

# Bioinspired NiCoO<sub>2</sub> nanocomposites derived from *Moringa oleifera* as a recyclable catalyst for multicomponent reactions with potent antimicrobial efficiency

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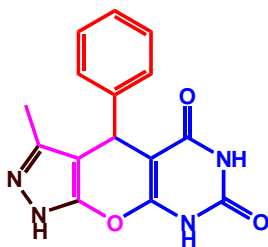
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**General:****Synthesis of pyrazolopyrano[2,3-d]pyrimidine:**

In 50 ml round bottom flask, equimolar amounts of aromatic aldehyde (1mmol), ethylacetoacetate (1mmol), hydrazine hydrate (1mmol) and barbuteric acid (1mmol) were combined with NiCoO<sub>2</sub>nanocomposite (5 mol%) and dissolved this mixture in 10 ml of solvent system (1:1 water : ethanol) and reaction carried out under ultrasonication. The progress of reaction was monitored by TLC. After completion of reaction the ensuing product was subjected to structural analysis using FT-IR, <sup>1</sup>H NMR, and <sup>13</sup>C NMR spectroscopy.



[TableNo.3,Entry-2]3-methyl-4-phenyl-4,8-dihydropyrazolo[4',3':5,6]pyrano[2,3-d]pyrimidine-5,7(1H,6H)-dione

FTIR–500cm<sup>-1</sup>, 1000cm<sup>-1</sup>,1450cm<sup>-1</sup>,1600cm<sup>-1</sup>,2900cm<sup>-1</sup>,3400cm<sup>-1</sup>.

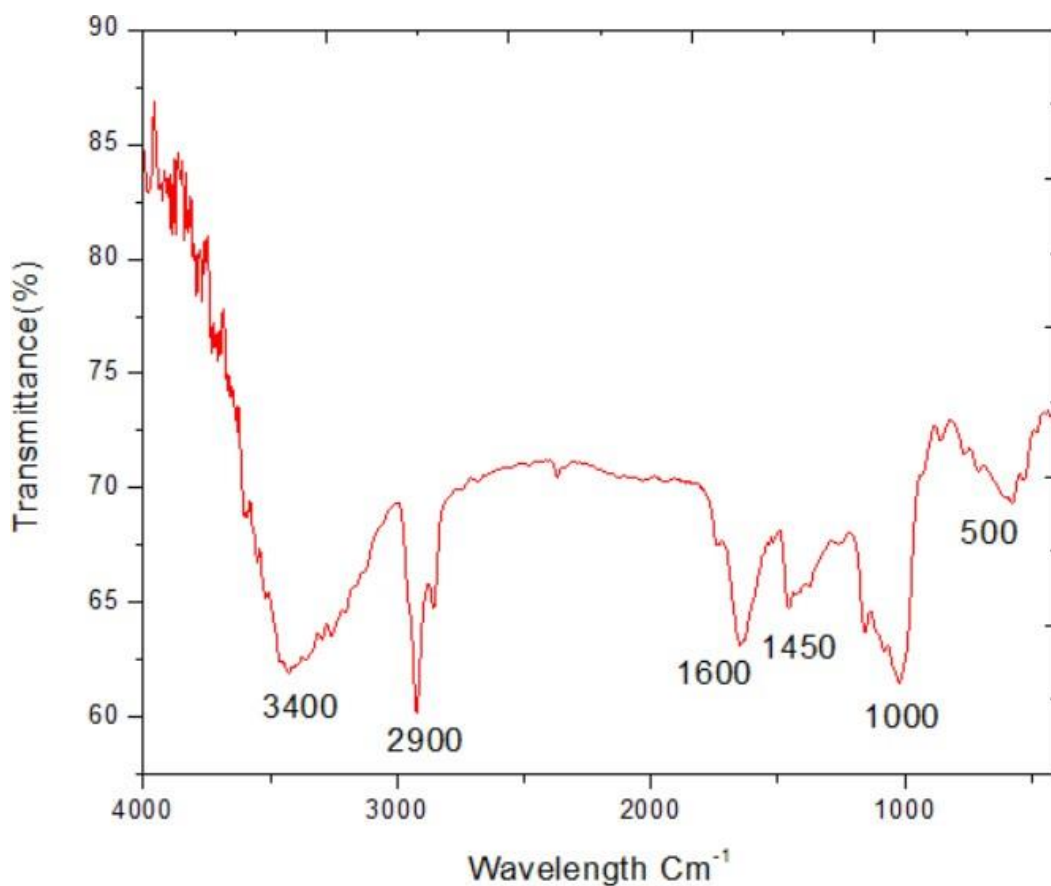


Figure1.FTIRspectrumof3-methyl-4-phenyl-4,8-dihydropyrazolo[4',3':5,6]pyrano[2,3-d]pyrimidine-5,7(1H,6H)-dione

