JerÃ´nimo Lameira

List of Publications by Year
in descending order

80 papers	1,459 citations	331670 21 h-index	395702 33 g-index
82 all docs	82 docs citations	82 times ranked	1914 citing authors

#	Article	IF	Citations
1	Application of Mangifera indica (mango) seeds as a biosorbent for removal of Victazol Orange 3R dye from aqueous solution and study of the biosorption mechanism. Chemical Engineering Journal, 2012, 209, 577-588.	12.7	114
2	Quantitative exploration of the molecular origin of the activation of GTPase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 20509-20514.	7.1	73
3	Exploring the Potentiality of Natural Products from Essential Oils as Inhibitors of Odorant-Binding Proteins: A Structure- and Ligand-Based Virtual Screening Approach To Find Novel Mosquito Repellents. ACS Omega, 2019, 4, 22475-22486.	3.5	63
4	Methyltransferases do not work by compression, cratic, or desolvation effects, but by electrostatic preorganization. Proteins: Structure, Function and Bioinformatics, 2015, 83, 318-330.	2.6	58
5	Structural and functional features of enzymes of Mycobacterium tuberculosis peptidoglycan biosynthesis as targets for drug development. Tuberculosis, 2015, 95, 95-111.	1.9	54
6	Assessment of mutations on RBD in the Spike protein of SARS-CoV-2 Alpha, Delta and Omicron variants. Scientific Reports, 2022, 12, .	3.3	53
7	Mycobacterium abscessus <scp>l</scp> , <scp>d</scp> -Transpeptidases Are Susceptible to Inactivation by Carbapenems and Cephalosporins but Not Penicillins. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	50
8	A theoretical study of phenolic compounds with antioxidant properties. European Journal of Medicinal Chemistry, 2007, 42, 440-446.	5.5	46
9	Combined Kinetic Studies and Computational Analysis on Kojic Acid Analogs as Tyrosinase Inhibitors. Molecules, 2014, 19, 9591-9605.	3.8	41
10	Structureâ€“activity relationship study of flavone compounds with anti-HIV-1 integrase activity: A density functional theory study. Bioorganic and Medicinal Chemistry, 2006, 14, 7105-7112.	3.0	39
11	A density functional study ofÂflavonoid compounds with anti-HIV activity. European Journal of Medicinal Chemistry, 2006, 41, 616-623.	5.5	38
12	Experimental study and computational modelling of cruzain cysteine protease inhibition by dipeptidyl nitriles. Physical Chemistry Chemical Physics, 2018, 20, 24317-24328.	2.8	38
13	Applications of Virtual Screening in Bioprospecting: Facts, Shifts, and Perspectives to Explore the Chemo-Structural Diversity of Natural Products. Frontiers in Chemistry, 2021, 9, 662688.	3.6	38
14	Assessment of the<scp>PETase</scp>conformational changes induced by poly(ethylene terephthalate) binding. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1340-1352.	2.6	32
15	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from Trypanosoma cruzi elucidated via the QM/MM approach. Physical Chemistry Chemical Physics, 2013, 15, 3772.	2.8	30
16	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ^'Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. Journal of Physical Chemistry B, 2008, 112, 14260-14266.	2.6	27
17	Assessment of the Cruzain Cysteine Protease Reversible and Irreversible Covalent Inhibition Mechanism. Journal of Chemical Information and Modeling, 2020, 60, 1666-1677.	5.4	26
18	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of O-GlcNAcase. Journal of Physical Chemistry B, 2011, 115, 6764-6775.	2.6	24

