Rosivaldo Borges

List of Publications by Year
in descending order

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93 papers	1,216 citations	430874 18 h-index	434195 31 g-index
94 all docs	94 docs citations	94 times ranked	1541 citing authors

#	Article	IF	Citations
1	Essential features for antioxidant capacity of ascorbic acid (vitamin C). Journal of Molecular Modeling, 2022, 28, 1.	1.8	45
2	Euterpe oleracea fruit (AÃ§ai)-enriched diet suppresses the development of experimental cerebral malaria induced by Plasmodium berghei (ANKA) infection. BMC Complementary Medicine and Therapies, 2022, 22, 11.	2.7	4
3	Identification of Potential Antiviral Inhibitors from Hydroxychloroquine and 1,2,4,5-Tetraoxanes Analogues and Investigation of the Mechanism of Action in SARS-CoV-2. International Journal of Molecular Sciences, 2022, 23, 1781.	4.1	11
4	Molecular modeling approaches of selective adenosine receptor type 2A agonists as potential anti-inflammatory drugs. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1-13.	3.5	30
5	An asymmetric performance between mangiferin and isomangiferin as antioxidants. Chemical Data Collections, 2021, 31, 100602.	2.3	1
6	A comparative theoretical mechanism on simplified flavonoid derivatives and isoxazolone analogous as Michael system inhibitor. Journal of Molecular Modeling, 2021, 27, 26.	1.8	3
7	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. Molecular Simulation, 2021, 47, 762-770.	2.0	2
8	Revisiting the Proposition of Binding Pockets and Bioactive Poses for GSK-3Î² Allosteric Modulators Addressed to Neurodegenerative Diseases. International Journal of Molecular Sciences, 2021, 22, 8252.	4.1	9
9	Molecular modifications on Î²-nitro-styrene derivatives increase their antioxidant capacities. Journal of Molecular Structure, 2021, 1243, 130853.	3.6	1
10	Hormones Nanofiltration in Carbon Nanotubes and Boron Nitride Nanotubes Using Uniform External Electric Field Through Molecular Dynamics. Journal of Nanoscience and Nanotechnology, 2021, 21, 5499-5509.	0.9	0
11	Interactions of Ozone-Functionalized Activated Charcoal with SARS-Cov-2 Proteases Using Molecular Docking and Dynamics. Journal of Nanoscience and Nanotechnology, 2021, 21, 6060-6072.	0.9	3
12	Natural Products-Based Drug Design against SARS-CoV-2 Mpro 3CLpro. International Journal of Molecular Sciences, 2021, 22, 11739.	4.1	24
13	Theoretical and practical study of the cefoxitinâ€Escherichia coli PBP5 complex interaction by molecular dynamics to obtain computational prototype of antimicrobial susceptibility to Gram negative bacteria. Chemical Biology and Drug Design, 2020, 96, 1095-1102.	3.2	2
14	New nanocarried phenobarbital formulation: Maintains better control of pentylenetetrazole-Induced seizures. Biotechnology Reports (Amsterdam, Netherlands), 2020, 28, e00539.	4.4	4
15	Alkylated Sesamol Derivatives as Potent Antioxidants. Molecules, 2020, 25, 3300.	3.8	6
16	Molecular modification approach on kojic acid derivatives as antioxidants related to ascorbic acid. Journal of Molecular Modeling, 2020, 26, 318.	1.8	7
17	Identification of New Rofecoxib-Based Cyclooxygenase-2 Inhibitors: A Bioinformatics Approach. Pharmaceuticals, 2020, 13, 209.	3.8	52
18	A comparative study between kojic acid and its methylated derivatives as antioxidant related to maltol and alomaltol. Chemical Data Collections, 2020, 28, 100464.	2.3	7

