

Antnio Jm Ribeiro

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

30
papers

929
citations

17
h-index

30
g-index

34
ext. papers

1,149
ext. citations

7.7
avg, IF

4.25
L-index

#	Paper	IF	Citations
30	Protein-ligand docking in the new millennium--a retrospective of 10 years in the field. <i>Current Medicinal Chemistry</i> , 2013 , 20, 2296-314	4.3	160
29	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017 , 7, e1281	7.9	104
28	Mechanism and Catalytic Site Atlas (M-CSA): a database of enzyme reaction mechanisms and active sites. <i>Nucleic Acids Research</i> , 2018 , 46, D618-D623	20.1	78
27	Benchmarking of DFT Functionals for the Hydrolysis of Phosphodiester Bonds. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2281-92	6.4	62
26	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. <i>ACS Catalysis</i> , 2015 , 5, 5617-5626	5.26	53
25	Emerging concepts in pseudoenzyme classification, evolution, and signaling. <i>Science Signaling</i> , 2019 , 12,	8.8	51
24	PDBe-KB: a community-driven resource for structural and functional annotations. <i>Nucleic Acids Research</i> , 2020 , 48, D344-D353	20.1	50
23	The catalytic mechanism of HIV-1 integrase for DNA 3'end processing established by QM/MM calculations. <i>Journal of the American Chemical Society</i> , 2012 , 134, 13436-47	16.4	47
22	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. <i>Chemistry - A European Journal</i> , 2013 , 19, 14081-9	4.8	42
21	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. <i>Bioconjugate Chemistry</i> , 2017 , 28, 590-599	6.3	36
20	A global analysis of function and conservation of catalytic residues in enzymes. <i>Journal of Biological Chemistry</i> , 2020 , 295, 314-324	5.4	28
19	Insight into Enzymatic Nitrile Reduction: QM/MM Study of the Catalytic Mechanism of QueF Nitrile Reductase. <i>ACS Catalysis</i> , 2015 , 5, 3740-3751	13.1	28
18	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2079-90	3.5	27
17	Benchmarking of density functionals for the kinetics and thermodynamics of the hydrolysis of glycosidic bonds catalyzed by glycosidases. <i>International Journal of Quantum Chemistry</i> , 2017 , 117, e25409	2.1	23
16	Improving the Biodesulfurization of Crude Oil and Derivatives: A QM/MM Investigation of the Catalytic Mechanism of NADH-FMN Oxidoreductase (DszD). <i>Journal of Physical Chemistry A</i> , 2016 , 120, 5300-6	2.8	22
15	Synthesis and Hydrolytic Studies on the Air-Stable [(4-CN-PhO)(E)P(EN(t)Bu)] ₂ (E = O, S, and Se) Cyclodiphosphazanes. <i>Inorganic Chemistry</i> , 2015 , 54, 6423-32	5.1	20
14	New insights in the catalytic mechanism of tyrosine ammonia-lyase given by QM/MM and QM cluster models. <i>Archives of Biochemistry and Biophysics</i> , 2015 , 582, 107-15	4.1	19

13	HMG-CoA Reductase inhibitors: an updated review of patents of novel compounds and formulations (2011-2015). <i>Expert Opinion on Therapeutic Patents</i> , 2016 , 26, 1257-1272	6.8	16
12	cuRRBS: simple and robust evaluation of enzyme combinations for reduced representation approaches. <i>Nucleic Acids Research</i> , 2017 , 45, 11559-11569	20.1	9
11	Identifying pseudoenzymes using functional annotation: pitfalls of common practice. <i>FEBS Journal</i> , 2020 , 287, 4128-4140	5.7	8
10	Ranking Enzyme Structures in the PDB by Bound Ligand Similarity to Biological Substrates. <i>Structure</i> , 2018 , 26, 565-571.e3	5.2	7
9	Exploring Chemical Biosynthetic Design Space with Transform-MinER. <i>ACS Synthetic Biology</i> , 2019 , 8, 2494-2506	5.7	7
8	A DFT study of the applicability of the charge balance model in two-metal enzymes: The case of cAMP-dependent protein kinase. <i>Chemical Physics Letters</i> , 2013 , 571, 66-70	2.5	7
7	Binding free energy calculations on E-selectin complexes with sLe oligosaccharide analogs. <i>Chemical Biology and Drug Design</i> , 2017 , 89, 114-123	2.9	6
6	Transform-MinER: transforming molecules in enzyme reactions. <i>Bioinformatics</i> , 2018 , 34, 3597-3599	7.2	6
5	Divalent metal ion-based catalytic mechanism of the Nudix hydrolase Orf153 (YmfB) from <i>Escherichia coli</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 1297-310		5
4	Catalytic Mechanism of Retroviral Integrase for the Strand Transfer Reaction Explored by QM/MM Calculations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5458-66	6.4	4
3	Analyses of cobalt-ligand and potassium-ligand bond lengths in metalloproteins: trends and patterns. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2271	2	2
2	GRaSP: a graph-based residue neighborhood strategy to predict binding sites. <i>Bioinformatics</i> , 2020 , 36, i726-i734	7.2	2
1	Conformational Variation in Enzyme Catalysis: A Structural Study on Catalytic Residues.. <i>Journal of Molecular Biology</i> , 2022 , 434, 167517	6.5	0