

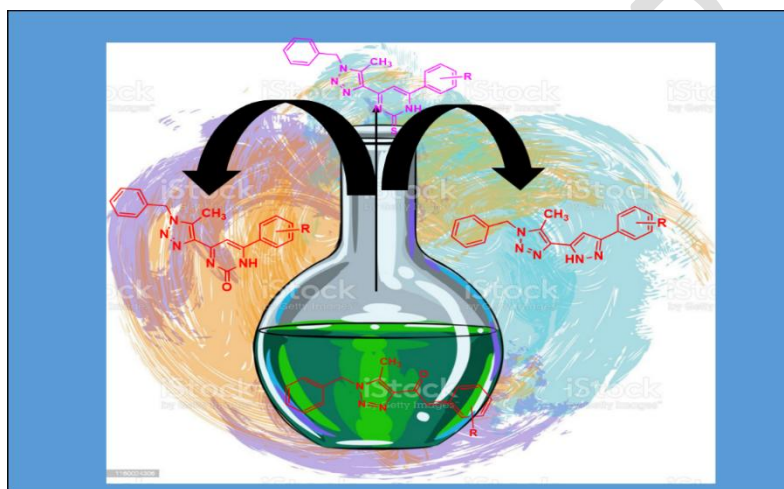
# A Novel Synthesis of 1,2,3triazole substituted pyrimidine, pyrazole by using 1,2,3triazolchalcone

## Abstract:

A series of 1- benzyl-5-methyl 1,2,3 triazole pyrimidine , 1- benzyl-5-methyl 1,2,3 triazole pyrazole were synthesised by using intermediate as phenyl Substituted prop-2-en-1-one .We obtained pyrazole when we treated propenones by using hydrazine hydrate and we obtained pyrimidine by using urea and thiourea .Conformations of the compounds were done by <sup>1</sup>HNMR and C<sup>13</sup> NMR analysis and these compounds were screened for antimicrobial activities .

**Keywords :** phenyl Substituted prop-2-en-1-one,urea, thiourea, hydrazine hydrate.

## Graphical Abstract



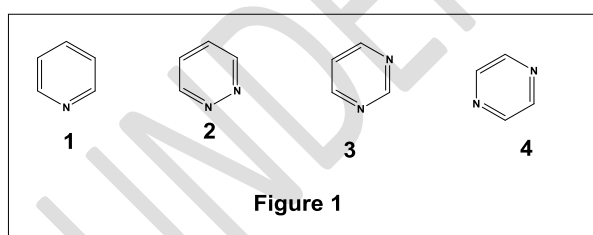
## Introduction:

Antimicrobial resistance has become a rapidly growing global issue. Among the two million people who become infected with bacterial infections in hospital every year, 70% of cases today involve strains that resist at least one drug.[1] In communities and hospitals around the world, the number of people suffering from antibiotic-resistant infections continues to grow.[2] A major cause for concern in the UK is methicillin-resistant *Staphylococcus aureus* (MRSA), which was at low levels a decade ago, but now accounts for ca. 50% of all *S. aureus* isolates.[3] Significant investments and research in the field of anti-infectious drugs are now desperately needed to prevent a public health crisis. The main cause for antibiotic resistance is antibiotic use. In the case of an antibiotic, it has been well

documented that resistance is primarily caused by continued dependence and careless use of these antibacterial.[4] and more and more proof is obtained suggesting that the same can be true for the emergence of resistance .[5][6] The potential cross-resistance of antibiotics and its bias due to the common resistance mechanism are particularly concerning.[7][8] Metal strength is observed due to contaminated environments.[9][10] The result of continued exposure to the antibacterial environment is an enrichment of bacteria that are inherently resistant to antimicrobials or have developed a resistance mechanism to these substances.[11][12] Structural modification of the antimicrobial drugs to which resistance has developed has proven to be an effective way to extend the life of antifungal agents like axles.[13] Antiviral agents like non-nucleoside reverse transcriptase inhibitors.[14]

Heterocyclic compounds are abundant in nature and they are of great importance, to live because of their structural sub units exist in a number of natural products such as vitamins, hormones and antibiotics.[15][16]. As a result, they have brought desirable attention to the design of biologically active molecules.[17][18] As well as advanced organic chemistry[19][20] Additionally in heterocyclic compounds nitrogen containing heterocyclic are an vital elegance of compounds in the medicinal chemistry and additionally contributed to the society from organic and commercial factor which helps to recognize significant procedures.[21] Totally unsaturated membered six-ring containing nitrogen is called azine [22] or pyridine (1) with two nitrogen atoms is known as diazine [23], and with a nitrogen at 1,2-position, it is known as pyridine (2), at 1,three-function as pyrimidine (3), and at 1,4-position is known as pyrazine (4) [figure1].However our main focus is on biological activities of pyrimidine as well as pyrazole .

