



# CLEAN AND EFFICIENT MICROWAVE ASSISTED SYNTHESIS OF SOME NEW PYRIMIDINE, PYRAZOLINE AND ISOXAZOLINE DERIVATIVES FROM 3-(3-NITROPHENYL)-N- PHENYL-PROP-2-ENAMIDE

Urvashi Tiwari<sup>[a]</sup>, Chetna Ameta<sup>[a]</sup>, Sanyogita Sharma<sup>[b]</sup>, Meenakshi Sharma<sup>[c]</sup>, Arpit Kumar Pathak<sup>[a]</sup>, Pinki B. Punjabi<sup>[a]\*</sup>

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A rapid and efficient method for the preparation of some new pyrimidine, pyrazoline and isoxazoline derivatives by the reaction of chalcones with hydroxylamine, urea and hydrazine hydrate under microwave exposure has been reported. The products have been isolated, purified and characterized by spectral methods like IR, NMR and mass spectrometry. The antibacterial and antifungal activities of the final products against various bacteria and fungi have also been reported.

\*Corresponding Authors

\*E-mail: [pb\\_punjabi@yahoo.com](mailto:pb_punjabi@yahoo.com)

- [a] Microwave Chemistry Laboratory, Department of Chemistry, Mohanlal Sukhadia University, Udaipur - 313 001, Rajasthan, India  
[b] Department of Chemistry, Pacific Institute of Technology, "Pacific Hills" Pratapnagar Extension, Airport Road, Debari, Udaipur, India  
[c] Department of Chemistry, Banasthali Vidyapeeth, Banasthali, Rajasthan, India

## Introduction

Increasing globalization and industrialization is causing harm to our ecosystem, which is gradually getting polluted. The implementation of green chemistry and green manufacturing technologies will help to decrease the causes for these climate changes which are dreadful for environmental and human health challenges that we are facing and feeling now-a-days. Green chemistry techniques are now being used across the world to develop new materials in every field of chemistry. MAOS (Microwave Assisted Organic Synthesis)<sup>1</sup> strategies offer feasible solutions to minimize environmental deterioration as their benefits are manifold: it frequently leads to dramatically reduction in reaction time, higher yields, cleaner reaction profiles and above all, eco-friendliness. This is a technique which gives "yes or no answer" for a particular chemical transformation within 5 to 10 minutes as compared to several hours in conventional protocol in industry and academia.<sup>2,3</sup> A heterocyclic compound is one which possesses a cyclic structure with hetero atoms in the ring in addition to c- atom. Nitrogen and oxygen containing heterocyclic compounds have received considerable attention due to their wide range of pharmacological activities.<sup>4-8</sup>

As our interest is to synthesize heterocyclic templates capable of bearing some potential pharmacophores which can enhance the inherent biological activity, Therefore systematic propagation of heterocyclic rings in chalcones

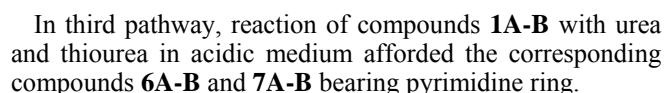
with the installation of biological active heterocyclic units such as isoxazoles, pyrimidines and pyrazoles has been carried out. Pyrimidines are found to be endowed with potential biological activity such as antitumor,<sup>9</sup> antiviral,<sup>10</sup> anticancer,<sup>11</sup> antibacterial,<sup>12</sup> antimicrobial<sup>13</sup> and many others.

Isoxazoles have been reported to possess bactericidal,<sup>14</sup> fungicidal<sup>15</sup> and antimicrobial activity.<sup>16</sup> Pyrazoles display a number of antimicrobial activities like anticancer,<sup>17</sup> antidiabetic<sup>18</sup> and antidepressant.<sup>19</sup> Therefore, it was thought worthwhile to synthesize these nuclei from 3-(substituted phenyl)-N-phenyl prop-2-enamide, in order to explore the pharmacological activities of these compounds.

