David R. Slochower

Curriculum Vitae

April 2019

Skaggs School of Pharmacy and Pharmaceutical Sciences
University of California, San Diego
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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 Pennsvylvania
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

- New methods for computing binding free energies
- Using computational chemistry to advance drug design
- Improving force fields using open source science
- Nonequilibrium statistical mechanics of molecular motors

Previous research

2017- **Force field development with the Open Force Field Group**
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)

2015-2016 **Inhibitors of prion protein**
Advisors: Michael K. Gilson, M.D., Ph.D. and Christina Sigurdson, D.V.M, 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)

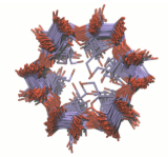
2009-2014 **Quantum, all-atom, and coarse-grained molecular dynamics of membranes**
Advisor: Paul A. Janmey, Ph.D. (University of Pennsylvania)

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)

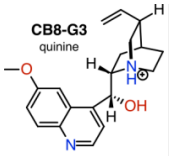
2007 **Experimental single molecule biophysics**
Advisor: Yale E. Goldman, M.D., Ph.D. (University of Pennsylvania)

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)

Preprints and working manuscripts



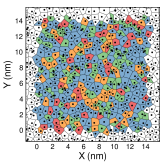
1. **Slochower DR**, Henriksen NM, Chodera JD, Mobley DL, Gilson MK. "Binding thermodynamics of host-guest systems with SMIRNOFF99Frosst from the Open Force Field Group" · Manuscript · GitHub (analysis code) · GitHub (parameterization code)



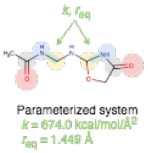
2. Rizzi A, Jensen T, **Slochower DR**, Aldeghi M, Gapsys V, Bosisio S, Henriksen NM, de Groot BL, Dickson A, Michel J, Gilson MK, Shirts MR, Mobley DL, Chodera JD. "The SAMPL6 SAMPLing challenge: Assessing the reliability and efficiency of binding free energy calculations" · GitHub (challenge information) · GitHub (results)

Peer-reviewed publications

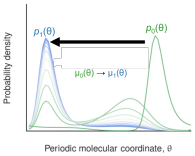
3. Himmelstein DS, **Slochower DR**, Malladi VS, Greene CS, Gitter, A. "Open Collaborative Writing with Manubot" *Accepted with minor revisions at PLOS Computational Biology* 2019 · GitHub (code) · GitHub (manuscript) · Nature TechBlog



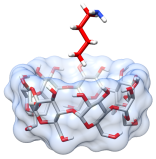
4. Bradley RP*, **Slochower DR***, Janmey PA, Radhakrishan R. "Molecular modeling of divalent cation-specific nano-clusters of phosphoinositides in physiologically-composed bilayers" *Under Review at JACS* 2018 · GitHub



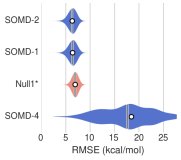
5. Mobley DL, Bannan CC, Bayly CI, Rizzi A, Chodera JD, Lim VT, Lim NM, Beauchamp KA, **Slochower DR**, Shirts MR, Gilson MK, Eastman PK. "Escaping Atom Types in Force Fields Using Direct Chemical Perception" *Journal of Chemical Theory and Computation*, 14 6706-6092, 2018 · GitHub



6. **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

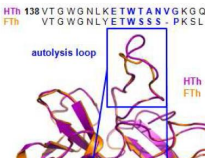


7. Yin J, Henriksen NM, **Slochower DR**, Gilson MK. "The SAMPL5 host-guest challenge: computing binding free energies and enthalpies from explicit solvent simulations by the attach-pull-release (APR) method" *Journal of Computer-Aided Molecular Design* 1:31 133-145, 2017 · DOI

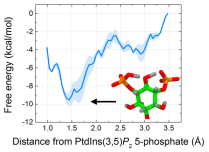


8. Yin J, Henriksen NM, **Slochower DR**, Shirts MR, Chiu MW, Mobley DL, Gilson MK. "Overview of the SAMPL5 host-guest challenge: Are we doing better?" *Journal of Computer-Aided Molecular Design* 1:31 1-19, 2017 · DOI · GitHub

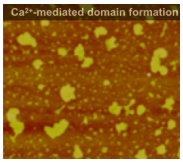
9. Smith JR, Galie PA, **Slochower DR**, Weisshaar CL, Janmey PA, Winkelstein BA. "Salmon-derived thrombin inhibits development of chronic pain through an endothelial barrier protective mechanism dependent on APC" *Biomaterials* 80 96-105, 2016 · DOI



