Bruno A C Horta

List of Publications by Year
in descending order

64	1,527	394421 19	330143 37
papers	citations	h-index	g-index

68	68	68	2135
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computer Modeling Explains the Structural Reasons for the Difference in Reactivity of Amine Transaminases Regarding Prochiral Methylketones. International Journal of Molecular Sciences, 2022, 23, 777.	4.1	2
2	Simultaneous parametrization of torsional and thirdâ€neighbor interaction terms in forceâ€field development: The LLSâ€SC algorithm. Journal of Computational Chemistry, 2022, , .	3.3	1
3	Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes? 2. A systematic study considering different chain lengths. Journal of Molecular Liquids, 2022, 354, 118829.	4.9	5
4	Targeting Nsp9 as an anti-SARS-CoV-2 strategy. New Journal of Chemistry, 2021, 45, 522-525.	2.8	9
5	Effects of paraffin, fatty acid and long alkyl chain phenol on the solidification of n-hexadecane under harsh subcooling condition: A molecular dynamics simulation study. Fuel, 2021, 285, 119029.	6.4	5
6	Drug-Loading Capacity of PAMAM Dendrimers Encapsulating Quercetin Molecules: A Molecular Dynamics Study with the 2016H66 Force Field. Journal of Chemical Information and Modeling, 2021, 61, 987-1000.	5.4	5
7	pyPolyBuilder: Automated Preparation of Molecular Topologies and Initial Configurations for Molecular Dynamics Simulations of Arbitrary Supramolecules. Journal of Chemical Information and Modeling, 2021, 61, 1539-1544.	5.4	8
8	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bioâ€Molecular Systems: Overview and Perspective on Issues. ChemPhysChem, 2021, 22, 264-282.	2.1	12
9	Self-diffusion coefficients of methane/n-hexane mixtures at high pressures: An evaluation of the finite-size effect and a comparison of force fields. Journal of Supercritical Fluids, 2020, 155, 104639.	3.2	14
10	Dinuclear copper(<scp>ii</scp>) complexes containing oxamate and blocking ligands: crystal structure, magnetic properties, and DFT calculations. New Journal of Chemistry, 2020, 44, 2597-2608.	2.8	6
11	Unimodal optimization using a genetic-programming-based method with periodic boundary conditions. Genetic Programming and Evolvable Machines, 2020, 21, 503-523.	2.2	3
12	Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes?. Journal of Molecular Modeling, 2020, 26, 296.	1.8	21
13	Systematic Optimization of a Fragment-Based Force Field against Experimental Pure-Liquid Properties Considering Large Compound Families: Application to Saturated Haloalkanes. Journal of Chemical Theory and Computation, 2020, 16, 7525-7555.	5.3	21
14	Emission redshift in DCM2-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Alq</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> caused by nonlinear Stark shifts and FÃ¶rster-mediated exciton diffusion. Physical Review B, 2020, 102, .	3.2	11
15	Evaluating Classical Force Fields against Experimental Cross-Solvation Free Energies. Journal of Chemical Theory and Computation, 2020, 16, 7556-7580.	5.3	28
16	Predicting the Miscibility and Rigidity of Poly(lactic-co-glycolic acid)/Polyethylene Glycol Blends via Molecular Dynamics Simulations. Macromolecules, 2020, 53, 3643-3654.	4.8	21
17	On the development of a nucleophilic methylthiolation methodology. Organic and Biomolecular Chemistry, 2020, 18, 5420-5426.	2.8	10
18	Effects of additives on oil displacement in nanocapillaries: A mesoscale simulation study. Journal of Molecular Liquids, 2020, 312, 112953.	4.9	4

