Eduardo Borges de Melo

List of Publications by Year
in descending order

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38 papers	936 citations	623734 14 h-index	454955 30 g-index
42 all docs	42 docs citations	42 times ranked	1508 citing authors

#	Article	IF	Citations
1	Quantitative structure-activity relationship and machine learning studies of 2-thiazolylhydrazone derivatives with anti-Cryptococcus neoformans activity. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9789-9800.	3.5	2
2	SMILES-based 2D-QSAR and similarity search for identification of potential new scaffolds for development of SARS-CoV-2 MPRO inhibitors. Structural Chemistry, 2022, 33, 1691-1706.	2.0	10
3	Insights on 3D Structures of Potential Drugâ€targeting Proteins of SARSâ€CoVâ€2: Application of Cavity Search and Molecular Docking. Molecular Informatics, 2021, 40, e2000096.	2.5	13
4	O potencial uso dos inibidores da proteÃna transportadora de dopamina no tratamento de transtornos neuropsiquiÃ¡tricos / The potential use of dopamine transport inhibitors in the treatment of neuropsychiatric disorders. Brazilian Journal of Health Review, 2021, 4, 12105-12128.	0.1	0
5	Synthesis and anti-Mycobacterium tuberculosis activity of imide-Î²-carboline and carbomethoxy-Î²-carboline derivatives. European Journal of Medicinal Chemistry, 2020, 187, 111935.	5.5	15
6	Novel coumarins active against Trypanosoma cruzi and toxicity assessment using the animal model Caenorhabditis elegans. BMC Pharmacology & Toxicology, 2019, 20, 76.	2.4	7
7	In silico study toward the identification of new and safe potential inhibitors of photosynthetic electron transport. Ecotoxicology and Environmental Safety, 2018, 153, 175-180.	6.0	1
8	Development and characterization of lipid-polymeric nanoparticles for oral insulin delivery. Expert Opinion on Drug Delivery, 2018, 15, 213-222.	5.0	35
9	Synthesis of Nerol Derivatives Containing a 1,2,3-Triazole Moiety and Evaluation of Their Activities against Cancer Cell Lines. Journal of the Brazilian Chemical Society, 2018, , .	0.6	1
10	Synthesis and SAR of new isoxazole-triazole bis-heterocyclic compounds as analogues of natural lignans with antiparasitic activity. Bioorganic and Medicinal Chemistry, 2018, 26, 4850-4862.	3.0	27
11	Influence of hyaluronic acid on the formation of isolated poly(vinyl acetate) films for oral solid coatings. Journal of Applied Polymer Science, 2017, 134, .	2.6	4
12	A QSAR study of integrase strand transfer inhibitors based on a large set of pyrimidine, pyrimidone, and pyridopyrazine carboxamide derivatives. Journal of Molecular Structure, 2017, 1141, 252-260.	3.6	9
13	Synthesis and 2D-QSAR studies of neolignan-based diaryl-tetrahydrofuran and -furan analogues with remarkable activity against Trypanosoma cruzi and assessment of the trypanothione reductase activity. European Journal of Medicinal Chemistry, 2017, 140, 187-199.	5.5	20
14	A QSAR Study of Human Thymidine Phosphorylase Inhibitors with SMILES-Based Descriptors. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 85-100.	0.5	0
15	COMPUTACIONAL STUDY OF 1H-IMIDAZOL-2-YL-PYRIMIDINE-4,6-DIAMINES FOR IDENTIFICATION OF POTENTIAL PARENT COMPOUNDS OF NEW ANTIMALARIAL AGENTS. Quimica Nova, 2016, , .	0.3	2
16	A bestâ€‹ comprehension about the toxicity of phenylsulfonyl carboxylates in Vibrio fischeri using quantitative structure activity/property relationship methods. Journal of Hazardous Materials, 2016, 304, 233-241.	12.4	6
17	A structureâ€“activity relationship study of the toxicity of ionic liquids using an adapted Ferreiraâ€“Kiralj hydrophobicity parameter. Physical Chemistry Chemical Physics, 2015, 17, 4516-4523.	2.8	14
18	1,2,3-Triazole-based analogue of benznidazole displays remarkable activity against Trypanosoma cruzi. Bioorganic and Medicinal Chemistry, 2015, 23, 6815-6826.	3.0	26

