Lauren Wickstrom

List of Publications by Year
in descending order

18	7,988	623574	839398
papers	citations	14 h-index	18 g-index

19	19	19	12291
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ff14SB: Improving the Accuracy of Protein Side Chain and Backbone Parameters from ff99SB. Journal of Chemical Theory and Computation, 2015, 11, 3696-3713.	2.3	7,322
2	Improved Efficiency of Replica Exchange Simulations through Use of a Hybrid Explicit/Implicit Solvation Model. Journal of Chemical Theory and Computation, 2006, 2, 420-433.	2.3	126
3	Secondary Structure Bias in Generalized Born Solvent Models:Â Comparison of Conformational Ensembles and Free Energy of Solvent Polarization from Explicit and Implicit Solvation. Journal of Physical Chemistry B, 2007, 111, 1846-1857.	1.2	121
4	Large Scale Affinity Calculations of Cyclodextrin Hostâ€“Guest Complexes: Understanding the Role of Reorganization in the Molecular Recognition Process. Journal of Chemical Theory and Computation, 2013, 9, 3136-3150.	2.3	77
5	Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 475-490.	1.3	53
6	The Unfolded State of the Villin Headpiece Helical Subdomain: Computational Studies of the Role of Locally Stabilized Structure. Journal of Molecular Biology, 2006, 360, 1094-1107.	2.0	46
7	Evaluation of Salt Bridge Structure and Energetics in Peptides Using Explicit, Implicit, and Hybrid Solvation Models. Journal of Chemical Theory and Computation, 2008, 4, 488-498.	2.3	35
8	Resolving the Ligand-Binding Specificity in c-MYC G-Quadruplex DNA: Absolute Binding Free Energy Calculations and SPR Experiment. Journal of Physical Chemistry B, 2017, 121, 10484-10497.	1.2	34
9	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. Journal of Physical Chemistry B, 2016, 120, 8743-8756.	1.2	33
10	The linear interaction energy method for the prediction of protein stability changes upon mutation. Proteins: Structure, Function and Bioinformatics, 2012, 80, 111-125.	1.5	27
11	Parameterization of an effective potential for proteinâ€“ligand binding from hostâ€“guest affinity data. Journal of Molecular Recognition, 2016, 29, 10-21.	1.1	27
12	Thermodynamic Decomposition of Solvation Free Energies with Particle Mesh Ewald and Long-Range Lennard-Jones Interactions in Grid Inhomogeneous Solvation Theory. Journal of Chemical Theory and Computation, 2021, 17, 2714-2724.	2.3	19
13	A combined treatment of hydration and dynamical effects for the modeling of hostâ€“guest binding thermodynamics: the SAMPL5 blinded challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 29-44.	1.3	18
14	Combining Alchemical Transformation with a Physical Pathway to Accelerate Absolute Binding Free Energy Calculations of Charged Ligands to Enclosed Binding Sites. Journal of Chemical Theory and Computation, 2020, 16, 2803-2813.	2.3	17
15	Exploring the Free-Energy Landscape and Thermodynamics of Protein-Protein Association. Biophysical Journal, 2020, 119, 1226-1238.	0.2	12
16	Ligand Selectivity in the Recognition of Protoberberine Alkaloids by Hybrid-2 Human Telomeric G-Quadruplex: Binding Free Energy Calculation, Fluorescence Binding, and NMR Experiments. Molecules, 2019, 24, 1574.	1.7	10
17	Role of Displacing Confined Solvent in the Conformational Equilibrium of Î²-Cyclodextrin. Journal of Physical Chemistry B, 2019, 123, 8378-8386.	1.2	6
18	Developing end-point methods for absolute binding free energy calculation using the Boltzmann-quasiharmonic model. Physical Chemistry Chemical Physics, 2022, 24, 6037-6052.	1.3	5