

# Marcelo Zaldini Hernandez

## List of Publications by Year in descending order

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57  
papers

2,127  
citations

236925

25  
h-index

233421

45  
g-index

58  
all docs

58  
docs citations

58  
times ranked

3338  
citing authors

#	ARTICLE	IF	CITATIONS
1	Halogen Atoms in the Modern Medicinal Chemistry: Hints for the Drug Design. <i>Current Drug Targets</i> , 2010, 11, 303-314.	2.1	528
2	Rotational features of carbon-nitrogen bonds in axially chiral o-tert-butyl anilides and related molecules. Potential substrates for the "prochiral auxiliary" approach to asymmetric synthesis. <i>Tetrahedron: Asymmetry</i> , 1997, 8, 3955-3975.	1.8	112
3	Synthesis, docking, and in vitro activity of thiosemicarbazones, aminoacyl-thiosemicarbazides and acyl-thiazolidones against <i>Trypanosoma cruzi</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 3749-3757.	3.0	98
4	Synthesis and anti-inflammatory activity of new arylidene-thiazolidine-2,4-diones as PPAR $\beta$ ligands. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 3805-3811.	3.0	86
5	2-Pyridyl thiazoles as novel anti- <i>Trypanosoma cruzi</i> agents: Structural design, synthesis and pharmacological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2014, 86, 48-59.	5.5	86
6	Quercetin as an inhibitor of snake venom secretory phospholipase A2. <i>Chemico-Biological Interactions</i> , 2011, 189, 9-16.	4.0	62
7	Selective and mild oxidation of sulfides to sulfoxides by oxodiperoxo molybdenum complexes adsorbed onto silica gel. <i>Tetrahedron</i> , 2001, 57, 9669-9676.	1.9	60
8	The encapsulation of $\beta$ -lapachone in 2-hydroxypropyl- $\beta$ -cyclodextrin inclusion complex into liposomes: A physicochemical evaluation and molecular modeling approach. <i>European Journal of Pharmaceutical Sciences</i> , 2011, 44, 332-340.	4.0	59
9	Structural Investigation of Anti- <i>Trypanosoma cruzi</i> 2-Iminothiazolidin-4-ones Allows the Identification of Agents with Efficacy in Infected Mice. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 10918-10936.	6.4	55
10	The Use of Solid Dispersion Systems in Hydrophilic Carriers to Increase Benznidazole Solubility. <i>Journal of Pharmaceutical Sciences</i> , 2011, 100, 2443-2451.	3.3	53
11	Synthesis, Cruzain Docking, and in vitro Studies of Aryloxythiazolyhydrazones Against <i>Trypanosoma cruzi</i> . <i>ChemMedChem</i> , 2007, 2, 1339-1345.	3.2	50
12	Combination of In Silico Methods in the Search for Potential CD4+ and CD8+ T Cell Epitopes in the Proteome of <i>Leishmania braziliensis</i> . <i>Frontiers in Immunology</i> , 2016, 7, 327.	4.8	47
13	Synthesis, biological evaluation and molecular modeling studies of arylidene-thiazolidinediones with potential hypoglycemic and hypolipidemic activities. <i>European Journal of Medicinal Chemistry</i> , 2007, 42, 1263-1271.	5.5	46
14	Studies toward the structural optimization of novel thiazolyhydrazone-based potent antitrypanosomal agents. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 7826-7835.	3.0	46
15	New 1,3-thiazole derivatives and their biological and ultrastructural effects on <i>Trypanosoma cruzi</i> . <i>European Journal of Medicinal Chemistry</i> , 2016, 121, 387-398.	5.5	46
16	Structural Design, Synthesis and Structure-Activity Relationships of Thiazolidinones with Enhanced Anti- <i>Trypanosoma cruzi</i> Activity. <i>ChemMedChem</i> , 2014, 9, 177-188.	3.2	39
17	A theoretical study of red-shifting and blue-shifting hydrogen bonds occurring between imidazolidine derivatives and PEG/PVP polymers. <i>Journal of Molecular Modeling</i> , 2010, 16, 119-127.	1.8	38
18	Thiosemicarbazones as <i>Aedes aegypti</i> larvicidal. <i>European Journal of Medicinal Chemistry</i> , 2015, 100, 162-175.	5.5	36

