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

#	Article	IF	Citations
19	How AI for Synthesis Can Help Tackle Challenges in Molecular Discovery. Chimia, 2021, 75, 677-678.	0.3	2