Yogesh Todarwal

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Career Goal

As I transition from academia to industry, I am keen to employ my profound expertise in programming, 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.

Work Experience

KTH Royal Institute of Technology — Dec. 2018 – Jan. 2024

Ph.D. Researcher — *Stockholm, Sweden*

Overview: Primarily focused on computational studies of protein-ligand interactions and self-assembly systems, I have made significant contributions to over nine projects (link). My work involved advancing multiscale simulation strategies by enhancing the accuracy of force fields used in simulations. This enhancement is crucial for understanding non-covalent interactions and ensuring reliability in spectroscopic studies and conformational analysis. Additionally, my PhD work encompassed rigorous data analysis and interpretation, writing research articles, collaborating with diverse research groups, and presenting our findings at international forums.

Key Achievements:

- Developed and refined force field 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.
- Utilized 3 million-atom MD simulations to characterize binding of various ligands to amyloid fibrils. This work contributes to the method development for early stage detection of Alzheimer's disease and is corroborated by experimental data.
- Elucidated the selective fluorescence of bTVBT4 ligand in Alzheimer's versus Pick's disease by identifying a unique binding mechanism: an accessible site in AD-tau and a blocked one in Pick's-tau.
- Devised a computational atomistic model for fibrillar structures, clarifying the self-assembly of low molecular weight gels. This model offers key insights into molecular-level gel formation processes.

Radboud University — May 2016 – July 2016

Summer Internship — *Nijmegen, Netherlands*

Overview: Internship focused on two key research areas: 1) Investigating allosteric modulations in a novel double-cage porphyrin system to understand molecular communication; 2) Advancing virtual screening techniques in supramolecular chemistry using the Autodock program and machine learning algorithms, particularly linear regression, to establish Quantitative Structure–Property Relationship (QSPR) models. This project offered a deep dive into the predictive modeling of the behaviors of chemical compounds, linking molecular structure with observed properties.

Key Achievements:

- Efficiently analyzed conformations of double cage porphyrin systems with limited computational resources using Monte-Carlo algorithm and MMFF force field, followed by semi-empirical PM6 optimization.
- Developed a QSPR using linear regression, revealing a strong correlation between binding energy and the interaction of pyridyl group of viologen (guest) with the porphyrin cage system (host).

Volunteer Research Contributions

Indian Institute of Technology Bombay — Mar. 2018 – Aug. 2018

Research Assistant — *Nijmegen, Netherlands*

Overview: Development of machine learning techniques for the diastereoselectivity of oxazole catalyzed asymmetric reactions under the guidance of Prof. Raghavan B. Sunoj. The project involved a novel approach using feature selection and neural networks to model and predict enantioselectivity in chemical catalysis. My responsibilities included assembling a detailed dataset from validated experiments and computations, building neural network models, fine-tuning hyper-parameters, and conducting a 5-fold cross-validation to affirm the reliability and accuracy.

Key Achievements:

- Enhanced model accuracy by applying feature selection with random forest algorithm to identify key chemical parameters.
- Efficiently predicted enantioselectivity, leading to expanded reaction library and discovery of highly selective ligands.
- Contributed to creating a versatile machine learning approach for solving a wide range of chemical problems.

Education

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

Indian Institute of Technology Bombay **Aug. 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

Selected Presentation Opportunities

- Poster presentation in a multiscale molecular dynamics workshop at the EPFL, Switzerland. 2022
- Research presentation to Master students taking the course BB2280 (Molecular modeling). 2021
- Poster presentation in Computing π-Conjugated Compounds conference. 2021
- ITN-COSINE workshop at the Trieste, Italy. 2019
- Wavefunction based methods workshop at Heidelberg University, Germany. 2019
- Ph.D. secondment at the SDU, Denmark. 2019

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

Scholastic Achievements and Awards

- A research article published with 1st author was highlighted by CBH school news within KTH (Link). 2021
- Undergraduate Research Award (URA 01) for outstanding contribution to academic research in the year 2016-2017 2017
- INSPIRE SCHOLARSHIP by the Department of Science and Technology, Govt. of India. This fellowship with the worth of INR 320,000 has been awarded to the top 1% of the Indian students pursuing basic sciences. 2013
- Ranked in the top 1% of the country in the Joint Entrance Exam (JEE) taken by about 900,000 students. 2013

Personal Interest

My days often begin with enriching my mind through inspiring podcasts and self-help books. As evening approaches, I switch gears to physical activities for a healthy balance. 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!