Leonardo Bruno Federico

List of Publications by Year
in descending order

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		1162367	940134
21	271	8	16
papers	citations	h-index	g-index

21	21	21	411
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Virtual screening, ADME/Tox predictions and the drug repurposing concept for future use of old drugs against the COVID-19. Life Sciences, 2020, 256, 117963.	2.0	58
2	Novel chalcones derivatives with potential antineoplastic activity investigated by docking and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2204-2216.	2.0	53
3	Pharmacophore and structure-based drug design, molecular dynamics and admet/tox studies to design novel potential pad4 inhibitors. Journal of Biomolecular Structure and Dynamics, 2019, 37, 966-981.	2.0	30
4	Molecular modeling and statistical analysis in the design of derivatives of human dipeptidyl peptidase IV. Journal of Biomolecular Structure and Dynamics, 2018, 36, 318-334.	2.0	18
5	Hierarchical Virtual Screening of Potential Insectides Inhibitors of Acetylcholinesterase and Juvenile Hormone from Temephos. Pharmaceuticals, 2019, 12, 61.	1.7	18
6	Identification of New Inhibitors with Potential Antitumor Activity from Polypeptide Structures via Hierarchical Virtual Screening. Molecules, 2019, 24, 2943.	1.7	16
7	In silico development of new acetylcholinesterase inhibitors. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1007-1021.	2.0	15
8	Revisiting the Proposition of Binding Pockets and Bioactive Poses for GSK-3Î² Allosteric Modulators Addressed to Neurodegenerative Diseases. International Journal of Molecular Sciences, 2021, 22, 8252.	1.8	9
9	GRIND2-based 3D-QSAR and prediction of activity spectra for symmetrical bis-pyridinium salts with promastigote antileishmanial activity. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2430-2440.	2.0	8
10	Identification of known drugs as potential SARS-CoV-2 Mpro inhibitors using ligand- and structure-based virtual screening. Future Medicinal Chemistry, 2021, 13, 1353-1366.	1.1	8
11	Identification of novel Î±Î²-tubulin modulators with antiproliferative activity directed to cancer therapy using ligand and structure-based virtual screening. International Journal of Biological Macromolecules, 2020, 165, 3040-3050.	3.6	7
12	Potential colchicine binding site inhibitors unraveled by virtual screening, molecular dynamics and MM/PBSA. Computers in Biology and Medicine, 2021, 137, 104817.	3.9	7
13	Prediction of the Three-Dimensional Structure of Phosphate-6-mannose PMI Present in the Cell Membrane of Xanthomonas citri subsp. citri of Interest for the Citrus Canker Control. Engineering Materials, 2020, , 259-276.	0.3	6
14	Structure-Based Drug Design of Novel MARK-3 Inhibitors in Cancer. Current Bioactive Compounds, 2014, 10, 131-138.	0.2	4
15	Ligand and Structure-Based Drug Design as Strategies for the Screening of New BACE1 Inhibitor Candidates. Current Physical Chemistry, 2016, 5, 253-262.	0.1	4
16	Key Aspects for Achieving Hits by Virtual Screening Studies. Engineering Materials, 2021, , 455-487.	0.3	3
17	In Silico Methods to Predict Relevant Toxicological Endpoints of Bioactive Substances. Engineering Materials, 2021, , 649-676.	0.3	2
18	Ligand- and Structure-Based Drug Design of Novel Calcium Channel Blockers. Journal of Computational and Theoretical Nanoscience, 2017, 14, 3489-3502.	0.4	2

#	Article	IF	Citations
19	A MLR and ADME/Tox Study of New Dihydroartemisinin Compounds with Antimalarial Activity. Journal of Computational and Theoretical Nanoscience, 2018, 15, 1785-1794.	0.4	2
20	ADME/Tox Study and Molecular Dynamics Simulations Applied in the Design of New Potential GABA-AT Inhibitors. Engineering Materials, 2021, , 719-738.	0.3	1
21	Discovery of Novel Leishmanicidal Drugs with Potential L-type Calcium Channel Blockage, Designed by Similarity-Based Virtual Screening Approaches. , 2017, , 01-06.		0