Karthikeyan Muthusamy

List of Publications by Citations

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	Homology modeling, molecular dynamics, e-pharmacophore mapping and docking study of Chikungunya virus nsP2 protease. *Journal of Molecular Modeling*, **2012**, 18, 39-51	2	70
60	Plant Isoquinoline Alkaloid Berberine Exhibits Chromatin Remodeling by Modulation of Histone Deacetylase To Induce Growth Arrest and Apoptosis in the A549 Cell Line. *Journal of Agricultural and Food Chemistry*, **2016**, 64, 9542-9550	5.7	42
59	Tannic acid attenuates TGF-β1-induced epithelial-to-mesenchymal transition by effectively intervening TGF-β signaling in lung epithelial cells. *Journal of Cellular Physiology*, **2018**, 233, 2513-2525	7	42
58	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. *Acta Pharmacologica Sinica*, **2013**, 34, 1592-606	8	41
57	Pharmacophore filtering and 3D-QSAR in the discovery of new JAK2 inhibitors. *Journal of Molecular Graphics and Modelling*, **2011**, 30, 186-97	2.8	39
56	Tannic acid prevents macrophage-induced pro-fibrotic response in lung epithelial cells via suppressing TLR4-mediated macrophage polarization. *Inflammation Research*, **2019**, 68, 1011-1024	7.2	19
55	Antidiabetic, antihyperlipidaemic, and antioxidant activity of Syzygium densiflorum fruits in streptozotocin and nicotinamide-induced diabetic rats. *Pharmaceutical Biology*, **2016**, 54, 1716-26	3.8	18
54	High throughput virtual screening and E-pharmacophore filtering in the discovery of new BACE-1 inhibitors. *Interdisciplinary Sciences, Computational Life Sciences*, **2013**, 5, 119-26	3.5	17
53	Identification of potent inhibitors against snake venom metalloproteinase (SVMP) using molecular docking and molecular dynamics studies. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 1516-27	3.6	16
52	Sighting of tankyrase inhibitors by structure- and ligand-based screening and in vitro approach. *Molecular BioSystems*, **2014**, 10, 2699-712		15
51	Molecular insights on TNKS1/TNKS2 and inhibitor-IWR1 interactions. *Molecular BioSystems*, **2014**, 10, 281-93		14
50	Ligand-based Pharmacophore Modeling; Atom-based 3D-QSAR Analysis and Molecular Docking Studies of Phosphoinositide-Dependent Kinase-1 Inhibitors. *Indian Journal of Pharmaceutical Sciences*, **2012**, 74, 141-51	1.5	14
49	insights on tankyrase protein: A potential target for colorectal cancer. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 3637-3648	3.6	14
48	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. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 2599-2618	3.6	13
47	E-Pharmacophore mapping and docking studies on Vitamin D receptor (VDR). *Bioinformation*, **2012**, 8, 705-10	1.1	13
46	Myocilin mutations among POAG patients from two populations of Tamil Nadu, South India, a comparative analysis. *Molecular Vision*, **2011**, 17, 3243-53	2.3	13
45	Zn2+ ion of the snake venom metalloproteinase (SVMP) plays a critical role in ligand binding: a molecular dynamics simulation study. *RSC Advances*, **2015**, 5, 70566-70576	3.7	12

