Yaoqi Zhou

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7161299/publications.pdf

Version: 2024-02-01

243 papers	14,447 citations	16411 64 h-index	28224 105 g-index
299 all docs	299 docs citations	299 times ranked	11815 citing authors

#	Article	IF	Citations
1	Distance-scaled, finite ideal-gas reference state improves structure-derived potentials of mean force for structure selection and stability prediction. Protein Science, 2009, 11, 2714-2726.	3.1	836
2	Real-time reliable determination of binding kinetics of DNA hybridization using a multi-channel graphene biosensor. Nature Communications, 2017, 8, 14902.	5.8	303
3	Capturing non-local interactions by long short-term memory bidirectional recurrent neural networks for improving prediction of protein secondary structure, backbone angles, contact numbers and solvent accessibility. Bioinformatics, 2017, 33, 2842-2849.	1.8	300
4	Improving prediction of secondary structure, local backbone angles and solvent accessible surface area of proteins by iterative deep learning. Scientific Reports, 2015, 5, 11476.	1.6	290
5	Improving protein fold recognition and template-based modeling by employing probabilistic-based matching between predicted one-dimensional structural properties of query and corresponding native properties of templates. Bioinformatics, 2011, 27, 2076-2082.	1.8	288
6	A Knowledge-Based Energy Function for Proteinâ^'Ligand, Proteinâ^'Protein, and Proteinâ^'DNA Complexes. Journal of Medicinal Chemistry, 2005, 48, 2325-2335.	2.9	264
7	Improving protein disorder prediction by deep bidirectional long short-term memory recurrent neural networks. Bioinformatics, 2017, 33, 685-692.	1.8	235
8	Protein binding site prediction using an empirical scoring function. Nucleic Acids Research, 2006, 34, 3698-3707.	6.5	223
9	Specific interactions for ab initio folding of protein terminal regions with secondary structures. Proteins: Structure, Function and Bioinformatics, 2008, 72, 793-803.	1.5	219
10	RNA secondary structure prediction using an ensemble of two-dimensional deep neural networks and transfer learning. Nature Communications, 2019, 10, 5407.	5.8	214
11	Fold recognition by combining sequence profiles derived from evolution and from depth-dependent structural alignment of fragments. Proteins: Structure, Function and Bioinformatics, 2004, 58, 321-328.	1.5	211
12	Interpreting the folding kinetics of helical proteins. Nature, 1999, 401, 400-403.	13.7	209
13	SPINE X: Improving protein secondary structure prediction by multistep learning coupled with prediction of solvent accessible surface area and backbone torsion angles. Journal of Computational Chemistry, 2012, 33, 259-267.	1.5	209
14	The distance fluctuation criterion for melting: Comparison of square-well and Morse potential models for clusters and homopolymers. Journal of Chemical Physics, 2002, 116, 2323-2329.	1.2	204
15	Reactivation of Dihydroorotate Dehydrogenase-Driven Pyrimidine Biosynthesis Restores Tumor Growth of Respiration-Deficient Cancer Cells. Cell Metabolism, 2019, 29, 399-416.e10.	7.2	190
16	Equilibrium thermodynamics of homopolymers and clusters: Molecular dynamics and Monte Carlo simulations of systems with square-well interactions. Journal of Chemical Physics, 1997, 107, 10691-10708.	1.2	189
17	Single-body residue-level knowledge-based energy score combined with sequence-profile and secondary structure information for fold recognition. Proteins: Structure, Function and Bioinformatics, 2004, 55, 1005-1013.	1.5	180
18	Structural insights into the histone H1-nucleosome complex. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 19390-19395.	3.3	178

#	Article	IF	Citations
19	First-Order Disorder-to-Order Transition in an Isolated Homopolymer Model. Physical Review Letters, 1996, 77, 2822-2825.	2.9	177
20	A physical reference state unifies the structure-derived potential of mean force for protein folding and binding. Proteins: Structure, Function and Bioinformatics, 2004, 56, 93-101.	1.5	176
21	Folding Rate Prediction Using Total Contact Distance. Biophysical Journal, 2002, 82, 458-463.	0.2	171
22	Sixty-five years of the long march in protein secondary structure prediction: the final stretch?. Briefings in Bioinformatics, 2018, 19, bbw129.	3.2	168
23	Folding thermodynamics of a model three-helix-bundle protein. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 14429-14432.	3.3	158
24	Accurate prediction of protein contact maps by coupling residual two-dimensional bidirectional long short-term memory with convolutional neural networks. Bioinformatics, 2018, 34, 4039-4045.	1.8	155
25	Native proteins are surface-molten solids: application of the lindemann criterion for the solid versus liquid state 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1999, 285, 1371-1375.	2.0	154
26	An accurate, residue-level, pair potential of mean force for folding and binding based on the distance-scaled, ideal-gas reference state. Protein Science, 2004, 13, 400-411.	3.1	153
27	SPINE-D: Accurate Prediction of Short and Long Disordered Regions by a Single Neural-Network Based Method. Journal of Biomolecular Structure and Dynamics, 2012, 29, 799-813.	2.0	150
28	Improving prediction of protein secondary structure, backbone angles, solvent accessibility and contact numbers by using predicted contact maps and an ensemble of recurrent and residual convolutional neural networks. Bioinformatics, 2019, 35, 2403-2410.	1.8	145
29	SPIDER2: A Package to Predict Secondary Structure, Accessible Surface Area, and Main-Chain Torsional Angles by Deep Neural Networks. Methods in Molecular Biology, 2017, 1484, 55-63.	0.4	137
30	Predicting backbone CÎ± angles and dihedrals from protein sequences by stacked sparse autoâ€encoder deep neural network. Journal of Computational Chemistry, 2014, 35, 2040-2046.	1.5	133
31	Chemical association in simple models of molecular and ionic fluids. Journal of Chemical Physics, 1989, 91, 3618-3623.	1.2	132
32	Ab initio folding of terminal segments with secondary structures reveals the fine difference between two closely related allâ€atom statistical energy functions. Protein Science, 2008, 17, 1212-1219.	3.1	131
33	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
34	Improving the prediction accuracy of residue solvent accessibility and realâ€value backbone torsion angles of proteins by guidedâ€learning through a twoâ€layer neural network. Proteins: Structure, Function and Bioinformatics, 2009, 74, 847-856.	1.5	125
35	Quantifying the effect of burial of amino acid residues on protein stability. Proteins: Structure, Function and Bioinformatics, 2003, 54, 315-322.	1.5	116
36	Achieving 80% ten-fold cross-validated accuracy for secondary structure prediction by large-scale training. Proteins: Structure, Function and Bioinformatics, 2006, 66, 838-845.	1.5	114

