SUMAN SAMANTRAY

Computational Chemist/Scientist

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SUMMARY

- Experienced computational chemist with over a decade of expertise across molecular simulation, bioinformatics, and biochemical engineering in high-performance computing environments. Extensive expertise in molecular dynamics (MD), quantum mechanics (QM) with density functional theory (DFT), and Monte Carlo (MC) simulations. Achievements include authoring 10+ publications, presenting at 10+ international conferences, and earning multiple prestigious fellowships and grants.

Key contributions:

- Built a Python interface to track protein aggregation pathways, aiding therapeutic drug design for neurodegenerative diseases.
- Created a Python module to estimate the chemical potential of molecular species in allosteric sites of large enzymes, assessing their toxicity and absorption.
- Formulated protocols for alchemical free energy perturbations and molecular simulations to improve transport efficiency and metabolism estimation within protein complexes.

Areas of Expertise: **Molecular Simulation, Protein-protein interactions, BioPolymers, Catalysis, Metalloenzymes, Small/Large molecule design, Gas adsorption and transport, Lipid membranes, Liquid interfaces, Physics-based modeling, protein-ligand complex**

TECHNICAL SKILLS & EXPERTISE

Languages and Tools:	Proficient:	**Python, Bash, Awk, Scikit, LaTeX, Git, JIRA/Agile, Docker, Slurm**	★★★★★
	Intermediate:	**C++, C, TensorFlow, RDKit, R, Julia**	★★★★☆
Computational packages:	Proficient:	**GROMACS, ORCA, PLUMED, MOE, Spartan, MATLAB, HADDOCK, AutoDock, OpenMM**	★★★★★
	Intermediate:	**Maestro, Gaussian, LAMMPS, CP2K, NWChem, AnSYS, COMSOL**	★★★★☆
Research Skills:	Proficient:	**Molecular dynamics (MD) and Montecarlo (MC) simulation, Structural Biology, Homology modeling, Forcefield development, Replica-exchange MD, Metadynamics, Free-energy perturbations, Thermodynamic integration, High-Performance computing and High-Throughput computing, Computer-aided molecule (drug or substrate) design, Structure-based drug design (SBDD)**	★★★★★
	Intermediate:	**Coarse-grained MD, Density function theory (DFT), Quantum Mechanics (QM) modelling, Bayesian maximum entropy (BME), Artificial Intelligence (AI) and ML/DL, big data analysis**	★★★★☆

WORK EXPERIENCE

Pacific Northwest National Laboratory **– Physical Biosciences Team** — ***Richland, WA, USA***
Research Associate — **08/2022 — Present**

- Contributed to a DOE-funded project on enzymatic catalysis, and artificial catalysts in metalloprotein complexes for converting greenhouse gases to biomass, enhancing energy efficiency.
- Performed DFT-based QM calculations and derived MD force field parameters for redox-active iron-sulfur sites in a tetrameric protein complex.
- Applied graph learning and Dijkstra's algorithm to optimize network paths and discover hidden tunnel architectures within protein complexes.
- Developed tunnel architecture models using free energy perturbations and MD simulations to enhance gas substrate transport efficiency.
- Created a Python program for Grand Canonical MC/MD simulations to estimate chemical potential and substrate occupancy in protein alcoves.
- Utilized metadynamics MD simulations for enhanced conformational sampling of protein complex for efficient docking of methyltransferase

RWTH Aachen University **– Institute of Biotechnology** — ***Aachen, Germany***
Postdoctoral Fellow/Sub-group Leader — **10/2021 — 03/2022**

- Participated in the NMRlipids project, simulating heterogeneous lipid membranes and published related findings.
- Developed simulation protocols to study dynamic binding of anchor peptides on polymer surfaces and improved protein thermophilic performance through mutations.

Juelich Research Center **– Institute of Biological Information Processing** — ***Juelich, Germany***
PhD Researcher — **03/2019 — 08/2021**

- Developed an Intrinsically disordered proteins (IDP)-specific MD force field for studying structure-activity relationships (SAR) of amyloid-beta, advancing Alzheimer's research.
- Designed a Python program to analyze protein aggregation pathways and aggregate size for therapeutic drug design targeting amyloid diseases.
- Implemented Markov state models and BME frameworks to identify metastable states in IDP aggregation pathways.
- Conducted multi-scale modeling of glycosaminoglycans to study their impact on IDP aggregation upon binding.
- Co-authored 8 journal articles and 2 book chapters on IDPs, forcefields, and computational modeling.

University of Galway **– School of Biological and Chemical Sciences** — ***Galway, Ireland***
Research Fellow — **01/2017 — 07/2018**

- Led a project on protein adsorption at liquid interfaces using molecular simulation, resulting in 2 published articles.
- Implemented bias-exchange metadynamics and replica exchange MD to study IDP denaturation at air-water interfaces.

NBCUniversal Media **– Digital Products and Interactive Media** — ***New York, USA***
Senior Software Engineer — **11/2015 — 05/2016**

- Co-developed an iOS SDK for real-time ad display during the 2016 Rio Olympics.
- Developed the iPadOS version of the NBCUView App for internal content review by NBCUniversal staff and clients.