<sup>1</sup>HNMR-(400MHz,CDCl<sub>3</sub>)-δppm:δ2.31(s,3H,CH<sub>3</sub>),δ5.50(2,1H,CH),δ7.13(d, J=7.2Hz, 2H,Ar-H), δ 7.40(t, J=7.8Hz, 1H,Ar-H), δ 7.82(t, J=7.3Hz, 2H,Ar-H), δ 10.50(s, 2H, NH), 13.50 (br s,1H NH)

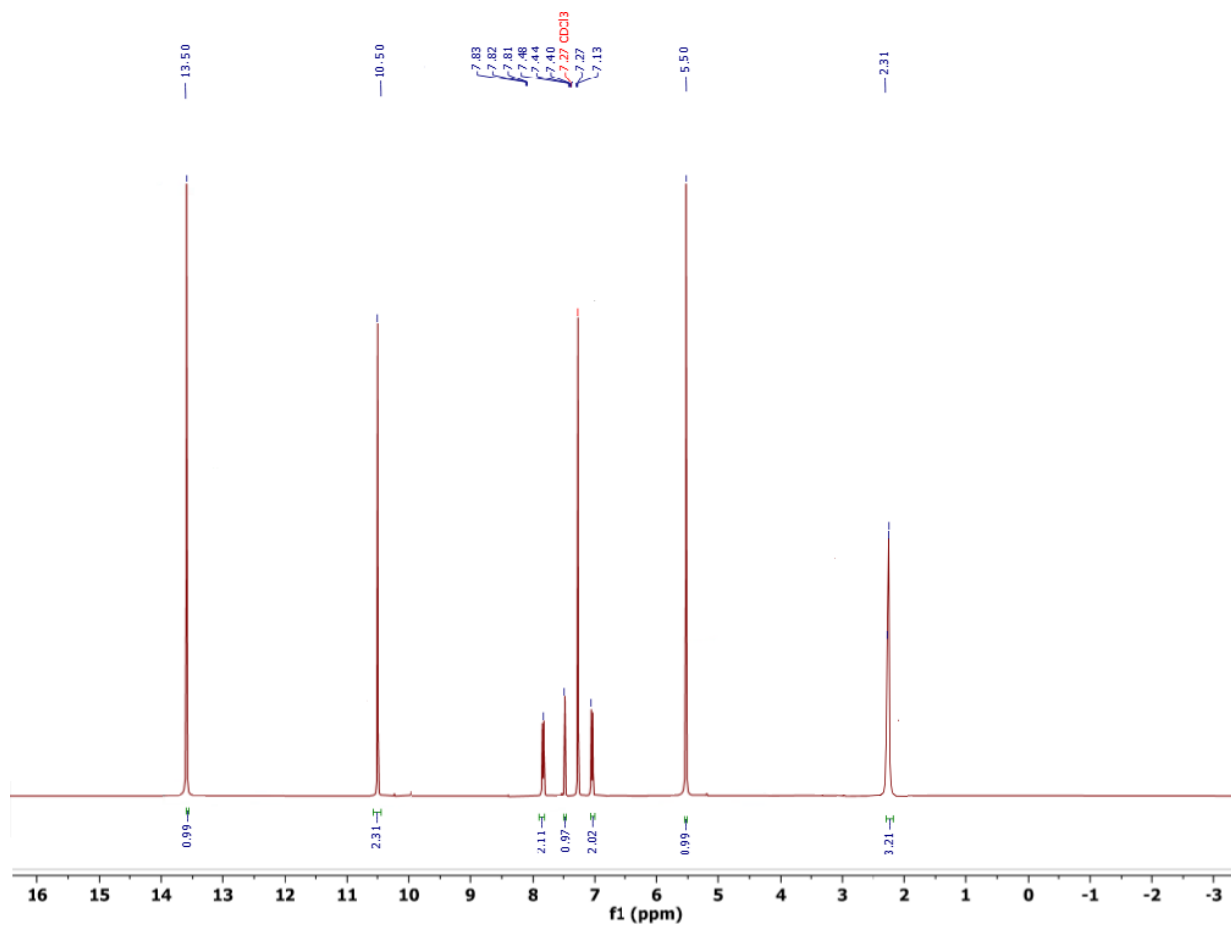
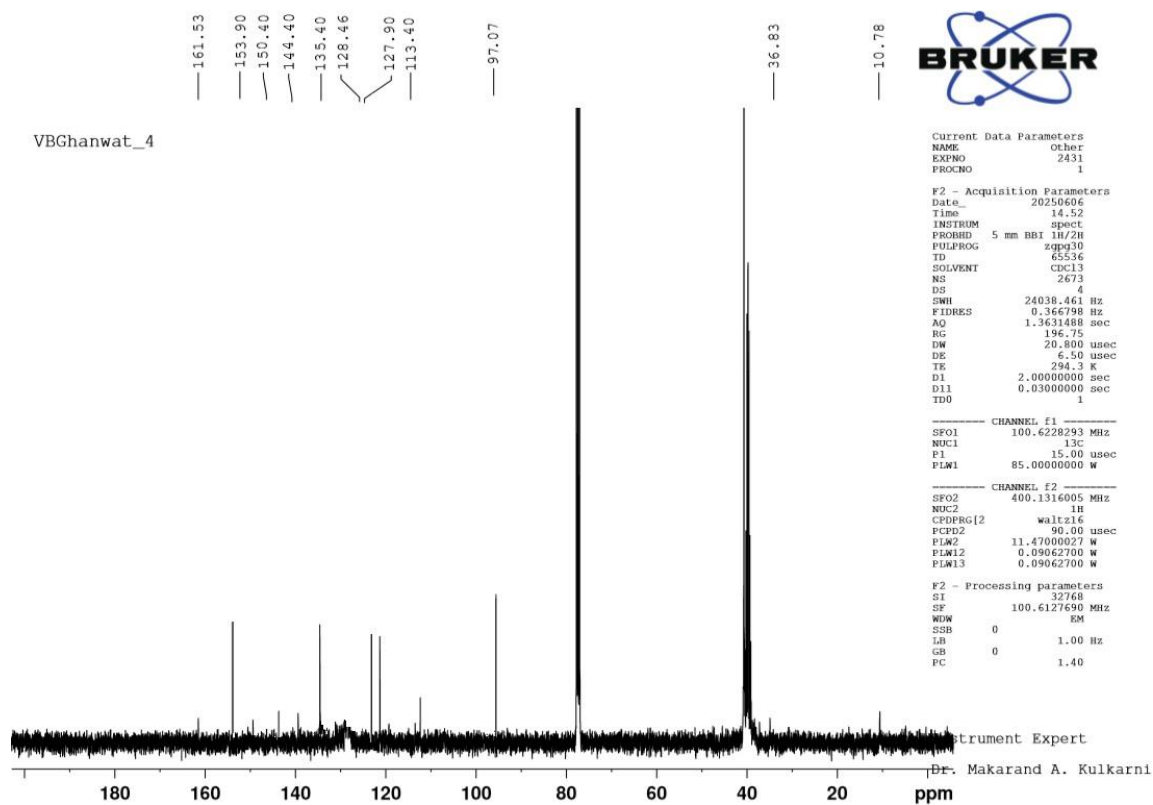
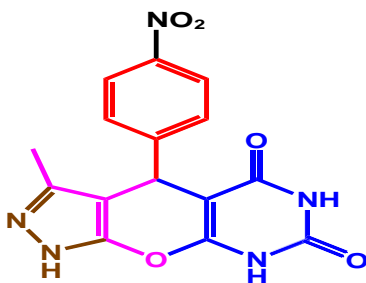


