

Cláudio Nahum Alves

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/754282/publications.pdf>

Version: 2024-02-01

141
papers

2,411
citations

218381

26
h-index

301761

39
g-index

143
all docs

143
docs citations

143
times ranked

3184
citing authors

#	ARTICLE	IF	CITATIONS
1	Application of <i>Mangifera indica</i> (mango) seeds as a biosorbent for removal of Victazol Orange 3R dye from aqueous solution and study of the biosorption mechanism. <i>Chemical Engineering Journal</i> , 2012, 209, 577-588.	6.6	114
2	Application of Acai Stalks as Biosorbents for the Removal of the Dye Procion Blue MX-R from Aqueous Solution. <i>Separation Science and Technology</i> , 2012, 47, 513-526.	1.3	79
3	Exploring the Potentiality of Natural Products from Essential Oils as Inhibitors of Odorant-Binding Proteins: A Structure- and Ligand-Based Virtual Screening Approach To Find Novel Mosquito Repellents. <i>ACS Omega</i> , 2019, 4, 22475-22486.	1.6	63
4	Structural and functional features of enzymes of <i>Mycobacterium tuberculosis</i> peptidoglycan biosynthesis as targets for drug development. <i>Tuberculosis</i> , 2015, 95, 95-111.	0.8	54
5	Assessment of mutations on RBD in the Spike protein of SARS-CoV-2 Alpha, Delta and Omicron variants. <i>Scientific Reports</i> , 2022, 12, .	1.6	53
6	Evaluation of total mercury concentrations in fish consumed in the municipality of Itaituba, Tapaj�s River Basin, Par�, Brazil. <i>Science of the Total Environment</i> , 2000, 261, 1-8.	3.9	50
7	<i>Mycobacterium abscessus</i> <scp>l</scp> , <scp>d</scp> -Transpeptidases Are Susceptible to Inactivation by Carbapenems and Cephalosporins but Not Penicillins. <i>Antimicrobial Agents and Chemotherapy</i> , 2017, 61, .	1.4	50
8	Mercury Contamination in Fish from Santar�m, Par�, Brazil. <i>Environmental Research</i> , 2000, 83, 117-122.	3.7	49
9	Kojic acid, a secondary metabolite from <i>Aspergillus</i> sp., acts as an inducer of macrophage activation. <i>Cell Biology International</i> , 2011, 35, 335-343.	1.4	49
10	Structure of Dihydrochalcones and Related Derivatives and Their Scavenging and Antioxidant Activity against Oxygen and Nitrogen Radical Species. <i>Molecules</i> , 2011, 16, 1749-1760.	1.7	48
11	A theoretical study of phenolic compounds with antioxidant properties. <i>European Journal of Medicinal Chemistry</i> , 2007, 42, 440-446.	2.6	46
12	Mercury levels assessment in hair of riverside inhabitants of the Tapaj�s River, Par� State, Amazon, Brazil: Fish consumption as a possible route of exposure. <i>Journal of Trace Elements in Medicine and Biology</i> , 2015, 30, 66-76.	1.5	46
13	Variability in essential oil composition of <i>Piper dilatatum</i> L.C. Rich. <i>Biochemical Systematics and Ecology</i> , 2011, 39, 669-675.	0.6	41
14	Combined Kinetic Studies and Computational Analysis on Kojic Acid Analogs as Tyrosinase Inhibitors. <i>Molecules</i> , 2014, 19, 9591-9605.	1.7	41
15	Structure-activity relationship study of flavone compounds with anti-HIV-1 integrase activity: A density functional theory study. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 7105-7112.	1.4	39
16	Three-dimensional model for analysis of spatial and temporal patterns of phytoplankton in Tucuru� reservoir, Par�, Brazil. <i>Ecological Modelling</i> , 2013, 253, 28-43.	1.2	39
17	A density functional study of flavonoid compounds with anti-HIV activity. <i>European Journal of Medicinal Chemistry</i> , 2006, 41, 616-623.	2.6	38
18	A Quantum Mechanics/Molecular Mechanics Study of the Protein-Ligand Interaction for Inhibitors of HIV-1 Integrase. <i>Chemistry - A European Journal</i> , 2007, 13, 7715-7724.	1.7	38

