

Notification no.: 548
Notification date: 06-11-2023
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Title: **Design, Synthesis and Biological Applications of Some Heterocyclic Analogues**
Keywords: Heterocyclic Analogs, Pyrazole, Oxadiazole, Antibacterial, DNA Binding, Molecular Docking

ABSTRACT

The thesis entitled “**Design, Synthesis and Biological Applications of Some Heterocyclic Analogues**” consists of six chapters. In this thesis we have mainly focused on design, synthesis and characterization of heterocyclic analogs and their biological applications. In **Chapter I**, we have focused on biologically active heterocyclic analogs in the field of pharmaceuticals and medicinal chemistry. In **Chapter II**, we describe the synthesized derivatives **3a-3j** and their *in-vitro* antibacterial activities against gram-positive and gram-negative bacterial strains. The most active analog **3d** showed potent antibacterial activity with MIC value of 64 µg/mL against *B. subtilis*. The interaction of compound **3d** with CT-DNA was found to be groove binding. The **Chapter III** deals with the synthesized of analogs **4a-4m** and their antibacterial, DNA binding and molecular modelling were also done. The active analog **4c** displayed highest antibacterial activity against *E. coli* (MIC = 64 µg/mL). The interaction between CT-DNA and the lead compound **4c** was found to be a groove binding mode of interaction. In **Chapter IV**, the oxadiazole derivatives **5a-5p** were synthesized and evaluated for antibacterial activity against bacterial strains. The most active analogs **5e** and **5f** showed potent antibacterial activity, with MIC values of 16 µg/mL against *E. coli* and *B. subtilis*. In **Chapter V**, oxadiazole based chemosensor **2** was synthesised and characterised by employing various spectroscopic studies. The compound **2** showed selective detection towards Ni²⁺ ion among the other competitive metal cations. The detection limit and association constant of oxadiazole compound **2** towards Ni²⁺ ion was found to be 9.4 µM and 1.04 x 10⁵, respectively. The intercalative mode of interaction of oxadiazole compound **2** toward CT-DNA was examined by various DNA binding studies. In **Chapter VI**, the pyrazole-based derivatives **7a-7o** were synthesized and evaluated for antibacterial activity against bacterial strains. The most active analog **7k** showed potent antibacterial activity, with MIC values of 128 µg/mL against *E. coli*, *S. aureus*, and *B. subtilis*. The molecule **7k** was considered for investigate for the interaction property with CT-DNA by various methods and the results were found to be electrostatic or groove binding.