# Yue Yang

List of Publications by Year
in descending order



| 18 | 1,037 | 777949 13 | 1051228 16 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 20 | 20 | 20 | 2134 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Machine learningâ€“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<sub>2</sub> 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 Substrateâ€™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<sup>2+</sup> 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 â€œ6-31+G** + LANL2DZâ€•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 |