Yang Zhang

List of Publications by Year
in descending order

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135 papers	37,643 citations	19636 61 h-index	11928 134 g-index
159 all docs	159 docs citations	159 times ranked	37100 citing authors

#	Article	IF	Citations
1	I-TASSER: a unified platform for automated protein structure and function prediction. Nature Protocols, 2010, 5, 725-738.	5.5	5,594
2	The I-TASSER Suite: protein structure and function prediction. Nature Methods, 2015, 12, 7-8.	9.0	4,923
3	I-TASSER server for protein 3D structure prediction. BMC Bioinformatics, 2008, 9, 40.	1.2	4,415
4	TM-align: a protein structure alignment algorithm based on the TM-score. Nucleic Acids Research, 2005, 33, 2302-2309.	6.5	2,634
5	I-TASSER server: new development for protein structure and function predictions. Nucleic Acids Research, 2015, 43, W174-W181.	6.5	1,897
6	Scoring function for automated assessment of protein structure template quality. Proteins: Structure, Function and Bioinformatics, 2004, 57, 702-710.	1.5	1,697
7	Improving the Physical Realism and Structural Accuracy of Protein Models by a Two-Step Atomic-Level Energy Minimization. Biophysical Journal, 2011, 101, 2525-2534.	0.2	871
8	Ab initio protein structure assembly using continuous structure fragments and optimized knowledgeâ€based force field. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1715-1735.	1.5	744
9	Proteinâ€“ligand binding site recognition using complementary binding-specific substructure comparison and sequence profile alignment. Bioinformatics, 2013, 29, 2588-2595.	1.8	739
10	LOMETS: A local meta-threading-server for protein structure prediction. Nucleic Acids Research, 2007, 35, 3375-3382.	6.5	734
11	How significant is a protein structure similarity with TM-score = 0.5?. Bioinformatics, 2010, 26, 889-895.	1.8	674
12	COFACTOR: an accurate comparative algorithm for structure-based protein function annotation. Nucleic Acids Research, 2012, 40, W471-W477.	6.5	582
13	BioLiP: a semi-manually curated database for biologically relevant ligandâ€“protein interactions. Nucleic Acids Research, 2012, 41, D1096-D1103.	6.5	568
14	Ab initio modeling of small proteins by iterative TASSER simulations. BMC Biology, 2007, 5, 17.	1.7	439
15	Progress and challenges in protein structure prediction. Current Opinion in Structural Biology, 2008, 18, 342-348.	2.6	437
16	COFACTOR: improved protein function prediction by combining structure, sequence and proteinâ€“protein interaction information. Nucleic Acids Research, 2017, 45, W291-W299.	6.5	424
17	Template-based modeling and free modeling by I-TASSER in CASP7. Proteins: Structure, Function and Bioinformatics, 2007, 69, 108-117.	1.5	410
18	Iâ€TASSER: Fully automated protein structure prediction in CASP8. Proteins: Structure, Function and Bioinformatics, 2009, 77, 100-113.	1.5	384

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19	SPICKER: A clustering approach to identify near-native protein folds. Journal of Computational Chemistry, 2004, 25, 865-871.	1.5	380
20	MUSTER: Improving protein sequence profileâ€“profile alignments by using multiple sources of structure information. Proteins: Structure, Function and Bioinformatics, 2008, 72, 547-556.	1.5	341
21	Automated structure prediction of weakly homologous proteins on a genomic scale. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 7594-7599.	3.3	324
22	Atomic-Level Protein Structure Refinement Using Fragment-Guided Molecular Dynamics Conformation Sampling. Structure, 2011, 19, 1784-1795.	1.6	309
23	STRUM: structure-based prediction of protein stability changes upon single-point mutation. Bioinformatics, 2016, 32, 2936-2946.	1.8	275
24	Folding non-homologous proteins by coupling deep-learning contact maps with I-TASSER assembly simulations. Cell Reports Methods, 2021, 1, 100014.	1.4	272
