

Katarzyna Åwiderek

List of Publications by Year in descending order

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69
papers

1,431
citations

279487

23
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377514

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all docs

74
docs citations

74
times ranked

1794
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational design of an amidase by combining the best electrostatic features of two promiscuous hydrolases. <i>Chemical Science</i> , 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. <i>ACS Catalysis</i> , 2022, 12, 698-708.	5.5	17
3	Covalent Inhibition of the Human 20S Proteasome with Homobelactosin C Inquired by QM/MM Studies. <i>Pharmaceuticals</i> , 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. <i>Chemical Science</i> , 2021, 12, 1433-1444.	3.7	87
5	Transfer hydrogenations catalyzed by streptavidin-hosted secondary amine organocatalysts. <i>Chemical Communications</i> , 2021, 57, 1919-1922.	2.2	10
6	Nature of Irreversible Inhibition of <i>Human</i> 20S Proteasome by Salinosporamide A. The Critical Role of Lys ⁴⁸ Asp Dyad Revealed from Electrostatic Effects Analysis. <i>ACS Catalysis</i> , 2021, 11, 3575-3589.	5.5	9
7	Caught in Action: X-ray Structure of Thymidylate Synthase with Noncovalent Intermediate Analog. <i>Biochemistry</i> , 2021, 60, 1243-1247.	1.2	1
8	Enzymatic ¹³ C-Dehydrogenation of 3-Ketosteroids – Reconciliation of Kinetic Isotope Effects with the Reaction Mechanism. <i>ACS Catalysis</i> , 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. <i>ACS Catalysis</i> , 2021, 11, 8635-8644.	5.5	6
10	Computational Studies Suggest Promiscuous <i>Candida antarctica</i> Lipase B as an Environmentally Friendly Alternative for the Production of Epoxides. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3604-3614.	2.5	5
11	Fundamental Insight into Glycoside Hydrolase-Catalyzed Hydrolysis of the Universal Koshland Substrates – Glycopyranosyl Fluorides. <i>ACS Catalysis</i> , 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 <i>Human</i> 20S Proteasome. <i>ACS Catalysis</i> , 2021, 11, 11806-11819.	5.5	5
13	Discovery of SARS-CoV-2 M ^{pro} peptide inhibitors from modelling substrate and ligand binding. <i>Chemical Science</i> , 2021, 12, 13686-13703.	3.7	54
14	The role of streptavidin and its variants in catalysis by biotinylated secondary amines. <i>Organic and Biomolecular Chemistry</i> , 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. <i>ACS Catalysis</i> , 2020, 10, 1938-1946.	5.5	19
17	Influence of Dielectric Environment upon Isotope Effects on Glycoside Heterolysis: Computational Evaluation and Atomic Hessian Analysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 1556-1563.	6.6	3
18	Glycoside hydrolase stabilization of transition state charge: new directions for inhibitor design. <i>Chemical Science</i> , 2020, 11, 10488-10495.	3.7	12

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19	Discovery of a Histidine-Based Scaffold as an Inhibitor of Gut Microbial Choline Trimethylamine-Lyase. <i>ChemMedChem</i> , 2020, 15, 2273-2279.	1.6	8
20	Electric Field Measurements Reveal the Pivotal Role of Cofactor-Substrate Interaction in Dihydrofolate Reductase Catalysis. <i>ACS Catalysis</i> , 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. <i>Chemical Science</i> , 2020, 11, 10626-10630.	3.7	130
22	Examination of the performance of semiempirical methods in QM/MM studies of the SN ₂ -like reaction of an adenylyl group transfer catalysed by ANT4. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	1
23	Molecular Insights into the Substrate-Assisted Mechanism of Viral DNA 3'-End Processing in Intasome of Prototype Foamy Virus Integrase from Molecular Dynamic and QM/MM Studies. <i>Journal of Chemical Information and Modeling</i> , 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. <i>Antibiotics</i> , 2019, 8, 25.	1.5	32
25	Theoretical study of the inhibition mechanism of human 20S proteasome by dihydroepone mycin. <i>European Journal of Medicinal Chemistry</i> , 2019, 164, 399-407.	2.6	12
26	Insights on the Origin of Catalysis on Glycine N-Methyltransferase from Computational Modeling. <i>Journal of the American Chemical Society</i> , 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. <i>Journal of Physical Chemistry A</i> , 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. <i>ACS Omega</i> , 2018, 3, 18613-18622.	1.6	14
29	Parallel reaction pathways and noncovalent intermediates in thymidylate synthase revealed by experimental and computational tools. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 10311-10314.	3.3	8
30	Experimental and Computational Studies Delineate the Role of Asparagine 177 in Hydride Transfer for E. coli Thymidylate Synthase. <i>ACS Catalysis</i> , 2018, 8, 10241-10253.	5.5	2
31	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 12478-12482.	7.2	38
32	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. <i>Angewandte Chemie</i> , 2018, 130, 12658-12662.	1.6	14
33	Revealing the mechanism for covalent inhibition of glycoside hydrolases by carbasugars at an atomic level. <i>Nature Communications</i> , 2018, 9, 3243.	5.8	28
34	Theoretical Studies on Mechanism of Inactivation of Kanamycin A by 4-O-Nucleotidyltransferase. <i>Frontiers in Chemistry</i> , 2018, 6, 660.	1.8	10
35	Benchmarking Quantum Mechanics/Molecular Mechanics (QM/MM) Methods on the Thymidylate Synthase-Catalyzed Hydride Transfer. <i>Journal of Chemical Theory and Computation</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 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 HG3.17 by Comparison with the Former Developed HG3. 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 Diels-Alderses. 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 <i>o</i> -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 enzymes—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. <i>Chemical Reviews</i> , 2013, 113, 7851-7879.	23.0	72
56	Role of Solvent on Nonenzymatic Peptide Bond Formation Mechanisms and Kinetic Isotope Effects. <i>Journal of the American Chemical Society</i> , 2013, 135, 8708-8719.	6.6	23
57	A theoretical study of carbon-carbon bond formation by a Michael-type addition. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 5598.	1.5	13
58	Extending Limits of Chlorine Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2012, 77, 5120-5124.	1.7	23
59	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. <i>Chemical Communications</i> , 2012, 48, 11253.	2.2	8
60	Theoretical studies of HIV-1 reverse transcriptase inhibition. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Journal of Molecular Modeling</i> , 2012, 18, 843-849.	0.8	10
62	Binding Ligands and Cofactor to L-Lactate Dehydrogenase from Human Skeletal and Heart Muscles. <i>Journal of Physical Chemistry B</i> , 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. <i>Archives of Biochemistry and Biophysics</i> , 2011, 505, 33-41.	1.4	16
64	A new scheme to calculate isotope effects. <i>Journal of Molecular Modeling</i> , 2011, 17, 2175-2182.	0.8	3
65	Importance of the Lactate Dehydrogenase Quaternary Structure in Theoretical Calculations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3393-3397.	1.2	15
66	Modeling excitation properties of iridium complexes. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 845-856.	0.9	26
67	Modeling of Isotope Effects on Binding Oxamate to Lactic Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 12782-12789.	1.2	36
68	Carbon and secondary deuterium kinetic isotope effects on S _N 2 methyl transfer reactions. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 1114-1120.	0.9	2
69	Theoretical Studies of the Self Cleavage Pistol Ribozyme Mechanism. <i>Topics in Catalysis</i> , 0, , 1.	1.3	3