RITANKAR BHATTACHARYA, Ph.D.

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Chemical Engineer ● Computational Chemist ● Protein Engineer ● (+91)90382-68721

SUMMARY

- Dr. Bhattacharya is a dedicated researcher with expertise in rational protein design and engineering, focusing on sequence design and alignment, structure prediction, epitope mapping, molecular docking, and fine-tuning their physicochemical properties, such as solubility, thermostability, immunogenicity, and mutation analysis - all based on chemical engineering thermodynamics. He is proficient in leveraging advanced **industry-standard** tools, such as **Rosetta, AlphaFold, RosettaFold, ProteinMPNN,** and **RFdiffusion** to develop innovative solutions in designing and optimizing therapeutic protein binders. Currently, he is **training** in **AI/ML** to apply to such fields. He has consistently demonstrated his ability to contribute to impactful scientific work, for which he was **awarded the GSC Travel Award for presenting at international conferences like AIChE and ACS**. He has always tried to connect computational and experimental research for which he participated in a workshop and earned an **NEB Molecular Biologist (CMB)** certification. With his research experience, he plans to develop a quick, cost-effective, innovative methodology to design on-demand therapeutic binders. As an undergraduate researcher, he gained experience in polymer membrane science. His work was recognized, and he was awarded a **full scholarship as a summer research intern at CNR-ITM, University of Calabria, Cosenza, Italy** to work with PVDF hollow fibers and flat sheet membranes for their application in membrane distillation. His works have been published in journals, such as **ACS Synthetic Biology, Scientific Reports,** and **Materials Today**.

- His strong communication skills, such as experience in grant proposal writing (**NIH NRSA F31**), scientific reports, reviewing articles, managing simultaneous projects (**funded by NIGMS, NIH: MIRA $1.75M**), and assisting his peers in research makes him an effective team player. He can simplistically articulate complex scientific concepts to present the audience with an interesting and engaging topic. He can efficiently plan, execute, and record projects independently.

SKILLS

Technical Skills

- **Protein Engineering**: Protein design and structure prediction using RosettaDesign, RFdiffusion, ProteinMPNN, AlphaFold, and RosettaFold; Molecular Docking, Sequence alignment
- **Molecular Mechanics Force fields**: CHARMM, Rosetta for energy calculation and data analysis
- **Molecular Dynamics Simulation**: VMD, NAMD for molecular dynamics simulation to investigate molecular behavior such as protein – ligand interactions
- **Optimization**: Solubility (SoluProt, CamSol), Thermostability (SCooP, PoPMuSiC, HoTMuSiC), De-immunization (IEDB), Visualization tools (UCSF Chimera/ PyMol)
- **Protein Databases**: RCSB PDB, UniProt, IMGT, SKEMPI for using the PDB files
- **Command-line Interfaces**: Linux, Windows Terminal for running short Python scripts and super-computing clusters (HPC, Easley) for running simulations and efficient data analysis
- **Molecular Biology:** New England Biolabs Certified Molecular Biologist (CMB), 2022
- **Immune Epitope Database** and Analysis Resource User Workshop (IEDB), 2022
- **Artificial Intelligence/Machine Learning:** Currently training in AI/ML applications
- **Computational expertise:** Python, Anaconda, MS Office, Jupyter notebook, Adobe Lightroom

Soft Skills

- **Leadership and Collaboration**: Proven experience in mentoring students and managing projects in cross-functional environments
- **Problem-solving and Presentation**: : Solved complex protein design challenges using data-driven approaches and advanced protein modeling tools, and presented in international conferences
- **Project Management and Communication**: Efficient in managing timelines and ensuring the successful delivery of research and development milestones
- **Critical thinking and Experimental Design**: Proposed and successfully executed the entire protein design pipeline with concrete evidence. The designs are being tested in the lab currently

EDUCATION

Auburn University, Auburn, AL, USA   **Aug 2017 – Aug 2024**
Doctor of Philosophy in Chemical Engineering
Thesis: Application of *In-Silico* Protein Engineering and Optimization Methods to Design Target-Specific Antibody Mimetics

Heritage Institute of Technology, Kolkata, WB, India   **July 2012 – June 2016**
Bachelor of Technology in Chemical Engineering

PROFESSIONAL EXPERIENCE

Senior Researcher, Indian Institute of Technology – Kharagpur, WB, India   **Sept 2025 – Present**

Researcher, Auburn University, AL, USA   **Dec 2024 – April 2025**
- Used protein modeling techniques to solve for Sars-Cov2 Nsp8 protein binding sites.

