

Khairul Bariyyah Abd Halim

List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Interactions of the EGFR juxtamembrane domain with PIP2-containing lipid bilayers: Insights from multiscale molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 1017-1025.	2.4	66
2	Sidekick for Membrane Simulations: Automated Ensemble Molecular Dynamics Simulations of Transmembrane Helices. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2165-2175.	5.3	27
3	Molecular Dynamic Simulation of Space and Earth-Grown Crystal Structures of Thermostable T1 Lipase <i>Geobacillus zalihae</i> Revealed a Better Structure. <i>Molecules</i> , 2017, 22, 1574.	3.8	25
4	Molecular docking and molecular dynamics simulations studies on Î²-glucosidase and xylanase <i>Trichoderma asperellum</i> to predict degradation order of cellulosic components in oil palm leaves for nanocellulose preparation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 2628-2641.	3.5	24
5	Molecular docking and molecular dynamics simulations of a mutant <i>Acinetobacter haemolyticus</i> alkaline-stable lipase against tributyrin. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 2079-2091.	3.5	19
6	<i>In silico</i> mutation on a mutant lipase from <i>Acinetobacter haemolyticus</i> towards enhancing alkaline stability. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4493-4507.	3.5	12
7	Homology modeling and docking studies of a Î²9-fatty acid desaturase from a Cold-tolerant <i>Pseudomonas</i> sp. AMS8. <i>PeerJ</i> , 2018, 6, e4347.	2.0	11
8	The mechanistic role of active site residues in non-stereo haloacid dehalogenase E (DehE). <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 219-225.	2.4	10
9	In silico study of carvone derivatives as potential neuraminidase inhibitors. <i>Journal of Molecular Modeling</i> , 2018, 24, 93.	1.8	9
10	Substrate docking and molecular dynamic simulation for prediction of fungal enzymes from <i>Trichoderma</i> species-assisted extraction of nanocellulose from oil palm leaves. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4246-4258.	3.5	7
11	Interaction of monomeric Ebola VP40 protein with a plasma membrane: A coarse-grained molecular dynamics (CGMD) simulation study. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 82, 137-144.	2.4	5