Imesh Ranaweera

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PROFILE

PhD student in Chemistry at the University of Florida, specializing in theoretical and computational chemistry. Research interests span computational methods for drug discovery, machine learning-guided molecular property prediction, and the application of artificial intelligence to chemical and biological systems. Currently contributing to the Molecular Dynamics Data Bank America (MDDBa) project the first MDDB node outside Europe and in the United States and actively engaged in developing and machine learning models to integrate experimental data for protein ensemble prediction.

RESEARCH INTERESTS

Keywords: Computational Chemistry · Drug Development · Machine Learning · Artificial Intelligence · Molecular Dynamics · Force Field Development

EDUCATION

University of Florida, College of Liberal Arts and Sciences
2024 – 2029 (Expected)

Doctor of Philosophy (Reading) in Chemistry — Gainesville, FL, USA

- **GPA**: 4.00/4.00
- **Coursework**: Chemical Bonding and Spectra, Computational Chemistry, Statistical Thermodynamics, Biological System Modeling, AI in Biology, AI in Agricultural and Life Sciences

University of Colombo, Faculty of Science
2019 – 2023

Bachelor of Science (Honors) in Computational Chemistry — Colombo, Sri Lanka

- **GPA**: 3.70/4.00 | **Class**: First Class Honors
- **Chemistry Coursework**: Computational Chemistry, Computational Programming in Chemistry, Advanced Molecular Modeling, Physical Chemistry, Biochemistry, Organic Chemistry, Inorganic Chemistry, Spectroscopy, Organometallic Chemistry
- **Computing/Data Coursework**: Machine Learning and Neural Computing, Data Structures and Algorithms, Database Systems, Fundamentals of Software Engineering, Data Analytics, Computational Biology, Logic Programming

Ananda College
2014 – 2017

G.C.E. Advanced and Ordinary Level Examinations — Colombo, Sri Lanka

- **A/L (2017)**: Biology – A, Chemistry – B, Physics – B | Z Score: 1.6644
- **O/L (2014)**: Nine Distinctions

RESEARCH EXPERIENCE

Molecular Dynamics Data Bank America (MDDBa)
2024 – Present

Graduate Research, Molecular Recognition Group (Perez Lab) — University of Florida, USA

- Contributing to the establishment of MDDBa, the **first MDDB node outside Europe** and the first in the United States, as part of the Perez Lab at the University of Florida

- Involved in data curation, infrastructure development, automation and interoperability efforts to expand global access to molecular dynamics simulation data

Undergraduate Research Project 2022 – 2023

Supervisor: Prof. Samantha Weerasinghe, Dept. of Chemistry University of Colombo, Sri Lanka

- Studied hydrotrope-driven solubility enhancement of drug-like molecules from Sri Lankan flora using **GROMACS** molecular dynamics simulations.
- Built **Fortran 95** tools for automated analysis and comapared hydrotropic effects of pyrogallol and resorcinol.

PUBLICATIONS

Journal Article 2026

- Imesh Ranaweera, Alberto Perez. *Beyond Classical Force Fields: Physics-Driven Assessment of the Grappa Machine-Learned Force Field on the FoldBind Dataset*. *ChemPhysChem*, 2025. https://doi.org/10.1002/cphc.202500815

Conference Abstract 2023

- I.C.M. Ranaweera, S. Weerasinghe. *Investigation of the effects of selected hydrotropes on the solubility of drug-like molecules from Sri Lankan flora: a computational approach*. 79th Annual Scientific Sessions, Sri Lanka Association for the Advancement of Science (SLAAS).

TEACHING & ACADEMIC EXPERIENCE

Graduate Research Assistant May 2026 – Present

Department of Chemistry, Molecular Recognition Group (Perez Lab) University of Florida, USA

- Conducting computational chemistry research focused on molecular dynamics, machine-learned force fields, and drug discovery applications

Graduate Teaching Assistant Aug. 2024 – May 2026

Department of Chemistry University of Florida, USA

- Assisted faculty with lecture delivery and course coordination for undergraduate chemistry courses
- Conducted weekly discussion and recitation sessions for undergraduate students
- Held regular office hours to provide individualized academic support
- Proctored examinations and evaluated assignments, problem sets, and laboratory reports

Teaching Assistant (Visiting) 2023 – 2024

Department of Chemistry CINEC Campus, Sri Lanka

- Assisted in delivering a Certificate Course in Computational Chemistry: Computer Aided Drug Design

Teaching Assistant Aug. 2023 – Jul. 2024

Dept. of Computation and Intelligent Systems, UCSC University of Colombo, Sri Lanka

