Jie Liang

List of Publications by Year in descending order

141 papers	9,273 citations	125106 35 h-index	53065 89 g-index
150 all docs	150 docs citations	150 times ranked	11096 citing authors

#	Article	IF	Citations
1	Modeling and simulation of cell nuclear architecture reorganization process. Journal of Computational Physics, 2022, 449, 110808.	1.9	2
2	Prevalence of Malnutrition, Its Risk Factors, and the Use of Nutrition Support in Patients with Inflammatory Bowel Disease. Inflammatory Bowel Diseases, 2022, 28, S59-S66.	0.9	15
3	Thermodynamics of unfolding mechanisms of mouse mammary tumor virus pseudoknot from a coarse-grained loop-entropy model. Journal of Biological Physics, 2022, 48, 129-150.	0.7	1
4	High-resolution single-cell 3D-models of chromatin ensembles during Drosophila embryogenesis. Nature Communications, 2021, 12, 205.	5.8	17
5	Exact Topology of the Dynamic Probability Surface of an Activated Process by Persistent Homology. Journal of Physical Chemistry B, 2021, 125, 4667-4680.	1.2	9
6	Exact Probability Landscapes of Stochastic Phenotype Switching in Feed-Forward Loops: Phase Diagrams of Multimodality. Frontiers in Genetics, 2021, 12, 645640.	1.1	6
7	Minimalistic 3D chromatin models: Sparse interactions in single cells drive the chromatin fold and form many-body units. Current Opinion in Structural Biology, 2021, 71, 200-214.	2.6	4
8	Simulation of pH-Dependent, Loop-Based Membrane Protein Gating Using Pretzel. Methods in Molecular Biology, 2021, 2186, 159-169.	0.4	0
9	Inferring initial state of the ancestral network of cellular fate decision: a case study of phage lambda. , 2021, 2021, 4436-4439.		0
10	GeTFEP: A general transfer free energy profile of transmembrane proteins. Protein Science, 2020, 29, 469-479.	3.1	5
11	Q-Nuc: a bioinformatics pipeline for the quantitative analysis of nucleosomal profiles. Interdisciplinary Sciences, Computational Life Sciences, 2020, 12, 69-81.	2.2	6
12	The structure of the TOM core complex in the mitochondrial outer membrane. Biological Chemistry, 2020, 401, 687-697.	1.2	15
13	Cellâ€“substrate mechanics guide collective cell migration through intercellular adhesion: a dynamic finite element cellular model. Biomechanics and Modeling in Mechanobiology, 2020, 19, 1781-1796.	1.4	11
14	CHROMATIX: computing the functional landscape of many-body chromatin interactions in transcriptionally active loci from deconvolved single cells. Genome Biology, 2020, 21, 13.	3.8	22
15	Structure-based Method for Predicting Deleterious Missense SNPs. , 2019, 2019, .		2
16	Predicting Oncogenic Missense Mutations. , 2019, 2019, .		0
17	Alterations in Chromatin Folding Patterns in Cancer Variant-Enriched Loci. , 2019, 2019, .		5
18	Guest Editorial on the Special Issue on Integrating Informatics and Technology for Precision Medicine. IEEE Journal of Biomedical and Health Informatics, 2019, 23, 12-13.	3.9	6

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19	Mating yeast cells use an intrinsic polarity site to assemble a pheromone-gradient tracking machine. Journal of Cell Biology, 2019, 218, 3730-3752.	2.3	24
20	Sensitivities of Regulation Intensities in Feed-Forward Loops with Multistability. , 2019, 2019, 1969-1972.		1
21	Discrete and continuous models of probability flux of switching dynamics: Uncovering stochastic oscillations in a toggle-switch system. Journal of Chemical Physics, 2019, 151, 185104.	1.2	5
22	Evolution of coagulation-fragmentation stochastic processes using accurate chemical master equation approach. Communications in Information and Systems, 2019, 19, 37-55.	0.3	0
23	High-resolution structure prediction of Î² -barrel membrane proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1511-1516.	3.3	32
24	Mechanism of OmpG pH-Dependent Gating from Loop Ensemble and Single Channel Studies. Journal of the American Chemical Society, 2018, 140, 1105-1115.	6.6	37
