JerÃ´nimo Lameira

List of Publications by Year
in descending order

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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	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
2	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
3	Host-Guest Inclusion Complexes of Natural Products and Nanosystems: Applications in the Development of Repellents. Molecules, 2022, 27, 2519.	3.8	4
4	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
5	Metabolic Processing of Selenium-Based Bioisosteres of meso-Diaminopimelic Acid in Live Bacteria. Biochemistry, 2022, 61, 1404-1414.	2.5	9
6	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
7	Design, synthesis and stepwise optimization of nitrile-based inhibitors of cathepsins B and L. Bioorganic and Medicinal Chemistry, 2021, 29, 115827.	3.0	6
8	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
9	OBTENÃ‡ÃƒO E CARACTERIZAÃ‡ÃƒO DE COMPLEXO DE INCLUSÃƒO DE Î²-CICLODEXTRINA E EUGENOL / PREPARATION AND CHARACTERIZATION OF Î²-CYCLODEXTRIN INCLUSION COMPLEX OF EUGENOL. Brazilian Journal of Development, 2021, 7, 33056-33070.	0.1	2
10	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
11	QM/MM Study of the Fosfomycin Resistance Mechanism Involving FosB Enzyme. ACS Omega, 2021, 6, 12507-12512.	3.5	3
12	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. Molecular Simulation, 2021, 47, 762-770.	2.0	2
13	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
14	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
15	Structural, energetic and lipophilic analysis of SARS-CoV-2 non-structural protein 9 (NSP9). Scientific Reports, 2021, 11, 23003.	3.3	11
16	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
17	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
18	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

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19	On the intrinsic reactivity of highly potent trypanocidal cruzain inhibitors. RSC Medicinal Chemistry, 2020, 11, 1275-1284.	3.9	7
20	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
21	Optimization strategy of single-digit nanomolar cross-class inhibitors of mammalian and protozoa cysteine proteases. Bioorganic Chemistry, 2020, 101, 104039.	4.1	7
22	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
23	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
24	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
25	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
26	Computational Investigation of Bisphosphate Inhibitors of 3-Deoxy-d-manno-octulosonate 8-phosphate Synthase. Molecules, 2019, 24, 2370.	3.8	8
27	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
28	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
29	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
30	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
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	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
33	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
34	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
35	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
36	Experimental study and computational modelling of cruzain cysteine protease inhibition by dipeptidyl nitriles. Physical Chemistry Chemical Physics, 2018, 20, 24317-24328.	2.8	38

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37	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
38	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
39	Unraveling the Additionâ€“Elimination Mechanism of EPSP Synthase through Computer Modeling. Journal of Physical Chemistry B, 2017, 121, 8626-8637.	2.6	9
40	Structural and evolutionary analysis of Leishmania Alba proteins. Molecular and Biochemical Parasitology, 2017, 217, 23-31.	1.1	12
41	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
42	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
43	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
44	Enhancing Paradynamics for QM/MM Sampling of Enzymatic Reactions. Journal of Physical Chemistry B, 2016, 120, 2155-2164.	2.6	22
45	Exploring the origin of the catalytic power and product specificity of SET domain protein methyltransferase. Molecular BioSystems, 2016, 12, 2980-2983.	2.9	5
46	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
47	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
48	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
49	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
50	Structural and functional features of enzymes of Mycobacterium tuberculosis peptidoglycan biosynthesis as targets for drug development. Tuberculosis, 2015, 95, 95-111.	1.9	54
51	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
52	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
53	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
54	Combined Kinetic Studies and Computational Analysis on Kojic Acid Analogs as Tyrosinase Inhibitors. Molecules, 2014, 19, 9591-9605.	3.8	41

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55	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
56	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
57	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
58	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
59	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
60	Proteinâ€“Ligand Interaction Study of CpOGA in Complex with GlcNAcstatin. Chemical Biology and Drug Design, 2013, 81, 284-290.	3.2	4
61	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
62	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
63	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
64	Structure modeling of a metalloendopeptidase from Corynebacterium pseudotuberculosis. Computers in Biology and Medicine, 2012, 42, 538-541.	7.0	2
65	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
66	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
67	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
68	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
69	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
70	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
71	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
72	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

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73	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
74	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
75	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
76	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
77	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
78	A theoretical study of phenolic compounds with antioxidant properties. European Journal of Medicinal Chemistry, 2007, 42, 440-446.	5.5	46
79	A density functional study ofÂflavonoid compounds with anti-HIV activity. European Journal of Medicinal Chemistry, 2006, 41, 616-623.	5.5	38
80	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