Tharindu Nuwan Senapathi, PhD, MSc, BSc (Hon)

Address: **Department of Chemistry,**
University of Sri Jayewardenepura,
Nugegoda, Sri Lanka.
Telephone: **+94717385385**
Email: **tharindu@sci.sjp.ac.lk**
Website: **http://science.sjp.ac.lk/che/dr-tharindu-senapathi/**
http://www.scientificomputing.uct.ac.za/
Google Scholar: **https://scholar.google.com/citations?hl=en&user=Vv7CYHYAAAAJ**

Professional Profile

Trained as a physical and computational chemist with expertise in developing and applying free energy and hybrid classical/quantum mechanical methods for application to chemical, life, and biomedical sciences. My primary research focuses on bringing computational chemistry and bioinformatics methods together to study chemical biology and reimagine how we develop small molecules in drug discovery.

Education

January 2017 – January 2020 **University of Cape Town, South Africa**
PhD (Chemistry)

Advisor: Professor Kevin Naidoo
Thesis Title: Development of a Computational Platform for System Based High Throughput Drug Discovery Illustrated on Pneumococcal Sialidases.

March 2015 – November 2016 **University of Cape Town, South Africa**
M.Sc. (Computational Science)

Advisor: Professor Kevin Naidoo
Thesis Title: The Catalytic Mechanism of ST6Gal-I Discovered by Using Parallel Reaction Dynamics Computation.

July 2009 – December 2013 **University of Sri Jayewardenepura, Sri Lanka**
B.Sc. Special Degree (Chemistry) Second Class Honours (Upper Division)

Advisor: Professor Nilwala Kottegoda
Thesis Title: Agrowaste-Based Dietary Fibres as a Nutraceutical Encapsulant.

Research and Work Experience

- **Senior Lecturer (Grade II)** - University of Sri Jayewardenepura – *January 2022 - Present*

- **Senior Lecturer (on contract)** - University of Sri Jayewardenepura – *October 2020 –January 2022* Research co-supervisor for two undergraduate students and one PhD student.

- **Research Associate** - University of Cape Town – *March 2021 – Present*
  - Reaction dynamics and inhibitor design for sialic acid related enzymes.

- **PhD Student -** University of Cape Town – *January 2017 – January 2020*
  - Development of a Computational Platform for System Based High Throughput Drug Discovery.
  - Developments in statistical mechanical and quantum mechanical methods and applications.
  - Free energy simulations using classical and QM/MM methods.
  - Highly experienced in software development for computational chemistry and bioinformatics.
  - Proficient in Bash, Python, R, JavaScript, MATLAB, Fortran, C, C++, XML, HTML, and Web Servers.

- **M.Sc. Student -** University of Cape Town - *March 2015 – November 2016*
  - Computational science – application of applied mathematics, physics, and computer science to solve chemical and biochemical problems.
  - Accelerating and benchmarking classical and ab initio molecular simulations on Graphics Processing Units (GPUs).

- **Systems Administrator** - University of Cape Town – *August 2016 – January 2020*
  - Develop and maintain a high-performance computing cluster and queue management.

- **Intern -** Sri Lanka Institute of Nanotechnology- *January 2012 – January 2014*
  - Research in advanced agriculture and technology
  - Experienced in FTIR, SEM, UV-Vis, TGA, DSC, PXRD

Teaching Experience

- **Senior Lecturer (Grade II)**
  Physical chemistry theory and practical classes for undergraduate students.
  University of Sri Jayewardenepura
  January 2022 – Present

Undergraduate Teaching: Currently Teaching

- *CHE 106 1.0 Structure and Properties of Matter*
- *CHE 350 0.0 Mathematics for Chemistry*
- *CHE 361 1.0 Advanced Chemical Kinetics*
- *CHE 457 1.0 Molecular Spectroscopy*

- *CHE 207 2.0 Chemistry Practical Unit (Physical Chemistry)*
- *CHE 315 2.0 Chemistry Practical Unit (Physical Chemistry)*
- *ICH 355 1.0 Solid State Chemistry*
- *ICH 373 2.0 Advanced Chemical Kinetics and Thermodynamics*
- *ICH 484 2.0 Quality Assurance, Accreditation, and Project Management (Statistical Methods)*
- *GMB 351 1.0 Advanced Bioinformatics*
- *GMB 422 2.0 Drug Discovery and Development*
- *FST 166 1.0 Structure and Properties of Matter*

Undergraduate Teaching: Previously Taught

- *CHE 103 1.0 Chemical Thermodynamics*
- *CHE 204 1.0 Electrochemistry*

➢ **Senior Lecturer (on contract)**
Physical chemistry theory and practical classes for 1st, 2nd, and 3rd year undergraduate students.
University of Sri Jayewardenepura
October 2020 – January 2022

Undergraduate Teaching: *CHE 106 1.0 Structure and Properties of Matter*
ICH 355 1.0 Solid State Chemistry
CHE 209 2.0 Chemistry Practical (Physical Chemistry)

➢ **Tutor and Demonstrator**
Physical chemistry practical and theory classes for 2nd and 3rd year undergraduate students.
University of Cape Town
January 2016 – December 2019

➢ **Temporary Demonstrator**
Physical chemistry practical classes for 1st, 2nd, and 3rd year undergraduate students.
Inorganic chemistry special degree practical classes for 3rd year chemistry special degree students.
University of Sri Jayewardenepura
February 2014 – February 2015

Publications

An in vitro one-pot synthetic biology approach to simulating diverging Golgi O-glycosylation of tumor-associated MUC1 from normal tissue MUC1 – **In review**

