

Akhil Kumar

List of Publications by Citations

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19
papers

289
citations

11
h-index

16
g-index

19
ext. papers

338
ext. citations

3.5
avg, IF

3.52
L-index

#	Paper	IF	Citations
19	Molecular docking based virtual screening of natural compounds as potential BACE1 inhibitors: 3D QSAR pharmacophore mapping and molecular dynamics analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 239-49	3.6	36
18	Virtual screening, ADMET profiling, molecular docking and dynamics approaches to search for potent selective natural molecules based inhibitors against metallothionein-III to study Alzheimer's disease. <i>Methods</i> , 2015 , 83, 105-10	4.6	28
17	Molecular insight into amyloid oligomer destabilizing mechanism of flavonoid derivative 2-(4' benzyloxyphenyl)-3-hydroxy-chromen-4-one through docking and molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 1252-63	3.6	27
16	The flavonoid derivative 2-(4' Benzyloxyphenyl)-3-hydroxy-chromen-4-one protects against A β 2-induced neurodegeneration in transgenic Drosophila: insights from in silico and in vivo studies. <i>Neurotoxicity Research</i> , 2014 , 26, 331-50	4.3	27
15	Docking, molecular dynamics, binding energy-MM-PBSA studies of naphthofuran derivatives to identify potential dual inhibitors against BACE-1 and GSK-3 β <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 275-290	3.6	26
14	Determination of potential inhibitors based on isatin derivatives against SARS-CoV-2 main protease (m): a molecular docking, molecular dynamics and structure-activity relationship studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-19	3.6	24
13	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. <i>Current Neuropharmacology</i> , 2018 , 16, 726-739	7.6	23
12	Gallic acid-based indanone derivative interacts synergistically with tetracycline by inhibiting efflux pump in multidrug resistant E. coli. <i>Applied Microbiology and Biotechnology</i> , 2016 , 100, 2311-25	5.7	21
11	Molecular investigation of active binding site of isoniazid (INH) and insight into resistance mechanism of S315T-MtKatG in Mycobacterium tuberculosis. <i>Tuberculosis</i> , 2017 , 105, 18-27	2.6	16
10	Investigation of naphthofuran moiety as potential dual inhibitor against BACE-1 and GSK-3 β molecular dynamics simulations, binding energy, and network analysis to identify first-in-class dual inhibitors against Alzheimer's disease. <i>Journal of Molecular Modeling</i> , 2017 , 23, 239	2	14
9	Molecular docking and simulation studies to give insight of surfactin amyloid interaction for destabilizing Alzheimer's A β 2 protofibrils. <i>Medicinal Chemistry Research</i> , 2016 , 25, 1616-1622	2.2	14
8	The effect of Benzothiazolone-2 on the expression of Metallothionein-3 in modulating Alzheimer's disease. <i>Brain and Behavior</i> , 2017 , 7, e00799	3.4	11
7	Structural investigations into the binding mode of novel neolignans Cmp10 and Cmp19 microtubule stabilizers by in silico molecular docking, molecular dynamics, and binding free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 1232-40	3.6	6
6	A physicochemical descriptor based method for effective and rapid screening of dual inhibitors against BACE-1 and GSK-3 β as targets for Alzheimer's disease. <i>Computational Biology and Chemistry</i> , 2017 , 71, 1-9	3.6	4
5	Screening of Anti-mycobacterial Phytochemical Compounds for Potential Inhibitors against Mycobacterium Tuberculosis Isocitrate Lyase. <i>Current Topics in Medicinal Chemistry</i> , 2019 , 19, 600-608	3	4
4	Molecular insight into multiple RpoB clinical mutants of Mycobacterium tuberculosis: An attempt to probe structural variations in rifampicin binding site underlying drug resistance. <i>International Journal of Biological Macromolecules</i> , 2018 , 120, 2200-2214	7.9	4
3	Computational Modeling of Multi-target-Directed Inhibitors Against Alzheimer's Disease. <i>Neuromethods</i> , 2018 , 533-571	0.4	3

2	Current Trends in Docking Methodologies. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , 2016 , 320-338	0.3	1
1	Current Trends in Docking Methodologies 2017 , 829-847		0