Conrado Pedebos

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7361810/publications.pdf

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18	226	933447 10	1058476 14
papers	citations	h-index	g-index

25	25	25	273
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Simulations of the spike: molecular dynamics and SARS-CoV-2. Nature Reviews Microbiology, 2022, 20, 192-192.	28.6	11
2	Rocio Virus Encephalitis: In Silico Evidence for Drug Repurposing. Macromol, 2022, 2, 100-112.	4.4	1
3	Uncovering cryptic pockets in the SARS-CoV-2 spike glycoprotein. Structure, 2022, 30, 1062-1074.e4.	3.3	21
4	The hitchhiker's guide to the periplasm: Unexpected molecular interactions of polymyxin B1 in E. coli. Structure, 2021, 29, 444-456.e2.	3.3	20
5	Modifying the catalytic preference of alphaâ€amylase toward nâ€alkanes for bioremediation purposes using in silico strategies. Journal of Computational Chemistry, 2021, 42, 1540-1551.	3.3	2
6	Making it Rain: Cloud-Based Molecular Simulations for Everyone. Journal of Chemical Information and Modeling, 2021, 61, 4852-4856.	5.4	41
7	Structural Basis for Silicic Acid Uptake by Higher Plants. Journal of Molecular Biology, 2021, 433, 167226.	4.2	18
8	Polymyxin B1 within the E. coli cell envelope: insights from molecular dynamics simulations. Biophysical Reviews, 2021, 13, 1061-1070.	3.2	7
9	The Lazy Life of Lipid-Linked Oligosaccharides in All Life Domains. Journal of Chemical Information and Modeling, 2020, 60, 631-643.	5.4	4
10	Evolution of an Amniote-Specific Mechanism for Modulating Ubiquitin Signaling via Phosphoregulation of the E2 Enzyme UBE2D3. Molecular Biology and Evolution, 2020, 37, 1986-2001.	8.9	2
11	Development of GROMOS-Compatible Parameter Set for Simulations of Chalcones and Flavonoids. Journal of Physical Chemistry B, 2019, 123, 994-1008.	2.6	7
12	CoCo-MD: A Simple and Effective Method for the Enhanced Sampling of Conformational Space. Journal of Chemical Theory and Computation, 2019, 15, 2587-2596.	5.3	20
13	Dynamics of DDB2-DDB1 complex under different naturally-occurring mutants in Xeroderma Pigmentosum disease. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 2579-2589.	2.4	7
14	The role of Zn2+, dimerization and N-glycosylation in the interaction of Auxin-Binding Protein 1 (ABP1) with different auxins. Glycobiology, 2017, 27, 1109-1119.	2.5	4
15	In silicoInvestigation of the PglB Active Site Reveals Transient Catalytic States and Octahedral Metal Ion Coordination. Glycobiology, 2015, 25, 1183-1195.	2.5	13
16	Atomic Model and Micelle Dynamics of QS-21 Saponin. Molecules, 2014, 19, 3744-3760.	3.8	21
17	Improving the Thrombin Inhibitory Activity of Glycyrrhizin, a Triterpenic Saponin, Through a Molecular Simplification of the Carbohydrate Moiety. Chemical Biology and Drug Design, 2013, 82, 756-760.	3.2	10
18	Unrestrained Conformational Characterization ofStenocereus erucaSaponins in Aqueous and Nonaqueous Solvents. Journal of Natural Products, 2012, 75, 1196-1200.	3.0	11