Chandrabose Selvaraj

List of Publications by Citations

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	Identification of new anti-nCoV drug chemical compounds from Indian spices exploiting SARS-CoV-2 main protease as target. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-9	3.6	88
85	Targeting COVID-19 (SARS-CoV-2) main protease through active phytochemicals of ayurvedic medicinal plants - (Ashwagandha), (Giloy) and (Tulsi) - a molecular docking study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-14	3.6	83
84	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
83	Phytoremediation of metal-contaminated soils by the hyperaccumulator canola (Brassica napus L.) and the use of its biomass for ethanol production. *Fuel*, **2016**, 183, 107-114	7.1	50
82	Enhancement of methanol production from synthetic gas mixture by Methylosinus sporium through covalent immobilization. *Applied Energy*, **2016**, 171, 383-391	10.7	46
81	Potential of Immobilized Whole-Cell Methylocella tundrae as a Biocatalyst for Methanol Production from Methane. *Journal of Microbiology and Biotechnology*, **2016**, 26, 1234-41	3.3	44
80	Molecular dynamics simulations and applications in computational toxicology and nanotoxicology. *Food and Chemical Toxicology*, **2018**, 112, 495-506	4.7	43
79	Computational investigation on Andrographis paniculata phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-12	3.6	41
78	Structure-based virtual screening and molecular dynamics simulation of SARS-CoV-2 Guanine-N7 methyltransferase (nsp14) for identifying antiviral inhibitors against COVID-19. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 4582-4593	3.6	41
77	A highly efficient sorbitol dehydrogenase from Gluconobacter oxydans G624 and improvement of its stability through immobilization. *Scientific Reports*, **2016**, 6, 33438	4.9	36
76	Exploring the selectivity of a ligand complex with CDK2/CDK1: a molecular dynamics simulation approach. *Journal of Molecular Recognition*, **2012**, 25, 504-12	2.6	31
75	Validation of potential inhibitors for SrtA against Bacillus anthracis by combined approach of ligand-based and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1333-49	3.6	30
74	In silico and in vitro studies of cinnamaldehyde and their derivatives against LuxS in Streptococcus pyogenes: effects on biofilm and virulence genes. *Journal of Molecular Recognition*, **2014**, 27, 106-16	2.6	30
73	In silico and in vitro studies on the protein-protein interactions between Brugia malayi immunomodulatory protein calreticulin and human C1q. *PLoS ONE*, **2014**, 9, e106413	3.7	28
72	Exploration of the binding of DNA binding ligands to Staphylococcal DNA through QM/MM docking and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, **2013**, 31, 561-71	3.6	27
71	In silico screening of indinavir-based compounds targeting proteolytic activity in HIV PR: binding pocket fit approach. *Medicinal Chemistry Research*, **2012**, 21, 4060-4068	2.2	27
70	Pharmacophore modelling and atom-based 3D-QSAR studies on N-methyl pyrimidones as HIV-1 integrase inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2012**, 27, 339-47	5.6	26

69	Identification of potential HIV-1 integrase strand transfer inhibitors: in silico virtual screening and QM/MM docking studies. *SAR and QSAR in Environmental Research*, **2013**, 24, 581-95	3.5	26
68	Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14□demethylase inhibitors. *Journal of Receptor and Signal Transduction Research*, **2013**, 33, 234-43	2.6	26
67	Targeting Multidrug Resistant Mycobacterium tuberculosis HtrA2 with Identical Chemical Entities of Fluoroquinolones. *Indian Journal of Pharmaceutical Sciences*, **2012**, 74, 217-22	1.5	26
66	Structural insights into the binding mode of d-sorbitol with sorbitol dehydrogenase using QM-polarized ligand docking and molecular dynamics simulations. *Biochemical Engineering Journal*, **2016**, 114, 244-256	4.2	25
