Chandrabose Selvaraj

List of Publications by Year
in descending order

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91 papers	2,119 citations	218592 26 h-index	276775 41 g-index
96 all docs	96 docs citations	96 times ranked	2402 citing authors

#	Article	IF	Citations
1	Targeting COVID-19 (SARS-CoV-2) main protease through active phytochemicals of ayurvedic medicinal plants â€“ Withania somnifera (Ashwagandha), Tinospora cordifolia (Giloy) and Ocimum sanctum (Tulsi) â€“ a molecular docking study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 190-203.	2.0	181
2	Understanding the biological role of PqqB in Pseudomonas stutzeri using molecular dynamics simulation approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4237-4249.	2.0	10
3	Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. Molecular Diversity, 2022, 26, 1893-1913.	2.1	35
4	Molecular interaction analysis of Î²-1, 3 glucan binding protein with Bacillus licheniformis and evaluation of its immunostimulant property in Oreochromis mossambicus. Fish and Shellfish Immunology, 2022, 121, 183-196.	1.6	2
5	Immunological insights of selectins in human disease mechanism. Advances in Protein Chemistry and Structural Biology, 2022, 129, 163-188.	1.0	2
6	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.	1.0	5
7	Editorial: Novel Therapeutic Interventions Against Infectious Diseases: COVID-19. Frontiers in Pharmacology, 2022, 13, 852078.	1.6	0
8	Molecular Insights into Agonist/Antagonist Effects on Macromolecules Involved in Human Disease Mechanisms. Current Molecular Pharmacology, 2022, 15, 263-264.	0.7	2
9	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.	1.9	17
10	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, 2021, 39, 4415-4426.	2.0	73
11	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.	2.0	73
12	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.	2.0	18
13	Investigating into the molecular interactions of flavonoids targeting NS2B-NS3 protease from ZIKA virus through in-silico approaches. Journal of Biomolecular Structure and Dynamics, 2021, 39, 272-284.	2.0	26
14	Eco-friendly Microbial Biopolymers: Recent Development, Biodegradation, and Applications. , 2021, , 547-577.		0
15	Chemoinformatics and QSAR. , 2021, , 183-212.		1
16	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.	1.0	5
17	Pan-selectin inhibitors as potential therapeutics for COVID-19 treatment: in silico screening study. Glycobiology, 2021, 31, 975-987.	1.3	9
18	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. International Journal of Molecular Sciences, 2021, 22, 7071.	1.8	22

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19	Synthesis, antibacterial, anti-oxidant and molecular docking studies of imidazoquinolines. Heliyon, 2021, 7, e07484.	1.4	5
20	Interrogation of Bacillus anthracis 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.	1.8	5
21	Elucidation of Agonist and Antagonist Dynamic Binding Patterns in ER-Î± by Integration of Molecular Docking, Molecular Dynamics Simulations and Quantum Mechanical Calculations. International Journal of Molecular Sciences, 2021, 22, 9371.	1.8	9
22	Molecular Features of Potential Herbal Products in Enhancing Human Immune System. , 2021, , 301-362.		0
23	Editorial: Molecular Studies of Covid-19 Chemistry. Frontiers in Chemistry, 2021, 9, 729142.	1.8	0
24	Structural Understanding of SARS-CoV-2 Drug Targets, Active Site Contour Map Analysis and COVID-19 Therapeutics. Current Molecular Pharmacology, 2021, 14, .	0.7	4
25	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.	2.0	28
26	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.	3.6	30
27	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.	0.9	2
28	Selectinsâ€"The Two Dr. Jekyll and Mr. Hyde Faces of Adhesion Moleculesâ€"A Review. Molecules, 2020, 25, 2835.	1.7	38
29	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
30	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.	2.0	132
31	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.	1.0	1
32	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.	1.8	32
33	Computational Studies Reveal Piperine, the Predominant Oleoresin of Black Pepper (<i>Piper) Tj ETQq1 1 0.784314 rgBT /Overlock	0.4	16
34	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. Current Drug Targets, 2020, 21, 132-147.	1.0	7
35	Computational Advances in Chronic Diseases Diagnostics and Therapy - II. Current Drug Targets, 2020, 21, 103-104.	1.0	5
36	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.	1.0	28

