Akanksha Yadav

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Education

2015-2019 **Bachelor of Science in Chemistry (4 Year BS)**
Along with a Minor degree in Biosciences
Indian Institute of Technology Bombay, Mumbai
CGPA: 8.86/10

2019-2021 (Ongoing) **Master of Science in Molecular Biology**
International Max Planck Research School-Molecular Biology, Göttingen

Research Experience

May-June 2020 **Rotation III - Investigating Ubiquitin dynamics using NMR-based relaxation dispersion**
Guide: Prof. Christian Griesinger, NMR-based Structural Biology group, MPI-BPC

- Analyzed ^{1}H-^{15}N **TROSY** experiments of 15N-labeled ubiquitin in water/d8-glycerol, 900MHz
- Calculated τ_c for ubiquitin samples from R_1 and R_2 relaxation data using Ccp-Nmr Analysis
- Analyzed ^{1}H-^{15}N **CPMG** relaxation dispersion data and wrote scripts to fit into two/three-state fast-exchange **Luz-Meiboom** model

Mar-Apr 2020 **Rotation II - Analyzing MD simulations of ArfB in solution v/s in ribosome complex**
Guide: Prof. Helmut Grubmüller, Theoretical and Computational Biophysics group, MPI-BPC

- Performed 600ns of molecular dynamics simulation of free protein ArfB in explicit solvent starting from a cryo-EM derived structure in ribosome complex, using **GROMACS**
- Analyzed secondary structure composition along trajectories and performed principal component analysis (**PCA**) with respect to different domains to identify dominant modes of motion
- Investigated mechanism of C-terminal of ArfB helping to position N-terminal, in the ribosome, for catalyzing **peptidyl-tRNA hydrolysis** using RMSF, RMSD and distance analyses

Jan-Feb 2020 **Rotation I - Prediction of gene expression measurements using cis and trans-eQTLs**
Guide: Dr. Johannes Söding, Quantitative and Computational Biology group, MPI-BPC

- Modified the PredictDB pipeline from PrediXcan to build **gene expression prediction** models using cis- and trans-eQTLs (discovered from **Tejaas**)
- Compared models' (different methods for **confounder correction** used on gene expression input data) performance using summary statistics
- Compared models' predictive performance across different races using nested cross-validation

2017-2019 **Molecular Dynamics Studies of Small Molecule Ligands with G-Quadruplex DNA**
Guide: Prof. Pradeepkumar P.I., Dept. of Chemistry, IIT Bombay

- Modelled and **optimized** potential G-quadruplex binding ligands using **Gaussian 09**
- Performed **rigid docking** of ligand with receptor G4 DNA in silico using **Autodock 4.2**
- Performed **molecular dynamics** simulations of ligand-DNA complex using AMBER 16
- Assisted performing biophysical assays to study interactions of ligands with G-quadruplexes
- Kumari, B.; **Yadav, A.**; Pany, S.P.; Pradeepkumar P.I; Kanvah, S.; Cationic red emitting fluorophore: A light up NIR fluorescent probe for G4-DNA. *J. Photochem. Photobiol., B*, 2019, 190, 128-136

Summer 2018 **GUI development for a data-based chemical modelling software suite, CANDIY**
Guide: Prof. Gaurav Chopra, Dept. of Chemistry, Purdue University

- Studied features of CANDOCK, part of CANDIY, designed for **docking** of small molecule ligands with biomolecules, coded in C++ for adding in the GUI
- Integrated 3D molecule renderer from **Avogadro** (open source) into **Qt**-based GUI of CANDOCK
- Parsed atomic and bond information from CANDOCK to Avogadro for visualization of input molecule integrated with the functions to run the program from the GUI

Scholastic Achievements

2019-2021	Recipient of stipend by the International Max Planck Research School **(IMPRS)**
2015-2019	Granted **INSPIRE Scholar Award** by the Dept. of Science and Technology, Govt. of India
2018	Recipient of summer stipend under **Purdue Undergraduate Research Experience** program
2016,2017	Awarded the **Institute Academic Prize** for two consecutive years Ranked **2nd** (SPI:10.0 in Spring semester 2016-17) in the 2015 batch, Department of Chemistry
2011-2015	Qualified the **National Talent Search Examination** and received a scholarship
2013	Selected for the **Indian National Mathematical Olympiad** from Mumbai zone conducted by HBCSE under the National Board of Higher Mathematics
2009	Among top 50 scholarship holders in state-level two-tier **Mathematics Prodigy Competition**

Academic Projects

Apr 2019 **Macro-molecular Crystallography course project - raw data processing**
Guide: Prof. Ruchi Anand, Dept. of Chemistry

- Processed diffraction data starting from raw images on **iMOSFLM** including peak picking, indexing, refining, integration, merging and scaling
- Determined space group, unit cell parameters, mosaicity and processing parameters
- Used **COOT** to visualize a given electron density and predict structure of putative ligand

Oct 2018 **Bioinformatics course project - Understanding de novo DNA synthesis**
Guide: Prof. Prasenjit Bhaumik, Dept. of Biosciences and Bioengineering

