

Ursula Kahler

List of Publications by Year in descending order

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Version: 2024-02-01

11
papers

266
citations

1039880

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1281743

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all docs

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docs citations

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times ranked

351
citing authors

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