

Luiz Carlos Alves de Oliveira

List of Publications by Year in descending order

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49
papers

786
citations

567247

15
h-index

552766

26
g-index

50
all docs

50
docs citations

50
times ranked

1019
citing authors

#	ARTICLE	IF	CITATIONS
1	Photocatalytic degradation of methylene blue dye by TiO ₂ supported on magnetic core shell (Si@Fe) surface. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 921-935.	2.2	14
2	Selective visible-light-driven toxicity breakdown of nerve agent simulant methyl paraoxon over a photoactive nanofabric. <i>Applied Catalysis B: Environmental</i> , 2021, 285, 119774.	20.2	9
3	Computational evidence for nitro derivatives of quinoline and quinoline N-oxide as low-cost alternative for the treatment of SARS-CoV-2 infection. <i>Scientific Reports</i> , 2021, 11, 6397.	3.3	11
4	Cathepsin K inhibitors based on 2-amino-1,3,4-oxadiazole derivatives. <i>Bioorganic Chemistry</i> , 2021, 109, 104662.	4.1	5
5	Bulk and surface theoretical investigation of Nb-doped γ -FeOOH as a promising bifunctional catalyst. <i>Journal of Molecular Modeling</i> , 2021, 27, 249.	1.8	2
6	Doping effect of Cu (II) in the adsorption of CrO ₄ ²⁻ by the Fe ₃ O ₄ (1 1 1) surface: A theoretical study. <i>Chemical Physics Letters</i> , 2021, 781, 138984.	2.6	6
7	Effect of drug metabolism in the treatment of SARS-CoV-2 from an entirely computational perspective. <i>Scientific Reports</i> , 2021, 11, 19998.	3.3	6
8	Theoretical insights into the effect of halogenated substituent on the electronic structure and spectroscopic properties of the favipiravir tautomeric forms and its implications for the treatment of COVID-19. <i>RSC Advances</i> , 2021, 11, 35228-35244.	3.6	9
9	Oxime K074 <i>in vitro</i> and <i>in silico</i> reactivation of acetylcholinesterase inhibited by nerve agents and pesticides. <i>Toxin Reviews</i> , 2020, 39, 157-166.	3.4	5
10	Understanding the Interaction Modes and Reactivity of Trimedoxime toward MmAChE Inhibited by Nerve Agents: Theoretical and Experimental Aspects. <i>International Journal of Molecular Sciences</i> , 2020, 21, 6510.	4.1	2
11	Trends in the Recent Patent Literature on Cholinesterase Reactivators (2016-2019). <i>Biomolecules</i> , 2020, 10, 436.	4.0	14
12	Experimental and theoretical affinity and catalysis studies between halogenated phenols and peroxidases: Understanding the bioremediation potential. <i>Ecotoxicology and Environmental Safety</i> , 2020, 202, 110895.	6.0	7
13	Asymmetric biodegradation of the nerve agents Sarin and VX by human dUTPase: chemometrics, molecular docking and hybrid QM/MM calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 2154-2164.	3.5	11
14	Methane Activation by (n=0, 1, 2; m= 1, 2): Reactivity Parameters, Electronic Properties and Binding Energy Analysis. <i>ChemistrySelect</i> , 2019, 4, 7912-7921.	1.5	0
15	Disarming <i>Pseudomonas aeruginosa</i> Virulence by the Inhibitory Action of 1,10-Phenanthroline-5,6-Dione-Based Compounds: Elastase B (LasB) as a Chemotherapeutic Target. <i>Frontiers in Microbiology</i> , 2019, 10, 1701.	3.5	41
16	Slight difference in the isomeric oximes K206 and K203 makes huge difference for the reactivation of organophosphorus-inhibited AChE: Theoretical and experimental aspects. <i>Chemico-Biological Interactions</i> , 2019, 309, 108671.	4.0	12
17	Development of technologies applied to the biodegradation of warfare nerve agents: Theoretical evidence for asymmetric homogeneous catalysis. <i>Chemico-Biological Interactions</i> , 2019, 308, 323-331.	4.0	14
18	Non-conventional compounds with potential therapeutic effects against Alzheimer's disease. <i>Expert Review of Neurotherapeutics</i> , 2019, 19, 375-395.	2.8	12