**Figure 1: pyrazine**



## Experimental Section

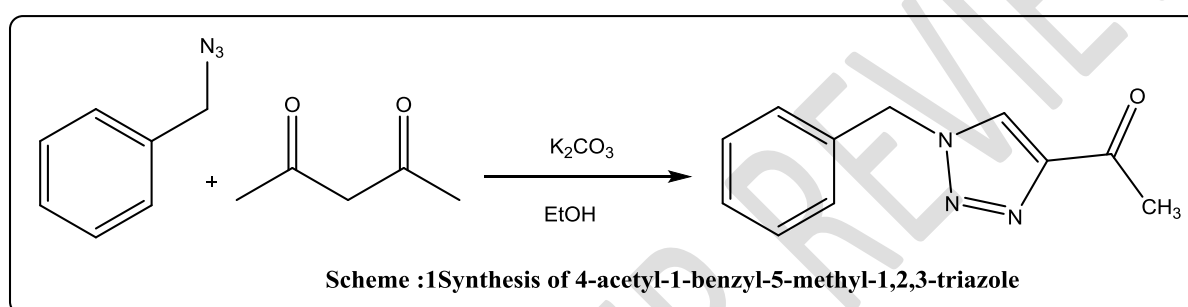
All chemicals, reagents and solvents were of commercially high purity grade purchased from Avra Synthesis Pvt. Ltd. and Merck Pvt. Ltd. India.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded in  $\text{CDCl}_3$  on Bruker Avance 300 MHz spectrometer and the chemical shifts are reported as  $\delta$  values in parts per million (ppm) relative to TMS , with coupling constant (J) values in Hertz (Hz). In  $^1\text{H}$  NMR, the abbreviation of splitting refers

as s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet, dd=doublet of doublet and bs=broad singlet.

## Materials and Methods

### 1. General procedure for Synthesis of 4-acetyl-1-benzyl-5-methyl-1,2,3-triazole

**Fig 2: Synthesis of 4-acetyl-1-benzyl-5-methyl-1,2,3-triazole**

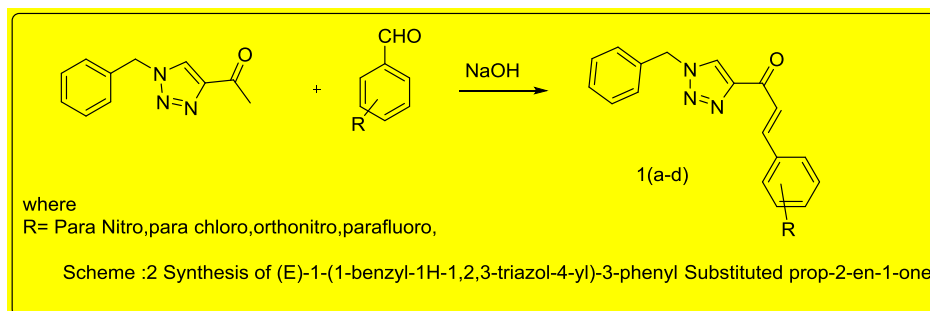


A mixture of benzyl azide (3.00 g, 0.022mole) , acetyl acetone (2.25 g, 0.0225mole), potassium carbonate (6.23 g, 0.045mole ) and absolute ethanol (95%, 15 ml) was taken in a round bottomed flask which was equipped with stirrer. The reaction mixture was stirred at 75°C for 30 min. The progress of the reaction was monitored by TLC. After the completion of the reaction, the solvent was removed under vacuum residual mass obtained excess of ice-water was added and neutralized with 10% HCl (20 ml). The product was extracted with diethyl ether (20 ml) and the extract was dried over anhydrous sodium sulphate. Evaporation of the solvent gave the crude product, which was purified by column chromatography using petroleum ether: ethylacetate (98:3) as eluent and recrystallized from absolute ethanol.[24]

### 2. Genral procedure for Synthesis of (E)-1-(1-benzyl-1H-1,2,3-triazol-4-yl)-3-phenyl Substituted prop-2-en-1-one [1]

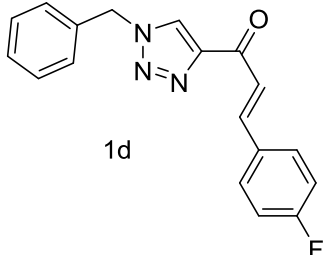
A mixture of 4-acetyl-1-benzyl-5-methyl-1,2,3-triazole,(0.2 g,0.009mole) and aromatic/hetero aromatic aldehydes, (1.0 eq) and 50% aqueous sodium hydroxide solution (1 ml) was stirred for 4–7 min at room temperature and poured into excess of crushed ice and neutralized with dilute hydrochloric acid. The chalcone derivatives which precipitated as solids were filtered and recrystallized from ethanol.[25]

**Fig 3 :** Synthesis of (E)-1-(1-benzyl-1H-1,2,3-triazol-4-yl)-3-phenyl Substituted prop-2-en-1-one



**Table:1** Characterisation data of Synthesised phenyl Substituted prop-2-en-1-one

Product	Colour	Yield and Melting Point
<p>1a</p>	Yellowish ur	70% 191 <sup>0</sup> C
<p>1b</p>	White colour	85% 170 <sup>0</sup> C
<p>1c</p>	Yellowish vn Colour	72% 193 <sup>0</sup> C

