

# John D. Chodera



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## Education and positions

2012-	<b>Assistant Member, Computational Biology Program, Sloan Kettering Institute</b>
2012-	<b>Assistant Member, Memorial Sloan Kettering Cancer Center</b>
2013-	<b>Assistant Professor, Physiology, Biophysics, and Systems Biology Program, Weill Cornell Graduate School of Medical Sciences</b>
2008–2012	<b>Independent Distinguished Postdoctoral Fellow, California Institute for Quantitative Biosciences (QB3), University of California, Berkeley</b>
2006–2008	<b>Postdoctoral researcher, Department of Chemistry, Stanford University</b> With <a href="#">Vijay S. Pande</a> (founder, <a href="#">Folding@Home</a> distributed computing project)
1999–2006	<b>Ph.D. in Biophysics, University of California, San Francisco</b> Committee: <a href="#">Ken A. Dill</a> (thesis advisor), <a href="#">Matthew P. Jacobson</a> , <a href="#">Vijay S. Pande</a>
1995–1999	<b>B.S. in Biology, California Institute of Technology</b> Undergraduate research with <a href="#">Paul H. Patterson</a> (experimental molecular neurobiology) and Jerry E. Solomon (computational chemistry)

## Fellowships and awards

2013–2016	Louis V. Gerstner Young Investigator Award
2013–2014	Google Exacycle for External Faculty
2008–2012	QB3-Berkeley Distinguished Postdoctoral Fellowship, University of California, Berkeley
2005–2006	IBM Predoctoral Fellowship
2005	Frank M. Goyan Award for outstanding work in physical chemistry, University of California, San Francisco
2000–2005	Howard Hughes Medical Institute Predoctoral Fellowship

## Research Interests

Rational computational design of allosteric small-molecule inhibitors and therapeutics  
Kinase inhibitor selectivity and evolution of therapeutic resistance in cancer  
Biomolecular dynamics and conformational heterogeneity  
Error and uncertainty in biophysical measurements  
Computational chemistry, molecular modeling, and forcefield development  
Multiscale modeling of the effects of small molecules on biochemical pathways

## Publications

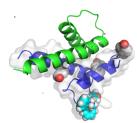
Google Scholar statistics: <http://goo.gl/qO0JW>

MyNCBI Bibliography: <http://goo.gl/e3kjgK>

*h-index: 31 / i10-index: 46 / citations: 5130 (6 Nov 2016)*

\* asterisk denotes equal contributions

## Submitted and Under Review

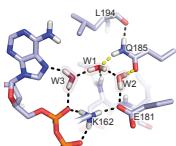


Wojnarowicz P, Desai B, Chin Y, Lima e Silva R, Ohnaka M, Lee SB, Cao MG, Ouerfelli O, Xu S, Goldgur Y, Miller M, Chaudhary J, Garland W, Stoller G, Albanese SA, Soni R, Philip J, Healey J, Vinagolu R, Norton L, Rosen N, Hendrickson R, Iavarone A, Dannenberg A, Chodera JD, Pavletich N, Lasorella A, Campochiaro P, Benzezra R

### **A small-molecule pan Id antagonist, AGX51, shows strong anti-tumor and anti-neovascular activity**

*Under review at Nature .*

*We identify the binding site of a new small-molecule pan-Id antagonist prior to its confirmation by mass spectrometry crosslinking data*



Cyphers S, Ruff E, Behr JM, Chodera JD, and Levinson NM

### **A conserved water-mediated hydrogen bond network governs allosteric activation in Aurora kinase A**

*Under review at Nature Chemical Biology .*

*Over 50 microseconds of aggregate simulation data on Folding@home reveal a surprisingly stable hydrogen bond network that underlies allosteric activation at Tpx2.*

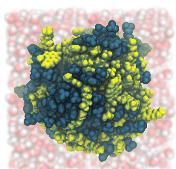


Intlekofer A, Wang B, Liu H, Shah H, Carmona-Fontaine C, Rustenburg AS, Salah S, Gunner MR, Chodera JD, Cross JR, and Thompson CB

