

# Claudio Nahum Alves

## List of Publications by Citations

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126  
papers

1,855  
citations

24  
h-index

34  
g-index

143  
ext. papers

2,121  
ext. citations

3.2  
avg, IF

4.51  
L-index

#	Paper	IF	Citations
126	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> , <b>2012</b> , 209, 577-588	14.7	92
125	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> , <b>2012</b> , 47, 513-526	2.5	72
124	Structural and functional features of enzymes of <i>Mycobacterium tuberculosis</i> peptidoglycan biosynthesis as targets for drug development. <i>Tuberculosis</i> , <b>2015</b> , 95, 95-111	2.6	47
123	Structure of dihydrochalcones and related derivatives and their scavenging and antioxidant activity against oxygen and nitrogen radical species. <i>Molecules</i> , <b>2011</b> , 16, 1749-60	4.8	43
122	Mercury contamination in fish from Santar^ m, Par^ ªBrazil. <i>Environmental Research</i> , <b>2000</b> , 83, 117-22	7.9	42
121	A theoretical study of phenolic compounds with antioxidant properties. <i>European Journal of Medicinal Chemistry</i> , <b>2007</b> , 42, 440-6	6.8	40
120	Evaluation of total mercury concentrations in fish consumed in the municipality of Itaituba, Tapaj^ ª River Basin, Par^ ªBrazil. <i>Science of the Total Environment</i> , <b>2000</b> , 261, 1-8	10.2	40
119	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> , <b>2019</b> , 4, 22475-22486	3.9	40
118	Mercury levels assessment in hair of riverside inhabitants of the Tapaj^ ª River, Par^ ªState, Amazon, Brazil: fish consumption as a possible route of exposure. <i>Journal of Trace Elements in Medicine and Biology</i> , <b>2015</b> , 30, 66-76	4.1	38
117	Structure-activity relationship study of flavone compounds with anti-HIV-1 integrase activity: a density functional theory study. <i>Bioorganic and Medicinal Chemistry</i> , <b>2006</b> , 14, 7105-12	3.4	38
116	A density functional study of flavonoid compounds with anti-HIV activity. <i>European Journal of Medicinal Chemistry</i> , <b>2006</b> , 41, 616-23	6.8	37
115	A quantum mechanics/molecular mechanics study of the protein-ligand interaction for inhibitors of HIV-1 integrase. <i>Chemistry - A European Journal</i> , <b>2007</b> , 13, 7715-24	4.8	36
114	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> , <b>2006</b> , 62, 5502-5509	2.4	35
113	<i>Mycobacterium abscessus</i> l,d-Transpeptidases Are Susceptible to Inactivation by Carbapenems and Cephalosporins but Not Penicillins. <i>Antimicrobial Agents and Chemotherapy</i> , <b>2017</b> , 61,	5.9	33
112	Three-dimensional model for analysis of spatial and temporal patterns of phytoplankton in Tucuru^ ª reservoir, Par^ ªBrazil. <i>Ecological Modelling</i> , <b>2013</b> , 253, 28-43	3	33
111	Combined kinetic studies and computational analysis on kojic acid analogous as tyrosinase inhibitors. <i>Molecules</i> , <b>2014</b> , 19, 9591-605	4.8	31
110	Variability in essential oil composition of <i>Piper dilatatum</i> L.C. Rich. <i>Biochemical Systematics and Ecology</i> , <b>2011</b> , 39, 669-675	1.4	31

