Mahesh Jethalia

Aspiring scientist interested in computational biology, structural biology, and applied ML

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EDUCATION

Indian Institute of Technology Kharagpur (IIT KGP), India *Aug 2015 – Feb 2021*

B.Tech and M.Tech (Dual Degree student)

Biotechnology and Biochemical Engineering (CGPA: 6.99/10, Additional CGPA: 8.5/10)

AWARDS & ACHIEVEMENTS

- UARE scholarship from the University of Alberta to work with Professor Jay Newby in 2019.
- All-India-Rank of 4539 (General) in JEE Advanced 2015 among 15 lakh candidates.
- Scholarship from All India Talent Search Examination by CETMSI in 2010.

PROFESSIONAL EXPERIENCE

Independent Researcher in Bioinformatics *Feb 2022-present*

Advised by Raghvendra Mall *St Jude Children's Research Hospital, TN, USA*

Master Regulator Analysis on cancers with different Invasiveness.

- Identified Enriched Pathways using common Master Regulator analysis.
- Invasiveness score ranking of different types of cancers visualized using violin plot on R.
- Measuring level of activity of common Master Regulators across the set of different cancers with different and varying invasiveness.
- Identified drugs that affect the enriched pathways using DrugBank and PubChem.

Independent Researcher in Structural biology *Feb 2022-present*

Advised by Gourab Bhattacharya *Indian Institute of Technology Kharagpur*

A study on Antitoxin-toxin interactions o*f Neisseria gonorrhoeae*

- Generated Graphs for Potential Energy, Temperature, Pressure, Density, RMSD, Radius of Gyration, and RMSF varies with time for the complex using GROMACS and Grace.
- Narrowed down the number of interactions to a few critical residues using (1) distance cutoffs (in Å) & (2) differences in the binding energy (ΔΔG in kJ/mole) of hotspot residues found using Alanine Scanning.
- Rendered Interface Residues of different chains of Antitoxin-toxin complex using Python & PyMoL.
- Rendered publication-quality photos of the toxin-antitoxin complex using PyMoL and UCSF ChimeraX.

Department of Mathematics and Statistical Sciences, University of Alberta, Canada

Research Intern under Professor Jay Newby, Biomathematics *June 2019-Aug 2019*

- Implemented a novel Particle Tracking algorithm (particularly using R-CNNs) in Python for tracking GEMs (Genetically Encoded Multimeric nanoparticles) using Tensorflow and Google Collab using video-based biological datasets & synthetic data to enable the measurement of cytoplasmic properties like molecular diffusion constants and viscosity. [Link: here]

Prakshep Pvt. Ltd, Bengaluru, India (Acquired by **Agro.ai**)

Operations Intern *May 2018 - July 2018*

- Project to (a) Identify plant species using photos captured from a smartphone, (b) Predict the shape, size, and color of the leaves a month in the future.
- Learned about Generative Adversarial Networks (GANs) and refined them (particularly, the pix2pix model) to do the above task for 3 different plants.

Engine: Generated images with desired segments with minimum missing patches to segment a plant for identification and future prediction.

- Lead the team of interns, to study various ways in which the data collection during the ground survey can be improved to provide better quality images quickly.

The Chatterjee Group (TCG) Life Sciences Pvt. Ltd, Kolkata, India
Intern *May 2017-July 2017*

- Project to evaluate Indian market size to identify the top 20 Drug APIs (Active Pharmaceutical Ingredients) of interest.
  -Surveyed multiple existing reports from Mckinsey, PwC, etc to identify common drugs
  -Figured out the APIs common among them and exclusive to a particular drug using the NIH website, & estimated & ranked them based on market size.

Conferences Attended:

- Conference on *Reinforcement Learning for Real Life*, at the University of Alberta, Canada in 2019.
- *Microbiology in the new Millennium: from Molecules to Communities* (October 2017)
  Attended a talk by Prof. Victor de Lorenzo on using *Pseudomonas putida* to recreate and build circuits for new-to-nature biological activities that will have an environmental impact by interacting with chemical waste.

ADVISORY / VOLUNTEER EXPERIENCE

- NCC ARMY EME cadet with Indian Army Corps, IIT Kharagpur.
- Associate member of Business Club, IIT Kharagpur.
- Member of Journal Club, IIT Kharagpur Association of Biotechnologists

SKILLS

PROGRAMMING:
Proficient in: ● Python ● R ●MATLAB ● C ● C++ ● Java ● Git ● LATEX
Familiar with these: ● Docker ● GPU/CUDA ● MySQL

MACHINE LEARNING / DEEP LEARNING
● Jupyter Notebook ● Scikit-learn ● Keras ● Tensorflow ● Google Collab

BIOINFORMATICS & STRUCTURAL BIOLOGY
● Bioconductor ● Biopython ● Single-cell transcriptomics ● RNA-SEQ ● NCBI BLAST ● RCSB PDB ● PyMoL ● GROMACS ● CHARMM ● AMBER ● ClusPro 2.0 ● Rosetta ● VMD ● UCSF ChimeraX

Technical Reports (Full list: here)

1. Prediction of structure, finding critical residue and interacting sites of antitoxin toxin pairs of *Neisseria lactamica*, and study dynamics of proteins using Molecular Dynamics Simulations. (Link to associated presentation, Link to thesis)
2. Prediction of structure, finding critical residue and interacting sites of antitoxin toxin pairs of *Neisseria gonorrhoeae*, and study dynamics of proteins using Molecular Dynamics Simulations & peptide design for the same.(*manuscript in preparation)
3. Network Based Identification of Top Key Master Regulators associated with Invasiveness Cancers (*manuscript in preparation)