25	On quantification of geometry and topology of protein pockets and channels for assessing mutation effects. , 2018, 2018, 263-266.		3
26	Folding-Degradation Relationship of a Membrane Protein Mediated by the Universally Conserved ATP-Dependent Protease FtsH. Journal of the American Chemical Society, 2018, 140, 4656-4665.	6.6	25
27	Discrete flux and velocity fields of probability and their global maps in reaction systems. Journal of Chemical Physics, 2018, 149, 185101.	1.2	6
28	Probabilistic control of HIV latency and transactivation by the Tat gene circuit. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 12453-12458.	3.3	23
29	A general method for predicting amino acid residues experiencing hydrogen exchange. , 2018, 2018, 341-344.		1
30	CASTp 3.0: computed atlas of surface topography of proteins. Nucleic Acids Research, 2018, 46, W363-W367.	6.5	1,341
31	Dynamic cellular finite-element method for modelling large-scale cell migration and proliferation under the control of mechanical and biochemical cues: a study of re-epithelialization. Journal of the Royal Society Interface, 2017, 14, 20160959.	1.5	17
32	Engineering a Novel Porin OmpGF Via Strand Replacement from Computational Analysis of Sequence Motif. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1180-1189.	1.4	7
33	Distance-Guided Forward and Backward Chain-Growth Monte Carlo Method for Conformational Sampling and Structural Prediction of Antibody CDR-H3 Loops. Journal of Chemical Theory and Computation, 2017, 13, 380-388.	2.3	4
34	Efficient computation of transfer free energies of amino acids in beta-barrel membrane proteins. Bioinformatics, 2017, 33, 1664-1671.	1.8	3
35	PRODIGEN: visualizing the probability landscape of stochastic gene regulatory networks in state and time space. BMC Bioinformatics, 2017, 18, 24.	1.2	4
36	A Knot Polynomial Invariant for Analysis of Topology of RNA Stems and Protein Disulfide Bonds. Computational and Mathematical Biophysics, 2017, 5, 21-30.	0.6	7

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37	Computational construction of 3D chromatin ensembles and prediction of functional interactions of alpha-globin locus from 5C data. Nucleic Acids Research, 2017, 45, 11547-11558.	6.5	28
38	Spatial organization of the budding yeast genome in the cell nucleus and identification of specific chromatin interactions from multi-chromosome constrained chromatin model. PLoS Computational Biology, 2017, 13, e1005658.	1.5	22
39	Global Nonlinear Fitness Function for Protein Structures. Health Information Science, 2017, , 1-35.	0.3	0
40	Mechanisms of stochastic focusing and defocusing in biological reaction networks: Insight from accurate Chemical Master Equation (ACME) solutions. , 2016, 2016, 1480-1483.		2
41	Gî² promotes pheromone receptor polarization and yeast chemotropism by inhibiting receptor phosphorylation. Science Signaling, 2016, 9, ra38.	1.6	22
42	Three-dimensional chromosome structures from energy landscape. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11991-11993.	3.3	7
43	Accurate Chemical Master Equation Solution Using Multi-Finite Buffers. Multiscale Modeling and Simulation, 2016, 14, 923-963.	0.6	35
44	State Space Truncation with Quantified Errors for Accurate Solutions to Discrete Chemical Master Equation. Bulletin of Mathematical Biology, 2016, 78, 617-661.	0.9	31
45	Challenges in structural approaches to cell modeling. Journal of Molecular Biology, 2016, 428, 2943-2964.	2.0	51
46	Outer Membrane Protein Folding and Topology from a Computational Transfer Free Energy Scale. Journal of the American Chemical Society, 2016, 138, 2592-2601.	6.6	23
47	Unique Toll-Like Receptor 4 Activation by NAMPT/PBEF Induces NFÎºB Signaling and Inflammatory Lung Injury. Scientific Reports, 2015, 5, 13135.	1.6	126
