

Mercedes Alfonso-Prieto

List of Publications by Year in descending order

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Version: 2024-02-01

48
papers

1,635
citations

361413

20
h-index

289244

40
g-index

49
all docs

49
docs citations

49
times ranked

2309
citing authors

#	ARTICLE	IF	CITATIONS
1	The Molecular Mechanism of the Catalase Reaction. <i>Journal of the American Chemical Society</i> , 2009, 131, 11751-11761.	13.7	325
2	Catalytic Metal Ions and Enzymatic Processing of DNA and RNA. <i>Accounts of Chemical Research</i> , 2015, 48, 220-228.	15.6	130
3	The Effect of a Water Molecule on the Mechanism of Formation of Compound O in Horseradish Peroxidase. <i>Journal of the American Chemical Society</i> , 2007, 129, 6346-6347.	13.7	99
4	High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 14260-14265.	7.1	92
5	On the Role of Water in Peroxidase Catalysis: A Theoretical Investigation of HRP Compound I Formation. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5161-5169.	2.6	89
6	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. <i>Journal of the American Chemical Society</i> , 2015, 137, 11170-11178.	13.7	86
7	Modulation of $\text{A}\hat{1}^2$ β -brillogenesis by glycosaminoglycan structure. <i>FASEB Journal</i> , 2010, 24, 4250-4261.	0.5	66
8	The Structures and Electronic Configuration of Compound I Intermediates of <i>Helicobacter pylori</i> and <i>Penicillium vitale</i> Catalases Determined by X-ray Crystallography and QM/MM Density Functional Theory Calculations. <i>Journal of the American Chemical Society</i> , 2007, 129, 4193-4205.	13.7	58
9	The reaction mechanisms of heme catalases: An atomistic view by ab initio molecular dynamics. <i>Archives of Biochemistry and Biophysics</i> , 2012, 525, 121-130.	3.0	57
10	Versatility of the Electronic Structure of Compound I in Catalase-Peroxidases. <i>Journal of the American Chemical Society</i> , 2007, 129, 13436-13446.	13.7	47
11	Catalases versus peroxidases: DFT investigation of H ₂ O ₂ oxidation in models systems and implications for heme protein engineering. <i>Journal of Inorganic Biochemistry</i> , 2012, 117, 292-297.	3.5	43
12	Agonist Binding to Chemosensory Receptors: A Systematic Bioinformatics Analysis. <i>Frontiers in Molecular Biosciences</i> , 2017, 4, 63.	3.5	36
13	An Integrated Biological Approach to Guide the Development of Metal-Chelating Inhibitors of Influenza Virus PA Endonuclease. <i>Molecular Pharmacology</i> , 2015, 87, 323-337.	2.3	33
14	Reductive Cleavage Mechanism of Co ^{III} -C Bond in Cobalamin-Dependent Methionine Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 12965-12971.	2.6	32
15	Predicting ligand binding poses for low-resolution membrane protein models: Perspectives from multiscale simulations. <i>Biochemical and Biophysical Research Communications</i> , 2018, 498, 366-374.	2.1	32
16	Role of the Axial Base in the Modulation of the Cob(II)alamin Electronic Properties: Insight from QM/MM, DFT, and CASSCF Calculations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1541-1551.	5.3	31
17	Dual binding mode of α -bitter sugars to their human bitter taste receptor target. <i>Scientific Reports</i> , 2019, 9, 8437.	3.3	31
18	Understanding Ligand Binding to G-Protein Coupled Receptors Using Multiscale Simulations. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 29.	3.5	30

