Jose Carneiro

List of Publications by Year
in descending order

157 papers	2,740 citations	236925 25 h-index	243625 44 g-index
159 all docs	159 docs citations	159 times ranked	3195 citing authors

#	Article	IF	Citations
1	Transesterification of Jatropha curcas oil glycerides: Theoretical and experimental studies of biodiesel reaction. Fuel, 2008, 87, 2286-2295.	6.4	186
2	Unified Mechanistic Concept of Electrophilic Aromatic Nitration:â€‰ Convergence of Computational Results and Experimental Data. Journal of the American Chemical Society, 2003, 125, 4836-4849.	13.7	142
3	The tert-butyl cation (C4H9+) potential energy surface. Journal of the American Chemical Society, 1993, 115, 259-270.	13.7	126
4	Density Functional Theory Investigation of the Contributions of Ï€â€“Ï€ Stacking and Hydrogen-Bonding Interactions to the Aggregation of Model Asphaltene Compounds. Energy & Fuels, 2012, 26, 2727-2735.	5.1	113
5	Adsorption of CO₂ on amine-functionalised MCM-41: experimental and theoretical studies. Physical Chemistry Chemical Physics, 2015, 17, 11095-11102.	2.8	93
6	Electrophilic Aromatic Nitration:Â Understanding Its Mechanism and Substituent Effectsâ€. Journal of Organic Chemistry, 2006, 71, 6192-6203.	3.2	81
7	Protonated Ethane. A Theoretical Investigation of C2H7+ Structures and Energies. Journal of the American Chemical Society, 1994, 116, 3483-3493.	13.7	76
8	Quantitative structureâ€“activity relationship in aziridinyl-1,4-naphthoquinone antimalarials: study of theoretical correlations by the PM3 method. Bioorganic and Medicinal Chemistry, 2004, 12, 87-93.	3.0	64
9	Does CHâ€‰5+ prefer a C2vrather than a Csstructure?. Journal of Computational Chemistry, 1992, 13, 997-1003.	3.3	59
10	Axial and Equatorial 1-Methyl-1-cyclohexyl Cation Isomers Both Have Chair Conformations but Differ in Cî”C and Cî”H Hyperconjugation Modes. Journal of the American Chemical Society, 1996, 118, 3761-3762.	13.7	59
11	Distortion toward bridging accompanying hyperconjugation in a simple tertiary alkyl carbocation. Journal of the American Chemical Society, 1991, 113, 3990-3992.	13.7	55
12	Exploring the DNA binding/cleavage, cellular accumulation and topoisomerase inhibition of 2-hydroxy-3-(aminomethyl)-1,4-naphthoquinone Mannich bases and their platinum(II) complexes. Journal of Inorganic Biochemistry, 2013, 119, 54-64.	3.5	55
13	Computational Study of the Effect of Dispersion Interactions on the Thermochemistry of Aggregation of Fused Polycyclic Aromatic Hydrocarbons as Model Asphaltene Compounds in Solution. Journal of Physical Chemistry A, 2014, 118, 896-908.	2.5	47
14	Hyperconjugative distortions and the cyclopentyl cation structure. Journal of the American Chemical Society, 1989, 111, 5475-5477.	13.7	46
15	Structural characterisation of natural products by means of quantum chemical calculations of NMR parameters: new insights. Organic Chemistry Frontiers, 2021, 8, 2019-2058.	4.5	45
16	Synthesis of Photosynthesis-Inhibiting Nostoclide Analogues. Journal of Agricultural and Food Chemistry, 2008, 56, 2321-2329.	5.2	41
17	3D-RISM-KH molecular theory of solvation and density functional theory investigation of the role of water in the aggregation of model asphaltenes. Physical Chemistry Chemical Physics, 2012, 14, 3922.	2.8	41
18	Semisynthetic Phenol Derivatives Obtained from Natural Phenols: Antimicrobial Activity and Molecular Properties. Journal of Agricultural and Food Chemistry, 2018, 66, 323-330.	5.2	37

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19	Density Functional Theory Study of Benzene Adsorption on Small Pd and Pt Clusters. Journal of Physical Chemistry C, 2007, 111, 11068-11076.	3.1	35
20	Structure of the 2-butyl cation. Hydrogen bridged or methyl bridged?. Journal of the American Chemical Society, 1990, 112, 4064-4066.	13.7	33