Selvaraj, Saranya, Monali Perera, Piumika Yapa, Imalka Munaweera, Inoka C. Perera, **Tharindu Senapathi**, and Laksiri Weerasinghe: In vitro analysis of XLAsp-P2 peptide loaded cellulose acetate nanofiber for wound healing. Journal of Pharmaceutical Sciences **2025**; DOI: https://doi.org/10.1016/j.xphs.2024.10.050. **Impact Factor 3.7**

Kevin Naidoo, Tomas Bruce-Chwatt, **Tharindu Senapathi**, and Malcolm Hillebrand: *Multidimensional Free Energy and Accelerated Quantum Library Methods Provide a Gateway to Glycoenzyme Conformational, Electronic and Reaction Mechanisms:* Accounts of Chemical Research **2021**; DOI: 10.1021/acs.accounts.1c00477. **Impact Factor: 22.38**

Simon Bray, **Tharindu Senapathi**, Christopher B. Barnett, and Björn Grüning: *Intuitive, reproducible high-throughput molecular dynamics in Galaxy: a tutorial*. Journal of Cheminformatics **2020,** *12* (1), 1-13; DOI: 10.1186/s13321-020-00451-6. **Impact Factor: 5.514**

Tharindu Senapathi, Miroslav Suruzhon, Christopher B. Barnett, Jonathan Essex, and Kevin J. Naidoo: *BRIDGE an open platform for reproducible high throughput free energy simulations*. Journal of Chemical Information and Modeling **2020,** *10* (17), e3731-e3731; DOI:10.1021/acs.jcim.0c00206. **Impact Factor: 4.549**

Christopher B. Barnett, **Tharindu Senapathi**, and Kevin J. Naidoo: *Conformational play in the binding of variably glycosylated MUC1 antigen to AR20.5 antibody*. Beilstein Journal of Organic Chemistry **2020,** *16* (1), 2540-2550 ; DOI: 10.3762/bjoc.16.206. **Impact Factor: 2.622**

Miroslav Suruzhon, **Tharindu Senapathi**, Michael Steven Bodnarchuk, Russell Viner, Ian Wall, Christopher B. Barnett, Kevin J. Naidoo, and Jonathan W. Essex: *ProtoCaller: Robust Automation of Binding Free Energy Calculations*. Journal of Chemical Information and Modeling **2020,** *60* (4), 1917-1921; DOI:10.1021/acs.jcim.9b01158. **Impact Factor: 4.549**

Tharindu Senapathi, Simon Bray, Christopher B. Barnett, Björn Grüning, and Kevin J Naidoo: *Biomolecular Reaction and Interaction Dynamics Global Environment (BRIDGE)*. Bioinformatics **2019,** *35* (18), 3508-3509; DOI:10.1093/bioinformatics/btz107. **Impact Factor: 6.937**

Upendra A. Rathnayake, **Tharindu Senapathi**, Chanaka Sandaruwan, Sanja Gunawardene, Veranja Karunaratne, and Nilwala Kottegoda: *Rice bran nanofiber composites for stabilization of phytase*. Chemistry Central Journal **2018,** *12* (1), 1-7; DOI:10.1186/s13065-018-0400-y. **Impact Factor: 4.215**

Book Chapters

Naidoo, Kevin J., Tomás Bruce-Chwatt, and **Tharindu Senapathi**. Enzyme Reaction Dynamics from Adaptive Reaction Coordinate Forces. Elsevier **2024**.

Conferences and Workshops

- **Worksop – participated in the workshop series for training the trainers – Sri Lanka (2021)**
  Title: Developing Academic Literacy in the State Universities.

- **Workshop - conducted at the Bioinformatics Community Conference - Germany (2021)**
  Title: High-throughput molecular dynamics and analysis.

- **Workshop - conducted at the Bioinformatics Community Conference - Germany (2020)**
  Title: High-throughput molecular dynamics with Galaxy.

- **Workshop -conducted at The Centre for High-Performance Computing National Conference – South Africa (2019)**
  Title: Accelerated free energy calculations using open-source tools.

- **Poster Presentation - The Centre for High-Performance Computing National Conference South Africa (2019)**
  Title: BRIDGE: High throughput Free Energy Calculations for Drug Discovery.

- **Workshop - conducted at The Centre for High-Performance Computing National Conference South Africa (2018)**
  Title: Biomolecular Reaction and Interaction Dynamics Global Environment (BRIDGE).

- **Poster Presentation - The Centre for High-Performance Computing National Conference South Africa (2018)**
  Title: Biomolecular Reaction and Interaction Dynamics Global Environment (BRIDGE).

- **Poster presentation at ACI Inorganic Conference & Carman Physical Chemistry Symposium South Africa (2017)**
  Title: A Study of Substrate Selectivity of ST6Gal-I Enzyme.

References

- **Nilwala Kottegoda (PhD), FRSC**
  Professor in Chemistry
  Head, Department of Chemistry
  University of Sri Jayewardenepura
  Sri Lanka
  Email: nilawla@sjp.ac.lk

- **Dr Chris Barnett (PhD)**
  Scientific Computing Research Unit
  Department of Chemistry
  University of Cape Town
  South Africa
  Email: chris.barnett@uct.ac.za

- **Kevin Naidoo (PhD), FRSSAf**
  South African Research Chair in Scientific Computing
  Director: Scientific Computing Research Unit
  Professor: Physical Chemistry
  Department of Chemistry
  University of Cape Town
  South Africa
  Email: kevin.naidoo@uct.ac.za