Yogesh Todarwal

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Carrier Goal

As I transition from academia to industry, I am keen to employ my profound expertise in theoretical model development, advanced simulations, and machine learning methodologies. I am driven by the prospect of harnessing these skills to tackle pressing industry-centric challenges, pushing the boundaries of innovation and achieving meaningful results. (Add two lines connecting to position that I am applying)

Work Experience

KTH Royal Institute of Technology   Dec. 2018 – Present
Ph.D. Researcher   *Stockholm, Sweden*

Outlook: Here is my example sentence in typewriter text: `This is an example sentence.`

Key Responsiblities:

- **Developed and refined force field (FF) parameters** to enhance the accuracy of Molecular Dynamics (MD) simulations for complex supramolecular systems, achieving less than 1 kcal/mol error in dihedral potential and under 0.1 eV discrepancy in transition energies.
- **Validated the refined FF parameters** by conducting comparative studies with Density Functional Theory (DFT) calculations, assessing conformers' relative energies and examining transition wavelengths for optimized geometries, ensuring enhanced predictive accuracy.
- **Conducted comprehensive research** on host-guest chemistry related to neurodegenerative diseases, pinpointing strong binding sites and modes for proteins like amyloid-beta, tau, and transthyretin (TTR) and proposing binding energy estimates for various fluorescent ligands.
- **Identified a unique binding site** for the bTVBT4 ligand specific to Alzheimer's Disease (AD) tau, providing insights into its non-reactivity with tau associated with Pick's Disease (PiD) and contributing to disease-specific detection.
- **Investigated self-assembly systems** for material development, delivering insights on spectral alterations due to side chain substitutions in oligothiophenes, establishing stable self-assembly models, and analyzing solvent effects on the spectroscopic properties of various molecular structures.

Radboud University   May 2016 – July 2016
Research Intern   *Nijmegen, Netherlands*

- **Conducted molecular modeling studies** on porphyrin systems, employing a range of software tools, enhancing the comprehension of allosteric behaviors within these systems.
- **Delved deep into allosteric modulations**, enhancing the broader understanding of molecular information transfer, inter-site communications, and the intricate dynamics of molecular interactions.
- **Employed virtual screening techniques** in the domain of supramolecular chemistry to pinpoint molecules exhibiting a heightened affinity, achieving a strong correlation between computational predictions and experimental results.

Education

KTH Royal Institute of Technology   Dec. 2018 – Jan. 2024
PhD in Theoretical Chemistry and Biology   *Stockholm, Sweden*

Indian Institute of Technology Bombay   June 2013 – May 2018
Integrated M.Sc. in Chemistry. (With focus on Computational Chemistry)   *Bombay, India*

Relevant Coursework

- Linear Algebra
- Data Analysis
- Differential Equations
- Calculus
- Advance Quantum Chemistry
- Computer Programming and Utilization (C++ and bash)
- Programming in Python
- Introduction to High-Performance Computing.

Technical Skills

Languages   : Python, Bash, C++, SQL
Operating Systems: Linux, Windows, MacOS
Software/Library : Pandas, NumPy, Matplotlib, Keras, Scipy, scikit-learn, SQL, Gromacs, Github/Gitlab, Gauss view, Gaussian16, Gamess, AIM2000, MultiWfn, Spartan, Autodock, Gold, ChemOffice, Chemissian, CYlview, MDAnalysis, Ambertools

Volunteer Positions

Assistant Manager of 50th inter-IIT sports Meet 2014   Aug. 2014 – Dec. 2014
Food and Beverage department
- Leadership: Administrated the allocation and execution of a refreshment budget of INR 1.5 million
- Planning: Formulated tendering process for messing facility to be provided for 1700 participants and 200 officials

Coordinator, MOOD INDIGO 2014   Apr. 2014 – Dec. 2014
Asia's largest cultural festival, Food and Beverages Department
- Cooperation: Worked in a team of 15 members
- Negotiation: Involved in helping the Core Group Members in fixing deals with various food vendors
- Management: Responsible for the food court set up on the campus during the festival

Phonathon volunteer conducted by Student Alumni Relations Cell (SARC)   June 2014
IIT Bombay Representation and Networking
- Networking: Represented IIT Bombay to establish strong relations with IITB Alumni
- Communication: Called 100+ IIT Bombay alumni for their reunion and alumni-student mentorship program

Personal Interest

I'm a huge fan of self-help books and frequently tune into inspiring podcasts. In the evenings, you'll often find me doing Zumba, out running to catch my breath, or relaxing with some comedy movies. Trekking, hiking, and camping? Count me in for all those outdoor adventures!