

# Dinesh Ravindra Raju

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## EDUCATION

**Georgia Institute of Technology | Atlanta, GA**

**Expected Fall 2022**

- *Master of Science (Bioinformatics)*. GPA: 3.5
- Relevant Graduate Coursework: Genomics and Applied Bioinformatics, Introduction to Database Systems, and Programming for Bioinformatics

**Sir M. Visvesvaraya Institute of Technology | Bangalore, India**

**August 2018**

- *Bachelor of Engineering (Biotechnology)*. Graduated in First Class with Distinction
- Relevant Undergraduate Coursework: Biostatistics and Biomodeling, Genomics and Proteomics, and Data Structures and Algorithms

## EXPERIENCE

**Emory University School of Medicine | Graduate Researcher | Atlanta, GA**

**Aug 2021 - Present**

- Currently working on structural and functional characterization of three highly potent Spike-mAb complexes isolated from SARS-COV-2 patients
- Desired result of the research is to correlate the **effect of mutations** on the SARS-COV-2 Spike protein, specifically in the receptor-binding domain (RBD), on antibody binding affinity via **QM/MM studies**

**Kcat Enzymatic Private Limited | Research Scientist | Bengaluru, India**

**Feb 2019 - July 2021**

- Engineered and 3d modelled a membrane bound CYP450 enzyme catalyzing C-22 desaturation reaction for the biocatalytic synthesis of an Active Pharmaceutical Ingredient (API), which is expected to **increase the client's revenue by 8.5 million dollars**
- Develop, optimize, and apply pipelines for processing and analyzing **Molecular Dynamics** trajectory data
- Spearheaded the development of an algorithm that quantifies the interactions between the substrate and amino acid residues during protein structural transformations
- Collaborated with the **University of St. Andrews** to identify plausible drug-binding pockets in the domains of SaTrmK and design small ligand compounds that inhibited the **binding of tRNA to Trmk**, resulting in decreased SaTrmK A22-methylation activity in Methicillin-resistant *Staphylococcus aureus* (MRSA).

## PROJECTS

**Exome Variant Analysis Project**

**Fall 2021**

- Developed and implemented a pipeline for variant analysis of exome sequencing data to determine variants(SNP) in an individual chosen from the 1000 Genomes Project
- Identified non-synonymous, deletion mutations resulting in a pathogenic mutation in the selected individual by checking for protein models and literature review

**RNA-Seq Analysis of ciprofloxacin treated Pseudomonas aeruginosa and Escherichia coli**

**Fall 2021**

- Developed a multi-tool pipeline for comparative gene expression analysis of differential gene expression profiles of *Pseudomonas aeruginosa* and *Escherichia coli* treated by ciprofloxacin
- The SOS response to ciprofloxacin in *P. aeruginosa* and *E. coli* was found to be similar.
- <https://gtbinf.wordpress.com/2021/11/04/11223/>

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## PUBLICATIONS

**Raju, D. R.**, Kumar, A., BK, N., Shetty, A., PS, A., Kumar, R. P., Lalitha, R., & Sigamani, G. (2021). Extensive modelling and quantum chemical study of sterol C-22 desaturase mechanism: A commercially important cytochrome P450 family. *Catalysis Today*.

<https://doi.org/10.1016/j.cattod.2021.12.004>

*Accepted*

Sweeney P, Crowe A, Kumar A, **Raju D**, Krishna NB, Sutherland E, Leo CJ, Fisher G, Lalitha R, Muthuraj L, Sigamani G, Oehler V, Synowsky S, Shirran SL, Gloster TM, Czekster CM, Kumar P, da Silva RG. Structure, dynamics, and inhibition of *Staphylococcus aureus* m1A22-tRNA methyltransferase.

<https://doi.org/10.1101/2021.12.24.474102>

## PATENTS

**Patent Application No: 202141000858 patented as per Indian Patent Act**

**08-01-2021**

A process to identify if a given 3D structure of a Transaminase enzyme complexed with PLP is S-selective or R-selective and to calculate the enantiomeric excess of the product of a Transaminase-Substrate reaction.

**Patent Application No: 202041038649 patented as per Indian Patent Act**

**08-08-2020**

Covalent Modulators of Spike Protein of Covid-19 and Compound that Challenges the Pockets that Stabilizes the Interchain Interaction of Spike Protein of Covid-19 and New Covalent Modulators Against MPRO of SARS-COV-2.

## SKILLS

**Programming Languages:** Python, Bash, awk, SQL, **VMD Tcl scripting**

**QM/MM Tools:** GROMACS, NAMD, AMBER, CPMD, GAMESS, Avogadro, CP2K, VMD, MDTraj

**Drug design:** AutoDock, CAVER, Autosite, MM/PBSA, MM/GBSA, MOPAC, Pymol

**Protein Modelling:** ISOLDE, COOT, PHENIX, ChimeraX, Modeller, Robetta, I-TASSER

**Tools, Packages, Platforms:** DESeq2, GATK, BWA Aligner, Kallisto, FastQC, BLAST, NCBI Toolkit, Ensembl Variant Effect Predictor (VEP), GATK, Galaxy Server, GEO2R

**Bioinformatics Experience:** Exome Variant analysis, RNA-Seq analysis

**Databases:** UCSC Genome Browser, Ensembl, NCBI, Entrez, dbSNP, RefSeq, 1000 Genomes Project

**Operating Systems:** macOS, Windows, \*nix environment

**Others:** MS Office Suite, Adobe Photoshop, GraphPad Prism

## AWARDS & HONORS

- Awarded the Computational Biology Faculty Award, Georgia Institute of Technology, Spring 2022
- All India Rank 681, Graduate Aptitude Test For Engineering (GATE), 2016
- Recognized as the best employee of the quarter (September – December 2020) for leading and completing two client projects successfully