ClÃ¡udio Nahum Alves

List of Publications by Year
in descending order

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	Exploring the Catalytic Mechanism of the RNA Cap Modification by nsp16-nsp10 Complex of SARS-CoV-2 through a QM/MM Approach. International Journal of Molecular Sciences, 2022, 23, 300.	1.8	4
2	Host-Guest Inclusion Complexes of Natural Products and Nanosystems: Applications in the Development of Repellents. Molecules, 2022, 27, 2519.	1.7	4
3	Assessment of mutations on RBD in the Spike protein of SARS-CoV-2 Alpha, Delta and Omicron variants. Scientific Reports, 2022, 12, .	1.6	53
4	Metabolic Processing of Selenium-Based Bioisosteres of meso-Diaminopimelic Acid in Live Bacteria. Biochemistry, 2022, 61, 1404-1414.	1.2	9
5	Unraveling the conformational dynamics of glycerol 3-phosphate dehydrogenase, a nicotinamide adenine dinucleotide-dependent enzyme of Leishmania mexicana. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2044-2055.	2.0	10
6	Layered double hydroxideâ€“indomethacin hybrid: A promising biocompatible compound for the treatment of neuroinflammatory diseases. Journal of Drug Delivery Science and Technology, 2021, 61, 102190.	1.4	2
7	OBTENÃ‡ÃƒO E CARACTERIZAÃ‡ÃƒO DE COMPLEXO DE INCLUSÃƒO DE Î²-CICLODEXTRINA E EUGENOL / PREPARATION AND CHARACTERIZATION OF Î²-CYCLODEXTRIN INCLUSION COMPLEX OF EUGENOL. Brazilian Journal of Development, 2021, 7, 33056-33070.	0.0	2
8	QM/MM Study of the Fosfomycin Resistance Mechanism Involving FosB Enzyme. ACS Omega, 2021, 6, 12507-12512.	1.6	3
9	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. Molecular Simulation, 2021, 47, 762-770.	0.9	2
10	Analysis of Kojic Acid Derivatives as Competitive Inhibitors of Tyrosinase: A Molecular Modeling Approach. Molecules, 2021, 26, 2875.	1.7	16
11	A molecular model to study FosA enzyme inhibition. Journal of Molecular Graphics and Modelling, 2021, 107, 107978.	1.3	0
12	Assessment of the<scp>PETase</scp>conformational changes induced by poly(ethylene terephthalate) binding. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1340-1352.	1.5	32
13	Structural, energetic and lipophilic analysis of SARS-CoV-2 non-structural protein 9 (NSP9). Scientific Reports, 2021, 11, 23003.	1.6	11
14	Facile Synthesis and Metabolic Incorporation of m-DAP Bioisosteres Into Cell Walls of Live Bacteria. ACS Chemical Biology, 2020, 15, 2966-2975.	1.6	21
15	Evaluating the Performance of a Non-Bonded Cu2+ Model Including Jahnâ^'Teller Effect into the Binding of Tyrosinase Inhibitors. International Journal of Molecular Sciences, 2020, 21, 4783.	1.8	14
16	Exploring Chloride Selectivity and Halogenase Regioselectivity of the SalL Enzyme through Quantum Mechanical/Molecular Mechanical Modeling. Journal of Chemical Information and Modeling, 2020, 60, 738-746.	2.5	14
17	Investigation of the target-site resistance of EPSP synthase mutants P106T and T102I/P106S against glyphosate. RSC Advances, 2020, 10, 44352-44360.	1.7	12
18	Computational Investigation of Bisphosphate Inhibitors of 3-Deoxy-d-manno-octulosonate 8-phosphate Synthase. Molecules, 2019, 24, 2370.	1.7	8

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19	Ferulate Anion Intercalated into Zn/Al Layered Double Hydroxide: A Promising Intercalation Compound for Inhibition of Leishmania (L.) amazonensis. Journal of the Brazilian Chemical Society, 2019, , .	0.6	1
20	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. ACS Omega, 2019, 4, 22475-22486.	1.6	63