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37	Phage Protein Interactions in the Inhibition Mechanism of Bacterial Cell. , 2020, , 121-142.		2
38	Applications of Polyhydroxyalkanoates Based Nanovehicles as Drug Carriers. , 2019, , 125-169.		2
39	Competitive Inhibition of Quercetin and Apigenin at the ATP Binding site of D-Alanine-D-Alanine Ligase of Helicobacter pylori â€“ A Molecular Modeling Approach. Current Biotechnology, 2019, 7, 340-348.	0.2	5
40	Computational Advances in Chronic Diseases Diagnostics and Therapy - I. Current Drug Targets, 2019, 21, 1-2.	1.0	6
41	Computational and Experimental Binding Mechanism of DNA-drug Interactions. Current Pharmaceutical Design, 2019, 24, 3739-3757.	0.9	7
42	Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview. Current Pharmaceutical Design, 2019, 25, 3390-3405.	0.9	13
43	Exploring the Biology and Structural Architecture of Sortase Role on Biofilm Formation in Gram Positive Pathogens. Current Topics in Medicinal Chemistry, 2019, 18, 2462-2480.	1.0	6
44	Molecular Modeling and Drug Design Techniques in Microbial Drug Discovery. , 2019, , 185-231.		0
45	Molecular dynamics simulations and applications in computational toxicology and nanotoxicology. Food and Chemical Toxicology, 2018, 112, 495-506.	1.8	59
46	Competitive docking model for prediction of the human nicotinic acetylcholine receptor Î±7 binding of tobacco constituents. Oncotarget, 2018, 9, 16899-16916.	0.8	7
47	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.	1.1	6
48	Development of estrogen receptor beta binding prediction model using large sets of chemicals. Oncotarget, 2017, 8, 92989-93000.	0.8	24
49	Protein Engineering Approaches in the Post-Genomic Era. Current Protein and Peptide Science, 2017, 19, 5-15.	0.7	14
50	Advantages of Structure-Based Drug Design Approaches in Neurological Disorders. Current Neuropharmacology, 2017, 15, 1136-1155.	1.4	23
51	Consensus Modeling for Prediction of Estrogenic Activity of Ingredients Commonly Used in Sunscreen Products. International Journal of Environmental Research and Public Health, 2016, 13, 958.	1.2	17
52	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, 186-198.	1.1	6
53	Modeling of macromolecular proteins in prophenoloxidase cascade through experimental and computational approaches. Biotechnology and Applied Biochemistry, 2016, 63, 779-788.	1.4	7
54	A highly efficient sorbitol dehydrogenase from Gluconobacter oxydans G624 and improvement of its stability through immobilization. Scientific Reports, 2016, 6, 33438.	1.6	42

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55	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.	1.8	31
56	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.	3.4	72
57	Enhancement of methanol production from synthetic gas mixture by Methylosinus sporium through covalent immobilization. Applied Energy, 2016, 171, 383-391.	5.1	53
58	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.	1.4	4
59	Potential of Immobilized Whole-Cell Methylocella tundrae as a Biocatalyst for Methanol Production from Methane. Journal of Microbiology and Biotechnology, 2016, 26, 1234-1241.	0.9	53
60	Explicit Drug Re-positioning. Advances in Protein Chemistry and Structural Biology, 2015, 100, 89-112.	1.0	4
61	Molecular cloning, relative expression, and structural analysis of pattern recognition molecule Î²â€glucan binding protein from mangrove crab Episesarma tetragonum. Biotechnology and Applied Biochemistry, 2015, 62, 416-423.	1.4	2
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, 1686-1697.	2.5	25
63	Mechanistic insights of SrtAâ€"LPXTG blockers targeting the transpeptidase mechanism in Streptococcus mutans. RSC Advances, 2015, 5, 100498-100510.	1.7	15
64	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, 178-189.	2.9	34
65	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.	1.1	38
66	Exploration of proteinâ€"protein interaction effects on Î±-2-macroglobulin in an inhibition of serine protease through gene expression and molecular simulations studies. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1841-1854.	2.0	7
67	Validation of potential inhibitors for SrtA againstBacillus anthracisby combined approach of ligand-based and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1333-1349.	2.0	35
68	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, 106-116.	1.1	41
69	Virtual screening based on pharmacophoric features of known calpain inhibitors to identify potent inhibitors of calpain. Medicinal Chemistry Research, 2014, 23, 2445-2455.	1.1	14
70	Investigations on the Interactions of Î»Phage-Derived Peptides Against the SrtA Mechanism in Bacillus anthracis. Applied Biochemistry and Biotechnology, 2014, 172, 1790-1806.	1.4	11
71	Structural elucidation of SrtA enzyme in Enterococcus faecalis: an emphasis on screening of potential inhibitors against the biofilm formation. Molecular BioSystems, 2014, 10, 1775-1789.	2.9	24
72	Ligand-based pharmacophore modelling and screening of DNA minor groove binders targetingStaphylococcus aureus. Journal of Molecular Recognition, 2014, 27, 429-437.	1.1	6