Figure2. <sup>1</sup>HNMR of 3-methyl-4-phenyl-4,8-dihydropyrazolo[4',3':5,6]pyrano[2,3d]pyrimidine-5,7(1H,6H)-dione

<sup>13</sup>CNMR: 89.75(1C,s), 36.24(1C,s), 97.07(1C,s), 113.40(1C,s), 127.90(1C,d), 135.40(1C,s), 144.40(1C,s), 150.40(1C,s), 153.90(1C,s), 161.53(1C,s), 153.90(1C,s), 144.40(1C,s), 135.40(1C,s), 128.46(1C,s), 127.90(1C,d), 113.40(1C,s), 97.07(1C,s), 36.24(1C,s), 10.78(1C,s)



**Figure 3.** <sup>13</sup>CNMR spectrum of 3-methyl-4-phenyl-4,8-dihydropyrazolo[4',3':5,6]pyrano[2,3-d]pyrimidine-5,7(1H,6H)-dione



[TableNo.3,Entry-3]3-Methyl-4-(4-nitrophenyl)-4,8-dihydropyrazolo[3',4':5,6] Pyrano [2,3-d] pyrimidine 5,7(1H,6H)-dione

FTIR:500cm<sup>-1</sup>,1000cm<sup>-1</sup>,1450,1600cm<sup>-1</sup>,2900cm<sup>-1</sup>,3400cm<sup>-1</sup>.

