Nobuaki Yasuo

List of Publications by Year
in descending order

19	409	933447 10	888059 17
papers	citations	h-index	g-index

24	24	24	570
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improved Method of Structure-Based Virtual Screening via Interaction-Energy-Based Learning. Journal of Chemical Information and Modeling, 2019, 59, 1050-1061.	5.4	89
2	Identification of key interactions between SARS-CoV-2 main protease and inhibitor drug candidates. Scientific Reports, 2020, 10, 12493.	3.3	85
3	Identification of potential inhibitors based on compound proposal contest: Tyrosine-protein kinase Yes as a target. Scientific Reports, 2015, 5, 17209.	3.3	33
4	Pharmacophore Modeling for Anti-Chagas Drug Design Using the Fragment Molecular Orbital Method. PLoS ONE, 2015, 10, e0125829.	2.5	33
5	An iterative compound screening contest method for identifying target protein inhibitors using the tyrosine-protein kinase Yes. Scientific Reports, 2017, 7, 12038.	3.3	28
6	Exploring the selectivity of inhibitor complexes with Bcl-2 and Bcl-XL: A molecular dynamics simulation approach. Journal of Molecular Graphics and Modelling, 2018, 79, 166-174.	2.4	27
7	Molecular Dynamics Simulation reveals the mechanism by which the Influenza Cap-dependent Endonuclease acquires resistance against Baloxavir marboxil. Scientific Reports, 2019, 9, 17464.	3.3	23
8	In silico, in vitro, X-ray crystallography, and integrated strategies for discovering spermidine synthase inhibitors for Chagas disease. Scientific Reports, 2017, 7, 6666.	3.3	21
9	A prospective compound screening contest identified broader inhibitors for Sirtuin 1. Scientific Reports, 2019, 9, 19585.	3.3	15
10	Screening for Inhibitors of Main Protease in SARS-CoV-2: In Silico and In Vitro Approach Avoiding Peptidyl Secondary Amides. Journal of Chemical Information and Modeling, 2022, 62, 350-358.	5.4	15
11	CoDe-DTI: Collaborative Deep Learning-based Drug-Target Interaction Prediction. , 2018, , .		11
12	MERMAID: an open source automated hit-to-lead method based on deep reinforcement learning. Journal of Cheminformatics, 2021, 13, 94.	6.1	10
13	Compound property enhancement by virtual compound synthesis. Journal of Bioinformatics and Computational Biology, 2018, 16, 1840016.	0.8	5
14	Bayesian statistics-based analysis of AC impedance spectra. AIP Advances, 2020, 10, .	1.3	3
15	Computer aided drug discovery review for infectious diseases with case study of anti-Chagas project. Parasitology International, 2021, 83, 102366.	1.3	3
16	Effect of charged mutation on aggregation of a pentapeptide: Insights from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2022, 90, 405-417.	2.6	2
17	Tuning of Bayesian optimization for materials synthesis: simulation of the one-dimensional case. Science and Technology of Advanced Materials Methods, 2022, 2, 119-128.	1.3	2
18	Application for Evaluating and Visualizing the Sequence Conservation of Ligand-binding Sites. IPSJ Transactions on Bioinformatics, 2015, 8, 9-13.	0.2	1

#	Article	IF	Citations
19	Statistical potentials for RNA-protein interactions optimized by CMA-ES. Journal of Molecular Graphics and Modelling, 2022, 110, 108044.	2.4	0