## Janet M Thornton

List of Publications by Year in descending order

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408 papers 63,035 citations

110 h-index 239 g-index

541 all docs

541 docs citations

541 times ranked

58363 citing authors

#	Article	IF	CITATIONS
1	The rapid generation of mutation data matrices from protein sequences. Bioinformatics, 1992, 8, 275-282.	1.8	4,891
2	AQUA and PROCHECK-NMR: Programs for checking the quality of protein structures solved by NMR. Journal of Biomolecular NMR, 1996, 8, 477-86.	1.6	4,736
3	LIGPLOT: a program to generate schematic diagrams of protein-ligand interactions. Protein Engineering, Design and Selection, 1995, 8, 127-134.	1.0	4,648
4	Satisfying Hydrogen Bonding Potential in Proteins. Journal of Molecular Biology, 1994, 238, 777-793.	2.0	2,001
5	Stereochemical quality of protein structure coordinates. Proteins: Structure, Function and Bioinformatics, 1992, 12, 345-364.	1.5	1,436
6	Main-chain Bond Lengths and Bond Angles in Protein Structures. Journal of Molecular Biology, 1993, 231, 1049-1067.	2.0	1,142
7	Influence of proline residues on protein conformation. Journal of Molecular Biology, 1991, 218, 397-412.	2.0	1,071
8	Ribosomal Protein S6 Kinase 1 Signaling Regulates Mammalian Life Span. Science, 2009, 326, 140-144.	6.0	1,009
9	PROMOTIF—A program to identify and analyze structural motifs in proteins. Protein Science, 1996, 5, 212-220.	3.1	955
10	A revised set of potentials for βâ€turn formation in proteins. Protein Science, 1994, 3, 2207-2216.	3.1	918
10		3.1	918
	A revised set of potentials for βâ€ŧurn formation in proteins. Protein Science, 1994, 3, 2207-2216.		
11	A revised set of potentials for βâ€turn formation in proteins. Protein Science, 1994, 3, 2207-2216.  PDBsum: Structural summaries of PDB entries. Protein Science, 2018, 27, 129-134.  Metal ions in biological catalysis: from enzyme databases to general principles. Journal of Biological	3.1	910
11 12	A revised set of potentials for βâ€turn formation in proteins. Protein Science, 1994, 3, 2207-2216.  PDBsum: Structural summaries of PDB entries. Protein Science, 2018, 27, 129-134.  Metal ions in biological catalysis: from enzyme databases to general principles. Journal of Biological Inorganic Chemistry, 2008, 13, 1205-1218.	3.1	910
11 12 13	A revised set of potentials for βâ€turn formation in proteins. Protein Science, 1994, 3, 2207-2216.  PDBsum: Structural summaries of PDB entries. Protein Science, 2018, 27, 129-134.  Metal ions in biological catalysis: from enzyme databases to general principles. Journal of Biological Inorganic Chemistry, 2008, 13, 1205-1218.  Protein superfamilles and domain superfolds. Nature, 1994, 372, 631-634.  NEW EMBO MEMBER'S REVIEW: Diversity of protein-protein interactions. EMBO Journal, 2003, 22,	3.1 1.1 13.7	910 868 783
11 12 13	A revised set of potentials for βâ€turn formation in proteins. Protein Science, 1994, 3, 2207-2216.  PDBsum: Structural summaries of PDB entries. Protein Science, 2018, 27, 129-134.  Metal ions in biological catalysis: from enzyme databases to general principles. Journal of Biological Inorganic Chemistry, 2008, 13, 1205-1218.  Protein superfamilles and domain superfolds. Nature, 1994, 372, 631-634.  NEW EMBO MEMBER'S REVIEW: Diversity of protein-protein interactions. EMBO Journal, 2003, 22, 3486-3492.  Evolution of function in protein superfamilies, from a structural perspective 1 1Edited by A. R. Fersht.	3.1 1.1 13.7 3.5	910 868 783
11 12 13 14	A revised set of potentials for βâ€ŧurn formation in proteins. Protein Science, 1994, 3, 2207-2216.  PDBsum: Structural summaries of PDB entries. Protein Science, 2018, 27, 129-134.  Metal ions in biological catalysis: from enzyme databases to general principles. Journal of Biological Inorganic Chemistry, 2008, 13, 1205-1218.  Protein superfamilles and domain superfolds. Nature, 1994, 372, 631-634.  NEW EMBO MEMBER'S REVIEW: Diversity of protein-protein interactions. EMBO Journal, 2003, 22, 3486-3492.  Evolution of function in protein superfamilies, from a structural perspective 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 2001, 307, 1113-1143.  ππ interactions: the geometry and energetics of phenylalanine-phenylalanine interactions in proteins.	3.1 1.1 13.7 3.5	910 868 783 739