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19	Discovery of Phthalimides as Immunomodulatory and Antitumor Drug Prototypes. <i>ChemMedChem</i> , 2010, 5, 523-528.	3.2	35
20	Design, synthesis and structure-activity relationship of phthalimides endowed with dual antiproliferative and immunomodulatory activities. <i>European Journal of Medicinal Chemistry</i> , 2015, 96, 491-503.	5.5	34
21	Interaction of Morphine With a New $\mu$ -2-Adrenoceptor Agonist in Mice. <i>Journal of Pain</i> , 2010, 11, 71-78.	1.4	31
22	Molecular Structure of the Molybdenum Oxo-Diperoxo Compound $\text{MoO}(\text{O}_2)_2(\text{OPy})(\text{H}_2\text{O})$ : A Computational and X-ray Study. <i>Inorganic Chemistry</i> , 2001, 40, 6022-6025.	4.0	28
23	Solute relaxation on the solvatochromism of ortho-betaine dyes. A sequential Monte Carlo/quantum mechanics study. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2088.	2.8	27
24	A theoretical study of the solvent effects in ethylene oxide: Hydrofluoric acid complex using continuum and new discrete models. <i>Computational and Theoretical Chemistry</i> , 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. <i>AAPS PharmSciTech</i> , 2012, 13, 1355-1366.	3.3	26
26	New PPAR $\beta$ partial agonist improves obesity-induced metabolic alterations and atherosclerosis in LDLr $^{-/-}$ mice. <i>Pharmacological Research</i> , 2016, 104, 49-60.	7.1	26
27	Synthesis and in vitro anticancer activity of novel thiazacridine derivatives. <i>Medicinal Chemistry Research</i> , 2013, 22, 2421-2429.	2.4	23
28	Solid Dispersions of Imidazolidinedione by PEG and PVP Polymers with Potential Antischistosomal Activities. <i>AAPS PharmSciTech</i> , 2011, 12, 401-410.	3.3	22
29	Chemometric study of liquid water simulations. I. The parameters of the TIP4P model potential. <i>Journal of Computational Chemistry</i> , 2003, 24, 973-981.	3.3	19
30	Chemical synthesis, docking studies and biological effects of a pan peroxisome proliferator-activated receptor agonist and cyclooxygenase inhibitor. <i>European Journal of Pharmaceutical Sciences</i> , 2013, 48, 689-697.	4.0	18
31	Synthesis, in vitro anticancer activity and in silico study of new disubstituted thiazolidinedione derivatives. <i>Medicinal Chemistry Research</i> , 2014, 23, 3220-3226.	2.4	18
32	Chagas disease: Immunology of the disease at a glance. <i>Cytokine and Growth Factor Reviews</i> , 2021, 62, 15-22.	7.2	18
33	Elucidation of the mechanism of complexation between oncolyxone A and cyclodextrins by isothermal titration calorimetry and molecular modeling. <i>Journal of Molecular Liquids</i> , 2019, 274, 165-172.	4.9	17
34	Estrutura, reatividade e propriedades biológicas de hidantoínas. <i>Quimica Nova</i> , 2008, 31, 614-622.	0.3	15
35	Molecular modeling and cytotoxicity of diffractaic acid: HP- $\beta$ -CD inclusion complex encapsulated in microspheres. <i>International Journal of Biological Macromolecules</i> , 2016, 92, 494-503.	7.5	15
36	A docking-based structural analysis of geldanamycin-derived inhibitor binding to human or Leishmania Hsp90. <i>Scientific Reports</i> , 2019, 9, 14756.	3.3	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 ( <i>Tityus serrulatus</i> ). <i>Toxicon</i> , 2013, 74, 19-26.	1.6	14
38	Coordination Chemistry of Br <sub>2</sub> InCH <sub>2</sub> Br: Coordination at the Metal Center. <i>Organometallics</i> , 1999, 18, 99-105.	2.3	13
