

# R Gregor Weir

## List of Publications by Year in descending order

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281  
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#	ARTICLE	IF	CITATIONS
1	Confined Water Determines Transport Properties of Guest Molecules in Narrow Pores. ACS Nano, 2016, 10, 7646-7656.	14.6	66
2	Curvature Dependence of Hydrophobic Hydration Dynamics. Physical Review Letters, 2015, 114, 187802.	7.8	17
3	Glycan-protein interactions determine kinetics of N-glycan remodeling. RSC Chemical Biology, 2021, 2, 917-931.	4.1	16
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	Principles for Tuning Hydrophobic Ligand-Receptor Binding Kinetics. Journal of Chemical Theory and Computation, 2017, 13, 3012-3019.	5.3	13
6	Variational implicit-solvent predictions of the dry-wet transition pathways for ligand-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	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
8	Solvent Fluctuations Induce Non-Markovian Kinetics in Hydrophobic Pocket-Ligand Binding. Journal of Physical Chemistry B, 2016, 120, 8127-8136.	2.6	8
9	Volume-scaled common nearest neighbor clustering algorithm with free-energy hierarchy. Journal of Chemical Physics, 2021, 154, 084106.	3.0	8
10	Connecting dynamic reweighting Algorithms: Derivation of the dynamic reweighting family tree. Journal of Chemical Physics, 2020, 153, 234106.	3.0	5
11	Affinity, kinetics, and pathways of anisotropic ligands binding to hydrophobic model pockets. Journal of Chemical Physics, 2018, 149, 094902.	3.0	1