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	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
2	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
3	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
4	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
5	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
6	In Silico Methods to Predict Relevant Toxicological Endpoints of Bioactive Substances. Engineering Materials, 2021, , 649-676.	0.3	2
7	Key Aspects for Achieving Hits by Virtual Screening Studies. Engineering Materials, 2021, , 455-487.	0.3	3
8	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
9	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
10	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
11	Identification of New Inhibitors with Potential Antitumor Activity from Polypeptide Structures via Hierarchical Virtual Screening. Molecules, 2019, 24, 2943.	1.7	16
12	Hierarchical Virtual Screening of Potential Insectides Inhibitors of Acetylcholinesterase and Juvenile Hormone from Temephos. Pharmaceuticals, 2019, 12, 61.	1.7	18
13	In silico development of new acetylcholinesterase inhibitors. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1007-1021.	2.0	15
14	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
15	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
16	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
17	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
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	Discovery of Novel Leishmanicidal Drugs with Potential L-type Calcium Channel Blockage, Designed by Similarity-Based Virtual Screening Approaches. , 2017, , 01-06.		0
20	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
21	Structure-Based Drug Design of Novel MARK-3 Inhibitors in Cancer. Current Bioactive Compounds, 2014, 10, 131-138.	0.2	4