44	In silico identification and screening of CYP24A1 inhibitors: 3D QSAR pharmacophore mapping and molecular dynamics analysis. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 1700-1714	3.6	12
43	In silico structural and functional analysis of the human TOPK protein by structure modeling and molecular dynamics studies. *Journal of Molecular Modeling*, **2013**, 19, 407-19	2	11
42	Epitope-based immunoinformatics and molecular docking studies of nucleocapsid protein and ovarian tumor domain of crimean-congo hemorrhagic Fever virus. *Frontiers in Genetics*, **2011**, 2, 72	4.5	11
41	Structural insights on vitamin D receptor and screening of new potent agonist molecules: structure and ligand-based approach. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 4148-4159	3.6	10
40	E-pharmacophore filtering and molecular dynamics simulation studies in the discovery of potent drug-like molecules for chronic kidney disease. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 2233-2250	3.6	9
39	Homology modeling, molecular dynamics, and molecular docking studies of Trichomonas vaginalis carbamate kinase. *Medicinal Chemistry Research*, **2012**, 21, 2105-2116	2.2	9
38	In silico studies on marine actinomycetes as potential inhibitors for Glioblastoma multiforme. *Bioinformation*, **2011**, 6, 100-6	1.1	9
37	Design and synthesis of imidazole based zinc binding groups as novel small molecule inhibitors targeting Histone deacetylase enzymes in lung cancer. *Journal of Molecular Structure*, **2020**, 1214, 128177	3.4	8
36	Investigation of Drug Interaction Potentials and Binding Modes on Direct Renin Inhibitors: A Computational Modeling Studies. *Letters in Drug Design and Discovery*, **2019**, 16, 919-938	0.8	8
35	A theoretical insight to understand the molecular mechanism of dual target ligand CTA-018 in the chronic kidney disease pathogenesis. *PLoS ONE*, **2018**, 13, e0203194	3.7	8
34	Pharmacophore modeling, 3D-QSAR and DFT studies of IWR small-molecule inhibitors of Wnt response. *Journal of Receptor and Signal Transduction Research*, **2013**, 33, 276-85	2.6	7
33	In vitro evaluation of antioxidant and antidiabetic activities of Syzygium densiflorum fruits. *Asian Pacific Journal of Tropical Disease*, **2015**, 5, 912-917		7
32	The Binding Mode Prediction and Similar Ligand Potency in the Active Site of Vitamin D Receptor with QM/MM Interaction, MESP, and MD Simulation. *Chemical Biology and Drug Design*, **2016**, 88, 272-80	2.9	7
31	Isolation and characterization of bioactive compounds of Clematis gouriana Roxb. ex DC against snake venom phospholipase A (PLA) computational and in vitro insights. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 1936-1949	3.6	5
30	Exploring the Carbamazepine Interaction with Human Pregnane X Receptor and Effect on ABCC2 Using in Vitro and in Silico Approach. *Pharmaceutical Research*, **2017**, 34, 1444-1458	4.5	5
29	Combined sequence and sequence-structure based methods for analyzing FGF23, CYP24A1 and VDR genes. *Meta Gene*, **2016**, 9, 26-36	0.7	5
28	Understanding the evolutionary relationship of hemagglutinin protein from influenza viruses using phylogenetic and molecular modeling studies. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 816-30	3.6	5
27	Jak2 inhibitor--a jackpot for pharmaceutical industries: a comprehensive computational method in the discovery of new potent Jak2 inhibitors. *Molecular BioSystems*, **2014**, 10, 2146-59		5

