Alberico Borges Ferreira da Silva

List of Publications by Year
in descending order

165 papers	2,994 citations	218592 26 h-index	233338 45 g-index
165 all docs	165 docs citations	165 times ranked	3670 citing authors

#	Article	IF	Citations
1	A mechanistic view of the reaction between phosphine and fluorine atom: Insights into PH3F isomers. Computational and Theoretical Chemistry, 2022, 1214, 113769.	1.1	0
2	Drug design of new sigma-1 antagonists against neuropathic pain: A QSAR study using partial least squares and artificial neural networks. Journal of Molecular Structure, 2021, 1223, 129156.	1.8	5
3	New D2R partial agonist candidates: an in silico approach from statistical models, molecular docking, and ADME/Tox properties. Structural Chemistry, 2021, 32, 2019-2033.	1.0	1
4	Drug design of new 5-HT6R antagonists aided by artificial neural networks. Journal of Molecular Graphics and Modelling, 2021, 104, 107844.	1.3	3
5	A partial least squares and artificial neural network study for a series of arylpiperazines as antidepressant agents. Journal of Molecular Modeling, 2021, 27, 297.	0.8	5
6	Generation, contraction, and polarisation of Gaussian basis sets for atomic and molecular calculations using the generator coordinate method with polynomial discretisation: atoms from Na through Cl. Physical Chemistry Chemical Physics, 2021, 23, 16989-16997.	1.3	0
7	On polarization functions for Gaussian basis sets. Journal of Molecular Modeling, 2020, 26, 293.	0.8	3
8	Microwave-Driven Hexagonal-to-Monoclinic Transition in BiPO₄: An In-Depth Experimental Investigation and First-Principles Study. Inorganic Chemistry, 2020, 59, 7453-7468.	1.9	24
9	Experimental and theoretical study on structure-tautomerism among edaravone, isoxazolone, and their heterocycles derivatives as antioxidants. Saudi Pharmaceutical Journal, 2020, 28, 819-827.	1.2	8
10	Drug design of new 5-HT6 antagonists: a QSAR study of arylsulfonamide derivatives. Structural Chemistry, 2020, 31, 1585-1597.	1.0	4
11	Accurate atomic electron affinities calculated by using anionic Gaussian basis sets. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	0
12	Crystal packing of a zinc(II)-azide complex with a N,N,S-tridentate thiosemicarbazone ligand: An experimental and computational study. Journal of Molecular Structure, 2019, 1197, 393-400.	1.8	9
13	A Proposal for the Mechanism of the CH + CO2 Reaction. ACS Omega, 2019, 4, 17843-17849.	1.6	5
14	A molecular modeling study of combretastatin-like chalcones as anticancer agents using PLS, ANN and consensus models. Structural Chemistry, 2018, 29, 957-965.	1.0	5
15	Sugar moiety has a synergistic effect on hydroxylated xanthone for better antioxidant activity of mangiferin. Medicinal Chemistry Research, 2018, 27, 1276-1282.	1.1	13
16	A mechanistic study of the electrochemical behavior of pendimethalin herbicide. Journal of Electroanalytical Chemistry, 2018, 826, 157-163.	1.9	2
17	Relativistic Prolapse-Free Gaussian Basis Sets of Quadruple-Î¶ Quality: (aug-)RPF-4Z. III. The f-Block Elements. Journal of Chemical Theory and Computation, 2017, 13, 1094-1101.	2.3	4
18	Accurate Calculations of Rate Constants for the Forward and Reverse H₂O + CO â†" HCOOH Reactions. ChemistrySelect, 2017, 2, 7267-7272.	0.7	8

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19	New consensus multivariate models based on PLS and ANN studies of sigma-1 receptor antagonists. Journal of Molecular Modeling, 2017, 23, 302.	0.8	4
20	Photodynamic Efficiency of Xanthene Dyes and Their Phototoxicity against a Carcinoma Cell Line: A Computational and Experimental Study. Journal of Chemistry, 2017, 2017, 1-9.	0.9	30
21	An antioxidant mechanism of morphine and related derivatives. Medicinal Chemistry Research, 2016, 25, 852-857.	1.1	11