25	The protein structure prediction problem could be solved using the current PDB library. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 1029-1034.	3.3	269
26	The CAFA challenge reports improved protein function prediction and new functional annotations for hundreds of genes through experimental screens. Genome Biology, 2019, 20, 244.	3.8	261
27	TOUCHSTONE II: A New Approach to Ab Initio Protein Structure Prediction. Biophysical Journal, 2003, 85, 1145-1164.	0.2	243
28	Protein Structure and Sequence Reanalysis of 2019-nCoV Genome Refutes Snakes as Its Intermediate Host and the Unique Similarity between Its Spike Protein Insertions and HIV-1. Journal of Proteome Research, 2020, 19, 1351-1360.	1.8	242
29	Protein structure prediction: when is it useful?. Current Opinion in Structural Biology, 2009, 19, 145-155.	2.6	234
30	A Novel Side-Chain Orientation Dependent Potential Derived from Random-Walk Reference State for Protein Fold Selection and Structure Prediction. PLoS ONE, 2010, 5, e15386.	1.1	216
31	Toward optimal fragment generations for ab initio protein structure assembly. Proteins: Structure, Function and Bioinformatics, 2013, 81, 229-239.	1.5	191
32	Deepâ€learning contactâ€map guided protein structure prediction in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1149-1164.	1.5	180
33	DockRMSD: an open-source tool for atom mapping and RMSD calculation of symmetric molecules through graph isomorphism. Journal of Cheminformatics, 2019, 11, 40.	2.8	174
34	A comparative assessment and analysis of 20 representative sequence alignment methods for protein structure prediction. Scientific Reports, 2013, 3, 2619.	1.6	171
35	A comprehensive assessment of sequence-based and template-based methods for protein contact prediction. Bioinformatics, 2008, 24, 924-931.	1.8	165
36	COACH-D: improved proteinâ€“ligand binding sites prediction with refined ligand-binding poses through molecular docking. Nucleic Acids Research, 2018, 46, W438-W442.	6.5	164

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37	GPCR-I-TASSER: A Hybrid Approach to G Protein-Coupled Receptor Structure Modeling and the Application to the Human Genome. Structure, 2015, 23, 1538-1549.	1.6	153
38	Development and large scale benchmark testing of the PROSPECTOR_3 threading algorithm. Proteins: Structure, Function and Bioinformatics, 2004, 56, 502-518.	1.5	152
39	DeepMSA: constructing deep multiple sequence alignment to improve contact prediction and fold-recognition for distant-homology proteins. Bioinformatics, 2020, 36, 2105-2112.	1.8	147
40	ResPRE: high-accuracy protein contact prediction by coupling precision matrix with deep residual neural networks. Bioinformatics, 2019, 35, 4647-4655.	1.8	142
41	Automated protein structure modeling in CASP9 by Iâ€TASSER pipeline combined with QUARKâ€based ab initio folding and FGâ€MDâ€based structure refinement. Proteins: Structure, Function and Bioinformatics, 2011, 79, 147-160.	1.5	139
42	Local energy landscape flattening: Parallel hyperbolic Monte Carlo sampling of protein folding. Proteins: Structure, Function and Bioinformatics, 2002, 48, 192-201.	1.5	130
43	MM-align: a quick algorithm for aligning multiple-chain protein complex structures using iterative dynamic programming. Nucleic Acids Research, 2009, 37, e83-e83.	6.5	126
44	Predicting the Effect of Mutations on Protein-Protein Binding Interactions through Structure-Based Interface Profiles. PLoS Computational Biology, 2015, 11, e1004494.	1.5	122
45	ResQ: An Approach to Unified Estimation of B -Factor and Residue-Specific Error in Protein Structure Prediction. Journal of Molecular Biology, 2016, 428, 693-701.	2.0	119
46	LOMETS2: improved meta-threading server for fold-recognition and structure-based function annotation for distant-homology proteins. Nucleic Acids Research, 2019, 47, W429-W436.	6.5	118
