Akhil Kumar

List of Publications by Year in Descending Order

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	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. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-19	3.6	24
18	Screening of Anti-mycobacterial Phytochemical Compounds for Potential Inhibitors against Mycobacterium Tuberculosis Isocitrate Lyase. *Current Topics in Medicinal Chemistry*, **2019**, 19, 600-608	3	4
17	Docking, molecular dynamics, binding energy-MM-PBSA studies of naphthofuran derivatives to identify potential dual inhibitors against BACE-1 and GSK-3β. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 275-290	3.6	26
16	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	7.6	23
15	Computational Modeling of Multi-target-Directed Inhibitors Against Alzheimer's Disease. *Neuromethods*, **2018**, 533-571	0.4	3
14	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	7.9	4
13	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	2.6	16
12	The effect of Benzothiazolone-2 on the expression of Metallothionein-3 in modulating Alzheimer's disease. *Brain and Behavior*, **2017**, 7, e00799	3.4	11
11	A physicochemical descriptor based method for effective and rapid screening of dual inhibitors against BACE-1 and GSK-3β as targets for Alzheimer's disease. *Computational Biology and Chemistry*, **2017**, 71, 1-9	3.6	4
10	Investigation of naphthofuran moiety as potential dual inhibitor against BACE-1 and GSK-3β molecular dynamics simulations, binding energy, and network analysis to identify first-in-class dual inhibitors against Alzheimer's disease. *Journal of Molecular Modeling*, **2017**, 23, 239	2	14
9	Current Trends in Docking Methodologies **2017**, 829-847		0
8	Molecular insight into amyloid oligomer destabilizing mechanism of flavonoid derivative 2-(4' benzyloxyphenyl)-3-hydroxy-chromen-4-one through docking and molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 1252-63	3.6	27
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. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 1232-40	3.6	6
6	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, 239-49	3.6	36
5	Gallic acid-based indanone derivative interacts synergistically with tetracycline by inhibiting efflux pump in multidrug resistant E. coli. *Applied Microbiology and Biotechnology*, **2016**, 100, 2311-25	5.7	21
4	Current Trends in Docking Methodologies. *Advances in Medical Technologies and Clinical Practice Book Series*, **2016**, 320-338	0.3	1
3	Molecular docking and simulation studies to give insight of surfactin amyloid interaction for destabilizing Alzheimer's Aβ42 protofibrils. *Medicinal Chemistry Research*, **2016**, 25, 1616-1622	2.2	14

2	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. *Methods*, **2015**, 83, 105-10	4.6	28
1	The flavonoid derivative 2-(4' Benzyloxyphenyl)-3-hydroxy-chromen-4-one protects against Aβ42-induced neurodegeneration in transgenic Drosophila: insights from in silico and in vivo studies. *Neurotoxicity Research*, **2014**, 26, 331-50	4.3	27