PART C

Biginelli type reactions and synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition
IIIIC. 1.  INTRODUCTION

The most common route for the synthesis of dihydropyrimidone (DHPM) employs the
cyclocondensation of aromatic aldehydes, acetoacetate and urea in presence of HCl as catalyst,
which is one of the most well known and representatives multi component reaction is the
Biginelli reaction.[1]

In the Beginelli reaction 1,3-diketones are the most commonly employed counterparts and use of
acetophenone derivatives in this type of process is rare. Wang et al., in 2004 remarkably
broadened the application of Biginelli reaction wherein a one-pot cyclocondensation of ketones,
instead of 1,3-diketone with aldehydes and urea was reported to give substituted
diarylpyrimidinones.

In recent years synthesis of biological active compounds is in great demand. Pyrimidine nucleus
is found in many natural bioactive products possessing multiple biological and medical
properties. Some of these compounds serve as antihypertensive, antibacterial, and anti-
inflammatory agents.[3] The batzelladine alkaloids containing 3,4-DHPM isolated from marine
sources inhibits the binding of HIV envelope protein gp-120 to human CD4 cells.[4] Such
properties make these pyrimidones highly important.

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Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition

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IIIC. 2. SOME INTERESTING AND USEFUL EXAMPLES FROM THE LITERATURE

A novel and efficient one-pot method for the preparation of fused ring 3,4-dihydropyrimidin-2(1H)-ones and thiones from cyclocondensation of aldehydes, cyclic ketones and urea or thiourea using a catalytic amount of cupric chloride under mild condition is described. This new method has the advantage to give high yields, to be completed in short reaction times and simple product isolation procedure (Scheme IIIC.1).[22]

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\begin{center}
\includegraphics[width=0.8\textwidth]{scheme_iiic1.png}
\end{center}
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**Scheme IIIC.1.**

Synthesis of pyrimido[1,2-a]benzimidazole derivatives is based on the Biginelli like cyclocondensation of aromatic aldehydes and acetoacetamide derivatives with 2-amino benzimidazole containing a guanidine fragment. An efficient synthesis of novel pyrimido[1,2-a]benzimidazoles was achieved. The cyclocondensations were achieved by heating of the starting materials in dimethylformamide (DMF) under reflux conditions (Scheme IIIC.2).[23]

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\begin{center}
\includegraphics[width=0.8\textwidth]{scheme_iiic2.png}
\end{center}
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**Scheme IIIC.2.**

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*Synthesis of 4,6-diarylpymidin-2(1H)-ones (DAPMs) under sonic condition*
An efficient synthesis of 3,4-dihydropyrimidin-2(1H)-one derivatives has been described by Tu and co-workers using potassium hydrogen sulfate as the promoter in glycol solution for the Biginelli reaction. It can be applied not only to open-chained 1,3-dicarbonyl compounds, but also to cyclic 1,3-dicarbonyl compounds. Bifunctional compounds containing two dihydropyrimidinone units have also been synthesized using isophthalaldehyde and terephthalaldehyde (Scheme III.C.3).[24,25]

$$\begin{align*}
R - O & + \begin{array}{c}
\text{NH} \\
\text{NH}
\end{array}
\begin{array}{c}
\text{O} \\
\text{O}
\end{array}
\rightarrow
\begin{array}{c}
\text{NH} \\
\text{NH}
\end{array}
\begin{array}{c}
\text{O} \\
\text{O}
\end{array} \\
\text{KHSO}_4 \\
\text{ethylene glycol}
\end{align*}$$

$R = \text{aryl}; \; \text{R}^1 = \text{OEt, OMe, Me}$

Scheme III.C.3.

Salehi and Guo have reported a magnesium bromide-catalyzed facile and efficient one-pot synthesis of dihydropyrimidinones under solvent-free conditions. Besides $\beta$ ketoesters, $\beta$-diketones have also been employed and thiourea/N-methylurea were also used to furnish the corresponding dihydropyrimidinones, which are also of much interest from a biological activity point of view (Scheme III.C.4).[26]

$$\begin{align*}
R - O & + \begin{array}{c}
\text{NH} \\
\text{NH}
\end{array}
\begin{array}{c}
\text{O} \\
\text{O}
\end{array}
\rightarrow
\begin{array}{c}
\text{NH} \\
\text{NH}
\end{array}
\begin{array}{c}
\text{O} \\
\text{O}
\end{array} \\
\text{MgBr}_2 \\
45-90 \text{ min} \\
100 \degree \text{C}
\end{align*}$$

$R = \text{aryl}; \; \text{R}^1 = \text{OEt, OMe, Me, Ph; R}^2 = \text{H, Me}$

$X = \text{O, S}$

Scheme III.C.4.


