Manuel N Melo

List of Publications by Year in descending order

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MANUEL N MELO

#	Article	IF	CITATIONS
1	Two decades of Martini: Better beads, broader scope. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	58
2	Coarse-Grain Simulations of Membrane-Adsorbed Helical Peptides. Methods in Molecular Biology, 2022, 2405, 137-150.	0.4	0
3	Improved Parameterization of Phosphatidylinositide Lipid Headgroups for the Martini 3 Coarse-Grain Force Field. Journal of Chemical Theory and Computation, 2022, 18, 357-373.	2.3	24
4	Parainfluenza Fusion Peptide Promotes Membrane Fusion by Assembling into Oligomeric Porelike Structures. ACS Chemical Biology, 2022, 17, 1831-1843.	1.6	3
5	Overlapping Properties of the Short Membrane-Active Peptide BP100 With (i) Polycationic TAT and (ii) α-helical Magainin Family Peptides. Frontiers in Cellular and Infection Microbiology, 2021, 11, 609542.	1.8	9
6	Coarse-Grained Parameterization of Nucleotide Cofactors and Metabolites: Protonation Constants, Partition Coefficients, and Model Topologies. Journal of Chemical Information and Modeling, 2021, 61, 335-346.	2.5	9
7	Acyl-chain saturation regulates the order of phosphatidylinositol 4,5-bisphosphate nanodomains. Communications Chemistry, 2021, 4, .	2.0	4
8	Localization Preference of Antimicrobial Peptides on Liquid-Disordered Membrane Domains. Frontiers in Cell and Developmental Biology, 2020, 8, 350.	1.8	25
9	Charge-dependent interactions of monomeric and filamentous actin with lipid bilayers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5861-5872.	3.3	35
10	Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460.	2.3	159
11	Ceramides bind VDAC2 to trigger mitochondrial apoptosis. Nature Communications, 2019, 10, 1832.	5.8	144
12	Self-assembly Stability Compromises the Efficacy of Tryptophan-Containing Designed Anti-measles Virus Peptides. , 2019, 10, .		2
13	The N-terminal amphipathic helix of Pex11p self-interacts to induce membrane remodelling during peroxisome fission. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1292-1300.	1.4	28
14	Structure–Stability–Function Mechanistic Links in the Anti-Measles Virus Action of Tocopherol-Derivatized Peptide Nanoparticles. ACS Nano, 2018, 12, 9855-9865.	7.3	13
15	Lipid–Protein Interactions Are Unique Fingerprints for Membrane Proteins. ACS Central Science, 2018, 4, 709-717.	5.3	274
16	High-Throughput Simulations Reveal Membrane-Mediated Effects of Alcohols on MscL Gating. Journal of the American Chemical Society, 2017, 139, 2664-2671.	6.6	41
17	Exchange pathways of plastoquinone and plastoquinol in the photosystem II complex. Nature Communications, 2017, 8, 15214.	5.8	71
18	Prediction of Thylakoid Lipid Binding Sites on Photosystem II. Biophysical Journal, 2017, 113, 2669-2681.	0.2	37

