

Structure based virtual screening, 3D-QSAR, molecular
selection of natural inhibitors against structural and non-structural protein
Chikungunya

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Antimicrobial cell penetrating peptides with bacterial cell specificity: pharmacophore modelling, quantitative structure activity relationship and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2370-2380.	3.5	4
2	Structure based virtual screening, 3D-QSAR, molecular dynamics and ADMET studies for selection of natural inhibitors against structural and non-structural targets of Chikungunya. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3150-3161.	3.5	24
3	Pharmacophore modeling, molecular docking and molecular dynamics simulation for screening and identifying anti-dengue phytocompounds. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1-15.	3.5	28
4	Characterization of medicinal plant-associated biocontrol <i>Bacillus subtilis</i> (SSL2) by liquid chromatography-mass spectrometry and evaluation of compounds by in silico and in vitro methods. Journal of Biomolecular Structure and Dynamics, 2020, 38, 500-510.	3.5	5
5	Hit identification and drug repositioning of potential non-nucleoside reverse transcriptase inhibitors by structure-based approach using computational tools (part II). Journal of Biomolecular Structure and Dynamics, 2020, 38, 3772-3789.	3.5	11
6	Targeting Chikungunya virus by computational approaches: from viral biology to the development of therapeutic strategies. Expert Opinion on Therapeutic Targets, 2020, 24, 63-78.	3.4	4
7	Computational guided identification of a citrus flavonoid as potential inhibitor of SARS-CoV-2 main protease. Molecular Diversity, 2020, 25, 1745-1759.	3.9	31
8	Antiviral therapeutics for chikungunya virus. Expert Opinion on Therapeutic Patents, 2020, 30, 467-480.	5.0	19
9	The role of natural and nature-based compounds against Chikungunya and Mayaro alphaviruses and their vectors. Studies in Natural Products Chemistry, 2021, 68, 459-497.	1.8	3
10	Multi-conformation representation of Mpro identifies promising candidates for drug repurposing against COVID-19. Journal of Molecular Modeling, 2021, 27, 128.	1.8	9
11	Artificial Intelligence, Big Data and Machine Learning Approaches in Precision Medicine & Drug Discovery. Current Drug Targets, 2021, 22, 631-655.	2.1	32
12	Targeting Chikungunya Virus Entry: alternatives for new inhibitors in drug discovery. Current Medicinal Chemistry, 2021, 28, .	2.4	2
13	Structure-based virtual screening and molecular dynamics simulation for the identification of sphingosine kinase-2 inhibitors as potential analgesics. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12472-12490.	3.5	8
15	Identification of lactoferrin-derived peptides as potential inhibitors against the main protease of SARS-CoV-2. LWT - Food Science and Technology, 2022, 154, 112684.	5.2	19
16	Virtual Combinatorial Chemistry and Pharmacological Screening: A Short Guide to Drug Design. International Journal of Molecular Sciences, 2022, 23, 1620.	4.1	17
17	Drug Repurposing for Identification of S1P1 agonists with Potential Application in Multiple Sclerosis Using in Silico Drug Design Approaches. Advanced Pharmaceutical Bulletin, 2022, , .	1.4	2
18	Exploration of Structure-Activity Relationship Using Integrated Structure and Ligand Based Approach: Hydroxamic Acid-Based HDAC Inhibitors and Cytotoxic Agents. Turkish Journal of Pharmaceutical Sciences, 2023, 20, 270-284.	1.4	1
19	Graph theoretical network analysis, in silico exploration, and validation of bioactive compounds from <i>Cynodon dactylon</i> as potential neuroprotective agents against β -synuclein. BiImpacts, 0, , .	1.5	1

#	ARTICLE	IF	CITATIONS
20	Computational screening of phytochemicals for anti-parasitic drug discovery. , 2023, , 257-283.		0
21	Pan-Genomics of Escherichia albertii for Antibiotic Resistance Profiling in Different Genome Fractions and Natural Product Mediated Intervention: In Silico Approach. Life, 2023, 13, 541.	2.4	3
22	Computational Prediction of 3,5-Diaryl-1H-Pyrazole and spiropyrazolines derivatives as potential acetylcholinesterase inhibitors for alzheimer disease treatment by 3D-QSAR, molecular docking, molecular dynamics simulation, and ADME-Tox. Journal of Biomolecular Structure and Dynamics, 0, , 1-14.	3.5	3
23	Design of new small molecules derived from indolin-2-one as potent TRKs inhibitors using a computer-aided drug design approach. Journal of Biomolecular Structure and Dynamics, 0, , 1-18.	3.5	1
24	Virtual screening and molecular dynamics investigations using natural compounds against autotaxin for the treatment of chronic pain. Journal of Biomolecular Structure and Dynamics, 0, , 1-21.	3.5	0