

KATUKOLIYA GAMAGE ANUTHTHARA SAMADHI

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Objective

With a background in Medical Laboratory Science, Chemistry, and Computer Science, I use my research experience to solve scientific challenges. I enjoy teaching and support scientists in starting businesses by assisting with their research and connecting them with resources. Additionally, I have a strong passion for open-source projects, managing and maintaining open-source communities.

Research Interest: A.I-Driven Drug Discovery, Computational Chemistry, Cheminformatics, Natural Product Chemistry, Material Science, Quantum Chemistry, Nanobiotechnology and Toxicology

Tech Skills: HTML, Python, Office, Adobe, Git, Git-Hub, Data Analytics, Linux and Azure Infrastructure

Laboratory Science Skills: Medical Laboratory Instrumentation and Medical Laboratory Testing

Industrial Experience

Department of Nuclear Medicine, Faculty of Medicine, University of Ruhuna
Clinical Laboratory Scientist - on site (full-time)

Galle, S.L
Jan 2021 – April 2021

Under the guidance of Prof. Manjula Hettiarachchi

- Managed the laboratory during Covid-19 time period, conducted various ELISA techniques, handled radioactive chemicals, analyzed and interpreted the results related to neonatal TSH and Growth Hormone tests.

Government Hospitals

S.L

Medical Laboratories: Teaching Hospital Karapitiya, Teaching Hospital Mahamodara,
District General Hospital Mathara and National Institute of Health Sciences

Clinical Laboratory Scientist Intern - on site (full-time)

Aug 2021 – Aug 2022

- Managed the laboratories and conducted various types of clinical laboratory tests and interpreted results related to Molecular Biology, Clinical Biochemistry, Clinical Microbiology, Virology, Hematology, Genetics, Histopathology and Cytopathology.
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Research Experience

South Asian Clinical Toxicology Research Collaboration [SACTRC]
Clinical Research Assistant - on site (full-time)

Colombo, S.L
Feb 2023 – Aug 2024

Under the guidance of Prof. Eranga, Prof. Lalindra & Prof. Ariarane

- Determining the pathophysiology of hump-nosed pit-viper bite associated thrombotic microangiopathy.

Clinical Medicine Academic and Research Center [NHSL], Faculty of Medicine, University of Colombo **S.L**
Graduate Research Assistant - on site (full-time) *Feb 2023 – Aug 2024*

Under the guidance of Prof. Eranga, Prof. Lalindra & Prof Ariaranee

- Determining the pathophysiology of hump-nosed pit-viper bite associated thrombotic microangiopathy
- Characteristics, outcomes, and factors associated with outcomes of severe leptospirosis: a prospective study in a tertiary care hospital in Sri Lanka

Sul's Research Group, Global-Chem **Texas, Austin, U.S.A**
Research Scientist - remote (part-time) *June 2023 – Nov 2024*

Under the guidance of Mr. Suliman Sharif

- **Projects that collaborated: Ongoing**
 - Speculative method for gin production efficiency with Artificial Intelligence.
 - Exploring Comprehensive Approaches to Snake Venom Analysis: Implications for Anti-venom Development through Molecular Dynamics Simulations.
 - AI and Quantum Chemistry-Powered Solutions for Challenges in the Gemstone Industry: Crystal Structure Analysis of Diamond Using Psi4 Quantum Methods.
- Implemented GitHub Actions CI pipelines to automate molecular dynamics simulation software, integrating it seamlessly with the advanced CPU and GPU capabilities provided by the Warp build and Azure infrastructure (Amber, Gromacs).
- **Curating Essential Chemical Data**
 - Targeting compounds in areas like Warfare, Sexual Health, Cannabis, Medicine, Vaccines, Narcotics, and Food Chemistry to build a relevant, impactful dataset.
- **Open Source Data Governance**
 - Establishing a decentralized, community-governed model for ethical chemical data sharing across sectors.
- **Standardized Artificial Chemical Intelligence**
 - Creating interactive, AI-driven interfaces that foster continuous community input, evolving intelligence through shared knowledge.

