Rajnish Kumar

List of Publications by Year
in descending order

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54 papers	1,098 citations	393982 19 h-index	476904 29 g-index
55 all docs	55 docs citations	55 times ranked	1294 citing authors

#	Article	IF	Citations
1	Epigenetic Modifications by Estrogen and Androgen in Alzheimerâ€™s Disease. CNS and Neurological Disorders - Drug Targets, 2023, 22, 6-17.	0.8	2
2	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, 2022, 40, 3609-3625.	2.0	25
3	DeepOlf: Deep Neural Network Based Architecture for Predicting Odorants and Their Interacting Olfactory Receptors. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2022, 19, 418-428.	1.9	20
4	Recent Applications of Artificial Intelligence in the Detection of Gastrointestinal, Hepatic and Pancreatic Diseases. Current Medicinal Chemistry, 2022, 29, 66-85.	1.2	7
5	OlfactionBase: a repository to explore odors, odorants, olfactory receptorsÂand odorantâ€“receptor interactions. Nucleic Acids Research, 2022, 50, D678-D686.	6.5	15
6	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, 2022, 40, 12472-12490.	2.0	8
7	Screening of potential antigens from whole proteome and development of multi-epitope vaccine against Rhizopus delemar using immunoinformatics approaches. Journal of Biomolecular Structure and Dynamics, 2022, , 1-28.	2.0	4
8	Recent Applications of Artificial Intelligence in Early Cancer Detection. Current Medicinal Chemistry, 2022, 29, 4410-4435.	1.2	6
9	Deep learning tools for advancing drug discovery and development. 3 Biotech, 2022, 12, 110.	1.1	39
10	DeePred-BBB: A Blood Brain Barrier Permeability Prediction Model With Improved Accuracy. Frontiers in Neuroscience, 2022, 16, 858126.	1.4	17
11	Decoding Seven Basic Odors by Investigating Pharmacophores and Molecular Features of Odorants. Current Bioinformatics, 2022, 17, 759-774.	0.7	1
12	Allosteric Binding Sites of AÎ² Peptides on the Acetylcholine Synthesizing Enzyme ChAT as Deduced by In Silico Molecular Modeling. International Journal of Molecular Sciences, 2022, 23, 6073.	1.8	21
13	Small molecule therapeutics for tauopathy in Alzheimerâ€™s disease: Walking on the path of most resistance. European Journal of Medicinal Chemistry, 2021, 209, 112915.	2.6	48
14	Dissecting Sex-Related Cognition between Alzheimerâ€™s Disease and Diabetes: From Molecular Mechanisms to Potential Therapeutic Strategies. Oxidative Medicine and Cellular Longevity, 2021, 2021, 1-19.	1.9	6
15	A deep neural networkâ€“based approach for prediction of mutagenicity of compounds. Environmental Science and Pollution Research, 2021, 28, 47641-47650.	2.7	17
16	Tozasertib Attenuates Neuropathic Pain by Interfering with Aurora Kinase and KIF11 Mediated Nociception. ACS Chemical Neuroscience, 2021, 12, 1948-1960.	1.7	19
17	Multi-Omics Approach in the Identification of Potential Therapeutic Biomolecule for COVID-19. Frontiers in Pharmacology, 2021, 12, 652335.	1.6	17
18	Recent trends in stem cell-based therapies and applications of artificial intelligence in regenerative medicine. World Journal of Stem Cells, 2021, 13, 521-541.	1.3	16

