Dr. Rajendra Kumar

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https://github.com/rjdkmr

ABOUT ME
Scientist, Engineer, Pharmacist, Rapid Learner, Knowledge Explorer, Problem Hunter, Determined and Focused, Innovative and Creative Thinker.

Research Areas

- Computational Chemistry
- Computational Biochemistry
- Chemoinformatics
- Bioinformatics
- Computational Biophysics
- Computational Biology

Technical Skills

- C/C++
- Python, C/C++ and Python Binding
- Javascript/Typescript
- Full stack development
- Backend
  - NodeJS - Express.js, Apollo GraphQL
  - Python - Flask, FastAPI, Pydantic
- Front-end – React, MUI, knockout.js
- Database – SQL, SQLAlchemy
- CI/CD – Jenkins, Kubernetes, Docker
- UIs – QT Designer, PyQt5, HTML/CSS
- Data analysis - numpy, scipy, matplotlib, pandas, h5py
- Machine Learning – scikit-learn
- Other: git, CMake, Vite, Rollup, pytest
- AWS (familiar) – S3, ECR, EC2, ElasticCache

Experience

05/02/2025 TO PRESENT

Associate Professor / Dept. of Pharmacoinformatics, NIPER, SAS Nagar (Mohali), Punjab, 160062

My research interests are in methods and AI development for therapeutic design at molecular level. My research areas include computational biophysics with focus on MD simulations, computational chemistry , chemoinformatics, structural bioinformatics and computational biology.

20/06/2022 TO 31/12/2025

Senior Scientific Software Developer - Associate Principal Data Engineer / AstraZeneca UK Ltd, Cambridge, United Kingdom

My role is to design and develop web-application, libraries, methods, and tools to augment and accelerate drug-design and discovery in AstraZeneca.

- **Technical Lead** for the project "**CAG Explorer**" - it is a **chemistry search engine** with a user-friendly interface only available inside AstraZeneca as like PubChem.
  - Designed and developed both front-end (**React/MUI/Vite**) user interface **(UI/UX)** and backend GraphQL server (**Apollo-GraphQL/NodeJS/ExpressJS**).

- In my role as a Technical Lead, I facilitated stakeholder meetings, gathered requirements, and allocated tasks to team members during each sprint.

- Contributed to Predictive Insight Platform (PIP) project under A-DMTA platform (**Augmenting DMTA using predictive AI modelling at AstraZeneca,** *Drug Discovery Today, Volume 29, Issue 4, April 2024, 103945*)**.**
  - **Advanced Python** programming – **concurrency**, **multiprocessing** etc.
- Microservices with OpenAPI (**swagger**) documentation – Python **Flask**/**FastAPI**-**Pydantic**
- CI/CD on AWS using **Docker**, **Jenkins**, **ArgoCD** and **Kubernetes** (familiar)
- Built **Grafana** dashboard for monitoring app usage and health.
- I designed, developed, and implemented **a new algorithm** for **the fastest yet accurate binary vector search** employed for **fingerprint chemical similarity search** – **Python**/**C**/**C++**.
- Familiarity with **ElasticSearch**/**OpenSearch** – built search queries.

30/09/2019 TO 15/06/2022

Senior Scientific Software Developer – Senior Research Associate / Astex Pharmaceutical, Cambridge, UK

My key role was to integrate my expertise in chemoinformatics, molecular modeling, simulations, and computational chemistry with programming and problem-solving abilities. I had designed and developed methods, tools, and software to accelerate drug-design and discovery in Astex.

- Designed and developed new methods and web-applications for computational drug-design
  - PDB/EMDB visualizer (**KnockoutJS**/**JQuery**/**Flask**/**SQLAlchemy**) – A NGL based web-app to search, browse and visualize PDB and EMDB structures
  - A web-app (**KnockoutJS**/**JQuery**/**Flask**) for Pharmacophore-based ligand clustering.
  - Automated pipeline for MD simulations using GROMACS – through **Python**.
  - Contributed in Overlay-pages (https://astx.com/interactive/F2L-2022/) development – **KnockoutJs**/**JQuery**/**Flask**/ **SQLAlchemy**
  - Designed and developed several small web-apps and libraries including **Python/C binding**.
- Actively contributed to the development of NGL (https://nglviewer.org/ngl/).
- Rewriting and retraining ESP Charge model for chemical compound with **TensorFlow**/**Python**.
- Developed a **new method for prediction of absolute binding free energy** by combining Molecular Dynamics Simulations and **Machine Learning** models.

