Rajnish Kumar

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

37 papers	450 citations	13 h-index	20 g-index
40 ext. papers	603 ext. citations	3.8 avg, IF	4.15 L-index

#	Paper	IF	Citations
37	Design, synthesis, biological evaluations and in silico studies of sulfonate ester derivatives of 2-(2-benzylidenehydrazono)thiazolidin-4-one as potential -glucosidase inhibitors. *Journal of Molecular Structure*, **2022**, 1247, 131266	3.4	1
36	Deep learning tools for advancing drug discovery and development.. *3 Biotech*, **2022**, 12, 110	2.8	2
35	Allosteric Binding Sites of Ab Peptides on the Acetylcholine Synthesizing Enzyme ChAT as Deduced by In Silico Molecular Modeling. *International Journal of Molecular Sciences*, **2022**, 23, 6073	6.3	2
34	Urea-thiazole/benzothiazole hybrids with a triazole linker: synthesis, antimicrobial potential, pharmacokinetic profile and in silico mechanistic studies. *Molecular Diversity*, **2021**, 1	3.1	2
33	Synthesis and studies of thiazolidinedione-isatin hybrids as -glucosidase inhibitors for management of diabetes. *Future Medicinal Chemistry*, **2021**, 13, 457-485	4.1	4
32	Tozasertib Attenuates Neuropathic Pain by Interfering with Aurora Kinase and KIF11 Mediated Nociception. *ACS Chemical Neuroscience*, **2021**, 12, 1948-1960	5.7	9
31	Hydroxytyrosol as anti-parkinsonian molecule: Assessment using in-silico and MPTP-induced Parkinson's disease model. *Biomedicine and Pharmacotherapy*, **2021**, 139, 111525	7.5	3
30	Small molecule therapeutics for tauopathy in Alzheimer's disease: Walking on the path of most resistance. *European Journal of Medicinal Chemistry*, **2021**, 209, 112915	6.8	16
29	Structure-based virtual screening and molecular dynamics simulation for the identification of sphingosine kinase-2 inhibitors as potential analgesics. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-19	3.6	0
28	FKBP51-Hsp90 complex as a novel therapeutic target for Alzheimer disease. *Alzheimer's and Dementia*, **2020**, 16, e042684	1.2	1
27	Proton pump inhibitors act with unprecedented potencies as inhibitors of the acetylcholine biosynthesizing enzyme-A plausible missing link for their association with incidence of dementia. *Alzheimer's and Dementia*, **2020**, 16, 1031-1042	1.2	16
26	Metal Binding by GMP-1 and Its Pyrimido [1, 2]benzimidazole Analogs Confirms Protection Against Amyloid-Associated Neurotoxicity. *Journal of Alzheimer's Disease*, **2020**, 73, 695-705	4.3	5
25	Esomeprazole reduces sperm motility index by targeting the spermic cholinergic machinery: A mechanistic study for the association between use of proton pump inhibitors and reduced sperm motility index. *Biochemical Pharmacology*, **2020**, 182, 114212	6	2
24	Targeting SARS-CoV-2 main protease: structure based virtual screening, in silico ADMET studies and molecular dynamics simulation for identification of potential inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-17	3.6	10
23	Computational Outlook of Marine Compounds as Anti-Cancer Representatives Targeting BCL-2 and Survivin. *Current Computer-Aided Drug Design*, **2019**, 15, 265-276	1.4	2
22	Hsp90 as a Member of Dicarboxylate Clamp TPR Protein Interaction Network: Implication in Human Diseases and Prospect as a Drug Target. *Heat Shock Proteins*, **2019**, 281-295	0.2	0
21	Exploring sulfonate esters of 5-arylidene thiazolidine-2,4-diones as PTP1B inhibitors with anti-hyperglycemic activity. *Medicinal Chemistry Research*, **2018**, 27, 476-487	2.2	7

