Anna Pabis

List of Publications by Year
in descending order

22 papers	744 citations	516215 16 h-index	642321 23 g-index
25 all docs	25 docs citations	25 times ranked	1291 citing authors

#	Article	IF	Citations
1	Evolution of chalcone isomerase from a noncatalytic ancestor. Nature Chemical Biology, 2018, 14, 548-555.	3.9	113
2	Cooperativity and flexibility in enzyme evolution. Current Opinion in Structural Biology, 2018, 48, 83-92.	2.6	81
3	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. Journal of Chemical Theory and Computation, 2013, 9, 153-164.	2.3	76
4	Influenza hemagglutinin drives viral entry via two sequential intramembrane mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 7200-7207.	3.3	46
5	Promiscuity and electrostatic flexibility in the alkaline phosphatase superfamily. Current Opinion in Structural Biology, 2016, 37, 14-21.	2.6	44
6	GTP Hydrolysis Without an Active Site Base: A Unifying Mechanism for Ras and Related GTPases. Journal of the American Chemical Society, 2019, 141, 10684-10701.	6.6	44
7	Cryptic genetic variation shapes the adaptive evolutionary potential of enzymes. ELife, 2019, 8, .	2.8	35
8	Extending the Nonbonded Cationic Dummy Model to Account for Ion-Induced Dipole Interactions. Journal of Physical Chemistry Letters, 2017, 8, 5408-5414.	2.1	33
9	Promiscuity in the Enzymatic Catalysis of Phosphate and Sulfate Transfer. Biochemistry, 2016, 55, 3061-3081.	1.2	32
10	A DFT Study of the cis-Dihydroxylation of Nitroaromatic Compounds Catalyzed by Nitrobenzene Dioxygenase. Journal of Physical Chemistry B, 2014, 118, 3245-3256.	1.2	30
11	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2246-2254.	2.3	27
12	Substrate and Enzyme Specificity of the Kinetic Isotope Effects Associated with the Dioxygenation of Nitroaromatic Contaminants. Environmental Science & Technology, 2016, 50, 6708-6716.	4.6	27
13	Molecular dynamics study of the hydration of the hydroxyl radical at body temperature. Physical Chemistry Chemical Physics, 2011, 13, 9458.	1.3	26
14	Probing the mechanisms for the selectivity and promiscuity of methyl parathion hydrolase. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160150.	1.6	23
15	A DFT Study of the Kinetic Isotope Effects on the Competing S_N2 and E2 Reactions between Hypochlorite Anion and Ethyl Chloride. Journal of Chemical Theory and Computation, 2009, 5, 33-36.	2.3	20
16	Measurements of Heavy-Atom Isotope Effects Using ¹H NMR Spectroscopy. Journal of Organic Chemistry, 2011, 76, 8033-8035.	1.7	19
17	Density and temperature effect on hydrogen-bonded clusters in water - MD simulation study. Open Chemistry, 2008, 6, 555-561.	1.0	16
18	A theoretical study of carbonâ€“carbon bond formation by a Michael-type addition. Organic and Biomolecular Chemistry, 2012, 10, 5598.	1.5	13

#	Article	IF	Citations
19	The structure of cyclolinopeptide A in chloroform refined by RDC measurements. Journal of Peptide Science, 2014, 20, 901-907.	0.8	11
20	Bifunctional Substrate Activation via an Arginine Residue Drives Catalysis in Chalcone Isomerases. ACS Catalysis, 2019, 9, 8388-8396.	5.5	11
21	Enhancing the Steroid Sulfatase Activity of the Arylsulfatase from Pseudomonas aeruginosa. ACS Catalysis, 2018, 8, 8902-8914.	5.5	10
22	Simulating the reactions of substituted pyridinio-N-phosphonates with pyridine as a model for biological phosphoryl transfer. Organic and Biomolecular Chemistry, 2017, 15, 7308-7316.	1.5	5