

Conrado Pedebos

List of Publications by Year in descending order

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Version: 2024-02-01

18
papers

226
citations

933447

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h-index

1058476

14
g-index

25
all docs

25
docs citations

25
times ranked

273
citing authors

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