Pedro Jorge Silva

List of Publications by Year in descending order

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37 papers	688 citations	623574 14 h-index	580701 25 g-index
49 all docs	49 docs citations	49 times ranked	1066 citing authors

#	Article	IF	Citations
1	Enzymes of hydrogen metabolism in Pyrococcus furiosus. FEBS Journal, 2000, 267, 6541-6551.	0.2	118
2	Two W-containing formate dehydrogenases (CO2-reductases) involved in syntrophic propionate oxidation by Syntrophobacter fumaroxidans. FEBS Journal, 2003, 270, 2476-2485.	0.2	101
3	Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. Journal of Chemical Theory and Computation, 2011, 7, 3898-3908.	2.3	45
4	Novel structure and redox chemistry of the prosthetic groups of the iron-sulfur flavoprotein sulfide dehydrogenase from Pyrococcus furiosus; evidence for a [2Fe-2S] cluster with Asp(Cys)3 ligands. Journal of Biological Inorganic Chemistry, 2000, 5, 527-534.	1.1	44
5	Reinvestigation of the Steady-State Kinetics and Physiological Function of the Soluble NiFe-Hydrogenase I of Pyrococcus furiosus. Journal of Bacteriology, 2008, 190, 1584-1587.	1.0	40
6	On the prosthetic groups of the NiFe sulfhydrogenase from Pyrococcus furiosus: topology, structure, and temperature-dependent redox chemistry. Journal of Biological Inorganic Chemistry, 1999, 4, 284-291.	1.1	31
7	Inductive and Resonance Effects on the Acidities of Phenol, Enols, and Carbonyl Î±-Hydrogens. Journal of Organic Chemistry, 2009, 74, 914-916.	1.7	24
8	Successes and failures of DFT functionals in acid/base and redox reactions of organic and biochemical interest. Computational and Theoretical Chemistry, 2011, 966, 120-126.	1.1	22
9	A theoretical study of radical-only and combined radical/carbocationic mechanisms of arachidonic acid cyclooxygenation by prostaglandin H synthase. Theoretical Chemistry Accounts, 2003, 110, 345-351.	0.5	18
10	A comparative density-functional study of the reaction mechanism of the O2-dependent coproporphyrinogen III oxidase. Bioorganic and Medicinal Chemistry, 2008, 16, 2726-2733.	1.4	18
11	Computational Studies on the Reactivity of Substituted 1,2-Dihydro-1,2-azaborines. Journal of Organic Chemistry, 2009, 74, 6120-6129.	1.7	18
12	Refining the reaction mechanism of O₂towards its co-substrate in cofactor-free dioxygenases. PeerJ, 2016, 4, e2805.	0.9	18
13	A Tale of Two Acids: When Arginine Is a More Appropriate Acid than H3O+. Journal of Physical Chemistry B, 2010, 114, 8994-9001.	1.2	17
14	Reaction Mechanism of the Vitamin K-Dependent Glutamate Carboxylase:Â A Computational Study. Journal of Physical Chemistry B, 2007, 111, 12883-12887.	1.2	15
15	Comparative Density Functional Study of Models for the Reaction Mechanism of Uroporphyrinogen III Synthase. Journal of Physical Chemistry B, 2008, 112, 3144-3148.	1.2	15
16	Density-Functional Study of Mechanisms for the Cofactor-Free Decarboxylation Performed by Uroporphyrinogen III Decarboxylase. Journal of Physical Chemistry B, 2005, 109, 18195-18200.	1.2	13
17	Isolation and spectroscopic characterization of the membrane-bound nitrate reductase from Pseudomonas chlororaphis DSM 50135. Biochimica Et Biophysica Acta - General Subjects, 2005, 1723, 151-162.	1.1	13
18	Assessing the reliability of sequence similarities detected through hydrophobic cluster analysis. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1588-1594.	1.5	13

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19	Influence of Alkyne and Azide Substituents on the Choice of the Reaction Mechanism of the Cu⁺-Catalyzed Addition of Azides to Iodoalkynes. Journal of Physical Chemistry A, 2018, 122, 7497-7507.	1.1	12
20	BBr₃â€Assisted Cleavage of Most Ethers Does Not Follow the Commonly Assumed Mechanism. European Journal of Organic Chemistry, 2013, 2013, 5195-5199.	1.2	11
21	Computational Characterization of the Substrate-Binding Mode in Coproporphyrinogen III Oxidase. Journal of Physical Chemistry B, 2011, 115, 1903-1910.	1.2	9
22	Computational development of rubromycin-based lead compounds for HIV-1 reverse transcriptase inhibition. PeerJ, 2014, 2, e470.	0.9	9
23	Evaluation of density functional methods on the geometric and energetic descriptions of species involved in Cu+-promoted catalysis. Journal of Molecular Modeling, 2013, 19, 5457-5467.	0.8	8
24	An Alternative Proposal for the Reaction Mechanism of Light-Dependent Protochlorophyllide Oxidoreductase. ACS Catalysis, 2022, 12, 2589-2605.	5.5	8
25	New insights into the mechanism of Schiff base synthesis from aromatic amines in the absence of acid catalyst or polar solvents. , 0, 2, e4.		7
26	Unravelling the Reaction Mechanism of the Reductive Ring Contraction of 1,2-Pyridazines. Journal of Organic Chemistry, 2012, 77, 4653-4659.	1.7	6
27	Improving the study of proton transfers between amino acid side chains in solution: choosing appropriate DFT functionals and avoiding hidden pitfalls. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	6
28	Computational insights into the photochemical step of the reaction catalyzed by protochlorophylide oxidoreductase. International Journal of Quantum Chemistry, 2011, 111, 1472-1479.	1.0	5
29	Chemiosmotic misunderstandings. Biophysical Chemistry, 2020, 264, 106424.	1.5	5
30	With or without light: comparing the reaction mechanism of dark-operative protochlorophyllide oxidoreductase with the energetic requirements of the light-dependent protochlorophyllide oxidoreductase. PeerJ, 2014, 2, e551.	0.9	5
31	Computational exploration of the reaction mechanism of the Cu ⁺ -catalysed synthesis of indoles from N -aryl enaminones. Royal Society Open Science, 2016, 3, 150582.	1.1	4
32	Mechanistic pathways of mercury removal from the organomercurial lyase active site. PeerJ, 2015, 3, e1127.	0.9	4
33	Response to â€œMolecular-level understanding of biological energy coupling and transduction: Response to â€œChemiosmotic misunderstandingsâ€â€. Biophysical Chemistry, 2021, 269, 106512.	1.5	2
34	Computational improvement of small-molecule inhibitors of Bacillus anthracis protective antigen activation through isostere-based substitutions. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5579-5587.	2.0	1
35	Will 1,2-dihydro-1,2-azaborine-based drugs resist metabolism by cytochrome P450 compound I?. PeerJ, 2016, 4, e2299.	0.9	1
36	Computational Development of Inhibitors of Plasmid-Borne Bacterial Dihydrofolate Reductase. Antibiotics, 2022, 11, 779.	1.5	1

#	Article	IF	Citations
37	Unveiling the Reaction Mechanism of the Das/Chechik/Marek Synthesis of Stereodefined Quaternary Carbon Centers. Applied Sciences (Switzerland), 2021, 11, 5002.	1.3	0