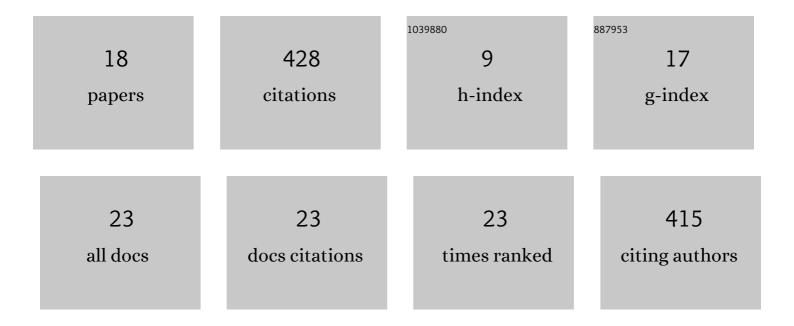
## Ariane Nunes-Alves

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/5023417/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. Processes, 2021, 9, 71.	1.3	162
2	Recent progress in molecular simulation methods for drug binding kinetics. Current Opinion in Structural Biology, 2020, 64, 126-133.	2.6	61
3	Escape of a Small Molecule from Inside T4ÂLysozyme by Multiple Pathways. Biophysical Journal, 2018, 114, 1058-1066.	0.2	44
4	Structure-kinetic relationship reveals the mechanism of selectivity of FAK inhibitors over PYK2. Cell Chemical Biology, 2021, 28, 686-698.e7.	2.5	36
5	Ligand unbinding mechanisms and kinetics for T4 lysozyme mutants from τRAMD simulations. Current Research in Structural Biology, 2021, 3, 106-111.	1.1	31
6	Mechanical Unfolding of Macromolecules Coupled to Bond Dissociation. Journal of Chemical Theory and Computation, 2018, 14, 282-290.	2.3	18
7	Ligand–Receptor Affinities Computed by an Adapted Linear Interaction Model for Continuum Electrostatics and by Protein Conformational Averaging. Journal of Chemical Information and Modeling, 2014, 54, 2309-2319.	2.5	17
8	Line-FRAP, A Versatile Method to Measure Diffusion Rates In Vitro and In Vivo. Journal of Molecular Biology, 2021, 433, 166898.	2.0	14
9	Structural characterization of an Arf dimer interface: molecular mechanism of Arfâ€dependent membrane scission. FEBS Letters, 2020, 594, 2240-2253.	1.3	12
10	Prediction of the Drug–Target Binding Kinetics for Flexible Proteins by Comparative Binding Energy Analysis. Journal of Chemical Information and Modeling, 2021, 61, 3708-3721.	2.5	12
11	Myotubularin-related protein 7 activates peroxisome proliferator-activated receptor-gamma. Oncogenesis, 2020, 9, 59.	2.1	6
12	Tobacco Nitrosamine N-nitrosonornicotine as Inhibitor of Neuronal Nicotinic Acetylcholine Receptors. Journal of Molecular Neuroscience, 2013, 49, 52-61.	1.1	5
13	Impact of the <i>Journal of Chemical Information and Modeling</i> Special Issue on Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2020, 60, 3328-3330.	2.5	5
14	The Non-phosphorylating Glyceraldehyde-3-Phosphate Dehydrogenase GapN Is a Potential New Drug Target in Streptococcus pyogenes. Frontiers in Microbiology, 2022, 13, 802427.	1.5	2
15	From Brazil to Germany: Challenges and Advantages. Journal of Chemical Information and Modeling, 2020, 60, 449-451.	2.5	1
16	A Protocol to Use Comparative Binding Energy Analysis to Estimate Drug-Target Residence Time. Methods in Molecular Biology, 2021, 2266, 171-186.	0.4	1
17	What Makes a Paper Be Highly Cited? 60 Years of the <i>Journal of Chemical Information and Modeling</i> . Journal of Chemical Information and Modeling, 2020, 60, 5866-5867.	2.5	1
18	Neurotransmitters as Main Players in the Neural Differentiation and Fate Determination Game. , 2010, ,		0

<sup>18</sup> 115-134.