

Chandrabose Selvaraj

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.

86

papers

1,414

citations

22

h-index

32

g-index

96

ext. papers

1,701

ext. citations

3.6

avg, IF

5.22

L-index

#	Paper	IF	Citations
86	Immunological insights of selectins in human disease mechanism.. <i>Advances in Protein Chemistry and Structural Biology</i> , 2022 , 129, 163-188	5.3	0
85	Structure and chemistry of enzymatic active sites that play a role in the switch and conformation mechanism.. <i>Advances in Protein Chemistry and Structural Biology</i> , 2022 , 130, 59-83	5.3	
84	Molecular Insights into Agonist/Antagonist Effects on Macromolecules Involved in Human Disease Mechanisms. <i>Current Molecular Pharmacology</i> , 2022 , 15, 263-264	3.7	1
83	Structure-based virtual screening and molecular dynamics simulation of SARS-CoV-2 Guanine-N7 methyltransferase (nsp14) for identifying antiviral inhibitors against COVID-19. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 4582-4593	3.6	41
82	Bacterial protein azurin and derived peptides as potential anti-SARS-CoV-2 agents: insights from molecular docking and molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 5706-5721	3.6	12
81	Molecular interaction analysis of E1, 3 glucan binding protein with <i>Bacillus licheniformis</i> and evaluation of its immunostimulant property in <i>Oreochromis mossambicus</i> .. <i>Fish and Shellfish Immunology</i> , 2021 , 121, 183-183	4.3	
80	Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. <i>Molecular Diversity</i> , 2021 , 1	3.1	10
79	High-Throughput Screening and Quantum Mechanics for Identifying Potent Inhibitors Against Mac1 Domain of SARS-CoV-2 Nsp3. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2021 , 18, 1262-1270	3	10
78	Pan-selectin inhibitors as potential therapeutics for COVID-19 treatment: in silico screening study. <i>Glycobiology</i> , 2021 , 31, 975-987	5.8	6
77	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	7
76	Synthesis, antibacterial, anti-oxidant and molecular docking studies of imidazoquinolines. <i>Heliyon</i> , 2021 , 7, e07484	3.6	1
75	Investigating into the molecular interactions of flavonoids targeting NS2B-NS3 protease from ZIKA virus through approaches. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 272-284	3.6	16
74	Eco-friendly Microbial Biopolymers: Recent Development, Biodegradation, and Applications 2021 , 547-577		
73	Chemoinformatics and QSAR 2021 , 183-212		0
72	Structural insights of macromolecules involved in bacteria-induced apoptosis in the pathogenesis of human diseases. <i>Advances in Protein Chemistry and Structural Biology</i> , 2021 , 126, 1-38	5.3	3
71	Interrogation of SrtA active site loop forming open/close lid conformations through extensive MD simulations for understanding binding selectivity of SrtA inhibitors. <i>Saudi Journal of Biological Sciences</i> , 2021 , 28, 3650-3659	4	3
70	Elucidation of Agonist and Antagonist Dynamic Binding Patterns in ER- β by Integration of Molecular Docking, Molecular Dynamics Simulations and Quantum Mechanical Calculations. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	4

