David L Mobley

List of Publications by Year
in descending order

119 papers	12,227 citations	41627 51 h-index	32181 105 g-index
186 all docs	186 docs citations	186 times ranked	10513 citing authors

#	Article	IF	Citations
1	Enhancing Sampling of Water Rehydration on Ligand Binding: A Comparison of Techniques. Journal of Chemical Theory and Computation, 2022, 18, 1359-1381.	2.3	22
2	Pre-Exascale Computing of Proteinâ€“Ligand Binding Free Energies with Open Source Software for Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1172-1177.	2.5	22
3	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
4	Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties. Journal of Chemical Theory and Computation, 2022, 18, 3577-3592.	2.3	9
5	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
6	Reversibly Sampling Conformations and Binding Modes Using Molecular Darting. Journal of Chemical Theory and Computation, 2021, 17, 302-314.	2.3	4
7	Structural and Molecular Dynamics of Mycobacterium tuberculosis Malic Enzyme, a Potential Anti-TB Drug Target. ACS Infectious Diseases, 2021, 7, 174-188.	1.8	3
8	Enhancing water sampling of buried binding sites using nonequilibrium candidate Monte Carlo. Journal of Computer-Aided Molecular Design, 2021, 35, 167-177.	1.3	22
9	Improving small molecule force fields by identifying and characterizing small molecules with inconsistent parameters. Journal of Computer-Aided Molecular Design, 2021, 35, 271-284.	1.3	12
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	A Benchmark of Electrostatic Method Performance in Relative Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 1048-1052.	2.5	12
12	Challenges Encountered Applying Equilibrium and Nonequilibrium Binding Free Energy Calculations. Journal of Physical Chemistry B, 2021, 125, 4241-4261.	1.2	33
13	Evaluation of logÂP, pKa, and logÂD predictions from the SAMPL7 blind challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 771-802.	1.3	42
14	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
15	Temperature artifacts in protein structures bias ligand-binding predictions. Chemical Science, 2021, 12, 11275-11293.	3.7	27
16	SAMPL7 Hostâ€“Guest Challenge Overview: assessing the reliability of polarizable and non-polarizable methods for binding free energy calculations. Journal of Computer-Aided Molecular Design, 2021, 35, 1-35.	1.3	45
17	Alchemical absolute proteinâ€“ligand binding free energies for drug design. Chemical Science, 2021, 12, 13958-13971.	3.7	48
18	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

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19	Enhancing Paraoxon Binding to Organophosphorus Hydrolase Active Site. International Journal of Molecular Sciences, 2021, 22, 12624.	1.8	2
20	Optimal designs for pairwise calculation: An application to free energy perturbation in minimizing prediction variability. Journal of Computational Chemistry, 2020, 41, 247-257.	1.5	26
21	Octanolâ€“water partition coefficient measurements for the SAMPL6 blind prediction challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 405-420.	1.3	40
22	D3R Grand Challenge 4: ligand similarity and MM-GBSA-based pose prediction and affinity ranking for BACE-1 inhibitors. Journal of Computer-Aided Molecular Design, 2020, 34, 163-177.	1.3	13
23	Kinetics and free energy of ligand dissociation using weighted ensemble milestoning. Journal of Chemical Physics, 2020, 153, 154117.	1.2	10
24	Insights on small molecule binding to the Hv1 proton channel from free energy calculations with molecular dynamics simulations. Scientific Reports, 2020, 10, 13587.	1.6	8
25	Fragment Pose Prediction Using Non-equilibrium Candidate Monte Carlo and Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 2778-2794.	2.3	9
26	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
27	Sampling Conformational Changes of Bound Ligands Using Nonequilibrium Candidate Monte Carlo and Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 1854-1865.	2.3	15
28	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
29	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). Communications Chemistry, 2020, 3, .	2.0	98
30	An optimized chemical-genetic method for cell-specific metabolic labeling of RNA. Nature Methods, 2020, 17, 311-318.	9.0	38
31	Benchmark assessment of molecular geometries and energies from small molecule force fields. F1000Research, 2020, 9, 1390.	0.8	30
32	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	2.2	125
33	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
34	Comparison of affinity ranking using AutoDock-GPU and MM-GBSA scores for BACE-1 inhibitors in the D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2019, 33, 1011-1020.	1.3	50
35	Structure of a Mycobacterium tuberculosis Heme-Degrading Protein, MhuD, Variant in Complex with Its Product. Biochemistry, 2019, 58, 4610-4620.	1.2	3
36	Enhancing Side Chain Rotamer Sampling Using Nonequilibrium Candidate Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 1848-1862.	2.3	18

