

Alberico Borges Ferreira da Silva

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

162
papers

2,534
citations

24
h-index

40
g-index

165
ext. papers

2,755
ext. citations

2.8
avg, IF

4.82
L-index

#	Paper	IF	Citations
162	A mechanistic view of the reaction between phosphine and fluorine atom: insights into PH ₃ F isomers. <i>Computational and Theoretical Chemistry</i> , 2022 , 113769	2	0
161	New D2R partial agonist candidates: an in silico approach from statistical models, molecular docking, and ADME/Tox properties. <i>Structural Chemistry</i> , 2021 , 32, 2019-2033	1.8	0
160	Drug design of new 5-HT ₂ antagonists aided by artificial neural networks. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 104, 107844	2.8	1
159	Drug design of new sigma-1 antagonists against neuropathic pain: A QSAR study using partial least squares and artificial neural networks. <i>Journal of Molecular Structure</i> , 2021 , 1223, 129156	3.4	2
158	A partial least squares and artificial neural network study for a series of arylpiperazines as antidepressant agents. <i>Journal of Molecular Modeling</i> , 2021 , 27, 297	2	1
157	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. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 16989-16997	3.6	0
156	Microwave-Driven Hexagonal-to-Monoclinic Transition in BiPO: An In-Depth Experimental Investigation and First-Principles Study. <i>Inorganic Chemistry</i> , 2020 , 59, 7453-7468	5.1	12
155	Experimental and theoretical study on structure-tautomerism among edaravone, isoxazolone, and their heterocycles derivatives as antioxidants. <i>Saudi Pharmaceutical Journal</i> , 2020 , 28, 819-827	4.4	3
154	Drug design of new 5-HT ₆ antagonists: a QSAR study of arylsulfonamide derivatives. <i>Structural Chemistry</i> , 2020 , 31, 1585-1597	1.8	2
153	Accurate atomic electron affinities calculated by using anionic Gaussian basis sets. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	0
152	On polarization functions for Gaussian basis sets. <i>Journal of Molecular Modeling</i> , 2020 , 26, 293	2	1
151	Crystal packing of a zinc(II)-azide complex with a N,N,S-tridentate thiosemicarbazone ligand: An experimental and computational study. <i>Journal of Molecular Structure</i> , 2019 , 1197, 393-400	3.4	6
150	A Proposal for the Mechanism of the CH + CO Reaction. <i>ACS Omega</i> , 2019 , 4, 17843-17849	3.9	2
149	A molecular modeling study of combretastatin-like chalcones as anticancer agents using PLS, ANN and consensus models. <i>Structural Chemistry</i> , 2018 , 29, 957-965	1.8	4
148	Sugar moiety has a synergistic effect on hydroxylated xanthone for better antioxidant activity of mangiferin. <i>Medicinal Chemistry Research</i> , 2018 , 27, 1276-1282	2.2	11
147	A mechanistic study of the electrochemical behavior of pendimethalin herbicide. <i>Journal of Electroanalytical Chemistry</i> , 2018 , 826, 157-163	4.1	2
146	Relativistic Prolapse-Free Gaussian Basis Sets of Quadruple-Quality: (aug-)RPF-4Z. III. The f-Block Elements. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1094-1101	6.4	4