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19	Binding Free Energy Calculations of Nine FDAâ€approved Protease Inhibitors Against HIVâ€1 Subtype C I36Tâ†'T Containing 100 Amino Acids Per Monomer. Chemical Biology and Drug Design, 2016, 87, 487-498.	3.2	23
20	A comparative modeling and molecular docking study onMycobacterium tuberculosistargets involved in peptidoglycan biosynthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2399-2417.	3.5	23
21	Enhancing Paradynamics for QM/MM Sampling of Enzymatic Reactions. Journal of Physical Chemistry B, 2016, 120, 2155-2164.	2.6	22
22	Facile Synthesis and Metabolic Incorporation of m-DAP Bioisosteres Into Cell Walls of Live Bacteria. ACS Chemical Biology, 2020, 15, 2966-2975.	3.4	21
23	Insights for design of Trypanosoma cruzi GAPDH inhibitors: A QM/MM MD study of 1,3â€bisphospoâ€<scp>D</scp>â€glyceric acid analogs. International Journal of Quantum Chemistry, 2012, 112, 3398-3402.	2.0	20
24	Computational Analysis of Human OGA Structure in Complex with PUGNAc and NAG-Thiazoline Derivatives. Journal of Chemical Information and Modeling, 2012, 52, 2775-2783.	5.4	19
25	Simulating the inhibition reaction of Mycobacterium tuberculosis<scp>l</scp>,<scp>d</scp>-transpeptidase 2 by carbapenems. Chemical Communications, 2015, 51, 12560-12562.	4.1	19
26	Evaluating QM/MM Free Energy Surfaces for Ranking Cysteine Protease Covalent Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 880-889.	5.4	19
27	Targeting the cell wall ofMycobacterium tuberculosis: a molecular modeling investigation of the interaction of imipenem and meropenem withL,D-transpeptidase 2. Journal of Biomolecular Structure and Dynamics, 2016, 34, 304-317.	3.5	18
28	Structural Analysis of Viral Infectivity Factor of HIV Type 1 and Its Interaction with A3G, EloC and EloB. PLoS ONE, 2014, 9, e89116.	2.5	18
29	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of CpNagJ in Complex with PUGNAc. Journal of Physical Chemistry B, 2010, 114, 7029-7036.	2.6	16
30	In silico identification of natural products with anticancer activity using a chemo-structural database of Brazilian biodiversity. Computational Biology and Chemistry, 2019, 83, 107102.	2.3	16
31	Predicting the affinity of halogenated reversible covalent inhibitors through relative binding free energy. Physical Chemistry Chemical Physics, 2019, 21, 24723-24730.	2.8	16
32	Molecular Modeling of T.Ârangeli, T.Âbrucei gambiense, and T.Âevansi Sialidases in Complex with the DANA Inhibitor. Chemical Biology and Drug Design, 2012, 80, 114-120.	3.2	15
33	Inhibition of tyrosinase by 4 H â€chromene analogs: Synthesis, kinetic studies, and computational analysis. Chemical Biology and Drug Design, 2017, 90, 804-810.	3.2	15
34	Evaluating the Performance of a Non-Bonded Cu2+ Model Including Jahnâ^'Teller Effect into the Binding of Tyrosinase Inhibitors. International Journal of Molecular Sciences, 2020, 21, 4783.	4.1	14
35	Exploring Chloride Selectivity and Halogenase Regioselectivity of the SalL Enzyme through Quantum Mechanical/Molecular Mechanical Modeling. Journal of Chemical Information and Modeling, 2020, 60, 738-746.	5.4	14
36	Pentacycloundecane lactam vs lactone norstatine type protease HIV inhibitors: binding energy calculations and DFT study. Journal of Biomedical Science, 2015, 22, 15.	7.0	13