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37	Binding Modes and Metabolism of Caffeine. Chemical Research in Toxicology, 2019, 32, 1374-1383.	1.7	18
38	Biomolecular Solvation Structure Revealed by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2019, 141, 4711-4720.	6.6	33
39	Infinite Dilution Activity Coefficients as Constraints for Force Field Parametrization and Method Development. Journal of Chemical Theory and Computation, 2019, 15, 3066-3074.	2.3	11
40	Assessing the Conformational Equilibrium of Carboxylic Acid via Quantum Mechanical and Molecular Dynamics Studies on Acetic Acid. Journal of Chemical Information and Modeling, 2019, 59, 1957-1964.	2.5	14
41	Liquid-like and rigid-body motions in molecular-dynamics simulations of a crystalline protein. Structural Dynamics, 2019, 6, 064704.	0.9	14
42	Toward Learned Chemical Perception of Force Field Typing Rules. Journal of Chemical Theory and Computation, 2019, 15, 402-423.	2.3	30
43	Why We Need the Living Journal of Computational Molecular Science. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	2
44	Best Practices for Foundations in Molecular Simulations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	105
45	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 2, .	2.2	3
46	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
47	Collaborative routes to clarifying the murky waters of aqueous supramolecular chemistry. Nature Chemistry, 2018, 10, 8-16.	6.6	143
48	Atomic Radius and Charge Parameter Uncertainty in Biomolecular Solvation Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 759-767.	2.3	13
49	Refining Protein Penetration into the Lipid Bilayer Using Fluorescence Quenching and Molecular Dynamics Simulations: The Case of Diphtheria Toxin Translocation Domain. Journal of Membrane Biology, 2018, 251, 379-391.	1.0	18
50	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
51	Overview of the SAMPL6 hostâ€“guest binding affinity prediction challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 937-963.	1.3	106
52	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. Journal of Chemical Theory and Computation, 2018, 14, 5567-5582.	2.3	66
53	Escaping Atom Types in Force Fields Using Direct Chemical Perception. Journal of Chemical Theory and Computation, 2018, 14, 6076-6092.	2.3	110
54	SAMPL6 challenge results from $$pK_a$$ predictions based on a general Gaussian process model. Journal of Computer-Aided Molecular Design, 2018, 32, 1165-1177.	1.3	20

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55	Hydration Free Energies in the FreeSolv Database Calculated with Polarized Iterative Hirshfeld Charges. Journal of Chemical Information and Modeling, 2018, 58, 1779-1797.	2.5	31
56	Challenges in the use of atomistic simulations to predict solubilities of drug-like molecules. F1000Research, 2018, 7, 686.	0.8	6
57	Challenges in the use of atomistic simulations to predict solubilities of drug-like molecules. F1000Research, 2018, 7, 686.	0.8	6
58	Predicting Binding Free Energies: Frontiers and Benchmarks. Annual Review of Biophysics, 2017, 46, 531-558.	4.5	265
59	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
60	Bayesian Model Averaging for Ensemble-Based Estimates of Solvation-Free Energies. Journal of Physical Chemistry B, 2017, 121, 3458-3472.	1.2	8
61	Overview of the SAMPL5 hostâ€“guest challenge: Are we doing better?. Journal of Computer-Aided Molecular Design, 2017, 31, 1-19.	1.3	140
62	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Journal of Computer-Aided Molecular Design, 2017, 31, 147-161.	1.3	187
63	A Critical Review of Validation, Blind Testing, and Real- World Use of Alchemical Protein-Ligand Binding Free Energy Calculations. Current Topics in Medicinal Chemistry, 2017, 17, 2577-2585.	1.0	88
64	Blind prediction of cyclohexaneâ€“water distribution coefficients from the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 927-944.	1.3	99
65	Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 945-958.	1.3	41
66	Sensitivity in Binding Free Energies Due to Protein Reorganization. Journal of Chemical Theory and Computation, 2016, 12, 4620-4631.	2.3	65
67	Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water. Journal of Chemical Theory and Computation, 2016, 12, 4015-4024.	2.3	137
68	Multiple binding modes of ibuprofen in human serum albumin identified by absolute binding free energy calculations. Physical Chemistry Chemical Physics, 2016, 18, 32358-32368.	1.3	75
69	Using MD Simulations To Calculate How Solvents Modulate Solubility. Journal of Chemical Theory and Computation, 2016, 12, 1930-1941.	2.3	34
70	Predicting the excess solubility of acetanilide, acetaminophen, phenacetin, benzocaine, and caffeine in binary water/ethanol mixtures via molecular simulation. Journal of Chemical Physics, 2015, 142, 044508.	1.2	37
71	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. Journal of the American Chemical Society, 2015, 137, 2695-2703.	6.6	931
72	Is Ring Breaking Feasible in Relative Binding Free Energy Calculations?. Journal of Chemical Information and Modeling, 2015, 55, 727-735.	2.5	42

