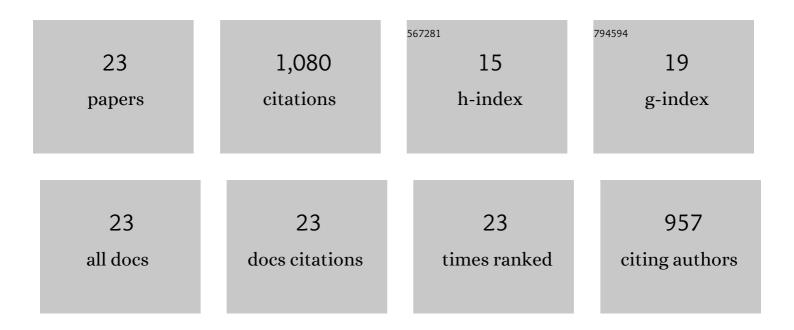
## Toyokazu Ishida

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Theoretical Perspectives on the Reaction Mechanism of Serine Proteases:  The Reaction Free Energy Profiles of the Acylation Process. Journal of the American Chemical Society, 2003, 125, 12035-12048.	13.7	154
2	Multilayer Formulation of the Fragment Molecular Orbital Method (FMO). Journal of Physical Chemistry A, 2005, 109, 2638-2646.	2.5	125
3	The Fragment Molecular Orbital Method for Geometry Optimizations of Polypeptides and Proteins. Journal of Physical Chemistry A, 2007, 111, 2722-2732.	2.5	117
4	Short Hydrogen Bond between Redox-Active Tyrosine Y <sub>Z</sub> and D1-His190 in the Photosystem II Crystal Structure. Biochemistry, 2011, 50, 9836-9844.	2.5	117
5	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
6	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
7	Low-Barrier Hydrogen Bond Hypothesis in the Catalytic Triad Residue of Serine Proteases:  Correlation between Structural Rearrangement and Chemical Shifts in the Acylation Process. Biochemistry, 2006, 45, 5413-5420.	2.5	64
8	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
9	Role of Asp102 in the Catalytic Relay System of Serine Proteases:  A Theoretical Study. Journal of the American Chemical Society, 2004, 126, 7111-7118.	13.7	58
10	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
11	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
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	Substrate Distortion Contributes to the Catalysis of Orotidine 5′-Monophosphate Decarboxylase. Journal of the American Chemical Society, 2013, 135, 17432-17443.	13.7	27
14	Probing protein environment in an enzymatic process: All-electron quantum chemical analysis combined with <i>ab initio</i> quantum mechanical/molecular mechanical modeling of chorismate mutase. Journal of Chemical Physics, 2008, 129, 125105.	3.0	23
15	Fragment molecular orbital study of the electronic excitations in the photosynthetic reaction center of <i>Blastochloris viridis</i> . Journal of Computational Chemistry, 2010, 31, 447-454.	3.3	23
16	Computational Modeling of Carbohydrate-Recognition Process in E-Selectin Complex: Structural Mapping of Sialyl Lewis X onto <i>Ab Initio</i> QM/MM Free Energy Surface. Journal of Physical Chemistry B, 2010, 114, 3950-3964.	2.6	15
17	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
18	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

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#	Article	IF	CITATIONS
19	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
20	Computational modeling of carbohydrate recognition in protein complex. AIP Conference Proceedings, 2017, , .	0.4	0
21	Modeling a Protein Enviorment in an Enzymatic Catalysis. , 2009, , 245-268.		Ο
22	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
23	Computational Molecular Design of Thermal Energy Storage Materials. Japanese Journal of Multiphase Flow, 2021, 35, 525-532.	0.3	0