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	DNA-Encoded Dynamic Chemical Library and Its Applications in Ligand Discovery. Journal of the American Chemical Society, 2018, 140, 15859-15867.	13.7	83
2	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
3	Improvement of Prediction Performance With Conjoint Molecular Fingerprint in Deep Learning. Frontiers in Pharmacology, 2020, 11, 606668.	3.5	29
4	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
5	High-throughput screening and rational design of biofunctionalized surfaces with optimized biocompatibility and antimicrobial activity. Nature Communications, 2021, 12, 3757.	12.8	20
6	Efficient free energy calculations by combining two complementary tempering sampling methods. Journal of Chemical Physics, 2017, 146, 024103.	3.0	15
7	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
8	Advances in L-Type Calcium Channel Structures, Functions and Molecular Modeling. Current Medicinal Chemistry, 2021, 28, 514-524.	2.4	10
9	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
10	Landscape Zooming toward the Prediction of RNA Cotranscriptional Folding. Journal of Chemical Theory and Computation, 2022, 18, 2002-2015.	5.3	8
11	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
12	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
13	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
14	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
15	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
16	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
17	Counterion distribution around a polyelectrolyte confined in a metalâ€“organic framework. Molecular Simulation, 0, , 1-9.	2.0	1
18	Isotopic Effect in Double Proton Transfer Process of Porphycene Investigated by Enhanced QM/MM Method. Journal of Visualized Experiments, 2019, , .	0.3	0