

Michael Levitt

List of Publications by Year in descending order

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172
papers

23,901
citations

15001

68
h-index

8878

150
g-index

186
all docs

186
docs citations

186
times ranked

16708
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural patterns in globular proteins. <i>Nature</i> , 1976, 261, 552-558.	13.7	1,288
2	Conformations of immunoglobulin hypervariable regions. <i>Nature</i> , 1989, 342, 877-883.	13.7	1,199
3	A simplified representation of protein conformations for rapid simulation of protein folding. <i>Journal of Molecular Biology</i> , 1976, 104, 59-107.	2.0	1,057
4	Computer simulation of protein folding. <i>Nature</i> , 1975, 253, 694-698.	13.7	978
5	Conformation of amino acid side-chains in proteins. <i>Journal of Molecular Biology</i> , 1978, 125, 357-386.	2.0	783
6	Protein normal-mode dynamics: Trypsin inhibitor, crambin, ribonuclease and lysozyme. <i>Journal of Molecular Biology</i> , 1985, 181, 423-447.	2.0	692
7	Aromatic rings act as hydrogen bond acceptors. <i>Journal of Molecular Biology</i> , 1988, 201, 751-754.	2.0	672
8	Conformational preferences of amino acids in globular proteins. <i>Biochemistry</i> , 1978, 17, 4277-4285.	1.2	670
9	Accurate modeling of protein conformation by automatic segment matching. <i>Journal of Molecular Biology</i> , 1992, 226, 507-533.	2.0	555
10	Helix to helix packing in proteins. <i>Journal of Molecular Biology</i> , 1981, 145, 215-250.	2.0	543
11	Automatic identification of secondary structure in globular proteins. <i>Journal of Molecular Biology</i> , 1977, 114, 181-239.	2.0	509
12	Calibration and Testing of a Water Model for Simulation of the Molecular Dynamics of Proteins and Nucleic Acids in Solution. <i>Journal of Physical Chemistry B</i> , 1997, 101, 5051-5061.	1.2	503
13	The ASTRAL Compendium in 2004. <i>Nucleic Acids Research</i> , 2004, 32, 189D-192.	6.5	480
14	Refinement of protein conformations using a macromolecular energy minimization procedure. <i>Journal of Molecular Biology</i> , 1969, 46, 269-279.	2.0	433
15	The ASTRAL compendium for protein structure and sequence analysis. <i>Nucleic Acids Research</i> , 2000, 28, 254-256.	6.5	432
16	Potential energy function and parameters for simulations of the molecular dynamics of proteins and nucleic acids in solution. <i>Computer Physics Communications</i> , 1995, 91, 215-231.	3.0	431
17	Detailed Molecular Model for Transfer Ribonucleic Acid. <i>Nature</i> , 1969, 224, 759-763.	13.7	411
18	Energy Functions that Discriminate X-ray and Near-native Folds from Well-constructed Decoys. <i>Journal of Molecular Biology</i> , 1996, 258, 367-392.	2.0	375

