NATESAN MANI

Boston, MA | mani.na@northeastern.edu | +17130417811 | www.linkedin.com/in/natesan-mani

SUMMARY

Computational biophysicist combining all-atom molecular dynamics simulations with data-driven analysis to solve problems in therapeutic antibody design. Industry experience at Genentech and Amgen developing predictive models for antibody viscosity, aggregation, and binding affinity. Published work on SARS-CoV-2 spike dynamics and glycan-mediated Antibody-receptor interactions.

EDUCATION

Northeastern University — Boston, MA
Ph.D. Candidate — Expected May 2026

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

- Leading a project to design high-affinity antibodies using computational strategies in collaboration with Amgen.
- Investigated conformational dynamics of SARS-CoV-2 and HIV spike proteins using microsecond-scale all-atom MD simulations, revealing allosteric mechanisms relevant to therapeutic targeting
- Developed custom analysis tools in Python, TCL, and Bash for processing multi-terabyte trajectory datasets and extracting mechanistic insights
- Mentored 3 undergraduate researchers in molecular dynamics simulation protocols and data analysis workflows
- Published 1 first-author manuscript along with 2 co-authored manuscripts and presented research at 5+ national conferences (BPS, AIChE, ACS).

WORK EXPERIENCE

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

- Developed computational workflow using custom coarse-grained molecular dynamics models (HOOMD-blue) to predict high-concentration behavior (viscosity, aggregation, solubility) for diverse therapeutic antibody formats
- Built in-silico screening platform to generate high-concentration property data across multiple antibody variants, designed to enable ML-based prediction for novel sequences and reduce experimental screening burden
- Validated computational predictions against experimental formulation data, informing portfolio decisions for high-profile therapeutic programs, work under consideration for patent application and joint publication
- Designed and executed GPU-accelerated CG-MD simulations on HPC infrastructure to model concentration-dependent antibody interactions at therapeutically relevant conditions (>150 mg/mL)

Amgen — **Cambridge, MA**
Process Development Intern – Antibody modeling — 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.
- Work contributed to 2 first-author manuscripts currently in preparation and multiple conference presentations.

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
- Organized 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 – December 2025

- Founded the Biophysical Society student chapter at Northeastern University to promote collaboration and engagement of graduate students and faculty performing biophysics-based research.
- Organized multiple research talks given by Doctoral and Postdoctoral students across multiple departments.
- Led VMD and PyMOL workshops for 25+ students

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.