Akio Kitao

List of Publications by Year
in descending order

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131 papers	5,290 citations	136950 32 h-index	98798 67 g-index
148 all docs	148 docs citations	148 times ranked	4602 citing authors

#	Article	IF	Citations
1	Multidimensional replica-exchange method for free-energy calculations. Journal of Chemical Physics, 2000, 113, 6042-6051.	3.0	775
2	Investigating protein dynamics in collective coordinate space. Current Opinion in Structural Biology, 1999, 9, 164-169.	5.7	445
3	The effects of solvent on the conformation and the collective motions of protein: Normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum. Chemical Physics, 1991, 158, 447-472.	1.9	369
4	Energy landscape of a native protein: Jumping-among-minima model. Proteins: Structure, Function and Bioinformatics, 1998, 33, 496-517.	2.6	242
5	Model-free methods of analyzing domain motions in proteins from simulation: A comparison of normal mode analysis and molecular dynamics simulation of lysozyme. , 1997, 27, 425-437.		241
6	Effect of Solvent on Collective Motions in Globular Protein. Journal of Molecular Biology, 1993, 234, 1207-1217.	4.2	198
7	Structure of the bacterial flagellar hook and implication for the molecular universal joint mechanism. Nature, 2004, 431, 1062-1068.	27.8	176
8	Harmonicity and anharmonicity in protein dynamics: A normal mode analysis and principal component analysis. Proteins: Structure, Function and Bioinformatics, 1995, 23, 177-186.	2.6	140
9	Principal component analysis of native ensembles of biomolecular structures (PCA_NEST): insights into functional dynamics. Bioinformatics, 2009, 25, 606-614.	4.1	120
10	Harmonic and anharmonic aspects in the dynamics of BPTI: A normal mode analysis and principal component analysis. Protein Science, 1994, 3, 936-943.	7.6	115
11	Parallel cascade selection molecular dynamics (PaCS-MD) to generate conformational transition pathway. Journal of Chemical Physics, 2013, 139, 035103.	3.0	110
12	TRPV4 channel activity is modulated by direct interaction of the ankyrin domain to PI(4,5)P2. Nature Communications, 2014, 5, 4994.	12.8	97
13	Delineating the conformational landscape of the adenosine A2A receptor during G protein coupling. Cell, 2021, 184, 1884-1894.e14.	28.9	97
14	Structure of the cytoplasmic domain of FlhA and implication for flagellar type III protein export. Molecular Microbiology, 2010, 76, 260-268.	2.5	80
15	Water Model Tuning for Improved Reproduction of Rotational Diffusion and NMR Spectral Density. Journal of Physical Chemistry B, 2012, 116, 6279-6287.	2.6	79
16	Picosecond fluctuating protein energy landscape mapped by pressure temperature molecular dynamics simulation. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 17261-17265.	7.1	71
17	Hydration Affects Both Harmonic and Anharmonic Nature of Protein Dynamics. Biophysical Journal, 2008, 95, 2916-2923.	0.5	62
18	Switch interactions control energy frustration and multiple flagellar filament structures. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 4894-4899.	7.1	60

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19	Eritoran inhibits S100A8-mediated TLR4/MD-2 activation and tumor growth by changing the immune microenvironment. Oncogene, 2016, 35, 1445-1456.	5.9	56
20	Conformational dynamics of polypeptides and proteins in the dihedral angle space and in the cartesian coordinate space: Normal mode analysis of deca-alanine. Journal of Computational Chemistry, 1991, 12, 359-368.	3.3	51
21	Exploring the Folding Free Energy Landscape of a Î²-Hairpin Miniprotein, Chignolin, Using Multiscale Free Energy Landscape Calculation Method. Journal of Physical Chemistry B, 2011, 115, 8806-8812.	2.6	45