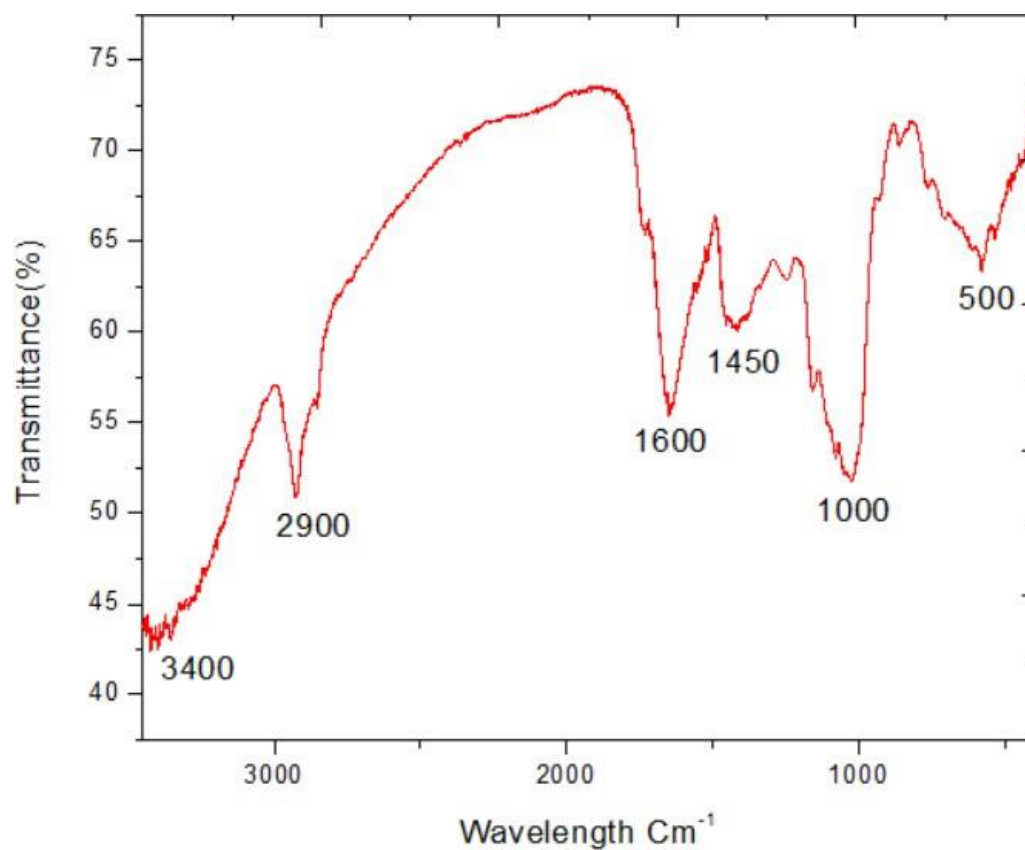


Figure4.FTIRspectrumof3-Methyl-4-(4-nitrophenyl)-4,8-dihydropyrazolo[3',4':5,6] Pyrano [2,3-d] pyrimidine 5,7(1H,6H)-dione

$^1\text{H NMR}$ (400MHz,  $\text{CDCl}_3$ ) - $\delta$ ppm:  $\delta$ 3.15(s, 3H,  $\text{CH}_3$ ),  $\delta$ 5.17(2, 1H, CH),  $\delta$ 7.28(d,  $J=7.2\text{Hz}$ , 2H, Ar-H),  $\delta$ 7.83(d,  $J=7.3\text{Hz}$ , 2H, Ar-H),  $\delta$ 10.32(s, 2H, NH), 13.20(brs, 1H NH)