21	Computational study of conformational changes in human 3-hydroxy-3-methylglutaryl coenzyme reductase induced by substrate binding. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4374-4383.	2.0	13
22	Theoretical study via DFT for prediction of 13C and 1H NMR data of two diterpenoids derived from the root of salvia grandifolia. Journal of the Serbian Chemical Society, 2019, 84, 591-598.	0.4	5
23	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.	1.5	3
24	Investigations into the flexibility of the 3D structure and rigid backbone of quinoline by fluorine addition to enhance its blue emission. CrystEngComm, 2018, 20, 2316-2323.	1.3	6
25	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.	2.0	6
26	Synthesis, antimalarial activity in vitro, and docking studies of novel neolignan derivatives. Chemical Biology and Drug Design, 2017, 90, 464-472.	1.5	3
27	Inhibition of tyrosinase by 4 H â€chromene analogs: Synthesis, kinetic studies, and computational analysis. Chemical Biology and Drug Design, 2017, 90, 804-810.	1.5	15
28	Structure and analgesic properties of layered double hydroxides intercalated with low amounts of ibuprofen. Journal of the American Ceramic Society, 2017, 100, 2712-2721.	1.9	7
29	Investigation of conventional and non-conventional hydrogen bonds: a comparison of fluorine-substituted and non-fluorine substituted compounds. Monatshefte FÃ¼r Chemie, 2017, 148, 2061-2068.	0.9	4
30	Unraveling the Additionâ€“Elimination Mechanism of EPSP Synthase through Computer Modeling. Journal of Physical Chemistry B, 2017, 121, 8626-8637.	1.2	9
31	Mycobacterium abscessus <scp>l</scp> , <scp>d</scp> -Transpeptidases Are Susceptible to Inactivation by Carbapenems and Cephalosporins but Not Penicillins. Antimicrobial Agents and Chemotherapy, 2017, 61, .	1.4	50
32	Computed insight into a peptide inhibitor preventing the induced fit mechanism of MurA enzyme from Pseudomonas aeruginosa. Chemical Biology and Drug Design, 2017, 89, 599-607.	1.5	10
33	Molecular Modeling Study of Acrylamides Derivatives as Inhibitors of the Dengue Virus Serine Proteases NS2/NS3B. Revista Virtual De Quimica, 2017, 9, 2272-2287.	0.1	0
34	Characterization of the Fruit Pulp of Camu-Camu (Myrciaria dubia) of Seven Different Genotypes and Their Rankings Using Statistical Methods PCA and HCA. Journal of the Brazilian Chemical Society, 2016, , .	0.6	1
35	Using LC and Hierarchical Cluster Analysis as Tools to Distinguish TimbÃ³ Collections into Two Deguelia Species: A Contribution to Chemotaxonomy. Molecules, 2016, 21, 569.	1.7	4
36	Exploring the origin of the catalytic power and product specificity of SET domain protein methyltransferase. Molecular BioSystems, 2016, 12, 2980-2983.	2.9	5

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37	Binding Free Energy Calculations of Nine FDAâ€approved Protease Inhibitors Against HIVâ€1 Subtype C I36Tâ†'T Containing 100 Amino Acids Per Monomer. Chemical Biology and Drug Design, 2016, 87, 487-498.	1.5	23
38	A comparative modeling and molecular docking study onMycobacterium tuberculosistargets involved in peptidoglycan biosynthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2399-2417.	2.0	23
39	Targeting the cell wall ofMycobacterium tuberculosis: a molecular modeling investigation of the interaction of imipenem and meropenem withL,D-transpeptidase 2. Journal of Biomolecular Structure and Dynamics, 2016, 34, 304-317.	2.0	18
40	A Computational Analysis of Indomethacin Derivative as Tubulin Inhibitor: Insights into Development of Chemotherapeutic Agents. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 431-436.	0.6	2