21	Synthesis of Rubrolide Analogues as New Inhibitors of the Photosynthetic Electron Transport Chain. Journal of Agricultural and Food Chemistry, 2012, 60, 10555-10563.	5.2	31
22	Density Functional Theory Study of the Adsorption of Formaldehyde on Pd₄ and on Pd₄/Î³-Al₂O₃ Clusters. Journal of Physical Chemistry A, 2008, 112, 8929-8937.	2.5	29
23	Insights into the interactions of CO₂ with amines: a DFT benchmark study. Physical Chemistry Chemical Physics, 2014, 16, 17213-17219.	2.8	29
24	Xanthenones: calixarenes-catalyzed syntheses, anticancer activity and QSAR studies. Organic and Biomolecular Chemistry, 2015, 13, 3280-3287.	2.8	29
25	Interaction between artemisinin and heme. A Density Functional Theory study of structures and interaction energies. Bioorganic and Medicinal Chemistry, 2008, 16, 5021-5029.	3.0	28
26	Ï*f*-Homoacenaphthylene andÏ€-Homoacenaphthene. Angewandte Chemie International Edition in English, 1991, 30, 683-686.	4.4	25
27	New copper(II)-radical one dimensional chain: Synthesis, crystal structure, EPR, magnetic properties and DFT calculations. Dalton Transactions, 2009, , 6816.	3.3	25
28	A New Method to Prepare 3-Alkyl-2-hydroxy-1,4-naphthoquinones: [nl]Synthesis of Lapachol and Phthiocol. Synlett, 2011, 2011, 1551-1554.	1.8	24
29	Adsorption of the herbicides diquat and difenzoquat on polyurethane foam: Kinetic, equilibrium and computational studies. Ecotoxicology and Environmental Safety, 2017, 145, 597-604.	6.0	24
30	Confirmation of the H-bridged structure of the 2-butyl cation by comparison of experimental and ab initio IR frequencies. Journal of the Chemical Society Chemical Communications, 1991, , 671-674.	2.0	23
31	DFT study of the reductive decomposition of artemisinin. Bioorganic and Medicinal Chemistry, 2006, 14, 1546-1557.	3.0	23
32	Modeling, kinetic, and equilibrium characterization of paraquat adsorption onto polyurethane foam using the ion-pairing technique. Journal of Environmental Management, 2015, 156, 200-208.	7.8	23
33	General method for the high yield preparation of 2-(4-X-phenylene)amine-1,4-naphthoquinones (X=ferrocenyl, OMe, Me, I, Cl, and NO2) from 2-methoxy-1,4-naphthoquinone and investigation of H+ and Mg2+ catalysts with DFT calculations. Journal of Molecular Structure, 2008, 891, 228-232.	3.6	22
34	Theoretical studies of the tautomerism in 3-(2-R-Phenylhydrazono)-naphthalene- 1,2,4-triones: synthesis of copper(II) complexes and studies of antibacterial and antitumor activities. Journal of the Brazilian Chemical Society, 2010, 21, 1293-1302.	0.6	22
35	Synthesis, structure-activity relationship and evaluation of new non-polymeric chemical additives based on naphthoquinone derivatives as wax precipitation inhibitors and pour point depressants to petroleum. Fuel, 2018, 220, 200-209.	6.4	21
36	Is tetrahedral H42+ a minimum? Anomalous behavior of popular basis sets with the standardp exponents on hydrogen. Journal of Computational Chemistry, 1993, 14, 285-294.	3.3	20

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37	Hostâ€“guest interactions and their role in enantioselective hydrogenation of Î±-keto esters. Journal of Molecular Catalysis A, 2001, 170, 235-243.	4.8	20
38	Synthesis, structure, electronic and magnetic properties of two new complexes obtained by coordination of Co(II) and Mn(II) phenyltrifluoroacetylacetonate with a nitronyl nitroxide radical. Inorganica Chimica Acta, 2008, 361, 4024-4030.	2.4	20
39	MNDO/d calculations on the interaction between artemisinin and heme. Computational and Theoretical Chemistry, 2001, 539, 267-272.	1.5	19
40	The role of C-centered radicals on the mechanism of action of artemisinin. Computational and Theoretical Chemistry, 2002, 580, 207-215.	1.5	19
41	Theoretical study on the adsorption of aromatic compounds on platinum clusters. International Journal of Quantum Chemistry, 2003, 92, 400-411.	2.0	18
42	Synthesis, electrochemical studies and anticancer activity of ferrocenyl oxindoles. Dalton Transactions, 2010, 39, 7338.	3.3	18
