Connor W Coley

List of Publications by Year
in descending order

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58 papers	6,158 citations	126907 33 h-index	138484 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. Journal of Chemical Information and Modeling, 2019, 59, 3370-3388.	5.4	773
2	A robotic platform for flow synthesis of organic compounds informed by AI planning. Science, 2019, 365, .	12.6	548
3	Prediction of Organic Reaction Outcomes Using Machine Learning. ACS Central Science, 2017, 3, 434-443.	11.3	477
4	Machine Learning in Computer-Aided Synthesis Planning. Accounts of Chemical Research, 2018, 51, 1281-1289.	15.6	430
5	A graph-convolutional neural network model for the prediction of chemical reactivity. Chemical Science, 2019, 10, 370-377.	7.4	430
6	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. Journal of Chemical Information and Modeling, 2017, 57, 1757-1772.	5.4	317
7	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. ACS Central Science, 2018, 4, 1465-1476.	11.3	245
8	Computer-Assisted Retrosynthesis Based on Molecular Similarity. ACS Central Science, 2017, 3, 1237-1245.	11.3	200
9	Autonomous Discovery in the Chemical Sciences Partâ€...I: Progress. Angewandte Chemie - International Edition, 2020, 59, 22858-22893.	13.8	180
10	SCScore: Synthetic Complexity Learned from a Reaction Corpus. Journal of Chemical Information and Modeling, 2018, 58, 252-261.	5.4	176
11	The Synthesizability of Molecules Proposed by Generative Models. Journal of Chemical Information and Modeling, 2020, 60, 5714-5723.	5.4	149
12	Autonomous Discovery in the Chemical Sciences Partâ€...II: Outlook. Angewandte Chemie - International Edition, 2020, 59, 23414-23436.	13.8	139
13	BigSMILES: A Structurally-Based Line Notation for Describing Macromolecules. ACS Central Science, 2019, 5, 1523-1531.	11.3	134
14	Uncertainty Quantification Using Neural Networks for Molecular Property Prediction. Journal of Chemical Information and Modeling, 2020, 60, 3770-3780.	5.4	129
15	Automated microfluidic platform for systematic studies of colloidal perovskite nanocrystals: towards continuous nano-manufacturing. Lab on A Chip, 2017, 17, 4040-4047.	6.0	118
16	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. Journal of Medicinal Chemistry, 2020, 63, 8667-8682.	6.4	118
17	Accelerating high-throughput virtual screening through molecular pool-based active learning. Chemical Science, 2021, 12, 7866-7881.	7.4	115
18	The Open Reaction Database. Journal of the American Chemical Society, 2021, 143, 18820-18826.	13.7	112

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19	Photoredox Iridiumâ€“Nickel Dual-Catalyzed Decarboxylative Arylation Cross-Coupling: From Batch to Continuous Flow via Self-Optimizing Segmented Flow Reactor. Organic Process Research and Development, 2018, 22, 542-550.	2.7	101
20	Learning Retrosynthetic Planning through Simulated Experience. ACS Central Science, 2019, 5, 970-981.	11.3	97
21	RDChiral: An RDKit Wrapper for Handling Stereochemistry in Retrosynthetic Template Extraction and Application. Journal of Chemical Information and Modeling, 2019, 59, 2529-2537.	5.4	96
22	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. Chemical Science, 2021, 12, 2198-2208.	7.4	75
23	Oscillatory Microprocessor for Growth and in Situ Characterization of Semiconductor Nanocrystals. Chemistry of Materials, 2015, 27, 6131-6138.	6.7	74
24	A segmented flow platform for on-demand medicinal chemistry and compound synthesis in oscillating droplets. Chemical Communications, 2017, 53, 6649-6652.	4.1	73
25	Evidential Deep Learning for Guided Molecular Property Prediction and Discovery. ACS Central Science, 2021, 7, 1356-1367.	11.3	73
26	Optimum catalyst selection over continuous and discrete process variables with a single droplet microfluidic reaction platform. Reaction Chemistry and Engineering, 2018, 3, 301-311.	3.7	69
27	Defining and Exploring Chemical Spaces. Trends in Chemistry, 2021, 3, 133-145.	8.5	60
28	Materialâ€Efficient Microfluidic Platform for Exploratory Studies of Visibleâ€Light Photoredox Catalysis. Angewandte Chemie - International Edition, 2017, 56, 9847-9850.	13.8	46
29	Data Augmentation and Pretraining for Template-Based Retrosynthetic Prediction in Computer-Aided Synthesis Planning. Journal of Chemical Information and Modeling, 2020, 60, 3398-3407.	5.4	44
30	Machine learning modeling of family wide enzyme-substrate specificity screens. PLoS Computational Biology, 2022, 18, e1009853.	3.2	41
31	Molecular Representation: Going Long on Fingerprints. CheM, 2020, 6, 1204-1207.	11.7	39
32	Quantum chemistry-augmented neural networks for reactivity prediction: Performance, generalizability, and explainability. Journal of Chemical Physics, 2022, 156, 084104.	3.0	37
33	Multitask prediction of site selectivity in aromatic Câ€“H functionalization reactions. Reaction Chemistry and Engineering, 2020, 5, 896-902.	3.7	35
34	Deep learning driven biosynthetic pathways navigation for natural products with BioNavi-NP. Nature Communications, 2022, 13, .	12.8	35
35	Inâ€Situ Microfluidic Study of Biphasic Nanocrystal Ligandâ€Exchange Reactions Using an Oscillatory Flow Reactor. Angewandte Chemie - International Edition, 2017, 56, 16333-16337.	13.8	34
36	Evaluating and clustering retrosynthesis pathways with learned strategy. Chemical Science, 2021, 12, 1469-1478.	7.4	34