41	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. Applied Biochemistry and Biotechnology, 2015, 176, 1709-1721.	1.4	13
42	A QM/MM Free Energy Study of the Oxidation Mechanism of Dihydroorotate Dehydrogenase (Class 1A) from Lactococcus lactis. Journal of Physical Chemistry B, 2015, 119, 1468-1473.	1.2	10
43	Mercury levels assessment in hair of riverside inhabitants of the TapajÃ³s River, ParÃ¡ State, Amazon, Brazil: Fish consumption as a possible route of exposure. Journal of Trace Elements in Medicine and Biology, 2015, 30, 66-76.	1.5	46
44	Structural and functional features of enzymes of Mycobacterium tuberculosis peptidoglycan biosynthesis as targets for drug development. Tuberculosis, 2015, 95, 95-111.	0.8	54
45	Insights into the mechanism of oxidation of dihydroorotate to orotate catalysed by human class 2 dihydroorotate dehydrogenase: a QM/MM free energy study. Physical Chemistry Chemical Physics, 2015, 17, 17790-17796.	1.3	8
46	Simulating the inhibition reaction of Mycobacterium tuberculosis<scp>l</scp>,<scp>d</scp>-transpeptidase 2 by carbapenems. Chemical Communications, 2015, 51, 12560-12562.	2.2	19
47	Pentacycloundecane lactam vs lactone norstatine type protease HIV inhibitors: binding energy calculations and DFT study. Journal of Biomedical Science, 2015, 22, 15.	2.6	13
48	Chemical Composition of the Bragantino Estuary Mangrove Sediment (PA) - Brazil. Revista Virtual De Quimica, 2015, 7, 1087-1101.	0.1	3
49	SPECTROSCOPIC DATA OF LABDANE DITERPENES: A THEORETICAL ANALYSIS VIA NMR AND DFT. Quimica Nova, 2015, , .	0.3	0
50	Antifungal Activity and Computational Study of Constituents from Piper divaricatum Essential Oil against Fusarium Infection in Black Pepper. Molecules, 2014, 19, 17926-17942.	1.7	36
51	The melatonin analog 5â€MCAâ€NAT increases endogenous dopamine levels by binding NRH:quinone reductase enzyme in the developing chick retina. International Journal of Developmental Neuroscience, 2014, 38, 119-126.	0.7	9
52	Mercury Speciation in Hair of Children in Three Communities of the Amazon, Brazil. BioMed Research International, 2014, 2014, 1-9.	0.9	22
53	Acetylcholinesterase Inhibitory Activity and Molecular Docking Study of 1â€Nitroâ€2â€Phenylethane, the Main Constituent of Aniba canelilla Essential Oil. Chemical Biology and Drug Design, 2014, 84, 192-198.	1.5	19
54	Catalytic Mechanism of L,D-Transpeptidase 2 from Mycobacterium tuberculosis Described by a Computational Approach: Insights for the Design of New Antibiotics Drugs. Journal of Chemical Information and Modeling, 2014, 54, 2402-2410.	2.5	23

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55	Combined Kinetic Studies and Computational Analysis on Kojic Acid Analogs as Tyrosinase Inhibitors. Molecules, 2014, 19, 9591-9605.	1.7	41
56	Structural Analysis of Viral Infectivity Factor of HIV Type 1 and Its Interaction with A3G, EloC and EloB. PLoS ONE, 2014, 9, e89116.	1.1	18
57	Analysis of the structure of calpain-10 and its interaction with the protease inhibitor SNJ-1715. Computers in Biology and Medicine, 2013, 43, 1334-1340.	3.9	4
58	Computational study of the mechanism of half-reactions in class 1A dihydroorotate dehydrogenase from Trypanosoma cruzi. Physical Chemistry Chemical Physics, 2013, 15, 18863.	1.3	7
59	Metal-dependent inhibition of HIV-1 integrase by 5CITEP inhibitor: A theoretical QM/MM approach. Chemical Physics Letters, 2013, 583, 175-179.	1.2	11
