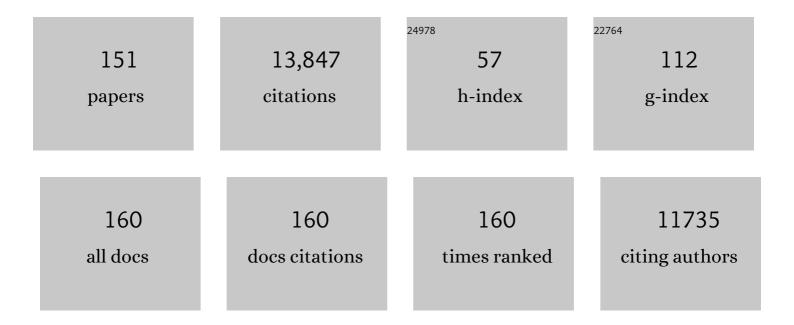
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	CACHE (Critical Assessment of Computational Hit-finding Experiments): A public–private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	13.8	22
2	MecCog: a knowledge representation framework for genetic disease mechanism. Bioinformatics, 2021, 37, 4180-4186.	1.8	1
3	Modeling SARSâ€CoVâ€2 proteins in the CASPâ€commons experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1987-1996.	1.5	24
4	Computational models in the service of Xâ€ray and <scp>cryoâ€</scp> electron microscopy structure determination. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1633-1646.	1.5	37
5	Target highlights in <scp>CASP14</scp> : Analysis of models by structure providers. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1647-1672.	1.5	27
6	Critical assessment of methods of protein structure prediction (CASP)—Round <scp>XIV</scp> . Proteins: Structure, Function and Bioinformatics, 2021, 89, 1607-1617.	1.5	281
7	Matching whole genomes to rare genetic disorders: Identification of potential causative variants using phenotypeâ€weighted knowledge in the CAGI SickKids5 clinical genomes challenge. Human Mutation, 2020, 41, 347-362.	1.1	4
8	CAGI SickKids challenges: Assessment of phenotype and variant predictions derived from clinical and genomic data of children with undiagnosed diseases. Human Mutation, 2019, 40, 1373-1391.	1.1	10
9	Assessing computational predictions of the phenotypic effect of cystathionineâ€betaâ€synthase variants. Human Mutation, 2019, 40, 1530-1545.	1.1	5
10	Assessment of predicted enzymatic activity of α― <i>N</i> â€acetylglucosaminidase variants of unknown significance for CAGI 2016. Human Mutation, 2019, 40, 1519-1529.	1.1	10
11	Performance of computational methods for the evaluation of pericentriolar material 1 missense variants in CAGlâ€5. Human Mutation, 2019, 40, 1474-1485.	1.1	8
12	Back Cover, Volume 40, Issue 9. Human Mutation, 2019, 40, ii.	1.1	0
13	Critical assessment of methods of protein structure prediction (CASP)—Round XIII. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1011-1020.	1.5	380
14	Target highlights in CASP13: Experimental target structures through the eyes of their authors. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1037-1057.	1.5	12
15	Assessment of methods for predicting the effects of PTEN and TPMT protein variants. Human Mutation, 2019, 40, 1495-1506.	1.1	16
16	Predicting venous thromboembolism risk from exomes in the Critical Assessment of Genome Interpretation (CAGI) challenges. Human Mutation, 2019, 40, 1314-1320.	1.1	10
17	Assessment of patient clinical descriptions and pathogenic variants from gene panel sequences in the CACIâ€5 intellectual disability challenge. Human Mutation, 2019, 40, 1330-1345.	1.1	11
18	Cover Image, Volume 87, Issue 12. Proteins: Structure, Function and Bioinformatics, 2019, 87, C4.	1.5	0

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19	latrogenic hypertension: a bioinformatic analysis. Pharmacogenomics Journal, 2019, 19, 337-346.	0.9	4
20	Target highlights from the first postâ€PSI CASP experiment (CASP12, May–August 2016). Proteins: Structure, Function and Bioinformatics, 2018, 86, 27-50.	1.5	11
21	A tribute to Anna Tramontano (1957–2017). Proteins: Structure, Function and Bioinformatics, 2018, 86, 5-6.	1.5	1
22	Critical assessment of methods of protein structure prediction (CASP)—Round XII. Proteins: Structure, Function and Bioinformatics, 2018, 86, 7-15.	1.5	296
23	Evaluation of the templateâ€based modeling in <scp>CASP12</scp> . Proteins: Structure, Function and Bioinformatics, 2018, 86, 321-334.	1.5	61
24	Harnessing formal concepts of biological mechanism to analyze human disease. PLoS Computational Biology, 2018, 14, e1006540.	1.5	14