22	The 1,2-hydrogen shift reaction for monohalogenophosphanes PH₂X and HPX (XÂ= F, Cl). Molecular Physics, 2016, 114, 2999-3014.	0.8	3
23	Vibrational spectroscopy, intramolecular CHâ‹¯O interaction and conformational analysis of 2,5-dimethyl-benzyl benzoate. Journal of Molecular Structure, 2016, 1125, 649-655.	1.8	2
24	THE H₂Â+ÂCOÂ ÂH₂CO REACTION: RATE CONSTANTS AND RELEVANCE TO HOT AND DENSE ASTROPHYSICAL MEDIA. Astrophysical Journal, Supplement Series, 2016, 225, 2.	3.0	10
25	Structure and toxicity of clozapine and olanzapine on agranulocytosis. Medicinal Chemistry Research, 2016, 25, 322-328.	1.1	5
26	Intramolecular interactions, isomerization and vibrational frequencies of two paracetamol analogues: A spectroscopic and a computational approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 162, 16-26.	2.0	11
27	PRECIPITATION REACTION OF CLAVULANIC ACID: THERMODYNAMIC AND ELECTRONIC STUDY. Quimica Nova, 2016, , .	0.3	0
28	Interaction between PH3 and small water clusters: Understanding the electronic and spectroscopic properties. Computational and Theoretical Chemistry, 2015, 1059, 35-44.	1.1	21
29	Electronic properties of the AsCO, AsSiO and AsGeO radicals: Linear or cyclic?. Polyhedron, 2015, 89, 160-167.	1.0	10
30	A computational study for the antioxidant capacity increases in hydroxy-derivatives of paracetamol and salicylic acid. Medicinal Chemistry Research, 2015, 24, 3453-3459.	1.1	6
31	Accurate Gaussian basis sets for atomic and molecular calculations obtained from the generator coordinate method with polynomial discretization. Journal of Molecular Modeling, 2015, 21, 274.	0.8	1
32	Theoretical study of dibenzotetraaza[14]annulene complexes with first row transition metals. Computational and Theoretical Chemistry, 2015, 1054, 93-99.	1.1	15
33	Molecular Features Related to HIV Integrase Inhibition Obtained from Structure- and Ligand-Based Approaches. PLoS ONE, 2014, 9, e81301.	1.1	6
34	Pattern Recognition Techniques Applied to the Study of Leishmanial Glyceraldehyde-3-Phosphate Dehydrogenase Inhibition. International Journal of Molecular Sciences, 2014, 15, 3186-3203.	1.8	4
35	Understanding the cytotoxicity or cytoprotective effects of biological and synthetic quinone derivatives by redox mechanism. Journal of Molecular Modeling, 2014, 20, 2541.	0.8	13
36	CO bonding in FeN4 complexes and the effect of the macrocycle ligand: A DFT study. Polyhedron, 2014, 67, 36-43.	1.0	11

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37	Molecular properties of the PCO radical: heat of formation and the isomerization pathways. Journal of Molecular Modeling, 2014, 20, 2074.	0.8	14
38	Quantum chemical DFT study of the interaction between molecular oxygen and FeN4 complexes, and effect of the macrocyclic ligand. Journal of Molecular Modeling, 2014, 20, 2131.	0.8	9
39	Relativistic Prolapse-Free Gaussian Basis Set of Quadruple-Î¶ Quality: (aug-)RPF-4Z. II. The d-Block Elements. Journal of Chemical Theory and Computation, 2014, 10, 4761-4764.	2.3	8
40	On the stability of the RuCl2(triphenylphosphine)2(amine) complexes: Ligand substituent effects of cyclic and acyclic amines. Polyhedron, 2014, 81, 661-667.	1.0	7
41	Relativistic Prolapse-Free Gaussian Basis Set of Quadruple-Î¶ Quality: (aug-)RPF-4Z. I. The s- and p-Block Elements. Journal of Chemical Theory and Computation, 2014, 10, 3800-3806.	2.3	15
42	The CH3PH2 and CH3PH isomers: isomerization, hydrogen release, thermodynamic, and spectroscopy properties. Journal of Molecular Modeling, 2014, 20, 2372.	0.8	8
43	A Structure and Antioxidant Activity Study of Paracetamol and Salicylic Acid. Pharmacology & Pharmacy, 2014, 05, 1185-1191.	0.2	10
44	A combined experimental and theoretical approach for radical-scavenging activity of edaravone and its related derivatives. Structural Chemistry, 2013, 24, 349-355.	1.0	9