60	Synthesis, 2D-NMR and molecular modelling studies of pentacycloundecane lactam-peptides and peptoids as potential HIV-1 wild type C-SA protease inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 78-88.	2.5	19
61	Proteinâ€“Ligand Interaction Study of CpOGA in Complex with GlcNAcstatin. Chemical Biology and Drug Design, 2013, 81, 284-290.	1.5	4
62	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from Trypanosoma cruzi elucidated via the QM/MM approach. Physical Chemistry Chemical Physics, 2013, 15, 3772.	1.3	30
63	Impact evaluation of a pisciculture in the TucuruÃ-reservoir (ParÃ¡, Brazil) using a two-dimensional water quality model. Journal of Hydrology, 2013, 487, 1-12.	2.3	38
64	Design and Evaluation of 4â€Aminophenol and Salicylate Derivatives as Freeâ€Radical Scavenger. Chemical Biology and Drug Design, 2013, 81, 414-419.	1.5	21
65	Three-dimensional model for analysis of spatial and temporal patterns of phytoplankton in TucuruÃ-reservoir, ParÃ¡, Brazil. Ecological Modelling, 2013, 253, 28-43.	1.2	39
66	Modelling Seagrass Biomass and Relative Nutrient Content. Journal of Coastal Research, 2013, 29, 1470.	0.1	6
67	Classification of Honeys from ParÃ¡ State (Amazon Region, Brazil) Produced by Three Different Species of Bees using Chemometric Methods. Journal of the Brazilian Chemical Society, 2013, , .	0.6	7
68	Application of Aqai Stalks as Biosorbents for the Removal of the Dye Procion Blue MX-R from Aqueous Solution. Separation Science and Technology, 2012, 47, 513-526.	1.3	79
69	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. Tetrahedron, 2012, 68, 6902-6907.	1.0	7
70	Computational Analysis of Human OGA Structure in Complex with PUGNAc and NAG-Thiazoline Derivatives. Journal of Chemical Information and Modeling, 2012, 52, 2775-2783.	2.5	19
71	Structure modeling of a metalloendopeptidase from Corynebacterium pseudotuberculosis. Computers in Biology and Medicine, 2012, 42, 538-541.	3.9	2
72	Application of Mangifera indica (mango) seeds as a biosorbent for removal of Victazol Orange 3R dye from aqueous solution and study of the biosorption mechanism. Chemical Engineering Journal, 2012, 209, 577-588.	6.6	114

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73	Ãcidos fenÃ³licos, flavonoides e atividade antioxidante em mÃ©is de Melipona fasciculata, M. flavolineata (Apidae, Meliponini) e Apis mellifera (Apidae, Apini) da AmazÃ´nia. Quimica Nova, 2012, 35, 1728-1732.	0.3	31
74	Diversity and three-dimensional structures of the alpha Mcr of the methanogenic Archaea from the anoxic region of TucuruÃ-Lake, in Eastern Brazilian Amazonia. Genetics and Molecular Biology, 2012, 35, 126-133.	0.6	2
75	Insights for design of Trypanosoma cruzi GAPDH inhibitors: A QM/MM MD study of 1,3â€bisphospoâ€<scp>D</scp>â€glyceric acid analogs. International Journal of Quantum Chemistry, 2012, 112, 3398-3402.	1.0	20
76	Molecular Modeling of T.Ârangeli, T.Âbrucei gambiense, and T.Âevansi Sialidases in Complex with the DANA Inhibitor. Chemical Biology and Drug Design, 2012, 80, 114-120.	1.5	15
77	Proteinâ€“ligand interaction of T. cruzi trans-sialidase inhibitors: a docking and QM/MM MD study. Structural Chemistry, 2012, 23, 147-152.	1.0	7
78	Homology modeling, molecular dynamics and QM/MM study of the regulatory protein PhoP from Corynebacterium pseudotuberculosis. Journal of Molecular Modeling, 2012, 18, 1219-1227.	0.8	7
79	Ab Initio correlated all electron Dirac-Fock calculations for eka-francium fluoride (E119F). Journal of the Brazilian Chemical Society, 2012, 23, 1104-1113.	0.6	9
