

Tobias Wulsdorf

List of Publications by Year in descending order

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Version: 2024-02-01

15
papers

337
citations

933264

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1058333

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docs citations

15
times ranked

565
citing authors

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