

# NITHISHWER MOUROUG ANAND

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

## EDUCATION

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**University of Oxford, DPhil in Computational Drug Discovery**

June 2026

**Indian Institute of Science Education and Research, Mohali, BS-MS, Physics & Data Science, GPA: 3.5**

Aug 2022

## SKILLS

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Languages Python, R, C++, HTML/CSS, SQL, Julia, Perl, Java, Matlab, Git

Research Software Tensorflow, Pytorch, Docker, OpenCV, Seurat, Gromacs, OpenFF, Scvelo, OpenMM, AutoDock

## RESEARCH EXPERIENCE

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**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 relevant 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

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1. Sivakumar, S., Jainarayanan, ..**Mouroug Anand, N.**. Distinct immune cell infiltration patterns in pancreatic ductal adenocarcinoma (PDAC) exhibit divergent immune cell selection and immunosuppressive mechanisms. *Nat Commun* 16, 1397 (2025). DOI:10.1038/s41467-024-55424-2
2. Cook, C., Alibay, I., **Mouroug Anand, N.**, Chudyk, E., Knegtel, R., & Biggin, P. (2024). Challenges of Absolute Binding Free Energies for Membrane Exposed Binding Pockets . *ChemRxiv*. doi:10.26434/chemrxiv-2024-9hwjs
3. Ries, B., Alibay, I., **Mouroug Anand, N.**...& Biggin, P. (2024) 'Automated absolute binding free energy calculation workflow for Drug Discovery', *Journal of Chemical Information and Modeling*, 64(14), pp. 5357–5364. doi:10.1021/acs.jcim.4c00343.
4. 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)
5. 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)
6. 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)

7. **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)
8. 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)
9. **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)
10. 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)
11. [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)

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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
Certificate 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

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<b>Junior Dean</b> , 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.	
<b>Vice President of Social Affairs</b> , 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	
<b>Co-Founder, Magnes Technologies</b> , 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.	
<b>Co-Founder, Oxtraits</b> , 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

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Your Entrepreneurs Scheme 24	Jan 2025
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