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19	Molecular modelling and quantitative structure-activity relationship studies of anatoxin-a and epibatidine derivatives with affinity to rodent nAChR receptors. Chemical Papers, 2014, 68, .	2.2	1
20	An alternative approach for the use of water solubility of nonionic pesticides in the modeling of the soil sorption coefficients. Water Research, 2014, 53, 191-199.	11.3	22
21	Multivariate SAR and QSAR of cucurbitacin derivatives as cytotoxic compounds in a human lung adenocarcinoma cell line. Journal of Molecular Graphics and Modelling, 2014, 48, 70-79.	2.4	15
22	Modeling structureâ€“activity relationships of prodiginines with antimalarial activity using GA/MLR and OPS/PLS. Journal of Molecular Graphics and Modelling, 2014, 54, 19-31.	2.4	24
23	The effect of different logÂP algorithms on the modeling of the soil sorption coefficient of nonionic pesticides. Water Research, 2013, 47, 5751-5759.	11.3	17
24	A new, fully validated and interpreted quantitative structure-activity relationship model of p-aminosalicylic acid derivatives as neuraminidase inhibitors. Chemical Papers, 2013, 67, .	2.2	2
25	A QSAR Study of Matrix Metalloproteinases Type 2 (MMP-2) Inhibitors with Cinnamoyl Pyrrolidine Derivatives. Scientia Pharmaceutica, 2012, 80, 265-281.	2.0	10
26	Modeling physical and toxicity endpoints of alkyl (1-phenylsulfonyl) cycloalkane-carboxylates using the Ordered Predictors Selection (OPS) for variable selection and descriptors derived with SMILES. Chemometrics and Intelligent Laboratory Systems, 2012, 118, 79-87.	3.5	7
27	A new quantitative structureâ€“property relationship model to predict bioconcentration factors of polychlorinated biphenyls (PCBs) in fishes using E-state index and topological descriptors. Ecotoxicology and Environmental Safety, 2012, 75, 213-222.	6.0	26
28	Four-Dimensional Structureâ€“Activity Relationship Model to Predict HIV-1 Integrase Strand Transfer Inhibition using LQTA-QSAR Methodology. Journal of Chemical Information and Modeling, 2012, 52, 1722-1732.	5.4	25
29	Multivariate QSAR study on the antimutagenic activity of flavonoids against 3-NFA on Salmonella typhimurium TA98. European Journal of Medicinal Chemistry, 2010, 45, 4562-4569.	5.5	22
30	Multivariate SAR/QSAR of 3-aryl-4-hydroxyquinolin-2(1H)-one derivatives as type I fatty acid synthase (FAS) inhibitors. European Journal of Medicinal Chemistry, 2010, 45, 5817-5826.	5.5	29
31	Nonequivalent Effects of Diverse LogP Algorithms in Three QSAR Studies. QSAR and Combinatorial Science, 2009, 28, 1156-1165.	1.4	5
32	Multivariate QSAR study of 4,5-dihydroxypyrimidine carboxamides as HIV-1 integrase inhibitors. European Journal of Medicinal Chemistry, 2009, 44, 3577-3583.	5.5	29
33	Inibidores da HIV-integrase: potencial abordagem farmacolÃ³gica para tratamento da AIDS. Quimica Nova, 2006, 29, 555-562.	0.3	1
34	Î±- and Î²-Glucosidase inhibitors: chemical structure and biological activity. Tetrahedron, 2006, 62, 10277-10302.	1.9	490
35	alfa e <FONT FACE=Symbol>b-</FONT>glucosidases como alvos moleculares para desenvolvimento de fÃ¡rmacos. Quimica Nova, 2006, 29, 840-843.	0.3	9
36	Synthesis of (+)-(2R,3S,4R)-2,3,4-trihydroxycyclohexanone from d-glucose. Carbohydrate Research, 2004, 339, 361-365.	2.3	2

#	Article	IF	Citations
37	4D-QSAR Study of 17Î²-Hydroxysteroid Dehydrogenase Type 3 Inhibitors. Journal of the Brazilian Chemical Society, 0, , .	0.6	0
38	In silico Risk Assessment Studies of New Psychoactive Substances Derived from Amphetamines and Cathinones. Journal of the Brazilian Chemical Society, 0, , .	0.6	0