22	Effects of solvent on the conformation and the collective motions of a protein. 3. Free energy analysis by the extended RISM theory. The Journal of Physical Chemistry, 1993, 97, 10231-10235.	2.9	43
23	Effects of Water Model and Simulation Box Size on Protein Diffusional Motions. Journal of Physical Chemistry B, 2007, 111, 11870-11872.	2.6	42
24	Evaluation of protein-protein docking model structures using all-atom molecular dynamics simulations combined with the solution theory in the energy representation. Journal of Chemical Physics, 2012, 137, 215105.	3.0	41
25	Nontargeted Parallel Cascade Selection Molecular Dynamics for Enhancing the Conformational Sampling of Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5493-5502.	5.3	41
26	Gate-controlled proton diffusion and protonation-induced ratchet motion in the stator of the bacterial flagellar motor. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7737-7742.	7.1	40
27	A Collective Motion Description of the 310-/.alpha.-Helix Transition: Implications for a Natural Reaction Coordinate. Journal of the American Chemical Society, 1994, 116, 6307-6315.	13.7	39
28	Improved protein free energy calculation by more accurate treatment of nonbonded energy: Application to chymotrypsin inhibitor 2, V57A. , 1998, 30, 388-400.		39
29	Structural Insights into the Substrate Specificity Switch Mechanism of the Type III Protein Export Apparatus. Structure, 2019, 27, 965-976.e6.	3.3	39
30	Collective Dynamics of Periplasmic Glutamine Binding Protein upon Domain Closure. Biophysical Journal, 2009, 97, 2541-2549.	0.5	37
31	Protein Boson Peak Originated from Hydration-Related Multiple Minima Energy Landscape. Journal of the American Chemical Society, 2005, 127, 8705-8709.	13.7	36
32	Dissociation Process of a MDM2/p53 Complex Investigated by Parallel Cascade Selection Molecular Dynamics and the Markov State Model. Journal of Physical Chemistry B, 2019, 123, 2469-2478.	2.6	36
33	Protein Electron Transfer Reorganization Energy Spectrum from Normal Mode Analysis. 2. Application to Ru-Modified Cytochromec. Journal of Physical Chemistry B, 1998, 102, 2085-2094.	2.6	34
34	Molecular Dynamics Simulations of NAD+-Induced Domain Closure in Horse Liver Alcohol Dehydrogenase. Biophysical Journal, 2006, 91, 1823-1831.	0.5	34
35	Proteinâ€“Ligand Dissociation Simulated by Parallel Cascade Selection Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 404-417.	5.3	34
36	Essential ion binding residues for Na+ flow in stator complex of the Vibrio flagellar motor. Scientific Reports, 2019, 9, 11216.	3.3	34

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37	Effects of solvent on the conformation and the collective motions of a protein. 2. Structure of hydration in melittin. The Journal of Physical Chemistry, 1993, 97, 10223-10230.	2.9	32
38	Comparison of normal mode analyses on a small globular protein in dihedral angle space and Cartesian coordinate space. Biophysical Chemistry, 1994, 52, 107-114.	2.8	32
39	Protein Electron Transfer Reorganization Energy Spectrum from Normal Mode Analysis. 1. Theory. Journal of Physical Chemistry B, 1998, 102, 2076-2084.	2.6	31
40	Inhibition of a type III secretion system by the deletion of a short loop in one of its membrane proteins. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 812-820.	2.5	31
41	Phagocytosis is mediated by two-dimensional assemblies of the F-BAR protein GAS7. Nature Communications, 2019, 10, 4763.	12.8	31
42	Vibrational Energy Transfer from Heme through Atomic Contacts in Proteins. Journal of Physical Chemistry B, 2018, 122, 5877-5884.	2.6	30
