Saad Naseem, PhD

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Permanent residence (sponsorship not required)

PROFESSIONAL SUMMARY

Biochemist and metabolic engineer with expertise spanning enzyme mechanism, strain engineering, and machine learning applied to biological systems. Currently leading rare earth element biorecovery and high-throughput bioprocess development at Lawrence Berkeley National Laboratory, integrating robotic liquid handling, statistical design of experiments, and computational approaches to accelerate microbial engineering. Pursuing an M.S. in Computer Science (Machine Learning) at Georgia Tech to deepen capabilities in predictive modeling, cheminformatics, and data-driven bioprocess optimization.

TECHNICAL SKILLS

Molecular Biology: PCR, cloning, Gibson assembly, Golden Gate assembly, CRISPR-Cpf1, CRAGE, gene insertion and deletion in *Pseudomonas putida* KT2440

Protein Biochemistry: Recombinant protein expression and purification (*E. coli*), enzyme kinetics, assay development, Western blot, AlphaFold, PyMOL, Scripps AutoDock Vina

Protein Crystallography: Screening and optimization of crystallization conditions, independent X-ray diffraction data collection

Analytical Chemistry & Instrumentation: HPLC, LC-MS method development, GC-MS (SRM/MRM), NMR, UV-Vis spectroscopy, FPLC (AKTA), plate reader

Computation & Data Science: Python, Java, object-oriented programming, machine learning (supervised, unsupervised), AutoML (AutoGluon), graph neural networks (Chemprop D-MPNN), cheminformatics, JMP statistical software

Automation & High-Throughput Screening: Hamilton Vantage liquid handling, 96-well plate assay development, Biolog PM phenotype microarray workflows

Synthetic Chemistry: Design, multi-step synthesis, purification, and characterization of small organic molecules

EDUCATION

Master of Science in Computer Science (Machine Learning Specialization) — 2024–2027
Georgia Institute of Technology, Atlanta, GA (Online/part-time)
Relevant coursework: CS 7641 Machine Learning, CS 6601 Artificial Intelligence, Introduction to Health Informatics

Ph.D. in Chemistry — 2016–2022
Texas A&M University, College Station, TX
Thesis: *Biochemical and Mechanistic Studies of Metalloenzymes in Lumichrome Catabolism and Chuangxinmycin Biosynthesis Pathway*

Bachelor of Science in Chemistry — 2012–2016
Lahore University of Management Sciences, Pakistan

RESEARCH EXPERIENCE

Lawrence Berkeley National Laboratory — Postdoctoral Scholar, Biochemist (Jan 2022–Present)

Rare Earth Element Biorecovery Using Methylobacterium extorquens AM1

- Developed a high-throughput colorimetric assay (Arsenazo III) for neodymium quantification in 96-well plate format, optimizing pH, matrix matching, and detection limits for complex biological matrices
- Developed automated liquid handling workflows on the Hamilton Vantage platform for media preparation, culture inoculation, and assay execution
- Built Python-based data analysis pipelines for high-throughput screening, including automated hit classification (three-tier system) and visualization

Metabolic Engineering of Pseudomonas putida KT2440

- Characterized C5 sugar catabolic pathways in *Pseudomonas* isolates for expanded carbon source utilization

- Engineered *P. putida* KT2440 using synthetic biology techniques (CRAGE) and CRISPR-Cpf1 systems for gene insertion and knockout
- Developed HPLC methods (Agilent Poroshell 120 EC-C18) for metabolite quantification and pathway analysis
- Mentored an undergraduate researcher in cloning and functional characterization of three enzymes in a xylose utilization pathway

Texas A&M University — Graduate Research Assistant (2016–2021)

Characterization of Metalloenzymes in the Lumichrome Catabolic Pathway

- Led a team of researchers to successfully characterize and develop assays for eight enzymes in the lumichrome catabolic pathway
- Discovered and characterized the first CYP450 to oxidize the C7-methyl of lumichrome
- Synthesized over 15 quinoxaline/isoalloxazine derivatives as substrate probes via multi-step organic synthesis
- Expressed and purified enzymes from diverse superfamilies: CYP450, Rieske dioxygenase, catechol dioxygenase, xanthine oxidase, amidohydrolases, dehydrogenases

Mechanistic Studies of C–S Bond-Forming Cytochrome P450 (CxnD)

- Elucidated the mechanism of C–S bond formation by trapping and analyzing reaction intermediates
- Designed and synthesized substrate analogs as mechanistic probes

