Umashankar Vetrivel

List of Publications by Year
in descending order

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43 papers	637 citations	623734 14 h-index	642732 23 g-index
43 all docs	43 docs citations	43 times ranked	907 citing authors

#	Article	IF	Citations
1	Structure-based design of small molecule and peptide inhibitors for selective targeting of ROCK1: an integrative computational approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7450-7468.	3.5	3
2	Hepatitis C Virus NS3/4A Inhibition and Host Immunomodulation by Tannins from Terminalia chebula: A Structural Perspective. Molecules, 2022, 27, 1076.	3.8	13
3	Coding-Complete Genome Sequences of NITMA1086 and NITMA1139, Two SARS-CoV-2 Isolates from Belagavi District, Karnataka State, India, Harboring the D614G Mutation. Microbiology Resource Announcements, 2021, 10, .	0.6	2
4	Membrane dynamics simulation and virtual screening reveals potential dual natural inhibitors of endothelin receptors for targeting glaucomatous condition. Life Sciences, 2021, 269, 119082.	4.3	3
5	Retinoschisis and Norrie disease: a missing link. BMC Research Notes, 2021, 14, 204.	1.4	2
6	Deciphering the structural and functional impact of missense mutations in Egr1-DNA interacting interface: an integrative computational approach. Journal of Biomolecular Structure and Dynamics, 2021, , 1-13.	3.5	0
7	Structure-based drug target prioritisation and rational drug design for targeting Chlamydia trachomatis eye infections. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3131-3143.	3.5	12
8	Understanding the Uptake Mechanism and Interaction Potential of the Designed Peptide and Preparation of Composite Fiber Matrix for Fungal Keratitis. ACS Omega, 2020, 5, 12090-12102.	3.5	3
9	Deciphering potential inhibitors targeting THI4 of Fusarium solani sp. to combat fungal keratitis: An integrative computational approach. Computational Biology and Chemistry, 2020, 88, 107350.	2.3	3
10	Microsecond scale sampling of Egr-1 conformational landscape to decipher the impact of its disorder regions on structureâ€“function relationship. Molecular Simulation, 2020, 46, 1255-1264.	2.0	2
11	KinomeRun: An interactive utility for kinome target screening and interaction fingerprint analysis towards holistic visualization on kinome tree. Chemical Biology and Drug Design, 2020, 96, 1162-1175.	3.2	2
12	Microsecond Simulation of the Proteoglycan-like Region of Carbonic Anhydrase IX and Design of Chemical Inhibitors Targeting pH Homeostasis in Cancer Cells. ACS Omega, 2020, 5, 4270-4281.	3.5	9
13	Mutational landscape screening of methylene tetrahydrofolate reductase to predict homocystinuria associated variants: An integrative computational approach. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 2020, 819-820, 111687.	1.0	11
14	PepVis: An integrated peptide virtual screening pipeline for ensemble and flexible docking protocols. Chemical Biology and Drug Design, 2019, 94, 2041-2050.	3.2	14
15	Designing and enhancing the antifungal activity of corneal specific cell penetrating peptide using gelatin hydrogel delivery system. International Journal of Nanomedicine, 2019, Volume 14, 605-622.	6.7	30
16	Structural insights on druggable hotspots in CD147: A bull's eye view. Life Sciences, 2019, 224, 76-87.	4.3	23
17	Identification of potential drugs targeting L,Lâ€diaminopimelate aminotransferase of Chlamydia trachomatis : An integrative pharmacoinformatics approach. Journal of Cellular Biochemistry, 2019, 120, 2271-2288.	2.6	14
18	Virtual screening of natural inhibitors targeting ornithine decarboxylase with pharmacophore scaffolding of DFMO and validation by molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 766-780.	3.5	19