### **Acidification enhances production of L-2-hydroxyglutarate through alternative substrate use by dehydrogenase enzymes**

*Under review at Nature Chemical Biology .*

*At low pH, metabolic enzymes lactate dehydrogenase and malate dehydrogenase undergo shifts in substrate selectivity due to surprisingly simple protonation state effects that have enormous ramifications for cancer metabolism.*



Shamay Y, Shah J, Tschaharganeh DF, Roxbury D, Budhathoki-Uprety J, Ijsik M, Mizrahi A, Nawaly K, Sugarman JL, Baut E, Neiman MR, Johnson DC, Sridharan R, Chu KL, Rajasekhar VK, Chodera JD, Lowe SW, and Heller DA

### **Quantitative self-assembly prediction yields targeted nanoparticles**

*Under revision for Nature Materials .*

*A decision tree based on predicted physical properties and molecular descriptors is capable of predicting the assembly of drug/dye nanoparticles that can be used in tumor-targeted selective kinase inhibitor therapy to minimize on- and off-pathway toxicity.*



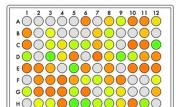
Eastman P, Swails J, Chodera JD, McGibbon RT, Zhao Y, Beauchamp KA, Wang LP, Simmonett AC, Harrigan MP, Brooks BR, and Pande VS

### **OpenMM 7: Rapid development of high performance algorithms for molecular dynamics**

*Under revision for PLoS Computational Biology .*

*The latest version of the GPU-accelerated molecular simulation OpenMM features a variety of incredibly flexible but fast tools for rapidly prototyping, evaluating, and deploying new simulation algorithms.*

## Preprints ahead of submission

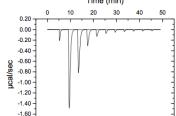


Parton DL, Hanson SM, Rodríguez-Laureano L, Albanese SK, Gradia S, Jeans C, Seeliger M, Chodera JD

### **An open library of human kinase domain constructs for automated bacterial expression**

*Preprint ahead of submission · bioRxv*

*We engineer a library of human kinase domains with useful bacterial expression using a novel phosphatase coexpression technique.*

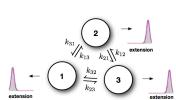


Boyce SE, Tellinghuisen JT, and Chodera JD

### **Avoiding accuracy-limiting pitfalls in the study of protein-ligand interactions with isothermal titration calorimetry**

*Preprint ahead of submission · bioRxv*

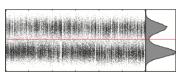
*We demonstrate how to avoid accuracy-limiting problems in standard isothermal calorimetry experiments as well as capture the primary sources of uncertainty in thermodynamic parameters.*



Chodera JD, Noé F, Hinrichs NS, Keller B, Elms PJ, Kaiser CM, Ewall-Wice A, Marqusee S, and Bustamante C  
**Bayesian hidden Markov model analysis of single-molecule biophysical experiments**

Preprint ahead of submission · [arXiv](#)

We present a Bayesian hidden Markov model analysis scheme that allows biomolecular conformational dynamics to be inferred from single-molecule trajectories.



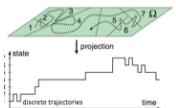
Chodera JD, Elms PJ, Swope WC, Prinz J-H, Marqusee S, Bustamante C, Noé F, and Pande VS

**A robust approach to estimating rates from time-correlation functions**

Preprint ahead of submission · [arXiv](#)

We present a simple, robust approach to estimating two-state rate constants from experimental or simulation data.

## Reviews and Commentaries

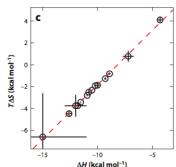


Chodera JD and Noé F

**Markov state models of biomolecular conformational dynamics**

Current Opinion in Structural Biology 25:135, 2014 · [DOI](#)

A review of the exciting developments in the stochastic modeling of biomolecular dynamics over the last few years.