Standard Seed Corporation **Delaware, Wilmington, U.S.A**
Cheminformatics Intern (Internship) - remote (part-time) *May 2024 – Oct 2024*

Under the guidance of Mr. Sul Sharif

- Conducted pharmacophore modeling and docking studies to support affordable extraction and characterization of 425 compounds in *Cannabis sativa*.
- Developed Machine Learning algorithms to analyze pharmacophore data and screened targets from a data base that consist with 2.5 million protein targets.
- Collaborated with scientists and business professionals to investigate the physiological effects of *Cannabis sativa* on human health.

Department of Biochemistry and Microbiology, Faculty of Medicine, University of Ruhuna **Galle, S.L**
Undergraduate Student Researcher - on site (full-time) *May 2022 – Jan 2023*

Under the guidance of Dr. P. Kalansuriya & Prof. W.M.D.G.B Wijerathna

- Enhancing Therapeutic Values of Plant Natural Products: Evaluation of in Vitro Antimicrobial Activities of Silver Nanoparticles Biosynthesized using Selected Medicinal Plant Extracts
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Publications and Presentations

- **Samadhi K.G.A¹**, Kalansuriya P², Wijerathna W.M.D.G.B³, Wasana KGP²
Faculty of Medicine UoR¹, Faculty of Allied Health Sciences UoR²
“Antimicrobial and Antifungal Activities of Silver Nanoparticles Biosynthesized by *Pothos scandens* and *Kaempferia galanga* Aqueous Extracts.”
International Conference in Medical Sciences, University of Jayawardanapura.(ICM-2023)
- **Samadhi K.G.A¹**, Kalansuriya P², Wijerathna W.M.D.G.B³, Wasana KGP² “Antimicrobial Activities of Silver Nanoparticles Biosynthesized by *Lannea coromandelica* Aqueous Extract.”
Faculty of Medicine UoR¹, Faculty of Allied Health Sciences UoR²
International Conference on Applied and Pure Sciences. University of Kelaniya. (ICAPS-2023)
- Damilola S. Bodun¹, Sulman Sharif¹, **Samadhi K.G.A²**
¹Standard Seed Corporation (Global Chemistry Inc), U.S.A
“Application of the LSTM-based deep generative model for de novo design of potential mitotic kinesin Eg5 inhibitors.” (Under Review)
- Suliman Sharif¹, Nishan Karassik², **Samadhi K.G.A¹**, Damilola Bodun¹
Standard Seed Corporation¹, Phylos Bioscience², Cambridge Crystallography Data Centre³
Development of New Pharmaceutical Standards for the Extraction, Identification, And Physiological Effects of the Constituents of *Cannabis Sativa* (Ongoing Research)
- Damilola S. Bodun¹, Sulman Sharif¹, **Samadhi K.G.A²**
¹Standard Seed Corporation (Global Chemistry Inc), U.S.A
Application of Artificial Intelligence For Gin Production (Ongoing Research)

Open Source Contributions and Teaching Experience

Global-Chem

Texas, Austin, U.S.A

A Generative AI Large Language Model Built on an Open-Source Chemical Database of Names and SMILES

Maintainer | DevOps - remote (part-time)

June 2023 – Pres

Under the guidance of Mr. Sul Sharif

- Engaging contributors in discussions on prioritizing key chemical spaces for exploration, providing essential resources, and transforming common chemical names into standardized 1-D molecular representations.
- Establishing a universal framework for recording and governance.
- Reviewing and managing pull requests through Git-Hub, for SMILES molecular representations, ensuring accuracy and consistency, while overseeing new releases of the Python package to maintain software quality.
- Additionally, sustaining scientific discussions, leading educational initiatives, and facilitating training to foster knowledge sharing and growth.

I.S.I Scientific Community

S.L

A startup open-source community, seeks to provide open-source education to the younger generation in Sri Lanka.

Community Manager - self-employed

March 2024– Pres

- Conducting scientific sessions to educate open source scientists.
- Subjects : Cheminformatics, Computational Chemistry and Computer Science.

- **Open Source Projects : Ongoing**
- **Trad-Chem** : A comprehensive chemical dictionary with SMILES notations for compounds used in traditional medicine systems, including Ayurveda, TCM, Homeopathy, and more.
- **Trad-Chem-LLM**: A chat-bot offering details on traditional medicinal compounds, including product names, benefits, target diseases, chemical compositions, and SMILES notations.

