Automated Quantum Mechanical Predictions of Enanti
Asymmetric Hydrogenation

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Citation Report

#	Article	IF	Citations
1	Rational Optimization of Supramolecular Catalysts for the Rhodiumâ€Catalyzed Asymmetric Hydrogenation Reaction. Angewandte Chemie, 2017, 129, 13236-13240.	1.6	6
2	Rational Optimization of Supramolecular Catalysts for the Rhodiumâ€Catalyzed Asymmetric Hydrogenation Reaction. Angewandte Chemie - International Edition, 2017, 56, 13056-13060.	7.2	30
3	Enantioselectivity in CPA-catalyzed Friedelâ€“Crafts reaction of indole and N-tosylimines: a challenge for guiding models. Organic and Biomolecular Chemistry, 2018, 16, 2225-2238.	1.5	11
4	The True Catalyst Revealed: The Intervention of Chiral Ca and Mg Phosphates in BrÃ¸nsted Acid Promoted Asymmetric Mannich Reactions. Journal of the American Chemical Society, 2018, 140, 5412-5420.	6.6	21
5	Mechanistically Guided Design of Ligands That Significantly Improve the Efficiency of CuH-Catalyzed Hydroamination Reactions. Journal of the American Chemical Society, 2018, 140, 13976-13984.	6.6	101
6	Comparing quantitative prediction methods for the discovery of small-molecule chiral catalysts. Nature Reviews Chemistry, 2018, 2, 290-305.	13.8	100
7	Computationally Assisted Mechanistic Investigation and Development of Pd-Catalyzed Asymmetric Suzukiâ€“Miyaura and Negishi Cross-Coupling Reactions for Tetra-ortho-Substituted Biaryl Synthesis. ACS Catalysis, 2018, 8, 10190-10209.	5.5	70
8	Rhodium-catalyzed asymmetric hydrogenation of Î²-branched enamides for the synthesis of Î²-stereogenic amines. Chemical Communications, 2018, 54, 6024-6027.	2.2	38
9	Expedited Screening of Active and Regioselective Catalysts for the Hydroformylation Reaction. Helvetica Chimica Acta, 2018, 101, e1800107.	1.0	19
10	AARON: An Automated Reaction Optimizer for New Catalysts. Journal of Chemical Theory and Computation, 2018, 14, 5249-5261.	2.3	103
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12	Questions in natural products synthesis research that can (and cannot) be answered using computational chemistry. Chemical Society Reviews, 2018, 47, 7845-7850.	18.7	28
13	Origin of the Selectivity and Activity in the Rhodium-Catalyzed Asymmetric Hydrogenation Using Supramolecular Ligands. ACS Catalysis, 2019, 9, 7535-7547.	5.5	18
15	Conformational Effects on Physical-Organic Descriptors: The Case of Sterimol Steric Parameters. ACS Catalysis, 2019, 9, 2313-2323.	5.5	96
16	Activity-Based Screening of Homogeneous Catalysts through the Rapid Assessment of Theoretically Derived Turnover Frequencies. ACS Catalysis, 2019, 9, 5716-5725.	5.5	48
17	Catalytic Homogeneous Asymmetric Hydrogenation: Successes and Opportunities. Organometallics, 2019, 38, 47-65.	1.1	184
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20	A Predictive Tool for Electrophilic Aromatic Substitutions Using Machine Learning. Journal of Organic Chemistry, 2019, 84, 4695-4703.	1.7	70

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21	Practical and efficient preparation of the chiral 4-bromotryptophan derivative by Rh-catalyzed hydrogenation. Tetrahedron Letters, 2020, 61, 151498.	0.7	2
22	Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. Organic Process Research and Development, 2020, 24, 1496-1507.	1.3	25
24	New Directions in the Modeling of Organometallic Reactions. Topics in Organometallic Chemistry, 2020, , .	0.7	1
25	Revealing the Strong Relationships between Ligand Conformers and Activation Barriers: A Case Study of Bisphosphine Reductive Elimination. ACS Catalysis, 2020, 10, 7136-7145.	5.5	25
26	Ligand Design for Asymmetric Catalysis: Combining Mechanistic and Chemoinformatics Approaches. Topics in Organometallic Chemistry, 2020, , 153-189.	0.7	1
27	Automated in Silico Design of Homogeneous Catalysts. ACS Catalysis, 2020, 10, 2354-2377.	5.5	119
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30	Scaffoldâ€Directed Face Selectivity Machineâ€Learned from Vectors of Nonâ€covalent Interactions. Angewandte Chemie - International Edition, 2021, 60, 15230-15235.	7.2	19
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32	Automated Construction and Optimization Combined with Machine Learning to Generate Pt(II) Methane Câ€“H Activation Transition States. Topics in Catalysis, 2022, 65, 312-324.	1.3	11
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34	Generating transition states of isomerization reactions with deep learning. Physical Chemistry Chemical Physics, 2020, 22, 23618-23626.	1.3	35
35	Computational insights into metal-catalyzed asymmetric hydrogenation. Advances in Catalysis, 2021, 68, 385-426.	0.1	1
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38	Virtual Ligand Strategy in Transition Metal Catalysis Toward Highly Efficient Elucidation of Reaction Mechanisms and Computational Catalyst Design. ACS Catalysis, 2023, 13, 5697-5711.	5.5	3