145	Accurate Calculations of Rate Constants for the Forward and Reverse H ₂ O + CO \leftrightarrow HCOOH Reactions. <i>ChemistrySelect</i> , 2017 , 2, 7267-7272	1.8	7
144	New consensus multivariate models based on PLS and ANN studies of sigma-1 receptor antagonists. <i>Journal of Molecular Modeling</i> , 2017 , 23, 302	2	2
143	Photodynamic Efficiency of Xanthene Dyes and Their Phototoxicity against a Carcinoma Cell Line: A Computational and Experimental Study. <i>Journal of Chemistry</i> , 2017 , 2017, 1-9	2.3	20
142	THE H ₂ + CO \rightarrow H ₂ CO REACTION: RATE CONSTANTS AND RELEVANCE TO HOT AND DENSE ASTROPHYSICAL MEDIA. <i>Astrophysical Journal, Supplement Series</i> , 2016 , 225, 2	8	8
141	Structure and toxicity of clozapine and olanzapine on agranulocytosis. <i>Medicinal Chemistry Research</i> , 2016 , 25, 322-328	2.2	3
140	Intramolecular interactions, isomerization and vibrational frequencies of two paracetamol analogues: A spectroscopic and a computational approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 162, 16-26	4.4	9
139	An antioxidant mechanism of morphine and related derivatives. <i>Medicinal Chemistry Research</i> , 2016 , 25, 852-857	2.2	8
138	The 1,2-hydrogen shift reaction for monohalogenophosphanes PH ₂ X and HPX (X = F, Cl). <i>Molecular Physics</i> , 2016 , 114, 2999-3014	1.7	3
137	Vibrational spectroscopy, intramolecular CH \cdots O interaction and conformational analysis of 2,5-dimethyl-benzyl benzoate. <i>Journal of Molecular Structure</i> , 2016 , 1125, 649-655	3.4	2
136	A computational study for the antioxidant capacity increases in hydroxy-derivatives of paracetamol and salicylic acid. <i>Medicinal Chemistry Research</i> , 2015 , 24, 3453-3459	2.2	6
135	Accurate Gaussian basis sets for atomic and molecular calculations obtained from the generator coordinate method with polynomial discretization. <i>Journal of Molecular Modeling</i> , 2015 , 21, 274	2	1
134	Theoretical study of dibenzotetraaza[14]annulene complexes with first row transition metals. <i>Computational and Theoretical Chemistry</i> , 2015 , 1054, 93-99	2	14
133	Interaction between PH ₃ and small water clusters: Understanding the electronic and spectroscopic properties. <i>Computational and Theoretical Chemistry</i> , 2015 , 1059, 35-44	2	16
132	Electronic properties of the AsCO, AsSiO and AsGeO radicals: Linear or cyclic?. <i>Polyhedron</i> , 2015 , 89, 1602-1607	1.67	9
131	Molecular properties of the PCO radical: heat of formation and the isomerization pathways. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2074	2	13
130	Quantum chemical DFT study of the interaction between molecular oxygen and FeN \cdots complexes, and effect of the macrocyclic ligand. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2131	2	8
129	Relativistic Prolapse-Free Gaussian Basis Set of Quadruple-Quality: (aug-)RPF-4Z. II. The d-Block Elements. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4761-4	6.4	8
128	On the stability of the RuCl ₂ (triphenylphosphine) ₂ (amine) complexes: Ligand substituent effects of cyclic and acyclic amines. <i>Polyhedron</i> , 2014 , 81, 661-667	2.7	7

