Alberico Borges Ferreira da Silva

List of Publications by Citations

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	Infrared Spectroscopy of Anionic, Cationic, and Zwitterionic Surfactants. *Advances in Physical Chemistry*, **2012**, 2012, 1-14		178
161	Universal Gaussian basis set for accurate ab initio /P relat ivistic Dirac-Fock calculations. *Physical Review A*, **1993**, 47, 143-146	2.6	165
160	Machine learning techniques and drug design. *Current Medicinal Chemistry*, **2012**, 19, 4289-97	4.3	100
159	The effects of solvation in the theoretical spectra of cationic dyes. *Theoretical Chemistry Accounts*, **2005**, 113, 274-280	1.9	67
158	Understanding the molecular aspects of tetrahydrocannabinol and cannabidiol as antioxidants. *Molecules*, **2013**, 18, 12663-74	4.8	61
157	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	1.7	58
156	Non-peptidic cruzain inhibitors with trypanocidal activity discovered by virtual screening and in vitro assay. *PLoS Neglected Tropical Diseases*, **2013**, 7, e2370	4.8	54
155	Complexation of the anti-Trypanosoma cruzi drug benznidazole improves solubility and efficacy. *Journal of Medicinal Chemistry*, **2008**, 51, 4104-14	8.3	53
154	The isomerization of dinitrogen tetroxide: O2N-NO2 --> ONO-NO2. *Journal of Physical Chemistry A*, **2007**, 111, 2913-20	2.8	52
153	Electrochemical Behavior of Nicotine Studied by Voltammetric Techniques at Boron-Doped Diamond Electrodes. *Analytical Letters*, **2005**, 38, 1587-1599	2.2	49
152	An AM1 study on the electron-donating and electron-accepting character of biomolecules. *International Journal of Quantum Chemistry*, **2003**, 95, 126-132	2.1	49
151	A structure-activity relationship study of quinone compounds with trypanocidal activity. *European Journal of Medicinal Chemistry*, **2005**, 40, 329-38	6.8	39
150	The origin of the molecular interaction between amino acids and gold nanoparticles: A theoretical and experimental investigation. *Chemical Physics Letters*, **2009**, 469, 186-190	2.5	38
149	Novel insights for dihydroorotate dehydrogenase class 1A inhibitors discovery. *European Journal of Medicinal Chemistry*, **2010**, 45, 5899-909	6.8	36
148	Use of Graphite Polyurethane Composite Electrode for Imipramine Oxidationâ€Mechanism Proposal and Electroanalytical Determination. *Analytical Letters*, **2006**, 39, 507-520	2.2	35
147	Propriedades quÃmico-quÃnticas empregadas em estudos das relaÃ§Ã£s estrutura-atividade. *Quimica Nova*, **2010**, 33, 694-699	1.6	31
146	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		31