25	The Product Guides the Process: Discovering Disease Mechanisms. Studies in Applied Philosophy, Epistemology and Rational Ethics, 2018, , 101-117.	0.2	4
26	Determination of disease phenotypes and pathogenic variants from exome sequence data in the CAGI 4 gene panel challenge. Human Mutation, 2017, 38, 1201-1216.	1.1	5
27	Performance of in silico tools for the evaluation of p16INK4a (CDKN2A) variants in CAGI. Human Mutation, 2017, 38, 1042-1050.	1.1	13
28	CAGI4 SickKids clinical genomes challenge: A pipeline for identifying pathogenic variants. Human Mutation, 2017, 38, 1169-1181.	1.1	11
29	CACI4 Crohn's exome challenge: Marker SNP versus exome variant models for assigning risk of Crohn disease. Human Mutation, 2017, 38, 1225-1234.	1.1	15
30	Working toward precision medicine: Predicting phenotypes from exomes in the Critical Assessment of Genome Interpretation (CAGI) challenges. Human Mutation, 2017, 38, 1182-1192.	1.1	39
31	Ensemble variant interpretation methods to predict enzyme activity and assign pathogenicity in the CACl4 <i>NAGLU</i> (Human Nâ€acetylâ€glucosaminidase) and <i>UBE2I</i> (Human SUMOâ€ligase) challenges. Human Mutation, 2017, 38, 1109-1122.	1.1	14
32	Matching phenotypes to whole genomes: Lessons learned from four iterations of the personal genome project community challenges. Human Mutation, 2017, 38, 1266-1276.	1.1	14
33	Reply to HU et al.: On the interpretation of gasdermin-B expression quantitative trait loci data. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E7863-E7864.	3.3	0
34	Reports from CAGI: The Critical Assessment of Genome Interpretation. Human Mutation, 2017, 38, 1039-1041.	1.1	38
35	Lessons from the CAGIâ€4 Hopkins clinical panel challenge. Human Mutation, 2017, 38, 1155-1168.	1.1	6
36	Mapping genetic variations to three-dimensional protein structures to enhance variant interpretation: a proposed framework. Genome Medicine, 2017, 9, 113.	3.6	47

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37	Critical assessment of methods of protein structure prediction: Progress and new directions in round XI. Proteins: Structure, Function and Bioinformatics, 2016, 84, 4-14.	1.5	198
38	Some of the most interesting <scp>CASP</scp> 11 targets through the eyes of their authors. Proteins: Structure, Function and Bioinformatics, 2016, 84, 34-50.	1.5	16
39	Consensus Genome-Wide Expression Quantitative Trait Loci and Their Relationship with Human Complex Trait Disease. OMICS A Journal of Integrative Biology, 2016, 20, 400-414.	1.0	46
40	Cover Image, Volume 84, Issue S1. Proteins: Structure, Function and Bioinformatics, 2016, 84, C1-C1.	1.5	2
41	Cover Image, Volume 84, Issue S1. Proteins: Structure, Function and Bioinformatics, 2016, 84, C4.	1.5	13
42	A bacteriophage endolysin that eliminates intracellular streptococci. ELife, 2016, 5, .	2.8	64
43	Insights from GWAS: emerging landscape of mechanisms underlying complex trait disease. BMC Genomics, 2015, 16, S4.	1.2	16
44	Increasing the stability of the bacteriophage endolysin PlyC using rationale-based FoldX computational modeling. Protein Engineering, Design and Selection, 2015, 28, 85-92.	1.0	32
45	Genetic Basis of Common Human Disease: Insight into the Role of Missense SNPs from Genome-Wide Association Studies. Journal of Molecular Biology, 2015, 427, 2271-2289.	2.0	44
46	Critical assessment of methods of protein structure prediction (CASP) — round x. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1-6.	1.5	366
47	Assessment of protein disorder region predictions in CASP10. Proteins: Structure, Function and Bioinformatics, 2014, 82, 127-137.	1.5	140
