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## The John Chodera Lab

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John Chodera, PhD

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The Chodera lab uses computation and experiments to develop quantitative, multiscale models of the effects of small molecules on biomolecular macromolecules and cellular pathways. To do this, the group utilizes physical models and rigorous statistical mechanics, with the overall goals of engineering novel therapeutics and tools for chemical biology, as well as understanding the physical driving forces behind ligand recognition the evolution of resistance mutations.

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## Featured News

### IN THE LAB



### [Computational “Hive Mind” Helps Scientists Solve an Enzyme’s Cryptic Movements](#)

The breakthrough gives an unprecedented look at the varied and shifting poses of a protein in action.

## Publications Highlights

[A dynamic mechanism for allosteric activation of Aurora kinase A by activation loop phosphorylation](#). Emily F. Ruff, Joseph M. Muretta, Andrew Thompson, Eric W. Lake, Soreen Cyphers, Steven K. Albanese, Sonya M. Hanson, Julie M. Behr, David D. Thomas, John D. Chodera, and Nicholas M. Levinson. *eLife*, in press. [[DOI](#)] [[bioRxiv](#)]

[Quantitative self-assembly prediction yields targeted nanomedicines](#). Yosi Shamay, Janki Shah, Mehtap Işık, Aviram Mizrahi, Josef Leibold, Darjus F. Tschaharganeh, Daniel Roxbury, Januka Budhathoki-Uprety, Karla Nawaly, James L. Sugarman, Emily Baut, Michelle R. Neiman, Megan Dacek, Kripa S. Ganesh, Darren C. Johnson, Ramya Sridharan, Karen L. Chu, Vinagolu K. Rajasekhar, Scott W. Lowe, John D. Chodera, and Daniel A. Heller. *Nature Materials*, in press. [DOI] [PDF] [Supporting Info] [nano-drugbank]

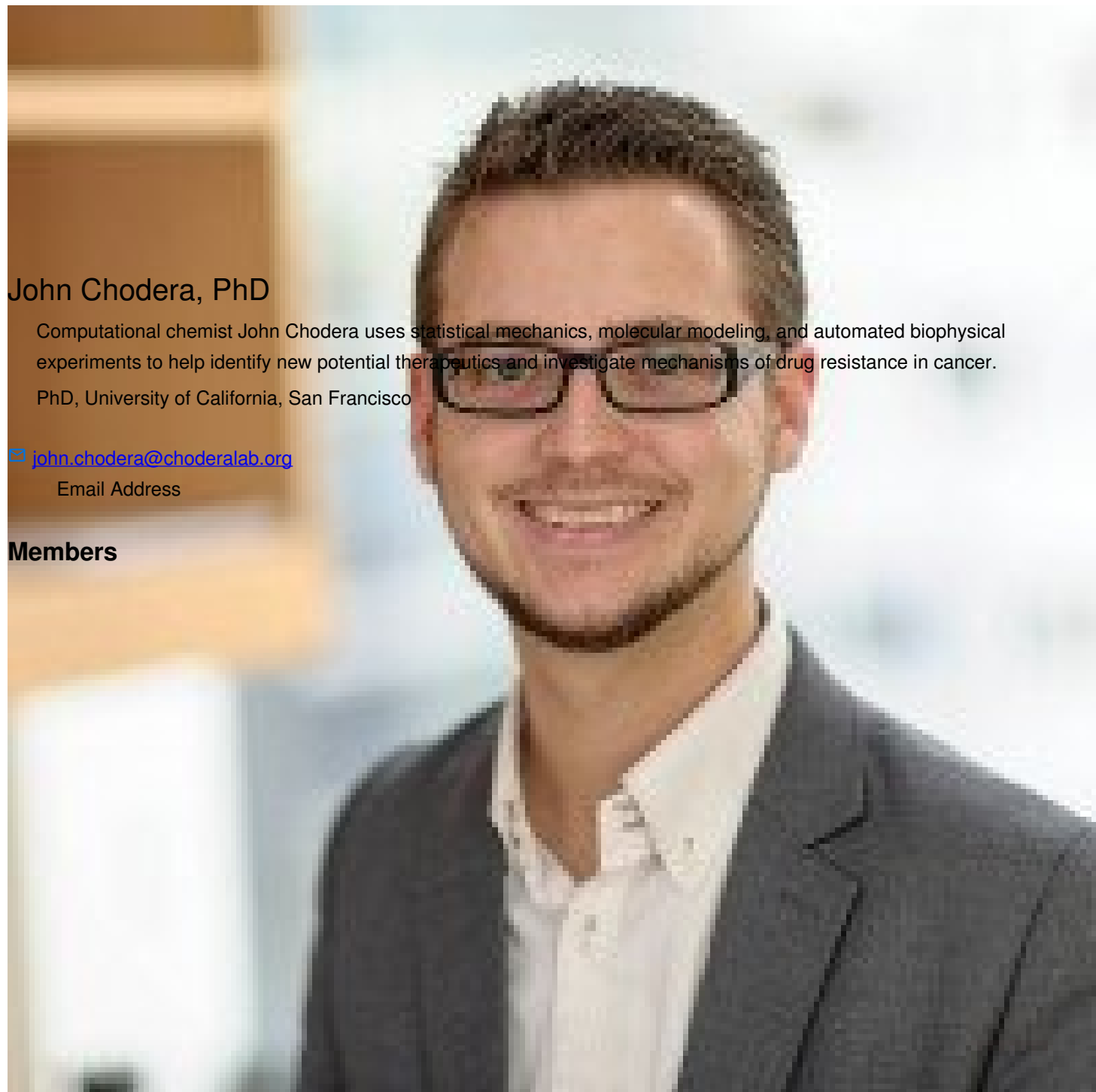
[Predicting resistance of clinical Abl mutations to targeted kinase inhibitors using alchemical free-energy calculations](#). Kevin Hauser, Christopher Negron, Steven K. Albanese, Soumya Ray, Thomas Steinbrecher, Robert Abel, John D. Chodera, and Lingle Wang. Manuscript prior to publication: [bioRxiv] [input files and analysis scripts]

