Robert Abel

List of Publications by Year
in descending order

18	4,347	567281 15	839539 18
papers	citations	h-index	g-index

19	19	19	6599
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring the Activity Profile of TbrPDEB1 and hPDE4 Inhibitors Using Free Energy Perturbation. ACS Medicinal Chemistry Letters, 2022, 13, 904-910.	2.8	1
2	Efficient Exploration of Chemical Space with Docking and Deep Learning. Journal of Chemical Theory and Computation, 2021, 17, 7106-7119.	5.3	75
3	Is Structure-Based Drug Design Ready for Selectivity Optimization?. Journal of Chemical Information and Modeling, 2020, 60, 6211-6227.	5.4	25
4	Reaction-Based Enumeration, Active Learning, and Free Energy Calculations To Rapidly Explore Synthetically Tractable Chemical Space and Optimize Potency of Cyclin-Dependent Kinase 2 Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 3782-3793.	5.4	81
5	Application of Free Energy Perturbation (FEP+) to Understanding Ligand Selectivity: A Case Study to Assess Selectivity Between Pairs of Phosphodiesterases (PDEâ€™s). Journal of Chemical Information and Modeling, 2019, 59, 2729-2740.	5.4	20
6	Rigorous Free Energy Perturbation Approach to Estimating Relative Binding Affinities between Ligands with Multiple Protonation and Tautomeric States. Journal of Chemical Theory and Computation, 2019, 15, 424-435.	5.3	36
7	Noncovalent inhibitors reveal BTK gatekeeper and auto-inhibitory residues that control its transforming activity. JCI Insight, 2019, 4, .	5.0	17
8	Accurate Calculation of Relative Binding Free Energies between Ligands with Different Net Charges. Journal of Chemical Theory and Computation, 2018, 14, 6346-6358.	5.3	77
9	Predicting resistance of clinical Abl mutations to targeted kinase inhibitors using alchemical free-energy calculations. Communications Biology, 2018, 1, 70.	4.4	66
10	Free Energy Perturbation Calculations of the Thermodynamics of Protein Side-Chain Mutations. Journal of Molecular Biology, 2017, 429, 923-929.	4.2	34
11	Prospective Evaluation of Free Energy Calculations for the Prioritization of Cathepsin L Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 2485-2497.	6.4	110
12	Accurate and Reliable Prediction of the Binding Affinities of Macrocycles to Their Protein Targets. Journal of Chemical Theory and Computation, 2017, 13, 6290-6300.	5.3	39
13	Advancing Drug Discovery through Enhanced Free Energy Calculations. Accounts of Chemical Research, 2017, 50, 1625-1632.	15.6	211
14	Accelerating drug discovery through tight integration of expert molecular design and predictive scoring. Current Opinion in Structural Biology, 2017, 43, 38-44.	5.7	62
15	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. Journal of Chemical Theory and Computation, 2017, 13, 42-54.	5.3	103
16	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	3.5	108
17	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. Journal of Chemical Theory and Computation, 2016, 12, 281-296.	5.3	2,349
18	Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. Journal of the American Chemical Society, 2015, 137, 2695-2703.	13.7	931