43	CO2 and H2 adsorption on 3D nitrogen-doped porous graphene: Experimental and theoretical studies. Journal of CO2 Utilization, 2021, 48, 101517.	6.8	18
44	Relative stability of radicals derived from artemisinin: A semiempirical and DFT study. International Journal of Quantum Chemistry, 2005, 103, 749-762.	2.0	17
45	DFT study of Li+ and Na+ positions in mordenites and hydration stability. Computational and Theoretical Chemistry, 2016, 1091, 115-121.	2.5	17
46	The effect of 2-exo and endo substituents on the geometry of norbornane. Computational and Theoretical Chemistry, 1987, 152, 281-291.	1.5	16
47	Density Functional Theory studies on interactions of phosphoryl ligands with the Ca2+ cation: Affinity and associated parameters. Computational and Theoretical Chemistry, 2009, 911, 46-51.	1.5	16
48	Interaction between alkaline earth cations and oxo-ligands. DFT study of the affinity of the Ca2+ cation for carbonyl ligands. Journal of Molecular Modeling, 2011, 17, 243-249.	1.8	16
49	Voltammetric and Theoretical Study of the Redox Properties of Rubrolide Analogues. Electrochimica Acta, 2014, 120, 334-343.	5.2	16
50	Combined theoretical and experimental studies on CO2 capture by amine-activated glycerol. Chemical Engineering Journal, 2021, 408, 128002.	12.7	16
51	Conformational effects on NMR chemical shifts of half-cage alcohols calculated by GIAO-DFT. Computational and Theoretical Chemistry, 2002, 579, 101-107.	1.5	15
52	Donorâ€“acceptor interactions in the enantioselective hydrogenation of Î±-ketoesters. Journal of Molecular Catalysis A, 2005, 226, 221-226.	4.8	15
53	Aminequinone-hydroxylquinoneimine tautomeric equilibrium revisited: molecular modeling study of the tautomeric equilibrium and substituent effects in 4-(4-R-phenylamino)naphthalene-1,2-diones. Journal of Molecular Modeling, 2010, 16, 825-830.	1.8	15
54	1,3-Butadiene hydrogenation on pd-supported systems: geometric effects. Brazilian Journal of Chemical Engineering, 2002, 19, 187-194.	1.3	14

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55	SYNTHESIS AND ANTIVIRAL ACTIVITY OF NEW 4- (PHENYLAMINO)THIENO[2,3-b]PYRIDINE DERIVATIVES. Heterocyclic Communications, 2004, 10, .	1.2	14
56	QSAR modeling of photosynthesisâ€inhibiting nostoclide derivatives. Pest Management Science, 2010, 66, 196-202.	3.4	14
57	Synthesis, characterization and catalytic activity of two novel cis-dioxovanadium(v) complexes: [VO2(L)] and [VO2(Hlox)]. Journal of the Brazilian Chemical Society, 2011, 22, 660-668.	0.6	14
58	Ab initio charge distributions in half-cage compounds. Computational and Theoretical Chemistry, 1990, 204, 183-192.	1.5	13
59	Experimental and theoretical studies on glucose hydrogenation to produce sorbitol. Reaction Kinetics and Catalysis Letters, 2007, 91, 341-352.	0.6	13
60	Interactions between alkaline earth cations and oxo ligands. DFT study of the affinity of the Mg2+ cation for phosphoryl ligands. Journal of Molecular Modeling, 2011, 17, 2061-2067.	1.8	13
61	Insight into and Computational Studies of the Selective Synthesis of 6H-Dibenzo[b,h]xanthenes. Journal of Organic Chemistry, 2016, 81, 5525-5537.	3.2	13
62	Modeling the Adsorption of CO on Small Pt, Fe and Co Clusters for the Fischerâ€“Tropsch Synthesis. Journal of Cluster Science, 2008, 19, 601-614.	3.3	12
63	Novel 2-(R-phenyl)amino-3-(2-methylpropenyl)-[1,4]-naphthoquinones: synthesis, characterization, electrochemical behavior and antitumor activity. Journal of the Brazilian Chemical Society, 2010, 21, 169-178.	0.6	12
64	A quantum chemical and chemometric study of sesquiterpene lactones with cytotoxicity against tumor cells. Journal of Chemometrics, 2011, 25, 401-407.	1.3	12
65	Mononuclear and dinuclear iron(III) compounds with Î²-diketonate ligands: Synthesis, magnetic behavior and DFT calculations. Solid State Sciences, 2013, 18, 10-16.	3.2	12
