ABSTRACT

In particular this thesis entitled “Design, Synthesis, Characterization and Biological Evaluation of Pharmacologically important Furan and its Derivatives” relates to the studies towards the synthesis of Benzofuran and its derivatives. The work represented in the thesis is divided into five chapters which can be summarized as below.

CHAPTER – 1

This chapter deals with introduction, literature review on important natural and synthetic molecules containing benzofuran motif and various synthetic approaches towards the synthesis of pharmacologically important benzofuran ring system.
CHAPTER – 2

Synthesis and characterization of Bis-tert-butyl-2-(di-6-hydroxybenzofuran-3-yl) ethylcarbamate [5a], 2-(6-hydroxy-1-benzofuran-3-yl) acetate [6a-c] and 2-(6-hydroxy-1-benzofuran-3-yl) acetamide derivatives [7a-d] have been discussed in this chapter under two sections viz., section-A and section-B respectively.

Section-A: This section describes the synthesis and characterization of Bis-tert-butyl-2-(di-6-hydroxybenzofuran-3-yl) ethylcarbamate [5a] through various functional group transformations.

![Structure of 5a]

Section-B: In this section synthesis and characterization of 2-(6-hydroxy-1-benzofuran-3-yl) acetate [6a-c] and 2-(6-hydroxy-1-benzofuran-3-yl)-N-4-substituted acetamide derivatives [7a-d] were carried out.

![Structures of 6a-c and 7a-d]

Newly synthesized intermediates and final compounds have been characterized to get structural confirmation by FTIR, \(^1^H\), \(^{13}\)C-NMR and MS techniques. Representative
spectra of FTIR, $^1$H, $^{13}$C-NMR and Mass are presented. Crystalline compounds [2a] and [3a] were characterized by X-ray crystallography.

**CHAPTER – 3**

In this chapter synthesis and characterization of 4-(1-benzofuran-2-yl)-2-methyl-6-substituted phenyl pyrimidine [3a-f] and 5-(4-$N$-alkyl-piperazin-1-yl)-1-benzofuran-2-yl)-3-phenylpropenone derivatives [5a-f] were carried out in section A and section B respectively.

**Section-A:** Detailed sequence of reaction carried out for the synthesis and characterization of 4-(1-benzofuran-2-yl)-2-methyl-6-substituted phenyl pyrimidine derivatives [3a-f] have been discussed in this section.

**Section-B:** This section describes the synthesis and characterization of 5-(4-$N$-alkyl-piperazin-1-yl)-1-benzofuran-2-yl)-3-phenylpropenone derivatives [5a-f] through three steps.
The spectroscopic techniques like FTIR, $^1$H, $^{13}$C-NMR and MS studies were used to establish the structures of the newly synthesized compounds. The compound [3a] was also characterized by single crystal x-ray diffraction studies. Representative spectra for the intermediates and final compounds have been presented.

CHAPTER – 4

This chapter presents the synthesis and characterization of symmetric (1, 1-dibenzofuran-2-yl) ethyl terephthalamide derivatives [4a-e].

The structures of the synthesized intermediates and final compounds were established by spectroscopic techniques. Representative spectra of FTIR, $^1$H, $^{13}$C-NMR and Mass spectra for the compounds have been presented. Single crystal X-ray crystallography diffraction study was carried out for the crystalline compounds [2a] and [2b].
CHAPTER – 5

This chapter deals with the in-vitro antibacterial and antifungal activity screening of the newly synthesized compounds of chapter-2, 3 and 4. The antibacterial activity of the synthesized compounds was tested against four bacterial strains such as Escherichia coli, K.aerogenes, P.desmolyticum and Staphylococcus aureus. While antifungal activity was carried out against two fungal strains such as A.niger and Candida albicans.

Additionally in-silico ADMET and molecular docking studies of the synthesized compounds were carried out on the target protein GlcN-6-P synthase using Autodock4.2 tool and Autodock Vina. The results have been discussed in detail and tabulated.