127	Relativistic Prolapse-Free Gaussian Basis Set of Quadruple-Quality: (aug-)RPF-4Z. I. The s- and p-Block Elements. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3800-6	6.4	14
126	The CH ₃ PH ₂ and CH ₃ PH isomers: isomerization, hydrogen release, thermodynamic, and spectroscopy properties. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2372	2	8
125	Molecular features related to HIV integrase inhibition obtained from structure- and ligand-based approaches. <i>PLoS ONE</i> , 2014 , 9, e81301	3.7	5
124	Pattern recognition techniques applied to the study of leishmanial glyceraldehyde-3-phosphate dehydrogenase inhibition. <i>International Journal of Molecular Sciences</i> , 2014 , 15, 3186-203	6.3	4
123	Understanding the cytotoxicity or cytoprotective effects of biological and synthetic quinone derivatives by redox mechanism. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2541	2	11
122	CO bonding in FeN ₄ complexes and the effect of the macrocycle ligand: A DFT study. <i>Polyhedron</i> , 2014 , 67, 36-43	2.7	8
121	A Structure and Antioxidant Activity Study of Paracetamol and Salicylic Acid. <i>Pharmacology & Pharmacy</i> , 2014 , 05, 1185-1191	0.3	6
120	A combined experimental and theoretical approach for radical-scavenging activity of edaravone and its related derivatives. <i>Structural Chemistry</i> , 2013 , 24, 349-355	1.8	8
119	4-hydroxy-2,5-dimethylphenyl-benzophenone: conformational stability, FT-IR and Raman investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 102, 386-92	4.4	10
118	Design and evaluation of 4-aminophenol and salicylate derivatives as free-radical scavenger. <i>Chemical Biology and Drug Design</i> , 2013 , 81, 414-9	2.9	18
117	The tautomerism influence on the antioxidant prediction of oxederavone. <i>Medicinal Chemistry Research</i> , 2013 , 22, 5617-5623	2.2	5
116	Identification of electronic and structural descriptors of adenosine analogues related to inhibition of leishmanial glyceraldehyde-3-phosphate dehydrogenase. <i>Molecules</i> , 2013 , 18, 5032-50	4.8	9
115	Coordination Ability of Polyether and Polyamine Ligands: A Density Functional Theory Study of First- and Second-Row Transition Metals. <i>Journal of Computational and Theoretical Nanoscience</i> , 2013 , 10, 2034-2040	0.3	7
114	Non-peptidic cruzain inhibitors with trypanocidal activity discovered by virtual screening and in vitro assay. <i>PLoS Neglected Tropical Diseases</i> , 2013 , 7, e2370	4.8	54
113	Evaluation and theoretical study on the anti-inflammatory mechanism of 1-nitro-2-phenylethane. <i>Planta Medica</i> , 2013 , 79, 628-33	3.1	14
112	A Theoretical Study of the Dapsone Derivatives on Methemoglobin. <i>Journal of Computational and Theoretical Nanoscience</i> , 2013 , 10, 2029-2033	0.3	4
111	Understanding the molecular aspects of tetrahydrocannabinol and cannabidiol as antioxidants. <i>Molecules</i> , 2013 , 18, 12663-74	4.8	61
110	A combined study using ligand-based design, synthesis, and pharmacological evaluation of analogues of the acetaminophen ortho-regioisomer with potent analgesic activity. <i>Chemical Biology and Drug Design</i> , 2012 , 80, 99-105	2.9	2

109	The basic antioxidant structure for flavonoid derivatives. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4073-80		30
108	Machine learning techniques and drug design. <i>Current Medicinal Chemistry</i> , 2012 , 19, 4289-97	4.3	100
107	Metal binding selectivity of oxa-aza macrocyclic ligand: a DFT study of first- and second-row transition metal for four coordination systems. <i>Structural Chemistry</i> , 2012 , 23, 1539-1545	1.8	7
106	Adsorption of sodium dodecyl sulfate on Ge substrate: the effect of a low-polarity solvent. <i>International Journal of Molecular Sciences</i> , 2012 , 13, 7980-93	6.3	22
105	Theoretical models for the antitrypanosomal activity of thiosemicarbazone derivatives. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 3364-3370	2.1	1
104	First- and second-row transition metal oxa-aza macrocyclic complexes: a DFT study of an octahedral conformation. <i>Journal of Molecular Modeling</i> , 2012 , 18, 3243-53	2	7
103	Density functional theory (DFT) study of edaravone derivatives as antioxidants. <i>International Journal of Molecular Sciences</i> , 2012 , 13, 7594-606	6.3	21
102	Infrared Spectroscopy of Anionic, Cationic, and Zwitterionic Surfactants. <i>Advances in Physical Chemistry</i> , 2012 , 2012, 1-14		178
101	Molecular Features for Antitrypanosomal Activity of Thiosemicarbazones Revealed by OPS-PLS QSAR Studies. <i>Medicinal Chemistry</i> , 2012 , 8, 1045-1056	1.8	1
100	Molecular features for antitrypanosomal activity of thiosemicarbazones revealed by OPS-PLS QSAR studies. <i>Medicinal Chemistry</i> , 2012 , 8, 1045-56	1.8	5
99	Structural and Electronic Properties of Dipyridamole and Derivatives. <i>Journal of Computational and Theoretical Nanoscience</i> , 2011 , 8, 69-73	0.3	2
98	Artificial neural networks and the study of the psychoactivity of cannabinoid compounds. <i>Chemical Biology and Drug Design</i> , 2010 , 75, 632-40	2.9	11
97	Insights into the molecular requirements for the anti-obesity activity of a series of CB1 ligands. <i>Chemical Biology and Drug Design</i> , 2010 , 76, 320-9	2.9	8
96	Propriedades químico-quânticas empregadas em estudos das relações estrutura-atividade. <i>Quimica Nova</i> , 2010 , 33, 694-699	1.6	31
95	Pharmacophore-based 3D QSAR studies on a series of high affinity 5-HT1A receptor ligands. <i>European Journal of Medicinal Chemistry</i> , 2010 , 45, 1508-14	6.8	24
94	The effect of the negative coupling parameter on the spectrum of a trapped Bose gas. <i>Journal of Mathematical Chemistry</i> , 2010 , 47, 636-646	2.1	
93	One-dimensional trapped atoms: critical coupling parameter and critical number of particles. <i>Journal of Mathematical Chemistry</i> , 2010 , 48, 687-696	2.1	
92	Novel insights for dihydroorotate dehydrogenase class 1A inhibitors discovery. <i>European Journal of Medicinal Chemistry</i> , 2010 , 45, 5899-909	6.8	36

