Shigetaka Yoneda

List of Publications by Year
in descending order

18	135	1163117 8	1281871 11
papers	citations	h-index	g-index

18	18	18	137
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Potential of mean force and umbrella sampling simulation for the transport of <scp>5â€oxazolidinone</scp> in heterotetrameric sarcosine oxidase. Proteins: Structure, Function and Bioinformatics, 2021, 89, 811-818.	2.6	5
2	Parallel Evolution of Two dmrt1-Derived Genes, dmy and dm-W, for Vertebrate Sex Determination. IScience, 2020, 23, 100757.	4.1	11
3	Visualizing the helical stacking of octahedral metallomesogens with a chiral core. Chemical Communications, 2020, 56, 12134-12137.	4.1	7
4	CAPLIB: A New Program Library for the Modeling and Analysis of Icosahedrally Symmetric Viral Capsids. ACS Omega, 2018, 3, 4458-4465.	3.5	0
5	Comprehensive Understanding of Host- and Guest-Dependent Helix Inversion in Chiral Nematic Liquid Crystals: Experimental and Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2018, 122, 10615-10626.	2.6	9
6	Molecular Dynamics Simulations to Determine the Structure and Dynamics of Hepatitis B Virus Capsid Bound to a Novel Anti-viral Drug. Chemical and Pharmaceutical Bulletin, 2016, 64, 1393-1396.	1.3	9
7	Analysis of water channels by molecular dynamics simulation of heterotetrameric sarcosine oxidase. Biophysics and Physicobiology, 2015, 12, 131-138.	1.0	4
8	Rotational Symmetry Boundary Condition. Seibutsu Butsuri, 2011, 51, 032-035.	0.1	0
9	Structure and dynamics of the GH loop of the foot-and-mouth disease virus capsid. Journal of Molecular Graphics and Modelling, 2009, 28, 278-286.	2.4	10
10	Analysis of Low-Frequency Phonons in Guanosine Dihydrate Based on Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2008, 112, 7055-7063.	2.5	3
11	Crystal Water Dynamics of Guanosine Dihydrate:Â Analysis of Atomic Displacement Parameters, Time Profile of Hydrogen-Bonding Probability, and Translocation of Water by MD Simulation. Journal of Physical Chemistry B, 2005, 109, 1304-1312.	2.6	13
12	Motion of an antiviral compound in a rhinovirus capsid under rotational symmetry boundary conditions. Journal of Molecular Graphics and Modelling, 2002, 21, 19-27.	2.4	8
13	A homology modeling method of an icosahedral viral capsid: inclusion of surrounding protein structures. Journal of Molecular Graphics and Modelling, 1999, 17, 114-119.	2.4	8
14	A Further Implementation of the Rotational Symmetry Boundary Conditions for Calculations of P43212 Symmetry Crystals. Journal of Molecular Graphics and Modelling, 1997, 15, 233-237.	2.4	7
15	Molecular dynamics simulation of a rhinovirus capsid under rotational symmetry boundary conditions. Journal of Computational Chemistry, 1996, 17, 191-203.	3.3	15
16	Free energy perturbation calculations on multiple mutation bases. Journal of Chemical Physics, 1992, 97, 6730-6736.	3.0	23
17	Molecular Dynamics and Free Energy Perturbation Calculations on the Mutation of Tyrosine 45 to Tryptophan in Ribonuclease T1.. Chemical and Pharmaceutical Bulletin, 1992, 40, 1303-1308.	1.3	3
18	A calculation by using semiempirical potentials of a complex of nucleotides and the cognate amino acid: A numerical approach to the amino acid recognition by tRNA for the ten typical cases. International Journal of Quantum Chemistry, 1985, 28, 201-208.	2.0	0