Cleydson Breno Rodrigues dos Santos

List of Publications by Year
in descending order

80 papers	1,433 citations	331670 21 h-index	377865 34 g-index
81 all docs	81 docs citations	81 times ranked	1326 citing authors

#	Article	IF	Citations
1	Identification of novel Aedes aegypti odorant-binding protein 1 modulators by ligand and structure-based approaches and bioassays. Journal of Biomolecular Structure and Dynamics, 2022, 40, 117-129.	3.5	8
2	Novel chalcones derivatives with potential antineoplastic activity investigated by docking and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2204-2216.	3.5	53
3	Methoxylated flavonols from Vellozia dasypus Seub ethyl acetate active myeloperoxidase extract: inÂvitro and in silico assays. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7574-7583.	3.5	44
4	The Role of Celecoxib as a Potential Inhibitor in the Treatment of Inflammatory Diseases - A Review. Current Medicinal Chemistry, 2022, 29, 3028-3049.	2.4	7
5	Identification of novel potential cyclooxygenase-2 inhibitors using ligand- and structure-based virtual screening approaches. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5386-5408.	3.5	5
6	Virtual screening and molecular docking of structures with potential inhibitor of the ebolavirus glycoprotein. Research, Society and Development, 2022, 11, e45311226034.	0.1	2
7	Identification of Potential Antiviral Inhibitors from Hydroxychloroquine and 1,2,4,5-Tetraoxanes Analogues and Investigation of the Mechanism of Action in SARS-CoV-2. International Journal of Molecular Sciences, 2022, 23, 1781.	4.1	11
8	Hierarchical Virtual Screening Based on Rocaglamide Derivatives to Discover New Potential Anti-Skin Cancer Agents. Frontiers in Molecular Biosciences, 2022, 9, .	3.5	9
9	Ethyl Acetate Fraction of Bixa orellana and Its Component Ellagic Acid Exert Antibacterial and Anti-Inflammatory Properties against Mycobacterium abscessus subsp. massiliense. Antibiotics, 2022, 11, 817.	3.7	5
10	A Computational Approach Applied to the Study of Potential Allosteric Inhibitors Protease NS2B/NS3 from Dengue Virus. Molecules, 2022, 27, 4118.	3.8	10
11	Identification of potential modulator of Anopheles gambiae odorant binding protein 1 by hierarchical virtual screening and molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6031-6043.	3.5	5
12	Pharmacophore-based virtual screening and molecular docking to identify promising dual inhibitors of human acetylcholinesterase and butyrylcholinesterase. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6021-6030.	3.5	35
13	Molecular modeling approaches of selective adenosine receptor type 2A agonists as potential anti-inflammatory drugs. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1-13.	3.5	30
14	Assessment of the hypoglycemic effect of Bixin in alloxan-induced diabetic rats: inÂvivo and in silico studies. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1017-1028.	3.5	4
15	A comparative theoretical mechanism on simplified flavonoid derivatives and isoxazolone analogous as Michael system inhibitor. Journal of Molecular Modeling, 2021, 27, 26.	1.8	3
16	ADME/Tox Study and Molecular Dynamics Simulations Applied in the Design of New Potential GABA-AT Inhibitors. Engineering Materials, 2021, , 719-738.	0.6	1
17	Revisiting the Proposition of Binding Pockets and Bioactive Poses for GSK-3Î² Allosteric Modulators Addressed to Neurodegenerative Diseases. International Journal of Molecular Sciences, 2021, 22, 8252.	4.1	9
18	Development of nano-emulsions based on Ayapana triplinervis essential oil for the control of Aedes aegypti larvae. PLoS ONE, 2021, 16, e0254225.	2.5	14

