ABSTRACT

The Present Thesis entitled as "**Metal free C- H Functionalization: a unique tool for library synthesis of functionalized 4-pyrimidiones**" has made some efforts to synthesize the diverse 4 pyrimidones with varied functional groups via different approaches and their applications in medicinal and pharmacological domains. Based on different direction and contents of the work; the thesis has been divided into four chapters.

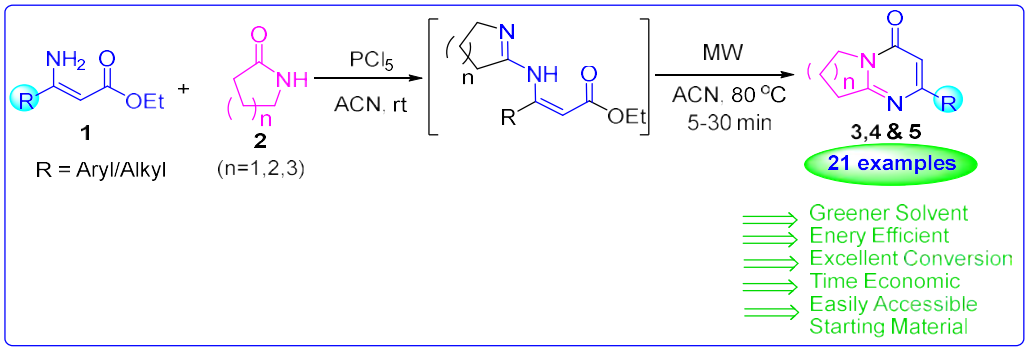
Chapter I: describes an introduction to present work, the **"A brief review on C-H functionalization/activation and a literature study regarding the synthesis of 4H-pyrido[1,2-a]pyrimidin-4-one derivatives"**

Summarizes a brief review on pyrimidines and it was further subdivided into following points:

1) Origin, background theory, importance and current status of C-H Functionalization.
2) Use of C-H functionalization techniques in selective functionalization of heterocycles.
3) Importance of 4-pyrimidiones and current literature status
4) Different approaches of its synthesis and further derivatization

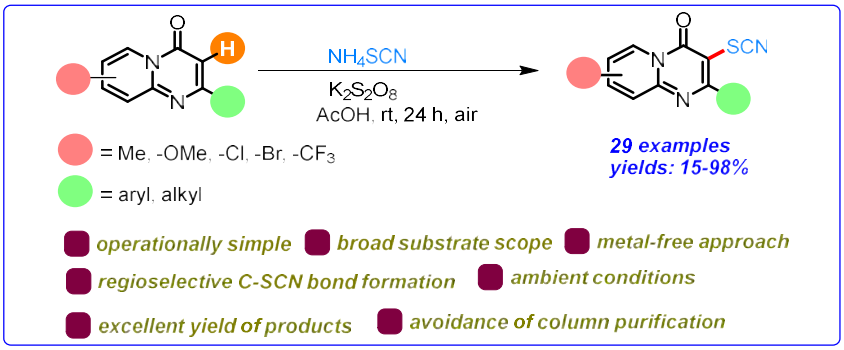
Chapter II: describes **"Microwave-assisted straight forward synthesis of 2-substituted alicyclic fused pyrimidone"**

We have divulged here a metal free- and MW assisted route to tetrahydro-4H-pyrido[1,2-a]pyrimidin-4-one and dihydropyrrolo[1,2-a]pyrimidin-4(6H)-one has been demonstrated by the reaction of aminoacrylates with lactams in presence of phosphorous pentachloride. This transformation comprises of the sequential formation of three new bonds to produce pyrimidone derivatives under mild reaction conditions and this strategy is well compatible for both electron deficient and electron rich amino-acrylates. This method is amenable for gram scale reaction.



Chapter III describes: "**Regioselective C(sp^2)3–H thiocyanation of substituted 4*H*-Pyrido[1,2-*a*]pyrimidin-4-ones and its late-stage deriovatization"**.

We demonstrate herein the first example of $K_2S_2O_8$ mediated direct C(sp^2)H thiocyanation of substituted 4H-pyrido[1,2-a]pyrimidin-4-ones at room temperature in the absence of a metal catalyst. This unique approach features a broad substrate scope with excellent functional group tolerance and substitution patterns, affording the target thiocyanated scaffolds lucrative yields with exclusive regioselectivity. Mechanistic investigations have also been conducted for better understanding of the reaction pathway. In addition, the synthetic utility of this protocol has been showcased through the construction of biologically relevant analogues.



Chapter IV describes: "**Regioselective substituted selenylation at (C-SP^3-H) of 4-pyrimidione under ambient condition''**

We have highlighted here regioselective selenylation at (C-SP3)-H of 4-pyrimidione under ambient condition. This is innovative work, and first work to install double bond at allylic position via dehydrogenative mechanistic pathway in open air. The mechanistic outline is proposed till now. This unique approach features a broad substrate scope with excellent functional group tolerance and substitution patterns, affording the target selenylated compounds with exclusive regioselectivity.