NATESAN MANI

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SUMMARY

Computational Scientist with expertise in the application of Molecular Dynamics to analyze protein systems. I possess the ability to lead cross-functional projects in collaboration with biotech leaders like Amgen and Genentech and I am passionate about translating scientific insights into real-world therapeutic solutions.

EDUCATION

Northeastern University   Boston, MA
Ph.D. Candidate   Expected 2025
University of Houston   Houston, TX
M.S. Chemical Engineering   2020
Osmania University   Hyderabad, India
B.S. Chemical Engineering   2019

RESEARCH EXPERIENCE

Northeastern University – *SimBioSys Lab*   Boston, MA
Doctoral Researcher – Protein Dynamics   January 2022 – Current

- Spearheading a project to design high-affinity antibodies using computational strategies in collaboration with Amgen.
- Investigated the dynamics of viral spike proteins such as SARS CoV-2 and HIV whose results contribute to potential therapeutics.
- Implemented custom analysis methods using Python, TCL and Bash to interpret simulation data.
- Utilized visualization tools such as VMD and PyMOL to analyze trajectories and structures.
- Developed expertise in utilizing software packages such as GROMACS, NAMD, or AMBER for molecular dynamics simulations and analysis.
- Presented posters and talks at several posters and talks at both national and regional conferences.
- Mentored undergraduate students in computational methods and molecular dynamics simulations.

WORK EXPERIENCE

Prescient Design, Genentech   **South San Francisco, CA**
Structural and Computational Biology Intern   June 2025-August 2025

- Using Physics based modelling and Machine learning towards applications in Large Molecule Drug Discovery.
- Developing an in-silico workflow to predict high concentration properties of complex antibody formats, relevant to several high-profile portfolio projects
- Using coarse grained Molecular Dynamics and design high concentration systems to help predict antibody viscosity and aggregation.
- Integrating ML models with physics-based predictions to accelerate therapeutic antibody developability assessment.

Amgen   **Cambridge, MA**
Process Development Intern – Antibody modelling   September 2023 - April 2024

- Modelled the antibody and NK receptor interface, with a focus on glycans in the Fc region of the antibody
- Calculated binding affinities using rigorous energy methods to train machine learning models for binding affinity prediction.
- Programmed analytical tools in Python to analyze simulation data and extract key interface dynamics that were used to gain molecular insight into the observed energy predictions
- Developed and optimized code for GPU-accelerated simulations and data analysis on high-performance computing clusters.
- Collaborated with experimental researchers from the Pivotal Attribute Sciences department and presented extensively at both Amgen and Northeastern.

TEACHING EXPERIENCE

Northeastern University   Boston, MA

Graduate Teaching Assistant   Sept 2021 – Dec 2021
- Advised approximately 40 graduate students on the topics of transport phenomena and fluid dynamics
- Graded exams, quizzes and projects and assisted in teaching the ANSYS software.

PUBLICATIONS

Mani, N., Suresh, R., & Chakraborty, S. (2025). Cleaved versus Uncleaved: How furin cleavage reshapes the conformational landscape of SARS-CoV-2 spike. *Protein Science*, 34(12), e70368. https://doi.org/10.1002/pro.70368

Mani, N., Polozova, A & Chakraborty, S. (2025) Deciphering the Role of Core Fucosylation in IgG1 Fc–CD16a Binding Through All-Atom Simulations, manuscript under preparation

Xiaoling Shi, Pardis Sadeghi,…**Natesan Mani** et al. "Novel, accurate pathogen sensors for fast detection of SARS-CoV-2 in the aerosol in seconds for a breathalyzer platform", *Biosensors and Bioelectronics,***2023, 14**

SELECT CONFERENCE PROCEEDINGS

Natesan Mani, Alla Polozova, Srirupa Chakraborty, "Impact of Glycan Architecture on IgG1 Fc-CD16a Binding: Insights from All-Atom Simulations." 2025 AIChE Annual Meeting, Abstract ID: 714688.

Natesan Mani, Alla Polozova, Srirupa Chakraborty, "Glycan-mediated regulation of IgG1 Fc-CD16a interactions: Insights from all-atom simulations.", Biophysical Journal, Vol 124, Issue 3, p428a.

Natesan Mani, Raghavendran Suresh, Srirupa Chakraborty, "Elucidating the role of Furin cleavage in SARS CoV-2 spike allostery using molecular dynamics simulations.", Biophysical Journal, Vol. 122, Issue 3, p188a.

LEADERSHIP AND SERVICE

ChemE Graduate Student Council (GSC)   Boston, MA
Treasurer   January 2024 – Current
- Budgeted for several academic and social events and acted as a liaison between the department and the graduate students
- Organised academic and social events such as Thesis Karaoke, Fall Formal and ChemE Jeopardy.
- Kickstarted the mentoring program and helped in matching incoming PhD students with mentors

Northeastern Biophysical Society   Boston, MA
President   January 2025 (expected)
- Founded the Biophysical Society student chapter at Northeastern University to promote collaboration and engagement of graduate students and faculty performing biophysics-based research.
- Organised multiple research talks given by Doctoral and Postdoctoral students across multiple departments.
- Organised workshops on software such as VMD and PyMOL

HONORS AND AWARDS

- **Broad Institute Prize** ($500) for "F.A.D.E: A Fully Agentic Drug Engine" research presentation (2025)
- **BPS Travel Award** to present research talk and poster at Biophysical Society Annual Meeting (2025)
- **LEADERs Fellowship** recognizing exceptional leadership and project management capabilities (2024)
- **PhD Network Travel Grant** for research presentation at Biophysical Society Annual Meeting (2023,2025)
- **ACS Travel Grant** for research presentation at ACS Northeast Regional Meeting (2023)
- **NSF ACCESS Award** providing 10,000 GPU hours of high-performance computing resources (2023)
- **Outstanding Service Award** for contributions to departmental initiatives and community engagement (2023)
- **Department Travel award** for presenting a talk at AIChE (2025).

SKILLS

Programming Languages: Python, R, TCL, Shell Script, Bash, Linux, LaTeX, WolframScript, MATLAB, SQL
Software: CHARMM, AMBER, GROMACS, Schrodinger, VMD, PyMOL, UCSF ChimeraX, SLURM, Git, VSCode, Rosetta, Tableau, COMSOL, ANSYS, Illustrator.
Engineering Leadership: Project Management, Grant Writing, Budget Planning, Mentoring, ROI analysis, Timeline Development.