65	Molecular insights of protein contour recognition with ligand pharmacophoric sites through combinatorial library design and MD simulation in validating HTLV-1 PR inhibitors. *Molecular BioSystems*, **2015**, 11, 178-89		23
64	Molecular docking, QPLD, and ADME prediction studies on HIV-1 integrase leads. *Medicinal Chemistry Research*, **2012**, 21, 4239-4251	2.2	22
63	Exploration of fluoroquinolone resistance in Streptococcus pyogenes: comparative structure analysis of wild-type and mutant DNA gyrase. *Journal of Molecular Recognition*, **2013**, 26, 276-85	2.6	22
62	Structure-Based Virtual Screening and Biological Evaluation of a Calpain Inhibitor for Prevention of Selenite-Induced Cataractogenesis in an in Vitro System. *Journal of Chemical Information and Modeling*, **2015**, 55, 1686-97	6.1	20
61	Selectins-The Two Dr. Jekyll and Mr. Hyde Faces of Adhesion Molecules-A Review. *Molecules*, **2020**, 25,	4.8	19
60	Structural elucidation of SrtA enzyme in Enterococcus faecalis: an emphasis on screening of potential inhibitors against the biofilm formation. *Molecular BioSystems*, **2014**, 10, 1775-89		19
59	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. *Journal of Molecular Recognition*, **2014**, 27, 696-706	2.6	19
58	Shape-based Machine Learning Models for the Potential Novel COVID-19 Protease Inhibitors Assisted by Molecular Dynamics Simulation. *Current Topics in Medicinal Chemistry*, **2020**, 20, 2146-2167	3	18
57	Combining in silico and in vitro approaches to identification of potent inhibitor against phospholipase A2 (PLA2). *International Journal of Biological Macromolecules*, **2020**, 144, 53-66	7.9	18
56	Comparative structural analysis of two proteins belonging to quorum sensing system in Vibrio cholerae. *Journal of Biomolecular Structure and Dynamics*, **2012**, 30, 574-84	3.6	17
55	Development of estrogen receptor beta binding prediction model using large sets of chemicals. *Oncotarget*, **2017**, 8, 92989-93000	3.3	17
54	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. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 4325-4335	3.6	17
53	Examine the characterization of biofilm formation and inhibition by targeting SrtA mechanism in Bacillus subtilis: a combined experimental and theoretical study. *Journal of Molecular Modeling*, **2014**, 20, 2364	2	16
52	Investigating into the molecular interactions of flavonoids targeting NS2B-NS3 protease from ZIKA virus through approaches. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 272-284	3.6	16

51	A three-dimensional chemical phase pharmacophore mapping, QSAR modelling and electronic feature analysis of benzofuran salicylic acid derivatives as LYP inhibitors. *SAR and QSAR in Environmental Research*, **2013**, 24, 1025-40	3.5	14
50	Virtual screening based on pharmacophoric features of known calpain inhibitors to identify potent inhibitors of calpain. *Medicinal Chemistry Research*, **2014**, 23, 2445-2455	2.2	13
49	Advantages of Structure-Based Drug Design Approaches in Neurological Disorders. *Current Neuropharmacology*, **2017**, 15, 1136-1155	7.6	13
48	Mechanistic insights of SrtA□PXTG blockers targeting the transpeptidase mechanism in Streptococcus mutans. *RSC Advances*, **2015**, 5, 100498-100510	3.7	12
47	Bacterial protein azurin and derived peptides as potential anti-SARS-CoV-2 agents: insights from molecular docking and molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5706-5721	3.6	12
46	Molecular modeling studies and comparative analysis on structurally similar HTLV and HIV protease using HIV-PR inhibitors. *Journal of Receptor and Signal Transduction Research*, **2014**, 34, 361-71	2.6	12
45	A database for the predicted pharmacophoric features of medicinal compounds. *Bioinformation*, **2011**, 6, 167-8	1.1	12