43	Molecular dynamics simulation of proteins under high pressure: Structure, function and thermodynamics. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129395.	2.4	30
44	Dependence of Protein Stability on the Structure of the Denatured State: Free Energy Calculations of I56V Mutation in Human Lysozyme. Biophysical Journal, 1998, 75, 2178-2187.	0.5	28
45	Hydration Effect on Low-Frequency Protein Dynamics Observed in Simulated Neutron Scattering Spectra. Biophysical Journal, 2008, 94, 4435-4443.	0.5	27
46	MuSTAR MD: Multi-scale sampling using temperature accelerated and replica exchange molecular dynamics. Journal of Chemical Physics, 2013, 139, 145105.	3.0	25
47	Salt Bridge Formation between the I-BAR Domain and Lipids Increases Lipid Density and Membrane Curvature. Scientific Reports, 2017, 7, 6808.	3.3	25
48	Enhancing Biomolecular Sampling with Reinforcement Learning: A Tree Search Molecular Dynamics Simulation Method. ACS Omega, 2019, 4, 13853-13862.	3.5	25
49	Impact of key residues within chloroplast thioredoxin-f on recognition for reduction and oxidation of target proteins. Journal of Biological Chemistry, 2019, 294, 17437-17450.	3.4	24
50	How can free energy component analysis explain the difference in protein stability caused by amino acid substitutions? Effect of three hydrophobic mutations at the 56th residue on the stability of human lysozyme. Protein Engineering, Design and Selection, 2003, 16, 665-671.	2.1	23
51	Ligand-Induced Protein Responses and Mechanical Signal Propagation Described by Linear Response Theories. Biophysical Journal, 2014, 107, 1415-1425.	0.5	23
52	Screw Motion Regulates Multiple Functions of T4 Phage Protein Gene Product 5 during Cell Puncturing. Journal of the American Chemical Society, 2011, 133, 13571-13576.	13.7	22
53	The Fast-Folding Mechanism of Villin Headpiece Subdomain Studied by Multiscale Distributed Computing. Journal of Chemical Theory and Computation, 2012, 8, 290-299.	5.3	22
54	Design, synthesis and structureâ€“activity relationship studies of novel sirtuin 2 (SIRT2) inhibitors with a benzamide skeleton. Bioorganic and Medicinal Chemistry, 2015, 23, 328-339.	3.0	22

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55	Parallel cascade selection molecular dynamics for efficient conformational sampling and free energy calculation of proteins. AIP Conference Proceedings, 2016, , .	0.4	22
56	Detecting coupled collective motions in protein by independent subspace analysis. Journal of Chemical Physics, 2010, 133, 185102.	3.0	21
57	Transform and relax sampling for highly anisotropic systems: Application to protein domain motion and folding. Journal of Chemical Physics, 2011, 135, 045101.	3.0	20
58	Functional Conversion of CPD and (6â€“4) Photolyases by Mutation. Biochemistry, 2016, 55, 4173-4183.	2.5	20
59	Mechanism of Deep-Sea Fish Î±-Actin Pressure Tolerance Investigated by Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e85852.	2.5	20
60	Gap compression/extension mechanism of bacterial flagellar hook as the molecular universal joint. Journal of Structural Biology, 2007, 157, 481-490.	2.8	19
61	Non-Gaussian behavior of elastic incoherent neutron scattering profiles of proteins studied by molecular dynamics simulation. Physical Review E, 2007, 75, 041912.	2.1	19
62	A theoretical study of the two binding modes between lysozyme and tri-NAG with an explicit solvent model based on the fragment molecular orbital method. Physical Chemistry Chemical Physics, 2013, 15, 3646.	2.8	18
63	Binding free energy of protein/ligand complexes calculated using dissociation Parallel Cascade Selection Molecular Dynamics and Markov state model. Biophysics and Physicobiology, 2021, 18, 305-316.	1.0	18
