

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Steered molecular dynamics and mechanical functions of proteins. Current Opinion in Structural Biology, 2001, 11, 224-230.	5.7	934
2	Structure and functional significance of mechanically unfolded fibronectin type III1 intermediates. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 14784-14789.	7.1	187
3	How the headpiece hinge angle is opened: new insights into the dynamics of integrin activation. Journal of Cell Biology, 2006, 175, 349-360.	5.2	181
4	Identifying Unfolding Intermediates of FN-III10 by Steered Molecular Dynamics. Journal of Molecular Biology, 2002, 323, 939-950.	4.2	159
5	DBD-Hunter: a knowledge-based method for the prediction of DNA–protein interactions. Nucleic Acids Research, 2008, 36, 3978-3992.	14.5	142
6	Structural space of protein–protein interfaces is degenerate, close to complete, and highly connected. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 22517-22522.	7.1	133
7	AF2Complex predicts direct physical interactions in multimeric proteins with deep learning. Nature Communications, 2022, 13, 1744.	12.8	128
8	Steered Molecular Dynamics Studies of Titin I1 Domain Unfolding. Biophysical Journal, 2002, 83, 3435-3445.	0.5	111
9	APoc: large-scale identification of similar protein pockets. Bioinformatics, 2013, 29, 597-604.	4.1	109
10	AlphaFold 2: Why It Works and Its Implications for Understanding the Relationships of Protein Sequence, Structure, and Function. Journal of Chemical Information and Modeling, 2021, 61, 4827-4831.	5.4	109
11	A Comprehensive Survey of Small-Molecule Binding Pockets in Proteins. PLoS Computational Biology, 2013, 9, e1003302.	3.2	103
12	Insights into Disease-Associated Mutations in the Human Proteome through Protein Structural Analysis. Structure, 2015, 23, 1362-1369.	3.3	103
13	Tuning the Mechanical Stability of Fibronectin Type III Modules through Sequence Variations. Structure, 2004, 12, 21-30.	3.3	98
14	Comprehensive prediction of drug-protein interactions and side effects for the human proteome. Scientific Reports, 2015, 5, 11090.	3.3	90
15	The distribution of ligand-binding pockets around protein-protein interfaces suggests a general mechanism for pocket formation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 3784-3789.	7.1	82
16	iAlign: a method for the structural comparison of protein–protein interfaces. Bioinformatics, 2010, 26, 2259-2265.	4.1	81
17	Molecular mechanisms of cellular mechanics. Physical Chemistry Chemical Physics, 2006, 8, 3692.	2.8	76
18	Structural Insights into How the MIDAS Ion Stabilizes Integrin Binding to an RGD Peptide under Force. Structure, 2004, 12, 2049-2058.	3.3	75

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19	A Threading-Based Method for the Prediction of DNA-Binding Proteins with Application to the Human Genome. PLoS Computational Biology, 2009, 5, e1000567.	3.2	74
20	Mechanical Strength of the Titin Z1Z2-Telethonin Complex. Structure, 2006, 14, 497-509.	3.3	70
21	Unfolding of titin domains studied by molecular dynamics simulations. Journal of Muscle Research and Cell Motility, 2002, 23, 513-521.	2.0	61
22	Interplay of physics and evolution in the likely origin of protein biochemical function. Proceedings of the United States of America, 2013, 110, 9344-9349.	7.1	59
23	Brain activity patterns in high-throughput electrophysiology screen predict bothÂdrug efficacies and side effects. Nature Communications, 2018, 9, 219.	12.8	55
24	Simulated Refolding of Stretched Titin Immunoglobulin Domains. Biophysical Journal, 2001, 81, 2268-2277.	0.5	48
25	DESTINI: A deep-learning approach to contact-driven protein structure prediction. Scientific Reports, 2019, 9, 3514.	3.3	44
26	From Nonspecific DNA–Protein Encounter Complexes to the Prediction of DNA–Protein Interactions. PLoS Computational Biology, 2009, 5, e1000341.	3.2	32
27	Large Scale Simulation of Protein Mechanics and Function. Advances in Protein Chemistry, 2003, 66, 195-247.	4.4	31
28	New benchmark metrics for proteinâ€protein docking methods. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1623-1634.	2.6	31
29	Repurposing FDA-approved drugs for anti-aging therapies. Biogerontology, 2016, 17, 907-920.	3.9	31
30	On the possible origin of protein homochirality, structure, and biochemical function. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26571-26579.	7.1	30
31	Are predicted protein structures of any value for binding site prediction and virtual ligand screening?. Current Opinion in Structural Biology, 2013, 23, 191-197.	5.7	29
32	Implications of the small number of distinct ligand binding pockets in proteins for drug discovery, evolution and biochemical function. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1163-1170.	2.2	27
33	The crystal structure of a tetrahydrofolate-bound dihydrofolate reductase reveals the origin of slow product release. Communications Biology, 2018, 1, 226.	4.4	23
34	ENTPRISE: An Algorithm for Predicting Human Disease-Associated Amino Acid Substitutions from Sequence Entropy and Predicted Protein Structures. PLoS ONE, 2016, 11, e0150965.	2.5	23
35	ENTPRISE-X: Predicting disease-associated frameshift and nonsense mutations. PLoS ONE, 2018, 13, e0196849.	2.5	20
36	A novel sequence alignment algorithm based on deep learning of the protein folding code. Bioinformatics, 2021, 37, 490-496.	4.1	19

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37	Onset of Anthrax Toxin Pore Formation. Biophysical Journal, 2006, 90, 3267-3279.	0.5	17
38	Why not consider a spherical protein? Implications of backbone hydrogen bonding for protein structure and function. Physical Chemistry Chemical Physics, 2011, 13, 17044.	2.8	16
39	Repurposed FDA-approved drugs targeting genes influencing aging can extend lifespan and healthspan in rotifers. Biogerontology, 2018, 19, 145-157.	3.9	16
40	Hurt, tired and queasy: Specific variants in the ATPase domain of the TRAP1 mitochondrial chaperone are associated with common, chronic "functional―symptomatology including pain, fatigue and gastrointestinal dysmotility. Mitochondrion, 2015, 23, 64-70.	3.4	15
41	The role of local versus nonlocal physicochemical restraints in determining protein native structure. Current Opinion in Structural Biology, 2021, 68, 1-8.	5.7	14
42	PSiFR: an integrated resource for prediction of protein structure and function. Bioinformatics, 2010, 26, 687-688.	4.1	13
43	On the Role of Physics and Evolution in Dictating Protein Structure and Function. Israel Journal of Chemistry, 2014, 54, 1176-1188.	2.3	10
44	How special is the biochemical function of native proteins?. F1000Research, 2016, 5, 207.	1.6	9
45	High-Performance Deep Learning Toolbox for Genome-Scale Prediction of Protein Structure and Function. , 2021, 2021, 46-57.		8
46	Integrin Activation In Vivo and In Silico. Structure, 2004, 12, 2096-2098.	3.3	7
47	Differential kinase activity of ACVR1 G328V and R206H mutations with implications to possible TβRI cross-talk in diffuse intrinsic pontine glioma. Scientific Reports, 2020, 10, 6140.	3.3	5
48	A General Framework to Learn Tertiary Structure for Protein Sequence Characterization. Frontiers in Bioinformatics, 2021, 1, .	2.1	3
49	On the emergence of homochirality and life itself. Biochemist, 2021, 43, 4-12.	0.5	2

50 Unfolding of titin domains studied by molecular dynamics simulations. , 2003, , 513-521.