Akhil Kumar

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9573946/publications.pdf

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19	397	840585 11	839398 18
papers	citations	h-index	g-index

19	19	19	683
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular docking based virtual screening of natural compounds as potential BACE1 inhibitors: 3D QSAR pharmacophore mapping and molecular dynamics analysis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 239-249.	2.0	44
2	Determination of potential inhibitors based on isatin derivatives against SARS-CoV-2 main protease (m^{pro}): a molecular docking, molecular dynamics and structure-activity relationship studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3110-3128.	2.0	41
3	Changing Paradigm from one Target one Ligand Towards Multi-target Directed Ligand Design for Key Drug Targets of Alzheimer Disease: An Important Role of In Silico Methods in Multi-target Directed Ligands Design. Current Neuropharmacology, 2018, 16, 726-739.	1.4	40
4	Molecular insight into amyloid oligomer destabilizing mechanism of flavonoid derivative 2-(4â€² Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 6 Journal of Biomolecular Structure and Dynamics, 2016, 34, 1252-1263.	2.0	37
5	Docking, molecular dynamics, binding energy-MM-PBSA studies of naphthofuran derivatives to identify potential dual inhibitors against BACE-1 and GSK-3Î². Journal of Biomolecular Structure and Dynamics, 2019, 37, 275-290.	2.0	37
6	The Flavonoid Derivative 2-(4â€² Benzyloxyphenyl)-3-hydroxy-chromen-4-one Protects Against AÎ²42-Induced Neurodegeneration in Transgenic Drosophila: Insights from In Silico and In Vivo Studies. Neurotoxicity Research, 2014, 26, 331-350.	1.3	34
7	Virtual screening, ADMET profiling, molecular docking and dynamics approaches to search for potent selective natural molecules based inhibitors against metallothionein-III to study Alzheimerâ€™s disease. Methods, 2015, 83, 105-110.	1.9	34
8	Gallic acid-based indanone derivative interacts synergistically with tetracycline by inhibiting efflux pump in multidrug resistant E. coli. Applied Microbiology and Biotechnology, 2016, 100, 2311-2325.	1.7	27
9	Investigation of naphthofuran moiety as potential dual inhibitor against BACE-1 and GSK-3Î²: molecular dynamics simulations, binding energy, and network analysis to identify first-in-class dual inhibitors against Alzheimerâ€™s disease. Journal of Molecular Modeling, 2017, 23, 239.	0.8	20
10	Molecular investigation of active binding site of isoniazid (INH) and insight into resistance mechanism of S315T-MtKatG in Mycobacterium tuberculosis. Tuberculosis, 2017, 105, 18-27.	0.8	19
11	Molecular docking and simulation studies to give insight of surfactin amyloid interaction for destabilizing Alzheimerâ€™s AÎ²42 protofibrils. Medicinal Chemistry Research, 2016, 25, 1616-1622.	1.1	18
12	The effect of Benzothiazoloneâ€2 on the expression of Metallothioneinâ€3 in modulating Alzheimer's disease. Brain and Behavior, 2017, 7, e00799.	1.0	11
13	Structural investigations into the binding mode of novel neolignans Cmp10 and Cmp19 microtubule stabilizers byin silicomolecular docking, molecular dynamics, and binding free energy calculations. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1232-1240.	2.0	8
14	Screening of Anti-mycobacterial Phytochemical Compounds for Potential Inhibitors against Mycobacterium Tuberculosis Isocitrate Lyase. Current Topics in Medicinal Chemistry, 2019, 19, 600-608.	1.0	8
15	A physicochemical descriptor based method for effective and rapid screening of dual inhibitors against BACE-1 and GSK-3Î² as targets for Alzheimerâ€™s disease. Computational Biology and Chemistry, 2017, 71, 1-9.	1.1	6
16	Computational Modeling of Multi-target-Directed Inhibitors Against Alzheimerâ€™s Disease. Neuromethods, 2018, , 533-571.	0.2	6
17	Molecular insight into multiple RpoB clinical mutants of Mycobacterium tuberculosis: An attempt to probe structural variations in rifampicin binding site underlying drug resistance. International Journal of Biological Macromolecules, 2018, 120, 2200-2214.	3.6	5
18	Current Trends in Docking Methodologies. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 320-338.	0.3	1

#	Article	IF	Citations
19	Current Trends in Docking Methodologies. , 2017, , 829-847.		1