Protein Crystallography and Kinetics of Chorismate Dehydratase (MqnA)

- Solved the apo-structure of MqnA and elucidated the first example of irreversible E1cb elimination in enzymology
- Determined enzyme mechanism through detailed kinetics (k_{cat}/K_m, pH-rate profiles)

LUMS — Research Assistant (2015–2016)

- Performed enzyme kinetics studies on dengue protease NS2B

COMPUTATIONAL RESEARCH & SELECTED PROJECTS

Machine Learning for Substrate Utilization Prediction (Georgia Tech / LBNL)

- Developed a graph neural network (D-MPNN, Chemprop) and AutoGluon-based pipeline for predicting *P. putida* KT2440 substrate utilization from a ~220-compound Biolog phenotype microarray dataset
- Engineered molecular descriptors including Morfeus 3D features and partial charge descriptors (Gasteiger, xTB) for improved model performance
- Implemented scaffold-split validation and Tanimoto k-NN baselines; evaluated cross-organism generalizability (*S. cerevisiae*, *E. coli* Nissle)
- Manuscript in preparation

PUBLICATIONS

Google Scholar Profile

1. Wang AL†, Eng T†, Rivier A, **Naseem S**, Codik A, Chen Y, Srinivasan A, Mukundan H, Tringe SG, Petzold CJ, Deutschbauer AM, Mukhopadhyay A*. Unraveling TNT Bioremediation: Redundant Nitroreductases and a Putative Non-Canonical Urea Pathway in *Pantoea* sp. MT58. *Manuscript in preparation.*
2. **Naseem S**, et al. Machine Learning-Driven Prediction of Substrate Utilization in *Pseudomonas putida* KT2440 Using Graph Neural Networks and Phenotype Microarray Data. *Manuscript in preparation.*
3. Sinha S, Jian X, Adak S, **Naseem S**, Steiner JL, Fedoseyenko D, Thiagarayaselvam A, Begley TP*. Vitamin B2 Catabolism: Nature's Route from Riboflavin to Acetoacetate and Pyruvate. *ACS Cent. Sci.* 2025, 11, 2353–2365.
4. Mahanta N, Hicks KA, **Naseem S**, Fedoseyenko D, Dairi T, Ealick SE, Begley TP*. Menaquinone Biosynthesis: Biochemical and Structural Studies on Chorismate Dehydratase. *Biochemistry* 2019, 58(14), 1837–1840.
5. Joshi S, Fedoseyenko D, Mahanta N, Manion H, **Naseem S**, Dairi T, Begley TP*. Novel Enzymology in Futalosine-dependent Menaquinone Biosynthesis. *Curr. Opin. Chem. Biol.* 2018, 47, 134–141.

6. **Naseem S**, Begley TP*. Mechanistic Studies of C–S Bond-Forming Cytochrome P450 Enzyme (CxnD) in Chuangxinmycin Biosynthesis Pathway. *Manuscript in preparation (Scooped)*

AWARDS

- Spot Award, Lawrence Berkeley National Laboratory (2023) — Recognized for presenting research technology advancing interdisciplinary innovation in industrial biotechnology and the bioeconomy
- Best Poster Award, EGSB Annual Meeting, Berkeley, CA (2023)
- Outstanding Teaching Assistant Award, Texas A&M University (2021)
- Nominated, Chemistry Life Processes Award, Texas A&M University (2021)

CERTIFICATIONS

- Deep Learning for Science Summer School, Lawrence Berkeley National Laboratory, Berkeley, CA (June 2025)
- From Artificial Intelligence and Machine Learning to Agent-based Science, EMSL Summer School, Richland, WA (July 2025)

POSTERS & TALKS

- Poster, Biosciences Area Annual Meeting, Berkeley, CA (2023)
- Poster, JGI Annual Meeting, Berkeley, CA (2023)
- Poster, Molecular Foundry Annual Meeting, Berkeley, CA (2023)
- Poster, SIMB Conference, Minneapolis, MN (2023)
- Poster, EGSB Annual Meeting (Best Poster Award), Berkeley, CA (2023)
- Poster, SBFC, Portland, OR (2023)
- Talk, Chemistry Life Sciences Symposium, College Station, TX (2021)
- Poster, Scott Symposium, College Station, TX (2018)

TEACHING EXPERIENCE

General Chemistry Laboratory, Texas A&M University (Fall 2016–Fall 2021)

- Delivered lectures and supervised experimental work for classes of approximately 20 students
- Received the Outstanding Teaching Assistant Award (2021)