EDUCATION

Ph.D. (Computational Science) | RWTH Aachen University, Aachen, Germany **|** ***(Honors:*** *magna cum laude*) **08/2018 — 11/2021**
Advisor: Prof. Birgit Strodel
Thesis: *Essays on the interplay between glycosaminoglycans and amyloid-β peptides.*

M.Eng. (Chemical Engineering) | University at Buffalo (SUNY), NY, USA **08/2013 — 08/2015**
Advisor: Prof. Jeffrey R. Errington
Thesis: *Calculation of saturation and interfacial properties of CO2-water-sillica system from grand canonical Montecarlo simulation.*

B.Tech. (Chemical Engineering) | Biju Patnaik University of Technology, Odisha, India **08/2009 — 06/2013**

SELECTED PUBLICATIONS (U: Upcoming, J: Journal, B: Book) * - Equal Contribution

J1. Kiirikki, A.M., & NMRLipids Consortium, et al. (2024). "Overlay databank unlocks data-driven analyses of biomolecules for all." *Nature Communications*, 15(1):1136.

J2. Samantray, S., & Strodel, B. (2021). "The effects of different glycosaminoglycans on the structure and aggregation of the amyloid (16–22) peptide." *Journal of Physical Chemistry B*, 125(21), 5511-5525.

J3. Samantray, S., & Cheung, D.L. (2021). "Effect of the air-water interface on the conformation of amyloid beta." *Biointerphases*, 15(6), 061011. (Selected as a Featured Article and highlighted in AIP Scilight)

J4. *Paul, A., *Samantray, S., et al. (2021). "Thermodynamics and kinetics of the amyloid-β peptide revealed by markov state models based on MD data in agreement with experiment." *Chemical Science*, 12(19), 6652-6669.

J5. Samantray, S., et al. (2020). "Different force fields give rise to different amyloid aggregation pathways in molecular dynamics simulations." *Journal of Chemical Information and Modeling*, 60(12), 6462–6475.

B1. Samantray, S., et al. (2022). "Molecular dynamics simulations of protein aggregation: protocols for simulation setup and analysis with Markov state models and transition networks." In *Methods in Molecular Biology*, Humana Press, ISBN 9781071615454, pp. 235-279.

B2. Olubiyi, O.O., Samantray, S., & Illig, A.-M. (2022). "Advances in structure-based virtual screening for drug discovery." In *Advances in Protein Molecular and Structural Biology Methods*, Academic Press, ISBN 9780323902649, pp. 387-404.

Manuscripts in preparation:

U1. "The hidden chokepoints: Exploring gas diffusion in the CODH/ACS enzyme complex using molecular simulations."

U2. "Insights into the catalytic mechanism of A-Cluster in the enzyme Acetyl-CoA synthase (ACS) from First Principles Calculations."

U3. "Thermodynamics and kinetics of gas substrates diffusing into A-Cluster in the enzyme Acetyl-CoA synthase (ACS) using hybrid Monte Carlo/Molecular Dynamics."

RESEARCH GRANTS/AWARDS/SCHOLARSHIPS

2024 Recipient of **Computational and Theoretical Chemistry Institute (CTCI) fellowship** at PNNL, USA. Awarded 10K USD for professional & research development.
2023 Awarded 4.32 million core-hours as Co-PI from Environmental Molecular Sciences Laboratory via PNNL (Office of U.S. DOE), USA.
2020 Awarded 1.70 million core-hours as Co-PI from Juelich Supercomputing Centre via Gauss Center for Computing, Germany.
2018 Recipient of **Aachen Institute for Computational Engineering Science (AICES) PhD fellowship** at RWTH Aachen University, Germany.
2018 Awarded 1.00 million core-hours as Co-PI from Irish Centre for High-End Computing (ICHEC), Ireland.
2017 Recipient of **College of Science and Engineering postgraduate fellowship** at University of Galway, Ireland.

SELECTED PRESENTATIONS/WORKSHOPS (V: Virtual)

2024 Oral and Poster presentation at "Enzymes, Coenzymes and Metabolic Pathways", Gordon Research Seminar and Conference, NH, USA.
2023 Oral and Poster presentation at 13th International Conference on Hydrogenases, Walla Walla, WA, USA.
2021 Oral presentation at 20th Huenfeld Conference: "Computer Simulation and Theory of Macromolecules", Huenfeld, Germany.
2020 Poster presentation at 5th Ulm meeting on "Biophysics of Amyloid Formation", Ulm University, Germany.
2018 Oral presentation at Nanoscale Simulators Meeting of Ireland, University of Limerick, Ireland.

Participant – "**2024** Clay Modelling Workshop" Edinburgh (**V**) | "**2022** CECAM Metadynamics Workshop", Lausanne (**V**) | "**2021** Martini Modelling Workshop", Groningen (**V**) |"**2019** PyEMMA Markov State Modelling Workshop", Berlin | "**2018** CECAM CHARMM-GUI Workshop", Lausanne.

TEACHING/ MENTORING/ VOLUNTEERING/ OUTREACH ACTIVITIES

2024 Reviewer- ACS Applied Materials & Interfaces, Molecular Pharmaceutics, International Journal of Molecular sciences, Molecules, Biomolecules, Frontiers in Molecular Biosciences, Physical Chemistry Chemical Physics.
2023 Volunteer/Curriculum developer- Next-Gen Bio Learning Network facilitated by Institute for Systems Biology, Seattle, USA.
2021 Co-Mentor of Graduate Students [1] Arghadwip Paul, MS Internship, currently pursuing PhD at University of Michigan, US. [2] Alexander-Maurice Illig, MS thesis, currently pursuing PhD at RWTH Aachen, Germany.
2020 Co-organizer, "Hands-on workshop on Molecular Dynamics Simulations of Proteins", Juelich Research Center, Germany.
2018 Served as Teaching Assistant, CH203: Biophysical Chemistry, CH332: Computational Approaches to Drug Design, U of Galway, Ireland.
2017 Instructor, Centre for Talented Youth, Dublin City University, Ireland.