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19	Recent Developments in Metal-Based Drugs and Chelating Agents for Neurodegenerative Diseases Treatments. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1829.	4.1	43
20	Future Therapeutic Perspectives into the Alzheimer's Disease Targeting the Oxidative Stress Hypothesis. <i>Molecules</i> , 2019, 24, 4410.	3.8	67
21	Use of iron ore tailing from tailing dam as catalyst in a fenton-like process for methylene blue oxidation in continuous flow mode. <i>Chemosphere</i> , 2019, 219, 328-334.	8.2	27
22	Carbon/Fe ₃ O ₄ magnetic composites obtained from PET and red mud residues: paracetamol and dye oxidation. <i>Environmental Technology (United Kingdom)</i> , 2019, 40, 2840-2852.	2.2	9
23	Anti-Virulence Strategy against the Multidrug-Resistant Bacterial Pathogen <i>Pseudomonas aeruginosa</i> : Pseudolysin (Elastase B) as a Potential Druggable Target. <i>Current Protein and Peptide Science</i> , 2019, 20, 471-487.	1.4	16
24	SYNTHESIS AND THEORETICAL STUDY OF HPW CATALYSTS SUPPORTED ON NIOBIA CALCINATED AT 500 AND 600 °C. <i>Quimica Nova</i> , 2019, , .	0.3	0
25	Peroxonioium inhibits leukemia cell growth. <i>RSC Advances</i> , 2018, 8, 10310-10313.	3.6	10
26	Identification of biotransformation products of disperse dyes with rat liver microsomes by LC-MS/MS and theoretical studies with DNA: Structure-mutagenicity relationship using <i>Salmonella</i> /microsome assay. <i>Science of the Total Environment</i> , 2018, 613-614, 1093-1103.	8.0	16
27	Interactions of cantharidin-like inhibitors with human protein phosphatase-5 in a Mg ²⁺ system: molecular dynamics and quantum calculations. <i>Journal of Molecular Modeling</i> , 2018, 24, 303.	1.8	0
28	Structure and bonding in NbX ₅ X = (F, Cl, Br and I) complexes: a molecular orbital perspective in the C-H bond activation. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	8
29	Influence of auxochrome group in disperse dyes bearing azo groups as chromophore center in the biotransformation and molecular docking prediction by reductase enzyme: Implications and assessment for environmental toxicity of xenobiotics. <i>Ecotoxicology and Environmental Safety</i> , 2018, 160, 114-126.	6.0	28
30	Insights into the pharmaceuticals and mechanisms of neurological orphan diseases: Current Status and future expectations. <i>Progress in Neurobiology</i> , 2018, 169, 135-157.	5.7	6
31	Theoretical Studies Applied to the Evaluation of the DFPase Bioremediation Potential against Chemical Warfare Agents Intoxication. <i>International Journal of Molecular Sciences</i> , 2018, 19, 1257.	4.1	22
32	Biotransformation of disperse dyes using nitroreductase immobilized on magnetic particles modified with tosyl group: Identification of products by LC-MS-MS and theoretical studies conducted with DNA. <i>Environmental Pollution</i> , 2018, 242, 863-871.	7.5	4
33	A newly developed oxime K203 is the most effective reactivator of tabun-inhibited acetylcholinesterase. <i>BMC Pharmacology & Toxicology</i> , 2018, 19, 8.	2.4	53
34	Insights into the Drug Repositioning Applied to the Alzheimer's Disease Treatment and Future Perspectives. <i>Current Alzheimer Research</i> , 2018, 15, 1161-1178.	1.4	16
35	Theoretical structural and electronic analyses with emphasis on the reactivity of iron oxide prototypes in methane C-H bond activation. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2017, 120, 195-208.	1.7	9
36	Biobased nanocomposites based on collagen, cellulose nanocrystals, and plasticizers. <i>Journal of Applied Polymer Science</i> , 2017, 134, .	2.6	8

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37	Synthesis and characterization of Fe_2O_3 (M = Co, Ni, Cu or Zn) photocatalysts for the degradation of the indigo carmine dye in water. <i>Hyperfine Interactions</i> , 2017, 238, 1.	0.5	9
38	Enzimas degradantes de organofosforados: Base molecular e perspectivas para biorremediação enzimática de agroquímicos. <i>Ciencia E Agrotecnologia</i> , 2017, 41, 471-482.	1.5	15
39	Computational enzymology for degradation of chemical warfare agents: promising technologies for remediation processes. <i>ALMS Microbiology</i> , 2017, 3, 108-135.	2.2	8
40	Iron Oxides Applied to Catalysis. , 2017, , 409-425.		2
41	Asymmetric biocatalysis of the nerve agent VX by human serum paraoxonase 1: molecular docking and reaction mechanism calculations. <i>Medicinal Chemistry Research</i> , 2016, 25, 2521-2533.	2.4	13
42	Insights into the value of statistical models and relativistic effects for the investigation of halogenated derivatives of fluorescent probes. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	7
43	Combined experimental and theoretical study on the removal of pollutant compounds by peroxidases: affinity and reactivity toward a bioremediation catalyst. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 1839-1848.	3.5	27
44	Computational Enzymology and Organophosphorus Degrading Enzymes: Promising Approaches Toward Remediation Technologies of Warfare Agents and Pesticides. <i>Current Medicinal Chemistry</i> , 2016, 23, 1041-1061.	2.4	50
45	Molecular Docking, Metal Substitution and Hydrolysis Reaction of Chiral Substrates of Phosphotriesterase. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2016, 19, 334-344.	1.1	22
46	Flexibility in the Molecular Design of Acetylcholinesterase Reactivators: Probing Representative Conformations by Chemometric Techniques and Docking/QM Calculations. <i>Letters in Drug Design and Discovery</i> , 2016, 13, 360-371.	0.7	52
47	Structure-based Drugs Design Studies on Spleen Tyrosine Kinase Inhibitors. <i>Letters in Drug Design and Discovery</i> , 2016, 13, 845-858.	0.7	1
48	Molecular insight into the inhibition mechanism of plant and rat 4-hydroxyphenylpyruvate dioxygenase by molecular docking and DFT calculations. <i>Medicinal Chemistry Research</i> , 2015, 24, 3958-3971.	2.4	25
49	Synergistic co-processing of Red Mud waste from the Bayer process and a crude untreated waste stream from bio-diesel production. <i>Green Chemistry</i> , 2013, 15, 496.	9.0	32