NITHISHWER MOUROUG ANAND

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Computational research scientist with expertise in AI-integrated immunogenomics and multi-scale physics

EDUCATION

University of Oxford, *DPhil in Computational Biochemistry* June 2026
Indian Institute of Science Education and Research, Mohali, *BS-MS, Physics & Data Science*, GPA: 3.5 Aug 2022

SKILLS

Languages	Python, R, C++, HTML/CSS, SQL, Julia, Perl, Java, Matlab, Git, Bash, LaTeX, Markdown
Research Software	Seurat, Gromacs, Scanpy, OpenFF, Scvelo, OpenMM, Velocyto, Dandelion, AMBER, AutoDock
Data Software	Tensorflow, Pytorch, Docker, OpenCV, Linux, Theano, HuggingFace

RESEARCH EXPERIENCE

Vertex Pharmaceuticals, *Visiting Research Scientist* Jan 2024 - Present

- Industrial Supervisors: Dr Ewa Chudyk, Dr Ronald Knegtel and Dr Fabio Zuccotto from Computational Chemistry.
- Implemented absolute binding free energy pipelines for compound potency prediction to membrane proteins.
- Applied the pipeline to pharmaceutically relevent Orexin Receptor (OX2R) agonists with an accuracy of 2 kcal/mol.

Department of Biochemistry, University of Oxford, *Doctoral Student* Oct 2022 - Present

- Academic Supervisors: Prof Philip Biggin and Prof Syma Khalid
- Investigating absolute binding free energy (ABFE) calculations for membrane targets in TRPC3/6 ion channels.
- Used metadynamics and ABFE calculations to investigate binding of GSK986, a novel TRPC3 inhibitor.

Institute of Immunology and Immunotherapy, University of Birmingham, *Bioinformatician* March 2023 - July 2023

- Academic Supervisors: Prof. Shivan Sivakumar and Prof. Rachel Bashford-Rogers
- Investigated pseudotime dynamics of T-cells in pancreatic ductal adenocarcinoma using scRNA-seq velocity analysis.
- Used dandelion, a computational scVDJ-seq pipeline to integrate V(D)J and pseudotime trajectory feature space

Department of Physical Chemistry, University of Oxford, *Master's Project Student* Mar 2021 - Mar 2022

- Academic Supervisors: Prof. Jonathan Doye, Prof. Ard Louis
- Investigated the free energy of DNA hairpins under nanoconfinement with Coarse Grained Molecular Dynamics
- Used oxDNA, oxView and Pymbar to visualize analyse and plot DNA origami trajectories from MD Simulations

School of Physics and Astronomy, University of Edinburgh, *Summer Research Intern* May 2020 - Aug 2020

- Supervisor: Prof. Andreas Hermann
- Used Ab-initio MD simulations to investigate plastic and superionic phases of mixtures at extreme conditions
- Performed quantum calculations in VASP using density functional theory (DFT) and Hartree–Fock exchange

Indian Institute of Technology, Madras, *ML Research Intern* May 2019 - Jul 2019

- Supervisors: Prof Lelitha Devi Vanajakshi, Dr Anil Kumar Bachu
- Developed a patented novel Deep-learning model for travel time prediction by incorporating domain knowledge with existing AI/ML techniques, outperforming Google Maps with an MAE of 5s

PUBLICATIONS AND PATENTS

1. Sivakumar, S., Jainarayanan, A., Arbe-Barnes, E., Sharma, P. K., Leathlobhair, M. N., Amin, S., ... **Mouroug Anand, N.** … Bashford-Rogers, R. (2023). Single-Cell Immune Multi-Omics and Repertoire Analyses in Pancreatic Ductal Adenocarcinoma Reveal Differential Immunosuppressive Mechanisms within Different Tumour Microenvironments. (DOI:10.1101/2023.08.31.555730)

2. Jainarayanan, A., **Mouroug Anand, N.**, Arbe-Barnes, E. H., Bush, A. J., Bashford-Rogers, R., Frampton, A., Heij, L., Middleton, M., Dustin, M. L., Abu-Shah, E., Sivakumar, S. (2023). Pseudotime dynamics of T-cells in pancreatic ductal adenocarcinoma inform distinct functional states within the regulatory and cytotoxic T-cells. IScience, 26(4), 106324. *(DOI:10.1016/j.isci.2023.106324)*

3. Haresh Liya, D., Elanchezhian, M., Pahari, M., **Mouroug Anand, N.**, Suresh, S., Balaji, N., and Jainarayanan, A. K., (2023) QPromoters: Sequence Based Prediction of Promoter Strength in Saccharomyces Cesrevisiae. *All Life 16, no. 1 (2023).* (DOI:10.1080/26895293.2023.2168304)

4. Liya, D. H., **Mouroug Anand, N.** , Jainarayanan, A. K., Elanchezhian, M., Seetharaman, M., Balakannan, D., & Pradhan, A. K. (2022). Drug repurposing and sequence analysis in S-glycoprotein variants reveals critical signature patterns and destabilization of receptor-binding domain in omicron variant. *Journal of Biomolecular Structure and Dynamics, 1-18.* (DOI:10.1080/07391102.2022.2127902)

