Tharindu Senapathi

PhD in Chemistry | Theoretical and Computational Chemist

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Department of Chemistry, University of Sri Jayewardenepura, Sri Lanka

RESEARCH PROFILE

Theoretical and computational chemist specializing in quantum chemistry, QM/MM reaction dynamics, and statistical-mechanical free-energy simulation methods. Research integrates computational chemistry, bioinformatics, first-principles materials simulation, and artificial intelligence to advance computer-aided drug discovery and materials design within a unified workflow. AI and machine-learning models are applied to small-molecule drug discovery, glycoenzyme chemistry, and the discovery of materials for battery systems, electrochemical interfaces, and next-generation energy storage. Creator of the BRIDGE open-source platform for reproducible, high-throughput free-energy simulations and co-developer of ProtoCaller. Committed to developing an independent research program at the intersection of quantum chemical theory, computational statistical mechanics, and AI-accelerated computer-aided drug discovery and materials design, with a proven record of high-impact publications, international collaboration, and teaching at the undergraduate and graduate levels.

RESEARCH INTERESTS

- Quantum chemistry and QM/MM reaction dynamics: enzyme catalysis, transition state theory, and ab initio and semiempirical methods applied to glycoenzymes and carbohydrate-active enzymes.
- Computational statistical mechanics: free energy methods (FEARCF) and molecular dynamics of biomolecular and materials systems.
- AI-driven computational chemistry: applying machine learning, generative models, and high-throughput automated free-energy workflows equally to computer-aided drug discovery and materials design, from small-molecule and glycoenzyme chemistry to the discovery and screening of battery, electrochemical, and energy-storage materials.
- Open-source software development for computational chemistry, HPC integration, GPU-accelerated simulation, and workflow automation (BRIDGE, ProtoCaller).
- Computational materials chemistry and materials design: first-principles simulations, molecular dynamics, and AI-assisted discovery of materials for battery systems, electrochemical interfaces, and next-generation energy storage technologies.

EDUCATION

PhD, Chemistry — University of Cape Town, South Africa ***Jan 2017 – Jan 2020***

Advisor: Professor Kevin Naidoo

Thesis: Development of a Computational Platform for System-Based High-Throughput Drug Discovery Illustrated on Pneumococcal Sialidases

M.Sc., Computational Science — University of Cape Town, South Africa ***Mar 2015 – Nov 2016***

Advisor: Professor Kevin Naidoo

Thesis: The Catalytic Mechanism of ST6Gal-I Discovered by Using Parallel Reaction Dynamics Computation

B.Sc. (Hons.) Special Degree, Chemistry — University of Sri Jayewardenepura, Sri Lanka *Jul 2009 – Dec 2013*

Advisor: Professor Nilwala Kottegoda

Thesis: Agrowaste-Based Dietary Fibers as a Nutraceutical Encapsulant

Certificate in Teaching in Higher Education (CTHE) — Staff Development Centre, University of Sri Jayewardenepura, Sri Lanka *Jun 2023*

Awarded by: Staff Development Center, University of Sri Jayewardenepura

Professional teaching qualification in higher education pedagogy, curriculum design, assessment, and reflective practice.

ACADEMIC AND RESEARCH EXPERIENCE

Senior Lecturer (Grade II) — Department of Chemistry, University of Sri Jayewardenepura *Jan 2022 – Present*

- Leading an independent research group in computational chemistry focused on computer-aided drug discovery and materials design.
- Supervising MSc and undergraduate research in first-principles simulations, molecular dynamics, and AI-assisted discovery of bioactive compounds and energy-storage materials.
- HPC resource development and administration for the research group.
- Undergraduate and postgraduate teaching.

Senior Lecturer (on contract) — Department of Chemistry, University of Sri Jayewardenepura *Oct 2020 – Jan 2022*

- Physical chemistry theory and practical instruction for 1st, 2nd, and 3rd year undergraduates, covering quantum chemistry, thermodynamics, kinetics, and spectroscopy.
- Supervised final-year undergraduate research projects applying molecular modeling and simulation to chemical and biochemical problems.
- Contributed to curriculum development and the introduction of computational methods into the undergraduate physical chemistry syllabus.