- Facilitated computer laboratory practical sessions and tutorials for first- and second-year undergraduates
- Co-supervised second- and third-year group projects, providing technical and research guidance
- Evaluated assignments, tutorials, and practical assessments across multiple modules

- **Subjects**: Introduction to Computing, Data Structures and Algorithms, Programming and Problem Solving, Rapid Application Development, Middleware Architecture
- Organizing Committee Member, **23rd ICTer International Conference**
- Organizing Committee Member, **I Am a Researcher Competition 2023**

AWARDS, CERTIFICATIONS & ACHIEVEMENTS

Achievements

Global Winning Team Member, BioML Challenge (Bits to Binders 2024–2025) 2025

- Member of PDNALab, the global winning team of the BioML Challenge: Bits to Binders competition

HiPerGator Pioneering Team Award 2025

- Team member recognized with the HiPerGator Pioneering Team Award at the University of Florida

Champions - Inter-University Chemistry Magic Competition 2022

- Led team to first-place finish in the inter-university chemistry magic competition

Certifications

Research Security Training (Combined), *CITI Program* 2026

Research Security Training, *CITI Program* 2026

Physical and Natural Sciences Responsible Conduct of Research, *CITI Program* 2026

Fundamentals of Deep Learning, *NVIDIA* 2026

Supervised Machine Learning: Regression and Classification, *DeepLearning.AI* 2024

Introduction to Artificial Intelligence, *IBM* 2023

Drug Discovery, *University of California San Diego* 2023

Introduction to Quantum Computing, *Udemy* 2023

Observation of Near-Earth Objects and Main Belt Asteroids via Pan-STARRS Image Analysis 2020, 2021, 2022

PRESENTATIONS & ACADEMIC ACTIVITIES

Oral: *Beyond Classical Force Fields: Physics-Driven Assessment of the Grappa Machine-Learned Force Field on the FoldBind Dataset*, CINEC International Research Symposium, CINEC Campus, Sri Lanka

Oral: *Beyond Classical Force Fields: Physics-Driven Assessment of the Grappa Machine-Learned Force Field on the FoldBind Dataset*, University of Florida, USA

Oral: *Investigation of the effects of selected hydrotropes on the solubility of drug-like molecules from Sri Lankan flora: a computational approach*, University of Florida, USA

Oral: *Biochemistry of Human Hair*, University of Colombo, Sri Lanka

Interview: Team interview of Prof. Rodolphe Barrangou for CH 4002 Seminar and Essay, University of Colombo, Sri Lanka

Project: Fortran 95 program to simulate a model salt in liquid argon for CH 3032 Computational Programming in Chemistry, University of Colombo, Sri Lanka

SKILLS

Programming : Python, Fortran, SQL

Scientific Software : AMBER, GROMACS, MELD, AlphaFold, BioEmu & aSAM, MDANCE, Gaussian 09W, GaussView 5.0, RasMol, RasWin, PyMOL, VMD, ChimeraX, Xmgrace, HyperChem Professional, WinMopac 7.21, ChemDraw, BURAI, ORCA

AI & LLM Tools : Claude Code / Codex / Opencode

Laboratory : Practical computational chemistry; qualitative and quantitative analysis of inorganic and organic compounds; basic synthetic organic chemistry techniques; basic characterization techniques; fundamental physical chemistry experiments

Instrumentation : Centrifuge machine, UV-Vis Spectrometer, pH meter, Water bath sonicator

Operating Systems : Linux, macOS, Windows

Languages : English, Sinhala

LEADERSHIP & SERVICE

Vice President, Chemical Society, University of Colombo 2022–2023

Member, Leo Club, University of Colombo 2019–2023

Member, Astronomical Society, University of Colombo 2019–2023

Senior Member, Science Union of Ananda College 2015–2017

Senior Member, Biological Society of Ananda College 2015–2017

Member, Saukyadana Unit, Ananda College 2011–2013

PROFESSIONAL MEMBERSHIPS

American Chemical Society (ACS)
Sri Lanka Association for the Advancement of Science (SLAAS)

SPORTS & OTHER ACTIVITIES

Cricket, Hockey, Swimming, Badminton

REFERENCES

Dr. Alberto Perez
Associate Professor and William R. Kenan, Jr. Term Professor
Associate Director, Quantum Theory Project
Department of Chemistry
University of Florida, USA
perez@chem.ufl.edu

Dr. Matt Gitzendanner
Manager, Training and Regulated Data Teams
UF Information Technology, Research Computing
University of Florida, USA
magitz@ufl.edu