Marwin H S Segler

List of Publications by Year
in descending order

13	4,598	759233 12	1125743 13
papers	citations	h-index	g-index

14	14	14	5733
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Opportunities and obstacles for deep learning in biology and medicine. Journal of the Royal Society Interface, 2018, 15, 20170387.	3.4	1,282
2	Planning chemical syntheses with deep neural networks and symbolic AI. Nature, 2018, 555, 604-610.	27.8	1,122
3	Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks. ACS Central Science, 2018, 4, 120-131.	11.3	908
4	GuacaMol: Benchmarking Models for de Novo Molecular Design. Journal of Chemical Information and Modeling, 2019, 59, 1096-1108.	5.4	383
5	Neuralâ€Symbolic Machine Learning for Retrosynthesis and Reaction Prediction. Chemistry - A European Journal, 2017, 23, 5966-5971.	3.3	334
6	Machine learning the ropes: principles, applications and directions in synthetic chemistry. Chemical Society Reviews, 2020, 49, 6154-6168.	38.1	148
7	Modelling Chemical Reasoning to Predict and Invent Reactions. Chemistry - A European Journal, 2017, 23, 6118-6128.	3.3	142
8	Artificial intelligence in drug discovery. Future Medicinal Chemistry, 2018, 10, 2025-2028.	2.3	74
9	Evaluation guidelines for machine learning tools in the chemical sciences. Nature Reviews Chemistry, 2022, 6, 428-442.	30.2	49
10	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
11	Silver-Catalyzed 1,3-Dipolar Cycloaddition of Azomethine Ylides with Î²-Boryl Acrylates. Journal of Organic Chemistry, 2011, 76, 1945-1948.	3.2	29
12	Dehydrogenative TEMPOâ€Mediated Formation of Unstable Nitrones: Easy Access to Nâ€Carbamoyl Isoxazolines. Chemistry - A European Journal, 2015, 21, 12053-12060.	3.3	23
13	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