*Synthesis of 4,6-diarylpymidin-2(1H)-ones (DAPMs) under sonic condition*
An efficient niobium(V) chloride-catalyzed synthesis of 3,4-dihydropyrimidinones has been described by Yadav and co-workers via the condensation reaction of an aldehyde, a β-keto ester, and urea or thiourea under ambient conditions. The study of this reaction using other Lewis acids such as indium(III) chloride, cerium(III) chloride, gadolinium(III) chloride, tantalum(V) chloride, and yttrium(III) chloride revealed that niobium(V) chloride was found to be superior in terms of conversion and reaction time. The other advantage of this catalyst is the reaction proceeded at room temperature where as the other Lewis acids required reflux conditions (Scheme IIIC.5).[27]

![Reaction Scheme IIIC.5.](image)

R = alkyl, aryl; R¹ = Me, Ph; R² = OEt, OMe, Me
X = O, S

(70-96 %)

Scheme IIIC.5.

Li et al. have reported a zinc-chloride, catalyzed, solvent-free protocol for the preparation of 3,4-dihydropyrimidin-2(1H)-ones by the condensation of an aldehyde, a 1,3-dicarbonyl compound, and urea or thiourea at 80 °C with shorter reaction times. The important feature of this method is that 2-furaldehyde furnished the desired products in 94–95% yields in 10 mins, which normally gives low yields (Scheme IIIC.6).[28]

![Reaction Scheme IIIC.6.](image)

R¹ = alkyl, aryl; R² = OEt, Me
X = O, S

(70-97 %)

Scheme IIIC.6.


Synthesis of 4,6-diarylpymridin-2(1H)-ones (DAPMs) under sonic condition
Trimethylsilyl triflate (1 mol %) mediated one-pot cyclocondensation reaction of aldehydes, β-keto esters and urea at room temperature in acetonitrile with shorter reaction times has been described by Bose et al. By using this procedure, a mitotickinesin Eg5 inhibitor monastrol has been prepared in 95% yield within 15 min. One mol% triethylsilyl triflate can also be used as a catalyst in acetonitrile at room temperature (Scheme IIC.7).[29]

\[
\begin{align*}
R = \text{alkyl, aryl; } R^1 = \text{Me, Et; } R^2 = \text{Me, Et, } ^1\text{Bu} \quad X = \text{O, S} \\
\text{Scheme IIC.7.}
\end{align*}
\]

A simplified green protocol for the Biginelli reaction catalyzed by p-toluenesulfonic acid using grindstone chemistry has been developed by Bose et al. This technique is convenient, time-saving, and also useful for kilogram scale operation (Scheme IIC.8).[30]

\[
\begin{align*}
R = \text{H, 4-OH, 4-OMe, 4-NO_2, 4-Cl} \quad X = \text{O, S} \\
\text{Scheme IIC.8.}
\end{align*}
\]

The facile preparation of these compounds by one-pot condensation of aldehydes, urea, and enolizable ketones has been reported by Sandhu et al. using bimetal system aluminum(III) chloride and potassium iodide in acetonitrile under reflux conditions.

Some other combinations of catalytic systems have also been studied and out of these, the most effective combination worked out to be the aluminum(III) chloride and potassium iodide system (Scheme III.C.9).[31]

![Chemical reaction diagram]

\[
\text{R} = \text{H, 4-OH, 4-OMe, 4-NO}_2, 4-\text{Cl}
\]

\[
\text{X} = \text{O, S}
\]

(82-90 %)

**Scheme III.C.9.**

Pan and co-workers have reported the use of trimethylsilyl chloride (TMSCl) as a facile and efficient reagent for the one-pot condensation of aldehydes, 1,3-dicarbonyl compounds, and urea (or thiourea) at room temperature to afford the corresponding dihydropyrimidinones. The advantages are a simple work-up by filtration, and aliphatic aldehydes also gave products in good yields (Scheme III.C.10).[32]

