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	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
2	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
3	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
4	Identification of New Rofecoxib-Based Cyclooxygenase-2 Inhibitors: A Bioinformatics Approach. Pharmaceuticals, 2020, 13, 209.	3.8	52
5	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
6	Identification of Potential COX-2 Inhibitors for the Treatment of Inflammatory Diseases Using Molecular Modeling Approaches. Molecules, 2020, 25, 4183.	3.8	45
7	Identification of Novel Chemical Entities for Adenosine Receptor Type 2A Using Molecular Modeling Approaches. Molecules, 2020, 25, 1245.	3.8	45
8	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
9	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
10	Identification of Potential Inhibitors from Pyriproxyfen with Insecticidal Activity by Virtual Screening. Pharmaceuticals, 2019, 12, 20.	3.8	42
11	A SAR and QSAR Study of New Artemisinin Compounds with Antimalarial Activity. Molecules, 2014, 19, 367-399.	3.8	38
12	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
13	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
14	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
15	Identification of Novel Protein Kinase Receptor Type 2 Inhibitors Using Pharmacophore and Structure-Based Virtual Screening. Molecules, 2018, 23, 453.	3.8	30
16	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
17	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
18	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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19	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
20	A QSAR, Pharmacokinetic and Toxicological Study of New Artemisinin Compounds with Anticancer Activity. Molecules, 2014, 19, 10670-10697.	3.8	24
21	Natural Products-Based Drug Design against SARS-CoV-2 Mpro 3CLpro. International Journal of Molecular Sciences, 2021, 22, 11739.	4.1	24
22	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
23	In Silico Evaluation of Ibuprofen and Two Benzoylpropionic Acid Derivatives with Potential Anti-Inflammatory Activity. Molecules, 2019, 24, 1476.	3.8	23
24	Acmella oleracea (L) R. K. Jansen Reproductive Toxicity in Zebrafish: AnIn VivoandIn SilicoAssessment. Evidence-based Complementary and Alternative Medicine, 2019, 2019, 1-19.	1.2	21
25	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
26	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
27	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
28	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
29	Hierarchical Virtual Screening of Potential Insectides Inhibitors of Acetylcholinesterase and Juvenile Hormone from Temephos. Pharmaceuticals, 2019, 12, 61.	3.8	18
30	Toward of Safer Phenylbutazone Derivatives by Exploration of Toxicity Mechanism. Molecules, 2019, 24, 143.	3.8	17
31	Application of Hartree-Fock Method for Modeling of Bioactive Molecules Using SAR and QSPR. Computational Molecular Bioscience, 2014, 04, 1-24.	0.4	17
32	Identification of New Inhibitors with Potential Antitumor Activity from Polypeptide Structures via Hierarchical Virtual Screening. Molecules, 2019, 24, 2943.	3.8	16
33	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
34	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
35	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
36	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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37	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
38	New PPARÎ±/Î³/Î´ Optimal Activator Rationally Designed by Computational Methods. Journal of the Brazilian Chemical Society, 2016, , .	0.6	11
39	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
40	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
41	A Computational Approach Applied to the Study of Potential Allosteric Inhibitors Protease NS2B/NS3 from Dengue Virus. Molecules, 2022, 27, 4118.	3.8	10
42	Antimalarial Artemisinins Derivatives Study: Molecular Modeling and Multivariate Analysis (PCA, HCA,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.4	9
43	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
44	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
45	Hierarchical Virtual Screening Based on Rocaglamide Derivatives to Discover New Potential Anti-Skin Cancer Agents. Frontiers in Molecular Biosciences, 2022, 9, .	3.5	9
46	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
47	ANTIOPHIDIAN ACTIVITY OF <i>BROSIMUM GUIANENSE</i> (AUBL) HUBER. American Journal of Pharmacology and Toxicology, 2014, 9, 148-156.	0.7	7
48	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
49	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
50	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
51	Alkylated Sesamol Derivatives as Potent Antioxidants. Molecules, 2020, 25, 3300.	3.8	6
52	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
53	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
54	Development of Monoamine Oxidase B Inhibitors with Antiparkinson Activity. Current Physical Chemistry, 2016, 6, 40-52.	0.2	5

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	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
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	Ligand- and Structure-Based Drug Design of Novel Calcium Channel Blockers. Journal of Computational and Theoretical Nanoscience, 2017, 14, 3489-3502.	0.4	2
65	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
66	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
67	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
68	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
69	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
70	Virtual screening and molecular docking of structures with potential inhibitor of the ebolavirus glycoprotein. Research, Society and Development, 2022, 11, e45311226034.	0.1	2
71	Physicochemical Characterization of Water Quality - Lagoa dos Ãndios in MacapÃ¡, Brazil. American Chemical Science Journal, 2015, 5, 122-134.	0.2	1
72	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

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73	The role of regioselective hydroxylation on toxicity of diclofenac and related derivatives. Molecular Simulation, 2019, 45, 1454-1458.	2.0	1
74	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
75	High-Throughput-Based Virtual Screening via Molecular Docking for Oxidative Stress Mediated by ROS Enzyme. Engineering Materials, 2021, , 489-513.	0.6	1
76	Pharmaceutical and Biological Potential of the Croton palanostigma Isolated Compounds. Journal of Computational and Theoretical Nanoscience, 2019, 16, 1773-1782.	0.4	1
77	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
78	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
79	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
80	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