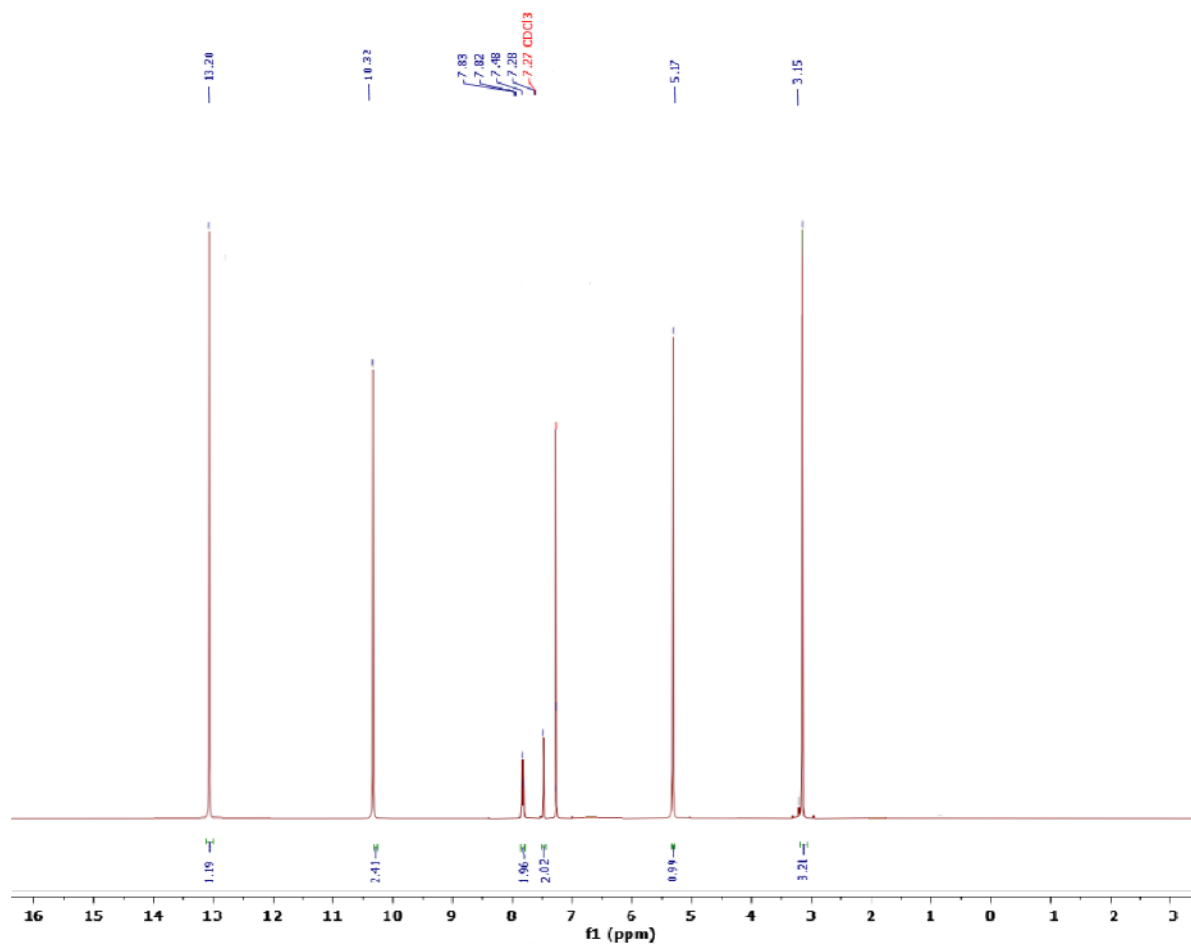


Figure 5.  $^1\text{H NMR}$  of 3-Methyl-4-(4-nitrophenyl)-4,8-dihydropyrazolo[3',4':5,6] Pyrano [2,3-d] pyrimidine 5,7(1H,6H)-dione

<sup>13</sup>CNMR(101MHz,CDCl<sub>3</sub>)-δ ppm: δ10.78,36.83,97.07,113.40,133.40,144.40,135.40,161.53