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19	OBPred: feature-fusion-based deep neural network classifier for odorant-binding protein prediction. Neural Computing and Applications, 2021, 33, 17633-17646.	3.2	5
20	Deep Learning in Disease Diagnosis: Models and Datasets. Current Bioinformatics, 2021, 16, 632-643.	0.7	4
21	Development of Machine Learning Based Blood-brain Barrier Permeability Prediction Models Using Physicochemical Properties, MACCS and Substructure Fingerprints. Current Bioinformatics, 2021, 16, 855-864.	0.7	7
22	SMILES to Smell: Decoding the Structureâ€“Odor Relationship of Chemical Compounds Using the Deep Neural Network Approach. Journal of Chemical Information and Modeling, 2021, 61, 676-688.	2.5	49
23	Hydroxychloroquine in COVID-19: therapeutic promises, current status, and environmental implications. Environmental Science and Pollution Research, 2021, 28, 40431-40444.	2.7	25
24	Crosstalk between epigenetics and mTOR as a gateway to new insights in pathophysiology and treatment of Alzheimer's disease. International Journal of Biological Macromolecules, 2021, 192, 895-903.	3.6	9
25	Available Compounds With Therapeutic Potential Against COVID-19: Antimicrobial Therapies, Supportive Care, and Probable Vaccines. Frontiers in Pharmacology, 2020, 11, 582025.	1.6	14
26	Therapeutic Promises of Chlorogenic Acid with Special Emphasis on its Anti-Obesity Property. Current Molecular Pharmacology, 2020, 13, 7-16.	0.7	37
27	Blood Brain Barrier Permeability Prediction Using Machine Learning Techniques: An Update. Current Pharmaceutical Biotechnology, 2019, 20, 1163-1171.	0.9	30
28	Sense of Smell: Structural, Functional, Mechanistic Advancements and Challenges in Human Olfactory Research. Current Neuropharmacology, 2019, 17, 891-911.	1.4	52
29	Computational Outlook of Marine Compounds as Anti-Cancer Representatives Targeting BCL-2 and Survivin. Current Computer-Aided Drug Design, 2019, 15, 265-276.	0.8	2
30	Prediction of Elimination of Compounds Using Artificial Intelligence Techniques. , 2018, , .		1
31	Prediction of Drug-Plasma Protein Binding Using Artificial Intelligence Based Algorithms. Combinatorial Chemistry and High Throughput Screening, 2018, 21, 57-64.	0.6	24
32	Promises of Machine Learning Approaches in Prediction of Absorption of Compounds. Mini-Reviews in Medicinal Chemistry, 2018, 18, 196-207.	1.1	21
33	Combined x-ray crystallography and computational modeling approach to investigate the Hsp90 C-terminal peptide binding to FKBP51. Scientific Reports, 2017, 7, 14288.	1.6	30
34	Discovery of novel choline acetyltransferase inhibitors using structure-based virtual screening. Scientific Reports, 2017, 7, 16287.	1.6	29
35	Prediction of Human Intestinal Absorption of Compounds Using Artificial Intelligence Techniques. Current Drug Discovery Technologies, 2017, 14, 244-254.	0.6	43
36	Prediction of catalytic site of proteins based on amino acid triads approach using non parametric function. , 2016, , .		0

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37	Prediction of Metabolism of Drugs using Artificial Intelligence: How far have we reached?. Current Drug Metabolism, 2016, 17, 129-141.	0.7	22
38	Zingerone silences quorum sensing and attenuates virulence of Pseudomonas aeruginosa. FÃ¬toterapÃ¬Ã¢, 2015, 102, 84-95.	1.1	100
39	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.	1.1	5
40	Design of potent human steroid 5Î±-reductase inhibitors: 3D-QSAR CoMFA, CoMSIA and docking studies. Medicinal Chemistry Research, 2013, 22, 4568-4580.	1.1	7
41	Advanced stage of breast cancer hoist alkaline phosphatase activity: risk factor for females in India. 3 Biotech, 2013, 3, 517-520.	1.1	19
42	3D-QSAR CoMFA and CoMSIA studies for design of potent human steroid 5Î±-reductase inhibitors. Medicinal Chemistry Research, 2013, 22, 105-114.	1.1	12
43	Prospects of Nanoâ€“Material in Breast Cancer Management. Pathology and Oncology Research, 2013, 19, 155-165.	0.9	5
44	Can we predict blood brain barrier permeability of ligands using computational approaches?. Interdisciplinary Sciences, Computational Life Sciences, 2013, 5, 95-101.	2.2	22
45	Application of microarray in breast cancer: An overview. Journal of Pharmacy and Bioallied Sciences, 2012, 4, 21.	0.2	52
46	Brain Region Specific Monoamine and Oxidative Changes During Restraint Stress. Canadian Journal of Neurological Sciences, 2012, 39, 311-318.	0.3	30
47	Accounting of ligandâ€“receptor interactions to explore and design novel architecture for PTP 1B inhibition: a legitimate approach. Journal of Chemometrics, 2012, 26, 576-584.	0.7	2
48	Pharmacological screening for anti-inflammatory, analgesic activity of pyrazolyl derivatives along with molecular docking studies. Medicinal Chemistry Research, 2012, 21, 3646-3655.	1.1	17
49	Novel Ocimumoside A and B as anti-stress agents: Modulation of brain monoamines and antioxidant systems in chronic unpredictable stress model in rats. Phytomedicine, 2012, 19, 639-647.	2.3	36
50	Classification of oral bioavailability of drugs by machine learning approaches: a comparative study.. Journal of Computational Interdisciplinary Sciences, 2012, 2, .	0.3	11
51	Purification, Characterization, Sequencing and Biological Chemistry of Galectin-1 Purified from Capra hircus (goat) Heart. Protein Journal, 2011, 30, 39-51.	0.7	16
52	A comparative study of support vector machine, artificial neural network and Bayesian classifier for mutagenicity prediction. Interdisciplinary Sciences, Computational Life Sciences, 2011, 3, 232-239.	2.2	21
53	A prediction model for oral bioavailability of drugs using physicochemical properties by support vector machine. Journal of Natural Science, Biology and Medicine, 2011, 2, 168.	1.0	25
54	Stem cells: An overview with respect to cardiovascular and renal disease. Journal of Natural Science, Biology and Medicine, 2010, 1, 43.	1.0	26