## Marcelo Zaldini Hernandes

List of Publications by Year in descending order

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236612 233125 2,127 57 25 45 citations g-index h-index papers 58 58 58 3338 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Halogen Atoms in the Modern Medicinal Chemistry: Hints for the Drug Design. Current Drug Targets, 2010, 11, 303-314.	1.0	528
2	Rotational features of carbon-nitrogen bonds in axially chiral o-tert-butyl anilides and related molecules. Potential substrates for the â€~prochiral auxiliary' approach to asymmetric synthesis. Tetrahedron: Asymmetry, 1997, 8, 3955-3975.	1.8	112
3	Synthesis, docking, and in vitro activity of thiosemicarbazones, aminoacyl-thiosemicarbazides and acyl-thiazolidones against Trypanosoma cruzi. Bioorganic and Medicinal Chemistry, 2006, 14, 3749-3757.	1.4	98
4	Synthesis and anti-inflammatory activity of new arylidene-thiazolidine-2,4-diones as PPAR $\hat{I}^3$ ligands. Bioorganic and Medicinal Chemistry, 2010, 18, 3805-3811.	1.4	86
5	2-Pyridyl thiazoles as novel anti-Trypanosoma cruzi agents: Structural design, synthesis and pharmacological evaluation. European Journal of Medicinal Chemistry, 2014, 86, 48-59.	2.6	86
6	Quercetin as an inhibitor of snake venom secretory phospholipase A2. Chemico-Biological Interactions, 2011, 189, 9-16.	1.7	62
7	Selective and mild oxidation of sulfides to sulfoxides by oxodiperoxo molybdenum complexes adsorbed onto silica gel. Tetrahedron, 2001, 57, 9669-9676.	1.0	60
8	The encapsulation of $\hat{l}^2$ -lapachone in 2-hydroxypropyl- $\hat{l}^2$ -cyclodextrin inclusion complex into liposomes: A physicochemical evaluation and molecular modeling approach. European Journal of Pharmaceutical Sciences, 2011, 44, 332-340.	1.9	59
9	Structural Investigation of Anti- <i>Trypanosoma cruzi</i> 2-Iminothiazolidin-4-ones Allows the Identification of Agents with Efficacy in Infected Mice. Journal of Medicinal Chemistry, 2012, 55, 10918-10936.	2.9	55
10	The Use of Solid Dispersion Systems in Hydrophilic Carriers to Increase Benznidazole Solubility. Journal of Pharmaceutical Sciences, 2011, 100, 2443-2451.	1.6	53
11	Synthesis, Cruzain Docking, and inâ€vitro Studies of Arylâ€4â€Oxothiazolylhydrazones Against <i>Trypanosoma cruzi</i> . ChemMedChem, 2007, 2, 1339-1345.	1.6	50
12	Combination of In Silico Methods in the Search for Potential CD4+ and CD8+ T Cell Epitopes in the Proteome of Leishmania braziliensis. Frontiers in Immunology, 2016, 7, 327.	2.2	47
13	Synthesis, biological evaluation and molecular modeling studies of arylidene-thiazolidinediones with potential hypoglycemic and hypolipidemic activities. European Journal of Medicinal Chemistry, 2007, 42, 1263-1271.	2.6	46
14	Studies toward the structural optimization of novel thiazolylhydrazone-based potent antitrypanosomal agents. Bioorganic and Medicinal Chemistry, 2010, 18, 7826-7835.	1.4	46
15	New 1,3-thiazole derivatives and their biological and ultrastructural effects on Trypanosoma cruzi. European Journal of Medicinal Chemistry, 2016, 121, 387-398.	2.6	46
16	Structural Design, Synthesis and Structure–Activity Relationships of Thiazolidinones with Enhanced Antiâ€∢i>Trypanosoma cruzi Activity. ChemMedChem, 2014, 9, 177-188.	1.6	39
17	A theoretical study of red-shifting and blue-shifting hydrogen bonds occurring between imidazolidine derivatives and PEG/PVP polymers. Journal of Molecular Modeling, 2010, 16, 119-127.	0.8	38
18	Thiosemicarbazones as Aedes aegypti larvicidal. European Journal of Medicinal Chemistry, 2015, 100, 162-175.	2.6	36

