

# AriÅ«n S Rustenburg

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4034179/publications.pdf>

Version: 2024-02-01

8  
papers

491  
citations

1163117

8  
h-index

1588992

8  
g-index

12  
all docs

12  
docs citations

12  
times ranked

989  
citing authors

#	ARTICLE	IF	CITATIONS
1	Overview of the SAMPL6 pKa challenge: evaluating small molecule microscopic and macroscopic pKa predictions. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 131-166.	2.9	23
2	Standard state free energies, not pKas, are ideal for describing small molecule protonation and tautomeric states. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 561-573.	2.9	20
3	Binding Modes of Ligands Using Enhanced Sampling (BLUES): Rapid Decorrelation of Ligand Binding Modes via Nonequilibrium Candidate Monte Carlo. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5579-5598.	2.6	53
4	Biomolecular Simulations under Realistic Macroscopic Salt Conditions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5466-5486.	2.6	63
5	pKa measurements for the SAMPL6 prediction challenge for a set of kinase inhibitor-like fragments. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1117-1138.	2.9	39
6	Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. <i>PLoS ONE</i> , 2018, 13, e0203224.	2.5	24
7	Acquired resistance to IDH inhibition through trans or cis dimer-interface mutations. <i>Nature</i> , 2018, 559, 125-129.	27.8	223
8	Measuring experimental cyclohexane-water distribution coefficients for the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 945-958.	2.9	41