Yunhui Ge

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4285074/publications.pdf

Version: 2024-02-01

20	189	1170033 9	1255698 13
papers	citations	h-index	g-index

34	34	34	227
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Enhancing Sampling of Water Rehydration on Ligand Binding: A Comparison of Techniques. Journal of Chemical Theory and Computation, 2022, 18, 1359-1381.	2.3	22
2	Estimation of binding rates and affinities from multiensemble Markov models and ligand decoupling. Journal of Chemical Physics, 2022, 156, 134115.	1.2	3
3	A Benchmark of Electrostatic Method Performance in Relative Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 1048-1052.	2.5	12
4	Solution-State Preorganization of Cyclic Î²-Hairpin Ligands Determines Binding Mechanism and Affinities for MDM2. Journal of Chemical Information and Modeling, 2021, 61, 2353-2367.	2.5	6
5	Reconciling Simulations and Experiments With BICePs: A Review. Frontiers in Molecular Biosciences, 2021, 8, 661520.	1.6	6
6	Metal Cation-Binding Mechanisms of Q-Proline Peptoid Macrocycles in Solution. Journal of Chemical Information and Modeling, 2021, 61, 2818-2828.	2.5	7
7	Temperature artifacts in protein structures bias ligand-binding predictions. Chemical Science, 2021, 12, 11275-11293.	3.7	27
8	Markov State Models to Elucidate Ligand Binding Mechanism. Methods in Molecular Biology, 2021, 2266, 239-259.	0.4	5
9	Efficient Estimation of Binding Kinetics using Scaled Non-Bonded Interactions and Harmonic Restraints. Biophysical Journal, 2020, 118, 140a.	0.2	0
10	BICePs 2.0: New Tools for Bayesian Inference of Conformational Populations from Theory and Experiment. Biophysical Journal, 2020, 118, 139a-140a.	0.2	0
11	Reconciling Simulated Ensembles of Apomyoglobin with Experimental Hydrogen/Deuterium Exchange Data Using Bayesian Inference and Multiensemble Markov State Models. Journal of Chemical Theory and Computation, 2020, 16, 1333-1348.	2.3	25
12	Exposing the Nucleation Site of Alpha Helix Folding: A Joint Experimental and Simulation Study. Biophysical Journal, 2019, 116, 310a.	0.2	0
13	Exposing the Nucleation Site in Î±-Helix Folding: A Joint Experimental and Simulation Study. Journal of Physical Chemistry B, 2019, 123, 1797-1807.	1.2	13
14	Using Computational Modeling to Understand the Binding Mechanism of Designed Cyclic Î²-Hairpin to MDM2. Biophysical Journal, 2019, 116, 193a.	0.2	0
15	Model Selection Using BICePs: A Bayesian Approach for Force Field Validation and Parameterization. Journal of Physical Chemistry B, 2018, 122, 5610-5622.	1.2	19
16	Reconciling Simulated Ensembles of Apomyoglobin with Experimental HDX Data. Biophysical Journal, 2018, 114, 680a-681a.	0.2	0
17	Simulations of the regulatory ACT domain of human phenylalanine hydroxylase (PAH) unveil its mechanism of phenylalanine binding. Journal of Biological Chemistry, 2018, 293, 19532-19543.	1.6	15
18	Elucidating the inhibition of peptidoglycan biosynthesis in Staphylococcus aureus by albocycline, a macrolactone isolated from Streptomyces maizeus. Bioorganic and Medicinal Chemistry, 2018, 26, 3453-3460.	1.4	15

#	Article	IF	Citations
19	Binding Pathways of Phenylalanine to the Dimeric Regulatory Domain of Human PAH Reveal a LID Gating Mechanism. Biophysical Journal, 2018, 114, 226a.	0.2	1
20	Computational and Experimental Evaluation of Designed Î²-Cap Hairpins Using Molecular Simulations and Kinetic Network Models. Journal of Chemical Information and Modeling, 2017, 57, 1609-1620.	2.5	9