Toyokazu Ishida

List of Publications by Year
in descending order

23 papers	1,080 citations	567281 15 h-index	794594 19 g-index
23 all docs	23 docs citations	23 times ranked	957 citing authors

#	Article	IF	Citations
1	Computational Molecular Design of Thermal Energy Storage Materials. Japanese Journal of Multiphase Flow, 2021, 35, 525-532.	0.3	0
2	Insight into the Catalytic Mechanism of GH11 Xylanase: Computational Analysis of Substrate Distortion Based on a Neutron Structure. Journal of the American Chemical Society, 2020, 142, 17966-17980.	13.7	13
3	Computational analysis of carbohydrate recognition based on hybrid QM/MM modeling: a case study of norovirus capsid protein in complex with Lewis antigen. Physical Chemistry Chemical Physics, 2018, 20, 4652-4665.	2.8	5
4	Computational modeling of carbohydrate recognition in protein complex. AIP Conference Proceedings, 2017, , .	0.4	0
5	Computational Analysis of Sugar Alcohols as Phase-Change Material: Insight into the Molecular Mechanism of Thermal Energy Storage. Journal of Physical Chemistry C, 2016, 120, 7903-7915.	3.1	38
6	Free energy based melting point prediction by NVT simulation with solid-liquid two-phase configuration. Chemical Physics Letters, 2016, 662, 273-279.	2.6	2
7	Substrate Distortion Contributes to the Catalysis of Orotidine 5â€²-Monophosphate Decarboxylase. Journal of the American Chemical Society, 2013, 135, 17432-17443.	13.7	27
8	Computational Study of Enzymatic Catalysis Based on Large Scale Quantum Chemical Calculations: Recent Progress and Future Prospects. Seibutsu Butsuri, 2013, 53, 326-327.	0.1	0
9	Short Hydrogen Bond between Redox-Active Tyrosine Y_Z and D1-His190 in the Photosystem II Crystal Structure. Biochemistry, 2011, 50, 9836-9844.	2.5	117
10	Fragment molecular orbital study of the electronic excitations in the photosynthetic reaction center of Blastochloris viridis. Journal of Computational Chemistry, 2010, 31, 447-454.	3.3	23
11	Computational Modeling of Carbohydrate-Recognition Process in E-Selectin Complex: Structural Mapping of Sialyl Lewis X onto Ab Initio QM/MM Free Energy Surface. Journal of Physical Chemistry B, 2010, 114, 3950-3964.	2.6	15
12	Effects of Point Mutation on Enzymatic Activity: Correlation between Protein Electronic Structure and Motion in Chorismate Mutase Reaction. Journal of the American Chemical Society, 2010, 132, 7104-7118.	13.7	36
13	Modeling a Protein Enviorment in an Enzymatic Catalysis. , 2009, , 245-268.		0
14	Probing protein environment in an enzymatic process: All-electron quantum chemical analysis combined with ab initio quantum mechanical/molecular mechanical modeling of chorismate mutase. Journal of Chemical Physics, 2008, 129, 125105.	3.0	23
15	The Fragment Molecular Orbital Method for Geometry Optimizations of Polypeptides and Proteins. Journal of Physical Chemistry A, 2007, 111, 2722-2732.	2.5	117
16	Accuracy of the three-body fragment molecular orbital method applied to MÃ¸ller-Plesset perturbation theory. Journal of Computational Chemistry, 2007, 28, 1476-1484.	3.3	79
17	Change in a protein's electronic structure induced by an explicit solvent: Anab initio fragment molecular orbital study of ubiquitin. Journal of Computational Chemistry, 2007, 28, 1750-1762.	3.3	69
18	Ab initio NMR chemical shift calculations on proteins using fragment molecular orbitals with electrostatic environment. Chemical Physics Letters, 2007, 445, 331-339.	2.6	59

#	Article	IF	Citations
19	Low-Barrier Hydrogen Bond Hypothesis in the Catalytic Triad Residue of Serine Proteases:â€‰ Correlation between Structural Rearrangement and Chemical Shifts in the Acylation Process. Biochemistry, 2006, 45, 5413-5420.	2.5	64
20	All Electron Quantum Chemical Calculation of the Entire Enzyme System Confirms a Collective Catalytic Device in the Chorismate Mutase Reaction. Journal of Physical Chemistry B, 2006, 110, 1457-1463.	2.6	56
21	Multilayer Formulation of the Fragment Molecular Orbital Method (FMO). Journal of Physical Chemistry A, 2005, 109, 2638-2646.	2.5	125
22	Role of Asp102 in the Catalytic Relay System of Serine Proteases:â€‰ A Theoretical Study. Journal of the American Chemical Society, 2004, 126, 7111-7118.	13.7	58
23	Theoretical Perspectives on the Reaction Mechanism of Serine Proteases:â€‰ The Reaction Free Energy Profiles of the Acylation Process. Journal of the American Chemical Society, 2003, 125, 12035-12048.	13.7	154