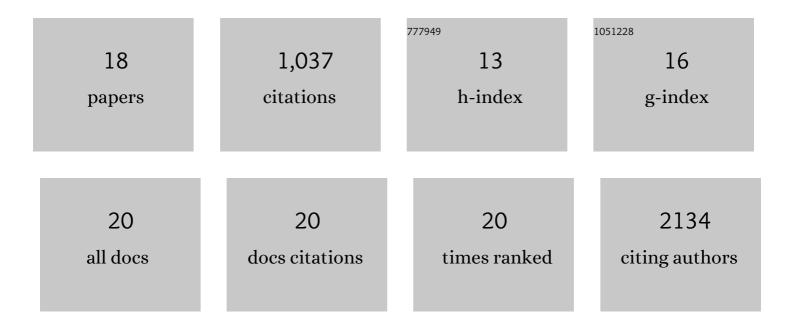
Yue Yang

List of Publications by Year in descending order

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YUE YANC

#	Article	IF	CITATIONS
1	Machine learning–driven multiscale modeling reveals lipid-dependent dynamics of RAS signaling proteins. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	44
2	Accelerators for Classical Molecular Dynamics Simulations of Biomolecules. Journal of Chemical Theory and Computation, 2022, 18, 4047-4069.	2.3	15
3	Discovery of Small-Molecule Inhibitors of SARS-CoV-2 Proteins Using a Computational and Experimental Pipeline. Frontiers in Molecular Biosciences, 2021, 8, 678701.	1.6	22
4	High-throughput virtual screening of small molecule inhibitors for SARS-CoV-2 protein targets with deep fusion models. , 2021, , .		7
5	Membrane interactions of the globular domain and the hypervariable region of KRAS4b define its unique diffusion behavior. ELife, 2020, 9, .	2.8	23
6	A massively parallel infrastructure for adaptive multiscale simulations. , 2019, , .		32
7	Structural Control of Nonnative Ligand Binding in Engineered Mutants of Phosphoenolpyruvate Carboxykinase. Biochemistry, 2018, 57, 6688-6700.	1.2	5
8	Mechanism of Formation of the Nonstandard Product in the Prenyltransferase Reaction of the G115T Mutant of FtmPT1: A Case of Reaction Dynamics Calling the Shots?. Biochemistry, 2017, 56, 2995-3007.	1.2	4
9	Carbonic anhydrase mimics for enhanced CO ₂ absorption in an amine-based capture solvent. Dalton Transactions, 2016, 45, 324-333.	1.6	23
10	Origin of Product Selectivity in a Prenyl Transfer Reaction from the Same Intermediate: Exploration of Multiple FtmPT1-Catalyzed Prenyl Transfer Pathways. Biochemistry, 2014, 53, 6126-6138.	1.2	7
11	Understanding a Substrate's Product Regioselectivity in a Family of Enzymes: A Case Study of Acetaminophen Binding in Cytochrome P450s. PLoS ONE, 2014, 9, e87058.	1.1	19
12	Approaches to efficiently estimate solvation and explicit water energetics in ligand binding: the use of WaterMap. Expert Opinion on Drug Discovery, 2013, 8, 277-287.	2.5	55
13	Catalytic Mechanism of Aromatic Prenylation by NphB. Biochemistry, 2012, 51, 2606-2618.	1.2	33
14	Insights into the Mechanistic Dichotomy of the Protein Farnesyltransferase Peptide Substrates CVIM and CVLS. Journal of the American Chemical Society, 2012, 134, 820-823.	6.6	15
15	Structural Survey of Zinc-Containing Proteins and Development of the Zinc AMBER Force Field (ZAFF). Journal of Chemical Theory and Computation, 2010, 6, 2935-2947.	2.3	378
16	Finding a Needle in the Haystack: Computational Modeling of Mg ²⁺ Binding in the Active Site of Protein Farnesyltransferase. Biochemistry, 2010, 49, 9658-9666.	1.2	27
17	Assessment of the CCSD and CCSD(T) Coupled-Cluster Methods in Calculating Heats of Formation for Zn Complexes. Journal of Physical Chemistry A, 2009, 113, 10081-10088.	1.1	13
18	Assessment of the "6-31+G** + LANL2DZ―Mixed Basis Set Coupled with Density Functional Theory Methods and the Effective Core Potential: Prediction of Heats of Formation and Ionization Potentials for First-Row-Transition-Metal Complexes. Journal of Physical Chemistry A, 2009, 113, 9843-9851.	1.1	313