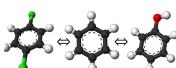


Chodera JD and Mobley DL

**Entropy-enthalpy compensation: Role and ramifications for rational ligand design**

Annual Reviews in Biophysics 42:121, 2013 · [DOI](#)

Entropy-enthalpy compensation is likely a universal phenomena, but not as severe as widely thought, and likely not of enormous concern for drug discovery and ligand design.

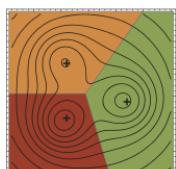


Chodera JD, Mobley DL, Shirts MR, Dixon RW, Branson KM, and Pande VS

**Free energy methods in drug discovery and design: Progress and challenges**

Current Opinion in Structural Biology 21:150, 2011 · [DOI](#)

A review of the opportunities and challenges for alchemical free energy calculations in drug discovery and design.

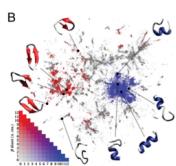


Prinz JH, Wu H, Sarich M, Keller B, Fischbach M, Held M, Chodera JD, Schütte, and Noé F

**Markov models of molecular kinetics: Generation and validation**

Journal of Chemical Physics 134:174105, 2011 · [DOI](#)

A review of current best practices for the generation and validation of Markov state models for describing the stochastic dynamics of biomolecular systems.

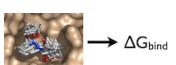


Chodera JD and Pande VS

**The Social Network (of protein conformations)**

Proceedings of the National Academy of Sciences 108:12969, 2011 · [DOI](#)

A new methodology for mapping protein conformational spaces is reminiscent of how we use two-dimensional maps to navigate a three-dimensional world.

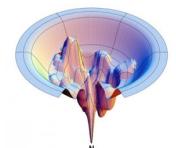


Shirts MR, Mobley DL, Chodera JD

**Alchemical free energy calculations: Ready for prime time?**

Annual Reports in Computational Chemistry 3:41, 2007 · [DOI](#)

A review of current alchemical free energy methodologies assessing whether they are ready for practical use in drug discovery and ligand design.



Dill KA, Ozkan SB, Weikl TR, Chodera JD, and Voelz VA

**The protein folding problem: When will it be solved?**

Current Opinion in Structural Biology 17(3):342, 2007 · [DOI](#)

A review of the current state of the protein folding problem.

## Published and In Press

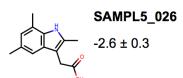


Xu J, Pham CG, Albanese SK, Dong Y, Oyama T, Lee CH, Rodrik-Outmezguine V, Yao Z, Han S, Chen D, Parton DL, Chodera JD, Rosen N, Cheng EH, and Hsieh JJ

### Mechanistically distinct cancer-associated mTOR activation clusters predict sensitivity to rapamycin

*Journal of Clinical Investigation* 126:3529, 2016 · DOI

We use massively parallel distributed molecular simulations on Foldinghome to probe the mechanism activating mutations of the mTOR kinase identified in clinical populations.

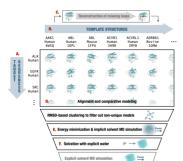


Rustenburg AS, Dancer J, Lin B, Ortwin D, Mobley DL, and Chodera JD

### Measuring cyclohexane-water distribution coefficients for the SAMPL5 challenge

*Journal of Computer Aided Molecular Design*, in press · DOI

To test the accuracy of physical modeling techniques in predicting free energies of transfer between aqueous and nonpolar solvents, we worked with Genentech to develop a new protocol to measure cyclohexane-water distribution coefficients for 53 druglike compounds at pH 7.4, fielding a blind community challenge as part of the SAMPL5 exercise.

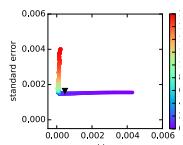


Parton DL, Grinaway PB, Hanson SM, Beauchamp KA, and Chodera JD

### Ensembler: Enabling high-throughput molecular simulations at the superfamily scale

*PLoS Computational Biology* 12:e1004728, 2016 · DOI

We demonstrate a new tool that enables—for the first time—massively parallel molecular simulation studies of biomolecular dynamics at the superfamily scale, illustrating its application to protein tyrosine kinases, an important class of drug targets in cancer.

