Katarzyna Åwiderek

List of Publications by Year
in descending order

69	1,431	279487 23	377514 34
papers	citations	h-index	g-index

74	74	74	1794
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Revealing the molecular mechanisms of proteolysis of SARS-CoV-2 M^{pro}by QM/MM computational methods. Chemical Science, 2020, 11, 10626-10630.	3.7	130
2	Mechanism of inhibition of SARS-CoV-2 M^{pro} by N3 peptidyl Michael acceptor explained by QM/MM simulations and design of new derivatives with tunable chemical reactivity. Chemical Science, 2021, 12, 1433-1444.	3.7	87
3	Binding Isotope Effects. Chemical Reviews, 2013, 113, 7851-7879.	23.0	72
4	Dynamic and Electrostatic Effects on the Reaction Catalyzed by HIV-1 Protease. Journal of the American Chemical Society, 2016, 138, 16283-16298.	6.6	68
5	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54
6	Computational strategies for the design of new enzymatic functions. Archives of Biochemistry and Biophysics, 2015, 582, 68-79.	1.4	49
7	Protein Conformational Landscapes and Catalysis. Influence of Active Site Conformations in the Reaction Catalyzed by L-Lactate Dehydrogenase. ACS Catalysis, 2015, 5, 1172-1185.	5.5	48
8	Insights on the Origin of Catalysis on Glycine N-Methyltransferase from Computational Modeling. Journal of the American Chemical Society, 2018, 140, 4327-4334.	6.6	48
9	Heavy enzymesâ€"experimental and computational insights in enzyme dynamics. Current Opinion in Chemical Biology, 2014, 21, 11-18.	2.8	39
10	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie - International Edition, 2018, 57, 12478-12482.	7.2	38
11	Modeling of Isotope Effects on Binding Oxamate to Lactic Dehydrogenase. Journal of Physical Chemistry B, 2009, 113, 12782-12789.	1.2	36
12	Peptide Bond Formation Mechanism Catalyzed by Ribosome. Journal of the American Chemical Society, 2015, 137, 12024-12034.	6.6	34
13	Binding Isotope Effects as a Tool for Distinguishing Hydrophobic and Hydrophilic Binding Sites of HIV-1 RT. Journal of Physical Chemistry B, 2015, 119, 917-927.	1.2	34
14	Predicting enzymatic reactivity: from theory to design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 407-421.	6.2	32
15	A Molecular Modeling Approach to Identify Novel Inhibitors of the Major Facilitator Superfamily of Efflux Pump Transporters. Antibiotics, 2019, 8, 25.	1.5	32
16	Theoretical Study of Primary Reaction of Pseudozyma antarctica Lipase B as the Starting Point To Understand Its Promiscuity. ACS Catalysis, 2014, 4, 426-434.	5.5	31
17	Unraveling the Reaction Mechanism of Enzymatic C5-Cytosine Methylation of DNA. A Combined Molecular Dynamics and QM/MM Study of Wild Type and Gln119 Variant. ACS Catalysis, 2016, 6, 3262-3276.	5.5	30
18	Protein Flexibility and Preorganization in the Design of Enzymes. The Kemp Elimination Catalyzed by HG3.17. ACS Catalysis, 2015, 5, 2587-2595.	5.5	28