44	Homology modeling, active site prediction, and targeting the anti hypertension activity through molecular docking on endothelin - B receptor domain. *Bioinformation*, **2012**, 8, 81-6	1.1	12
43	Consensus Modeling for Prediction of Estrogenic Activity of Ingredients Commonly Used in Sunscreen Products. *International Journal of Environmental Research and Public Health*, **2016**, 13,	4.6	12
42	Virtual screening of LPXTG competitive SrtA inhibitors targeting signal transduction mechanism in Bacillus anthracis: a combined experimental and theoretical study. *Journal of Receptor and Signal Transduction Research*, **2014**, 34, 221-32	2.6	11
41	Investigations on the interactions of □hage-derived peptides against the SrtA mechanism in Bacillus anthracis. *Applied Biochemistry and Biotechnology*, **2014**, 172, 1790-806	3.2	10
40	Computational Studies Reveal Piperine, the Predominant Oleoresin of Black Pepper (<i>Piper nigrum</i>) as a Potential Inhibitor of SARS-CoV-2 (COVID-19). *Current Science*, **2020**, 119, 1333	2.2	10
39	Protein Engineering Approaches in the Post-Genomic Era. *Current Protein and Peptide Science*, **2018**, 19, 5-15	2.8	10
38	Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. *Molecular Diversity*, **2021**, 1	3.1	10
37	High-Throughput Screening and Quantum Mechanics for Identifying Potent Inhibitors Against Mac1 Domain of SARS-CoV-2 Nsp3. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2021**, 18, 1262-1270	3	10
36	Microsecond MD Simulation and Multiple-Conformation Virtual Screening to Identify Potential Anti-COVID-19 Inhibitors Against SARS-CoV-2 Main Protease. *Frontiers in Chemistry*, **2020**, 8, 595273	5	10
35	Interaction investigations of crustacean □GBP recognition toward pathogenic microbial cell membrane and stimulate upon prophenoloxidase activation. *Journal of Molecular Recognition*, **2014** , 27, 173-83	2.6	7
34	Competitive docking model for prediction of the human nicotinic acetylcholine receptor □ binding of tobacco constituents. *Oncotarget*, **2018**, 9, 16899-16916	3.3	7

33	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	7
32	Ligand-based pharmacophore modelling and screening of DNA minor groove binders targeting Staphylococcus aureus. *Journal of Molecular Recognition*, **2014**, 27, 429-37	2.6	6
31	Computational and Experimental Binding Mechanism of DNA-drug Interactions. *Current Pharmaceutical Design*, **2018**, 24, 3739-3757	3.3	6
30	Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview. *Current Pharmaceutical Design*, **2019**, 25, 3390-3405	3.3	6
29	Pan-selectin inhibitors as potential therapeutics for COVID-19 treatment: in silico screening study. *Glycobiology*, **2021**, 31, 975-987	5.8	6
28	Modeling of macromolecular proteins in prophenoloxidase cascade through experimental and computational approaches. *Biotechnology and Applied Biochemistry*, **2016**, 63, 779-788	2.8	6
27	Exploring the Biology and Structural Architecture of Sortase Role on Biofilm Formation in Gram Positive Pathogens. *Current Topics in Medicinal Chemistry*, **2018**, 18, 2462-2480	3	5
26	Chemopreventive effect of saponin isolated from Gymnema sylevestre on prostate cancer through in silico and in vivo analysis. *Medicinal Chemistry Research*, **2017**, 26, 1915-1925	2.2	4
25	Understanding the biological role of PqqB in using molecular dynamics simulation approach. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-13	3.6	4
24	Communication of □phage lysin plyG enzymes binding toward SrtA for inhibition of Bacillus anthracis: protein-protein interaction and molecular dynamics study. *Cell Communication and Adhesion*, **2014**, 21, 257-65		4
23	Explicit Drug Re-positioning: Predicting Novel Drug-Target Interactions of the Shelved Molecules with QM/MM Based Approaches. *Advances in Protein Chemistry and Structural Biology*, **2015**, 100, 89-112	5.3	4
