Toru Ekimoto

List of Publications by Year in descending order

18 papers	227 citations	1040056 9 h-index	1058476 14 g-index
19 all docs	19 docs citations	19 times ranked	276 citing authors

#	Article	IF	Citations
1	A synthetic ion channel with anisotropic ligand response. Nature Communications, 2020, 11, 2924.	12.8	36
2	Apo- and Antagonist-Binding Structures of Vitamin D Receptor Ligand-Binding Domain Revealed by Hybrid Approach Combining Small-Angle X-ray Scattering and Molecular Dynamics. Journal of Medicinal Chemistry, 2016, 59, 7888-7900.	6.4	25
3	An accurate and rapid method for calculating hydration free energies of a variety of solutes including proteins. Journal of Chemical Physics, 2019, 150, 175101.	3.0	20
4	Multiscale molecular dynamics simulations of rotary motor proteins. Biophysical Reviews, 2018, 10, 605-615.	3.2	19
5	Moving toward generalizable NZ-1 labeling for 3D structure determination with optimized epitope-tag insertion. Acta Crystallographica Section D: Structural Biology, 2021, 77, 645-662.	2.3	18
6	Supramolecular Mechanosensitive Potassium Channel Formed by Fluorinated Amphiphilic Cyclophane. Journal of the American Chemical Society, 2022, 144, 11802-11809.	13.7	17
7	Allosteric Regulation of 3CL Protease of SARS-CoV-2 and SARS-CoV Observed in the Crystal Structure Ensemble. Journal of Molecular Biology, 2021, 433, 167324.	4.2	11
8	Rotation Mechanism of Molecular Motor V1-ATPase Studied by Multiscale Molecular Dynamics Simulation. Biophysical Journal, 2017, 112, 911-920.	0.5	10
9	Structural and dynamical insights into the PH domain of p62 in human TFIIH. Nucleic Acids Research, 2021, 49, 2916-2930.	14.5	10
10	Elimination of Finite-Size Effects on Binding Free Energies via the Warp-Drive Method. Journal of Chemical Theory and Computation, 2018, 14, 6544-6559.	5.3	9
11	Hybrid Methods for Modeling Protein Structures Using Molecular Dynamics Simulations and Small-Angle X-Ray Scattering Data. Advances in Experimental Medicine and Biology, 2018, 1105, 237-258.	1.6	9
12	Imidazoliniumâ€based Multiblock Amphiphile as Transmembrane Anion Transporter. Chemistry - an Asian Journal, 2021, 16, 147-157.	3.3	9
13	Serine 298 Phosphorylation in Linker 2 of UHRF1 Regulates Ligand-Binding Property of Its Tandem Tudor Domain. Journal of Molecular Biology, 2020, 432, 4061-4075.	4.2	8
14	Structure-based screening combined with computational and biochemical analyses identified the inhibitor targeting the binding of DNA Ligase 1 to UHRF1. Bioorganic and Medicinal Chemistry, 2021, 52, 116500.	3.0	8
15	Rotational Mechanism Model of the Bacterial V1 Motor Based on Structural and Computational Analyses. Frontiers in Physiology, 2019, 10, 46.	2.8	7
16	An accurate and efficient computation method of the hydration free energy of a large, complex molecule. Journal of Chemical Physics, 2015, 142, 175101.	3.0	6
17	Mechanism of Vitamin D Receptor Ligand-Binding Domain Regulation Studied by gREST Simulations. Journal of Chemical Information and Modeling, 2021, 61, 3625-3637.	5.4	3
18	Combination of coarse-grained molecular dynamics simulations and small-angle X-ray scattering experiments. Biophysics and Physicobiology, 2019, 16, 377-390.	1.0	2