Research Associate — Scientific Computing Research Unit, University of Cape Town *Mar 2021 – Present*

- Reaction dynamics and inhibitor design for sialic acid-related enzymes.
- Co-authoring publications and contributing to research in glycoenzyme chemistry.

PhD Researcher — Scientific Computing Research Unit, University of Cape Town *Jan 2017 – Jan 2020*

- Developed BRIDGE: an open-source Galaxy-based platform for reproducible high-throughput free energy simulations.
- QM/MM and classical free energy simulations of enzymatic catalysis and inhibitor binding.
- GPU acceleration of classical and ab initio molecular simulations.
- Programming: Python, Bash, R, JavaScript, MATLAB, Fortran, C, C++, XML, HTML.

Systems Administrator — Scientific Computing Research Unit, University of Cape Town *Aug 2016 – Jan 2020*

- Developed and maintained HPC cluster and SLURM/PBS queue management system.

M.Sc. Researcher — University of Cape Town *Mar 2015 – Nov 2016*

- Computational science — applied mathematics, physics, and computer science to chemical and biochemical problems.
- Benchmarked GPU acceleration of classical and ab initio molecular simulations.

Intern — Sri Lanka Institute of Nanotechnology *Jan 2012 – Jan 2014*

- Research in advanced agriculture and nanotechnology; instrumental techniques: FTIR, SEM, UV-Vis, TGA, DSC, PXRD.

TEACHING EXPERIENCE

Senior Lecturer (Grade II) — Department of Chemistry, University of Sri Jayewardenepura *Jan 2022 – Present*

Physical chemistry theory and practical instruction for undergraduate and postgraduate students; quantum chemistry, kinetics, spectroscopy, bioinformatics, and computer-aided drug discovery and materials design.

Undergraduate — Currently Teaching

Code	Course Title	Level
CHE 106 1.0	Structure and Properties of Matter	UG Year 1
CHE 208 1.0	Quantum Chemistry	UG Year 2
CHE 350 0.0	Mathematics for Chemistry	UG Year 3
CHE 361 1.0	Advanced Chemical Kinetics	UG Year 3
CHE 362 1.0	Advanced Quantum Chemistry	UG Year 3
CHE 363 1.0	Statistical Thermodynamics	UG Year 3
CHE 457 1.0	Molecular Spectroscopy	UG Year 4
CHE 207 2.0	Chemistry Practical Unit (Physical Chemistry)	UG Year 2
CHE 315 2.0	Chemistry Practical Unit (Physical Chemistry)	UG Year 3
ICH 373 2.0	Advanced Chemical Kinetics and Thermodynamics	UG Year 3
ICH 484 2.0	Quality Assurance, Accreditation and Project Management (Statistical Methods)	UG Year 4
GMB 351 1.0	Advanced Bioinformatics	UG Year 3
GMB 422 1.0	Drug Discovery and Development	UG Year 4
FST 166 1.0	Structure and Properties of Matter	UG Year 1
PHS 2702	Pharmaceutical Analysis:Electrochemical Analytical Methods	UG Year 2

Undergraduate — Previously Taught

Code	Course Title	Level
CHE 103 1.0	Chemical Thermodynamics	UG Year 1
CHE 204 1.0	Electrochemistry	UG Year 2
ICH 355 1.0	Solid State Chemistry	UG Year 3

Postgraduate

Code	Course Title	Level
MPST 527	Modelling and Simulation	PG
IAC 80303/100303	Electroanalytical Techniques	PG
IOC 90402/100401	Modern Medicinal Chemistry	PG
IAC 50430/100430	Analytical Techniques In Biomedical and Pharmaceutical Applications	PG

Tutor and Demonstrator — Physical Chemistry, University of Cape Town ***Jan 2016 – Dec 2019***

Physical chemistry practical and theory classes for 2nd and 3rd year undergraduate students.

Temporary Demonstrator — University of Sri Jayewardenepura ***Feb 2014 – Feb 2015***

Physical chemistry practical classes for 1st, 2nd, and 3rd year undergraduates; inorganic chemistry special degree practicals for 3rd year students.

PUBLICATIONS

Citations are listed in reverse chronological order.