80	Crystal Structure of Limonoid 6-<I>O</I>-Acetylswietephragmin <I>E</I> and Theoretical Study of Nuclear Magnetic Resonance Spectra of Phragmalin Limonoids. Advanced Science Letters, 2012, 18, 150-157.	0.2	0
81	The Role of Short-Range Disorder in BaWO₄ Crystals in the Intense Green Photoluminescence. Journal of Physical Chemistry C, 2011, 115, 12180-12186.	1.5	24
82	Kojic acid, a secondary metabolite fromAspergillussp., acts as an inducer of macrophage activation. Cell Biology International, 2011, 35, 335-343.	1.4	49
83	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of O-GlcNAcase. Journal of Physical Chemistry B, 2011, 115, 6764-6775.	1.2	24
84	Structure of Dihydrochalcones and Related Derivatives and Their Scavenging and Antioxidant Activity against Oxygen and Nitrogen Radical Species. Molecules, 2011, 16, 1749-1760.	1.7	48
85	Biotransformation of chalcones by the endophytic fungus Aspergillus flavus isolated from Paspalum maritimum trin. Journal of the Brazilian Chemical Society, 2011, 22, 1333-1338.	0.6	28
86	Fully Relativistic 4-Components DFT Investigation on Bonding and Dissociation Energy of HgO. Journal of Computational and Theoretical Nanoscience, 2011, 8, 38-42.	0.4	2
87	Structural and Electronic Properties of Dipyridamole and Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 69-73.	0.4	2
88	Assessment of surface water in two Amazonian rivers impacted by industrial wastewater, Barcarena City, ParÃ¡ State (Brazil). Journal of the Brazilian Chemical Society, 2011, 22, 1493-1504.	0.6	14
89	A theoretical study of the molecular mechanism of the GAPDH Trypanosoma cruzi enzyme involving iodoacetate inhibitor. Chemical Physics Letters, 2011, 514, 336-340.	1.2	12
90	Variability in essential oil composition of Piper dilatatum L.C. Rich. Biochemical Systematics and Ecology, 2011, 39, 669-675.	0.6	41

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91	Computational analysis of aspartic protease plasmepsin II complexed with EH58 inhibitor: a QM/MM MD study. Journal of Molecular Modeling, 2011, 17, 2631-2638.	0.8	8
92	A theoretical study of salicylate oxidation for ADME prediction. Medicinal Chemistry Research, 2011, 20, 269-273.	1.1	5
93	A quantum mechanical/molecular mechanical study of the aspartic protease plasmepsin IV complexed with allophenylnorstatine-based inhibitor. Chemical Physics Letters, 2011, 509, 169-174.	1.2	5
94	Identification of (â˚)(E)-N-[2(S)-Hydroxy-2-(4-hydroxyphenyl) ethyl]ferulamide, a Natural Product Isolated from Croton Pullei: Theoretical and Experimental Analysis. International Journal of Molecular Sciences, 2011, 12, 9389-9403.	1.8	4
95	A Theoretical Study for Oxidative Metabolism of Acetaminophen. Journal of Computational and Theoretical Nanoscience, 2010, 7, 1968-1972.	0.4	3
96	Homology modeling and molecular dynamics simulation of an alpha methyl coenzyme M reductase from methanogenic archea. International Journal of Quantum Chemistry, 2010, 110, 2067-2075.	1.0	1
97	Synthesis, X-ray crystal structure and theoretical calculations of antileishmanial neolignan analogues. Journal of the Brazilian Chemical Society, 2010, 21, 1825-1837.	0.6	6
98	ComposiÃ§Ã£o quÃmica e valor nutricional para grandes herbÃvoros das folhas e frutos de aninga (Montrichardia linifera, Araceae). Acta Amazonica, 2010, 40, 729-736.	0.3	11
99	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 Croton palanostigma Klotzsch. Journal of the Brazilian Chemical Society, 2010, 21, 731-739.	0.6	8
