Tyler Luchko

List of Publications by Year
in descending order

21	975	623734 14	713466 21
papers	citations	h-index	g-index

23	23	23	998
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. Journal of Chemical Theory and Computation, 2010, 6, 607-624.	5.3	232
2	An MM/3D-RISM Approach for Ligand Binding Affinities. Journal of Physical Chemistry B, 2010, 114, 8505-8516.	2.6	129
3	Ion Counting from Explicit-Solvent Simulations and 3D-RISM. Biophysical Journal, 2014, 106, 883-894.	0.5	102
4	The evolution of the structure of tubulin and its potential consequences for the role and function of microtubules in cells and embryos. International Journal of Developmental Biology, 2006, 50, 341-358.	0.6	68
5	Simple electrolyte solutions: Comparison of DRISM and molecular dynamics results for alkali halide solutions. Journal of Chemical Physics, 2013, 138, 044103.	3.0	63
6	Identification and Characterization of an Intermediate Taxol Binding Site Within Microtubule Nanopores and a Mechanism for Tubulin Isotype Binding Selectivity. Journal of Chemical Information and Modeling, 2009, 49, 424-436.	5.4	60
7	Competitive interaction of monovalent cations with DNA from 3D-RISM. Nucleic Acids Research, 2015, 43, 8405-8415.	14.5	47
8	Conformational Analysis of the Carboxy-Terminal Tails of Human Î²-Tubulin Isotypes. Biophysical Journal, 2008, 94, 1971-1982.	0.5	46
9	Structural Mass Spectrometry of the Î±Î²-Tubulin Dimer Supports a Revised Model of Microtubule Assembly. Biochemistry, 2009, 48, 4858-4870.	2.5	43
10	Molecular dynamics modeling of tubulin Câ€terminal tail interactions with the microtubule surface. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2968-2982.	2.6	38
11	Characterization of an inhibitory dynamic pharmacophore for the ERCC1â€“XPA interaction using a combined molecular dynamics and virtual screening approach. Journal of Molecular Graphics and Modelling, 2009, 28, 113-130.	2.4	36
12	SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling. Journal of Computer-Aided Molecular Design, 2016, 30, 1115-1127.	2.9	29
13	Closure for the Ornstein-Zernike equation with pressure and free energy consistency. Physical Review E, 2019, 99, 032130.	2.1	23
14	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
15	Integral Equation Theory of Biomolecules and Electrolytes. RSC Biomolecular Sciences, 2012, , 51-86.	0.4	15
16	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
17	Integral equation models for solvent in macromolecular crystals. Journal of Chemical Physics, 2022, 156, 014801.	3.0	5
18	Accelerating the 3D reference interaction site model theory of molecular solvation with treecode summation and cutâ€offs. Journal of Computational Chemistry, 2022, 43, 1251-1270.	3.3	4

#	Article	IF	Citations
19	Computational Analysis of Binding Interactions between the Ryanodine Receptor Type 2 and Calmodulin. Journal of Physical Chemistry B, 2021, 125, 10720-10735.	2.6	3
20	Electron Paramagnetic Resonance Measurements of Four Nitroxide Probes in Supercooled Water Explained by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 3962-3972.	2.6	1
21	Non-Gaussian statistics of the vibrational fluctuations of myoglobin and the thermal fluctuations of myoglobin hydration. , 2004, 5467, 1.		0