Rodolpho C Braga

List of Publications by Year
in descending order

57 papers	2,524 citations	201674 27 h-index	197818 49 g-index
67 all docs	67 docs citations	67 times ranked	3349 citing authors

#	Article	IF	Citations
1	STopTox: An in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012.	6.0	38
2	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267.	3.3	32
3	Applications of Virtual Screening in Bioprospecting: Facts, Shifts, and Perspectives to Explore the Chemo-Structural Diversity of Natural Products. Frontiers in Chemistry, 2021, 9, 662688.	3.6	38
4	BeeToxAI: An artificial intelligence-based web app to assess acute toxicity of chemicals to honey bees. Artificial Intelligence in the Life Sciences, 2021, 1, 100013.	2.2	8
5	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	5.4	21
6	Deep Learning-driven research for drug discovery: Tackling Malaria. PLoS Computational Biology, 2020, 16, e1007025.	3.2	34
7	DÃ©jÃ vu: Stimulating open drug discovery for SARS-CoV-2. Drug Discovery Today, 2020, 25, 928-941.	6.4	81
8	Discovery of new potent hits against intracellular Trypanosoma cruzi by QSAR-based virtual screening. European Journal of Medicinal Chemistry, 2019, 163, 649-659.	5.5	25
9	In Silico Chemogenomics Drug Repositioning Strategies for Neglected Tropical Diseases. Current Medicinal Chemistry, 2019, 26, 4355-4379.	2.4	24
10	Biological and Toxicological Evaluation of N-(4methyl-phenyl)-4-methylphthalimide on Bone Cancer in Mice. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 667-676.	1.7	0
11	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	6.7	35
12	Computational drug discovery for the Zika virus. Brazilian Journal of Pharmaceutical Sciences, 2018, 54, .	1.2	6
13	QSAR-Based Virtual Screening: Advances and Applications in Drug Discovery. Frontiers in Pharmacology, 2018, 9, 1275.	3.5	291
14	The Aâ€“Z of Zika drug discovery. Drug Discovery Today, 2018, 23, 1833-1847.	6.4	48
15	QSAR-Driven Design and Discovery of Novel Compounds With Antiplasmodial and Transmission Blocking Activities. Frontiers in Pharmacology, 2018, 9, 146.	3.5	22
16	In Vitro , In Silico , and In Vivo Analyses of Novel Aromatic Amidines against Trypanosoma cruzi. Antimicrobial Agents and Chemotherapy, 2018, 62, .	3.2	16
17	Design, synthesis, biological evaluation and X-ray structural studies of potent human dihydroorotate dehydrogenase inhibitors based on hydroxylated azole scaffolds. European Journal of Medicinal Chemistry, 2017, 129, 287-302.	5.5	46
18	QSAR-driven design, synthesis and discovery of potent chalcone derivatives with antitubercular activity. European Journal of Medicinal Chemistry, 2017, 137, 126-138.	5.5	96

#	Article	IF	Citations
19	Pred-Skin: A Fast and Reliable Web Application to Assess Skin Sensitization Effect of Chemicals. Journal of Chemical Information and Modeling, 2017, 57, 1013-1017.	5.4	79
20	Molecular dynamics simulations of Zika virus NS3 helicase: Insights into RNA binding site activity. Biochemical and Biophysical Research Communications, 2017, 492, 643-651.	2.1	32
21	Discovery of New Anti-Schistosomal Hits by Integration of QSAR-Based Virtual Screening and High Content Screening. Journal of Medicinal Chemistry, 2016, 59, 7075-7088.	6.4	67
22	Evaluation of cytotoxic effect of the combination of a pyridinyl carboxamide derivative and oxaliplatin on NCI-H1299 human non-small cell lung carcinoma cells. Biomedicine and Pharmacotherapy, 2016, 84, 1019-1028.	5.6	2
23	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	9.0	42
24	QSAR-Driven Discovery of Novel Chemical Scaffolds Active against Schistosoma mansoni. Journal of Chemical Information and Modeling, 2016, 56, 1357-1372.	5.4	47
25	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	9.0	103
26	Predâ€hERG: A Novel webâ€Accessible Computational Tool for Predicting Cardiac Toxicity. Molecular Informatics, 2015, 34, 698-701.	2.5	159
27	In Silico Repositioning-Chemogenomics Strategy Identifies New Drugs with Potential Activity against Multiple Life Stages of Schistosoma mansoni. PLoS Neglected Tropical Diseases, 2015, 9, e3435.	3.0	47
28	Advances in Methods for Predicting Phase I Metabolism of Polyphenols. Current Drug Metabolism, 2014, 15, 120-126.	1.2	22
29	Editorial (Thematic Issue: Drug Metabolism, Toxicology Experimental Determination and Theoretical) Tj ETQq1 1 0.784314 rgBT /Over Medicinal Chemistry, 2014, 14, 1323-1324.	2.1	1
30	In silico Prediction of Drug Metabolism by P450. Current Drug Metabolism, 2014, 15, 514-525.	1.2	27
31	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	2.1	82
32	Virtual Screening Strategies in Medicinal Chemistry: The State of the Art and Current Challenges. Current Topics in Medicinal Chemistry, 2014, 14, 1899-1912.	2.1	57
33	3D-QSAR Approaches in Drug Design: Perspectives to Generate Reliable CoMFA Models. Current Computer-Aided Drug Design, 2014, 10, 148-159.	1.2	45
34	Structural and chemical basis for enhanced affinity to a series of mycobacterial thymidine monophosphate kinase inhibitors: fragment-based QSAR and QM/MM docking studies. Journal of Molecular Modeling, 2013, 19, 179-192.	1.8	11
35	In silico metabolism studies of dietary flavonoids by CYP1A2 and CYP2C9. Food Research International, 2013, 50, 102-110.	6.2	26
36	Discovery of new potential hits of Plasmodium falciparum enoyl-ACP reductase through ligand- and structure-based drug design approaches. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 2436-2441.	2.2	14