![Chemical reaction diagram]

\[
\text{R}^1 = \text{alkyl, aryl; R}^2 = \text{OEt, Me}
\]

\[
\text{X} = \text{O, S}
\]

(76-97 %)

**Scheme III.C.10.**

**IIIC. 2.1. CONCLUSIONS**

The above reported methods suffer from drawbacks such as use of stoichiometric amounts of catalysts, expensive reagents, prolonged reaction time and varying yields of the products. Therefore, developing a general, mild and simple method for the synthesis of 4,6-diarylpyrimidin-2(1H)-ones is necessary.


*Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition*
IIIC. 3. PRESENT WORK: A ONE-POT THREE-COMPONENT SYNTHESIS OF 4,6-DIARYLPYRIMIDIN-2(1H)-ONES (DAPMs) USING ATOMIZED SODIUM IN THF UNDER SONIC CONDITION

IIIC. 3.1. INTRODUCTION

In the present work we are reporting an effective and simple protocol for the synthesis of 4,6-diarylpyrimidin-2(1H)-ones using atomized sodium in THF via a one-pot three-component cyclocondensation of methyl ketones and urea with various substituted aryl aldehydes under ultrasonic condition. This one-pot route is mild, energy efficient and inexpensive. The yields are high (up to 90 %) and the reactions go to completion within 10–15 minutes as shown in the (Scheme IIIC.11).

![Scheme IIIC.11.](image)

IIIC. 3.2. RESULTS AND DISCUSSION

We started our investigations with various catalysts, in various solvents under different reaction conditions in order to develop a new method for the synthesis of 4,6-diarylpyrimidin-2(1H)-ones via a one-pot three-component Biginelli-like cyclocondensation reaction. To standardize the conditions all the reactions were carried out with 4-(N,N-dimethylamino)benzaldehyde, acetophenone and urea as model substrates. Initially we selected a series of metals and conducted the above reaction to get high yield of the desired product in THF. The results of this study are presented in Table IIIC.1. In order to verify whether THF is a suitable solvent or not, the reaction was carried out in various solvents and under solvent-free condition and the results of these studies are presented in Table IIIC.2. It was found that, atomized sodium in THF is ideal in terms of yield and the time of the completion of the reaction. For optimizing the amount of atomized sodium, we then, worked with different amounts of atomized sodium required for the reaction and the results are given in the Table IIIC.3. From this Table it is clear that, equivalent

*Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition*
amount of the metal is essential for the present reaction. The amount of THF required to give the maximum yield of the product is found to be 2 mL Table IIIC.4. From the data provided in the Tables III.C.1–4 it is also clear that, synthesis of 4,6-diarylpyrimidin-2(1H)-ones using atomized sodium/THF via a three-component one-pot Biginelli-like cyclocondensation under the influence of ultrasound at 35 kHz is efficient and gives high yield of the product in short duration.

**Table IIIC.1:** A comparative study on the synthesis of 4f with different metals

<table>
<thead>
<tr>
<th>Entry</th>
<th>Metal(^a)</th>
<th>Time (min)</th>
<th>Yield (%)(^{b,c})</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>Sodium</td>
<td>30–40</td>
<td>70</td>
</tr>
<tr>
<td>b</td>
<td>Atomized sodium</td>
<td>10–20</td>
<td>90</td>
</tr>
<tr>
<td>c</td>
<td>Aluminium</td>
<td>12–20</td>
<td>10</td>
</tr>
<tr>
<td>d</td>
<td>Zinc</td>
<td>12–20</td>
<td>15</td>
</tr>
<tr>
<td>e</td>
<td>Iron</td>
<td>12–20</td>
<td>20</td>
</tr>
<tr>
<td>f</td>
<td>Copper</td>
<td>12–20</td>
<td>05</td>
</tr>
</tbody>
</table>

\(^a\) 2 mg atom; \(^b\) Isolated yields; \(^c\) Characterized by IR and comparison with authentic sample on TLC.