#	Article	IF	Citations
37	Accurate and efficient loop selections by the DFIRE-based all-atom statistical potential. Protein Science, 2004, 13, 391-399.	3.1	112
38	Title is missing!. Nature, 1999, 401, 400-403.	13.7	109
39	Predicting Continuous Local Structure and the Effect of Its Substitution for Secondary Structure in Fragment-Free Protein Structure Prediction. Structure, 2009, 17, 1515-1527.	1.6	108
40	The calorimetric criterion for a twoâ€state process revisited. Protein Science, 1999, 8, 1064-1074.	3.1	107
41	SPOT-Disorder2: Improved Protein Intrinsic Disorder Prediction by Ensembled Deep Learning. Genomics, Proteomics and Bioinformatics, 2019, 17, 645-656.	3.0	106
42	Folding of a model three-helix bundle protein: a thermodynamic and kinetic analysis 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1999, 293, 917-951.	2.0	103
43	Chemical association in simple models of molecular and ionic fluids. II. Thermodynamic properties. Journal of Chemical Physics, 1992, 96, 1504-1506.	1.2	102
44	Chemical association in simple models of molecular and ionic fluids. III. The cavity function. Journal of Chemical Physics, 1992, 96, 1507-1515.	1.2	102
45	EASE-MM: Sequence-Based Prediction of Mutation-Induced Stability Changes with Feature-Based Multiple Models. Journal of Molecular Biology, 2016, 428, 1394-1405.	2.0	101
46	Structure-based prediction of RNA-binding domains and RNA-binding sites and application to structural genomics targets. Nucleic Acids Research, 2011, 39, 3017-3025.	6.5	100
47	Ion solvation dynamics in an interaction-site model solvent. Chemical Physics, 1991, 152, 201-220.	0.9	93
48	SPEM: improving multiple sequence alignment with sequence profiles and predicted secondary structures. Bioinformatics, 2005, 21, 3615-3621.	1.8	92
49	Fluids inside a poreâ€”an integral-equation approach. Molecular Physics, 1989, 66, 767-789.	0.8	91
50	Fold recognition by concurrent use of solvent accessibility and residue depth. Proteins: Structure, Function and Bioinformatics, 2007, 68, 636-645.	1.5	87
51	Singleâ€sequenceâ€based prediction of protein secondary structures and solvent accessibility by deep wholeâ€sequence learning. Journal of Computational Chemistry, 2018, 39, 2210-2216.	1.5	84
52	Structure-based prediction of DNA-binding proteins by structural alignment and a volume-fraction corrected DFIRE-based energy function. Bioinformatics, 2010, 26, 1857-1863.	1.8	81
53	Sequenceâ€based prediction of proteinâ€“peptide binding sites using support vector machine. Journal of Computational Chemistry, 2016, 37, 1223-1229.	1.5	81
54	Real-SPINE: An integrated system of neural networks for real-value prediction of protein structural properties. Proteins: Structure, Function and Bioinformatics, 2007, 68, 76-81.	1.5	79