Graduate Research Assistant, Auburn University, AL, USA   **Jan 2021 – July 2024**
- Designed and analyzed over 2,000 monobody – tag epitope peptide complexes based on optimal binding interactions and excellent structural features. Found correlations between their binding metrics, performed post-analysis, and shortlisted the top 1% of designs for experiments. One-third of the selected designs bound experimentally. Published in *ACS Synthetic Biology, 2024*.
- Designed and characterized over 2100 **DARPins** to bind a **snake venom neurotoxin**. Analyzed and shortlisted 2% for **RosettaDesign** affinity maturation. The affinity-matured designs were examined and visually inspected (using **UCSF Chimera**) for optimal binding features, then the top 2% were subjected to **VMD** and **NAMD MD simulations** to assess structural integrity over time. The MD simulation data was analyzed both qualitatively and quantitatively, leading to a down-selection of the top 50 for experiments. Experiments are to begin in Fall 2025.
- Predicted three nanobodies (using **I-Tasser, Robetta, TrRosetta**) to bind canine CTLA4 protein. Employed **ZDOCK** for global docking of these predicted binders with the CTLA4 conserved epitope. Out of 90 predictions, 86 showed nanobodies interacting with the conserved epitope of canine CTLA4.. Published in *Scientific Reports, 2021*.
- Designed helical bundles from the **RCSB PDB** using **RosettaDesign** and optimized them with **CamSol** to enhance solubility, **HoTMuSiC** and **PoPMuSiC** for **thermostability**, and used the **IEDB De-immunization** tool to humanize the sequences and prepare them for engineering as protein binders. The top 15 structures, which folded successfully according to **AlphaFold** and **RosettaFold**, are currently undergoing experimental testing..
- Used **RFdiffusion** and **ProteinMPNN** to *de novo* design over 80,000 protein binders targeting different epitopes of a trimeric antigen. Due to some technical issues with the pae-interaction scores across multiple rounds and time constraints, a new hypothesis was formulated to analyze them later..

Graduate Teaching Assistant, Auburn University, AL, USA   **Aug 2017 – Dec 2020**
- Conducted independent research and taught UG students the fundamentals of computational protein engineering, and molecular visualization tools. Assisted over 50 students with assignments and quizzes (*Phase and Reaction Equilibria, and Computer Aided-Chemical Engineering*) during office hours. Proctored and graded assignments, take-home quizzes, and examinations.

Undergraduate Summer Research Intern   **June – July 2015**
Institute on Membrane Technology – National Research Council of Italy, Italy
- Synthesized and characterized PVDF hollow fiber and flat sheet membranes to analyze and improve viscosity, porosity, permeability, and mechanical strength under the supervision of Late **Dr. Enrico Drioli** (Founding Director) and **Dr. Alberto Figoli** (Director)

Undergraduate Researcher   **Jan 2013 - March 2016**
Heritage Institute of Technology, Kolkata, (HITK), India
- Directed the feasibility analysis of a 500 MW thermal power plant to enhance cost efficiency. Based on assumptions the plant efficiency to be **29%** and the generation cost was **4 cents/unit**.
- Removed arsenic to purify water using Micellar Enhanced Ultrafiltration.
- Purified carbohydrates using ultrafiltration membrane reactor (*95-97% recovery*).