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19	Discovery of Phthalimides as Immunomodulatory and Antitumor Drug Prototypes. ChemMedChem, 2010, 5, 523-528.	1.6	35
20	Design, synthesis and structure–activity relationship of phthalimides endowed with dual antiproliferative and immunomodulatory activities. European Journal of Medicinal Chemistry, 2015, 96, 491-503.	2.6	34
21	Interaction of Morphine With a New α2-Adrenoceptor Agonist in Mice. Journal of Pain, 2010, 11, 71-78.	0.7	31
22	Molecular Structure of the Molybdenum Oxo-Diperoxo Compound MoO(O2)2(OPy)(H2O):Â A Computational and X-ray Study. Inorganic Chemistry, 2001, 40, 6022-6025.	1.9	28
23	Solute relaxation on the solvatochromism of ortho-betaine dyes. A sequential Monte Carlo/quantum mechanics study. Physical Chemistry Chemical Physics, 2004, 6, 2088.	1.3	27
24	A theoretical study of the solvent effects in ethylene oxide: Hydrofluoric acid complex using continuum and new discrete models. Computational and Theoretical Chemistry, 2007, 802, 91-97.	1.5	27
25	Enhanced Antiproliferative Activity of the New Anticancer Candidate LPSF/AC04 in Cyclodextrin Inclusion Complexes Encapsulated into Liposomes. AAPS PharmSciTech, 2012, 13, 1355-1366.	1.5	26
26	New PPAR $\hat{1}^3$ partial agonist improves obesity-induced metabolic alterations and atherosclerosis in LDLr $\hat{1}^2$ mice. Pharmacological Research, 2016, 104, 49-60.	3.1	26
27	Synthesis and in vitro anticancer activity of novel thiazacridine derivatives. Medicinal Chemistry Research, 2013, 22, 2421-2429.	1.1	23
28	Solid Dispersions of Imidazolidinedione by PEG and PVP Polymers with Potential Antischistosomal Activities. AAPS PharmSciTech, 2011, 12, 401-410.	1.5	22
29	Chemometric study of liquid water simulations. I. The parameters of the TIP4P model potential. Journal of Computational Chemistry, 2003, 24, 973-981.	1.5	19
30	Chemical synthesis, docking studies and biological effects of a pan peroxisome proliferator-activated receptor agonist and cyclooxygenase inhibitor. European Journal of Pharmaceutical Sciences, 2013, 48, 689-697.	1.9	18
31	Synthesis, in vitro anticancer activity and in silico study of new disubstituted thiazolidinedione derivatives. Medicinal Chemistry Research, 2014, 23, 3220-3226.	1.1	18
32	Chagas disease: Immunology of the disease at a glance. Cytokine and Growth Factor Reviews, 2021, 62, 15-22.	3.2	18
33	Elucidation of the mechanism of complexation between oncocalyxone A and cyclodextrins by isothermal titration calorimetry and molecular modeling. Journal of Molecular Liquids, 2019, 274, 165-172.	2.3	17
34	Estrutura, reatividade e propriedades biológicas de hidantoÃnas. Quimica Nova, 2008, 31, 614-622.	0.3	15
35	Molecular modeling and cytotoxicity of diffractaic acid: HP-β-CD inclusion complex encapsulated in microspheres. International Journal of Biological Macromolecules, 2016, 92, 494-503.	3.6	15
36	A docking-based structural analysis of geldanamycin-derived inhibitor binding to human or Leishmania Hsp90. Scientific Reports, 2019, 9, 14756.	1.6	15

