## Kazuhiro Takemura

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	TRPV4 channel activity is modulated by direct interaction of the ankyrin domain to PI(4,5)P2. Nature Communications, 2014, 5, 4994.	12.8	97
2	Water Model Tuning for Improved Reproduction of Rotational Diffusion and NMR Spectral Density. Journal of Physical Chemistry B, 2012, 116, 6279-6287.	2.6	79
3	Effects of Water Model and Simulation Box Size on Protein Diffusional Motions. Journal of Physical Chemistry B, 2007, 111, 11870-11872.	2.6	42
4	Evaluation of protein-protein docking model structures using all-atom molecular dynamics simulations combined with the solution theory in the energy representation. Journal of Chemical Physics, 2012, 137, 215105.	3.0	41
5	Protein–Ligand Dissociation Simulated by Parallel Cascade Selection Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 404-417.	5.3	34
6	Phagocytosis is mediated by two-dimensional assemblies of the F-BAR protein GAS7. Nature Communications, 2019, 10, 4763.	12.8	31
7	Salt Bridge Formation between the I-BAR Domain and Lipids Increases Lipid Density and Membrane Curvature. Scientific Reports, 2017, 7, 6808.	3.3	25
8	Enhancing Biomolecular Sampling with Reinforcement Learning: A Tree Search Molecular Dynamics Simulation Method. ACS Omega, 2019, 4, 13853-13862.	3.5	25
9	Impact of key residues within chloroplast thioredoxin-f on recognition for reduction and oxidation of target proteins. Journal of Biological Chemistry, 2019, 294, 17437-17450.	3.4	24
10	Mechanism of Deep-Sea Fish α-Actin Pressure Tolerance Investigated by Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e85852.	2.5	20
11	Binding free energy analysis of protein-protein docking model structures by evERdock. Journal of Chemical Physics, 2018, 148, 105101.	3.0	16
12	Refining evERdock: Improved selection of good protein-protein complex models achieved by MD optimization and use of multiple conformations. Journal of Chemical Physics, 2018, 149, 195101.	3.0	15
13	ColDock: Concentrated Ligand Docking with All-Atom Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2018, 122, 7191-7200.	2.6	12
14	High anisotropy and frustration: the keys to regulating protein function efficiently in crowded environments. Current Opinion in Structural Biology, 2017, 42, 50-58.	5.7	9
15	Free-energy analysis of lysozyme–triNAC binding modes with all-atom molecular dynamics simulation combined with the solution theory in the energy representation. Chemical Physics Letters, 2013, 559, 94-98.	2.6	8
16	evERdock BAI: Machine-learning-guided selection of protein-protein complex structure. Journal of Chemical Physics, 2019, 151, 215104.	3.0	8
17	Regulation of caveolae through cholesterol-depletion dependent tubulation by PACSIN2/Syndapin II. Journal of Cell Science, 2020, 133, .	2.0	7
18	Motional coherency in chain dynamics of polybutadiene studied by molecular dynamics simulations. Polymer, 2006, 47, 5973-5978.	3.8	5

#	Article	IF	CITATIONS
19	More efficient screening of protein-protein complex model structures for reducing the number of candidates. Biophysics and Physicobiology, 2019, 16, 295-303.	1.0	4
20	An Efficient Timer and Sizer of Biomacromolecular Motions. Structure, 2020, 28, 259-269.e8.	3.3	4
21	Motional Coherency in Chain Dynamics of Class-Forming Polymers. Macromolecular Symposia, 2007, 249-250, 498-501.	0.7	0
22	Molecular Dynamics and Space Correlation of Atactic Poly(methyl methacrylate). Kobunshi Ronbunshu, 2010, 67, 39-44.	0.2	0
23	TRPV4 Channel Activity Is Modulated by Direct Interaction of the Ankyrin Domain to PI(4,5)P <sub>2</sub> . Seibutsu Butsuri, 2015, 55, 262-265.	0.1	ο