

# Michell de Oliveira Almeida

## List of Publications by Year in descending order

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Version: 2024-02-01

22  
papers

137  
citations

1307594

7  
h-index

1281871

11  
g-index

23  
all docs

23  
docs citations

23  
times ranked

200  
citing authors

#	ARTICLE	IF	CITATIONS
1	Study on molecular structure, spectroscopic properties (FTIR and UV-Vis), NBO, QTAIM, HOMO-LUMO energies and docking studies of 5-fluorouracil, a substance used to treat cancer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 184, 169-176.	3.9	21
2	An electronic point of view on the inhibition of ALK-5 by bioactive candidates related to cancer. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	18
3	Medicinal Electrochemistry: Integration of Electrochemistry, Medicinal Chemistry and Computational Chemistry. <i>Current Medicinal Chemistry</i> , 2014, 21, 2266-2275.	2.4	11
4	Tailoring the ORR selectivity for H <sub>2</sub> O <sub>2</sub> electrogeneration by modification of Printex L6 carbon with 1,4-naphthoquinone: a theoretical, experimental and environmental application study. <i>Materials Advances</i> , 2020, 1, 1318-1329.	5.4	10
5	Studies on the Dual Activity of EGFR and HER-2 Inhibitors Using Structure-Based Drug Design Techniques. <i>International Journal of Molecular Sciences</i> , 2018, 19, 3728.	4.1	9
6	Competition Between Phenothiazines and BH3 Peptide for the Binding Site of the Antiapoptotic BCL-2 Protein. <i>Frontiers in Chemistry</i> , 2020, 8, 235.	3.6	9
7	In silico studies on the interaction between bioactive ligands and ALK5, a biological target related to the cancer treatment. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 2045-2053.	3.5	7
8	Time dependent-density functional theory (TD-DFT) and experimental studies of UV-Visible spectra and cyclic voltammetry for Cu(II) complex with Et <sub>2</sub> DTC. <i>Journal of Molecular Structure</i> , 2018, 1157, 463-468.	3.6	7
9	Structure-Based Virtual Screening, Molecular Dynamics and Binding Free Energy Calculations of Hit Candidates as ALK-5 Inhibitors. <i>Molecules</i> , 2020, 25, 264.	3.8	7
10	Computational analyses of interactions between ALK-5 and bioactive ligands: insights for the design of potential anticancer agents. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 4010-4022.	3.5	6
11	Computational Study of the Alkylation Reaction of the Nitrogen Mustard Mechlorethamine Using NBO Model and the QTAIM Theory. <i>Open Journal of Physical Chemistry</i> , 2013, 03, 127-137.	0.6	6
12	Gas-phase errors affect DFT-based electrocatalysis models of oxygen reduction to hydrogen peroxide. <i>ChemElectroChem</i> , 2022, 9, .	3.4	6
13	Diamond electrodes applied to the voltammetric generation of nitro-anion radicals from methyl parathion in aqueous media. <i>Diamond and Related Materials</i> , 2020, 110, 108112.	3.9	4
14	Density functional theory studies of oxygen reduction reaction for hydrogen peroxide generation on Graphene-Based catalysts. <i>Journal of Electroanalytical Chemistry</i> , 2021, 895, 115429.	3.8	4
15	Molecular description of keto-based inhibitors of cruzain with activity against Chagas disease combining 3D-QSAR studies and molecular dynamics. <i>Chemical Biology and Drug Design</i> , 2018, 92, 1475-1487.	3.2	3
16	Computational investigation of the carmustine (BCNU) alkylation mechanism using the QTAIM, IQA, and NBO models. <i>Structural Chemistry</i> , 2021, 32, 79-96.	2.0	2
17	A study of possible substitutes for the endocrine disruptor DEHP in two hormone receptors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12516-12525.	3.5	2
18	Integrated Protocol to Design Potential Inhibitors of Dipeptidyl Peptidase-4 (DPP-4). <i>Current Topics in Medicinal Chemistry</i> , 2020, 20, 209-226.	2.1	2

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19	Gasâ€Phase Errors Affect DFTâ€Based Electrocatalysis Models of Oxygen Reduction to Hydrogen Peroxide. ChemElectroChem, 2022, 9, .	3.4	2
20	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
21	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
22	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