45	4-Hydroxy-2,5-dimethylphenyl-benzophenone: Conformational stability, FT-IR and Raman investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 102, 386-392.	2.0	10
46	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
47	The tautomerism influence on the antioxidant prediction of oxederavone. Medicinal Chemistry Research, 2013, 22, 5617-5623.	1.1	5
48	Identification of Electronic and Structural Descriptors of Adenosine Analogues Related to Inhibition of Leishmanial Glyceraldehyde-3-Phosphate Dehydrogenase. Molecules, 2013, 18, 5032-5050.	1.7	10
49	Coordination Ability of Polyether and Polyamine Ligands: A Density Functional Theory Study of First- and Second-Row Transition Metals. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2034-2040.	0.4	7
50	Non-peptidic Cruzain Inhibitors with Trypanocidal Activity Discovered by Virtual Screening and In Vitro Assay. PLoS Neglected Tropical Diseases, 2013, 7, e2370.	1.3	63
51	Evaluation and Theoretical Study on the Anti-inflammatory Mechanism of 1-Nitro-2-phenylethane. Planta Medica, 2013, 79, 628-633.	0.7	18
52	A Theoretical Study of the Dapsone Derivatives on Methemoglobin. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2029-2033.	0.4	4
53	Understanding the Molecular Aspects of Tetrahydrocannabinol and Cannabidiol as Antioxidants. Molecules, 2013, 18, 12663-12674.	1.7	95
54	Density Functional Theory (DFT) Study of Edaravone Derivatives as Antioxidants. International Journal of Molecular Sciences, 2012, 13, 7594-7606.	1.8	23

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55	Infrared Spectroscopy of Anionic, Cationic, and Zwitterionic Surfactants. Advances in Physical Chemistry, 2012, 2012, 1-14.	2.0	216
56	Molecular Features for Antitrypanosomal Activity of Thiosemicarbazones Revealed by OPS-PLS QSAR Studies. Medicinal Chemistry, 2012, 8, 1045-1056.	0.7	2
57	The basic antioxidant structure for flavonoid derivatives. Journal of Molecular Modeling, 2012, 18, 4073-4080.	0.8	37
58	Machine Learning Techniques and Drug Design. Current Medicinal Chemistry, 2012, 19, 4289-4297.	1.2	147
59	Metal binding selectivity of oxa-aza macrocyclic ligand: a DFT study of first- and second-row transition metal for four coordination systems. Structural Chemistry, 2012, 23, 1539-1545.	1.0	7
60	Adsorption of Sodium Dodecyl Sulfate on Ge Substrate: The Effect of a Low-Polarity Solvent. International Journal of Molecular Sciences, 2012, 13, 7980-7993.	1.8	24
61	Theoretical models for the antitrypanosomal activity of thiosemicarbazone derivatives. International Journal of Quantum Chemistry, 2012, 112, 3364-3370.	1.0	2
62	First- and second-row transition metal oxa-aza macrocyclic complexes: a DFT study of an octahedral conformation. Journal of Molecular Modeling, 2012, 18, 3243-3253.	0.8	8
63	A Combined Study Using Ligandâ€Based Design, Synthesis, and Pharmacological Evaluation of Analogues of the Acetaminophen Orthoâ€Regioisomer with Potent Analgesic Activity. Chemical Biology and Drug Design, 2012, 80, 99-105.	1.5	3
64	Molecular Features for Antitrypanosomal Activity of Thiosemicarbazones Revealed by OPS-PLS QSAR Studies. Medicinal Chemistry, 2012, 8, 1045-1056.	0.7	5
65	Structural and Electronic Properties of Dipyridamole and Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 69-73.	0.4	2
66	Propriedades quÃmico-quÃ¢nticas empregadas em estudos das relaÃ§Ãµes estrutura-atividade. Quimica Nova, 2010, 33, 694-699.	0.3	40
67	Pharmacophore-based 3D QSAR studies on a series of high affinity 5-HT1A receptor ligands. European Journal of Medicinal Chemistry, 2010, 45, 1508-1514.	2.6	29
68	The effect of the negative coupling parameter on the spectrum of a trapped Bose gas. Journal of Mathematical Chemistry, 2010, 47, 636-646.	0.7	0