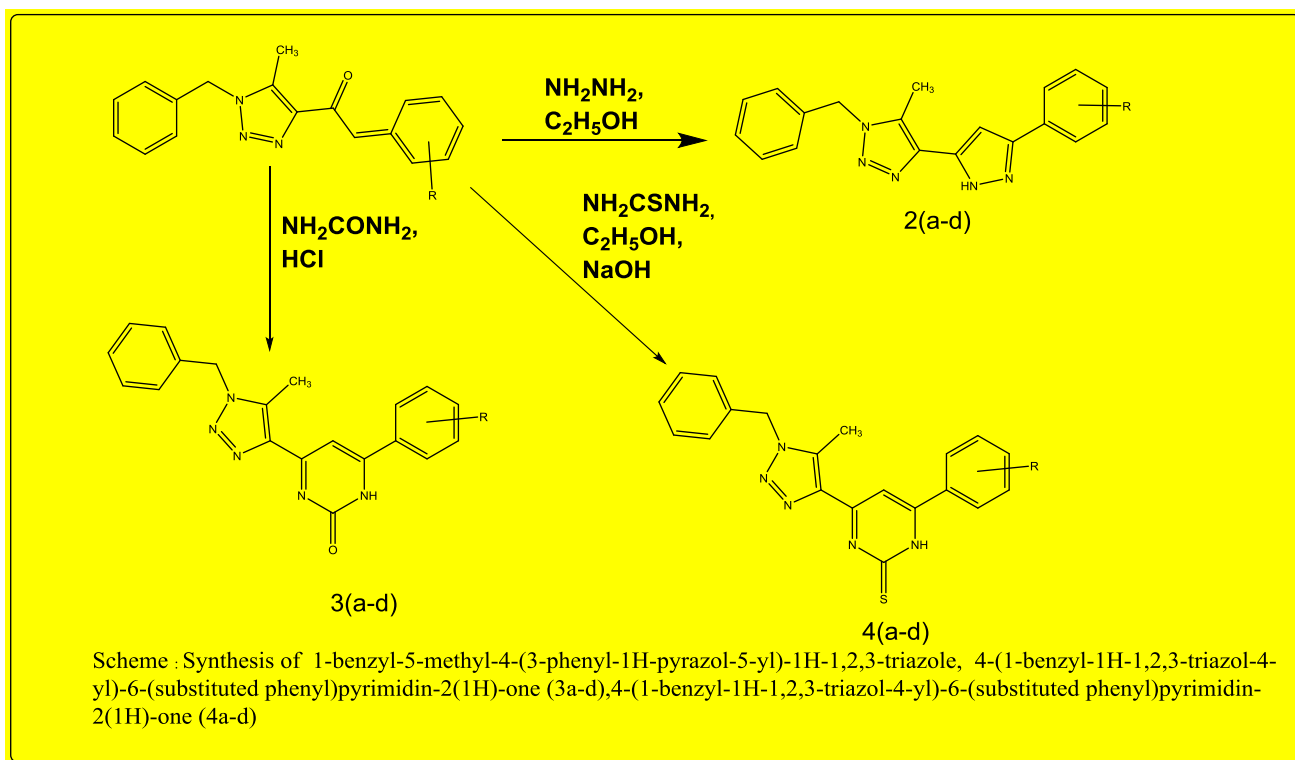
 <p>1d</p>	Brown Colour	75% 188 <sup>0</sup> C
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### 3. Genral procedure for synthesis of 1- benzyl-5-methyl 1,2,3triazole pyrimidine:

A mixture of chalcone (2.5 g, 10 mmol) and different nucleophilic reagents, like urea and thiourea (10 mmol), was dissolved in alcoholic sodium hydroxide (4 g NaOH and 10 mL ethanol) and was stirred for about 2-3 hours with a magnetic stirrer and it was then poured into 400 ml of cold water with continuous stirring for an hour, and after that, we kept the mixture in a refrigerator for 24 hours. Precipitate obtained was filtered, washed, and recrystallized (mostly in ethanol). [25]

### 4. General procedure for synthesis of 1- benzyl-5-methyl 1,2,3 triazole pyrazole

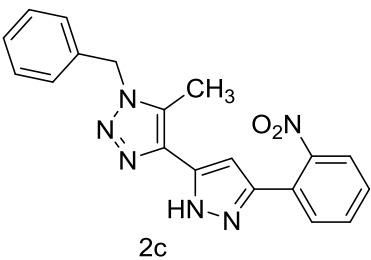
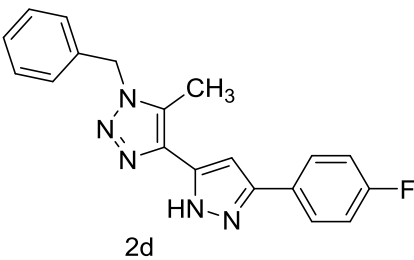
Here we dissolved a mixture of chalcone (2.5 g, 10 mmol) and different nucleophilic reagents, namely, hydrazine hydrate (10 mmol), 50 ml ethanol, and furthermore we added a few drops of conc. HCl, the reaction mixture was refluxed for 4 hrs and after that, we poured the mixture to crushed ice. Precipitate obtained was filtered, dried, and recrystallized from ethanol. [25]