47	REMO: A new protocol to refine full atomic protein models from Câ€alpha traces by optimizing hydrogenâ€bonding networks. Proteins: Structure, Function and Bioinformatics, 2009, 76, 665-676.	1.5	112
48	BindProfX: Assessing Mutation-Induced Binding Affinity Change by Protein Interface Profiles with Pseudo-Counts. Journal of Molecular Biology, 2017, 429, 426-434.	2.0	107
49	3DRobot: automated generation of diverse and well-packed protein structure decoys. Bioinformatics, 2016, 32, 378-387.	1.8	104
50	Assembling multidomain protein structures through analogous global structural alignments. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 15930-15938.	3.3	104
51	Recognizing Protein-Ligand Binding Sites by Global Structural Alignment and Local Geometry Refinement. Structure, 2012, 20, 987-997.	1.6	101
52	Interplay of Iâ€TASSER and QUARK for templateâ€based and ab initio protein structure prediction in CASP10. Proteins: Structure, Function and Bioinformatics, 2014, 82, 175-187.	1.5	98
53	Recognizing metal and acid radical ion-binding sites by integrating ab initio modeling with template-based transferals. Bioinformatics, 2016, 32, 3260-3269.	1.8	98
54	Ensembling multiple raw coevolutionary features with deep residual neural networks for contactâ€map prediction in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1082-1091.	1.5	96

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55	De novo design of protein peptides to block association of the SARS-CoV-2 spike protein with human ACE2. Aging, 2020, 12, 11263-11276.	1.4	89
56	Templateâ€based and free modeling of Iâ€TASSER and QUARK pipelines using predicted contact maps in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 136-151.	1.5	86
57	Effects of SARSâ€CoVâ€2 mutations on protein structures and intraviral proteinâ€“protein interactions. Journal of Medical Virology, 2021, 93, 2132-2140.	2.5	85
58	I-TASSER gateway: A protein structure and function prediction server powered by XSEDE. Future Generation Computer Systems, 2019, 99, 73-85.	4.9	80
59	ThreaDom: extracting protein domain boundary information from multiple threading alignments. Bioinformatics, 2013, 29, i247-i256.	1.8	79
60	Deep learning techniques have significantly impacted protein structure prediction and protein design. Current Opinion in Structural Biology, 2021, 68, 194-207.	2.6	77
61	BSPâ€SLIM: A blind lowâ€resolution ligandâ€protein docking approach using predicted protein structures. Proteins: Structure, Function and Bioinformatics, 2012, 80, 93-110.	1.5	75
62	ANGLOR: A Composite Machine-Learning Algorithm for Protein Backbone Torsion Angle Prediction. PLoS ONE, 2008, 3, e3400.	1.1	75
63	EvoEF2: accurate and fast energy function for computational protein design. Bioinformatics, 2020, 36, 1135-1142.	1.8	73
64	Toward the solution of the protein structure prediction problem. Journal of Biological Chemistry, 2021, 297, 100870.	1.6	73
65	NeBcon: protein contact map prediction using neural network training coupled with naÃ¯ve Bayes classifiers. Bioinformatics, 2017, 33, 2296-2306.	1.8	71
66	Deducing high-accuracy protein contact-maps from a triplet of coevolutionary matrices through deep residual convolutional networks. PLoS Computational Biology, 2021, 17, e1008865.	1.5	70
67	Mapping Monomeric Threading to Proteinâ€“Protein Structure Prediction. Journal of Chemical Information and Modeling, 2013, 53, 717-725.	2.5	67
68	Integration of <scp>QUARK</scp> and <scp>Iâ€TASSER</scp> for Ab Initio Protein Structure Prediction in <scp>CASP11</scp>. Proteins: Structure, Function and Bioinformatics, 2016, 84, 76-86.	1.5	63
69	Improving Protein Structure Prediction Using Multiple Sequence-Based Contact Predictions. Structure, 2011, 19, 1182-1191.	1.6	62
70	LS-align: an atom-level, flexible ligand structural alignment algorithm for high-throughput virtual screening. Bioinformatics, 2018, 34, 2209-2218.	1.8	62
