# John D Chodera

List of Publications by Year
in descending order



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|---|---|---|---|
| 111 papers | 17,051 citations | 41627 51 h-index | 29333 108 g-index |
| 172 all docs | 172 docs citations | 172 times ranked | 18886 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | INK4 Tumor Suppressor Proteins Mediate Resistance to CDK4/6 Kinase Inhibitors. Cancer Discovery, 2022, 12, 356-371. | 7.7 | 68 |
| 2 | Bayesian-Inference-Driven Model Parametrization and Model Selection for 2CLJQ Fluid Models. Journal of Chemical Information and Modeling, 2022, , . | 2.5 | 6 |
| 3 | GCN2 kinase activation by ATP-competitive kinase inhibitors. Nature Chemical Biology, 2022, 18, 207-215. | 3.9 | 19 |
| 4 | CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295. | 13.8 | 22 |
| 5 | SAMPL7 protein-ligand challenge: A community-wide evaluation of computational methods against fragment screening and pose-prediction. Journal of Computer-Aided Molecular Design, 2022, 36, 291-311. | 1.3 | 10 |
| 6 | Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties. Journal of Chemical Theory and Computation, 2022, 18, 3577-3592. | 2.3 | 9 |
| 7 | Open Force Field Evaluator: An Automated, Efficient, and Scalable Framework for the Estimation of Physical Properties from Molecular Simulation. Journal of Chemical Theory and Computation, 2022, 18, 3566-3576. | 2.3 | 19 |
| 8 | Fitting quantum machine learning potentials to experimental free energy data: predicting tautomer ratios in solution. Chemical Science, 2021, 12, 11364-11381. | 3.7 | 15 |
| 9 | Discovery of SARS-CoV-2 main protease inhibitors using a synthesis-directed de novo design model. Chemical Communications, 2021, 57, 5909-5912. | 2.2 | 30 |
| 10 | Overview of the SAMPL6 pKa challenge: evaluating small molecule microscopic and macroscopic pKa predictions. Journal of Computer-Aided Molecular Design, 2021, 35, 131-166. | 1.3 | 23 |
| 11 | Circulating SARS-CoV-2 spike N439K variants maintain fitness while evading antibody-mediated immunity. Cell, 2021, 184, 1171-1187.e20. | 13.5 | 541 |
| 12 | What Markov State Models Can and Cannot Do: Correlation versus Path-Based Observables in Protein-Folding Models. Journal of Chemical Theory and Computation, 2021, 17, 3119-3133. | 2.3 | 32 |
| 13 | SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. Nature Chemistry, 2021, 13, 651-659. | 6.6 | 190 |
| 14 | A white-knuckle ride of open COVID drug discovery. Nature, 2021, 594, 330-332. | 13.7 | 25 |
| 15 | SARS-CoV-2 RBD antibodies that maximize breadth and resistance to escape. Nature, 2021, 597, 97-102. | 13.7 | 385 |
| 16 | Development and Benchmarking of Open Force Field v1.0.0â€”the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280. | 2.3 | 80 |
| 17 | Automated high throughput pKa and distribution coefficient measurements of pharmaceutical compounds for the SAMPL8 blind prediction challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 1141-1155. | 1.3 | 6 |
| 18 | Mutation in Abl kinase with altered drug-binding kinetics indicates a novel mechanism of imatinib resistance. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 3.3 | 30 |

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|---|---|---|---|
| 19 | Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801. | 1.2 | 15 |
| 20 | Octanolâ€“water partition coefficient measurements for the SAMPL6 blind prediction challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 405-420. | 1.3 | 40 |
| 21 | Is Structure-Based Drug Design Ready for Selectivity Optimization?. Journal of Chemical Information and Modeling, 2020, 60, 6211-6227. | 2.5 | 25 |
| 22 | Crowdsourcing drug discovery for pandemics. Nature Chemistry, 2020, 12, 581-581. | 6.6 | 88 |
| 23 | Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. Journal of Chemical Theory and Computation, 2020, 16, 4757-4775. | 2.3 | 120 |
| 24 | Assessing the accuracy of octanolâ€“water partition coefficient predictions in the SAMPL6 Part II logÂP Challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 335-370. | 1.3 | 44 |
| 25 | Standard state free energies, not pKas, are ideal for describing small molecule protonation and tautomeric states. Journal of Computer-Aided Molecular Design, 2020, 34, 561-573. | 1.3 | 20 |
| 26 | The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633. | 1.3 | 86 |
| 27 | Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, . | 2.2 | 125 |
| 28 | Binding Thermodynamics of Hostâ€“Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. Journal of Chemical Theory and Computation, 2019, 15, 6225-6242. | 2.3 | 21 |
| 29 | Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099. | 2.5 | 26 |
| 30 | A Small-Molecule Pan-Id Antagonist Inhibits Pathologic Ocular Neovascularization. Cell Reports, 2019, 29, 62-75.e7. | 2.9 | 30 |
| 31 | Small-molecule targeting of MUSASHI RNA-binding activity in acute myeloid leukemia. Nature Communications, 2019, 10, 2691. | 5.8 | 93 |
| 32 | What Makes a Kinase Promiscuous for Inhibitors?. Cell Chemical Biology, 2019, 26, 390-399.e5. | 2.5 | 59 |
| 33 | OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes. Journal of Chemical Theory and Computation, 2019, 15, 837-856. | 2.3 | 34 |
| 34 | OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. Journal of Chemical Theory and Computation, 2019, 15, 813-836. | 2.3 | 45 |
| 35 | Toward Learned Chemical Perception of Force Field Typing Rules. Journal of Chemical Theory and Computation, 2019, 15, 402-423. | 2.3 | 30 |
| 36 | Ancestral reconstruction reveals mechanisms of ERK regulatory evolution. ELife, 2019, 8, . | 2.8 | 24 |