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19	An Overview of the Î±4Î²1 Integrin and the Potential Therapeutic Role of its Antagonists. Current Medicinal Chemistry, 2021, 28, 5884-5895.	2.4	4
20	Potential colchicine binding site inhibitors unraveled by virtual screening, molecular dynamics and MM/PBSA. Computers in Biology and Medicine, 2021, 137, 104817.	7.0	7
21	An in Silico Study of Natural Compounds as Potential MAO-B Inhibitors for the Treatment of Parkinsonâ€™s Disease. Engineering Materials, 2021, , 591-617.	0.6	3
22	High-Throughput-Based Virtual Screening via Molecular Docking for Oxidative Stress Mediated by ROS Enzyme. Engineering Materials, 2021, , 489-513.	0.6	1
23	Natural Products-Based Drug Design against SARS-CoV-2 Mpro 3CLpro. International Journal of Molecular Sciences, 2021, 22, 11739.	4.1	24
24	An In Silico and In Vitro Study of the Metal Complex di-Î¼-Chloro-Bis[Chlorine (4,7-Dimethyl-1,10-Phenanthroline) Cadmium(ii)] with Antibacterial Potential. Journal of Computational and Theoretical Nanoscience, 2021, 18, 1702-1713.	0.4	0
25	Potential inhibitors of the enzyme acetylcholinesterase and juvenile hormone with insecticidal activity: study of the binding mode via docking and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4687-4709.	3.5	51
26	Alkylated Sesamol Derivatives as Potent Antioxidants. Molecules, 2020, 25, 3300.	3.8	6
27	Identification of novel Î±Î²-tubulin modulators with antiproliferative activity directed to cancer therapy using ligand and structure-based virtual screening. International Journal of Biological Macromolecules, 2020, 165, 3040-3050.	7.5	7
28	Identification of New Rofecoxib-Based Cyclooxygenase-2 Inhibitors: A Bioinformatics Approach. Pharmaceuticals, 2020, 13, 209.	3.8	52
29	Chemometric methods in antimalarial drug design from 1,2,4,5-tetraoxanes analogues. SAR and QSAR in Environmental Research, 2020, 31, 677-695.	2.2	43
30	Identification of Potential COX-2 Inhibitors for the Treatment of Inflammatory Diseases Using Molecular Modeling Approaches. Molecules, 2020, 25, 4183.	3.8	45
31	Identification of Novel Chemical Entities for Adenosine Receptor Type 2A Using Molecular Modeling Approaches. Molecules, 2020, 25, 1245.	3.8	45
32	Chemical profiling of Curatella americana Linn leaves by UPLC-HRMS and its wound healing activity in mice. PLoS ONE, 2020, 15, e0225514.	2.5	6
33	Hydroethanolic extract from Endopleura uchi (Huber) Cuatrecasas and its marker bergenin: Toxicological and pharmacokinetic studies in silico and in vivo on zebrafish. Toxicology Reports, 2020, 7, 217-232.	3.3	14
34	Theoretical Study of Monoamine Oxidase B Inhibitors as Drug Candidates for Treatment of Parkinsonâ€™s Disease. Central Nervous System Agents in Medicinal Chemistry, 2020, 20, 128-143.	1.1	2
35	Application of Chemometric Techniques for Validation of Computational Methods Applied in Molecular Modeling of 6Î±-Hidroxyvouacapan-7Î², 17Î²-Lactone with Antiproliferative Activity in Leukemia Cells. Journal of Computational and Theoretical Nanoscience, 2020, 17, 4855-4865.	0.4	2
36	Identification of New Inhibitors with Potential Antitumor Activity from Polypeptide Structures via Hierarchical Virtual Screening. Molecules, 2019, 24, 2943.	3.8	16

