

David R. Slochower

Curriculum Vitae

September 2018

📍 Skaggs School of Pharmacy and Pharmaceutical Sciences
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Education and positions

- 2015- **Postdoctoral scholar**, University of California, San Diego
Advisor: Michael K. Gilson, M.D., Ph.D.
Topic: Biophysical modeling and computational chemistry
- 2014 **Instructor**, University of Pennsylvania
Course: “Molecular physiology and cellular engineering”
- 2007-2014 **Ph.D. in Biochemistry and Molecular Biophysics**, University of Pennsylvania
Advisor: Paul A. Janmey, Ph.D.
Thesis: Multiscale simulations of phosphatidylinositol bisphosphate: understanding its biological role through physical chemistry
- 2003-2007 **A.B. cum laude in Physics with distinction**, Kenyon College
Research: high energy nuclear imaging

Research interests

- Physical chemistry of biological membranes
- Nonequilibrium statistical mechanics of molecular motors
- New methods for computing binding free energies
- Improved simulation force fields based on open source science

Previous research

- 2017- **Force field development with the open force field consortium**
[Open Force Field Group](#)
- 2016- **Thermodynamics of host-guest molecular recognition**
Advisor: Michael K. Gilson, M.D., Ph.D. (University of California, San Diego)
- 2015- **Theory of molecular motors**
Advisor: Michael K. Gilson, M.D., Ph.D. (University of California, San Diego)
- 2014-2015 **Simulations and docking of macrocycles**
Advisors: Ravi Radhakrishnan, Ph.D. (University of Pennsylvania) and Mark A. Lemmon, Ph.D. (Yale University)
- 2009-2014 **Quantum, all-atom, and coarse-grained molecular dynamics of membranes**
Advisor: Paul A. Janmey, Ph.D. (University of Pennsylvania)
- 2008 **Simulations of viral entry into cells**
Advisors: William DeGrado, Ph.D. (University of California, San Francisco) and Michael L. Klein, Ph.D. (Temple University)
- 2007 **Experimental single molecule biophysics**
Advisor: Yale E. Goldman, M.D., Ph.D. (University of Pennsylvania)
- 2007 **Computational design of synthetic peptides**
Advisor: Jeffery Saven, Ph.D. (University of Pennsylvania)
- 2006-2008 **Coded aperture imaging**

Advisors: John Idoine, Ph.D. (Kenyon College), John Frangioni, M.D., Ph.D. (Harvard University), and Richard Lanza, Ph.D. (Massachusetts Institute of Technology)

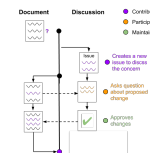
2005

Analysis of protein hydration shells in simulations

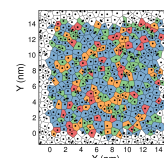
Advisor: Matthias Buck, Ph.D. (Case Western Reserve University)

Peer-reviewed publications

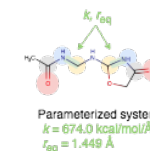
1. Himmelstein DS, **Slochower DR**, Malladi VS, Greene CS, Gitter, A. "Open Collaborative Writing with Manubot" *Under Review at eLife* 2018 · [GitHub](#) · [Nature TechBlog](#)



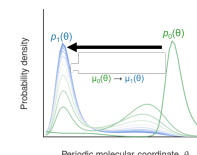
2. Bradley RP*, **Slochower DR***, Janmey PA, Radhakrishnan R. "Molecular modeling of divalent cation-specific nano-clusters of phosphoinositides in physiologically-composed bilayers" *Under Review at JACS* 2018 · [GitHub](#)



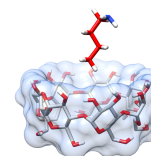
3. Mobley DL, Bannan CC, Bayly CI, Rizzi A, Chodera JD, Lim VT, Lim NM, Beauchamp KA, **Slochower DR**, Shirts MR, Gilson MK, Eastman PK. "Escaping Atom Types in Force Fields Using Direct Chemical Perception" *Under Review at JCTC* 2018 · [GitHub](#)



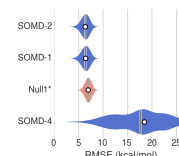
4. **Slochower DR**, Gilson MK. "Motor-like Properties of Nonmotor Enzymes" *Biophysical Journal* 114:9, 2018 · [bioRxiv](#) · [DOI](#) · [GitHub](#) · [New and Notable](#) · [UCSD In the News](#)



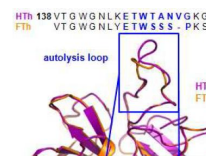
5. Yin J, Henriksen NM, **Slochower DR**, Gilson MK. "The SAMPL5 host-guest challenge: computing binding free energies and enthalpies from explicit solvent simulations by the attach-pull-release (APR) method" *Journal of Computer-Aided Molecular Design* 1:31 133-145, 2017 · [DOI](#)