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37	Computational study of conformational changes in human 3-hydroxy-3-methylglutaryl coenzyme reductase induced by substrate binding. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4374-4383.	3.5	13
38	A theoretical study of the molecular mechanism of the GAPDH Trypanosoma cruzi enzyme involving iodoacetate inhibitor. Chemical Physics Letters, 2011, 514, 336-340.	2.6	12
39	Structural and evolutionary analysis of Leishmania Alba proteins. Molecular and Biochemical Parasitology, 2017, 217, 23-31.	1.1	12
40	Catalysis by solvation rather than the desolvation effect: exploring the catalytic efficiency of SAM-dependent chlorinase. Physical Chemistry Chemical Physics, 2017, 19, 21350-21356.	2.8	12
41	Investigation of the target-site resistance of EPSP synthase mutants P106T and T102I/P106S against glyphosate. RSC Advances, 2020, 10, 44352-44360.	3.6	12
42	A combined X-ray and theoretical study of flavonoid compounds with anti-inflammatory activity. Computational and Theoretical Chemistry, 2008, 862, 16-20.	1.5	11
43	Metal-dependent inhibition of HIV-1 integrase by 5CITEP inhibitor: A theoretical QM/MM approach. Chemical Physics Letters, 2013, 583, 175-179.	2.6	11
44	Structural, energetic and lipophilic analysis of SARS-CoV-2 non-structural protein 9 (NSP9). Scientific Reports, 2021, 11, 23003.	3.3	11
45	Computed insight into a peptide inhibitor preventing the induced fit mechanism of MurA enzyme from Pseudomonas aeruginosa. Chemical Biology and Drug Design, 2017, 89, 599-607.	3.2	10
46	Understanding the Mechanism of Direct Activation of AMP-Kinase: Toward a Fine Allosteric Tuning of the Kinase Activity. Journal of Chemical Information and Modeling, 2019, 59, 2859-2870.	5.4	10
47	Unraveling the conformational dynamics of glycerol 3-phosphate dehydrogenase, a nicotinamide adenine dinucleotide-dependent enzyme of Leishmania mexicana. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2044-2055.	3.5	10
48	Targeting Peptidyl-prolyl Cis-trans Isomerase NIMA-interacting 1: A Structure-based Virtual Screening Approach to Find Novel Inhibitors. Current Computer-Aided Drug Design, 2020, 16, 605-617.	1.2	10
49	Unraveling the Additionâ€“Elimination Mechanism of EPSP Synthase through Computer Modeling. Journal of Physical Chemistry B, 2017, 121, 8626-8637.	2.6	9
50	First homology model of Plasmodium falciparum glucose-6-phosphate dehydrogenase: Discovery of selective substrate analog-based inhibitors as novel antimalarial agents. European Journal of Medicinal Chemistry, 2018, 146, 108-122.	5.5	9
51	Predicting the Relative Binding Affinity for Reversible Covalent Inhibitors by Free Energy Perturbation Calculations. Journal of Chemical Information and Modeling, 2021, 61, 4733-4744.	5.4	9
52	Metabolic Processing of Selenium-Based Bioisosteres of meso-Diaminopimelic Acid in Live Bacteria. Biochemistry, 2022, 61, 1404-1414.	2.5	9
53	Computational analysis of aspartic protease plasmepsin II complexed with EH58 inhibitor: a QM/MM MD study. Journal of Molecular Modeling, 2011, 17, 2631-2638.	1.8	8
54	Computational Investigation of Bisphosphate Inhibitors of 3-Deoxy-d-manno-octulosonate 8-phosphate Synthase. Molecules, 2019, 24, 2370.	3.8	8

