# Akanksha Yadav

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## Education

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| **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** | **Master of Science in Molecular Biology** |
| (Ongoing) | 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 $^1H$-$^{15}N$ **TROSY** experiments of 15N-labeled ubiquitin in water/d8-glycerol, 900MHz
- Calculated $\tau_c$ for ubiquitin samples from $R_1$ and $R_2$ relaxation data using Ccp-Nmr Analysis
- Analyzed $^1H$-$^{15}N$ **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: Prof. 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

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| 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

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| **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

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| Major (Chemistry) | **Organic:** Reactions of carbonyl compounds, Thermal and photochemical reactions <br> **Inorganic:** Magnetochemistry, Organometallic Chemistry <br> **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 <br> **Metabolic and Genetic Networks:** Enzyme Mechanisms and Regulation, Biological Membranes, Photosynthesis, Metabolic Networks, Signal Transduction, Microbiomes <br> **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

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| Misc. | - Member of **Hertha Sponer College** of Multiscale Bioimaging (MBExC) platform, Göttingen targeting select students to provide interdisciplinary training in natural sciences/biomedicine <br> - Attended **UK Biobank** Scientific Conference 2020, **Lindau** Online Science Days 2020 <br> - Joined **The Physics of Life** online summer school 2020 by Princeton University <br> - Successfully completed the workshop **Statistics for Life Scientists** conducted by the SIB, Basel <br> - Qualified for finals of **Bioinformatics Contest** 2018 organized by Stepik and Rosalind <br> - Completed courses on **Coursera**: Introduction to genomic technologies - JHU, Bioinformatics-I (with honors) - UC San Diego, Machine Learning - Stanford <br> - Cleared level A1.1 of **German language** course |
| Sports | - Secured **gold medal** in the 200m event at the annual athletic championship conducted by Bombay City District Amateur Athletic Association (BCDAAA) <br> - Bagged **bronze medal** in 4x100m relay at **Bombay YMCA** annual athletic meet <br> - Won **bronze medals** in the events 100,200m at the institute Athletic General Championship <br> - Part of the **IIT Bombay Athletics** team selected to participate in Inter IIT competition |