

Isabella Alvim Guedes

List of Publications by Year in descending order

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Version: 2024-02-01

21
papers

1,097
citations

759233

12
h-index

888059

17
g-index

22
all docs

22
docs citations

22
times ranked

1494
citing authors

#	ARTICLE	IF	CITATIONS
1	Receptor-ligand molecular docking. <i>Biophysical Reviews</i> , 2014, 6, 75-87.	3.2	324
2	Empirical Scoring Functions for Structure-Based Virtual Screening: Applications, Critical Aspects, and Challenges. <i>Frontiers in Pharmacology</i> , 2018, 9, 1089.	3.5	185
3	Highly Flexible Ligand Docking: Benchmarking of the DockThor Program on the LEADS-PEP Protein-Peptide Data Set. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 667-683.	5.4	144
4	New machine learning and physics-based scoring functions for drug discovery. <i>Scientific Reports</i> , 2021, 11, 3198.	3.3	91
5	Design, synthesis and evaluation of novel feruloyl-donepezil hybrids as potential multitarget drugs for the treatment of Alzheimer's disease. <i>European Journal of Medicinal Chemistry</i> , 2017, 130, 440-457.	5.5	67
6	Drug design and repurposing with DockThor-VS web server focusing on SARS-CoV-2 therapeutic targets and their non-synonym variants. <i>Scientific Reports</i> , 2021, 11, 5543.	3.3	63
7	Design, synthesis and pharmacological evaluation of N-benzyl-piperidinyl-aryl-acylhydrazone derivatives as donepezil hybrids: Discovery of novel multi-target anti-alzheimer prototype drug candidates. <i>European Journal of Medicinal Chemistry</i> , 2018, 147, 48-65.	5.5	52
8	Novel series of tacrine-tianeptine hybrids: Synthesis, cholinesterase inhibitory activity, S100B secretion and a molecular modeling approach. <i>European Journal of Medicinal Chemistry</i> , 2016, 121, 758-772.	5.5	39
9	Structural modeling and docking studies of ribose 5-phosphate isomerase from <i>Leishmania major</i> and <i>Homo sapiens</i> : A comparative analysis for Leishmaniasis treatment. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 55, 134-147.	2.4	23
10	Discovery of naphthyl-acylhydrazone p38 MAPK inhibitors with in vivo anti-inflammatory and anti-TNF activity. <i>Chemical Biology and Drug Design</i> , 2018, 91, 391-397.	3.2	22
11	Design, synthesis, cholinesterase inhibition and molecular modelling study of novel tacrine hybrids with carbohydrate derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 5566-5577.	3.0	21
12	Design, Synthesis and Biological Evaluation of Novel Triazole N-acylhydrazone Hybrids for Alzheimer's Disease. <i>Molecules</i> , 2020, 25, 3165.	3.8	14
13	Synthesis of new lophine-carbohydrate hybrids as cholinesterase inhibitors: cytotoxicity evaluation and molecular modeling. <i>MedChemComm</i> , 2019, 10, 2089-2101.	3.4	13
14	A unique SaeS allele overrides cell-density dependent expression of saeR and lukSF-PV in the ST30-SCCmecIV lineage of CA-MRSA. <i>International Journal of Medical Microbiology</i> , 2016, 306, 367-380.	3.6	10
15	LASSBio-1829 Hydrochloride: Development of a New Orally Active N-Acylhydrazone IKK2 Inhibitor with Anti-inflammatory Properties. <i>ChemMedChem</i> , 2016, 11, 234-244.	3.2	7
16	Cinnamoyl-N-Acylhydrazone-Donepezil Hybrids: Synthesis and Evaluation of Novel Multifunctional Ligands Against Neurodegenerative Diseases. <i>Neurochemical Research</i> , 2020, 45, 3003-3020.	3.3	7
17	Isobenzofuran-1(3H)-ones as new tyrosinase inhibitors: Biological activity and interaction studies by molecular docking and NMR. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2021, 1869, 140580.	2.3	6
18	Chiral Bistacrine Analogues: Synthesis, Cholinesterase Inhibitory Activity and a Molecular Modeling Approach. <i>Journal of the Brazilian Chemical Society</i> , 0, , .	0.6	5

#	ARTICLE	IF	CITATIONS
19	Expedient Microwave-Assisted Synthesis of Bis(n)-lophine Analogues as Selective Butyrylcholinesterase Inhibitors: Cytotoxicity Evaluation and Molecular Modelling. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
20	Design, synthesis, and biological evaluation of new thalidomideâ€“donepezil hybrids as neuroprotective agents targeting cholinesterases and neuroinflammation. RSC Medicinal Chemistry, 0, , .	3.9	1
21	An Expedient Synthesis of Tacrine-Squaric Hybrids as Potent, Selective and Dualâ€“Binding Cholinesterase Inhibitors. Journal of the Brazilian Chemical Society, 0, , .	0.6	0