AntÃ³nio Jm Ribeiro

List of Publications by Year
in descending order

32 papers	1,345 citations	430442 18 h-index	414034 32 g-index
34 all docs	34 docs citations	34 times ranked	2314 citing authors

#	Article	IF	Citations
1	Conformational Variation in Enzyme Catalysis: A Structural Study on Catalytic Residues. Journal of Molecular Biology, 2022, 434, 167517.	2.0	17
2	GRaSP-web: a machine learning strategy to predict binding sites based on residue neighborhood graphs. Nucleic Acids Research, 2022, 50, W392-W397.	6.5	7
3	The Enzyme Portal: an integrative tool for enzyme information and analysis. FEBS Journal, 2021, , .	2.2	2
4	PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Research, 2020, 48, D344-D353.	6.5	87
5	Identifying pseudoenzymes using functional annotation: pitfalls of common practice. FEBS Journal, 2020, 287, 4128-4140.	2.2	19
6	A global analysis of function and conservation of catalytic residues in enzymes. Journal of Biological Chemistry, 2020, 295, 314-324.	1.6	68
7	GRaSP: a graph-based residue neighborhood strategy toÂpredict binding sites. Bioinformatics, 2020, 36, i726-i734.	1.8	10
8	Emerging concepts in pseudoenzyme classification, evolution, and signaling. Science Signaling, 2019, 12, .	1.6	80
9	Exploring Chemical Biosynthetic Design Space with Transform-MinER. ACS Synthetic Biology, 2019, 8, 2494-2506.	1.9	16
10	Mechanism and Catalytic Site Atlas (M-CSA): a database of enzyme reaction mechanisms and active sites. Nucleic Acids Research, 2018, 46, D618-D623.	6.5	151
11	Ranking Enzyme Structures in the PDB by Bound Ligand Similarity to Biological Substrates. Structure, 2018, 26, 565-571.e3.	1.6	23
12	Transform-MinER: transforming molecules in enzyme reactions. Bioinformatics, 2018, 34, 3597-3599.	1.8	10
13	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.	1.0	37
14	Unique Triphenylphosphonium Derivatives for Enhanced Mitochondrial Uptake and Photodynamic Therapy. Bioconjugate Chemistry, 2017, 28, 590-599.	1.8	46
15	cuRRBS: simple and robust evaluation of enzyme combinations for reduced representation approaches. Nucleic Acids Research, 2017, 45, 11559-11569.	6.5	14
16	Binding free energy calculations on Eâ€selectin complexes with <scp>sL</scp>e^x oligosaccharide analogs. Chemical Biology and Drug Design, 2017, 89, 114-123.	1.5	8
17	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1281.	6.2	137
18	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, 5300-5306.	1.1	24

#	Article	IF	Citations
19	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.	2.4	19
20	Insight into Enzymatic Nitrile Reduction: QM/MM Study of the Catalytic Mechanism of QueF Nitrile Reductase. ACS Catalysis, 2015, 5, 3740-3751.	5.5	28
21	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, 107-115.	1.4	24
22	Synthesis and Hydrolytic Studies on the Air-Stable [(4-CN-PhO)(E)P(Î¼-N^tBu)]₂ (E = O, S, and Se) Cyclodiphosphazanes. Inorganic Chemistry, 2015, 54, 6423-6432.	1.9	25
23	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. ACS Catalysis, 2015, 5, 5617-5626.	5.5	72
24	Catalytic Mechanism of Retroviral Integrase for the Strand Transfer Reaction Explored by QM/MM Calculations. Journal of Chemical Theory and Computation, 2014, 10, 5458-5466.	2.3	6
25	Analyses of cobaltâ€“ligand and potassiumâ€“ligand bond lengths in metalloproteins: trends and patterns. Journal of Molecular Modeling, 2014, 20, 2271.	0.8	4
26	Divalent metal ion-based catalytic mechanism of the Nudix hydrolase Orf153 (YmfB) fromEscherichia coli. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1297-1310.	2.5	5
27	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, 2079-2090.	1.5	38
28	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.	1.2	7
29	The Catalytic Mechanism of Protein Phosphataseâ€…5 Established by DFT Calculations. Chemistry - A European Journal, 2013, 19, 14081-14089.	1.7	44
30	Protein-Ligand Docking in the New Millennium â€“ A Retrospective of 10 Years in the Field. Current Medicinal Chemistry, 2013, 20, 2296-2314.	1.2	197
31	The Catalytic Mechanism of HIV-1 Integrase for DNA 3â€²-End Processing Established by QM/MM Calculations. Journal of the American Chemical Society, 2012, 134, 13436-13447.	6.6	51
32	Benchmarking of DFT Functionals for the Hydrolysis of Phosphodiester Bonds. Journal of Chemical Theory and Computation, 2010, 6, 2281-2292.	2.3	69