Minoru Sakurai

List of Publications by Year
in descending order

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64 papers	1,942 citations	236925 25 h-index	254184 43 g-index
66 all docs	66 docs citations	66 times ranked	1868 citing authors

#	Article	IF	Citations
1	Molecular mechanism underlying the selective attack of trehalose lipids on cancer cells as revealed by coarse-grained molecular dynamics simulations. Biochemistry and Biophysics Reports, 2021, 25, 100913.	1.3	3
2	Group 3 LEA Protein Model Peptides Suppress Heat-Induced Lysozyme Aggregation. Elucidation of the Underlying Mechanism Using Coarse-Grained Molecular Simulations. Journal of Physical Chemistry B, 2020, 124, 2747-2759.	2.6	7
3	Development of an ATP force field for coarseâ€grained simulation of ATPases and its application to the maltose transporter. Journal of Computational Chemistry, 2019, 40, 2096-2102.	3.3	5
4	Replica exchange molecular dynamics simulation study on the mechanism of desiccation-induced structuralization of an intrinsically disordered peptide as a model of LEA proteins. Biophysics and Physicobiology, 2019, 16, 196-204.	1.0	4
5	A LEA model peptide protects the function of a red fluorescent protein in the dry state. Biochemistry and Biophysics Reports, 2019, 17, 27-31.	1.3	10
6	The mechanism of nucleotideâ€binding domain dimerization in the intact maltose transporter as studied by allâ€atom molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2018, 86, 237-247.	2.6	7
7	Physicochemical Aspects of the Biological Functions of Trehalose and Group 3 LEA Proteins as Desiccation Protectants. Advances in Experimental Medicine and Biology, 2018, 1081, 271-286.	1.6	9
8	Functional Mechanisms of ABC Transporters as Revealed by Molecular Simulations. , 2018, , 179-201.		1
9	Structural Dynamics of the Heterodimeric ABC Transporter TM287/288 Induced by ATP and Substrate Binding. Biochemistry, 2016, 55, 6730-6738.	2.5	10
10	Group 3 LEA protein model peptides protect enzymes against desiccation stress. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2016, 1864, 1237-1243.	2.3	27
11	Mechanism for the Transport of ABC Transporters by Experimental and Simulation Studies. Seibutsu Butsuri, 2016, 56, 005-008.	0.1	1
12	The Dry Preservation of Giant Vesicles Using a Group 3 LEA Protein Model Peptide and Its Molecular Mechanism. Bulletin of the Chemical Society of Japan, 2016, 89, 1493-1499.	3.2	10
13	Thermal fluctuations enable rapid proteinâ€“protein associations in aqueous solution by lowering the reaction barrier. Chemical Physics Letters, 2016, 643, 114-118.	2.6	3
14	Analysis of the Free Energy Landscapes for the Openingâ€“Closing Dynamics of the Maltose Transporter ATPase MalK₂ Using Enhanced-Sampling Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2015, 119, 9717-9725.	2.6	14
15	Water-mediated forces between the nucleotide binding domains generate the power stroke in an ABC transporter. Chemical Physics Letters, 2014, 616-617, 165-170.	2.6	6
16	Group 3 LEA protein model peptides protect liposomes during desiccation. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2757-2766.	2.6	38
17	ATP-Induced Conformational Changes of Nucleotide-Binding Domains in an ABC Transporter. Importance of the Water-Mediated Entropic Force. Journal of Physical Chemistry B, 2014, 118, 12612-12620.	2.6	17
18	The Power Stroke Driven by ATP Binding in CFTR As Studied by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 83-93.	2.6	32