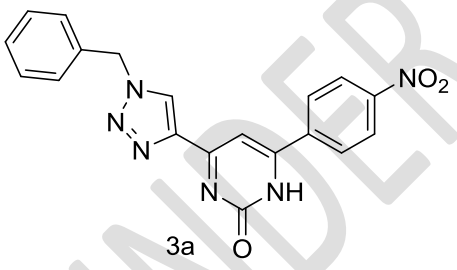
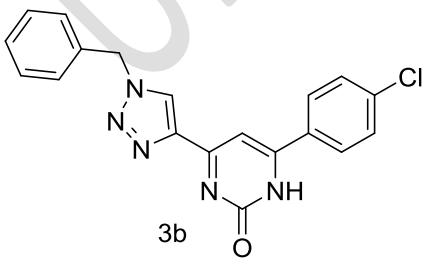
**Fig 4: synthesis of 1- benzyl-5-methyl 1,2,3 triazole pyrazole**

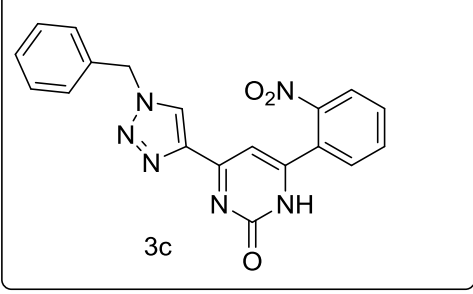
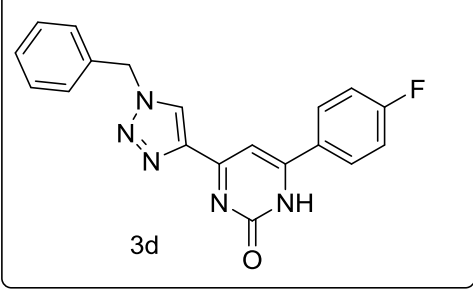
**Table:2 Characterisation data of Synthesised 1-benzyl-5-methyl-4-(3-phenyl-1H-pyrazol-5-yl)-1H-1,2,3-triazole(2a-d)**

Product	Colour	Yield and Melting pt
<p>2a</p>	Yellowish colour	65% 167 <sup>0</sup> C
<p>2b</p>	White colour	70% 165 <sup>0</sup> C

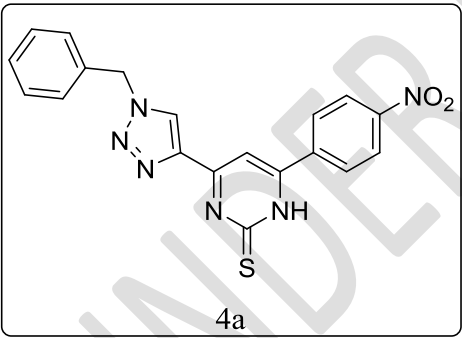
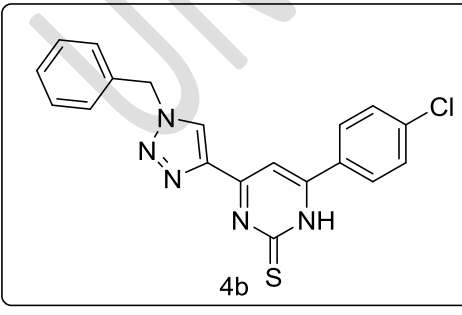
 <p>2c</p>	Brownish colour	75% 163 <sup>0</sup> C
 <p>2d</p>	Yellow colour	70% 167 <sup>0</sup> C

**Table: 3 Characterisation data of Synthesised 4-(1-benzyl-1H-1,2,3-triazol-4-yl)-6-(substituted phenyl)pyrimidin-2(1H)-one (3a-d)**

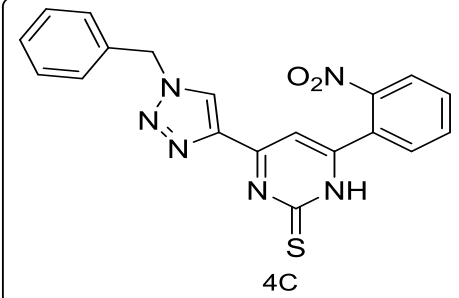
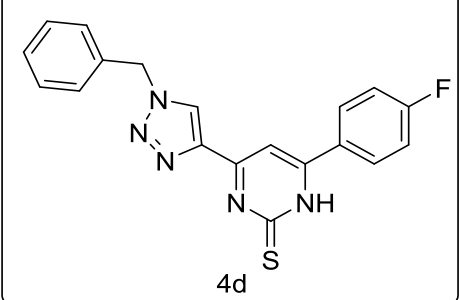
Product	Colour	Yield and Melting nt
 <p>3a</p>	Yellowish flakes	70% 173 <sup>0</sup> C
 <p>3b</p>	White flakes	75% 178 <sup>0</sup> C

