

David R. Slochower

Curriculum Vitae

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Education and positions

- 2019- **Open Force Field Postdoctoral Fellow**
Topic: Force Field Development
- 2015- **Postdoctoral scholar**, University of California, San Diego
Advisor: Michael K. Gilson, M.D., Ph.D.
Topic: Computational chemistry and biophysics
- 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

- 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

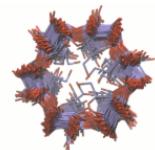
Previous research

- 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)

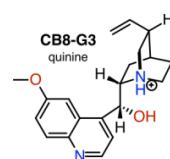
- 2007 **Experimental single molecule biophysics**
Advisor: Yale E. Goldman, M.D., Ph.D. (University of Pennsylvania)
- 2007 **Computational design of synthetic peptides**
Advisor: Jeffery Saven, Ph.D. (University of Pennsylvania)
- 2006-2008 **Coded aperture imaging**
Advisors: John Idoine, Ph.D. (Kenyon 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 \(parameterization code\)](#)

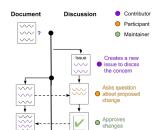


2. Rizzi A, Jensen T, **Slochower DR**, Aldeghi M, Gapsys V, Bosisio S, Henriksen NM, de Groot BL, Dickson A, Michel J, Gilson MK, Shirts MR, Mobley DL, Chodera JD. "The SAMPL6 SAMPLing challenge: Assessing the reliability and efficiency of binding free energy calculations" · [GitHub \(challenge information\)](#)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

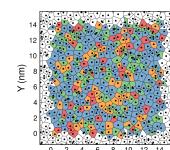


Peer-reviewed publications

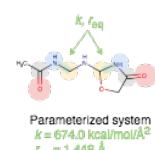
3. Himmelstein DS, **Slochower DR**, Malladi VS, Greene CS, Gitter, A. "Open Collaborative Writing with Manubot" *Accepted with minor revisions at PLOS Computational Biology* 2019 · [GitHub \(code\)](#) · [GitHub \(manuscript\)](#) · [Nature TechBlog](#)



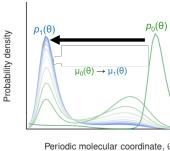
4. Bradley RP*, **Slochower DR***, Janmey PA, Radhakrishnan R. "Molecular modeling of divalent cation-specific nano-clusters of phosphoinositides in physiologically-composed bilayers" *Under Review at JACS* 2018 · [GitHub](#)



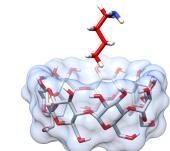
5. Mobley DL, Bannan CC, Bayly CI, Rizzi A, Chodera JD, Lim VT, Lim NM, Beauchamp KA, **Slochower DR**, Shirts MR, Gilson MK, Eastman PK. "Escaping Atom Types in Force Fields Using Direct Chemical Perception" *Journal of Chemical Theory and Computation*, 14 6706-6092, 2018 · [GitHub](#)



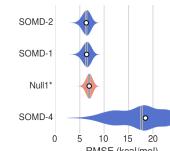
6. **Slochower DR**, Gilson MK. "Motor-like Properties of Nonmotor Enzymes" *Biophysical Journal* 114:9, 2018 · [bioRxiv](#) · [DOI](#) · [GitHub](#) · [New and Notable](#) · [UCSD In the News](#)



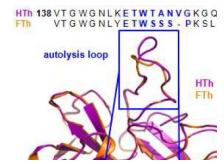
7. Yin J, Henriksen NM, **Slochower DR**, Gilson MK. "The SAMPL5 host-guest challenge: computing binding free energies and enthalpies from explicit solvent simulations by the attach-pull-release (APR) method" *Journal of Computer-Aided Molecular Design* 1:31 133-145, 2017 · [DOI](#)



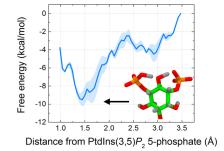
8. Yin J, Henriksen NM, **Slochower DR**, Shirts MR, Chiu MW, Mobley DL, Gilson MK. "Overview of the SAMPL5 host-guest challenge: Are we doing better?" *Journal of Computer-Aided Molecular Design* 1:31 1-19, 2017 · [DOI](#) · [GitHub](#)