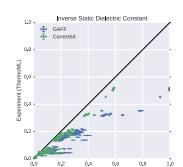


Chodera JD

### A simple method for automated equilibration detection in molecular simulations

*Journal of Chemical Theory and Computation* 12:1799, 2016 · DOI

We present a simple approach to automatically determining the equilibrated region of a molecular simulation, a longstanding challenge formerly without a good solution.

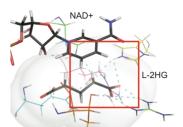


Beauchamp KA, Behr JM, Rustenburg AS, Bayly CI, Kroenlein K, and Chodera JD.

### Towards automated benchmarking of atomistic forcefields: Neat liquid densities and static dielectric constants from the ThermoML data archive

*Journal of Physical Chemistry B* 199:12912, 2015 · DOI

Molecular mechanics forcefields are critical to computer-guide drug design, but the benchmarking and improvement of these forcefields has been hindered by the lack of high-quality machine-readable physical property datasets. We show how the NIST-curated ThermoML Archive, which stores physical property data in an IUPAC-standard XML format, can eliminate these roadblocks and reveal issues with current generation forcefields.

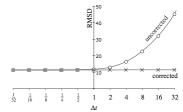


Intlekofer AM, Dematteo RG, Venetti S, Finley LWS, Lu Chao, Judkins AR, Rutenberg AS, Grinaway PB, Chodera JD, Cross JR, and Thompson CB

### Hypoxia introduces production of L-2-Hydroxyglutarate

*Cell Metabolism* 22:1–8, 2015 · DOI

Molecular docking is used to demonstrate the potential for alternative substrate usage by isocitrate dehydrogenases under hypoxic conditions in cancer.

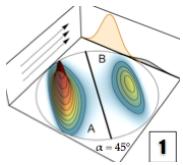


Sivak DA, Chodera JD, and Crooks GE

### Time step rescaling recovers continuous-time dynamical properties for discrete-time Langevin integration of nonequilibrium systems

*Journal of Physical Chemistry B*, 118:6466–6474, 2014. William C. Swope Festschrift · DOI

We derive a simple, easy-to-implement Langevin integrator that has universally useful properties in molecular simulations.

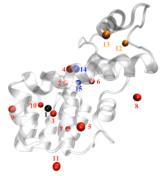


Prinz J-H, Chodera JD, and Noé F

### Spectral rate theory for two-state kinetics

*Physical Review X* 4:011020, 2014 · DOI

We present a new mathematical framework for unifying various two-state rate theories presented in the physical chemistry literature over many decades, and provide a quantitative way to measure reaction coordinate quality.

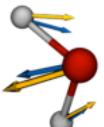


Wang K, Chodera JD, Yang Y, and Shirts MR

### Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics

*Journal of Computer Aided Molecular Design* 27:989–1007, 2013 · DOI

We show how bound ligand poses can be identified even when the location of the binding sites are unknown using the machinery of alchemical modern free energy calculations on graphics processors.

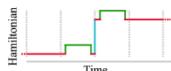


Wang L-P, Head-Gordon TL, Ponder JW, Ren P, Chodera JD, Eastman PK, Martinez TJ, and Pande VS

### Systematic improvement of a classical molecular model of water

*Journal of Physical Chemistry B* 117:9956–9972, 2013 · DOI

Water is the most important molecule in biology, and accurate treatment of its interactions is critical to accurate modeling for drug discovery. While polarizable models of water can achieve very high accuracies, they are both difficult to parameterize and expensive to employ. Here, we show how a high quality inexpensive polarizable model of liquid water can be derived using an automated parameterization engine.



Sivak DA, Chodera JD, and Crooks GE

### Using nonequilibrium fluctuation theorems to understand and correct errors in equilibrium and nonequilibrium discrete Langevin dynamics simulations

*Physical Review X* 3:011007, 2013 · DOI

All molecular dynamics simulations introduce error into the sampled distribution by virtue of the finite timestep used to integrate the equations of motion on a digital computer. While traditional approaches to analyzing this error are extremely complicated, we show how interpreting finite-timestep integrators as a form of nonequilibrium driving leads to simple, straightforward schemes for assessing the impact of these errors, as well as correcting for them.