#	Article	IF	Citations
55	BEST: Improved Prediction of B-Cell Epitopes from Antigen Sequences. PLoS ONE, 2012, 7, e40104.	1.1	79
56	Highly accurate sequence-based prediction of half-sphere exposures of amino acid residues in proteins. Bioinformatics, 2016, 32, 843-849.	1.8	79
57	Predicting the topology of transmembrane helical proteins using mean burial propensity and a hidden-Markov-model-based method. Protein Science, 2003, 12, 1547-1555.	3.1	77
58	SPARKS 2 and SP3 servers in CASP6. Proteins: Structure, Function and Bioinformatics, 2005, 61, 152-156.	1.5	76
59	Energy Functions in De Novo Protein Design: Current Challenges and Future Prospects. Annual Review of Biophysics, 2013, 42, 315-335.	4.5	75
60	EVLncRNAs: a manually curated database for long non-coding RNAs validated by low-throughput experiments. Nucleic Acids Research, 2018, 46, D100-D105.	6.5	75
61	Recent advances in glycoinformatic platforms for glycomics and glycoproteomics. Current Opinion in Structural Biology, 2020, 62, 56-69.	2.6	74
62	Stability scale and atomic solvation parameters extracted from 1023 mutation experiments. Proteins: Structure, Function and Bioinformatics, 2002, 49, 483-492.	1.5	73
63	A new sizeâ€‐independent score for pairwise protein structure alignment and its application to structure classification and nucleicâ€‐acid binding prediction. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2080-2088.	1.5	69
64	Criticality of charged systems. I. The restricted primitive model. Journal of Chemical Physics, 1995, 102, 5785-5795.	1.2	68
65	SP5: Improving Protein Fold Recognition by Using Torsion Angle Profiles and Profile-Based Gap Penalty Model. PLoS ONE, 2008, 3, e2325.	1.1	68
66	DDOMAIN: Dividing structures into domains using a normalized domain-domain interaction profile. Protein Science, 2007, 16, 947-955.	3.1	67
67	Accurate Single-Sequence Prediction of Protein Intrinsic Disorder by an Ensemble of Deep Recurrent and Convolutional Architectures. Journal of Chemical Information and Modeling, 2018, 58, 2369-2376.	2.5	67
68	Realâ€‐value prediction of backbone torsion angles. Proteins: Structure, Function and Bioinformatics, 2008, 72, 427-433.	1.5	66
69	Structure-aware proteinâ€“protein interaction site prediction using deep graph convolutional network. Bioinformatics, 2021, 38, 125-132.	1.8	64
70	Assembly and Kinetic Folding Pathways of a Tetrameric Î²-Sheet Complex: Molecular Dynamics Simulations on Simplified Off-Lattice Protein Models. Biophysical Journal, 2004, 86, 31-49.	0.2	63
71	DDIG-in: discriminating between disease-associated and neutral non-frameshifting micro-indels. Genome Biology, 2013, 14, R23.	13.9	63
72	SPIN2: Predicting sequence profiles from protein structures using deep neural networks. Proteins: Structure, Function and Bioinformatics, 2018, 86, 629-633.	1.5	62

#	Article	IF	Citations
73	Structure-based prediction of proteinâ€“ peptide binding regions using Random Forest. Bioinformatics, 2018, 34, 477-484.	1.8	62
74	A simple reference state makes a significant improvement in nearâ€native selections from structurally refined docking decoys. Proteins: Structure, Function and Bioinformatics, 2007, 69, 244-253.	1.5	59
75	Sequence-Based Prediction of Proteinâ€“Carbohydrate Binding Sites Using Support Vector Machines. Journal of Chemical Information and Modeling, 2016, 56, 2115-2122.	2.5	59
76	Intrinsically Semi-disordered State and Its Role in Induced Folding and Protein Aggregation. Cell Biochemistry and Biophysics, 2013, 67, 1193-1205.	0.9	57
77	Temperature Dependence of the Distribution of the First Passage Time:â€‰ Results from Discontinuous Molecular Dynamics Simulations of an All-Atom Model of the Second Î²-Hairpin Fragment of Protein G. Journal of the American Chemical Society, 2003, 125, 6300-6305.	6.6	56
78	Highly accurate and high-resolution function prediction of RNA binding proteins by fold recognition and binding affinity prediction. RNA Biology, 2011, 8, 988-996.	1.5	53
79	Transcriptome profiling of lentil (Lens culinaris) through the first 24 hours of Ascochyta lentis infection reveals key defence response genes. BMC Genomics, 2018, 19, 108.	1.2	53
80	Nucleotide Sugar Transporter SLC35 Family Structure and Function. Computational and Structural Biotechnology Journal, 2019, 17, 1123-1134.	1.9	53
81	DDIG-in: detecting disease-causing genetic variations due to frameshifting indels and nonsense mutations employing sequence and structural properties at nucleotide and protein levels. Bioinformatics, 2015, 31, 1599-1606.	1.8	52
82	RegSNPs-intron: a computational framework for predicting pathogenic impact of intronic single nucleotide variants. Genome Biology, 2019, 20, 254.	3.8	52
83	Role of hydrophilic and hydrophobic contacts in folding of the second ?-hairpin fragment of protein G: Molecular dynamics simulation studies of an all-atom model. Proteins: Structure, Function and Bioinformatics, 2002, 47, 154-162.	1.5	51
84	What is a Desirable Statistical Energy Function for Proteins and How Can It Be Obtained?. Cell Biochemistry and Biophysics, 2006, 46, 165-174.	0.9	50
85	Accurate single-sequence prediction of solvent accessible surface area using local and global features. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3170-3176.	1.5	50
86	Trends in template/fragment-free protein structure prediction. Theoretical Chemistry Accounts, 2011, 128, 3-16.	0.5	48
87	SPRINT-Gly: predictingN-andO-linked glycosylation sites of human and mouse proteins by using sequence and predicted structural properties. Bioinformatics, 2019, 35, 4140-4146.	1.8	48
88	Exploring the Molecular Design of Protein Interaction Sites with Molecular Dynamics Simulations and Free Energy Calculations. Biochemistry, 2009, 48, 399-414.	1.2	47
89	Improved RNA secondary structure and tertiary base-pairing prediction using evolutionary profile, mutational coupling and two-dimensional transfer learning. Bioinformatics, 2021, 37, 2589-2600.	1.8	47
90	An allâ€atom knowledgeâ€based energy function for proteinâ€DNA threading, docking decoy discrimination, and prediction of transcriptionâ€factor binding profiles. Proteins: Structure, Function and Bioinformatics, 2009, 76, 718-730.	1.5	46