145	The basic antioxidant structure for flavonoid derivatives. *Journal of Molecular Modeling*, **2012**, 18, 4073-80		30
144	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. *International Journal of Quantum Chemistry*, **2006**, 106, 2617-2623	2.1	30
143	A multivariate study on flavonoid compounds scavenging the peroxynitrite free radical. *Computational and Theoretical Chemistry*, **2007**, 808, 25-33		28
142	The asymmetric dimerization of nitrogen dioxide. *Chemical Physics Letters*, **2007**, 436, 47-50	2.5	28
141	Universal Gaussian basis set for relativistic calculations on atoms and molecules. *Chemical Physics Letters*, **1993**, 201, 37-40	2.5	27
140	Relativistic universal Gaussian basis set for DiracâHockâCoulomb and DiracâHockâBreit SCF calculations on heavy atoms. *Chemical Physics Letters*, **1993**, 203, 201-204	2.5	26
139	The nuclear electric quadrupole moment of antimony from the molecular method. *Journal of Chemical Physics*, **2006**, 125, 64301	3.9	25
138	Pharmacophore-based 3D QSAR studies on a series of high affinity 5-HT1A receptor ligands. *European Journal of Medicinal Chemistry*, **2010**, 45, 1508-14	6.8	24
137	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	2.1	24
136	The generator coordinate Hartree-Fock method for molecular systems. Formalism and first applications to H2, LiH and Li2. *Chemical Physics*, **1991**, 154, 379-384	2.3	24
135	Adsorption of sodium dodecyl sulfate on Ge substrate: the effect of a low-polarity solvent. *International Journal of Molecular Sciences*, **2012**, 13, 7980-93	6.3	22
134	Deactivation of triplet-excited riboflavin by purine derivatives: important role of uric acid in light-induced oxidation of milk sensitized by riboflavin. *Journal of Agricultural and Food Chemistry*, **2005**, 53, 3679-84	5.7	22
133	A structureâActivity relationship study of HEPT-analog compounds with anti-HIV activity. *Computational and Theoretical Chemistry*, **2000**, 530, 39-47		22
132	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. *Computational and Theoretical Chemistry*, **1999**, 491, 123-131		22
131	Density functional theory (DFT) study of edaravone derivatives as antioxidants. *International Journal of Molecular Sciences*, **2012**, 13, 7594-606	6.3	21
130	A partial least squares and principal component regression study of quinone compounds with trypanocidal activity. *Structural Chemistry*, **2007**, 18, 49-57	1.8	21
129	A multiple linear regression and partial least squares study of flavonoid compounds with anti-HIV activity. *Computational and Theoretical Chemistry*, **2001**, 541, 81-88		21
128	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	2.3	20

127	A polynomial version of the generator coordinate Dirac-Fock method. *Journal of Computational Chemistry*, **2004**, 25, 1904-9	3.5	20
126	A quantum chemical and statistical study of flavonoid compounds (flavones) with anti-HIV activity. *European Journal of Medicinal Chemistry*, **2003**, 38, 929-38	6.8	20
125	A study on the influence of molecular properties in the psychoactivity of cannabinoid compounds. *Journal of Molecular Modeling*, **2005**, 11, 200-9	2	19
124	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	2.1	19
123	Design and evaluation of 4-aminophenol and salicylate derivatives as free-radical scavenger. *Chemical Biology and Drug Design*, **2013**, 81, 414-9	2.9	18
122	The use of classification methods for modeling the antioxidant activity of flavonoid compounds. *Journal of Molecular Modeling*, **2006**, 12, 915-20	2	18
121	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		18
120	Generator coordinate method in time-dependent density-functional theory: memory made simple. *Journal of Chemical Physics*, **2007**, 127, 124101	3.9	17
119	A partial least squares regression study with antioxidant flavonoid compounds. *Structural Chemistry* , **2006**, 17, 307-313	1.8	17
118	A Structure-Activity Relationship (SAR) Study of Neolignan Compounds with Anti-schistosomiasis Activity. *Journal of the Brazilian Chemical Society*, **2002**, 13, 300-307	1.5	17
117	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, 932-40	3.5	17
116	Interaction between PH3 and small water clusters: Understanding the electronic and spectroscopic properties. *Computational and Theoretical Chemistry*, **2015**, 1059, 35-44	2	16
115	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	3.5	16
114	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, 1970-9	3.5	16
113	A chemometric study of the 5-HT(1A) receptor affinities presented by arylpiperazine compounds. *European Journal of Medicinal Chemistry*, **2008**, 43, 364-72	6.8	15
112	Theoretical study of dibenzotetraaza[14]annulene complexes with first row transition metals. *Computational and Theoretical Chemistry*, **2015**, 1054, 93-99	2	14
111	Relativistic Prolapse-Free Gaussian Basis Set of Quadruple-□Quality: (aug-)RPF-4Z. I. The s- and p-Block Elements. *Journal of Chemical Theory and Computation*, **2014**, 10, 3800-6	6.4	14
110	Evaluation and theoretical study on the anti-inflammatory mechanism of 1-nitro-2-phenylethane. *Planta Medica*, **2013**, 79, 628-33	3.1	14

