Marcelo C R Melo

List of Publications by Year
in descending order

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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	Mining for encrypted peptide antibiotics in the human proteome. Nature Biomedical Engineering, 2022, 6, 67-75.	22.5	64
2	Fundamental behaviors emerge from simulations of a living minimal cell. Cell, 2022, 185, 345-360.e28.	28.9	66
3	A tethered ligand assay to probe SARS-CoV-2:ACE2 interactions. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2114397119.	7.1	38
4	Impact of natural selection on global patterns of genetic variation and association with clinical phenotypes at genes involved in SARS-CoV-2 infection. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2123000119.	7.1	7
5	Accelerating antibiotic discovery through artificial intelligence. Communications Biology, 2021, 4, 1050.	4.4	68
6	Generalized correlation-based dynamical network analysis: a new high-performance approach for identifying allosteric communications in molecular dynamics trajectories. Journal of Chemical Physics, 2020, 153, 134104.	3.0	81
7	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
8	Modelling the Genetic Information Processes of a Genetically Minimal Cell. Biophysical Journal, 2020, 118, 461a.	0.5	0
9	Modelling the Nucleotide Metabolic Network of a Genetically Minimal Cell. Biophysical Journal, 2020, 118, 460a-461a.	0.5	0
10	Understanding and modelling the interactions of peptides with membranes: from partitioning to self-assembly. Current Opinion in Structural Biology, 2020, 61, 160-166.	5.7	31
11	10.1063/5.0018980.1. , 2020, , .		0
12	Dynamical Network Analysis of Protein:RNA Complexes Made Easy. Biophysical Journal, 2019, 116, 562a-563a.	0.5	0
13	Kinetic Modeling of the Genetic Information Processes in a Minimal Cell. Frontiers in Molecular Biosciences, 2019, 6, 130.	3.5	13
14	Direction Matters: Monovalent Streptavidin/Biotin Complex under Load. Nano Letters, 2019, 19, 3415-3421.	9.1	53
15	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	19.0	149
16	Population FBA predicts metabolic phenotypes in yeast. PLoS Computational Biology, 2017, 13, e1005728.	3.2	18
17	Enhanced sampling techniques in molecular dynamics simulations of biological systems. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 872-877.	2.4	537
18	Large Scale Structure Sampling for Protein Fold Prediction using the Generalized Simulated Annealing. Biophysical Journal, 2013, 104, 228a-229a.	0.5	1

#	Article	IF	Citations
19	QM/MM Molecular Dynamics Methods Applied to Investigate Cellulose Fibers Hydration. Biophysical Journal, 2012, 102, 735a.	0.5	0
20	GSAFold: A new application of GSA to protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2305-2310.	2.6	11