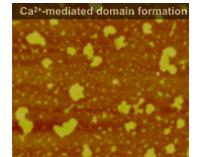
9. Smith JR, Galie PA, **Slochower DR**, Weisshaar CL, Janmey PA, Winkelstein BA. "Salmon-derived thrombin inhibits development of chronic pain through an endothelial barrier protective mechanism dependent on APC" *Biomaterials* 80 96-105, 2016 · [DOI](#)



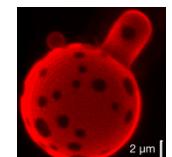
10. **Slochower DR**, Wang Y-H, Radhakrishnan R, Janmey PA. "Physical chemistry and membrane properties of two phosphatidylinositol bisphosphate isomers" *Physical Chemistry Chemical Physics* 17:19 12608-12615, 2015 · [DOI](#)



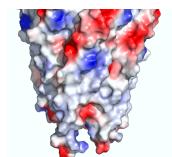
11. Wang Y-H, **Slochower DR**, Janmey PA. "Counterion-mediated cluster formation by polyphosphoinositides" *Chemistry and Physics of Lipids* 182 38-51, 2014 · [DOI](#)



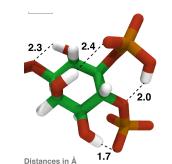
12. **Slochower DR**, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. "Counterion-mediated pattern formation in membranes containing anionic lipids" *Advances in Colloid and Interface Science* 208 177-188, 2014 · [DOI](#)



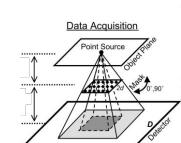
13. Janmey PA, **Slochower DR**, Wang Y-H, Wen Q, Ceber A. "Polyelectrolyte properties of filamentous biopolymers and their consequences in biological fluids" *Soft Matter* 10:10 1439-1449, 2014 · [DOI](#)



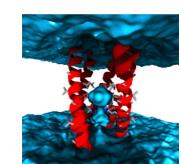
14. **Slochower DR**, Huwe PJ, Radhakrishnan R, Janmey PA. "Quantum and All-Atom Molecular Dynamics Simulations of Protonation and Divalent Ion Binding to Phosphatidylinositol 4,5-Bisphosphate (PIP₂)" *The Journal of Physical Chemistry B* 117:28 8322-8329, 2013 · [DOI](#)



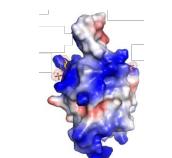
15. Fujii, H, Idoine JD, Gioux S, Accorsi R, **Slochower DR**, Lanza R, Frangioni JV. "Optimization of Coded Aperture Radioscintigraphy for Sentinel Lymph Node Mapping" *Molecular Imaging and Biology* 14:2 173-182, 2012 · [DOI](#)



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](#)



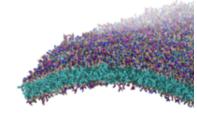
17. Moravcevic K, Mendrola JM, Schmitz KR, Wang Y-H, **Slochower DR**, Janmey PA, Lemmon MA. "Kinase Associated-1 Domains Drive MARK/PAR1 Kinases to Membrane Targets by Binding Acidic Phospholipids" *Cell* 143:6 966-977, 2010 · [DOI](#)



* These authors contributed equally.

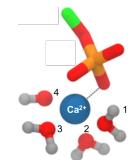
Book chapters

1. **Slochower DR**, Wang Y-H, 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 authored and co-authored

pAPRika	GitHub	Free energy calculations with AMBER and OpenMM	
speakeasy	GitHub	Automates the conversion of SMIRNOFF parameters to AMBER force field files	
taproom	GitHub	Host-guest (and soon, protein-ligand) benchmark systems for free energy calculations, with support for SMIRNOFF parameter coverage	
smirnovert	GitHub	Convert host-guest systems into SMIRNOFF force fields	

manubot	GitHub	Automated scholarly publishing	
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BioPhysCode	GitHub	Tools for building and analyzing membrane simulations	
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Software skills

- Proficient programming in Python (extensive use of notebooks) with knowledge of Bash, C++, FORTRAN, Perl, and R.
- 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.
- Experience working with Schrödinger and Chemical Computing Group software suites.
- Accomplished using OpenEye Toolkits; familiar with KNIME and RDKit.

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

- 2019 Talk **Benchmarking emerging force fields from the Open Force Field Initiative**
2019 American Chemical Society meeting
- 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 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 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 **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

- 2019 Open Force Field Initiative Postdoctoral Fellow
- 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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