Vinicius G Maltarollo

List of Publications by Year
in descending order

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26	466	687363 13	713466 21
papers	citations	h-index	g-index

26	26	26	597
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Transfer and Multi-task Learning in QSAR Modeling: Advances and Challenges. Frontiers in Pharmacology, 2018, 9, 74.	3.5	87
2	Advances and Perspectives in Applying Deep Learning for Drug Design and Discovery. Frontiers in Robotics and AI, 2019, 6, 108.	3.2	60
3	Recent Advances in the Prediction of Pharmacokinetics Properties in Drug Design Studies: A Review. ChemMedChem, 2022, 17, .	3.2	44
4	Advanced QSAR studies on PPARÎ´ ligands related to metabolic diseases. Journal of the Brazilian Chemical Society, 2012, 23, 78-84.	0.6	23
5	Structure-Based Virtual Screening and Discovery of New PPARÎ´/Î³ Dual Agonist and PPARÎ´ and Î³ Agonists. PLoS ONE, 2015, 10, e0118790.	2.5	21
6	Theoretical study of tautomers and photoisomers of avobenzone by DFT methods. Journal of Molecular Modeling, 2015, 21, 319.	1.8	20
7	Computational studies of TGF-Î²RI (ALK-5) inhibitors: Analysis of the binding interactions between ligandâ€“receptor using 2D and 3D techniques. European Journal of Pharmaceutical Sciences, 2013, 49, 542-549.	4.0	18
8	Quantitative structureâ€“activity relationships (HQSAR, CoMFA, and CoMSIA) studies for COX-2 selective inhibitors. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1436-1445.	3.5	17
9	Antibacterial activity of synthetic 1,3â€bis(aryloxy)propanâ€2â€amines against Gramâ€positive bacteria. MicrobiologyOpen, 2019, 8, e814.	3.0	16
10	Knowing and combating the enemy: a brief review on SARS-CoV-2 and computational approaches applied to the discovery of drug candidates. Bioscience Reports, 2021, 41, .	2.4	16
11	Theoretical study on the molecular and electronic properties of some substances used for diabetes mellitus treatment. Journal of Molecular Modeling, 2010, 16, 799-804.	1.8	15
12	Hologram QSAR Studies of Antiprotozoal Activities of Sesquiterpene Lactones. Molecules, 2014, 19, 10546-10562.	3.8	15
13	GQ-11: A new PPAR agonist improves obesity-induced metabolic alterations in LDLrâ^'/â^' mice. International Journal of Obesity, 2018, 42, 1062-1072.	3.4	15
14	Application of bioisosterism in design of the semicarbazone derivatives as cruzain inhibitors: a theoretical and experimental study. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1244-1259.	3.5	14
15	Role of physicochemical properties in the activation of peroxisome proliferator-activated receptor Î´. Journal of Molecular Modeling, 2011, 17, 2549-2558.	1.8	12
16	Hologram quantitative structureâ€“activity relationship and comparative molecular interaction field analysis of aminothiazole and thiazolesulfonamide as reversible LSD1 inhibitors. Future Medicinal Chemistry, 2015, 7, 1381-1394.	2.3	12
17	Synthesis of arylfuran derivatives as potential antibacterial agents. Medicinal Chemistry Research, 2021, 30, 1074-1086.	2.4	9
18	Ligandâ€•and Structureâ€Based Drug Design Strategies and PPARÎ´/Î± Selectivity. Chemical Biology and Drug Design, 2012, 80, 533-544.	3.2	8

#	Article	IF	Citations
19	Current trends in quantitative structureâ€“activity relationship validation and applications on drug discovery. Future Science OA, 2017, 3, FSO214.	1.9	8
20	In silico studies on the interaction between bioactive ligands and ALK5, a biological target related to the cancer treatment. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2045-2053.	3.5	7
21	Structure-Based Virtual Screening, Molecular Dynamics and Binding Free Energy Calculations of Hit Candidates as ALK-5 Inhibitors. Molecules, 2020, 25, 264.	3.8	7
22	The Role of QSAR and Virtual Screening Studies in Type 2 Diabetes Drug Discovery. Medicinal Chemistry, 2017, 13, 706-720.	1.5	7
23	Molecular Features Related to HIV Integrase Inhibition Obtained from Structure- and Ligand-Based Approaches. PLoS ONE, 2014, 9, e81301.	2.5	6
24	On the relationship of anthranilic derivatives structure and the FXR (Farnesoid X receptor) agonist activity. Journal of Biomolecular Structure and Dynamics, 2018, 36, 4378-4391.	3.5	5
25	Understanding electrostatic and steric requirements related to hypertensive action of AT1 antagonists using molecular modeling techniques. Journal of Molecular Modeling, 2014, 20, 2231.	1.8	2
26	Understanding PPAR-Î´ affinity and selectivity using hologram quantitative structureâ€“activity modeling, molecular docking and GRID calculations. Future Medicinal Chemistry, 2016, 8, 1913-1926.	2.3	2