Roberto Dias Lins Neto

List of Publications by Year
in descending order

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79 papers	3,694 citations	172443 29 h-index	133244 59 g-index
86 all docs	86 docs citations	86 times ranked	5165 citing authors

#	Article	IF	Citations
1	Identification of potential Staphylococcus aureus dihydrofolate reductase inhibitors using QSAR, molecular docking, dynamics simulations and free energy calculation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3835-3846.	3.5	2
2	Spread of Gamma (P.1) Sub-Lineages Carrying Spike Mutations Close to the Furin Cleavage Site and Deletions in the N-Terminal Domain Drives Ongoing Transmission of SARS-CoV-2 in Amazonas, Brazil. Microbiology Spectrum, 2022, 10, e0236621.	3.0	28
3	GM2/GM3 controls the organizational status of CD82/Met microdomains: further studies in GM2/GM3 complexation. Glycoconjugate Journal, 2022, , .	2.7	0
4	Differential Frequencies of HLA-DRB1, DQA1, and DQB1 Alleles and Haplotypes Are Observed in the Arbovirus-Related Neurological Syndromes. Journal of Infectious Diseases, 2021, 224, 517-525.	4.0	2
5	Immune evasion of SARS-CoV-2 variants of concern is driven by low affinity to neutralizing antibodies. Chemical Communications, 2021, 57, 6094-6097.	4.1	18
6	Characterizing Binding Kinetics and Thermodynamics of Computer-Designed Nanobodies Targeting SARS-CoV-2 RBD. Biophysical Journal, 2021, 120, 21a-22a.	0.5	0
7	Repositioning Lopinavir, an HIV Protease Inhibitor, as a Promising Antifungal Drug: Lessons Learned from Candida albicansâ€"In Silico, In Vitro and In Vivo Approaches. Journal of Fungi (Basel,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	3.5	11
8	The ongoing evolution of variants of concern and interest of SARS-CoV-2 in Brazil revealed by convergent indels in the amino (N)-terminal domain of the spike protein. Virus Evolution, 2021, 7, veab069.	4.9	31
9	Are Zika virus cross-reactive antibodies against aquaporin-4 associated to Neuromyelitis Optica Spectrum Disorder?. Journal of Neuroimmunology, 2021, 360, 577697.	2.3	1
10	Identification of a Zika NS2B epitope as a biomarker for severe clinical phenotypes. RSC Medicinal Chemistry, 2021, 12, 1525-1539.	3.9	2
11	SARS-CoV-2 recombinant proteins stimulate distinct cellular and humoral immune response profiles in samples from COVID-19 convalescent patients. Clinics, 2021, 76, e3548.	1.5	3
12	SuAVE: A Tool for Analyzing Curvature-Dependent Properties in Chemical Interfaces. Journal of Chemical Information and Modeling, 2020, 60, 473-484.	5.4	24
13	Rotational Profiler: A Fast, Automated, and Interactive Server to Derive Torsional Dihedral Potentials for Classical Molecular Simulations. Journal of Chemical Information and Modeling, 2020, 60, 5923-5927.	5.4	4
14	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
15	Unraveling the Role of Nanobodies Tetrad on Their Folding and Stability Assisted by Machine and Deep Learning Algorithms. Lecture Notes in Computer Science, 2020, , 93-104.	1.3	0
16	Influence of directional positive Darwinian selection-driven evolution on arboviruses Dengue and Zika virulence and pathogenesis. Molecular Phylogenetics and Evolution, 2019, 140, 106607.	2.7	1
17	The influence of biotinylation on the ability of a computer designed protein to detect B-cells producing anti-HIV-1 2F5 antibodies. Journal of Molecular Graphics and Modelling, 2019, 93, 107442.	2.4	4
18	Study protocol for the multicentre cohorts of Zika virus infection in pregnant women, infants, and acute clinical cases in Latin America and the Caribbean: the ZIKAlliance consortium. BMC Infectious Diseases, 2019, 19, 1081.	2.9	11

