

**Dedicated to**  
***Maa and Baba***

## **List of Publications**

### **Sections of the work presented in this thesis are reported in the following publications**

1. **Saha, D.** and Nath Jha, A. Computational multi-target approach to target essential enzymes of *Leishmania donovani* using comparative molecular dynamic simulations and MMPBSA analysis. *Phytochemical Analysis*, 34(7):842-854, 2023
2. **Saha, D.**, Borah, N. J. and Jha, A. N. Molecular scaffold recognition of drug molecules against essential genes of *Leishmania donovani* using biocomputing approach. *South African Journal of Botany*, 162:52-63, 2023
3. **Saha, D.** and Jha, A. N. Integrated subtractive genomics and structure-based approach to unravel the therapeutic drug target of *Leishmania* species. *Archives of Microbiology*, 206(10):1-17, 2024

### **Other Publications**

1. Quraishi, S., **Saha, D.**, Kumari, K., Jha, A. N. and Roy, A. S. Non-covalent binding interaction of bioactive coumarin esculetin with calf thymus DNA and yeast transfer RNA: A detailed investigation to decipher the binding affinities, binding location, interacting forces and structural alterations at a molecular level. *International Journal of Biological Macromolecules*, 257,128568, 2024.
2. Rather, M. A., **Saha, D.**, Bhuyan, S., Jha, A. N. and Mandal, M. Quorum quenching: A drug discovery approach against *Pseudomonas aeruginosa*. *Microbiological Research*, 127173, 2022.

### **Conference Proceeding**

1. **Saha, D.** and Jha, A. N. Multi-target approach on *Leishmania donovani* and finding out potent inhibitors for essential enzymes. In *Proceedings of the XXXVIII Symposium of Bioinformatics and Computer-Aided Drug Discovery pp*, 2022.

### **Book Chapter**

1. **Saha, D.**, Khataniar, A., Singh, A. K. and Jha, A. N. Review of methods for encapsulation of nutraceutical compounds. In *Nutraceuticals* (pp. 127-156). Academic Press, 2023.

# Declaration

I, hereby, declare that the thesis entitled, “**Study on Genomic Sequences and Proteins of *Leishmania donovani* by Sequence and Structure-Based Approach**” has been submitted to the **Department of Molecular Biology and Biotechnology, Tezpur University** under the School of Sciences in partial fulfillment for the award of the degree of Doctor of Philosophy in Molecular Biology and Biotechnology. The work reported in this thesis is original and was carried out by me during my tenure as a PhD student at the Department of Molecular Biology and Biotechnology, Tezpur University, Napaam. This thesis work has not been previously considered for the award of any degree, diploma, associateship, membership or similar title of any university or institution or organization.

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### Certificate of the Supervisor

This is to certify that the thesis entitled, “**Study on Genomic Sequences and Proteins of *Leishmania donovani* by Sequence and Structure-Based Approach**”, submitted to the School of Sciences, Tezpur University in partial fulfillment for the award of the degree of Doctor of Philosophy in **Molecular Biology and Biotechnology** is a record of research work carried out by **Mr. Debanjan Saha** under my supervision and guidance.

All help received by him from various sources have been duly acknowledged. No part of this thesis has been submitted elsewhere for award of any other degree.

Date: 6<sup>th</sup> Jan, 2025

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## **List of Abbreviation**

2D	Two dimensional
3D	Three dimensional
Ag <sub>2</sub> O	Silver oxide
AmB	Amphotericin B
AAH	Adenine aminohydrolase
Ade	Adenine,
Ado	Adenosine
ADMET	Absorption, Distribution, Metabolism, Excretion and Toxicity
ADSL	Adenylosuccinate Lyase
ADSS	Adenylosuccinate synthetase
AMBER	Assisted Model Building with Energy Refinement
AML	Acute Myeloid Leukaemia
AMP	Adenosine Monophosphate
AMPDA	AMP deaminase
APRT	Adenine phosphoribosyltransferase
ATB	Automated Topology Builder
BCG	Bacillus Calmette-Guérin
BLAST	Basic Local Alignment Search Tool
COM	Centre of Mass
CL	Cutaneous Leishmaniasis
CHARMM	Chemistry at Harvard Macromolecular Mechanics
DNA	Deoxyribonucleic acid
DHODH	Dihydroorotate dehydrogenase
FDA	Food and Drug Administration
FFT	Fast Fourier transform
GDH	Glutamate dehydrogenase
GLOII	Glyoxalase II
GAPDH	Glyceraldehyde-3-phosphate dehydrogenase
GMP	Guanosine Monophosphate
GMPS	Guanosine monophosphate synthetase
GROMACS	GRONingen MACHine for Chemical Simulations
GROMOS	GRONingen MOlecular Simulation
GR	glutathione reductase
GUI	Graphical User Interface
LMT	Leishmania miltefosine transporter
UniProt	Universal Protein Resource

IL	Interleukin
(IFN)- $\gamma$	Interferon
IDRI	Infectious Disease Research Institute
KEGG	Kyoto Encyclopedia of Genes and Genomes
LGA	Lamarckian genetic algorithm
MDR	Multidrug-resistant
MD	Molecular Dynamics
MCL	Mucocutaneous leishmaniasis
MLR	Multiple Linear Regression
MMPBSA	Molecular Mechanics Poisson-Boltzmann Surface Area
MSA	Multiple Sequence Alignment
NVBDCP	National Vector Borne Disease Control Programme
NAMD	Nanoscale Molecular Dynamics
NCBI	National Center for Biotechnology Information
NMR	Nuclear Magnetic Resonance
NTDs	Neglected Tropical Diseases
PME	Particle mesh Ewald
PASS	Prediction of Activity Spectra for Substances
PK	Pyridoxal kinase
PCA	Principal Component Analysis
PDB	Protein Data Bank
PIN	Protein Interaction Network
PME	Particle Mesh Ewald
QSAR	Quantitative Structure Activity Relationship
RCSB	Research Collaboratory for Structural Bioinformatics
RMSD	Root Mean Square Deviation
RMSF	Root mean square fluctuation
RNA	Ribonucleic acid
SCOP	Structural Classification of Proteins
SDM	Sterol alpha-14 demethylase
SLN	Solid lipid nanoparticles
SMILES	Simplified Molecular Input Line Entry System
SPC	Single Point Charge
TB	Tuberculosis
TNF- $\alpha$	tumor- necrosis factor- $\alpha$
TiO <sub>2</sub>	Titanium dioxide
VL	Visceral Leishmaniasis
VS	Virtual Screening
WHO	World Health Organization
XMP	Xanthine Monophosphate
XPRT	Xanthine phosphoribosyltransferase