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	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
2	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
3	Advancing Drug Discovery through Enhanced Free Energy Calculations. Accounts of Chemical Research, 2017, 50, 1625-1632.	15.6	211
4	Prospective Evaluation of Free Energy Calculations for the Prioritization of Cathepsin L Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 2485-2497.	6.4	110
5	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	3.5	108
6	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. Journal of Chemical Theory and Computation, 2017, 13, 42-54.	5.3	103
7	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
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	Efficient Exploration of Chemical Space with Docking and Deep Learning. Journal of Chemical Theory and Computation, 2021, 17, 7106-7119.	5.3	75
10	Predicting resistance of clinical Abl mutations to targeted kinase inhibitors using alchemical free-energy calculations. Communications Biology, 2018, 1, 70.	4.4	66
11	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
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	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
14	Free Energy Perturbation Calculations of the Thermodynamics of Protein Side-Chain Mutations. Journal of Molecular Biology, 2017, 429, 923-929.	4.2	34
15	Is Structure-Based Drug Design Ready for Selectivity Optimization?. Journal of Chemical Information and Modeling, 2020, 60, 6211-6227.	5.4	25
16	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
17	Noncovalent inhibitors reveal BTK gatekeeper and auto-inhibitory residues that control its transforming activity. JCI Insight, 2019, 4, .	5.0	17
18	Exploring the Activity Profile of TbrPDEB1 and hPDE4 Inhibitors Using Free Energy Perturbation. ACS Medicinal Chemistry Letters, 2022, 13, 904-910.	2.8	1