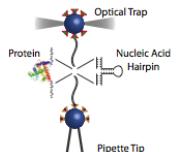


Eastman P, Friedrichs MS, Chodera JD, Radmer RJ, Bruns CM, Ku JP, Beauchamp KA, Lane TJ, Wang L, Shukla D, Tye T, Houston M, Stich T, Klein C, Shirts MR, and Pande VS

### OpenMM 4: A reusable, extensible, hardware independent library for high performance molecular simulation

*Journal of Chemical Theory and Computation* 9:461, 2012 · DOI

Inexpensive consumer GPUs promise a 100-fold increase in simulation power by problems that can effectively exploit their highly specialized structure. Here, we describe the latest advances in an extremely high performance, open-source, extensible GPU-accelerated library and toolkit for molecular simulation.

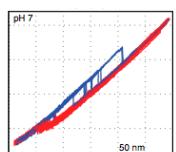


Elms PJ, Chodera JD, Bustamante CJ, Marqusee S

### The limitations of constant-force-feedback experiments

*Biophysical Journal* 103:1490, 2012 · DOI

Popular constant-force-feedback single-molecule experiments can cause severe artifacts in single-molecule force spectroscopy data. We demonstrate a simple alternative that eliminates these artifacts.



Elms PJ, Chodera JD, Bustamante C, Marqusee S

### The molten globule state is unusually deformable under mechanical force

*Proceedings of the National Academy of Sciences* 109:3796, 2012 · DOI

We measure the physical properties of the molten globule state of apo-myoglobin, and show that it is unusually deformable compared to typical protein native states.

$$f_{\text{exp}} = \int d\vec{r} f(\vec{r}) p_1(\vec{r})$$

Pitera JW and Chodera JD

### On the use of experimental observations to bias simulated ensembles

*Journal of Chemical Theory and Computation* 8:3445, 2012 · DOI

We show how the concept of maximum entropy can be used to recover unbiased conformational distributions from experimental data, and how this concept relates to the popular ‘ensemble refinement’ schemes for NMR data analysis.

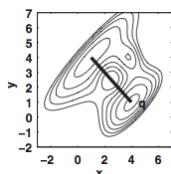


Kaiser CM, Goldman DH, Chodera JD, Tinoco I, Jr., and Bustamante C

### The ribosome modulates nascent protein folding

*Science* 334:1723, 2011 · DOI

Using single-molecule force spectroscopy, we show how the ribosome itself modulates the folding dynamics of nascent protein chains emerging from the exit tunnel.

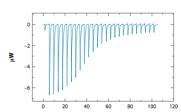


Chodera JD and Pande VS

### **Splitting probabilities as a test of reaction coordinate choice in single-molecule experiments**

Physical Review Letters 107:098102, 2011 · [DOI](#)

We demonstrate a simple test for identifying poor reaction coordinates in single-molecule experiments.

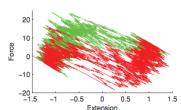


Tellinghuisen JT and Chodera JD

### **Systematic errors in isothermal titration calorimetry: Concentrations and baselines**

Analytical Biochemistry 414:297, 2011 · [DOI](#)

A word of caution about large errors in isothermal titration calorimetry measurements arising from ligand concentration errors.

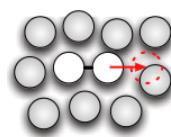


Minh DDL, Chodera JD

### **Estimating equilibrium ensemble averages using multiple time slices from driven nonequilibrium processes: Theory and application to free energies, moments, and thermodynamic length in single-molecule pulling experiments**

Journal of Chemical Physics 134:024111, 2011 · [DOI](#)

We derive a new estimator for estimating equilibrium expectations from nonequilibrium experiments, and show how it can be used to estimate a variety of useful quantities in simulated single-molecule force spectroscopy experiments.

