R Gregor WeiÃ

List of Publications by Year
in descending order

11	173	1307594 7	1281871 11
papers	citations	h-index	g-index

12	12	12	281
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Relative free-energy calculations for scaffold hopping-type transformations with an automated RE-EDS sampling procedure. Journal of Computer-Aided Molecular Design, 2022, 36, 117-130.	2.9	10
2	Glycanâ€“protein interactions determine kinetics of N-glycan remodeling. RSC Chemical Biology, 2021, 2, 917-931.	4.1	16
3	Volume-scaled common nearest neighbor clustering algorithm with free-energy hierarchy. Journal of Chemical Physics, 2021, 154, 084106.	3.0	8
4	N-Glycosylation Enhances Conformational Flexibility of Protein Disulfide Isomerase Revealed by Microsecond Molecular Dynamics and Markov State Modeling. Journal of Physical Chemistry B, 2021, 125, 9467-9479.	2.6	16
5	Connecting dynamic reweighting Algorithms: Derivation of the dynamic reweighting family tree. Journal of Chemical Physics, 2020, 153, 234106.	3.0	5
6	Variational implicit-solvent predictions of the dryâ€“wet transition pathways for ligandâ€“receptor binding and unbinding kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14989-14994.	7.1	12
7	Affinity, kinetics, and pathways of anisotropic ligands binding to hydrophobic model pockets. Journal of Chemical Physics, 2018, 149, 094902.	3.0	1
8	Principles for Tuning Hydrophobic Ligandâ€“Receptor Binding Kinetics. Journal of Chemical Theory and Computation, 2017, 13, 3012-3019.	5.3	13
9	Confined Water Determines Transport Properties of Guest Molecules in Narrow Pores. ACS Nano, 2016, 10, 7646-7656.	14.6	66
10	Solvent Fluctuations Induce Non-Markovian Kinetics in Hydrophobic Pocket-Ligand Binding. Journal of Physical Chemistry B, 2016, 120, 8127-8136.	2.6	8
11	Curvature Dependence of Hydrophobic Hydration Dynamics. Physical Review Letters, 2015, 114, 187802.	7.8	17