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	Infrared Spectroscopy of Anionic, Cationic, and Zwitterionic Surfactants. Advances in Physical Chemistry, 2012, 2012, 1-14.	2.0	216
2	Universal Gaussian basis set for accurateab initio/PrelativisticDirac-Fockcalculations. Physical Review A, 1993, 47, 143-146.	1.0	175
3	Machine Learning Techniques and Drug Design. Current Medicinal Chemistry, 2012, 19, 4289-4297.	1.2	147
4	Understanding the Molecular Aspects of Tetrahydrocannabinol and Cannabidiol as Antioxidants. Molecules, 2013, 18, 12663-12674.	1.7	95
5	The effects of solvation in the theoretical spectra of cationic dyes. Theoretical Chemistry Accounts, 2005, 113, 274-280.	0.5	74
6	Electrochemical Behavior of Nicotine Studied by Voltammetric Techniques at Boronâ€Doped Diamond Electrodes. Analytical Letters, 2005, 38, 1587-1599.	1.0	64
7	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
8	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
9	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
10	Complexation of the anti-Trypanosoma cruzi Drug Benznidazole Improves Solubility and Efficacy. Journal of Medicinal Chemistry, 2008, 51, 4104-4114.	2.9	57
11	The Isomerization of Dinitrogen Tetroxide:â€‰ O2Nâ^'NO2 â†' ONOâ^'NO2. Journal of Physical Chemistry A, 2007, 111, 2913-2920.	1.1	54
12	A structureâ€“activity relationship study of quinone compounds with trypanocidal activity. European Journal of Medicinal Chemistry, 2005, 40, 329-338.	2.6	48
13	Novel insights for dihydroorotate dehydrogenase class 1A inhibitors discovery. European Journal of Medicinal Chemistry, 2010, 45, 5899-5909.	2.6	47
14	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
15	Use of Graphite Polyurethane Composite Electrode for Imipramine Oxidationâ€"Mechanism Proposal and Electroanalytical Determination. Analytical Letters, 2006, 39, 507-520.	1.0	40
16	Propriedades quÃmico-quÃ¢nticas empregadas em estudos das relaÃ§Ãµes estrutura-atividade. Quimica Nova, 2010, 33, 694-699.	0.3	40
17	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
18	The basic antioxidant structure for flavonoid derivatives. Journal of Molecular Modeling, 2012, 18, 4073-4080.	0.8	37

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19	A multivariate study on flavonoid compounds scavenging the peroxynitrite free radical. Computational and Theoretical Chemistry, 2007, 808, 25-33.	1.5	36
20	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. International Journal of Quantum Chemistry, 2006, 106, 2617-2623.	1.0	32
21	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
22	The nuclear electric quadrupole moment of antimony from the molecular method. Journal of Chemical Physics, 2006, 125, 064301.	1.2	29
23	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
24	Universal Gaussian basis set for relativistic calculations on atoms and molecules. Chemical Physics Letters, 1993, 201, 37-40.	1.2	28
25	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
26	The asymmetric dimerization of nitrogen dioxide. Chemical Physics Letters, 2007, 436, 47-50.	1.2	28
27	A structureâ€“activity relationship study of HEPT-analog compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2000, 530, 39-47.	1.5	26
28	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
29	A partial least squares regression study with antioxidant flavonoid compounds. Structural Chemistry, 2006, 17, 307-313.	1.0	25
30	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
31	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 1999, 491, 123-131.	1.5	24
32	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
33	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
34	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
35	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
36	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

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37	A partial least squares and principal component regression study of quinone compounds with trypanocidal activity. Structural Chemistry, 2007, 18, 49-57.	1.0	23
38	Density Functional Theory (DFT) Study of Edaravone Derivatives as Antioxidants. International Journal of Molecular Sciences, 2012, 13, 7594-7606.	1.8	23
39	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
40	A polynomial version of the generator coordinate Dirac-Fock method. Journal of Computational Chemistry, 2004, 25, 1904-1909.	1.5	22
41	The use of classification methods for modeling the antioxidant activity of flavonoid compounds. Journal of Molecular Modeling, 2006, 12, 915-920.	0.8	21
42	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
43	Interaction between PH3 and small water clusters: Understanding the electronic and spectroscopic properties. Computational and Theoretical Chemistry, 2015, 1059, 35-44.	1.1	21
44	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
45	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
46	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
47	Generator coordinate method in time-dependent density-functional theory: Memory made simple. Journal of Chemical Physics, 2007, 127, 124101.	1.2	19
48	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
49	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
50	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
51	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
52	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
53	Evaluation and Theoretical Study on the Anti-inflammatory Mechanism of 1-Nitro-2-phenylethane. Planta Medica, 2013, 79, 628-633.	0.7	18
54	Cationic dye dimers: a theoretical study. Theoretical Chemistry Accounts, 2007, 118, 305-314.	0.5	17

