

Nicholas Leioatts

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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

Undergraduate Research/Internships

- Detector Physics, Summer 2005 - Spring 2009.
Muon Tomography (Designed & built scintillation and gaseous-based particle detectors)
- 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

Teaching

- Mentor for research students: Hanna Shebert (2012), Pooja Suresh (2013-2014).
- 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. (1 year/\$20,000)
- William F. Neuman Award, 2013.
- Training Grant, NIH T32 GM068411, 2011-2012. (1 year/\$26,000)
- 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-.
- Departmental service:
 - Organizer - Biophysics Program Retreat, 2010 & 2011.

Invited Seminars

- Weill Cornell Medical College, New York, NY, USA, 22 November 2013.
Title: *Capturing the Multiple Scales of Rhodopsin Activation*.
- KTH (Royal Institute of Technology) Stockholm, Sweden, 9 April 2014.
Title: *Unravelling Allostery with Simulations of the Dim-Light Receptor Rhodopsin*.
- Max Plank Institute for Biophysical Chemistry, Goettingen, Germany, 14 April 2014.
Title: *Unravelling Allostery with Simulations of the Dim-Light Receptor Rhodopsin*.

Conference Presentations

- *Ensemble Dynamics of Opsin and Rhodopsin*.
58th Annual Biophysical Society Meeting. San Francisco, CA, USA, 15-19 February 2014.
- *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, USA, 2-6 February 2013.
- *Unraveling Allostery with Simulations of Rhodopsin and Opsin*.
Computational Chemistry Gordon Research Conference. Mount Snow, VT, USA, 22-27 July 2012.
- *Elucidating Elastic Network Model Robustness by Parameterization with Molecular Dynamics*.
56th Annual Biophysical Society Meeting. San Diego, CA, USA, 25-29 February 2012.
- *Validating and Improving Elastic Network Models with Microsecond Scale Molecular Dynamics*.
55th Annual Biophysical Society Meeting. Baltimore, MD, USA, 5-9 March 2011.

Publications

1. **Leioatts, N.**, Suresh, P., Romo, T., and Grossfield, A., *Structure-Based Simulations Reveal Concerted Dynamics of GPCR Activation*, Proteins, 2014, DOI: 10.1002/prot.24617
2. Mnpotra, J., Qiao, Z., Cai, J., Lynch, D.L., Grossfield, A., **Leioatts, N.**, Hurst, D.P., Pitman, M.C., Song, Z.-H., and Reggio, P.H., *Structural Basis of G Protein-Coupled Receptor-G_i Protein Interaction: Formation of the Cannabinoid CB2 Receptor/G_i Protein Complex*, J. Biol. Chem., 2014, DOI: 10.1074/jbc.M113.539916
3. **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)
4. **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
5. 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
6. **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