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|---|---|---|---|
| 37 | The dynamic conformational landscape of the protein methyltransferase SETD8. ELife, 2019, 8, . | 2.8 | 38 |
| 38 | Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 2, . | 2.2 | 3 |
| 39 | Binding Modes of Ligands Using Enhanced Sampling (BLUES): Rapid Decorrelation of Ligand Binding Modes via Nonequilibrium Candidate Monte Carlo. Journal of Physical Chemistry B, 2018, 122, 5579-5598. | 1.2 | 53 |
| 40 | Biomolecular Simulations under Realistic Macroscopic Salt Conditions. Journal of Physical Chemistry B, 2018, 122, 5466-5486. | 1.2 | 63 |
| 41 | Quantitative self-assembly prediction yields targeted nanomedicines. Nature Materials, 2018, 17, 361-368. | 13.3 | 141 |
| 42 | Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278. | 0.2 | 318 |
| 43 | Quantifying Configuration-Sampling Error in Langevin Simulations of Complex Molecular Systems. Entropy, 2018, 20, 318. | 1.1 | 29 |
| 44 | pKaÂmeasurements for the SAMPL6 prediction challenge for a set of kinase inhibitor-like fragments. Journal of Computer-Aided Molecular Design, 2018, 32, 1117-1138. | 1.3 | 39 |
| 45 | Overview of the SAMPL6 hostâ€“guest binding affinity prediction challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 937-963. | 1.3 | 106 |
| 46 | Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. PLoS ONE, 2018, 13, e0203224. | 1.1 | 24 |
| 47 | Escaping Atom Types in Force Fields Using Direct Chemical Perception. Journal of Chemical Theory and Computation, 2018, 14, 6076-6092. | 2.3 | 110 |
| 48 | A dynamic mechanism for allosteric activation of Aurora kinase A by activation loop phosphorylation. ELife, 2018, 7, . | 2.8 | 62 |
| 49 | Acquired resistance to IDH inhibition through trans or cis dimer-interface mutations. Nature, 2018, 559, 125-129. | 13.7 | 223 |
| 50 | Predicting resistance of clinical Abl mutations to targeted kinase inhibitors using alchemical free-energy calculations. Communications Biology, 2018, 1, 70. | 2.0 | 66 |
| 51 | An Open Library of Human Kinase Domain Constructs for Automated Bacterial Expression. Biochemistry, 2018, 57, 4675-4689. | 1.2 | 37 |
| 52 | A water-mediated allosteric network governs activation of Aurora kinase A. Nature Chemical Biology, 2017, 13, 402-408. | 3.9 | 53 |
| 53 | L-2-Hydroxyglutarate production arises from noncanonical enzyme function at acidic pH. Nature Chemical Biology, 2017, 13, 494-500. | 3.9 | 190 |
| 54 | Approaches for Calculating Solvation Free Energies and Enthalpies Demonstrated with an Update of the FreeSolv Database. Journal of Chemical & Engineering Data, 2017, 62, 1559-1569. | 1.0 | 164 |