48	Challenging the state of the art in protein structure prediction: Highlights of experimental target structures for the 10th Critical Assessment of Techniques for Protein Structure Prediction Experiment CASP10. Proteins: Structure, Function and Bioinformatics, 2014, 82, 26-42.	1.5	53
49	CASP10 results compared to those of previous CASP experiments. Proteins: Structure, Function and Bioinformatics, 2014, 82, 164-174.	1.5	91
50	GWAS and drug targets. BMC Genomics, 2014, 15, S5.	1.2	56
51	Neighbor Overlap Is Enriched in the Yeast Interaction Network: Analysis and Implications. PLoS ONE, 2012, 7, e39662.	1.1	2
52	Protein stability and <i>in vivo</i> concentration of missense mutations in phenylalanine hydroxylase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 61-70.	1.5	29
53	Genetic basis of common human disease: insight into the role of nonsynonymous SNPs from genome-wide association studies. Genome Biology, 2011, 12, .	13.9	0
54	Structural and Functional Impact of Cancer-Related Missense Somatic Mutations. Journal of Molecular Biology, 2011, 413, 495-512.	2.0	35

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55	Protein Characterization of a Candidate Mechanism SNP for Crohn's Disease: The Macrophage Stimulating Protein R689C Substitution. PLoS ONE, 2011, 6, e27269.	1.1	24
56	Evaluation of disorder predictions in CASP9. Proteins: Structure, Function and Bioinformatics, 2011, 79, 107-118.	1.5	102
57	CASP9 results compared to those of previous casp experiments. Proteins: Structure, Function and Bioinformatics, 2011, 79, 196-207.	1.5	91
58	Target highlights in CASP9: Experimental target structures for the critical assessment of techniques for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2011, 79, 6-20.	1.5	19
59	Critical assessment of methods of protein structure prediction (CASP)—round IX. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1-5.	1.5	187
60	Composition bias and the origin of ORFan genes. Bioinformatics, 2010, 26, 996-999.	1.8	16
61	Structural Basis for the Mechanism and Substrate Specificity of Glycocyamine Kinase, a Phosphagen Kinase Family Member [,] . Biochemistry, 2010, 49, 2031-2041.	1.2	22
62	Stochastic noise in splicing machinery. Nucleic Acids Research, 2009, 37, 4873-4886.	6.5	157
63	Structural implication of splicing stochastics. Nucleic Acids Research, 2009, 37, 4862-4872.	6.5	31
64	Evaluation of templateâ€based models in CASP8 with standard measures. Proteins: Structure, Function and Bioinformatics, 2009, 77, 18-28.	1.5	114
65	CASP8 results in context of previous experiments. Proteins: Structure, Function and Bioinformatics, 2009, 77, 217-228.	1.5	38
66	Critical assessment of methods of protein structure prediction—Round VIII. Proteins: Structure, Function and Bioinformatics, 2009, 77, 1-4.	1.5	229
67	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. Nature Reviews Drug Discovery, 2009, 8, 455-463.	21.5	260
68	A survey of proteins encoded by non-synonymous single nucleotide polymorphisms reveals a significant fraction with altered stability and activity. Biochemical Journal, 2009, 424, 15-26.	1.7	43
69	Comparative Modeling in Structural Genomics. Structure, 2008, 16, 14-16.	1.6	25
70	Flexibility of Aromatic Residues in the Active-Site Gorge of Acetylcholinesterase: X-ray versus Molecular Dynamics. Biophysical Journal, 2008, 95, 2500-2511.	0.2	104
71	Proteopedia - a scientific 'wiki' bridging the rift between 3D structure and function of biomacromolecules. Genome Biology, 2008, 9, R121.	13.9	98
72	Comparative Modeling in Structural Genomics. , 2008, , 121-134.		2

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73	Critical assessment of methods of protein structure prediction—Round VII. Proteins: Structure, Function and Bioinformatics, 2007, 69, 3-9.	1.5	199
74	Progress from CASP6 to CASP7. Proteins: Structure, Function and Bioinformatics, 2007, 69, 194-207.	1.5	60