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19	Experimental and theoretical study on structure-tautomerism among edaravone, isoxazolone, and their heterocycles derivatives as antioxidants. Saudi Pharmaceutical Journal, 2020, 28, 819-827.	2.7	8
20	Identification of Novel Chemical Entities for Adenosine Receptor Type 2A Using Molecular Modeling Approaches. Molecules, 2020, 25, 1245.	3.8	45
21	Impact of conformational and solubility properties on psycho-activity of cannabidiol (CBD) and tetrahydrocannabinol (THC). Chemical Data Collections, 2020, 26, 100345.	2.3	6
22	The role of regioselective hydroxylation on toxicity of diclofenac and related derivatives. Molecular Simulation, 2019, 45, 1454-1458.	2.0	1
23	Toward of Safer Phenylbutazone Derivatives by Exploration of Toxicity Mechanism. Molecules, 2019, 24, 143.	3.8	17
24	In Silico Evaluation of Ibuprofen and Two Benzoylpropionic Acid Derivatives with Potential Anti-Inflammatory Activity. Molecules, 2019, 24, 1476.	3.8	23
25	Mechanisms underlying the vasorelaxant effect of trans-4-methoxy-Î²-nitrostyrene in the rat mesenteric resistance arteries. European Journal of Pharmacology, 2019, 853, 201-209.	3.5	5
26	Sugar moiety has a synergistic effect on hydroxylated xanthone for better antioxidant activity of mangiferin. Medicinal Chemistry Research, 2018, 27, 1276-1282.	2.4	13
27	An In Silico Study of the Antioxidant Ability for Two Caffeine Analogs Using Molecular Docking and Quantum Chemical Methods. Molecules, 2018, 23, 2801.	3.8	38
28	Time-Dependent Density Functional Theory Analysis of Triphenylamine-Functionalized Graphene Doped with Transition Metals for Photocatalytic Hydrogen Production. Journal of Nanoscience and Nanotechnology, 2018, 18, 4987-4991.	0.9	6
29	Influence of piperidine ring on stability and reactivity of piperine. Chemical Data Collections, 2018, 17-18, 138-142.	2.3	6
30	AVANÃ‡OS QUÃMICOS NO PLANEJAMENTO E DESENVOLVIMENTO DE DERIVADOS DO PARACETAMOL. Quimica Nova, 2018, , .	0.3	1
31	Mauritia flexuosa L. protects against deficits in memory acquisition and oxidative stress in rat hippocampus induced by methylmercury exposure. Nutritional Neuroscience, 2017, 20, 297-304.	3.1	20
32	Diet enriched with the Amazon fruit aÃ§aÃ-(Euterpe oleracea) prevents electrophysiological deficits and oxidative stress induced by methyl-mercury in the rat retina. Nutritional Neuroscience, 2017, 20, 265-272.	3.1	12
33	Edaravone toxicity can be related to redox properties of their oxidized derivatives. Chemical Data Collections, 2017, 7-8, 51-57.	2.3	3
34	Sesamol is a related antioxidant to the vitamin E. Chemical Data Collections, 2017, 11-12, 77-83.	2.3	13
35	Isolating toxicophoric scaffold on trans -dehydrocrotonin. Chemical Data Collections, 2017, 11-12, 211-219.	2.3	1
36	Thermodynamic DFT analysis of natural gas. Journal of Molecular Modeling, 2017, 23, 224.	1.8	4