66	Adsorption of Bitumen Model Compounds on Kaolinite in Liquid and Supercritical Carbon Dioxide Solvents: A Study by Periodic Density Functional Theory and Molecular Theory of Solvation. Energy & Fuels, 2015, 29, 2853-2863.	5.1	12
67	A New, Simple and Efficient Method of Steglich Esterification of Juglone with Long-Chain Fatty Acids: Synthesis of a New Class of Non-Polymeric Wax Deposition Inhibitors for Crude Oil. Journal of the Brazilian Chemical Society, 2014, , .	0.6	11
68	Mechanism of the Catalytic Carboxylation of Alkylboronates with CO₂ Using Niâ^'NHC Complexes: A DFT Study. Chemistry - A European Journal, 2017, 23, 14954-14961.	3.3	11
69	Stereo-electronic effects on carbon-13 and hydrogen chemical shifts of bicyclic alcohols. Computational and Theoretical Chemistry, 2001, 539, 163-169.	1.5	10
70	Steric and electronic contributions to conformational effects on chemical shifts of acyclic alcohols. Computational and Theoretical Chemistry, 2002, 580, 75-83.	1.5	10
71	A general approach for the synthesis of 5-substituted-4-amino-pyrrolidin-2-ones and 5-substituted-4-amino-3-pyrrolin-2-ones. Tetrahedron Letters, 2009, 50, 2402-2404.	1.4	10
72	Solvent assisted decomposition of the tetrahedral intermediate of the transesterification reaction to biodiesel production. A density functional study. Fuel, 2010, 89, 685-690.	6.4	10

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73	The effect of the molecular structures of dicyanomethylene compounds on their supramolecular assembly, photophysical and electrochemical properties. Physical Chemistry Chemical Physics, 2013, 15, 13013.	2.8	10
74	Computational study of the interaction between the [Pb(H2O)3]2+ cation and ligands containing oxygen, nitrogen and sulfur donor atoms. Polyhedron, 2015, 102, 193-200.	2.2	10
75	DFT study of ethanol dehydration catalysed by hematite. RSC Advances, 2016, 6, 40408-40417.	3.6	10
76	Conformational effects on properties of half-cage compounds. Computational and Theoretical Chemistry, 1999, 488, 151-156.	1.5	9
77	Hyperconjugation effects of hydroxyl and amine groups on chemical shifts of neighboring carbon nuclei. International Journal of Quantum Chemistry, 2003, 95, 322-328.	2.0	9
78	Solvent effects on the relative stability of radicals derived from artemisinin: DFT study using the PCM/COSMO approach. International Journal of Quantum Chemistry, 2006, 106, 2804-2810.	2.0	9
79	Interaction between alkaline earth cations and oxo ligands: a DFT study of the affinity of Mg2+ for carbonyl ligands. Journal of Molecular Modeling, 2012, 18, 4389-4396.	1.8	9
80	Density functional theory investigation of the binding interactions between phosphoryl, carbonyl, imino, and thiocarbonyl ligands and the pentaaqua nickel(II) complex: Coordination affinity and associated parameters. International Journal of Quantum Chemistry, 2013, 113, 2621-2628.	2.0	9
81	Experimental and DFT evaluation of the 1H and 13C NMR chemical shifts for calix[4]arenes. Journal of Molecular Structure, 2018, 1157, 97-105.	3.6	9
82	Unraveling the helianane family: a complementary quantum mechanical study. New Journal of Chemistry, 2020, 44, 8055-8060.	2.8	9
83	Hyperconjugation and charge distribution in alicyclic alcohols and exo- and endo-norbornol. Computational and Theoretical Chemistry, 1994, 306, 101-113.	1.5	8
84	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.	1.8	8
85	DFT studies of imino and thiocarbonyl ligands with the pentaaqua Mg2+ cation: affinity and associated parameters. Journal of Molecular Modeling, 2013, 19, 2669-2677.	1.8	8
86	Dynamic behaviour of carbocations on zeolites: mobility and rearrangement of the C4H7+ system. Chemical Communications, 2013, 49, 4480.	4.1	8
87	DFT studies of the interactions between the [Ca(H 2 O) 5] 2+ cation and monofunctional oxo, aza, sulfur and phosphorous ligands. Computational and Theoretical Chemistry, 2016, 1075, 104-110.	2.5	8