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73	Guidelines for the analysis of free energy calculations. Journal of Computer-Aided Molecular Design, 2015, 29, 397-411.	1.3	375
74	A Python tool to set up relative free energy calculations in GROMACS. Journal of Computer-Aided Molecular Design, 2015, 29, 1007-1014.	1.3	30
75	Interrogating HIV integrase for compounds that bind- a SAMPL challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 347-362.	1.3	25
76	Box size effects are negligible for solvation free energies of neutral solutes. Journal of Computer-Aided Molecular Design, 2014, 28, 825-829.	1.3	18
77	Blind prediction of solvation free energies from the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 135-150.	1.3	131
78	Blind prediction of HIV integrase binding from the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 327-345.	1.3	53
79	The SAMPL4 hostâ€“guest blind prediction challenge: an overview. Journal of Computer-Aided Molecular Design, 2014, 28, 305-317.	1.3	162
80	FreeSolv: a database of experimental and calculated hydration free energies, with input files. Journal of Computer-Aided Molecular Design, 2014, 28, 711-720.	1.3	284
81	A Fixed-Charge Model for Alcohol Polarization in the Condensed Phase, and Its Role in Small Molecule Hydration. Journal of Physical Chemistry B, 2014, 118, 6438-6446.	1.2	54
82	Blind Prediction of Charged Ligand Binding Affinities in a Model Binding Site. Journal of Molecular Biology, 2013, 425, 4569-4583.	2.0	53
83	Lead optimization mapper: automating free energy calculations for lead optimization. Journal of Computer-Aided Molecular Design, 2013, 27, 755-770.	1.3	105
84	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. Journal of Chemical Physics, 2013, 139, 184103.	1.2	187
85	Separated topologiesâ€”A method for relative binding free energy calculations using orientational restraints. Journal of Chemical Physics, 2013, 138, 085104.	1.2	25
86	Entropy-Enthalpy Compensation: Role and Ramifications in Biomolecular Ligand Recognition and Design. Annual Review of Biophysics, 2013, 42, 121-142.	4.5	416
87	An Introduction to Best Practices in Free Energy Calculations. Methods in Molecular Biology, 2013, 924, 271-311.	0.4	84
88	3-Aryl-3-arylmethoxyazetidines. A new class of high affinity ligands for monoamine transporters. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 4404-4407.	1.0	7
89	Triazoleâ€“Dithiocarbamate Based Selective Lysine Specific Demethylase 1 (LSD1) Inactivators Inhibit Gastric Cancer Cell Growth, Invasion, and Migration. Journal of Medicinal Chemistry, 2013, 56, 8543-8560.	2.9	198
90	Calculating the Sensitivity and Robustness of Binding Free Energy Calculations to Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 3072-3083.	2.3	26

