

Johannes Kraml

List of Publications by Year in descending order

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493
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#	ARTICLE	IF	CITATIONS
1	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
2	CDR-H3 loop ensemble in solution – conformational selection upon antibody binding. <i>MAbs</i> , 2019, 11, 1077-1088.	2.6	49
3	Catalytic Site p <i>K</i> _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
4	Solvation Free Energy as a Measure of Hydrophobicity: Application to Serine Protease Binding Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5872-5882.	2.3	42
5	Late-Stage Functionalization of Drug-Like Molecules Using Diversinates. <i>ChemMedChem</i> , 2018, 13, 983-987.	1.6	32
6	Polarizable and non-polarizable force fields: Protein folding, unfolding, and misfolding. <i>Journal of Chemical Physics</i> , 2020, 153, 185102.	1.2	26
7	Conformational Ensembles of Antibodies Determine Their Hydrophobicity. <i>Biophysical Journal</i> , 2021, 120, 143-157.	0.2	23
8	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
9	X-Entropy: A Parallelized Kernel Density Estimator with Automated Bandwidth Selection to Calculate Entropy. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1533-1538.	2.5	16
10	Macrocyclic 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
11	Electrostatic recognition in substrate binding to serine proteases. <i>Journal of Molecular Recognition</i> , 2018, 31, e2727.	1.1	13
12	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
13	Charge Anisotropy of Nitrogen: Where Chemical Intuition Fails. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4443-4453.	2.3	8
14	Sodium-induced population shift drives activation of thrombin. <i>Scientific Reports</i> , 2020, 10, 1086.	1.6	8
15	Explicit solvation thermodynamics in ionic solution: extending grid inhomogeneous solvation theory to solvation free energy of salt-water mixtures. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 101-116.	1.3	8
16	pH-Induced Local Unfolding of the Phl p 6 Pollen Allergen From cpH-MD. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 603644.	1.6	5
17	Grid inhomogeneous solvation theory for cross-solvation in rigid solvents. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	3
18	Hydration thermodynamics of cytosolic phospholipase A2 GIVA predict its membrane-associated parts and its highly hydrated binding site. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 953-959.	2.0	1