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	Recent Advances in the Prediction of Pharmacokinetics Properties in Drug Design Studies: A Review. ChemMedChem, 2022, 17, .	3.2	44
2	Synthesis of arylfuran derivatives as potential antibacterial agents. Medicinal Chemistry Research, 2021, 30, 1074-1086.	2.4	9
3	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
4	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
5	Advances and Perspectives in Applying Deep Learning for Drug Design and Discovery. Frontiers in Robotics and AI, 2019, 6, 108.	3.2	60
6	Antibacterial activity of synthetic 1,3â€bis(aryloxy)propanâ€2â€amines against Gramâ€positive bacteria. MicrobiologyOpen, 2019, 8, e814.	3.0	16
7	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
8	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
9	Transfer and Multi-task Learning in QSAR Modeling: Advances and Challenges. Frontiers in Pharmacology, 2018, 9, 74.	3.5	87
10	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
11	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
12	Current trends in quantitative structureâ€“activity relationship validation and applications on drug discovery. Future Science OA, 2017, 3, FSO214.	1.9	8
13	The Role of QSAR and Virtual Screening Studies in Type 2 Diabetes Drug Discovery. Medicinal Chemistry, 2017, 13, 706-720.	1.5	7
14	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
15	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
16	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
17	Theoretical study of tautomers and photoisomers of avobenzone by DFT methods. Journal of Molecular Modeling, 2015, 21, 319.	1.8	20
18	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

#	Article	IF	Citations
19	Molecular Features Related to HIV Integrase Inhibition Obtained from Structure- and Ligand-Based Approaches. PLoS ONE, 2014, 9, e81301.	2.5	6
20	Hologram QSAR Studies of Antiprotozoal Activities of Sesquiterpene Lactones. Molecules, 2014, 19, 10546-10562.	3.8	15
21	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
22	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
23	Advanced QSAR studies on PPARÎ´ ligands related to metabolic diseases. Journal of the Brazilian Chemical Society, 2012, 23, 78-84.	0.6	23
24	Ligandâ€•and Structureâ€Based Drug Design Strategies and PPARÎ´/Î± Selectivity. Chemical Biology and Drug Design, 2012, 80, 533-544.	3.2	8
25	Role of physicochemical properties in the activation of peroxisome proliferator-activated receptor Î´. Journal of Molecular Modeling, 2011, 17, 2549-2558.	1.8	12
26	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