

Karthikeyan Muthusamy

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.

61
papers

615
citations

13
h-index

21
g-index

62
ext. papers

702
ext. citations

3.1
avg, IF

4.26
L-index

#	Paper	IF	Citations
61	Structural exploration of common pharmacophore based berberine derivatives as novel histone deacetylase inhibitor targeting HDACs enzymes.. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022 , 1-14	3.6	
60	Computational Study on the Inhibitory Effect of Natural Compounds against the SARS-CoV-2 Proteins.. <i>Bioinorganic Chemistry and Applications</i> , 2022 , 2022, 8635054	4.2	3
59	Structural insights on vitamin D receptor and screening of new potent agonist molecules: structure and ligand-based approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 4148-4159	3.6	10
58	Targeting renin receptor for the inhibition of renin angiotensin aldosterone system: An alternative approach through in silico drug discovery. <i>Computational and Theoretical Chemistry</i> , 2021 , 1208, 113541 ²		
57	Computational prediction of small molecules with predicted binding to FGFR3 and testing biological effects in bone cells. <i>Experimental Biology and Medicine</i> , 2021 , 246, 1660-1667	3.7	
56	Mechanistic insights on nsSNPs on binding site of renin and cytochrome P450 proteins: A computational perceptual study for pharmacogenomics evaluation. <i>Journal of Cellular Biochemistry</i> , 2021 , 122, 1460-1474	4.7	4
55	In Silico Analysis of Drug Repurposing Strategy for the Identification of Potential NS3 Helicase Inhibitors Against Zika Virus. <i>Current Chinese Science</i> , 2021 , 1, 373-385	0.2	
54	Structural and functional insights on vitamin D receptor and CYP24A1 deleterious single nucleotide polymorphisms: A computational and pharmacogenomics perpetual approach. <i>Cell Biochemistry and Function</i> , 2021 , 39, 874-885	4.2	0
53	In silico drug designing for the identification of promising antagonist hit molecules against bradykinin receptor. <i>Computational and Theoretical Chemistry</i> , 2021 , 1202, 113334	2	
52	Virtual screening assisted discovery of novel natural products to inhibit the catalytic mechanism of Mycobacterium tuberculosis InhA. <i>Journal of Molecular Liquids</i> , 2021 , 335, 116204	6	4
51	Design and synthesis of imidazole based zinc binding groups as novel small molecule inhibitors targeting Histone deacetylase enzymes in lung cancer. <i>Journal of Molecular Structure</i> , 2020 , 1214, 12817-12834	3.4	8
50	Computational study on cross-talking cancer signalling mechanism of ring finger protein 146, AXIN and Tankyrase protein complex. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 5173-5185	3.6	1
49	TRAF2 and NCK-Interacting Kinase Inhibitors for Colorectal Cancer: In Vitro and Theoretical Validations. <i>ACS Combinatorial Science</i> , 2020 , 22, 608-616	3.9	3
48	Computational and Pharmacogenomic Insights on Hypertension Treatment: Rational Drug Design and Optimization Strategies. <i>Current Drug Targets</i> , 2020 , 21, 18-33	3	4
47	Inhibitory potential of Hydroxychavicol on Ehrlich ascites carcinoma model and interaction on cancer targets. <i>Natural Product Research</i> , 2020 , 34, 1591-1596	2.3	3
46	Tannic acid prevents macrophage-induced pro-fibrotic response in lung epithelial cells via suppressing TLR4-mediated macrophage polarization. <i>Inflammation Research</i> , 2019 , 68, 1011-1024	7.2	19
45	Investigation of Drug Interaction Potentials and Binding Modes on Direct Renin Inhibitors: A Computational Modeling Studies. <i>Letters in Drug Design and Discovery</i> , 2019 , 16, 919-938	0.8	8