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19	Duffy binding-like 1Î± adhesin from Plasmodium falciparum recognizes ABH histo-blood group saccharide in a type specific manner. Carbohydrate Polymers, 2019, 207, 266-275.	10.2	0
20	Rational Zika vaccine design via the modulation of antigen membrane anchors in chimpanzee adenoviral vectors. Nature Communications, 2018, 9, 2441.	12.8	69
21	Aromatic Rings Commonly Used in Medicinal Chemistry: Force Fields Comparison and Interactions With Water Toward the Design of New Chemical Entities. Frontiers in Pharmacology, 2018, 9, 395.	3.5	40
22	Amino acid polymorphisms in the fibronectin-binding repeats of fibronectin-binding protein A affect bond strength and fibronectin conformation. Journal of Biological Chemistry, 2017, 292, 8797-8810.	3.4	16
23	Conformational stability of the epidermal growth factor (EGF) receptor as influenced by glycosylation, dimerization and EGF hormone binding. Proteins: Structure, Function and Bioinformatics, 2017, 85, 561-570.	2.6	18
24	Cover Image, Volume 85, Issue 4. Proteins: Structure, Function and Bioinformatics, 2017, 85, C4.	2.6	0
25	Significant Performance Enhancement of Polymer Resins by Bioinspired Dynamic Bonding. Advanced Materials, 2017, 29, 1703026.	21.0	63
26	Polymyxin Binding to the Bacterial Outer Membrane Reveals Cation Displacement and Increasing Membrane Curvature in Susceptible but Not in Resistant Lipopolysaccharide Chemotypes. Journal of Chemical Information and Modeling, 2017, 57, 2181-2193.	5.4	54
27	Mapping Putative B-Cell Zika Virus NS1 Epitopes Provides Molecular Basis for Anti-NS1 Antibody Discrimination between Zika and Dengue Viruses. ACS Omega, 2017, 2, 3913-3920.	3.5	41
28	De Novo Design and Biophysical Characterization of an Affinity-Enhanced Protein Displaying the Structure of the Broadly Neutralizing HIV-1 2F5 Antibody Epitope. Biophysical Journal, 2016, 110, 346a.	0.5	0
29	Molecularly Smooth Self-Assembled Monolayer for High-Mobility Organic Field-Effect Transistors. Nano Letters, 2016, 16, 6709-6715.	9.1	31
30	Endovascular Infections Caused by Methicillin-Resistant Staphylococcus aureus Are Linked to Clonal Complex-Specific Alterations in Binding and Invasion Domains of Fibronectin-Binding Protein A as Well as the Occurrence of fnbB. Infection and Immunity, 2015, 83, 4772-4780.	2.2	24
31	Comparative hazard analysis and toxicological modeling of diverse nanomaterials using the embryonic zebrafish (EZ) metric of toxicity. Journal of Nanoparticle Research, 2015, 17, 250.	1.9	30
32	Assessing protein conformational sampling and structural stability via de novo design and molecular dynamics simulations. Biopolymers, 2015, 103, 351-361.	2.4	7
33	Desorption/ionization efficiencies of triacylglycerols and phospholipids via EASIâ€MS. Journal of Mass Spectrometry, 2014, 49, 335-341.	1.6	7
34	Anionic Form of Usnic Acid Promotes Lamellar to Nonlamellar Transition in DPPC and DOPC Membranes. Journal of Physical Chemistry B, 2014, 118, 3881-3886.	2.6	5
35	Hydration, ionic valence and cross-linking propensities of cations determine the stability of lipopolysaccharide (LPS) membranes. Chemical Communications, 2014, 50, 231-233.	4.1	43
36	PITOMBA: Parameter Interface for Oligosaccharide Molecules Based on Atoms. Journal of Chemical Theory and Computation, 2014, 10, 5068-5080.	5.3	20