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19	One Fold with Many Functions: The Evolutionary Relationships between TIM Barrel Families Based on their Sequences, Structures and Functions. Journal of Molecular Biology, 2002, 321, 741-765.	2.0	568
20	The Catalytic Site Atlas: a resource of catalytic sites and residues identified in enzymes using structural data. Nucleic Acids Research, 2004, 32, 129D-133.	6.5	541
21	Structural Characterisation and Functional Significance of Transient Protein–Protein Interactions. Journal of Molecular Biology, 2003, 325, 991-1018.	2.0	537
22	PDBsum: a web-based database of summaries and analyses of all PDB structures. Trends in Biochemical Sciences, 1997, 22, 488-490.	3.7	536
23	An overview of the structures of protein-DNA complexes. Genome Biology, 2000, 1, reviews001.1.	13.9	531
24	Analysis of Catalytic Residues in Enzyme Active Sites. Journal of Molecular Biology, 2002, 324, 105-121.	2.0	529
25	Protein-protein interactions: A review of protein dimer structures. Progress in Biophysics and Molecular Biology, 1995, 63, 31-65.	1.4	507
26	Conformation of Î <sup>2</sup> -hairpins in protein structures. Journal of Molecular Biology, 1989, 206, 759-777.	2.0	490
27	Evidence for lifespan extension and delayed age–related biomarkers in insulin receptor substrate 1 null mice. FASEB Journal, 2008, 22, 807-818.	0.2	487
28	Antibody-antigen Interactions: Contact Analysis and Binding Site Topography. Journal of Molecular Biology, 1996, 262, 732-745.	2.0	456
29	Protein promiscuity and its implications for biotechnology. Nature Biotechnology, 2009, 27, 157-167.	9.4	434
30	Prediction of protein-protein interaction sites using patch analysis 1 1Edited by G. von Heijne. Journal of Molecular Biology, 1997, 272, 133-143.	2.0	411
31	CATH: comprehensive structural and functional annotations for genome sequences. Nucleic Acids Research, 2015, 43, D376-D381.	6.5	399
32	Protein-DNA interactions: a structural analysis. Journal of Molecular Biology, 1999, 287, 877-896.	2.0	397
33	Genome-wide Responses to Mitochondrial Dysfunction. Molecular Biology of the Cell, 2001, 12, 297-308.	0.9	391
34	Analysis of Main Chain Torsion Angles in Proteins: Prediction of NMR Coupling Constants for Native and Random Coil Conformations. Journal of Molecular Biology, 1996, 255, 494-506.	2.0	379
35	PDBsum more: new summaries and analyses of the known 3D structures of proteins and nucleic acids. Nucleic Acids Research, 2004, 33, D266-D268.	6.5	373
36	Predicting Protein Ligand Binding Sites by Combining Evolutionary Sequence Conservation and 3D Structure. PLoS Computational Biology, 2009, 5, e1000585.	1.5	356

