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 Scientist, 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`

📖 PROFESSIONAL TRAINING

Data engineering

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`

AI/ML

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`

Management	Agile project management

GOOGLE | Coursera

Agile, Scrum workflow, Product Backlog, Implementing scrum, Applying Agile in the organization

Project management · Agile · Scrum

🎓 EDUCATION

Nov 2022 Oct 2017	**PhD	Computational Chemistry**

UNIVERSITY OF GRONINGEN | Groningen, the Netherlands

<u>Thesis</u> : *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

<u>Thesis</u> : *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

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

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

🏆 AWARDS

🎓 Awarded integrated **MS-PhD scholarship** at Indian Institute of Scientific Education and Research, Trivandrum [2012-2014]

🏆 **S.N. Bhatt Memorial Excellence fellowship**, International Center for Theoretical Sciences, Bangalore [2015]

⧖ Junior Research Fellowship, Tata Institute of Fundamental Research, Mumbai, India [2017]

🎓 Secured a competitive **PhD Scholarship** ($\sim$ 100K €) by writing a scientific proposal [2017-2021]

🚲 LEISURE

> Indian-classical (Carnatic) Music
> Reading (non-fiction)
> Cooperative Board Games
> Swimming

🔭 INTERESTS

> Behavioral sciences
> Machine learning
> Theoretical chemistry
> Portrait Photography