 <p>3c</p>	Orange flakes	78% 173 <sup>o</sup> C
 <p>3d</p>	White Flakes	80% 169 <sup>o</sup> C

**Table: 4** Characterisation data of Synthesised 4-(1-benzyl-1H-1,2,3-triazol-4-yl)-6-(substituted phenyl)pyrimidin-2(1H)-one (4a-d)

Product	Colour	Yield and Melting pt
 <p>4a</p>	Brownish Crystals	80% 178 <sup>o</sup> C
 <p>4b</p>	White crystals	85% 177 <sup>o</sup> C



 <p>4c</p>	<b>Orange stals</b>	<b>Colour</b>  <b>80% 170<sup>0</sup>C</b>
 <p>4d</p>	<b>White Crystals</b>	<b>75% 168<sup>0</sup>C</b>

### Spectral data of Synthesised compounds

#### Compound 1a:

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):**  $\delta$  5.27 (2H, s), 5.73 (1H, d,  $J = 10.0$  Hz), 6.82 (2H, d,  $J = 8.0$ , 1.1, 0.5 Hz), 7.18-7.45 (6H, 7.25 (d,  $J = 10.0$  Hz), 7.28 (d,  $J = 7.8$ , 1.6, 1.3, 0.5 Hz), 7.32 (t,  $J = 7.4$ , 1.5 Hz), 7.39 (t,  $J = 7.6$ , 1.8, 0.5 Hz)), 7.62 (2H, d,  $J = 8.1$ , 1.6, 0.5 Hz), 7.83 (1H, s).

**<sup>13</sup>C NMR:**  $\delta$  52.7 (1C, s), 114.3 (2C, s), 124.3 (1C, s), 126.3 (1C, s), 127.7-127.8 (3C), 127.7 (s), 127.8 (s)), 128.4 (2C, s), 128.6 (2C, s), 130.0 (1C, s), 131.0 (1C, s), 133.7 (1C, s), 135.9 (1C, s), 148.4 (1C, s), 178.4 (1C, s).

**m/z:** 334(100%), 335(19.5%)

#### Compound 1b:

**<sup>1</sup>H NMR: (DMSO-d<sup>6</sup>)**  $\delta$  5.28 (2H, s), 5.81 (1H, d,  $J = 9.7$  Hz), 7.22-7.46 (6H, 7.28 (d,  $J = 7.8$ , 1.6, 1.3, 0.5 Hz), 7.32 (t,  $J = 7.7$ , 1.6 Hz), 7.39 (t,  $J = 7.7$ , 1.8, 0.5 Hz), 7.40 (d,  $J = 9.7$  Hz)), 7.47-7.62 (4H, 7.54 (d,  $J = 8.1$ , 1.5, 0.5 Hz), 7.56 (d,  $J = 8.1$ , 1.4, 0.5 Hz)), 7.84 (1H, s).

**<sup>13</sup>C NMR:**  $\delta$  52.7 (1C, s), 124.3 (1C, s), 126.3 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 128.7 (2C, s), 129.8-130.1 (3C, 129.9 (s), 130.0 (s)), 131.0 (1C, s), 133.6-133.8 (2C, 133.7 (s), 133.7 (s)), 135.9 (1C, s), 178.4 (1C, s).

**m/z:** 323(100%), 324(19.5%), 325(32%)

**Compound 1c:**

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.28 (2H, s), 5.87 (1H, d, J = 9.5 Hz), 7.18-7.48 (10H), 7.25 (d, J = 8.3, 1.4, 1.3 Hz), 7.24 (t, J = 1.5, 0.5 Hz), 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.32 (t, J = 7.7, 1.6 Hz), 7.34 (d, J = 7.8, 1.5, 1.3 Hz), 7.39 (t, J = 7.7, 1.8, 0.5 Hz), 7.40 (d, J = 9.5 Hz), 7.41 (d, J = 8.3, 7.8, 0.5 Hz), 7.85 (1H, s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 115.0 (1C, s), 115.4 (1C, s), 124.3 (1C, s), 126.3 (1C, s), 127.2 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 130.2 (1C, s), 130.6 (1C, s), 131.0 (1C, s), 133.7 (1C, s), 135.9 (1C, s), 161.2 (1C, s), 178.4 (1C, s).

