Philippe Schwaller

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8639473/publications.pdf

Version: 2024-02-01

19	3,066	567144 15	839398 18
papers	citations	h-index	g-index

50	50	50	3899
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reaction classification and yield prediction using the differential reaction fingerprint DRFP. , 2022, 1, 91-97.		45
2	Machine intelligence for chemical reaction space. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	30
3	Predicting enzymatic reactions with a molecular transformer. Chemical Science, 2021, 12, 8648-8659.	3.7	43
4	Prediction of chemical reaction yields using deep learning. Machine Learning: Science and Technology, 2021, 2, 015016.	2.4	106
5	Unassisted noise reduction of chemical reaction datasets. Nature Machine Intelligence, 2021, 3, 485-494.	8.3	24
6	Extraction of organic chemistry grammar from unsupervised learning of chemical reactions. Science Advances, 2021, 7, .	4.7	98
7	Inferring experimental procedures from text-based representations of chemical reactions. Nature Communications, 2021, 12, 2573.	5.8	28
8	How AI for Synthesis Can Help Tackle Challenges in Molecular Discovery. Chimia, 2021, 75, 677-678.	0.3	2
9	Mapping the space of chemical reactions using attention-based neural networks. Nature Machine Intelligence, 2021, 3, 144-152.	8.3	121
10	Transfer learning enables the molecular transformer to predict regio- and stereoselective reactions on carbohydrates. Nature Communications, 2020, 11, 4874.	5.8	107
11	Automated extraction of chemical synthesis actions from experimental procedures. Nature Communications, 2020, 11, 3601.	5.8	89
12	Exploring chemical space using natural language processing methodologies for drug discovery. Drug Discovery Today, 2020, 25, 689-705.	3.2	68
13	Predicting retrosynthetic pathways using transformer-based models and a hyper-graph exploration strategy. Chemical Science, 2020, 11, 3316-3325.	3.7	176
14	Molecular Transformer: A Model for Uncertainty-Calibrated Chemical Reaction Prediction. ACS Central Science, 2019, 5, 1572-1583.	5.3	424
15	Data-driven Chemical Reaction Prediction and Retrosynthesis. Chimia, 2019, 73, 997.	0.3	19
16	Data-Driven Learning Systems for Chemical Reaction Prediction: An Analysis of Recent Approaches. ACS Symposium Series, 2019, , 61-79.	0.5	11
17	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotechnology, 2018, 13, 246-252.	15.6	1,317
18	Insights into photovoltaic properties of ternary organic solar cells from phase diagrams. Science and Technology of Advanced Materials, 2018, 19, 669-682.	2.8	13

#	Article	IF	Citations
19	â€œFound in Translationâ€: predicting outcomes of complex organic chemistry reactions using neural sequence-to-sequence models. Chemical Science, 2018, 9, 6091-6098.	3.7	269