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37	Flow chemistry-enabled studies of rhodium-catalyzed hydroformylation reactions. Chemical Communications, 2018, 54, 8567-8570.	4.1	32
38	Towards efficient discovery of green synthetic pathways with Monte Carlo tree search and reinforcement learning. Chemical Science, 2020, 11, 10959-10972.	7.4	31
39	Multiphase Oscillatory Flow Strategy forin SituMeasurement and Screening of Partition Coefficients. Analytical Chemistry, 2015, 87, 11130-11136.	6.5	26
40	Automated Chemical Reaction Extraction from Scientific Literature. Journal of Chemical Information and Modeling, 2022, 62, 2035-2045.	5.4	26
41	Autonomous platforms for data-driven organic synthesis. Nature Communications, 2022, 13, 1075.	12.8	25
42	Machine Learning on DNA-Encoded Library Count Data Using an Uncertainty-Aware Probabilistic Loss Function. Journal of Chemical Information and Modeling, 2022, 62, 2316-2331.	5.4	20
43	Ligand-Mediated Nanocrystal Growth. Langmuir, 2018, 34, 3307-3315.	3.5	19
44	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. Frontiers in Chemical Engineering, 2020, 2, .	2.7	16
45	Materialâ€Efficient Microfluidic Platform for Exploratory Studies of Visibleâ€Light Photoredox Catalysis. Angewandte Chemie, 2017, 129, 9979-9982.	2.0	11
46	Autonome Entdeckung in den chemischen Wissenschaften, Teilâ€…I: Fortschritt. Angewandte Chemie, 2020, 132, 23054-23091.	2.0	11
47	Improving the performance of models for one-step retrosynthesis through re-ranking. Journal of Cheminformatics, 2022, 14, 15.	6.1	10
48	Similarity based enzymatic retrosynthesis. Chemical Science, 2022, 13, 6039-6053.	7.4	10
49	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. Journal of Chemical Information and Modeling, 2021, 61, 4949-4961.	5.4	7
50	Inâ€Situ Microfluidic Study of Biphasic Nanocrystal Ligandâ€Exchange Reactions Using an Oscillatory Flow Reactor. Angewandte Chemie, 2017, 129, 16551-16555.	2.0	5
51	Combining retrosynthesis and mixed-integer optimization for minimizing the chemical inventory needed to realize a WHO essential medicines list. Reaction Chemistry and Engineering, 2020, 5, 367-376.	3.7	5
52	Direct Optimization across Computer-Generated Reaction Networks Balances Materials Use and Feasibility of Synthesis Plans for Molecule Libraries. Journal of Chemical Information and Modeling, 2021, 61, 493-504.	5.4	5
53	A focus on simulation and machine learning as complementary tools for chemical space navigation. Chemical Science, 2022, 13, 8221-8223.	7.4	5
54	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. Angewandte Chemie, 2020, 132, 23620-23643.	2.0	4

#	Article	IF	Citations
55	Machine learned prediction of reaction template applicability for data-driven retrosynthetic predictions of energetic materials. AIP Conference Proceedings, 2020, , .	0.4	3
56	A Modular Microfluidic Technology for Systematic Studies of Colloidal Semiconductor Nanocrystals. Journal of Visualized Experiments, 2018, , .	0.3	2
57	pyscreener: A Python Wrapper for Computational Docking Software. Journal of Open Source Software, 2022, 7, 3950.	4.6	2
58	Editorial overview: Understanding, predicting, and optimizing biomolecular interactions with machine learning. Current Opinion in Chemical Biology, 2021, 65, A1-A3.	6.1	0