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	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
2	Elucidating degradation mechanisms of florfenicol in soil by stable-isotope assisted nontarget screening. Journal of Hazardous Materials, 2021, 403, 123974.	12.4	17
3	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
4	Gaussian accelerated molecular dynamics: Principles and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1521.	14.6	127
5	Multiscale computational study of ligand binding pathways: Case of p38 MAP kinase and its inhibitors. Biophysical Journal, 2021, 120, 3881-3892.	0.5	13
6	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
7	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
8	Ligand Binding Pathways and Conformational Transitions of the HIV Protease. Biochemistry, 2018, 57, 1533-1541.	2.5	52
9	Brownian dynamic study of an enzyme metabolon in the TCA cycle: Substrate kinetics and channeling. Protein Science, 2018, 27, 463-471.	7.6	29
10	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
11	Investigation of Structural Dynamics of Enzymes and Protonation States of Substrates Using Computational Tools. Catalysts, 2016, 6, 82.	3.5	12
12	Protonation states and catalysis: Molecular dynamics studies of intermediates in tryptophan synthase. Protein Science, 2016, 25, 166-183.	7.6	23
13	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
14	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
15	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
16	Electrostatic steering enhances the rate of cAMP binding to phosphodiesterase: Brownian dynamics modeling. Protein Science, 2015, 24, 1884-1889.	7.6	15
17	Switches of hydrogen bonds during ligandâ€“protein association processes determine binding kinetics. Journal of Molecular Recognition, 2014, 27, 537-548.	2.1	21
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	Insights from Free-Energy Calculations: Protein Conformational Equilibrium, Driving Forces, and Ligand-Binding Modes. Biophysical Journal, 2012, 103, 342-351.	0.5	30
20	Mechanism of PhosphoThreonine/Serine Recognition and Specificity for Modular Domains from All-atom Molecular Dynamics. BMC Biophysics, 2011, 4, 12.	4.4	12
21	Molecular Modeling of ABHD5 Structure and Ligand Recognition. Frontiers in Molecular Biosciences, 0, 9, .	3.5	4