71	EvoDesign: Designing Proteinâ€“Protein Binding Interactions Using Evolutionary Interface Profiles in Conjunction with an Optimized Physical Energy Function. Journal of Molecular Biology, 2019, 431, 2467-2476.	2.0	60
72	MetaGO: Predicting Gene Ontology of Non-homologous Proteins Through Low-Resolution Protein Structure Prediction and Proteinâ€“Protein Network Mapping. Journal of Molecular Biology, 2018, 430, 2256-2265.	2.0	58

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73	ATPbind: Accurate Proteinâ€“ATP Binding Site Prediction by Combining Sequence-Profiling and Structure-Based Comparisons. Journal of Chemical Information and Modeling, 2018, 58, 501-510.	2.5	57
74	FASPR: an open-source tool for fast and accurate protein side-chain packing. Bioinformatics, 2020, 36, 3758-3765.	1.8	54
75	Protein structure prediction using deep learning distance and hydrogenâ€bonding restraints in <scp>CASP14</scp>. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1734-1751.	1.5	53
76	Templateâ€based protein structure prediction in <scp>CASP11</scp> and retrospect of <scp>Iâ€TASSER</scp> in the last decade. Proteins: Structure, Function and Bioinformatics, 2016, 84, 233-246.	1.5	48
77	Detecting distant-homology protein structures by aligning deep neural-network based contact maps. PLoS Computational Biology, 2019, 15, e1007411.	1.5	45
78	EDock: blind proteinâ€“ligand docking by replica-exchange monte carlo simulation. Journal of Cheminformatics, 2020, 12, 37.	2.8	45
79	An Evolution-Based Approach to De Novo Protein Design and Case Study on Mycobacterium tuberculosis. PLoS Computational Biology, 2013, 9, e1003298.	1.5	44
80	EvoDesign: de novo protein design based on structural and evolutionary profiles. Nucleic Acids Research, 2013, 41, W273-W280.	6.5	44
81	FUpred: detecting protein domains through deep-learning-based contact map prediction. Bioinformatics, 2020, 36, 3749-3757.	1.8	44
82	Improving fragment-based ab initio protein structure assembly using low-accuracy contact-map predictions. Nature Communications, 2021, 12, 5011.	5.8	44
83	Ab Initio structure prediction for Escherichia coli: towards genome-wide protein structure modeling and fold assignment. Scientific Reports, 2013, 3, 1895.	1.6	43
84	SSIPe: accurately estimating proteinâ€“protein binding affinity change upon mutations using evolutionary profiles in combination with an optimized physical energy function. Bioinformatics, 2020, 36, 2429-2437.	1.8	42
85	I-TASSER-MR: automated molecular replacement for distant-homology proteins using iterative fragment assembly and progressive sequence truncation. Nucleic Acids Research, 2017, 45, W429-W434.	6.5	37
86	Potential of Three Ethnomedicinal Plants as Antisickling Agents. Molecular Pharmaceutics, 2017, 14, 172-182.	2.3	37
87	CGLFold: a contact-assistedde novoprotein structure prediction using global exploration and loop perturbation sampling algorithm. Bioinformatics, 2020, 36, 2443-2450.	1.8	36
88	Computational Protein Design and Large-Scale Assessment by I-TASSER Structure Assembly Simulations. Journal of Molecular Biology, 2011, 407, 764-776.	2.0	34
89	Improving Protein Template Recognition by Using Small-Angle X-Ray Scattering Profiles. Biophysical Journal, 2011, 101, 2770-2781.	0.2	33
90	CR-I-TASSER: assemble protein structures from cryo-EM density maps using deep convolutional neural networks. Nature Methods, 2022, 19, 195-204.	9.0	33

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91	LabCaS: Labeling calpain substrate cleavage sites from amino acid sequence using conditional random fields. Proteins: Structure, Function and Bioinformatics, 2013, 81, 622-634.	1.5	29
92	Fueling ab initio folding with marine metagenomics enables structure and function predictions of new protein families. Genome Biology, 2019, 20, 229.	3.8	28
93	Structure and Protein Interaction-Based Gene Ontology Annotations Reveal Likely Functions of Uncharacterized Proteins on Human Chromosome 17. Journal of Proteome Research, 2018, 17, 4186-4196.	1.8	27