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37	The SDR (short-chain dehydrogenase/reductase and related enzymes) nomenclature initiative. Chemico-Biological Interactions, 2009, 178, 94-98.	1.7	329
38	Amino/Aromatic Interactions in Proteins: Is the Evidence Stacked Against Hydrogen Bonding?. Journal of Molecular Biology, 1994, 239, 315-331.	2.0	319
39	Protein-protein interfaces: Analysis of amino acid conservation in homodimers. Proteins: Structure, Function and Bioinformatics, 2001, 42, 108-124.	1.5	299
40	Tess: A geometric hashing algorithm for deriving 3D coordinate templates for searching structural databases. Application to enzyme active sites. Protein Science, 1997, 6, 2308-2323.	3.1	297
41	PROTEIN FAMILIES AND THEIR EVOLUTION—A STRUCTURAL PERSPECTIVE. Annual Review of Biochemistry, 2005, 74, 867-900.	5.0	295
42	Buried waters and internal cavities in monomeric proteins. Protein Science, 1994, 3, 1224-1235.	3.1	293
43	Predicting protein function from sequence and structural data. Current Opinion in Structural Biology, 2005, 15, 275-284.	2.6	280
44	PDBsum additions. Nucleic Acids Research, 2014, 42, D292-D296.	6.5	279
45	The CATH domain structure database: new protocols and classification levels give a more comprehensive resource for exploring evolution. Nucleic Acids Research, 2007, 35, D291-D297.	6.5	274
46	Construction, Visualisation, and Clustering of Transcription Networks from Microarray Expression Data. PLoS Computational Biology, 2007, 3, e206.	1.5	261
47	Structural Families in Loops of Homologous Proteins: Automatic Classification, Modelling and Application to Antibodies. Journal of Molecular Biology, 1996, 263, 800-815.	2.0	257
48	Protein–DNA Interactions: Amino Acid Conservation and the Effects of Mutations on Binding Specificity. Journal of Molecular Biology, 2002, 320, 991-1009.	2.0	243
49	Prepublication data sharing. Nature, 2009, 461, 168-170.	13.7	243
50	Solvent-induced distortions and the curvature of α-helices. Nature, 1983, 306, 281-283.	13.7	235
51	Derivation of 3D coordinate templates for searching structural databases: Application to serâ€Hisâ€Asp catalytic triads in the serine proteinases and lipases. Protein Science, 1996, 5, 1001-1013.	3.1	229
52	From protein structure to function. Current Opinion in Structural Biology, 1999, 9, 374-382.	2.6	229
53	The CATH Domain Structure Database and related resources Gene3D and DHS provide comprehensive domain family information for genome analysis. Nucleic Acids Research, 2004, 33, D247-D251.	6.5	226
54	Intrinsic φ,Ï^ propensities of amino acids, derived from the coil regions of known structures. Nature Structural Biology, 1995, 2, 596-603.	9.7	225

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55	Mitochondria-to-Nuclear Signaling Is Regulated by the Subcellular Localization of the Transcription Factors Rtg1p and Rtg3p. Molecular Biology of the Cell, 2000, 11, 2103-2115.	0.9	223
56	Discriminating between homodimeric and monomeric proteins in the crystalline state. Proteins: Structure, Function and Bioinformatics, 2000, 41, 47-57.	1.5	217
57	Protein folds and functions. Structure, 1998, 6, 875-884.	1.6	207
58	The implications of alternative splicing in the ENCODE protein complement. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5495-5500.	3.3	206
59	Amino and carboxy-terminal regions in globular proteins. Journal of Molecular Biology, 1983, 167, 443-460.	2.0	198
60	The European dimension for the mouse genome mutagenesis program. Nature Genetics, 2004, 36, 925-927.	9.4	195
61	Protein Function Prediction Using Local 3D Templates. Journal of Molecular Biology, 2005, 351, 614-626.	2.0	195
62	BLEEP?potential of mean force describing protein-ligand interactions: I. Generating potential. Journal of Computational Chemistry, 1999, 20, 1165-1176.	1.5	194
63	From structure to function: approaches and limitations. Nature Structural Biology, 2000, 7, 991-994.	9.7	193
64	Identification, classification, and analysis of betaâ€bulges in proteins. Protein Science, 1993, 2, 1574-1590.	3.1	191
65	An algorithm for constraint-based structural template matching: application to 3D templates with statistical analysis. Bioinformatics, 2003, 19, 1644-1649.	1.8	191
66	Shape Variation in Protein Binding Pockets and their Ligands. Journal of Molecular Biology, 2007, 368, 283-301.	2.0	188
67	New functional families (FunFams) in CATH to improve the mapping of conserved functional sites to 3D structures. Nucleic Acids Research, 2012, 41, D490-D498.	6.5	188
68	Structural and Chemical Profiling of the Human Cytosolic Sulfotransferases. PLoS Biology, 2007, 5, e97.	2.6	187
69	The structural basis of allosteric regulation in proteins. FEBS Letters, 2009, 583, 1692-1698.	1.3	187
70	SIRIUS. Journal of Molecular Biology, 1990, 211, 595-615.	2.0	186
71	Using electrostatic potentials to predict DNA-binding sites on DNA-binding proteins. Nucleic Acids Research, 2003, 31, 7189-7198.	6.5	186
72	Determinants of strand register in antiparallel βâ€sheets of proteins. Protein Science, 1998, 7, 2287-2300.	3.1	182