#	ARTICLE	IF	CITATIONS
19	Protein folding by restrained energy minimization and molecular dynamics. <i>Journal of Molecular Biology</i> , 1983, 170, 723-764.	2.0	349
20	Molecular dynamics of native protein. <i>Journal of Molecular Biology</i> , 1983, 168, 595-617.	2.0	348
21	Within the twilight zone: a sensitive profile-profile comparison tool based on information theory. <i>Journal of Molecular Biology</i> , 2002, 315, 1257-1275.	2.0	267
22	Super-resolution biomolecular crystallography with low-resolution data. <i>Nature</i> , 2010, 464, 1218-1222.	13.7	267
23	Comprehensive Evaluation of Protein Structure Alignment Methods: Scoring by Geometric Measures. <i>Journal of Molecular Biology</i> , 2005, 346, 1173-1188.	2.0	260
24	Energy refinement of hen egg-white lysozyme. <i>Journal of Molecular Biology</i> , 1974, 82, 393-420.	2.0	259
25	Nature of the protein universe. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 11079-11084.	3.3	254
26	The Volume of Atoms on the Protein Surface: Calculated from Simulation, using Voronoi Polyhedra. <i>Journal of Molecular Biology</i> , 1995, 249, 955-966.	2.0	243
27	Molecular dynamics simulations of helix denaturation. <i>Journal of Molecular Biology</i> , 1992, 223, 1121-1138.	2.0	231
28	Water: now you see it, now you don't. <i>Structure</i> , 1993, 1, 223-226.	1.6	231
29	Extreme conformational flexibility of the furanose ring in DNA and RNA. <i>Journal of the American Chemical Society</i> , 1978, 100, 2607-2613.	6.6	225
30	Structural Basis of Transcription: Backtracked RNA Polymerase II at 3.4 Angstrom Resolution. <i>Science</i> , 2009, 324, 1203-1206.	6.0	225
31	The complexity and accuracy of discrete state models of protein structure. <i>Journal of Molecular Biology</i> , 1995, 249, 493-507.	2.0	222
32	Decoys \tilde{R} Us: A database of incorrect conformations to improve protein structure prediction. <i>Protein Science</i> , 2000, 9, 1399-1401.	3.1	215
33	Combining Efficient Conformational Sampling with a Deformable Elastic Network Model Facilitates Structure Refinement at Low Resolution. <i>Structure</i> , 2007, 15, 1630-1641.	1.6	213
34	Mechanism of folding chamber closure in a group II chaperonin. <i>Nature</i> , 2010, 463, 379-383.	13.7	196
35	Molecular dynamics of native protein. <i>Journal of Molecular Biology</i> , 1983, 168, 621-657.	2.0	195
36	Comprehensive assessment of automatic structural alignment against a manual standard, the scop classification of proteins. <i>Protein Science</i> , 1998, 7, 445-456.	3.1	190

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37	Accurate prediction of the stability and activity effects of site-directed mutagenesis on a protein core. <i>Nature</i> , 1991, 352, 448-451.	13.7	188
38	PROTEIN FOLDING:The Endgame. <i>Annual Review of Biochemistry</i> , 1997, 66, 549-579.	5.0	184
39	Protein Unfolding Pathways Explored Through Molecular Dynamics Simulations. <i>Journal of Molecular Biology</i> , 1993, 232, 600-619.	2.0	178
40	Small Libraries of Protein Fragments Model Native Protein Structures Accurately. <i>Journal of Molecular Biology</i> , 2002, 323, 297-307.	2.0	170
41	Ab initio construction of protein tertiary structures using a hierarchical approach. <i>Journal of Molecular Biology</i> , 2000, 300, 171-185.	2.0	162
42	Factors affecting the ability of energy functions to discriminate correct from incorrect folds. <i>Journal of Molecular Biology</i> , 1997, 266, 831-846.	2.0	159
43	Subunit order of eukaryotic TRiC/CCT chaperonin by cross-linking, mass spectrometry, and combinatorial homology modeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 2884-2889.	3.3	158
44	Exploring conformational space with a simple lattice model for protein structure. <i>Journal of Molecular Biology</i> , 1994, 243, 668-682.	2.0	153
45	Effect of proline residues on protein folding. <i>Journal of Molecular Biology</i> , 1981, 145, 251-263.	2.0	146
46	Growth of novel protein structural data. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 3183-3188.	3.3	145
47	Architecture of an RNA Polymerase II Transcription Pre-Initiation Complex. <i>Science</i> , 2013, 342, 1238724.	6.0	143
48	Nonpolar solutes enhance water structure within hydration shells while reducing interactions between them. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6777-6782.	3.3	141
49	Recognizing Native Folds by the Arrangement of Hydrophobic and Polar Residues. <i>Journal of Molecular Biology</i> , 1995, 252, 709-720.	2.0	134
50	Near-native structure refinement using in vacuo energy minimization. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 3177-3182.	3.3	134
51	Millisecond dynamics of RNA polymerase II translocation at atomic resolution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 7665-7670.	3.3	127
52	KoBaMIN: a knowledge-based minimization web server for protein structure refinement. <i>Nucleic Acids Research</i> , 2012, 40, W323-W328.	6.5	124
53	De novo protein design. I. in search of stability and specificity 1 Edited by F. E. Cohen. <i>Journal of Molecular Biology</i> , 1999, 293, 1161-1181.	2.0	122
54	ASTRAL compendium enhancements. <i>Nucleic Acids Research</i> , 2002, 30, 260-263.	6.5	117

