Mercedes Alfonso-Prieto

List of Publications by Year
in descending order

48 papers	1,635 citations	361045 20 h-index	301761 39 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. Journal of the American Chemical Society, 2009, 131, 11751-11761.	6.6	325
2	Catalytic Metal Ions and Enzymatic Processing of DNA and RNA. Accounts of Chemical Research, 2015, 48, 220-228.	7.6	130
3	The Effect of a Water Molecule on the Mechanism of Formation of Compound 0 in Horseradish Peroxidase. Journal of the American Chemical Society, 2007, 129, 6346-6347.	6.6	99
4	High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14260-14265.	3.3	92
5	On the Role of Water in Peroxidase Catalysis: A Theoretical Investigation of HRP Compound I Formation. Journal of Physical Chemistry B, 2010, 114, 5161-5169.	1.2	89
6	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. Journal of the American Chemical Society, 2015, 137, 11170-11178.	6.6	86
7	Modulation of AÎ² ₄₂ fÃ¬brillogenesis by glycosaminoglycan structure. FASEB Journal, 2010, 24, 4250-4261.	0.2	66
8	The Structures and Electronic Configuration of Compound I Intermediates ofHelicobacterpyloriandPenicillium vitaleCatalases Determined by X-ray Crystallography and QM/MM Density Functional Theory Calculations. Journal of the American Chemical Society, 2007, 129, 4193-4205.	6.6	58
9	The reaction mechanisms of heme catalases: An atomistic view by ab initio molecular dynamics. Archives of Biochemistry and Biophysics, 2012, 525, 121-130.	1.4	57
10	Versatility of the Electronic Structure of Compound I in Catalase-Peroxidases. Journal of the American Chemical Society, 2007, 129, 13436-13446.	6.6	47
11	Catalases versus peroxidases: DFT investigation of H2O2 oxidation in models systems and implications for heme protein engineering. Journal of Inorganic Biochemistry, 2012, 117, 292-297.	1.5	43
12	Agonist Binding to Chemosensory Receptors: A Systematic Bioinformatics Analysis. Frontiers in Molecular Biosciences, 2017, 4, 63.	1.6	36
13	An Integrated Biological Approach to Guide the Development of Metal-Chelating Inhibitors of Influenza Virus PA Endonuclease. Molecular Pharmacology, 2015, 87, 323-337.	1.0	33
14	Reductive Cleavage Mechanism of Coâ^'C Bond in Cobalamin-Dependent Methionine Synthase. Journal of Physical Chemistry B, 2010, 114, 12965-12971.	1.2	32
15	Predicting ligand binding poses for low-resolution membrane protein models: Perspectives from multiscale simulations. Biochemical and Biophysical Research Communications, 2018, 498, 366-374.	1.0	32
16	Role of the Axial Base in the Modulation of the Cob(I)alamin Electronic Properties: Insight from QM/MM, DFT, and CASSCF Calculations. Journal of Chemical Theory and Computation, 2011, 7, 1541-1551.	2.3	31
17	Dual binding mode of â€œbitter sugarsâ€•to their human bitter taste receptor target. Scientific Reports, 2019, 9, 8437.	1.6	31
18	Understanding Ligand Binding to G-Protein Coupled Receptors Using Multiscale Simulations. Frontiers in Molecular Biosciences, 2019, 6, 29.	1.6	30

