Lochana C. Menikarachchi Ph.D.

Senior Lecturer,
Department of Pharmacy, Faculty of Allied Health Sciences,
University of Peradeniya, Peradeniya

Experience

Senior Lecturer Gr. II
Department of Pharmacy, University of Peradeniya – February 2015, Present

Research Specialist in Pharmacology and Toxicology
School of Pharmacy, University of Connecticut - November 2015, Present

Senior Technical Lead
WSO2 Inc, 20, Palm Grove, Colombo: August 2014 - January 2015

- Machine Learning and Big Data Technologies

Postdoctoral Research Fellow
University of Connecticut: September 2011 - July 2014

- Development of computational chemistry techniques and software for metabolomics (LC-MS) research.

Graduate Assistant
University of Connecticut: September 2006 - August 2011

- Worked as a teaching assistant for CHEM 1126, 1127 and 1128
- Teaching duties included demonstrating lab experiments, supervising two lab classes, grading lab reports and teaching discussion classes

Temporary Assistant Lecturer
University of Peradeniya: May 2005 - May 2006

- Conducted 100 level General Chemistry labs
- Duties included demonstrating lab experiments, grading and supervising 3 lab sessions
- Worked as an instructor for 100 level discussion classes and CH201 (Organometallic Chemistry)

Education

Microsoft Certified Professional - Microsoft Inc.
2002 - 2002

- Windows Server Administration

ACS Examination in Information Technology - Australian Computer Society
2000 - 2002

BSc. (Chemistry Special) – University of Peradeniya
September 2001 - June 2005

- B.Sc. (Chemistry Special) - 1st Class
  GPA : 3.80 / 4.00
  Minor : Computer Science, Statistics
- **Awards and Honors**

(1) B.F. Khan Gold Medal for Best Overall Performance in Chemistry at the Undergraduate Level (2001-2005) - University of Peradeniya, Sri lanka

(2) Hayleys Award for Best Performance in Chemistry (2002, 2003)

(3) University Award for Academic Excellence (2004, 2005) - University of Peradeniya, Sri lanka

(4) Silver Medal – Inter University Chemistry Competition (Royal Society of Chemistry, 2006)

Ph.D. (Computational Biochemistry) - University of Connecticut
September 2006 - June 2011

- Thesis on Fragmentation and Moving Domain Methods for the Computation of Electrostatic Potentials in Proteins
  GPA : 4.00 / 4.00
- **Awards and Honors**

Contact me

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About Me

A highly multidisciplinary research scientist / engineer with expertise in chemistry, biology, pharmaceutical sciences, statistics and computer science

Interest Areas

Cheminformatics
Metabolomics
Drug discovery

(1) NIH-NCRR Travel Grant to attend a workshop titled Methods and Applications of Hybrid QM/MM Simulations to Biomolecular Systems, National Resource for Biomedical Supercomputing(NRBSC)-Pittsburgh Supercomputing Center(PSC), Sep 2007

(2) Partnership for Excellence in Structural Biology Fellowship - University of Connecticut, USA 2007

(3) R.T. Major Poster Award University of Connecticut 2008

Publications

(1) Menikarachchi, L. C.; Gascón, J. A. Optimization of Cutting Schemes for the Evaluation of Molecular Electrostatic Potentials in Proteins via Moving-Domain QM/MM. J. Mol. Model. 2008, 14, 479–487, 10.1007/s00894-008-0306-z

(2) Menikarachchi, L. C.; Gascón, J. A. QM/MM Approaches in Medicinal Chemistry Research. Curr. Top. Med. Chem. 2010, 10, 46–54, http://dx.doi.org/10.2174/156802610790232297

(3) Menikarachchi, L. C.; Gascón, J. a. An Extrapolation Method for Computing Protein Solvation Energies Based on Density Fragmentation of a Graphical Surface Tessellation. J. Mol. Graph. Model. 2011, 30, 38–45, 10.1016/j.jmgm.2011.06.001

(4) Beshir, A. B.; Argueta, C. E.; Menikarachchi, L. C.; Gascón, J. A.; & Gabriel Fenteany. Locostatin Disrupts Association of Raf Kinase Inhibitor Protein With Binding Proteins by Modifying a Conserved Histidine Residue in the Ligand-Binding Pocket. For. Immunopathol. Dis. Therap. 2011, 2, 47–58, 10.1615/ForumImmunDisTher.v2.i1.60

(5) Menikarachchi, L. C.; Cawley, S.; Hill, D. W.; Hall, L. M.; Hall, L.; Lai, S.; Wilder, J.; Grant, D. F. MolFind: A Software Package Enabling HPLC/MS-Based Identification of Unknown Chemical Structures. Anal. Chem. 2012, 84, 9388–93394, 10.1021/ac302048x

(6) Menikarachchi, L. C.; Hill, D. W.; Hamdalla, M. a; Mandoiu, I. I.; Grant, D. F. In Silico Enzymatic Synthesis of a 400 000 Compound Biochemical Database for Nontargeted Metabolomics. J. Chem. Inf. Model. 2013, 53, 2483–2492, http://pubs.acs.org/doi/abs/10.1021/ci400368v