**Table IIIC.2:** Effect of nature of solvent on the synthesis of 4f

<table>
<thead>
<tr>
<th>Entry</th>
<th>Solvent(^a)</th>
<th>Time (min)</th>
<th>Yield (%)(^{b,c,d})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>At 25°C</td>
<td>MW</td>
<td>) ) ) )</td>
</tr>
<tr>
<td>a</td>
<td>No solvent</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>b</td>
<td>Acetone</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>c</td>
<td>Acetonitrile</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>d</td>
<td>Chloroform</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>e</td>
<td>DCE</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>f</td>
<td>DCM</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>g</td>
<td>Ethanol</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>h</td>
<td>Ether</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>i</td>
<td>Hexane</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>j</td>
<td>Methanol</td>
<td>360–480</td>
<td>60–80</td>
</tr>
<tr>
<td>k</td>
<td>THF</td>
<td>360–480</td>
<td>60–80</td>
</tr>
</tbody>
</table>

\(^a\) Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition
### Table III.C.3: Amount of sodium required for the synthesis of 4f

<table>
<thead>
<tr>
<th>Entry</th>
<th>Amount of atomized sodium (mg atom)</th>
<th>Time (min))</th>
<th>Yield (%)$^{a,b}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0.0</td>
<td>50</td>
<td>ND</td>
</tr>
<tr>
<td>b</td>
<td>0.5</td>
<td>30</td>
<td>70</td>
</tr>
<tr>
<td>c</td>
<td>1.0</td>
<td>20</td>
<td>75</td>
</tr>
<tr>
<td>d</td>
<td>1.5</td>
<td>20</td>
<td>80$^{c}$</td>
</tr>
<tr>
<td>e</td>
<td>2.0</td>
<td>10</td>
<td>90</td>
</tr>
<tr>
<td>f</td>
<td>2.5</td>
<td>10</td>
<td>90</td>
</tr>
<tr>
<td>g</td>
<td>3.0</td>
<td>10</td>
<td>90</td>
</tr>
</tbody>
</table>

$^{a}$Isolated yields; after silica gel column chromatography;  
$^{b}$Characterized by IR and by comparison with authentic samples on TLC. ND: not detected;  
$^{c}$4-(N,N-dimethylamino)benzaldehyde (2.0 mmol), acetophenone (2.0 mmol), and urea (3.0 mmol) in THF (5.0 mL) under sonic condition (35 kHz).

### Table III.C.4: Amount of THF required for the synthesis of 4f

<table>
<thead>
<tr>
<th>Entry</th>
<th>THF (mL)</th>
<th>Time (min))</th>
<th>Yield (%)$^{a,b,c}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0.5</td>
<td>50</td>
<td>80</td>
</tr>
<tr>
<td>b</td>
<td>1.0</td>
<td>50</td>
<td>80</td>
</tr>
<tr>
<td>c</td>
<td>1.5</td>
<td>50</td>
<td>85</td>
</tr>
<tr>
<td>d</td>
<td>2</td>
<td>50</td>
<td>90</td>
</tr>
<tr>
<td>e</td>
<td>2</td>
<td>40</td>
<td>90</td>
</tr>
<tr>
<td>f</td>
<td>2</td>
<td>35</td>
<td>90</td>
</tr>
<tr>
<td>g</td>
<td>2</td>
<td>30</td>
<td>90</td>
</tr>
<tr>
<td>h</td>
<td>2</td>
<td>25</td>
<td>90</td>
</tr>
<tr>
<td>i</td>
<td>2</td>
<td>20</td>
<td>90</td>
</tr>
</tbody>
</table>

*Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition*
In order to find the generality of the use of atomized sodium in THF for the cyclocondensation of benzaldehyde, acetonaphone, and urea under sonic condition, different substituted aromatic aldehydes were selected and the reaction was carried out in a sonic bath working at 35 kHz (constant frequency) maintained at 25 °C by circulating water. The results of this study are presented in Table III.C.5. It can be seen that, the reaction is not influenced by neither electron donating nor electron withdrawing substituents on the aromatic ring of aldehydes and ketone at different positions.

