Shigehiko Hayashi

List of Publications by Year
in descending order

50	2,745	218381	276539
papers	citations	26 h-index	41 g-index

55	55	55	2409
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hybrid QM/MM Free-Energy Evaluation of Drug-Resistant Mutational Effect on the Binding of an Inhibitor Indinavir to HIV-1 Protease. Journal of Chemical Information and Modeling, 2022, 62, 1328-1344.	2.5	5
2	Ab Initio Evaluation of the Redox Potential of Cytochrome c. Journal of Chemical Theory and Computation, 2021, 17, 1194-1207.	2.3	2
3	A computational method to simulate global conformational changes of proteins induced by cosolvent. Journal of Computational Chemistry, 2021, 42, 552-563.	1.5	4
4	Time-resolved serial femtosecond crystallography reveals early structural changes in channelrhodopsin. ELife, 2021, 10, .	2.8	41
5	An Atomistic Model of a Precursor State of Light-Induced Channel Opening of Channelrhodopsin. Biophysical Journal, 2018, 115, 1281-1291.	0.2	15
6	QM/MM Geometry Optimization on Extensive Free-Energy Surfaces for Examination of Enzymatic Reactions and Design of Novel Functional Properties of Proteins. Annual Review of Physical Chemistry, 2017, 68, 135-154.	4.8	15
7	Photoactivation Intermediates of a G-Protein Coupled Receptor Rhodopsin Investigated by a Hybrid Molecular Simulation. Journal of Physical Chemistry B, 2017, 121, 3842-3852.	1.2	7
8	A polyaromatic nanocapsule as a sucrose receptor in water. Science Advances, 2017, 3, e1701126.	4.7	98
9	Atomistic modeling of alternating access of a mitochondrial ADP/ATP membrane transporter with molecular simulations. PLoS ONE, 2017, 12, e0181489.	1.1	17
10	X-ray Crystallographic Structure of Thermophilic Rhodopsin. Journal of Biological Chemistry, 2016, 291, 12223-12232.	1.6	38
11	Molecular Dynamics of Channelrhodopsin at the Early Stages of Channel Opening. PLoS ONE, 2015, 10, e0131094.	1.1	33
12	Atomistic design of microbial opsin-based blue-shifted optogenetics tools. Nature Communications, 2015, 6, 7177.	5.8	78
13	Key Chemical Factors of Arginine Finger Catalysis of F₁-ATPase Clarified by an Unnatural Amino Acid Mutation. Biochemistry, 2015, 54, 472-480.	1.2	14
14	Linear Response Path Following: A Molecular Dynamics Method To Simulate Global Conformational Changes of Protein upon Ligand Binding. Journal of Chemical Theory and Computation, 2015, 11, 2900-2917.	2.3	17
15	Molecular Mechanism of Wide Photoabsorption Spectral Shifts of Color Variants of Human Cellular Retinol Binding Protein II. Journal of the American Chemical Society, 2015, 137, 13362-13370.	6.6	26
16	Role of Bulk Water Environment in Regulation of Functional Hydrogen-Bond Network in Photoactive Yellow Protein. Journal of Physical Chemistry B, 2015, 119, 15537-15549.	1.2	6
17	Silencing Neurons with Light. Science, 2014, 344, 369-370.	6.0	5
18	1SBA-04 Crucial Role of Protein Flexibility in Enzymatic Catalysis(1SBA Regulating structure formation) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.0	0