91	Photophysical properties and quantum chemical studies of poly(2,7-9,9-dihexylfluorene-diyil). <i>Journal of the Brazilian Chemical Society</i> , 2009 , 20, 160-166	1.5	13
90	Docking and molecular dynamics simulation of quinone compounds with trypanocidal activity. <i>Journal of Molecular Modeling</i> , 2009 , 15, 1175-84	2	11
89	A chemometric study on the analgesic activity of cannabinoid compounds using SDA, KNN and SIMCA methods. <i>Structural Chemistry</i> , 2009 , 20, 577-585	1.8	7
88	The origin of the molecular interaction between amino acids and gold nanoparticles: A theoretical and experimental investigation. <i>Chemical Physics Letters</i> , 2009 , 469, 186-190	2.5	38
87	Excitation energies from ground-state density-functionals by means of generator coordinates. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 4564-9	3.6	3
86	Complexation of the anti-Trypanosoma cruzi drug benznidazole improves solubility and efficacy. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 4104-14	8.3	53
85	A prática docente na formação do pós-graduando em química. <i>Química Nova</i> , 2008 , 31, 1888-1891	1.6	2
84	A neural networks study of quinone compounds with trypanocidal activity. <i>Journal of Molecular Modeling</i> , 2008 , 14, 975-85	2	13
83	Crystal structure and theoretical calculations of Julocrotine, a natural product with antileishmanial activity. <i>International Journal of Quantum Chemistry</i> , 2008 , 108, 513-520	2.1	9
82	A chemometric study of the 5-HT(1A) receptor affinities presented by arylpiperazine compounds. <i>European Journal of Medicinal Chemistry</i> , 2008 , 43, 364-72	6.8	15
81	A theoretical study on the XeF ₂ molecule. <i>Chemical Physics</i> , 2008 , 348, 89-96	2.3	13
80	A combined X-ray and theoretical study of flavonoid compounds with anti-inflammatory activity. <i>Computational and Theoretical Chemistry</i> , 2008 , 862, 16-20		10
79	Two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT(1A) receptor ligands. <i>Medicinal Chemistry</i> , 2008 , 4, 328-35	1.8	10
78	Generator coordinate method in time-dependent density-functional theory: memory made simple. <i>Journal of Chemical Physics</i> , 2007 , 127, 124101	3.9	17
77	Photoinduced electron-transfer processes based on novel bipyridine-Ru(II) complex: properties of cis-[Ru(2,2'-bipyridine) ₂ (5,6-bis(3-amidopyridine)-7-oxanorbornene)](PF ₆) ₂ and cis-[Ru(2,2'-bipyridine) ₂ (3-aminopyridine) ₂](PF ₆) ₂ complexes. <i>Inorganic Chemistry</i> , 2007 , 46, 5744-53	5.1	11
76	The isomerization of dinitrogen tetroxide: O ₂ N-NO ₂ → ONO-NO ₂ . <i>Journal of Physical Chemistry A</i> , 2007 , 111, 2913-20	2.8	52
75	1,4- Addition of diazomethane to a heterodiene: a direct preparation of the oxazolic ring. <i>Anais Da Academia Brasileira De Ciencias</i> , 2007 , 79, 29-33	1.4	6
74	A multivariate study on flavonoid compounds scavenging the peroxynitrite free radical. <i>Computational and Theoretical Chemistry</i> , 2007 , 808, 25-33		28