69	One-dimensional trapped atoms: critical coupling parameter and critical number of particles. Journal of Mathematical Chemistry, 2010, 48, 687-696.	0.7	0
70	Novel insights for dihydroorotate dehydrogenase class 1A inhibitors discovery. European Journal of Medicinal Chemistry, 2010, 45, 5899-5909.	2.6	47
71	Artificial Neural Networks and the Study of the Psychoactivity of Cannabinoid Compounds. Chemical Biology and Drug Design, 2010, 75, 632-640.	1.5	17
72	Research Article: Insights into the Molecular Requirements for the Antiâ€obesity Activity of a Series of CB1 Ligands. Chemical Biology and Drug Design, 2010, 76, 320-329.	1.5	8

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73	Photophysical properties and quantum chemical studies of poly(2,7-9,9'-dihexylfluorene-dyil). Journal of the Brazilian Chemical Society, 2009, 20, 160-166.	0.6	13
74	Docking and molecular dynamics simulation of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2009, 15, 1175-1184.	0.8	12
75	A chemometric study on the analgesic activity of cannabinoid compounds using SDA, KNN and SIMCA methods. Structural Chemistry, 2009, 20, 577-585.	1.0	7
76	The origin of the molecular interaction between amino acids and gold nanoparticles: A theoretical and experimental investigation. Chemical Physics Letters, 2009, 469, 186-190.	1.2	42
77	Excitation energies from ground-state density-functionals by means of generator coordinates. Physical Chemistry Chemical Physics, 2009, 11, 4564.	1.3	3
78	A neural networks study of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2008, 14, 975-985.	0.8	14
79	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
80	A chemometric study of the 5-HT1A receptor affinities presented by arylpiperazine compounds. European Journal of Medicinal Chemistry, 2008, 43, 364-372.	2.6	19
81	A theoretical study on the XeF2 molecule. Chemical Physics, 2008, 348, 89-96.	0.9	14
82	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
83	Complexation of the anti-Trypanosoma cruzi Drug Benznidazole Improves Solubility and Efficacy. Journal of Medicinal Chemistry, 2008, 51, 4104-4114.	2.9	57
84	A prÃ¡tica docente na formaÃ§Ã£o do pÃ³s-graduando em quÃmica. Quimica Nova, 2008, 31, 1888-1891.	0.3	4
85	Two-Dimensional QSAR Studies on Arylpiperazines as High-Affinity 5-HT1A Receptor Ligands. Medicinal Chemistry, 2008, 4, 328-335.	0.7	10
86	Generator coordinate method in time-dependent density-functional theory: Memory made simple. Journal of Chemical Physics, 2007, 127, 124101.	1.2	19
87	Photoinduced Electron-Transfer Processes Based on Novel Bipyridineâ˜Ru(II) Complex:Â Properties ofcis-[Ru(2,2â€˜-bipyridine)2(5,6-bis(3-amidopyridine)-7-oxanorbornene)](PF6)2andcis-[Ru(2,2â€˜-bipyridine)2(3-aminopyridine)2](PF6)2. Inorganic Chemistry, 2007, 46, 5744-5753.	4.9	12
88	The Isomerization of Dinitrogen Tetroxide:â€‰ O2Nâ˜NO2 â† ONOâ˜NO2. Journal of Physical Chemistry A, 2007, 111, 2913-2920.	1.1	54
89	1,4- Addition of diazomethane to a heterodiene: a direct preparation of the oxazolic ring. Anais Da Academia Brasileira De Ciencias, 2007, 79, 29-33.	0.3	6
90	A multivariate study on flavonoid compounds scavenging the peroxynitrite free radical. Computational and Theoretical Chemistry, 2007, 808, 25-33.	1.5	36

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91	The asymmetric dimerization of nitrogen dioxide. Chemical Physics Letters, 2007, 436, 47-50.	1.2	28
92	The nuclear electric quadrupole moment of lutetium from the molecular method. Chemical Physics Letters, 2007, 445, 95-98.	1.2	11
93	Prolapse-free relativistic Gaussian basis sets for the superheavy elements up to Uuo (Z=118) and Lr (Z=103). Atomic Data and Nuclear Data Tables, 2007, 93, 931-961.	0.9	13