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73	Protein function annotation by homology-based inference. Genome Biology, 2009, 10, 207.	13.9	182
74	A method for localizing ligand binding pockets in protein structures. Proteins: Structure, Function and Bioinformatics, 2005, 62, 479-488.	1.5	181
75	Understanding nature's catalytic toolkit. Trends in Biochemical Sciences, 2005, 30, 622-629.	3.7	177
76	The CATH classification revisited-architectures reviewed and new ways to characterize structural divergence in superfamilies. Nucleic Acids Research, 2009, 37, D310-D314.	6.5	174
77	Evolutionary conservation of regulated longevity assurance mechanisms. Genome Biology, 2007, 8, R132.	13.9	173
78	Validation of protein models derived from experiment. Current Opinion in Structural Biology, 1998, 8, 631-639.	2.6	172
79	Real spherical harmonic expansion coefficients as 3D shape descriptors for protein binding pocket and ligand comparisons. Bioinformatics, 2005, 21, 2347-2355.	1.8	170
80	The Catalytic Site Atlas 2.0: cataloging catalytic sites and residues identified in enzymes. Nucleic Acids Research, 2014, 42, D485-D489.	6.5	168
81	Using A Neural Network and Spatial Clustering to Predict the Location of Active Sites in Enzymes. Journal of Molecular Biology, 2003, 330, 719-734.	2.0	167
82	Deviations from Planarity of the Peptide Bond in Peptides and Proteins. Journal of Molecular Biology, 1996, 264, 1180-1195.	2.0	163
83	Protein folds, functions and evolution. Journal of Molecular Biology, 1999, 293, 333-342.	2.0	163
84	Lithium Promotes Longevity through GSK3/NRF2-Dependent Hormesis. Cell Reports, 2016, 15, 638-650.	2.9	163
85	Plasticity of enzyme active sites. Trends in Biochemical Sciences, 2002, 27, 419-426.	3.7	162
86	Conservation helps to identify biologically relevant crystal contacts. Journal of Molecular Biology, 2001, 313, 399-416.	2.0	159
87	Alpha plus beta folds revisited: some favoured motifs. Structure, 1993, 1, 105-120.	1.6	156
88	Conformational Changes Observed in Enzyme Crystal Structures upon Substrate Binding. Journal of Molecular Biology, 2005, 346, 21-28.	2.0	153
89	Mechanism and Catalytic Site Atlas (M-CSA): a database of enzyme reaction mechanisms and active sites. Nucleic Acids Research, 2018, 46, D618-D623.	6.5	151
90	Domain assignment for protein structures using a consensus approach: Characterization and analysis. Protein Science, 1998, 7, 233-242.	3.1	147

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91	Heme proteinsâ€"Diversity in structural characteristics, function, and folding. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2349-2368.	1.5	147
92	PoreWalker: A Novel Tool for the Identification and Characterization of Channels in Transmembrane Proteins from Their Three-Dimensional Structure. PLoS Computational Biology, 2009, 5, e1000440.	1.5	146
93	Elucidating Human Phosphatase-Substrate Networks. Science Signaling, 2013, 6, rs10.	1.6	145
94	Potential energy functions for threading. Current Opinion in Structural Biology, 1996, 6, 210-216.	2.6	144
95	Searching for functional sites in protein structures. Current Opinion in Chemical Biology, 2004, 8, 3-7.	2.8	138
96	Progress of Structural Genomics Initiatives: An Analysis of Solved Target Structures. Journal of Molecular Biology, 2005, 348, 1235-1260.	2.0	136
97	Quantifying the Similarities within Fold Space. Journal of Molecular Biology, 2002, 323, 909-926.	2.0	133
98	CATH: expanding the horizons of structure-based functional annotations for genome sequences. Nucleic Acids Research, 2019, 47, D280-D284.	6.5	131
99	Recognition of super-secondary structure in proteins. Journal of Molecular Biology, 1984, 173, 487-514.	2.0	128
100	Sequence and Structural Differences between Enzyme and Nonenzyme Homologs. Structure, 2002, 10, 1435-1451.	1.6	127
101	Extending CATH: increasing coverage of the protein structure universe and linking structure with function. Nucleic Acids Research, 2011, 39, D420-D426.	6.5	126
102	Protein Recognition of Adenylate: An Example of a Fuzzy Recognition Template. Journal of Molecular Biology, 1996, 263, 486-500.	2.0	125
103	Integrating mutation data and structural analysis of the TP53 tumor-suppressor protein. Human Mutation, 2002, 19, 149-164.	1.1	122
104	Retrograde Signaling Is Regulated by the Dynamic Interaction between Rtg2p and Mks1p. Molecular Cell, 2003, 12, 401-411.	4.5	122
105	Using a Library of Structural Templates to Recognise Catalytic Sites and Explore their Evolution in Homologous Families. Journal of Molecular Biology, 2005, 347, 565-581.	2.0	122
106	DamID in <i>C. elegans</i> reveals longevityâ€associated targets of DAFâ€16/FoxO. Molecular Systems Biology, 2010, 6, 399.	3.2	122
107	Small Molecule Subgraph Detector (SMSD) toolkit. Journal of Cheminformatics, 2009, 1, 12.	2.8	117
108	Understanding the Functional Roles of Amino Acid Residues in Enzyme Catalysis. Journal of Molecular Biology, 2009, 390, 560-577.	2.0	117