109	A DFT study for paracetamol and 3,5-disubstituted analogues. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 673, 93-97		31
108	Impact evaluation of a pisciculture in the Tucuru^ reservoir (Par^ Brazil) using a two-dimensional water quality model. <i>Journal of Hydrology</i> , <b>2013</b> , 487, 1-12	6	30
107	Kojic acid, a secondary metabolite from <i>Aspergillus</i> sp., acts as an inducer of macrophage activation. <i>Cell Biology International</i> , <b>2011</b> , 35, 335-43	4.5	30
106	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. <i>International Journal of Quantum Chemistry</i> , <b>2006</b> , 106, 2617-2623	2.1	30
105	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> , <b>2014</b> , 19, 17926-42	4.8	25
104	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> , <b>2013</b> , 15, 3772-85	3.6	24
103	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> , <b>2008</b> , 112, 14260-6	3.4	24
102	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> , <b>2011</b> , 22, 1333-1338	1.5	23
101	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> , <b>2014</b> , 54, 2402-10	6.1	22
100	A quantum mechanic/molecular mechanic study of the wild-type and N155S mutant HIV-1 integrase complexed with diketo acid. <i>Biophysical Journal</i> , <b>2008</b> , 94, 2443-51	2.9	22
99	A structure-activity relationship study of HEPT-analog compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , <b>2000</b> , 530, 39-47		22
98	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , <b>1999</b> , 491, 123-131		22
97	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> , <b>2016</b> , 34, 2399-417	3.6	21
96	Enzyme molecular mechanism as a starting point to design new inhibitors: a theoretical study of O-GlcNAcase. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 6764-75	3.4	21
95	The Role of Short-Range Disorder in BaWO4 Crystals in the Intense Green Photoluminescence. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 12180-12186	3.8	21
94	A multiple linear regression and partial least squares study of flavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , <b>2001</b> , 541, 81-88		21
93	Mercury speciation in hair of children in three communities of the Amazon, Brazil. <i>BioMed Research International</i> , <b>2014</b> , 2014, 945963	3	18
92	Design and evaluation of 4-aminophenol and salicylate derivatives as free-radical scavenger. <i>Chemical Biology and Drug Design</i> , <b>2013</b> , 81, 414-9	2.9	18

91	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> , <b>2002</b> , 583, 105-116		18
90	Targeting the cell wall of <i>Mycobacterium tuberculosis</i> : a molecular modeling investigation of the interaction of imipenem and meropenem with L,D-transpeptidase 2. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2016</b> , 34, 304-17	3.6	17
89	Computational analysis of human OGA structure in complex with PUGNAc and NAG-thiazoline derivatives. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 2775-83	6.1	17
88	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> , <b>2007</b> , 15, 3818-24	3.4	17
87	A QSAR study of 8-O-4'-neolignans with antifungal activity. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 672, 215-219		17
86	A Structure-Activity Relationship (SAR) Study of Neolignan Compounds with Anti-schistosomiasis Activity. <i>Journal of the Brazilian Chemical Society</i> , <b>2002</b> , 13, 300-307	1.5	17
85	Simulating the inhibition reaction of <i>Mycobacterium tuberculosis</i> L,D-transpeptidase 2 by carbapenems. <i>Chemical Communications</i> , <b>2015</b> , 51, 12560-2	5.8	16
84	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> , <b>2013</b> , 28, 78-88	5.6	16
83	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 <sup>2+</sup> Lewis Acid Catalyst and Water Solvent. <i>European Journal of Organic Chemistry</i> , <b>2002</b> , 2002, 2557	3.2	16
82	Structural analysis of viral infectivity factor of HIV type 1 and its interaction with A3G, EloC and EloB. <i>PLoS ONE</i> , <b>2014</b> , 9, e89116	3.7	16
81	^ Eidos fen^ lcos, flavonoides e atividade antioxidante em m^ ls de <i>Melipona fasciculata</i> , M. <i>flavolineata</i> (Apidae, Meliponini) e <i>Apis mellifera</i> (Apidae, Apini) da Amaz^ bia. <i>Quimica Nova</i> , <b>2012</b> , 35, 1728-1732	1.6	15
80	Quantum mechanical/molecular mechanical molecular dynamics simulation of wild-type and seven mutants of CpNagJ in complex with PUGNAc. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 7029-36	3.4	15
79	Structure-Activity Relationship of Compounds which are Anti-Schistosomiasis Active. <i>Journal of the Brazilian Chemical Society</i> , <b>1998</b> , 9, 577-582	1.5	15
78	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> , <b>2012</b> , 112, 3398-3402 <sup>2.1</sup>		14
77	An AM1 theoretical study on the effect of Zn <sup>2+</sup> Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. <i>Tetrahedron</i> , <b>2002</b> , 58, 2695-2700	2.4	14
76	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> , <b>2014</b> , 84, 192-8	2.9	13
75	Theoretical calculations on dipyridamole structure allow to explain experimental properties associated to electrochemical oxidation and protonation. <i>Chemical Physics Letters</i> , <b>2001</b> , 349, 146-152	2.5	13
74	A theoretical study of the intramolecular hetero Diels-Alder cycloaddition reactions of azoalkenes. <i>Computational and Theoretical Chemistry</i> , <b>2001</b> , 535, 165-169		13