22	Exploration of protein-protein interaction effects on □2-macroglobulin in an inhibition of serine protease through gene expression and molecular simulations studies. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1841-54	3.6	4
21	In vitro and in silico studies on cell adhesion protein peroxinectin from Fenneropenaeus indicus and screening of heme blockers against activity. *Journal of Molecular Recognition*, **2016**, 29, 186-98	2.6	4
20	Competitive Inhibition of Quercetin and Apigenin at the ATP Binding site of D-Alanine-D-Alanine Ligase of Helicobacter pylori □A Molecular Modeling Approach. *Current Biotechnology*, **2019**, 7, 340-348	0.6	4
19	Elucidation of Agonist and Antagonist Dynamic Binding Patterns in ER-□by Integration of Molecular Docking, Molecular Dynamics Simulations and Quantum Mechanical Calculations. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	4
18	Understanding the importance of conservative hypothetical protein LdBPK_070020 in Leishmania donovani and its role in subsistence of the parasite. *Archives of Biochemistry and Biophysics*, **2016**, 596, 10-21	4.1	3
17	Structural insights of macromolecules involved in bacteria-induced apoptosis in the pathogenesis of human diseases. *Advances in Protein Chemistry and Structural Biology*, **2021**, 126, 1-38	5.3	3
16	Interrogation of SrtA active site loop forming open/close lid conformations through extensive MD simulations for understanding binding selectivity of SrtA inhibitors. *Saudi Journal of Biological Sciences*, **2021**, 28, 3650-3659	4	3

15	Structural Understanding of SARS-CoV-2 Drug Targets, Active Site Contour Map Analysis and COVID-19 Therapeutics. *Current Molecular Pharmacology*, **2021**,	3.7	3
14	Molecular cloning, relative expression, and structural analysis of pattern recognition molecule glucan binding protein from mangrove crab Episesarma tetragonum. *Biotechnology and Applied Biochemistry*, **2015**, 62, 416-23	2.8	2
13	Phage Protein Interactions in the Inhibition Mechanism of Bacterial Cell **2020**, 121-142		2
12	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. *Current Drug Targets*, **2020**, 21, 132-147	3	2
11	Effect of Amino Acid Substitution in the Penaeus monodon LGBP and Specificity Through Mutational Analysis. *International Journal of Peptide Research and Therapeutics*, **2020**, 26, 1789-1801	2.1	2
10	Applications of Polyhydroxyalkanoates Based Nanovehicles as Drug Carriers **2019**, 125-169		1
9	Synthesis, antibacterial, anti-oxidant and molecular docking studies of imidazoquinolines. *Heliyon*, **2021**, 7, e07484	3.6	1
8	Molecular Insights into Agonist/Antagonist Effects on Macromolecules Involved in Human Disease Mechanisms. *Current Molecular Pharmacology*, **2022**, 15, 263-264	3.7	1
7	Immunological insights of selectins in human disease mechanism.. *Advances in Protein Chemistry and Structural Biology*, **2022**, 129, 163-188	5.3	0
6	Chemoinformatics and QSAR **2021**, 183-212		0
5	Characterization and structural analysis of prophenoloxidase in mud crab Scylla serrata and discovering novel chemical inhibitors through virtual screening. *Structural Chemistry*, **2020**, 31, 1563-1584	1.8	
4	Molecular interaction analysis of 1, 3 glucan binding protein with Bacillus licheniformis and evaluation of its immunostimulant property in Oreochromis mossambicus.. *Fish and Shellfish Immunology*, **2021**, 121, 183-183	4.3	
3	Molecular Modeling and Drug Design Techniques in Microbial Drug Discovery **2019**, 185-231		
2	Eco-friendly Microbial Biopolymers: Recent Development, Biodegradation, and Applications **2021**, 547-577		
1	Structure and chemistry of enzymatic active sites that play a role in the switch and conformation mechanism.. *Advances in Protein Chemistry and Structural Biology*, **2022**, 130, 59-83	5.3	