

Markus K Dahlgren

List of Publications by Year in descending order

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13
papers

4,884
citations

933447

10
h-index

1125743

13
g-index

13
all docs

13
docs citations

13
times ranked

7517
citing authors

#	ARTICLE	IF	CITATIONS
1	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 281-296.	5.3	2,349
2	Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. <i>Journal of the American Chemical Society</i> , 2015, 137, 2695-2703.	13.7	931
3	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1863-1874.	5.3	698
4	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4291-4300.	5.3	582
5	Characterization of Biaryl Torsional Energetics and its Treatment in OPLS All-Atom Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1191-1199.	5.4	84
6	Design, Synthesis, and Multivariate Quantitative Structure-Activity Relationship of Salicylanilides Potent Inhibitors of Type III Secretion in <i>Yersinia</i> . <i>Journal of Medicinal Chemistry</i> , 2007, 50, 6177-6188.	6.4	66
7	Statistical molecular design of a focused salicylidene acylhydrazide library and multivariate QSAR of inhibition of type III secretion in the Gram-negative bacterium <i>Yersinia</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 2686-2703.	3.0	63
8	Pre-clinical pharmacokinetics and anti-chlamydial activity of salicylidene acylhydrazide inhibitors of bacterial type III secretion. <i>Journal of Antibiotics</i> , 2012, 65, 397-404.	2.0	39
9	Virtual Screening and Optimization Yield Low-Nanomolar Inhibitors of the Tautomerase Activity of <i>Plasmodium falciparum</i> Macrophage Migration Inhibitory Factor. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 10148-10159.	6.4	33
10	Illuminating HIV gp120-ligand recognition through computationally-driven optimization of antibody-recruiting molecules. <i>Chemical Science</i> , 2014, 5, 2311-2317.	7.4	19
11	Virtual screening reveals allosteric inhibitors of the <i>Toxoplasma gondii</i> thymidylate synthase dihydrofolate reductase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2014, 24, 1232-1235.	2.2	9
12	Synthesis of 2-(2-Aminopyrimidine)-2,2-difluoroethanols as Potential Bioisosters of Salicylidene Acylhydrazides. <i>Molecules</i> , 2010, 15, 4423-4438.	3.8	7
13	Synthesis of [4-(2-Hydroxyphenyl)thiazol-2-yl]methanones as Potential Bioisosteres of Salicylidene Acylhydrazides. <i>Molecules</i> , 2010, 15, 6019-6034.	3.8	4