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55	Artificial Neural Networks and the Study of the Psychoactivity of Cannabinoid Compounds. Chemical Biology and Drug Design, 2010, 75, 632-640.	1.5	17
56	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
57	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
58	A quantum chemical and photophysical study of acridine-9-N-methacrylamide. Computational and Theoretical Chemistry, 2004, 674, 213-225.	1.5	15
59	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
60	Theoretical study of dibenzotetraaza[14]annulene complexes with first row transition metals. Computational and Theoretical Chemistry, 2015, 1054, 93-99.	1.1	15
61	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
62	A theoretical study of the intramolecular hetero Dielsâ€“Alder cycloaddition reactions of azoalkenes. Computational and Theoretical Chemistry, 2001, 535, 165-169.	1.5	14
63	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
64	A neural networks study of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2008, 14, 975-985.	0.8	14
65	A theoretical study on the XeF2 molecule. Chemical Physics, 2008, 348, 89-96.	0.9	14
66	Molecular properties of the PCO radical: heat of formation and the isomerization pathways. Journal of Molecular Modeling, 2014, 20, 2074.	0.8	14
67	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
68	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.	1.9	13
69	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
70	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
71	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
72	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

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73	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
74	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
75	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
76	Docking and molecular dynamics simulation of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2009, 15, 1175-1184.	0.8	12
77	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
78	The nuclear electric quadrupole moment of lutetium from the molecular method. Chemical Physics Letters, 2007, 445, 95-98.	1.2	11
79	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
80	CO bonding in FeN4 complexes and the effect of the macrocycle ligand: A DFT study. Polyhedron, 2014, 67, 36-43.	1.0	11
81	An antioxidant mechanism of morphine and related derivatives. Medicinal Chemistry Research, 2016, 25, 852-857.	1.1	11
82	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
83	Electronic structures and electronic spectra of the linkage isomers NSOâ¯ and SNOâ¯. Journal of Molecular Structure, 1987, 162, 351-357.	1.8	10
84	Generator coordinate gaussian expanded natural orbitals. Computational and Theoretical Chemistry, 1990, 210, 63-70.	1.5	10
85	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
86	Rate Coefficient for the Reaction SiO + Si2O2atT= 10â¯1000 K. Journal of Physical Chemistry A, 2006, 110, 13221-13226.	1.1	10
87	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
88	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
89	Electronic properties of the AsCO, AsSiO and AsGeO radicals: Linear or cyclic?. Polyhedron, 2015, 89, 160-167.	1.0	10
90	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

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91	Two-Dimensional QSAR Studies on Arylpiperazines as High-Affinity 5-HT1A Receptor Ligands. Medicinal Chemistry, 2008, 4, 328-335.	0.7	10
92	A Structure and Antioxidant Activity Study of Paracetamol and Salicylic Acid. Pharmacology & Pharmacy, 2014, 05, 1185-1191.	0.2	10
93	Molecular orbital description of the polythiazyl polymer. Computational and Theoretical Chemistry, 1986, 139, 327-332.	1.5	9
94	Theoretical and conformational studies of a series of cannabinoids. Journal of Molecular Structure, 1995, 356, 247-256.	1.8	9
95	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
96	A quantum chemical study on the psychoactivity of cannabinoid compounds. Computational and Theoretical Chemistry, 2001, 538, 99-106.	1.5	9
97	A theoretical study on the analgesic activity of cannabinoid compounds. Computational and Theoretical Chemistry, 2004, 709, 223-229.	1.5	9
98	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
99	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
100	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
101	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
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	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
104	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
105	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
106	The CH3PH2 and CH3PH isomers: isomerization, hydrogen release, thermodynamic, and spectroscopy properties. Journal of Molecular Modeling, 2014, 20, 2372.	0.8	8
107	Accurate Calculations of Rate Constants for the Forward and Reverse H₂O + CO â†” HCOOH Reactions. ChemistrySelect, 2017, 2, 7267-7272.	0.7	8
108	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

