

# Yue Yang

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/320989/publications.pdf>

Version: 2024-02-01

18  
papers

1,037  
citations

687363

13  
h-index

940533

16  
g-index

20  
all docs

20  
docs citations

20  
times ranked

1887  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural Survey of Zinc-Containing Proteins and Development of the Zinc AMBER Force Field (ZAFF). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2935-2947.	5.3	378
2	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. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9843-9851.	2.5	313
3	Approaches to efficiently estimate solvation and explicit water energetics in ligand binding: the use of WaterMap. <i>Expert Opinion on Drug Discovery</i> , 2013, 8, 277-287.	5.0	55
4	Machine learning-driven multiscale modeling reveals lipid-dependent dynamics of RAS signaling proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	7.1	44
5	Catalytic Mechanism of Aromatic Prenylation by NphB. <i>Biochemistry</i> , 2012, 51, 2606-2618.	2.5	33
6	A massively parallel infrastructure for adaptive multiscale simulations. , 2019, , .		32
7	Finding a Needle in the Haystack: Computational Modeling of $Mg^{2+}$ Binding in the Active Site of Protein Farnesyltransferase. <i>Biochemistry</i> , 2010, 49, 9658-9666.	2.5	27
8	Carbonic anhydrase mimics for enhanced $CO_2$ absorption in an amine-based capture solvent. <i>Dalton Transactions</i> , 2016, 45, 324-333.	3.3	23
9	Membrane interactions of the globular domain and the hypervariable region of KRAS4b define its unique diffusion behavior. <i>ELife</i> , 2020, 9, .	6.0	23
10	Discovery of Small-Molecule Inhibitors of SARS-CoV-2 Proteins Using a Computational and Experimental Pipeline. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 678701.	3.5	22
11	Understanding a Substrate's Product Regioselectivity in a Family of Enzymes: A Case Study of Acetaminophen Binding in Cytochrome P450s. <i>PLoS ONE</i> , 2014, 9, e87058.	2.5	19
12	Insights into the Mechanistic Dichotomy of the Protein Farnesyltransferase Peptide Substrates CVIM and CVLS. <i>Journal of the American Chemical Society</i> , 2012, 134, 820-823.	13.7	15
13	Accelerators for Classical Molecular Dynamics Simulations of Biomolecules. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4047-4069.	5.3	15
14	Assessment of the CCSD and CCSD(T) Coupled-Cluster Methods in Calculating Heats of Formation for Zn Complexes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10081-10088.	2.5	13
15	Origin of Product Selectivity in a Prenyl Transfer Reaction from the Same Intermediate: Exploration of Multiple FtmPT1-Catalyzed Prenyl Transfer Pathways. <i>Biochemistry</i> , 2014, 53, 6126-6138.	2.5	7
16	High-throughput virtual screening of small molecule inhibitors for SARS-CoV-2 protein targets with deep fusion models. , 2021, , .		7
17	Structural Control of Nonnative Ligand Binding in Engineered Mutants of Phosphoenolpyruvate Carboxykinase. <i>Biochemistry</i> , 2018, 57, 6688-6700.	2.5	5
18	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?. <i>Biochemistry</i> , 2017, 56, 2995-3007.	2.5	4