Sivasudhan Rathnachalam, PhD

Computational Scientist & Data Enthusiast

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PhD in (bio) computational chemistry with **multidisciplinary background** and fascination with innovations in computational sciences. About two years of experience in protein engineering linked to Biotech industry. Proficient and interested in developing challenging computational programs to solve scientific problems with machine learning approaches. I enjoy inter-team and client communications of complex scientific results in a technically diverse teams.

Work Experience

Ongoing
November 2021

Protein Modeller, Operations division
EV Biotech | Groningen, the Netherlands

Modelling/Computational Chemistry

- Rationalizing experiments through atomistic (molecular dynamics) simulations
- Quantum chemistry/Physics calculations to study molecular interactions
- Inter-team communication of scientific results to diverse audience
- Technical expert in dealing with client queries related to proteins
- Successfully completed 4 internal R&D projects as a project lead and 3 other projects as co-lead.

Selected research projects

- Deep-learning driven bio-synthetic pathway search for natural products
- Protein thermal stability prediction using deep-learning approach
- Automatizing (Python) of molecular dynamics workflow for enzyme engineering
- Workflow for protein-ligand/protein-protein binding free energy computations

Position history

- In Nov 2021 joined the company as molecular dynamics analyst in computational teams
- In Apr 2022 promoted as a protein modeller
- In June 2022 Nov promoted as protein scientist in the Operations division

Industrial research | Data analysis and engineering | Comp. chemistry | Enzyme engineering | Deep-learning | Project management | Bioinformatics

Ongoing
Jan 2023

Guest Researcher
University of Groningen | Groningen, the Netherlands

- Reactive Martini forcefield for protein structure prediction.

Python | method development | Coarse-grained simulations

July 2017
October 2013

Research fellow
Institute of Plant Physiology, Russian Academy of Sciences | Moscow, Russian Federation
Full-time since September 2016

- Planned and conducted molecular biology experiments with inhibitory analysis
- Processed experiment samples for RT-PCR/RT-qPCR
- Analysed the experimental data
- Contributed to the assessment of cyanobacterial culture collection by analysing various strains
- Created new hypothesis about cyanobacterial calcium signalling system based on my experiments

Molecular biology | Plant physiology | Microbiology | mRNA | DNA | Gene regulation

Courses

On-going

Datascience Specialization
University of California, Davis | Coursera
SQL, Data wrangling, analysis & AB testing, Distributed computing with PySpark SQL, SQL for data science Capstone project
SQL | PySpark | Data engineering | Complex data management | AB testing

On-going | **Deep learning Specialization**
Stanford University | Coursera
Neural networks and deep learning, hyperparameter tuning, regularization, optimization, convolutional neural networks, sequence models

Deep learning | optimization | CNN | Neural network | machine learning

Education

Nov 2022 – Oct 2017 | **PhD | Computational Chemistry**
Zernike Institute for Advanced Materials, University of Groningen | Groningen, the Netherlands
Thesis : *Excited-state processes in biomolecules* - a computational study of biomolecular interactions with light.

Computational chemistry | Protein-ligand docking | Molecular dynamics | Quantum dynamics | Excited-state processes | Electronic structure methods | Soft X-ray absorption simulations

July 2016 – September 2014 | **Master | Physical Chemistry**
University of Pune | Pune, India
Thesis : *Effect of Au-nanoparticles in absorbing radioactive waste- a computational study*

DNA-Au binding | Computational Chemistry | Nanoscience

Skills

Programming Languages	**Python**, Bash/shell, Fortran90, Julia, MATLAB
Python libraries	Numpy, Pandas, Scikit learn, **RDkit**, MDAnalysis, Cobrapy, Pytorch
Computational programs	Q-Chem, Gaussian, ORCA, DFTB, **XTB**, MOPAC, GROMACS, NAMD, OpenMM, High performance computing
Communication	Presentation, Public speaking, **Networking**, Science communication
Management	**Project development**, Project management (Agile), Teamwork
Languages	English(fluent), **Dutch(A2)**, Bengali, Hindi, Tamil (Native)

Extracurricular activities

September 2021 – July 2019 | **Founder and organiser**
Academic lunches in Groningen | Groningen, the Netherlands
Academic lunches in Groningen was a social group that allows researchers to share their work/expertise to the diverse audience.

Public speaking | Communication | Networking | Leadership

August 2016 – Dec 2014 | **Founder, member**
Student Science Club | Pune, Maharashtra, India
The student science club aimed at organising lectures from the state-of-the art scientific topics by veteran scientist, and facilitating debates of scientific interest.

Communication | Public outreach

Leisure

- Classical Music
- Reading (non-fiction)
- Cooperative Board Games
- Swimming

Interests

- Data Science
- Machine learning
- Theoretical chemistry
- Street Photography