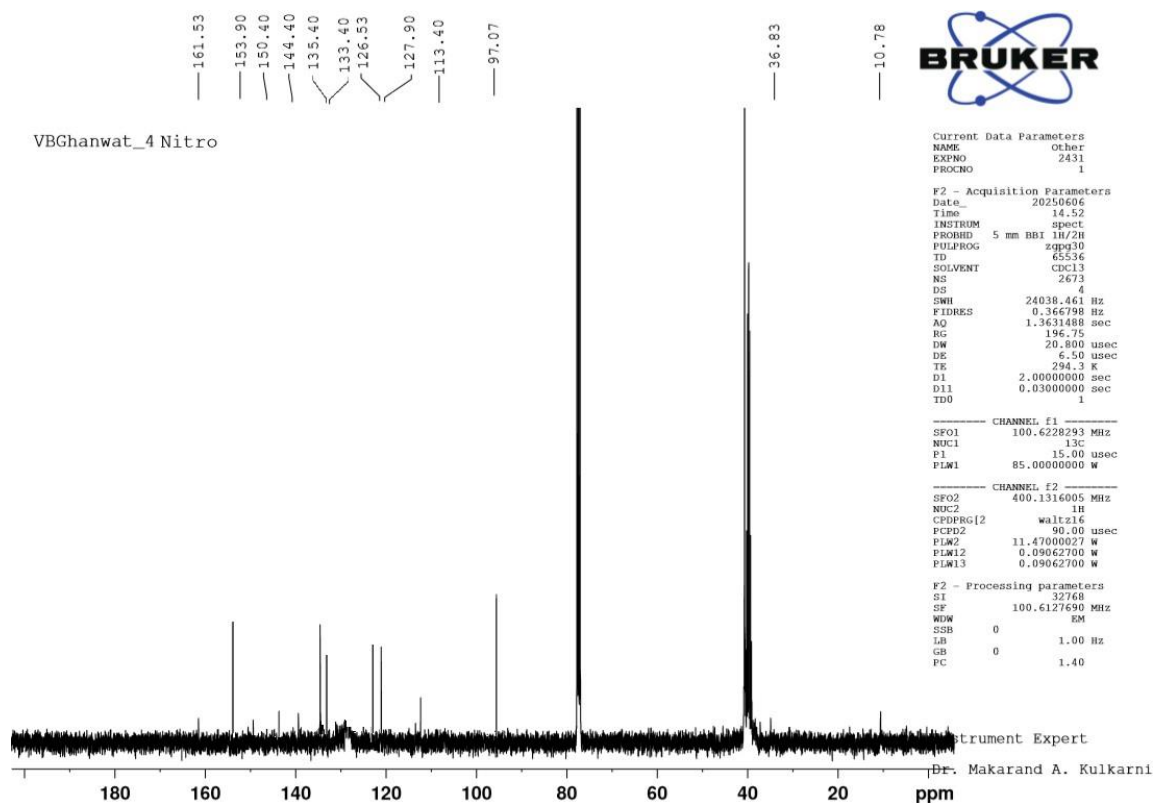
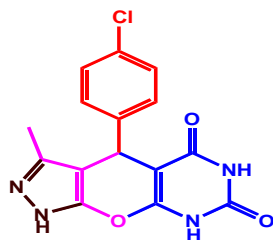


Figure6. <sup>13</sup>CNMR of 3-Methyl-4-(4-nitrophenyl)-4,8-dihydropyrazolo[3',4':5,6]pyrano[2,3-d]pyrimidine 5,7(1H,6H)-dione





[TableNo.3,Entry-5]5-(2-hydroxyphenyl)-1,2,4-triazolidine-3-thione

FTIR: 500  $\text{cm}^{-1}$ , 1000  $\text{cm}^{-1}$ , 1400, 1600  $\text{cm}^{-1}$ , 2900  $\text{cm}^{-1}$ , 3450  $\text{cm}^{-1}$ .

