COMPUTATIONAL & SYSTEMS BIOLOGY PROGRAM

The John Chodera Lab

Research

John Chodera, PhD

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.

View Lab Overview →

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 Mizrachi, 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. Na *ture 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]

View All Publications

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

Email Address

Members

Viktor Belay

Graduate Student

David Dotson

Software Scientist

Erica Goldberger

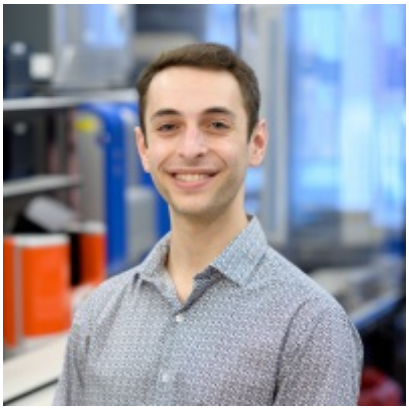
Research Technician

Michael Henry

Software Scientist

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

Graduate Student

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

john.chodera@choderalab.org
Lab Head Email

Disclosures

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John Chodera discloses the following relationships and financial interests:

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Professional Services and Activities

Interline Therapeutics LLC

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MPM Capital

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