#	ARTICLE	IF	CITATIONS
19	Impact evaluation of a pisciculture in the Tucuruá-reservoir (Pará, Brazil) using a two-dimensional water quality model. <i>Journal of Hydrology</i> , 2013, 487, 1-12.	2.3	38
20	A DFT study for paracetamol and 3,5-disubstituted analogues. <i>Computational and Theoretical Chemistry</i> , 2004, 673, 93-97.	1.5	37
21	Antifungal Activity and Computational Study of Constituents from <i>Piper divaricatum</i> Essential Oil against <i>Fusarium</i> Infection in Black Pepper. <i>Molecules</i> , 2014, 19, 17926-17942.	1.7	36
22	A DFT study of the Diels-Alder reaction between methyl acrolein derivatives and cyclopentadiene. Understanding the effects of Lewis acids catalysts based on sulfur containing boron heterocycles. <i>Tetrahedron</i> , 2006, 62, 5502-5509.	1.0	35
23	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2617-2623.	1.0	32
24	Assessment of the PETase conformational changes induced by poly(ethylene terephthalate) binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1340-1352.	1.5	32
25	Ácidos fenólicos, flavonoides e atividade antioxidante em <i>Melipona fasciculata</i> , <i>M. flavolineata</i> (Apidae, Meliponini) e <i>Apis mellifera</i> (Apidae, Apini) da Amazônia. <i>Química Nova</i> , 2012, 35, 1728-1732.	0.3	31
26	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from <i>Trypanosoma cruzi</i> elucidated via the QM/MM approach. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3772.	1.3	30
27	Biotransformation of chalcones by the endophytic fungus <i>Aspergillus flavus</i> isolated from <i>Paspalum maritimum</i> trin. <i>Journal of the Brazilian Chemical Society</i> , 2011, 22, 1333-1338.	0.6	28
28	A Quantum Mechanics/Molecular Mechanics Study of the Protein-Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14260-14266.	1.2	27
29	A structure-activity relationship study of HEPT-analog compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 2000, 530, 39-47.	1.5	26
30	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 1999, 491, 123-131.	1.5	24
31	A multiple linear regression and partial least squares study of flavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 2001, 541, 81-88.	1.5	24
32	The Role of Short-Range Disorder in BaWO ₄ Crystals in the Intense Green Photoluminescence. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12180-12186.	1.5	24
33	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of <i>O</i> -GlcNAcase. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6764-6775.	1.2	24
34	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. <i>Biophysical Journal</i> , 2008, 94, 2443-2451.	0.2	23
35	Catalytic Mechanism of L,D-Transpeptidase 2 from <i>Mycobacterium tuberculosis</i> Described by a Computational Approach: Insights for the Design of New Antibiotics Drugs. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2402-2410.	2.5	23
36	Binding Free Energy Calculations of Nine FDA-Approved Protease Inhibitors Against HIV-1 Subtype C136T Containing 100 Amino Acids Per Monomer. <i>Chemical Biology and Drug Design</i> , 2016, 87, 487-498.	1.5	23

