Nicholas Leioatts

Department of Biochemistry and Biophysics
University of Rochester Medical Center
Box 712, 601 Elmwood Ave.
Rochester, NY 14642

Phone: (772) 633-1719
Email: Nicholas_Leioatts@urmc.rochester.edu

Research Interests

- Structure and dynamics of allosteric macromolecules.
- Computational methods, especially those that allow modeling at various scales of time and resolution.
- Analysis methods for directly comparing computational results to *experimental observables*.

Education

Ph.D. Biophysics, University of Rochester Medical Center, (**expected 2014**).
M.S. Biophysics, University of Rochester Medical Center, 2012.
B.S. Physics, Florida Institute of Technology, 2009.

Research Experience

Graduate Research

- University of Rochester Medical Center

  Focus: ***Understanding allostery in GPCRs using computer simulation at multiple resolutions***
  Advisor: Dr. Alan Grossfield

REU/Internships

- Amertron Inc., Spring 2007 - Spring 2008.

  Manufacturing Engineer (Designing/Testing RF connectors)
- Fermi National Accelerator Lab, Summer 2006.

  Performed monte carlo simulations of particle accelerator beamline

Undergraduate Research

- Detector Physics, Summer 2005 - Spring 2009.

  Muon Tomography (Designed & built scintillation and gaseous-based particle detectors)

Teaching

- Mentor for research students: Hanna Shebert (2012), Pooja Suresh (2013).
- GRE Quantitative Preparatory Class, Instructor, Fall 2010 & 2012.
- General Biochemistry (Ph.D.), Teaching Assistant, Fall 2010.

Honors, Awards, & Fellowships

- Elon H. Hooker fellowship, 2013-2014.
- William F. Neuman Award, 2013.
- Training Grant, NIH T32 GM068411, 2011-2012.
- Biochemistry Department Retreat Poster Presentation Award, 2012.
- Departmental Seminar Award, 2011 & 2012.
- Departmental Travel Award, 2011.

Professional Activities and Service

- **Associate Chair for Gordon Research Seminar** in Computational Chemistry, 2014.
- Host for annual "T32 student-invited speaker" seminar, 2013.
- **Reviewer**
  - Chem. Phys. Lipids, 2013.
  - J. Chem. Theor. & Comp., 2012-2013.
- Departmental service:
  - Organizer - Biophysics Program Retreat, 2010 & 2011.

Conference and Seminar Presentations

- *Retinal Changes Conformation During the Early Stages of Rhodopsin Activation.*
- *Understanding the Rhodopsin Activation Mechanism with Molecular Dynamics.*
  57th Annual Biophysical Society Meeting. Philadelphia, PA, 2-6 February 2013.
- *Unraveling Allostery with Simulations of Rhodopsin and Opsin.*
  Computational Chemistry Gordon Research Conference. Mount Snow, VT, 22-27 July 2012.
- *Elucidating Elastic Network Model Robustness by Parameterization with Molecular Dynamics.*
  56th Annual Biophysical Society Meeting. San Diego, CA, 25-29 February 2012.
- *Validating and Improving Elastic Network Models with Microsecond Scale Molecular Dynamics.*
  55th Annual Biophysical Society Meeting. Baltimore, MD, 5-9 March 2011.

Publications

1. **Leioatts, N.**, Suresh, P., and Grossfield, A., *Tracking the Activation of Two Model GPCRs using Structure-Based Dynamics*, (in preparation, submission planned February 2014)
2. **Leioatts, N.**, Mertz, B., Martínez-Mayorga, K., Romo, T.D., Pitman, M.C., Feller, S.E., Grossfield, A., and Brown, M.F., *Retinal dynamics explained by a concerted transition early in rhodopsin activation*, Biochemistry, 2013, DOI: 10.1021/bi4013947
3. Seckler, J.M., **Leioatts, N.**, Mao, H., and Grossfield, A., *The interplay of structure and dynamics in the function of HIV-1 Reverse Transcriptase*, Proteins: Struc. Func. Bioinf., 2013, DOI: 10.1002/prot.24325
4. **Leioatts, N.**, and Grossfield, A., *Molecular Dynamics Simulations of Membranes and Membrane Proteins* in "Molecular Modeling at the Atomic Scale", ed. Ruhong Zhou, CRC Press (in press, June 2014)
5. **Leioatts, N.**, Romo, T.D., and Grossfield, A., *Elastic network models are robust to variations in formalism*, J. Chem. Theor. Comput., 2012, DOI:10.1021/ct3000316