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	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
2	Statistical potentials for RNA-protein interactions optimized by CMA-ES. Journal of Molecular Graphics and Modelling, 2022, 110, 108044.	2.4	0
3	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
4	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
5	Computer aided drug discovery review for infectious diseases with case study of anti-Chagas project. Parasitology International, 2021, 83, 102366.	1.3	3
6	MERMAID: an open source automated hit-to-lead method based on deep reinforcement learning. Journal of Cheminformatics, 2021, 13, 94.	6.1	10
7	Identification of key interactions between SARS-CoV-2 main protease and inhibitor drug candidates. Scientific Reports, 2020, 10, 12493.	3.3	85
8	Bayesian statistics-based analysis of AC impedance spectra. AIP Advances, 2020, 10, .	1.3	3
9	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
10	A prospective compound screening contest identified broader inhibitors for Sirtuin 1. Scientific Reports, 2019, 9, 19585.	3.3	15
11	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
12	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
13	CoDe-DTI: Collaborative Deep Learning-based Drug-Target Interaction Prediction. , 2018, , .		11
14	Compound property enhancement by virtual compound synthesis. Journal of Bioinformatics and Computational Biology, 2018, 16, 1840016.	0.8	5
15	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
16	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
17	Identification of potential inhibitors based on compound proposal contest: Tyrosine-protein kinase Yes as a target. Scientific Reports, 2015, 5, 17209.	3.3	33
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	Pharmacophore Modeling for Anti-Chagas Drug Design Using the Fragment Molecular Orbital Method. PLoS ONE, 2015, 10, e0125829.	2.5	33