109	Cationic dye dimers: a theoretical study. *Theoretical Chemistry Accounts*, **2007**, 118, 305-314	1.9	14
108	A quantum chemical and photophysical study of acridine-9-N-methacrylamide. *Computational and Theoretical Chemistry*, **2004**, 674, 213-225		14
107	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	2.4	14
106	Molecular properties of the PCO radical: heat of formation and the isomerization pathways. *Journal of Molecular Modeling*, **2014**, 20, 2074	2	13
105	Photophysical properties and quantum chemical studies of poly(2,7-9,9Ndihexylfluorene-dyil). *Journal of the Brazilian Chemical Society*, **2009**, 20, 160-166	1.5	13
104	A neural networks study of quinone compounds with trypanocidal activity. *Journal of Molecular Modeling*, **2008**, 14, 975-85	2	13
103	A theoretical study on the XeF2 molecule. *Chemical Physics*, **2008**, 348, 89-96	2.3	13
102	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, 1153-61		13
101	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, 3103-11	4.4	13
100	Theoretical calculations on dipyridamole structure allow to explain experimental properties associated to electrochemical oxidation and protonation. *Chemical Physics Letters*, **2001**, 349, 146-152	2.5	13
99	A theoretical study of the intramolecular hetero DielsâĂŞAlder cycloaddition reactions of azoalkenes. *Computational and Theoretical Chemistry*, **2001**, 535, 165-169		13
98	Microwave-Driven Hexagonal-to-Monoclinic Transition in BiPO: An In-Depth Experimental Investigation and First-Principles Study. *Inorganic Chemistry*, **2020**, 59, 7453-7468	5.1	12
97	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	1.5	12
96	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	1.7	12
95	Sugar moiety has a synergistic effect on hydroxylated xanthone for better antioxidant activity of mangiferin. *Medicinal Chemistry Research*, **2018**, 27, 1276-1282	2.2	11
94	Understanding the cytotoxicity or cytoprotective effects of biological and synthetic quinone derivatives by redox mechanism. *Journal of Molecular Modeling*, **2014**, 20, 2541	2	11
93	Artificial neural networks and the study of the psychoactivity of cannabinoid compounds. *Chemical Biology and Drug Design*, **2010**, 75, 632-40	2.9	11
92	Docking and molecular dynamics simulation of quinone compounds with trypanocidal activity. *Journal of Molecular Modeling*, **2009**, 15, 1175-84	2	11

91	Photoinduced electron-transfer processes based on novel bipyridine-Ru(II) complex: properties of cis-[Ru(2,2Ñbipyridine)2(5,6-bis(3-amidopyridine)-7-oxanorbornene)](PF6)2 and cis-[Ru(2,2Ñbipyridine)2(3-aminopyridine)2](PF6)2 complexes. *Inorganic Chemistry*, **2007**, 46, 5744-53	5.1	11
90	The nuclear electric quadrupole moment of lutetium from the molecular method. *Chemical Physics Letters*, **2007**, 445, 95-98	2.5	11
89	4-hydroxy-2,5-dimethylphenyl-benzophenone: conformational stability, FT-IR and Raman investigation. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 102, 386-92	4.4	10
88	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	2	10
87	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	4.1	10
86	A combined X-ray and theoretical study of flavonoid compounds with anti-inflammatory activity. *Computational and Theoretical Chemistry*, **2008**, 862, 16-20		10
85	The influence of electronic and steric effects in the structureâ□ctivity relationship (SAR) study of quinone compounds with biological activity against Trypanosoma cruzi. *Computational and Theoretical Chemistry*, **2003**, 634, 271-280		10
84	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	2.1	10
83	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	2.5	10
82	Generator coordinate gaussian expanded natural orbitals. *Computational and Theoretical Chemistry*, **1990**, 210, 63-70		10
81	Two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT(1A) receptor ligands. *Medicinal Chemistry*, **2008**, 4, 328-35	1.8	10
80	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	4.4	9
79	Electronic properties of the AsCO, AsSiO and AsGeO radicals: Linear or cyclic?. *Polyhedron*, **2015**, 89, 160-167	2.1	9
78	Identification of electronic and structural descriptors of adenosine analogues related to inhibition of leishmanial glyceraldehyde-3-phosphate dehydrogenase. *Molecules*, **2013**, 18, 5032-50	4.8	9
77	Crystal structure and theoretical calculations of Julocrotine, a natural product with antileishmanial activity. *International Journal of Quantum Chemistry*, **2008**, 108, 513-520	2.1	9
76	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	2.4	9
75	A quantum chemical study on the psychoactivity of cannabinoid compounds. *Computational and Theoretical Chemistry*, **2001**, 538, 99-106		9
74	THE H 2 + CO $leftrightarrow $ H 2 CO REACTION: RATE CONSTANTS AND RELEVANCE TO HOT AND DENSE ASTROPHYSICAL MEDIA. *Astrophysical Journal, Supplement Series*, **2016**, 225, 2	8	8