(7) Menikarachchi, L. C.; Hamdalla, M. A.; Hill, D. W.; Grant, D. F. Chemical Structure Identification in Metabolomics: Computational Modeling of Experimental Features. Comput. Struct. Biotechnol. J. 2013, 5, 10.5936/csbj.201302005

(8) Giuseppe Paglia, Jonathan P. Williams, Lochana Menikarachchi, J. Will Thompson, Richard Tyldesley-Worster, Skarphédinn Halldórsson, Ottar Rolfsson, Arthur Moseley, David Grant, James Langridge, Bernhard O. Palsson, and Giuseppe Astarita, Ion Mobility Derived Collision Cross Sections to Support Metabolomics Applications, Anal. Chem. **2014** *86* (8), 3985-3993, http://dx.doi.org/10.1021/ac500405x

(9) Giuseppe Paglia, Peggi Angel, Jonathan P. Williams, Keith Richardson, Hernando J. Olivos, J. Will Thompson, Lochana Menikarachchi, Steven Lai, Callee Walsh, Arthur Moseley, Robert S. Plumb, David F. Grant, Bernhard O. Palsson, James Langridge, Scott Geromanos, and Giuseppe Astarita, Ion Mobility-Derived Collision Cross Section As an Additional Measure for Lipid Fingerprinting and Identification, Anal. Chem. 2015 87 (2), 1137-1144, 10.1021/ac503715v

(10) Paglia G, Menikarachchi LC, Langridge J, Astarita G. Travelling-wave ion mobility-mass spectrometry in metabolomics: workflows and bioinformatic tools. In: Identification and Data Processing Methods in Metabolomics. Rudaz S (Ed). Future Medicine, London, UK. DOI 10.4155/FSEB2013.14.224.

(11) M. L. Hall, Menikarachchi, L. C., Chen, M. - H., and Grant, D. F., Optimizing Artificial Neural Network models for metabolomics and systems biology: an example using HPLC retention index data, Bioanalysis. doi: 10.4155/bio.15.1

(12) L.C. Menikarachchi, R. Dubey, D.W. Hill, D.N. Brush, D.F. Grant, Development of Database Assisted Structure Identification (DASI) Methods for Nontargeted Metabolomics, Metabolites 6 (2), 17, doi:10.3390/metabo6020017

Conference Proceedings

(1) Menikarachchi, L. C.; Gascon, J. A. Implicit Solvation in QM/MM, a Density Domain Fragmentation Approach. In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY; 2010; Vol. 239.

(2) Rudnitskaya, A. N.; Menikarachchi, L. C.; Fenteany, G.; Gascon, J. A. Mechanistic Study of the Reaction Between Locostatin and Raf Kinase Inhibitor Protein (RKIP). In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY; 2011; Vol. 242.

(3) Menikarachchi, L. C.; Gascon, J. A. Moving Domain QM/MM Method to Describe Polarization Effects in Protein Electrostatics. In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY; 2009; Vol. 237.

(4) Menikarachchi, L. C.; Gascon, J. A. PHYS 447-Moving Domain QM/MM Method for Accurate Description of Molecular Electrostatic Potentials in Proteins. In ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY; 2007; Vol. 234.

Copyrighted Software

(1) MolFind : MolFind is a java based software package for identifying unknown chemical structures in complex mixtures using HPLC/MS data.
http://metabolomics.pharm.uconn.edu/software

(2) IIMDB : A large (~ 400, 000) web accessible NOSQL database with a Restful web service
http://metabolomics.pharm.uconn.edu/iimdb/

(3) IIMDBAdmin : JavaFX based admin interface for building and administering IIMDB

(4) PUGRest : JavaFX based client for downloading compounds from PubChem

(5) SDF2Excel : Java/Swing based utility for converting structure data files to excel format

(6) PMG-Seed : A tool for in silico biochemical structure generation

Skills

Life Sciences / Chemistry

- Metabolomics : Development of computational chemistry techniques and software for metabolomics (LC-MS) research
- Biological Chemistry
- Analytical Chemistry
- Physical Pharmacy
- Pharmaceutical Chemistry
- Medicinal Chemistry
- Cheminformatics
- Computational Chemistry

Computer Science / Statistics

- Computer Languages : Java, C/C++, Perl, Python, Fortran
- GUI Toolkits : Swing, JavaFX
- Predictive Modeling / Machine Learning Techniques (Random Forests, ANN etc.) : Apache Spark, R, PMML and JPMML
- Cheminformatics (Java) APIs : Chemaxon, CDK, Jmol, Ambit
- Web Development : HTML5, CSS3, Javascript / JQuery
- Content Management : Drupal 7
  e.g.
  http://metabolomics.pharm.uconn.edu
- Web Servers : Apache
- Project Management / Build Tools : Maven, Ant
- DBMS : OrientDB, H2, MYSQL
- Software Testing and Quality Assurance : SonarQube, JaCoCo, PMD, Find Bugs, TestNG and JUnit-4
- Computational Chemistry Software : Gaussian03, Shrodinger Suite, Desmond, Tinker
- Operating Systems : Windows, OSX and Many Flavors of Linux (Suse, RedHat, Ubuntu)
- Building and Configuring Rocks Based Linux Clusters
  e.g.
  http://gardel.chem.uconn.edu
  http://powder.uconn.edu
  http://helios.chem.uconn.edu