#	Article	IF	Citations
91	Direct prediction of profiles of sequences compatible with a protein structure by neural networks with fragment-based local and energy-based nonlocal profiles. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2565-2573.	1.5	46
92	DEPICTER: Intrinsic Disorder and Disorder Function Prediction Server. Journal of Molecular Biology, 2020, 432, 3379-3387.	2.0	46
93	DescribePROT: database of amino acid-level protein structure and function predictions. Nucleic Acids Research, 2021, 49, D298-D308.	6.5	46
94	The role of sidechain packing and native contact interactions in folding: Discontinuous molecular dynamics folding simulations of an all-atom GÅ•model of fragment B of Staphylococcal protein A. Journal of Chemical Physics, 2002, 117, 8983-8995.	1.2	45
95	In-silico prediction of disorder content using hybrid sequence representation. BMC Bioinformatics, 2011, 12, 245.	1.2	45
96	Molecular Dynamics Simulations of Human Antimicrobial Peptide LL-37 in Model POPC and POPG Lipid Bilayers. International Journal of Molecular Sciences, 2018, 19, 1186.	1.8	45
97	Systems-level understanding of ethanol-induced stresses and adaptation in E. coli. Scientific Reports, 2017, 7, 44150.	1.6	43
98	A survey of Type III restriction-modification systems reveals numerous, novel epigenetic regulators controlling phase-variable regulons; phasevarions. Nucleic Acids Research, 2018, 46, 3532-3542.	6.5	43
99	EVLncRNAs 2.0: an updated database of manually curated functional long non-coding RNAs validated by low-throughput experiments. Nucleic Acids Research, 2021, 49, D86-D91.	6.5	42
100	The Dependence of All-Atom Statistical Potentials on Structural Training Database. Biophysical Journal, 2004, 86, 3349-3358.	0.2	41
101	Phase Separation of Ionic Fluids:Â An Extended Ebelingâ^'Grigo Approach. The Journal of Physical Chemistry, 1996, 100, 1415-1419.	2.9	39
102	SPOT-Seq-RNA: Predicting Proteinâ€“RNA Complex Structure and RNA-Binding Function by Fold Recognition and Binding Affinity Prediction. Methods in Molecular Biology, 2014, 1137, 119-130.	0.4	39
103	Predicting residueâ€“residue contact maps by a twoâ€layer, integrated neuralâ€network method. Proteins: Structure, Function and Bioinformatics, 2009, 76, 176-183.	1.5	38
104	Small Open Reading Frames: Current Prediction Techniques and Future Prospect. Current Protein and Peptide Science, 2011, 12, 503-507.	0.7	38
105	Prediction of RNA binding proteins comes of age from low resolution to high resolution. Molecular BioSystems, 2013, 9, 2417.	2.9	37
106	Natural protein sequences are more intrinsically disordered than random sequences. Cellular and Molecular Life Sciences, 2016, 73, 2949-2957.	2.4	37
107	Investigating DNA-, RNA-, and protein-based features as a means to discriminate pathogenic synonymous variants. Human Mutation, 2017, 38, 1336-1347.	1.1	37
108	Identifying molecular recognition features in intrinsically disordered regions of proteins by transfer learning. Bioinformatics, 2020, 36, 1107-1113.	1.8	37

#	Article	IF	Citations
109	Nonlocal integralâ€equation approximations. I. The zeroth order (hydrostatic) approximation with applications. Journal of Chemical Physics, 1990, 92, 5533-5543.	1.2	36
110	Cooperativity in Scapharca Dimeric Hemoglobin: Simulation of Binding Intermediates and Elucidation of the Role of Interfacial Water. Journal of Molecular Biology, 2003, 326, 593-606.	2.0	36
111	Consensus scoring for enriching nearâ€native structures from proteinâ€“protein docking decoys. Proteins: Structure, Function and Bioinformatics, 2009, 75, 397-403.	1.5	36
112	Analytical approach to molecular liquids. IV. Solvation dynamics and electronâ€transfer reactions. Journal of Chemical Physics, 1989, 91, 4885-4890.	1.2	35
113	Folding processes of the B domain of protein A to the native state observed in all-atom ab initio folding simulations. Journal of Chemical Physics, 2008, 128, 235105.	1.2	35
114	Protein side chain modeling with orientationâ€dependent atomic force fields derived by series expansions. Journal of Computational Chemistry, 2011, 32, 1680-1686.	1.5	35
115	Optimal secretion of alkali-tolerant xylanase in Bacillus subtilis by signal peptide screening. Applied Microbiology and Biotechnology, 2016, 100, 8745-8756.	1.7	35
116	DLIGAND2: an improved knowledge-based energy function for proteinâ€“ligand interactions using the distance-scaled, finite, ideal-gas reference state. Journal of Cheminformatics, 2019, 11, 52.	2.8	35
117	Thermodynamic perturbation theory for fused hardâ€sphere and hardâ€disk chain fluids. Journal of Chemical Physics, 1995, 103, 2688-2695.	1.2	34
118	Docking prediction using biological information, ZDOCK sampling technique, and clustering guided by the DFIRE statistical energy function. Proteins: Structure, Function and Bioinformatics, 2005, 60, 314-318.	1.5	34
119	LEAP: Highly accurate prediction of protein loop conformations by integrating coarseâ€grained sampling and optimized energy scores with allâ€atom refinement of backbone and side chains. Journal of Computational Chemistry, 2014, 35, 335-341.	1.5	34
120	Advancing the Accuracy of Protein Fold Recognition by Utilizing Profiles From Hidden Markov Models. IEEE Transactions on Nanobioscience, 2015, 14, 761-772.	2.2	34
121	Critical nucleation size in the folding of small apparently two-state proteins. Protein Science, 2004, 13, 1173-1181.	3.1	33
122	Pairing a high-resolution statistical potential with a nucleobase-centric sampling algorithm for improving RNA model refinement. Nature Communications, 2021, 12, 2777.	5.8	33
123	Assessing secondary structure assignment of protein structures by using pairwise sequenceâ€alignment benchmarks. Proteins: Structure, Function and Bioinformatics, 2008, 71, 61-67.	1.5	32
124	Predicting DNA-Binding Proteins and Binding Residues by Complex Structure Prediction and Application to Human Proteome. PLoS ONE, 2014, 9, e96694.	1.1	32
125	Repurposing clinically approved drugs for COVID-19 treatment targeting SARS-CoV-2 papain-like protease. International Journal of Biological Macromolecules, 2021, 188, 137-146.	3.6	32
126	Thermodynamics and stability of a Â-sheet complex: Molecular dynamics simulations on simplified off-lattice protein models. Protein Science, 2004, 13, 40-53.	3.1	31

