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Title of Thesis: Synthesis of some Novel Compounds and their Biological Studies

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ABSTRACT

The present research work deals with the synthesis and characterization of some Heterocyclic compounds and their biological evaluation. The thesis comprises of five chapters.

Chapter 1- deals with the general introduction and literature review of heterocyclic compounds. The application of heterocycles in medicinal chemistry has lead to many breakthroughs and further research in this field is ongoing.

Chapter 2- deals with the synthesis of fifteen hybrid molecules containing 1, 2, 4- triazoles and quinazolin-4-(3*H*)-one and their characterization with various spectroscopic techniques such as NMR, mass, IR. They were evaluated against HM1: 1MSS strain of *E. histolytica.* Compound 4 showed better results than the standard drugs. Toxicity of the hybrids was measured cervical cancer cell line, HeLa cells. Majority of the compound had low toxicity.

Chapter 3- 4-aryl-5-cyano-2-methylthio-6-oxo-1, 6-dihydropyrimidine derivatives were synthesized and screened *in vitro* against the HM1:IMSS strain of *E. histolytica*. All the compounds were characterized by various spectroscopic techniques like NMR, IR, elemental analysis, mass etc. Out of the nine synthesized compounds, five showed better anti-amoebic activity than the standard drug metronidazole (IC_{50} 1.8 µM).

Chapter 4- deals with the general synthesis of 4-Oxo Quinazoline and synthesis and characterization of a series of 2-methyl-4(5)-nitro-1*H*-imidazole and quinazolin-4(3*H*)-one

Schiff base hybrids. Twelve compounds (2-13) were synthesized and characterised by spectroscopic techniques. *In vitro* antiamoebic activity was performed for all the compounds. They showed IC_{50} values in the range (0.14-9.65μM). Six compounds (**2, 3, 5, 6, 8** and **11**) were found to be better inhibitors than the standard drug Metronidazole (IC_{50} = 1.80μM) and showed low cytotoxicity on human embryonic kidney - 293(HEK-293) cells. The docking results are also found to be in agreement with the observed *in vitro* data and affirm the antiamoebic potential of the most active antiamoebic molecule.

Chapter 5- general synthesis 2-methyl-4-nitro-1*H*-imidazole is reported also 2-methyl-4-nitro-1*H*-imidazole linked *N*-acetamide derivatives have been synthesized and evaluated for their antiamoebic potential. The structure elucidation of all the synthesized compounds was done by various spectral studies. All the compounds were screened against HM1: IMSS strain of *Entamoeba histolytica.* Out of nine compounds synthesized, four showed better activity then the standard drug metronidazole. Cytotoxicity of the compounds on human embryonic kidney – 293 (HEK-293) normal cells was measured by MTT assay. Based on percentage of cell viability IC_{50} values of each compound was determined. The compound 15, 16, 17 and 18 showed good cell viability and the least toxicity.