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| 55 | OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659. | 1.5 | 1,561 |
| 56 | Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 945-958. | 1.3 | 41 |
| 57 | Simulating mTOR Hyperactivating Mutations to Understand Functionally Significant Structural Rearrangements. Biophysical Journal, 2016, 110, 207a. | 0.2 | 0 |
| 58 | A Simple Method for Automated Equilibration Detection in Molecular Simulations. Journal of Chemical Theory and Computation, 2016, 12, 1799-1805. | 2.3 | 133 |
| 59 | Mechanistically distinct cancer-associated mTOR activation clusters predict sensitivity to rapamycin. Journal of Clinical Investigation, 2016, 126, 3526-3540. | 3.9 | 82 |
| 60 | Ensembler: Enabling High-Throughput Molecular Simulations at the Superfamily Scale. PLoS Computational Biology, 2016, 12, e1004728. | 1.5 | 20 |
| 61 | Modeling error in experimental assays using the bootstrap principle: understanding discrepancies between assays using different dispensing technologies. Journal of Computer-Aided Molecular Design, 2015, 29, 1073-1086. | 1.3 | 12 |
| 62 | Introduction to the special issue: Data Part 2: Experimental Data. Journal of Computer-Aided Molecular Design, 2015, 29, 777-777. | 1.3 | 0 |
| 63 | Hypoxia Induces Production of L-2-Hydroxyglutarate. Cell Metabolism, 2015, 22, 304-311. | 7.2 | 374 |
| 64 | Toward Automated Benchmarking of Atomistic Force Fields: Neat Liquid Densities and Static Dielectric Constants from the ThermoML Data Archive. Journal of Physical Chemistry B, 2015, 119, 12912-12920. | 1.2 | 30 |
| 65 | Spectral Rate Theory for Two-State Kinetics. Physical Review X, 2014, 4, . | 2.8 | 16 |
| 66 | Time Step Rescaling Recovers Continuous-Time Dynamical Properties for Discrete-Time Langevin Integration of Nonequilibrium Systems. Journal of Physical Chemistry B, 2014, 118, 6466-6474. | 1.2 | 56 |
| 67 | Systematic Improvement on the Classical Molecular Model of Water. Biophysical Journal, 2014, 106, 403a. | 0.2 | 0 |
| 68 | Markov state models of biomolecular conformational dynamics. Current Opinion in Structural Biology, 2014, 25, 135-144. | 2.6 | 628 |
| 69 | Estimation and Validation of Markov Models. Advances in Experimental Medicine and Biology, 2014, 797, 45-60. | 0.8 | 3 |
| 70 | Uncertainty Estimation. Advances in Experimental Medicine and Biology, 2014, 797, 61-74. | 0.8 | 1 |
| 71 | Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972. | 1.2 | 279 |
| 72 | Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics. Journal of Computer-Aided Molecular Design, 2013, 27, 989-1007. | 1.3 | 100 |

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| 73 | OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 461-469. | 2.3 | 583 |
| 74 | Entropy-Enthalpy Compensation: Role and Ramifications in Biomolecular Ligand Recognition and Design. Annual Review of Biophysics, 2013, 42, 121-142. | 4.5 | 416 |
| 75 | Using Nonequilibrium Fluctuation Theorems to Understand and Correct Errors in Equilibrium and Nonequilibrium Simulations of Discrete Langevin Dynamics. Physical Review X, 2013, 3, . | 2.8 | 43 |
| 76 | The molten globule state is unusually deformable under mechanical force. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 3796-3801. | 3.3 | 81 |
| 77 | On the Use of Experimental Observations to Bias Simulated Ensembles. Journal of Chemical Theory and Computation, 2012, 8, 3445-3451. | 2.3 | 222 |
| 78 | Limitations of Constant-Force-Feedback Experiments. Biophysical Journal, 2012, 103, 1490-1499. | 0.2 | 42 |
| 79 | Splitting Probabilities as a Test of Reaction Coordinate Choice in Single-Molecule Experiments. Physical Review Letters, 2011, 107, 098102. | 2.9 | 46 |
| 80 | The Ribosome Modulates Nascent Protein Folding. Science, 2011, 334, 1723-1727. | 6.0 | 268 |
| 81 | Optimal use of data in parallel tempering simulations for the construction of discrete-state Markov models of biomolecular dynamics. Journal of Chemical Physics, 2011, 134, 244108. | 1.2 | 46 |
| 82 | Alchemical free energy methods for drug discovery: progress and challenges. Current Opinion in Structural Biology, 2011, 21, 150-160. | 2.6 | 468 |
| 83 | Replica exchange and expanded ensemble simulations as Gibbs sampling: Simple improvements for enhanced mixing. Journal of Chemical Physics, 2011, 135, 194110. | 1.2 | 137 |
| 84 | Systematic errors in isothermal titration calorimetry: Concentrations and baselines. Analytical Biochemistry, 2011, 414, 297-299. | 1.1 | 64 |
| 85 | 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, 2011, 134, 024111. | 1.2 | 15 |
| 86 | Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, E1009-18. | 3.3 | 91 |
| 87 | Dynamical fingerprints for probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4822-4827. | 3.3 | 105 |
| 88 | The social network (of protein conformations). Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 12969-12970. | 3.3 | 11 |
| 89 | Dynamical reweighting: Improved estimates of dynamical properties from simulations at multiple temperatures. Journal of Chemical Physics, 2011, 134, 244107. | 1.2 | 55 |
| 90 | Markov models of molecular kinetics: Generation and validation. Journal of Chemical Physics, 2011, 134, 174105. | 1.2 | 968 |