48	Mechanical Model of Geometric Cell and Topological Algorithm for Cell Dynamics from Single-Cell to Formation of Monolayered Tissues with Pattern. PLoS ONE, 2015, 10, e0126484.	1.1	13
49	Multiscale Modeling of Cellular Epigenetic States: Stochasticity in Molecular Networks, Chromatin Folding in Cell Nuclei, and Tissue Pattern Formation of Cells. Critical Reviews in Biomedical Engineering, 2015, 43, 323-346.	0.5	4
50	Guest Editorial EMBC 2014. IEEE Journal of Biomedical and Health Informatics, 2015, 19, 1291-1292.	3.9	0
51	Conformational sampling and structure prediction of multiple interacting loops in soluble and Î²-barrel membrane proteins using multi-loop distance-guided chain-growth Monte Carlo method. Bioinformatics, 2015, 31, 2646-2652.	1.8	16
52	Mechanisms of Regulating Tissue Elongation in Drosophila Wing: Impact of Oriented Cell Divisions, Oriented Mechanical Forces, and Reduced Cell Size. PLoS ONE, 2014, 9, e86725.	1.1	16
53	On Simplified Global Nonlinear Function for Fitness Landscape: A Case Study of Inverse Protein Folding. PLoS ONE, 2014, 9, e104403.	1.1	2
54	Roles of regulated internalization in the polarization of cell surface receptors. , 2014, 2014, 1166-9.		2

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55	Fast Protein Loop Sampling and Structure Prediction Using Distance-Guided Sequential Chain-Growth Monte Carlo Method. PLoS Computational Biology, 2014, 10, e1003539.	1.5	49
56	Spatial confinement is a major determinant of the folding landscape of human chromosomes. Nucleic Acids Research, 2014, 42, 8223-8230.	6.5	55
57	Computational predictions of structures of multichromosomes of budding yeast. , 2014, 2014, 3945-8.		4
58	Lysine carboxylation: unveiling a spontaneous post-translational modification. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 48-57.	2.5	24
59	Weakly Stable Regions and Protein-Protein Interactions in Beta-Barrel Membrane Proteins. Current Pharmaceutical Design, 2014, 20, 1268-1273.	0.9	13
60	GPU-Based Steady-State Solution of the Chemical Master Equation. , 2013, , .		7
61	Adaptively biased sequential importance sampling for rare events in reaction networks with comparison to exact solutions from finite buffer dCME method. Journal of Chemical Physics, 2013, 139, 025101.	1.2	21
62	Dynamic mechanical finite element model of biological cells for studying cellular pattern formation. , 2013, 2013, 4517-20.		7
63	Structure-based Analysis of VDAC1 Protein. Journal of Biological Chemistry, 2012, 287, 2179-2190.	1.6	73
64	Predicting Three-Dimensional Structures of Transmembrane Domains of Î²-Barrel Membrane Proteins. Journal of the American Chemical Society, 2012, 134, 1775-1781.	6.6	41
65	Engineered Oligomerization State of OmpF Protein through Computational Design Decouples Oligomer Dissociation from Unfolding. Journal of Molecular Biology, 2012, 419, 89-101.	2.0	28
66	Computational studies of membrane proteins: Models and predictions for biological understanding. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 927-941.	1.4	36
67	Ionizable side chains at catalytic active sites of enzymes. European Biophysics Journal, 2012, 41, 449-460.	1.2	25
68	Mechanisms of Regulating Cell Topology in Proliferating Epithelia: Impact of Division Plane, Mechanical Forces, and Cell Memory. PLoS ONE, 2012, 7, e43108.	1.1	27
69	Lipid-binding surfaces of membrane proteins: Evidence from evolutionary and structural analysis. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1092-1102.	1.4	68
70	Structural Signatures of Enzyme Binding Pockets from Order-Independent Surface Alignment: A Study of Metalloendopeptidase and NAD Binding Proteins. Journal of Molecular Biology, 2011, 406, 713-729.	2.0	49
71	Improving the Resistance of a Eukaryotic Î²-Barrel Protein to Thermal and Chemical Perturbations. Journal of Molecular Biology, 2011, 413, 150-161.	2.0	21