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19	Dynamics and structural changes induced by ATP and/or substrate binding in the inward-facing conformation state of P-glycoprotein. Chemical Physics Letters, 2013, 557, 145-149.	2.6	13
20	An abundant LEA protein in the anhydrobiotic midge, PvLEA4, acts as a molecular shield by limiting growth of aggregating protein particles. Insect Biochemistry and Molecular Biology, 2013, 43, 1055-1067.	2.7	65
21	Full-Quantum chemical calculation of the absorption maximum of bacteriorhodopsin: a comprehensive analysis of the amino acid residues contributing to the opsin shift. Biophysics (Nagoya-shi, Japan), 2012, 8, 115-125.	0.4	4
22	Evaluation of proteinâ€ligand binding free energy focused on its entropic components. Journal of Computational Chemistry, 2012, 33, 550-560.	3.3	26
23	Effects of Group 3 LEA protein model peptides on desiccation-induced protein aggregation. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 891-897.	2.3	49
24	Experimental and Theoretical Study on the Intermolecular Complex Formation Between Trehalose and Benzene Compounds in Aqueous Solution. Journal of Physical Chemistry B, 2011, 115, 9823-9830.	2.6	22
25	Salt Effects on the Structural and Thermodynamic Properties of a Group 3 LEA Protein Model Peptide. Biochemistry, 2011, 50, 7093-7103.	2.5	35
26	Theoretical study on the absorption maxima of real GFPs. Chemical Physics Letters, 2010, 484, 324-329.	2.6	8
27	Multivariate analysis of properties of amino acid residues in proteins from a viewpoint of functional site prediction. Chemical Physics Letters, 2010, 488, 81-85.	2.6	7
28	Desiccation-Induced Structuralization and Glass Formation of Group 3 Late Embryogenesis Abundant Protein Model Peptides. Biochemistry, 2010, 49, 1093-1104.	2.5	102
29	Effects of Trehalose on the Swelling Behavior of Hydrogel â€"Visualization of the Preferential Hydration of Disaccharidesâ€". Chemistry Letters, 2009, 38, 264-265.	1.3	2
30	AM1, PM3, and PM5 calculations of the absorption maxima of basic organic dyes. Computational and Theoretical Chemistry, 2008, 860, 119-127.	1.5	41
31	Structures of the Chromophore Binding Sites in BLUF Domains as Studied by Molecular Dynamics and Quantum Chemical Calculations^{â€}. Photochemistry and Photobiology, 2008, 84, 1003-1010.	2.5	36
32	Vitrification is essential for anhydrobiosis in an African chironomid, Polypedilum vanderplanki. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5093-5098.	7.1	217
33	Parallelized integral-direct CIS(D) calculations with multilayer fragment molecular orbital scheme. Theoretical Chemistry Accounts, 2007, 117, 541-553.	1.4	71
34	Thermodynamic functions of Î±,Î±-trehalose dihydrate and of Î±,Î²-trehalose monohydrate at temperatures from 13K to 300K. Journal of Chemical Thermodynamics, 2006, 38, 1612-1619.	2.0	10
35	Linear-scaling molecular orbital calculations for the pKa values of ionizable residues in proteins. Journal of Computational Chemistry, 2006, 27, 906-916.	3.3	10
36	Accurate evaluation of the absorption maxima of retinal proteins based on a hybrid QM/MM method. Journal of Computational Chemistry, 2006, 27, 1623-1630.	3.3	26

