Johannes Kraml

List of Publications by Year
in descending order

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18	404	840119 11	839053 18
papers	citations	h-index	g-index

19	19	19	493
all docs	docs citations	times ranked	citing authors

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