72	Accuracy of functional surfaces on comparatively modeled protein structures. Journal of Structural and Functional Genomics, 2011, 12, 97-107.	1.2	10

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73	GPU-accelerated Chemical Similarity Assessment for Large Scale Databases. Procedia Computer Science, 2011, 4, 2007-2016.	1.2	9
74	Constrained proper sampling of conformations of transition state ensemble of protein folding. Journal of Chemical Physics, 2011, 134, 075103.	1.2	13
75	Computational Cellular Dynamics Based on the Chemical Master Equation: A Challenge for Understanding Complexity. Journal of Computer Science and Technology, 2010, 25, 154-168.	0.9	35
76	Nonlinear Langevin model with product stochasticity for biological networks: The case of the Schnakenberg model. Journal of Systems Science and Complexity, 2010, 23, 896-905.	1.6	2
77	Probability landscape of heritable and robust epigenetic state of lysogeny in phage lambda. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 18445-18450.	3.3	74
78	Combinatorial Analysis for Sequence and Spatial Motif Discovery in Short Sequence Fragments. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2010, 7, 524-536.	1.9	15
79	Geometry of protein shape and its evolutionary pattern for function prediction and characterization. , 2009, 2009, 2324-7.		1
80	Predicting weakly stable regions, oligomerization state, and proteinâ€“protein interfaces in transmembrane domains of outer membrane proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 12735-12740.	3.3	62
81	Perturbation-based Markovian Transmission Model for Probing Allosteric Dynamics of Large Macromolecular Assembling: A Study of GroEL-GroES. PLoS Computational Biology, 2009, 5, e1000526.	1.5	15
82	Prediction of geometrically feasible three-dimensional structures of pseudoknotted RNA through free energy estimation. Rna, 2009, 15, 2248-2263.	1.6	46
83	Structural model of ï‌ GABA_C receptor based on evolutionary analysis: Testing of predicted proteinâ€“protein interactions involved in receptor assembly and function. Protein Science, 2009, 18, 2371-2383.	3.1	17
84	Predicting Protein Function and Binding Profile via Matching of Local Evolutionary and Geometric Surface Patterns. Journal of Molecular Biology, 2009, 387, 451-464.	2.0	65
85	A model study of protein nascent chain and cotranslational folding using hydrophobicâ€polar residues. Proteins: Structure, Function and Bioinformatics, 2008, 70, 442-449.	1.5	13
86	Predicting protein folding rates from geometric contact and amino acid sequence. Protein Science, 2008, 17, 1256-1263.	3.1	98
87	Optimal enumeration of state space of finitely buffered stochastic molecular networks and exact computation of steady state landscape probability. BMC Systems Biology, 2008, 2, 30.	3.0	60
88	Novel Approach to Structure-Based Pharmacophore Search Using Computational Geometry and Shape Matching Techniques. Journal of Chemical Information and Modeling, 2008, 48, 889-901.	2.5	54
89	Predicting and Characterizing Protein Functions Through Matching Geometric and Evolutionary Patterns of Binding Surfaces. Advances in Protein Chemistry and Structural Biology, 2008, 75, 107-141.	1.0	4
90	Stochastic probability landscape model for switching efficiency, robustness, and differential threshold for induction of genetic circuit in phage Î». , 2008, 2008, 611-4.		5

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91	Discrete state model and accurate estimation of loop entropy of RNA secondary structures. Journal of Chemical Physics, 2008, 128, 125107.	1.2	46
92	Generating properly weighted ensemble of conformations of proteins from sparse or indirect distance constraints. Journal of Chemical Physics, 2008, 129, 094101.	1.2	15