94	Identifying the Zoonotic Origin of SARS-CoV-2 by Modeling the Binding Affinity between the Spike Receptor-Binding Domain and Host ACE2. Journal of Proteome Research, 2020, 19, 4844-4856.	1.8	27
95	A New Protocol for Atomic-Level Protein Structure Modeling and Refinement Using Low-to-Medium Resolution Cryo-EM Density Maps. Journal of Molecular Biology, 2020, 432, 5365-5377.	2.0	26
96	Exploring the speed and performance of molecular replacement withAMPLEusingQUARK ab initioprotein models. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 338-343.	2.5	25
97	ThreaDomEx: a unified platform for predicting continuous and discontinuous protein domains by multiple-threading and segment assembly. Nucleic Acids Research, 2017, 45, W400-W407.	6.5	25
98	Progressive assembly of multi-domain protein structures from cryo-EM density maps. Nature Computational Science, 2022, 2, 265-275.	3.8	25
99	Functions of Essential Genes and a Scale-Free Protein Interaction Network Revealed by Structure-Based Function and Interaction Prediction for a Minimal Genome. Journal of Proteome Research, 2021, 20, 1178-1189.	1.8	23
100	Protein interâ€residue contact and distance prediction by coupling complementary coevolution features with deep residual networks in <scp>CASP14</scp>. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1911-1921.	1.5	23
101	Improving accuracy of protein contact prediction using balanced network deconvolution. Proteins: Structure, Function and Bioinformatics, 2015, 83, 485-496.	1.5	22
102	Underestimation-Assisted Global-Local Cooperative Differential Evolution and the Application to Protein Structure Prediction. IEEE Transactions on Evolutionary Computation, 2019, 24, 1-1.	7.5	22
103	MMpred: a distance-assisted multimodal conformation sampling for de novo protein structure prediction. Bioinformatics, 2021, 37, 4350-4356.	1.8	22
104	Artificial intelligence-based multi-objective optimization protocol for protein structure refinement. Bioinformatics, 2020, 36, 437-448.	1.8	21
105	Endoplasmic reticulumâ€“associated degradation is required for nephrin maturation and kidney glomerular filtration function. Journal of Clinical Investigation, 2021, 131, .	3.9	21
106	Mechanism for DPY30 and ASH2L intrinsically disordered regions to modulate the MLL/SET1 activity on chromatin. Nature Communications, 2021, 12, 2953.	5.8	21
107	Blinded Testing of Function Annotation for uPE1 Proteins by I-TASSER/COFACTOR Pipeline Using the 2018â€“2019 Additions to neXtProt and the CAFA3 Challenge. Journal of Proteome Research, 2019, 18, 4154-4166.	1.8	20
108	DAMpred: Recognizing Disease-Associated nsSNPs through Bayes-Guided Neural-Network Model Built on Low-Resolution Structure Prediction of Proteins and Proteinâ€“Protein Interactions. Journal of Molecular Biology, 2019, 431, 2449-2459.	2.0	19

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109	Virtual Screening of Human Class-A GPCRs Using Ligand Profiles Built on Multiple Ligandâ€“Receptor Interactions. Journal of Molecular Biology, 2020, 432, 4872-4890.	2.0	19
110	Computational design of SARS-CoV-2 spike glycoproteins to increase immunogenicity by T cell epitope engineering. Computational and Structural Biotechnology Journal, 2021, 19, 518-529.	1.9	19
111	Landscape of variable domain of heavyâ€chainâ€only antibody repertoire from alpaca. Immunology, 2020, 161, 53-65.	2.0	17
112	The Human DNA Mismatch Repair Protein MSH3 Contains Nuclear Localization and Export Signals That Enable Nuclear-Cytosolic Shuttling in Response to Inflammation. Molecular and Cellular Biology, 2020, 40, .	1.1	17
113	LOMETS3: integrating deep learning and profile alignment for advanced protein template recognition and function annotation. Nucleic Acids Research, 2022, 50, W454-W464.	6.5	17