**Table III.C.5:** Three-component cyclocondensation of aldehyde, urea with aromatic ketone by atomized sodium in dry THF under sonic condition (35 kHz constant frequency at 25 °C).

| Entry | Ketone R<sub>1</sub> (1) | Aldehyde R<sub>2</sub> | Product (4) | Time (min) | Yield (%)<sup>a,b</sup> | Melting point (°C) | Found | Reported<sup>c,d</sup> |
|-------|------------------|------------------|--------------|------------|-----------------|-----------------|--------|----------------|---|
| a     | H                | H                | 4a           | 10         | 90              | 235             |        | 233–240<sup>f</sup> |
| b     | H                | 4-CH<sub>3</sub> | 4b           | 14         | 88              | 288             |        | 287–290<sup>e</sup> |
| c     | H                | 4-Cl             | 4c           | 13         | 86              | 255–257         | 258–260<sup>f</sup> |
| d     | H                | 4-OH             | 4d           | 13         | 86              | 258–261         | 260–263<sup>e</sup> |
| e     | H                | 4-OCH<sub>3</sub>| 4e           | 12         | 88              | 258             | 258–260<sup>f</sup> |
| f     | H                | 4-<sub>N,N</sub>-(CH<sub>3</sub>)<sub>2</sub> | 4f           | 10         | 90              | 292             |        | 290–293<sup>d</sup> |
| g     | 4-Cl             | H                | 4g           | 10         | 88              | 250–253         | 251–254<sup>e</sup> |
| h     | 4-NO<sub>2</sub>| 4-Cl             | 4h           | 11         | 88              | 310             |        | 308–310<sup>e</sup> |

<sup>a</sup> Isolated yields.
<sup>b</sup> Characterized by IR and by comparison with authentic samples on TLC.
<sup>c</sup> 4-(N,N-dimethylamino)benzaldehyde (2.0 mmol), acetonaphone (2.0 mmol), atomized sodium (2 mg atom) and urea (3.0 mmol) under sonic condition (35 kHz).

*Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition*
IIIC. 3.3. EFFECT OF ULTRASOUND ON THE REACTION

The phenomenon of acoustic cavitation attributes to the accomplishment of the organic reactions under sonic condition.[35] The primary chemical reactions are due to the transient state of immense temperature, pressure and extraordinary heating rates which are generated due the cavitation bubble collapse.[36] The present reaction is an example of a three-phase system: the liquid phase (reagents in solvents), solid phase (atomized sodium and solid substrates), and the gas phase (dissolved gases in the liquids and gases on the inner-surface of the vessel). Under sonication the attractive forces of the molecule is disturbed by a series of compression and rarefaction cycles due to which cavitation bubbles will be formed.

The reaction is a liquid-solid heterogenous reaction, and the bubble collapse becomes non-spherical near solid surface i.e, near the surface of the solid atomized sodium and solid substrates which drag the liquid high-speed jets near the surface creating shockwave damage to the surface. Most of the energy available is transferred to the accelerating jet and not completely to the bubble wall itself which creates the high-speed jet reach velocities of hundreds of metres per second. Also, in addition to this, the starting materials get fragmented due to the shockwaves created by cavity collapse in the liquid. The formation of these micro-jets and shockwaves on the surface creates the localized erosion responsible for most of the sonochemical effects on the present heterogeneous reaction.

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*Synthesis of 4,6-diarylpurin-2(1H)-ones (DAPMs) under sonic condition*
IIIC. 3.4. EXPERIMENTAL

All the chemicals used were commercially available reagents. All the solvents were distilled before use. THF was distilled and dried over sodium. All the reactions were studied using SIDILU Indian make sonic bath working at 35 kHz (constant frequency) maintained at 25 °C (by circulating water). The completion of the reaction was monitored on TLC (eluent: 8–10 % ethyl acetate in light petrol), by comparison with the authentic samples. Melting points of the obtained products were determined using a Büchi apparatus. Nuclear magnetic resonance spectra were obtained on a 400 MHz Bruker AMX spectrometer in DMSO-d₆ using TMS as a standard. GC-Mass spectra were obtained using a Shimadzu GC-MS QP 5050A instrument equipped with a 30 m length and 0.32 mm dia BP-5 column with the column temperature 80 – 15 – 250 °C. Infrared spectra were recorded using Shimadzu FT-IR-8400s Spectrometer as KBr pellets for solids.