## Results and Discussion

Acetanilide on condensation with substituted aldehydes in presence of 30% NaOH afforded compound **1A-B**, which were used as intermediates for the synthesis of pyrazolines, pyrimidines and isoxazolines following three different pathways. Compounds **1A-B** gave characteristics IR bands in the region between 3310-3315 cm<sup>-1</sup> for (N-H str.), 3014 – 3018 cm<sup>-1</sup> (C-H str., Ar-H), 1660 -1666 cm<sup>-1</sup> (C=O str.), 1595 -1605 cm<sup>-1</sup> (C=C str.) and <sup>1</sup>H NMR signals for multiplet of nine integrating aromatic protons at (δ) 6.20 - 7.40, doublet of C-H vinyl group at (δ) 6.302 -5.20, singlet at (δ) 5.24 – 5.95 for N-H group and signal at (δ) 3.5 for OCH<sub>3</sub>. Further, compounds **1A** and **1B** were confirmed by the characteristics IR bands at 1540, 1499 cm<sup>-1</sup> (NO<sub>2</sub> str.) and 1218 cm<sup>-1</sup> (C-O-C str.).

Chalcones are convenient starting material for the synthesis of pyrazolines, pyrimidines and isoxazolines due to their α, β-unsaturated moiety. The absence of carbonyl stretching frequency in the region of 1665 cm<sup>-1</sup> confirms the formation of products. In the first path way compound **1A** and **1B** were treated with hydrazides of benzotriazole, mercaptobenzthiazole and phenylhydrazine hydrate resulting in the formation of pyrazoline containing nuclei



**Table 1.** Physical and analytical data of synthesized compounds

Compound	Molecular Formula	Mol. weight	M.P., °C	Yield, %	Elemental analysis, calculated/(found) %		
					C	H	N
<b>1A</b>	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	268	92	70	67.16 (67.06)	4.51 (4.44)	10.44(10.36)
<b>1B</b>	C <sub>16</sub> H <sub>15</sub> NO <sub>2</sub>	253	76	75	75.87(75.79)	5.97(5.90)	5.53(5.45)
<b>2A</b>	C <sub>23</sub> H <sub>19</sub> N <sub>7</sub> O <sub>3</sub>	441	210	68	62.58(62.49)	4.34(4.25)	22.21(22.16)
<b>2B</b>	C <sub>24</sub> H <sub>22</sub> N <sub>6</sub> O <sub>2</sub>	426	228	72	67.59(67.50)	5.20(5.11)	19.71(19.63)
<b>3A</b>	C <sub>24</sub> H <sub>19</sub> N <sub>5</sub> O <sub>3</sub> S <sub>2</sub>	489	182	78	58.88(58.79)	3.91(3.82)	14.31(14.22)
<b>3B</b>	C <sub>25</sub> H <sub>22</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	474	210	65	63.27(63.18)	4.67(4.58)	11.81(11.73)
<b>4A</b>	C <sub>21</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	358	158	77	70.38(70.30)	5.06(5.00)	15.63(15.56)
<b>4B</b>	C <sub>22</sub> H <sub>21</sub> N <sub>3</sub> O	343	160	70	76.94(76.85)	6.16(6.09)	12.24(12.14)
<b>5A</b>	C <sub>15</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub>	283	196	75	63.60(63.51)	4.63(4.55)	14.83(14.74)
<b>5B</b>	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	268	206	80	71.62(71.56)	6.01(5.92)	10.44(10.32)
<b>6A</b>	C <sub>16</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub>	310	208	64	61.93(61.84)	4.55(4.42)	18.06(17.93)
<b>6B</b>	C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>	295	210	69	69.14(69.05)	5.80(5.70)	14.23(14.14)
<b>7A</b>	C <sub>16</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S	326	160	71	58.88(58.79)	4.32(4.22)	17.17(17.09)
<b>7B</b>	C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> OS	311	156	67	65.57(65.48)	5.50(5.41)	13.49(13.38)

