Wenjun Zheng

List of Publications by Year
in descending order

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72 papers	2,698 citations	172457 29 h-index	197818 49 g-index
75 all docs	75 docs citations	75 times ranked	2374 citing authors

#	Article	IF	Citations
1	Low-frequency normal modes that describe allosteric transitions in biological nanomachines are robust to sequence variations. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 7664-7669.	7.1	248
2	A comparative study of motor-protein motions by using a simple elastic-network model. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 13253-13258.	7.1	202
3	Protein conformational transitions explored by mixed elastic network models. Proteins: Structure, Function and Bioinformatics, 2007, 69, 43-57.	2.6	132
4	Network of Dynamically Important Residues in the Open/Closed Transition in Polymerases Is Strongly Conserved. Structure, 2005, 13, 565-577.	3.3	117
5	Identification of Dynamical Correlations within the Myosin Motor Domain by the Normal Mode Analysis of an Elastic Network Model. Journal of Molecular Biology, 2005, 346, 745-759.	4.2	113
6	Allosteric Transitions in the Chaperonin GroEL are Captured by a Dominant Normal Mode that is Most Robust to Sequence Variations. Biophysical Journal, 2007, 93, 2289-2299.	0.5	111
7	Probing the Local Dynamics of Nucleotide-Binding Pocket Coupled to the Global Dynamics: Myosin versus Kinesin. Biophysical Journal, 2005, 89, 167-178.	0.5	93
8	Normal-Modes-Based Prediction of Protein Conformational Changes Guided by Distance Constraints. Biophysical Journal, 2005, 88, 3109-3117.	0.5	86
9	Electrostatically Biased Binding of Kinesin to Microtubules. PLoS Biology, 2011, 9, e1001207.	5.6	64
10	Accurate Flexible Fitting of High-Resolution Protein Structures into Cryo-Electron Microscopy Maps Using Coarse-Grained Pseudo-Energy Minimization. Biophysical Journal, 2011, 100, 478-488.	0.5	61
11	Vibrational subsystem analysis: A method for probing free energies and correlations in the harmonic limit. Journal of Chemical Physics, 2008, 129, 214109.	3.0	58
12	Accurate Flexible Fitting of High-Resolution Protein Structures to Small-Angle X-Ray Scattering Data Using a Coarse-Grained Model withÂImplicit Hydration Shell. Biophysical Journal, 2011, 101, 2981-2991.	0.5	58
13	Large-scale evaluation of dynamically important residues in proteins predicted by the perturbation analysis of a coarse-grained elastic model. BMC Structural Biology, 2009, 9, 45.	2.3	56
14	Evidence of Protein Collective Motions on the Picosecond Timescale. Biophysical Journal, 2011, 100, 1058-1065.	0.5	56
15	Molecular mechanisms underlying menthol binding and activation of TRPM8 ion channel. Nature Communications, 2020, 11, 3790.	12.8	54
16	Predicting order of conformational changes during protein conformational transitions using an interpolated elastic network model. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2469-2481.	2.6	49
17	Toward the mechanism of dynamical couplings and translocation in hepatitis C virus NS3 helicase using elastic network model. Proteins: Structure, Function and Bioinformatics, 2007, 67, 886-896.	2.6	48
18	A Unification of the Elastic Network Model and the Gaussian Network Model for Optimal Description of Protein Conformational Motions and Fluctuations. Biophysical Journal, 2008, 94, 3853-3857.	0.5	48

