Muthukumaran Jayaraman

List of Publications by Year
in descending order

55 papers	788 citations	623574 14 h-index	552653 26 g-index
56 all docs	56 docs citations	56 times ranked	1280 citing authors

#	Article	IF	Citations
1	Isolation and biological evaluation 7-hydroxy flavone fromAvicennia officinalisL: insights from extensiveinÂvitro, DFT, molecular docking and molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2848-2860.	2.0	5
2	Identification and prioritization of promising lead molecules fromSyzygium aromaticumagainst Sortase C fromStreptococcus pyogenes: anin silicoinvestigation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5418-5435.	2.0	1
3	In silicoandin vitroinvestigations on the proteinâ€“protein interactions of glutathione S-transferases with mitogen-activated protein kinase 8 and apoptosis signal-regulating kinase 1. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1430-1440.	2.0	6
4	Identification of promising antiviral drug candidates against non-structural protein 15 (NSP15) from SARS-CoV-2: an in silico assisted drug-repurposing study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 438-448.	2.0	24
5	Experimental and computational investigation on the binding of anticancer drug gemcitabine with bovine serum albumin. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9144-9157.	2.0	10
6	Biological evaluation of gallic acid and quercetin derived fromCeriops tagal: insights from extensiveinÂvitroandin silicostudies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1490-1502.	2.0	19
7	Identifying the natural compound Catechin from tropical mangrove plants as a potential lead candidate against 3CL^{pro}from SARS-CoV-2: An integratedin silicoapproach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13392-13411.	2.0	6
8	A potential implication of UDP-glucuronosyltransferase 2B10 in the detoxification of drugs used in pediatric hematopoietic stem cell transplantation setting: an in silico investigation. BMC Molecular and Cell Biology, 2022, 23, 5.	1.0	1
9	An extensive computational study to identify potential inhibitors of Acyl-homoserine-lactone synthase from Acinetobacter baumannii (strain AYE). Journal of Molecular Graphics and Modelling, 2022, 114, 108168.	1.3	8
10	Comparative structural and functional analysis of STL and SLL, chitin-binding lectins from Solanum spp.. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4907-4922.	2.0	5
11	Targeting SARS-CoV-2: a systematic drug repurposing approach to identify promising inhibitors against 3C-like proteinase and 2â€²-O-ribose methyltransferase. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2679-2692.	2.0	209
12	Structural and functional characterization of chitin binding lectin from Datura stramonium: insights from phylogenetic analysis, protein structure prediction, molecular docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1698-1716.	2.0	4
13	A comprehensive in silico and inÂvitro studies on quinizarin: a promising phytochemical derived from Rhizophora mucronata Lam. Journal of Biomolecular Structure and Dynamics, 2021, , 1-12.	2.0	10
14	Experimental and in silico investigation on the interaction of indomethacin with bovine serum albumin: Effect of sodium dodecyl sulfate surfactant monomers on the binding. Journal of Molecular Liquids, 2021, 336, 116858.	2.3	7
15	Molecular interactions of cefoperazone with bovine serum albumin: Extensive experimental and computational investigations. Journal of Molecular Liquids, 2021, 337, 116354.	2.3	37
16	A Comprehensive In Silico Study Towards Understanding the Inhibitory Mechanism of Lactoperoxidase by Dapsone and Propofol. Current Computer-Aided Drug Design, 2021, 17, 550-559.	0.8	0
17	Isolation, characterisation, anticancer and anti-oxidant activities of 2-methoxy mucic acid from Rhizophora apiculata: an in vitro and in silico studies. Journal of Biomolecular Structure and Dynamics, 2021, , 1-13.	2.0	3
18	Screening of promising molecules against MurG as drug target in multi-drug-resistant-Acinetobacter baumannii - insights from comparative protein modeling, molecular docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5230-5252.	2.0	13

