Yu-Ming M Huang

List of Publications by Year
in descending order

21 papers	615 citations	687363 13 h-index	752698 20 g-index
21 all docs	21 docs citations	21 times ranked	939 citing authors

#	Article	IF	Citations
1	Endosidin2 targets conserved exocyst complex subunit EXO70 to inhibit exocytosis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E41-50.	7.1	129
2	Gaussian accelerated molecular dynamics: Principles and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1521.	14.6	127
3	Ligand Binding Pathways and Conformational Transitions of the HIV Protease. Biochemistry, 2018, 57, 1533-1541.	2.5	52
4	Insights from Free-Energy Calculations: Protein Conformational Equilibrium, Driving Forces, and Ligand-Binding Modes. Biophysical Journal, 2012, 103, 342-351.	0.5	30
5	Mechanism of the Association Pathways for a Pair of Fast and Slow Binding Ligands of HIV-1 Protease. Biochemistry, 2017, 56, 1311-1323.	2.5	30
6	Replica Exchange Gaussian Accelerated Molecular Dynamics: Improved Enhanced Sampling and Free Energy Calculation. Journal of Chemical Theory and Computation, 2018, 14, 1853-1864.	5.3	29
7	Brownian dynamic study of an enzyme metabolon in the TCA cycle: Substrate kinetics and channeling. Protein Science, 2018, 27, 463-471.	7.6	29
8	Molecular dynamic study of MlaC protein in Gramâ€negative bacteria: conformational flexibility, solvent effect and proteinâ€phospholipid binding. Protein Science, 2016, 25, 1430-1437.	7.6	26
9	Protonation states and catalysis: Molecular dynamics studies of intermediates in tryptophan synthase. Protein Science, 2016, 25, 166-183.	7.6	23
10	Switches of hydrogen bonds during ligandâ€“protein association processes determine binding kinetics. Journal of Molecular Recognition, 2014, 27, 537-548.	2.1	21
11	Characterization of Promiscuous Binding of Phosphor Ligands to Breast-Cancer-Gene 1 (BRCA1) C-Terminal (BRCT): Molecular Dynamics, Free Energy, Entropy and Inhibitor Design. PLoS Computational Biology, 2016, 12, e1005057.	3.2	21
12	Elucidating degradation mechanisms of florfenicol in soil by stable-isotope assisted nontarget screening. Journal of Hazardous Materials, 2021, 403, 123974.	12.4	17
13	Electrostatic steering enhances the rate of cAMP binding to phosphodiesterase: Brownian dynamics modeling. Protein Science, 2015, 24, 1884-1889.	7.6	15
14	Multiscale computational study of ligand binding pathways: Case of p38 MAP kinase and its inhibitors. Biophysical Journal, 2021, 120, 3881-3892.	0.5	13
15	Mechanism of PhosphoThreonine/Serine Recognition and Specificity for Modular Domains from All-atom Molecular Dynamics. BMC Biophysics, 2011, 4, 12.	4.4	12
16	Investigation of Structural Dynamics of Enzymes and Protonation States of Substrates Using Computational Tools. Catalysts, 2016, 6, 82.	3.5	12
17	Enhanced Disrupting Effect of Benzophenone-1 Chlorination Byproducts to the Androgen Receptor: Cell-Based Assays and Gaussian Accelerated Molecular Dynamics Simulations. Chemical Research in Toxicology, 2021, 34, 1140-1149.	3.3	12
18	Mechanistic Insights into Phosphopeptideâ€“BRCT Domain Association: Preorganization, Flexibility, and Phosphate Recognition. Journal of Physical Chemistry B, 2012, 116, 10247-10258.	2.6	6

#	Article	IF	Citations
19	Docking simulation and antibiotic discovery targeting the MlaC protein in Gramâ€negative bacteria. Chemical Biology and Drug Design, 2019, 93, 647-652.	3.2	5
20	Molecular Modeling of ABHD5 Structure and Ligand Recognition. Frontiers in Molecular Biosciences, 0, 9, .	3.5	4
21	An Integrated Pharmacological, Structural, and Genetic Analysis of Extracellular Versus Intracellular ROS Production in Neutrophils. Journal of Molecular Biology, 2022, 434, 167533.	4.2	2