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37	Isolation, homology modeling and renal effects of a C-type natriuretic peptide from the venom of the Brazilian yellow scorpion (Tityus serrulatus). Toxicon, 2013, 74, 19-26.	0.8	14
38	Coordination Chemistry of Br2InCH2Br:  Coordination at the Metal Center. Organometallics, 1999, 18, 99-105.	1.1	13
39	Sulfonamide–metal complexes endowed with potent anti-Trypanosoma cruzi activity. Journal of Enzyme Inhibition and Medicinal Chemistry, 2014, 29, 230-236.	2.5	13
40	Preparation, crystal structure determination, and properties of adducts of halogenomethyl compounds of indium with Group 16 donors. Journal of Organometallic Chemistry, 2001, 626, 68-75.	0.8	12
41	Inhibition of Neurotoxic Secretory Phospholipases A2Enzymatic, Edematogenic, and Myotoxic Activities by Harpalycin 2, an Isoflavone Isolated fromHarpalyce brasilianaBenth. Evidence-based Complementary and Alternative Medicine, 2012, 2012, 1-9.	0.5	12
42	Preparation, crystal structure determination and properties of adducts of indium methylene compounds with Group 15 donors. Journal of Organometallic Chemistry, 2000, 603, 203-212.	0.8	10
43	The use of the generator coordinate method for designing basis set. Application to oxo-diperoxo molybdenum complexes. Computational and Theoretical Chemistry, 2002, 589-590, 251-264.	1.5	10
44	Supramolecular interactions between βâ€lapachone with cyclodextrins studied using isothermal titration calorimetry and molecular modeling. Journal of Molecular Recognition, 2017, 30, e2646.	1.1	10
45	Chagas Disease Treatment and Rational Drug Discovery: A Challenge That Remains. Frontiers in Pharmacology, 2019, 10, 873.	1.6	9
46	Biological Evaluation of Arylsemicarbazone Derivatives as Potential Anticancer Agents. Pharmaceuticals, 2019, 12, 169.	1.7	9
47	CycloMolder software: building theoretical cyclodextrin derivatives models and evaluating their host:guest interactions. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2019, 93, 301-308.	0.9	9
48	AIPAR: ab initio parametrization of intermolecular potentials for computer simulations. Journal of Molecular Modeling, 2005, 11, 61-68.	0.8	7
49	Design, Synthesis and In Vitro Trypanocidal and Leishmanicidal Activities of 2â€(2â€Arylidene)hydrazonoâ€4â€oxothiazolidineâ€5â€acetic Acid Derivatives. ChemistrySelect, 2019, 4, 13163	-P3 <sup>7</sup> 172.	7
50	AGOA: A Hydration Procedure and Its Application to the 1-Phenyl-beta-Carboline Molecule. Journal of the Brazilian Chemical Society, 2002, 13, 36-42.	0.6	7
51	Novel Nitrofurazone Derivatives Endowed with Antimicrobial Activity. Archiv Der Pharmazie, 2008, 341, 655-660.	2.1	5
52	Anti-hypersensitivity effects of the phthalimide derivative N-(4methyl-phenyl)-4-methylphthalimide in different pain models in mice. Biomedicine and Pharmacotherapy, 2017, 96, 503-512.	2.5	5
53	Synthesis, antitrypanosomal activity and molecular docking studies of pyrimidine derivatives. Medicinal Chemistry Research, 2018, 27, 2512-2522.	1.1	5
54	Immunogenicity of Potential CD4+ and CD8+ T Cell Epitopes Derived From the Proteome of Leishmania braziliensis. Frontiers in Immunology, 2020, 10, 3145.	2.2	4

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55	Streptomyces hygroscopicus UFPEDA 3370: A valuable source of the potent cytotoxic agent nigericin and its evaluation against human colorectal cancer cells. Chemico-Biological Interactions, 2021, 333, 109316.	1.7	2
56	NPCdc, a synthetic natriuretic peptide, is a substrate to neprilysin and enhances blood pressure-lowering induced by enalapril in 5/6 nephrectomized rats. Toxicon, 2021, 203, 30-39.	0.8	2
57	Principal component analysis of the effects of wavefunction modification on the electrostatic potential of indole. International Journal of Quantum Chemistry, 2005, 102, 379-386.	1.0	1