Connor W Coley

List of Publications by Citations

53 papers	2,959 citations	25 h-index	54 g-index
71 ext. papers	4,455 ext. citations	9.5 avg, IF	6.21 L-index

#	Paper	IF	Citations
53	Prediction of Organic Reaction Outcomes Using Machine Learning. *ACS Central Science*, **2017**, 3, 434-443	16.8	325
52	A robotic platform for flow synthesis of organic compounds informed by AI planning. *Science*, **2019**, 365,	33.3	271
51	Machine Learning in Computer-Aided Synthesis Planning. *Accounts of Chemical Research*, **2018**, 51, 1281-1289	14.9	255
50	Analyzing Learned Molecular Representations for Property Prediction. *Journal of Chemical Information and Modeling*, **2019**, 59, 3370-3388	6.1	247
49	A graph-convolutional neural network model for the prediction of chemical reactivity. *Chemical Science*, **2019**, 10, 370-377	9.4	237
48	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. *Journal of Chemical Information and Modeling*, **2017**, 57, 1757-1772	6.1	191
47	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Central Science*, **2018**, 4, 1465-1476	16.8	131
46	Computer-Assisted Retrosynthesis Based on Molecular Similarity. *ACS Central Science*, **2017**, 3, 1237-1245	16.8	112
45	SCScore: Synthetic Complexity Learned from a Reaction Corpus. *Journal of Chemical Information and Modeling*, **2018**, 58, 252-261	6.1	90
44	Automated microfluidic platform for systematic studies of colloidal perovskite nanocrystals: towards continuous nano-manufacturing. *Lab on A Chip*, **2017**, 17, 4040-4047	7.2	80
43	Autonomous Discovery in the Chemical Sciences Part I: Progress. *Angewandte Chemie - International Edition*, **2020**, 59, 22858-22893	16.4	75
42	Photoredox Iridium–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	3.9	67
41	Autonomous Discovery in the Chemical Sciences Part II: Outlook. *Angewandte Chemie - International Edition*, **2020**, 59, 23414-23436	16.4	62
40	Oscillatory Microprocessor for Growth and in Situ Characterization of Semiconductor Nanocrystals. *Chemistry of Materials*, **2015**, 27, 6131-6138	9.6	61
39	The Synthesizability of Molecules Proposed by Generative Models. *Journal of Chemical Information and Modeling*, **2020**, 60, 5714-5723	6.1	60
38	BigSMILES: A Structurally-Based Line Notation for Describing Macromolecules. *ACS Central Science*, **2019**, 5, 1523-1531	16.8	58
37	Learning Retrosynthetic Planning through Simulated Experience. *ACS Central Science*, **2019**, 5, 970-981	16.8	54