44	insights on tankyrase protein: A potential target for colorectal cancer. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 3637-3648	3.6	14
43	In silico identification and screening of CYP24A1 inhibitors: 3D QSAR pharmacophore mapping and molecular dynamics analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 1700-1714	3.6	12
42	Vitamin D receptor (VDR) non-synonymous single nucleotide polymorphisms (nsSNPs) affect the calcitriol drug response - A theoretical insight. <i>Journal of Molecular Graphics and Modelling</i> , 2018 , 81, 14-24	2.8	3
41	Current Scenario in Structure and Ligand-Based Drug Design on Anti-colon Cancer Drugs. <i>Current Pharmaceutical Design</i> , 2018 , 24, 3829-3841	3.3	5
40	Atom-based and Pharmacophore-based 3D - QSAR Studies on Vitamin D Receptor (VDR). <i>Combinatorial Chemistry and High Throughput Screening</i> , 2018 , 21, 329-343	1.3	3
39	Computational and in vitro insights on snake venom phospholipase A inhibitor of phytocompound ikshusterol-3-O-glucoside of <i>Clematis gouriana</i> Roxb. ex DC. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018 , 36, 4197-4208	3.6	3
38	Tannic acid attenuates TGF- β -induced epithelial-to-mesenchymal transition by effectively intervening TGF- β signaling in lung epithelial cells. <i>Journal of Cellular Physiology</i> , 2018 , 233, 2513-2525	7	42
37	A theoretical insight to understand the molecular mechanism of dual target ligand CTA-018 in the chronic kidney disease pathogenesis. <i>PLoS ONE</i> , 2018 , 13, e0203194	3.7	8
36	Isolation and characterization of bioactive compounds of <i>Clematis gouriana</i> Roxb. ex DC against snake venom phospholipase A (PLA) computational and in vitro insights. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 1936-1949	3.6	5
35	Exploring the Carbamazepine Interaction with Human Pregnane X Receptor and Effect on ABC2 Using In Vitro and In Silico Approach. <i>Pharmaceutical Research</i> , 2017 , 34, 1444-1458	4.5	5
34	Combined sequence and sequence-structure based methods for analyzing FGF23, CYP24A1 and VDR genes. <i>Meta Gene</i> , 2016 , 9, 26-36	0.7	5
33	Antidiabetic, antihyperlipidaemic, and antioxidant activity of <i>Syzygium densiflorum</i> fruits in streptozotocin and nicotinamide-induced diabetic rats. <i>Pharmaceutical Biology</i> , 2016 , 54, 1716-26	3.8	18
32	A computational study on role of 6-(hydroxymethyl)-3-[3,4,5-trihydroxy-6-[(3,4,5-trihydroxyoxan-2-yl)oxymethyl]oxan-2-yl]oxyoxane-2,4,5-triol in the regulation of blood glucose level. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 2599-2618	3.6	13
31	High-affinity selective inhibitor against phospholipase A2 (PLA2): a computational study. <i>Journal of Receptor and Signal Transduction Research</i> , 2016 , 36, 111-8	2.6	4
30	E-pharmacophore filtering and molecular dynamics simulation studies in the discovery of potent drug-like molecules for chronic kidney disease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 2233-2250	3.6	9
29	Computational prediction of immunodominant antigenic regions & potential protective epitopes for dengue vaccination. <i>Indian Journal of Medical Research</i> , 2016 , 144, 587-591	2.9	3
28	The Binding Mode Prediction and Similar Ligand Potency in the Active Site of Vitamin D Receptor with QM/MM Interaction, MESP, and MD Simulation. <i>Chemical Biology and Drug Design</i> , 2016 , 88, 272-80	2.9	7
27	Plant Isoquinoline Alkaloid Berberine Exhibits Chromatin Remodeling by Modulation of Histone Deacetylase To Induce Growth Arrest and Apoptosis in the A549 Cell Line. <i>Journal of Agricultural and Food Chemistry</i> , 2016 , 64, 9542-9550	5.7	42

