Gaspar P Pinto

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6662520/publications.pdf

Version: 2024-02-01

16 papers	617 citations	840119 11 h-index	940134 16 g-index
18 all docs	18 docs citations	18 times ranked	693 citing authors

#	Article	IF	Citations
1	Caver Web 1.0: identification of tunnels and channels in proteins and analysis of ligand transport. Nucleic Acids Research, 2019, 47, W414-W422.	6.5	138
2	Engineering enzyme access tunnels. Biotechnology Advances, 2019, 37, 107386.	6.0	128
3	Transcription and Translation Inhibitors in Cancer Treatment. Frontiers in Chemistry, 2020, 8, 276.	1.8	54
4	Engineering theÂprotein dynamics of anÂancestral luciferase. Nature Communications, 2021, 12, 3616.	5.8	54
5	Computational design of enzymes for biotechnological applications. Biotechnology Advances, 2021, 47, 107696.	6.0	51
6	Light-Emitting Dehalogenases: Reconstruction of Multifunctional Biocatalysts. ACS Catalysis, 2019, 9, 4810-4823.	5.5	33
7	Establishing the Catalytic Mechanism of Human Pancreatic Î±-Amylase with QM/MM Methods. Journal of Chemical Theory and Computation, 2015, 11, 2508-2516.	2.3	32
8	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
9	Triesterase and Promiscuous Diesterase Activities of a Diâ€Co^{II}â€Containing Organophosphate Degrading Enzyme Reaction Mechanisms. Chemistry - A European Journal, 2015, 21, 3736-3745.	1.7	19
10	Fast Screening of Inhibitor Binding/Unbinding Using Novel Software Tool CaverDock. Frontiers in Chemistry, 2019, 7, 709.	1.8	19
11	Exploiting enzyme evolution for computational protein design. Trends in Biochemical Sciences, 2022, 47, 375-389.	3.7	15
12	The impact of tunnel mutations on enzymatic catalysis depends on the tunnel-substrate complementarity and the rate-limiting step. Computational and Structural Biotechnology Journal, 2020, 18, 805-813.	1.9	14
13	Screening of world approved drugs against highly dynamical spike glycoprotein of SARS-CoV-2 using CaverDock and machine learning. Computational and Structural Biotechnology Journal, 2021, 19, 3187-3197.	1.9	11
14	LoopGrafter: a web tool for transplanting dynamical loops for protein engineering. Nucleic Acids Research, 2022, 50, W465-W473.	6.5	11
15	Trimethylphosphate and Dimethylphosphate Hydrolysis by Binuclear Cd^{II}, Mn^{II}, and Zn^{II}â€“Fe^{II} Promiscuous Organophosphateâ€Đegrading Enzyme: Reaction Mechanisms. Chemistry - A European Journal, 2017, 23, 13742-13753.	1.7	8
16	Virtual screening of potential anticancer drugs based on microbial products. Seminars in Cancer Biology, 2022, 86, 1207-1217.	4.3	6