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37	The role of regioselective hydroxylation on toxicity of diclofenac and related derivatives. Molecular Simulation, 2019, 45, 1454-1458.	2.0	1
38	Identification of Potential Inhibitors from Pyriproxyfen with Insecticidal Activity by Virtual Screening. Pharmaceuticals, 2019, 12, 20.	3.8	42
39	Toward of Safer Phenylbutazone Derivatives by Exploration of Toxicity Mechanism. Molecules, 2019, 24, 143.	3.8	17
40	Hierarchical Virtual Screening of Potential Insectides Inhibitors of Acetylcholinesterase and Juvenile Hormone from Temephos. Pharmaceuticals, 2019, 12, 61.	3.8	18
41	In Silico Evaluation of Ibuprofen and Two Benzoylpropionic Acid Derivatives with Potential Anti-Inflammatory Activity. Molecules, 2019, 24, 1476.	3.8	23
42	Acmella oleracea (L) R. K. Jansen Reproductive Toxicity in Zebrafish: An In Vivo and In Silico Assessment. Evidence-based Complementary and Alternative Medicine, 2019, 2019, 1-19.	1.2	21
43	In Silico Study to Identify New Antituberculosis Molecules from Natural Sources by Hierarchical Virtual Screening and Molecular Dynamics Simulations. Pharmaceuticals, 2019, 12, 36.	3.8	55
44	Studies of NMR, molecular docking, and molecular dynamics simulation of new promising inhibitors of cruzaine from the parasite Trypanosoma cruzi. Medicinal Chemistry Research, 2019, 28, 246-259.	2.4	15
45	Pharmacophore and structure-based drug design, molecular dynamics and admet/tox studies to design novel potential pad4 inhibitors. Journal of Biomolecular Structure and Dynamics, 2019, 37, 966-981.	3.5	30
46	Pharmaceutical and Biological Potential of the Croton palanostigma Isolated Compounds. Journal of Computational and Theoretical Nanoscience, 2019, 16, 1773-1782.	0.4	1
47	Evaluation of Computational Method from Crystallographic Structure of Galantamine for Molecular Modeling of Drug Candidates Anti-Alzheimerâ€™s Disease. Journal of Computational and Theoretical Nanoscience, 2019, 16, 2673-2686.	0.4	2
48	Oil from the fruits of Pterodon emarginatus Vog.: A traditional anti-inflammatory. Study combining in vivo and in silico. Journal of Ethnopharmacology, 2018, 222, 107-120.	4.1	23
49	Molecular modeling and statistical analysis in the design of derivatives of human dipeptidyl peptidase IV. Journal of Biomolecular Structure and Dynamics, 2018, 36, 318-334.	3.5	18
50	An In Silico Study of the Antioxidant Ability for Two Caffeine Analogs Using Molecular Docking and Quantum Chemical Methods. Molecules, 2018, 23, 2801.	3.8	38
51	Alzheimer's Disease: A Review from the Pathophysiology to Diagnosis, New Perspectives for Pharmacological Treatment. Current Medicinal Chemistry, 2018, 25, 3141-3159.	2.4	193
52	An Antioxidant Potential, Quantum-Chemical and Molecular Docking Study of the Major Chemical Constituents Present in the Leaves of Curatella americana Linn. Pharmaceuticals, 2018, 11, 72.	3.8	33
53	Identification of Novel Protein Kinase Receptor Type 2 Inhibitors Using Pharmacophore and Structure-Based Virtual Screening. Molecules, 2018, 23, 453.	3.8	30
54	Virtual Screening and Statistical Analysis in the Design of New Caffeine Analogues Molecules with Potential Epithelial Anticancer Activity. Current Pharmaceutical Design, 2018, 24, 576-594.	1.9	28

