In memory of my parents

Late Tushar Kanti Sarkar

Late Deepali Sarkar

DECLARATION

I, **Subhajit Sarkar,** hereby declare that the work presented in this thesis entitled **"VIRTUAL SCREENING, MOLECULAR DOCKING STUDIES, ADMET PROPERTIES, DENSITY FUNCTIONAL THEORY AND 2D-QSAR MODELING TO DESIGN POTENTIAL INHIBITORS"** is an authentic record of research work done by me under the supervision of Dr. Rajesh Kumar Das, Assistant Professor, Department of Chemistry, University of North Bengal, Darjeeling, West Bengal, India

The research work in this thesis (in part or in full) has not been submitted elsewhere earlier, for the award of any other degree, diploma and fellowship to this or any other University/Institute.

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ENLIGHTENMENT TO PERFECTION
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CERTIFICATE

This is to certify that the thesis entitled **"VIRTUAL SCREENING, MOLECULAR DOCKING STUDIES, ADMET PROPERTIES, DENSITY FUNCTIONAL THEORY AND 2D-QSAR MODELING TO DESIGN POTENTIAL INHIBITORS"** is an authentic record of research work carried out by **Mr. Subhajit Sarkar** for partial fulfilment of the requirements for the degree of "DOCTOR OF PHILOSOPHY IN CHEMISTRY" under my supervision at University of North Bengal, Darjeeling, West Bengal, India. I further certify that this research work is original, and no part of this thesis has been submitted for the award of any degree or diploma to this or any other University/Institute.

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PREFACE

Wet lab based drug design processes use trial and error methods for screening natural and synthetic compounds. It costs millions of dollars and very long time approximately 10-15 years. To meet these severe challenges nowadays pharmaceutical companies rely very much on computer-aided design techniques to discover potential drugs.

The thesis starts with ***Chapter I*** *where a detailed study of different types of QSIs and inhibition mechanisms are described.* ***Chapter II*** *discusses all the methodologies associated with computer aided drug design techniques in detail.* ***Chapter III*** *comprises 14 derivative compounds of hamamelitannin (HAM) could be developed as effective inhibitors of S. aureus biofilm formation and considered for in vitro and in vivo analysis.* ***Chapter IV*** *encompasses computer assisted drug design study on the natural product oroidin (ODN) and its derivatives and found that some of them could be used as potent inhibitors of heat shock protein 90 (Hsp90).* ***Chapter V*** *describes a QSAR study to develop a standard model on a dataset of sixty-six significant phosphodiesterase-4A (PDE4A) inhibitors. The study revealed that the eight compounds possessed potent PDE4A inhibitory activity and might be considered as future drugs subject to the viability of in situ and in vivo proceedings. C****hapter VI****, quantitative structure activity relationship (QSAR) model was built from a dataset of 44 compounds as lysine-specific demethylase (LSD1) inhibitors, out of which 10 compounds have fully satisfied all the criteria of drug-like properties and these designed lead molecules would have more potency to treat LSD1 target after going through in vivo and in vitro analysis.* ***Chapter VII*** *includes the future possibilities of designing potential inhibitors of many critical diseases along with 3D-QSAR and ANN validation for better lead compounds.*

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Subhajit Sarkar

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