

Lauren Wickstrom

List of Publications by Year in descending order

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Version: 2024-02-01

18
papers

7,988
citations

623734

14
h-index

839539

18
g-index

19
all docs

19
docs citations

19
times ranked

12291
citing authors

#	ARTICLE	IF	CITATIONS
1	ff14SB: Improving the Accuracy of Protein Side Chain and Backbone Parameters from ff99SB. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3696-3713.	5.3	7,322
2	Improved Efficiency of Replica Exchange Simulations through Use of a Hybrid Explicit/Implicit Solvation Model. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 420-433.	5.3	126
3	Secondary Structure Bias in Generalized Born Solvent Models: A Comparison of Conformational Ensembles and Free Energy of Solvent Polarization from Explicit and Implicit Solvation. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1846-1857.	2.6	121
4	Large Scale Affinity Calculations of Cyclodextrin Host-Guest Complexes: Understanding the Role of Reorganization in the Molecular Recognition Process. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3136-3150.	5.3	77
5	Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 475-490.	2.9	53
6	The Unfolded State of the Villin Headpiece Helical Subdomain: Computational Studies of the Role of Locally Stabilized Structure. <i>Journal of Molecular Biology</i> , 2006, 360, 1094-1107.	4.2	46
7	Evaluation of Salt Bridge Structure and Energetics in Peptides Using Explicit, Implicit, and Hybrid Solvation Models. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 488-498.	5.3	35
8	Resolving the Ligand-Binding Specificity in c-MYC G-Quadruplex DNA: Absolute Binding Free Energy Calculations and SPR Experiment. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10484-10497.	2.6	34
9	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8743-8756.	2.6	33
10	The linear interaction energy method for the prediction of protein stability changes upon mutation. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 111-125.	2.6	27
11	Parameterization of an effective potential for protein-ligand binding from host-guest affinity data. <i>Journal of Molecular Recognition</i> , 2016, 29, 10-21.	2.1	27
12	Thermodynamic Decomposition of Solvation Free Energies with Particle Mesh Ewald and Long-Range Lennard-Jones Interactions in Grid Inhomogeneous Solvation Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2714-2724.	5.3	19
13	A combined treatment of hydration and dynamical effects for the modeling of host-guest binding thermodynamics: the SAMPL5 blinded challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 29-44.	2.9	18
14	Combining Alchemical Transformation with a Physical Pathway to Accelerate Absolute Binding Free Energy Calculations of Charged Ligands to Enclosed Binding Sites. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2803-2813.	5.3	17
15	Exploring the Free-Energy Landscape and Thermodynamics of Protein-Protein Association. <i>Biophysical Journal</i> , 2020, 119, 1226-1238.	0.5	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. <i>Molecules</i> , 2019, 24, 1574.	3.8	10
17	Role of Displacing Confined Solvent in the Conformational Equilibrium of β -Cyclodextrin. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8378-8386.	2.6	6
18	Developing end-point methods for absolute binding free energy calculation using the Boltzmann-quasi-harmonic model. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6037-6052.	2.8	5