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| 91 | Probability distributions of molecular observables computed from Markov models. II. Uncertainties in observables and their time-evolution. Journal of Chemical Physics, 2010, 133, 105102. | 1.2 | 38 |
| 92 | The Mechanical Properties of PCNA: Implications for the Loading and Function of a DNA Sliding Clamp. Biophysical Journal, 2010, 98, 3062-3069. | 0.2 | 19 |
| 93 | Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564. | 1.2 | 1,093 |
| 94 | The Mechanical Properties of PCNA: Implications for the Loading and Function of Sliding Clamps. Biophysical Journal, 2010, 98, 630a. | 0.2 | 0 |
| 95 | Optimal estimators and asymptotic variances for nonequilibrium path-ensemble averages. Journal of Chemical Physics, 2009, 131, 134110. | 1.2 | 48 |
| 96 | Bayesian comparison of Markov models of molecular dynamics with detailed balance constraint. Journal of Chemical Physics, 2009, 131, 045106. | 1.2 | 52 |
| 97 | Statistically optimal analysis of samples from multiple equilibrium states. Journal of Chemical Physics, 2008, 129, 124105. | 1.2 | 1,328 |
| 98 | Predicting Small-Molecule Solvation Free Energies: An Informal Blind Test for Computational Chemistry. Journal of Medicinal Chemistry, 2008, 51, 769-779. | 2.9 | 248 |
| 99 | Treating Entropy and Conformational Changes in Implicit Solvent Simulations of Small Molecules. Journal of Physical Chemistry B, 2008, 112, 938-946. | 1.2 | 106 |
| 100 | Protein folding by zipping and assembly. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 11987-11992. | 3.3 | 141 |
| 101 | Predicting Absolute Ligand Binding Free Energies to a Simple Model Site. Journal of Molecular Biology, 2007, 371, 1118-1134. | 2.0 | 269 |
| 102 | Automatic discovery of metastable states for the construction of Markov models of macromolecular conformational dynamics. Journal of Chemical Physics, 2007, 126, 155101. | 1.2 | 567 |
| 103 | Comparison of Charge Models for Fixed-Charge Force Fields:Â Small-Molecule Hydration Free Energies in Explicit Solvent. Journal of Physical Chemistry B, 2007, 111, 2242-2254. | 1.2 | 245 |
| 104 | Chapter 4 Alchemical Free Energy Calculations: Ready for Prime Time?. Annual Reports in Computational Chemistry, 2007, 3, 41-59. | 0.9 | 175 |
| 105 | Use of the Weighted Histogram Analysis Method for the Analysis of Simulated and Parallel Tempering Simulations. Journal of Chemical Theory and Computation, 2007, 3, 26-41. | 2.3 | 416 |
| 106 | Accurate and Efficient Corrections for Missing Dispersion Interactions in Molecular Simulations. Journal of Physical Chemistry B, 2007, 111, 13052-13063. | 1.2 | 181 |
| 107 | Confine-and-Release Method:â€‰ Obtaining Correct Binding Free Energies in the Presence of Protein Conformational Change. Journal of Chemical Theory and Computation, 2007, 3, 1231-1235. | 2.3 | 168 |
| 108 | Longâ€Time Protein Folding Dynamics from Shortâ€Time Molecular Dynamics Simulations. Multiscale Modeling and Simulation, 2006, 5, 1214-1226. | 0.6 | 204 |

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| 109 | On the use of orientational restraints and symmetry corrections in alchemical free energy calculations. Journal of Chemical Physics, 2006, 125, 084902. | 1.2 | 253 |
| 110 | MOPED: Method for optimizing physical energy parameters using decoys. Journal of Computational Chemistry, 2003, 24, 89-97. | 1.5 | 18 |
| 111 | An Alternative Explanation for the Catalytic Proficiency of Orotidine 5â€˜-Phosphate Decarboxylase. Journal of the American Chemical Society, 2001, 123, 12837-12848. | 6.6 | 41 |