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19	gem â€Dichlorocyclopropanation of Dicarbonyl Derivatives. Chemistry - A European Journal, 2019, 25, 16555-16563.	3.3	7
20	Influence of the Treatment of Nonbonded Interactions on the Thermodynamic and Transport Properties of Pure Liquids Calculated Using the 2016H66 Force Field. Journal of Chemical Theory and Computation, 2019, 15, 1806-1826.	5.3	28
21	Molecular Dynamics Simulations of PAMAM and PPI Dendrimers Using the GROMOS-Compatible 2016H66 Force Field. Journal of Chemical Information and Modeling, 2019, 59, 1444-1457.	5.4	24
22	Frontispiece: gemâ€Dichlorocyclopropanation of Dicarbonyl Derivatives. Chemistry - A European Journal, 2019, 25, .	3.3	0
23	Continuousâ€Flow Synthesis of (R)â€Propylene Carbonate: An Important Intermediate in the Synthesis of Tenofovir. European Journal of Organic Chemistry, 2018, 2018, 2931-2938.	2.4	17
24	Multi-Modal Optimization by Multi-Gene Genetic Programming. , 2018, , .		3
25	Experimental and theoretical studies of a greener catalytic system for saturated hydrocarbon chlorination composed by trichloroisocyanuric acid and a copper(II) compound. Applied Catalysis A: General, 2018, 562, 150-158.	4.3	1
26	Solvent effects on the decarboxylation of trichloroacetic acid: insights from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 21988-21998.	2.8	15
27	Insights into CC Chemokine Ligand 2/Chemokine Receptor 2 Molecular Recognition: A Step Forward toward Antichemotactic Agents. Biochemistry, 2017, 56, 3197-3210.	2.5	10
28	Front Cover: Methylsulfenylation of Electrophilic Carbon Atoms: Reaction Development, Scope, and Mechanism (Eur. J. Org. Chem. 12/2017). European Journal of Organic Chemistry, 2017, 2017, 1566-1566.	2.4	0
29	Methylsulfenylation of Electrophilic Carbon Atoms: Reaction Development, Scope, and Mechanism. European Journal of Organic Chemistry, 2017, 2017, 1578-1582.	2.4	16
30	New insights into flavivirus biology: the influence of pH over interactions between prM and E proteins. Journal of Computer-Aided Molecular Design, 2017, 31, 1009-1019.	2.9	15
31	Simulating Bilayers of Nonionic Surfactants with the GROMOS-Compatible 2016H66 Force Field. Langmuir, 2017, 33, 10225-10238.	3.5	12
32	The flavivirus capsid protein: Structure, function and perspectives towards drug design. Virus Research, 2017, 227, 115-123.	2.2	67
33	Feature importance calculation and protein quality assessment on the decoy discrimination problem. , 2017, , .		0
34	Langmuir films and mechanical properties of polyethyleneglycol fatty acid esters at the air-water interface. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 498, 50-57.	4.7	16
35	Anti-biofilm potential of phenolic acids: the influence of environmental pH and intrinsic physico-chemical properties. Biofouling, 2016, 32, 853-860.	2.2	15
36	The mechanism by which P250L mutation impairs flavivirus-NS1 dimerization: an investigation based on molecular dynamics simulations. European Biophysics Journal, 2016, 45, 573-580.	2.2	6

