\Data\SR-239\_13C1NON\_E6.als  
SR-239 13C Mr.sunil Rai



Compound (8a):  $^{13}\text{C}$  NMR



C:\WINNMR98\Data\SR-239\_13C2BCM\_E6.als  
 SR-239 13C Mr.sunil Rai



### 3. Single Crystal X-ray data:

The X-ray diffraction data of compounds **1d**, **1e**, **1g** and **2d** was collected on Bruker SMART APEX CCD area detector diffractometer. The structure was solved and refined by using SHELXS program.<sup>1</sup> Molecular graphics were designed by using Mercury version-3.2.<sup>2</sup>

**Table S1.** Crystal data and structure refinement parameters for compound **1d**.

compound name	5,6-dimethyl-2-oxo-4-phenyl-1,2-dihydropyridine-3-carbonitrile
CCDC Number	981162
empirical Formula	C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O
formula weight	224.26
temperature	293 K
wavelength	0.71073 Å
crystal system	Triclinic
space group	P-1
unit cell dimensions	a = 7.4066 (7) Å, α = 116.399 (13) ° b = 9.4392 (12) Å, β = 97.846 (9) ° c = 9.7203 (13) Å, γ = 90.409 (9) °
cell volume	601.24 (12) Å <sup>3</sup>
D <sub>calculated</sub>	1.239 mg/ m <sup>3</sup>
F(000)	236
crystal size	0.40 × 0.38 × 0.36 mm
Z	2
R factor (%)	6.31
theta range	3.4 to 32.6°
limiting Indices	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14
μ(Mo KR)/mm-1	0.08
R <sub>int</sub>	0.021
measured reflections	6568
independent refln	3913
reflections with $I > 2\sigma(I)$	2298
parameters	158
goodness of fit	1.0

$R[F^2 > 2\sigma(F^2)]$	0.063
wR(F <sup>2</sup> )	0.200

**Table S2.** Crystal data and structure refinement parameters for compound **1e**.

compound name	(6-ethyl-2-oxo-4-phenyl-1,2-dihydropyridine-3-carbonitrile)
CCDC Number	981163
empirical Formula	C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O
formula weight	224.26
temperature	293 K
wavelength	0.71073 Å
crystal system	Monoclinic
space group	P2 <sub>1</sub> /c
unit cell dimensions	a = 7.3809 (6) Å, α = 90 ° b = 8.0626 (6) Å, β = 98.378 (6)° c = 19.9265 (12) Å, γ = 90°
cell volume	1173.16 (15) Å <sup>3</sup>
D <sub>calculated</sub>	1.270 mg/ m <sup>3</sup>
F(000)	472
crystal size	0.45 × 0.43 × 0.41 mm
Z	4
R factor (%)	6.83
theta range	3.2 to 29.0°
limiting Indices	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -27 ≤ l ≤ 27
μ(Mo KR)/mm-1	0.08
R <sub>int</sub>	0.022
measured reflections	5083
independent refln	2686
reflections with $I > 2\sigma(I)$	1537
parameters	158
goodness of fit	1.02

$R[F^2 > 2\sigma(F^2)]$	0.068
wR(F <sup>2</sup> )	0.191

**Table S3.** Crystal data and structure refinement parameters for compound **1g**.

compound name	<i>2-oxo-4-phenyl-6-propyl-1,2-dihydropyridine-3-carbonitrile</i>
CCDC Number	981430
empirical Formula	C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O
formula weight	238.28
temperature	293 K
wavelength	0.71073 Å
crystal system	Triclinic
space group	P-1
unit cell dimensions	a = 9.7064 (10) Å, α = 82.404 (8)° b = 9.7294 (10) Å, β = 77.082 (9)° c = 14.4315 (14) Å, γ = 75.690 (9)°
cell volume	1282.9 (2) Å <sup>3</sup>
D <sub>calculated</sub>	1.234 mg/ m <sup>3</sup>
F(000)	504
crystal size	0.52 × 0.50 × 0.48 mm
Z	4
R factor (%)	5.74
theta range	3.3 to 29.1°
limiting Indices	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -19 ≤ l ≤ 19
μ(Mo KR)/mm-1	0.08
R <sub>int</sub>	0.022
measured reflections	10237
independent refln	5798
reflections with $I > 2\sigma(I)$	2362
parameters	335
goodness of fit	1.03

$R[F^2 > 2\sigma(F^2)]$	0.057
wR(F <sup>2</sup> )	0.156

**Table S4.** Crystal data and structure refinement parameters for compound **2d**.

compound name	<i>4-(4-chlorophenyl)-5,6-dimethyl-2-oxo-1,2-dihydropyridine-3-carbonitrile</i>
CCDC Number	981164
empirical Formula	C <sub>14</sub> H <sub>11</sub> ClN <sub>2</sub> O
formula weight	258.70
temperature	293 K
wavelength	0.71073 Å
crystal system	Triclinic
space group	P-1
unit cell dimensions	a = 9.3937 (10) Å, α = 61.217 (12)° b = 17.428 (2) Å, β = 78.071 (9)° c = 18.0482 (18) Å, γ = 87.092 (9)°
cell volume	2529.7 (5) Å <sup>3</sup>
D <sub>calculated</sub>	1.359 mg/m <sup>3</sup>
F(000)	1072
crystal size	0.54 × 0.53 × 0.52 mm
Z	8
R factor (%)	9.09
theta range	3.2 to 29.2°
limiting Indices	-12 ≤ h ≤ 12, -23 ≤ k ≤ 23, -24 ≤ l ≤ 24
μ(Mo KR)/mm-1	0.08
R <sub>int</sub>	0.040
measured reflections	21373
independent refln	11464
reflections with $I > 2\sigma(I)$	5232
parameters	665
goodness of fit	1.00
$R[F^2 > 2\sigma(F^2)]$	0.091
wR(F <sup>2</sup> )	0.250

#### **4. References**

1. G. M. Sheldrick, *Acta Cryst A* 2008, A64, 112-122.
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