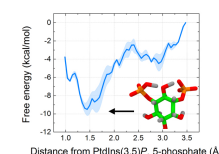
6. Yin J, Henriksen NM, **Slochower DR**, Shirts MR, Chiu MW, Mobley DL, Gilson MK. "Overview of the SAMPL5 host-guest challenge: Are we doing better?" *Journal of Computer-Aided Molecular Design* 1:31 1-19, 2017 · [DOI](#) · [GitHub](#)



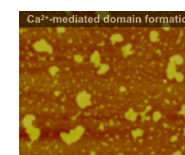
7. Smith JR, Galie PA, **Slochower DR**, Weisshaar CL, Janmey PA, Winkelstein BA. "Salmon-derived thrombin inhibits development of chronic pain through an endothelial barrier protective mechanism dependent on APC" *Biomaterials* 80 96-105, 2016 · [DOI](#)



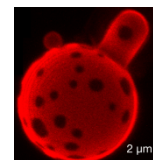
8. **Slochower DR**, Wang Y-H, Radhakrishnan R, Janmey PA. "Physical chemistry and membrane properties of two phosphatidylinositol biphosphate isomers" *Physical Chemistry Chemical Physics* 17:19 12608-12615, 2015 · [DOI](#)



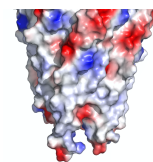
9. Wang Y-H, **Slochower DR**, Janmey PA. "Counterion-mediated cluster formation by polyphosphoinositides" *Chemistry and Physics of Lipids* 182 38-51, 2014 · [DOI](#)



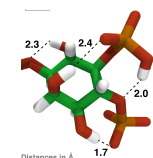
10. **Slochower DR**, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. "Counterion-mediated pattern formation in membranes containing anionic lipids" *Advances in Colloid and Interface Science* 208 177-188, 2014 · [DOI](#)



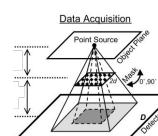
11. Janmey PA, **Slochower DR**, Wang Y-H, Wen Q, Ceber A. "Polyelectrolyte properties of filamentous biopolymers and their consequences in biological fluids" *Soft Matter* 10:10 1439-1449, 2014 · [DOI](#)



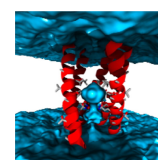
12. **Slochower DR**, Huwe PJ, Radhakrishnan R, Janmey PA. "Quantum and All-Atom Molecular Dynamics Simulations of Protonation and Divalent Ion Binding to Phosphatidylinositol 4,5-Bisphosphate (PIP₂)" *The Journal of Physical Chemistry B* 117:28 8322-8329, 2013 · [DOI](#)



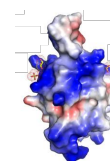
13. Fujii, H, Idoine JD, Gioux S, Accorsi R, **Slochower DR**, Lanza R, Frangioni JV. "Optimization of Coded Aperture Radioscintigraphy for Sentinel Lymph Node Mapping" *Molecular Imaging and Biology* 14:2 173-182, 2012 · [DOI](#)



14. Donald JE, Zhang Y, Fiorin G, Carnevale V, **Slochower DR**, Gai F, Klein ML, De-Grado WF. "Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion" *Proceedings of the National Academy of Sciences* 108:10 3958-3963, 2011 · [DOI](#)



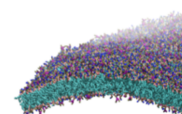
15. Moravcevic K, Mendrola JM, Schmitz KR, Wang Y-H, **Slochower DR**, Janmey PA, Lemmon MA. "Kinase Associated-1 Domains Drive MARK/PAR1 Kinases to Membrane Targets by Binding Acidic Phospholipids" *Cell* 143:6 966-977, 2010 · [DOI](#)



* These authors contributed equally.

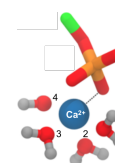
Book chapters

1. **Slochower DR**, Wang Y-H, Radhakrishnan R, Janmey PA. "Lipid membrane shape evolution and the actin cytoskeleton" in *Handbook of Lipid Membranes, Molecular and Materials Aspects*, Eds. Safinya C, Rädler, J. (2018)



Ph.D. thesis

Slochower DR. "Multiscale simulations of phosphatidylinositol bisphosphate: understanding its biological role through physical chemistry" *University of Pennsylvania*, 2014