5. **Mouroug Anand, N.**, B. Anil Kumar, Vanajakshi, L. , et al. (2021): Deep learning– just data or domain related knowledge adds value?: bus travel time prediction as a case study *The International Journal of Transportation Research* (DOI:10.1080/19427867.2021.1952042)

6. Beal, J., Farny, N.G., Haddock-Angelli, T. ,Selvarajah, V. , Baldwin, G. S., Buckley-Taylor, R., Gershater M., Kiga, D., Marken, J., Sanchania, V., Sison A., Workman C. T. & **iGEM Interlab Study Contributors** et al. (2020) Robust estimation of bacterial cell count from optical density. Commun Biol 3, 512. *Communications Biology* (DOI:10.1038/s42003-020-01127-5)

7. **Mouroug Anand, N.**, Haresh Liya, D., Pradhan, A. K., Tayal, N., Bansal, A., Donakonda, S., et al. (2020): A Comprehensive SARS-CoV-2 Genomic Analysis Identifies Potential Targets for Drug Repurposing. *Plos One* (DOI:10.1371/journal.pone.0248553)

8. Surana, P., Jainarayanan, A. K., **Mouroug Anand, N.** and Sharma, M. (2019) Analysing non-synonymous mutations in Multidrug-Resistant tuberculosis drugs. *Journal of Clinical Tuberculosis and Other Mycobacterial Diseases. (JCTUBE)* (DOI:10.1016/j.jctube.2019.100124)

9. **[PATENT] Mouroug Anand, N. (2020)**. A method and system for predicting a vehicle travel time (Indian Patent number: 202141005606). The Indian Patent Office (IPO), Office of the Controller General of Patents, Designs and Trademarks (CGPDTM) , Government of India.

AWARDS & GRANTS (TOTALLING 165K USD)

Runner Up, HDR UK-Roche Hackathon	Apr 2024
Reuben Public Engagement with Research Innovation Award, Reuben College	Mar 2024
Enspire All-Innovate entrepreneurship award, Oxford University Innovation	Feb 2024
Industrial Cooperative Award in Science & Technology (iCASE), Vertex Pharmaceuticals	Oct 2022
Oxford Reuben Scholarship, Reuben Foundation	Oct 2022
Certficate of academic excellence, IISER Mohali	Dec 2021
Indian Biological Engineering Competition (iBEC) - 2018, Department of Biotechnology, Govt. of India	Aug 2018
Indian Biological Engineering Competition (iBEC) - 2017, Department of Biotechnology, Govt. of India	Aug 2017
Innovation in Science Pursuit for Inspired Research Fellowship, Department of Science & Technology	Aug 2017

LEADERSHIP

Junior Dean, Hertford College, Oxford, UK — Jan 2024 - Present

- Head of the college welfare team at the Hertford College Graduate Center, South Oxford.
- Managed the discipline and welfare of over 100 students while maintaining essential health and safety standards.

Vice President of Social Affairs, Reuben College GCR, Oxford, UK — Dec 2022 - Present

- Organized social events, formal dinners, and intercollegiate exchanges in collaboration with the social secretaries
- Represented the Student body (GCR) on Graduate Provision Committee (GPC) and College General Body meetings

Co-Founder, Magnes Technologies, Enspire Student Entrepreneurs' Programme (StEP) — Mar 2023 - Present

- Founded a startup based on patented University of Oxford IP for haptic technology with Prof. Jeroen Bergmann
- Recognized a market opportunity and led a team of skilled scientists and engineers to develop innovative technology currently incubated at Oxford University Innovation. Won £500 in pre-seed funding at Enspire All-Innovate.

Consultant, Olga's Fine Foods, The Oxford Strategy Challenge — Sept 2023 - Dec 2023

- Developed a comprehensive 5-year AI strategy aimed at optimizing cost reduction initiatives across critical areas such as marketing and product innovation by analysing over 1000 offerings across more than 5 supermarket chains

Co-Founder, Oxtraits, Nucleate Catalyse programme, Cancer Tech Accelerator, OX1 incubator — Nov 2022 - Mar 2023

- Founded a startup for next-gen, cloud-based, non-invasive genetic risk assessment using patented dermatoglyphics technology.

CONFERENCES AND WORKSHOPS

HDR-UK Roche Hackathon	April 2024
European Biophysical Societies' Association Congress, Stockholm	Aug 2023
SteP student entrepreneurship programme	Jun 2023
OX1 Startup Incubator - EnSpire, Oxford	May 2023
Nucleate Catalyse entrepreneurship programme, Oxford	Mar 2023
Vertex chemistry PhD student day, Oxford	Feb 2023
Cancer Tech Accelerator, London	Feb 2023
ESMO Immuno-Oncology Congress, Geneva	Dec 2022
23nd EMBL PhD Symposium | The Big Picture: Zooming Into Life, Virtual	Dec 2021
International Genetically Engineered Machines (iGEM), Boston	Oct 2018