

David L Mobley

List of Publications by Year in descending order

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137
papers

11,333
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25047

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docs citations

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times ranked

10001
citing authors

#	ARTICLE	IF	CITATIONS
1	The Need for Continuing Blinded Pose- and Activity Prediction Benchmarks. <i>Journal of Chemical Information and Modeling</i> , 2025, 65, 2180-2190.	4.9	0
2	IMERGE-FEP: Improving Relative Free Energy Calculation Convergence with Chemical Intermediates. <i>Journal of Physical Chemistry B</i> , 2025, 129, 2370-2379.	2.9	0
3	A Fast, Convenient, Polarizable Electrostatic Model for Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2024, 20, 1293-1305.	5.5	2
4	The SAMPL9 host-guest blind challenge: an overview of binding free energy predictive accuracy. <i>Physical Chemistry Chemical Physics</i> , 2024, 26, 9207-9225.	2.8	5
5	Impact of protein conformations on binding free energy calculations in the beta-secretase 1 system. <i>Journal of Computational Chemistry</i> , 2024, 45, 2024-2033.	4.9	2
6	Building Block-Centric Approach to DNA-Encoded Library Design. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 4661-4672.	4.9	1
7	Machine-learned molecular mechanics force fields from large-scale quantum chemical data. <i>Chemical Science</i> , 2024, 15, 12861-12878.	7.5	7
8	Current State of Open Source Force Fields in Protein-Ligand Binding Affinity Predictions. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 5063-5076.	4.9	10
9	The Open Force Field Initiative: Open Software and Open Science for Molecular Modeling. <i>Journal of Physical Chemistry B</i> , 2024, 128, 7043-7067.	2.9	5
10	Benchmarking Quantum Mechanical Levels of Theory for Valence Parametrization in Force Fields. <i>Journal of Physical Chemistry B</i> , 2024, 128, 7888-7902.	2.9	1
11	Konnektor: A Framework for Using Graph Theory to Plan Networks for Free Energy Calculations. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 8396-8403.	4.9	0
12	Kinetics-Based State Definitions for Discrete Binding Conformations of T4 L99A in MD via Markov State Modeling. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 8870-8879.	4.9	0
13	Leveraging a Separation of States Method for Relative Binding Free Energy Calculations in Systems with Trapped Waters. <i>Journal of Chemical Theory and Computation</i> , 2024, 20, 11013-11031.	5.5	1
14	Molecular-dynamics simulation methods for macromolecular crystallography. <i>Acta Crystallographica Section D: Structural Biology</i> , 2023, 79, 50-65.	3.4	12
15	Enhanced Grand Canonical Sampling of Occluded Water Sites Using Nonequilibrium Candidate Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1050-1062.	5.5	14
16	To Design Scalable Free Energy Perturbation Networks, Optimal Is Not Enough. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1776-1793.	4.9	11
17	Development and Benchmarking of Open Force Field 2.0.0: The Sage Small Molecule Force Field. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 3251-3275.	5.5	67
18	A transferable double exponential potential for condensed phase simulations of small molecules. <i>Digital Discovery</i> , 2023, 2, 1178-1187.	5.5	8