100	Biotransformation of sucrose into 5-hydroxy-2-hydroxymethyl-Î³-pirone by Aspergillus flavus. Anais Da Academia Brasileira De Ciencias, 2010, 82, 569-576.	0.3	4
101	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of CpNagJ in Complex with PUGNAc. Journal of Physical Chemistry B, 2010, 114, 7029-7036.	1.2	16
102	Levels of As, Cd, Pb and Hg found in the hair from people living in Altamira, ParÃ¡, Brazil: environmental implications in the Belo Monte area. Journal of the Brazilian Chemical Society, 2009, 20, .	0.6	8
103	Essential oil composition of Croton palanostigma Klotzsch from north Brazil. Journal of the Brazilian Chemical Society, 2009, 20, 1188-1192.	0.6	11
104	AvaliaÃ§Ã£o de minerais em plantas medicinais amazÃ´nicas. Revista Brasileira De Farmacognosia, 2009, 19, 621-625.	0.6	1
105	A QM/MM study of the reaction mechanism for the 3â€²-processing step catalyzed by HIV-1 integrase. Computational and Theoretical Chemistry, 2009, 898, 115-120.	1.5	8
106	Crystal structure and theoretical calculations of Julocrotine, a natural product with antileishmanial activity. International Journal of Quantum Chemistry, 2008, 108, 513-520.	1.0	12
107	Crystal structure and theoretical study of IR and ¹H and ¹³C NMR spectra of cordatin, a natural product with antiulcerogenic activity. International Journal of Quantum Chemistry, 2008, 108, 2564-2575.	1.0	10
108	A combined X-ray and theoretical study of flavonoid compounds with anti-inflammatory activity. Computational and Theoretical Chemistry, 2008, 862, 16-20.	1.5	11

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109	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. Biophysical Journal, 2008, 94, 2443-2451.	0.2	23
110	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ^'Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. Journal of Physical Chemistry B, 2008, 112, 14260-14266.	1.2	27
111	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ€"Ligand Interaction for Inhibitors of HIV-1 Integrase. Chemistry - A European Journal, 2007, 13, 7715-7724.	1.7	38
112	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. Bioorganic and Medicinal Chemistry, 2007, 15, 3818-3824.	1.4	17
113	A theoretical study of phenolic compounds with antioxidant properties. European Journal of Medicinal Chemistry, 2007, 42, 440-446.	2.6	46
114	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. International Journal of Quantum Chemistry, 2006, 106, 2617-2623.	1.0	32
115	Theoretical and experimental study of aparisthman: A natural product with anti-ulcer activity. International Journal of Quantum Chemistry, 2006, 106, 2706-2713.	1.0	8
116	A density functional study ofÂflavonoid compounds with anti-HIV activity. European Journal of Medicinal Chemistry, 2006, 41, 616-623.	2.6	38
117	Structureâ€"activity relationship study of flavone compounds with anti-HIV-1 integrase activity: A density functional theory study. Bioorganic and Medicinal Chemistry, 2006, 14, 7105-7112.	1.4	39
118	A DFT study of the Dielsâ€"Alder reaction between methyl acrolein derivatives and cyclopentadiene. Understanding the effects of Lewis acids catalysts based on sulfur containing boron heterocycles. Tetrahedron, 2006, 62, 5502-5509.	1.0	35
119	Lead Optimisation: Improving the Affinity of the Antiretrovirals Nelfinavir and Amprenavir for HIV-1 Protease. Letters in Drug Design and Discovery, 2006, 3, 383-389.	0.4	1
120	A QSAR study of 8.O.4â€²-neolignans with antifungal activity. Computational and Theoretical Chemistry, 2004, 672, 215-219.	1.5	19
