Asghar Razavi

Curriculum Vitae

Education

- 2011–2015 **Doctor of Philosophy**, *Department of Chemistry*, Temple University, Philadelphia. *GPA – 3.96*
- Advisor Prof. Vincent Voelz
- 2008–2010 **Master of Science**, *Department of Chemistry*, Sharif University of Technology, Tehran, Iran. *GPA – 3.43*
 - Advisor Prof. Gholamabbas Parsafar
- 2004–2008 **Bachelor of Science**, *Department of Chemistry*, University of Tabriz, Tabriz, Iran. *GPA – 3.18*

Research Experience

Postdoctoral Associate, Weill Cornell Medical College of Cornell University, New York.

- 2016-present Computational: Membrane Transporters, Markov State Models
 - Advisor Prof. Harel Weinstein

Graduate Research Assistant, Temple University, Philadelphia.

- 2012-2015 Computational: Protein Folding, Membrane Transporters, Markov State Models, Small Molecule Drug Design
 - Advisor Prof. Vincent Voelz
- 2011-2012 Experimental: Ultrafast Lasers, Atomic Force Microscopy

Advisor Prof. Eric Borguet

Graduate Research Assistant, Sharif University of Technology, Tehran, Iran.

- 2008-2010 Theoretical: Ionic Liquids, Equations of State
 - Advisor Prof. Gholamabbas Parsafar

Teaching/Mentoring Experience

Graduate Teaching Assistant, Temple University, Philadelphia.

- 2011-2015 General Chemistry One
- 2013-2014 Physical Chemistry of Biomolecules
 - 2013 Physical Chemistry One
 - 2012 General Chemistry Two

Research Mentor, Temple University, Philadelphia.

2012-2014 Helped new members of the Voelz lab with Molecular Dynamics simulations and analysis techniques including Python programming language and building Markov State Models

Teaching Mentor, Sharif University of Technology, Tehran, Iran.

2009 Statistical Thermodynamics

Research Interests

Discover, quantitatively understand, and leverage mechanisms of the complex molecular machinery involved in neurotransmission and intercellular communication ; Advance methods of molecular biophysics in the area of dimensionality reduction and kinetic network models of large biological systems ; Quantify kinetics, thermodynamics, and molecular pathways of substrate transport and efflux in neurotransmitter transporters ; Design small molecules/peptidomimetics targeting specific functional aspects of neurotransmitter transporters such as ion and substrate binding sites, allosteric sites, phosphorylation and palmitoylation sites ; Develop next generation analytics methods for on-the-fly annotation and identification of rare events in molecular dynamics simulations

Professional Organizations

- 2015-present Member of Biophysical Society
- 2014-2016 Member of American Chemical Society

Awards

- 2015 Biophysical Society Educational Committee Travel Award
- 2015 XSEDE15 Student Program Travel Grant award
- 2015 Daniel Swern Fellowship from Temple University for Outstanding Research

Journal Publications

Trilce Estrada, Jeremy Benson, Hector Carrillo-Cabada, **Asghar M. Razavi**, Michel A. Cuendet, Harel Weinstein, Ewa Deelman, Michela Taufer: Graphic Encoding of Macromolecules for Efficient High-Throughput Analysis, *Proceedings of the 2018 ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics*, pp 315-324, 2018

Asghar M. Razavi, George Khelashvili, Harel Weinstein: How structural elements evolving from bacterial to human SLC6 transporters enabled new functional properties, *BMC Biology*, 16:31, 2018

Giulia Morra, **Asghar M. Razavi**, Kalpana Pandey, Harel Weinstein, Anant K. Menon, George Khelashvili: Mechanisms of lipid scrambling by the G protein-coupled receptor opsin, *Structure*, Vol. 26, pp 1-12, 2018

Michael V. LeVine, Michel A. Cuendet, **Asghar M. Razavi**, George Khelashvili, Harel Weinstein: Thermodynamic Coupling Function Analysis of Allosteric Mechanisms in the Human Dopamine Transporter, *Biophysical Journal*, Vol. 114, pp 1-5, 2018