**Table 2.** Antimicrobial activity of synthesized compounds (500 ppm)

Compound	Code	Antibacterial activity (Activity index)				Antifungal activity (Activity index)	
		<i>K.pneumoniae</i>	<i>P. aeruginosa</i>	<i>E.Coli</i>	<i>B.subtilis</i>	<i>C.albicans</i>	<i>A. fumigatus</i>
<b>2A</b>	A	14	14	20	10	15	16
<b>2B</b>	B	22	12	18	15	12	-
<b>3A</b>	C	12	20	22	19	18	12
<b>3B</b>	D	18	14	16	17	-	17
<b>4A</b>	E	23	-	12	21	12	-
<b>4B</b>	F	20	-	14	16	-	11
<b>5A</b>	G	-	18	08	19	12	08
<b>5B</b>	H	10	24	13	18	10	-
<b>6A</b>	I	-	15	23	20	16	-
<b>6B</b>	J	14	20	18	16	10	15
<b>7A</b>	K	13	-	16	22	11	12
<b>7B</b>	L	16	18	19	14	-	-
Standard 1	1	24	25	25	24	-	-
Standard 2	2	-	-	-	-	20	NA

Standard: 1 = Ciprofloxacin, 2 = Fluconazole dispersible; NA: Nil activity

Their IR, <sup>1</sup>H NMR and mass spectral studies confirmed the structure of these compounds. **6A-B** gave IR bands at 1692 cm<sup>-1</sup> (CONH str.), 1618 cm<sup>-1</sup> (C=N str.), 1728 cm<sup>-1</sup> (C=O str.) and 1350 & 1487 cm<sup>-1</sup> (NO<sub>2</sub> str.) and <sup>1</sup>H NMR signals at (δ) 6.06 (dd, 1H, H<sub>c</sub>), 5.30 (s, 1H, NH), 3.30 (dd, 1H, H<sub>b</sub>), 4.26 (dd, 1H, H<sub>a</sub>) and 5.8 (d, 1H, CONH) confirmed the synthesis of compound **6A-B** and pyrimidine ring. Similarly, compound **7A-B** gave some characteristic bands in the region between 3370 – 3380 cm<sup>-1</sup> (N-H str.), 1670 -1672 cm<sup>-1</sup> (CSNH str.), 3080 -3090 cm<sup>-1</sup> (C–H str., Ar–H), 1608 -1612 cm<sup>-1</sup> (C=N str.) and <sup>1</sup>H NMR signals at (δ) 6.06 -6.08 (dd, 1H, H<sub>c</sub>), 4.20 -4.30 (dd, 1H, H<sub>a</sub>), 3.28 -3.32 (dd, 1H, H<sub>b</sub>) and 5.0 -5.4 (s, 1H, CSNH) which, further confirmed the synthesis of compounds **7A-B**.

The synthesized compounds have also been characterized by their mass spectral and elemental analysis studies.

### Antimicrobial activity

The antimicrobial activity of synthesized compounds has been investigated against four bacterial strains i.e., *E. coli*, *B. subtilis*, *K. pneumoniae* and *P. aeruginosa* and two fungal strains *C. albicans* and *A. fumigatus*. (**Table 2**)

Sabourad dextrose agar media following agar well diffusion method at 500 µg / mL using DMSO as solvent. The zone of inhibition was measured in mm. Standard drugs used were ciprofloxacin (antibacterial) and fluconazole dispersible (antifungal). Compounds **3A**, **6A**, **7B** and **4A**, **6A**, **7A** showed better activity against *E.coli* and *B. subtilis*, respectively. The rest compounds shows moderate to good activity. Compounds **2B**, **4A**, **4B** and **3A**, **5B**, **6B** showed significant activity against *K. pneumoniae* and *P. aeruginosa*, respectively. Compounds **3A**, **6A** showed good activity against *C. albicans* and all synthesized compounds showed moderate to good activity against *A. fumigatus* as compared to standard drug, which was active against *A. fumigatus*.