PUBLICATIONS/CONFERENCES

Journal

- *Extracellular Peptide-Ligand Dimerization Actuator Receptor Design for Reversible and Spatially Dosed 3D Cell-Material Communication*, by M. Recktenwald*, R. Bhattacharya*, Md. M. Benmassaoud, J. MacAulay, V. M. Chauhan, L. Davis, E. Hutt, P. A. Galie, M. M. Staehle, N. M. Daringer, R. J. Pantazes, S. L. Vega, **ACS Synthetic Biology**, 2024, *equal contribution
- *Nanobody based CTLA4 inhibitors for immune checkpoint blockade therapy of canine cancer patients*, J. Marable, D. Ruiz, A. K. Jaiswal, R. Bhattacharya, R. Pantazes, P. Agarwal, A. S. Suryawanshi, D. Bedi, A. Mishra, B. F. Smith, and M. Sandey, **Scientific Reports**, 2021
- *Studies On hydrolysis of skimmed milk using immobilized β-galactosidase in a membrane reactor*, P. Sen, N. Choudhury, M. Dutta, R. Bhattacharya, **Materials Today**, 2016

Conference

- Biomedical Engineering Society (**BMES**), 2024 (Co-author - Peptide-Ligand Responsive Receptors that Enable 3D Cell-Material Communication, M. Recktenwald, R. Bhattacharya, J. MacAulay, N. Daringer, R. J. Pantazes, S. Vega)
- American Institute of Chemical Engineers (**AIChE**), 2023 (Oral - The in-silico Design and Analysis of DARPin – α-Cobratoxin Complexes, R. Bhattacharya, A. Richard, R. Pantazes)
- **AIChE** Annual Meeting, 2021 (Oral - Computationally-Designed 10th Type III Fibronectin Domains for Peptide Binding, Bhattacharya R., Chauhan V., Pantazes R.)
- American Chemical Society (**ACS**), 2021 (Oral - Overview of an algorithm for the rapid de novo design of binding proteins, R. Bhattacharya, V. Chauhan, R. Pantazes)
- **AIChE** Annual Meeting, 2019 (Poster - Therapeutic Applications of an Algorithm for Ultra-Rapid Binding Interaction Engineering, Bhattacharya R., Chauhan V., Pantazes R.)
- Several departmental open house and university (interdepartmental) presentations

AWARDS/HONORS and ACHIEVEMENTS

- **Awarded** $300 Graduate Student Council (GSC) Travel Grant, USA — 2022
- **Reviewer** for Graduate School Best Mentor and Frank Strum Memorial Fellowship, USA — 2021
- **Judge** for the UG Auburn Annual Research Symposium, USA — 2021
- **Elected Senator** (Finance team), Graduate Student Council, USA — 2020 – 2021
- **AIChE Student Member,** volunteered in graduate student recruitment, USA — 2019, 21
- **Awarded** the Doctoral student fellowship, USA — 2017 – 2024
- **Qualifed** Graduate Aptitude Test in Engineering (GATE), India — 2017
- **Awarded** the Summer Internship Scholarship at CNR – ITM, Italy — 2015
- **Internshala Student Partner** of my Undergraduate institution HIT, Kolkata, India — 2015 – 2016
- **Peer Mentor** to fellow UG students, assisted with mental health awareness, India — 2012 – 2016

ORGANIZATIONAL ROLES

- Student Member, American Institute of Chemical Engineers — 2019 – 2024
- Student Member, American Chemical Society — 2021 – 2022
- Student Member, Indian Institute of Chemical Engineers — 2012 – 2016
- Official Photographer, Cultural and Tech Fest, HIT, Kolkata, India — 2013 – 2015
- Senior member, Photography club 'Pravasana', HIT, Kolkata, India — 2013 – 2015
- Event Organizer and Coordinator, Students' Council, HIT, Kolkata, India — 2012 – 2015
- Event transportation in-charge, Indian Science Congress Association, India — 2013

RESEARCH INTEREST

- *In-silico* protein sequence design, optimization, structure prediction and fine-tuning.
- Future interests include but not limited to protein purification, expression, binding, biological instruments, CRISPR-CAS9, Next-gen sequencing, cancer therapy, infectious diseases, neurotoxins, genomics, and deep learning.

SUBJECT KNOWLEDGE

- **Technical**: Transport Phenomena; Thermodynamics; Protein Engineering and Therapeutics
- **Soft skill development**: Use of AI; Presentation; Problem solving, critical thinking and writing tasks