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109	Integrating Structure, Bioinformatics, and Enzymology to Discover Function. Journal of Biological Chemistry, 2003, 278, 26039-26045.	1.6	115
110	Evolution of protein function, from a structural perspective. Current Opinion in Chemical Biology, 1999, 3, 548-556.	2.8	114
111	Prediction of protein structure from amino acid sequence. Nature, 1978, 271, 15-20.	13.7	112
112	Prediction of the location and type of βâ€ŧurns in proteins using neural networks. Protein Science, 1999, 8, 1045-1055.	3.1	112
113	BLEEP?potential of mean force describing protein-ligand interactions: II. Calculation of binding energies and comparison with experimental data. Journal of Computational Chemistry, 1999, 20, 1177-1185.	1.5	112
114	Genomeâ€wide dFOXO targets and topology of the transcriptomic response to stress and insulin signalling. Molecular Systems Biology, 2011, 7, 502.	3.2	112
115	EC-BLAST: a tool to automatically search and compare enzyme reactions. Nature Methods, 2014, 11, 171-174.	9.0	112
116	Coordinated multitissue transcriptional and plasma metabonomic profiles following acute caloric restriction in mice. Physiological Genomics, 2006, 27, 187-200.	1.0	109
117	AlphaFold heralds a data-driven revolution in biology and medicine. Nature Medicine, 2021, 27, 1666-1669.	15.2	108
118	The impact of AlphaFold2 one year on. Nature Methods, 2022, 19, 15-20.	9.0	107
119	Protein Superfamily Evolution and the Last Universal Common Ancestor (LUCA). Journal of Molecular Evolution, 2006, 63, 513-525.	0.8	105
120	Longevity GWAS Using the <i>Drosophila </i> A Biological Sciences and Medical Sciences, 2015, 70, 1470-1478.	1.7	105
121	HERA—A program to draw schematic diagrams of protein secondary structures. Proteins: Structure, Function and Bioinformatics, 1990, 8, 203-212.	1.5	104
122	Structures of Nâ€termini of helices in proteins. Protein Science, 1997, 6, 147-155.	3.1	104
123	Towards an understanding of the arginine-aspartate interaction. Journal of Molecular Biology, 1992, 226, 251-262.	2.0	103
124	A Structure-based Anatomy of the E.coli Metabolome. Journal of Molecular Biology, 2003, 334, 697-719.	2.0	103
125	Conformational Diversity of Ligands Bound to Proteins. Journal of Molecular Biology, 2006, 356, 928-944.	2.0	103
126	Direct Keap1-Nrf2 disruption as a potential therapeutic target for Alzheimer's disease. PLoS Genetics, 2017, 13, e1006593.	1.5	102