## Experimental Section

### General Procedure

All reactions were carried out in a domestic microwave oven (Kenstar, Model No. OM-26 EGO). Melting points are uncorrected and determined in open capillaries. Reactions were monitored by thin layer chromatography using silica gel-G as adsorbent using ethyl acetate: n-hexane (7: 3) as

eluent and products were detected by iodine vapors. IR spectra (KBr pellets) were recorded on Perkin-Elmer 1800 (FTIR) spectrometer.  $^1\text{H}$  NMR spectra ( $\text{DMSO}-d_6$ ) were taken on a Bruker DRX spectrometer (300 MHz FT NMR) using TMS as internal standard and chemical shift were expressed in  $\delta$ . Mass spectra were taken on a Jeol SX-102/PA-6000 (EI) spectrometer. Elemental analysis was carried out on C, H, N analyzer (Elemental Vario Carlo Alba 1108). The results were found to be in good agreement with the calculated values ( $\pm 0.2\%$ ).

#### Synthesis of **1A** and **1B**

It is prepared by the reaction of mixture of acetanilide (0.01 mol), aldehydes (0.01 mol), aqueous NaOH (30%) in methanol (50 mL). The reaction mixture was stirred for 1 hr. Then the reaction mixture was irradiated for 6-8 minutes in MW at 600 W. After completion of reaction, the viscous mass was poured into ice cold water with vigorous stirring and left over night for complete precipitation. The resultant solid was dried and recrystallized from ethanol.

#### Synthesis of **2A**, **2B**, **3A**, **3B**, **4A** and **4B**

Equimolar amounts of chalcone 1A-B (0.01 mol), substituted hydrazides (0.01 mol) in ethanol (50 mL) were taken in an Erlenmeyer flask and 2-3 mL of glacial acetic acid was added to it. The reaction mixture was mixed thoroughly and irradiated for 6-8 minutes at 720 W with intermitted irradiation for 30 sec. interval. On completion of reaction (as monitored by TLC) resultant mass was poured into ice cold water with vigorous stirring. The solid obtained was filtered, washed with ethanol and recrystallized from ethanol.

#### Synthesis of **5A** and **5B**

It is prepared by reacting purified mixture of chalcone (0.01 mol), hydroxylamine hydrochloride (0.01 mol) and of NaOH (30%) in ethanol (50 mL) under microwave irradiation for 4-6 minutes at 720W. Completion of reaction was monitored by TLC. Excess of solvent was removed by evaporation; obtained mass was poured into ice water with vigorous stirring. It was kept over night. The resultant solid product was filtered, washed and recrystallized from acetone.

#### Synthesis of **6A**, **6B**, **7A** and **7B**

It is prepared by reacting purified mixture of chalcone (1A-B) (0.01 mol), compounds urea or thiourea (0.01 mol) in ethanol (50 mL) and 2-3 drops of conc. HCl. Reaction mass was irradiated for 7-10 minute in microwave at 960 W. Excess of solvent was removed, poured in ice-cold water, filtered, recrystallized from ethanol.

### Spectral Data

#### 3-(3-Nitrophenyl)-N-phenyl prop-2-enamide (**1A**)

IR (KBr,  $\text{cm}^{-1}$ ): 3315 (NH), 3018 (C-H str. Ar-H), 1666 (C=O), 1602 (C=C), 1540, 1499 ( $\text{NO}_2$ );  $^1\text{H}$  NMR ( $\delta$ ): 6.35-7.40 (m, 9H, Ar), 6.30 (d, 1H, CH vinyl), 5.95 (d, 1H, CH vinyl), 5.26 (s, 1H, NH); Mass ( $m/z$ ): 268 [ $\text{M}$ ] $^{+}$ .

#### 3-(4-Methoxyphenyl)-N-phenyl prop-2-enamide (**1B**)

IR (KBr,  $\text{cm}^{-1}$ ): 3311 (NH), 3014 (C-H str., ArH), 1599 (C=O), 1218 (C-O-C);  $^1\text{H}$  NMR ( $\delta$ ): 6.20-7.30 (m, 9H Ar-H), 6.10 (d, 1H, CH vinyl), 5.92 (d, 1H, CH vinyl), 5.24 (s, 1H, NH), 3.5 (s, 3H,  $\text{OCH}_3$ ); Mass ( $M/Z$ ): 253 [ $\text{M}$ ] $^{+}$ .