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55	Alignment of the amino acid sequences of distantly related proteins using variable gap penalties. <i>Protein Engineering, Design and Selection</i> , 1986, 1, 77-78.	1.0	108
56	Can Morphing Methods Predict Intermediate Structures?. <i>Journal of Molecular Biology</i> , 2009, 385, 665-674.	2.0	104
57	The birth of computational structural biology. , 2001, 8, 392-393.		101
58	Solvent dramatically affects protein structure refinement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 20239-20244.	3.3	99
59	Keeping the shape but changing the charges: A simulation study of urea and its isoœsteric analogs. <i>Journal of Chemical Physics</i> , 1996, 104, 9417-9430.	1.2	95
60	Protein topology and stability define the space of allowed sequences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 1280-1285.	3.3	94
61	Hierarchy of structure loss in MD simulations of src SH3 domain unfolding. <i>Journal of Molecular Biology</i> , 1999, 291, 215-225.	2.0	91
62	Birth and Future of Multiscale Modeling for Macromolecular Systems (Nobel Lecture). <i>Angewandte Chemie - International Edition</i> , 2014, 53, 10006-10018.	7.2	91
63	Simulating protein evolution in sequence and structure space. <i>Current Opinion in Structural Biology</i> , 2004, 14, 202-207.	2.6	89
64	Modeling nucleic acids. <i>Current Opinion in Structural Biology</i> , 2012, 22, 273-278.	2.6	85
65	A Novel Approach to Decoy Set Generation: Designing a Physical Energy Function Having Local Minima with Native Structure Characteristics. <i>Journal of Molecular Biology</i> , 2003, 329, 159-174.	2.0	83
66	Fully differentiable coarse-grained and all-atom knowledge-based potentials for RNA structure evaluation. <i>Rna</i> , 2011, 17, 1066-1075.	1.6	81
67	Symmetry-free cryo-EM structures of the chaperonin TRiC along its ATPase-driven conformational cycle. <i>EMBO Journal</i> , 2012, 31, 720-730.	3.5	80
68	Finite-difference solution of the Poisson-Boltzmann equation: Complete elimination of self-energy. <i>Journal of Computational Chemistry</i> , 1996, 17, 1344-1351.	1.5	77
69	De novo protein design. II. plasticity in sequence space 1 Edited by F. E. Cohen. <i>Journal of Molecular Biology</i> , 1999, 293, 1183-1193.	2.0	74
70	Induced peptide conformations in different antibody complexes: molecular modeling of the three-dimensional structure of peptide-antibody complexes using NMR-derived distance restraints. <i>Biochemistry</i> , 1992, 31, 6884-6897.	1.2	73
71	On the Universe of Protein Folds. <i>Annual Review of Biophysics</i> , 2013, 42, 559-582.	4.5	73
72	RNA polymerase II trigger loop residues stabilize and position the incoming nucleotide triphosphate in transcription. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 15745-15750.	3.3	70