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73	Molecular insights on analogs of HIV PR inhibitors toward HTLVâ€1 PR through QM/MM interactions and molecular dynamics studies: comparative structure analysis of wild and mutant HTLVâ€1 PR. Journal of Molecular Recognition, 2014, 27, 696-706.	1.1	22
74	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.	0.8	20
75	Virtual screening of LPXTG competitive SrtA inhibitors targeting signal transduction mechanism inBacillus anthracis: a combined experimental and theoretical study. Journal of Receptor and Signal Transduction Research, 2014, 34, 221-232.	1.3	14
76	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, 361-371.	1.3	16
77	Interaction investigations of crustacean Î²â€GBP recognition toward pathogenic microbial cell membrane and stimulate upon prophenoloxidase activation. Journal of Molecular Recognition, 2014, 27, 173-183.	1.1	8
78	Communication of Î³ Phage Lysin plyG Enzymes Binding toward SrtA for Inhibition ofBacillus Anthracis: Proteinâ€"Protein Interaction and Molecular Dynamics Study. Cell Communication and Adhesion, 2014, 21, 257-265.	1.0	5
79	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, 1025-1040.	1.0	14
80	Exploration of the binding of DNA binding ligands toStaphylococcalDNA through QM/MM docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2013, 31, 561-571.	2.0	38
81	Identification of potential HIV-1 integrase strand transfer inhibitors:In silicovirtual screening and QM/MM docking studies. SAR and QSAR in Environmental Research, 2013, 24, 581-595.	1.0	33
82	Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14Î±-demethylase inhibitors. Journal of Receptor and Signal Transduction Research, 2013, 33, 234-243.	1.3	32
83	Exploration of fluoroquinolone resistance in Streptococcus pyogenes: comparative structure analysis of wildâ€type and mutant DNA gyrase. Journal of Molecular Recognition, 2013, 26, 276-285.	1.1	28
84	Molecular docking, QPLD, and ADME prediction studies on HIV-1 integrase leads. Medicinal Chemistry Research, 2012, 21, 4239-4251.	1.1	28
85	In silico screening of indinavir-based compounds targeting proteolytic activity in HIV PR: binding pocket fit approach. Medicinal Chemistry Research, 2012, 21, 4060-4068.	1.1	33
86	Comparative structural analysis of two proteins belonging to quorum sensing system inVibrio cholerae. Journal of Biomolecular Structure and Dynamics, 2012, 30, 574-584.	2.0	24
87	Exploring the selectivity of a ligand complex with CDK2/CDK1: a molecular dynamics simulation approach. Journal of Molecular Recognition, 2012, 25, 504-512.	1.1	39
88	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, 339-347.	2.5	33
89	Targeting multidrug resistant Mycobacterium tuberculosis htra2 with identical chemical entities of fluoroquinolones. Indian Journal of Pharmaceutical Sciences, 2012, 74, 217.	1.0	32
90	Homology modeling, active site prediction, and targeting the anti hypertension activity through molecular docking on endothelin â€" B receptor domain. Bioinformation, 2012, 8, 81-86.	0.2	16

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91	A database for the predicted pharmacophoric features of medicinal compounds. Bioinformation, 2011, 6, 167-168.	0.2	19