Michell de Oliveira Almeida

List of Publications by Year
in descending order

22	137	1307594 7	1281871 11
papers	citations	h-index	g-index

23	23	23	200
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A study of possible substitutes for the endocrine disruptor DEHP in two hormone receptors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12516-12525.	3.5	2
2	Gasâ€Phase Errors Affect DFTâ€Based Electrocatalysis Models of Oxygen Reduction to Hydrogen Peroxide. ChemElectroChem, 2022, 9, .	3.4	2
3	Gasâ€phase errors affect DFTâ€based electrocatalysis models of oxygen reduction to hydrogen peroxide. ChemElectroChem, 2022, 9, .	3.4	6
4	Computational investigation of the carmustine (BCNU) alkylation mechanism using the QTAIM, IQA, and NBO models. Structural Chemistry, 2021, 32, 79-96.	2.0	2
5	In silico Studies on the Interaction Between Bioactive Ligands and DPPIV: Insights on Potential Candidates for the Treatment of type 2 Diabetes Mellitus. Medicinal Chemistry, 2021, 17, 247-263.	1.5	0
6	Flavonoid derivatives targeting BCR-ABL kinase: Semisynthesis, Molecular dynamic simulations and Enzymatic inhibition.. Current Topics in Medicinal Chemistry, 2021, 21, 1999-2017.	2.1	1
7	Density functional theory studies of oxygen reduction reaction for hydrogen peroxide generation on Graphene-Based catalysts. Journal of Electroanalytical Chemistry, 2021, 895, 115429.	3.8	4
8	Virtual Screening of Adenylate Kinase 3 Inhibitors Employing Pharmacophoric Model, Molecular Docking, and Molecular Dynamics Simulations as Potential Therapeutic Target in Chronic Lymphocytic Leukemia. Future Pharmacology, 2021, 1, 60-79.	1.8	0
9	Diamond electrodes applied to the voltammetric generation of nitro-anion radicals from methyl parathion in aqueous media. Diamond and Related Materials, 2020, 110, 108112.	3.9	4
10	Tailoring the ORR selectivity for H₂O₂ electrogeneration by modification of Printex L6 carbon with 1,4-naphthoquinone: a theoretical, experimental and environmental application study. Materials Advances, 2020, 1, 1318-1329.	5.4	10
11	Structure-Based Virtual Screening, Molecular Dynamics and Binding Free Energy Calculations of Hit Candidates as ALK-5 Inhibitors. Molecules, 2020, 25, 264.	3.8	7
12	Competition Between Phenothiazines and BH3 Peptide for the Binding Site of the Antiapoptotic BCL-2 Protein. Frontiers in Chemistry, 2020, 8, 235.	3.6	9
13	Integrated Protocol to Design Potential Inhibitors of Dipeptidyl Peptidase- 4 (DPP-4). Current Topics in Medicinal Chemistry, 2020, 20, 209-226.	2.1	2
14	An electronic point of view on the inhibition of ALK-5 by bioactive candidates related to cancer. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	18
15	Molecular description of Î±â€ketoâ€based inhibitors of cruzain with activity against Chagas disease combining 3Dâ€QSAR studies and molecular dynamics. Chemical Biology and Drug Design, 2018, 92, 1475-1487.	3.2	3
16	Time dependent-density functional theory (TD-DFT) and experimental studies of UVâ€“Visible spectra and cyclic voltammetry for Cu(II) complex with Et2DTC. Journal of Molecular Structure, 2018, 1157, 463-468.	3.6	7
17	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
18	Studies on the Dual Activity of EGFR and HER-2 Inhibitors Using Structure-Based Drug Design Techniques. International Journal of Molecular Sciences, 2018, 19, 3728.	4.1	9

#	Article	IF	Citations
19	Study on molecular structure, spectroscopic properties (FTIR and UVâ€“Vis), NBO, QTAIM, HOMO-LUMO energies and docking studies of 5-fluorouracil, a substance used to treat cancer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 184, 169-176.	3.9	21
20	In silico studies on the interaction between bioactive ligands and ALK5, a biological target related to the cancer treatment. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2045-2053.	3.5	7
21	Medicinal Electrochemistry: Integration of Electrochemistry, Medicinal Chemistry and Computational Chemistry. Current Medicinal Chemistry, 2014, 21, 2266-2275.	2.4	11
22	Computational Study of the Alkylation Reaction of the Nitrogen Mustard Mechlorethamine Using NBO Model and the QTAIM Theory. Open Journal of Physical Chemistry, 2013, 03, 127-137.	0.6	6