88	Synthesis, characterization, and thermal and computational investigations of the l-histidine bis(fluoride) crystal. Journal of Molecular Modeling, 2022, 28, .	1.8	8
89	Ab initio and density functional study of the 5-pentacyclo[6.2.1.13,6.02,7.04,10]dodecyl cation. A symmetrical Î¼-hydride bridged carbocation. Chemical Physics Letters, 2001, 345, 189-194.	2.6	7
90	Through space hyperconjugation in half-cage alcohols. Computational and Theoretical Chemistry, 2004, 677, 51-54.	1.5	7

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91	Synthesis, structural characterization and conformational aspects of nostoclide analogues. Journal of Molecular Structure, 2009, 917, 1-9.	3.6	7
92	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.	2.0	7
93	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
94	Tautomerism in Quinoxalines Derived from the 1,4-Naphthoquinone Nucleus: Acid Mediated Synthesis, X-ray Molecular Structure of 5-Chlorobenzo[f]quinoxalin-6-ol and Density Functional Theory Calculations. Journal of the Brazilian Chemical Society, 2013, 24, 219-229.	0.6	7
95	Natural polyprenylated benzophenone: keto-enol tautomerism from density functional calculations and the AIM theory. Journal of Molecular Modeling, 2017, 23, 140.	1.8	7
96	Single step mechanism for nucleophilic substitution of 2,3-dichloro naphthoquinone using nitrogen, oxygen and sulfur nucleophiles: A DFT approach. Tetrahedron, 2017, 73, 4363-4370.	1.9	7
97	Formation of Dimethyl Carbonate from CO₂ and Methanol Catalyzed by Me₂SnO: A Density Functional Theory Approach. Journal of Physical Chemistry A, 2021, 125, 2413-2424.	2.5	7
98	A semiempirical study of the conformational behavior of cinchonidine and its interaction with methyl pyruvate. Brazilian Journal of Chemical Engineering, 2001, 18, 287-298.	1.3	7
99	Ab initio charge distribution in tetracyclic norbornyl derivatives. Chemical Physics Letters, 1990, 175, 182-186.	2.6	6
100	The interaction between amines and methyl pyruvate involving protonated species. Catalysis Today, 2005, 107-108, 31-39.	4.4	6
101	Vibrational spectroscopy of lapachol, Î±- and Î²-lapachone: Theoretical and experimental elucidation of the Raman and infrared spectra. Vibrational Spectroscopy, 2016, 86, 311-323.	2.2	6
102	Î±â€•and Î²â€Łapachone Isomerization in Acidic Media: Insights from Experimental and Implicit/Explicit Solvation Approaches. ChemPlusChem, 2019, 84, 52-61.	2.8	6
103	The mechanism for H2S scavenging by 1,3,5-hexahydrotriazines explored by DFT. Tetrahedron, 2020, 76, 131112.	1.9	6
104	The effects of lone pairs on charge distribution in the tetracyclic norbornyl derivatives. Chemical Physics Letters, 1993, 202, 278-283.	2.6	5
105	Ab initio studies of hyperconjugation effects on charge distribution in tetracyclododecane alcohols. Chemical Physics Letters, 1995, 237, 33-38.	2.6	5
106	Ab initio study of hyperconjugation effects on charge distribution in representative polycyclic alcohols. Chemical Physics Letters, 1996, 248, 158-164.	2.6	5
107	Supramolecular assembly of (Z)-ethyl 2-cyano-3-((4-fluorophenyl)amino) acrylate, crystal structure, Hirshfeld surface analysis and DFT studies. Journal of Molecular Structure, 2016, 1120, 333-340.	3.6	5
108	Regioâ€•and Stereoselectivity in 1,3â€Đipolar Cycloadditions: Activation Strain Analyses for Reactions of Hydrazoic Acid with Substituted Alkenes. European Journal of Organic Chemistry, 2017, 2017, 4313-4318.	2.4	5

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109	A DFT study of the interaction between [Cd(H2O)3]2+ and monodentate O-, N-, and S-donor ligands: bond interaction analysis. Journal of Molecular Modeling, 2018, 24, 39.	1.8	5
110	DFT analysis of the interaction between Hg2+ and monodentate neutral ligands using NBO, EDA, and QTAIM. Journal of Molecular Modeling, 2020, 26, 146.	1.8	5
