Kerly Pasqualoto

List of Publications by Year in descending order

43 papers	945 citations	471509 17 h-index	477307 29 g-index
43 all docs	43 docs citations	43 times ranked	1509 citing authors

#	Article	IF	Citations
1	4D-QSAR: Perspectives in Drug Design. Molecules, 2010, 15, 3281-3294.	3.8	83
2	LQTA-QSAR: A New 4D-QSAR Methodology. Journal of Chemical Information and Modeling, 2009, 49, 1428-1436.	5.4	70
3	Mastoparan induces apoptosis in B16F10-Nex2 melanoma cells via the intrinsic mitochondrial pathway and displays antitumor activity in vivo. Peptides, 2015, 68, 113-119.	2.4	55
4	Rational Design of New Antituberculosis Agents:Â Receptor-Independent Four-Dimensional Quantitative Structureâ"Activity Relationship Analysis of a Set of Isoniazid Derivatives. Journal of Medicinal Chemistry, 2004, 47, 3755-3764.	6.4	53
5	Design, synthesis, antimicrobial activity and molecular modeling studies of novel benzofuroxan derivatives against Staphylococcus aureus. Bioorganic and Medicinal Chemistry, 2009, 17, 3028-3036.	3.0	47
6	Apoptotic effect of eugenol envolves G2/M phase abrogation accompanied by mitochondrial damage and clastogenic effect on cancer cell in vitro. Phytomedicine, 2016, 23, 725-735.	5.3	43
7	RPF101, a new capsaicin-like analogue, disrupts the microtubule network accompanied by arrest in the G2/M phase, inducing apoptosis and mitotic catastrophe in the MCF-7 breast cancer cells. Toxicology and Applied Pharmacology, 2013, 266, 385-398.	2.8	37
8	Synthesis, molecular modeling and preliminary biological evaluation of a set of 3-acetyl-2,5-disubstituted-2,3-dihydro-1,3,4-oxadiazole as potential antibacterial, anti-Trypanosoma cruzi and antifungal agents. Bioorganic and Medicinal Chemistry, 2011, 19, 6292-6301.	3.0	35
9	Rational Design and 3D-Pharmacophore Mapping of 5â€²-Thiourea-Substituted Î±-Thymidine Analogues as Mycobacterial TMPK Inhibitors. Journal of Chemical Information and Modeling, 2009, 49, 1070-1078.	5.4	33
10	An Approach for the Rational Design of New Antituberculosis Agents. Current Drug Targets, 2001, 2, 427-437.	2.1	32
11	Dillapiole as Antileishmanial Agent: Discovery, Cytotoxic Activity and Preliminary SAR Studies of Dillapiole Analogues. Archiv Der Pharmazie, 2012, 345, 934-944.	4.1	30
12	Exploring 5-nitrofuran derivatives against nosocomial pathogens: Synthesis, antimicrobial activity and chemometric analysis. Bioorganic and Medicinal Chemistry, 2014, 22, 2844-2854.	3.0	29
13	Cytotoxic effects of dillapiole on MDA-MB-231 cells involve the induction of apoptosis through the mitochondrial pathway by inducing an oxidative stress while altering the cytoskeleton network. Biochimie, 2014, 99, 195-207.	2.6	25
14	Fragment-based and classical quantitative structureâ€“activity relationships for a series of hydrazides as antituberculosis agents. Molecular Diversity, 2008, 12, 47-59.	3.9	24
15	Novel benzofuroxan derivatives against multidrug-resistant Staphylococcus aureus strains: Design using Toplissâ€™ decision tree, synthesis and biological assay. Bioorganic and Medicinal Chemistry, 2011, 19, 5031-5038.	3.0	23
16	5-Nitro-2-furfuriliden derivatives as potential anti-Trypanosoma cruzi agents: Design, synthesis, bioactivity evaluation, cytotoxicity and exploratory data analysis. Bioorganic and Medicinal Chemistry, 2013, 21, 5395-5406.	3.0	21
17	Molecular modeling studies and in vitro bioactivity evaluation of a set of novel 5-nitro-heterocyclic derivatives as anti-T. cruzi agents. Bioorganic and Medicinal Chemistry, 2009, 17, 2673-2679.	3.0	18
18	Ligand-based design, synthesis, and experimental evaluation of novel benzofuroxan derivatives as anti-Trypanosoma cruzi agents. European Journal of Medicinal Chemistry, 2013, 64, 200-214.	5.5	18

