Nicholas Leioatts, Ph.D.

Dept. of Theoretical & Computational Biophysics
Max Planck Institute for Biophysical Chemistry
Am Fassberg 11, Göttingen, Germany, 37077.
Phone: +49 551 201-2325
Email: Nicholas.Leioatts@mpibpc.mpg.de

Education

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

Research Experience

Postdoctoral Research

- Max Planck Institute for Biophysical Chemistry, 2014 - .

  Focus: ***Determining the driving forces behind F1-ATPase function***
  Advisor: Dr. Helmut Grubmüller

Graduate Research

- University of Rochester Medical Center, 2009 - 2014.

  Focus: ***Understanding the dynamic process of GPCR activity using computer simulation***
  Advisor: Dr. Alan Grossfield

Undergraduate Research/Internships

- Detector Physics, 2005 - 2009.
  Muon Tomography (Designed & built scintillation and gaseous-based particle detectors)
- Amertron Inc., 2007 - 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

- George V. Metzger Doctoral Dissertation Award, 2015.
- German Biophysical Society (DGfB) Travel Award, 2015.
- Elon H. Hooker Fellowship, 2013-2014.
- William F. Neuman Award, 2013.
- Training Grant, NIH T32 GM068411, 2011-2012.

Professional Activities and Service

- **Chair for Gordon Research Seminar** on Computational Chemistry, 2016.
- Associate Chair for Gordon Research Seminar on Computational Chemistry, 2014.
- Reviewer for: Chem. Phys. Lipids, J. Chem. Theor. & Comp., Biophys. J.

Invited Seminars

- Florida Institute of Technology, Melbourne, Florida, 22 August 2014.
  Title: *All Science is Physics, or: Unravelling Signal Transduction in the Biomedically Important Membrane Protein, Rhodopsin.*
- Max Plank Institute for Biophysical Chemistry, Goettingen, Germany, 14 April 2014.
  Title: *Unravelling Allostery with Simulations of the Dim-Light Receptor Rhodopsin.*
- KTH (Royal Institute of Technology) Stockholm, Sweden, 9 April 2014.
  Title: *Unravelling Allostery with Simulations of the Dim-Light Receptor Rhodopsin.*
- Weill Cornell Medical College, New York, NY, USA, 22 November 2013.
  Title: *Capturing the Multiple Scales of Rhodopsin Activation.*

Publications

1. **Leioatts, N.**, Romo, T., Danial, S.A., and Grossfield, A., *Retinal Conformation Changes Rhodopsin's Dynamic Ensemble*, Biophys. J, 2015, DOI: 10.1016/j.bpj.2015.06.046

2. Romo, T., **Leioatts, N.**, and Grossfield, A., *Lightweight Object Oriented Structure Analysis: Tools for Building Tools to Analyze Molecular Dynamics Simulations*, J. Comput. Chem., 2014, DOI: 10.1002/jcc.23753

3. **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

4. 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

5. **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 2014, ISBN: 9781466562950

6. **Leioatts, N.**, Mertz, B., Martínez-Mayorga, K., Romo, T.D., Pitman, M.C., Feller, S.E., Grossfield, A., and Brown, M.F., *Retinal Ligand Mobility Explains Internal Hydration and Reconciles Active Rhodopsin Structures*, Biochemistry, 2013, DOI: 10.1021/bi4013947

7. 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

8. **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