

TABLE OF CONTENTS

Topics	Page No.
Abstract	i
Preface	iv
Acknowledgments	v
Table of Contents	vi
List of Tables	viii
List of Figures	x
List of Appendices	xiii
<hr/>	
Chapter I: Introduction	1
1.1 Quorum Sensing	2
1.2 Quorum Sensing Inhibition	4
1.3 Quorum-Sensing regulation in <i>S. aureus</i>	9
1.4 Heat Shock Protein (HSP)	12
1.5 Background of QSAR	13
1.6 Phosphodiesterase-4 (PDE4)	15
1.7 Lysine-Specific Demethylase 1 (LSD1)	17
1.8 Aims and Objectives	19
1.9 References	20
<hr/>	
Chapter II: Methodology	31
2.1 Computational approach in drug discovery	32
2.2 Density Functional theory	32
2.3 Molecular Docking	34
2.4 Molecular Dynamics Simulation	37
2.5 Free energy calculation using MM-PBSA	41
2.6 ADMET prediction	42
2.7 QSAR approach in QSARINS	43
2.8 Half maximal inhibitory concentration	47
2.9 References	48
<hr/>	
Chapter III: Screening of Some Hamamelitannin Derivatives against Staphylococcus Aureus: A Computational Perspective	51
3.1 Introduction	52
3.2 Materials and methods	54
3.3 Results and discussion	58
3.4 Conclusion	67
3.5 References	67
3.6 Supporting information	71

Chapter IV: Selection the Drug Efficacy of Oroidin Derivatives as Hsp90 Inhibitors by Computer Aided Drug Design Method	79
4.1 Introduction	80
4.2 Materials and methods	81
4.3 Results and discussion	86
4.4 Conclusion	107
4.5 References	108
4.6 Supporting information	111
<hr/>	
Chapter V: Validation of Some Heterocyclic Compound Derivatives as Phosphodiesterase-4 Inhibitors- A QSAR Perspective	131
5.1 Introduction	132
5.2 Materials and methods	133
5.3 Results and discussion	140
5.4 Conclusion	150
5.5 References	151
5.6 Supporting information	153
<hr/>	
Chapter VI: QSAR modeling for anti-histone lysine-specific demethylase 1 activity of substituted N-(2-Phenylcyclopropyl) Piperidin-4-Amine derivatives	160
6.1 Introduction	161
6.2 Materials and methods	163
6.3 Results and discussion	166
6.4 Conclusion	176
6.5 References	177
6.6 Supporting information	181
<hr/>	
Chapter VII: Scope for Future work	189
Summary of the Thesis	191
Appendix-I	196
Appendix-II	197
Appendix-III	198
Bibliography	199
Index	224
<hr/>	