39	Sulfonamide-metal complexes endowed with potent anti- <i>Trypanosoma cruzi</i> activity. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2014, 29, 230-236.	5.2	13
40	Preparation, crystal structure determination, and properties of adducts of halogenomethyl compounds of indium with Group 16 donors. <i>Journal of Organometallic Chemistry</i> , 2001, 626, 68-75.	1.8	12
41	Inhibition of Neurotoxic Secretory Phospholipases A <sub>2</sub> Enzymatic, Edematogenic, and Myotoxic Activities by Harpalycin 2, an Isoflavone Isolated from <i>Harpalyce brasiliensis</i> . <i>Evidence-based Complementary and Alternative Medicine</i> , 2012, 2012, 1-9.	1.2	12
42	Preparation, crystal structure determination and properties of adducts of indium methylene compounds with Group 15 donors. <i>Journal of Organometallic Chemistry</i> , 2000, 603, 203-212.	1.8	10
43	The use of the generator coordinate method for designing basis set. Application to oxo-diperoxo molybdenum complexes. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 251-264.	1.5	10
44	Supramolecular interactions between $\beta$ -cyclodextrin with cyclodextrins studied using isothermal titration calorimetry and molecular modeling. <i>Journal of Molecular Recognition</i> , 2017, 30, e2646.	2.1	10
45	Chagas Disease Treatment and Rational Drug Discovery: A Challenge That Remains. <i>Frontiers in Pharmacology</i> , 2019, 10, 873.	3.5	9
46	Biological Evaluation of Arylsemicarbazone Derivatives as Potential Anticancer Agents. <i>Pharmaceuticals</i> , 2019, 12, 169.	3.8	9
47	CycloMolder software: building theoretical cyclodextrin derivatives models and evaluating their host:guest interactions. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2019, 93, 301-308.	1.6	9
48	AIPAR: ab initio parametrization of intermolecular potentials for computer simulations. <i>Journal of Molecular Modeling</i> , 2005, 11, 61-68.	1.8	7
49	Design, Synthesis and In Vitro Trypanocidal and Leishmanicidal Activities of $\beta$ -(2-Arylidene)hydrazone-4-thiazolidine-5-acetic Acid Derivatives. <i>ChemistrySelect</i> , 2019, 4, 13163-13172.	1.5	7
50	AGOA: A Hydration Procedure and Its Application to the 1-Phenyl-beta-Carboline Molecule. <i>Journal of the Brazilian Chemical Society</i> , 2002, 13, 36-42.	0.6	7
51	Novel Nitrofurazone Derivatives Endowed with Antimicrobial Activity. <i>Archiv Der Pharmazie</i> , 2008, 341, 655-660.	4.1	5
52	Anti-hypersensitivity effects of the phthalimide derivative N-(4-methyl-phenyl)-4-methylphthalimide in different pain models in mice. <i>Biomedicine and Pharmacotherapy</i> , 2017, 96, 503-512.	5.6	5
53	Synthesis, antitrypanosomal activity and molecular docking studies of pyrimidine derivatives. <i>Medicinal Chemistry Research</i> , 2018, 27, 2512-2522.	2.4	5
54	Immunogenicity of Potential CD4 <sup>+</sup> and CD8 <sup>+</sup> T Cell Epitopes Derived From the Proteome of <i>Leishmania braziliensis</i> . <i>Frontiers in Immunology</i> , 2020, 10, 3145.	4.8	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. <i>Chemico-Biological Interactions</i> , 2021, 333, 109316.	4.0	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. <i>Toxicol</i> , 2021, 203, 30-39.	1.6	2
57	Principal component analysis of the effects of wavefunction modification on the electrostatic potential of indole. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 379-386.	2.0	1