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19	Coupling between Normal Modes Drives Protein Conformational Dynamics: Illustrations Using Allosteric Transitions in Myosin II. Biophysical Journal, 2009, 96, 2128-2137.	0.5	47
20	Modeling Protein Conformational Changes by Iterative Fitting of Distance Constraints Using Reoriented Normal Modes. Biophysical Journal, 2006, 90, 4327-4336.	0.5	45
21	Protein structure prediction constrained by solution X-ray scattering data and structural homology identification. Journal of Molecular Biology, 2002, 316, 173-187.	4.2	43
22	Allosteric Transitions in Biological Nanomachines are Described by Robust Normal Modes of Elastic Networks. Current Protein and Peptide Science, 2009, 10, 128-132.	1.4	43
23	Decrypting the Sequence of Structural Events during the Gating Transition of Pentameric Ligand-Gated Ion Channels Based on an Interpolated Elastic Network Model. PLoS Computational Biology, 2011, 7, e1001046.	3.2	41
24	A combined coarse-grained and all-atom simulation of TRPV1 channel gating and heat activation. Journal of General Physiology, 2015, 145, 443-456.	1.9	37
25	Probing the Flexibility of Tropomyosin and Its Binding to Filamentous Actin Using Molecular Dynamics Simulations. Biophysical Journal, 2013, 105, 1882-1892.	0.5	35
26	Heat activation mechanism of TRPV1: New insights from molecular dynamics simulation. Temperature, 2019, 6, 120-131.	3.0	34
27	Conformational Changes and Flexibility of DNA Devices Observed by Small-Angle X-ray Scattering. Nano Letters, 2016, 16, 4871-4879.	9.1	33
28	Probing the Structural Dynamics of the NMDA Receptor Activation by Coarse-Grained Modeling. Biophysical Journal, 2017, 112, 2589-2601.	0.5	33
29	Investigating the effects of tropomyosin mutations on its flexibility and interactions with filamentous actin using molecular dynamics simulation. Journal of Muscle Research and Cell Motility, 2016, 37, 131-147.	2.0	32
30	Probing the Structural and Energetic Basis of Kinesinâ€“Microtubule Binding Using Computational Alanine-Scanning Mutagenesis. Biochemistry, 2011, 50, 8645-8655.	2.5	30
31	Decrypting the Heat Activation Mechanism of TRPV1 Channel by Molecular Dynamics Simulation. Biophysical Journal, 2018, 114, 40-52.	0.5	30
32	Anharmonic Normal Mode Analysis of Elastic Network Model Improves theÂModeling of Atomic Fluctuations in Protein Crystal Structures. Biophysical Journal, 2010, 98, 3025-3034.	0.5	28
33	Coarse-grained modeling of the structural states and transition underlying the powerstroke of dynein motor domain. Journal of Chemical Physics, 2012, 136, 155103.	3.0	25
34	Fold recognition aided by constraints from small angle X-ray scattering data. Protein Engineering, Design and Selection, 2005, 18, 209-219.	2.1	24
35	Multiscale modeling of structural dynamics underlying force generation and product release in actomyosin complex. Proteins: Structure, Function and Bioinformatics, 2010, 78, 638-660.	2.6	23
36	Functional differences between neurotransmitter binding sites of muscle acetylcholine receptors. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17660-17665.	7.1	22

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37	A survey of coarse-grained methods for modeling protein conformational transitions. Current Opinion in Structural Biology, 2017, 42, 24-30.	5.7	22
38	Normalâ€modeâ€based modeling of allosteric couplings that underlie cyclic conformational transition in F₁ ATPase. Proteins: Structure, Function and Bioinformatics, 2009, 76, 747-762.	2.6	21
39	Optimal modeling of atomic fluctuations in protein crystal structures for weak crystal contact interactions. Journal of Chemical Physics, 2010, 132, 014111.	3.0	21
40	Toward elucidating the heat activation mechanism of the TRPV1 channel gating by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1938-1949.	2.6	21
41	Pathogenic mechanism of a catecholaminergic polymorphic ventricular tachycardia causing-mutation in cardiac calcium release channel RyR2. Journal of Molecular and Cellular Cardiology, 2018, 117, 26-35.	1.9	21
42	Langevin Network Model of Myosinâ€. Journal of Physical Chemistry B, 2008, 112, 6274-6281.	2.6	18
43	All-Atom Structural Investigation of Kinesinâ€“Microtubule Complex Constrained by High-Quality Cryo-Electron-Microscopy Maps. Biochemistry, 2012, 51, 5022-5032.	2.5	18
44	Coarseâ€grained and allâ€atom modeling of structural states and transitions in hemoglobin. Proteins: Structure, Function and Bioinformatics, 2013, 81, 240-252.	2.6	18
45	Predicting cryptic ligand binding sites based on normal modes guided conformational sampling. Proteins: Structure, Function and Bioinformatics, 2021, 89, 416-426.	2.6	18
46	Coarseâ€grained modeling of conformational transitions underlying the processive stepping of myosin V dimer along filamentous actin. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2291-2305.	2.6	17
47	All-Atom Molecular Dynamics Simulations of Actinâ€“Myosin Interactions: A Comparative Study of Cardiac Î± Myosin, Î² Myosin, and Fast Skeletal Muscle Myosin. Biochemistry, 2013, 52, 8393-8405.	2.5	17
48	Toward decrypting the allosteric mechanism of the ryanodine receptor based on coarseâ€grained structural and dynamic modeling. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2307-2318.	2.6	17
49	Probing the structural dynamics of the CRISPRâ€Cas9 RNAâ€guided DNAâ€cleavage system by coarseâ€grained modeling. Proteins: Structure, Function and Bioinformatics, 2017, 85, 342-353.	2.6	16
50	Allâ€atom and coarseâ€grained simulations of the forced unfolding pathways of the SNARE complex. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1376-1386.	2.6	15
51	A single molecular distance predicts agonist binding energy in nicotinic receptors. Journal of General Physiology, 2019, 151, 452-464.	1.9	15
52	Decrypting the Structural, Dynamic, and Energetic Basis of a Monomeric Kinesin Interacting with a Tubulin Dimer in Three ATPase States by All-Atom Molecular Dynamics Simulation. Biochemistry, 2015, 54, 859-869.	2.5	14
53	Structural correlates of affinity in fetal versus adult endplate nicotinic receptors. Nature Communications, 2016, 7, 11352.	12.8	14
54	Congenital myopathyâ€related mutations in tropomyosin disrupt regulatory function through altered actin affinity and tropomodulin binding. FEBS Journal, 2019, 286, 1877-1893.	4.7	14

