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List of Publications by Year in descending order

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Version: 2024-02-01

58
papers

6,158
citations

126708

33
h-index

138251

58
g-index

71
all docs

71
docs citations

71
times ranked

4224
citing authors

#	ARTICLE	IF	CITATIONS
1	Analyzing Learned Molecular Representations for Property Prediction. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3370-3388.	2.5	773
2	A robotic platform for flow synthesis of organic compounds informed by AI planning. <i>Science</i> , 2019, 365, .	6.0	548
3	Prediction of Organic Reaction Outcomes Using Machine Learning. <i>ACS Central Science</i> , 2017, 3, 434-443.	5.3	477
4	Machine Learning in Computer-Aided Synthesis Planning. <i>Accounts of Chemical Research</i> , 2018, 51, 1281-1289.	7.6	430
5	A graph-convolutional neural network model for the prediction of chemical reactivity. <i>Chemical Science</i> , 2019, 10, 370-377.	3.7	430
6	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1757-1772.	2.5	317
7	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. <i>ACS Central Science</i> , 2018, 4, 1465-1476.	5.3	245
8	Computer-Assisted Retrosynthesis Based on Molecular Similarity. <i>ACS Central Science</i> , 2017, 3, 1237-1245.	5.3	200
9	Autonomous Discovery in the Chemical Sciences Partâ€¦I: Progress. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 22858-22893.	7.2	180
10	SCScore: Synthetic Complexity Learned from a Reaction Corpus. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 252-261.	2.5	176
11	The Synthesizability of Molecules Proposed by Generative Models. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5714-5723.	2.5	149
12	Autonomous Discovery in the Chemical Sciences Partâ€¦II: Outlook. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23414-23436.	7.2	139
13	BigSMILES: A Structurally-Based Line Notation for Describing Macromolecules. <i>ACS Central Science</i> , 2019, 5, 1523-1531.	5.3	134
14	Uncertainty Quantification Using Neural Networks for Molecular Property Prediction. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3770-3780.	2.5	129
15	Automated microfluidic platform for systematic studies of colloidal perovskite nanocrystals: towards continuous nano-manufacturing. <i>Lab on A Chip</i> , 2017, 17, 4040-4047.	3.1	118
16	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 8667-8682.	2.9	118
17	Accelerating high-throughput virtual screening through molecular pool-based active learning. <i>Chemical Science</i> , 2021, 12, 7866-7881.	3.7	115
18	The Open Reaction Database. <i>Journal of the American Chemical Society</i> , 2021, 143, 18820-18826.	6.6	112

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19	Photoredox Iridium–Nickel Dual-Catalyzed Decarboxylative Arylation Cross-Coupling: From Batch to Continuous Flow via Self-Optimizing Segmented Flow Reactor. <i>Organic Process Research and Development</i> , 2018, 22, 542-550.	1.3	101
20	Learning Retrosynthetic Planning through Simulated Experience. <i>ACS Central Science</i> , 2019, 5, 970-981.	5.3	97
21	RDChiral: An RDKit Wrapper for Handling Stereochemistry in Retrosynthetic Template Extraction and Application. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2529-2537.	2.5	96
22	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. <i>Chemical Science</i> , 2021, 12, 2198-2208.	3.7	75
23	Oscillatory Microprocessor for Growth and in Situ Characterization of Semiconductor Nanocrystals. <i>Chemistry of Materials</i> , 2015, 27, 6131-6138.	3.2	74
24	A segmented flow platform for on-demand medicinal chemistry and compound synthesis in oscillating droplets. <i>Chemical Communications</i> , 2017, 53, 6649-6652.	2.2	73
25	Evidential Deep Learning for Guided Molecular Property Prediction and Discovery. <i>ACS Central Science</i> , 2021, 7, 1356-1367.	5.3	73
26	Optimum catalyst selection over continuous and discrete process variables with a single droplet microfluidic reaction platform. <i>Reaction Chemistry and Engineering</i> , 2018, 3, 301-311.	1.9	69
27	Defining and Exploring Chemical Spaces. <i>Trends in Chemistry</i> , 2021, 3, 133-145.	4.4	60
28	Material–Efficient Microfluidic Platform for Exploratory Studies of Visible–Light Photoredox Catalysis. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9847-9850.	7.2	46
29	Data Augmentation and Pretraining for Template-Based Retrosynthetic Prediction in Computer-Aided Synthesis Planning. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3398-3407.	2.5	44
30	Machine learning modeling of family wide enzyme-substrate specificity screens. <i>PLoS Computational Biology</i> , 2022, 18, e1009853.	1.5	41
31	Molecular Representation: Going Long on Fingerprints. <i>CheM</i> , 2020, 6, 1204-1207.	5.8	39
32	Quantum chemistry-augmented neural networks for reactivity prediction: Performance, generalizability, and explainability. <i>Journal of Chemical Physics</i> , 2022, 156, 084104.	1.2	37
33	Multitask prediction of site selectivity in aromatic C–H functionalization reactions. <i>Reaction Chemistry and Engineering</i> , 2020, 5, 896-902.	1.9	35
34	Deep learning driven biosynthetic pathways navigation for natural products with BioNavi-NP. <i>Nature Communications</i> , 2022, 13, .	5.8	35
35	In–Situ Microfluidic Study of Biphasic Nanocrystal Ligand–Exchange Reactions Using an Oscillatory Flow Reactor. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 16333-16337.	7.2	34
36	Evaluating and clustering retrosynthesis pathways with learned strategy. <i>Chemical Science</i> , 2021, 12, 1469-1478.	3.7	34

