AARON: An Automated Reaction Optimizer for New Ca

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Citation Report

#	Article	IF	Citations
1	Importance of thorough conformational analysis in modelling transition metal-mediated reactions: Case studies on pincer complexes containing phosphine groups. Journal of Saudi Chemical Society, 2019, 23, 1206-1218.	2.4	6
2	Automatic Conformational Search of Transition States for Catalytic Reactions Using Genetic Algorithm. Journal of Physical Chemistry A, 2019, 123, 10303-10314.	1.1	11
3	Computational assessment on the Tolman cone angles for P-ligands. Dalton Transactions, 2019, 48, 15036-15048.	1.6	62
4	Relative Strength of Common Directing Groups in Palladium-Catalyzed Aromatic Câ^'H Activation. IScience, 2019, 20, 373-391.	1.9	34
5	Integration of machine learning approaches for accelerated discovery of transition-metal dichalcogenides as Hg0 sensing materials. Applied Energy, 2019, 254, 113651.	5.1	21
6	A Computational Study on the Stereo- and Regioselective Formation of the C4Î±â€“C6â€² Bond of Tethered Catechin Moieties by an Exhaustive Search of the Transition States. Journal of Organic Chemistry, 2019, 84, 2840-2849.	1.7	3
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9	Automatic Proposal of Multistep Reaction Mechanisms using a Graph-Driven Search. Journal of Physical Chemistry A, 2019, 123, 3407-3417.	1.1	35
10	Computational Ligand Descriptors for Catalyst Design. Chemical Reviews, 2019, 119, 6561-6594.	23.0	254
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18	Established and Emerging Computational Tools to Study Homogeneous Catalysisâ€”From Quantum Mechanics to Machine Learning. CheM, 2020, 6, 1904-1913.	5.8	44

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20	How does the nickel catalyst control the doubly enantioconvergent coupling of racemic alkyl nucleophiles and electrophiles? The rebound mechanism. Organic Chemistry Frontiers, 2020, 7, 3411-3419.	2.3	8
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