73	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> , <b>2015</b> , 176, 1709-21	3.2	12
72	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> , <b>2003</b> , 14, 809-814	1.5	12
71	Inhibition of tyrosinase by 4H-chromene analogs: Synthesis, kinetic studies, and computational analysis. <i>Chemical Biology and Drug Design</i> , <b>2017</b> , 90, 804-810	2.9	11
70	Exploring Chloride Selectivity and Halogenase Regioselectivity of the SalL Enzyme through Quantum Mechanical/Molecular Mechanical Modeling. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 738-746	6.1	11
69	Determination of total mercury in workers' urine in gold shops of Itaituba, Par� State, Brazil. <i>Science of the Total Environment</i> , <b>2000</b> , 261, 169-76	10.2	11
68	Molecular modeling of <i>T. rangeli</i> , <i>T. brucei gambiense</i> , and <i>T. evansi</i> sialidases in complex with the DANA inhibitor. <i>Chemical Biology and Drug Design</i> , <b>2012</b> , 80, 114-20	2.9	10
67	Crystal structure and theoretical study of IR and <sup>1</sup> H and <sup>13</sup> C NMR spectra of cordatin, a natural product with antiulcerogenic activity. <i>International Journal of Quantum Chemistry</i> , <b>2008</b> , 108, 2564-2575	2.1	10
66	A combined X-ray and theoretical study of flavonoid compounds with anti-inflammatory activity. <i>Computational and Theoretical Chemistry</i> , <b>2008</b> , 862, 16-20		10
65	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> , <b>2019</b> , 37, 4374-4383	2.6	10
64	A theoretical study of the molecular mechanism of the GAPDH <i>Trypanosoma cruzi</i> enzyme involving iodoacetate inhibitor. <i>Chemical Physics Letters</i> , <b>2011</b> , 514, 336-340	2.5	9
63	Composi� qu�nica e valor nutricional para grandes herb�oras das folhas e frutos de aninga ( <i>Montrichardia linifera</i> , Araceae). <i>Acta Amazonica</i> , <b>2010</b> , 40, 729-736	0.8	9
62	Crystal structure and theoretical calculations of Julocrotine, a natural product with antileishmanial activity. <i>International Journal of Quantum Chemistry</i> , <b>2008</b> , 108, 513-520	2.1	9
61	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> , <b>2001</b> , 57, 6877-6883	2.4	9
60	Assessment of the PETase conformational changes induced by poly(ethylene terephthalate) binding. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2021</b> , 89, 1340-1352	4.2	9
59	Unraveling the Addition-Elimination Mechanism of EPSP Synthase through Computer Modeling. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 8626-8637	3.4	8
58	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> , <b>2017</b> , 89, 599-607	2.9	8
57	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> , <b>2015</b> , 119, 1468-73	3.4	8
56	Assessment of surface water in two Amazonian rivers impacted by industrial wastewater, Barcarena City, Par� State (Brazil). <i>Journal of the Brazilian Chemical Society</i> , <b>2011</b> , 22, 1493-1504	1.5	8

