

Marcelo C R Melo

List of Publications by Year in descending order

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Version: 2024-02-01

20
papers

2,702
citations

840776

11
h-index

996975

15
g-index

26
all docs

26
docs citations

26
times ranked

3465
citing authors

#	ARTICLE	IF	CITATIONS
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. <i>Journal of Chemical Physics</i> , 2020, 153, 044130.	3.0	1,548
2	Enhanced sampling techniques in molecular dynamics simulations of biological systems. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 872-877.	2.4	537
3	NAMD goes quantum: an integrative suite for hybrid simulations. <i>Nature Methods</i> , 2018, 15, 351-354.	19.0	149
4	Generalized correlation-based dynamical network analysis: a new high-performance approach for identifying allosteric communications in molecular dynamics trajectories. <i>Journal of Chemical Physics</i> , 2020, 153, 134104.	3.0	81
5	Accelerating antibiotic discovery through artificial intelligence. <i>Communications Biology</i> , 2021, 4, 1050.	4.4	68
6	Fundamental behaviors emerge from simulations of a living minimal cell. <i>Cell</i> , 2022, 185, 345-360.e28.	28.9	66
7	Mining for encrypted peptide antibiotics in the human proteome. <i>Nature Biomedical Engineering</i> , 2022, 6, 67-75.	22.5	64
8	Direction Matters: Monovalent Streptavidin/Biotin Complex under Load. <i>Nano Letters</i> , 2019, 19, 3415-3421.	9.1	53
9	A tethered ligand assay to probe SARS-CoV-2:ACE2 interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2114397119.	7.1	38
10	Understanding and modelling the interactions of peptides with membranes: from partitioning to self-assembly. <i>Current Opinion in Structural Biology</i> , 2020, 61, 160-166.	5.7	31
11	Population FBA predicts metabolic phenotypes in yeast. <i>PLoS Computational Biology</i> , 2017, 13, e1005728.	3.2	18
12	Kinetic Modeling of the Genetic Information Processes in a Minimal Cell. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 130.	3.5	13
13	GSAFold: A new application of GSA to protein structure prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 2305-2310.	2.6	11
14	Impact of natural selection on global patterns of genetic variation and association with clinical phenotypes at genes involved in SARS-CoV-2 infection. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2123000119.	7.1	7
15	Large Scale Structure Sampling for Protein Fold Prediction using the Generalized Simulated Annealing. <i>Biophysical Journal</i> , 2013, 104, 228a-229a.	0.5	1
16	QM/MM Molecular Dynamics Methods Applied to Investigate Cellulose Fibers Hydration. <i>Biophysical Journal</i> , 2012, 102, 735a.	0.5	0
17	Dynamical Network Analysis of Protein:RNA Complexes Made Easy. <i>Biophysical Journal</i> , 2019, 116, 562a-563a.	0.5	0
18	Modelling the Genetic Information Processes of a Genetically Minimal Cell. <i>Biophysical Journal</i> , 2020, 118, 461a.	0.5	0

#	ARTICLE	IF	CITATIONS
19	Modelling the Nucleotide Metabolic Network of a Genetically Minimal Cell. Biophysical Journal, 2020, 118, 460a-461a.	0.5	0
20	10.1063/5.0018980.1., 2020,,.		0