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37	Mechanism of the vasorelaxant effect induced by transâ€4â€methylâ€Î²â€nitrostyrene, a synthetic nitroderivative, in rat thoracic aorta. Clinical and Experimental Pharmacology and Physiology, 2017, 44, 787-794.	1.9	7
38	Trans-4-methoxy-Î²-nitrostyrene relaxes rat thoracic aorta through a sGC-dependent pathway. European Journal of Pharmacology, 2017, 807, 182-189.	3.5	9
39	Anti-Inflammatory Potential of 1-Nitro-2-Phenylethylene. Molecules, 2017, 22, 1977.	3.8	7
40	Study of anti-inflammatory and analgesic properties of 3-benzoyl-propionic acid. ParÃ¡ Research Medical Journal, 2017, 1, .	0.2	1
41	An antioxidant mechanism of morphine and related derivatives. Medicinal Chemistry Research, 2016, 25, 852-857.	2.4	11
42	Structure and toxicity of clozapine and olanzapine on agranulocytosis. Medicinal Chemistry Research, 2016, 25, 322-328.	2.4	5
43	Involvement of electron and hydrogen transfers through redox metabolism on activity and toxicity of the nimesulide. Journal of Molecular Modeling, 2015, 21, 166.	1.8	10
44	Theoretical Thermodynamics Study of Polyamidoamine Deposited Around a Nanotube as Motor Controlled by Light and Under Temperature Effect. Journal of Nanoscience and Nanotechnology, 2015, 15, 2840-2844.	0.9	0
45	The antioxidant properties of salicylate derivatives: A possible new mechanism of anti-inflammatory activity. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4808-4811.	2.2	33
46	A computational study for the antioxidant capacity increases in hydroxy-derivatives of paracetamol and salicylic acid. Medicinal Chemistry Research, 2015, 24, 3453-3459.	2.4	6
47	In Vitro Protective Effect and Antioxidant Mechanism of Resveratrol Induced by Dapsone Hydroxylamine in Human Cells. PLoS ONE, 2015, 10, e0134768.	2.5	39
48	Clinical Oxidative Stress during Leprosy Multidrug Therapy: Impact of Dapsone Oxidation. PLoS ONE, 2014, 9, e85712.	2.5	18
49	Understanding the cytotoxicity or cytoprotective effects of biological and synthetic quinone derivatives by redox mechanism. Journal of Molecular Modeling, 2014, 20, 2541.	1.8	13
50	Vasorelaxant effects of 1-nitro-2-phenylethene in rat isolated aortic rings. Vascular Pharmacology, 2014, 63, 55-62.	2.1	17
51	Flagella Interacting with a Carbon Nanowire with the Variation of Time and Initial Temperature. Journal of Nanoscience and Nanotechnology, 2014, 14, 4590-4594.	0.9	0
52	Molecular Simulation of Nicotine-Related Alkaloids Interaction with Human DNA. Journal of Computational and Theoretical Nanoscience, 2014, 11, 1797-1801.	0.4	0
53	Thermodynamics Study of the Parallel Gold Nanowires Matrices. Journal of Computational and Theoretical Nanoscience, 2014, 11, 856-859.	0.4	0
54	A Structure and Antioxidant Activity Study of Paracetamol and Salicylic Acid. Pharmacology & Pharmacy, 2014, 05, 1185-1191.	0.7	10

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55	A combined experimental and theoretical approach for radical-scavenging activity of edaravone and its related derivatives. Structural Chemistry, 2013, 24, 349-355.	2.0	9
56	Design and Evaluation of 4â€Aminophenol and Salicylate Derivatives as Freeâ€Radical Scavenger. Chemical Biology and Drug Design, 2013, 81, 414-419.	3.2	21
57	The tautomerism influence on the antioxidant prediction of oxederavone. Medicinal Chemistry Research, 2013, 22, 5617-5623.	2.4	5
58	Evaluation and Theoretical Study on the Anti-inflammatory Mechanism of 1-Nitro-2-phenylethane. Planta Medica, 2013, 79, 628-633.	1.3	18
59	A Theoretical Study of the Dapsone Derivatives on Methemoglobin. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2029-2033.	0.4	4
60	Understanding the Molecular Aspects of Tetrahydrocannabinol and Cannabidiol as Antioxidants. Molecules, 2013, 18, 12663-12674.	3.8	95
61	Antioxidant factors, nitric oxide levels, and cellular damage in leprosy patients. Revista Da Sociedade Brasileira De Medicina Tropical, 2013, 46, 645-649.	0.9	9
62	Density Functional Theory (DFT) Study of Edaravone Derivatives as Antioxidants. International Journal of Molecular Sciences, 2012, 13, 7594-7606.	4.1	23
63	The basic antioxidant structure for flavonoid derivatives. Journal of Molecular Modeling, 2012, 18, 4073-4080.	1.8	37
64	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. Tetrahedron, 2012, 68, 6902-6907.	1.9	7
65	An electronic study of pyrazolones drugs on agranulocytosis. Medicinal Chemistry Research, 2012, 21, 1389-1394.	2.4	3
66	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.	3.2	3
67	Structure of Dihydrochalcones and Related Derivatives and Their Scavenging and Antioxidant Activity against Oxygen and Nitrogen Radical Species. Molecules, 2011, 16, 1749-1760.	3.8	48
68	A Conformational Study of (<I>E</I>)- and (<I>Z</I>)-Pyridine-2-Carbaldehyde-2â€²-Pyridylhydrazone. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2058-2060.	0.4	1
69	An Electronic Study for Metronidazole Metabolism. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1274-1277.	0.4	0
70	Structural and Electronic Properties of Dipyridamole and Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 69-73.	0.4	2
71	Stability and Reactivity of Benzopyranones Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 97-101.	0.4	1
72	An Electronic Study of Biphenyl Derivatives Chlorinated. Journal of Computational and Theoretical Nanoscience, 2011, 8, 216-219.	0.4	1