#	Article	IF	Citations
127	Note on standard free energy of transfer and partitioning of ionic species between two fluid phases. Journal of Chemical Physics, 1988, 89, 3836-3839.	1.2	30
128	Predicting lysineâ€malonylation sites of proteins using sequence and predicted structural features. Journal of Computational Chemistry, 2018, 39, 1757-1763.	1.5	30
129	DNA sequence repeats identify numerous Type I restrictionâ€modification systems that are potential epigenetic regulators controlling phaseâ€variable regulons; phasevarions. FASEB Journal, 2020, 34, 1038-1051.	0.2	29
130	The theory of semipermeable vesicles and membranes: An integralâ€equation approach. I. General formalism and application to a hardâ€sphere mixture. Journal of Chemical Physics, 1988, 89, 7010-7019.	1.2	28
131	Fluids inside a poreâ€”an integral-equation approach. Molecular Physics, 1989, 66, 791-796.	0.8	28
132	Protein Motions at Zero-Total Angular Momentum: The Importance of Long-Range Correlations. Biophysical Journal, 2000, 79, 2902-2908.	0.2	28
133	Genome-scale characterization of RNA tertiary structures and their functional impact by RNA solvent accessibility prediction. Rna, 2017, 23, 14-22.	1.6	28
134	The hard-sphere fluid: New exact results with applications. Journal of Statistical Physics, 1988, 52, 1389-1412.	0.5	27
135	Fluctuations of backbone torsion angles obtained from NMRâ€determined structures and their prediction. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3353-3362.	1.5	27
136	Impact of human pathogenic micro-insertions and micro-deletions on post-transcriptional regulation. Human Molecular Genetics, 2014, 23, 3024-3034.	1.4	27
137	regSNPs-splicing: a tool for prioritizing synonymous single-nucleotide substitution. Human Genetics, 2017, 136, 1279-1289.	1.8	27
138	RNAcmap: a fully automatic pipeline for predicting contact maps of RNAs by evolutionary coupling analysis. Bioinformatics, 2021, 37, 3494-3500.	1.8	27
139	Thermodynamics of an All-Atom Off-Lattice Model of the Fragment B of Staphylococcal Protein A:â€‰ Implication for the Origin of the Cooperativity of Protein Folding. Journal of Physical Chemistry B, 2002, 106, 1481-1485.	1.2	26
140	Design and Evaluation of a Novel Peptideâ€“Drug Conjugate Covalently Targeting SARS-CoV-2 Papain-like Protease. Journal of Medicinal Chemistry, 2022, 65, 876-884.	2.9	26
141	Predicting the errors of predicted local backbone angles and non-local solvent- accessibilities of proteins by deep neural networks. Bioinformatics, 2016, 32, 3768-3773.	1.8	25
142	Improved fragment sampling for ab initio protein structure prediction using deep neural networks. Nature Machine Intelligence, 2019, 1, 347-355.	8.3	25
143	SPOT-Contact-LM: improving single-sequence-based prediction of protein contact map using a transformer language model. Bioinformatics, 2022, 38, 1888-1894.	1.8	25
144	Characterizing the Existing and Potential Structural Space of Proteins by Large-Scale Multiple Loop Permutations. Journal of Molecular Biology, 2011, 408, 585-595.	2.0	24