#	Article	IF	Citations
19	Proton Transfer Drives Protein Radical Formation in Helicobacter pylori Catalase but Not in Penicillium vitale Catalase. Journal of the American Chemical Society, 2011, 133, 4285-4298.	6.6	25
20	Oxazoline or Oxazolinium Ion? The Protonation State and Conformation of the Reaction Intermediate of Chitinase Enzymes Revisited. Chemistry - A European Journal, 2018, 24, 19258-19265.	1.7	24
21	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. Nature Communications, 2019, 10, 2222.	5.8	20
22	A photoswitchable GABA receptor channel blocker. British Journal of Pharmacology, 2019, 176, 2661-2677.	2.7	20
23	Magnesium-Dependent RNA Binding to the PA Endonuclease Domain of the Avian Influenza Polymerase. Journal of Physical Chemistry B, 2014, 118, 873-889.	1.2	19
24	Structure-function relationships of the disease-linked A218T oxytocin receptor variant. Molecular Psychiatry, 2022, 27, 907-917.	4.1	17
25	The dynamic role of distal side residues in heme hydroperoxidase catalysis. Interplay between X-ray crystallography and ab initio MD simulations. Archives of Biochemistry and Biophysics, 2010, 500, 37-44.	1.4	16
26	Photocontrol of Endogenous Glycine Receptors InÂVivo. Cell Chemical Biology, 2020, 27, 1425-1433.e7.	2.5	16
27	Electronic State of the Molecular Oxygen Released by Catalase. Journal of Physical Chemistry A, 2008, 112, 12842-12848.	1.1	14
28	Characterization of cancer-associated IDH2 mutations that differ in tumorigenicity, chemosensitivity and 2-hydroxyglutarate production. Oncotarget, 2019, 10, 2675-2692.	0.8	13
29	Substrate Recognition in the Escherichia coli Ammonia Channel AmtB: A QM/MM Investigation. Journal of Physical Chemistry B, 2010, 114, 11859-11865.	1.2	12
30	Reâ€engineering specificity in 1,3â€1, 4â€Î²â€glucanase to accept branched xyloglucan substrates. Proteins: Structure, Function and Bioinformatics, 2011, 79, 365-375.	1.5	12
31	Combined computational and experimental analysis of a complex of ribonuclease III and the regulatory macrodomain protein, YmdB. Proteins: Structure, Function and Bioinformatics, 2015, 83, 459-472.	1.5	12
32	A first principles study of the binding of formic acid in catalase complementing high resolution X-ray structures. Chemical Physics, 2006, 323, 129-137.	0.9	11
33	Mechanism of Ribonuclease III Catalytic Regulation by Serine Phosphorylation. Scientific Reports, 2016, 6, 25448.	1.6	11
34	Multi-scale simulations of membrane proteins: The case of bitter taste receptors. Journal of Science: Advanced Materials and Devices, 2017, 2, 15-21.	1.5	11
35	Robust principal component analysisâ€based prediction of <scp>proteinâ€protein</scp> interaction hot spots. Proteins: Structure, Function and Bioinformatics, 2021, 89, 639-647.	1.5	11
36	Mechanisms Underlying Proton Release in CLC-type F^{â€“}/H⁺ Antiporters. Journal of Physical Chemistry Letters, 2021, 12, 4415-4420.	2.1	10

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37	Multiscale simulations on human Frizzled and Taste2 GPCRs. Current Opinion in Structural Biology, 2019, 55, 8-16.	2.6	9
38	Ligand Pose Predictions for Human G Protein-Coupled Receptors: Insights from the Amber-Based Hybrid Molecular Mechanics/Coarse-Grained Approach. Journal of Chemical Information and Modeling, 2020, 60, 5103-5116.	2.5	9
39	Subunit-Specific Photocontrol of Glycine Receptors by Azobenzene-Nitrazepam Photoswitcher. ENeuro, 2021, 8, ENEURO.0294-20.2020.	0.9	9
40	Hybrid MM/CG Webserver: Automatic Set Up of Molecular Mechanics/Coarse-Grained Simulations for Human G Protein-Coupled Receptor/Ligand Complexes. Frontiers in Molecular Biosciences, 2020, 7, 576689.	1.6	7
41	Photopharmacology of Ion Channels through the Light of the Computational Microscope. International Journal of Molecular Sciences, 2021, 22, 12072.	1.8	6
42	Bitter Taste and Olfactory Receptors: Beyond Chemical Sensing in the Tongue and the Nose. Journal of Membrane Biology, 2021, 254, 343-352.	1.0	4
43	PIP2-Mediated Gating of the Inward Rectifier Potassium Channel Kir2.2. Biophysical Journal, 2013, 104, 431a.	0.2	0
44	Interaction of the Inward Rectifier Potassium Channel Kir 2.2 with Phosphatidylserine. Biophysical Journal, 2014, 106, 99a.	0.2	0
45	Interaction of Ribonuclease III with the Regulatory Macrodomain Protein YmdB Analyzed by Docking Calculations and SPR Experiments. Biophysical Journal, 2015, 108, 225a.	0.2	0
46	Neprilysin-neuropeptide Y axis as a target for treatment of liver fibrosis and portal hypertension. Journal of Hepatology, 2020, 73, S29.	1.8	0
47	Neprilysin-Dependent Neuropeptide Y Cleavage in the Liver Promotes Fibrosis by Blocking Npy-Receptor 1. SSRN Electronic Journal, 0, , .	0.4	0
48	Density Functional Theory-Based Treatments of Metal-Binding Sites in Metalloenzymes: Challenges and Opportunities. , 2015, , 95-116.		0