Zhaoxi Sun

List of Publications by Year
in descending order

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Version: 2024-02-01

36	781	535685 17	591227 27
papers	citations	h-index	g-index

81	81	81	541
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Seeding the multi-dimensional nonequilibrium pulling for Hamiltonian variation: indirect nonequilibrium free energy simulations at QM levels. Physical Chemistry Chemical Physics, 2022, 24, 8800-8819.	1.3	11
2	Multiple Poses and Thermodynamics of Ligands Targeting Protein Surfaces: The Case of Furosemide Binding to mitoNEET in Aqueous Solution. Frontiers in Cell and Developmental Biology, 2022, 10, 886568.	1.8	3
3	More is simpler: Decomposition of <scp>ligandâ€binding</scp> affinity for proteins being disordered. Protein Science, 2022, 31, .	3.1	4
4	Molecular Modeling of Ionic Liquids: Forceâ€Field Validation and Thermodynamic Perspective from Largeâ€Scale Fastâ€Growth Solvation Free Energy Calculations. Advanced Theory and Simulations, 2022, 5, .	1.3	6
5	SAMPL7 TrimerTrip hostâ€“guest binding affinities from extensive alchemical and end-point free energy calculations. Journal of Computer-Aided Molecular Design, 2021, 35, 117-129.	1.3	27
6	Binding Thermodynamics and Interaction Patterns of Inhibitor-Major Urinary Protein-I Binding from Extensive Free-Energy Calculations: Benchmarking AMBER Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 284-297.	2.5	19
7	SAMPL7 TrimerTrip hostâ€“guest binding poses and binding affinities from spherical-coordinates-biased simulations. Journal of Computer-Aided Molecular Design, 2021, 35, 105-115.	1.3	20
8	Thermodynamic Insights of Base Flipping in TNA Duplex: Force Fields, Salt Concentrations, and Free-Energy Simulation Methods. CCS Chemistry, 2021, 3, 1026-1039.	4.6	23
9	Binding thermodynamics and interaction patterns of human purine nucleoside phosphorylase-inhibitor complexes from extensive free energy calculations. Journal of Computer-Aided Molecular Design, 2021, 35, 643-656.	1.3	9
10	Ion dynamics and selectivity of Nav channels from molecular dynamics simulation. Chemical Physics, 2021, 548, 111245.	0.9	19
11	BARâ€Based Multiâ€Dimensional Nonequilibrium Pulling for Indirect Construction of QM/MM Free Energy Landscapes: Varying the QM Region. Advanced Theory and Simulations, 2021, 4, 2100185.	1.3	14
12	Titration of Adenine in a GA Mismatch with Grand Canonical Simulations. Journal of Computational Biophysics and Chemistry, 2021, 20, 165-173.	1.0	6
13	A General Picture of Cucurbit[8]uril Hostâ€“Guest Binding. Journal of Chemical Information and Modeling, 2021, 61, 6107-6134.	2.5	35
14	Extensive numerical tests of leapfrog integrator in middle thermostat scheme in molecular simulations. Chinese Journal of Chemical Physics, 2021, 34, 932-948.	0.6	2
15	Theoretical understanding of the thermodynamics and interactions in transcriptional regulator TtgRâ€“ligand binding. Physical Chemistry Chemical Physics, 2020, 22, 1511-1524.	1.3	13
16	Model-based process design of a ternary protein separation using multi-step gradient ion-exchange SMB chromatography. Computers and Chemical Engineering, 2020, 138, 106851.	2.0	7
17	SAMPL6 hostâ€“guest binding affinities and binding poses from spherical-coordinates-biased simulations. Journal of Computer-Aided Molecular Design, 2020, 34, 589-600.	1.3	23
18	Thermodynamics of Helix formation in small peptides of varying lengthin vacuo, implicit solvent and explicit solvent: Comparison between AMBER force fields. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950015.	1.8	7

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19	Thermodynamics of helix formation in small peptides of varying length in vacuo, in implicit solvent, and in explicit solvent. Journal of Molecular Modeling, 2019, 25, 3.	0.8	36
20	Determination of Base-Flipping Free-Energy Landscapes from Nonequilibrium Stratification. Journal of Chemical Information and Modeling, 2019, 59, 2980-2994.	2.5	17
21	Sulfur-substitution-induced base flipping in the DNA duplex. Physical Chemistry Chemical Physics, 2019, 21, 14923-14940.	1.3	21
22	Understanding Aldose Reductase-Inhibitors interactions with free energy simulation. Journal of Molecular Graphics and Modelling, 2019, 91, 10-21.	1.3	10
23	Understanding PIM-1 kinase inhibitor interactions with free energy simulation. Physical Chemistry Chemical Physics, 2019, 21, 7544-7558.	1.3	16
24	BAR-based multi-dimensional nonequilibrium pulling for indirect construction of a QM/MM free energy landscape. Physical Chemistry Chemical Physics, 2019, 21, 6672-6688.	1.3	19
25	BARâ€based optimum adaptive steered MD for configurational sampling. Journal of Computational Chemistry, 2019, 40, 1270-1289.	1.5	22
26	Determination of binding affinities of 3-Hydroxy-3-Methylglutaryl Coenzyme A reductase inhibitors from free energy calculation. Chemical Physics Letters, 2019, 723, 1-10.	1.2	11
27	BAR-based multi-dimensional nonequilibrium pulling for indirect construction of QM/MM free energy landscapes: from semi-empirical to ab initio. Physical Chemistry Chemical Physics, 2019, 21, 21942-21959.	1.3	14
28	BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation: the nonequilibrium stratification. Physical Chemistry Chemical Physics, 2018, 20, 2009-2021.	1.3	31
29	Interaction entropy for computational alanine scanning in protein-protein binding. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1342.	6.2	51
30	Interaction entropy for protein-protein binding. Journal of Chemical Physics, 2017, 146, 124124.	1.2	92
31	Optimization of convergence criteria for fragmentation methods. Chemical Physics Letters, 2017, 687, 163-170.	1.2	18
32	Extensive Assessment of Various Computational Methods for Aspartateâ€™s pK_a Shift. Journal of Chemical Information and Modeling, 2017, 57, 1621-1639.	2.5	42
33	Protonation-dependent base flipping in the catalytic triad of a small RNA. Chemical Physics Letters, 2017, 684, 239-244.	1.2	28
34	Proteinâ€“Ligand Empirical Interaction Components for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1793-1806.	2.5	51
35	BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation. Physical Chemistry Chemical Physics, 2017, 19, 15005-15020.	1.3	41
36	Titration of Adenine in a GA mismatch with Grand Canonical Simulations. Journal of Theoretical and Computational Chemistry, 0, , .	1.8	0