**m/z:** 334.11 (100.0%), 335.11 (19.5%), 336.11 (1.8%).

**Compound 1d:**

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.28 (2H, s), 5.91 (1H, d, J = 9.5 Hz), 7.22-7.61 (9H), 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.38 (t, J = 8.0, 0.5 Hz), 7.39 (t, J = 7.7, 1.8, 0.5 Hz), 7.40 (d, J = 9.5 Hz), 7.43 (d, J = 8.0, 1.6, 1.2 Hz), 7.54 (d, J = 8.1, 1.7, 1.2 Hz), 7.79-7.90 (2H), 7.84 (d, J = 1.7, 1.6, 0.5 Hz), 7.85 (s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 124.3 (1C, s), 126.3 (1C, s), 127.0 (1C, s), 127.2 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 128.7 (1C, s), 130.0 (1C, s), 130.4 (1C, s), 130.6 (1C, s), 131.0 (1C, s), 133.7 (1C, s), 135.9 (1C, s), 178.4 (1C, s).

**m/z:** 307.11 (100.0%), 308.12 (19.5%).

**Compound 2a**

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 2.52 (3H, s), 5.28 (2H, s), 6.70 (2H, d, J = 8.2, 1.2, 0.5 Hz), 6.81-7.02 (3H), 6.87 (d, J = 8.2, 1.4, 0.5 Hz), 6.97 (s), 7.24-7.45 (3H), 7.30 (t, J = 7.3, 1.5, 1.2 Hz), 7.38 (d, J = 7.9, 7.3, 1.1, 0.4 Hz), 7.82 (2H, d, J = 7.9, 1.4, 0.4 Hz).

**<sup>13</sup>C NMR:** δ 9.6 (1C, s), 52.8 (1C, s), 108.1 (1C, s), 114.3 (2C, s), 127.3 (2C, s), 127.8 (1C, s), 128.4 (2C, s), 129.4 (2C, s), 133.5 (1C, s), 133.6-133.8 (2C, 133.7 (s), 133.7 (s)), 135.9 (1C, s), 137.1 (1C, s), 148.3-148.6 (2C, s), 148.4 (s), 148.5 (s).

**m/z:** 360.13 (100.0%), 361.14 (20.5%)

**Compound 2b**

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 2.54 (3H, s), 5.37 (2H, s), 6.97 (1H, s), 7.24-7.53 (5H, 7.30 (tdd, J = 7.3, 1.5, 1.2 Hz), 7.38 (dddd, J = 7.9, 7.3, 1.1, 0.4 Hz), 7.46 (ddd, J = 8.4, 1.4, 0.5 Hz)), 7.60 (2H, ddd, J = 8.4, 1.4, 0.5 Hz), 7.82 (2H, dtd, J = 7.9, 1.4, 0.4 Hz).

**<sup>13</sup>C NMR:** δ 9.6 (1C, s), 52.8 (1C, s), 108.1 (1C, s), 127.3 (2C, s), 127.8 (1C, s), 128.4 (2C, s), 128.6-128.8 (4C, 128.7 (s), 128.7 (s)), 133.5 (1C, s), 133.6-133.8 (3C, 133.7 (s), 133.7 (s), 133.7 (s)), 135.9 (1C, s), 137.1 (1C, s), 148.5 (1C, s).

**m/z:** 349.11 (100.0%), 351.11 (32.0%), 350.11 (20.5%).

### Compound 2c

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 2.54 (3H, s), 5.22 (2H, s), 6.53-6.76 (2H, 6.60 (d, J = 7.9, 7.6, 1.2 Hz), 6.70 (d, J = 8.1, 1.2, 0.5 Hz)), 6.81-7.03 (3H, 6.87 (d, J = 7.9, 1.3, 0.5 Hz), 6.95 (d, J = 8.1, 7.6, 1.3 Hz), 6.97 (s)), 7.24-7.45 (3H, 7.30 (t, J = 7.3, 1.5, 1.2 Hz), 7.38 (d, J = 7.9, 7.3, 1.1, 0.4 Hz)), 7.82 (2H, d, J = 7.9, 1.4, 0.4 Hz).

**<sup>13</sup>C NMR:** δ 9.6 (1C, s), 52.4 (1C, s), 108.1 (1C, s), 115.8 (1C, s), 121.2 (1C, s), 127.3-127.3 (3C, 127.3 (s), 127.3 (s)), 127.8 (1C, s), 128.2 (1C, s), 128.3-128.5 (3C, 128.4 (s), 128.4 (s)), 133.5 (1C, s), 133.6-133.8 (2C, 133.7 (s), 133.7 (s)), 137.1 (1C, s), 144.3 (1C, s), 148.5 (1C, s).

**m/z:** 360.13 (100.0%), 361.14 (20.5%).

### Compound 2d

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 2.52 (3H, s), 5.37 (2H, s), 6.87-7.02 (3H, 6.93 (d, J = 8.5, 1.2, 0.6 Hz), 6.97 (s)), 7.19-7.45 (5H, 7.25 (d, J = 8.5, 1.2, 0.6 Hz), 7.30 (t, J = 7.3, 1.5, 1.2 Hz), 7.38 (d, J = 7.9, 7.3, 1.1, 0.4 Hz)), 7.82 (2H, d, J = 7.9, 1.4, 0.4 Hz).