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127	The evolution and structural anatomy of the small molecule metabolic pathways in Escherichia coli. Journal of Molecular Biology, 2001, 311, 693-708.	2.0	101
128	Protein structural topology: Automated analysis and diagrammatic representation. Protein Science, 1999, 8, 897-904.	3.1	101
129	Knowledge-based validation of protein structure coordinates derived by X-ray crystallography and NMR spectroscopy. Current Opinion in Structural Biology, 1994, 4, 731-737.	2.6	100
130	Analysis and prediction of carbohydrate binding sites. Protein Engineering, Design and Selection, 2000, 13, 89-98.	1.0	100
131	Identifying DNA-binding proteins using structural motifs and the electrostatic potential. Nucleic Acids Research, 2004, 32, 4732-4741.	6.5	100
132	Diapause-associated metabolic traits reiterated in long-lived daf-2 mutants in the nematode Caenorhabditis elegans. Mechanisms of Ageing and Development, 2006, 127, 458-472.	2.2	99
133	Small binding proteins selected from a combinatorial repertoire of knottins displayed on phage. Journal of Molecular Biology, 1998, 277, 317-332.	2.0	98
134	Successful protein fold recognition by optimal sequence threading validated by rigorous blind testing. Proteins: Structure, Function and Bioinformatics, 1995, 23, 387-397.	1.5	97
135	Catalysing New Reactions during Evolution: Economy of Residues and Mechanism. Journal of Molecular Biology, 2003, 331, 829-860.	2.0	96
136	Evolution of Protein Superfamilies and Bacterial Genome Size. Journal of Molecular Biology, 2004, 336, 871-887.	2.0	95
137	The Classification and Evolution of Enzyme Function. Biophysical Journal, 2015, 109, 1082-1086.	0.2	95
138	Molecular basis of inherited diseases: a structural perspective. Trends in Genetics, 2003, 19, 505-513.	2.9	92
139	Wavelet transforms for the characterization and detection of repeating motifs. Journal of Molecular Biology, 2002, 316, 341-363.	2.0	91
140	The European Bioinformatics Institute's data resources. Nucleic Acids Research, 2010, 38, D17-D25.	6.5	90
141	X-SITE: Use of Empirically Derived Atomic Packing Preferences to Identify Favourable Interaction Regions in the Binding Sites of Proteins. Journal of Molecular Biology, 1996, 259, 175-201.	2.0	89
142	Detection of 3D atomic similarities and their use in the discrimination of small molecule protein-binding sites. Bioinformatics, 2008, 24, i105-i111.	1.8	89
143	Rebuilding flavodoxin from $\hat{\text{Cl}}$ coordinates: A test study. Proteins: Structure, Function and Bioinformatics, 1989, 5, 170-182.	1.5	88
144	Three-dimensional structure analysis of PROSITE patterns 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1999, 286, 1673-1691.	2.0	88

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145	Automatic inference of protein quaternary structure from crystals. Journal of Applied Crystallography, 2003, 36, 1116-1122.	1.9	88
146	The CATH protein family database: A resource for structural and functional annotation of genomes. Proteomics, 2002, 2, 11-21.	1.3	87
147	PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Research, 2020, 48, D344-D353.	6.5	87
148	Conformational change in substrate binding, catalysis and product release: an open and shut case?. FEBS Letters, 2004, 567, 67-73.	1.3	86
149	Assessment of comparative modeling in CASP2. Proteins: Structure, Function and Bioinformatics, 1997, 29, 14-28.	1.5	85
150	The European Bioinformatics Institute's data resources: towards systems biology. Nucleic Acids Research, 2004, 33, D46-D53.	6.5	85
151	Protein fold recognition. Journal of Computer-Aided Molecular Design, 1993, 7, 439-456.	1.3	83
152	Accommodating Sequence Changes in $\hat{l}^2$ -Hairpins in Proteins. Journal of Molecular Biology, 1993, 229, 428-447.	2.0	82
153	[5] Conformation of $\hat{l}^2$ hairpins in protein structures: Classification and diversity in homologous structures. Methods in Enzymology, 1991, 202, 59-82.	0.4	81
154	RTG-dependent Mitochondria-to-Nucleus Signaling Is Regulated by MKS1 and Is Linked to Formation of Yeast Prion [URE3]. Molecular Biology of the Cell, 2002, 13, 795-804.	0.9	80
155	Ligand selectivity and competition between enzymes in silico. Nature Biotechnology, 2004, 22, 1039-1045.	9.4	80
156	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	21.5	80
157	Exploring the Evolution of Novel Enzyme Functions within Structurally Defined Protein Superfamilies. PLoS Computational Biology, 2012, 8, e1002403.	1.5	80
158	Emerging concepts in pseudoenzyme classification, evolution, and signaling. Science Signaling, 2019, 12, .	1.6	80
159	Recognizing the fold of a protein structure. Bioinformatics, 2003, 19, 1748-1759.	1.8	79
160	Towards Fully Automated Structure-based Function Prediction in Structural Genomics: A Case Study. Journal of Molecular Biology, 2007, 367, 1511-1522.	2.0	79
161	Correlation of observed fold frequency with the occurrence of local structural motifs. Journal of Molecular Biology, 1999, 287, 969-981.	2.0	78
162	Retrograde Response to Mitochondrial Dysfunction Is Separable from TOR1/2 Regulation of Retrograde Gene Expression. Journal of Biological Chemistry, 2005, 280, 42528-42535.	1.6	78