#	Article	IF	Citations
145	The theory of semipermeable vesicles and membranes: An integralâ€equation approach. II. Donnan equilibrium. Journal of Chemical Physics, 1988, 89, 7020-7029.	1.2	23
146	Criticality of charged systems. II. The binary mixture of hard spheres and ions. Journal of Chemical Physics, 1995, 102, 5796-5802.	1.2	23
147	Folding Thermodynamics of Model Four-Strand Antiparallel Î²-Sheet Proteins. Biophysical Journal, 2002, 82, 646-659.	0.2	23
148	Temperature-Dependent Folding Pathways of Pin1 WW Domain: An All-Atom Molecular Dynamics Simulation of a GÅ•Model. Biophysical Journal, 2007, 93, 2152-2161.	0.2	23
149	Improving computational protein design by using structureâ€derived sequence profile. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2338-2348.	1.5	23
150	Outer-sphere electron-transfer reactions in model molecular solvents: the mean spherical approximation. Chemical Physics, 1991, 152, 185-200.	0.9	22
151	Fast and Accurate Method for Identifying High-Quality Protein-Interaction Modules by Clique Merging and Its Application to Yeast. Journal of Proteome Research, 2006, 5, 801-807.	1.8	22
152	Prediction and validation of the unexplored RNAâ€binding protein atlas of the human proteome. Proteins: Structure, Function and Bioinformatics, 2014, 82, 640-647.	1.5	22
153	SPOT-1D-Single: improving the single-sequence-based prediction of protein secondary structure, backbone angles, solvent accessibility and half-sphere exposures using a large training set and ensembled deep learning. Bioinformatics, 2021, 37, 3464-3472.	1.8	22
154	Single-sequence and profile-based prediction of RNA solvent accessibility using dilated convolutional neural network. Bioinformatics, 2021, 36, 5169-5176.	1.8	21
155	Fused hardâ€sphere chain molecules: Comparison between Monte Carlo simulation for the bulk pressure and generalized Flory theories. Journal of Chemical Physics, 1995, 102, 6212-6223.	1.2	20
156	Folding mechanisms of individual Î²-hairpins in a GÅ•model of Pin1 WW domain by all-atom molecular dynamics simulations. Journal of Chemical Physics, 2008, 128, 225103.	1.2	20
157	The dual role of a loop with low loop contact distance in folding and domain swapping. Protein Science, 2009, 11, 1695-1701.	3.1	20
158	Carbohydrate-binding protein identification by coupling structural similarity searching with binding affinity prediction. Journal of Computational Chemistry, 2014, 35, 2177-2183.	1.5	20
159	Equations of state for hard-sphere fluids. International Journal of Thermophysics, 1988, 9, 953-963.	1.0	19
160	Nonlocal integralâ€equation approximations. II. Lennardâ€Jones fluids. Journal of Chemical Physics, 1990, 92, 5544-5550.	1.2	19
161	Linear dependence on chain length for the thermodynamic properties of tangent hard-sphere chains. Molecular Physics, 1995, 86, 1157-1172.	0.8	19
162	Solute excluded-volume effects on the stability of globular proteins: A statistical thermodynamic theory. , 1998, 38, 273-284.		19

#	Article	IF	Citations
163	Protein flexibility prediction by an all-atom mean-field statistical theory. Protein Science, 2005, 14, 1772-1777.	3.1	19
164	Fast and accurate non-sequential protein structure alignment using a new asymmetric linear sum assignment heuristic. Bioinformatics, 2016, 32, 370-377.	1.8	19
165	SPOT-Peptide: Template-Based Prediction of Peptide-Binding Proteins and Peptide-Binding Sites. Journal of Chemical Information and Modeling, 2019, 59, 924-930.	2.5	19
166	Analytical approach to molecular liquids. I. Siteâ€“site interaction model using an extended meanâ€spherical approximation. Journal of Chemical Physics, 1989, 91, 4861-4868.	1.2	18
167	Microscopic modelling of association. Fluid Phase Equilibria, 1992, 79, 1-20.	1.4	18
168	QBES: Predicting real values of solvent accessibility from sequences by efficient, constrained energy optimization. Proteins: Structure, Function and Bioinformatics, 2006, 63, 961-966.	1.5	18
169	SPOT-ligand 2: improving structure-based virtual screening by binding-homology search on an expanded structural template library. Bioinformatics, 2017, 33, 1238-1240.	1.8	18
170	Argonaute proteins: structures and their endonuclease activity. Molecular Biology Reports, 2021, 48, 4837-4849.	1.0	18
171	Web-based toolkits for topology prediction of transmembrane helical proteins, fold recognition, structure and binding scoring, folding-kinetics analysis and comparative analysis of domain combinations. Nucleic Acids Research, 2005, 33, W193-W197.	6.5	17
172	Grid-based prediction of torsion angle probabilities of protein backbone and its application to discrimination of protein intrinsic disorder regions and selection of model structures. BMC Bioinformatics, 2018, 19, 29.	1.2	17
173	Systematic Analysis of REBASE Identifies Numerous Type I Restriction-Modification Systems with Duplicated, Distinct hsdS Specificity Genes That Can Switch System Specificity by Recombination. MSystems, 2020, 5, .	1.7	17
174	From â€œDark Matterâ€•to â€œStarâ€• Insight Into the Regulation Mechanisms of Plant Functional Long Non-Coding RNAs. Frontiers in Plant Science, 2021, 12, 650926.	1.7	17
175	Analytical approach to molecular liquids. II. Solvation of ions in molecular fluids. Journal of Chemical Physics, 1989, 91, 4869-4878.	1.2	16
176	Chemical association in simple models of molecular and ionic fluids. IV. New approximation for the cavity function and an application to the theory of weak electrolytes. Journal of Chemical Physics, 1995, 102, 8089-8093.	1.2	16
177	SCUD: Fast structure clustering of decoys using reference state to remove overall rotation. Journal of Computational Chemistry, 2005, 26, 1189-1192.	1.5	16
178	s<scp>DFIRE</scp>: Sequenceâ€specific statistical energy function for protein structure prediction by decoy selections. Journal of Computational Chemistry, 2016, 37, 1119-1124.	1.5	16
179	Evaluating the predictions of the protein stability change upon single amino acid substitutions for the FXN CAGI5 challenge. Human Mutation, 2019, 40, 1392-1399.	1.1	16
180	Assessment of methods for predicting the effects of PTEN and TPMT protein variants. Human Mutation, 2019, 40, 1495-1506.	1.1	16