**<sup>13</sup>C NMR:** δ 9.6 (1C, s), 52.8 (1C, s), 108.1 (1C, s), 115.4 (2C, s), 127.3 (2C, s), 127.8 (1C, s), 128.4 (2C, s), 130.1 (2C, s), 133.5 (1C, s), 133.6-133.8 (2C, 133.7 (s), 133.7 (s)), 135.9 (1C, s), 137.1 (1C, s), 148.5 (1C, s), 162.5 (1C, s).

**m/z:** 333.14 (100.0%), 334.14 (20.5%)

### Compound 3a

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.34 (2H, s), 6.47 (1H, s), 6.80 (2H, d, J = 8.0, 1.1, 0.4 Hz), 7.23-7.40 (5H, 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz)), 7.77-7.92 (3H, 7.83 (d, J = 8.0, 1.5, 0.4 Hz), 7.87 (s)).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 97.5 (1C, s), 114.3 (2C, s), 124.3 (1C, s), 127.1 (2C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 132.3 (1C, s), 133.7 (1C, s), 135.9 (1C, s), 146.0 (1C, s), 148.4 (1C, s), 151.7 (1C, s), 157.7 (1C, s).

**m/z:** 363.09 (100.0%), 365.09 (32.0%), 364.09 (20.5%).

### Compound 3b

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.34 (2H, s), 6.67 (1H, s), 7.22-7.40 (5H, 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz), 7.49-7.66 (4H, 7.55 (d, J = 8.7, 1.6, 0.5 Hz), 7.60 (d, J = 8.7, 1.5, 0.5 Hz)), 7.89 (1H, s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 97.5 (1C, s), 124.3 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 128.5 (2C, s), 128.7 (2C, s), 132.3 (1C, s), 133.6-133.8 (2C, 133.7 (s), 133.7 (s)), 135.9 (1C, s), 146.0 (1C, s), 151.7 (1C, s), 157.7 (1C, s).

**m/z:** 363.09 (100.0%), 365.09 (32.0%), 364.09 (20.5%), 366.09 (6.6%).

### Compound 3c

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.34 (2H, s), 6.48 (1H, s), 7.00-7.40 (7H, 7.06 (d, J = 8.3, 1.2, 0.5 Hz), 7.16 (d, J = 7.7, 7.6, 1.2 Hz), 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz)), 7.65-7.80 (2H, 7.73 (d, J = 8.3, 7.6, 1.4 Hz), 7.72 (d, J = 7.7, 1.4, 0.5 Hz)), 7.87 (1H, s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 97.5 (1C, s), 115.8 (1C, s), 121.5 (1C, s), 124.3 (1C, s), 124.9 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.2 (1C, s), 128.3-128.5 (3C, 128.4 (s), 128.4 (s)), 133.7 (1C, s), 135.9 (1C, s), 145.5 (1C, s), 146.0 (1C, s), 151.7 (1C, s), 157.7 (1C, s).

**m/z:** 374.11 (100.0%), 375.12 (20.5%), 375.11 (2.2%).

### Compound 3d

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.34 (2H, s), 6.70 (1H, s), 7.22-7.48 (7H, 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz), 7.42 (d, J = 8.4, 1.2, 0.5 Hz), 7.77-7.94 (3H, 7.83 (d, J = 8.4, 1.5, 0.5 Hz), 7.89 (s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 97.5 (1C, s), 115.4 (2C, s), 124.3 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 131.9 (2C, s), 132.3 (1C, s), 133.7 (1C, s), 135.9 (1C, s), 146.0 (1C, s), 151.7 (1C, s), 157.7 (1C, s), 162.5 (1C, s).

**m/z:** 347.12 (100.0%), 348.12 (20.5%).

### Compound 4a

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.31 (2H, s), 6.29 (1H, s), 6.86 (2H, d, J = 8.0, 1.1, 0.5 Hz), 7.22-7.40 (5H, 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz)), 7.64 (2H, d, J = 8.0, 1.6, 0.5 Hz), 7.81 (1H, s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 97.5 (1C, s), 114.3 (2C, s), 124.3 (1C, s), 127.1 (2C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 132.3 (1C, s), 133.7 (1C, s), 135.9 (1C, s), 146.0 (1C, s), 148.4 (1C, s), 151.7 (1C, s), 178.8 (1C, s).

**m/z:** 390.09 (100.0%), 391.09 (20.5%), 392.09 (4.5%)

### Compound 4b:

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.33 (2H, s), 6.48 (1H, s), 7.22-7.40 (5H, 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz), 7.47-7.73 (4H), 7.54 (d, J = 8.6, 1.5, 0.5 Hz), 7.66 (d, J = 8.6, 1.7, 0.5 Hz)), 7.83 (1H, s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 97.5 (1C, s), 124.3 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 128.5 (2C, s), 128.7 (2C, s), 132.3 (1C, s), 133.6-133.8 (2C, 133.7 (s), 133.7 (s)), 135.9 (1C, s), 146.0 (1C, s), 151.7 (1C, s), 178.8 (1C, s).

