

Kerly Pasqualoto

List of Publications by Year in descending order

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43
papers

945
citations

471509

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477307

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1509
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#	ARTICLE	IF	CITATIONS
1	Apoptotic effect of eugenol involves G2/M phase abrogation accompanied by mitochondrial damage and clastogenic effect on cancer cell in vitro. <i>Phytomedicine</i> , 2016, 23, 725-735.	5.3	43
2	Tick salivary gland as potential natural source for the discovery of promising antitumor drug candidates. <i>Biomedicine and Pharmacotherapy</i> , 2016, 77, 14-19.	5.6	17
3	BFD-22 a new potential inhibitor of BRAF inhibits the metastasis of B16F10 melanoma cells and simultaneously increased the tumor immunogenicity. <i>Toxicology and Applied Pharmacology</i> , 2016, 295, 56-67.	2.8	13
4	<i>In silico</i> study to analyse the disassembly of quercetin-targeted dendrimers potentially leishmanicide. <i>Molecular Simulation</i> , 2015, 41, 1495-1508.	2.0	3
5	RPF151, a novel capsaicin-like analogue: in vitro studies and in vivo preclinical antitumor evaluation in a breast cancer model. <i>Tumor Biology</i> , 2015, 36, 7251-7267.	1.8	18
6	Synthesis, characterization, in silico approach and in vitro antiproliferative activity of RPF151, a benzodioxole sulfonamide analogue designed from capsaicin scaffold. <i>Journal of Molecular Structure</i> , 2015, 1088, 138-146.	3.6	13
7	Designing and exploring active N ⁺ -(5-nitrofuranyl) methylene substituted hydrazides against three <i>Trypanosoma cruzi</i> strains more prevalent in Chagas disease patients. <i>European Journal of Medicinal Chemistry</i> , 2015, 96, 330-339.	5.5	17
8	Transcripts involved in hemostasis: Exploring salivary complexes from <i>Haementeria vizottoi</i> leeches through transcriptomics, phylogenetic studies and structural features. <i>Toxicon</i> , 2015, 106, 20-29.	1.6	12
9	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. <i>Applied Radiation and Isotopes</i> , 2015, 96, 91-101.	1.5	13
10	Mastoparan induces apoptosis in B16F10-Nex2 melanoma cells via the intrinsic mitochondrial pathway and displays antitumor activity in vivo. <i>Peptides</i> , 2015, 68, 113-119.	2.4	55
11	To Be Drug or Prodrug: Structure-Property Exploratory Approach Regarding Oral Bioavailability. <i>Journal of Pharmacy and Pharmaceutical Sciences</i> , 2014, 17, 532.	2.1	14
12	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. <i>Biochimie</i> , 2014, 99, 195-207.	2.6	25
13	Exploring 5-nitrofuranyl derivatives against nosocomial pathogens: Synthesis, antimicrobial activity and chemometric analysis. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 2844-2854.	3.0	29
14	Alkylphosphocholines as Promising Antitumor Agents: Exploring the Role of Structural Features on the Hemolytic Potential. <i>Molecular Informatics</i> , 2014, 33, 53-64.	2.5	4
15	Novel Capsaicin Analogues as Potential Anticancer Agents: Synthesis, Biological Evaluation, and <i>In Silico</i> Approach. <i>Archiv Der Pharmazie</i> , 2014, 347, 885-895.	4.1	14
16	Structural Findings and Molecular Modeling Approach of a TFPI-Like Inhibitor. <i>Protein and Peptide Letters</i> , 2014, 21, 452-457.	0.9	11
17	Design and exploratory data analysis of a second generation of dendrimer prodrugs potentially antichagasic and leishmanicide. <i>Molecular Diversity</i> , 2013, 17, 711-720.	3.9	13
18	5-Nitro-2-furfuriliden derivatives as potential anti- <i>Trypanosoma cruzi</i> agents: Design, synthesis, bioactivity evaluation, cytotoxicity and exploratory data analysis. <i>Bioorganic and Medicinal Chemistry</i> , 2013, 21, 5395-5406.	3.0	21