26	Current Scenario in Structure and Ligand-Based Drug Design on Anti-colon Cancer Drugs. *Current Pharmaceutical Design*, **2018**, 24, 3829-3841	3.3	5
25	High-affinity selective inhibitor against phospholipase A2 (PLA2): a computational study. *Journal of Receptor and Signal Transduction Research*, **2016**, 36, 111-8	2.6	4
24	Theoretical studies on benzimidazole derivatives as E. coli biotin carboxylase inhibitors. *Medicinal Chemistry Research*, **2012**, 21, 2169-2180	2.2	4
23	Docking Studies of Adenosine Analogues with NS5 Methyltransferase of Yellow Fever Virus. *Indian Journal of Microbiology*, **2012**, 52, 28-34	3.7	4
22	In silico genome analysis and drug efficacy test of influenza A virus (H1N1) 2009. *Indian Journal of Microbiology*, **2009**, 49, 358-64	3.7	4
21	Mechanistic insights on nsSNPs on binding site of renin and cytochrome P450 proteins: A computational perceptual study for pharmacogenomics evaluation. *Journal of Cellular Biochemistry*, **2021**, 122, 1460-1474	4.7	4
20	Computational and Pharmacogenomic Insights on Hypertension Treatment: Rational Drug Design and Optimization Strategies. *Current Drug Targets*, **2020**, 21, 18-33	3	4
19	Virtual screening assisted discovery of novel natural products to inhibit the catalytic mechanism of Mycobacterium tuberculosis InhA. *Journal of Molecular Liquids*, **2021**, 335, 116204	6	4
18	Vitamin D receptor (VDR) non-synonymous single nucleotide polymorphisms (nsSNPs) affect the calcitriol drug response - A theoretical insight. *Journal of Molecular Graphics and Modelling*, **2018**, 81, 14-24	2.8	3
17	Structure-based drug discovery of ApoE4 inhibitors from the plant compounds. *Medicinal Chemistry Research*, **2012**, 21, 825-833	2.2	3
16	Atom-based and Pharmacophore-based 3D - QSAR Studies on Vitamin D Receptor (VDR). *Combinatorial Chemistry and High Throughput Screening*, **2018**, 21, 329-343	1.3	3
15	Computational prediction of immunodominant antigenic regions & potential protective epitopes for dengue vaccination. *Indian Journal of Medical Research*, **2016**, 144, 587-591	2.9	3
14	TRAF2 and NCK-Interacting Kinase Inhibitors for Colorectal Cancer: In Vitro and Theoretical Validations. *ACS Combinatorial Science*, **2020**, 22, 608-616	3.9	3
13	Inhibitory potential of Hydroxychavicol on Ehrlich ascites carcinoma model and interaction on cancer targets. *Natural Product Research*, **2020**, 34, 1591-1596	2.3	3
12	Computational and in vitro insights on snake venom phospholipase A inhibitor of phytocompound ikshusterol3-O-glucoside of Clematis gouriana Roxb. ex DC. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 4197-4208	3.6	3
11	Computational Study on the Inhibitory Effect of Natural Compounds against the SARS-CoV-2 Proteins.. *Bioinorganic Chemistry and Applications*, **2022**, 2022, 8635054	4.2	3
10	Pharmacophore modeling, 3D-QSAR, and molecular docking study on naphthyridine derivatives as inhibitors of 3-phosphoinositide-dependent protein kinase-1. *Medicinal Chemistry Research*, **2013**, 22, 3812-3822	2.2	2
9	Computational insights into the inhibition of influenza viruses by rupestonic acid derivatives: pharmacophore modeling, 3D-QSAR, CoMFA and COMSIA studies. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 63-74	1.3	2

8	Computational study on cross-talking cancer signalling mechanism of ring finger protein 146, AXIN and Tankyrase protein complex. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 5173-5185	3.6	1
7	Structural and functional insights on vitamin D receptor and CYP24A1 deleterious single nucleotide polymorphisms: A computational and pharmacogenomics perpetual approach. *Cell Biochemistry and Function*, **2021**, 39, 874-885	4.2	0
6	ACE DD genotype associated with the female Chronic Kidney Disease patients of Tamilnadu population. *Egyptian Journal of Medical Human Genetics*, **2015**, 16, 29-33	2	
5	Structural exploration of common pharmacophore based berberine derivatives as novel histone deacetylase inhibitor targeting HDACs enzymes.. *Journal of Biomolecular Structure and Dynamics*, **2022**, 1-14	3.6	
4	Targeting renin receptor for the inhibition of renin angiotensin aldosterone system: An alternative approach through in silico drug discovery. *Computational and Theoretical Chemistry*, **2021**, 1208, 113541	2	
3	Computational prediction of small molecules with predicted binding to FGFR3 and testing biological effects in bone cells. *Experimental Biology and Medicine*, **2021**, 246, 1660-1667	3.7	
2	In Silico Analysis of Drug Repurposing Strategy for the Identification of Potential NS3 Helicase Inhibitors Against Zika Virus. *Current Chinese Science*, **2021**, 1, 373-385	0.2	
1	In silico drug designing for the identification of promising antagonist hit molecules against bradykinin receptor. *Computational and Theoretical Chemistry*, **2021**, 1202, 113334	2	