IIIC. 3.5. GENERAL PROCEDURE FOR THE SYNTHESIS OF 4f

A mixture of 4-(dimethylamino)benzaldehyde (0.274 g, 2.0 mmol), acetophenone (0.24 g, 2.0 mmol), urea (0.18 g, 3.0 mmol), atomized sodium (2.0 mg atom), THF (2 ml) were sonicated in a sonic bath working at 35 kHz (constant frequency) maintained at 25 °C (by circulating water) for 10 minutes. At the end of the reaction, liquefied reaction mixture suddenly becomes solid, to which water was added and shaken for few minutes. This was filtered through a sintered funnel to afford the crude product, which was further purified by recrystallization using absolute ethanol.

IIIC. 3.6. CONCLUSIONS

In conclusion we have developed an efficient synthesis of 4,6-diarylpyrimidin-2(1H)-ones by a one-pot three component cyclocondensation reaction between an aldehyde, a methyl ketone and urea under solvent-free condition using atomized sodium in THF under sonic condition. This new protocol has advantages include: (i) the use of cheap, easy to handle and commercially available sodium metal; (ii) short reaction time (10–15 min); and (iii) high yield (91–96%).
III. 3.7. SPECTRAL DATA

4,6-Diphenyl-pyrimidin-2(1H)-one (Table III.5, entry 4a)

m.p. 235 °C; IR (KBr) v = 3358, 3159, 2960, 1612, 1502 cm⁻¹; ¹H NMR (DMSO, 300 MHz): δ 7.1–7.15 (d, J =15 Hz, 2H, HAr and CH), 7.3–7.6 (m, 7H, HAr), 7.88–7.92 (d, J =12 Hz, 2H, HAr), 7.99 (s, 1H, NH) ppm; MS (70 ev), m/z: 248 [M⁺]

4-(4’-Tolyl)-6-phenyl-pyrimidin-2(1H)-one (Table III.5, entry 4b)

m.p. 288 °C; IR (KBr) v = 3449, 3099, 2923, 1620, 1513, 1460 cm⁻¹; ¹H NMR (DMSO, 300 MHz): δ 2.39 (s, 3H, CH₃), 7.36 (d, J =7.5 Hz, 2H, HAr), 7.53–7.57 (m, 4H, H-5 and HAr), 8.07 (d, J = 7.6 Hz, 2H, HAr), 8.15 (d, J = 5.75 Hz, 2H, HAr) ppm; MS (70 ev), m/z: 262 [M⁺].

4-(4’-Chlorophenyl)-6-phenyl-pyrimidin-2(1H)-one (Table III.5, entry 4c)

m.p. 255-257 °C; IR (KBr) v = 3429, 3230, 3083, 1605, 1549, 1509 cm⁻¹; ¹H NMR (DMSO, 500 MHz): δ 7.59 (d, J = 7.33 Hz, 2H, HAr), 7.60–7.69 (m, 4H, HAr and H-5), 8.16 (d, J = 7.45 Hz, 2H, HAr), 8.22 (d, J = 8.32 Hz, 2H, HAr) ppm; MS (70 ev), m/z: 282 [M⁺]

4-(4’-Hydroxyphenyl)-6-phenyl-pyrimidin-2(1H)-one (Table III.5, entry 4d)

m.p. 258-261 °C; IR (KBr) v = 3389, 2922, 1613, 1515, 1450 cm⁻¹; ¹H NMR (DMSO, 500 MHz): δ 6.96–7.04 (m, 3H, NH and H-4), 7.52–7.71 (m, 5H, HAr and H-5), 8.05–8.16 (m, 5H, HAr), 11 (s, 1H, OH) ppm; MS (70 ev), m/z: 264 [M⁺]

4-(4’-Methoxyphenyl)-6-phenyl-pyrimidin-2(1H)-one (Table III.5, entry 4e)

m.p. 258 °C; IR (KBr) v = 3440, 3095, 2930, 1608, 1514, 1458 cm⁻¹; ¹H NMR (DMSO, 400MHz): δ 3.9 (s, 3H, CH₃), 7.2–8.2 (m, 10H, H-5 and HAr), 11.95 (s, 1H, NH) ppm; MS (70 ev), m/z: 278 [M⁺]

