Connor W Coley

List of Publications by Year in Descending Order

Source: https://exaly.com/author-pdf/9578715/connor-w-coley-publications-by-year.pdf
Version: 2024-04-25

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Machine learning modeling of family wide enzyme-substrate specificity screens.. *PLoS Computational Biology*, **2022**, 18, e1009853	5	0
52	Autonomous platforms for data-driven organic synthesis.. *Nature Communications*, **2022**, 13, 1075	17.4	1
51	Quantum chemistry-augmented neural networks for reactivity prediction: Performance, generalizability, and explainability.. *Journal of Chemical Physics*, **2022**, 156, 084104	3.9	5
50	Improving the performance of models for one-step retrosynthesis through re-ranking.. *Journal of Cheminformatics*, **2022**, 14, 15	8.6	1
49	pyscreener: A Python Wrapper for Computational Docking Software. *Journal of Open Source Software*, **2022**, 7, 3950	5.2	0
48	The Open Reaction Database. *Journal of the American Chemical Society*, **2021**, 143, 18820-18826	16.4	18
47	Evidential Deep Learning for Guided Molecular Property Prediction and Discovery. *ACS Central Science*, **2021**, 7, 1356-1367	16.8	12
46	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
45	Accelerating high-throughput virtual screening through molecular pool-based active learning. *Chemical Science*, **2021**, 12, 7866-7881	9.4	25
44	Defining and Exploring Chemical Spaces. *Trends in Chemistry*, **2021**, 3, 133-145	14.8	16
43	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
42	Molecular Representation: Going Long on Fingerprints. *CheM*, **2020**, 6, 1204-1207	16.2	14
41	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. *Journal of Medicinal Chemistry*, **2020**, 63, 8667-8682	8.3	53
40	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. *Frontiers in Chemical Engineering*, **2020**, 2,	1	7
39	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
38	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
37	Machine learned prediction of reaction template applicability for data-driven retrosynthetic predictions of energetic materials **2020**,		1

36	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. *Angewandte Chemie*, **2020**, 132, 23620-23643	3.6	0
35	Uncertainty Quantification Using Neural Networks for Molecular Property Prediction. *Journal of Chemical Information and Modeling*, **2020**, 60, 3770-3780	6.1	47
34	Towards efficient discovery of green synthetic pathways with Monte Carlo tree search and reinforcement learning. *Chemical Science*, **2020**, 11, 10959-10972	9.4	12
33	Autonomous Discovery in the Chemical Sciences Part I: Progress. *Angewandte Chemie - International Edition*, **2020**, 59, 22858-22893	16.4	75
32	Autonomous Discovery in the Chemical Sciences Part II: Outlook. *Angewandte Chemie - International Edition*, **2020**, 59, 23414-23436	16.4	62
31	Autonome Entdeckung in den chemischen Wissenschaften, Teil I: Fortschritt. *Angewandte Chemie*, **2020**, 132, 23054-23091	3.6	5
30	The Synthesizability of Molecules Proposed by Generative Models. *Journal of Chemical Information and Modeling*, **2020**, 60, 5714-5723	6.1	60
29	Multitask prediction of site selectivity in aromatic C–H functionalization reactions. *Reaction Chemistry and Engineering*, **2020**, 5, 896-902	4.9	16
28	Evaluating and clustering retrosynthesis pathways with learned strategy. *Chemical Science*, **2020**, 12, 1469-1478	9.4	10
27	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
26	BigSMILES: A Structurally-Based Line Notation for Describing Macromolecules. *ACS Central Science*, **2019**, 5, 1523-1531	16.8	58
25	A graph-convolutional neural network model for the prediction of chemical reactivity. *Chemical Science*, **2019**, 10, 370-377	9.4	237
24	Learning Retrosynthetic Planning through Simulated Experience. *ACS Central Science*, **2019**, 5, 970-981	16.8	54
23	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
22	A robotic platform for flow synthesis of organic compounds informed by AI planning. *Science*, **2019**, 365,	33.3	271
21	Analyzing Learned Molecular Representations for Property Prediction. *Journal of Chemical Information and Modeling*, **2019**, 59, 3370-3388	6.1	247
20	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
19	Ligand-Mediated Nanocrystal Growth. *Langmuir*, **2018**, 34, 3307-3315	4	16

18	SCScore: Synthetic Complexity Learned from a Reaction Corpus. *Journal of Chemical Information and Modeling*, **2018**, 58, 252-261	6.1	90
17	Machine Learning in Computer-Aided Synthesis Planning. *Accounts of Chemical Research*, **2018**, 51, 1281-1289	14.9	255
16	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
15	A Modular Microfluidic Technology for Systematic Studies of Colloidal Semiconductor Nanocrystals. *Journal of Visualized Experiments*, **2018**,	1.6	1
14	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. *ACS Central Science*, **2018**, 4, 1465-1476	16.8	131
13	Flow chemistry-enabled studies of rhodium-catalyzed hydroformylation reactions. *Chemical Communications*, **2018**, 54, 8567-8570	5.8	25
12	Prediction of Organic Reaction Outcomes Using Machine Learning. *ACS Central Science*, **2017**, 3, 434-443	16.8	325
11	A segmented flow platform for on-demand medicinal chemistry and compound synthesis in oscillating droplets. *Chemical Communications*, **2017**, 53, 6649-6652	5.8	53
10	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
9	In-Situ Microfluidic Study of Biphasic Nanocrystal Ligand-Exchange Reactions Using an Oscillatory Flow Reactor. *Angewandte Chemie*, **2017**, 129, 16551-16555	3.6	5
8	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
7	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. *Journal of Chemical Information and Modeling*, **2017**, 57, 1757-1772	6.1	191
6	Computer-Assisted Retrosynthesis Based on Molecular Similarity. *ACS Central Science*, **2017**, 3, 1237-1245	16.8	112
5	Material-Efficient Microfluidic Platform for Exploratory Studies of Visible-Light Photoredox Catalysis. *Angewandte Chemie - International Edition*, **2017**, 56, 9847-9850	16.4	33
4	Material-Efficient Microfluidic Platform for Exploratory Studies of Visible-Light Photoredox Catalysis. *Angewandte Chemie*, **2017**, 129, 9979-9982	3.6	9
3	Multiphase Oscillatory Flow Strategy for in Situ Measurement and Screening of Partition Coefficients. *Analytical Chemistry*, **2015**, 87, 11130-6	7.8	23
2	Oscillatory Microprocessor for Growth and in Situ Characterization of Semiconductor Nanocrystals. *Chemistry of Materials*, **2015**, 27, 6131-6138	9.6	61
1	A Graph-Convolutional Neural Network Model for the Prediction of Chemical Reactivity		2