55	Computational analysis of aspartic protease plasmepsin II complexed with EH58 inhibitor: a QM/MM MD study. <i>Journal of Molecular Modeling</i> , <b>2011</b> , 17, 2631-8	2	8
54	Theoretical and experimental study of aparisthman: A natural product with anti-ulcer activity. <i>International Journal of Quantum Chemistry</i> , <b>2006</b> , 106, 2706-2713	2.1	8
53	Ab Initio correlated all electron Dirac-Fock calculations for eka-francium fluoride (E119F). <i>Journal of the Brazilian Chemical Society</i> , <b>2012</b> , 23, 1104-1113	1.5	8
52	Pentacycloundecane lactam vs lactone norstatine type protease HIV inhibitors: binding energy calculations and DFT study. <i>Journal of Biomedical Science</i> , <b>2015</b> , 22, 15	13.3	7
51	Homology modeling, molecular dynamics and QM/MM study of the regulatory protein PhoP from <i>Corynebacterium pseudotuberculosis</i> . <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 1219-27	2	7
50	Computational study of the mechanism of half-reactions in class 1A dihydroorotate dehydrogenase from <i>Trypanosoma cruzi</i> . <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 18863-71	3.6	7
49	Metal-dependent inhibition of HIV-1 integrase by 5CITEP inhibitor: A theoretical QM/MM approach. <i>Chemical Physics Letters</i> , <b>2013</b> , 583, 175-179	2.5	7
48	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> , <b>2014</b> , 38, 119-26	2.7	7
47	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. <i>Tetrahedron</i> , <b>2012</b> , 68, 6902-6907	2.4	7
46	Isolation, X-ray crystal structure and theoretical calculations of the new compound 8-Eepicordatin 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> , <b>2010</b> , 21, 731-739	1.5	7
45	Essential oil composition of <i>Croton palanostigma</i> Klotzsch from north Brazil. <i>Journal of the Brazilian Chemical Society</i> , <b>2009</b> , 20, 1188-1192	1.5	7
44	A QM/MM study of the reaction mechanism for the 3'-processing step catalyzed by HIV-1 integrase. <i>Computational and Theoretical Chemistry</i> , <b>2009</b> , 898, 115-120		7
43	Structure and analgesic properties of layered double hydroxides intercalated with low amounts of ibuprofen. <i>Journal of the American Ceramic Society</i> , <b>2017</b> , 100, 2712-2721	3.8	6
42	Protein-ligand interaction of <i>T. cruzi</i> trans-sialidase inhibitors: a docking and QM/MM MD study. <i>Structural Chemistry</i> , <b>2012</b> , 23, 147-152	1.8	6
41	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> , <b>2018</b> , 36, 4010-4022	3.6	6
40	Modelling Seagrass Biomass and Relative Nutrient Content. <i>Journal of Coastal Research</i> , <b>2013</b> , 29, 1470	0.6	5
39	A theoretical study of salicylate oxidation for ADME prediction. <i>Medicinal Chemistry Research</i> , <b>2011</b> , 20, 269-273	2.2	5
38	A quantum mechanical/molecular mechanical study of the aspartic protease plasmepsin IV complexed with allophenylnorstatine-based inhibitor. <i>Chemical Physics Letters</i> , <b>2011</b> , 509, 169-174	2.5	5

37	A density functional theory study on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. <i>Chemical Physics</i> , <b>2004</b> , 306, 35-41	2.3	5
36	A quantum chemical and statistical study of biflavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , <b>2002</b> , 577, 187-195		5
35	Theoretical study via DFT for prediction of <sup>13</sup> C and <sup>1</sup> H NMR data of two diterpenoids derived from the root of <i>salvia grandifolia</i> . <i>Journal of the Serbian Chemical Society</i> , <b>2019</b> , 84, 591-598	0.9	5
34	Evaluating the Performance of a Non-Bonded Cu Model Including Jahn-Teller Effect into the Binding of Tyrosinase Inhibitors. <i>International Journal of Molecular Sciences</i> , <b>2020</b> , 21,	6.3	5
33	Exploring the origin of the catalytic power and product specificity of SET domain protein methyltransferase. <i>Molecular BioSystems</i> , <b>2016</b> , 12, 2980-3		5
32	Investigation of conventional and non-conventional hydrogen bonds: a comparison of fluorine-substituted and non-fluorine substituted compounds. <i>Monatshefte für Chemie</i> , <b>2017</b> , 148, 2061-2068	1.4	4
31	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> , <b>2015</b> , 17, 17790-6	3.6	4
30	Investigations into the flexibility of the 3D structure and rigid backbone of quinoline by fluorine addition to enhance its blue emission. <i>CrystEngComm</i> , <b>2018</b> , 20, 2316-2323	3.3	4
29	Computational Investigation of Bisphosphate Inhibitors of 3-Deoxy-d--octulosonate 8-phosphate Synthase. <i>Molecules</i> , <b>2019</b> , 24,	4.8	4
28	Protein-ligand interaction study of CpOGA in complex with GlcNAcstatin. <i>Chemical Biology and Drug Design</i> , <b>2013</b> , 81, 284-90	2.9	4
27	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> , <b>2009</b> , 20,	1.5	4
26	A study on the anti-HIV activity of biflavonoid compounds by using quantum chemical and chemometric methods. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 674, 191-197		4
25	A semi-empirical study of biflavonoid compounds with biological activity against tuberculosis. <i>Computational and Theoretical Chemistry</i> , <b>2004</b> , 676, 83-87		4
24	Theoretical study on the stereochemistry of intramolecular hetero Diels-Alder cycloaddition reactions of azoalkenes. <i>International Journal of Quantum Chemistry</i> , <b>2003</b> , 95, 133-136	2.1	4
23	Facile Synthesis and Metabolic Incorporation of -DAP Bioisosteres Into Cell Walls of Live Bacteria. <i>ACS Chemical Biology</i> , <b>2020</b> , 15, 2966-2975	4.9	4
22	Synthesis, antimalarial activity in vitro, and docking studies of novel neolignan derivatives. <i>Chemical Biology and Drug Design</i> , <b>2017</b> , 90, 464-472	2.9	3
21	Analysis of the structure of calpain-10 and its interaction with the protease inhibitor SNJ-1715. <i>Computers in Biology and Medicine</i> , <b>2013</b> , 43, 1334-40	7	3
20	Synthesis, X-ray crystal structure and theoretical calculations of antileishmanial neolignan analogues. <i>Journal of the Brazilian Chemical Society</i> , <b>2010</b> , 21, 1825-1837	1.5	3