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19	Broadening the Scope of Binding Free Energy Calculations Using a Separated Topologies Approach. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 5058-5076.	5.5	17
20	Building Block-Based Binding Predictions for DNA-Encoded Libraries. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 5120-5132.	4.9	7
21	Enhancing Sampling of Water Rehydration on Ligand Binding: A Comparison of Techniques. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1359-1381.	5.5	29
22	Pre-Exascale Computing of Protein-Ligand Binding Free Energies with Open Source Software for Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1172-1177.	4.9	35
23	SAMPL7 protein-ligand challenge: A community-wide evaluation of computational methods against fragment screening and pose-prediction. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 291-311.	3.1	12
24	Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3577-3592.	5.5	12
25	Open Force Field Evaluator: An Automated, Efficient, and Scalable Framework for the Estimation of Physical Properties from Molecular Simulation. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3566-3576.	5.5	25
26	Best Practices for Constructing, Preparing, and Evaluating Protein-Ligand Binding Affinity Benchmarks [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2022, 4, .	10.9	41
27	Absolute Binding Free Energy Calculations for Buried Water Molecules. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6482-6499.	5.5	4
28	An overview of the SAMPL8 host-guest binding challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 707-734.	3.1	34
29	Reversibly Sampling Conformations and Binding Modes Using Molecular Darting. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 302-314.	5.5	3
30	Structural and Molecular Dynamics of <i>Mycobacterium tuberculosis</i> Malic Enzyme, a Potential Anti-TB Drug Target. <i>ACS Infectious Diseases</i> , 2021, 7, 174-188.	3.8	5
31	Improving small molecule force fields by identifying and characterizing small molecules with inconsistent parameters. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 271-284.	3.1	15
32	Overview of the SAMPL6 pKa challenge: evaluating small molecule microscopic and macroscopic pKa predictions. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 131-166.	3.1	32
33	A Benchmark of Electrostatic Method Performance in Relative Binding Free Energy Calculations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1048-1052.	4.9	12
34	Challenges Encountered Applying Equilibrium and Nonequilibrium Binding Free Energy Calculations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4241-4261.	2.9	37
35	Evaluation of log $\hat{A}P$, pKa, and log $\hat{A}D$ predictions from the SAMPL7 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 771-802.	3.1	56
36	Development and Benchmarking of Open Force Field v1.0.0—the Parsley Small-Molecule Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6262-6280.	5.5	98

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37	Temperature artifacts in protein structures bias ligand-binding predictions. <i>Chemical Science</i> , 2021, 12, 11275-11293.	7.5	25
38	SAMPL7 Host-Guest Challenge Overview: assessing the reliability of polarizable and non-polarizable methods for binding free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 1-35.	3.1	55
39	Automated high throughput pKa and distribution coefficient measurements of pharmaceutical compounds for the SAMPL8 blind prediction challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 1141-1155.	3.1	11
40	Enhancing Paraoxon Binding to Organophosphorus Hydrolase Active Site. <i>International Journal of Molecular Sciences</i> , 2021, 22, 12624.	4.5	6
41	Optimal designs for pairwise calculation: An application to free energy perturbation in minimizing prediction variability. <i>Journal of Computational Chemistry</i> , 2020, 41, 247-257.	4.9	29
42	Kinetics and free energy of ligand dissociation using weighted ensemble milestoning. <i>Journal of Chemical Physics</i> , 2020, 153, .	3.0	10
43	Insights on small molecule binding to the Hv1 proton channel from free energy calculations with molecular dynamics simulations. <i>Scientific Reports</i> , 2020, 10, .	3.7	10
44	Fragment Pose Prediction Using Non-equilibrium Candidate Monte Carlo and Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2778-2794.	5.5	9
45	Assessing the accuracy of octanol-water partition coefficient predictions in the SAMPL6 Part II log \hat{P} Challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 335-370.	3.1	45
46	Sampling Conformational Changes of Bound Ligands Using Nonequilibrium Candidate Monte Carlo and Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1854-1865.	5.5	19
47	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 601-633.	3.1	91
48	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). <i>Communications Chemistry</i> , 2020, 3, .	5.8	163
49	Enhancing water sampling of buried binding sites using nonequilibrium candidate Monte Carlo. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 35, 167-177.	3.1	21
50	An optimized chemical-genetic method for cell-specific metabolic labeling of RNA. <i>Nature Methods</i> , 2020, 17, 311-318.	14.5	45
51	Benchmark assessment of molecular geometries and energies from small molecule force fields. <i>F1000Research</i> , 2020, 9, 1390.	0.6	33
52	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2020, 2, .	10.9	158
53	Binding Thermodynamics of Host-Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6225-6242.	5.5	24
54	Comparison of affinity ranking using AutoDock-GPU and MM-GBSA scores for BACE-1 inhibitors in the D3R Grand Challenge 4. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 1011-1020.	3.1	55