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163	ELIXIR: a distributed infrastructure for European biological data. Trends in Biotechnology, 2012, 30, 241-242.	4.9	78
164	Prediction of progress at last. Nature, 1991, 354, 105-106.	13.7	77
165	A study into the effects of protein binding on nucleotide conformation. Nucleic Acids Research, 1993, 21, 1369-1380.	6.5	77
166	VarSite: Disease variants and protein structure. Protein Science, 2020, 29, 111-119.	3.1	77
167	A bioinformatician's view of the metabolome. BioEssays, 2006, 28, 534-545.	1.2	76
168	The Greek key motif: extraction, classification and analysis. Protein Engineering, Design and Selection, 1993, 6, 233-245.	1.0	75
169	Regulation of Lifespan, Metabolism, and Stress Responses by the Drosophila SH2B Protein, Lnk. PLoS Genetics, 2010, 6, e1000881.	1.5	75
170	Chopping and Changing: the Evolution of the Flavin-dependent Monooxygenases. Journal of Molecular Biology, 2016, 428, 3131-3146.	2.0	75
171	Pathway evolution, structurally speaking. Current Opinion in Structural Biology, 2002, 12, 374-382.	2.6	73
172	Metal-MACiE: a database of metals involved in biological catalysis. Bioinformatics, 2009, 25, 2088-2089.	1.8	73
173	Reaction Decoder Tool (RDT): extracting features from chemical reactions. Bioinformatics, 2016, 32, 2065-2066.	1.8	<b>7</b> 3
174	From protein structure to biochemical function?. Journal of Structural and Functional Genomics, 2003, 4, 167-177.	1.2	72
175	Conformational analysis of protein structures derived from NMR data. Proteins: Structure, Function and Bioinformatics, 1993, 17, 232-251.	1.5	71
176	The European Bioinformatics Institute's data resources 2014. Nucleic Acids Research, 2014, 42, D18-D25.	6.5	71
177	Prediction of strand pairing in antiparallel and parallel ?-sheets using information theory. Proteins: Structure, Function and Bioinformatics, 2002, 48, 178-191.	1.5	70
178	Analysis of protein main-chain solvation as a function of secondary structure. Journal of Molecular Biology, 1991, 221, 669-691.	2.0	69
179	Understanding the molecular machinery of genetics through 3D structures. Nature Reviews Genetics, 2008, 9, 141-151.	7.7	69
180	Structural and sequence patterns in the loops of $\hat{l}^2\hat{l}\pm\hat{l}^2$ units. Protein Engineering, Design and Selection, 1987, 1, 173-181.	1.0	68

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181	Analysis of Domain Structural Class Using an Automated Class Assignment Protocol. Journal of Molecular Biology, 1996, 262, 168-185.	2.0	68
182	A global analysis of function and conservation of catalytic residues in enzymes. Journal of Biological Chemistry, 2020, 295, 314-324.	1.6	68
183	Morphological aspects of oligomeric protein structures. Progress in Biophysics and Molecular Biology, 2005, 89, 9-35.	1.4	67
184	Screening for genes that accelerate the epigenetic aging clock in humans reveals a role for the H3K36 methyltransferase NSD1. Genome Biology, 2019, 20, 146.	3.8	66
185	Barrel structures in proteins: Automatic identification and classification including a sequence analysis of TIM barrels. Protein Science, 1999, 8, 2072-2084.	3.1	65
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