Tom Kurtzman

List of Publications by Year
in descending order

21 papers	815 citations	567281 15 h-index	713466 21 g-index
27 all docs	27 docs citations	27 times ranked	1034 citing authors

#	Article	IF	Citations
1	Application of the alchemical transfer and potential of mean force methods to the SAMPL8 host-guest blinded challenge. Journal of Computer-Aided Molecular Design, 2022, 36, 63-76.	2.9	8
2	Developing end-point methods for absolute binding free energy calculation using the Boltzmann-quasiharmonic model. Physical Chemistry Chemical Physics, 2022, 24, 6037-6052.	2.8	5
3	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.	5.3	19
4	An online repository of solvation thermodynamic and structural maps of SARS-CoV-2 targets. Journal of Computer-Aided Molecular Design, 2020, 34, 1219-1228.	2.9	7
5	A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site. PLoS ONE, 2019, 14, e0219473.	2.5	22
6	Hidden bias in the DUD-E dataset leads to misleading performance of deep learning in structure-based virtual screening. PLoS ONE, 2019, 14, e0220113.	2.5	144
7	Role of Displacing Confined Solvent in the Conformational Equilibrium of Î²-Cyclodextrin. Journal of Physical Chemistry B, 2019, 123, 8378-8386.	2.6	6
8	Inclusion of enclosed hydration effects in the binding free energy estimation of dopamine D3 receptor complexes. PLoS ONE, 2019, 14, e0222902.	2.5	9
9	Simulating Water Exchange to Buried Binding Sites. Journal of Chemical Theory and Computation, 2019, 15, 2684-2691.	5.3	33
10	Solvation Structure and Thermodynamic Mapping (SSTMap): An Open-Source, Flexible Package for the Analysis of Water in Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2018, 14, 418-425.	5.3	40
11	New Dopamine D3-Selective Receptor Ligands Containing a 6-Methoxy-1,2,3,4-tetrahydroisoquinolin-7-ol Motif. ACS Medicinal Chemistry Letters, 2018, 9, 990-995.	2.8	8
12	Water Pharmacophore: Designing Ligands using Molecular Dynamics Simulations with Water. Scientific Reports, 2018, 8, 10400.	3.3	25
13	Testing inhomogeneous solvation theory in structure-based ligand discovery. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6839-E6846.	7.1	65
14	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.	2.9	18
15	Solvation thermodynamic mapping of molecular surfaces in AmberTools: GIST. Journal of Computational Chemistry, 2016, 37, 2029-2037.	3.3	95
16	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. Journal of Physical Chemistry B, 2016, 120, 8743-8756.	2.6	33
17	Parameterization of an effective potential for proteinâ€“ligand binding from hostâ€“guest affinity data. Journal of Molecular Recognition, 2016, 29, 10-21.	2.1	27
18	Spatial Decomposition of Translational Waterâ€“Water Correlation Entropy in Binding Pockets. Journal of Chemical Theory and Computation, 2016, 12, 414-429.	5.3	34

#	Article	IF	Citations
19	Estimation of Solvation Entropy and Enthalpy via Analysis of Water Oxygenâ€“Hydrogen Correlations. Journal of Chemical Theory and Computation, 2015, 11, 5090-5102.	5.3	31
20	Thermodynamics of Water in an Enzyme Active Site: Grid-Based Hydration Analysis of Coagulation Factor Xa. Journal of Chemical Theory and Computation, 2014, 10, 2769-2780.	5.3	117
21	Dewetting transitions in protein cavities. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1856-1869.	2.6	64