ERANDIKA KARUNARATNE

Ames, IA USA
+16174706525
erandikarunaratne44@gmail.com
https://www.linkedin.com/in/erandika-k

SUMMARY

- Computational chemist with 8+ years of research experience.
- Extensive experience in cheminformatics, machine learning, database handling, molecular dynamics, and DFT calculations.
- Self-starter and excellent team player with proven ability to work in an interdisciplinary work environment as evidenced by 7+ long-lasting research projects and collaborative publications.
- Excellent interpersonal, and communication skills with the ability to understand, interpret, and communicate complex scientific data as evidenced by over 10 national and international conference presentations and 7+ years of teaching and mentoring experience.

EDUCATION

PhD, Chemistry, 2019
University of Connecticut, Storrs, CT USA

BSc, Chemistry, 2010
University of Peradeniya, Peradeniya, Sri Lanka

SKILLS

- Experience with computational chemistry simulation suites (Schrodinger, MOE)
- Experience with Molecular Dynamics (Materials Studio, LAMMPS)
- Experience with quantum chemistry software packages (Gaussian, TURBOMOLE)
- Skilled with Cheminformatics toolkits (RDKit, OpenBabel, ChemAxon) and expertise in chemical informatics projects
- Proficiency in Python and the PyData stack (numpy, pandas, scipy, scikit-learn, etc.)
- Experience with Machine Learning techniques (Scikit-learn, TensorFlow, Chemprop)
- Familiar with R programming and data analysis with SQL
- Experience with data visualization and dimensionality reduction algorithms
- Experience in managing and analyzing large datasets
- Experience with Linux and high-performance computing (HPC) environments
- Exceptional analytical and problem-solving skills
- Experience working in multidisciplinary teams that include experimentalists
- Familiar with medicinal chemistry
- Familiar with structure-based and ligand-based drug design
- Strong team player, excellent communicator, and continuous learner

EXPERIENCE

Postdoctoral Research Associate, 11/2022 – present
Ames National Laboratory, Ames, IA USA

- Utilized Python, RDkit, Scikitlearn to organize and curate large datasets, and trained neural network machine learning models using Chemprop software, resulting in a 90% accuracy in predicting binding affinities of metal-ligand complexes.

- Utilized chemometric techniques to successfully predict metal-ligand binding affinities using IR spectroscopic data, resulting in more efficient and cost-effective research processes.
- Developed a convolutional neural network model for image analysis enabling experimentalists to make informed decisions with ease and precision.

Postdoctoral Research Associate*, 02/*2019 – 09/2022
University of Connecticut, Storrs, CT USA

- Achieved a 59% correct identification rate of unknown metabolites through teamwork with multidisciplinary researchers in building a computational workflow using DFT calculations and cheminformatics techniques. This advancement allowed for more precise analysis and interpretation of mass and IR spectral data, leading to a deeper understanding of biofluid composition.
- Utilized Python programming, RDKit, and ChemAxon to clean and analyze data, as well as calculate properties of datasets extracted from the PubChem database.

Graduate Research Assistant, 08/2012 – 12/2018
University of Connecticut, Storrs, CT USA

- Collaborated with multidisciplinary researchers to calculate the conformational space of flavin-C60 (FC60) molecule using molecular dynamics, leading to the demonstration of its charge transfer characteristics around single-walled carbon nanotubes (SWNTs).
- Utilized molecular dynamics and DFT calculations to uncover the preferential C60 localization around flavin-wrapped nanotubes. This discovery enhanced the understanding of molecular interactions in flavin helices.
- Characterized the XRD pattern of SWNT nucleated FMN (flavin mononucleotide) crystals and simulated its crystal packing. Interpreted the underlying notion of selective flavin assemblies on specific chiral nanotubes leading to the identification of optimal crystal packing conditions. Contributed to a deeper understanding of selective flavin assemblies on specific chiral nanotubes.
- Established the stability and structural organization of diverse flavin derivatives around SWNTs by integrating spectroscopic techniques with computational modeling, enhancing the knowledge of their interactions.
- Led student research projects, resulting in poster presentations at research symposiums elevating the visibility of our research and fostering collaboration.

