Sean M Colby

List of Publications by Year
in descending order

17 papers	407 citations	1040056 9 h-index	940533 16 g-index
17 all docs	17 docs citations	17 times ranked	549 citing authors

#	Article	IF	Citations
1	A Practical Guide to Metabolomics Software Development. Analytical Chemistry, 2021, 93, 1912-1923.	6.5	30
2	Ligand- and Structure-Based Analysis of Deep Learning-Generated Potential α2a Adrenoceptor Agonists. Journal of Chemical Information and Modeling, 2021, 61, 481-492.	5.4	1
3	Exploring the Impacts of Conformer Selection Methods on Ion Mobility Collision Cross Section Predictions. Analytical Chemistry, 2021, 93, 3830-3838.	6.5	8
4	Quantum Chemistry Calculations for Metabolomics. Chemical Reviews, 2021, 121, 5633-5670.	47.7	47
5	Application and assessment of deep learning for the generation of potential NMDA receptor antagonists. Physical Chemistry Chemical Physics, 2021, 23, 1197-1214.	2.8	9
6	Deep Learning to Generate *in Silico* Chemical Property Libraries and Candidate Molecules for Small Molecule Identification in Complex Samples. Analytical Chemistry, 2020, 92, 1720-1729.	6.5	62
7	Who Is Metabolizing What? Discovering Novel Biomolecules in the Microbiome and the Organisms Who Make Them. Frontiers in Cellular and Infection Microbiology, 2020, 10, 388.	3.9	6
8	Water-dispersible nanocolloids and higher temperatures promote the release of carbon from riparian soil. Vadose Zone Journal, 2020, 19, e20077.	2.2	2
9	Machine Learning Approaches for Analysis of Multiscale Imaging Data for Atmospheric and Soil Particles. Microscopy and Microanalysis, 2019, 25, 194-195.	0.4	0
10	Relative permeability for water and gas through fractures in cement. PLoS ONE, 2019, 14, e0210741.	2.5	7
11	ISiCLE: A Quantum Chemistry Pipeline for Establishing in Silico Collision Cross Section Libraries. Analytical Chemistry, 2019, 91, 4346-4356.	6.5	74
12	Efficient discrimination of natural stereoisomers of chicoric acid, an HIV-1 integrase inhibitor. Journal of Photochemistry and Photobiology B: Biology, 2018, 189, 258-266.	3.8	13
13	An automated framework for NMR chemical shift calculations of small organic molecules. Journal of Cheminformatics, 2018, 10, 52.	6.1	37
14	The state of rhizospheric science in the era of multi-omics: A practical guide to omics technologies. Rhizosphere, 2017, 3, 212-221.	3.0	66
15	From data to knowledge: The future of multi-omics data analysis for the rhizosphere. Rhizosphere, 2017, 3, 222-229.	3.0	30
16	Comparison of realistic and idealized breathing patterns in computational models of airflow and vapor dosimetry in the rodent upper respiratory tract. Inhalation Toxicology, 2016, 28, 192-202.	1.6	5
17	In situ casting and imaging of the rat airway tree for accurate 3D reconstruction. Experimental Lung Research, 2013, 39, 249-257.	1.2	10