73	Quantum chemical DFT study of the interaction between molecular oxygen and FeNâ□complexes, and effect of the macrocyclic ligand. *Journal of Molecular Modeling*, **2014**, 20, 2131	2	8
72	Relativistic Prolapse-Free Gaussian Basis Set of Quadruple-□Quality: (aug-)RPF-4Z. II. The d-Block Elements. *Journal of Chemical Theory and Computation*, **2014**, 10, 4761-4	6.4	8
71	The CH3PH2 and CH3PH isomers: isomerization, hydrogen release, thermodynamic, and spectroscopy properties. *Journal of Molecular Modeling*, **2014**, 20, 2372	2	8
70	A combined experimental and theoretical approach for radical-scavenging activity of edaravone and its related derivatives. *Structural Chemistry*, **2013**, 24, 349-355	1.8	8
69	CO bonding in FeN4 complexes and the effect of the macrocycle ligand: A DFT study. *Polyhedron*, **2014**, 67, 36-43	2.7	8
68	Insights into the molecular requirements for the anti-obesity activity of a series of CB1 ligands. *Chemical Biology and Drug Design*, **2010**, 76, 320-9	2.9	8
67	Rate coefficient for the reaction SiO + Si2O2 at T = 10-1000 K. *Journal of Physical Chemistry A*, **2006**, 110, 13221-6	2.8	8
66	The employment of relativistic adapted Gaussian basis sets in DouglasâKrollâHess scalar calculations with diatomic molecules. *Chemical Physics*, **2006**, 331, 173-177	2.3	8
65	A theoretical study on the analgesic activity of cannabinoid compounds. *Computational and Theoretical Chemistry*, **2004**, 709, 223-229		8
64	Theoretical and conformational studies of a series of cannabinoids. *Journal of Molecular Structure*, **1995**, 356, 247-256	3.4	8
63	Electronic structures and electronic spectra of the linkage isomers NSOâ□and SNOâ□*Journal of Molecular Structure*, **1987**, 162, 351-357	3.4	8
62	Molecular orbital description of the polythiazyl polymer. *Computational and Theoretical Chemistry*, **1986**, 139, 327-332		8
61	An antioxidant mechanism of morphine and related derivatives. *Medicinal Chemistry Research*, **2016** , 25, 852-857	2.2	8
60	On the stability of the RuCl2(triphenylphosphine)2(amine) complexes: Ligand substituent effects of cyclic and acyclic amines. *Polyhedron*, **2014**, 81, 661-667	2.7	7
59	Accurate Calculations of Rate Constants for the Forward and Reverse H2O + CO <-> HCOOH Reactions. *ChemistrySelect*, **2017**, 2, 7267-7272	1.8	7
58	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	1.8	7
57	First- and second-row transition metal oxa-aza macrocyclic complexes: a DFT study of an octahedral conformation. *Journal of Molecular Modeling*, **2012**, 18, 3243-53	2	7
56	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	0.3	7