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37	Quantum chemical study on the affinity maturation of 48G7 antibody. Computational and Theoretical Chemistry, 2005, 722, 203-211.	1.5	7
38	De- and rehydration behavior of Î±,Î±-trehalose dihydrate under humidity-controlled atmospheres. Carbohydrate Research, 2005, 340, 429-438.	2.3	34
39	A quantum chemical method for rapid optimization of protein structures. Journal of Computational Chemistry, 2005, 26, 160-168.	3.3	18
40	Decisive Role of Electronic Polarization of the Protein Environment in Determining the Absorption Maximum of Halorhodopsin. Journal of the American Chemical Society, 2003, 125, 3108-3112.	13.7	27
41	NMR and Quantum Chemical Study on the OHÂ·Â·Â·Ï€ and CHÂ·Â·Â·O Interactions between Trehalose and Unsaturated Fatty Acids:Â Implication for the Mechanism of Antioxidant Function of Trehalose. Journal of the American Chemical Society, 2003, 125, 12739-12748.	13.7	120
42	Quantum Chemical Study of the pKaControl Mechanism for the Active Center in Bacteriorhodopsin and Its M Intermediate. Journal of Physical Chemistry B, 2003, 107, 2867-2874.	2.6	16
43	Effect of Protein Environment on pKaShifts in the Active Site of Photoactive Yellow Protein. Journal of Physical Chemistry B, 2003, 107, 14569-14575.	2.6	32
44	Study of the Opsin Shift of Bacteriorhodopsin:â€‰ Insight from QM/MM Calculations with Electronic Polarization Effects of the Protein Environment. Journal of Physical Chemistry B, 2001, 105, 867-879.	2.6	85
45	Effects of Hydration on the Electronic Structure of an Enzyme:Â Implications for the Catalytic Function. Journal of the American Chemical Society, 2001, 123, 8161-8162.	13.7	17
46	Spectral Tuning of Photoactive Yellow Protein. Theoretical and Experimental Analysis of Medium Effects on the Absorption Spectrum of the Chromophore. Journal of Physical Chemistry B, 2001, 105, 9887-9895.	2.6	51
47	Infrared spectroscopic study on the properties of the anhydrous form II of trehalose. Implications for the functional mechanism of trehalose as a biostabilizer. Carbohydrate Research, 2001, 334, 233-241.	2.3	62
48	Local Structure of Phosphate/Amine Polyion Complexes in Phospholipid/Polypeptide Mixtures by Solid State NMR and ab Initio Chemical Shielding Calculation. Journal of Physical Chemistry A, 2000, 104, 2716-2723.	2.5	5
49	13C Chemical Shift-Conformation Relationship in the Chromophores of Rhodopsin and Bacteriorhodopsin. ACS Symposium Series, 1999, , 148-161.	0.5	0
50	13C chemical shift tensors and secondary structure of poly-L-alanine by solid-state two-dimensional spin-echo NMR andab initio chemical shielding calculation. Magnetic Resonance in Chemistry, 1999, 37, 303-311.	1.9	13
51	Structural Study of Acidic Phospholipidâ^'Basic Homopolypeptide Complexes by31P and13C Solid-State NMR Chemical Shifts. Journal of Physical Chemistry B, 1998, 102, 3073-3076.	2.6	4
52	Physical Origin of the Opsin Shift of Bacteriorhodopsin. Comprehensive Analysis Based on Medium Effect Theory of Absorption Spectra. Journal of the American Chemical Society, 1998, 120, 4459-4470.	13.7	52
53	Infrared Spectroscopic Study on the Structural Property of a Trehalose-Water Complex. Chemistry Letters, 1998, 27, 759-760.	1.3	18
54	Theoretical evaluation of medium effects on absorption maxima of molecular solutes. I. Formulation of a new method based on the self-consistent reaction field theory. Journal of Chemical Physics, 1997, 107, 5652-5660.	3.0	24

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55	Theoretical Study of Intermolecular Interaction at the Lipidâ^'Water Interface. 1. Quantum Chemical Analysis Using a Reaction Field Theory. Journal of Physical Chemistry B, 1997, 101, 4810-4816.	2.6	111
56	Density Functional Study of the Radical Reactions of 3-Methyl-1-phenyl-2-pyrazolin-5-one (MCI-186):â€‰Implication for the Biological Function of MCI-186 as a Highly Potent Antioxidative Radical Scavenger. Journal of Physical Chemistry A, 1997, 101, 3769-3775.	2.5	47
57	Theoretical Study of Intermolecular Interaction at the Lipidâ^'Water Interface. 2. Analysis Based on the Poissonâ^'Boltzmann Equation. Journal of Physical Chemistry B, 1997, 101, 4817-4825.	2.6	90
58	Hydration characteristics of carbohydrates and physiological functions of trehalose.. Seibutsu Butsuri, 1997, 37, 326-330.	0.1	4
59	Ab InitioStudy of13C Shieldings for Linear Ï€-Conjugated Systems. Theoretical Determination of the C12â^'C13 Conformation in the Chromophore of Rhodopsin. Journal of the American Chemical Society, 1996, 118, 8904-8915.	13.7	8
60	Ab initio study of the13C nuclear shieldings for some polyenals and their schiff bases using LORG theory. Magnetic Resonance in Chemistry, 1995, 33, 453-457.	1.9	9
61	Crystallization and compatibility of poly(vinyl alcohol)/poly(3-hydroxybutyrate) blends: Influence of blend composition and tacticity of poly(vinyl alcohol). Journal of Applied Polymer Science, 1995, 56, 17-24.	2.6	90
62	An application of the reaction field theory to hydrated metal cations in the framework of the MNDO, AM1, and PM3 methods. Journal of Computational Chemistry, 1995, 16, 378-384.	3.3	18
63	General parameterization of a reaction field theory combined with the boundary element method. Journal of Computational Chemistry, 1994, 15, 90-104.	3.3	25
64	Increasing Packing Density of Hydrated Dipalmitoylphosphatidylcholine Unilamellar Vesicles Induced by Trehalose. Chemistry Letters, 1990, 19, 1841-1844.	1.3	6