69	Structural Understanding of SARS-CoV-2 Drug Targets, Active Site Contour Map Analysis and COVID-19 Therapeutics. <i>Current Molecular Pharmacology</i> , 2021 ,	3.7	3
68	Understanding the biological role of PqqB in using molecular dynamics simulation approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-13	3.6	4
67	Computational investigation on <i>Andrographis paniculata</i> phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-12	3.6	41
66	Selectins-The Two Dr. Jekyll and Mr. Hyde Faces of Adhesion Molecules-A Review. <i>Molecules</i> , 2020 , 25,	4.8	19
65	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. <i>Environmental Health Perspectives</i> , 2020 , 128, 27002	8.4	70
64	Identification of new anti-nCoV drug chemical compounds from Indian spices exploiting SARS-CoV-2 main protease as target. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-9	3.6	88
63	Characterization and structural analysis of prophenoloxidase in mud crab <i>Scylla serrata</i> and discovering novel chemical inhibitors through virtual screening. <i>Structural Chemistry</i> , 2020 , 31, 1563-1584 ^{1,8}		
62	Computational Studies Reveal Piperine, the Predominant Oleoresin of Black Pepper (&i>Piper nigrum&i>) as a Potential Inhibitor of SARS-CoV-2 (COVID-19). <i>Current Science</i> , 2020 , 119, 1333	2.2	10
61	Phage Protein Interactions in the Inhibition Mechanism of Bacterial Cell 2020 , 121-142		2
60	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. <i>Current Drug Targets</i> , 2020 , 21, 132-147		2
59	Shape-based Machine Learning Models for the Potential Novel COVID-19 Protease Inhibitors Assisted by Molecular Dynamics Simulation. <i>Current Topics in Medicinal Chemistry</i> , 2020 , 20, 2146-2167	3	18
58	Combining in silico and in vitro approaches to identification of potent inhibitor against phospholipase A2 (PLA2). <i>International Journal of Biological Macromolecules</i> , 2020 , 144, 53-66	7.9	18
57	Effect of Amino Acid Substitution in the <i>Penaeus monodon</i> LGBP and Specificity Through Mutational Analysis. <i>International Journal of Peptide Research and Therapeutics</i> , 2020 , 26, 1789-1801	2.1	2
56	Targeting COVID-19 (SARS-CoV-2) main protease through active phytochemicals of ayurvedic medicinal plants - (Ashwagandha), (Giloy) and (Tulsi) - a molecular docking study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-14	3.6	83
55	Molecular docking and molecular dynamics simulation studies to identify potent AURKA inhibitors: assessing the performance of density functional theory, MM-GBSA and mass action kinetics calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 4325-4335	3.6	17
54	Microsecond MD Simulation and Multiple-Conformation Virtual Screening to Identify Potential Anti-COVID-19 Inhibitors Against SARS-CoV-2 Main Protease. <i>Frontiers in Chemistry</i> , 2020 , 8, 595273	5	10
53	Applications of Polyhydroxyalkanoates Based Nanovehicles as Drug Carriers 2019 , 125-169		1
52	Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview. <i>Current Pharmaceutical Design</i> , 2019 , 25, 3390-3405	3.3	6

51	Molecular Modeling and Drug Design Techniques in Microbial Drug Discovery 2019 , 185-231		
50	Competitive Inhibition of Quercetin and Apigenin at the ATP Binding site of D-Alanine-D-Alanine Ligase of <i>Helicobacter pylori</i> – A Molecular Modeling Approach. <i>Current Biotechnology</i> , 2019 , 7, 340-348	0.6	4
49	Molecular dynamics simulations and applications in computational toxicology and nanotoxicology. <i>Food and Chemical Toxicology</i> , 2018 , 112, 495-506	4.7	43
48	Competitive docking model for prediction of the human nicotinic acetylcholine receptor $\alpha 7$ binding of tobacco constituents. <i>Oncotarget</i> , 2018 , 9, 16899-16916	3.3	7
47	Computational and Experimental Binding Mechanism of DNA-drug Interactions. <i>Current Pharmaceutical Design</i> , 2018 , 24, 3739-3757	3.3	6
46	Protein Engineering Approaches in the Post-Genomic Era. <i>Current Protein and Peptide Science</i> , 2018 , 19, 5-15	2.8	10
45	Exploring the Biology and Structural Architecture of Sortase Role on Biofilm Formation in Gram Positive Pathogens. <i>Current Topics in Medicinal Chemistry</i> , 2018 , 18, 2462-2480	3	5
44	Chemopreventive effect of saponin isolated from <i>Gymnema sylevestre</i> on prostate cancer through in silico and in vivo analysis. <i>Medicinal Chemistry Research</i> , 2017 , 26, 1915-1925	2.2	4
43	Development of estrogen receptor beta binding prediction model using large sets of chemicals. <i>Oncotarget</i> , 2017 , 8, 92989-93000	3.3	17
42	Advantages of Structure-Based Drug Design Approaches in Neurological Disorders. <i>Current Neuropharmacology</i> , 2017 , 15, 1136-1155	7.6	13
41	Structural insights into the binding mode of d-sorbitol with sorbitol dehydrogenase using QM-polarized ligand docking and molecular dynamics simulations. <i>Biochemical Engineering Journal</i> , 2016 , 114, 244-256	4.2	25
40	Phytoremediation of metal-contaminated soils by the hyperaccumulator canola (<i>Brassica napus</i> L.) and the use of its biomass for ethanol production. <i>Fuel</i> , 2016 , 183, 107-114	7.1	50
39	Enhancement of methanol production from synthetic gas mixture by <i>Methylosinus sporium</i> through covalent immobilization. <i>Applied Energy</i> , 2016 , 171, 383-391	10.7	46
38	Understanding the importance of conservative hypothetical protein LdBPK_070020 in <i>Leishmania donovani</i> and its role in subsistence of the parasite. <i>Archives of Biochemistry and Biophysics</i> , 2016 , 596, 10-21	4.1	3
37	Potential of Immobilized Whole-Cell <i>Methylocella tundrae</i> as a Biocatalyst for Methanol Production from Methane. <i>Journal of Microbiology and Biotechnology</i> , 2016 , 26, 1234-41	3.3	44
36	Consensus Modeling for Prediction of Estrogenic Activity of Ingredients Commonly Used in Sunscreen Products. <i>International Journal of Environmental Research and Public Health</i> , 2016 , 13,	4.6	12
35	In vitro and in silico studies on cell adhesion protein peroxinectin from <i>Fenneropenaeus indicus</i> and screening of heme blockers against activity. <i>Journal of Molecular Recognition</i> , 2016 , 29, 186-98	2.6	4
34	Modeling of macromolecular proteins in prophenoxidase cascade through experimental and computational approaches. <i>Biotechnology and Applied Biochemistry</i> , 2016 , 63, 779-788	2.8	6