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55	Investigating the interâ€subunit/subdomain interactions and motions relevant to disease mutations in the Nâ€terminal domain of ryanodine receptors by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1633-1644.	2.6	13
56	Functional effects of substitutions I92T and V95A in actin-binding period 3 of tropomyosin. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 558-568.	2.3	13
57	Approximate normal mode analysis based on vibrational subsystem analysis with high accuracy and efficiency. Journal of Chemical Physics, 2009, 130, 194111.	3.0	12
58	Structure-Based Simulations of the Translocation Mechanism of the Hepatitis C Virus NS3 Helicase along Single-Stranded Nucleic Acid. Biophysical Journal, 2012, 103, 1343-1353.	0.5	11
59	Probing the Energetics of Dynactin Filament Assembly and the Binding of Cargo Adaptor Proteins Using Molecular Dynamics Simulation and Electrostatics-Based Structural Modeling. Biochemistry, 2017, 56, 313-323.	2.5	10
60	Cross-subunit interactions that stabilize open states mediate gating in NMDA receptors. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	10
61	All-atom modeling of anisotropic atomic fluctuations in protein crystal structures. Journal of Chemical Physics, 2011, 135, 144114.	3.0	9
62	Probing the structural dynamics of the <scp>SNARE</scp> recycling machine based on coarseâ€grained modeling. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1055-1066.	2.6	7
63	Investigating the structural dynamics of the PIEZO1 channel activation and inactivation by coarseâ€grained modeling. Proteins: Structure, Function and Bioinformatics, 2017, 85, 2198-2208.	2.6	7
64	Unzipping of neuronal snare protein with steered molecular dynamics occurs in three steps. Journal of Molecular Modeling, 2014, 20, 2381.	1.8	6
65	Probing the folded state and mechanical unfolding pathways of T4 lysozyme using all-atom and coarse-grained molecular simulation. Journal of Chemical Physics, 2015, 142, 035101.	3.0	6
66	Analysis of Protein Conformational Transitions Using Elastic Network Model. Methods in Molecular Biology, 2014, 1084, 159-172.	0.9	5
67	High-Resolution Modeling of Protein Structures Based on Flexible Fitting of Low-Resolution Structural Data. Advances in Protein Chemistry and Structural Biology, 2014, 96, 267-284.	2.3	4
68	Investigating dual Ca²⁺ modulation of the ryanodine receptor 1 by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1528-1539.	2.6	4
69	Computer Modeling of Helicases Using Elastic Network Model. Methods in Molecular Biology, 2009, 587, 235-243.	0.9	2
70	All-Atom Simulations of Actin-Myosin Interactions --- A Comparative Study of Cardiac Alpha Myosin, Beta Myosin and Skeletal Muscle Myosin. Biophysical Journal, 2013, 104, 308a.	0.5	1
71	Predicting lipid and ligand binding sites in TRPV1 channel by molecular dynamics simulation and machine learning. Proteins: Structure, Function and Bioinformatics, 2021, 89, 966-977.	2.6	1
72	Molecular dynamics simulation of tropomyosin bound to actins/myosin in the closed and open states. Proteins: Structure, Function and Bioinformatics, 2019, 87, 805-814.	2.6	0