

Marwin H S Segler

List of Publications by Year in descending order

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Version: 2024-02-01

13
papers

4,598
citations

759233

12
h-index

1125743

13
g-index

14
all docs

14
docs citations

14
times ranked

5733
citing authors

#	ARTICLE	IF	CITATIONS
1	Improving Few- and Zero-Shot Reaction Template Prediction Using Modern Hopfield Networks. Journal of Chemical Information and Modeling, 2022, 62, 2111-2120.	5.4	30
2	RetroGNN: Fast Estimation of Synthesizability for Virtual Screening and De Novo Design by Learning from Slow Retrosynthesis Software. Journal of Chemical Information and Modeling, 2022, 62, 2293-2300.	5.4	12
3	Evaluation guidelines for machine learning tools in the chemical sciences. Nature Reviews Chemistry, 2022, 6, 428-442.	30.2	49
4	Machine learning the ropes: principles, applications and directions in synthetic chemistry. Chemical Society Reviews, 2020, 49, 6154-6168.	38.1	148
5	GuacaMol: Benchmarking Models for de Novo Molecular Design. Journal of Chemical Information and Modeling, 2019, 59, 1096-1108.	5.4	383
6	Opportunities and obstacles for deep learning in biology and medicine. Journal of the Royal Society Interface, 2018, 15, 20170387.	3.4	1,282
7	Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks. ACS Central Science, 2018, 4, 120-131.	11.3	908
8	Planning chemical syntheses with deep neural networks and symbolic AI. Nature, 2018, 555, 604-610.	27.8	1,122
9	Artificial intelligence in drug discovery. Future Medicinal Chemistry, 2018, 10, 2025-2028.	2.3	74
10	Neural-Symbolic Machine Learning for Retrosynthesis and Reaction Prediction. Chemistry - A European Journal, 2017, 23, 5966-5971.	3.3	334
11	Modelling Chemical Reasoning to Predict and Invent Reactions. Chemistry - A European Journal, 2017, 23, 6118-6128.	3.3	142
12	Dehydrogenative TEMPO-Mediated Formation of Unstable Nitrones: Easy Access to <i>N</i> -Carbamoyl Isoxazolines. Chemistry - A European Journal, 2015, 21, 12053-12060.	3.3	23
13	Silver-Catalyzed 1,3-Dipolar Cycloaddition of Azomethine Ylides with β -Boryl Acrylates. Journal of Organic Chemistry, 2011, 76, 1945-1948.	3.2	29