Subhash Chandra

List of Publications by Year in Descending Order

49 papers	422 citations	12 h-index	18 g-index
56 ext. papers	595 ext. citations	3 avg, IF	4.43 L-index

#	Paper	IF	Citations
49	Assessment of activity of chalcone compounds as inhibitors of 3-chymotrypsin like protease (3CL) of SARS-CoV-2: in silico study.. *Structural Chemistry*, **2022**, 1-17	1.8	1
48	Identification of Zinc-Binding Inhibitors of Matrix Metalloproteinase-9 to Prevent Cancer Through Deep Learning and Molecular Dynamics Simulation Approach.. *Frontiers in Molecular Biosciences*, **2022**, 9, 857430	5.6	
47	Identification of Putative Elicitors From Plant Root Exudates Responsible for PsoR Activation in Plant-Beneficial spp. by Docking and Molecular Dynamics Simulation Approaches to Decipher Plant-Microbe Interaction.. *Frontiers in Plant Science*, **2022**, 13, 875494	6.2	3
46	identification of natural fungicide from against isocitrate lyase of. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 4816-4834	3.6	4
45	Identification of luteolin -7-glucoside and epicatechin gallate from , as novel EGFR L858R kinase inhibitors against lung cancer: Docking and simulation-based study. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5048-5057	3.6	3
44	Structure-based screening of novel lichen compounds against SARS Coronavirus main protease (Mpro) as potentials inhibitors of COVID-19. *Molecular Diversity*, **2021**, 25, 1665-1677	3.1	27
43	screening of natural compounds to inhibit interaction of human ACE2 receptor and spike protein of SARS-CoV-2 for the prevention of COVID-19. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-13	3.6	1
42	Identification of SARS-CoV-2 RNA dependent RNA polymerase inhibitors using pharmacophore modelling, molecular docking and molecular dynamics simulation approaches. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-12	3.6	
41	Computational investigation of drug bank compounds against 3C-like protease (3CL) of SARS-CoV-2 using deep learning and molecular dynamics simulation. *Molecular Diversity*, **2021**, 1	3.1	3
40	Identification of Berbamine, Oxyacanthine and Rutin from Berberis asiatica as anti-SARS-CoV-2 compounds: An in silico study. *Journal of Molecular Graphics and Modelling*, **2021**, 109, 108028	2.8	4
39	Using Chouś 5-steps rule to study pharmacophore-based virtual screening of SARS-CoV-2 Mpro inhibitors. *Molecular Diversity*, **2021**, 25, 1731-1744	3.1	4
38	Molecular dynamics simulation for screening phytochemicals as □amylase inhibitors from medicinal plants. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 6524-6538	3.6	8
37	Predictive modeling by deep learning, virtual screening and molecular dynamics study of natural compounds against SARS-CoV-2 main protease. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 6728-6746	3.6	16
36	Deep-learning based repurposing of FDA-approved drugs against dihydrofolate reductase and molecular dynamics study. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-17	3.6	2
35	Antimicrobial activity of methanolic extracts of Vernonia cinerea against Xanthomonas oryzae and identification of their compounds using in silico techniques. *PLoS ONE*, **2021**, 16, e0252759	3.7	2
34	Screening of potential bio-molecules from against SARS-CoV-2 main protease using computational approaches. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-12	3.6	4
33	identification of antidiabetic target for phytochemicals of and mechanistic insights by molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-18	3.6	2