20	In silico modelling and molecular dynamics simulation studies of thiazolidine based PTP1B inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 1195-1211	3.6	17
19	identification and biochemical characterization of the human dicarboxylate clamp TPR protein interaction network. *FEBS Open Bio*, **2018**, 8, 1830-1843	2.7	3
18	Soluble A□2 Acts as Allosteric Activator of the Core Cholinergic Enzyme Choline Acetyltransferase. *Frontiers in Molecular Neuroscience*, **2018**, 11, 327	6.1	5
17	Synthesis, crystal structure and antimicrobial potential of some fluorinated chalcone-1,2,3-triazole conjugates. *European Journal of Medicinal Chemistry*, **2018**, 155, 263-274	6.8	65
16	Synthesis, biological evaluation and in silico studies of 5-(3-methoxybenzylidene)thiazolidine-2,4-dione analogues as PTP1B inhibitors. *Bioorganic Chemistry*, **2017**, 71, 1-9	5.1	14
15	N-alkylated thiazolidine-2,4-dione analogs as PTP1B inhibitors: synthesis, biological activity, and docking studies. *Medicinal Chemistry Research*, **2017**, 26, 1176-1183	2.2	8
14	Combined x-ray crystallography and computational modeling approach to investigate the Hsp90 C-terminal peptide binding to FKBP51. *Scientific Reports*, **2017**, 7, 14288	4.9	15
13	Discovery of novel choline acetyltransferase inhibitors using structure-based virtual screening. *Scientific Reports*, **2017**, 7, 16287	4.9	21
12	Evaluation of potential flavonoid inhibitors of glyoxalase-I based on virtual screening and in vitro studies. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 993-1007	3.6	19
11	Novel ligands of Choline Acetyltransferase designed by in silico molecular docking, hologram QSAR and lead optimization. *Scientific Reports*, **2016**, 6, 31247	4.9	20
10	Amyloid-□peptides act as allosteric modulators of cholinergic signalling through formation of soluble BA□ACs. *Brain*, **2016**, 139, 174-92	11.2	24
9	Zingerone silences quorum sensing and attenuates virulence of Pseudomonas aeruginosa. *F□toterap□* **2015**, 102, 84-95	3.2	64
8	In silico accounting of novel pyridazine analogues as h-PTP 1B inhibitors: pharmacophore modelling, atom-based 3D QSAR and docking studies. *Medicinal Chemistry Research*, **2014**, 23, 2701-2711	2.2	5
7	A paradigm for development of novel PTP 1B inhibitors: Pharmacophore modelling, atom-based 3D-QSAR and docking studies. *Medicinal Chemistry Research*, **2014**, 23, 927-938	2.2	4
6	Validation of formylchromane derivatives as protein tyrosine phosphatase 1B inhibitors by pharmacophore modeling, atom-based 3D-QSAR and docking studies. *Chemical Biology and Drug Design*, **2013**, 82, 71-80	2.9	8
5	Design of potent human steroid 5□reductase inhibitors: 3D-QSAR CoMFA, CoMSIA and docking studies. *Medicinal Chemistry Research*, **2013**, 22, 4568-4580	2.2	6
4	3D-QSAR CoMFA and CoMSIA studies for design of potent human steroid 5□reductase inhibitors. *Medicinal Chemistry Research*, **2013**, 22, 105-114	2.2	12
3	Accounting of ligand□eceptor interactions to explore and design novel architecture for PTP 1B inhibition: a legitimate approach. *Journal of Chemometrics*, **2012**, 26, 576-584	1.6	2

2	Pharmacological screening for anti-inflammatory, analgesic activity of pyrazolyl derivatives along with molecular docking studies. *Medicinal Chemistry Research*, **2012**, 21, 3646-3655	2.2	13
1	Synthesis, antibacterial evaluation and QSAR studies of 7-[4-(5-aryl-1,3,4-oxadiazole-2-yl)piperazinyl] quinolone derivatives. *European Journal of Medicinal Chemistry*, **2011**, 46, 3543-50	6.8	43