Thereza A Soares

List of Publications by Year
in descending order

80 papers	2,964 citations	218381 26 h-index	174990 52 g-index
81 all docs	81 docs citations	81 times ranked	4689 citing authors

#	Article	IF	Citations
1	Validation of the 53A6 GROMOS force field. European Biophysics Journal, 2005, 34, 273-284.	1.2	443
2	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
3	Cytotoxicity and slow release of the anti-cancer drug doxorubicin from ZIF-8. RSC Advances, 2012, 2, 9437.	1.7	247
4	An improved nucleic acid parameter set for the GROMOS force field. Journal of Computational Chemistry, 2005, 26, 725-737.	1.5	161
5	A Glycam-Based Force Field for Simulations of Lipopolysaccharide Membranes: Parametrization and Validation. Journal of Chemical Theory and Computation, 2012, 8, 4719-4731.	2.3	96
6	Validation of the GROMOS force-field parameter set 45A3 against nuclear magnetic resonance data of hen egg lysozyme. Journal of Biomolecular NMR, 2004, 30, 407-422.	1.6	87
7	A combined experimental and computational study of novel nanocage-based metalâ€“organic frameworks for drug delivery. Dalton Transactions, 2015, 44, 19370-19382.	1.6	83
8	Myricetin protects Galleria mellonella against Staphylococcus aureus infection and inhibits multiple virulence factors. Scientific Reports, 2017, 7, 2823.	1.6	83
9	Enzyme specific activity in functionalized nanoporous supports. Nanotechnology, 2008, 19, 125102.	1.3	59
10	Characterization of the outer membrane protein OprF of Pseudomonas aeruginosa in a lipopolysaccharide membrane by computer simulation. Proteins: Structure, Function and Bioinformatics, 2009, 74, 475-488.	1.5	56
11	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.	2.5	54
12	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.	2.3	52
13	Two isoreticular metalâ€“organic frameworks with CdSO₄-like topology: selective gas sorption and drug delivery. Dalton Transactions, 2014, 43, 17265-17273.	1.6	51
14	Metal organic frameworks for drug delivery and environmental remediation: A molecular docking approach. International Journal of Quantum Chemistry, 2012, 112, 3346-3355.	1.0	47
15	Hydration, ionic valence and cross-linking propensities of cations determine the stability of lipopolysaccharide (LPS) membranes. Chemical Communications, 2014, 50, 231-233.	2.2	43
16	Designed Benzothiadiazole Fluorophores for Selective Mitochondrial Imaging and Dynamics. Chemistry - A European Journal, 2014, 20, 15360-15374.	1.7	43
17	Gramâ€Negative Bacteria Targeting Mediated by Carbohydrateâ€“Carbohydrate Interactions Induced by Surfaceâ€Modified Nanoparticles. Advanced Functional Materials, 2019, 29, 1904216.	7.8	43
18	Bioimaging, cellular uptake and dynamics in living cells of a lipophilic fluorescent benzothiadiazole at low temperature (4 Â°C). Chemical Science, 2014, 5, 3995.	3.7	41