#	Article	IF	Citations
19	Binding Analysis of Some Classical Acetylcholinesterase Inhibitors: Insights for a Rational Design Using Free Energy Perturbation Method Calculations with QM/MM MD Simulations. Journal of Chemical Information and Modeling, 2017, 57, 958-976.	2.5	28
20	Revealing the mechanism for covalent inhibition of glycoside hydrolases by carbasugars at an atomic level. Nature Communications, 2018, 9, 3243.	5.8	28
21	Modeling excitation properties of iridium complexes. Journal of Physical Organic Chemistry, 2009, 22, 845-856.	0.9	26
22	Theoretical studies of HIV-1 reverse transcriptase inhibition. Physical Chemistry Chemical Physics, 2012, 14, 12614.	1.3	24
23	Extending Limits of Chlorine Kinetic Isotope Effects. Journal of Organic Chemistry, 2012, 77, 5120-5124.	1.7	23
24	Role of Solvent on Nonenzymatic Peptide Bond Formation Mechanisms and Kinetic Isotope Effects. Journal of the American Chemical Society, 2013, 135, 8708-8719.	6.6	23
25	Reaction Mechanism of Organocatalytic Michael Addition of Nitromethane to Cinnamaldehyde: A Case Study on Catalyst Regeneration and Solvent Effects. Journal of Physical Chemistry A, 2018, 122, 451-459.	1.1	20
26	Exploring the Origin of Amidase Substrate Promiscuity in CALB by a Computational Approach. ACS Catalysis, 2020, 10, 1938-1946.	5.5	19
27	Catalytic enantioselective epoxidation of nitroalkenes. Chemical Communications, 2016, 52, 10060-10063.	2.2	18
28	Benchmarking Quantum Mechanics/Molecular Mechanics (QM/MM) Methods on the Thymidylate Synthase-Catalyzed Hydride Transfer. Journal of Chemical Theory and Computation, 2017, 13, 1375-1388.	2.3	17
29	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M^{pro} Explored by QM/MM Simulations. ACS Catalysis, 2022, 12, 698-708.	5.5	17
30	Differences and similarities in binding of pyruvate and l-lactate in the active site of M4 and H4 isoforms of human lactate dehydrogenase. Archives of Biochemistry and Biophysics, 2011, 505, 33-41.	1.4	16
31	Revealing the Origin of the Efficiency of the De Novo Designed Kemp Eliminase HGâ€3.17 by Comparison with the Former Developed HGâ€3. Chemistry - A European Journal, 2017, 23, 7582-7589.	1.7	16
32	Importance of the Lactate Dehydrogenase Quaternary Structure in Theoretical Calculations. Journal of Physical Chemistry B, 2010, 114, 3393-3397.	1.2	15
33	The influence of active site conformations on the hydride transfer step of the thymidylate synthase reaction mechanism. Physical Chemistry Chemical Physics, 2015, 17, 30793-30804.	1.3	15
34	Computational Study of the Michaelis Complex Formation and the Effect on the Reaction Mechanism of Cruzain Cysteine Protease. ACS Omega, 2018, 3, 18613-18622.	1.6	14
35	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie, 2018, 130, 12658-12662.	1.6	14
36	Binding Ligands and Cofactor to<scp>L</scp>-Lactate Dehydrogenase from Human Skeletal and Heart Muscles. Journal of Physical Chemistry B, 2011, 115, 6366-6376.	1.2	13

#	Article	IF	Citations
37	A theoretical study of carbonâ€“carbon bond formation by a Michael-type addition. Organic and Biomolecular Chemistry, 2012, 10, 5598.	1.5	13
38	Theoretical study of the inhibition mechanism of human 20S proteasome by dihydroeponemycin. European Journal of Medicinal Chemistry, 2019, 164, 399-407.	2.6	12
39	Glycoside hydrolase stabilization of transition state charge: new directions for inhibitor design. Chemical Science, 2020, 11, 10488-10495.	3.7	12
40	Problems with molecular mechanics implementations on the example of 4-benzoyl-1-(4-methyl-imidazol-5-yl)-carbonylthiosemicarbazide. Journal of Molecular Modeling, 2012, 18, 843-849.	0.8	10
41	Is Promiscuous CALB a Good Scaffold for Designing New Epoxidases?. Molecules, 2015, 20, 17789-17806.	1.7	10
42	Theoretical Studies on Mechanism of Inactivation of Kanamycin A by 4â€²-O-Nucleotidyltransferase. Frontiers in Chemistry, 2018, 6, 660.	1.8	10
43	Transfer hydrogenations catalyzed by streptavidin-hosted secondary amine organocatalysts. Chemical Communications, 2021, 57, 1919-1922.	2.2	10
44	Enzymatic Î”¹-Dehydrogenation of 3-Ketosteroidsâ€”Reconciliation of Kinetic Isotope Effects with the Reaction Mechanism. ACS Catalysis, 2021, 11, 8211-8225.	5.5	10
45	Nature of Irreversible Inhibition of Human 20S Proteasome by Salinosporamide A. The Critical Role of Lysâ€“Asp Dyad Revealed from Electrostatic Effects Analysis. ACS Catalysis, 2021, 11, 3575-3589.	5.5	9
46	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. Chemical Communications, 2012, 48, 11253.	2.2	8
47	Parallel reaction pathways and noncovalent intermediates in thymidylate synthase revealed by experimental and computational tools. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10311-10314.	3.3	8
48	Discovery of a Histidineâ€Based Scaffold as an Inhibitor of Gut Microbial Choline Trimethylamineâ€Lyase. ChemMedChem, 2020, 15, 2273-2279.	1.6	8
49	Enzyme Promiscuity in Enolase Superfamily. Theoretical Study of o-Succinylbenzoate Synthase Using QM/MM Methods. Journal of Physical Chemistry B, 2015, 119, 1899-1911.	1.2	6
50	Molecular mechanism of the site-specific self-cleavage of the RNA phosphodiester backbone by a twister ribozyme. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
51	Combined Theoretical and Experimental Study to Unravel the Differences in Promiscuous Amidase Activity of Two Nonhomologous Enzymes. ACS Catalysis, 2021, 11, 8635-8644.	5.5	6
52	Computational design of an amidase by combining the best electrostatic features of two promiscuous hydrolases. Chemical Science, 2022, 13, 4779-4787.	3.7	6
53	Computational Studies of Candida Antarctica Lipase B to Test Its Capability as a Starting Point To Redesign New Dielsâ€“Alderases. Journal of Physical Chemistry B, 2016, 120, 2053-2070.	1.2	5
54	Theoretical studies of energetics and binding isotope effects of binding a triazole-based inhibitor to HIV-1 reverse transcriptase. Physical Chemistry Chemical Physics, 2016, 18, 310-317.	1.3	5