55	A chemometric study on the analgesic activity of cannabinoid compounds using SDA, KNN and SIMCA methods. *Structural Chemistry*, **2009**, 20, 577-585	1.8	7
54	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		7
53	A computational study for the antioxidant capacity increases in hydroxy-derivatives of paracetamol and salicylic acid. *Medicinal Chemistry Research*, **2015**, 24, 3453-3459	2.2	6
52	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	3.4	6
51	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	1.4	6
50	Contracted Gaussian bases for the first-row atoms applied to neutral and charged diatomic molecules. *Computational and Theoretical Chemistry*, **2001**, 539, 29-34		6
49	On the helium ground-state Hartree-Fock energy. *Chemical Physics Letters*, **1991**, 183, 31-33	2.5	6
48	A Structure and Antioxidant Activity Study of Paracetamol and Salicylic Acid. *Pharmacology & Pharmacy*, **2014**, 05, 1185-1191	0.3	6
47	Molecular features related to HIV integrase inhibition obtained from structure- and ligand-based approaches. *PLoS ONE*, **2014**, 9, e81301	3.7	5
46	The tautomerism influence on the antioxidant prediction of oxederavone. *Medicinal Chemistry Research*, **2013**, 22, 5617-5623	2.2	5
45	A density functional theory study on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. *Chemical Physics*, **2004**, 306, 35-41	2.3	5
44	A quantum chemical and statistical study of biflavonoid compounds with anti-HIV activity. *Computational and Theoretical Chemistry*, **2002**, 577, 187-195		5
43	Molecular features for antitrypanosomal activity of thiosemicarbazones revealed by OPS-PLS QSAR studies. *Medicinal Chemistry*, **2012**, 8, 1045-56	1.8	5
42	Relativistic Prolapse-Free Gaussian Basis Sets of Quadruple-Quality: (aug-)RPF-4Z. III. The f-Block Elements. *Journal of Chemical Theory and Computation*, **2017**, 13, 1094-1101	6.4	4
41	A molecular modeling study of combretastatin-like chalcones as anticancer agents using PLS, ANN and consensus models. *Structural Chemistry*, **2018**, 29, 957-965	1.8	4
40	Pattern recognition techniques applied to the study of leishmanial glyceraldehyde-3-phosphate dehydrogenase inhibition. *International Journal of Molecular Sciences*, **2014**, 15, 3186-203	6.3	4
39	A Theoretical Study of the Dapsone Derivatives on Methemoglobin. *Journal of Computational and Theoretical Nanoscience*, **2013**, 10, 2029-2033	0.3	4
38	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		4

37	Theoretical study on the stereochemistry of intramolecular hetero DielsâÅAlder cycloaddition reactions of azoalkenes. *International Journal of Quantum Chemistry*, **2003**, 95, 133-136	2.1	4
36	Accurate adapted Gaussian basis sets for helium- and beryllium-like atomic species to be used in DiracâFock calculations. *Computational and Theoretical Chemistry*, **1999**, 464, 1-6		4
35	Experimental and theoretical study on structure-tautomerism among edaravone, isoxazolone, and their heterocycles derivatives as antioxidants. *Saudi Pharmaceutical Journal*, **2020**, 28, 819-827	4.4	3
34	Structure and toxicity of clozapine and olanzapine on agranulocytosis. *Medicinal Chemistry Research* , **2016**, 25, 322-328	2.2	3
33	Excitation energies from ground-state density-functionals by means of generator coordinates. *Physical Chemistry Chemical Physics*, **2009**, 11, 4564-9	3.6	3
32	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	2.1	3
31	Influence of confining anisotropy on the unstable behavior of a Bose gas with attractive interaction. *Physical Review A*, **2004**, 70,	2.6	3
30	Quantum chemical and statistical study of megazol-derived compounds with trypanocidal activity. *International Journal of Quantum Chemistry*, **2005**, 103, 738-748	2.1	3
29	The 1,2-hydrogen shift reaction for monohalogenophosphanes PH2X and HPX (X = F, Cl). *Molecular Physics*, **2016**, 114, 2999-3014	1.7	3
28	Drug design of new 5-HT6 antagonists: a QSAR study of arylsulfonamide derivatives. *Structural Chemistry*, **2020**, 31, 1585-1597	1.8	2
27	A mechanistic study of the electrochemical behavior of pendimethalin herbicide. *Journal of Electroanalytical Chemistry*, **2018**, 826, 157-163	4.1	2
26	A Proposal for the Mechanism of the CH + CO Reaction. *ACS Omega*, **2019**, 4, 17843-17849	3.9	2
25	A combined study using ligand-based design, synthesis, and pharmacological evaluation of analogues of the acetaminophen ortho-regioisomer with potent analgesic activity. *Chemical Biology and Drug Design*, **2012**, 80, 99-105	2.9	2
24	New consensus multivariate models based on PLS and ANN studies of sigma-1 receptor antagonists. *Journal of Molecular Modeling*, **2017**, 23, 302	2	2
23	Structural and Electronic Properties of Dipyridamole and Derivatives. *Journal of Computational and Theoretical Nanoscience*, **2011**, 8, 69-73	0.3	2
22	A prï¿½tica docente na formaï¿½ do pï¿½-graduando em quï¿½mica. *Quimica Nova*, **2008**, 31, 1888-1891	1.6	2
21	Relativistic Gaussian basis sets obtained with a polynomial version of the generator coordinate DiracâFock method: Ionization energies of some closed-shell atomic systems. *International Journal of Quantum Chemistry*, **2005**, 103, 529-536	2.1	2
20	N-Acetyl-cysteine Increases Chemical Stability of Hydroquinone in Pharmaceutical Formulations: a Theoretical and Experimental Approach. *Journal of the Brazilian Chemical Society*,	1.5	2