64	DTA: dihedral transition analysis for characterization of the effects of large main-chain dihedral changes in proteins. Bioinformatics, 2009, 25, 628-635.	4.1	17
65	Using molecular dynamics simulations to prioritize and understand AI-generated cell penetrating peptides. Scientific Reports, 2021, 11, 10630.	3.3	17
66	Binding free energy analysis of protein-protein docking model structures by evERdock. Journal of Chemical Physics, 2018, 148, 105101.	3.0	16
67	Molecular dynamics simulation shows large volume fluctuations of proteins. European Biophysics Journal, 2000, 29, 472-480.	2.2	15
68	Refining evERdock: Improved selection of good protein-protein complex models achieved by MD optimization and use of multiple conformations. Journal of Chemical Physics, 2018, 149, 195101.	3.0	15
69	Haptic-Assisted Interactive Molecular Docking Incorporating Receptor Flexibility. Journal of Chemical Information and Modeling, 2019, 59, 2900-2912.	5.4	15
70	Computational analysis of thermal stability: effect of Ileâ†'Val mutations in human lysozyme. Folding & Design, 1998, 3, 173-181.	4.5	14
71	Kinetic Selection and Relaxation of the Intrinsically Disordered Region of a Protein upon Binding. Journal of Chemical Theory and Computation, 2020, 16, 2835-2845.	5.3	14
72	Hydration-Dependent Protein Dynamics Revealed by Molecular Dynamics Simulation of Crystalline Staphylococcal Nuclease. Journal of Physical Chemistry B, 2008, 112, 3522-3528.	2.6	13

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73	Computational Assignment of the Histidine Protonation State in (6-4) Photolyase Enzyme and Its Effect on the Protonation Step. ACS Catalysis, 2016, 6, 5500-5507.	11.2	13
74	Hydration-coupled protein boson peak measured by incoherent neutron scattering. Physica B: Condensed Matter, 2006, 385-386, 871-873.	2.7	12
75	Monte Carlo Sampling with Linear Inverse Kinematics for Simulation of Protein Flexible Regions. Journal of Chemical Theory and Computation, 2015, 11, 3895-3905.	5.3	12
76	ColDock: Concentrated Ligand Docking with All-Atom Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2018, 122, 7191-7200.	2.6	12
77	High pressure inhibits signaling protein binding to the flagellar motor and bacterial chemotaxis through enhanced hydration. Scientific Reports, 2020, 10, 2351.	3.3	12
78	Electron Fate and Mutational Robustness in the Mechanism of (6-4)Photolyase-Mediated DNA Repair. ACS Catalysis, 2017, 7, 4835-4845.	11.2	11
79	Origins of biological function in DNA and RNA hairpin loop motifs from replica exchange molecular dynamics simulation. Physical Chemistry Chemical Physics, 2018, 20, 2990-3001.	2.8	11
80	Principal Component Analysis and Related Methods for Investigating the Dynamics of Biological Macromolecules. J, 2022, 5, 298-317.	0.9	11
81	Thermal Unfolding Simulations of Bacterial Flagellin: Insight into its Refolding Before Assembly. Biophysical Journal, 2008, 94, 3858-3871.	0.5	10
82	Multi-Scale Free Energy Landscape calculation method by combination of coarse-grained and all-atom models. Chemical Physics Letters, 2011, 503, 145-152.	2.6	10
83	Multiple Markov transition matrix method: Obtaining the stationary probability distribution from multiple simulations. Journal of Computational Chemistry, 2009, 30, 1850-1858.	3.3	9
84	CyClus: A fast, comprehensive cylindrical interface approximation clustering/reranking method for rigidâ€body proteinâ€“protein docking decoys. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1005-1016.	2.6	9
85	Molecular Dynamics Study of Nitrogen-Pyramidalized Bicyclic Î²-Proline Oligomers: Length-Dependent Convergence to Organized Structures. Journal of Physical Chemistry B, 2017, 121, 100-109.	2.6	9
