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	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
2	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
3	Solvation thermodynamic mapping of molecular surfaces in AmberTools: GIST. Journal of Computational Chemistry, 2016, 37, 2029-2037.	3.3	95
4	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
5	Dewetting transitions in protein cavities. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1856-1869.	2.6	64
6	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
7	Spatial Decomposition of Translational Waterâ€“Water Correlation Entropy in Binding Pockets. Journal of Chemical Theory and Computation, 2016, 12, 414-429.	5.3	34
8	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. Journal of Physical Chemistry B, 2016, 120, 8743-8756.	2.6	33
9	Simulating Water Exchange to Buried Binding Sites. Journal of Chemical Theory and Computation, 2019, 15, 2684-2691.	5.3	33
10	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
11	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
12	Water Pharmacophore: Designing Ligands using Molecular Dynamics Simulations with Water. Scientific Reports, 2018, 8, 10400.	3.3	25
13	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
14	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
15	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
16	Inclusion of enclosed hydration effects in the binding free energy estimation of dopamine D3 receptor complexes. PLoS ONE, 2019, 14, e0222902.	2.5	9
17	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
18	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

#	Article	IF	Citations
19	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
20	Role of Displacing Confined Solvent in the Conformational Equilibrium of Î²-Cyclodextrin. Journal of Physical Chemistry B, 2019, 123, 8378-8386.	2.6	6
21	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