

Patrick F Riley

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7562400/publications.pdf>

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12
papers

2,289
citations

759233

12
h-index

1125743

13
g-index

13
all docs

13
docs citations

13
times ranked

2810
citing authors

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