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	A theoretical antioxidant pharmacophore for resveratrol. European Journal of Medicinal Chemistry, 2009, 44, 1644-1649.	5.5	148
2	Understanding the Molecular Aspects of Tetrahydrocannabinol and Cannabidiol as Antioxidants. Molecules, 2013, 18, 12663-12674.	3.8	95
3	Identification of New Rofecoxib-Based Cyclooxygenase-2 Inhibitors: A Bioinformatics Approach. Pharmaceuticals, 2020, 13, 209.	3.8	52
4	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
5	Identification of Novel Chemical Entities for Adenosine Receptor Type 2A Using Molecular Modeling Approaches. Molecules, 2020, 25, 1245.	3.8	45
6	Essential features for antioxidant capacity of ascorbic acid (vitamin C). Journal of Molecular Modeling, 2022, 28, 1.	1.8	45
7	In Vitro Protective Effect and Antioxidant Mechanism of Resveratrol Induced by Dapsone Hydroxylamine in Human Cells. PLoS ONE, 2015, 10, e0134768.	2.5	39
8	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
9	A DFT study for paracetamol and 3,5-disubstituted analogues. Computational and Theoretical Chemistry, 2004, 673, 93-97.	1.5	37
10	The basic antioxidant structure for flavonoid derivatives. Journal of Molecular Modeling, 2012, 18, 4073-4080.	1.8	37
11	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
12	Density functional theory study of metabolic derivatives of the oxidation of paracetamol. International Journal of Quantum Chemistry, 2006, 106, 2617-2623.	2.0	32
13	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
14	Natural Products-Based Drug Design against SARS-CoV-2 Mpro 3CLpro. International Journal of Molecular Sciences, 2021, 22, 11739.	4.1	24
15	Density Functional Theory (DFT) Study of Edaravone Derivatives as Antioxidants. International Journal of Molecular Sciences, 2012, 13, 7594-7606.	4.1	23
16	In Silico Evaluation of Ibuprofen and Two Benzoylpropionic Acid Derivatives with Potential Anti-Inflammatory Activity. Molecules, 2019, 24, 1476.	3.8	23
17	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
18	Mauritia flexuosaL. 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

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19	A QSAR study of 8.O.4â€²-neolignans with antifungal activity. Computational and Theoretical Chemistry, 2004, 672, 215-219.	1.5	19
20	Evaluation and Theoretical Study on the Anti-inflammatory Mechanism of 1-Nitro-2-phenylethane. Planta Medica, 2013, 79, 628-633.	1.3	18
21	Clinical Oxidative Stress during Leprosy Multidrug Therapy: Impact of Dapsone Oxidation. PLoS ONE, 2014, 9, e85712.	2.5	18
22	Vasorelaxant effects of 1-nitro-2-phenylethene in rat isolated aortic rings. Vascular Pharmacology, 2014, 63, 55-62.	2.1	17
23	Toward of Safer Phenylbutazone Derivatives by Exploration of Toxicity Mechanism. Molecules, 2019, 24, 143.	3.8	17
24	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
25	Tautomerism and Radical-Scavenging Activity of Edaravone by DFT Methods. Journal of Computational and Theoretical Nanoscience, 2010, 7, 153-156.	0.4	13
26	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
27	Sesamol is a related antioxidant to the vitamin E. Chemical Data Collections, 2017, 11-12, 77-83.	2.3	13
28	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
29	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
30	An antioxidant mechanism of morphine and related derivatives. Medicinal Chemistry Research, 2016, 25, 852-857.	2.4	11
31	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
32	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
33	A Structure and Antioxidant Activity Study of Paracetamol and Salicylic Acid. Pharmacology & Pharmacy, 2014, 05, 1185-1191.	0.7	10
34	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
35	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
36	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

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37	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
38	A Geometric and Electronic Study of Dapsone. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1428-1431.	0.4	8
39	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
40	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. Tetrahedron, 2012, 68, 6902-6907.	1.9	7
41	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
42	Anti-Inflammatory Potential of 1-Nitro-2-Phenylethylene. Molecules, 2017, 22, 1977.	3.8	7
43	Molecular modification approach on kojic acid derivatives as antioxidants related to ascorbic acid. Journal of Molecular Modeling, 2020, 26, 318.	1.8	7
44	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
45	A Theoretical Study for Oxidative Metabolism of Salicylates. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1140-1142.	0.4	6
46	R-(-)Linalool UV Spectroscopy: The Experimental and Theoretical Study. Journal of Computational and Theoretical Nanoscience, 2010, 7, 414-417.	0.4	6
47	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
48	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
49	Influence of piperidine ring on stability and reactivity of piperine. Chemical Data Collections, 2018, 17-18, 138-142.	2.3	6
50	Alkylated Sesamol Derivatives as Potent Antioxidants. Molecules, 2020, 25, 3300.	3.8	6
51	Impact of conformational and solubility properties on psycho-activity of cannabidiol (CBD) and tetrahydrocannabinol (THC). Chemical Data Collections, 2020, 26, 100345.	2.3	6
52	A Theoretical Study of Resveratrol Oxidation. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1637-1639.	0.4	5
53	A DFT Study of Aminophenol Stability. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1694-1696.	0.4	5
54	A theoretical study of salicylate oxidation for ADME prediction. Medicinal Chemistry Research, 2011, 20, 269-273.	2.4	5