75	Rigorous performance evaluation in protein structure modelling and implications for computational biology. Philosophical Transactions of the Royal Society B: Biological Sciences, 2006, 361, 453-458.	1.8	34
76	Identification and Analysis of Deleterious Human SNPs. Journal of Molecular Biology, 2006, 356, 1263-1274.	2.0	237
77	Towards computing with proteins. Proteins: Structure, Function and Bioinformatics, 2006, 63, 53-64.	1.5	87
78	Detection of operons. Proteins: Structure, Function and Bioinformatics, 2006, 64, 615-628.	1.5	14
79	Outcome of a Workshop on Archiving Structural Models of Biological Macromolecules. Structure, 2006, 14, 1211-1217.	1.6	60
80	SNPs3D: candidate gene and SNP selection for association studies. BMC Bioinformatics, 2006, 7, 166.	1.2	383
81	A decade of CASP: progress, bottlenecks and prognosis in protein structure prediction. Current Opinion in Structural Biology, 2005, 15, 285-289.	2.6	435
82	Critical assessment of methods of protein structure prediction (CASP)—Round 6. Proteins: Structure, Function and Bioinformatics, 2005, 61, 3-7.	1.5	162
83	Progress over the first decade of CASP experiments. Proteins: Structure, Function and Bioinformatics, 2005, 61, 225-236.	1.5	172
84	The psychrophilic lifestyle as revealed by the genome sequence of Colwellia psychrerythraea 34H through genomic and proteomic analyses. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 10913-10918.	3.3	529
85	Loss of Protein Structure Stability as a Major Causative Factor in Monogenic Disease. Journal of Molecular Biology, 2005, 353, 459-473.	2.0	438
86	Protein Family Clustering for Structural Genomics. Journal of Molecular Biology, 2005, 353, 744-759.	2.0	27
87	Molecular modeling of protein function regions. Proteins: Structure, Function and Bioinformatics, 2004, 55, 942-961.	1.5	43
88	CAPRI: A Critical Assessment of PRedicted Interactions. Proteins: Structure, Function and Bioinformatics, 2003, 52, 2-9.	1.5	586
89	Three-dimensional structural location and molecular functional effects of missense SNPs in the T cell receptor V? domain. Proteins: Structure, Function and Bioinformatics, 2003, 53, 748-757.	1.5	25
90	Assessment of progress over the CASP experiments. Proteins: Structure, Function and Bioinformatics, 2003, 53, 585-595.	1.5	110

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91	Evaluation of disorder predictions in CASP5. Proteins: Structure, Function and Bioinformatics, 2003, 53, 561-565.	1.5	90
92	Critical assessment of methods of protein structure prediction (CASP)-round V. Proteins: Structure, Function and Bioinformatics, 2003, 53, 334-339.	1.5	221
93	The Significance of Performance Ranking in CASP—Response to Marti-Renom et al Structure, 2002, 10, 291-292.	1.6	5
94	A unifold, mesofold, and superfold model of protein fold use. Proteins: Structure, Function and Bioinformatics, 2002, 46, 61-71.	1.5	85
95	Assisting Functional Assignment for Hypothetical Heamophilus influenzae Gene Products through Structural Genomics. Current Drug Targets Infectious Disorders, 2002, 2, 339-353.	2.1	7
96	Processing and evaluation of predictions in CASP4. Proteins: Structure, Function and Bioinformatics, 2001, 45, 13-21.	1.5	131
97	Comparison of performance in successive CASP experiments. Proteins: Structure, Function and Bioinformatics, 2001, 45, 163-170.	1.5	62
98	Critical assessment of methods of protein structure prediction (CASP): Round IV. Proteins: Structure, Function and Bioinformatics, 2001, 45, 2-7.	1.5	146
99	SNPs, protein structure, and disease. Human Mutation, 2001, 17, 263-270.	1.1	649
100	Completeness in structural genomics. Nature Structural Biology, 2001, 8, 559-566.	9.7	336
101	We need both computer models and experiments. Nature, 2001, 409, 558-558.	13.7	13