#### 2-(1H-benzotriazol-1-yl)-1-[5-(3-nitrophenyl)-3-(phenylamino)-4,5-dihydro-1H-pyrazol-1-yl]ethanone (**2A**)

IR (KBr,  $\text{cm}^{-1}$ ): 3348 (NH), 3022 (C-H str., ArH), 2962 ( $\text{CH}_2$ ), 1815 (C=O), 1683 (C=N), 1606, 1415 ( $\text{NO}_2$ );  $^1\text{H}$ NMR ( $\delta$ ): 6.64-7.96 (m, 13H, Ar), 6.40 (dd, 1H,  $\text{H}_c$ ), 5.33 (s, 1H, NH), 4.54 (dd, 1H,  $\text{H}_a$ ), 3.48 (dd, 1H,  $\text{H}_b$ ), 3.24 (s, 2H,  $\text{CH}_2$ ); Mass ( $m/z$ ): 441 [ $\text{M}$ ] $^{+}$ .

#### 2-(1H-benzotriazol-1-yl)-1-[5-(4-methoxyphenyl)-3-(phenylamino)-4,5-dihydro-1H-pyrazol-1-yl]ethanone (**2B**)

IR (KBr,  $\text{cm}^{-1}$ ): 3345 (NH), 3018 (C-H str., Ar-H), 2954 ( $\text{CH}_2$ ), 1812 (C=O), 1678 (C=N), 1225 (C-O-C);  $^1\text{H}$  NMR ( $\delta$ ): 6.50-7.86 (m, 13H, Ar), 6.36 (dd, 1H,  $\text{H}_a$ ), 3.46 (dd, 1H,  $\text{H}_b$ ), 3.22 (s, 2H,  $\text{CH}_2$ ), 3.60 (s, 3H,  $-\text{OCH}_3$ ); Mass ( $m/z$ ): 426 [ $\text{M}$ ] $^{+}$ .

#### 2-(1,3-Benzothiazol-2-yl sulfanyl)-1-[5-(3-nitrophenyl)-3-(phenylamino)-4,5-dihydro-1H-pyrazol-1-yl] ethanone (**3A**)

IR (KBr,  $\text{cm}^{-1}$ ): 3348 (NH), 3018 (C-H str. Ar-H), 2950 ( $\text{CH}_2$ ), 1820 (C=O), 1650 (C=N), 1600, 1410 ( $\text{NO}_2$ );  $^1\text{H}$  NMR ( $\delta$ ): 6.65-7.35 (m, 13H, Ar-H), 6.21 (dd, 1H,  $\text{H}_c$ ), 5.22 (s, 1H, NH), 4.40 (dd, 1H,  $\text{H}_a$ ), 3.20 (dd, 1H,  $\text{H}_b$ ), 2.78 (t, 1H,  $\text{H}_c$ ), 2.89 (s, 2H,  $\text{CH}_2$ ); Mass ( $m/z$ ): 489 [ $\text{M}$ ] $^{+}$ .

#### 2-(1,3-Benzothiazol-2-yl-sulfanyl)-1-[5-(4-methoxyphenyl)-3-(phenylamino)-4,5-dihydro-1H-pyrazol-1-yl]ethanone (**3B**)

IR (KBr,  $\text{cm}^{-1}$ ): 3344 (NH), 3015 (C-H str., Ar-H), 2946 ( $\text{CH}_2$ ), 1816 (C=O), 1647 (C=N), 1220 (C-O-C);  $^1\text{H}$ NMR ( $\delta$ ): 6.42-7.98 (m, 13H, Ar-H), 6.15 (dd, 1H,  $\text{H}_c$ ), 5.18 (s, 1H, NH), 4.32 (dd, 1H,  $\text{H}_a$ ), 3.14 (dd, 1H,  $\text{H}_b$ ), 2.84 (s, 2H,  $\text{CH}_2$ ), 3.80 (s, 3H,  $\text{OCH}_3$ ); Mass ( $m/z$ ): 474 [ $\text{M}$ ] $^{+}$ .

