TABLE OF CONTENTS

Certificate i
Declaration ii
Acknowledgments iii
Abbreviations/Formulae Commonly Used vi
List of Tables viii
List of Figures ix
List of Spectra xi

CHAPTER-1 INTRODUCTION TO MALARIA 1-31
1.1 INTRODUCTION
1.2 HISTORY
1.3 MALARIA TODAY AND GLOBAL BURDEN
1.4 MALARIA BURDEN IN INDIA
1.5 FACTORS INFLUENCING MALARIA DISTRIBUTION
1.6 PROGRESS IN DECREASING MALARIA BURDEN SINCE 2000
1.7 MALARIA PARASITE AND LIFE CYCLE
1.8 PATHOLOGY
  1.8.1 Pathology of Plasmodium falciparum
1.9 CONTROL OF MALARIA
  1.9.1 Vector control
  1.9.2 Disease control
    1.9.1.1 Antimalarial Drugs
      1.9.1.1.1 Quinolines
      1.9.1.1.2 Hydroxynapthoquinones
      1.9.1.1.3 Folate antagonists
      1.9.1.1.4 Antibiotics
      1.9.1.1.5 Artemisinins
1.10 ANTIMALARIAL DRUG RESISTANCE
1.11 ORIGIN OF THE CURRENT STUDY
REFERENCES
CHAPTER-2 LITERATURE REVIEW

2.1 BRIEF REVIEW ON HETEROCYCLIC COMPOUNDS AS ANTIMALARIALS

2.2 RECENT RESEARCH CONDUCTED IN ANTIMALARIALS

REFERENCES

CHAPTER-3 DESIGNING OF COMPOUNDS USING IN SILICO APPROACHES

3.1 INTRODUCTION

3.2 MATERIAL AND METHODS
   3.2.1 Library generation of ligands
   3.2.2 ADME and toxicity studies
      3.2.2.1 ADME prediction studies
      3.2.2.2 Toxicity prediction
   3.2.3 Molecular docking analysis
      3.2.3.1 Target preparation
      3.2.3.2 Ligand preparation
      3.2.3.3 Docking studies on MVD
      3.2.3.4 Docking energy calculation
   3.2.4 Validation of docking score of MVD by re-docking studies on Autodock 4.2

3.3 RESULTS AND DISCUSSION
   3.3.1 Virtual Screening workflow
   3.3.2 ADME and Toxicity prediction
   3.3.3 Prediction of binding site
   3.3.4 Binding mode analysis
   3.3.5 Docking studies on the library of furanone bearing quinoline moiety
   3.3.6 Docking studies on the library of furanone bearing pyrazole moiety

3.4 CONCLUSIONS

REFERENCES
CHAPTER-4 SYNTHESIS AND CHARACTERIZATION

4.1 CHEMISTRY

4.2 SYNTHESIS

4.2.1 Synthetic Scheme

4.3 EXPERIMENTAL

REFERENCES

CHAPTER-5 EVALUATION OF ANTIMALARIAL ACTIVITY

5.1 INTRODUCTION

5.1.1 Schizont maturation assay (SMI)

5.1.2 Lactate dehydrogenase inhibition (LDH) assay

5.2 MATERIALS AND METHODS

5.2.1 In vitro cultivation of Plasmodium parasite

5.2.1.1 Preparation of culture medium for cultivation of Plasmodium falciparum

5.2.1.1.1 Preparation of RPMI medium

5.2.1.1.2 Preparation of washing medium

5.2.1.1.3 Preparation of serum

5.2.1.1.4 Preparation of complete media

5.2.1.1.5 Preparation of erythrocytes for culture

5.2.1.1.6 Initiation of culture

5.2.2 Maintenance of Plasmodium falciparum culture

5.2.2.1 Monitoring culture growth

5.2.2.2 Smear preparation

5.2.2.3 Subculturing

5.2.3 Estimation of antimalarial activity

5.2.3.1 Synchronization of Plasmodium falciparum

5.2.3.1.1 Procedure of synchronization

5.2.3.1.2 Preparation of drug solution

5.2.3.3 In vitro antimalarial activity of synthesized derivatives

5.2.3.3.1 Schizont maturation assay

5.2.3.3.1.1 Microscopic analysis and counting of parasite
5.2.3.3.1.2 Calculation of IC$_{50}$ and data analysis

5.2.3.3.2 Plasmodium lactate dehydrogenase (pLDH) inhibition assay

5.2.3.3.2.1 Measurement of pLDH activity

5.2.3.3.2.2 Calculation of IC$_{50}$ and data analysis

5.3 RESULTS AND DISCUSSION

5.4 CONCLUSIONS

REFERENCES

CHAPTER-6 SUMMARY AND CONCLUSIONS  133-136

LIST OF PUBLICATIONS & PRESENTATION  137-138