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37	Extension and validation of the GROMOS 53A6_{<scp>glyc</scp>} parameter set for glycoproteins. Journal of Computational Chemistry, 2014, 35, 2087-2095.	3.3	42
38	MDWiZ: A platform for the automated translation of molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2014, 48, 80-86.	2.4	10
39	IMSPeptider: A computational peptide collision crossâ€section area calculator based on a novel molecular dynamics simulation protocol. Journal of Computational Chemistry, 2013, 34, 1707-1718.	3.3	5
40	De novo design of immunoreactive conformation-specific HIV-1 epitopes based on Top7 scaffold. RSC Advances, 2013, 3, 11790.	3.6	14
41	Aspartic Proteolytic Inhibitors Induce Cellular and Biochemical Alterations in Fungal Cells. , 2013, , 89-119.		3
42	Influence of Scaffold Stability and Electrostatics on Top7-Based Engineered Helical HIV-1 Epitopes. Lecture Notes in Computer Science, 2013, , 94-103.	1.3	2
43	A Glycam-Based Force Field for Simulations of Lipopolysaccharide Membranes: Parametrization and Validation. Journal of Chemical Theory and Computation, 2012, 8, 4719-4731.	5.3	96
44	GROMOS 53A6_{GLYC}, an Improved GROMOS Force Field for Hexopyranose-Based Carbohydrates. Journal of Chemical Theory and Computation, 2012, 8, 4681-4690.	5.3	132
45	The Effect of Temperature, Cations, and Number of Acyl Chains on the Lamellar to Non-Lamellar Transition in Lipid-A Membranes: A Microscopic View. Journal of Chemical Theory and Computation, 2012, 8, 3830-3838.	5.3	52
46	Conformational Variability of Organophosphorus Hydrolase upon Soman and Paraoxon Binding. Journal of Physical Chemistry B, 2011, 115, 15389-15398.	2.6	9
47	Modeling the Nanophase Structural Dynamics of Phenylated Sulfonated Poly Ether Ether Ketone Ketone (Ph-SPEEKK) Membranes As a Function of Hydration. Journal of Physical Chemistry B, 2011, 115, 1817-1824.	2.6	15
48	Chitosan molecular structure as a function of Nâ€acetylation. Biopolymers, 2011, 95, 448-460.	2.4	88
49	Polymorphisms in fibronectin binding protein A of Staphylococcus aureus are associated with infection of cardiovascular devices. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 18372-18377.	7.1	69
50	Prebiotic chemical kinetics imprint on positional codon usage. Journal of the Brazilian Chemical Society, 2010, 21, 1117-1120.	0.6	0
51	The Role of Nonbonded Interactions in the Conformational Dynamics of Organophosphorous Hydrolase Adsorbed onto Functionalized Mesoporous Silica Surfaces. Journal of Physical Chemistry B, 2010, 114, 531-540.	2.6	37
52	Interaction between the CBM of Cel9A from Thermobifida fusca and cellulose fibers. Journal of Molecular Recognition, 2009, 22, 38-45.	2.1	22
53	Electrostatic Cooperativity of Hydroxyl Groups at Metal Oxide Surfaces. Journal of Physical Chemistry C, 2009, 113, 16568-16570.	3.1	6
54	Characterization of Chitin and Chitosan Molecular Structure in Aqueous Solution. Journal of Chemical Theory and Computation, 2008, 4, 2141-2149.	5.3	142