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19	Structure based drug designing and discovery of promising lead molecules against UDP-N-acetylenolpyruvoylglucosamine reductase (MurB): A potential drug target in multi-drug resistant Acinetobacter baumannii. Journal of Molecular Graphics and Modelling, 2020, 100, 107675.	1.3	12
20	Identification of promising molecules against MurD ligase from Acinetobacter baumannii: insights from comparative protein modelling, virtual screening, molecular dynamics simulations and MM/PBSA analysis. Journal of Molecular Modeling, 2020, 26, 304.	0.8	11
21	Molecular interactions of ceftazidime with bovine serum albumin: Spectroscopic, molecular docking, and DFT analyses. Journal of Molecular Liquids, 2020, 313, 113490.	2.3	40
22	Computer aided ligand based screening for identification of promising molecules against enzymes involved in peptidoglycan biosynthetic pathway from Acinetobacter baumannii. Microbial Pathogenesis, 2020, 147, 104205.	1.3	13
23	Prioritization of Mur family drug targets against A. baumannii and identification of their homologous proteins through molecular phylogeny, primary sequence, and structural analysis. Journal of Genetic Engineering and Biotechnology, 2020, 18, 33.	1.5	6
24	A comprehensive review on promising anti-viral therapeutic candidates identified against main protease from SARS-CoV-2 through various computational methods. Journal of Genetic Engineering and Biotechnology, 2020, 18, 69.	1.5	41
25	Crystal structure analysis of ethyl 3-(4-chlorophenyl)-1,6-dimethyl-4-methylsulfanyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 443-445.	0.2	2
26	Crystal structure analysis of ethyl 6-(4-methoxyphenyl)-1-methyl-4-methylsulfanyl-3-phenyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1209-1212.	0.2	1
27	Shedding Light on the Interaction of Human Anti-Apoptotic Bcl-2 Protein with Ligands through Biophysical and in Silico Studies. International Journal of Molecular Sciences, 2019, 20, 860.	1.8	25
28	Systematic exploration of predicted destabilizing nonsynonymous single nucleotide polymorphisms (nsSNPs) of human aldehyde oxidase: A Bioâ€informatics study. Pharmacology Research and Perspectives, 2019, 7, e00538.	1.1	9
29	Association of CTH variant with sinusoidal obstruction syndrome in children receiving intravenous busulfan and cyclophosphamide before hematopoietic stem cell transplantation. Pharmacogenomics Journal, 2018, 18, 64-69.	0.9	13
30	Genotype Distribution of Dihydrofolatereductase Variants and their Role in Disease Susceptibility to Acute Lymphoblastic Leukemia in Indian Population: An Experimental and Computational Analysis. Journal of Leukemia (Los Angeles, Calif), 2016, 04, .	0.1	3
31	Synthesis, in vitro and in silico anti-proliferative activity of 4-aryl-4H-chromene derivatives. Medicinal Chemistry Research, 2016, 25, 1308-1315.	1.1	23
32	In vitro and in vivo biological characterization of the anti-proliferative potential of a cyclic trinuclear organotin(<scp>iv</scp>) complex. Molecular BioSystems, 2016, 12, 1015-1023.	2.9	17
33	Synthesis, in vitro and in silico antimalarial activity of 7-chloroquinoline and 4H-chromene conjugates. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4657-4663.	1.0	41
34	Design, synthesis, in vitro and in silico anti-cancer activity of 4H-chromenes with C4-active methine groups. Medicinal Chemistry Research, 2015, 24, 1226-1240.	1.1	22
35	Exploring the structural features of Aspartate Trans Carbamoylase (TtATCase) fromThermus thermophilusHB8 through in silico approaches: a potential drug target for inborn error of pyrimidine metabolism. Journal of Biomolecular Structure and Dynamics, 2014, 32, 591-601.	2.0	6
36	Design, synthesis, molecular docking, and biological evaluation of N-methyl-3-nitro-4-(nitromethyl)-4H-chromen-2-amine derivatives as potential anti-cancer agents. Medicinal Chemistry Research, 2014, 23, 642-659.	1.1	22

