

# Gustavo Pierdominici-Sottile

## List of Publications by Year in descending order

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20  
papers

190  
citations

1162889

8  
h-index

1058333

14  
g-index

20  
all docs

20  
docs citations

20  
times ranked

212  
citing authors

#	ARTICLE	IF	CITATIONS
1	Free Energy Study of the Catalytic Mechanism of <i>Trypanosoma cruzi</i> trans-Sialidase. From the Michaelis Complex to the Covalent Intermediate. <i>Biochemistry</i> , 2011, 50, 10150-10158.	1.2	40
2	Proton Transfer Facilitated by Ligand Binding. An Energetic Analysis of the Catalytic Mechanism of <i>Trypanosoma cruzi</i> Trans-Sialidase. <i>Biochemistry</i> , 2011, 50, 836-842.	1.2	33
3	Consistent Principal Component Modes from Molecular Dynamics Simulations of Proteins. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 826-834.	2.5	20
4	Unraveling the Differences of the Hydrolytic Activity of <i>Trypanosoma cruzi</i> trans-Sialidase and <i>Trypanosoma rangeli</i> Sialidase: A Quantum Mechanicsâ€“Molecular Mechanics Modeling Study. <i>Journal of Physical Chemistry B</i> , 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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 424-435.	1.5	10
6	The Dynamic Behavior of the P2X4 Ion Channel in the Closed Conformation. <i>Biophysical Journal</i> , 2016, 111, 2642-2650.	0.2	10
7	Molecular Dynamics Study of the Active Site of Methylamine Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11592-11599.	1.2	9
8	New insights into the meaning and usefulness of principal component analysis of concatenated trajectories. <i>Journal of Computational Chemistry</i> , 2015, 36, 424-432.	1.5	9
9	Quantum study of the structure of the active site of methylamine dehydrogenase. <i>International Journal of Quantum Chemistry</i> , 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. <i>Advances in Quantum Chemistry</i> , 2010, , 247-282.	0.4	7
11	Evaluation of the kinetic isotope effect in methylamine dehydrogenase using the wave function propagation approach. <i>Chemical Physics</i> , 2009, 363, 59-64.	0.9	6
12	QM/MM Molecular Dynamics Study of the Galactopyranose â†’ Galactofuranose Reaction Catalysed by <i>Trypanosoma cruzi</i> UDP-Galactopyranose Mutase. <i>PLoS ONE</i> , 2014, 9, e109559.	1.1	6
13	Molecular Dynamics Simulations of Substrate Release from <i>Trypanosoma cruzi</i> UDP-Galactopyranose Mutase. <i>Journal of Chemical Information and Modeling</i> , 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. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3045-3056.	1.2	4
15	Steric Control of the Rate-Limiting Step of UDP-Galactopyranose Mutase. <i>Biochemistry</i> , 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. <i>Chemical Physics Letters</i> , 2008, 456, 243-246.	1.2	2
17	Charge Discrimination in P2X4 Receptors Occurs in Two Consecutive Stages. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1017-1025.	1.2	2
18	Recognition and Binding of RsmE to an AGGAC Motif of RsmZ: Insights from Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 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