114	Structure and Location of the Regulatory Î² Subunits in the (Î±Î²Î³Î´)4 Phosphorylase Kinase Complex. Journal of Biological Chemistry, 2012, 287, 36651-36661.	1.6	16
115	Changing the Apoptosis Pathway through Evolutionary Protein Design. Journal of Molecular Biology, 2019, 431, 825-841.	2.0	16
116	Toward the Accuracy and Speed of Protein Side-Chain Packing: AÂSystematic Study on Rotamer Libraries. Journal of Chemical Information and Modeling, 2020, 60, 410-420.	2.5	15
117	ADDRESS: A Database of Disease-associated Human Variants Incorporating Protein Structure and Folding Stabilities. Journal of Molecular Biology, 2021, 433, 166840.	2.0	15
118	DEMO2: Assemble multi-domain protein structures by coupling analogous template alignments with deep-learning inter-domain restraint prediction. Nucleic Acids Research, 2022, 50, W235-W245.	6.5	15
119	Structural Bioinformatics Inspection of neXtProt PE5 Proteins in the Human Proteome. Journal of Proteome Research, 2015, 14, 3750-3761.	1.8	13
120	Decoding the link of microbiome niches with homologous sequences enables accurately targeted protein structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	12
121	Accurate multistage prediction of protein crystallization propensity using deep-cascade forest with sequence-based features. Briefings in Bioinformatics, 2021, 22, .	3.2	11
122	Detecting Gene Ontology misannotations using taxon-specific rate ratio comparisons. Bioinformatics, 2020, 36, 4383-4388.	1.8	10
123	Identification of 13 Guanidinobenzoyl- or Aminidinobenzoyl-Containing Drugs to Potentially Inhibit TMPRSS2 for COVID-19 Treatment. International Journal of Molecular Sciences, 2021, 22, 7060.	1.8	10
124	Crystal structure of designed PX domain from cytokine-independent survival kinase and implications on evolution-based protein engineering. Journal of Structural Biology, 2015, 191, 197-206.	1.3	9
125	Using iterative fragment assembly and progressive sequence truncation to facilitate phasing and crystal structure determination of distantly related proteins. Acta Crystallographica Section D: Structural Biology, 2016, 72, 616-628.	1.1	9
126	Integrating Multimeric Threading With High-throughput Experiments for Structural Interactome of Escherichia coli. Journal of Molecular Biology, 2021, 433, 166944.	2.0	9

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127	Deep learning geometrical potential for high-accuracy ab initio protein structure prediction. IScience, 2022, 25, 104425.	1.9	7
128	Approaches toab initiomolecular replacement of Î±-helical transmembrane proteins. Acta Crystallographica Section D: Structural Biology, 2017, 73, 985-996.	1.1	6
129	Fitting Low-Resolution Protein Structures into Cryo-EM Density Maps by Multiobjective Optimization of Global and Local Correlations. Journal of Physical Chemistry B, 2021, 125, 528-538.	1.2	4
130	Protein structural features predict responsiveness to pharmacological chaperone treatment for three lysosomal storage disorders. PLoS Computational Biology, 2021, 17, e1009370.	1.5	4
131	The structure of the large regulatory Î± subunit of phosphorylase kinase examined by modeling and hydrogenâ€deuterium exchange. Protein Science, 2018, 27, 472-484.	3.1	3
132	RTL8 promotes nuclear localization of UBQLN2 to subnuclear compartments associated with protein quality control. Cellular and Molecular Life Sciences, 2022, 79, 176.	2.4	3
133	MR-REX: molecular replacement by cooperative conformational search and occupancy optimization on low-accuracy protein models. Acta Crystallographica Section D: Structural Biology, 2018, 74, 606-620.	1.1	2
134	Function Prediction for G Protein-Coupled Receptors through Text Mining and Induction Matrix Completion. ACS Omega, 2019, 4, 3045-3054.	1.6	2
135	Accurate flexible refinement for atomic-level protein structure using cryo-EM density maps and deep learning. Briefings in Bioinformatics, 2022, , .	3.2	2