## Rajnish Kumar

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Zingerone silences quorum sensing and attenuates virulence of Pseudomonas aeruginosa. Fìtoterapìâ, 2015, 102, 84-95.	2.2	100
2	Application of microarray in breast cancer: An overview. Journal of Pharmacy and Bioallied Sciences, 2012, 4, 21.	0.6	52
3	Sense of Smell: Structural, Functional, Mechanistic Advancements and Challenges in Human Olfactory Research. Current Neuropharmacology, 2019, 17, 891-911.	2.9	52
4	SMILES to Smell: Decoding the Structure–Odor Relationship of Chemical Compounds Using the Deep Neural Network Approach. Journal of Chemical Information and Modeling, 2021, 61, 676-688.	5.4	49
5	Small molecule therapeutics for tauopathy in Alzheimer's disease: Walking on the path of most resistance. European Journal of Medicinal Chemistry, 2021, 209, 112915.	5.5	48
6	Prediction of Human Intestinal Absorption of Compounds Using Artificial Intelligence Techniques. Current Drug Discovery Technologies, 2017, 14, 244-254.	1.2	43
7	Deep learning tools for advancing drug discovery and development. 3 Biotech, 2022, 12, 110.	2.2	39
8	Therapeutic Promises of Chlorogenic Acid with Special Emphasis on its Anti-Obesity Property. Current Molecular Pharmacology, 2020, 13, 7-16.	1.5	37
9	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.	5.3	36
10	Brain Region Specific Monoamine and Oxidative Changes During Restraint Stress. Canadian Journal of Neurological Sciences, 2012, 39, 311-318.	0.5	30
11	Combined x-ray crystallography and computational modeling approach to investigate the Hsp90 C-terminal peptide binding to FKBP51. Scientific Reports, 2017, 7, 14288.	3.3	30
12	Blood Brain Barrier Permeability Prediction Using Machine Learning Techniques: An Update. Current Pharmaceutical Biotechnology, 2019, 20, 1163-1171.	1.6	30
13	Discovery of novel choline acetyltransferase inhibitors using structure-based virtual screening. Scientific Reports, 2017, 7, 16287.	3.3	29
14	Stem cells: An overview with respect to cardiovascular and renal disease. Journal of Natural Science, Biology and Medicine, 2010, 1, 43.	1.0	26
15	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.	3.5	25
16	Hydroxychloroquine in COVID-19: therapeutic promises, current status, and environmental implications. Environmental Science and Pollution Research, 2021, 28, 40431-40444.	5.3	25
17	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
18	Prediction of Drug-Plasma Protein Binding Using Artificial Intelligence Based Algorithms. Combinatorial Chemistry and High Throughput Screening, 2018, 21, 57-64.	1.1	24