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19	Proton Transfer Drives Protein Radical Formation in <i>Helicobacter pylori</i> Catalase but Not in <i>Penicillium vitale</i> Catalase. <i>Journal of the American Chemical Society</i> , 2011, 133, 4285-4298.	13.7	25
20	Oxazoline or Oxazolium Ion? The Protonation State and Conformation of the Reaction Intermediate of Chitinase Enzymes Revisited. <i>Chemistry - A European Journal</i> , 2018, 24, 19258-19265.	3.3	24
21	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. <i>Nature Communications</i> , 2019, 10, 2222.	12.8	20
22	A photoswitchable GABA receptor channel blocker. <i>British Journal of Pharmacology</i> , 2019, 176, 2661-2677.	5.4	20
23	Magnesium-Dependent RNA Binding to the PA Endonuclease Domain of the Avian Influenza Polymerase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 873-889.	2.6	19
24	Structure-function relationships of the disease-linked A218T oxytocin receptor variant. <i>Molecular Psychiatry</i> , 2022, 27, 907-917.	7.9	17
25	The dynamic role of distal side residues in heme hydroperoxidase catalysis. Interplay between X-ray crystallography and ab initio MD simulations. <i>Archives of Biochemistry and Biophysics</i> , 2010, 500, 37-44.	3.0	16
26	Photocontrol of Endogenous Glycine Receptors In Vivo. <i>Cell Chemical Biology</i> , 2020, 27, 1425-1433.e7.	5.2	16
27	Electronic State of the Molecular Oxygen Released by Catalase. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12842-12848.	2.5	14
28	Characterization of cancer-associated IDH2 mutations that differ in tumorigenicity, chemosensitivity and 2-hydroxyglutarate production. <i>Oncotarget</i> , 2019, 10, 2675-2692.	1.8	13
29	Substrate Recognition in the <i>Escherichia coli</i> Ammonia Channel AmtB: A QM/MM Investigation. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11859-11865.	2.6	12
30	Re-engineering specificity in 1,3- α -D-glucanase to accept branched xyloglucan substrates. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 365-375.	2.6	12
31	Combined computational and experimental analysis of a complex of ribonuclease III and the regulatory macrodomain protein, YmdB. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 459-472.	2.6	12
32	A first principles study of the binding of formic acid in catalase complementing high resolution X-ray structures. <i>Chemical Physics</i> , 2006, 323, 129-137.	1.9	11
33	Mechanism of Ribonuclease III Catalytic Regulation by Serine Phosphorylation. <i>Scientific Reports</i> , 2016, 6, 25448.	3.3	11
34	Multi-scale simulations of membrane proteins: The case of bitter taste receptors. <i>Journal of Science: Advanced Materials and Devices</i> , 2017, 2, 15-21.	3.1	11
35	Robust principal component analysis-based prediction of protein-protein interaction hot spots. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 639-647.	2.6	11
36	Mechanisms Underlying Proton Release in CLC-type F ⁺ /H ⁺ Antiporters. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4415-4420.	4.6	10

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37	Multiscale simulations on human Frizzled and Taste2 GPCRs. <i>Current Opinion in Structural Biology</i> , 2019, 55, 8-16.	5.7	9
38	Ligand Pose Predictions for Human G Protein-Coupled Receptors: Insights from the Amber-Based Hybrid Molecular Mechanics/Coarse-Grained Approach. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5103-5116.	5.4	9
39	Subunit-Specific Photocontrol of Glycine Receptors by Azobenzene-Nitrazepam Photoswitcher. <i>ENeuro</i> , 2021, 8, ENEURO.0294-20.2020.	1.9	9
40	Hybrid MM/CG Webserver: Automatic Set Up of Molecular Mechanics/Coarse-Grained Simulations for Human G Protein-Coupled Receptor/Ligand Complexes. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 576689.	3.5	7
41	Photopharmacology of Ion Channels through the Light of the Computational Microscope. <i>International Journal of Molecular Sciences</i> , 2021, 22, 12072.	4.1	6
42	Bitter Taste and Olfactory Receptors: Beyond Chemical Sensing in the Tongue and the Nose. <i>Journal of Membrane Biology</i> , 2021, 254, 343-352.	2.1	4
43	PIP2-Mediated Gating of the Inward Rectifier Potassium Channel Kir2.2. <i>Biophysical Journal</i> , 2013, 104, 431a.	0.5	0
44	Interaction of the Inward Rectifier Potassium Channel Kir 2.2 with Phosphatidylserine. <i>Biophysical Journal</i> , 2014, 106, 99a.	0.5	0
45	Interaction of Ribonuclease III with the Regulatory Macrodomein Protein YmdB Analyzed by Docking Calculations and SPR Experiments. <i>Biophysical Journal</i> , 2015, 108, 225a.	0.5	0
46	Nepriylsin-neuropeptide Y axis as a target for treatment of liver fibrosis and portal hypertension. <i>Journal of Hepatology</i> , 2020, 73, S29.	3.7	0
47	Nepriylsin-Dependent Neuropeptide Y Cleavage in the Liver Promotes Fibrosis by Blocking Npy-Receptor 1. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
48	Density Functional Theory-Based Treatments of Metal-Binding Sites in Metalloenzymes: Challenges and Opportunities. , 2015, , 95-116.		0