Katarzyna Åwiderek

List of Publications by Year
in descending order

69	1,431	318942	425179
papers	citations	23 h-index	34 g-index

74	74	74	1969
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational design of an amidase by combining the best electrostatic features of two promiscuous hydrolases. Chemical Science, 2022, 13, 4779-4787.	3.7	6
2	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
3	Covalent Inhibition of the Human 20S Proteasome with Homobelactosin C Inquired by QM/MM Studies. Pharmaceuticals, 2022, 15, 531.	1.7	1
4	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
5	Transfer hydrogenations catalyzed by streptavidin-hosted secondary amine organocatalysts. Chemical Communications, 2021, 57, 1919-1922.	2.2	10
6	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
7	Caught in Action: X-ray Structure of Thymidylate Synthase with Noncovalent Intermediate Analog. Biochemistry, 2021, 60, 1243-1247.	1.2	1
8	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
9	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
10	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
11	Fundamental Insight into Glycoside Hydrolase-Catalyzed Hydrolysis of the Universal Koshland Substratesâ€“Glycopyranosyl Fluorides. ACS Catalysis, 2021, 11, 10383-10393.	5.5	3
12	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
13	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54
14	The role of streptavidin and its variants in catalysis by biotinylated secondary amines. Organic and Biomolecular Chemistry, 2021, 19, 10424-10431.	1.5	2
15	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0
16	Exploring the Origin of Amidase Substrate Promiscuity in CALB by a Computational Approach. ACS Catalysis, 2020, 10, 1938-1946.	5.5	19
17	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
18	Glycoside hydrolase stabilization of transition state charge: new directions for inhibitor design. Chemical Science, 2020, 11, 10488-10495.	3.7	12

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19	Discovery of a Histidineâ€Based Scaffold as an Inhibitor of Gut Microbial Choline Trimethylamineâ€Lyase. ChemMedChem, 2020, 15, 2273-2279.	1.6	8
20	Electric Field Measurements Reveal the Pivotal Role of Cofactorâ€“Substrate Interaction in Dihydrofolate Reductase Catalysis. ACS Catalysis, 2020, 10, 7907-7914.	5.5	2
21	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
22	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
23	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
24	A Molecular Modeling Approach to Identify Novel Inhibitors of the Major Facilitator Superfamily of Efflux Pump Transporters. Antibiotics, 2019, 8, 25.	1.5	32
25	Theoretical study of the inhibition mechanism of human 20S proteasome by dihydroeponemycin. European Journal of Medicinal Chemistry, 2019, 164, 399-407.	2.6	12
26	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
27	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
28	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
29	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
30	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
31	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie - International Edition, 2018, 57, 12478-12482.	7.2	38
32	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie, 2018, 130, 12658-12662.	1.6	14
33	Revealing the mechanism for covalent inhibition of glycoside hydrolases by carbasugars at an atomic level. Nature Communications, 2018, 9, 3243.	5.8	28
34	Theoretical Studies on Mechanism of Inactivation of Kanamycin A by 4â€²-O-Nucleotidyltransferase. Frontiers in Chemistry, 2018, 6, 660.	1.8	10
35	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
36	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

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37	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
38	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
39	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
40	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
41	Catalytic enantioselective epoxidation of nitroalkenes. Chemical Communications, 2016, 52, 10060-10063.	2.2	18
42	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
43	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
44	Is Promiscuous CALB a Good Scaffold for Designing New Epoxidases?. Molecules, 2015, 20, 17789-17806.	1.7	10
45	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
46	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
47	Computational strategies for the design of new enzymatic functions. Archives of Biochemistry and Biophysics, 2015, 582, 68-79.	1.4	49
48	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
49	Peptide Bond Formation Mechanism Catalyzed by Ribosome. Journal of the American Chemical Society, 2015, 137, 12024-12034.	6.6	34
50	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
51	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
52	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
53	Predicting enzymatic reactivity: from theory to design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 407-421.	6.2	32
54	Heavy enzymesâ€”experimental and computational insights in enzyme dynamics. Current Opinion in Chemical Biology, 2014, 21, 11-18.	2.8	39

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55	Binding Isotope Effects. Chemical Reviews, 2013, 113, 7851-7879.	23.0	72
56	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
57	A theoretical study of carbonâ€“carbon bond formation by a Michael-type addition. Organic and Biomolecular Chemistry, 2012, 10, 5598.	1.5	13
58	Extending Limits of Chlorine Kinetic Isotope Effects. Journal of Organic Chemistry, 2012, 77, 5120-5124.	1.7	23
59	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. Chemical Communications, 2012, 48, 11253.	2.2	8
60	Theoretical studies of HIV-1 reverse transcriptase inhibition. Physical Chemistry Chemical Physics, 2012, 14, 12614.	1.3	24
61	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
62	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
63	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
64	A new scheme to calculate isotope effects. Journal of Molecular Modeling, 2011, 17, 2175-2182.	0.8	3
65	Importance of the Lactate Dehydrogenase Quaternary Structure in Theoretical Calculations. Journal of Physical Chemistry B, 2010, 114, 3393-3397.	1.2	15
66	Modeling excitation properties of iridium complexes. Journal of Physical Organic Chemistry, 2009, 22, 845-856.	0.9	26
67	Modeling of Isotope Effects on Binding Oxamate to Lactic Dehydrogenase. Journal of Physical Chemistry B, 2009, 113, 12782-12789.	1.2	36
68	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
69	Theoretical Studies of the Self Cleavage Pistol Ribozyme Mechanism. Topics in Catalysis, 0, , 1.	1.3	3