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	QSAR-Based Virtual Screening: Advances and Applications in Drug Discovery. Frontiers in Pharmacology, 2018, 9, 1275.	3.5	291
2	Predâ€hERG: A Novel webâ€Accessible Computational Tool for Predicting Cardiac Toxicity. Molecular Informatics, 2015, 34, 698-701.	2.5	159
3	Dihydropyrimidin-(2H)-ones obtained byÂultrasound irradiation: aÂnew class ofÂpotential antioxidant agents. European Journal of Medicinal Chemistry, 2006, 41, 513-518.	5.5	132
4	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
5	Catalytic Applications of Chiral Organoselenium Compounds in Asymmetric Synthesis. Synlett, 2006, 2006, 1453-1466.	1.8	115
6	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	9.0	103
7	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
8	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
9	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
10	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	2.1	82
11	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
12	DÃ©jÃ vu: Stimulating open drug discovery for SARS-CoV-2. Drug Discovery Today, 2020, 25, 928-941.	6.4	81
13	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
14	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
15	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
16	The Aâ€“Z of Zika drug discovery. Drug Discovery Today, 2018, 23, 1833-1847.	6.4	48
17	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
18	QSAR-Driven Discovery of Novel Chemical Scaffolds Active against Schistosoma mansoni. Journal of Chemical Information and Modeling, 2016, 56, 1357-1372.	5.4	47

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19	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
20	3D-QSAR Approaches in Drug Design: Perspectives to Generate Reliable CoMFA Models. Current Computer-Aided Drug Design, 2014, 10, 148-159.	1.2	45
21	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	9.0	42
22	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
23	STopTox: An in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity. Environmental Health Perspectives, 2022, 130, 27012.	6.0	38
24	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	6.7	35
25	Deep Learning-driven research for drug discovery: Tackling Malaria. PLoS Computational Biology, 2020, 16, e1007025.	3.2	34
26	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
27	Pred-Skin: A Web Portal for Accurate Prediction of Human Skin Sensitizers. Chemical Research in Toxicology, 2021, 34, 258-267.	3.3	32
28	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
29	In silico Prediction of Drug Metabolism by P450. Current Drug Metabolism, 2014, 15, 514-525.	1.2	27
30	In silico metabolism studies of dietary flavonoids by CYP1A2 and CYP2C9. Food Research International, 2013, 50, 102-110.	6.2	26
31	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
32	In Silico Chemogenomics Drug Repositioning Strategies for Neglected Tropical Diseases. Current Medicinal Chemistry, 2019, 26, 4355-4379.	2.4	24
33	QSAR and QM/MM Approaches Applied to Drug Metabolism Prediction. Mini-Reviews in Medicinal Chemistry, 2012, 12, 573-582.	2.4	23
34	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
35	Advances in Methods for Predicting Phase I Metabolism of Polyphenols. Current Drug Metabolism, 2014, 15, 120-126.	1.2	22
36	QSAR-Driven Design and Discovery of Novel Compounds With Antiplasmodial and Transmission Blocking Activities. Frontiers in Pharmacology, 2018, 9, 146.	3.5	22

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37	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	5.4	21
38	Development of Web and Mobile Applications for Chemical Toxicity Prediction. Journal of the Brazilian Chemical Society, 0, , .	0.6	18
39	In Vitro , In Silico , and In Vivo Analyses of Novel Aromatic Amidines against Trypanosoma cruzi. Antimicrobial Agents and Chemotherapy, 2018, 62, .	3.2	16
40	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
41	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
42	New Tuberculostatic Agents Targeting Nucleic Acid Biosynthesis: Drug Design using QSAR Approaches. Current Pharmaceutical Design, 2013, 20, 4474-4485.	1.9	12
43	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
44	Aspectos toxicolÃ³gicos e quÃmicos da Anatoxina-a e seus anÃ¡logos. Quimica Nova, 2006, 29, 1365-1371.	0.3	8
45	Microbial Î²-glycosylation of entacapone by Cunninghamella echinulata ATCC 9245. Journal of Bioscience and Bioengineering, 2012, 113, 611-613.	2.2	8
46	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
47	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
48	QUIMIOINFORMÃ‡TICA: UMA INTRODUÃ‡ÃƒO. Quimica Nova, 0, , .	0.3	7
49	Computational drug discovery for the Zika virus. Brazilian Journal of Pharmaceutical Sciences, 2018, 54, .	1.2	6
50	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
51	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
52	Automated Framework for Developing Predictive Machine Learning Models for Data-Driven Drug Discovery. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
53	Development of QSAR models for identification of CYP3A4 substrates and inhibitors. , 0, , .		1
54	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

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55	PIPELINE COMPUTACIONAL PARA O DESENHO DE PROTEÃNAS IMUNOGÃŠNICAS MULTI-EPITOPO DO VÃRUS NIPAH VISANDO O DESENVOLVIMENTO DE VACINAS. , 0, , .		0
56	Fragment-based approach for affinity and selectivity for dUTPase: Insights for design of new anti-malarial agents. , 0, , .		0
57	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