19	Biotransformation of sucrose into 5-hydroxy-2-hydroxymethyl- $\beta$ -irone by <i>Aspergillus flavus</i> . <i>Anais Da Academia Brasileira De Ciencias</i> , <b>2010</b> , 82, 569-76	1.4	3
18	Identification of (-)(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> , <b>2011</b> , 12, 9389-403	6.3	3
17	A Theoretical Study for Oxidative Metabolism of Acetaminophen. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2010</b> , 7, 1968-1972	0.3	3
16	Unraveling the conformational dynamics of glycerol 3-phosphate dehydrogenase, a nicotinamide adenine dinucleotide-dependent enzyme of. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 39, 2044-2055	3.6	3
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> , <b>2018</b> , 92, 1475-1487	2.9	2
14	Structure modeling of a metalloendopeptidase from <i>Corynebacterium pseudotuberculosis</i> . <i>Computers in Biology and Medicine</i> , <b>2012</b> , 42, 538-41	7	2
13	Diversity and three-dimensional structures of the alpha Mcr of the methanogenic Archaea from the anoxic region of Tucuru <sup>^</sup> Lake, in Eastern Brazilian Amazonia. <i>Genetics and Molecular Biology</i> , <b>2012</b> , 35, 126-33	2	2
12	Structural and Electronic Properties of Dipyridamole and Derivatives. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2011</b> , 8, 69-73	0.3	2
11	A Computational Analysis of Indomethacin Derivative as Tubulin Inhibitor: Insights into Development of Chemotherapeutic Agents. <i>Combinatorial Chemistry and High Throughput Screening</i> , <b>2016</b> , 19, 431-6	1.3	2
10	Classification of Honeys from Par <sup>^</sup> State (Amazon Region, Brazil) Produced by Three Different Species of Bees using Chemometric Methods. <i>Journal of the Brazilian Chemical Society</i> , <b>2013</b> ,	1.5	2
9	Investigation of the target-site resistance of EPSP synthase mutants P106T and T102I/P106S against glyphosate.. <i>RSC Advances</i> , <b>2020</b> , 10, 44352-44360	3.7	2
8	Analysis of Kojic Acid Derivatives as Competitive Inhibitors of Tyrosinase: A Molecular Modeling Approach. <i>Molecules</i> , <b>2021</b> , 26,	4.8	2
7	Using LC and Hierarchical Cluster Analysis as Tools to Distinguish Timb <sup>^</sup> Collections into Two <i>Deguelia</i> Species: A Contribution to Chemotaxonomy. <i>Molecules</i> , <b>2016</b> , 21,	4.8	2
6	Structural, energetic and lipophilic analysis of SARS-CoV-2 non-structural protein 9 (NSP9). <i>Scientific Reports</i> , <b>2021</b> , 11, 23003	4.9	0
5	QM/MM Study of the Fosfomycin Resistance Mechanism Involving FosB Enzyme. <i>ACS Omega</i> , <b>2021</b> , 6, 12507-12512	3.9	0
4	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. <i>Molecular Simulation</i> , <b>2021</b> , 47, 762-770	2	0
3	Layered double hydroxide/indomethacin hybrid: A promising biocompatible compound for the treatment of neuroinflammatory diseases. <i>Journal of Drug Delivery Science and Technology</i> , <b>2021</b> , 61, 102190	4.5	0
2	OBTEN <sup>^</sup> M E CARACTERIZA <sup>^</sup> M DE COMPLEXO DE INCLUS <sup>^</sup> M DE ECICLODEXTRINA E EUGENOL / PREPARATION AND CHARACTERIZATION OF ECYCLODEXTRIN INCLUSION COMPLEX OF EUGENOL. <i>Brazilian Journal of Development</i> , <b>2021</b> , 7, 33056-33070	0	0



- 1 A molecular model to study FosA enzyme inhibition. *Journal of Molecular Graphics and Modelling*, **2021**, 107, 107978 2.8