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55	Proteinâ€“ligand interaction of T. cruzi trans-sialidase inhibitors: a docking and QM/MM MD study. Structural Chemistry, 2012, 23, 147-152.	2.0	7
56	Homology modeling, molecular dynamics and QM/MM study of the regulatory protein PhoP from Corynebacterium pseudotuberculosis. Journal of Molecular Modeling, 2012, 18, 1219-1227.	1.8	7
57	Computational study of the mechanism of half-reactions in class 1A dihydroorotate dehydrogenase from Trypanosoma cruzi. Physical Chemistry Chemical Physics, 2013, 15, 18863.	2.8	7
58	Structure and analgesic properties of layered double hydroxides intercalated with low amounts of ibuprofen. Journal of the American Ceramic Society, 2017, 100, 2712-2721.	3.8	7
59	On the intrinsic reactivity of highly potent trypanocidal cruzain inhibitors. RSC Medicinal Chemistry, 2020, 11, 1275-1284.	3.9	7
60	Optimization strategy of single-digit nanomolar cross-class inhibitors of mammalian and protozoa cysteine proteases. Bioorganic Chemistry, 2020, 101, 104039.	4.1	7
61	Computational analyses of interactions between ALK-5 and bioactive ligands: insights for the design of potential anticancer agents. Journal of Biomolecular Structure and Dynamics, 2018, 36, 4010-4022.	3.5	6
62	Crystal structure of Leishmania mexicana cysteine protease B in complex with a high-affinity azadipeptide nitrile inhibitor. Bioorganic and Medicinal Chemistry, 2020, 28, 115743.	3.0	6
63	Design, synthesis and stepwise optimization of nitrile-based inhibitors of cathepsins B and L. Bioorganic and Medicinal Chemistry, 2021, 29, 115827.	3.0	6
64	A quantum mechanical/molecular mechanical study of the aspartic protease plasmepsin IV complexed with allophenylnorstatine-based inhibitor. Chemical Physics Letters, 2011, 509, 169-174.	2.6	5
65	Exploring the origin of the catalytic power and product specificity of SET domain protein methyltransferase. Molecular BioSystems, 2016, 12, 2980-2983.	2.9	5
66	Analysis of the structure of calpain-10 and its interaction with the protease inhibitor SNJ-1715. Computers in Biology and Medicine, 2013, 43, 1334-1340.	7.0	4
67	Proteinâ€“Ligand Interaction Study of CpOGA in Complex with GlcNAcstatin. Chemical Biology and Drug Design, 2013, 81, 284-290.	3.2	4
68	A patent review on cathepsin K inhibitors to treat osteoporosis (2011 â€“ 2021). Expert Opinion on Therapeutic Patents, 2022, 32, 561-573.	5.0	4
69	Exploring the Catalytic Mechanism of the RNA Cap Modification by nsp16-nsp10 Complex of SARS-CoV-2 through a QM/MM Approach. International Journal of Molecular Sciences, 2022, 23, 300.	4.1	4
70	Host-Guest Inclusion Complexes of Natural Products and Nanosystems: Applications in the Development of Repellents. Molecules, 2022, 27, 2519.	3.8	4
71	QM/MM Study of the Fosfomycin Resistance Mechanism Involving FosB Enzyme. ACS Omega, 2021, 6, 12507-12512.	3.5	3
72	Density Functional Theory Calculations of the Nuclear Magnetic Resonance Parameters for Two Dihydrochalcones. Journal of Computational and Theoretical Nanoscience, 2012, 9, 953-956.	0.4	2

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73	Structure modeling of a metalloendopeptidase from Corynebacterium pseudotuberculosis. Computers in Biology and Medicine, 2012, 42, 538-541.	7.0	2
74	Layered double hydroxideâ€“indomethacin hybrid: A promising biocompatible compound for the treatment of neuroinflammatory diseases. Journal of Drug Delivery Science and Technology, 2021, 61, 102190.	3.0	2
75	OBTENÃ‡ÃƒO E CARACTERIZAÃ‡ÃƒO DE COMPLEXO DE INCLUSÃƒO DE Î'-CICLODEXTRINA E EUGENOL / PREPARATION AND CHARACTERIZATION OF Î'-CYCLODEXTRIN INCLUSION COMPLEX OF EUGENOL. Brazilian Journal of Development, 2021, 7, 33056-33070.	0.1	2
76	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. Molecular Simulation, 2021, 47, 762-770.	2.0	2
77	A Computational Analysis of Indomethacin Derivative as Tubulin Inhibitor: Insights into Development of Chemotherapeutic Agents. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 431-436.	1.1	2
78	Homology modeling and molecular dynamics simulation of an alpha methyl coenzyme M reductase from methanogenic archea. International Journal of Quantum Chemistry, 2010, 110, 2067-2075.	2.0	1
79	Ferulate Anion Intercalated into Zn/Al Layered Double Hydroxide: A Promising Intercalation Compound for Inhibition of Leishmania (L.) amazonensis. Journal of the Brazilian Chemical Society, 2019, , .	0.6	1
80	Understanding the Mechanism of Direct Activation of AMP-Kinase: Towards a Fine Allosteric Tuning of the Kinase Activity. Proceedings (mdpi), 2019, 22, .	0.2	0