Gustavo Pierdominici-Sottile

List of Publications by Year
in descending order

20 papers	190 citations	1163065 8 h-index	1058452 14 g-index
20 all docs	20 docs citations	20 times ranked	212 citing authors

#	Article	IF	Citations
1	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.	5.4	2
2	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.	2.6	4
3	Ion Selectivity in P2X Receptors: A Comparison between hP2X3 and zfP2X4. Journal of Physical Chemistry B, 2021, , .	2.6	1
4	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.	5.4	1
5	Molecular Dynamics Simulations of Substrate Release from Trypanosoma cruzi UDP-Galactopyranose Mutase. Journal of Chemical Information and Modeling, 2019, 59, 809-817.	5.4	4
6	Charge Discrimination in P2X4 Receptors Occurs in Two Consecutive Stages. Journal of Physical Chemistry B, 2019, 123, 1017-1025.	2.6	2
7	Steric Control of the Rate-Limiting Step of UDP-Galactopyranose Mutase. Biochemistry, 2018, 57, 3713-3721.	2.5	3
8	Consistent Principal Component Modes from Molecular Dynamics Simulations of Proteins. Journal of Chemical Information and Modeling, 2017, 57, 826-834.	5.4	20
9	The Dynamic Behavior of the P2X4 Ion Channel in the Closed Conformation. Biophysical Journal, 2016, 111, 2642-2650.	0.5	10
10	New insights into the meaning and usefulness of principal component analysis of concatenated trajectories. Journal of Computational Chemistry, 2015, 36, 424-432.	3.3	9
11	QM/MM Molecular Dynamics Study of the Galactopyranose â†' Galactofuranose Reaction Catalysed by Trypanosoma cruzi UDP-Galactopyranose Mutase. PLoS ONE, 2014, 9, e109559.	2.5	6
12	Freeâ€energy computations identify the mutations required to confer transâ€sialidase activity into Trypanosoma rangeli sialidase. Proteins: Structure, Function and Bioinformatics, 2014, 82, 424-435.	2.6	10
13	Unraveling the Differences of the Hydrolytic Activity of Trypanosoma cruzi trans-Sialidase and Trypanosoma rangeli Sialidase: A Quantum Mechanicsâ€"Molecular Mechanics Modeling Study. Journal of Physical Chemistry B, 2014, 118, 5807-5816.	2.6	13
14	Free Energy Study of the Catalytic Mechanism of Trypanosoma cruzitrans-Sialidase. From the Michaelis Complex to the Covalent Intermediate. Biochemistry, 2011, 50, 10150-10158.	2.5	40
15	Proton Transfer Facilitated by Ligand Binding. An Energetic Analysis of the Catalytic Mechanism ofTrypanosoma cruziTrans-Sialidase. Biochemistry, 2011, 50, 836-842.	2.5	33
16	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.	0.8	7
17	Evaluation of the kinetic isotope effect in methylamine dehydrogenase using the wave function propagation approach. Chemical Physics, 2009, 363, 59-64.	1.9	6
18	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.	2.6	2

#	Article	IF	Citations
19	Molecular Dynamics Study of the Active Site of Methylamine Dehydrogenase. Journal of Physical Chemistry B, 2006, 110, 11592-11599.	2.6	9
20	Quantum study of the structure of the active site of methylamine dehydrogenase. International Journal of Quantum Chemistry, 2005, 105, 937-945.	2.0	8