94	Cationic dye dimers: a theoretical study. Theoretical Chemistry Accounts, 2007, 118, 305-314.	0.5	17
95	A partial least squares and principal component regression study of quinone compounds with trypanocidal activity. Structural Chemistry, 2007, 18, 49-57.	1.0	23
96	Studies of the electrochemical reduction of atrazine on a mercury electrode in acid medium: An electrochemical and NMR approach. Journal of Electroanalytical Chemistry, 2007, 608, 47-51.	1.9	12
97	The Generator Coordinate Diracâ€“Fock Method and Relativistic Calculations for Atoms and Molecules. , 2007, , 79-150.		0
98	Use of Graphite Polyurethane Composite Electrode for Imipramine Oxidationâ€”Mechanism Proposal and Electroanalytical Determination. Analytical Letters, 2006, 39, 507-520.	1.0	40
99	Rate Coefficient for the Reaction SiO + Si2O2atT= 10â^'1000 K. Journal of Physical Chemistry A, 2006, 110, 13221-13226.	1.1	10
100	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. International Journal of Quantum Chemistry, 2006, 106, 2617-2623.	1.0	32
101	Adapted relativistic prolapse-free Gaussian basis sets for closed shell atoms up to nobelium and to be used with the uniform sphere nucleus model. International Journal of Quantum Chemistry, 2006, 106, 2790-2803.	1.0	3
102	The employment of relativistic adapted Gaussian basis sets in Douglasâ€“Krollâ€“Hess scalar calculations with diatomic molecules. Chemical Physics, 2006, 331, 173-177.	0.9	8
103	A partial least squares regression study with antioxidant flavonoid compounds. Structural Chemistry, 2006, 17, 307-313.	1.0	25
104	The use of classification methods for modeling the antioxidant activity of flavonoid compounds. Journal of Molecular Modeling, 2006, 12, 915-920.	0.8	21
105	Accurate relativistic adapted Gaussian basis sets for hydrogen through xenon without variational prolapse and to be used with both uniform sphere and Gaussian nucleus models. Journal of Computational Chemistry, 2006, 27, 61-71.	1.5	18
106	Accurate relativistic adapted Gaussian basis sets for Cesium through Radon without variational prolapse and to be used with both uniform sphere and Gaussian nucleus models. Journal of Computational Chemistry, 2006, 27, 1970-1979.	1.5	18
107	The nuclear electric quadrupole moment of antimony from the molecular method. Journal of Chemical Physics, 2006, 125, 064301.	1.2	29
108	A chemometric study of megazol derivatives with activity againstTrypanosoma equiperdum. SAR and QSAR in Environmental Research, 2006, 17, 533-547.	1.0	1

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109	A structureâ€“activity relationship study of quinone compounds with trypanocidal activity. European Journal of Medicinal Chemistry, 2005, 40, 329-338.	2.6	48
110	An accurate relativistic universal Gaussian basis set for hydrogen through Nobelium without variational prolapse and to be used with both uniform sphere and Gaussian nucleus models. Journal of Computational Chemistry, 2005, 26, 932-940.	1.5	18
111	The effects of solvation in the theoretical spectra of cationic dyes. Theoretical Chemistry Accounts, 2005, 113, 274-280.	0.5	74
112	A study on the influence of molecular properties in the psychoactivity of cannabinoid compounds. Journal of Molecular Modeling, 2005, 11, 200-209.	0.8	20
113	Highly accurate relativistic universal Gaussian basis set for Dirac-Fock-Breit calculations. International Journal of Quantum Chemistry, 2005, 102, 1-7.	1.0	1
114	Selection of quantum chemical descriptors by chemometric methods in the study of antioxidant activity of flavonoid compounds. International Journal of Quantum Chemistry, 2005, 103, 731-737.	1.0	23
115	Quantum chemical and statistical study of megazol-derived compounds with trypanocidal activity. International Journal of Quantum Chemistry, 2005, 103, 738-748.	1.0	4
