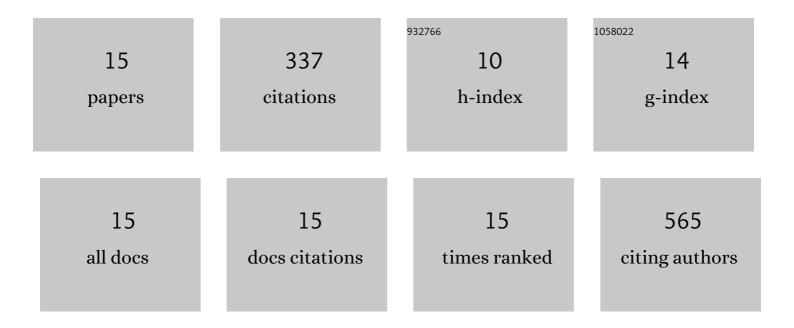
Tobias Wulsdorf

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Intriguing role of water in protein-ligand binding studied by neutron crystallography on trypsin complexes. Nature Communications, 2018, 9, 3559.	5.8	140
2	Paradoxically, Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on Drug–Kinase Binding. Journal of Medicinal Chemistry, 2018, 61, 5922-5933.	2.9	36
3	Impact of Surface Water Layers on Protein–Ligand Binding: How Well Are Experimental Data Reproduced by Molecular Dynamics Simulations in a Thermolysin Test Case?. Journal of Chemical Information and Modeling, 2016, 56, 223-233.	2.5	29
4	Price for Opening the Transient Specificity Pocket in Human Aldose Reductase upon Ligand Binding: Structural, Thermodynamic, Kinetic, and Computational Analysis. ACS Chemical Biology, 2017, 12, 1397-1415.	1.6	23
5	Protein–Ligand Complex Solvation Thermodynamics: Development, Parameterization, and Testing of GIST-Based Solvent Functionals. Journal of Chemical Information and Modeling, 2020, 60, 1409-1423.	2.5	17
6	Conformational Changes in Alkyl Chains Determine the Thermodynamic and Kinetic Binding Profiles of Carbonic Anhydrase Inhibitors. ACS Chemical Biology, 2020, 15, 675-685.	1.6	16
7	Strategies for Late-Stage Optimization: Profiling Thermodynamics by Preorganization and Salt Bridge Shielding. Journal of Medicinal Chemistry, 2019, 62, 9753-9771.	2.9	15
8	Elucidating the Origin of Long Residence Time Binding for Inhibitors of the Metalloprotease Thermolysin. ACS Chemical Biology, 2017, 12, 225-233.	1.6	14
9	A Falseâ€Positive Screening Hit in Fragmentâ€Based Lead Discovery: Watch out for the Red Herring. Angewandte Chemie - International Edition, 2017, 56, 1908-1913.	7.2	12
10	Role of Water Molecules in Protein–Ligand Dissociation and Selectivity Discrimination: Analysis of the Mechanisms and Kinetics of Biomolecular Solvation Using Molecular Dynamics. Journal of Chemical Information and Modeling, 2020, 60, 1818-1832.	2.5	11
11	On the Implication of Water on Fragmentâ€ŧo‣igand Growth in Kinase Binding Thermodynamics. ChemMedChem, 2018, 13, 1988-1996.	1.6	8
12	Diamondoid Amino Acidâ€Based Peptide Kinaseâ€A Inhibitor Analogues. ChemMedChem, 2019, 14, 663-672.	1.6	7
13	Advancing GIST-Based Solvent Functionals through Multiobjective Optimization of Solvent Enthalpy and Entropy Scoring Terms. Journal of Chemical Information and Modeling, 2020, 60, 6654-6665.	2.5	5
14	Fragment Screening Hit Draws Attention to a Novel Transient Pocket Adjacent to the Recognition Site of the tRNA-Modifying Enzyme TGT. Journal of Medicinal Chemistry, 2020, 63, 6802-6820.	2.9	4
15	Falschâ€positiver Treffer im Fragmentâ€basierten Wirkstoffdesign: Lass Dich nicht auf die falsche Färte locken!. Angewandte Chemie, 2017, 129, 1934-1940.	1.6	0