73	The asymmetric dimerization of nitrogen dioxide. <i>Chemical Physics Letters</i> , 2007 , 436, 47-50	2.5	28
72	The nuclear electric quadrupole moment of lutetium from the molecular method. <i>Chemical Physics Letters</i> , 2007 , 445, 95-98	2.5	11
71	Prolapse-free relativistic Gaussian basis sets for the superheavy elements up to Uuo (Z=118) and Lr (Z=103). <i>Atomic Data and Nuclear Data Tables</i> , 2007 , 93, 931-961	2	10
70	Cationic dye dimers: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2007 , 118, 305-314	1.9	14
69	A partial least squares and principal component regression study of quinone compounds with trypanocidal activity. <i>Structural Chemistry</i> , 2007 , 18, 49-57	1.8	21
68	Studies of the electrochemical reduction of atrazine on a mercury electrode in acid medium: An electrochemical and NMR approach. <i>Journal of Electroanalytical Chemistry</i> , 2007 , 608, 47-51	4.1	10
67	The Generator Coordinate Dirac-Hock Method and Relativistic Calculations for Atoms and Molecules 2007 , 79-150		
66	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. <i>Journal of Computational Chemistry</i> , 2006 , 27, 61-71	3.5	16
65	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. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1970-9	3.5	16
64	The nuclear electric quadrupole moment of antimony from the molecular method. <i>Journal of Chemical Physics</i> , 2006 , 125, 64301	3.9	25
63	A chemometric study of megazol derivatives with activity against Trypanosoma equiperdum. <i>SAR and QSAR in Environmental Research</i> , 2006 , 17, 533-47	3.5	1
62	Use of Graphite Polyurethane Composite Electrode for Imipramine Oxidation-Mechanism Proposal and Electroanalytical Determination. <i>Analytical Letters</i> , 2006 , 39, 507-520	2.2	35
61	Rate coefficient for the reaction SiO + Si2O2 at T = 10-1000 K. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 13221-6	2.8	8
60	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. <i>International Journal of Quantum Chemistry</i> , 2006 , 106, 2617-2623	2.1	30
59	Adapted relativistic prolapse-free Gaussian basis sets for closed shell atoms up to nobelium and to be used with the uniform sphere nucleus model. <i>International Journal of Quantum Chemistry</i> , 2006 , 106, 2790-2803	2.1	3
58	The employment of relativistic adapted Gaussian basis sets in Douglas-Kroll-Hess scalar calculations with diatomic molecules. <i>Chemical Physics</i> , 2006 , 331, 173-177	2.3	8
57	A partial least squares regression study with antioxidant flavonoid compounds. <i>Structural Chemistry</i> , 2006 , 17, 307-313	1.8	17
56	The use of classification methods for modeling the antioxidant activity of flavonoid compounds. <i>Journal of Molecular Modeling</i> , 2006 , 12, 915-20	2	18