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55	Structure of a <i>Mycobacterium tuberculosis</i> Heme-Degrading Protein, MhuD, Variant in Complex with Its Product. <i>Biochemistry</i> , 2019, 58, 4610-4620.	2.9	5
56	Enhancing Side Chain Rotamer Sampling Using Nonequilibrium Candidate Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1848-1862.	5.5	23
57	Binding Modes and Metabolism of Caffeine. <i>Chemical Research in Toxicology</i> , 2019, 32, 1374-1383.	3.9	20
58	Biomolecular Solvation Structure Revealed by Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2019, 141, 4711-4720.	15.7	30
59	Infinite Dilution Activity Coefficients as Constraints for Force Field Parametrization and Method Development. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3066-3074.	5.5	14
60	Assessing the Conformational Equilibrium of Carboxylic Acid via Quantum Mechanical and Molecular Dynamics Studies on Acetic Acid. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1957-1964.	4.9	16
61	Liquid-like and rigid-body motions in molecular-dynamics simulations of a crystalline protein. <i>Structural Dynamics</i> , 2019, 6, .	2.3	12
62	Toward Learned Chemical Perception of Force Field Typing Rules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 402-423.	5.5	30
63	Octanol-water partition coefficient measurements for the SAMPL6 blind prediction challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 34, 405-420.	3.1	42
64	D3R Grand Challenge 4: ligand similarity and MM-GBSA-based pose prediction and affinity ranking for BACE-1 inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 34, 163-177.	3.1	13
65	Challenges in the use of atomistic simulations to predict solubilities of drug-like molecules. <i>F1000Research</i> , 2019, 7, 686.	0.6	6
66	Why We Need the Living Journal of Computational Molecular Science. <i>Living Journal of Computational Molecular Science</i> , 2019, 1, .	10.9	2
67	Best Practices for Foundations in Molecular Simulations [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019, 1, .	10.9	130
68	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019, 2, .	10.9	4
69	Binding Modes of Ligands Using Enhanced Sampling (BLUES): Rapid Decorrelation of Ligand Binding Modes via Nonequilibrium Candidate Monte Carlo. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5579-5598.	2.9	56
70	Atomic Radius and Charge Parameter Uncertainty in Biomolecular Solvation Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 759-767.	5.5	14
71	Refining Protein Penetration into the Lipid Bilayer Using Fluorescence Quenching and Molecular Dynamics Simulations: The Case of Diphtheria Toxin Translocation Domain. <i>Journal of Membrane Biology</i> , 2018, 251, 379-391.	2.6	17
72	pKa measurements for the SAMPL6 prediction challenge for a set of kinase inhibitor-like fragments. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1117-1138.	3.1	39

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73	Overview of the SAMPL6 host-guest binding affinity prediction challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 937-963.	3.1	113
74	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5567-5582.	5.5	69
75	Escaping Atom Types in Force Fields Using Direct Chemical Perception. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6076-6092.	5.5	116
76	SAMPL6 challenge results from ΔG_{bind} predictions based on a general Gaussian process model. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1165-1177.	3.1	20
77	Hydration Free Energies in the FreeSolv Database Calculated with Polarized Iterative Hirshfeld Charges. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1779-1797.	4.9	37
78	Challenges in the use of atomistic simulations to predict solubilities of drug-like molecules. <i>Frontiers in Molecular Sciences</i> , 2018, 7, 686.	0.6	6
79	Predicting Binding Free Energies: Frontiers and Benchmarks. <i>Annual Review of Biophysics</i> , 2017, 46, 531-558.	13.3	274
80	Approaches for Calculating Solvation Free Energies and Enthalpies Demonstrated with an Update of the FreeSolv Database. <i>Journal of Chemical & Engineering Data</i> , 2017, 62, 1559-1569.	2.2	182
81	Bayesian Model Averaging for Ensemble-Based Estimates of Solvation-Free Energies. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3458-3472.	2.9	7
82	Collaborative routes to clarifying the murky waters of aqueous supramolecular chemistry. <i>Nature Chemistry</i> , 2017, 10, 8-16.	13.9	149
83	A Critical Review of Validation, Blind Testing, and Real-World Use of Alchemical Protein-Ligand Binding Free Energy Calculations. <i>Current Topics in Medicinal Chemistry</i> , 2017, 17, 2577-2585.	2.7	85
84	Blind prediction of cyclohexane-water distribution coefficients from the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 927-944.	3.1	93
85	Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 945-958.	3.1	39
86	Sensitivity in Binding Free Energies Due to Protein Reorganization. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4620-4631.	5.5	64
87	Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4015-4024.	5.5	143
88	Multiple binding modes of ibuprofen in human serum albumin identified by absolute binding free energy calculations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32358-32368.	2.8	80
89	Using MD Simulations To Calculate How Solvents Modulate Solubility. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1930-1941.	5.5	39
90	Overview of the SAMPL5 host-guest challenge: Are we doing better?. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 31, 1-19.	3.1	138