Lecturer*, *2011 – 2012
University of Rajarata, Mihintale, Sri Lanka

- Implemented innovative teaching methods to engage 120 undergraduate students in 2 physical chemistry courses, resulting in a 15% increase in student satisfaction and course ratings.

Teaching Assistant/ Undergraduate Research*, *2009 – 2011
University of Peradeniya, Peradeniya, Sri Lanka

- Improved efficiency in managing physical chemistry laboratories for 230 students by implementing new organizational systems, resulting in smoother operations and enhanced learning experiences.
- Synthesized, modified, and characterized iron oxide nanoparticles for targeted drug delivery, utilizing skills in chemistry and nanotechnology.

PROFESSIONAL DEVELOPMENT

- Google Data Analytics Certificate - Coursera (2022)

- Machine Learning, Stanford University - Coursera (2019)
- Deep Learning in Python – DataCamp (2019)
- Data Science Methodology – Coursera (2019)
- Open-Source tools for Data Science, IBM – Coursera (2019)

AWARDS

- Recognized as an excellent teaching assistant by Provost, University of Connecticut, CT (2018)
- Doctoral Research Award, University of Connecticut, CT (2018)
- University award for Academic Excellence 2010/2011, University of Peradeniya, Sri Lanka

PUBLICATIONS

- Prediction of stability constants of metal-ligand complexes by machine learning for the design of ligands with optimal metal ion selectivity, *J. Chem. Phys*, 160, 042502 (2024)
- Combining experimental with computational infrared and mass spectra for high throughput non-targeted chemical structure identification, *Anal Chem* 95, 11901−11907 (2023)
- High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectroscopy. *Anal Chem* 93, 10688-10696 (2021)
- Fullerene-Assisted Photoinduced Charge Transfer of Single-Walled Carbon Nanotubes through a Flavin Helix. *J. Am. Chem. Soc* 138, 5904-5915 (2016)

PRESENTATIONS

- Determination of Metal-Ligand Binding Strength using IR Spectroscopy, *CMI Meeting at Mines*, 2024
- Prediction of Stability Constants of Metal-Ligand Complexes by Machine Learning and de Novo design of ligands for metal ion selectivity, *11th Annual Japan-US Bilateral Meeting on Rare Metals*, 2023
- Harnessing the Power of Data, *Research SLAM*, Ames National Laboratory, 2023
- Data-Driven Approach to Predict Stability Constants of Metal-Ligand Complexes, *ACS Fall National Meeting*, 2023
- High-throughput non-targeted chemical structure identification by searching chemical databases using gas-phase infrared spectra, *ACS Fall National Meeting*, 2021
- Selection and enrichment of carbon nanotubes, *Three Minute Thesis*, UConn, 2018
- Theoretical insights into Flavin-C_{60} complexes *via* molecular mechanics and molecular dynamics, *254th ACS National Meeting*, 2017
- Designing self-assemblies towards chiral enrichment of single-walled carbon nanotubes, *254th ACS National Meeting*, 2017
- Flavin-C_{60} complex assisted photo induced charge transfer of single-walled carbon nanotubes, *Connecticut symposium on Microelectronics & Optoelectronics (CMOC),* 2017
- Perfluoro-functionalized flavin and its effect on stability of flavin helices around single-walled carbon nanotubes, *254th ACS National Meeting*, 2017
- Computational study of Lumazine assembly around single-walled carbon nanotubes, *251st ACS National Meeting*, 2016
- Theoretical Insights into Photo induced charge transfer of flavin-C_{60} complexes via molecular mechanics and molecular dynamics, *MRS Fall Meeting*, 2016
- Theoretical study of flavin-C_{60} complexes *via* molecular mechanics and molecular dynamics calculations, *MRS Fall Meeting*, 2015