111	Molecular properties of cationic antitrypanosomal drugs: a Principal Component Analysis study of 2-phenylimidazo[1,2-a]pyridinium salts. Computational and Theoretical Chemistry, 1995, 335, 255-266.	1.5	4
112	NitraÃ§Ã£o aromÃ¡tica: substituiÃ§Ã£o eletrofÃlica ou reaÃ§Ã£o com transferÃªncia de elÃ©trons?. Quimica Nova, 2001, 24, 381-389.	0.3	4
113	17O NMR investigation of rigid polycyclic systems: experimental and calculated chemical shifts. Journal of Molecular Structure, 2004, 702, 71-76.	3.6	4
114	Conformational and vibrational study of di-n-propyl and di-i-propylphosphonates by MM/QM method. International Journal of Quantum Chemistry, 2005, 103, 763-774.	2.0	4
115	Interpretation of Conformational Effects on 2-endo-Norborneol by Natural Chemical Shielding Analysis. Journal of Physical Chemistry A, 2005, 109, 802-806.	2.5	4
116	DFT studies of structure and vibrational frequencies of isotopically substituted diamin uranyl nitrate using relativistic effective core potentials. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1140-1145.	3.9	4
117	Dimethyl sulfoxide oxidation mediated by a copper(II) diamine complex: A possible source of problem in the synthesis of molecular magnetic compounds. Polyhedron, 2009, 28, 2026-2028.	2.2	4
118	Analysis of anisotropic effects in trinuclear metal carbonyl compounds by visualization of through-space NMR shielding. Journal of Molecular Modeling, 2010, 16, 1415-1420.	1.8	4
119	Ab Initio, DFT and semi-empirical studies on interactions of phosphoryl, carbonyl, imino and thiocarbonyl ligands with the li+ cation: affinity and associated parameters. Journal of the Brazilian Chemical Society, 2012, , .	0.6	4
120	Spectroscopic and dynamic NMR study, X-ray crystallography and DFT calculations of two phosphoramidates: (C4H3O2)P(O)(Cl)C6H14N and (C4H3O2)P(O)(C6H11NH)2. Journal of Molecular Structure, 2013, 1046, 64-73.	3.6	4
121	A density functional theory investigation of the interaction of the tetraaqua calcium cation with bidentate carbonyl ligands. Journal of Molecular Modeling, 2017, 23, 60.	1.8	4
122	Computational and Experimental Investigations of the Role of Water and Alcohols in the Desorption of Heterocyclic Aromatic Compounds from Kaolinite in Toluene. Journal of Physical Chemistry C, 2018, 122, 10377-10391.	3.1	4
123	MP2 versus density functional theory calculations in CO 2 â€sequestration reactions with anions: Basis set extrapolation and solvent effects. International Journal of Quantum Chemistry, 2021, 121, e26583.	2.0	4
124	2,5-Diketopiperazines via Intramolecular N-Alkylation of Ugi Adducts: A Contribution to the Synthesis, Density Functional Theory Study, X-ray Characterization, and Potential Herbicide Application. Journal of Agricultural and Food Chemistry, 2022, 70, 1799-1809.	5.2	4
125	Conformational characterization of a camphor-based chiral Î³-amino alcohol. Journal of Molecular Structure, 2007, 827, 121-125.	3.6	3
126	Docking between natural peroxides and heme group by parametric method 6. International Journal of Quantum Chemistry, 2012, 112, 3390-3397.	2.0	3

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127	Evaluation of some density functional methods for the estimation of hydrogen and carbon chemical shifts of phosphoramidates. Computational and Theoretical Chemistry, 2016, 1090, 218-224.	2.5	3
128	Reactivity and regioselectivity in reactions of methyl and ethyl azides with cyclooctynes: activation strain model and energy decomposition analysis. Journal of Molecular Modeling, 2017, 23, 14.	1.8	3
129	Effect of the Metalâ€“Support Interaction on the Adsorption of NO on Pd₄/Î³-Al₂O₃: A Density Functional Theory and Natural Bond Orbital Study. Journal of Physical Chemistry C, 2017, 121, 14147-14155.	3.1	3
130	Study on the regioselectivity of the N-ethylation reaction of N-benzyl-4-oxo-1,4-dihydroquinoline-3-carboxamide. Beilstein Journal of Organic Chemistry, 2019, 15, 388-400.	2.2	3
