Ursula Kahler

List of Publications by Year
in descending order

11 papers	266 citations	1039880 9 h-index	1281743 11 g-index
11 all docs	11 docs citations	11 times ranked	351 citing authors

#	Article	IF	Citations
1	Characterizing the Diversity of the CDR-H3 Loop Conformational Ensembles in Relationship to Antibody Binding Properties. Frontiers in Immunology, 2018, 9, 3065.	2.2	73
2	Catalytic Site pK_a Values of Aspartic, Cysteine, and Serine Proteases: Constant pH MD Simulations. Journal of Chemical Information and Modeling, 2020, 60, 3030-3042.	2.5	44
3	Polarizable and non-polarizable force fields: Protein folding, unfolding, and misfolding. Journal of Chemical Physics, 2020, 153, 185102.	1.2	26
4	Dynamics Govern Specificity of a Protein-Protein Interface: Substrate Recognition by Thrombin. PLoS ONE, 2015, 10, e0140713.	1.1	24
5	Localization of Millisecond Dynamics: Dihedral Entropy from Accelerated MD. Journal of Chemical Theory and Computation, 2016, 12, 3449-3455.	2.3	23
6	Protein-Protein Binding as a Two-Step Mechanism: Preselection of Encounter Poses during the Binding of BPTI and Trypsin. Biophysical Journal, 2020, 119, 652-666.	0.2	22
7	Macrocycle Cell Permeability Measured by Solvation Free Energies in Polar and Apolar Environments. Journal of Chemical Information and Modeling, 2020, 60, 3508-3517.	2.5	15
8	Electrostatic recognition in substrate binding to serine proteases. Journal of Molecular Recognition, 2018, 31, e2727.	1.1	13
9	Solvation Thermodynamics in Different Solvents: Waterâ€“Chloroform Partition Coefficients from Grid Inhomogeneous Solvation Theory. Journal of Chemical Information and Modeling, 2020, 60, 3843-3853.	2.5	11
10	Sodium-induced population shift drives activation of thrombin. Scientific Reports, 2020, 10, 1086.	1.6	8
11	An unexpected switch in peptide binding mode: from simulation to substrate specificity. Journal of Biomolecular Structure and Dynamics, 2018, 36, 4072-4084.	2.0	7