Patrick F Riley

List of Publications by Year
in descending order

12	2,289	759233 12	1125743 13
papers	citations	h-index	g-index

13	13	13	2810
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	30.2	22
2	Defining Levels of Automated Chemical Design. Journal of Medicinal Chemistry, 2022, 65, 7073-7087.	6.4	20
3	Deep diversification of an AAV capsid protein by machine learning. Nature Biotechnology, 2021, 39, 691-696.	17.5	165
4	Using simulation to accelerate autonomous experimentation: A case study using mechanics. IScience, 2021, 24, 102262.	4.1	35
5	Kohn-Sham Equations as Regularizer: Building Prior Knowledge into Machine-Learned Physics. Physical Review Letters, 2021, 126, 036401.	7.8	89
6	Machine Learning on DNA-Encoded Libraries: A New Paradigm for Hit Finding. Journal of Medicinal Chemistry, 2020, 63, 8857-8866.	6.4	81
7	A Bayesian experimental autonomous researcher for mechanical design. Science Advances, 2020, 6, eaaz1708.	10.3	127
8	Message Passing Neural Networks. Lecture Notes in Physics, 2020, , 199-214.	0.7	32
9	Quantum optimization with a novel Gibbs objective function and ansatz architecture search. Physical Review Research, 2020, 2, .	3.6	48
10	Optimization of Molecules via Deep Reinforcement Learning. Scientific Reports, 2019, 9, 10752.	3.3	243
11	Prediction Errors of Molecular Machine Learning Models Lower than Hybrid DFT Error. Journal of Chemical Theory and Computation, 2017, 13, 5255-5264.	5.3	435
12	Molecular graph convolutions: moving beyond fingerprints. Journal of Computer-Aided Molecular Design, 2016, 30, 595-608.	2.9	991