#	Article	IF	Citations
181	Analytical approach to molecular liquids. III. The Born solvation free energy of two fixed ions in a dipolar solvent. Journal of Chemical Physics, 1989, 91, 4879-4884.	1.2	15
182	Fluids inside a poreâ€"An integral equation approach. Molecular Physics, 1989, 68, 1265-1275.	0.8	15
183	Analytical approach to molecular liquids. V. Symmetric dissociative dipolar dumbbells with the bonding length Ïƒ/3â‰Lâ‰Ïƒ/2 and related systems. Journal of Chemical Physics, 1993, 98, 5777-5787.	1.2	15
184	Protein Folding Pathways and Kinetics: Molecular Dynamics Simulations of Î²-Strand Motifs. Biophysical Journal, 2002, 83, 819-835.	0.2	15
185	The helix-coil transition revisited. Proteins: Structure, Function and Bioinformatics, 2007, 69, 58-68.	1.5	15
186	SPOTâ€Ligand: Fast and effective structureâ€based virtual screening by binding homology search according to ligand and receptor similarity. Journal of Computational Chemistry, 2016, 37, 1734-1739.	1.5	15
187	Large expert-curated database for benchmarking document similarity detection in biomedical literature search. Database: the Journal of Biological Databases and Curation, 2019, 2019, .	1.4	15
188	Getting to Know Your Neighbor: Protein Structure Prediction Comes of Age with Contextual Machine Learning. Journal of Computational Biology, 2020, 27, 796-814.	0.8	15
189	Accurate inference of the full base-pairing structure of RNA by deep mutational scanning and covariation-induced deviation of activity. Nucleic Acids Research, 2020, 48, 1451-1465.	6.5	15
190	All-Atom Knowledge-Based Potential for RNA Structure Discrimination Based on the Distance-Scaled Finite Ideal-Gas Reference State. Journal of Computational Biology, 2020, 27, 856-867.	0.8	15
191	Structural signatures of thermal adaptation of bacterial ribosomal RNA, transfer RNA, and messenger RNA. PLoS ONE, 2017, 12, e0184722.	1.1	15
192	Investigation the Possibility of Using Peptides with a Helical Repeating Pattern of Hydro-Phobic and Hydrophilic Residues to Inhibit IL-10. PLoS ONE, 2016, 11, e0153939.	1.1	14
193	Infectivity of Plasmodium falciparum in Malaria-Naive Individuals Is Related to Knob Expression and Cytoadherence of the Parasite. Infection and Immunity, 2016, 84, 2689-2696.	1.0	14
194	Bias-Exchange Metadynamics Simulation of Membrane Permeation of 20 Amino Acids. International Journal of Molecular Sciences, 2018, 19, 885.	1.8	14
195	Reaching alignment-profile-based accuracy in predicting protein secondary and tertiary structural properties without alignment. Scientific Reports, 2022, 12, 7607.	1.6	14
196	Predicting RNA distance-based contact maps by integrated deep learning on physics-inferred secondary structure and evolutionary-derived mutational coupling. Bioinformatics, 2022, 38, 3900-3910.	1.8	14
197	Performance of in silico tools for the evaluation of p16INK4a (CDKN2A) variants in CAGI. Human Mutation, 2017, 38, 1042-1050.	1.1	13
198	Bâ€factor profile prediction for RNA flexibility using support vector machines. Journal of Computational Chemistry, 2018, 39, 407-411.	1.5	13

#	Article	IF	Citations
199	Detecting Proline and Non-Proline Cis Isomers in Protein Structures from Sequences Using Deep Residual Ensemble Learning. Journal of Chemical Information and Modeling, 2018, 58, 2033-2042.	2.5	13
200	Different effects of cholesterol on membrane permeation of arginine and tryptophan revealed by bias-exchange metadynamics simulations. Journal of Chemical Physics, 2019, 150, 084106.	1.2	13
201	Probing RNA structures and functions by solvent accessibility: an overview from experimental and computational perspectives. Briefings in Bioinformatics, 2022, 23, .	3.2	13
202	ExonImpact: Prioritizing Pathogenic Alternative Splicing Events. Human Mutation, 2017, 38, 16-24.	1.1	12
203	RNA Backbone Torsion and Pseudotorsion Angle Prediction Using Dilated Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2021, 61, 2610-2622.	2.5	12
204	Solute excluded-volume effects on the stability of globular proteins: A statistical thermodynamic theory. , 1996, 38, 273.		12
205	FOLD HELICAL PROTEINS BY ENERGY MINIMIZATION IN DIHEDRAL SPACE AND A DFIRE-BASED STATISTICAL ENERGY FUNCTION. Journal of Bioinformatics and Computational Biology, 2005, 03, 1151-1170.	0.3	11
206	Templateâ€based structure prediction and classification of transcription factors in Arabidopsis thaliana. Protein Science, 2012, 21, 828-838.	3.1	11
207	Domain Graph ofArabidopsisProteome by Comparative Analysis. Journal of Proteome Research, 2005, 4, 435-444.	1.8	10
208	Refining nearâ€native proteinâ€“protein docking decoys by local resampling and energy minimization. Proteins: Structure, Function and Bioinformatics, 2009, 76, 309-316.	1.5	10
209	LRFragLib: an effective algorithm to identify fragments for de novo protein structure prediction. Bioinformatics, 2017, 33, 677-684.	1.8	10
210	Assessment of predicted enzymatic activity of Î±â€•N â€acetylglucosaminidase variants of unknown significance for CAGI 2016. Human Mutation, 2019, 40, 1519-1529.	1.1	10
211	Interplay of hydrophobic and hydrophilic interactions in sequence-dependent cell penetration of spontaneous membrane-translocating peptides revealed by bias-exchange metadynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183402.	1.4	10
212	DisBind: A database of classified functional binding sites in disordered and structured regions of intrinsically disordered proteins. BMC Bioinformatics, 2017, 18, 206.	1.2	9
213	SPOTâ€Fold: Fragmentâ€Free Protein Structure Prediction Guided by Predicted Backbone Structure and Contact Map. Journal of Computational Chemistry, 2020, 41, 745-750.	1.5	9
214	Exact results for isolated sticky chains. Molecular Physics, 1995, 86, 1485-1492.	0.8	8
215	Intrinsic Disorder and Semi-disorder Prediction by SPINE-D. Methods in Molecular Biology, 2017, 1484, 159-174.	0.4	8
216	Quantitative mapping of genetic similarity in human heritable diseases by shared mutations. Human Mutation, 2018, 39, 292-301.	1.1	8