#	ARTICLE	IF	CITATIONS
37	A comparative modeling and molecular docking study on <i>Mycobacterium tuberculosis</i> targets involved in peptidoglycan biosynthesis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 2399-2417.	2.0	23
38	Mercury Speciation in Hair of Children in Three Communities of the Amazon, Brazil. <i>BioMed Research International</i> , 2014, 2014, 1-9.	0.9	22
39	Design and Evaluation of 4-Aminophenol and Salicylate Derivatives as Free Radical Scavenger. <i>Chemical Biology and Drug Design</i> , 2013, 81, 414-419.	1.5	21
40	Facile Synthesis and Metabolic Incorporation of <i>m</i> -DAP Bioisosteres Into Cell Walls of Live Bacteria. <i>ACS Chemical Biology</i> , 2020, 15, 2966-2975.	1.6	21
41	Insights for design of <i>Trypanosoma cruzi</i> GAPDH inhibitors: A QM/MM MD study of 1,3-bisphospho-D-glyceric acid analogs. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3398-3402.	1.0	20
42	A structure-activity relationship (SAR) study of synthetic neolignans and related compounds with biological activity against <i>Escherichia coli</i> . <i>Computational and Theoretical Chemistry</i> , 2002, 583, 105-116.	1.5	19
43	A study of neolignan compounds with biological activity against <i>Paracoccidioides brasiliensis</i> by using quantum chemical and chemometric methods. <i>Journal of the Brazilian Chemical Society</i> , 2003, 14, 809-814.	0.6	19
44	A QSAR study of 8-O- β -neolignans with antifungal activity. <i>Computational and Theoretical Chemistry</i> , 2004, 672, 215-219.	1.5	19
45	Computational Analysis of Human OGA Structure in Complex with PUGNAc and NAG-Thiazoline Derivatives. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2775-2783.	2.5	19
46	Synthesis, 2D-NMR and molecular modelling studies of pentacycloundecane lactam-peptides and peptoids as potential HIV-1 wild type C-SA protease inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2013, 28, 78-88.	2.5	19
47	Acetylcholinesterase Inhibitory Activity and Molecular Docking Study of 1-Nitro-2-Phenylethane, the Main Constituent of <i>Aniba canelilla</i> Essential Oil. <i>Chemical Biology and Drug Design</i> , 2014, 84, 192-198.	1.5	19
48	Simulating the inhibition reaction of <i>Mycobacterium tuberculosis</i> , <i>d</i> -transpeptidase 2 by carbapenems. <i>Chemical Communications</i> , 2015, 51, 12560-12562.	2.2	19
49	A Structure-Activity Relationship (SAR) Study of Neolignan Compounds with Anti-schistosomiasis Activity. <i>Journal of the Brazilian Chemical Society</i> , 2002, 13, 300-307.	0.6	18
50	Targeting the cell wall of <i>Mycobacterium tuberculosis</i> : a molecular modeling investigation of the interaction of imipenem and meropenem with <i>L</i> -, <i>D</i> -transpeptidase 2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 304-317.	2.0	18
51	Structural Analysis of Viral Infectivity Factor of HIV Type 1 and Its Interaction with A3G, EloC and EloB. <i>PLoS ONE</i> , 2014, 9, e89116.	1.1	18
52	Structure-Activity Relationship of Compounds which are Anti-Schistosomiasis Active. <i>Journal of the Brazilian Chemical Society</i> , 1998, 9, 577-582.	0.6	17
53	A DFT Study of the Molecular Mechanisms of the Diels-Alder Reaction between Cyclopentadiene and 3-Phenyl-1-(2-pyridyl)-2-propen-1-one - Role of the Zn ²⁺ Lewis Acid Catalyst and Water Solvent. <i>European Journal of Organic Chemistry</i> , 2002, 2002, 2557.	1.2	17
54	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 3818-3824.	1.4	17