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37	A GROMOS-Compatible Force Field for Small Organic Molecules in the Condensed Phase: The 2016H66 Parameter Set. Journal of Chemical Theory and Computation, 2016, 12, 3825-3850.	5.3	118
38	Association of the anti-tuberculosis drug rifampicin with a PAMAM dendrimer. Journal of Molecular Graphics and Modelling, 2015, 60, 34-42.	2.4	69
39	Chiral Chlorohydrins from the Biocatalyzed Reduction of Chloroketones: Chiral Building Blocks for Antiretroviral Drugs. ChemCatChem, 2015, 7, 984-992.	3.7	28
40	Long-timescale motions in glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2015, 55, 48-64.	2.4	6
41	Effect of the cosolutes trehalose and methanol on the equilibrium and phase-transition properties of glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulations. European Biophysics Journal, 2014, 43, 517-544.	2.2	10
42	Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle. Journal of the American Chemical Society, 2014, 136, 3842-3851.	13.7	42
43	MDWiZ: A platform for the automated translation of molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2014, 48, 80-86.	2.4	10
44	Phase-transition properties of glycerol-monopalmitate lipid bilayers investigated by molecular dynamics simulation: influence of the system size and force-field parameters. Molecular Simulation, 2013, 39, 563-583.	2.0	10
45	A GROMOS Parameter Set for Vicinal Diether Functions: Properties of Polyethyleneoxide and Polyethyleneglycol. Journal of Chemical Theory and Computation, 2012, 8, 3943-3963.	5.3	61
46	Reoptimized interaction parameters for the peptideâ€backbone model compound Nâ€methylacetamide in the GROMOS force field: Influence on the folding properties of two betaâ€peptides in methanol. Journal of Computational Chemistry, 2012, 33, 1907-1917.	3.3	13
47	Temperature Dependence of the Dielectric Permittivity of Acetic Acid, Propionic Acid and Their Methyl Esters: A Molecular Dynamics Simulation Study. ChemPhysChem, 2012, 13, 1182-1190.	2.1	19
48	The role of helices 5 and 6 on the human Î²1-adrenoceptor activation mechanism. Molecular Simulation, 2012, 38, 236-240.	2.0	8
49	New functionalities in the GROMOS biomolecular simulation software. Journal of Computational Chemistry, 2012, 33, 340-353.	3.3	98
50	Enantiomeric Segregation in the Gel Phase of Lipid Bilayers. Journal of the American Chemical Society, 2011, 133, 8464-8466.	13.7	11
51	GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. Journal of Chemical Theory and Computation, 2011, 7, 3379-3390.	5.3	180
52	Dynamical behaviour of the human Î²1-adrenoceptor under agonist binding. Molecular Simulation, 2011, 37, 907-913.	2.0	10
53	New Interaction Parameters for Oxygen Compounds in the GROMOS Force Field: Improved Pure-Liquid and Solvation Properties for Alcohols, Ethers, Aldehydes, Ketones, Carboxylic Acids, and Esters. Journal of Chemical Theory and Computation, 2011, 7, 1016-1031.	5.3	112
54	Structural and dynamic effects of changing the pattern of disulfide bonds in the vascular endothelial growth factor. Revista Virtual De Quimica, 2011, 3, .	0.4	0

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55	Interaction of the disaccharides trehalose and gentiobiose with lipid bilayers: A comparative molecular dynamics study. Journal of Molecular Graphics and Modelling, 2010, 29, 331-346.	2.4	33
56	Simulating the Transition between Gel and Liquid-Crystal Phases of Lipid Bilayers: Dependence of the Transition Temperature on the Hydration Level. Journal of Chemical Theory and Computation, 2010, 6, 2488-2500.	5.3	26
57	Investigating the differential activation of vascular endothelial growth factor (VEGF) receptors. Journal of Molecular Graphics and Modelling, 2009, 28, 287-296.	2.4	9
58	ProteÃnas quinases: caracterÃsticas estruturais e inibidores quÃmicos. Quimica Nova, 2009, 32, 453-462.	0.3	10
59	On the structure, interactions, and dynamics of bound VEGF. Journal of Molecular Graphics and Modelling, 2008, 26, 1091-1103.	2.4	8
60	Deamination process in the formation of a copper(II) complex with glutamic acid and a new ligand derived from guanidinoacetic acid: Synthesis, characterization, and molecular modeling studies. Polyhedron, 2008, 27, 2386-2394.	2.2	10
61	MKTOP: a program for automatic construction of molecular topologies. Journal of the Brazilian Chemical Society, 2008, 19, 1433-1435.	0.6	135
62	Engineered Monomeric Human Histidine Triad Nucleotide-binding Protein 1 Hydrolyzes Fluorogenic Acyl-adenylate and Lysyl-tRNA Synthetase-generated Lysyl-adenylate. Journal of Biological Chemistry, 2007, 282, 15137-15147.	3.4	33
63	Dynamical behavior of the vascular endothelial growth factor: Biological implications. Proteins: Structure, Function and Bioinformatics, 2007, 67, 517-525.	2.6	9
64	The Isobutyleneâ"Isobutane Alkylation Process in Liquid HF Revisited. Journal of Physical Chemistry B, 2005, 109, 12946-12955.	2.6	10