Andrew F Zahrt

List of Publications by Year
in descending order

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11 papers	869 citations	933447 10 h-index	1281871 11 g-index
13 all docs	13 docs citations	13 times ranked	1049 citing authors

#	Article	IF	Citations
1	Prediction of higher-selectivity catalysts by computer-driven workflow and machine learning. Science, 2019, 363, .	12.6	335
2	Structural, Kinetic, and Computational Characterization of the Elusive Arylpalladium(II)boronate Complexes in the Suzukiâ€“Miyaura Reaction. Journal of the American Chemical Society, 2017, 139, 3805-3821.	13.7	138
3	Quantitative Structureâ€“Selectivity Relationships in Enantioselective Catalysis: Past, Present, and Future. Chemical Reviews, 2020, 120, 1620-1689.	47.7	117
4	Elucidating the Role of the Boronic Esters in the Suzukiâ€“Miyaura Reaction: Structural, Kinetic, and Computational Investigations. Journal of the American Chemical Society, 2018, 140, 4401-4416.	13.7	109
5	Development of a Computer-Guided Workflow for Catalyst Optimization. Descriptor Validation, Subset Selection, and Training Set Analysis. Journal of the American Chemical Society, 2020, 142, 11578-11592.	13.7	48
6	Dreams, False Starts, Dead Ends, and Redemption: A Chronicle of the Evolution of a Chemoinformatic Workflow for the Optimization of Enantioselective Catalysts. Accounts of Chemical Research, 2021, 54, 2041-2054.	15.6	31
7	Evaluating continuous chirality measure as a 3D descriptor in chemoinformatics applied to asymmetric catalysis. Tetrahedron, 2019, 75, 1841-1851.	1.9	25
8	Cautionary Guidelines for Machine Learning Studies with Combinatorial Datasets. ACS Combinatorial Science, 2020, 22, 586-591.	3.8	25
9	Continuous stirred-tank reactor cascade platform for self-optimization of reactions involving solids. Reaction Chemistry and Engineering, 2022, 7, 1315-1327.	3.7	22
10	Computational methods for training set selection and error assessment applied to catalyst design: guidelines for deciding which reactions to run first and which to run next. Reaction Chemistry and Engineering, 2021, 6, 694-708.	3.7	12
11	A Conformerâ€Dependent, Quantitative Quadrant Model. European Journal of Organic Chemistry, 2021, 2021, 2343-2354.	2.4	7