#	Article	IF	Citations
19	Structural and spectral characterizations of C1C2 channelrhodopsin and its mutants by molecular simulations. Chemical Physics Letters, 2013, 556, 266-271.	1.2	18
20	Adenosine Triphosphate Hydrolysis Mechanism in Kinesin Studied by Combined Quantum-Mechanical/Molecular-Mechanical Metadynamics Simulations. Journal of the American Chemical Society, 2013, 135, 8908-8919.	6.6	56
21	Crucial Role of Protein Flexibility in Formation of a Stable Reaction Transition State in an Î±-Amylase Catalysis. Journal of the American Chemical Society, 2012, 134, 7045-7055.	6.6	52
22	Crystal structure of the channelrhodopsin light-gated cation channel. Nature, 2012, 482, 369-374.	13.7	503
23	QM/MM Reweighting Free Energy SCF for Geometry Optimization on Extensive Free Energy Surface of Enzymatic Reaction. Journal of Chemical Theory and Computation, 2012, 8, 322-334.	2.3	45
24	Molecular Mechanism of ATP Hydrolysis in F₁-ATPase Revealed by Molecular Simulations and Single-Molecule Observations. Journal of the American Chemical Society, 2012, 134, 8447-8454.	6.6	95
25	2SG-05 Molecular mechanism of enzymatic reaction studied by the QM/MM reweighting free energy SCF method(2SG New approaches for probing biomolecular fluctuations,The 49th Annual Meeting of) Tj ETQq1 1 0.784314 rgBT /Ov		
26	3C1112 Theoretical Study of Structural Flexibility upon a Chemical Reaction in a Psychrophilic Enzyme(3C Protein: Funcrion 2,The 49th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2011, 51, S114.	0.0	0
27	Local entropy difference upon a substrate binding of a psychrophilic Î±-amylase and a mesophilic homologue. Chemical Physics Letters, 2011, 501, 517-522.	1.2	5
28	3P084 Theoretical study of flexibility and catalytic activity in psychrophilic enzymes(Protein:) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 382	0.0	0
29	Protein Collective Motions Coupled to Ligand Migration in Myoglobin. Biophysical Journal, 2010, 98, 1649-1657.	0.2	14
30	Electronic Coulombic Coupling of Excitation-Energy Transfer in Xanthorhodopsin. Journal of the American Chemical Society, 2009, 131, 14152-14153.	6.6	50
31	Photochemical Reaction Dynamics of the Primary Event of Vision Studied by Means of a Hybrid Molecular Simulation. Biophysical Journal, 2009, 96, 403-416.	0.2	106
32	A search for ligand diffusion pathway in myoglobin using a metadynamics simulation. Chemical Physics Letters, 2008, 464, 220-225.	1.2	35
33	2P-060 Structual flexibility and catalytic activity in psychrophilic and mesophilic enzymes(The 46th) Tj ETQq1 1 0.784314 rgBT /Overl	0.0	0
34	3P-251 The theoretical invesitigation about the proton transfer reaction mechanism in the photosynthetic reaction center of Rh. Sphaeroides(The 46th Annual Meeting of the Biophysical Society) Tj ETQq0 0 0 rgBT /Overlock 10		
35	3P-164 Molecular mechanism of ATP hydrolysis reaction in F_1-ATPase molecular motor(The 46th) Tj ETQq1 1 0.784314 rgBT /Overlo	0.0	0
36	Geometry optimization based on linear response free energy with quantum mechanical/molecular mechanical method: Applications to Menshutkin-type and Claisen rearrangement reactions in aqueous solution. Journal of Chemical Physics, 2007, 126, 144503.	1.2	34

#	Article	IF	Citations
37	S09A6 Mechanism of chemical-mechanical energy conversion of FrATPase molecular motor studied by hybrid molecular simulations(Mechanism of F_1-ATPase Molecular Motor-A Cross Talk among Single) Tj ETQq1 1 0.784314 rgBT /Ove	0.0	0
38	Theoretical Studies on the Color-Tuning Mechanism in Retinal Proteins. Journal of Chemical Theory and Computation, 2007, 3, 605-618.	2.3	134
39	Chemical Reactions in Biological Systems Studied by Hybrid QM/MM Simulations. Seibutsu Butsuri, 2006, 46, 76-81.	0.0	0
40	Mechanism of color tuning in retinal protein: SAC-CI and QM/MM study. Chemical Physics Letters, 2005, 414, 239-242.	1.2	67
41	Role of Hydrogen-Bond Network in Energy Storage of Bacteriorhodopsin's Light-Driven Proton Pump Revealed by ab Initio Normal-Mode Analysis. Journal of the American Chemical Society, 2004, 126, 10516-10517.	6.6	65
42	ATP Hydrolysis in the Î²TP and Î²DP Catalytic Sites of F1-ATPase. Biophysical Journal, 2004, 87, 2954-2967.	0.2	84
43	Molecular Dynamics Simulation of Bacteriorhodopsin's Photoisomerization Using Ab Initio Forces for the Excited Chromophore. Biophysical Journal, 2003, 85, 1440-1449.	0.2	141
44	On the Mechanism of ATP Hydrolysis in F1-ATPase. Biophysical Journal, 2003, 85, 2253-2266.	0.2	130
45	Structural Changes during the Formation of Early Intermediates in the Bacteriorhodopsin Photocycle. Biophysical Journal, 2002, 83, 1281-1297.	0.2	134
46	Molecular Dynamics Investigation of Primary Photoinduced Eventsin the Activation of Rhodopsin. Biophysical Journal, 2002, 83, 3097-3112.	0.2	174
47	Structural Determinants of Spectral Tuning in Retinal ProteinsBacteriorhodopsin vs Sensory Rhodopsin II#. Journal of Physical Chemistry B, 2001, 105, 10124-10131.	1.2	111
48	Proton Transfer in Bacteriorhodopsin:â€‰ Structure, Excitation, IR Spectra, and Potential Energy Surface Analyses by an ab Initio QM/MM Method. Journal of Physical Chemistry B, 2000, 104, 10678-10691.	1.2	203
49	Solvent Effect on Intramolecular Long-Range Electron-Transfer Reactions between Porphyrin and Benzoquinone in an Acetonitrile Solution:â€‰ Molecular Dynamics Calculations of Reaction Rate Constants. Journal of Physical Chemistry A, 1998, 102, 3333-3342.	1.1	16
50	Reaction Dynamics of Charge-Transfer State Formation of 4-(N,N-Dimethylamino)benzonitrile in a Methanol Solution: Theoretical Analyses. The Journal of Physical Chemistry, 1995, 99, 955-964.	2.9	52