**m/z:** 379.07 (100.0%), 381.06 (32.0%), 380.07 (20.5%), 382.07 (6.6%)

### Compound 4c:

**<sup>1</sup>H NMR(DMSO-d<sup>6</sup>):** δ 5.31 (2H, s), 6.34 (1H, s), 6.80-7.04 (2H, 6.86 (d, J = 8.1, 1.1, 0.5 Hz), 6.97 (d J = 7.8, 7.4, 1.1 Hz), 7.22-7.40 (5H, 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz)), 7.57-7.74 (2H, 7.64 (d, J = 8.1, 7.4, 1.4 Hz), 7.68 (d, J = 7.8, 1.4, 0.5 Hz)), 7.81 (1H, s).

**<sup>13</sup>C NMR:** δ 52.7 (1C, s), 97.5 (1C, s), 115.8 (1C, s), 121.5 (1C, s), 124.3 (1C, s), 124.9 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.2 (1C, s), 128.3-128.5 (3C, 128.4 (s), 128.4 (s)), 133.7 (1C, s), 135.9 (1C, s), 145.5 (1C, s), 146.0 (1C, s), 151.7 (1C, s), 178.8 (1C, s).

**m/z:** 390.09 (100.0%), 391.09 (20.5%), 392.09 (4.5%).

### Compound 4d:

**<sup>1</sup>H NMR:** δ 5.33 (2H, s), 6.45 (1H, s), 7.17-7.40 (7H, 7.23 (d, J = 8.4, 1.2, 0.5 Hz), 7.28 (d, J = 7.8, 1.6, 1.3, 0.5 Hz), 7.30 (t, J = 7.7, 1.6 Hz), 7.34 (t, J = 7.7, 1.8, 0.5 Hz), 7.74-7.87 (3H, 7.80 (d, J = 8.4, 1.5, 0.5 Hz), 7.82 (s).

**$^{13}\text{C}$  NMR:**  $\delta$  52.7 (1C, s), 97.5 (1C, s), 115.4 (2C, s), 124.3 (1C, s), 127.7-127.8 (3C, 127.7 (s), 127.8 (s)), 128.4 (2C, s), 131.9 (2C, s), 132.3 (1C, s), 133.7 (1C, s), 135.9 (1C, s), 146.0 (1C, s), 151.7 (1C, s), 162.5 (1C, s), 178.8 (1C, s).

**m/z:** 363.10 (100.0%), 364.10 (20.5%), 365.09 (4.5%).

### Biological activity :

All recently pre-arranged mixtures were evaluated for antibacterial activity against *B. Subtilis* and *A. aerogenes* by utilizing plate dispersion method .[26] The circles of every fixation were put in three-fold on supplement agar medium cultivated with new bacterial societies separately. The brooding was completed at 37<sup>0</sup>c for 24 hrs.

**Results of the examination has been accounted for in the Table 5**

Compound Number	Minimum Inhibitory concentration Mg/disk meter of Zone of inhibition in mm)	
	B.s	A.nor
<b>2a</b>	5(10.2)	5(9.7)
<b>2b</b>	<5(7.4)	5(8.2)
<b>2c</b>	5(11.4)	10(10.2)
<b>2d</b>	10(9.2)	<5(7.1)
<b>3a</b>	<5(7.8)	5(9.1)
<b>3b</b>	5(9.1)	5(8.6)
<b>3c</b>	5(9.2)	5(8.7)
<b>3d</b>	5(9.1)	5(8.2)
<b>4a</b>	5(10.1)	5(9.7)
<b>4b</b>	<5(7.3)	<b>5(8.1)</b>
<b>4c</b>	<b>5(11.3)</b>	<b>10(10.3)</b>
<b>4d</b>	<b>10(9.3)</b>	<5(7.2)

## RESULTS AND DISCUSSION:

A series of 1-benzyl-5-methyl 1,2,3 triazole pyrazole, 4-(1-benzyl-1H-1,2,3-triazol-4-yl)-6-(substituted phenyl)pyrimidin-2(1H)-one derivatives were synthesised by using the intermediate as (E)-1-(1-benzyl-1H-1,2,3-triazol-4-yl)-3-phenyl Substituted prop-2-en-1-one. Upon reacting with hydrazine hydrate we obtained pyrazole and same intermediate upon reacting with urea and thiourea we obtained Pyrimidiene. Hence these compounds were Confirmed by spectral analysis and these compounds were Screened for pharmacological activities like antimicrobial by using B.Subtilis and A.aerogenes. Nitro substituted derivatives showed promising results than other derivatives.

## Conclusion :

In conclusion, the present method demonstrates an operationally simple and clean procedure for the synthesis of pyrazole and pyrimidiene using a catalytic amount of hydrazine hydrate, urea and thiourea. Moreover, the catalyst used is of low cost, recyclable, less toxic and moisture compatible. The yields of products were excellent within short reaction time. Therefore, this methodology is one of the valid contributions to the field of pyrazole and pyrimidiene synthesis. Most of the synthesized compounds have displayed potent biological activities. Pharmacological activities of the nitro substituted compounds gave good results.

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