Chapter 5

Conclusion and Future Scopes

CONCLUSION

The work presented in the thesis can be summarized as the development of six (06) different methodologies for the synthesis of *N*- and *O*- heterocycles using alkyl/arylidene barbiturates as the key intermediate in all the processes. Also, the reactions were developed as “on-water” multicomponent protocols. Overall, it can be commented that the reaction schemes were highly efficient in serving the purpose of being atom economic, pot-economic and less hazardous in nature. The high specificity and selectivity achieved led to almost no side product generation. The library of compounds designed contains widely accepted and extensively used bioactive heterocyclic segments, which make them potential candidates for application in the field of pharmaceutics. The chapter wise concluding remarks are as follows:

Conclusions from Chapter 2

a. Two efficient and novel methodologies, first a base mediated and second a $FeCl_3.6H_2O$ catalysed MCR synthesis of aryl substituted unsymmetrical pyrano-dipyrimidines were developed.

b. The domino reactions were chemoselective and the formation of desired products was highly selective and isolated in good-excellent yields. No by-products were formed in the reactions.

c. No chromatographic methods of isolation of products were used. The solid products formed were collected by simple filtration and purified by washing with appropriate solvents.

d. The plausible mechanism for the formation of the mentioned class of compounds have been discussed in details

e. Initially, the reaction was developed as a base mediated reaction but in the subsequent section it was modified into a catalysis protocol. This also shows the modifications done to an already green procedure to make it greener.

Conclusions from Chapter 3

a. Two protocols, firstly a base mediated selective synthesis of barbiturate functionalised chromeno[2,3-*d*]pyrimidine and symmetrical pyranodipyrimidines and secondly, molecular iodine –acetic acid catalysed synthesis of three different classes of compounds, namely, barbiturate functionalised chromeno[2,3-*d*]pyrimidines, 4-hydroxycoumarin functionalised chromeno[2,3-*d*]pyrimidines, and 6-aminouracil functionalised chromeno[2,3-*d*]pyrimidines were developed through simple yet highly efficient methods.

b. The first reaction protocol was developed from the observations made in chapter 2 and was further successfully modified in to a catalysis scheme in the subsequent section.

c. High selectivity for the formation of products was achieved through the MCRs. Additionally, the products were obtained as solids and no chromatographic methods of isolation and purification were used. The compounds formed were collected by simple filtration followed by washing with appropriate solvents for purification.

d. The plausible mechanisms for the formation of all the classes of compounds have been thoroughly discussed and the observations have been reasoned in the best possible way.

Conclusions from Chapter 4

a. Two highly efficient, firstly a base mediated and secondly, trisodium citrate dihydrate catalysed green methods for the synthesis of 1,2,4-triazolidine-thiones have been developed.

b. Application of greener methods i.e. mechanochemical and sonochemical, were discussed in both the developments.

c. The products were isolated *via* chromatography free method and were obtained in excellent yield with high purity.

d. The reaction mechanism was established according to experimental findings and thereby a new mechanistic approach has also been proposed.

FUTURE SCOPE

The developed reaction protocols hold high prospects of further studies.

a. The plausible mechanism can be further studied and verified with the aid of computational studies and the reasons for the transformations and selectivity can be explained in better ways.

b. The libraries of compound synthesized bear biologically potent heterocyclic segments. Many show resemblance to pharmaceutical compounds under trial. Therefore, the concerned compounds can be modified by further functionalization and a thorough biological study could be carried out to deduce the applicability of the molecules formed.

c. The molecules synthesized also contain reactive sites, which can be explored to study the limitations of already established protocols such as coupling reactions.