19	Vibrational spectroscopy, intramolecular CH?O interaction and conformational analysis of 2,5-dimethyl-benzyl benzoate. *Journal of Molecular Structure*, **2016**, 1125, 649-655	3.4	2
18	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	3.4	2
17	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	2	1
16	Theoretical models for the antitrypanosomal activity of thiosemicarbazone derivatives. *International Journal of Quantum Chemistry*, **2012**, 112, 3364-3370	2.1	1
15	Molecular Features for Antitrypanosomal Activity of Thiosemicarbazones Revealed by OPS-PLS QSAR Studies. *Medicinal Chemistry*, **2012**, 8, 1045-1056	1.8	1
14	A correlation between geometric features and analgesic activity for a series of cannabinoid compounds. *Journal of Molecular Structure*, **1998**, 441, 97-100	3.4	1
13	A chemometric study of megazol derivatives with activity against Trypanosoma equiperdum. *SAR and QSAR in Environmental Research*, **2006**, 17, 533-47	3.5	1
12	Highly accurate relativistic universal Gaussian basis set for DiracâHockâBreit calculations. *International Journal of Quantum Chemistry*, **2005**, 102, 1-7	2.1	1
11	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	2.1	1
10	On polarization functions for Gaussian basis sets. *Journal of Molecular Modeling*, **2020**, 26, 293	2	1
9	Drug design of new 5-HTR antagonists aided by artificial neural networks. *Journal of Molecular Graphics and Modelling*, **2021**, 104, 107844	2.8	1
8	A partial least squares and artificial neural network study for a series of arylpiperazines as antidepressant agents. *Journal of Molecular Modeling*, **2021**, 27, 297	2	1
7	New D2R partial agonist candidates: an in silico approach from statistical models, molecular docking, and ADME/Tox properties. *Structural Chemistry*, **2021**, 32, 2019-2033	1.8	0
6	Accurate atomic electron affinities calculated by using anionic Gaussian basis sets. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	
5	The effect of the negative coupling parameter on the spectrum of a trapped Bose gas. *Journal of Mathematical Chemistry*, **2010**, 47, 636-646	2.1	
4	One-dimensional trapped atoms: critical coupling parameter and critical number of particles. *Journal of Mathematical Chemistry*, **2010**, 48, 687-696	2.1	
3	The Generator Coordinate DiracâHock Method and Relativistic Calculations for Atoms and Molecules **2007**, 79-150		
2	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	3.6	

List of Publications

1 A mechanistic view of the reaction between phosphine and fluorine atom: insights into PH3F isomers. *Computational and Theoretical Chemistry*, **2022**, 113769 2