#### 5-(3-Nitrophenyl)-N,1-diphenyl-4,5-dihydro-1H-pyrazol-3-amine (**4A**)

IR (KBr,  $\text{cm}^{-1}$ ): 3351 (NH), 3096 (C-H str., Ar-H), 2949 ( $\text{CH}_2$ ), 1610 (C=N), 1338, 1487 ( $\text{NO}_2$ );  $^1\text{H}$ NMR ( $\delta$ ): 6.25-7.40 (m, 14H, Ar-H), 6.34 (dd, 1H,  $\text{H}_c$ ), 5.1 (s, 1H, NH), 4.50 (dd, 1H,  $\text{H}_a$ ), 3.46 (dd, 1H,  $\text{H}_b$ ); Mass ( $m/z$ ): 358 [ $\text{M}$ ] $^{+}$ .

#### 5-(4-Methoxyphenyl)-N,1-diphenyl-4,5-dihydro-1H-pyrazol-3-amine (**4B**)

IR (KBr,  $\text{cm}^{-1}$ ): 3350 (NH), 3090 (C-H str., Ar-H), 2946 ( $\text{CH}_2$ ), 1615 (C=N), 1214 (C-O-C);  $^1\text{H}$  NMR ( $\delta$ ): 6.30-7.20 (m, 14H, Ar-H), 6.20 (dd, 1H,  $\text{H}_c$ ), 5.5 (s, 1H, NH), 4.40 (dd, 1H,  $\text{H}_a$ ), 3.42 (dd, 1H,  $\text{H}_b$ ), 3.3 (s, 3H,  $-\text{OCH}_3$ ); Mass ( $m/z$ ): 343 [ $\text{M}$ ] $^{+}$ .



**5-(3-Nitrophenyl)-N-phenyl-4,5-dihydro-1,2-oxazol-3-amine (5A)**

IR (KBr,  $\text{cm}^{-1}$ ): 3348 (NH), 3089 (C-H str., Ar-H), 2931 ( $\text{CH}_2$ ), 1638 ( $\text{C}=\text{N}$ ), 1450, 1352 ( $\text{NO}_2$ );  $^1\text{H}$ NMR ( $\delta$ ): 6.82-7.39 (m, 9H, Ar), 6.16 (dd, 1H,  $\text{H}_c$ ), 5.4 (s, 1H, NH), 4.38 (dd, 1H,  $\text{H}_a$ ), 3.40 (dd, 1H,  $\text{H}_b$ ); Mass ( $m/z$ ): 283  $[\text{M}]^+$ .

**5-(4-Methoxyphenyl)-N-phenyl-4,5-dihydro-1,2-oxazol-3-amine (5B)**

IR (KBr,  $\text{cm}^{-1}$ ): 3344 (NH), 3080 (C-H str., Ar-H), 2930 ( $\text{CH}_2$ ), 1630 ( $\text{C}=\text{N}$ ), 1210 ( $\text{C}-\text{O}-\text{C}$ );  $^1\text{H}$ NMR ( $\delta$ ): 6.95-7.25 (m, 9H, Ar-H), 6.10 (dd, 1H,  $\text{H}_c$ ), 4.9 (s, 1H, NH), 4.30 (dd, 1H,  $\text{H}_a$ ), 3.36 (dd, 1H,  $\text{H}_b$ ), 3.3 (s, 3H,  $-\text{OCH}_3$ ); Mass ( $m/z$ ): 268  $[\text{M}]^+$ .