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91	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 31, 147-161.	3.1	214
92	Predicting the excess solubility of acetanilide, acetaminophen, phenacetin, benzocaine, and caffeine in binary water/ethanol mixtures via molecular simulation. <i>Journal of Chemical Physics</i> , 2015, 142, .	3.0	38
93	Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. <i>Journal of the American Chemical Society</i> , 2015, 137, 2695-2703.	15.7	937
94	Is Ring Breaking Feasible in Relative Binding Free Energy Calculations?. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 727-735.	4.9	40
95	Guidelines for the analysis of free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 397-411.	3.1	386
96	A Python tool to set up relative free energy calculations in GROMACS. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 1007-1014.	3.1	34
97	Interrogating HIV integrase for compounds that bind- a SAMPL challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 347-362.	3.1	24
98	Box size effects are negligible for solvation free energies of neutral solutes. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 825-829.	3.1	19
99	Blind prediction of solvation free energies from the SAMPL4 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 135-150.	3.1	127
100	Blind prediction of HIV integrase binding from the SAMPL4 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 327-345.	3.1	48
101	The SAMPL4 host-guest blind prediction challenge: an overview. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 305-317.	3.1	155
102	FreeSolv: a database of experimental and calculated hydration free energies, with input files. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 711-720.	3.1	326
103	A Fixed-Charge Model for Alcohol Polarization in the Condensed Phase, and Its Role in Small Molecule Hydration. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6438-6446.	2.9	55
104	Blind Prediction of Charged Ligand Binding Affinities in a Model Binding Site. <i>Journal of Molecular Biology</i> , 2013, 425, 4569-4583.	4.2	51
105	Lead optimization mapper: automating free energy calculations for lead optimization. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 755-770.	3.1	116
106	Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects. <i>Journal of Chemical Physics</i> , 2013, 139, .	3.0	190
107	Separated topologies—a method for relative binding free energy calculations using orientational restraints. <i>Journal of Chemical Physics</i> , 2013, 138, .	3.0	30
108	Entropy-Enthalpy Compensation: Role and Ramifications in Biomolecular Ligand Recognition and Design. <i>Annual Review of Biophysics</i> , 2013, 42, 121-142.	13.3	412