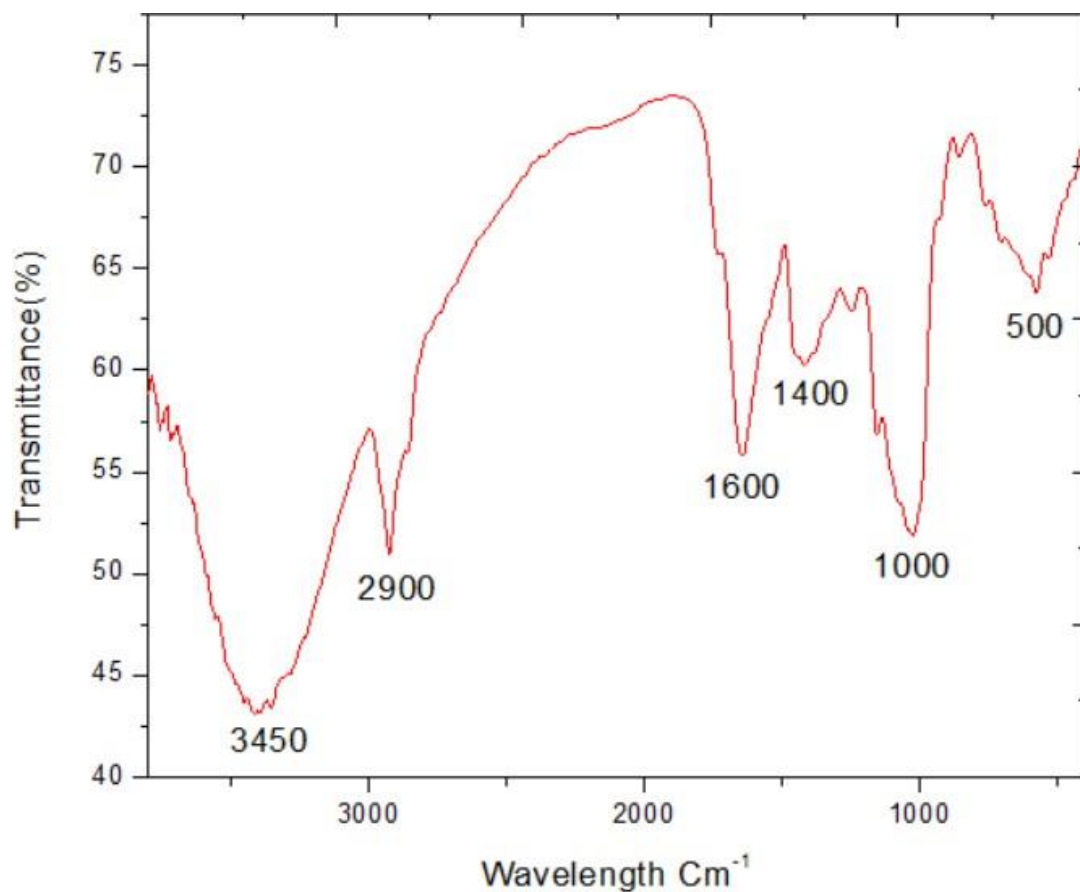
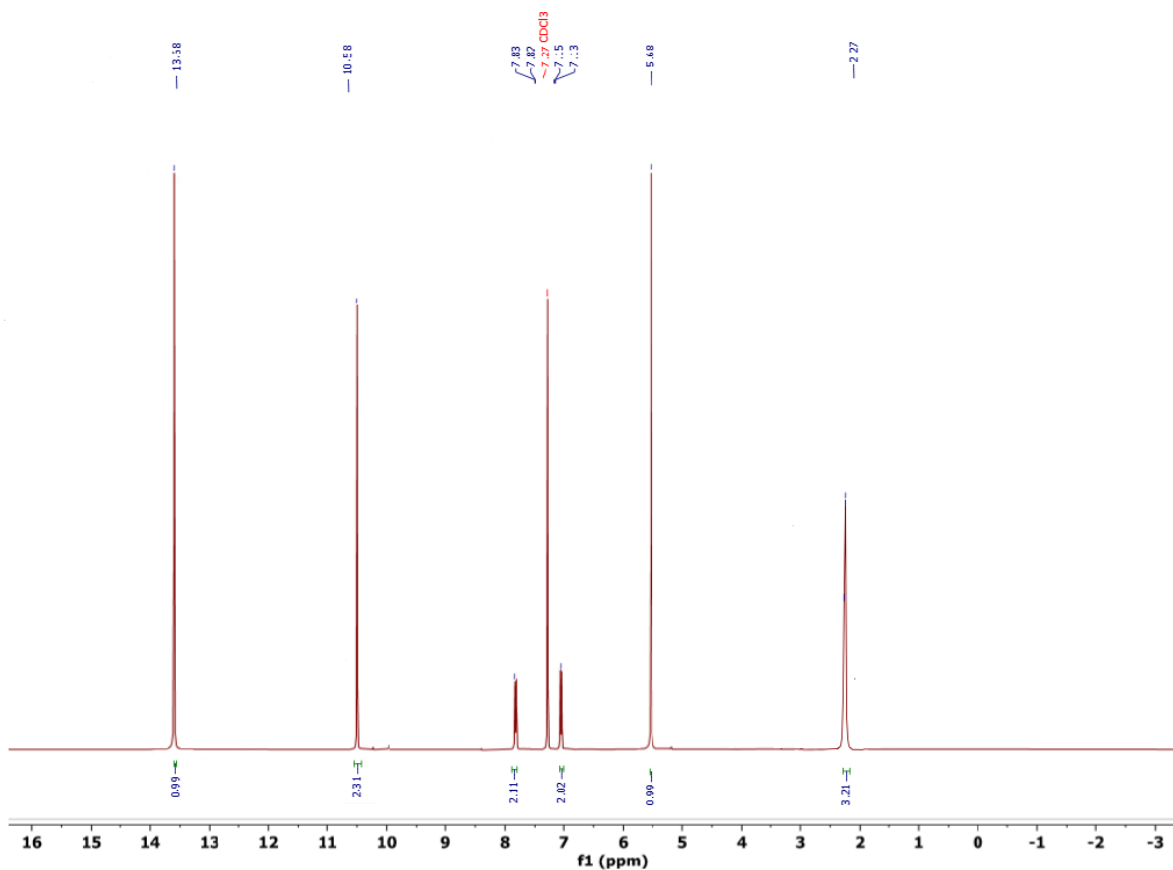