116	New adapted Gaussian basis sets for the relativistic closed shell atoms from helium to barium generated with the generator coordinate Dirac-Fock method. International Journal of Quantum Chemistry, 2005, 103, 523-528.	1.0	1
117	Energy lowering of current-carrying single-particle states in open-shell atoms due to an exchange-correlation vector potential. International Journal of Quantum Chemistry, 2005, 103, 516-522.	1.0	10
118	Relativistic Gaussian basis sets obtained with a polynomial version of the generator coordinate Dirac-Fock method: Ionization energies of some closed-shell atomic systems. International Journal of Quantum Chemistry, 2005, 103, 529-536.	1.0	2
119	A chemometric study on the accumulation of heavy metals along the Mogi GuaÃ§u river basin. Journal of the Brazilian Chemical Society, 2005, 16, 1104.	0.6	3
120	Deactivation of Triplet-Excited Riboflavin by Purine Derivatives:â€‰ Important Role of Uric Acid in Light-Induced Oxidation of Milk Sensitized by Riboflavin. Journal of Agricultural and Food Chemistry, 2005, 53, 3679-3684.	2.4	23
121	Electrochemical Behavior of Nicotine Studied by Voltammetric Techniques at Boronâ€Doped Diamond Electrodes. Analytical Letters, 2005, 38, 1587-1599.	1.0	64
122	Influence of confining anisotropy on the unstable behavior of a Bose gas with attractive interaction. Physical Review A, 2004, 70, .	1.0	5
123	A polynomial version of the generator coordinate Dirac-Fock method. Journal of Computational Chemistry, 2004, 25, 1904-1909.	1.5	22
124	A Study on the Antipicornavirus Activity of Flavonoid Compounds (Flavones) by Using Quantum Chemical and Chemometric Methods.. ChemInform, 2004, 35, no.	0.1	0
125	A theoretical study on the analgesic activity of cannabinoid compounds. Computational and Theoretical Chemistry, 2004, 709, 223-229.	1.5	9
126	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

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127	A quantum chemical and photophysical study of acridine-9-N-methacrylamide. Computational and Theoretical Chemistry, 2004, 674, 213-225.	1.5	15
128	The influence of electronic, steric and hydrophobic properties of flavonoid compounds in the inhibition of the xanthine oxidase. Computational and Theoretical Chemistry, 2004, 684, 1-7.	1.5	37
129	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
130	A Study on the Antipicornavirus Activity of Flavonoid Compounds (Flavones) by Using Quantum Chemical and Chemometric Methods. Journal of Chemical Information and Computer Sciences, 2004, 44, 1153-1161.	2.8	14
131	A quantum chemical and statistical study of flavonoid compounds (flavones) with anti-HIV activity. European Journal of Medicinal Chemistry, 2003, 38, 929-938.	2.6	22
132	The influence of electronic and steric effects in the structureâ€“activity relationship (SAR) study of quinone compounds with biological activity against Trypanosoma cruzi. Computational and Theoretical Chemistry, 2003, 634, 271-280.	1.5	11
133	An AM1 study on the electron-donating and electron-accepting character of biomolecules. International Journal of Quantum Chemistry, 2003, 95, 126-132.	1.0	62
134	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
135	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
136	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
137	A quantum chemical and statistical study of biflavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2002, 577, 187-195.	1.5	5
138	A theoretical study on the influence of the frontier orbitals HOMO and LUMO and the size of C4 and C2 substituents in the psychoactivity of cannabinoid compounds. Computational and Theoretical Chemistry, 2002, 578, 111-117.	1.5	8
139	Synthesis, structure, electronic and vibrational spectra of 9-(Diethylamino)-benzo(a)phenoxazin-7-ium-5-N-methacrylamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 3103-3111.	2.0	15