32	Molecular docking and molecular dynamics simulation approach to screen natural compounds for inhibition of by targeting peptide deformylase. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 823-840	3.6	22
31	Identification of potent Antigen 85C inhibitors of Mycobacterium tuberculosis via in-house lichen library and binding free energy studies Part-II. *Journal of Molecular Graphics and Modelling*, **2021**, 103, 107822	2.8	2
30	Molecular basis for the repurposing of histamine H2-receptor antagonist to treat COVID-19. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-18	3.6	4
29	Recent advances on computational approach towards potential drug discovery against leishmaniasis **2021**, 63-84		1
28	QSAR modeling and pharmacoinformatics of SARS coronavirus 3C-like protease inhibitors. *Computers in Biology and Medicine*, **2021**, 134, 104483	7	2
27	Molecular docking and molecular dynamics simulation approaches for evaluation of laccase-mediated biodegradation of various industrial dyes. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-11	3.6	4
26	Identification of natural inhibitors against Mpro of SARS-CoV-2 by molecular docking, molecular dynamics simulation, and MM/PBSA methods. *Journal of Biomolecular Structure and Dynamics*, **2020** , 1-12	3.6	11
25	Identification of potential Mycolyltransferase Ag85C inhibitors of Mycobacterium tuberculosis H37Rv via Virtual High Throughput Screening and Binding free energy studies. *Journal of Molecular Graphics and Modelling*, **2020**, 98, 107584	2.8	10
24	A spotlight on the recent advances in bacterial plant diseases and their footprint on crop production **2020**, 37-69		1
23	In silico screening of natural compounds against COVID-19 by targeting Mpro and ACE2 using molecular docking. *European Review for Medical and Pharmacological Sciences*, **2020**, 24, 4529-4536	2.9	71
22	screening of anti-inflammatory compounds from Lichen by targeting cyclooxygenase-2. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3544-3562	3.6	17
21	Virtual screening of anti-HIV1 compounds against SARS-CoV-2: machine learning modeling, chemoinformatics and molecular dynamics simulation based analysis. *Scientific Reports*, **2020**, 10, 20397	4.9	15
20	Repurposing of FDA approved drugs against serovar Typhi by targeting dihydrofolate reductase: an study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-14	3.6	2
19	A dynamic simulation study of FDA drug from zinc database against COVID-19 main protease receptor. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-17	3.6	10
18	In silico screening of potential antidiabetic phytochemicals from Phyllanthus emblica against therapeutic targets of type 2 diabetes. *Journal of Ethnopharmacology*, **2020**, 248, 112268	5	17
17	Foliar Application of Iron Fortified Bacteriosiderophore Improves Growth and Grain Fe Concentration in Wheat and Soybean. *Indian Journal of Microbiology*, **2019**, 59, 344-350	3.7	7
16	Foliar application of organic and inorganic iron formulation induces differential detoxification response to improve growth and biofortification in soybean. *Plant Physiology Reports*, **2019**, 24, 119-128	1.4	12
15	Comparative analysis of machine learning based QSAR models and molecular docking studies to screen potential anti-tubercular inhibitors against InhA of mycobacterium tuberculosis. *International Journal of Computational Biology and Drug Design*, **2018**, 11, 209	0.4	3

14	Enolase of Mycobacterium tuberculosis is a surface exposed plasminogen binding protein. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 3355-3364	4	19
13	In silico prediction and evaluation of interaction between protein arginine N-methyltransferase 5 cancer target and curcumin derivatives by molecular docking and simulation. *International Journal of Computational Biology and Drug Design*, **2017**, 10, 79	0.4	
12	Evaluation of predictive models based on random forest, decision tree and support vector machine classifiers and virtual screening of anti-mycobacterial compounds. *International Journal of Computational Biology and Drug Design*, **2017**, 10, 248	0.4	3
11	High Throughput Virtual Screening to Identify Novel natural product Inhibitors for MethionyltRNA-Synthetase of Brucella melitensis. *Bioinformation*, **2017**, 13, 8-16	1.1	5
10	IN SILICO IDENTIFICATION OF NOVEL EGFR TYROSINE KINASE INHIBITORS ASSOCIATED WITH NON-SMALL CELL LUNG CANCER FROM PHYTOCHEMICAL LIBRARY. *International Research Journal of Pharmacy*, **2016**, 7, 22-25	0.2	
9	Virtual screening of natural compounds as inhibitors of EGFR 696-1022 T790M associated with non-small cell lung cancer. *Bioinformation*, **2016**, 12, 311-317	1.1	8
8	3D QSAR, pharmacophore and molecular docking studies of known inhibitors and designing of novel inhibitors for M18 aspartyl aminopeptidase of Plasmodium falciparum. *BMC Structural Biology*, **2016**, 16, 12	2.7	18
7	In silico prediction of anti-malarial hit molecules based on machine learning methods. *International Journal of Computational Biology and Drug Design*, **2015**, 8, 40-53	0.4	3
6	Immune response and protective efficacy of live attenuated Salmonella vaccine expressing antigens of Mycobacterium avium subsp. paratuberculosis against challenge in mice. *Vaccine*, **2012**, 31, 242-51	4.1	9
5	A plant based protective antigen [PA(dIV)] vaccine expressed in chloroplasts demonstrates protective immunity in mice against anthrax. *Vaccine*, **2011**, 29, 4521-33	4.1	26
4	Identification and characterization of immunodominant B-cell epitope of the C-terminus of protective antigen of Bacillus anthracis. *Molecular Immunology*, **2009**, 46, 2107-15	4.3	25
3	Induction of cytotoxic T lymphocyte response against Mycobacterial antigen using domain I of anthrax edema factor as antigen delivery system. *Biochemical and Biophysical Research Communications*, **2007**, 357, 50-5	3.4	2
2	Evaluation of the ability of N-terminal fragment of lethal factor of Bacillus anthracis for delivery of Mycobacterium T cell antigen ESAT-6 into cytosol of antigen presenting cells to elicit effective cytotoxic T lymphocyte response. *Biochemical and Biophysical Research Communications*, **2006**, 351, 702-7	3.4	6
1	Molecular Docking Study of drug molecules from Drug Bank database against COVID-19 Mpro protein		2