Matteo Aldeghi

List of Publications by Year
in descending order

34 papers	2,417 citations	257101 24 h-index	395343 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. Chemical Science, 2016, 7, 207-218.	3.7	248
2	Twoâ€•and Threeâ€dimensional Rings in Drugs. Chemical Biology and Drug Design, 2014, 83, 450-461.	1.5	235
3	Nanoparticle synthesis assisted by machine learning. Nature Reviews Materials, 2021, 6, 701-716.	23.3	179
4	Data-Driven Strategies for Accelerated Materials Design. Accounts of Chemical Research, 2021, 54, 849-860.	7.6	168
5	Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152.	3.7	147
6	Predictions of Ligand Selectivity from Absolute Binding Free Energy Calculations. Journal of the American Chemical Society, 2017, 139, 946-957.	6.6	132
7	Selective targeting of the BRG/PB1 bromodomains impairs embryonic and trophoblast stem cell maintenance. Science Advances, 2015, 1, e1500723.	4.7	112
8	Statistical Analysis on the Performance of Molecular Mechanics Poissonâ€“Boltzmann Surface Area versus Absolute Binding Free Energy Calculations: Bromodomains as a Case Study. Journal of Chemical Information and Modeling, 2017, 57, 2203-2221.	2.5	108
9	Machine learning directed drug formulation development. Advanced Drug Delivery Reviews, 2021, 175, 113806.	6.6	99
10	The Fragment Molecular Orbital Method Reveals New Insight into the Chemical Nature of GPCRâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2016, 56, 159-172.	2.5	97
11	A molecular mechanism for transthyretin amyloidogenesis. Nature Communications, 2019, 10, 925.	5.8	92
12	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	1.3	86
13	Accurate Estimation of Ligand Binding Affinity Changes upon Protein Mutation. ACS Central Science, 2018, 4, 1708-1718.	5.3	82
14	Fragment Molecular Orbital Method Applied to Lead Optimization of Novel Interleukin-2 Inducible T-Cell Kinase (ITK) Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 4352-4363.	2.9	69
15	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Applied Physics Reviews, 2021, 8, .	5.5	61
16	Selfâ€Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. Advanced Functional Materials, 2021, 31, 2106725.	7.8	57
17	Large-scale analysis of water stability in bromodomain binding pockets with grand canonical Monte Carlo. Communications Chemistry, 2018, 1, .	2.0	52
18	Accurate absolute free energies for ligandâ€“protein binding based on non-equilibrium approaches. Communications Chemistry, 2021, 4, .	2.0	49

#	Article	IF	Citations
19	Alchemical absolute proteinâ€“ligand binding free energies for drug design. Chemical Science, 2021, 12, 13958-13971.	3.7	48
20	Predicting Kinase Inhibitor Resistance: Physics-Based and Data-Driven Approaches. ACS Central Science, 2019, 5, 1468-1474.	5.3	40
21	Absolute Alchemical Free Energy Calculations for Ligand Binding: A Beginnerâ€™s Guide. Methods in Molecular Biology, 2018, 1762, 199-232.	0.4	38
22	Assigning confidence to molecular property prediction. Expert Opinion on Drug Discovery, 2021, 16, 1009-1023.	2.5	34
23	Accurate Calculation of Free Energy Changes upon Amino Acid Mutation. Methods in Molecular Biology, 2019, 1851, 19-47.	0.4	32
24	Olympus: a benchmarking framework for noisy optimization and experiment planning. Machine Learning: Science and Technology, 2021, 2, 035021.	2.4	31
25	Using the fragment molecular orbital method to investigate agonistâ€“orexin-2 receptor interactions. Biochemical Society Transactions, 2016, 44, 574-581.	1.6	27
26	Exploring GPCR-Ligand Interactions with the Fragment Molecular Orbital (FMO) Method. Methods in Molecular Biology, 2018, 1705, 179-195.	0.4	15
27	Characterising GPCRâ€“ligand interactions using a fragment molecular orbital-based approach. Current Opinion in Structural Biology, 2019, 55, 85-92.	2.6	13
28	Structural basis for antibiotic action of the B1 antivitamin 2â€²-methoxy-thiamine. Nature Chemical Biology, 2020, 16, 1237-1245.	3.9	13
29	Characterizing Interhelical Interactions of G-Protein Coupled Receptors with the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2020, 16, 2814-2824.	2.3	13
30	Golem: an algorithm for robust experiment and process optimization. Chemical Science, 2021, 12, 14792-14807.	3.7	12
31	Application of an Integrated GPCR SAR-Modeling Platform To Explain the Activation Selectivity of Human 5-HT_{2C} over 5-HT_{2B}. ACS Chemical Biology, 2016, 11, 1372-1382.	1.6	11
32	A focus on simulation and machine learning as complementary tools for chemical space navigation. Chemical Science, 2022, 13, 8221-8223.	3.7	5
33	Beyond Membrane Protein Structure: Drug Discovery, Dynamics and Difficulties. Advances in Experimental Medicine and Biology, 2016, 922, 161-181.	0.8	4
34	Advances in Molecular Simulation. , 2017, , 14-33.		1