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Memorial Sloan Kettering Cancer Center

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The John Chodera Lab

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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 (https://www.mskcc.org/research/ski/labs/john-chodera/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](#)]

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People
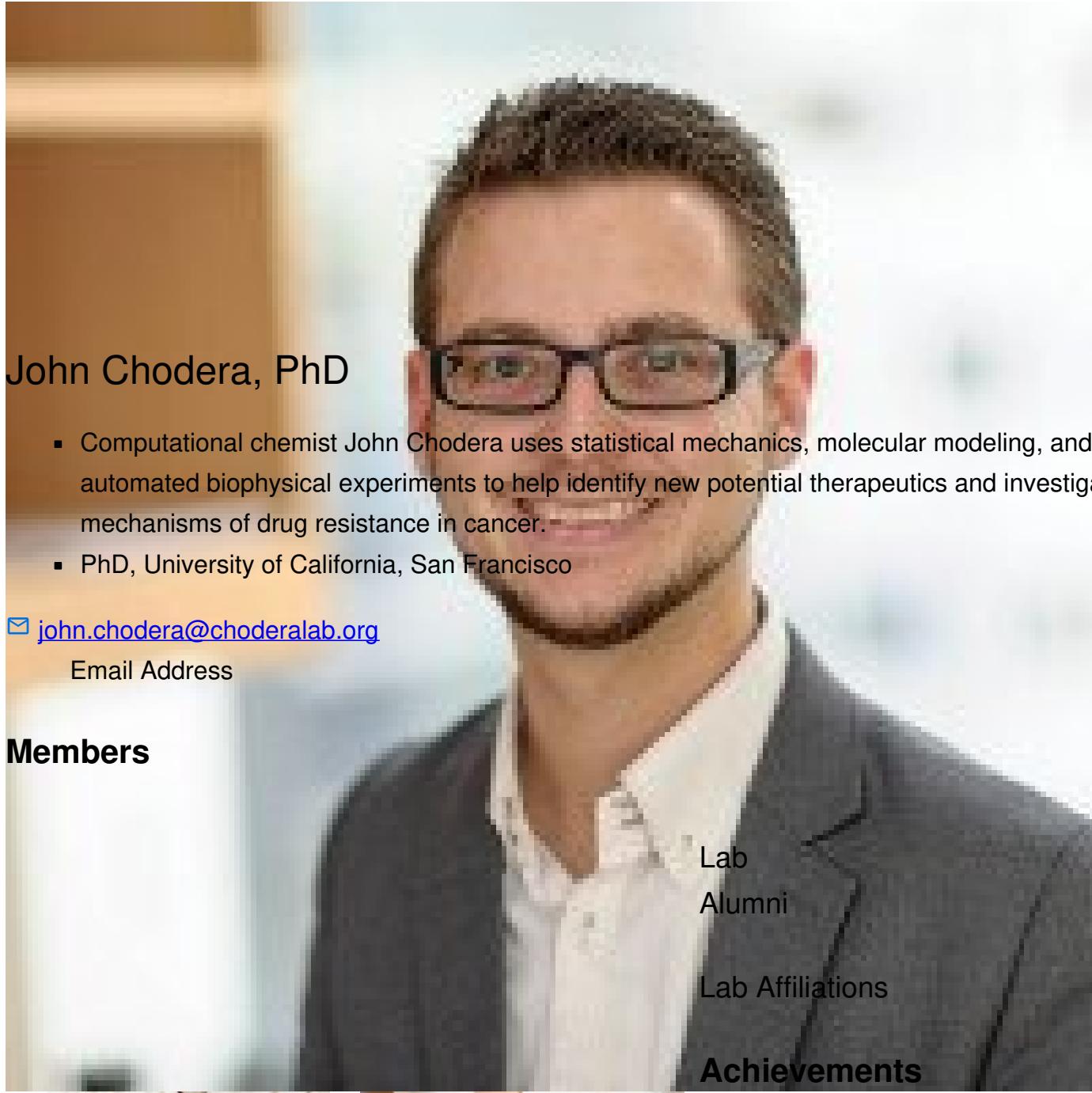
John Chodera, PhD

- 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

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Lab Affiliations

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Viktor Belay
Graduate Student

Maria A. Castellanos
Postdoctoral Research Fellow

- Louis V. Gerstner Young Investigator Award (2013)
  QB3-Berkeley Distinguished Postdoctoral Fellowship, University of

-
   California, Berkeley (2008)
- IBM Predoctoral Fellowship (2005)
-
   Predoctoral Fellowship (2000)

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Ariana Clerkin
Postdoctoral Research Fellow

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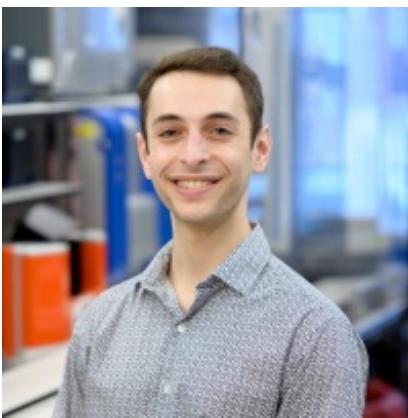
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Disclosures

Members of the MSK Community often work with pharmaceutical, device, biotechnology, and life sciences companies, and other organizations outside of MSK, to find safe and effective cancer treatments, to improve patient care, and to educate the health care community. These activities outside of MSK further our mission, provide productive collaborations, and promote the practical application of scientific discoveries.

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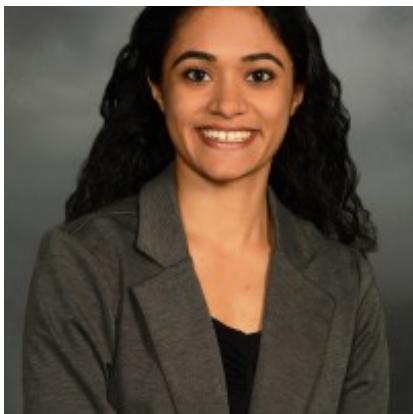
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- **Achira, Inc.**
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