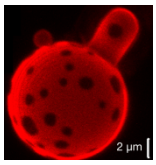
10. **Slochower DR**, Wang Y-H, Radhakrishnan R, Janmey PA. "Physical chemistry and membrane properties of two phosphatidylinositol bisphosphate isomers" *Physical Chemistry Chemical Physics* 17:19 12608-12615, 2015 · DOI



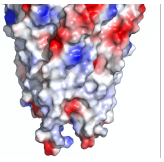
11. Wang Y-H, **Slochower DR**, Janmey PA. "Counterion-mediated cluster formation by polyphosphoinositides" *Chemistry and Physics of Lipids* 182 38-51, 2014 · DOI



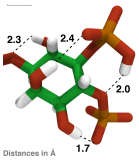
12. **Slochower DR**, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. "Counterion-mediated pattern formation in membranes containing anionic lipids" *Advances in Colloid and Interface Science* 208 177-188, 2014 · DOI



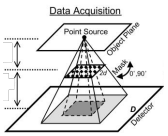
13. Janmey PA, **Slochower DR**, Wang Y-H, Wen Q, Ceber A. "Polyelectrolyte properties of filamentous biopolymers and their consequences in biological fluids" *Soft Matter* 10:10 1439-1449, 2014 · DOI



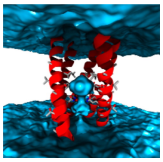
14. **Slochower DR**, Huwe PJ, Radhakrishnan R, Janmey PA. "Quantum and All-Atom Molecular Dynamics Simulations of Protonation and Divalent Ion Binding to Phosphatidylinositol 4,5-Bisphosphate (PIP_2)" *The Journal of Physical Chemistry B* 117:28 8322-8329, 2013 · DOI



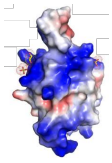
15. Fujii, H, Idoine JD, Gioux S, Accorsi R, **Slochower DR**, Lanza R, Frangioni JV. "Optimization of Coded Aperture Radioscintigraphy for Sentinel Lymph Node Mapping" *Molecular Imaging and Biology* 14:2 173-182, 2012 · DOI



16. Donald JE, Zhang Y, Fiorin G, Carnevale V, **Slochower DR**, Gai F, Klein ML, DeGrado 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



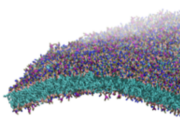
17. Moravcevic K, Mendrola JM, Schmitz KR, Wang Y-H, **Slochower DR**, Janmey PA, Lemmon MA. "Kinase Associated-1 Domains Drive MARK/PAR1 Kinases to Membrane Targets by Binding Acidic Phospholipids" *Cell* 143:6 966-977, 2010 · DOI



* These authors contributed equally.

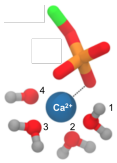
Book chapters

1. **Slochower DR**, Wang Y-H, Radhakrishan 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

Software skills

- Proficient programming in Python and Jupyter Notebooks with knowledge of Bash, C++, FORTRAN, and Perl.
- Active user of GitHub and continuous integration platforms; experienced writing unit, integration, and regression tests.
- Expert with molecular dynamics simulations using AMBER and OpenMM; familiar with Gromacs, CHARMM, and LAMMPS.
- Used Schrödinger and MOE software suites
- Accomplished using OpenEye Toolkits; familiar with KNIME and RDKit

Invited talks, posters, abstracts, and workshops (selected)

2019 Talk **Binding free energy calculations using the attach-pull-release method**
2019 AMBER developers' meeting

2019 Talk **Benchmarking emerging force fields with binding thermodynamics calculations**
2019 University of California Chemical Symposium

2017 Talk **Directional motion in chiral molecules out of equilibrium**
253rd 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 chemisty 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 (PIP_2)**
57th Biophysical Society Meeting

2012 Talk **Molecular Dynamics Simulations of Ion Binding and Protonation of Phosphatidylinositol Bisphosphate (PIP_2)**
244th American Chemical Society Meeting

2012 Talk **Simulations of membrane electrostatics with PtdInsP_2**
George W. Raiziss 30th Annual Retreat

2012 Poster **Molecular Dynamics Simulations of Phosphatidylinositol Bisphosphate (PIP_2)**
American Physical Society, March Meeting

2011 Talk **Molecular Dynamics Simulations of Membranes**
47th New England Complex Fluids Workshop

2011 Poster **Molecular Dynamics Simulations of Monolayers and Membranes with Phosphatidylinositol Bisphosphate**
55th Biophysical Society Meeting

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

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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