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19	PocketPipe: A computational pipeline for integrated Pocketome prediction and comparison. Bioinformation, 2019, 15, 295-298.	0.5	3
20	POAP: A GNU parallel based multithreaded pipeline of open babel and AutoDock suite for boosted high throughput virtual screening. Computational Biology and Chemistry, 2018, 74, 39-48.	2.3	60
21	Genome-wide codon usage profiling of ocular infective Chlamydia trachomatis serovars and drug target identification. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1979-2003.	3.5	9
22	Design of inhibitory peptide targeting Toxoplasma gondii RON4â€human Î²â€tubulin interactions by implementing structural bioinformatics methods. Journal of Cellular Biochemistry, 2018, 119, 3236-3246.	2.6	8
23	Insights on ornithine decarboxylase silencing as a potential strategy for targeting retinoblastoma. Biomedicine and Pharmacotherapy, 2018, 98, 23-28.	5.6	5
24	Deciphering ophthalmic adaptive inhibitors targeting RON4 of Toxoplasma gondii: An integrative in silico approach. Life Sciences, 2018, 213, 82-93.	4.3	5
25	Demystifying the pH dependent conformational changes of human heparanase pertaining to structureâ€“function relationships: an in silico approach. Journal of Computer-Aided Molecular Design, 2018, 32, 821-840.	2.9	9
26	Comparative docking of dual conformations in human fatty acid synthase thioesterase domain reveals potential binding cavity for virtual screening of ligands. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1350-1366.	3.5	7
27	Virtual screening, molecular dynamics, and binding free energy calculations on human carbonic anhydrase IX catalytic domain for deciphering potential leads. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2155-2168.	3.5	27
28	Probing the intermolecular interactions of PPARÎ³-LBD with polyunsaturated fatty acids and their anti-inflammatory metabolites to infer most potential binding moieties. Lipids in Health and Disease, 2017, 16, 17.	3.0	37
29	Ornithine and its role in metabolic diseases: An appraisal. Biomedicine and Pharmacotherapy, 2017, 86, 185-194.	5.6	70
30	Multilevel Precision-Based Rational Design of Chemical Inhibitors Targeting the Hydrophobic Cleft ofToxoplasma gondiiApical Membrane Antigen 1 (AMA1). Genomics and Informatics, 2016, 14, 53.	0.8	8
31	PCOSDB: PolyCystic Ovary Syndrome DataBase for manually curated genes associated with the disease. Bioinformation, 2016, 12, 4-8.	0.5	11
32	In silico analysis and prioritization of drug targets in Fusarium solani. Medical Hypotheses, 2015, 84, 81-84.	1.5	8
33	Importance of ABC transporters in different tissues. Drug Metabolism and Drug Interactions, 2014, 29, 65-66.	0.3	1
34	Modulation of multidrug resistance 1 expression and function in retinoblastoma cells by curcumin. Journal of Pharmacology and Pharmacotherapeutics, 2013, 4, 103-109.	0.4	17
35	Virtual screening studies reveal linarin as a potential natural inhibitor targeting CDK4 in retinoblastoma. Journal of Pharmacology and Pharmacotherapeutics, 2013, 4, 256-264.	0.4	13
36	Agonistic effect of polyunsaturated fatty acids (PUFAs) and its metabolites on brain-derived neurotrophic factor (BDNF) through molecular docking simulation. Lipids in Health and Disease, 2012, 11, 109.	3.0	25

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37	In vitro and In silico studies on inhibitory effects of curcumin on multi drug resistance associated protein (MRP1) in retinoblastoma cells. Bioinformation, 2012, 8, 13-19.	0.5	21
38	A novel in silico approach to identify potential therapeutic targets in human bacterial pathogens. The HUGO Journal, 2011, 5, 25-34.	4.1	40
39	InPACdb - Indian plant anticancer compounds database. Bioinformation, 2009, 4, 71-74.	0.5	21
40	Open discovery: An integrated live Linux platform of Bioinformatics tools. Bioinformation, 2008, 3, 144-146.	0.5	8
41	ACUA: A software tool for automated codon usage analysis. Bioinformation, 2007, 2, 62-63.	0.5	55
42	Deciphering novel potential antibacterial targets in tomato pathogen Ralstonia solanacearum GMI1000 through integration of in silico subtractive genomics, codon usage and proteinâ€“protein interaction analyses. Australasian Plant Pathology, 0, , 1.	1.0	1
43	Elucidating the Therapeutic Potential of Cell-Penetrating Peptides in Human Tenon Fibroblast Cells. ACS Omega, 0, , .	3.5	3