

# Markus K Dahlgren

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/10392210/publications.pdf>

Version: 2024-02-01

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  | 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       |
| 2  | 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       |
| 3  | 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     |
| 4  | 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       |
| 5  | 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         |
| 6  | Illuminating HIV gp120-ligand recognition through computationally-driven optimization of antibody-recruiting molecules. <i>Chemical Science</i> , 2014, 5, 2311-2317.  | 7.4  | 19        |
| 7  | 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        |
| 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 | 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         |
| 11 | 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        |
| 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 | 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        |