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19	Impact of the Molecular Environment on Thiolâ€“Ene Coupling For Biofunctionalization and Conjugation. Bioconjugate Chemistry, 2016, 27, 2111-2123.	1.8	39
20	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.	1.2	37
21	A thermo-responsive adsorbent-heater-thermometer nanomaterial for controlled drug release: (ZIF-8,EuxTby)@AuNP core-shell. Materials Science and Engineering C, 2019, 102, 578-588.	3.8	36
22	Toward Chemically Resolved Computer Simulations of Dynamics and Remodeling of Biological Membranes. Journal of Physical Chemistry Letters, 2017, 8, 3586-3594.	2.1	35
23	Assessment of the convergence of molecular dynamics simulations of lipopolysaccharide membranes. Molecular Simulation, 2008, 34, 295-307.	0.9	33
24	Probing deep into the interaction of a fluorescent chalcone derivative and bovine serum albumin (BSA): an experimental and computational study. Organic and Biomolecular Chemistry, 2013, 11, 4764.	1.5	31
25	Ionization state and molecular docking studies for the macrophage migration inhibitory factor: the role of lysine 32 in the catalytic mechanism. Journal of Molecular Recognition, 2000, 13, 146-156.	1.1	30
26	Electrostatics and flexibility drive membrane recognition and early penetration by the antimicrobial peptide dendrimer bH1. Chemical Communications, 2013, 49, 8821.	2.2	29
27	Single-Amino Acid Modifications Reveal Additional Controls on the Proton Pathway of [FeFe]-Hydrogenase. Biochemistry, 2016, 55, 3165-3173.	1.2	29
28	Docking of 4-oxalocrotonate tautomerase substrates: Implications for the catalytic mechanism. , 1999, 50, 319-328.		26
29	SuAVE: A Tool for Analyzing Curvature-Dependent Properties in Chemical Interfaces. Journal of Chemical Information and Modeling, 2020, 60, 473-484.	2.5	24
30	Engineering an ultra-stable affinity reagent based on Top7. Protein Engineering, Design and Selection, 2009, 22, 325-332.	1.0	23
31	Outer Membrane Remodeling: The Structural Dynamics and Electrostatics of Rough Lipopolysaccharide Chemotypes. Journal of Chemical Theory and Computation, 2014, 10, 2488-2497.	2.3	23
32	Conformational Dynamics and Responsiveness of Weak and Strong Polyelectrolyte Brushes: Atomistic Simulations of Poly(dimethyl aminoethyl methacrylate) and Poly(2-(methacryloyloxy)ethyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 217 Td	1.6	23
33	Investigations on human immunodeficiency virus type 1 integrase/DNA binding interactions via molecular dynamics and electrostatics calculations. , 2000, 85, 123-131.		22
34	Editorial: Method and Data Sharing and Reproducibility of Scientific Results. Journal of Chemical Information and Modeling, 2020, 60, 5868-5869.	2.5	22
35	Correlatos bioquÃmicos da depressÃ£o em crianÃ§as. Arquivos De Neuro-Psiquiatria, 1991, 49, 418-425.	0.3	21
36	Alpha- and beta-polypeptides show a different stability of helical secondary structure. Tetrahedron, 2004, 60, 7775-7780.	1.0	20

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37	Molecular dynamics studies of alanine racemase: A structural model for drug design. Biopolymers, 2003, 70, 186-200.	1.2	19
38	Molecular Dynamics of Organophosphorous Hydrolases Bound to the Nerve Agent Soman. Journal of Chemical Theory and Computation, 2007, 3, 1569-1579.	2.3	19
39	The enzyme 3-hydroxykynurenine transaminase as potential target for 1,2,4-oxadiazoles with larvicide activity against the dengue vector Aedes aegypti. Bioorganic and Medicinal Chemistry, 2013, 21, 6996-7003.	1.4	18
40	Modeling the electrostatic potential of asymmetric lipopolysaccharide membranes: The MEMPOT algorithm implemented in DelPhi. Journal of Computational Chemistry, 2014, 35, 1418-1429.	1.5	17
41	Internal dynamics and ionization states of the macrophage migration inhibitory factor: Comparison between wild-type and mutant forms. Biopolymers, 2002, 65, 313-323.	1.2	16
42	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
43	Effect of dimerization on the mechanism of action of aurein 1.2. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1129-1138.	1.4	16
44	Phospholamban Modulates the Functional Coupling between Nucleotide Domains in Ca-ATPase Oligomeric Complexes in Cardiac Sarcoplasmic Reticulum. Biochemistry, 2009, 48, 2411-2421.	1.2	15
45	The â€œpre-assembled stateâ€•of magainin 2 lysine-linked dimer determines its enhanced antimicrobial activity. Colloids and Surfaces B: Biointerfaces, 2018, 167, 432-440.	2.5	15
46	Aggregation of Lipid A Variants: A Hybrid Particle-Field Model. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129570.	1.1	15
47	De novo design of immunoreactive conformation-specific HIV-1 epitopes based on Top7 scaffold. RSC Advances, 2013, 3, 11790.	1.7	14
48	Revisiting the structural flexibility of the complex p21ras-GTP: The catalytic conformation of the molecular switch II. Proteins: Structure, Function and Bioinformatics, 2001, 45, 297-312.	1.5	13
49	Antimicrobial peptide induced colloidal transformations in bacteria-mimetic vesicles: Combining in silico tools and experimental methods. Journal of Colloid and Interface Science, 2021, 596, 352-363.	5.0	13
50	Mulheres em ciÃªncia e tecnologia: ascensÃ£o limitada. Quimica Nova, 2001, 24, 281-285.	0.3	13
51	Molecular basis of the structural stability of a Top7-based scaffold at extreme pH and temperature conditions. Journal of Molecular Graphics and Modelling, 2010, 28, 755-765.	1.3	12
52	Molecular Dynamics Simulations of Cetyltrimethylammonium Bromide (CTAB) Micelles and their Interactions with a Gold Surface in Aqueous Solution. Journal of the Brazilian Chemical Society, 0, , .	0.6	12
53	Discovery of 1,2,4-oxadiazole derivatives as a novel class of noncompetitive inhibitors of 3-hydroxykynurenine transaminase (HKT) from Aedes aegypti. Bioorganic and Medicinal Chemistry, 2020, 28, 115252.	1.4	12
54	Conformational Variability of Organophosphorus Hydrolase upon Soman and Paraoxon Binding. Journal of Physical Chemistry B, 2011, 115, 15389-15398.	1.2	9