Peer-Reviewed Journal Articles

1. Nashed, A.; Dilsook, K.; **Senapathi, T.**; Naidoo, K. J. An In Vitro Approach for Simulating Divergent Golgi O-Glycosylation of Tumor-Associated MUC1 from Normal MUC1. Nature Communications 2026, 17, 3619. https://doi.org/10.1038/s41467-026-72151-y
2. Selvaraj, S.; Perera, M.; Yapa, P.; Munaweera, I.; Perera, I. C.; **Senapathi, T.**; Weerasinghe, L. In Vitro Analysis of XLAsp-P2 Peptide-Loaded Cellulose Acetate Nanofiber for Wound Healing. Journal of Pharmaceutical Sciences 2025, 114 (2), 911–922. https://doi.org/10.1016/j.xphs.2024.10.050
3. Sigera, S.; Theekshana, K. D.; Dinanja, S. G.; Eranga, P.; Karunathilake, N.; Abeywardhana, S.; Weerasinghe, L.; **Senapathi, T.**; Peiris, D. C. Molecular Docking and Molecular Dynamics Simulations Reveal the Antidiabetic Potential of a Novel Fucoxanthin Derivative from Chnoospora minima. Marine Drugs 2025, 23, 471. https://doi.org/10.3390/md23120471
4. Naidoo, K. J.; Bruce-Chwatt, T.; **Senapathi, T.**; Hillebrand, M. Multidimensional Free Energy and Accelerated Quantum Library Methods Provide a Gateway to Glycoenzyme Conformational, Electronic and Reaction Mechanisms. Accounts of Chemical Research 2021, 54 (22), 4120–4130. https://doi.org/10.1021/acs.accounts.1c00477
5. Barnett, C. B.; **Senapathi, T.**; Naidoo, K. J. Conformational Play in the Binding of Variably Glycosylated MUC1 Antigen to AR20.5 Antibody. Beilstein Journal of Organic Chemistry 2020, 16, 2540–2550. https://doi.org/10.3762/bjoc.16.206
6. Bray, S.; **Senapathi, T.**; Barnett, C. B.; Grüning, B. Intuitive, Reproducible High-Throughput Molecular Dynamics in Galaxy: A Tutorial. Journal of Cheminformatics 2020, 12, 1–13. https://doi.org/10.1186/s13321-020-00451-6
7. **Senapathi, T.**; Barnett, C. B.; Naidoo, K. J. BRIDGE: An Open Platform for Reproducible Protein-Ligand Simulations and Free Energy of Binding Calculations. Bio-protocol 2020, 10 (17), e3731. https://doi.org/10.21769/BioProtoc.3731

8. **Senapathi, T.**; Suruzhon, M.; Barnett, C. B.; Essex, J. W.; Naidoo, K. J. BRIDGE: An Open Platform for Reproducible High-Throughput Free Energy Simulations. Journal of Chemical Information and Modeling 2020, 60 (8), 3731–3740. https://doi.org/10.1021/acs.jcim.0c00206

9. Suruzhon, M.; **Senapathi, T.**; Bodnarchuk, M. S.; Viner, R.; Wall, I.; Barnett, C. B.; Naidoo, K. J.; Essex, J. W. ProtoCaller: Robust Automation of Binding Free Energy Calculations. Journal of Chemical Information and Modeling 2020, 60 (4), 1917–1921. https://doi.org/10.1021/acs.jcim.9b01158

10. **Senapathi, T.**; Bray, S.; Barnett, C. B.; Grüning, B.; Naidoo, K. J. Biomolecular Reaction and Interaction Dynamics Global Environment (BRIDGE). Bioinformatics 2019, 35 (18), 3508–3509. https://doi.org/10.1093/bioinformatics/btz107

11. Rathnayake, U. A.; **Senapathi, T.**; Sandaruwan, C.; Gunawardene, S.; Karunaratne, V.; Kottegoda, N. Rice Bran Nanofiber Composites for Stabilization of Phytase. Chemistry Central Journal 2018, 12, 1–7. https://doi.org/10.1186/s13065-018-0400-y

Book Chapters

1. Naidoo, K. J.; Bruce-Chwatt, T.; **Senapathi, T.** Enzyme Reaction Dynamics from Adaptive Reaction Coordinate Forces. In Comprehensive Computational Chemistry; Elsevier, 2024; pp 544–558. https://doi.org/10.1016/B978-0-12-821978-2.00124-0

SOFTWARE DEVELOPMENT

BRIDGE — Biomolecular Reaction and Interaction Dynamics Global Environment ***2019 – Present***

Open-source, Galaxy-based platform integrating GROMACS, AMBER, and FESetup for reproducible high-throughput free-energy simulations on HPC and cloud, supporting computer-aided drug discovery and materials design workflows. Published in Bioinformatics and the Journal of Chemical Information and Modeling.