102	From fold to function. Current Opinion in Structural Biology, 2000, 10, 384-389.	2.6	72
103	Local electrostatic optimization in proteins. Protein Engineering, Design and Selection, 1999, 12, 727-735.	1.0	4
104	Predicting protein three-dimensional structure. Current Opinion in Biotechnology, 1999, 10, 583-588.	3.3	79
105	Low Frequency Motion in Proteins. Journal of Computational Physics, 1999, 151, 169-189.	1.9	27
106	Critical assessment of methods of protein structure prediction (CASP): Round III. Proteins: Structure, Function and Bioinformatics, 1999, 37, 2-6.	1.5	137
107	Processing and analysis of CASP3 protein structure predictions. Proteins: Structure, Function and Bioinformatics, 1999, 37, 22-29.	1.5	206
108	Some measures of comparative performance in the three CASPs. Proteins: Structure, Function and Bioinformatics, 1999, 37, 231-237.	1.5	39

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109	Processing and analysis of CASP3 protein structure predictions. Proteins: Structure, Function and Bioinformatics, 1999, 37, 22-29.	1.5	54
110	Critical assessment of methods of protein structure prediction (CASP): Round III. Proteins: Structure, Function and Bioinformatics, 1999, 37, 2-6.	1.5	27
111	Processing and analysis of CASP3 protein structure predictions. Proteins: Structure, Function and Bioinformatics, 1999, Suppl 3, 22-9.	1.5	142
112	Critical assessment of methods of protein structure prediction (CASP): Round III. , 1999, 37, 2.		103
113	Conformation of the sebacyl β1Lys82–β2Lys82 crosslink in T-state human hemoglobin. , 1998, 30, 309-320.		5
114	pKaShifts in Small Molecules and HIV Protease:Â Electrostatics and Conformation. Journal of the American Chemical Society, 1998, 120, 6138-6146.	6.6	55
115	An all-atom distance-dependent conditional probability discriminatory function for protein structure prediction 1 1Edited by F. Cohen. Journal of Molecular Biology, 1998, 275, 895-916.	2.0	429
116	A graph-theoretic algorithm for comparative modeling of protein structure. Journal of Molecular Biology, 1998, 279, 287-302.	2.0	133
117	Dielectric Screening Treatment of Electrostatic Solvation. Journal of Physical Chemistry B, 1997, 101, 11226-11236.	1.2	37
118	Protein folding simulations with genetic algorithms and a detailed molecular description. Journal of Molecular Biology, 1997, 269, 240-259.	2.0	128
119	Ab initio protein folding simulations with genetic algorithms: Simulations on the complete sequence of small proteins. Proteins: Structure, Function and Bioinformatics, 1997, 29, 179-184.	1.5	20
120	Critical assessment of methods of protein structure prediction (CASP): Round II. , 1997, 29, 2-6.		114
121	Handling context-sensitivity in protein structures using graph theory: Bona fide prediction. Proteins: Structure, Function and Bioinformatics, 1997, 29, 43-49.	1.5	15
122	Criteria for evaluating protein structures derived from comparative modeling. Proteins: Structure, Function and Bioinformatics, 1997, 29, 7-13.	1.5	28
123	Chaos in protein dynamics. Proteins: Structure, Function and Bioinformatics, 1997, 29, 417-425.	1.5	63
124	Ab initio protein folding simulations with genetic algorithms: Simulations on the complete sequence of small proteins. Proteins: Structure, Function and Bioinformatics, 1997, 29, 179-184.	1.5	5
125	Critical assessment of methods of protein structure prediction (CASP): Round II. Proteins: Structure, Function and Bioinformatics, 1997, 29, 2-6.	1.5	22
126	Ab initio protein folding simulations with genetic algorithms: Simulations on the complete sequence of small proteins. Proteins: Structure, Function and Bioinformatics, 1997, 29, 179-184.	1.5	2