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37	Molecular dynamic simulations of the tubulinâ€“human gamma synuclein complex: structural insight into the regulatory mechanism involved in inducing resistance against Taxol. Molecular BioSystems, 2013, 9, 1470.	2.9	9
38	6-Ethyl-N-methyl-3-nitro-4-nitromethyl-4H-chromen-2-amine. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o180-o181.	0.2	1
39	Structural insights into interacting mechanism of ID1 protein with an antagonist ID1/3-PA7 and agonist ETS-1 in treatment of ovarian cancer: molecular docking and dynamics studies. Journal of Molecular Modeling, 2012, 18, 4865-4884.	0.8	6
40	Synthesis and in silico evaluation of 1N-methyl-1S-methyl-2-nitroethylene (NMSM) derivatives against Alzheimer disease: to understand their interacting mechanism with acetylcholinesterase. Journal of Chemical Biology, 2012, 5, 151-166.	2.2	4
41	An X-Ray Crystallographic Study of N-Methyl-3-nitro-4-(nitromethyl)-4H-chromen-2-amine. Journal of Chemical Crystallography, 2011, 41, 1927-1934.	0.5	3
42	Insight into residues involved in the structure and function of the breast cancer associated protein human gamma synuclein. Journal of Molecular Modeling, 2011, 17, 251-263.	0.8	13
43	1-(2-Naphthyl)-3-phenyl-3-(4,5,6,7-tetrahydro-1,2,3-benzoselenadiazol-4-yl)propan-1-one. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2010-o2011.	0.2	2
44	4-[4-(Diethylamino)phenyl]-N-methyl-3-nitro-4H-chromen-2-amine. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o1395-o1396.	0.2	0
45	3-(4-Methylphenyl)-1-phenyl-3-(4,5,6,7-tetrahydro-1,2,3-benzoselenadiazol-4-yl)propan-1-one. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o1660-o1661.	0.2	1
46	6,8-Dichloro-N-methyl-3-nitro-4-nitromethyl-4H-chromen-2-amine. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o898-o899.	0.2	3
47	4-{(4-Chlorophenyl)[4-(4-methylphenyl)-1,2,3-selenadiazol-5-yl]methyl}-4,5,6,7-tetrahydro-1,2,3-benzoselenadiazole. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o1421-o1422.	0.2	0
48	6-Methoxy-N-methyl-3-nitro-4-nitromethyl-4H-chromen-2-amine. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o1276-o1277.	0.2	3
49	2,2â€²-[Naphthalene-1,5-diylbis(nitrilomethanylylidene)]diphenol. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o1765-o1766.	0.2	0
50	Butane-1,4-diyl bis(pyridine-4-carboxylate). Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o1803-o1803.	0.2	0
51	Analysis of CYP3A4-HIV-1 protease drugs interactions by computational methods for Highly Active Antiretroviral Therapy in HIV/AIDS. Journal of Molecular Graphics and Modelling, 2010, 28, 455-463.	1.3	20
52	Bis(Î¼-phenyltellurido-Îº2Te:Te)bis[tetracarbonylrhenium(I)]. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, m558-m559.	0.2	3
53	Heptacarbonyl-1Îº³C,2Îº⁴C-(4-phenylpyridine-1ÎºN)di-Î¼-phenyltellurido-1:2Îº⁴< Acta Crystallographica Section E: Structure Reports Online, 2010, 66, m518-m519.	0.2	1
54	ZifBASE: a database of zinc finger proteins and associated resources. BMC Genomics, 2009, 10, 421.	1.2	32

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55	Influence of the Genetic Polymorphisme in the 5â€² Flanking and Exonic Regions of CYP2C19 on Proguanil Oxidation. Drug Metabolism and Pharmacokinetics, 2009, 24, 537-548.	1.1	12