86	High anisotropy and frustration: the keys to regulating protein function efficiently in crowded environments. Current Opinion in Structural Biology, 2017, 42, 50-58.	5.7	9
87	Principal component analysis of native ensembles of biomolecular structures (PCA_NEST): insights into functional dynamics. Bioinformatics, 2009, 25, 2147-2147.	4.1	8
88	Free-energy analysis of lysozymeâ€“triNAG binding modes with all-atom molecular dynamics simulation combined with the solution theory in the energy representation. Chemical Physics Letters, 2013, 559, 94-98.	2.6	8
89	Molecular dynamics simulation of bacterial flagella. Biophysical Reviews, 2018, 10, 617-629.	3.2	8
90	evERdock BAI: Machine-learning-guided selection of protein-protein complex structure. Journal of Chemical Physics, 2019, 151, 215104.	3.0	8

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91	Dynamic profile analysis to characterize dynamics-driven allosteric sites in enzymes. Biophysics and Physicobiology, 2016, 13, 117-126.	1.0	7
92	Regulation of caveolae through cholesterol-depletion dependent tubulation by PACSIN2/Syndapin II. Journal of Cell Science, 2020, 133, .	2.0	7
93	Amplitudes and directions of internal protein motions from a JAM analysis of15N relaxation data. Magnetic Resonance in Chemistry, 2006, 44, S130-S142.	1.9	6
94	Conformational transition pathway and free energy analyses of proteins by parallel cascade selection molecular dynamics (PaCS-MD). AIP Conference Proceedings, 2014, , .	0.4	6
95	Regulatory Switching by Concerted Motions on the Microsecond Time Scale of the Oxygen Sensor Protein FixL. Journal of Physical Chemistry B, 2021, 125, 6847-6856.	2.6	6
96	Drug Targeting Based on a New Concept-Targeting Against TLR4 as an Example. Endocrine, Metabolic and Immune Disorders - Drug Targets, 2015, 15, 83-87.	1.2	6
97	Dynamical heterogeneity of protein dynamics studied by elastic incoherent neutron scattering and molecular simulations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 442, 356-360.	5.6	5
98	Mechanical unfolding of bacterial flagellar filament protein by molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2010, 28, 548-554.	2.4	5
99	The Effect of End Constraints on Protein Loop Kinematics. Biophysical Journal, 2010, 98, 1976-1985.	0.5	5
100	Inhibition of the hexamerization of SARS-CoV-2 endoribonuclease and modeling of RNA structures bound to the hexamer. Scientific Reports, 2022, 12, 3860.	3.3	5
101	Molecular simulation study to examine the possibility of detecting collective motion in protein by inelastic neutron scattering. Physica B: Condensed Matter, 2004, 350, E627-E630.	2.7	4
102	High quality rendering of protein dynamics in space filling mode. Journal of Molecular Graphics and Modelling, 2017, 78, 158-167.	2.4	4
103	More efficient screening of protein-protein complex model structures for reducing the number of candidates. Biophysics and Physicobiology, 2019, 16, 295-303.	1.0	4
104	An Efficient Timer and Sizer of Biomacromolecular Motions. Structure, 2020, 28, 259-269.e8.	3.3	4
105	Edge expansion parallel cascade selection molecular dynamics simulation for investigating large-amplitude collective motions of proteins. Journal of Chemical Physics, 2020, 152, 225101.	3.0	4
106	Energy landscape of a native protein: Jumpingâ€amongâ€minima model. Proteins: Structure, Function and Bioinformatics, 1998, 33, 496-517.	2.6	4
107	Universality and Structural Implications of the Boson Peak in Proteins. Biophysical Journal, 2019, 117, 229-238.	0.5	3
108	Dissociation Pathways of the p53 DNA Binding Domain from DNA and Critical Roles of Key Residues Elucidated by dPaCS-MD/MSM. Journal of Chemical Information and Modeling, 2022, 62, 1294-1307.	5.4	3