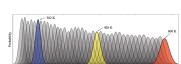


Nilmeier JP, Crooks GE, Minh DDL, and Chodera JD

### **Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation**

Proceedings of the National Academy of Sciences 108:E1009, 2011 · [DOI](#)

We present a significant generalization of Monte Carlo methods that provide an enormously useful tool for enhancing the efficiency of molecular simulations and enabling molecular design.

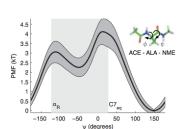


Prinz J-H, Chodera JD, Pande VS, Smith JC, and Noé F

### **Optimal use of data in parallel tempering simulations for the construction of discrete-state Markov models of biomolecular dynamics**

Journal of Chemical Physics 134:244108, 2011 · [DOI](#)

We demonstrate how multitemperature data from parallel tempering simulations can be used to construct fully temperature-dependent models of the dynamics of biomolecular systems.

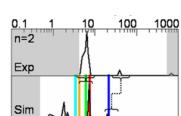


Chodera JD, Swope WC, Noé F, Prinz J-H, Shirts MR, and Pande VS

### **Dynamical reweighting: Improved estimates for dynamical properties from simulations at multiple temperatures**

Journal of Chemical Physics 134:244107, 2011 · [DOI](#)

We describe how reweighing techniques can provide optimal estimates of temperature-dependent dynamical properties from simulations conducted at multiple temperatures.

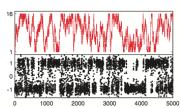


Noé F, Doose S, Daidone I, Löllmann M, Sauer M, Chodera JD, and Smith JC

### **Dynamical fingerprints: A theoretical framework for understanding biomolecular processes by combination of simulation and kinetic experiments**

Proceedings of the National Academy of Sciences 108:4822, 2011 · [DOI](#)

We present a new framework for comparing essential features of the dynamics between experiment and simulation to identify the kinetics processes contributing to individual relaxation timescales in perturbation-response or correlation spectroscopy experiments.

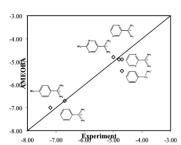


Chodera JD and Shirts MR

### **Replica exchange and expanded ensemble simulations as Gibbs sampling: Simple improvements for enhanced mixing**

Journal of Chemical Physics 135:194110, 2011 · [DOI](#)

We show how a simple change to the way exchanges are handled in the popular replica-exchange simulation methodology can astronomically increase efficiency at no increase in computational cost.

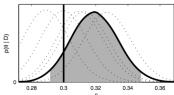


Ponder JW, Wu C, Ren P, Pande VS, Chodera JD, Mobley DL, Schnieders MJ, Haque I, Lambrecht DS, DiStasio RA Jr., Head-Gordon M, Clark GNL, Johnson ME, and Head-Gordon T

### **Current status of the AMOEBA polarizable force field**

Journal of Physical Chemistry B 114:2549, 2010 · [DOI](#)

The AMOEBA polarizable force field is able to reproduce a diverse set of physical chemical phenomenon to high accuracy.



Chodera JD and Noé F

## Probability distributions of molecular observables computed from Markov models.

### II. Uncertainties in observables and their time-evolution

*Journal of Chemical Physics* 133:105102, 2010 · [DOI](#)

A simple Bayesian approach for the modeling of statistical uncertainties in kinetic and equilibrium quantities computed from Markov state models of biomolecular dynamics.

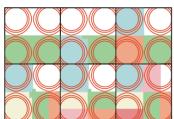


Adelman JL, Chodera JD, Kuo IW, Miller TF, and Barsky D

## The mechanical properties of PCNA: Implications for the loading and function of a DNA sliding clamp

*Biophysical Journal* 98:3062, 2010 · [DOI](#)

Molecular simulations of the PCNA clamp responsible for DNA polymerase processivity show a surprisingly small energetic penalty for the deformation required for clamp loading. Featured on issue cover.