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109	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
110	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
111	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
112	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
113	On the helium ground-state Hartree-Fock energy. Chemical Physics Letters, 1991, 183, 31-33.	1.2	6
114	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
115	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
116	Molecular Features Related to HIV Integrase Inhibition Obtained from Structure- and Ligand-Based Approaches. PLoS ONE, 2014, 9, e81301.	1.1	6
117	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
118	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
119	A quantum chemical and statistical study of biflavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2002, 577, 187-195.	1.5	5
120	Influence of confining anisotropy on the unstable behavior of a Bose gas with attractive interaction. Physical Review A, 2004, 70, .	1.0	5
121	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
122	The tautomerism influence on the antioxidant prediction of oxederavone. Medicinal Chemistry Research, 2013, 22, 5617-5623.	1.1	5
123	Structure and toxicity of clozapine and olanzapine on agranulocytosis. Medicinal Chemistry Research, 2016, 25, 322-328.	1.1	5
124	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
125	A Proposal for the Mechanism of the CH + CO2 Reaction. ACS Omega, 2019, 4, 17843-17849.	1.6	5
126	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

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127	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
128	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
129	Molecular Features for Antitrypanosomal Activity of Thiosemicarbazones Revealed by OPS-PLS QSAR Studies. Medicinal Chemistry, 2012, 8, 1045-1056.	0.7	5
130	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
131	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
132	Quantum chemical and statistical study of megazol-derived compounds with trypanocidal activity. International Journal of Quantum Chemistry, 2005, 103, 738-748.	1.0	4
133	A prÃ¡tica docente na formaÃ§Ã£o do pÃ³s-graduando em quÃmica. Quimica Nova, 2008, 31, 1888-1891.	0.3	4
134	A Theoretical Study of the Dapsone Derivatives on Methemoglobin. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2029-2033.	0.4	4
135	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
136	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
137	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
138	Drug design of new 5-HT6 antagonists: a QSAR study of arylsulfonamide derivatives. Structural Chemistry, 2020, 31, 1585-1597.	1.0	4
139	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
140	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
141	Excitation energies from ground-state density-functionals by means of generator coordinates. Physical Chemistry Chemical Physics, 2009, 11, 4564.	1.3	3
142	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
143	The 1,2-hydrogen shift reaction for monohalogenophosphanes PH₂X and HPX (XÂ= F, Cl). Molecular Physics, 2016, 114, 2999-3014.	0.8	3
144	On polarization functions for Gaussian basis sets. Journal of Molecular Modeling, 2020, 26, 293.	0.8	3

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145	Drug design of new 5-HT6R antagonists aided by artificial neural networks. Journal of Molecular Graphics and Modelling, 2021, 104, 107844.	1.3	3
146	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
147	Structural and Electronic Properties of Dipyridamole and Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 69-73.	0.4	2
148	Molecular Features for Antitrypanosomal Activity of Thiosemicarbazones Revealed by OPS-PLS QSAR Studies. Medicinal Chemistry, 2012, 8, 1045-1056.	0.7	2
149	Theoretical models for the antitrypanosomal activity of thiosemicarbazone derivatives. International Journal of Quantum Chemistry, 2012, 112, 3364-3370.	1.0	2
150	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
151	A mechanistic study of the electrochemical behavior of pendimethalin herbicide. Journal of Electroanalytical Chemistry, 2018, 826, 157-163.	1.9	2
152	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
153	Highly accurate relativistic universal Gaussian basis set for Dirac-Fock-Breit calculations. International Journal of Quantum Chemistry, 2005, 102, 1-7.	1.0	1
154	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
155	A chemometric study of megazol derivatives with activity againstTrypanosoma equiperdum. SAR and QSAR in Environmental Research, 2006, 17, 533-547.	1.0	1
156	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
157	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
158	A Study on the Antipicornavirus Activity of Flavonoid Compounds (Flavones) by Using Quantum Chemical and Chemometric Methods.. ChemInform, 2004, 35, no.	0.1	0
159	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
160	One-dimensional trapped atoms: critical coupling parameter and critical number of particles. Journal of Mathematical Chemistry, 2010, 48, 687-696.	0.7	0
161	Accurate atomic electron affinities calculated by using anionic Gaussian basis sets. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	0
162	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

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163	The Generator Coordinate Diracâ€“Fock Method and Relativistic Calculations for Atoms and Molecules. , 2007, , 79-150.		0
164	PRECIPITATION REACTION OF CLAVULANIC ACID: THERMODYNAMIC AND ELECTRONIC STUDY. Quimica Nova, 2016, , .	0.3	0
165	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