121	A DFT study for paracetamol and 3,5-disubstituted analogues. Computational and Theoretical Chemistry, 2004, 673, 93-97.	1.5	37
122	A study on the anti-HIV activity of biflavonoid compounds by using quantum chemical and chemometric methods. Computational and Theoretical Chemistry, 2004, 674, 191-197.	1.5	4
123	A semi-empirical study of biflavonoid compounds with biological activity against tuberculosis. Computational and Theoretical Chemistry, 2004, 676, 83-87.	1.5	5
124	A density functional theory study on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. Chemical Physics, 2004, 306, 35-41.	0.9	5
125	Theoretical study on the stereochemistry of intramolecular hetero Diels-Alder cycloaddition reactions of azoalkenes. International Journal of Quantum Chemistry, 2003, 95, 133-136.	1.0	4
126	A study of neolignan compounds with biological activity against Paracoccidioides brasiliensis by using quantum chemical and chemometric methods. Journal of the Brazilian Chemical Society, 2003, 14, 809-814.	0.6	19

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127	A Structure-Activity Relationship (SAR) Study of Neolignan Compounds with Anti-schistosomiasis Activity. Journal of the Brazilian Chemical Society, 2002, 13, 300-307.	0.6	18
128	A quantum chemical and statistical study of biflavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2002, 577, 187-195.	1.5	5
129	A DFT Study of the Molecular Mechanisms of the Dielsâ^'Alder Reaction between Cyclopentadiene and 3-Phenyl-1-(2-pyridyl)-2-propen-1-one â^' Role of the Zn2+ Lewis Acid Catalyst and Water Solvent. European Journal of Organic Chemistry, 2002, 2002, 2557.	1.2	17
130	A structureâ€“activity relationship (SAR) study of synthetic neolignans and related compounds with biological activity against Escherichia coli. Computational and Theoretical Chemistry, 2002, 583, 105-116.	1.5	19
131	An AM1 theoretical study on the effect of Zn2+ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. Tetrahedron, 2002, 58, 2695-2700.	1.0	15
132	A study on the effect of Lewis acid catalysis on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. Tetrahedron, 2001, 57, 6877-6883.	1.0	9
133	Theoretical calculations on dipyridamole structure allow to explain experimental properties associated to electrochemical oxidation and protonation. Chemical Physics Letters, 2001, 349, 146-152.	1.2	14
134	A theoretical study of the intramolecular hetero Dielsâ€“Alder cycloaddition reactions of azoalkenes. Computational and Theoretical Chemistry, 2001, 535, 165-169.	1.5	14
135	A multiple linear regression and partial least squares study of flavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2001, 541, 81-88.	1.5	24
136	A structureâ€“activity relationship study of HEPT-analog compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2000, 530, 39-47.	1.5	26
137	Mercury Contamination in Fish from SantarÃ©m, ParÃ¡, Brazil. Environmental Research, 2000, 83, 117-122.	3.7	49
138	Evaluation of total mercury concentrations in fish consumed in the municipality of Itaituba, TapajÃƒÂ³s River Basin, ParÃƒÂ¡, Brazil. Science of the Total Environment, 2000, 261, 1-8.	3.9	50
139	Determination of total mercury in workers' urine in gold shops of Itaituba, ParÃƒÂ¡ State, Brazil. Science of the Total Environment, 2000, 261, 169-176.	3.9	15
140	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 1999, 491, 123-131.	1.5	24
141	Structure-Activity Relationship of Compounds which are Anti-Schistosomiasis Active. Journal of the Brazilian Chemical Society, 1998, 9, 577-582.	0.6	17