#	ARTICLE	IF	CITATIONS
55	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of <i>CpNagI</i> in Complex with PUGNAc. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7029-7036.	1.2	16
56	Analysis of Kojic Acid Derivatives as Competitive Inhibitors of Tyrosinase: A Molecular Modeling Approach. <i>Molecules</i> , 2021, 26, 2875.	1.7	16
57	Determination of total mercury in workers' urine in gold shops of Itaituba, Pará State, Brazil. <i>Science of the Total Environment</i> , 2000, 261, 169-176.	3.9	15
58	An AM1 theoretical study on the effect of Zn ²⁺ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. <i>Tetrahedron</i> , 2002, 58, 2695-2700.	1.0	15
59	Molecular Modeling of <i>T. Arangeli, T. Abrupei gambiense</i> and <i>T. Evansi</i> Sialidases in Complex with the DANA Inhibitor. <i>Chemical Biology and Drug Design</i> , 2012, 80, 114-120.	1.5	15
60	Inhibition of tyrosinase by 4 H chromene analogs: Synthesis, kinetic studies, and computational analysis. <i>Chemical Biology and Drug Design</i> , 2017, 90, 804-810.	1.5	15
61	Theoretical calculations on dipyradamole structure allow to explain experimental properties associated to electrochemical oxidation and protonation. <i>Chemical Physics Letters</i> , 2001, 349, 146-152.	1.2	14
62	A theoretical study of the intramolecular hetero Diels-Alder cycloaddition reactions of azoalkenes. <i>Computational and Theoretical Chemistry</i> , 2001, 535, 165-169.	1.5	14
63	Assessment of surface water in two Amazonian rivers impacted by industrial wastewater, Barcarena City, Pará State (Brazil). <i>Journal of the Brazilian Chemical Society</i> , 2011, 22, 1493-1504.	0.6	14
64	Evaluating the Performance of a Non-Bonded Cu ²⁺ Model Including Jahn-Teller Effect into the Binding of Tyrosinase Inhibitors. <i>International Journal of Molecular Sciences</i> , 2020, 21, 4783.	1.8	14
65	Exploring Chloride Selectivity and Halogenase Regioselectivity of the SalI Enzyme through Quantum Mechanical/Molecular Mechanical Modeling. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 738-746.	2.5	14
66	Virtual Screening and Molecular Dynamics Simulations from a Bank of Molecules of the Amazon Region Against Functional NS3-4A Protease-Helicase Enzyme of Hepatitis C Virus. <i>Applied Biochemistry and Biotechnology</i> , 2015, 176, 1709-1721.	1.4	13
67	Pentacycloundecane lactam vs lactone norstatine type protease HIV inhibitors: binding energy calculations and DFT study. <i>Journal of Biomedical Science</i> , 2015, 22, 15.	2.6	13
68	Computational study of conformational changes in human 3-hydroxy-3-methylglutaryl coenzyme reductase induced by substrate binding. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 4374-4383.	2.0	13
69	Crystal structure and theoretical calculations of Julocrotine, a natural product with antileishmanial activity. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 513-520.	1.0	12
70	A theoretical study of the molecular mechanism of the GAPDH <i>Trypanosoma cruzi</i> enzyme involving iodoacetate inhibitor. <i>Chemical Physics Letters</i> , 2011, 514, 336-340.	1.2	12
71	Investigation of the target-site resistance of EPSP synthase mutants P106T and T102I/P106S against glyphosate. <i>RSC Advances</i> , 2020, 10, 44352-44360.	1.7	12
72	A combined X-ray and theoretical study of flavonoid compounds with anti-inflammatory activity. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 16-20.	1.5	11