93	Knowledge-Based Energy Functions for Computational Studies of Proteins. , 2007, , 71-123.		9
94	Topology independent protein structural alignment. BMC Bioinformatics, 2007, 8, 388.	1.2	25
95	Predicting Enzyme Functional Surfaces and Locating Key Residues Automatically from Structures. Annals of Biomedical Engineering, 2007, 35, 1037-1042.	1.3	13
96	Computation of Protein Geometry and Its Applications: Packing and Function Prediction. , 2007, , 181-206.		3
97	CASTp: computed atlas of surface topography of proteins with structural and topographical mapping of functionally annotated residues. Nucleic Acids Research, 2006, 34, W116-W118.	6.5	1,541
98	Sequence Motifs and Antimotifs in Î²-Barrel Membrane Proteins from a Genome-Wide Analysis: The Ala-Tyr Dichotomy and Chaperone Binding Motifs. Journal of Molecular Biology, 2006, 363, 611-623.	2.0	26
99	Prediction of transmembrane helix orientation in polytopic membrane proteins. , 2006, 6, 13.		77
100	Empirical potential function for simplified protein models: Combining contact and local sequence-structure descriptors. Proteins: Structure, Function and Bioinformatics, 2006, 63, 949-960.	1.5	33
101	Prediction of buried helices in multispan alpha helical membrane proteins. Proteins: Structure, Function and Bioinformatics, 2006, 63, 1-5.	1.5	14
102	Monte Carlo sampling of near-native structures of proteins with applications. Proteins: Structure, Function and Bioinformatics, 2006, 66, 61-68.	1.5	20
103	Evolutionary Patterns of Retinal-Binding Pockets of Type I Rhodopsins and Their Functions. Photochemistry and Photobiology, 2006, 82, 1426-1435.	1.3	12
104	Combinatorial model for sequence and spatial motif discovery in short sequence fragments: Examples from ÃŸ-barrel membrane proteins. , 2006, 2006, 3470-3.		4
105	Estimation of Amino Acid Residue Substitution Rates at Local Spatial Regions and Application in Protein Function Inference: A Bayesian Monte Carlo Approach. Molecular Biology and Evolution, 2006, 23, 421-436.	3.5	70
106	Protein Folding Dynamics via Quantification of Kinematic Energy Landscape. Physical Review Letters, 2006, 96, 058106.	2.9	20
107	Combinatorial model for sequence and spatial motif discovery in short sequence fragments: Examples from ÃŸ-barrel membrane proteins. Annual International Conference of the IEEE Engineering in Medicine and Biology Society, 2006, , .	0.5	0
108	Automated method for predicting enzyme functional surfaces and locating key residues with accuracy and specificity. Annual International Conference of the IEEE Engineering in Medicine and Biology Society, 2006, , .	0.5	0

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109	Protein surface analysis for function annotation in high-throughput structural genomics pipeline. Protein Science, 2005, 14, 2972-2981.	3.1	70
110	The membraneâ€“water interface region of membrane proteins: structural bias and the anti-snorkeling effect. Trends in Biochemical Sciences, 2005, 30, 355-357.	3.7	31
111	Geometric cooperativity and anticooperativity of three-body interactions in native proteins. Proteins: Structure, Function and Bioinformatics, 2005, 60, 46-65.	1.5	41
112	Empirical lipid propensities of amino acid residues in multispan alpha helical membrane proteins. Proteins: Structure, Function and Bioinformatics, 2005, 59, 496-509.	1.5	85
113	Interstrand Pairing Patterns in Î²-Barrel Membrane Proteins: The Positive-outside Rule, Aromatic Rescue, and Strand Registration Prediction. Journal of Molecular Biology, 2005, 354, 979-993.	2.0	93
114	Importance of chirality and reduced flexibility of protein side chains: A study with square and tetrahedral lattice models. Journal of Chemical Physics, 2004, 121, 592.	1.2	17
115	Developing optimal non-linear scoring function for protein design. Bioinformatics, 2004, 20, 3080-3098.	1.8	33