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37	Flow chemistry-enabled studies of rhodium-catalyzed hydroformylation reactions. <i>Chemical Communications</i> , 2018, 54, 8567-8570.	2.2	32
38	Towards efficient discovery of green synthetic pathways with Monte Carlo tree search and reinforcement learning. <i>Chemical Science</i> , 2020, 11, 10959-10972.	3.7	31
39	Multiphase Oscillatory Flow Strategy for In Situ Measurement and Screening of Partition Coefficients. <i>Analytical Chemistry</i> , 2015, 87, 11130-11136.	3.2	26
40	Automated Chemical Reaction Extraction from Scientific Literature. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2035-2045.	2.5	26
41	Autonomous platforms for data-driven organic synthesis. <i>Nature Communications</i> , 2022, 13, 1075.	5.8	25
42	Machine Learning on DNA-Encoded Library Count Data Using an Uncertainty-Aware Probabilistic Loss Function. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2316-2331.	2.5	20
43	Ligand-Mediated Nanocrystal Growth. <i>Langmuir</i> , 2018, 34, 3307-3315.	1.6	19
44	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. <i>Frontiers in Chemical Engineering</i> , 2020, 2, .	1.3	16
45	Material-Efficient Microfluidic Platform for Exploratory Studies of Visible-Light Photoredox Catalysis. <i>Angewandte Chemie</i> , 2017, 129, 9979-9982.	1.6	11
46	Autonome Entdeckung in den chemischen Wissenschaften, Teil I: Fortschritt. <i>Angewandte Chemie</i> , 2020, 132, 23054-23091.	1.6	11
47	Improving the performance of models for one-step retrosynthesis through re-ranking. <i>Journal of Cheminformatics</i> , 2022, 14, 15.	2.8	10
48	Similarity based enzymatic retrosynthesis. <i>Chemical Science</i> , 2022, 13, 6039-6053.	3.7	10
49	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4949-4961.	2.5	7
50	In Situ Microfluidic Study of Biphasic Nanocrystal Ligand-Exchange Reactions Using an Oscillatory Flow Reactor. <i>Angewandte Chemie</i> , 2017, 129, 16551-16555.	1.6	5
51	Combining retrosynthesis and mixed-integer optimization for minimizing the chemical inventory needed to realize a WHO essential medicines list. <i>Reaction Chemistry and Engineering</i> , 2020, 5, 367-376.	1.9	5
52	Direct Optimization across Computer-Generated Reaction Networks Balances Materials Use and Feasibility of Synthesis Plans for Molecule Libraries. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 493-504.	2.5	5
53	A focus on simulation and machine learning as complementary tools for chemical space navigation. <i>Chemical Science</i> , 2022, 13, 8221-8223.	3.7	5
54	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. <i>Angewandte Chemie</i> , 2020, 132, 23620-23643.	1.6	4

#	ARTICLE	IF	CITATIONS
55	Machine learned prediction of reaction template applicability for data-driven retrosynthetic predictions of energetic materials. AIP Conference Proceedings, 2020, , .	0.3	3
56	A Modular Microfluidic Technology for Systematic Studies of Colloidal Semiconductor Nanocrystals. Journal of Visualized Experiments, 2018, , .	0.2	2
57	pyscreener: A Python Wrapper for Computational Docking Software. Journal of Open Source Software, 2022, 7, 3950.	2.0	2
58	Editorial overview: Understanding, predicting, and optimizing biomolecular interactions with machine learning. Current Opinion in Chemical Biology, 2021, 65, A1-A3.	2.8	0