

Matteo Aldeghi

List of Publications by Year in descending order

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Version: 2024-02-01

34
papers

2,417
citations

257450

24
h-index

395702

33
g-index

35
all docs

35
docs citations

35
times ranked

2740
citing authors

#	ARTICLE	IF	CITATIONS
1	Accurate calculation of the absolute free energy of binding for drug molecules. <i>Chemical Science</i> , 2016, 7, 207-218.	7.4	248
2	Two- and Three-dimensional Rings in Drugs. <i>Chemical Biology and Drug Design</i> , 2014, 83, 450-461.	3.2	235
3	Nanoparticle synthesis assisted by machine learning. <i>Nature Reviews Materials</i> , 2021, 6, 701-716.	48.7	179
4	Data-Driven Strategies for Accelerated Materials Design. <i>Accounts of Chemical Research</i> , 2021, 54, 849-860.	15.6	168
5	Large scale relative protein ligand binding affinities using non-equilibrium alchemy. <i>Chemical Science</i> , 2020, 11, 1140-1152.	7.4	147
6	Predictions of Ligand Selectivity from Absolute Binding Free Energy Calculations. <i>Journal of the American Chemical Society</i> , 2017, 139, 946-957.	13.7	132
7	Selective targeting of the BRG/PB1 bromodomains impairs embryonic and trophoblast stem cell maintenance. <i>Science Advances</i> , 2015, 1, e1500723.	10.3	112
8	Statistical Analysis on the Performance of Molecular Mechanics Poisson-Boltzmann Surface Area versus Absolute Binding Free Energy Calculations: Bromodomains as a Case Study. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2203-2221.	5.4	108
9	Machine learning directed drug formulation development. <i>Advanced Drug Delivery Reviews</i> , 2021, 175, 113806.	13.7	99
10	The Fragment Molecular Orbital Method Reveals New Insight into the Chemical Nature of GPCR-Ligand Interactions. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 159-172.	5.4	97
11	A molecular mechanism for transthyretin amyloidogenesis. <i>Nature Communications</i> , 2019, 10, 925.	12.8	92
12	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 601-633.	2.9	86
13	Accurate Estimation of Ligand Binding Affinity Changes upon Protein Mutation. <i>ACS Central Science</i> , 2018, 4, 1708-1718.	11.3	82
14	Fragment Molecular Orbital Method Applied to Lead Optimization of Novel Interleukin-2 Inducible T-Cell Kinase (ITK) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 4352-4363.	6.4	69
15	G _{ryffin} : An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. <i>Applied Physics Reviews</i> , 2021, 8, .	11.3	61
16	Self-Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. <i>Advanced Functional Materials</i> , 2021, 31, 2106725.	14.9	57
17	Large-scale analysis of water stability in bromodomain binding pockets with grand canonical Monte Carlo. <i>Communications Chemistry</i> , 2018, 1, .	4.5	52
18	Accurate absolute free energies for ligand-protein binding based on non-equilibrium approaches. <i>Communications Chemistry</i> , 2021, 4, .	4.5	49

#	ARTICLE	IF	CITATIONS
19	Alchemical absolute protein–ligand binding free energies for drug design. <i>Chemical Science</i> , 2021, 12, 13958-13971.	7.4	48
20	Predicting Kinase Inhibitor Resistance: Physics-Based and Data-Driven Approaches. <i>ACS Central Science</i> , 2019, 5, 1468-1474.	11.3	40
21	Absolute Alchemical Free Energy Calculations for Ligand Binding: A Beginner’s Guide. <i>Methods in Molecular Biology</i> , 2018, 1762, 199-232.	0.9	38
22	Assigning confidence to molecular property prediction. <i>Expert Opinion on Drug Discovery</i> , 2021, 16, 1009-1023.	5.0	34
23	Accurate Calculation of Free Energy Changes upon Amino Acid Mutation. <i>Methods in Molecular Biology</i> , 2019, 1851, 19-47.	0.9	32
24	Olympus: a benchmarking framework for noisy optimization and experiment planning. <i>Machine Learning: Science and Technology</i> , 2021, 2, 035021.	5.0	31
25	Using the fragment molecular orbital method to investigate agonist–orexin-2 receptor interactions. <i>Biochemical Society Transactions</i> , 2016, 44, 574-581.	3.4	27
26	Exploring GPCR-Ligand Interactions with the Fragment Molecular Orbital (FMO) Method. <i>Methods in Molecular Biology</i> , 2018, 1705, 179-195.	0.9	15
27	Characterising GPCR–ligand interactions using a fragment molecular orbital-based approach. <i>Current Opinion in Structural Biology</i> , 2019, 55, 85-92.	5.7	13
28	Structural basis for antibiotic action of the B1 antivitamin 2–methoxy-thiamine. <i>Nature Chemical Biology</i> , 2020, 16, 1237-1245.	8.0	13
29	Characterizing Interhelical Interactions of G-Protein Coupled Receptors with the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2814-2824.	5.3	13
30	Golem: an algorithm for robust experiment and process optimization. <i>Chemical Science</i> , 2021, 12, 14792-14807.	7.4	12
31	Application of an Integrated GPCR SAR-Modeling Platform To Explain the Activation Selectivity of Human 5-HT _{2C} over 5-HT _{2B} . <i>ACS Chemical Biology</i> , 2016, 11, 1372-1382.	3.4	11
32	A focus on simulation and machine learning as complementary tools for chemical space navigation. <i>Chemical Science</i> , 2022, 13, 8221-8223.	7.4	5
33	Beyond Membrane Protein Structure: Drug Discovery, Dynamics and Difficulties. <i>Advances in Experimental Medicine and Biology</i> , 2016, 922, 161-181.	1.6	4
34	<i>Advances in Molecular Simulation</i> , 2017, , 14-33.		1