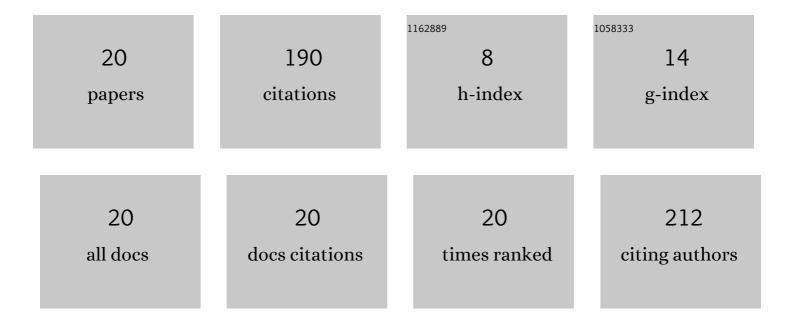
Gustavo Pierdominici-Sottile

List of Publications by Year in descending order

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Gustavo

#	Article	IF	CITATIONS
1	Free Energy Study of the Catalytic Mechanism of <i>Trypanosoma cruzitrans</i> -Sialidase. From the Michaelis Complex to the Covalent Intermediate. Biochemistry, 2011, 50, 10150-10158.	1.2	40
2	Proton Transfer Facilitated by Ligand Binding. An Energetic Analysis of the Catalytic Mechanism of Trypanosoma cruziTrans-Sialidase. Biochemistry, 2011, 50, 836-842.	1.2	33
3	Consistent Principal Component Modes from Molecular Dynamics Simulations of Proteins. Journal of Chemical Information and Modeling, 2017, 57, 826-834.	2.5	20
4	Unraveling the Differences of the Hydrolytic Activity of <i>Trypanosoma cruzi</i> <i>trans</i> -Sialidase and <i>Trypanosoma rangeli</i> Sialidase: A Quantum Mechanics–Molecular Mechanics Modeling Study. Journal of Physical Chemistry B, 2014, 118, 5807-5816.	1.2	13
5	Freeâ€energy computations identify the mutations required to confer transâ€sialidase activity into <i>Trypanosoma rangeli</i> sialidase. Proteins: Structure, Function and Bioinformatics, 2014, 82, 424-435.	1.5	10
6	The Dynamic Behavior of the P2X4 Ion Channel in the Closed Conformation. Biophysical Journal, 2016, 111, 2642-2650.	0.2	10
7	Molecular Dynamics Study of the Active Site of Methylamine Dehydrogenase. Journal of Physical Chemistry B, 2006, 110, 11592-11599.	1.2	9
8	New insights into the meaning and usefulness of principal component analysis of concatenated trajectories. Journal of Computational Chemistry, 2015, 36, 424-432.	1.5	9
9	Quantum study of the structure of the active site of methylamine dehydrogenase. International Journal of Quantum Chemistry, 2005, 105, 937-945.	1.0	8
10	Applications of Mixed-Quantum/Classical Trajectories to the Study of Nuclear Quantum Effects in Chemical Reactions and Vibrational Relaxation Processes. Advances in Quantum Chemistry, 2010, , 247-282.	0.4	7
11	Evaluation of the kinetic isotope effect in methylamine dehydrogenase using the wave function propagation approach. Chemical Physics, 2009, 363, 59-64.	0.9	6
12	QM/MM Molecular Dynamics Study of the Galactopyranose → Galactofuranose Reaction Catalysed by Trypanosoma cruzi UDP-Galactopyranose Mutase. PLoS ONE, 2014, 9, e109559.	1.1	6
13	Molecular Dynamics Simulations of Substrate Release from <i>Trypanosoma cruzi</i> UDP-Galactopyranose Mutase. Journal of Chemical Information and Modeling, 2019, 59, 809-817.	2.5	4
14	Molecular Dynamics Simulations Unveil the Basis of the Sequential Binding of RsmE to the Noncoding RNA RsmZ. Journal of Physical Chemistry B, 2021, 125, 3045-3056.	1.2	4
15	Steric Control of the Rate-Limiting Step of UDP-Galactopyranose Mutase. Biochemistry, 2018, 57, 3713-3721.	1.2	3
16	The role of residue Thr122 of methylamine dehydrogenase on the proton transfer from the iminoquinone intermediate to residue Asp76. Chemical Physics Letters, 2008, 456, 243-246.	1.2	2
17	Charge Discrimination in P2X4 Receptors Occurs in Two Consecutive Stages. Journal of Physical Chemistry B, 2019, 123, 1017-1025.	1.2	2
18	Recognition and Binding of RsmE to an AGGAC Motif of RsmZ: Insights from Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2022, 62, 6614-6627.	2.5	2

#	Article	IF	CITATIONS
19	Positively Charged Residues in the Head Domain of P2X4 Receptors Assist the Binding of ATP. Journal of Chemical Information and Modeling, 2020, 60, 923-932.	2.5	1
20	Ion Selectivity in P2X Receptors: A Comparison between hP2X3 and zfP2X4. Journal of Physical Chemistry B, 2021, , .	1.2	1