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127	Critical assessment of methods of protein structure prediction (CASP): Round II. , 1997, 29, 2.		82
128	Chaos in protein dynamics. , 1997, 29, 417.		1
129	Chaos in protein dynamics. Proteins: Structure, Function and Bioinformatics, 1997, 29, 417-425.	1.5	2
130	Local Interactions Dominate Folding in a Simple Protein Model. Journal of Molecular Biology, 1996, 259, 988-994.	2.0	95
131	The current state of the art in protein structure prediction. Current Opinion in Biotechnology, 1996, 7, 422-427.	3.3	61
132	Determination of the conformation of folding initiation sites in proteins by computer simulation. Proteins: Structure, Function and Bioinformatics, 1995, 23, 129-141.	1.5	43
133	A large-scale experiment to assess protein structure prediction methods. Proteins: Structure, Function and Bioinformatics, 1995, 23, ii-iv.	1.5	440
134	Confronting the problem of interconnected structural changes in the comparative modeling of proteins. Proteins: Structure, Function and Bioinformatics, 1995, 23, 327-336.	1.5	25
135	Ab initio structure prediction for small polypeptides and protein fragments using genetic algorithms. Proteins: Structure, Function and Bioinformatics, 1995, 23, 454-460.	1.5	60
136	Structure, Dynamics and Energetics of Initiation Sites in Protein Folding: I. Analysis of a 1 ns Molecular Dynamics Trajectory of an Early Folding Unit in Water: The Helix I/Loop I-Fragment of Barnase. Journal of Molecular Biology, 1995, 250, 239-257.	2.0	11
137	Comparison of systematic search and database methods for constructing segments of protein structure. Protein Engineering, Design and Selection, 1994, 7, 953-960.	1.0	113
138	An accurate simulation of the protein Streptomyces griseus protease A. Journal of Molecular Graphics, 1993, 11, 62-63.	1.7	0
139	Troponin-C mutants with increased calcium affinity. FEBS Journal, 1993, 213, 599-604.	0.2	34
140	Finding the lowest free energy conformation of a protein is an NP-hard problem: Proof and implications. Bulletin of Mathematical Biology, 1993, 55, 1183-1198.	0.9	109
141	Genetic Algorithms for Protein Folding Simulations. Journal of Molecular Biology, 1993, 231, 75-81.	2.0	484
142	Protein design on computers. Five new proteins: Shpilka, grendel, fingerclasp, leather, and aida. Proteins: Structure, Function and Bioinformatics, 1992, 12, 105-110.	1.5	26
143	Docking by least-squares fitting of molecular surface patterns. Journal of Molecular Biology, 1992, 225, 849-858.	2.0	93
144	The crystal packing interactions of two different crystal forms of bovine Ribonuclease A. Journal of Crystal Growth, 1991, 110, 119-130.	0.7	14

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145	Analysis of the steric strain in the polypeptide backbone of protein molecules. Proteins: Structure, Function and Bioinformatics, 1991, 11, 223-229.	1.5	216
146	Comparative molecular model building of two serine proteinases from cytotoxic T lymphocytes. Proteins: Structure, Function and Bioinformatics, 1988, 4, 190-204.	1.5	78
147	[46] molecular structure of troponin C and its implications for the Ca2+ triggering of muscle contraction. Methods in Enzymology, 1987, 139, 610-632.	0.4	18
148	Crystal structure of demetallized concanavalin A: the metal-binding region. Journal of Molecular Biology, 1979, 131, 137-155.	2.0	57
149	The effect of binding of metal ions on the three-dimensional structure of demetallized concanavalin A. FEBS Letters, 1978, 95, 54-56.	1.3	8
150	Binding of divalent copper ions to aspartic acid residue 52 in hen egg-white lysozyme. Journal of Molecular Biology, 1974, 87, 357-368.	2.0	38
151	The identification by X-ray crystallography of the site of attachment of an affinity label to hen egg-white lysozyme. Journal of Molecular Biology, 1973, 75, 1-4.	2.0	41