#	ARTICLE	IF	CITATIONS
73	Essential oil composition of <i>Croton palanostigma</i> Klotzsch from north Brazil. <i>Journal of the Brazilian Chemical Society</i> , 2009, 20, 1188-1192.	0.6	11
74	Composição química e valor nutricional para grandes herbívoros das folhas e frutos de aninga (<i>Montrichardia linifera</i> , Araceae). <i>Acta Amazonica</i> , 2010, 40, 729-736.	0.3	11
75	Metal-dependent inhibition of HIV-1 integrase by 5CITEP inhibitor: A theoretical QM/MM approach. <i>Chemical Physics Letters</i> , 2013, 583, 175-179.	1.2	11
76	Structural, energetic and lipophilic analysis of SARS-CoV-2 non-structural protein 9 (NSP9). <i>Scientific Reports</i> , 2021, 11, 23003.	1.6	11
77	Crystal structure and theoretical study of IR and ¹ H and ¹³ C NMR spectra of cordatin, a natural product with antiulcerogenic activity. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2564-2575.	1.0	10
78	A QM/MM Free Energy Study of the Oxidation Mechanism of Dihydroorotate Dehydrogenase (Class 1A) from <i>Lactococcus lactis</i> . <i>Journal of Physical Chemistry B</i> , 2015, 119, 1468-1473.	1.2	10
79	Computed insight into a peptide inhibitor preventing the induced fit mechanism of MurA enzyme from <i>Pseudomonas aeruginosa</i> . <i>Chemical Biology and Drug Design</i> , 2017, 89, 599-607.	1.5	10
80	Unraveling the conformational dynamics of glycerol 3-phosphate dehydrogenase, a nicotinamide adenine dinucleotide-dependent enzyme of <i>Leishmania mexicana</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 2044-2055.	2.0	10
81	A study on the effect of Lewis acid catalysis on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. <i>Tetrahedron</i> , 2001, 57, 6877-6883.	1.0	9
82	The melatonin analog 5-MCA-NAT increases endogenous dopamine levels by binding NRH:quinone reductase enzyme in the developing chick retina. <i>International Journal of Developmental Neuroscience</i> , 2014, 38, 119-126.	0.7	9
83	Unraveling the Addition-Elimination Mechanism of EPSP Synthase through Computer Modeling. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8626-8637.	1.2	9
84	Ab Initio correlated all electron Dirac-Fock calculations for eka-francium fluoride (E119F). <i>Journal of the Brazilian Chemical Society</i> , 2012, 23, 1104-1113.	0.6	9
85	Metabolic Processing of Selenium-Based Bioisosteres of <i>meso</i> -Diaminopimelic Acid in Live Bacteria. <i>Biochemistry</i> , 2022, 61, 1404-1414.	1.2	9
86	Theoretical and experimental study of aparisthman: A natural product with anti-ulcer activity. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2706-2713.	1.0	8
87	Levels of As, Cd, Pb and Hg found in the hair from people living in Altamira, Pará, Brazil: environmental implications in the Belo Monte area. <i>Journal of the Brazilian Chemical Society</i> , 2009, 20, .	0.6	8
88	A QM/MM study of the reaction mechanism for the 3'-processing step catalyzed by HIV-1 integrase. <i>Computational and Theoretical Chemistry</i> , 2009, 898, 115-120.	1.5	8
89	Isolation, X-ray crystal structure and theoretical calculations of the new compound 8-Epicordatin and identification of others terpenes and steroids from the bark and leaves of <i>Croton palanostigma</i> Klotzsch. <i>Journal of the Brazilian Chemical Society</i> , 2010, 21, 731-739.	0.6	8
90	Computational analysis of aspartic protease plasmepsin II complexed with EH58 inhibitor: a QM/MM MD study. <i>Journal of Molecular Modeling</i> , 2011, 17, 2631-2638.	0.8	8

#	ARTICLE	IF	CITATIONS
91	Insights into the mechanism of oxidation of dihydroorotate to orotate catalysed by human class 2 dihydroorotate dehydrogenase: a QM/MM free energy study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17790-17796.	1.3	8
92	Computational Investigation of Bisphosphate Inhibitors of 3-Deoxy-d-manno-octulosonate 8-phosphate Synthase. <i>Molecules</i> , 2019, 24, 2370.	1.7	8
93	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. <i>Tetrahedron</i> , 2012, 68, 6902-6907.	1.0	7
94	Protein-ligand interaction of <i>T. cruzi</i> trans-sialidase inhibitors: a docking and QM/MM MD study. <i>Structural Chemistry</i> , 2012, 23, 147-152.	1.0	7
95	Homology modeling, molecular dynamics and QM/MM study of the regulatory protein PhoP from <i>Corynebacterium pseudotuberculosis</i> . <i>Journal of Molecular Modeling</i> , 2012, 18, 1219-1227.	0.8	7
96	Computational study of the mechanism of half-reactions in class 1A dihydroorotate dehydrogenase from <i>Trypanosoma cruzi</i> . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18863.	1.3	7
97	Structure and analgesic properties of layered double hydroxides intercalated with low amounts of ibuprofen. <i>Journal of the American Ceramic Society</i> , 2017, 100, 2712-2721.	1.9	7
98	Classification of Honeys from Pará State (Amazon Region, Brazil) Produced by Three Different Species of Bees using Chemometric Methods. <i>Journal of the Brazilian Chemical Society</i> , 2013, , .	0.6	7
99	Synthesis, X-ray crystal structure and theoretical calculations of antileishmanial neolignan analogues. <i>Journal of the Brazilian Chemical Society</i> , 2010, 21, 1825-1837.	0.6	6
100	Modelling Seagrass Biomass and Relative Nutrient Content. <i>Journal of Coastal Research</i> , 2013, 29, 1470.	0.1	6
101	Investigations into the flexibility of the 3D structure and rigid backbone of quinoline by fluorine addition to enhance its blue emission. <i>CrystEngComm</i> , 2018, 20, 2316-2323.	1.3	6
102	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.	2.0	6
103	A quantum chemical and statistical study of biflavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 2002, 577, 187-195.	1.5	5
104	A semi-empirical study of biflavonoid compounds with biological activity against tuberculosis. <i>Computational and Theoretical Chemistry</i> , 2004, 676, 83-87.	1.5	5
105	A density functional theory study on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. <i>Chemical Physics</i> , 2004, 306, 35-41.	0.9	5
106	A theoretical study of salicylate oxidation for ADME prediction. <i>Medicinal Chemistry Research</i> , 2011, 20, 269-273.	1.1	5
107	A quantum mechanical/molecular mechanical study of the aspartic protease plasmepsin IV complexed with allophenylnorstatine-based inhibitor. <i>Chemical Physics Letters</i> , 2011, 509, 169-174.	1.2	5
108	Exploring the origin of the catalytic power and product specificity of SET domain protein methyltransferase. <i>Molecular BioSystems</i> , 2016, 12, 2980-2983.	2.9	5