33	A highly efficient sorbitol dehydrogenase from <i>Gluconobacter oxydans</i> G624 and improvement of its stability through immobilization. <i>Scientific Reports</i> , 2016 , 6, 33438	4.9	36
32	Molecular cloning, relative expression, and structural analysis of pattern recognition molecule Eglucan binding protein from mangrove crab <i>Episesarma tetragonum</i> . <i>Biotechnology and Applied Biochemistry</i> , 2015 , 62, 416-23	2.8	2
31	Structure-Based Virtual Screening and Biological Evaluation of a Calpain Inhibitor for Prevention of Selenite-Induced Cataractogenesis in an in Vitro System. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1686-97	6.1	20
30	Mechanistic insights of SrtA Π PXTG blockers targeting the transpeptidase mechanism in <i>Streptococcus mutans</i> . <i>RSC Advances</i> , 2015 , 5, 100498-100510	3.7	12
29	Molecular insights of protein contour recognition with ligand pharmacophoric sites through combinatorial library design and MD simulation in validating HTLV-1 PR inhibitors. <i>Molecular BioSystems</i> , 2015 , 11, 178-89		23
28	Explicit Drug Re-positioning: Predicting Novel Drug-Target Interactions of the Shelved Molecules with QM/MM Based Approaches. <i>Advances in Protein Chemistry and Structural Biology</i> , 2015 , 100, 89-112 ^{5:3}		4
27	Virtual screening based on pharmacophoric features of known calpain inhibitors to identify potent inhibitors of calpain. <i>Medicinal Chemistry Research</i> , 2014 , 23, 2445-2455	2.2	13
26	Investigations on the interactions of Φ hage-derived peptides against the SrtA mechanism in <i>Bacillus anthracis</i> . <i>Applied Biochemistry and Biotechnology</i> , 2014 , 172, 1790-806	3.2	10
25	Structural elucidation of SrtA enzyme in <i>Enterococcus faecalis</i> : an emphasis on screening of potential inhibitors against the biofilm formation. <i>Molecular BioSystems</i> , 2014 , 10, 1775-89		19
24	Ligand-based pharmacophore modelling and screening of DNA minor groove binders targeting <i>Staphylococcus aureus</i> . <i>Journal of Molecular Recognition</i> , 2014 , 27, 429-37	2.6	6
23	Molecular insights on analogs of HIV PR inhibitors toward HTLV-1 PR through QM/MM interactions and molecular dynamics studies: comparative structure analysis of wild and mutant HTLV-1 PR. <i>Journal of Molecular Recognition</i> , 2014 , 27, 696-706	2.6	19
22	Examine the characterization of biofilm formation and inhibition by targeting SrtA mechanism in <i>Bacillus subtilis</i> : a combined experimental and theoretical study. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2364	2	16
21	Virtual screening of LPXTG competitive SrtA inhibitors targeting signal transduction mechanism in <i>Bacillus anthracis</i> : a combined experimental and theoretical study. <i>Journal of Receptor and Signal Transduction Research</i> , 2014 , 34, 221-32	2.6	11
20	Molecular modeling studies and comparative analysis on structurally similar HTLV and HIV protease using HIV-PR inhibitors. <i>Journal of Receptor and Signal Transduction Research</i> , 2014 , 34, 361-71	2.6	12
19	Interaction investigations of crustacean EGBP recognition toward pathogenic microbial cell membrane and stimulate upon prophenoloxidase activation. <i>Journal of Molecular Recognition</i> , 2014 , 27, 173-83	2.6	7
18	Communication of Φ hage lysin plyG enzymes binding toward SrtA for inhibition of <i>Bacillus anthracis</i> : protein-protein interaction and molecular dynamics study. <i>Cell Communication and Adhesion</i> , 2014 , 21, 257-65		4
17	In silico and in vitro studies on the protein-protein interactions between <i>Brugia malayi</i> immunomodulatory protein calreticulin and human C1q. <i>PLoS ONE</i> , 2014 , 9, e106413	3.7	28
16	Exploration of protein-protein interaction effects on Φ -macroglobulin in an inhibition of serine protease through gene expression and molecular simulations studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014 , 32, 1841-54	3.6	4