High Point Academy Sri Lanka
Education Institute That Provides Primary and Secondary Educational Services
Assistant Coordinator - self-employed

S.L

Oct 2024– Pres

- Organizing entertainment events and teaching for primary and secondary students.

Event Hosted

- As the founder president of Ruhuna Medical Laboratory Science Student's Society, I organized 07 career guidance webinars for M.L.S students. 100-150 students, University of Ruhuna. S.L, Dec 2022

Awards

- Sri Lankan University Games (SLUG) Entertainment committee : Appreciation Award **UOR, 2019**
- IEEE Green Innovation: All island digital art competition, Most popular category, 1st Place **SLTC, 2020**

Extra Skills

- **DevOps Engineering and Programming** : Linux, Git, Git-Hub, CI pipelines, HTML, Python, PyPi, Pytest, PyCharm, Pandas, NumPy, Warp-build, CPUs, GPUs, Chat-Gpt, Microsoft Azure, VS Code, IntelliJ IDEA, Google-Colab, Jupyter Notebooks, Netlify, Conda, Cuda, Lucidspark, Matplotlib, Cloudy
- **Cheminformatics** : Chimera, AlphaFold, H++, PropKa, Gromacs, Amber, Charm-gui, SMIELS, SMARTS, STOUT, VMD, PyMol, RDkit, Pytraj, MD Analysis, Swissprot, Uniprot, RCSB PDB, CCDC, Schrodinger
- **Science** : Flowcytometry, ROTEM, BacT/ALERT, BS-800M, Coatron A6, BC-5380, URIT-1600+1280.
- **Art** : Graphic Designer and a Video editor. (Adobe Products: Photoshop, Illustrator, Premiere-Pro, Lightroom) Photographer and a Videographer. (Canon and Nikon DSLR series, Ronin S, Gopro Hero series)
- **Music** : Vocalist, Rhythm guitarist and a Bass guitarist.
- **Social Media** :
 - **Linkedin** : 336 followers
 - **Medium** : 3 followers (Science blog)
 - **YouTube** : A.W Storytellers (Travel Vlog), 51 subscribers, 5 Videos
 - **Facebook** :
 - Rainbow Feathers Design Labs (803 followers)
 - Capturra Studio (318 followers)
 - Films by Capturra Studio (1200 followers)
- **Business** :
 - Rainbow Feathers Design Labs (since 2020)
 - Capturra Studio (since 2020)

Extra-Curricular Activities

- **Involvements within School :**

- Was a senior scout of Kelaniya President's Collage scout troops and participated in leadership programs.
- Was a senior cadet of Nalanda Collage Eastern Cadet Band and participated in the assessment camp in Rantambe 2013.
- Former member of Nalanda Collage Environmental Society.
- Former member of Nalanda Collage Symphony Orchestra.
- Active participation in Nalanda Collage cultural and social events.

- **Involvements within University:**

- Was the founder president of Ruhuna Medical Laboratory Science Students' Society. (RMLSSS: 2022-2023)
- Was a senior member of Art Society, Faculty of Allied Health Sciences, University of Ruhuna.
- Active participation in First Inter Faculty Competition in Instrumental and Vocal Music (ICIVM) 2018, University of Ruhuna.
- Was a team member of University of Ruhuna Rugby team and participated in Sri Lankan University Games (SLUG) 2019.
- Active participation in University of Ruhuna cultural and social events.

Education

- Elementary School Sacramento Westfield School, California, U.S.A, Sep 2006 – Dec 2006
- Ordinary Level : 07 A Grades Kelaniya President's Collage, S.L (2001-2011)
- Advance Level : Chemistry-A, Biology-B, Physics-B Nalanda Collage, S.L (2012-2014)
- B.sc Honors in Medical Laboratory Science Faculty of A.H.S, UOR, S.L (2018-2023)

Referees

- **Mr. Suliman Sharif**

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- **Dr. Pabasara Kalansuriya**

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Contact : 0773294912

LinkedIn : <https://www.linkedin.com/in/pabasara-kalansuriya-phd-31647933/>

- **Dr. Kalani Gunawardana**

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Contact : 0702721122

I do hereby declare that the above particulars furnished by me are true and correct to the best of my knowledge.

K.G.A Samadhi, 2024.11.05