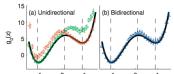


Bacallado S, Chodera JD, and Pande VS

## Bayesian comparison of Markov models of molecular dynamics with detailed balance constraint

*Journal of Chemical Physics* 131:045106, 2009 · [DOI](#)

A Bayesian scheme for comparing state space decompositions for Markov state models of biomolecular dynamics that incorporates the fact that physical systems must obey detailed balance. This paper utilizes recent results from Markov chain theory on edge-reinforced random walks.



Minh DDL, Chodera JD

## Optimal estimators and asymptotic variances for nonequilibrium path-ensemble averages

*Journal of Chemical Physics* 131:134110, 2009 · [DOI](#)

We derive an optimal estimator and corresponding statistical uncertainties for inferring expectations of bidirectional nonequilibrium processes. These estimators have widespread applicability in single-molecule biophysical force-spectroscopy experiments and nonequilibrium molecular simulations.

Shirts MR, Chodera JD

## Statistically optimal analysis of samples from multiple equilibrium states

*Journal of Chemical Physics* 129:124105, 2008 · [DOI](#)

We present a highly general, statistically optimal approach for producing estimates of free energies and equilibrium expectations from multiple simulations that provably extracts all useful information from the data.



Nicholls A\*, Mobley DL\*, Guthrie JP, Chodera JD, and Pande VS

## Predicting small-molecule solvation free energies: A blind challenge test for computational chemistry

*Journal of Medicinal Chemistry* 51:769, 2008 · [DOI](#)

A blind evaluation of the accuracy of alchemical free energy methods for computing gas-to-water transfer free energies (solvation free energies) of small molecules demonstrates that modern forcefields are likely sufficiently accurate to be useful in drug design.

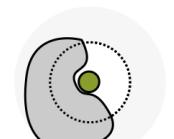


Mobley DL, Dill KA, and Chodera JD

## Treating entropy and conformational changes in implicit solvent simulations of small molecules

*Journal of Physical Chemistry B* 112:938, 2008 · [DOI](#)

An quantitative examination of how much conformational entropy contributes to hydration free energies of small molecules, with implications for ligand binding.

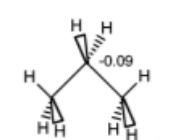


Shirts MR\*, Mobley DL\*, Chodera JD, and Pande VS

## Accurate and efficient corrections for missing dispersion interactions in molecular simulations

*Journal of Physical Chemistry B* 111:13052, 2007 · [DOI](#)

We identify a major source of systematic error in absolute alchemical free energy calculations of ligand binding and show how a simple procedure can inexpensively and accurately eliminate it.

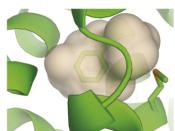


Mobley DL, Dumont E, Chodera JD, Bayly CI, Cooper MD, and Dill KA

## Comparison of charge models for fixed-charge force fields: Small-molecule hydration free energies in explicit solvent

*Journal of Physical Chem B* 111:2242, 2007 · [DOI](#)

We compare a number of popular methods for deriving charge models for small molecules, deriving lessons about best practices for accurate simulations.

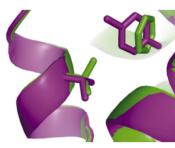


Mobley DL, Graves AP, Chodera JD, McReynolds AC, Shoichet BK, and Dill KA

### Predicting absolute ligand binding free energies to a simple model site

Journal of Molecular Biology 371:1118, 2007 · [DOI](#)

We show how alchemical free energy calculations are capable of accurate blind prediction of small-molecule binding affinities to a simple model protein binding site.



Mobley DL, Chodera JD, and Dill KA

### Confine-and-release method: Obtaining correct binding free energies in the presence of protein conformational change

Journal of Chemical and Theoretical Computation 3:1231, 2007 · [DOI](#)

We present a general scheme for obtaining correct ligand binding affinities when protein conformational change is implicated in ligand binding.



Chodera JD\*, Singhal N\*, Swope WC, Pitera JW, Pande VS, and Dill KA

### Automatic discovery of metastable states for the construction of Markov models of macromolecular conformational dynamics

Journal of Chemical Physics 126:155101, 2007 · [DOI](#)

Proposing one of the first automated algorithms for discovering kinetically metastable states of biomolecules from molecular simulations, this paper shows how many biomolecules can possess numerous distinct long-lived conformational states even though the equilibrium populations of these states may be too small for standard structural biology techniques to detect.