36	A segmented flow platform for on-demand medicinal chemistry and compound synthesis in oscillating droplets. *Chemical Communications*, **2017**, 53, 6649-6652	5.8	53
35	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. *Journal of Medicinal Chemistry*, **2020**, 63, 8667-8682	8.3	53
34	Uncertainty Quantification Using Neural Networks for Molecular Property Prediction. *Journal of Chemical Information and Modeling*, **2020**, 60, 3770-3780	6.1	47
33	RDChiral: An RDKit Wrapper for Handling Stereochemistry in Retrosynthetic Template Extraction and Application. *Journal of Chemical Information and Modeling*, **2019**, 59, 2529-2537	6.1	43
32	Optimum catalyst selection over continuous and discrete process variables with a single droplet microfluidic reaction platform. *Reaction Chemistry and Engineering*, **2018**, 3, 301-311	4.9	41
31	Material-Efficient Microfluidic Platform for Exploratory Studies of Visible-Light Photoredox Catalysis. *Angewandte Chemie - International Edition*, **2017**, 56, 9847-9850	16.4	33
30	In-Situ Microfluidic Study of Biphasic Nanocrystal Ligand-Exchange Reactions Using an Oscillatory Flow Reactor. *Angewandte Chemie - International Edition*, **2017**, 56, 16333-16337	16.4	27
29	Accelerating high-throughput virtual screening through molecular pool-based active learning. *Chemical Science*, **2021**, 12, 7866-7881	9.4	25
28	Flow chemistry-enabled studies of rhodium-catalyzed hydroformylation reactions. *Chemical Communications*, **2018**, 54, 8567-8570	5.8	25
27	Multiphase Oscillatory Flow Strategy for in Situ Measurement and Screening of Partition Coefficients. *Analytical Chemistry*, **2015**, 87, 11130-6	7.8	23
26	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. *Chemical Science*, **2020**, 12, 2198-2208	9.4	21
25	The Open Reaction Database. *Journal of the American Chemical Society*, **2021**, 143, 18820-18826	16.4	18
24	Ligand-Mediated Nanocrystal Growth. *Langmuir*, **2018**, 34, 3307-3315	4	16
23	Multitask prediction of site selectivity in aromatic C–H functionalization reactions. *Reaction Chemistry and Engineering*, **2020**, 5, 896-902	4.9	16
22	Defining and Exploring Chemical Spaces. *Trends in Chemistry*, **2021**, 3, 133-145	14.8	16
21	Data Augmentation and Pretraining for Template-Based Retrosynthetic Prediction in Computer-Aided Synthesis Planning. *Journal of Chemical Information and Modeling*, **2020**, 60, 3398-3407	6.1	15
20	Molecular Representation: Going Long on Fingerprints. *CheM*, **2020**, 6, 1204-1207	16.2	14
19	Towards efficient discovery of green synthetic pathways with Monte Carlo tree search and reinforcement learning. *Chemical Science*, **2020**, 11, 10959-10972	9.4	12

18	Evidential Deep Learning for Guided Molecular Property Prediction and Discovery. *ACS Central Science*, **2021**, 7, 1356-1367	16.8	12
17	Evaluating and clustering retrosynthesis pathways with learned strategy. *Chemical Science*, **2020**, 12, 1469-1478	9.4	10
16	Material-Efficient Microfluidic Platform for Exploratory Studies of Visible-Light Photoredox Catalysis. *Angewandte Chemie*, **2017**, 129, 9979-9982	3.6	9
15	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. *Frontiers in Chemical Engineering*, **2020**, 2,	1	7
14	In-Situ Microfluidic Study of Biphasic Nanocrystal Ligand-Exchange Reactions Using an Oscillatory Flow Reactor. *Angewandte Chemie*, **2017**, 129, 16551-16555	3.6	5
13	Autonome Entdeckung in den chemischen Wissenschaften, Teil I: Fortschritt. *Angewandte Chemie*, **2020**, 132, 23054-23091	3.6	5
12	Quantum chemistry-augmented neural networks for reactivity prediction: Performance, generalizability, and explainability.. *Journal of Chemical Physics*, **2022**, 156, 084104	3.9	5
11	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	4.9	3
10	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	6.1	3
9	A Graph-Convolutional Neural Network Model for the Prediction of Chemical Reactivity		2
8	A Modular Microfluidic Technology for Systematic Studies of Colloidal Semiconductor Nanocrystals. *Journal of Visualized Experiments*, **2018**,	1.6	1
7	Machine learned prediction of reaction template applicability for data-driven retrosynthetic predictions of energetic materials **2020**,		1
6	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. *Journal of Chemical Information and Modeling*, **2021**, 61, 4949-4961	6.1	1
5	Autonomous platforms for data-driven organic synthesis.. *Nature Communications*, **2022**, 13, 1075	17.4	1
4	Improving the performance of models for one-step retrosynthesis through re-ranking.. *Journal of Cheminformatics*, **2022**, 14, 15	8.6	1
3	Machine learning modeling of family wide enzyme-substrate specificity screens.. *PLoS Computational Biology*, **2022**, 18, e1009853	5	0
2	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. *Angewandte Chemie*, **2020**, 132, 23620-23643	3.6	0
1	pyscreener: A Python Wrapper for Computational Docking Software. *Journal of Open Source Software*, **2022**, 7, 3950	5.2	0