55	Deactivation of triplet-excited riboflavin by purine derivatives: important role of uric acid in light-induced oxidation of milk sensitized by riboflavin. <i>Journal of Agricultural and Food Chemistry</i> , 2005 , 53, 3679-84	5.7	22
54	Electrochemical Behavior of Nicotine Studied by Voltammetric Techniques at Boron-Doped Diamond Electrodes. <i>Analytical Letters</i> , 2005 , 38, 1587-1599	2.2	49
53	A structure-activity relationship study of quinone compounds with trypanocidal activity. <i>European Journal of Medicinal Chemistry</i> , 2005 , 40, 329-38	6.8	39
52	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. <i>Journal of Computational Chemistry</i> , 2005 , 26, 932-40	3.5	17
51	The effects of solvation in the theoretical spectra of cationic dyes. <i>Theoretical Chemistry Accounts</i> , 2005 , 113, 274-280	1.9	67
50	A study on the influence of molecular properties in the psychoactivity of cannabinoid compounds. <i>Journal of Molecular Modeling</i> , 2005 , 11, 200-9	2	19
49	Highly accurate relativistic universal Gaussian basis set for Dirac-Fock-Breit calculations. <i>International Journal of Quantum Chemistry</i> , 2005 , 102, 1-7	2.1	1
48	Selection of quantum chemical descriptors by chemometric methods in the study of antioxidant activity of flavonoid compounds. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 731-737	2.1	19
47	Quantum chemical and statistical study of megazol-derived compounds with trypanocidal activity. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 738-748	2.1	3
46	New adapted Gaussian basis sets for the relativistic closed shell atoms from helium to barium generated with the generator coordinate Dirac-Fock method. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 523-528	2.1	1
45	Energy lowering of current-carrying single-particle states in open-shell atoms due to an exchange-correlation vector potential. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 516-522	2.1	10
44	Relativistic Gaussian basis sets obtained with a polynomial version of the generator coordinate Dirac-Fock method: Ionization energies of some closed-shell atomic systems. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 529-536	2.1	2
43	Influence of confining anisotropy on the unstable behavior of a Bose gas with attractive interaction. <i>Physical Review A</i> , 2004 , 70,	2.6	3
42	A polynomial version of the generator coordinate Dirac-Fock method. <i>Journal of Computational Chemistry</i> , 2004 , 25, 1904-9	3.5	20
41	A theoretical study on the analgesic activity of cannabinoid compounds. <i>Computational and Theoretical Chemistry</i> , 2004 , 709, 223-229		8
40	A study on the anti-HIV activity of biflavonoid compounds by using quantum chemical and chemometric methods. <i>Computational and Theoretical Chemistry</i> , 2004 , 674, 191-197		4
39	A quantum chemical and photophysical study of acridine-9-N-methacrylamide. <i>Computational and Theoretical Chemistry</i> , 2004 , 674, 213-225		14
38	The influence of electronic, steric and hydrophobic properties of flavonoid compounds in the inhibition of the xanthine oxidase. <i>Computational and Theoretical Chemistry</i> , 2004 , 684, 1-7		31

