Liangxu Xie

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2686490/publications.pdf

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18	265	1163117 8	940533 16
papers	citations	h-index	g-index

19	19	19	393
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Landscape Zooming toward the Prediction of RNA Cotranscriptional Folding. Journal of Chemical Theory and Computation, 2022, 18, 2002-2015.	5.3	8
2	Advances in L-Type Calcium Channel Structures, Functions and Molecular Modeling. Current Medicinal Chemistry, 2021, 28, 514-524.	2.4	10
3	High-throughput screening and rational design of biofunctionalized surfaces with optimized biocompatibility and antimicrobial activity. Nature Communications, 2021, 12, 3757.	12.8	20
4	Multitask deep networks with grid featurization achieve improved scoring performance for proteinâ€“ligand binding. Chemical Biology and Drug Design, 2020, 96, 973-983.	3.2	9
5	Improvement of Prediction Performance With Conjoint Molecular Fingerprint in Deep Learning. Frontiers in Pharmacology, 2020, 11, 606668.	3.5	29
6	Isotopic Effect in Double Proton Transfer Process of Porphycene Investigated by Enhanced QM/MM Method. Journal of Visualized Experiments, 2019, , .	0.3	0
7	Highly Selective Transport of Alkali Metal Ions by Nanochannels of Polyelectrolyte Threaded MIL-53 Metal Organic Framework. Nano Letters, 2019, 19, 4990-4996.	9.1	31
8	Understanding the entropic effect in chorismate mutase reaction catalyzed by isochorismate-pyruvate lyase fromPseudomonas aeruginosa(PchB). Catalysis Science and Technology, 2019, 9, 957-965.	4.1	4
9	Mechanistic Insights and Rational Design of a Versatile Surface with Cells/Bacteria Recognition Capability via Orientated Fusion Peptides. Advanced Science, 2019, 6, 1801827.	11.2	11
10	Enhanced QM/MM sampling for free energy calculation of chemical reactions: A case study of double proton transfer. Journal of Chemical Physics, 2019, 150, 044111.	3.0	2
11	DNA-Encoded Dynamic Chemical Library and Its Applications in Ligand Discovery. Journal of the American Chemical Society, 2018, 140, 15859-15867.	13.7	83
12	Efficient free energy calculations by combining two complementary tempering sampling methods. Journal of Chemical Physics, 2017, 146, 024103.	3.0	15
13	Thermodynamic properties of solvated peptides from selective integrated tempering sampling with a new weighting factor estimation algorithm. Molecular Physics, 2017, 115, 885-894.	1.7	2
14	Multi-responsive, bidirectional, and large deformation bending actuators based on borax cross-linked polyvinyl alcohol derivative hydrogel. RSC Advances, 2017, 7, 40005-40014.	3.6	26
15	Poly(ethylene glycol) (PEG) in a Polyethylene (PE) Framework: A Simple Model for Simulation Studies of a Soluble Polymer in an Open Framework. Langmuir, 2017, 33, 11746-11753.	3.5	6
16	Enhanced molecular dynamics simulation of the transformation between Î±-helix and Î²-hairpin structures for peptide. Molecular Physics, 2016, 114, 2424-2431.	1.7	4
17	Double bond isomerization of butene catalyzed by 1-ethyl-3-methyl-imidazolium chloride: Concerted or stepwise mechanism?. Computational and Theoretical Chemistry, 2011, 963, 344-347.	2.5	4
18	Counterion distribution around a polyelectrolyte confined in a metalâ€“organic framework. Molecular Simulation, 0, , 1-9.	2.0	1