Wenjun Zheng

List of Publications by Year
in descending order

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	Predicting cryptic ligand binding sites based on normal modes guided conformational sampling. Proteins: Structure, Function and Bioinformatics, 2021, 89, 416-426.	2.6	18
2	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
3	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
4	Molecular mechanisms underlying menthol binding and activation of TRPM8 ion channel. Nature Communications, 2020, 11, 3790.	12.8	54
5	Investigating dual Ca^{2+} modulation of the ryanodine receptor 1 by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1528-1539.	2.6	4
6	A single molecular distance predicts agonist binding energy in nicotinic receptors. Journal of General Physiology, 2019, 151, 452-464.	1.9	15
7	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
8	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
9	Heat activation mechanism of TRPV1: New insights from molecular dynamics simulation. Temperature, 2019, 6, 120-131.	3.0	34
10	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
11	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
12	Decrypting the Heat Activation Mechanism of TRPV1 Channel by Molecular Dynamics Simulation. Biophysical Journal, 2018, 114, 40-52.	0.5	30
13	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
14	Probing the Structural Dynamics of the NMDA Receptor Activation by Coarse-Grained Modeling. Biophysical Journal, 2017, 112, 2589-2601.	0.5	33
15	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
16	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
17	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
18	A survey of coarse-grained methods for modeling protein conformational transitions. Current Opinion in Structural Biology, 2017, 42, 24-30.	5.7	22

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19	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
20	Conformational Changes and Flexibility of DNA Devices Observed by Small-Angle X-ray Scattering. Nano Letters, 2016, 16, 4871-4879.	9.1	33
21	Structural correlates of affinity in fetal versus adult endplate nicotinic receptors. Nature Communications, 2016, 7, 11352.	12.8	14
22	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
23	Probing the structural dynamics of the <scp>SNARE</scp> recycling machine based on coarse‐grained modeling. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1055-1066.	2.6	7
24	Toward decrypting the allosteric mechanism of the ryanodine receptor based on coarse‐grained structural and dynamic modeling. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2307-2318.	2.6	17
25	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
26	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
27	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
28	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
29	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
30	Analysis of Protein Conformational Transitions Using Elastic Network Model. Methods in Molecular Biology, 2014, 1084, 159-172.	0.9	5
31	All‐atom and coarse‐grained simulations of the forced unfolding pathways of the SNARE complex. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1376-1386.	2.6	15
32	Unzipping of neuronal snare protein with steered molecular dynamics occurs in three steps. Journal of Molecular Modeling, 2014, 20, 2381.	1.8	6
33	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
34	Probing the Flexibility of Tropomyosin and Its Binding to Filamentous Actin Using Molecular Dynamics Simulations. Biophysical Journal, 2013, 105, 1882-1892.	0.5	35
35	All-Atom Molecular Dynamics Simulations of Actin–Myosin Interactions: A Comparative Study of Cardiac α Myosin, β Myosin, and Fast Skeletal Muscle Myosin. Biochemistry, 2013, 52, 8393-8405.	2.5	17
36	Coarse‐grained and all‐atom modeling of structural states and transitions in hemoglobin. Proteins: Structure, Function and Bioinformatics, 2013, 81, 240-252.	2.6	18

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37	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
38	All-Atom Structural Investigation of Kinesin–Microtubule Complex Constrained by High-Quality Cryo-Electron-Microscopy Maps. Biochemistry, 2012, 51, 5022-5032.	2.5	18
39	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
40	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
41	Evidence of Protein Collective Motions on the Picosecond Timescale. Biophysical Journal, 2011, 100, 1058-1065.	0.5	56
42	Accurate Flexible Fitting of High-Resolution Protein Structures to Small-Angle X-Ray Scattering Data Using a Coarse-Grained Model with Implicit Hydration Shell. Biophysical Journal, 2011, 101, 2981-2991.	0.5	58
43	Probing the Structural and Energetic Basis of Kinesin–Microtubule Binding Using Computational Alanine-Scanning Mutagenesis. Biochemistry, 2011, 50, 8645-8655.	2.5	30
44	Electrostatically Biased Binding of Kinesin to Microtubules. PLoS Biology, 2011, 9, e1001207.	5.6	64
45	Coarse-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
46	All-atom modeling of anisotropic atomic fluctuations in protein crystal structures. Journal of Chemical Physics, 2011, 135, 144114.	3.0	9
47	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
48	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
49	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
50	Optimal modeling of atomic fluctuations in protein crystal structures for weak crystal contact interactions. Journal of Chemical Physics, 2010, 132, 014111.	3.0	21
51	Anharmonic Normal Mode Analysis of Elastic Network Model Improves the Modeling of Atomic Fluctuations in Protein Crystal Structures. Biophysical Journal, 2010, 98, 3025-3034.	0.5	28
52	Approximate normal mode analysis based on vibrational subsystem analysis with high accuracy and efficiency. Journal of Chemical Physics, 2009, 130, 194111.	3.0	12
53	Normal-mode-based modeling of allosteric couplings that underlie cyclic conformational transition in F_1 ATPase. Proteins: Structure, Function and Bioinformatics, 2009, 76, 747-762.	2.6	21
54	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

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55	Coupling between Normal Modes Drives Protein Conformational Dynamics: Illustrations Using Allosteric Transitions in Myosin II. Biophysical Journal, 2009, 96, 2128-2137.	0.5	47
56	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
57	Computer Modeling of Helicases Using Elastic Network Model. Methods in Molecular Biology, 2009, 587, 235-243.	0.9	2
58	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
59	Langevin Network Model of Myosinâ€. Journal of Physical Chemistry B, 2008, 112, 6274-6281.	2.6	18
60	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
61	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
62	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
63	Protein conformational transitions explored by mixed elastic network models. Proteins: Structure, Function and Bioinformatics, 2007, 69, 43-57.	2.6	132
64	Modeling Protein Conformational Changes by Iterative Fitting of Distance Constraints Using Reoriented Normal Modes. Biophysical Journal, 2006, 90, 4327-4336.	0.5	45
65	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
66	Network of Dynamically Important Residues in the Open/Closed Transition in Polymerases Is Strongly Conserved. Structure, 2005, 13, 565-577.	3.3	117
67	Fold recognition aided by constraints from small angle X-ray scattering data. Protein Engineering, Design and Selection, 2005, 18, 209-219.	2.1	24
68	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
69	Normal-Modes-Based Prediction of Protein Conformational Changes Guided by Distance Constraints. Biophysical Journal, 2005, 88, 3109-3117.	0.5	86
70	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
71	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
72	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