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73	A Geometric and Electronic Study of Dapsone. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1428-1431.	0.4	8
74	Structure and Reactivity of Imidazolin-Azabutadienes. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1129-1131.	0.4	1
75	A theoretical study of salicylate oxidation for ADME prediction. Medicinal Chemistry Research, 2011, 20, 269-273.	2.4	5
76	A Theoretical Study of Chloroquine Tautomerism. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1639-1642.	0.4	1
77	An Electronic Study of Tocopherol-Ring Regioisomers as Antioxidants. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2061-2065.	0.4	0
78	Structureâ€“Activity Relationship of Bergenin and Acetylated Derivatives as Anti-Inflammatory. Journal of Computational and Theoretical Nanoscience, 2011, 8, 550-553.	0.4	0
79	A Theoretical Study of Paracetamol Acyl-Ether Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 670-675.	0.4	2
80	A Theoretical Study for Oxidative Metabolism of Acetaminophen. Journal of Computational and Theoretical Nanoscience, 2010, 7, 1968-1972.	0.4	3
81	Tautomerism and Radical-Scavenging Activity of Edaravone by DFT Methods. Journal of Computational and Theoretical Nanoscience, 2010, 7, 153-156.	0.4	13
82	Conformational Studies on Rotenoid and Its Biosynthetic Implications. Journal of Computational and Theoretical Nanoscience, 2010, 7, 1486-1489.	0.4	0
83	R-(-)Linalool UV Spectroscopy: The Experimental and Theoretical Study. Journal of Computational and Theoretical Nanoscience, 2010, 7, 414-417.	0.4	6
84	Dihydroflavonols from the leaves of Derris urucu (Leguminosae): structural elucidation and DPPH radical-scavenging activity. Journal of the Brazilian Chemical Society, 2009, 20, .	0.6	14
85	A Theoretical Study of Resveratrol Oxidation. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1637-1639.	0.4	5
86	A Theoretical Study for Oxidative Metabolism of Salicylates. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1140-1142.	0.4	6
87	A theoretical antioxidant pharmacophore for resveratrol. European Journal of Medicinal Chemistry, 2009, 44, 1644-1649.	5.5	148
88	Theoretical Modeling of Parallel Matrix Gold Nanowires. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1546-1548.	0.4	0
89	A DFT Study of Aminophenol Stability. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1694-1696.	0.4	5
90	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. International Journal of Quantum Chemistry, 2006, 106, 2617-2623.	2.0	32

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91	A QSAR study of 8.O.4â€²-neolignans with antifungal activity. Computational and Theoretical Chemistry, 2004, 672, 215-219.	1.5	19
92	A DFT study for paracetamol and 3,5-disubstituted analogues. Computational and Theoretical Chemistry, 2004, 673, 93-97.	1.5	37
93	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