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109	Dependence of Vibrational Energy Transfer on Distance in a Four-Helix Bundle Protein: Equidistant Increments with the Periodicity of Î± Helices. Journal of Physical Chemistry B, 2022, 126, 3283-3290.	2.6	3
110	Enhanced resolution of molecular recognition to distinguish structurally similar molecules by different conformational responses of a protein upon ligand binding. Journal of Structural Biology, 2011, 173, 20-28.	2.8	2
111	Cancellation between auto- and mutual correlation contributions of protein/water dynamics in terahertz time-domain spectra. Biophysics and Physicobiology, 2019, 16, 240-247.	1.0	2
112	Structure of the MotA/B Proton Channel. Methods in Molecular Biology, 2017, 1593, 133-145.	0.9	1
113	Similarities and Differences between Thymine(6â€“4)Thymine/Cytosine DNA Lesion Repairs by Photolyases. Journal of Physical Chemistry B, 2018, 122, 8537-8547.	2.6	1
114	Multi-strand Î²-sheet of Alzheimer AÎ²(1â€“40) folds to Î²-strip helix: implication for protofilament formation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2143-2153.	3.5	1
115	The role of the half-turn in determining structures of Alzheimerâ€™s AÎ² wild-type and mutants. Journal of Structural Biology, 2021, 213, 107792.	2.8	1
116	Improved protein free energy calculation by more accurate treatment of nonbonded energy: Application to chymotrypsin inhibitor 2, V57A. Proteins: Structure, Function and Bioinformatics, 1998, 30, 388-400.	2.6	1
117	Energy landscape of a native protein: Jumping-among-minima model. , 0, .		1
118	Energy landscape of a native protein: Jumping-among-minima model. , 0, .		1
119	A Novel Method to Investigate Functionally-relevant Protein Dynamics.. Seibutsu Butsuri, 2000, 40, 167-172.	0.1	1
120	The effects of solvent on the conformation and the collective motions of protein. , 1993, , 1211-1214.		1
121	The Effects of Solvent and Anharmonicity on Incoherent Inelastic Neutron Scattering Spectra of Proteins. Journal of Neutron Research, 2002, 10, 143-147.	1.1	0
122	Slow Protein Dynamics to be Detected in Inelastic Neutron Scattering Spectra Studied by Molecular Simulation. AIP Conference Proceedings, 2004, , .	0.4	0
123	3P070 Multi-scale free energy calculation method with the combination of coarse-grained and all-atom models.(Protein: Property,The 48th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2010, 50, S157.	0.1	0
124	1PT174 Molecular Dynamics Simulation of Protein Using Robot Dynamics Algorithm(The 50th Annual) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.1	0
125	TRPV4 Channel Activity Is Modulated by Direct Interaction of the Ankyrin Domain to PI(4,5)P₂. Seibutsu Butsuri, 2015, 55, 262-265.	0.1	0
126	Complex molecular systems: a frontier of molecular science. Physical Chemistry Chemical Physics, 2018, 20, 2945-2946.	2.8	0

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127	Theoretical Studies on the Role of the Denatured State in Protein Stability. Seibutsu Butsuri, 2000, 40, 368-373.	0.1	0
128	Molecular Interaction and Energy Frustration Play Essential Roles in Polymorphic Supercoiling of Bacterial Flagellar Filament. Seibutsu Butsuri, 2008, 48, 011-017.	0.1	0
129	Molecular Simulation Methods to Enhance Soft Protein Motions. Seibutsu Butsuri, 2014, 54, 167-171.	0.1	0
130	Forewords to the special issue â€œProgress of theoretical and computational biophysicsâ€”in honor of Professor Nobuhiro Goâ€™s outstanding contribution on the occasion of his 80th birthdayâ€• Biophysics and Physicobiology, 2019, 16, 173-175.	1.0	0
131	Calculation of Binding Free Energy and Kinetic Rates with Flexible Protein Docking. Seibutsu Butsuri, 2021, 61, 398-399.	0.1	0