MANUEL N MELO

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19	Extending the Adress Multiscale Scheme for Protein and Bilayer Applications. Biophysical Journal, 2016, 110, 643a-644a.	0.2	0
20	Altered secondary structure of Dynorphin A associates with loss of opioid signalling and NMDA-mediated excitotoxicity in SCA23. Human Molecular Genetics, 2016, 25, ddw130.	1.4	9
21	Computational Lipidomics and the Lipid Organization of Cell Envelopes. Biophysical Journal, 2015, 108, 342a.	0.2	Ο
22	Adaptive resolution simulation of polarizable supramolecular coarse-grained water models. Journal of Chemical Physics, 2015, 142, 244118.	1.2	39
23	Hsc70-4 Deforms Membranes to Promote Synaptic Protein Turnover by Endosomal Microautophagy. Neuron, 2015, 88, 735-748.	3.8	140
24	Dry Martini, a Coarse-Grained Force Field for Lipid Membrane Simulations with Implicit Solvent. Journal of Chemical Theory and Computation, 2015, 11, 260-275.	2.3	236
25	Adaptive resolution simulation of an atomistic protein in MARTINI water. Journal of Chemical Physics, 2014, 140, 054114.	1.2	74
26	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	6.6	734
27	Adaptive Resolution Simulation of MARTINI Solvents. Journal of Chemical Theory and Computation, 2014, 10, 2591-2598.	2.3	46
28	The Mechanisms and Quantification of the Selective Permeability in Transport Across Biological Barriers: the Example of Kyotorphin. Mini-Reviews in Medicinal Chemistry, 2014, 14, 99-110.	1.1	5
29	Defined lipid analogues induce transient channels to facilitate drug-membrane traversal and circumvent cancer therapy resistance. Scientific Reports, 2013, 3, 1949.	1.6	22
30	Bacteriocin AS-48 binding to model membranes and pore formation as revealed by coarse-grained simulations. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2524-2531.	1.4	37
31	The Mechanism of Action of Antimicrobial Peptides: Lipid Vesicles vs. Bacteria. Frontiers in Immunology, 2012, 3, 236.	2.2	38
32	Relating Molecular-Level Events with Bacterial Killing by Antimicrobial Peptides. Biophysical Journal, 2012, 102, 91a.	0.2	0
33	Prediction of Antibacterial Activity from Physicochemical Properties of Antimicrobial Peptides. PLoS ONE, 2011, 6, e28549.	1.1	45
34	Using zeta-potential measurements to quantify peptide partition to lipid membranes. European Biophysics Journal, 2011, 40, 481-487.	1.2	64
35	Escherichia coli Cell Surface Perturbation and Disruption Induced by Antimicrobial Peptides BP100 and pepR. Journal of Biological Chemistry, 2010, 285, 27536-27544.	1.6	193
36	Drug–lipid interaction evaluation: why a 19th century solution?. Trends in Pharmacological Sciences, 2010, 31, 449-454.	4.0	31

MANUEL N MELO

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37	Antimicrobial peptides: linking partition, activity and high membrane-bound concentrations. Nature Reviews Microbiology, 2009, 7, 245-250.	13.6	568
38	Interaction of the Dengue Virus Fusion Peptide with Membranes Assessed by NMR: The Essential Role of the Envelope Protein Trp101 for Membrane Fusion. Journal of Molecular Biology, 2009, 392, 736-746.	2.0	45
39	Synergistic Effects of the Membrane Actions of Cecropin-Melittin Antimicrobial Hybrid Peptide BP100. Biophysical Journal, 2009, 96, 1815-1827.	0.2	83
40	Interaction between dengue virus fusion peptide and lipid bilayers depends on peptide clustering. Molecular Membrane Biology, 2008, 25, 128-138.	2.0	30
41	Characterization of glycoinositolphosphoryl ceramide structure mutant strains of Cryptococcus neoformans. Glycobiology, 2007, 17, 1C-1C.	1.3	36
42	Omiganan interaction with bacterial membranes and cell wall models. Assigning a biological role to saturation. Biochimica Et Biophysica Acta - Biomembranes, 2007, 1768, 1277-1290.	1.4	56
43	How to address CPP and AMP translocation? Methods to detect and quantify peptide internalizationin vitroandin vivo(Review). Molecular Membrane Biology, 2007, 24, 173-184.	2.0	34
44	Omiganan Pentahydrochloride in the Front Line of Clinical Applications of Antimicrobial Peptides. Recent Patents on Anti-infective Drug Discovery, 2006, 1, 201-207.	0.5	59
45	Cell-penetrating peptides and antimicrobial peptides: how different are they?. Biochemical Journal, 2006, 399, 1-7.	1.7	367