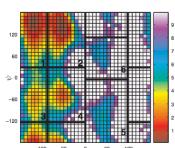


Ozkan SB, Wu GA, Chodera JD, and Dill KA

### Protein Folding by Zipping and Assembly

Proceedings of the National Academy of Sciences 104:11987, 2007 · [DOI](#)

A review of the utility of the proposed zipping and assembly mechanism for the concomitant formation of secondary and tertiary structure in protein folding for predicting folding pathways and native structures.

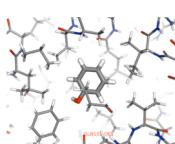


Chodera JD, W. C. Swope, J. W. Pitera, C. Seok, and K. A. Dill

### Use of the weighted histogram analysis method for the analysis of simulated and parallel tempering simulations

Journal of Chemical Theory and Computation 3:26, 2007 · [DOI](#)

The weighted histogram analysis method (WHAM), a mainstay of molecular dynamics simulation analysis, is thoroughly explained and modernized for the analysis of simulated and parallel tempering simulation data.



Mobley DL, Chodera JD, and Dill KA

### On the use of orientational restraints and symmetry corrections in alchemical free energy calculations

Journal of Chemical Physics 125:084902, 2006 · [DOI](#)

We illustrate how orientational restraints can be used to greatly reduce the computational effort in alchemical calculations of ligand binding free energies, and clarify how symmetry corrections are necessary when molecules contain symmetric or pseudosymmetric substituents.

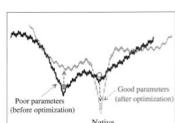


Chodera JD, Swope WC, Pitera JW, and Dill KA

### Long-time protein folding dynamics from short-time molecular dynamics simulations

Multiscale Modeling and Simulation 5:1214, 2006 · [DOI](#)

We show how the long-time dynamics of biomolecular systems can be recapitulated from statistics collected from short molecular simulations sampling transitions between kinetically metastable states.

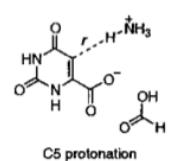


Seok C, Rosen JB, Chodera JD, Dill KA

### MOPED: Method for optimizing physical energy parameters using decoys

Journal of Computational Chemistry 24:89, 2003 · [DOI](#)

We propose a new way to optimize parameters for a physical energy function using decoy structures for protein folding studies.



Lee TS\*, Chong LT\*, Chodera JD, and Kollman PA

### An alternative explanation for the catalytic proficiency of orotidine 5'-phosphate decarboxylase

Journal of the American Chemical Society 123:12837, 2001 · [DOI](#)

A combined QM and MD analysis of potential plausible mechanisms to explain the enormous catalytic acceleration of one of the most proficient enzymes known.

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BOSTON MAY 2016	Free Energy Methods in Drug Design Workshop Vertex Pharmaceuticals, Boston, MA
CAMBRIDGE, MA MAY 2016	Markov State Models in Drug Design Workshop Novartis, Cambridge, MA
BERLIN SEP 2015	World Molecular Kinetics Workshop 2015 Freie Universität Berlin, Germany
BOSTON MAY 2014	Free Energy Methods in Drug Design Workshop Vertex Pharmaceuticals, Boston, MA
BERLIN SEP 2013	World Molecular Kinetics Workshop 2013 Freie Universität Berlin, Germany
CAMBRIDGE, MA MAY 2012	Free Energy Methods in Drug Design Workshop Vertex Pharmaceuticals, Cambridge, MA
BERLIN SEP 2011	World Molecular Kinetics Workshop 2011 Freie Universität Berlin, Germany
CAMBRIDGE, MA MAY 2010	Free Energy Methods in Drug Design Workshop Vertex Pharmaceuticals, Cambridge, MA
BERLIN MAY 2009	World Molecular Kinetics Workshop 2009 Freie Universität Berlin, Germany

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