David R. Slochower

Curriculum Vitae

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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

- 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)

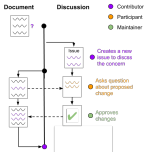
2007 **Computational design of synthetic peptides**
Advisor: Jeffery Saven, Ph.D. (University of Pennsylvania)

2006-2008 **Coded aperture imaging**

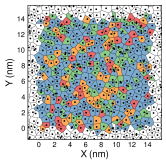
Advisors: John Idoine, Ph.D. (Kenyon College), John Frangioni, M.D., Ph.D. (Harvard University), and Richard Lanza, Ph.D. (Massachusetts Institute of Technology)

2005 **Analysis of protein hydration shells in simulations**
Advisor: Matthias Buck, Ph.D. (Case Western Reserve University)

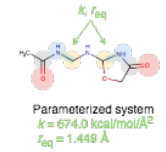
Peer-reviewed publications



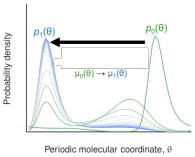
1. Himmelstein DS, **Slochower DR**, Malladi VS, Greene CS, Gitter, A. "Open Collaborative Writing with Manubot" *Accepted with minor revisions at PLOS Computational Biology* 2019 · GitHub (code) · GitHub (manuscript) · Nature TechBlog



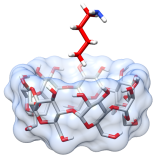
2. Bradley RP*, **Slochower DR***, Janmey PA, Radhakrishan R. "Molecular modeling of divalent cation-specific nano-clusters of phosphoinositides in physiologically-composed bilayers" *Under Review at JACS* 2018 · GitHub



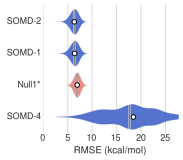
3. Mobley DL, Bannan CC, Bayly CI, Rizzi A, Chodera JD, Lim VT, Lim NM, Beauchamp KA, **Slochower DR**, Shirts MR, Gilson MK, Eastman PK. "Escaping Atom Types in Force Fields Using Direct Chemical Perception" *Journal of Chemical Theory and Computation*, 14 6706-6092, 2018 · GitHub



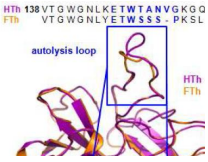
4. **Slochower DR**, Gilson MK. "Motor-like Properties of Nonmotor Enzymes" *Biophysical Journal* 114:9, 2018 · bioRxiv · DOI · GitHub · New and Notable · UCSD In the News



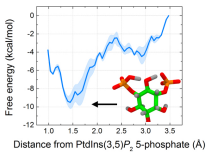
5. Yin J, Henriksen NM, **Slochower DR**, Gilson MK. "The SAMPL5 host-guest challenge: computing binding free energies and enthalpies from explicit solvent simulations by the attach-pull-release (APR) method" *Journal of Computer-Aided Molecular Design* 1:31 133-145, 2017 · DOI



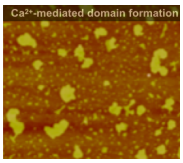
6. Yin J, Henriksen NM, **Slochower DR**, Shirts MR, Chiu MW, Mobley DL, Gilson MK. "Overview of the SAMPL5 host-guest challenge: Are we doing better?" *Journal of Computer-Aided Molecular Design* 1:31 1-19, 2017 · DOI · GitHub



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

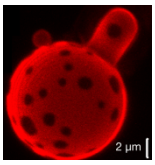


8. **Slochower DR**, Wang Y-H, Radhakrishnan R, Janmey PA. "Physical chemistry and membrane properties of two phosphatidylinositol bisphosphate isomers" *Physical Chemistry Chemical Physics* 17:19 12608-12615, 2015 · DOI

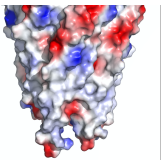


9. Wang Y-H, **Slochower DR**, Janmey PA. "Counterion-mediated cluster formation by polyphosphoinositides" *Chemistry and Physics of Lipids* 182 38-51, 2014 · DOI

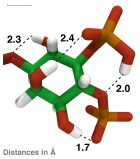
10. **Slochower DR**, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. "Counterion-mediated pattern formation in membranes containing anionic lipids" *Advances in Colloid and Interface Science* 208 177-188, 2014 · DOI



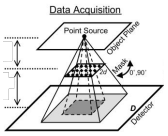
11. Janmey PA, **Slochower DR**, Wang Y-H, Wen Q, Ceber A. "Polyelectrolyte properties of filamentous biopolymers and their consequences in biological fluids" *Soft Matter* 10:10 1439-1449, 2014 · DOI



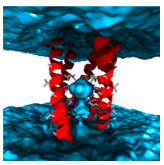
12. **Slochower DR**, Huwe PJ, Radhakrishnan R, Janmey PA. "Quantum and All-Atom Molecular Dynamics Simulations of Protonation and Divalent Ion Binding to Phosphatidylinositol 4,5-Bisphosphate (PIP_2)" *The Journal of Physical Chemistry B* 117:28 8322-8329, 2013 · DOI



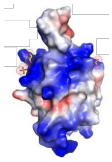
13. Fujii, H, Idoine JD, Gioux S, Accorsi R, **Slochower DR**, Lanza R, Frangioni JV. "Optimization of Coded Aperture Radioscintigraphy for Sentinel Lymph Node Mapping" *Molecular Imaging and Biology* 14:2 173-182, 2012 · DOI



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



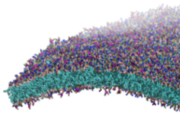
15. Moravcevic K, Mendrola JM, Schmitz KR, Wang Y-H, **Slochower DR**, Janmey PA, Lemmon MA. "Kinase Associated-1 Domains Drive MARK/PAR1 Kinases to Membrane Targets by Binding Acidic Phospholipids" *Cell* 143:6 966-977, 2010 · DOI



* These authors contributed equally.

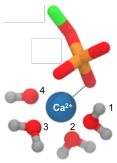
Book chapters

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

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 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	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 (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	**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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