ProtoCaller — Robust Automation of Binding Free Energy Calculations ***2020 – Present***

Co-developer. Python toolkit for automated binding free-energy calculations integrating GROMACS, AMBER, and OpenMM; applied to computer-aided drug discovery pipelines and extensible to host–guest and ligand–surface interactions relevant to materials design. Published in the Journal of Chemical Information and Modeling.

FEARCF — Free Energies From Adaptive Reaction Coordinate Forces ***2018 – Present***

Co-developer. Computational framework implementing adaptive reaction-coordinate force methods to compute multidimensional free-energy landscapes and reaction mechanisms across biomolecular and materials systems, enabling quantitative insight for computer-aided drug discovery and materials design.

GRANTS

PI — University Grant (ASP/01/RE/SCI/2021/24) *Completed*

PI — University Grant (RG/URG/SCI/2024/19) *Ongoing*

PI — University Grant (RG/URG/SCI/2026/13) *Ongoing*

POSTGRADUATE STUDENT SUPERVISION

Master's (by research)

- Mr. Shehan Jayasinghe *Completed 2026*
- Ms. Sranya Selvaraj *Completed 2025*
- Ms. Kanchana Harshani *Ongoing*
- Ms. Hansika Navarathne *Ongoing*

WORKSHOPS AND INVITED TALKS CONDUCTED

Invited Webinar (Resource Person) — Centre for Plant Materials and Herbal Products Research (CPMHPR), University of Sri Jayewardenepura — ***2025***

"Computational Strategies for Natural Products-Based Drug Discovery: From Virtual Screening to QM/MM Methods"

Resource Person — Annual Popularization of Chemistry Program, Royal Society of Chemistry — Sri Lanka Section, Badulla — ***2025***

"Advanced Level Teachers' Training Seminar in Chemistry"

Resource Person — A/L Teacher Training Program, Science Branch, Ministry of Education, Higher Education and Vocational Education, Sri Lanka — ***2024***

"Physical Chemistry Laboratory Training for A/L Chemistry Teachers"

Resource Person — Annual Popularization of Chemistry Program, Royal Society of Chemistry — Sri Lanka Section, Nuwara Eliya — ***2022***

"Popularization of Chemistry — Outreach"

Workshop (Instructor) — Bioinformatics Community Conference, Germany — ***2021***

"High-throughput molecular dynamics and analysis"

Workshop (Instructor) — Bioinformatics Community Conference, Germany — ***2020***

"High-throughput molecular dynamics with Galaxy"

Workshop (Instructor) — CHPC National Conference, South Africa — ***2019***

"Accelerated free energy calculations using open-source tools"

Workshop (Instructor) — CHPC National Conference, South Africa — ***2018***

"Biomolecular Reaction and Interaction Dynamics Global Environment (BRIDGE)"

REFERENCES

The following referees can be contacted to provide detailed assessments of my research, teaching, and academic service.

Professor Kevin J. Naidoo

PhD & M.Sc. Advisor

Professor of Chemistry
Scientific Computing Research Unit
Department of Chemistry
University of Cape Town, South Africa

Email: kevin.naidoo@uct.ac.za

Relationship: *Doctoral and Master's research supervisor (2015–2020); ongoing research collaborator.*

Senior Professor Upul Subhasighne

Dean, Faculty of Applied Sciences

Senior Professor
Faculty of Applied Sciences
University of Sri Jayewardenepura, Sri Lanka

Email: upuls@sjp.ac.lk

Relationship: *Dean of the faculty; can attest to my academic, teaching, and administrative service at the University of Sri Jayewardenepura.*

Professor Theshini Perera *Head of Department, Chemistry*

Professor of Chemistry

Department of Chemistry
Faculty of Applied Sciences
University of Sri Jayewardenepura, Sri Lanka

Email: theshi@sjp.ac.lk

Relationship: *Head of Department; can attest to my teaching, research, and departmental contributions.*