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55	In Vitro Evolution of a Peptide with a Hematite Binding Motif That May Constitute a Natural Metal-Oxide Binding Archetype. Environmental Science & Technology, 2008, 42, 3821-3827.	10.0	83
56	Computer Simulation of Uranyl Uptake by the Rough Lipopolysaccharide Membrane of Pseudomonas aeruginosa. Biomacromolecules, 2008, 9, 29-35.	5.4	33
57	Influence of the B-band O-antigen chain in the structure and electrostatics of the lipopolysaccharide membrane of Pseudomonas aeruginosa. Journal of the Brazilian Chemical Society, 2008, 19, 312-320.	0.6	16
58	Molecular Models to Emulate Confinement Effects on the Internal Dynamics of Organophosphorous Hydrolase. Lecture Notes in Computer Science, 2008, , 68-78.	1.3	2
59	Revisiting the internal conformational dynamics and solvation properties of cyclodextrins. Journal of the Brazilian Chemical Society, 2007, 18, 951-961.	0.6	8
60	Influence of Long-Range Electrostatic Treatments on the Folding of the N-Terminal H4 Histone Tail Peptide. Journal of Chemical Theory and Computation, 2006, 2, 246-250.	5.3	28
61	Protein under pressure: Molecular dynamics simulation of the arc repressor. Proteins: Structure, Function and Bioinformatics, 2006, 65, 136-144.	2.6	31
62	An improved nucleic acid parameter set for the GROMOS force field. Journal of Computational Chemistry, 2005, 26, 725-737.	3.3	161
63	A new GROMOS force field for hexopyranose-based carbohydrates. Journal of Computational Chemistry, 2005, 26, 1400-1412.	3.3	286
64	Variational Particle Number Approach for Rational Compound Design. Physical Review Letters, 2005, 95, 153002.	7.8	112
65	Trehalose-protein interaction in aqueous solution. Proteins: Structure, Function and Bioinformatics, 2004, 55, 177-186.	2.6	204
66	Prediction of HIV-1 Integrase/Viral DNA Interactions in the Catalytic Domain by Fast Molecular Docking. Journal of Medicinal Chemistry, 2004, 47, 821-828.	6.4	52
67	Interaction of the Disaccharide Trehalose with a Phospholipid Bilayer: A Molecular Dynamics Study. Biophysical Journal, 2004, 86, 2273-2285.	0.5	156
68	A consistent potential energy parameter set for lipids: dipalmitoylphosphatidylcholine as a benchmark of the GROMOS96 45A3 force field. European Biophysics Journal, 2003, 32, 67-77.	2.2	181
69	Internal dynamics and ionization states of the macrophage migration inhibitory factor: Comparison between wild-type and mutant forms. Biopolymers, 2002, 65, 313-323.	2.4	16
70	Computer Simulation of the Rough Lipopolysaccharide Membrane of Pseudomonas aeruginosa. Biophysical Journal, 2001, 81, 1037-1046.	0.5	107
71	Similarities in the HIV-1 and ASV integrase active sites upon metal cofactor binding. Biopolymers, 2000, 53, 308-315.	2.4	27
72	Developing a Dynamic Pharmacophore Model for HIV-1 Integrase. Journal of Medicinal Chemistry, 2000, 43, 2100-2114.	6.4	271

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73	Investigations on human immunodeficiency virus type 1 integrase/DNA binding interactions via molecular dynamics and electrostatics calculations. , 2000, 85, 123-131.		22
74	Solvent Accessibility to Aspartyl and Succinimidyl Residues at Positions 7 and 23 in the Amyloid Î² 1 - 28 Peptide. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 1999, 54, 264-270.	1.4	1
75	Molecular Dynamics Studies on the HIV-1 Integrase Catalytic Domain. Biophysical Journal, 1999, 76, 2999-3011.	0.5	78
76	Brownian and Essential Dynamics Studies of the HIV-1 Integrase Catalytic Domain. Journal of Biomolecular Structure and Dynamics, 1998, 16, 733-745.	3.5	17
77	The Molecular Structure and Conformational Dynamics of Chitosan Polymers: An Integrated Perspective from Experiments and Computational Simulations. , 0, , .		5
78	SUAVE: UMA FERRAMENTA PARA AVALIAÃ‡ÃƒO DE PROPRIEDADES DEPENDENTES DE CURVATURA EM SUPERFÃCIES GENÃ‰RICAS. , 0, , .		0
79	IMUNOREATIVIDADE DE APTÃ‚MEROS ENGENHEIRADOS IN SILICO CONTRA EPÃTOPO NEUTRALIZANTE DO VÃRUS ZIKA VIA TERMOFORESE EM MICROESCALA. , 0, , .		0