#	Article	IF	Citations
37	New Tuberculostatic Agents Targeting Nucleic Acid Biosynthesis: Drug Design using QSAR Approaches. Current Pharmaceutical Design, 2013, 20, 4474-4485.	1.9	12
38	Assessing the Performance of 3D Pharmacophore Models in Virtual Screening: How Good are They?. Current Topics in Medicinal Chemistry, 2013, 13, 1127-1138.	2.1	103
39	QSAR and QM/MM Approaches Applied to Drug Metabolism Prediction. Mini-Reviews in Medicinal Chemistry, 2012, 12, 573-582.	2.4	23
40	Cyclic voltammetry and computational chemistry studies on the evaluation of the redox behavior of parabens and other analogues. Journal of the Brazilian Chemical Society, 2012, 23, 565-572.	0.6	29
41	Combination of docking, molecular dynamics and quantum mechanical calculations for metabolism prediction of 3,4-methylenedioxybenzoyl-2-thienylhydrazone. Journal of Molecular Modeling, 2012, 18, 2065-2078.	1.8	23
42	Microbial Î²-glycosylation of entacapone by Cunninghamella echinulata ATCC 9245. Journal of Bioscience and Bioengineering, 2012, 113, 611-613.	2.2	8
43	Development of topotecan loaded lipid nanoparticles for chemical stabilization and prolonged release. European Journal of Pharmaceutics and Biopharmaceutics, 2011, 79, 189-196.	4.3	126
44	Determination of the cardioactive prototype LASSBio-294 and its metabolites in dog plasma by LCâ€“MS/MS: Application for a pharmacokinetic study. Journal of Pharmaceutical and Biomedical Analysis, 2011, 55, 1024-1030.	2.8	7
45	Structure-based prediction and biosynthesis of the major mammalian metabolite of the cardioactive prototype LASSBio-294. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3734-3736.	2.2	14
46	Aspectos toxicolÃ³gicos e quÃmicos da Anatoxina-a e seus anÃ¡logos. Quimica Nova, 2006, 29, 1365-1371.	0.3	8
47	Dihydropyrimidin-(2H)-ones obtained byÂultrasound irradiation: aÂnew class ofÂpotential antioxidant agents. European Journal of Medicinal Chemistry, 2006, 41, 513-518.	5.5	132
48	A Mild and Efficient Method for Halogenation of 3,5-Dimethyl Pyrazoles by Ultrasound Irradiation Using N-Halosuccinimides.. ChemInform, 2006, 37, no.	0.0	0
49	Catalytic Applications of Chiral Organoselenium Compounds in Asymmetric Synthesis. Synlett, 2006, 2006, 1453-1466.	1.8	115
50	A mild and efficient method for halogenation of 3,5-dimethyl pyrazoles by ultrasound irradiation using N-halosuccinimides. Tetrahedron Letters, 2005, 46, 6833-6837.	1.4	81
51	Efficient Synthesis of Chiral Î²-Seleno Amides via Ring-Opening Reaction of 2-Oxazolines and Their Application in the Palladium-Catalyzed Asymmetric Allylic Alkylation. Journal of Organic Chemistry, 2005, 70, 9021-9024.	3.2	84
52	Development of Web and Mobile Applications for Chemical Toxicity Prediction. Journal of the Brazilian Chemical Society, 0, , .	0.6	18
53	Automated Framework for Developing Predictive Machine Learning Models for Data-Driven Drug Discovery. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
54	PIPELINE COMPUTACIONAL PARA O DESENHO DE PROTEÃNAS IMUNOGÃŠNICAS MULTI-EPITOPO DO VÃRUS NIPAH VISANDO O DESENVOLVIMENTO DE VACINAS. , 0, , .		0

#	Article	IF	Citations
55	QUIMIOINFORMÃ‡TICA: UMA INTRODUÃ‡ÃƒO. Quimica Nova, 0, , .	0.3	7
56	Fragment-based approach for affinity and selectivity for dUTPase: Insights for design of new anti-malarial agents. , 0, , .		0
57	Development of QSAR models for identification of CYP3A4 substrates and inhibitors. , 0, , .		1