#	Article	IF	Citations
217	De novo protein design by an energy function based on series expansion in distance and orientation dependence. Bioinformatics, 2021, 38, 86-93.	1.8	8
218	Electron rearrangement and energy relaxation due to a core hole creation in molecules. The Journal of Physical Chemistry, 1992, 96, 2949-2952.	2.9	7
219	Salt Effects on Protein Titration and Binding. Journal of Physical Chemistry B, 1998, 102, 10615-10621.	1.2	7
220	Editorial [Hot Topic: Machine Learning Models in Protein Bioinformatics (Guest Editors: Lukasz) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62	0.7	7
221	Fast and Accurate Accessible Surface Area Prediction Without a Sequence Profile. Methods in Molecular Biology, 2017, 1484, 127-136.	0.4	7
222	YesU from Bacillus subtilis preferentially binds fucosylated glycans. Scientific Reports, 2018, 8, 13139.	1.6	7
223	Selfâ€derived structureâ€disrupting peptides targeting methionine aminopeptidase in pathogenic bacteria: a new strategy to generate antimicrobial peptides. FASEB Journal, 2019, 33, 2095-2104.	0.2	7
224	GM-DockZn: a geometry matching-based docking algorithm for zinc proteins. Bioinformatics, 2020, 36, 4004-4011.	1.8	7
225	Predicting functional long non-coding RNAs validated by low throughput experiments. RNA Biology, 2019, 16, 1555-1564.	1.5	6
226	The Role of Semidisorder in Temperature Adaptation of Bacterial FlgM Proteins. Biophysical Journal, 2013, 105, 2598-2605.	0.2	5
227	Computational Prediction of Carbohydrateâ€Binding Proteins and Binding Sites. Current Protocols in Protein Science, 2018, 94, e75.	2.8	5
228	Experimentally Validated Plant lncRNAs in EVLncRNAs Database. Methods in Molecular Biology, 2019, 1933, 431-437.	0.4	5
229	Moraxella catarrhalis phase-variable loci show differences in expression during conditions relevant to disease. PLoS ONE, 2020, 15, e0234306.	1.1	5
230	Design and Folding of a Multidomain Protein. Biochemistry, 2005, 44, 12107-12112.	1.2	4
231	Uneven size distribution of mammalian genes in the number of tissues expressed and in the number of co-expressed genes. Human Molecular Genetics, 2006, 15, 1313-1318.	1.4	4
232	A heuristic for the time constrained asymmetric linear sum assignment problem. Journal of Combinatorial Optimization, 2017, 33, 551-566.	0.8	4
233	Exact results for the effect of bond flexibility on the structure and the collapse transition of isolated square-well trimers. Molecular Physics, 1996, 89, 1707-1717.	0.8	4
234	The theory of semipermeable vesicles and membranes: An integralâ€equation approach. III. Vesicles with internal nonpermeating ions. Journal of Chemical Physics, 1989, 91, 3208-3211.	1.2	3

#	Article	IF	Citations
235	Effective protein conformational sampling based on predicted torsion angles. Journal of Computational Chemistry, 2016, 37, 976-980.	1.5	2
236	Testers wanted for article search tool. Nature, 2017, 549, 31-31.	13.7	2
237	Self-Inhibitory Peptides Targeting the Neisseria gonorrhoeae MtrCDE Efflux Pump Increase Antibiotic Susceptibility. Antimicrobial Agents and Chemotherapy, 2022, 66, AAC0154221.	1.4	2
238	Fast and accurate thermodynamics of square-well systems from umbrella-sampling simulations of hard-sphere systems. Journal of Chemical Physics, 2001, 115, 7550-7553.	1.2	1
239	SPOT-1D2: Improving Protein Secondary Structure Prediction using High Sequence Identity Training Set and an Ensemble of Recurrent and Residual-convolutional Neural Networks. , 2021, , .		1
240	DeepANIS: Predicting antibody paratope from concatenated CDR sequences by integrating bidirectional long-short-term memory and transformer neural networks. , 2021, , .		1
241	Computational Prediction of N- and O-Linked Glycosylation Sites for Human and Mouse Proteins. Methods in Molecular Biology, 2022, , 177-186.	0.4	1
242	Cooperativity inScapharca dimeric hemoglobin: Simulation of binding intermediates and elucidation of the role of interfacial water. Rendiconti Lincei, 2006, 17, 191-211.	1.0	0
243	High-throughput split-protein profiling by combining transposon mutagenesis and regulated protein-protein interactions with deep sequencing. International Journal of Biological Macromolecules, 2022, 203, 543-552.	3.6	0