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109	An Introduction to Best Practices in Free Energy Calculations. <i>Methods in Molecular Biology</i> , 2013, , 271-311.	0.0	79
110	3-Aryl-3-arylmethoxyazetidines. A new class of high affinity ligands for monoamine transporters. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 4404-4407.	2.1	7
111	Triazoleâ€“Dithiocarbamate Based Selective Lysine Specific Demethylase 1 (LSD1) Inactivators Inhibit Gastric Cancer Cell Growth, Invasion, and Migration. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 8543-8560.	6.9	199
112	Calculating the Sensitivity and Robustness of Binding Free Energy Calculations to Force Field Parameters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3072-3083.	5.5	27
113	Perspective: Alchemical free energy calculations for drug discovery. <i>Journal of Chemical Physics</i> , 2012, 137, .	3.0	183
114	Small Molecule Solvation Free Energy: Enhanced Conformational Sampling Using Expanded Ensemble Molecular Dynamics Simulation. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2910-2918.	5.5	40
115	Alchemical free energy methods for drug discovery: progress and challenges. <i>Current Opinion in Structural Biology</i> , 2011, 21, 150-160.	7.1	471
116	Alchemical prediction of hydration free energies for SAMPL. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 26, 551-562.	3.1	67
117	Predicting hydration free energies using all-atom molecular dynamics simulations and multiple starting conformations. <i>Journal of Computer-Aided Molecular Design</i> , 2010, 24, 307-316.	3.1	97
118	Synthesis and structureâ€“activity studies of benzyl ester meperidine and normeperidine derivatives as selective serotonin transporter ligands. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 8356-8364.	2.7	2
119	Free-energy calculations in structure-based drug design. , 2010, , 61-86.		64
120	Synthesis and monoamine transporter affinity of 3Î±-arylmethoxy-3Î²-arylnortropanes. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 6865-6868.	2.1	5
121	Quantifying Correlations Between Allosteric Sites in Thermodynamic Ensembles. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2486-2502.	5.5	187
122	Predictions of Hydration Free Energies from All-Atom Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4533-4537.	2.9	79
123	Predicting Ligand Binding Affinity with Alchemical Free Energy Methods in a Polar Model Binding Site. <i>Journal of Molecular Biology</i> , 2009, 394, 747-763.	4.2	150
124	Binding of Small-Molecule Ligands to Proteins: â€œWhat You Seeâ€“Is Not Always â€œWhat You Getâ€“. <i>Structure</i> , 2009, 17, 489-498.	3.9	470
125	Small Molecule Hydration Free Energies in Explicit Solvent: An Extensive Test of Fixed-Charge Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 350-358.	5.5	298
126	Predicting Small-Molecule Solvation Free Energies: An Informal Blind Test for Computational Chemistry. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 769-779.	6.9	240

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127	Treating Entropy and Conformational Changes in Implicit Solvent Simulations of Small Molecules. <i>Journal of Physical Chemistry B</i> , 2008, 112, 938-946.	2.9	104
128	Charge Asymmetries in Hydration of Polar Solutes. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2405-2414.	2.9	93
129	Nonlinear scaling schemes for Lennard-Jones interactions in free energy calculations. <i>Journal of Chemical Physics</i> , 2007, 127, .	3.0	259
130	Predicting Absolute Ligand Binding Free Energies to a Simple Model Site. <i>Journal of Molecular Biology</i> , 2007, 371, 1118-1134.	4.2	255
131	A Mathematical Model of Glioblastoma Tumor Spheroid Invasion in a Three-Dimensional In Vitro Experiment. <i>Biophysical Journal</i> , 2007, 92, 356-365.	0.4	197
132	Comparison of Charge Models for Fixed-Charge Force Fields: A Small-Molecule Hydration Free Energies in Explicit Solvent. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2242-2254.	2.9	234
133	Chapter 4 Alchemical Free Energy Calculations: Ready for Prime Time?. <i>Annual Reports in Computational Chemistry</i> , 2007, , 41-59.	0.0	170
134	Confine-and-Release Method: Obtaining Correct Binding Free Energies in the Presence of Protein Conformational Change. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1231-1235.	5.5	160
135	On the use of orientational restraints and symmetry corrections in alchemical free energy calculations. <i>Journal of Chemical Physics</i> , 2006, 125, 084902.	3.0	250
136	Modeling Amyloid β -Peptide Insertion into Lipid Bilayers. <i>Biophysical Journal</i> , 2004, 86, 3585-3597.	0.4	47
137	Simulations of Oligomeric Intermediates in Prion Diseases. <i>Biophysical Journal</i> , 2003, 85, 2213-2223.	0.4	9