Antnio Jm Ribeiro

List of Publications by Year in Descending Order

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	Conformational Variation in Enzyme Catalysis: A Structural Study on Catalytic Residues.. *Journal of Molecular Biology*, **2022**, 434, 167517	6.5	0
29	A global analysis of function and conservation of catalytic residues in enzymes. *Journal of Biological Chemistry*, **2020**, 295, 314-324	5.4	28
28	GRaSP: a graph-based residue neighborhood strategy to predict binding sites. *Bioinformatics*, **2020**, 36, i726-i734	7.2	2
27	Identifying pseudoenzymes using functional annotation: pitfalls of common practice. *FEBS Journal*, **2020**, 287, 4128-4140	5.7	8
26	PDBe-KB: a community-driven resource for structural and functional annotations. *Nucleic Acids Research*, **2020**, 48, D344-D353	20.1	50
25	Emerging concepts in pseudoenzyme classification, evolution, and signaling. *Science Signaling*, **2019**, 12,	8.8	51
24	Exploring Chemical Biosynthetic Design Space with Transform-MinER. *ACS Synthetic Biology*, **2019**, 8, 2494-2506	5.7	7
23	Mechanism and Catalytic Site Atlas (M-CSA): a database of enzyme reaction mechanisms and active sites. *Nucleic Acids Research*, **2018**, 46, D618-D623	20.1	78
22	Ranking Enzyme Structures in the PDB by Bound Ligand Similarity to Biological Substrates. *Structure*, **2018**, 26, 565-571.e3	5.2	7
21	Transform-MinER: transforming molecules in enzyme reactions. *Bioinformatics*, **2018**, 34, 3597-3599	7.2	6
20	Benchmarking of density functionals for the kinetics and thermodynamics of the hydrolysis of glycosidic bonds catalyzed by glycosidases. *International Journal of Quantum Chemistry*, **2017**, 117, e25409	2.1	23
19	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. *Bioconjugate Chemistry*, **2017**, 28, 590-599	6.3	36
18	cuRRBS: simple and robust evaluation of enzyme combinations for reduced representation approaches. *Nucleic Acids Research*, **2017**, 45, 11559-11569	20.1	9
17	Binding free energy calculations on E-selectin complexes with sLe oligosaccharide analogs. *Chemical Biology and Drug Design*, **2017**, 89, 114-123	2.9	6
16	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1281	7.9	104
15	HMG-CoA Reductase inhibitors: an updated review of patents of novel compounds and formulations (2011-2015). *Expert Opinion on Therapeutic Patents*, **2016**, 26, 1257-1272	6.8	16
14	Improving the Biodesulfurization of Crude Oil and Derivatives: A QM/MM Investigation of the Catalytic Mechanism of NADH-FMN Oxidoreductase (DszD). *Journal of Physical Chemistry A*, **2016**, 120, 5300-6	2.8	22

List of Publications

13	New insights in the catalytic mechanism of tyrosine ammonia-lyase given by QM/MM and QM cluster models. *Archives of Biochemistry and Biophysics*, **2015**, 582, 107-15	4.1	19
12	Synthesis and Hydrolytic Studies on the Air-Stable [(4-CN-PhO)(E)P(μN(t)Bu)]2 (E = O, S, and Se) Cyclodiphosphazanes. *Inorganic Chemistry*, **2015**, 54, 6423-32	5.1	20
11	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. *ACS Catalysis*, **2015**, 5, 5617-5626	9.1	53
10	Insight into Enzymatic Nitrile Reduction: QM/MM Study of the Catalytic Mechanism of QueF Nitrile Reductase. *ACS Catalysis*, **2015**, 5, 3740-3751	13.1	28
9	Catalytic Mechanism of Retroviral Integrase for the Strand Transfer Reaction Explored by QM/MM Calculations. *Journal of Chemical Theory and Computation*, **2014**, 10, 5458-66	6.4	4
8	Analyses of cobalt-ligand and potassium-ligand bond lengths in metalloproteins: trends and patterns. *Journal of Molecular Modeling*, **2014**, 20, 2271	2	2
7	Divalent metal ion-based catalytic mechanism of the Nudix hydrolase Orf153 (YmfB) from Escherichia coli. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 1297-310		5
6	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. *Journal of Computational Chemistry*, **2013**, 34, 2079-90	3.5	27
5	A DFT study of the applicability of the charge balance model in two-metal enzymes: The case of cAMP-dependent protein kinase. *Chemical Physics Letters*, **2013**, 571, 66-70	2.5	7
4	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. *Chemistry - A European Journal*, **2013**, 19, 14081-9	4.8	42
3	Protein-ligand docking in the new millennium--a retrospective of 10 years in the field. *Current Medicinal Chemistry*, **2013**, 20, 2296-314	4.3	160
2	The catalytic mechanism of HIV-1 integrase for DNA 3′-end processing established by QM/MM calculations. *Journal of the American Chemical Society*, **2012**, 134, 13436-47	16.4	47
1	Benchmarking of DFT Functionals for the Hydrolysis of Phosphodiester Bonds. *Journal of Chemical Theory and Computation*, **2010**, 6, 2281-92	6.4	62