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55	Membrane negative curvature induced by a hybrid peptide from pediocin PA-1 and plantaricin 149 as revealed by atomistic molecular dynamics simulations. Soft Matter, 2016, 12, 8884-8898.	1.2	9
56	Towards Simulations of Outer Membrane Proteins in Lipopolysaccharide Membranes. AIP Conference Proceedings, 2007, , .	0.3	7
57	Alpha-hemolysin nanopore allows discrimination of the microcystins variants. RSC Advances, 2019, 9, 14683-14691.	1.7	7
58	Out of Sight, Out of Mind: The Effect of the Equilibration Protocol on the Structural Ensembles of Charged Glycolipid Bilayers. Molecules, 2020, 25, 5120.	1.7	7
59	A second generation of 1,2,4-oxadiazole derivatives with enhanced solubility for inhibition of 3-hydroxykynurenine transaminase (HKT) from Aedes aegypti. RSC Medicinal Chemistry, 2021, 12, 222-236.	1.7	7
60	Plural Origins of the Molecular Homochirality in Our Biota. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 1996, 51, 70-74.	0.6	5
61	Metal Organic Frameworks for Selective Degradation of Amoxicillin in Biomedical Wastes. Journal of the Brazilian Chemical Society, 0, , .	0.6	5
62	Effect of the ligandâ€™s bulkiness on the shape of functionalized gold nanoparticles in aqueous solutions: A molecular dynamics study. Chemical Physics Letters, 2019, 731, 136576.	1.2	5
63	Compatibility of GROMOS-Derived Atomic Parameters for Lipopolysaccharide Membranes with the SPC/E Water Model and Alternative Long-Range Electrostatic Treatments Using Single Nonbonded Cutoff and Atom-Based Charge Schemes. Journal of the Brazilian Chemical Society, 0, , .	0.6	5
64	Advancing Women in Chemistry. Journal of Chemical Information and Modeling, 2021, 61, 5305-5306.	2.5	5
65	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.	2.5	4
66	Molecular Simulation in Latin America: Coming of Age. Journal of Chemical Information and Modeling, 2019, 59, 3601-3602.	2.5	3
67	AplicaÃ§Ã£o da equaÃ§Ã£o de Poisson-Boltzmann ao cÃ¡lculo de propriedades dependentes do pH em proteÃnas. Quimica Nova, 2004, 27, 640-647.	0.3	2
68	Computational Chemistry in Asia. Journal of Chemical Information and Modeling, 2021, 61, 547-547.	2.5	2
69	Molecular Models to Emulate Confinement Effects on the Internal Dynamics of Organophosphorous Hydrolase. Lecture Notes in Computer Science, 2008, , 68-78.	1.0	2
70	Bias Amplification in Gender, Gender Identity, and Geographical Affiliation. Journal of Chemical Information and Modeling, 2022, , .	2.5	2
71	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.	0.6	1
72	Fast and low-cost evaluation of hydroxykynurenine activity. MethodsX, 2020, 7, 100982.	0.7	1

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73	The tug of war between Al³⁺ and Na⁺ for orderâ€“disorder transitions in lipid-A membranes. Physical Chemistry Chemical Physics, 2021, 23, 15127-15137.	1.3	1
74	The Role of the Conformational Dynamics of Glutathione S-Transferase Epsilon Class on Insecticide Resistance inAnopheles gambiae. Journal of the Brazilian Chemical Society, 2016, , .	0.6	1
75	Plural origins of molecular homochirality in our biota Part II. The relative stabilities of homochiral and mixed oligoribotides and peptides. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 1997, 52, 89-96.	0.6	1
76	Frontispiece: Designed Benzothiadiazole Fluorophores for Selective Mitochondrial Imaging and Dynamics. Chemistry - A European Journal, 2014, 20, .	1.7	0
77	Study of the Mecanism of Action of a Hybrid Peptide in POPG:POPC Bilayers. Biophysical Journal, 2014, 106, 99a.	0.2	0
78	Can Biomimetic Zinc Compounds Assist a (3 + 2) Cycloaddition Reaction? A Theoretical Perspective. Journal of Chemical Theory and Computation, 2017, 13, 6382-6390.	2.3	0
79	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.	5.1	0
80	Outlook on the Development and Application of Molecular Simulations in Latin America. Journal of Chemical Information and Modeling, 2020, 60, 435-438.	2.5	0