15	Validation of potential inhibitors for SrtA against Bacillus anthracis by combined approach of ligand-based and molecular dynamics simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014 , 32, 1333-49	3.6	30
14	In silico and in vitro studies of cinnamaldehyde and their derivatives against LuxS in Streptococcus pyogenes: effects on biofilm and virulence genes. <i>Journal of Molecular Recognition</i> , 2014 , 27, 106-16	2.6	30
13	A three-dimensional chemical phase pharmacophore mapping, QSAR modelling and electronic feature analysis of benzofuran salicylic acid derivatives as LYP inhibitors. <i>SAR and QSAR in Environmental Research</i> , 2013 , 24, 1025-40	3.5	14
12	Exploration of the binding of DNA binding ligands to Staphylococcal DNA through QM/MM docking and molecular dynamics simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013 , 31, 561-71	3.6	27
11	Identification of potential HIV-1 integrase strand transfer inhibitors: in silico virtual screening and QM/MM docking studies. <i>SAR and QSAR in Environmental Research</i> , 2013 , 24, 581-95	3.5	26
10	Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14 α -demethylase inhibitors. <i>Journal of Receptor and Signal Transduction Research</i> , 2013 , 33, 234-43	2.6	26
9	Exploration of fluoroquinolone resistance in Streptococcus pyogenes: comparative structure analysis of wild-type and mutant DNA gyrase. <i>Journal of Molecular Recognition</i> , 2013 , 26, 276-85	2.6	22
8	Molecular docking, QPLD, and ADME prediction studies on HIV-1 integrase leads. <i>Medicinal Chemistry Research</i> , 2012 , 21, 4239-4251	2.2	22
7	In silico screening of indinavir-based compounds targeting proteolytic activity in HIV PR: binding pocket fit approach. <i>Medicinal Chemistry Research</i> , 2012 , 21, 4060-4068	2.2	27
6	Comparative structural analysis of two proteins belonging to quorum sensing system in Vibrio cholerae. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012 , 30, 574-84	3.6	17
5	Exploring the selectivity of a ligand complex with CDK2/CDK1: a molecular dynamics simulation approach. <i>Journal of Molecular Recognition</i> , 2012 , 25, 504-12	2.6	31
4	Pharmacophore modelling and atom-based 3D-QSAR studies on N-methyl pyrimidones as HIV-1 integrase inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2012 , 27, 339-47	5.6	26
3	Targeting Multidrug Resistant Mycobacterium tuberculosis HtrA2 with Identical Chemical Entities of Fluoroquinolones. <i>Indian Journal of Pharmaceutical Sciences</i> , 2012 , 74, 217-22	1.5	26
2	Homology modeling, active site prediction, and targeting the anti hypertension activity through molecular docking on endothelin - B receptor domain. <i>Bioinformation</i> , 2012 , 8, 81-6	1.1	12
1	A database for the predicted pharmacophoric features of medicinal compounds. <i>Bioinformation</i> , 2011 , 6, 167-8	1.1	12