#	Article	IF	Citations
55	Computational Studies Suggest Promiscuous Candida antarctica Lipase B as an Environmentally Friendly Alternative for the Production of Epoxides. Journal of Chemical Information and Modeling, 2021, 61, 3604-3614.	2.5	5
56	On the Origin of the Different Reversible Characters of Salinosporamide A and Homosalinosporamide A in the Covalent Inhibition of the Human 20S Proteasome. ACS Catalysis, 2021, 11, 11806-11819.	5.5	5
57	A new scheme to calculate isotope effects. Journal of Molecular Modeling, 2011, 17, 2175-2182.	0.8	3
58	Molecular Insights into the Substrate-Assisted Mechanism of Viral DNA 3â€²-End Processing in Intasome of Prototype Foamy Virus Integrase from Molecular Dynamic and QM/MM Studies. Journal of Chemical Information and Modeling, 2019, 59, 2995-3005.	2.5	3
59	Influence of Dielectric Environment upon Isotope Effects on Glycoside Heterolysis: Computational Evaluation and Atomic Hessian Analysis. Journal of the American Chemical Society, 2020, 142, 1556-1563.	6.6	3
60	Theoretical Studies of the Self Cleavage Pistol Ribozyme Mechanism. Topics in Catalysis, 0, , 1.	1.3	3
61	Fundamental Insight into Glycoside Hydrolase-Catalyzed Hydrolysis of the Universal Koshland Substratesâ€“Glycopyranosyl Fluorides. ACS Catalysis, 2021, 11, 10383-10393.	5.5	3
62	Carbon and secondary deuterium kinetic isotope effects on S_N2 methyl transfer reactions. Journal of Physical Organic Chemistry, 2007, 20, 1114-1120.	0.9	2
63	Experimental and Computational Studies Delineate the Role of Asparagine 177 in Hydride Transfer forE. coliThymidylate Synthase. ACS Catalysis, 2018, 8, 10241-10253.	5.5	2
64	Electric Field Measurements Reveal the Pivotal Role of Cofactorâ€“Substrate Interaction in Dihydrofolate Reductase Catalysis. ACS Catalysis, 2020, 10, 7907-7914.	5.5	2
65	The role of streptavidin and its variants in catalysis by biotinylated secondary amines. Organic and Biomolecular Chemistry, 2021, 19, 10424-10431.	1.5	2
66	Examination of the performance of semiempirical methods in QM/MM studies of the SN2-like reaction of an adenylyl group transfer catalysed by ANT4â€². Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	1
67	Caught in Action: X-ray Structure of Thymidylate Synthase with Noncovalent Intermediate Analog. Biochemistry, 2021, 60, 1243-1247.	1.2	1
68	Covalent Inhibition of the Human 20S Proteasome with Homobelactosin C Inquired by QM/MM Studies. Pharmaceuticals, 2022, 15, 531.	1.7	1
69	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0