26	Zn ²⁺ ion of the snake venom metalloproteinase (SVMP) plays a critical role in ligand binding: a molecular dynamics simulation study. <i>RSC Advances</i> , 2015 , 5, 70566-70576	3.7	12
25	Identification of potent inhibitors against snake venom metalloproteinase (SVMP) using molecular docking and molecular dynamics studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015 , 33, 1516-1527	3.6	16
24	Computational insights into the inhibition of influenza viruses by rupestonic acid derivatives: pharmacophore modeling, 3D-QSAR, CoMFA and COMSIA studies. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2015 , 18, 63-74	1.3	2
23	In vitro evaluation of antioxidant and antidiabetic activities of <i>Syzygium densiflorum</i> fruits. <i>Asian Pacific Journal of Tropical Disease</i> , 2015 , 5, 912-917		7
22	ACE DD genotype associated with the female Chronic Kidney Disease patients of Tamilnadu population. <i>Egyptian Journal of Medical Human Genetics</i> , 2015 , 16, 29-33	2	
21	Understanding the evolutionary relationship of hemagglutinin protein from influenza viruses using phylogenetic and molecular modeling studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014 , 32, 816-830	3.6	5
20	Sighting of tankyrase inhibitors by structure- and ligand-based screening and in vitro approach. <i>Molecular BioSystems</i> , 2014 , 10, 2699-712		15
19	Molecular insights on TNKS1/TNKS2 and inhibitor-IWR1 interactions. <i>Molecular BioSystems</i> , 2014 , 10, 281-93		14
18	Jak2 inhibitor--a jackpot for pharmaceutical industries: a comprehensive computational method in the discovery of new potent Jak2 inhibitors. <i>Molecular BioSystems</i> , 2014 , 10, 2146-59		5
17	High throughput virtual screening and E-pharmacophore filtering in the discovery of new BACE-1 inhibitors. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2013 , 5, 119-26	3.5	17
16	Pharmacophore modeling, 3D-QSAR and DFT studies of IWR small-molecule inhibitors of Wnt response. <i>Journal of Receptor and Signal Transduction Research</i> , 2013 , 33, 276-85	2.6	7
15	Pharmacophore modeling, 3D-QSAR, and molecular docking study on naphthyridine derivatives as inhibitors of 3-phosphoinositide-dependent protein kinase-1. <i>Medicinal Chemistry Research</i> , 2013 , 22, 3812-3822	2.2	2
14	Molecular modeling, quantum polarized ligand docking and structure-based 3D-QSAR analysis of the imidazole series as dual AT(1) and ET(A) receptor antagonists. <i>Acta Pharmacologica Sinica</i> , 2013 , 34, 1592-606	8	41
13	In silico structural and functional analysis of the human TOPK protein by structure modeling and molecular dynamics studies. <i>Journal of Molecular Modeling</i> , 2013 , 19, 407-19	2	11
12	Homology modeling, molecular dynamics, e-pharmacophore mapping and docking study of Chikungunya virus nsP2 protease. <i>Journal of Molecular Modeling</i> , 2012 , 18, 39-51	2	70
11	Theoretical studies on benzimidazole derivatives as <i>E. coli</i> biotin carboxylase inhibitors. <i>Medicinal Chemistry Research</i> , 2012 , 21, 2169-2180	2.2	4
10	E-Pharmacophore mapping and docking studies on Vitamin D receptor (VDR). <i>Bioinformatics</i> , 2012 , 8, 705-10	1.1	13
9	Structure-based drug discovery of ApoE4 inhibitors from the plant compounds. <i>Medicinal Chemistry Research</i> , 2012 , 21, 825-833	2.2	3

8	Homology modeling, molecular dynamics, and molecular docking studies of <i>Trichomonas vaginalis</i> carbamate kinase. <i>Medicinal Chemistry Research</i> , 2012 , 21, 2105-2116	2.2	9
7	Docking Studies of Adenosine Analogues with NS5 Methyltransferase of Yellow Fever Virus. <i>Indian Journal of Microbiology</i> , 2012 , 52, 28-34	3.7	4
6	Ligand-based Pharmacophore Modeling; Atom-based 3D-QSAR Analysis and Molecular Docking Studies of Phosphoinositide-Dependent Kinase-1 Inhibitors. <i>Indian Journal of Pharmaceutical Sciences</i> , 2012 , 74, 141-51	1.5	14
5	Epitope-based immunoinformatics and molecular docking studies of nucleocapsid protein and ovarian tumor domain of crimean-congo hemorrhagic Fever virus. <i>Frontiers in Genetics</i> , 2011 , 2, 72	4.5	11
4	Pharmacophore filtering and 3D-QSAR in the discovery of new JAK2 inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2011 , 30, 186-97	2.8	39
3	Myocilin mutations among POAG patients from two populations of Tamil Nadu, South India, a comparative analysis. <i>Molecular Vision</i> , 2011 , 17, 3243-53	2.3	13
2	In silico studies on marine actinomycetes as potential inhibitors for Glioblastoma multiforme. <i>Bioinformation</i> , 2011 , 6, 100-6	1.1	9
1	In silico genome analysis and drug efficacy test of influenza A virus (H1N1) 2009. <i>Indian Journal of Microbiology</i> , 2009 , 49, 358-64	3.7	4