Zheng Zheng

List of Publications by Year
in descending order

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26 papers	497 citations	759233 12 h-index	677142 22 g-index
29 all docs	29 docs citations	29 times ranked	697 citing authors

#	Article	IF	Citations
1	MovableType Software for Fast Free Energy-Based Virtual Screening: Protocol Development, Deployment, Validation, and Assessment. Journal of Chemical Information and Modeling, 2020, 60, 5437-5456.	5.4	7
2	Receptorâ€“Ligand Binding Free Energies from a Consecutive Histograms Monte Carlo Sampling Method. Journal of Chemical Theory and Computation, 2020, 16, 6645-6655.	5.3	4
3	Application of the Movable Type Free Energy Method to the Caspase-Inhibitor BindingAffinity Study. International Journal of Molecular Sciences, 2019, 20, 4850.	4.1	1
4	Random Forest Refinement of Pairwise Potentials for Proteinâ€“Ligand Decoy Detection. Journal of Chemical Information and Modeling, 2019, 59, 3305-3315.	5.4	14
5	Random Forest Refinement of the KECSA2 Knowledge-Based Scoring Function for Protein Decoy Detection. Journal of Chemical Information and Modeling, 2019, 59, 1919-1929.	5.4	10
6	Free-Energy-Based Protein Design: Re-Engineering Cellular Retinoic Acid Binding Protein II Assisted by the Moveable-Type Approach. Journal of the American Chemical Society, 2018, 140, 3483-3486.	13.7	5
7	The Role of the Active Site Flap in Streptavidin/Biotin Complex Formation. Journal of the American Chemical Society, 2018, 140, 5434-5446.	13.7	16
8	Generation of Pairwise Potentials Using Multidimensional Data Mining. Journal of Chemical Theory and Computation, 2018, 14, 5045-5067.	5.3	12
9	Detailed potential of mean force studies on hostâ€“guest systems from the SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1013-1026.	2.9	15
10	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727.	3.0	82
11	On the fly estimation of hostâ€“guest binding free energies using the movable type method: participation in the SAMPL5 blind challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 47-60.	2.9	13
12	Incorporation of side chain flexibility into protein binding pockets using MTflex. Bioorganic and Medicinal Chemistry, 2016, 24, 4978-4987.	3.0	7
13	KECSA-Movable Type Implicit Solvation Model (KMTISM). Journal of Chemical Theory and Computation, 2015, 11, 667-682.	5.3	19
14	A cascade reaction network mimicking the basic functional steps of adaptive immune response. Nature Chemistry, 2015, 7, 835-841.	13.6	95
15	Free Energy-Based Conformational Search Algorithm Using the Movable Type Sampling Method. Journal of Chemical Theory and Computation, 2015, 11, 5853-5864.	5.3	15
16	Bringing Clarity to the Prediction of Proteinâ€“Ligand Binding Free Energies via â€œBlurringâ€. Journal of Chemical Theory and Computation, 2014, 10, 1314-1325.	5.3	19
17	Development of the Knowledge-Based and Empirical Combined Scoring Algorithm (KECSA) To Score Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2013, 53, 1073-1083.	5.4	48
18	The Movable Type Method Applied to Proteinâ€“Ligand Binding. Journal of Chemical Theory and Computation, 2013, 9, 5526-5538.	5.3	28

#	Article	IF	Citations
19	Statistics-based model for basis set superposition error correction in large biomolecules. Physical Chemistry Chemical Physics, 2012, 14, 7795.	2.8	12
20	Prediction of trypsin/molecular fragment binding affinities by free energy decomposition and empirical scores. Journal of Computer-Aided Molecular Design, 2012, 26, 647-659.	2.9	11
21	Ligand Identification Scoring Algorithm (LISA). Journal of Chemical Information and Modeling, 2011, 51, 1296-1306.	5.4	25
22	Model for the fast estimation of basis set superposition error in biomolecular systems. Journal of Chemical Physics, 2011, 135, 144110.	3.0	31
23	Application of the HSAB principle for the quantitative analysis of nucleophilicity/basicity of organic compounds with lone-pair electrons. Journal of Chinese Pharmaceutical Sciences, 2011, 20, .	0.1	1
24	A Combined Method for Determining Reaction Transition State Geometry and Energy. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2009, 25, 1439-1442.	4.9	0
25	Fast, Routine Free Energy of Binding Estimation Using MovableType. ACS Symposium Series, 0, , 247-265.	0.5	1
26	The Conformational Transition Pathways and Hidden Intermediates in DFG-Flip Process of c-Met Kinase Revealed by Metadynamics Simulations. Journal of Chemical Information and Modeling, 0, , .	5.4	4