140	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
141	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
142	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
143	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
144	A theoretical study of the intramolecular hetero Dielsâ€“Alder cycloaddition reactions of azoalkenes. Computational and Theoretical Chemistry, 2001, 535, 165-169.	1.5	14

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145	A quantum chemical study on the psychoactivity of cannabinoid compounds. Computational and Theoretical Chemistry, 2001, 538, 99-106.	1.5	9
146	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
147	Contracted Gaussian bases for the first-row atoms applied to neutral and charged diatomic molecules. Computational and Theoretical Chemistry, 2001, 539, 29-34.	1.5	6
148	A structureâ€“activity relationship study of HEPT-analog compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2000, 530, 39-47.	1.5	26
149	Accurate adapted Gaussian basis sets for helium- and beryllium-like atomic species to be used in Diracâ€“Fock calculations. Computational and Theoretical Chemistry, 1999, 464, 1-6.	1.5	5
150	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 1999, 491, 123-131.	1.5	24
151	A correlation between geometric features and analgesic activity for a series of cannabinoid compounds. Journal of Molecular Structure, 1998, 441, 97-100.	1.8	1
152	Adapted Gaussian basis sets for the relativistic closed-shell atoms from helium to barium generated with the generator coordinate Dirac-Fock method. Chemical Physics Letters, 1996, 263, 775-782.	1.2	12
153	Theoretical and conformational studies of a series of cannabinoids. Journal of Molecular Structure, 1995, 356, 247-256.	1.8	9
154	Ab initio calculations of relativistic and electron correlation effects in polyatomics using the universal Gaussian basis set: XeF2. International Journal of Quantum Chemistry, 1995, 55, 213-225.	1.0	24
155	Universal Gaussian basis set for relativistic calculations on atoms and molecules. Chemical Physics Letters, 1993, 201, 37-40.	1.2	28
156	Relativistic universal Gaussian basis set for Diracâ€”Fockâ€”Coulomb and Diracâ€”Fockâ€”Breit SCF calculations on heavy atoms. Chemical Physics Letters, 1993, 203, 201-204.	1.2	28
157	Universal Gaussian basis set for accurateab initio/PrelativisticDirac-Fockcalculations. Physical Review A, 1993, 47, 143-146.	1.0	175
158	Universal Gaussian and slater-type bases for atoms H to Xe based on the generator coordinate Hartree-Fock method. Molecular Physics, 1993, 78, 1301-1307.	0.8	13
159	The generator coordinate Hartree-Fock method for molecular systems. Formalism and first applications to H2, LiH and Li2. Chemical Physics, 1991, 154, 379-384.	0.9	25
160	On the helium ground-state Hartree-Fock energy. Chemical Physics Letters, 1991, 183, 31-33.	1.2	6
161	Generator coordinate gaussian expanded natural orbitals. Computational and Theoretical Chemistry, 1990, 210, 63-70.	1.5	10
162	Universal gaussian and Slater-type bases for atoms H to Xe based on the generator coordinate Hartree-Fock method. Molecular Physics, 1989, 68, 433-445.	0.8	61

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163	Electronic structures and electronic spectra of the linkage isomers NSOâ¯ and SNOâ¯. Journal of Molecular Structure, 1987, 162, 351-357.	1.8	10
164	Molecular orbital description of the polythiazyl polymer. Computational and Theoretical Chemistry, 1986, 139, 327-332.	1.5	9
165	N-Acetyl-cysteine Increases Chemical Stability of Hydroquinone in Pharmaceutical Formulations: a Theoretical and Experimental Approach. Journal of the Brazilian Chemical Society, 0, , .	0.6	5