**6-(3-Nitrophenyl)-4-(phenylamino)-5,6-dihydropyrimidin-2-(1H)-one (6A)**

IR (KBr,  $\text{cm}^{-1}$ ): 3380 (NH), 3080 (C-H str., Ar-H), 1692 (CONH), 1618 ( $\text{C}=\text{N}$ ), 1350, 1487 ( $\text{NO}_2$ ), 1728 ( $\text{C}=\text{O}$ );  $^1\text{H}$ NMR ( $\delta$ ): 6.80-7.48 (m, 9H, Ar-H), 6.06 (dd, 1H,  $\text{H}_c$ ), 5.3 (s, 1H, NH), 3.30 (dd, 1H,  $\text{H}_b$ ), 4.26 (dd, 1H,  $\text{H}_a$ ), 5.8 (d, 1H, CONH); Mass ( $m/z$ ): 310  $[\text{M}]^+$ .

**6-(4-Methoxyphenyl)-4-(phenylamino)-5,6-dihydropyrimidin-2-(1H)-one (6B)**

IR (KBr,  $\text{cm}^{-1}$ ): 1680 (CONH), 3060 (C-H str., Ar-H), 1720 ( $\text{C}=\text{O}$ ), 1610 ( $\text{C}=\text{N}$ ), 1218 ( $\text{C}-\text{O}-\text{C}$ );  $^1\text{H}$ NMR ( $\delta$ ): 6.60-7.30 (m, 9H, Ar-H), 6.04 (dd, 1H,  $\text{H}_c$ ), 5.1 (s, 1H, NH), 3.28 (dd, 1H,  $\text{H}_b$ ), 4.20 (dd, 1H,  $\text{H}_a$ ), 5.6 (d, 1H, CONH); Mass ( $m/z$ ): 295  $[\text{M}]^+$ .

**6-(3-Nitrophenyl)-4-(phenylamino)-5,6-dihydropyrimidine-2-(1H)-thione (7A)**

IR (KBr,  $\text{cm}^{-1}$ ): 3387 (NH), 3089 (C-H str., Ar-H), 1672 (CSNH), 1612 ( $\text{C}=\text{N}$ ), 1389, 1428 ( $\text{NO}_2$ );  $^1\text{H}$ NMR ( $\delta$ ): 6.28-7.46 (m, 9H, Ar-H), 6.08 (dd, 1H,  $\text{H}_c$ ), 5.1 (s, 1H, NH), 3.32 (dd, 1H,  $\text{H}_b$ ), 4.30 (dd, 1H,  $\text{H}_a$ ), 5.0 (d, 1H, CSNH); Mass ( $m/z$ ): 326  $[\text{M}]^+$ .

**6-(4-Methoxyphenyl)-4-(phenylamino)-5,6-dihydropyrimidine-2-(1H)-thione (7B)**

IR (KBr,  $\text{cm}^{-1}$ ): 1670 (CSNH), 3080 (C-H str., Ar-H), 1608 ( $\text{C}=\text{N}$ ), 3378 (NH);  $^1\text{H}$ NMR ( $\delta$ ): 6.20-7.40 (m, 9H, Ar-H), 6.06 (dd, 1H,  $\text{H}_c$ ), 5.2 (s, 1H, NH), 4.20 (dd, 1H,  $\text{H}_a$ ), 3.28 (dd, 1H,  $\text{H}_b$ ), 5.4 (s, 1H, CSNH); Mass ( $m/z$ ): 311  $[\text{M}]^+$ .

**Conclusion**

The purpose of the research is the development of new potent bioactive molecules with less toxic, safer and easily available methods. From the literature survey it is evident that Microwave Induced Organic Reaction Enhancement (MORE) chemistry offers a simple, nonconventional technique for the synthesis of wide variety of compounds including biologically important heterocyclic compounds, co-ordination compounds etc.

The results of the antimicrobial screening indicated that the synthesized derivatives in which 3- $\text{NO}_2$  substituted

benzene rings attached to the pyrazoline moiety show excellent activity whereas 4- $\text{OCH}_3$  substituted benzene rings attached to the pyrimidine moiety show good activity against *K. pneumoniae* as compared to other compounds. Compounds containing isoxazole moiety are moderately active against both bacteria and fungi.

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