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55	The tautomerism influence on the antioxidant prediction of oxederavone. Medicinal Chemistry Research, 2013, 22, 5617-5623.	2.4	5
56	Structure and toxicity of clozapine and olanzapine on agranulocytosis. Medicinal Chemistry Research, 2016, 25, 322-328.	2.4	5
57	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
58	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
59	A Theoretical Study of the Dapsone Derivatives on Methemoglobin. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2029-2033.	0.4	4
60	Thermodynamic DFT analysis of natural gas. Journal of Molecular Modeling, 2017, 23, 224.	1.8	4
61	New nanocarried phenobarbital formulation: Maintains better control of pentylenetetrazole-Induced seizures. Biotechnology Reports (Amsterdam, Netherlands), 2020, 28, e00539.	4.4	4
62	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
63	A Theoretical Study for Oxidative Metabolism of Acetaminophen. Journal of Computational and Theoretical Nanoscience, 2010, 7, 1968-1972.	0.4	3
64	An electronic study of pyrazolones drugs on agranulocytosis. Medicinal Chemistry Research, 2012, 21, 1389-1394.	2.4	3
65	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
66	Edaravone toxicity can be related to redox properties of their oxidized derivatives. Chemical Data Collections, 2017, 7-8, 51-57.	2.3	3
67	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
68	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
69	Structural and Electronic Properties of Dipyridamole and Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 69-73.	0.4	2
70	A Theoretical Study of Paracetamol Acyl-Ether Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 670-675.	0.4	2
71	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
72	Experimental and theoretical approaches for the development of 4H-Chromene derivatives as inhibitors of tyrosinase. Molecular Simulation, 2021, 47, 762-770.	2.0	2

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73	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
74	Stability and Reactivity of Benzopyranones Derivatives. Journal of Computational and Theoretical Nanoscience, 2011, 8, 97-101.	0.4	1
75	An Electronic Study of Biphenyl Derivatives Chlorinated. Journal of Computational and Theoretical Nanoscience, 2011, 8, 216-219.	0.4	1
76	Structure and Reactivity of Imidazolin-Azabutadienes. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1129-1131.	0.4	1
77	A Theoretical Study of Chloroquine Tautomerism. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1639-1642.	0.4	1
78	Isolating toxicophoric scaffold on trans -dehydrocrotonin. Chemical Data Collections, 2017, 11-12, 211-219.	2.3	1
79	The role of regioselective hydroxylation on toxicity of diclofenac and related derivatives. Molecular Simulation, 2019, 45, 1454-1458.	2.0	1
80	An asymmetric performance between mangiferin and isomangiferin as antioxidants. Chemical Data Collections, 2021, 31, 100602.	2.3	1
81	Molecular modifications on Î²-nitro-styrene derivatives increase their antioxidant capacities. Journal of Molecular Structure, 2021, 1243, 130853.	3.6	1
82	Study of anti-inflammatory and analgesic properties of 3-benzoyl-propionic acid. ParÃ¡ Research Medical Journal, 2017, 1, .	0.2	1
83	AVANÃ‡OS QUÃMICOS NO PLANEJAMENTO E DESENVOLVIMENTO DE DERIVADOS DO PARACETAMOL. Quimica Nova, 2018, , .	0.3	1
84	Theoretical Modeling of Parallel Matrix Gold Nanowires. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1546-1548.	0.4	0
85	Conformational Studies on Rotenoid and Its Biosynthetic Implications. Journal of Computational and Theoretical Nanoscience, 2010, 7, 1486-1489.	0.4	0
86	An Electronic Study for Metronidazole Metabolism. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1274-1277.	0.4	0
87	An Electronic Study of Tocopherol-Ring Regioisomers as Antioxidants. Journal of Computational and Theoretical Nanoscience, 2011, 8, 2061-2065.	0.4	0
88	Structureâ€“Activity Relationship of Bergenin and Acetylated Derivatives as Anti-Inflammatory. Journal of Computational and Theoretical Nanoscience, 2011, 8, 550-553.	0.4	0
89	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
90	Molecular Simulation of Nicotine-Related Alkaloids Interaction with Human DNA. Journal of Computational and Theoretical Nanoscience, 2014, 11, 1797-1801.	0.4	0

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91	Thermodynamics Study of the Parallel Gold Nanowires Matrices. Journal of Computational and Theoretical Nanoscience, 2014, 11, 856-859.	0.4	0
92	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
93	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