116	pvSOAR: detecting similar surface patterns of pocket and void surfaces of amino acid residues on proteins. Nucleic Acids Research, 2004, 32, W555-W558.	6.5	68
117	Optimal nonlinear scoring function for global fitness landscape of protein design. , 2004, 2004, 2828-31.		0
118	Potential function of simplified protein models for discriminating native proteins from decoys: combining contact interaction and local sequence-dependent geometry. , 2004, 2004, 2976-9.		3
119	Are Residues in a Protein Folding Nucleus Evolutionarily Conserved?. Journal of Molecular Biology, 2004, 335, 869-880.	2.0	33
120	COMPUTATIONAL DESIGN OF COMBINATORIAL PEPTIDE LIBRARY FOR MODULATING PROTEIN-PROTEIN INTERACTIONS. , 2004, , .		3
121	Interhelical Hydrogen Bonds in Transmembrane Region Are Important for Function and Stability of Ca²⁺-Transporting ATPase. Cell Biochemistry and Biophysics, 2003, 39, 1-12.	0.9	5
122	Simplicial edge representation of protein structures and alpha contact potential with confidence measure. Proteins: Structure, Function and Bioinformatics, 2003, 53, 792-805.	1.5	52
123	Higher-order Interhelical Spatial Interactions in Membrane Proteins. Journal of Molecular Biology, 2003, 327, 251-272.	2.0	51
124	Structural Location of Disease-associated Single-nucleotide Polymorphisms. Journal of Molecular Biology, 2003, 327, 1021-1030.	2.0	74
125	Inferring Functional Relationships of Proteins from Local Sequence and Spatial Surface Patterns. Journal of Molecular Biology, 2003, 332, 505-526.	2.0	151
126	Origin of scaling behavior of protein packing density: A sequential Monte Carlo study of compact long chain polymers. Journal of Chemical Physics, 2003, 118, 6102-6109.	1.2	56

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127	CASTp: Computed Atlas of Surface Topography of proteins. Nucleic Acids Research, 2003, 31, 3352-3355.	6.5	936
128	Position-Dependence of Stabilizing Polar Interactions of Asparagine in Transmembrane Helical Bundlesâ€. Biochemistry, 2003, 42, 6400-6407.	1.2	70
129	Statistical geometry of packing defects of lattice chain polymer from enumeration and sequential Monte Carlo method. Journal of Chemical Physics, 2002, 117, 3511-3521.	1.2	36
130	Experimental and computational studies of determinants of membrane-protein folding. Current Opinion in Chemical Biology, 2002, 6, 878-884.	2.8	31
131	Interhelical hydrogen bonds and spatial motifs in membrane proteins: Polar clamps and serine zippers. Proteins: Structure, Function and Bioinformatics, 2002, 47, 209-218.	1.5	149
132	Helix-helix packing and interfacial pairwise interactions of residues in membrane proteins. Journal of Molecular Biology, 2001, 311, 891-907.	2.0	175
133	Are Proteins Well-Packed?. Biophysical Journal, 2001, 81, 751-766.	0.2	248
134	Analytical shape computation of macromolecules: I. molecular area and volume through alpha shape. , 1998, 33, 1-17.		258
135	Analytical shape computation of macromolecules: II. Inaccessible cavities in proteins. , 1998, 33, 18-29.		157
136	Anatomy of protein pockets and cavities: Measurement of binding site geometry and implications for ligand design. Protein Science, 1998, 7, 1884-1897.	3.1	949
137	On the definition and the construction of pockets in macromolecules. Discrete Applied Mathematics, 1998, 88, 83-102.	0.5	181
138	Hydration Structure of Antithrombin Conformers and Water Transfer during Reactive Loop Insertion. Biophysical Journal, 1998, 75, 573-582.	0.2	10
139	Analytical shape computation of macromolecules: II. Inaccessible cavities in proteins. Proteins: Structure, Function and Bioinformatics, 1998, 33, 18-29.	1.5	15
140	Analytical shape computation of macromolecules: I. molecular area and volume through alpha shape. Proteins: Structure, Function and Bioinformatics, 1998, 33, 1-17.	1.5	5
141	Measuring proteins and voids in proteins. , 0, , .		42