01/01/2018 TO 31/08/2019

Postdoctoral Research Associate / Department of Chemistry, Umeå university, Umeå, Sweden

My key role was to perform scientific research - to design compounds that selectively target certain, or even individual, G-quadruplexes to study their biological roles and investigate their potential as therapeutics.

- Designed and developed **a software tool** "gmx_clusterByFeatures" for feature-based clustering of molecular conformations from Molecular Dynamics trajectories.
  - Developed as **Python package by binding with C++** – used **pybind11**
  - Employed Python **scikit-learn** for K-Means and other clustering algorithm.
  - CLIs for users with no-programming experiences.
  - Documentation website using sphinx - https://gmx-clusterbyfeatures.readthedocs.io/
- Used several python libraries such as numpy, scipy, scikit-learn and matplotlib for data analysis

01/04/2015 TO 31/12/2017

Postdoctoral Research Associate / ICE Lab, Umeå university, Umeå, Sweden

- Development of a **platform for the comparison, interactive visualization and analysis of genome contact maps**. It is a large software package with GUI. It is **published** in **NAR** (https://doi.org/10.1093/nar/gkx644).
  - Designed and developed Genome Contact Map Explorer (gcMapExplorer)
  - Developed as a platform with **CLIs**, **APIs** and **UIs** for visualization and analysis – **Python/Cython/PyQt5**
  - Addressed the problem of visualizing and analyzing (calculations) huge matrix data.
  - Python modules such as numpy, scipy, scikit-learn, matplotlib, h5py, Cython etc. were used in this software.
  - Documentation website using Sphinx - https://gcmapexplorer.readthedocs.io/
- Performed **modelling and simulations of mitotic chromosomes** – data analysis using Python libraries (https://link.springer.com/article/10.1007/s00412-018-0684-7).

01/08/2014 TO 31/12/2015

Postdoctoral Research Research Associate / Max Planck Institute for Biophysical Chemistry, Goettingen, Germany

- **Design** and **developed** **do_x3dna and dnaMD** - tools to analyze structural fluctuations of dsDNA or dsRNA from molecular dynamics simulations.
  - Developed in Python and employed modules such as numpy, scipy, matplotlib, h5py etc.
  - Documentation website using Sphinx - https://do-x3dna.readthedocs.io/

Education

JULY 2014

PhD / Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany

- Dissertation title: "Molecular dynamics studies of the Phi29 Connector DNA complex"
- Supervisor: Prof. Dr. Helmut Grubmüller
- Specialization: Computational Biophysics and Biochemistry
- Grade: Magna cum laude

JUNE 2009

M. S. (Pharm.) / National Institute for Pharmaceutical Education and Research (NIPER), SAS Nagar, Punjab, India

- Specialization: Pharmacoinformatics
- Grade: 73.6%

JUNE 2007

B. Pharm. / Birla Institute of Technology (BIT), Mesra, Ranchi, Jharkhand, India

- Specialization: Pharmaceutical Sciences
- Grade: 81.8%

Academic Achievements

- Published **research papers in high impact factor journals** like JACS, NAR, RSC Chemical Science etc. and earned **> 4300 citations**.
- Qualified (**in top 100 rank**) **ICMR** Research-Fellowship Examination 2009.
- Qualified (**in top 10 rank**) **JNU** PhD Entrance Examination 2009, New Delhi, India.
- Achieved All India **65 rank** in **NIPER** Entrance Examination 2007.
- Achieved All India **485 rank** in **GATE** 2007 (Pharm. Sciences).
- Achieved All India **274 rank** in All India Engineering Entrance Examination 2003 (Pharmacy)

Research Publications

Google Scholar: https://scholar.google.com/citations?user=zYKuBCcAAAAJ