#	ARTICLE	IF	CITATIONS
109	Theoretical study via DFT for prediction of ¹³ C and ¹ H NMR data of two diterpenoids derived from the root of <i>salvia grandifolia</i> . <i>Journal of the Serbian Chemical Society</i> , 2019, 84, 591-598.	0.4	5
110	Theoretical study on the stereochemistry of intramolecular hetero Diels-Alder cycloaddition reactions of azoalkenes. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 133-136.	1.0	4
111	A study on the anti-HIV activity of biflavonoid compounds by using quantum chemical and chemometric methods. <i>Computational and Theoretical Chemistry</i> , 2004, 674, 191-197.	1.5	4
112	Biotransformation of sucrose into 5-hydroxy-2-hydroxymethyl- δ^3 -pirone by <i>Aspergillus flavus</i> . <i>Anais Da Academia Brasileira De Ciencias</i> , 2010, 82, 569-576.	0.3	4
113	Identification of ($\hat{\alpha}$)(E)-N-[2(S)-Hydroxy-2-(4-hydroxyphenyl) ethyl]ferulamide, a Natural Product Isolated from <i>Croton Pullei</i> : Theoretical and Experimental Analysis. <i>International Journal of Molecular Sciences</i> , 2011, 12, 9389-9403.	1.8	4
114	Analysis of the structure of calpain-10 and its interaction with the protease inhibitor SNJ-1715. <i>Computers in Biology and Medicine</i> , 2013, 43, 1334-1340.	3.9	4
115	Protein-Ligand Interaction Study of CpG in Complex with GlcNAcstatin. <i>Chemical Biology and Drug Design</i> , 2013, 81, 284-290.	1.5	4
116	Using LC and Hierarchical Cluster Analysis as Tools to Distinguish <i>Timbala</i> Collections into Two <i>Deguelia</i> Species: A Contribution to Chemotaxonomy. <i>Molecules</i> , 2016, 21, 569.	1.7	4
117	Investigation of conventional and non-conventional hydrogen bonds: a comparison of fluorine-substituted and non-fluorine substituted compounds. <i>Monatshefte für Chemie</i> , 2017, 148, 2061-2068.	0.9	4
118	Exploring the Catalytic Mechanism of the RNA Cap Modification by nsp16-nsp10 Complex of SARS-CoV-2 through a QM/MM Approach. <i>International Journal of Molecular Sciences</i> , 2022, 23, 300.	1.8	4
119	Host-Guest Inclusion Complexes of Natural Products and Nanosystems: Applications in the Development of Repellents. <i>Molecules</i> , 2022, 27, 2519.	1.7	4
120	A Theoretical Study for Oxidative Metabolism of Acetaminophen. <i>Journal of Computational and Theoretical Nanoscience</i> , 2010, 7, 1968-1972.	0.4	3
121	Synthesis, antimalarial activity <i>in vitro</i> and docking studies of novel neolignan derivatives. <i>Chemical Biology and Drug Design</i> , 2017, 90, 464-472.	1.5	3
122	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.	1.5	3
123	QM/MM Study of the Fosfomycin Resistance Mechanism Involving FosB Enzyme. <i>ACS Omega</i> , 2021, 6, 12507-12512.	1.6	3
124	Chemical Composition of the Bragantino Estuary Mangrove Sediment (PA) - Brazil. <i>Revista Virtual De Quimica</i> , 2015, 7, 1087-1101.	0.1	3
125	Fully Relativistic 4-Components DFT Investigation on Bonding and Dissociation Energy of HgO. <i>Journal of Computational and Theoretical Nanoscience</i> , 2011, 8, 38-42.	0.4	2
126	Structural and Electronic Properties of Dipyridamole and Derivatives. <i>Journal of Computational and Theoretical Nanoscience</i> , 2011, 8, 69-73.	0.4	2