[Biomolecular simulations under realistic macroscopic salt conditions](#). Gregory A. Ross, Ariën S. Rustenburg, Patrick B. Grinaway, Josh Fass, and John D. Chodera. Manuscript prior to publication: [bioRxiv] [simulation code] [results and analysis scripts]

[L-2-Hydroxyglutarate production arises from noncanonical enzyme function at acidic pH](#). Intlekofer A, Wang B, Liu H, Shah H, Carmona-Fontaine C, Rustenburg AS, Salah S, Gunner MR, Chodera JD, Cross JR, and Thompson CB. *Nature Chemical Biology* 13:494, 2017. [DOI] [PDF] [GitHub]

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## People



## John Chodera, PhD

Computational chemist John Chodera uses statistical mechanics, molecular modeling, and automated biophysical experiments to help identify new potential therapeutics and investigate mechanisms of drug resistance in cancer.

PhD, University of California, San Francisco

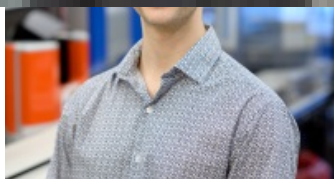
 [john.chodera@choderalab.org](mailto:john.chodera@choderalab.org)

Email Address

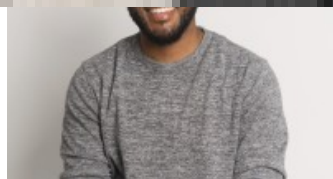
## Members



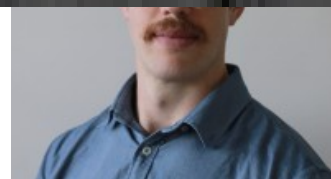
Christopher Iacovella  
Software Scientist



Benjamin Kaminow  
Graduate Student



Kendall Lemons  
Graduate Student

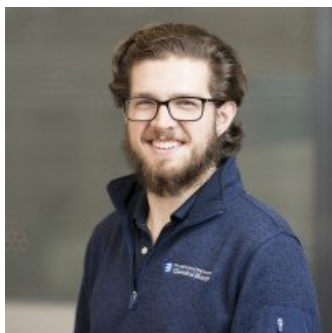


Hugo MacDermott-  
Opeskin  
Software Scientist





Ellen T.  
Mammen  
Senior Administrative  
Assistant



Alexander  
Payne  
Graduate Student



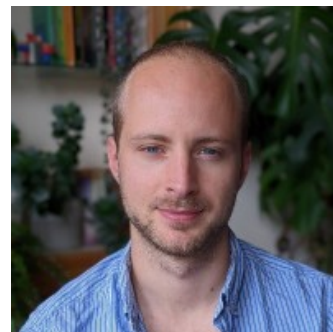
Iván Pulido  
Software Scientist



Michael Retchin  
Graduate Student



Dominic Rufa  
Graduate Student



Jenke Scheen  
Postdoctoral Research  
Scholar



Sukrit Singh  
Postdoctoral Research  
Fellow



Kenichiro Takaba  
Visiting Investigator



Andrea Volkamer  
Collaborator



Yuanqing Wang  
Research Fellow



Jessica White  
Graduate Student



Ivy  
Zhang

Lab Alumni

+

Lab Affiliations

+

## Achievements

Louis V. Gerstner Young Investigator Award (2013)

QB3-Berkeley Distinguished Postdoctoral Fellowship, University of California, Berkeley (2008)

IBM Predoctoral Fellowship (2005)

Howard Hughes Medical Institute Predoctoral Fellowship (2000)

## Get in Touch

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Lab Head Email

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John Chodera discloses the following relationships and financial interests:

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Professional Services and Activities

Interline Therapeutics LLC

Equity; Professional Services and Activities

MPM Capital

Professional Services and Activities

OpenEye Scientific Software, Inc.

Professional Services and Activities

Ventus Therapeutics

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