Asghar M Razavi, George Khelashvili, Harel Weinstein: A Markov State-based Quantitative Kinetic Model of Sodium Release from the Dopamine Transporter, *Nature Scientific Reports* 7:40076, 2017

Asghar M Razavi, Lucie Delemotte, Joshua R. Berlin, Vincenzo Carnevale, Vincent A. Voelz: Molecular simulations and free-energy calculations suggest conformation-dependent anion binding to a cytoplasmic site as a mechanism for Na+/K+-ATPase ion selectivity, *Journal of Biological Chemistry*, Vol. 292, pp 12412-12423, 2017

Asghar M Razavi, Vincent A Voelz: Kinetic network models of tryptophan mutations in β -hairpins reveal the importance of non-native interactions, *Journal of Chemical Theory and Computation*, Vol. 11, pp 2801-2812, 2015

Vincent A Voelz, Brandon Elmon, **Asghar M Razavi**, Guangfeng Zhou: Surprisal Metrics for Quantifying Perturbed Conformational Dynamics in Markov State Models. *Journal of Chemical Theory and Computation*, Vol. 10, pp 5716-5728, 2014

Asghar M Razavi, William M Wuest, Vincent A Voelz: Computational Screening and Selection of Cyclic Peptide Hairpin Mimetics by Molecular Simulation and Kinetic Network Models. *Journal of Chemical Information and Modeling*, Vol. 54, pp 1425-1432, 2014.

Conference Presentations

Talks

Asghar M Razavi, George Khelashvili, Michael V. LeVine, Michel A. Cuendet, Harel Weinstein: Allosteric networks in biological systems, *Distributed, Collective Computation in Biological and Artificial Systems conference, Janelia Research Campus, Ashburn, VA*, 03/2018

Asghar M Razavi*, **Lucie Delemotte, Vincenzo Carnevale, Vincent A Voelz**: Understanding Ion Selectivity of Na⁺,K⁺/ATPase by Computational Approach, *Biophysical Society 59th Annual Meeting*, 02/2015

* Recipient of BPS travel award

Selected Posters

Asghar M. Razavi, George Khelashvili, Harel Weinstein: Markov State-based Quantitative Kinetic Model of Sodium Release from the Dopamine Transporter, *Biophysical Society 61th Annual Meeting*, 02/2017

Asghar M. Razavi, Heinrich Roder, Vincent A. Voelz : Early Stages of Apomyoglobin Folding Probed by Experiment and H/D Restrained Simulations, *XSEDE15*, 07/2015

Asghar M Razavi, Lucie Delemotte, Vincenzo Carnevale, Vincent A Voelz: Understanding Ion Selectivity of Na⁺, K⁺/ATPase by Computational Approach, *Mechanisms of Membrane Transport, Gordon Research Conference*, 06/2015

Asghar M Razavi, Lucie Delemotte, Vincenzo Carnevale, Vincent A Voelz: Understanding Ion Selectivity of Na⁺, K⁺/ATPase by Computational Approach, *Protein Folding Consortium*, 05/2015

Vincent A Voelz, Asghar M Razavi: Using Kinetic Network Models to Understand Folding Mechanisms of GB1 Hairpin and its Trpzip Variants, *Biophysical Society 59th Annual Meeting*, 02/2015

Asghar M Razavi, William M Wuest, Vincent A Voelz: Computational Screening and Selection of Cyclic Peptide Hairpin Mimetics by Molecular Simulation and Kinetic Network Models, 248th ACS National Meeting 08/2014

M. H. Dinpajooh, A. Razavi Majarashin, and G. A. Parsafar: Equation of State of Nanoscale Solids and Macroscopic Solids, *5th Iranian Nanotechnology Conference* 07/2009

Invited Talks

Understanding Folding Landscapes Using the tICA Approach, Temple University, Philadelphia 04/2014

Markov State Models and Their Applications in Protein Folding, Temple University, Philadelphia 04/2013

Distillation and Vaporization Mechanisms of Ionic Liquids, Sharif University of Technology, Tehran, Iran 05/2009