#	ARTICLE	IF	CITATIONS
127	Structure modeling of a metalloendopeptidase from <i>Corynebacterium pseudotuberculosis</i> . <i>Computers in Biology and Medicine</i> , 2012, 42, 538-541.	3.9	2
128	Diversity and three-dimensional structures of the alpha Mcr of the methanogenic Archaea from the anoxic region of Tucuruá-Lake, in Eastern Brazilian Amazonia. <i>Genetics and Molecular Biology</i> , 2012, 35, 126-133.	0.6	2
129	Layered double hydroxide- <i>indomethacin</i> hybrid: A promising biocompatible compound for the treatment of neuroinflammatory diseases. <i>Journal of Drug Delivery Science and Technology</i> , 2021, 61, 102190.	1.4	2
130	OBTENÇÃO E CARACTERIZAÇÃO DE COMPLEXO DE INCLUSÃO DE β -CICLODEXTRINA E EUGENOL / PREPARATION AND CHARACTERIZATION OF β -CYCLODEXTRIN INCLUSION COMPLEX OF EUGENOL. <i>Brazilian Journal of Development</i> , 2021, 7, 33056-33070.	0.0	2
131	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. <i>Molecular Simulation</i> , 2021, 47, 762-770.	0.9	2
132	A Computational Analysis of Indomethacin Derivative as Tubulin Inhibitor: Insights into Development of Chemotherapeutic Agents. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2016, 19, 431-436.	0.6	2
133	Lead Optimisation: Improving the Affinity of the Antiretrovirals Nelfinavir and Amprenavir for HIV-1 Protease. <i>Letters in Drug Design and Discovery</i> , 2006, 3, 383-389.	0.4	1
134	Avaliação de minerais em plantas medicinais amazônicas. <i>Revista Brasileira De Farmacognosia</i> , 2009, 19, 621-625.	0.6	1
135	Homology modeling and molecular dynamics simulation of an alpha methyl coenzyme M reductase from methanogenic archaea. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2067-2075.	1.0	1
136	Characterization of the Fruit Pulp of Camu-Camu (<i>Myrciaria dubia</i>) of Seven Different Genotypes and Their Rankings Using Statistical Methods PCA and HCA. <i>Journal of the Brazilian Chemical Society</i> , 2016, , .	0.6	1
137	Ferulate Anion Intercalated into Zn/Al Layered Double Hydroxide: A Promising Intercalation Compound for Inhibition of <i>Leishmania (L.) amazonensis</i> . <i>Journal of the Brazilian Chemical Society</i> , 2019, , .	0.6	1
138	A molecular model to study FosA enzyme inhibition. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107978.	1.3	0
139	Crystal Structure of Limonoid 6-O-Acetylswietephragmin and Theoretical Study of Nuclear Magnetic Resonance Spectra of Phragmalin Limonoids. <i>Advanced Science Letters</i> , 2012, 18, 150-157.	0.2	0
140	SPECTROSCOPIC DATA OF LABDANE DITERPENES: A THEORETICAL ANALYSIS VIA NMR AND DFT. <i>Quimica Nova</i> , 2015, , .	0.3	0
141	Molecular Modeling Study of Acrylamides Derivatives as Inhibitors of the Dengue Virus Serine Proteases NS2/NS3B. <i>Revista Virtual De Quimica</i> , 2017, 9, 2272-2287.	0.1	0