37	A density functional theory study on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. <i>Chemical Physics</i> , 2004 , 306, 35-41	2.3	5
36	A study on the antipicornavirus activity of flavonoid compounds (flavones) by using quantum chemical and chemometric methods. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 1153-61		13
35	A study of neolignan compounds with biological activity against <i>Paracoccidioides brasiliensis</i> by using quantum chemical and chemometric methods. <i>Journal of the Brazilian Chemical Society</i> , 2003 , 14, 809-814	1.5	12
34	A quantum chemical and statistical study of flavonoid compounds (flavones) with anti-HIV activity. <i>European Journal of Medicinal Chemistry</i> , 2003 , 38, 929-38	6.8	20
33	The influence of electronic and steric effects in the structure-activity relationship (SAR) study of quinone compounds with biological activity against <i>Trypanosoma cruzi</i> . <i>Computational and Theoretical Chemistry</i> , 2003 , 634, 271-280		10
32	An AM1 study on the electron-donating and electron-accepting character of biomolecules. <i>International Journal of Quantum Chemistry</i> , 2003 , 95, 126-132	2.1	49
31	Theoretical study on the stereochemistry of intramolecular hetero Diels-Alder cycloaddition reactions of azoalkenes. <i>International Journal of Quantum Chemistry</i> , 2003 , 95, 133-136	2.1	4
30	A Structure-Activity Relationship (SAR) Study of Neolignan Compounds with Anti-schistosomiasis Activity. <i>Journal of the Brazilian Chemical Society</i> , 2002 , 13, 300-307	1.5	17
29	A quantum chemical and statistical study of biflavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 2002 , 577, 187-195		5
28	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. <i>Computational and Theoretical Chemistry</i> , 2002 , 578, 111-117		7
27	Synthesis, structure, electronic and vibrational spectra of 9-(Diethylamino)-benzo(a)phenoxazin-7-ium-5-N-methacrylamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002 , 58, 3103-11	4.4	13
26	A structure-activity relationship (SAR) study of synthetic neolignans and related compounds with biological activity against <i>Escherichia coli</i> . <i>Computational and Theoretical Chemistry</i> , 2002 , 583, 105-116		18
25	An AM1 theoretical study on the effect of Zn ²⁺ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. <i>Tetrahedron</i> , 2002 , 58, 2695-2700	2.4	14
24	A study on the effect of Lewis acid catalysis on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. <i>Tetrahedron</i> , 2001 , 57, 6877-6883	2.4	9
23	Theoretical calculations on dipyridamole structure allow to explain experimental properties associated to electrochemical oxidation and protonation. <i>Chemical Physics Letters</i> , 2001 , 349, 146-152	2.5	13
22	A theoretical study of the intramolecular hetero Diels-Alder cycloaddition reactions of azoalkenes. <i>Computational and Theoretical Chemistry</i> , 2001 , 535, 165-169		13
21	A quantum chemical study on the psychoactivity of cannabinoid compounds. <i>Computational and Theoretical Chemistry</i> , 2001 , 538, 99-106		9
20	A multiple linear regression and partial least squares study of flavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 2001 , 541, 81-88		21

19	Contracted Gaussian bases for the first-row atoms applied to neutral and charged diatomic molecules. <i>Computational and Theoretical Chemistry</i> , 2001 , 539, 29-34		6
18	A structure-activity relationship study of HEPT-analog compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 2000 , 530, 39-47		22
17	Accurate adapted Gaussian basis sets for helium- and beryllium-like atomic species to be used in Dirac-Fock calculations. <i>Computational and Theoretical Chemistry</i> , 1999 , 464, 1-6		4
16	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. <i>Computational and Theoretical Chemistry</i> , 1999 , 491, 123-131		22
15	A correlation between geometric features and analgesic activity for a series of cannabinoid compounds. <i>Journal of Molecular Structure</i> , 1998 , 441, 97-100	3-4	1
14	Adapted Gaussian basis sets for the relativistic closed-shell atoms from helium to barium generated with the generator coordinate Dirac-Fock method. <i>Chemical Physics Letters</i> , 1996 , 263, 775-782 ⁵		10
13	Ab initio calculations of relativistic and electron correlation effects in polyatomics using the universal Gaussian basis set: XeF ₂ . <i>International Journal of Quantum Chemistry</i> , 1995 , 55, 213-225	2.1	24
12	Theoretical and conformational studies of a series of cannabinoids. <i>Journal of Molecular Structure</i> , 1995 , 356, 247-256	3-4	8
11	Universal Gaussian basis set for accurate ab initio /P relativistic Dirac-Fock calculations. <i>Physical Review A</i> , 1993 , 47, 143-146	2.6	165
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5	Generator coordinate gaussian expanded natural orbitals. <i>Computational and Theoretical Chemistry</i> , 1990 , 210, 63-70		10
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