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19	Can we predict blood brain barrier permeability of ligands using computational approaches?. Interdisciplinary Sciences, Computational Life Sciences, 2013, 5, 95-101.	3.6	22
20	Prediction of Metabolism of Drugs using Artificial Intelligence: How far have we reached?. Current Drug Metabolism, 2016, 17, 129-141.	1.2	22
21	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.	3.6	21
22	Promises of Machine Learning Approaches in Prediction of Absorption of Compounds. Mini-Reviews in Medicinal Chemistry, 2018, 18, 196-207.	2.4	21
23	Allosteric Binding Sites of Al <sup>2</sup> Peptides on the Acetylcholine Synthesizing Enzyme ChAT as Deduced by In Silico Molecular Modeling. International Journal of Molecular Sciences, 2022, 23, 6073.	4.1	21
24	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.	3.0	20
25	Advanced stage of breast cancer hoist alkaline phosphatase activity: risk factor for females in India. 3 Biotech, 2013, 3, 517-520.	2.2	19
26	Tozasertib Attenuates Neuropathic Pain by Interfering with Aurora Kinase and KIF11 Mediated Nociception. ACS Chemical Neuroscience, 2021, 12, 1948-1960.	3.5	19
27	Pharmacological screening for anti-inflammatory, analgesic activity of pyrazolyl derivatives along with molecular docking studies. Medicinal Chemistry Research, 2012, 21, 3646-3655.	2.4	17
28	A deep neural network–based approach for prediction of mutagenicity of compounds. Environmental Science and Pollution Research, 2021, 28, 47641-47650.	5.3	17
29	Multi-Omics Approach in the Identification of Potential Therapeutic Biomolecule for COVID-19. Frontiers in Pharmacology, 2021, 12, 652335.	3.5	17
30	DeePred-BBB: A Blood Brain Barrier Permeability Prediction Model With Improved Accuracy. Frontiers in Neuroscience, 2022, 16, 858126.	2.8	17
31	Purification, Characterization, Sequencing and Biological Chemistry of Galectin-1 Purified from Capra hircus (goat) Heart. Protein Journal, 2011, 30, 39-51.	1.6	16
32	Recent trends in stem cell-based therapies and applications of artificial intelligence in regenerative medicine. World Journal of Stem Cells, 2021, 13, 521-541.	2.8	16
33	OlfactionBase: a repository to explore odors, odorants, olfactory receptorsÂand odorant–receptor interactions. Nucleic Acids Research, 2022, 50, D678-D686.	14.5	15
34	Available Compounds With Therapeutic Potential Against COVID-19: Antimicrobial Therapies, Supportive Care, and Probable Vaccines. Frontiers in Pharmacology, 2020, 11, 582025.	3.5	14
35	3D-QSAR CoMFA and CoMSIA studies for design of potent human steroid 5α-reductase inhibitors. Medicinal Chemistry Research, 2013, 22, 105-114.	2.4	12
36	Classification of oral bioavailability of drugs by machine learning approaches: a comparative study Journal of Computational Interdisciplinary Sciences, 2012, 2, .	0.3	11

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37	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.	7.5	9
38	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.	3.5	8
39	Design of potent human steroid 5α-reductase inhibitors: 3D-QSAR CoMFA, CoMSIA and docking studies. Medicinal Chemistry Research, 2013, 22, 4568-4580.	2.4	7
40	Recent Applications of Artificial Intelligence in the Detection of Gastrointestinal, Hepatic and Pancreatic Diseases. Current Medicinal Chemistry, 2022, 29, 66-85.	2.4	7
41	Development of Machine Learning Based Blood-brain Barrier Permeability Prediction Models Using Physicochemical Properties, MACCS and Substructure Fingerprints. Current Bioinformatics, 2021, 16, 855-864.	1.5	7
42	Dissecting Sex-Related Cognition between Alzheimer's Disease and Diabetes: From Molecular Mechanisms to Potential Therapeutic Strategies. Oxidative Medicine and Cellular Longevity, 2021, 2021, 1-19.	4.0	6
43	Recent Applications of Artificial Intelligence in Early Cancer Detection. Current Medicinal Chemistry, 2022, 29, 4410-4435.	2.4	6
44	Prospects of Nano–Material in Breast Cancer Management. Pathology and Oncology Research, 2013, 19, 155-165.	1.9	5
45	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.	2.4	5
46	OBPred: feature-fusion-based deep neural network classifier for odorant-binding protein prediction. Neural Computing and Applications, 2021, 33, 17633-17646.	5.6	5
47	Deep Learning in Disease Diagnosis: Models and Datasets. Current Bioinformatics, 2021, 16, 632-643.	1.5	4
48	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.	3.5	4
49	Accounting of ligand–receptor interactions to explore and design novel architecture for PTP 1B inhibition: a legitimate approach. Journal of Chemometrics, 2012, 26, 576-584.	1.3	2
50	Computational Outlook of Marine Compounds as Anti-Cancer Representatives Targeting BCL-2 and Survivin. Current Computer-Aided Drug Design, 2019, 15, 265-276.	1.2	2
51	Epigenetic Modifications by Estrogen and Androgen in Alzheimer's Disease. CNS and Neurological Disorders - Drug Targets, 2023, 22, 6-17.	1.4	2
52	Prediction of Elimination of Compounds Using Artificial Intelligence Techniques. , 2018, , .		1
53	Decoding Seven Basic Odors by Investigating Pharmacophores and Molecular Features of Odorants. Current Bioinformatics, 2022, 17, 759-774.	1.5	1
54	Prediction of catalytic site of proteins based on amino acid triads approach using non parametric function. , 2016, , .		0