- Literature review regarding DNA polymerase showing de novo synthesis activity
- Recognizing **primase** and **polymerase** active sites in available PDB structures, understanding the mechanism of action and comparing key residues involved
- Utilizing multiple sequence alignment, secondary and tertiary structure prediction and fold recognition tools to gain insight into structure of **PrimPol**

Sep 2016 **Molecular biology course project - Modelling a Genetic Switch**
Guide: Prof. Swati Patankar, Dept. of Biosciences and Bioengineering

- Designed a **hypothetical switch** to drive a **targeted** system for checking **cancer cell growth**
- Incorporated an **optoelectronic gate**, based on a **series of porphyrins**, stimulated using an input photon of green light produced by an intracellular GFP construct
- Applied **small molecule targeted therapy** strategy by utilizing the switch to activate a repressor ligand photochemically, which then binds to **promoter region** and arrests transcription

Nov 2015 **Computer Programming and Utilization course project - Text Processor**
Guide: Prof. Varsha Apte, Dept. of Computer Science and engineering

- Coded an editing software that took raw electronic text as input and used simple commands fed by the user to invoke desired utilities
- Utilized basic structures in C++ to create editing tools like Find and Replace, Encode, Decode

Skill set

Languages	C/C++, R, Python, Bash, LaTeX
Software	PyMol, Chimera, Coot, ClustalX, GROMACS, CCP4i, CcpNmr, Autodock, Gaussian, AMBER, Rosetta, 3DNA, Adobe Illustrator, AutoCAD, Solidworks
Wet lab	UV/Visible and IR spectroscopy, agarose gel electrophoresis, Gibson assembly, PCR and cloning, DNA quantification, protein purification, SDS-PAGE, cell culture, transfection, mRNA microinjection, fast kinetics using stopped flow, single-molecule FRET using TIRF microscopy, light microscopy, NMR and Mass Spectroscopy of proteins

Key Courses Undertaken

Major (Chemistry)	**Organic:** Reactions of carbonyl compounds, Thermal and photochemical reactions **Inorganic:** Magnetochemistry, Organometallic Chemistry **Physical:** Chemical Thermodynamics, Data Analysis, Introduction to computational quantum mechanics, Molecular energetics and dynamics, Molecular spectroscopy, Computational Chemistry
Others	Calculus, Linear Algebra, Differential equations, Quantum Physics, Basics of electricity/magnetism
Minor	Molecular Biology, Genetic Engineering, Introduction to Computational Biology, Metabolism and Bioenergetics, Molecular cell biology and Genetics, Bioinformatics, Molecular biophysics
Master (2 lectures each)	**DNA and Gene Expression:** DNA Structure, Replication and Repair, Genomics, Epigenetics, Transcription, Translation, RNA Splicing, RNA-based regulation, Protein Structures and Folding **Metabolic and Genetic Networks:** Enzyme Mechanisms and Regulation, Biological Membranes, Photosynthesis, Metabolic Networks, Signal Transduction, Microbiomes **Cell Biology, Immunology:** Protein Sorting and Processing, Ubiquitin, Nucleocytoplasmic Transport, Cytoskeleton, Cell Cycle, Meiosis, Apoptosis, Cancer, Infectious Diseases, Immunology: Innate Immunity, T Cell Development and Function, B Cells

Extracurricular Activities

Misc.
- Member of **Hertha Sponer College** of Multiscale Bioimaging (MBExC) platform, Göttingen targeting select students to provide interdisciplinary training in natural sciences/biomedicine
- Attended **UK Biobank** Scientific Conference 2020, **Lindau** Online Science Days 2020
- Joined **The Physics of Life** online summer school 2020 by Princeton University
- Successfully completed the workshop **Statistics for Life Scientists** conducted by the SIB, Basel
- Qualified for finals of **Bioinformatics Contest** 2018 organized by Stepik and Rosalind
- Completed courses on **Coursera**: Introduction to genomic technologies - JHU, Bioinformatics-I (with honors) - UC San Diego, Machine Learning - Stanford
- Cleared level A1.1 of **German language** course
- Volunteered to organize Asia-Pacific Conference of Theoretical and Computational Chemistry, 8

Sports
- Secured **gold medal** in the 200m event at the annual athletic championship conducted by Bombay City District Amateur Athletic Association (BCDAAA)
- Bagged **bronze medal** in 4x100m relay at **Bombay YMCA** annual athletic meet
- Won **bronze medals** in the events 100,200m at the institute Athletic General Championship
- Part of the **IIT Bombay Athletics** team selected to participate in Inter IIT competition

References

Email **Dr. Johannes Söding** | Quantitative and Computational Biology group, MPI-BPC
Email **Prof. Dr. Helmut Grubmüller** | Theoretical and Computational Biophysics group, MPI-BPC
Email **Prof. Dr. Christian Griesinger** | NMR-based Structural Biology group, MPI-BPC
Email **Prof. Anindya Dutta** | Department of Chemistry, IIT Bombay