THILIBAN MANIVARMA

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SUMMARY

I am pursuing a doctoral degree in computational biophysics and focusing on the discovery and development of novel therapeutics for life-threatening diseases using protein's sequence and structural data in the field of computational biophysics, machine learning, artificial intelligence, computer aided drug design. Specifically I am interested in protein-protein system, protein-membrane system, HOTSPOTS in protein-protein interface.

EDUCATION

- Ph.D., 2020-2024, Computational biophysics, Nicolaus Copernicus University in Torun, Poland.
- MTech., CGPA 9.58, 2018-2020, Computational biology, Anna University, India.
- BTech., CGPA 7.46, 2014-2018, Pharmaceutical technology, Anna University, India.
- State board of Tamil Nadu, 89%, Anderson Higher Secondary School, India.

EXPERIENCE

Ph.D. – Computational biophysics (SONATA15, National Science Centre (2019/35/D/ST4/02203; 2020-2023) grant obtained by Dr. Karolina Mikulska-Ruminska **08/2020-present**

- **Project name:** "Computational studies of regulatory mechanism and inhibition of ferroptotic cell death signal"
  Subject : Understanding the regulatory mechanism of 15LOX1/PEBP1 involved in ferroptosis and finding the potential inhibitors to stop the complex formation of 15LOX1/PEBP1.

  Key words : Molecular docking, Molecular dynamic simulation, protein-protein system, protein-membrane system, Virtual screening, Pharmacophore modelling, Hotspots prediction, NAMD, CHARMM-GUI.

Mtech Thesis – supported and funded (12500 RS per month) by Govt. of India **10/2018-05/2020**

- **Project name:** "*In-silico* studies on Nipah virus proteins and their host pathogen interaction studies"
  Subject : This study underlines an interacting mechanism of Nipah virus G protein to the host protein, Eph4. We found a motif in the interface of Nipah virus G and Eph4, which is using similar to host protein-protein interaction (EphB2 – ephrinB2 complex) for entry. We call this as *Structural mimicry*. Nipah virus acts like a host and it enters, replicates.

  Key words : Molecular docking, protein-protein interaction, Systems biology, Machine learning.

BTech Thesis **07/2017-10/2018**

- **Project name:** "*In-silico* docking studies on dengue protein (DEN 4)"
  Subject : Screening potential inhibitors against dengue virus type 4 protein which is common strain in humans.

  Key words : Molecular docking, protein-ligand interaction.

Teaching

- **Uresearcher, a research education company, 09/2021-05/2022:** I was an instructor and handled *"Python essentials for Drug Discovery"*.

- **University, Ph.D. course works**, **03/2023-now:** I have been teaching "Introduction to python programming" to the students of informatics (8) and several doctoral candidates (9) from different disciplines as a part of my Ph.D. studies.

PERSONAL PROJECTS

- **Predicting HOTSPOT residues in the protein-protein complex, 15LOX1/PEBP1 (Artificial intelligence):** - Protein-protein interface dataset, - Supervised learning, - Python, - Tensorflow, - Neural network, - Jupyter notebook.
- **Finding potential inhibitors for 15LOX1 in the chEMBL (Machine Learning/Artificial intelligence):** - Inhibitors, - Supervised learning, - chEMBL, - Python, - Machine learning, - Tensorflow, - Jupyter notebook.
- **Classifying sialic acid independent and dependent viruses (Machine learning):** - Protein sequence dataset, - supervised learning, -python, -scikit learn, -Jupyter notebook.
- **Drug Discovery Hackathon 2020, Govt of India** – Participated and guided a group of students in national wide competition to find potential inhibitors for Covid 19 -Molecular docking, -Structural bioinformatics, -Virtual screening
- **Phytochemical analysis on Rhizopora mangle:** -soxhlet extraction, -antioxidants, -cancer therapy.

AREA OF INTEREST

- Molecular docking and Molecular dynamics simulation analysis.
- Sequence analysis and Structural bioinformatics
- Motif and structure prediction
- Protein - Protein interaction studies
- Machine learning and artificial intelligence
- Computer aided drug design
- Pharmacophore modelling and virtual screening
- Data science and Database management

TECHNICAL SKILLS AND TOOLS

Programming languages: Python, tcl.
Database management: SQL.
OS handle: Windows, Linux.
Molecular dynamics simulations: NAMD, GROMACS. **Molecular docking analysis:** Autodock, SMINA.
Machine learning/Artificial intelligence: Sci-kit learn, Keras, Tensorflow, KNIME.
Computational chemistry: RDkit, PaDEL.
Visualization tools: PyMol, VMD, Chimera. **Virtual screening :** OpenEye scientific.

CONFERENCES, PRESENTATIONS, INTERNSHIPS

- **Investigating the membrane effect on the dynamics of 15LOX-1/PEBP1**, , K. Mikulska-Rumińska, T. Manivarma, 13 XII 2022 r. (online), Department of Environmental and Occupational Health, University of Pittsburgh , USA.
- **"Diverse roles of membrane in ferroptotic cell death. Insights from molecular dynamics study of 15LOX1-PEBP1 complex " (poster)**, Biophysics at the Dawn of Exascale Computers - Hamburg, Germany(May 16-20, 2022).
- **"Diverse roles of membrane in ferroptotic cell death. Insights from molecular dynamics study of 15LOX1-PEBP1 complex " (poster),** *Bioinformatics in Torun* 2022 (BIT22) conference, Torun, Poland June 24th 2022.
- "**Hot spots, proteins and machine learning" (flash talk, online),** *Bioinformatics in Torun* 2021 (BIT21) conference, June 24th 2021.
- Attended 7 days RUSA program about **MACHINEL EARNING AND ARTIFICIAL INTELIGENCE**, Anna University – Chennai,2019.
- Attended one month summer internship on **"Network modeling of components on protein secretion systems in Mycobacterium tuberculosis"** in Institute of Mathematical Sciences , Chennai, 2019.
- Attended 5 days' workshop on **Computer Aided Drug Design** in Tamil Nadu Veterinary and Animal Sciences University – Chennai,2017.

AWARDS AND ACHIEVEMENTS

- **Best Candidate Award** from National Cadet Crop (NCC) , Anna University, Chennai - 2015.
- **Roll of Honor award** for school topper ranking - 2013.
- **Best Speaker Award** from various speech rendition in Tamil – 2010.
- **Awarded district first** in Computer exam by Azim Premji Foundation – 2005.