Lucianna Helene Santos

List of Publications by Year
in descending order

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		1163117	752698
30	536	8	20
papers	citations	h-index	g-index

32	32	32	692
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rad5 HIRAN domain: Structural insights into its interaction with ssDNA through molecular modeling approaches. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3062-3075.	3.5	0
2	pH and non-covalent ligand binding modulate Zika virus NS2B/NS3 protease binding site residues: Discoveries from MD and constant pH MD simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10359-10372.	3.5	3
3	Bacterial 2â€²-Deoxyguanosine Riboswitch Classes as Potential Targets for Antibiotics: A Structure and Dynamics Study. International Journal of Molecular Sciences, 2022, 23, 1925.	4.1	3
4	Characterization of an Allosteric Pocket in Zika Virus NS2B-NS3 Protease. Journal of Chemical Information and Modeling, 2022, 62, 945-957.	5.4	4
5	Propedia: a database for proteinâ€“peptide identification based on a hybrid clustering algorithm. BMC Bioinformatics, 2021, 22, 1.	2.6	261
6	ToxAnalyzer: A user-friendly web tool for interactive data analysis and visualization of chemical compounds from the Comparative Toxicogenomics Database (CTD)â„¢. Computational Toxicology, 2021, 19, 100170.	3.3	1
7	Studying effects of different protonation states of His11 and His102 in ribose-5-phosphate isomerase of Trypanosoma cruzi: an example of cooperative behavior. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2047-2056.	3.5	4
8	Shared Binding Mode of Perrottetinene and Tetrahydrocannabinol Diastereomers inside the CB1 Receptor May Incentivize Novel Medicinal Drug Design: Findings from an in Silico Assay. ACS Chemical Neuroscience, 2020, 11, 4289-4300.	3.5	3
9	Profiling selectivity of chagasin mutants towards cysteine proteases cruzain or cathepsin L through molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-13.	3.5	1
10	Antigenic and Substrate Preference Differences between Scorpion and Spider Dermonecrotic Toxins, a Comparative Investigation. Toxins, 2020, 12, 631.	3.4	7
11	Insights into the Mechanism of Ethionamide Resistance in Mycobacterium tuberculosis through an in silico Structural Evaluation of EthA and Mutants Identified in Clinical Isolates. Catalysts, 2020, 10, 543.	3.5	4
12	Proteus: An algorithm for proposing stabilizing mutation pairs based on interactions observed in known protein 3D structures. BMC Bioinformatics, 2020, 21, 275.	2.6	6
13	GlutantÎ²ase: a database for improving the rational design of glucose-tolerant Î²-glucosidases. BMC Molecular and Cell Biology, 2020, 21, 50.	2.0	9
14	Structural insights into NS5B protein of novel equine hepaciviruses and pegiviruses complexed with polymerase inhibitors. Virus Research, 2020, 278, 197867.	2.2	8
15	A Brief History of Bioinformatics Told by Data Visualization. Lecture Notes in Computer Science, 2020, , 235-246.	1.3	0
16	Integrating Molecular Docking and Molecular Dynamics Simulations. Methods in Molecular Biology, 2019, 2053, 13-34.	0.9	87
17	Benzimidazole inhibitors of the major cysteine protease of Trypanosoma brucei. Future Medicinal Chemistry, 2019, 11, 1537-1551.	2.3	7
18	Introducing Programming Skills for Life Science Students. Biochemistry and Molecular Biology Education, 2019, 47, 288-295.	1.2	16

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19	A Computational Method to Propose Mutations in Enzymes Based on Structural Signature Variation (SSV). International Journal of Molecular Sciences, 2019, 20, 333.	4.1	11
20	Understanding Structureâ€“Activity Relationships for Trypanosomal Cysteine Protease Inhibitors by Simulations and Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 137-148.	5.4	17
21	Proteingo: Motivation, user experience, and learning of molecular interactions in biological complexes. Entertainment Computing, 2019, 29, 31-42.	2.9	10
22	nAPOLI: a graph-based strategy to detect and visualize conserved protein-ligand interactions in large-scale. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2019, 17, 1-1.	3.0	25
23	Thiophenacetamide as a potential modulator to NF-Î²B: structure and dynamics study using in silico and molecular biology assays. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4395-4406.	3.5	3
24	Characterization of glucose-tolerant Î²-glucosidases used in biofuel production under the bioinformatics perspective: a systematic review. Genetics and Molecular Research, 2017, 16, .	0.2	19
25	Computational drug design strategies applied to the modelling of human immunodeficiency virus-1 reverse transcriptase inhibitors. Memorias Do Instituto Oswaldo Cruz, 2015, 110, 847-864.	1.6	23
26	Global and Local Controllability. Boletim Da Sociedade Paranaense De Matematica, 2014, 32, 27.	0.4	0
27	A Brief View of Molecular Modeling Approaches to P2 Receptors. , 0, , .		0
28	Modelagem computacional de proteÃnas. , 0, , .		2
29	Docagem molecular: em busca do encaixe perfeito e acessÃvel. , 0, , .		1
30	Using Computers to Improve Biofuel Production. Frontiers for Young Minds, 0, 10, .	0.8	0