131	Dielectric behavior of water in [bmim] [$$hbox {Tf}_2$$N] room-temperature ionic liquid: molecular dynamic study. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	3
132	A DFT study on the mechanism for polymerization of Î´-valerolactone initiated by N-heterocyclic carbene (NHC) catalysts. Molecular Catalysis, 2021, 515, 111896.	2.0	3
133	Semi-empirical study of cycloaddition reactions to form Î²-lactams from 2-amino-Î²-D-arabine[1â€²,2â€²:4,5]oxazoline (ureid) and ketenes. Computational and Theoretical Chemistry, 1997, 394, 281-289.	1.5	2
134	Conformational and vibrational study of di-n-butyl and di-sec-butylphosphonates by MM/QM method. International Journal of Quantum Chemistry, 2006, 106, 2633-2642.	2.0	2
135	Density Functional Theory studies on interactions of phosphoryl ligands with a pentaaqua Ca2+ complex: Bond interaction analysis. Computational and Theoretical Chemistry, 2012, 999, 7-12.	2.5	2
136	Structural characterization of unusually stable polycyclic ozonides. Journal of Molecular Structure, 2015, 1082, 151-161.	3.6	2
137	The Effect of Gamma-Al2O3Support on the NO Adsorption on Pd4Cluster. Journal of the Brazilian Chemical Society, 2016, , .	0.6	2
138	Diradical-singlet character of 1,3-dipoles affects reactivity of 1,3-dipolar cycloaddition reactions and intramolecular cyclization. Journal of Molecular Modeling, 2019, 25, 306.	1.8	2
139	Hetero-Dielsâ€“Alder Reactions of Quinone Methides: The Origin of the Î±-Regioselectivity of 3-Methylene-1,2,4-naphthotriones. Journal of Organic Chemistry, 2020, 85, 7001-7013.	3.2	2
140	Study of the Chemical Structures of Helianuois G and H by Theoretical Calculations of 1H NMR Chemical Shifts. Revista Virtual De Quimica, 2021, 13, 1140-1146.	0.4	2
141	Absolute Configuration of (â^')-Cubebin, a Classical Lignan with Pharmacological Potential, Defined by Means of Chiroptical Spectroscopy. Journal of the Brazilian Chemical Society, 0, , .	0.6	2
142	Revisiting the structure of Heliannuol L: A computational approach. Magnetic Resonance in Chemistry, 2022, 60, 434-441.	1.9	2
143	Bioactivity and molecular properties of Phenoxyacetic Acids Derived from Eugenol and Guaiacol compared to the herbicide 2,4-D. Anais Da Academia Brasileira De Ciencias, 2021, 93, e20191368.	0.8	2
144	Supramolecular dimers drive the reaction between CO2 and alkanolamines towards carbonate formation. Journal of CO2 Utilization, 2022, 61, 102054.	6.8	2

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145	Fragmentation studies of tetrahydropyridocarbazole derivatives by EI, ESI-MS/MS and FAB. Spectroscopy, 2001, 15, 19-25.	0.8	1
146	Search for new antimalarial compounds obtained from natural sources by molecular modeling. International Journal of Quantum Chemistry, 2010, 110, 2057-2066.	2.0	1
147	Density Functional Theory as a tool to identify the dominant magnetic interactions in the [Cu(hfac)2(N3TEMPO)]n chain. Inorganic Chemistry Communication, 2012, 24, 67-69.	3.9	1
148	The structure of dichlorotris(triphenylphosphine)ruthenium(II): a DFT study of interaction energies and substitution mechanism. Molecular Simulation, 0, , 1-8.	2.0	1
149	Acid-Catalyzed Z-E Isomerization of Î³-Alkylidenebutenolides: An Experimental and DFT Study. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
150	Tautomerism in quinoxalines derived from the 1,4-naphthoquinone nucleus: acid mediated synthesis, X-ray molecular structure of 5-chlorobenzo[f]quinoxalin-6-ol and density functional theory calculations. Journal of the Brazilian Chemical Society, 2013, 24, 219-229.	0.6	1
151	Carbon-carbon and carbon-hydrogen hyperconjugation in neutral alcohols. Computational and Theoretical Chemistry, 1996, 388, 85-95.	1.5	1
152	TOP - um programa de cÃ¡lculo de descritores topolÃ³gicos para uso em correlaÃ§Ãµes entre estrutura e atividade. Quimica Nova, 1998, 21, 709-713.	0.3	0
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