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55	Computational design of new protein kinase 2 inhibitors for the treatment of inflammatory diseases using QSAR, pharmacophore-structure-based virtual screening, and molecular dynamics. Journal of Molecular Modeling, 2018, 24, 225.	1.8	26
56	A MLR and ADME/Tox Study of New Dihydroartemisinin Compounds with Antimalarial Activity. Journal of Computational and Theoretical Nanoscience, 2018, 15, 1785-1794.	0.4	2
57	Chemical Study, Predictions In Silico and Larvicide Activity of the Essential Oil of Root Philodendron deflexum Poepp. (Journal of Computational and Theoretical Nanoscience, Vol. 14(7),) Tj ETQq1 1 0.784314 rgBT /Ov	0.4	0
58	Cannabinoid Typeâ€…1 Receptor (CB1) Ligands with Therapeutic Potential for Withdrawal Syndrome in Chemical Dependents of Cannabis sativa. ChemMedChem, 2017, 12, 1408-1416.	3.2	12
59	In vivo and in vitro evaluation of antiplasmodial activity of Amasonia campestris (Aubl.) Moldenke. African Journal of Pharmacy and Pharmacology, 2017, 11, 377-384.	0.3	1
60	A Viability Study for the Production of Biofilms and In Silico Predictions of Major Compounds in Kefir. Journal of Computational and Theoretical Nanoscience, 2017, 14, 2915-2926.	0.4	9
61	Ligand- and Structure-Based Drug Design of Novel Calcium Channel Blockers. Journal of Computational and Theoretical Nanoscience, 2017, 14, 3489-3502.	0.4	2
62	Chemical Study, Predictions In Silico and Larvicide Activity of the Essential Oil of Root Philodendron deflexum Poepp.. Journal of Computational and Theoretical Nanoscience, 2017, 14, 3330-3337.	0.4	2
63	Molecular Modeling of Peptide Derivatives NS3 Protease Inhibitors of the Type 2 Dengue Virus. Current Physical Chemistry, 2016, 6, 28-39.	0.2	2
64	New PPARÎ±/Î³/Î´ Optimal Activator Rationally Designed by Computational Methods. Journal of the Brazilian Chemical Society, 2016, , .	0.6	11
65	Development of Monoamine Oxidase B Inhibitors with Antiparkinson Activity. Current Physical Chemistry, 2016, 6, 40-52.	0.2	5
66	Molecular Modeling as Motivating Tool in Teaching and Learning in Mechanisms of Diels-Alder Reactions. Revista Virtual De Quimica, 2016, 8, 2026-2041.	0.4	0
67	Physicochemical Characterization of Water Quality - Lagoa dos Ãndios in MacapÃ¡, Brazil. American Chemical Science Journal, 2015, 5, 122-134.	0.2	1
68	Antimalarial Artemisinins Derivatives Study: Molecular Modeling and Multivariate Analysis (PCA, HCA,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.4	9
69	Computational Investigation of Antifungal Compounds Using Molecular Modeling and Prediction of ADME/Tox Properties. Journal of Computational and Theoretical Nanoscience, 2015, 12, 3682-3691.	0.4	18
70	Production and characterization of absorbent heat from the bark of residual Brazil nut bark (Bertholletia Excelsa l.). Chemistry Central Journal, 2015, 9, 36.	2.6	4
71	Estudo FÃsico-QuÃmico e AvaliaÃ§Ã£o do Potencial Larvicida do Extrato EtanÃ³lico das Cascas do Caule de Licania macrophylla Benth. Biota AmazÃ´nia, 2015, 5, 74-78.	0.2	1
72	Rational Design of Antimalarial Drugs Using Molecular Modeling and Statistical Analysis. Current Pharmaceutical Design, 2015, 21, 4112-4127.	1.9	13

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73	A QSAR, Pharmacokinetic and Toxicological Study of New Artemisinin Compounds with Anticancer Activity. Molecules, 2014, 19, 10670-10697.	3.8	24
74	ANTIOPHIDIAN ACTIVITY OF <i>BROSIMUM GUIANENSE</i> (AUBL) HUBER. American Journal of Pharmacology and Toxicology, 2014, 9, 148-156.	0.7	7
75	Validation of Computational Methods Applied in Molecular Modeling of Artemisinin with Antimalarial Activity. Journal of Computational and Theoretical Nanoscience, 2014, 11, 553-561.	0.4	5
76	A SAR and QSAR Study of New Artemisinin Compounds with Antimalarial Activity. Molecules, 2014, 19, 367-399.	3.8	38
77	Molecular Modeling: Origin, Fundamental Concepts and Applications Using Structure-Activity Relationship and Quantitative Structure-Activity Relationship. Reviews in Theoretical Science, 2014, 2, 91-115.	0.5	21
78	Application of Hartree-Fock Method for Modeling of Bioactive Molecules Using SAR and QSPR. Computational Molecular Bioscience, 2014, 04, 1-24.	0.4	17
79	Computational Analysis of Physicochemical, Pharmacokinetic and Toxicological Properties of Deoxyhypusine Synthase Inhibitors with Antimalarial Activity. Computational Molecular Bioscience, 2014, 04, 47-57.	0.4	19
80	Evaluation of Quantum Chemical Methods and Basis Sets Applied in the Molecular Modeling of Artemisinin. Computational Molecular Bioscience, 2013, 03, 66-79.	0.4	10