Software packages and contributions

pAPRika	GitHub	Free energy calculations with AMBER and OpenMM
speakeasy	GitHub	Automates the conversion of SMIRNOFF parameters to AMBER force field files
smirnovert	GitHub	Convert host-guest systems into SMIRNOFF force fields
manubot	GitHub	Automated scholarly publishing
BioPhysCode	GitHub	Tools for building and analyzing membrane simulations

Invited talks, posters, abstracts, and workshops (since 2010)

- 2018 Talk **Using calorimetric data to drive accuracy in computer-aided drug design**
Presented by Michael K. Gilson at The North American Calorimetry Conference
- 2017 Talk **Directional motion in chiral molecules out of equilibrium**
253rd American Chemical Society Meeting
- 2017 Talk **Are all enzymes molecular motors? An effect of binding and catalysis out of equilibrium**
Presented by Michael K. Gilson at the 254th American Chemical Society Meeting
- 2017 Poster **Directional and driven motion in enzymes out of equilibrium**
61st Annual Biophysical Society Meeting
- 2014 Talk **Multiscale modeling of polyphosphoinositides**
University of California, San Diego
- 2014 Talk **Physical chemistry of phosphatidylinositol isomers**
University of California, Irvine
- 2013 Talk **Membranes: Polyphosphoinositides**
Friday Research Discussions, University of Pennsylvania
- 2013 Poster **Quantum and All-atom Molecular Dynamics Simulations of Proton Binding to Phosphatidylinositol 4,5-bisphosphate (PIP₂)**
57th Biophysical Society Meeting
- 2012 Poster **Multiscale modeling of membrane curvature induced by epsin**
Presented by Ryan Bradley at the 244th American Chemical Society Meeting
- 2012 Talk **Molecular Dynamics Simulations of Ion Binding and Protonation of Phosphatidylinositol Bisphosphate (PIP₂)**
244th American Chemical Society Meeting
- 2012 Talk **Simulations of membrane electrostatics with PtdInsP₂**
George W. Raiziss 30th Annual Retreat
- 2012 Poster **Molecular Dynamics Simulations of Phosphatidylinositol Bisphosphate (PIP₂)**
American Physical Society, March Meeting
- 2011 Talk **Molecular Dynamics Simulations of Membranes**
47th New England Complex Fluids Workshop
- 2011 Poster **Association of transmembrane helices in viral fusion peptides suggests a protein-centric mechanism of membrane fusion**
Presented by Giacomo Fiorin at the 55th Biophysical Society Meeting
- 2011 Poster **Molecular Dynamics Simulations of Monolayers and Membranes with Phosphatidylinositol Bisphosphate**
55th Biophysical Society Meeting
- 2011 Workshop **Demsond Workshops**
D. E. Shaw Research
- 2011 Workshop **Temple High Performance Computing (HPC)**
Axel Kohlmeyer, Temple University
- 2010 Talk **Simulating highly charged monolayers**
Mechanistic Studies in Membrane Biophysics: Experiments and Theory, Telluride Science and Research Workshop
- 2010 Poster **Simulations of Monolayers with Phosphatidylinositol Bisphosphate**
Gotham-Metro Condensed Matter Meeting
- 2010 Poster **Viral fusogenic peptides form transmembrane helical bundles: Implications for the mechanism of fusion**
Presented by Vincenzo Carnevale at the 239th American Chemical Society

Awards and grants

2012-2013 NIH T32 Structural Biology Training Grant
2011 Juan Grana Graduate Teaching Assistantship
2010-2012 NIH T32 Interdisciplinary Cardiovascular Training Grant
2007 Distinction in Physics (best research), Kenyon College
2007 Sigma Xi, The Scientific Honor Society
2004-2007 Dean's List, Kenyon College
2005 Best Summer Project (biophysics), Case Western Reserve University
2001 Science Olympiad, National Champion Team

Teaching and mentoring experience

Fall 2014 Molecular Physiology & Cellular Engineering – University of Pennsylvania
I was responsible for creating the syllabus, giving lectures, designing project assignments, and grading for one-half of this course.

Spring 2011 Macromolecular Biophysics II – University of Pennsylvania
I was in charge of arranging lectures, holding office hours and regular review sessions, grading homework and exams for first and second year graduate students.

2009- Mentored high school, undergraduate, and graduate students in research.

Spring 2005 Programming I – Kenyon College
I designed regression tests for weekly project assignments, graded, and then posted my own solutions to the class.

Service

- Reviewer for *Soft Matter*
- Reviewer for *European Biophysics Journal*
- Reviewer for *Scientific Reports*
- Reviewer for *Nature Structural & Molecular Biology*
- Member, Biophysical Society
- Member, American Chemical Society

References

Michael K. Gilson, M.D., Ph.D.
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Co-Director UC San Diego Center for Drug Discovery Innovation
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