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19	Molecular modelling as a tool for studying the disassembly of potentially leishmanicide-targeted dendrimer. <i>Molecular Simulation</i> , 2013, 39, 860-867.	2.0	5
20	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. <i>Toxicol</i> , 2013, 69, 200-210.	1.6	4
21	Ligand-based design, synthesis, and experimental evaluation of novel benzofuroxan derivatives as anti- <i>Trypanosoma cruzi</i> agents. <i>European Journal of Medicinal Chemistry</i> , 2013, 64, 200-214.	5.5	18
22	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. <i>Toxicology and Applied Pharmacology</i> , 2013, 266, 385-398.	2.8	37
23	Dillapiole as Antileishmanial Agent: Discovery, Cytotoxic Activity and Preliminary SAR Studies of Dillapiole Analogues. <i>Archiv Der Pharmazie</i> , 2012, 345, 934-944.	4.1	30
24	Preliminary in vitro evaluation of N ² -(benzofuroxan-5-yl)methylene benzohydrazide derivatives as potential anti- <i>Trypanosoma cruzi</i> agents. <i>MedChemComm</i> , 2012, 3, 824.	3.4	9
25	A novel set of biaryl ether sulfonamide hydroxamates as potential MMPs inhibitors: Molecular dynamics simulations and molecular properties evaluation. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3374-3389.	2.0	4
26	Molecular modeling approach to predict a binding mode for the complex methotrexate-carboxypeptidase G2. <i>Journal of Molecular Modeling</i> , 2012, 18, 1867-1875.	1.8	4
27	Molecular modeling study on the disassembly of dendrimers designed as potential antichagasic and antileishmanial prodrugs. <i>Journal of Molecular Modeling</i> , 2012, 18, 2257-2269.	1.8	14
28	Self-organizing maps and VolSurf approach to predict aldose reductase inhibition by flavonoid compounds. <i>Revista Brasileira De Farmacognosia</i> , 2011, 21, 170-180.	1.4	13
29	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- <i>Trypanosoma cruzi</i> and antifungal agents. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 6292-6301.	3.0	35
30	Molecular modeling and QSAR studies of a set of indole and benzimidazole derivatives as H4 receptor antagonists. <i>Journal of Molecular Modeling</i> , 2011, 17, 921-928.	1.8	9
31	Novel benzofuroxan derivatives against multidrug-resistant <i>Staphylococcus aureus</i> strains: Design using Topoliss TM decision tree, synthesis and biological assay. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 5031-5038.	3.0	23
32	4D-QSAR: Perspectives in Drug Design. <i>Molecules</i> , 2010, 15, 3281-3294.	3.8	83
33	Molecular modeling as a promising tool to study dendrimer prodrugs delivery. <i>Computational and Theoretical Chemistry</i> , 2010, 939, 133-138.	1.5	17
34	Molecular modeling studies and in vitro bioactivity evaluation of a set of novel 5-nitro-heterocyclic derivatives as anti- <i>T. cruzi</i> agents. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 2673-2679.	3.0	18
35	Design, synthesis, antimicrobial activity and molecular modeling studies of novel benzofuroxan derivatives against <i>Staphylococcus aureus</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 3028-3036.	3.0	47
36	LQTA-QSAR: A New 4D-QSAR Methodology. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1428-1436.	5.4	70

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37	Rational Design and 3D-Pharmacophore Mapping of 5-Thiourea-Substituted $\hat{\pm}$ -Thymidine Analogues as Mycobacterial TMPK Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1070-1078.	5.4	33
38	Fragment-based and classical quantitative structure-activity relationships for a series of hydrazides as antituberculosis agents. <i>Molecular Diversity</i> , 2008, 12, 47-59.	3.9	24
39	A study of physicochemical and biopharmaceutical properties of Amoxicillin tablets using full factorial design and PCA biplot. <i>Analytica Chimica Acta</i> , 2007, 595, 216-220.	5.4	10
40	Application of a Receptor Pruning Methodology to the Enoyl-ACP Reductase from <i>Escherichia coli</i> (FabI). <i>QSAR and Combinatorial Science</i> , 2006, 25, 629-636.	1.4	15
41	Molecular dynamics simulations of a set of isoniazid derivatives bound to InhA, the enoyl-ACP reductase from <i>M. tuberculosis</i> . <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2689-2699.	2.0	3
42	Rational Design of New Antituberculosis Agents: A Receptor-Independent Four-Dimensional Quantitative Structure-Activity Relationship Analysis of a Set of Isoniazid Derivatives. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 3755-3764.	6.4	53
43	An Approach for the Rational Design of New Antituberculosis Agents. <i>Current Drug Targets</i> , 2001, 2, 427-437.	2.1	32