4-(4’-N,N-Dimethylphenyl)-6-phenyl-pyrimidin-2(1H)-one (Table III.5, entry 4f)

m.p. 292 °C; IR (KBr) v = 3448, 3095, 2925, 1619, 1509 cm⁻¹; ¹H NMR (DMSO, 300 MHz): δ 3.04 (d, J = 6.63 Hz, 6H, CH₃), 6.79–6.81 (d, J = 6Hz, 2H, HAr), 7.36 (s, 1H, CH), 7.52–7.58 (m, 3H, HAr), 8.06–8.12 (m, 4H, HAr), 11.89 (s, br, 1H, NH) ppm; MS (70 ev), m/z: 291 [M⁺]
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4-(4'-Chlorophenyl)-6-phenyl-pyrimidin-2(1H)-one (Table IIIC.5, entry 4g)

m.p. 250-253 °C; IR (KBr) ν = 3320, 1608, 1532, 1488 cm⁻¹; ¹H NMR (DMSO, 300 MHz): δ 7.56 (d, J = 5.90 Hz, 3H, HAr), 7.82 (s, 1H, H-5), 8.17 (d, J = 6.62 Hz, 2H), 8.35 (d, J = 8.25 Hz, 2H, HAr), 8.46 (d, J = 8.16 Hz, 2H, HAr) ppm; MS (70 ev), m/z: 282 [M⁺]

4-(4'-Chlorophenyl)-6-(p-nitrophenyl)-pyrimidin-2(1H)-one (Table IIIC.5, entry 4h)

m.p. 310 °C; IR (KBr) ν = 3412, 3192, 2921, 1612, 1548, 1515, 1456, 1348 cm⁻¹; ¹H NMR (DMSO, 300 MHz): δ 6.90–7.83 (m, 9H, H-5 and HAr), 9.98 (s, 1H, NH) ppm; MS (70 ev), m/z: 327 [M⁺]

4-(4'-Chlorophenyl)-6-(p-methoxyphenyl)-pyrimidin-2(1H)-one (Table IIIC.5, entry 4i)

m.p. 311 °C; IR (KBr) ν = 3446, 3105, 2926, 1614, 1513 cm⁻¹; ¹H NMR (DMSO, 500 MHz): δ 3.86 (s, 3H, OCH₃), 7.094 (d, J = 8.85 Hz, 2H, HAr), 7.57 (s, 1H, H-5), 7.61 (d, J = 8.55 Hz, 2H, HAr), 8.16 (d, J = 8.16 Hz, 2H, HAr), 8.21 (d, J = 8.15 Hz, 2H, HAr), 11.96 (s, br, 1H, NH) ppm; MS (70 ev), m/z: 312 [M⁺]

4-(4'-N,N-Dimethylphenyl)-6-(p-methoxyphenyl)-pyrimidin-2(1H)-one (Table IIIC.5, entry 4j)

m.p. 285–289 °C; IR (KBr) ν = 3454, 3113, 2932, 1627, 1528 cm⁻¹; ¹H NMR (DMSO, 500 MHz): δ 1.23 (d, J = 6.63 Hz, 6H, CH₃), 3.88 (s, 3H, OCH₃), 7.101 (d, J = 8.86 Hz, 2H, HAr), 7.62 (s, 1H, H-5), 7.63 (d, J = 8.56 Hz, 2H, HAr), 8.19 (d, J = 8.17 Hz, 2H, HAr), 8.23 (d, J = 8.16 Hz, 2H, HAr), 11.97 (s, br, 1H, NH) ppm; MS (70 ev), m/z: 321 [M⁺]

Synthesis of 4,6-diarylpymidin-2(1H)-ones (DAPMs) under sonic condition

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Fig. IIC.1. $^1H$ NMR spectrum of 4,6-Diphenyl-pyrimidin-2(1H)-one
Fig. III.C. $^1H$ NMR spectrum of 4-(4’-Methoxyphenyl)-6-phenyl-pyrimidin-2(1H)-one

Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition
Fig. III.C.1. $^1H$ NMR spectrum of 4-($4^\prime$-N,N-Dimethylphenyl)-6-phenyl-pyrimidin-2(1H)-one

Synthesis of 4,6-diarylpyrimidin-2(1H)-ones (DAPMs) under sonic condition