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91	Perspective: Alchemical free energy calculations for drug discovery. Journal of Chemical Physics, 2012, 137, 230901.	1.2	181
92	Alchemical prediction of hydration free energies for SAMPL. Journal of Computer-Aided Molecular Design, 2012, 26, 551-562.	1.3	67
93	Letâ€™s get honest about sampling. Journal of Computer-Aided Molecular Design, 2012, 26, 93-95.	1.3	74
94	Small Molecule Solvation Free Energy: Enhanced Conformational Sampling Using Expanded Ensemble Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2011, 7, 2910-2918.	2.3	41
95	Alchemical free energy methods for drug discovery: progress and challenges. Current Opinion in Structural Biology, 2011, 21, 150-160.	2.6	468
96	Predicting hydration free energies using all-atom molecular dynamics simulations and multiple starting conformations. Journal of Computer-Aided Molecular Design, 2010, 24, 307-316.	1.3	98
97	Synthesis and structureâ€“activity studies of benzyl ester meperidine and normeperidine derivatives as selective serotonin transporter ligands. Bioorganic and Medicinal Chemistry, 2010, 18, 8356-8364.	1.4	2
98	Free-energy calculations in structure-based drug design. , 2010, , 61-86.		65
99	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	1.2	1,093
100	Synthesis and monoamine transporter affinity of 3Î±-arylmethoxy-3Î²-arylnortropanes. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6865-6868.	1.0	5
101	Quantifying Correlations Between Allosteric Sites in Thermodynamic Ensembles. Journal of Chemical Theory and Computation, 2009, 5, 2486-2502.	2.3	203
102	Predictions of Hydration Free Energies from All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 4533-4537.	1.2	86
103	Predicting Ligand Binding Affinity with Alchemical Free Energy Methods in a Polar Model Binding Site. Journal of Molecular Biology, 2009, 394, 747-763.	2.0	160
104	Binding of Small-Molecule Ligands to Proteins: â€œWhat You Seeâ€•Is Not Always â€œWhat You Getâ€• Structure, 2009, 17, 489-498.	1.6	500
105	Small Molecule Hydration Free Energies in Explicit Solvent: An Extensive Test of Fixed-Charge Atomistic Simulations. Journal of Chemical Theory and Computation, 2009, 5, 350-358.	2.3	302
106	Predicting Small-Molecule Solvation Free Energies: An Informal Blind Test for Computational Chemistry. Journal of Medicinal Chemistry, 2008, 51, 769-779.	2.9	248
107	Treating Entropy and Conformational Changes in Implicit Solvent Simulations of Small Molecules. Journal of Physical Chemistry B, 2008, 112, 938-946.	1.2	106
108	Charge Asymmetries in Hydration of Polar Solutes. Journal of Physical Chemistry B, 2008, 112, 2405-2414.	1.2	98

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109	Nonlinear scaling schemes for Lennard-Jones interactions in free energy calculations. Journal of Chemical Physics, 2007, 127, 214108.	1.2	269
110	Predicting Absolute Ligand Binding Free Energies to a Simple Model Site. Journal of Molecular Biology, 2007, 371, 1118-1134.	2.0	269
111	A Mathematical Model of Glioblastoma Tumor Spheroid Invasion in a Three-Dimensional In Vitro Experiment. Biophysical Journal, 2007, 92, 356-365.	0.2	211
112	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
113	Chapter 4 Alchemical Free Energy Calculations: Ready for Prime Time?. Annual Reports in Computational Chemistry, 2007, 3, 41-59.	0.9	175
114	Accurate and Efficient Corrections for Missing Dispersion Interactions in Molecular Simulations. Journal of Physical Chemistry B, 2007, 111, 13052-13063.	1.2	181
115	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
116	On the use of orientational restraints and symmetry corrections in alchemical free energy calculations. Journal of Chemical Physics, 2006, 125, 084902.	1.2	253
117	Hysteresis loops of Coâ€“Pt perpendicular magnetic multilayers. Journal of Physics Condensed Matter, 2004, 16, 5897-5906.	0.7	6
118	Modeling Amyloid Î²-Peptide Insertion into Lipid Bilayers. Biophysical Journal, 2004, 86, 3585-3597.	0.2	50
119	Simulations of Oligomeric Intermediates in Prion Diseases. Biophysical Journal, 2003, 85, 2213-2223.	0.2	11