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19	RPF151, a novel capsaicin-like analogue: in vitro studies and in vivo preclinical antitumor evaluation in a breast cancer model. Tumor Biology, 2015, 36, 7251-7267.	1.8	18
20	Molecular modeling as a promising tool to study dendrimer prodrugs delivery. Computational and Theoretical Chemistry, 2010, 939, 133-138.	1.5	17
21	Designing and exploring active Nâ€²-[(5-nitrofuran-2-yl) methylene] substituted hydrazides against three Trypanosoma cruzi strains more prevalent in Chagas disease patients. European Journal of Medicinal Chemistry, 2015, 96, 330-339.	5.5	17
22	Tick salivary gland as potential natural source for the discovery of promising antitumor drug candidates. Biomedicine and Pharmacotherapy, 2016, 77, 14-19.	5.6	17
23	Application of a Receptor Pruning Methodology to the Enoyl-ACP Reductase fromEscherichia coli (FabI). QSAR and Combinatorial Science, 2006, 25, 629-636.	1.4	15
24	Molecular modeling study on the disassembly of dendrimers designed as potential antichagasic and antileishmanial prodrugs. Journal of Molecular Modeling, 2012, 18, 2257-2269.	1.8	14
25	To Be Drug or Prodrug: Structure-Property Exploratory Approach Regarding Oral Bioavailability. Journal of Pharmacy and Pharmaceutical Sciences, 2014, 17, 532.	2.1	14
26	Novel Capsaicin Analogues as Potential Anticancer Agents: Synthesis, Biological Evaluation, and In Silico Approach. Archiv Der Pharmazie, 2014, 347, 885-895.	4.1	14
27	Self-organizing maps and VolSurf approach to predict aldose reductase inhibition by flavonoid compounds. Revista Brasileira De Farmacognosia, 2011, 21, 170-180.	1.4	13
28	Design and exploratory data analysis of a second generation of dendrimer prodrugs potentially antichagasic and leishmanicide. Molecular Diversity, 2013, 17, 711-720.	3.9	13
29	Synthesis, characterization, in silico approach and in vitro antiproliferative activity of RPF151, a benzodioxole sulfonamide analogue designed from capsaicin scaffold. Journal of Molecular Structure, 2015, 1088, 138-146.	3.6	13
30	Evaluation and comparison of a new DOTA and DTPA - bombesin agonist in vitro and in vivo in low and high GRPR expressing prostate and breast tumor models. Applied Radiation and Isotopes, 2015, 96, 91-101.	1.5	13
31	BFD-22 a new potential inhibitor of BRAF inhibits the metastasis of B16F10 melanoma cells and simultaneously increased the tumor immunogenicity. Toxicology and Applied Pharmacology, 2016, 295, 56-67.	2.8	13
32	Transcripts involved in hemostasis: Exploring salivary complexes from Haementeria vizottoi leeches through transcriptomics, phylogenetic studies and structural features. Toxicon, 2015, 106, 20-29.	1.6	12
33	Structural Findings and Molecular Modeling Approach of a TFPI-Like Inhibitor. Protein and Peptide Letters, 2014, 21, 452-457.	0.9	11
34	A study of physicochemical and biopharmaceutical properties of Amoxicillin tablets using full factorial design and PCA biplot. Analytica Chimica Acta, 2007, 595, 216-220.	5.4	10
35	Molecular modeling and QSAR studies of a set of indole and benzimidazole derivatives as H4 receptor antagonists. Journal of Molecular Modeling, 2011, 17, 921-928.	1.8	9
36	Preliminary in vitro evaluation of Nâ€²-(benzofuroxan-5-yl)methylene benzohydrazide derivatives as potential anti-Trypanosoma cruzi agents. MedChemComm, 2012, 3, 824.	3.4	9

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37	Molecular modelling as a tool for studying the disassembly of potentially leishmanicide-targeted dendrimer. Molecular Simulation, 2013, 39, 860-867.	2.0	5
38	A novel set of Î²â€Nâ€biaryl ether sulfonamide hydroxamates as potential MMPs inhibitors: Molecular dynamics simulations and molecular properties evaluation. International Journal of Quantum Chemistry, 2012, 112, 3374-3389.	2.0	4
39	Molecular modeling approach to predict a binding mode for the complex methotrexate-carboxypeptidase G2. Journal of Molecular Modeling, 2012, 18, 1867-1875.	1.8	4
40	Rational development of novel leads from animal secretion based on coagulation and cell targets: 1. In silico analysis to explore a peptide derivative as lipocalins' signature. Toxicon, 2013, 69, 200-210.	1.6	4
41	Alkylphosphocholines as Promising Antitumor Agents: Exploring the Role of Structural Features on the Hemolytic Potential. Molecular Informatics, 2014, 33, 53-64.	2.5	4
42	Molecular dynamics simulations of a set of isoniazid derivatives bound to InhA, the enoyl-acp reductase fromM. tuberculosis. International Journal of Quantum Chemistry, 2006, 106, 2689-2699.	2.0	3
43	In silicostudy to analyse the disassembly of quercetin-targeted dendrimers potentially leishmanicide. Molecular Simulation, 2015, 41, 1495-1508.	2.0	3