Figure7.FTIR spectrum of 4-(4-chlorophenyl)-3methyl-4,8-dihydropyrazolo[3',4': 5,6]Pyrano [2,3-d] pyrimidine 5,7(1H,6H)-dione

**$^1\text{H NMR}$ (400MHz,  $\text{CDCl}_3$ )- $\delta$  ppm:**  $\delta$ 2.27(s, 3H,  $\text{CH}_3$ ),  $\delta$ 5.68 (2, 1H, CH),  $\delta$ 7.15 (d,  $J=7.2\text{Hz}$ , 2H, Ar-H),  $\delta$ 7.82(d,  $J=7.3\text{Hz}$ , 2H, Ar-H),  $\delta$ 10.58(s, 2H, NH), 13.68(brs, 1HNH)



**Figure 8.**  $^1\text{H NMR}$  of 4-(4-chlorophenyl)-3-methyl-4,8-dihydropyrazolo[3',4':5,6]pyrano[2,3-d]pyrimidine 5,7(1H,6H)-dione

<sup>13</sup>CNMR(101MHz,CDCl<sub>3</sub>)-δppm:δ10.78, 36.83,97.07,113.40,127.90,135.40,144.40, 1150.40,153.90,161.53

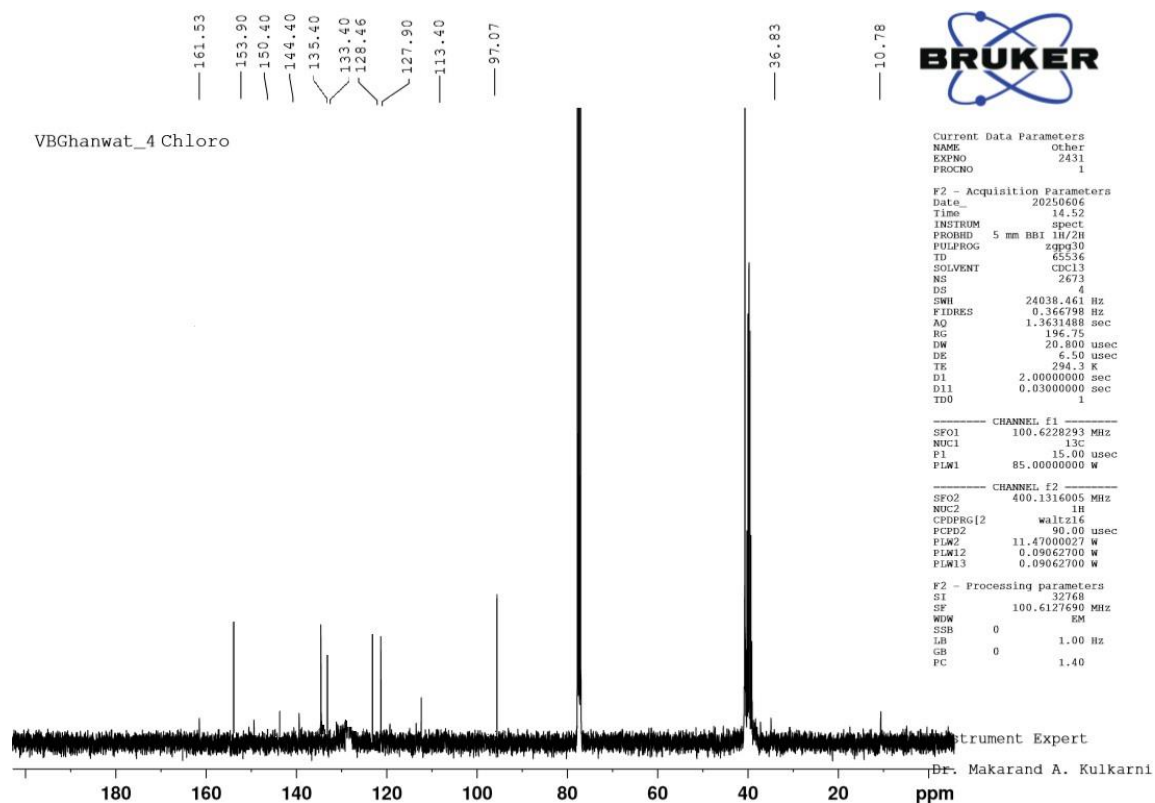


Figure9. <sup>13</sup>CNMR of 4-(4-chlorophenyl)-3methyl-4,8-dihydropyrazolo[3',4':5,6] Pyrano [2,3-d] pyrimidine 5,7(1H,6H)-dione