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73	Folding and stability of helical proteins: Carp myogen. <i>Journal of Molecular Biology</i> , 1976, 106, 421-437.	2.0	69
74	Using a Hydrophobic Contact Potential to Evaluate Native and Near-native Folds Generated by Molecular Dynamics Simulations. <i>Journal of Molecular Biology</i> , 1996, 257, 716-725.	2.0	68
75	Competitive assessment of protein fold recognition and alignment accuracy. <i>Proteins: Structure, Function and Bioinformatics</i> , 1997, 29, 92-104.	1.5	68
76	Ab initio protein structure prediction using a combined hierarchical approach. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 194-198.	1.5	66
77	Diffusion of nucleoside triphosphates and role of the entry site to the RNA polymerase II active center. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 17361-17364.	3.3	66
78	Roles of mutation and recombination in the evolution of protein thermodynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 10382-10387.	3.3	63
79	Molecular dynamics of hydrogen bonds in bovine pancreatic trypsin inhibitor protein. <i>Nature</i> , 1981, 294, 379-380.	13.7	61
80	Future of fundamental discovery in US biomedical research. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 6498-6503.	3.3	61
81	How Hydrophobic Buckminsterfullerene Affects Surrounding Water Structure. <i>Journal of Physical Chemistry B</i> , 2008, 112, 2981-2990.	1.2	60
82	An Atomic Environment Potential for use in Protein Structure Prediction. <i>Journal of Molecular Biology</i> , 2005, 352, 986-1001.	2.0	59
83	The Crystal Structures of the Eukaryotic Chaperonin CCT Reveal Its Functional Partitioning. <i>Structure</i> , 2013, 21, 540-549.	1.6	59
84	Probing antibody diversity by 2D NMR: comparison of amino acid sequences, predicted structures, and observed antibody-antigen interactions in complexes of two antipeptide antibodies. <i>Biochemistry</i> , 1989, 28, 7168-7175.	1.2	58
85	Sequence Variations within Protein Families are Linearly Related to Structural Variations. <i>Journal of Molecular Biology</i> , 2002, 323, 551-562.	2.0	57
86	Detailed Hydration Maps of Benzene and Cyclohexane Reveal Distinct Water Structures. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13492-13500.	1.2	57
87	Simulating Water and the Molecules of Life. <i>Scientific American</i> , 1998, 279, 100-105.	1.0	56
88	Improved protein structure selection using decoy-dependent discriminatory functions. <i>BMC Structural Biology</i> , 2004, 4, 8.	2.3	56
89	Protein folding and unfolding dynamics. <i>Current Opinion in Structural Biology</i> , 1994, 4, 291-295.	2.6	55
90	Evidence of turn and salt bridge contributions to β -hairpin stability: MD simulations of C-terminal fragment from the B1 domain of protein G. <i>Biophysical Chemistry</i> , 2002, 101-102, 187-201.	1.5	55

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91	Generalized ensemble methods for de novo structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 1415-1420.	3.3	52
92	Cryo-EM Structure of a Group II Chaperonin in the Prehydrolysis ATP-Bound State Leading to Lid Closure. Structure, 2011, 19, 633-639.	1.6	52
93	Insights on cross-species transmission of SARS-CoV-2 from structural modeling. PLoS Computational Biology, 2020, 16, e1008449.	1.5	52
94	The PRESAGE database for structural genomics. Nucleic Acids Research, 1999, 27, 251-253.	6.5	48
95	WeFold: A competition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	1.5	48
96	A comprehensive analysis of 40 blind protein structure predictions. , 2002, 2, 3.		47
97	Consistent refinement of submitted models at CASP using a knowledge-based potential. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2668-2678.	1.5	46
98	NMR-derived model for a peptide-antibody complex. Biochemistry, 1990, 29, 10032-10041.	1.2	45
99	Emerging β^2 -Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures. Journal of the American Chemical Society, 2017, 139, 8820-8827.	6.6	43
100	Accuracy of side-chain prediction upon near-native protein backbones generated by ab initio folding methods. , 1998, 33, 204-217.		42
101	Modeling and design by hierarchical natural moves. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 2890-2895.	3.3	42
102	Contribution of tryptophan residues to the combining site of a monoclonal anti-dinitrophenyl spin-label antibody. Biochemistry, 1987, 26, 6058-6064.	1.2	41
103	Simulating the minimum core for hydrophobic collapse in globular proteins. Protein Science, 1997, 6, 2606-2616.	3.1	40
104	Optimized Torsion-Angle Normal Modes Reproduce Conformational Changes More Accurately Than Cartesian Modes. Biophysical Journal, 2011, 101, 2966-2969.	0.2	37
105	Improving the Accuracy of Macromolecular Structure Refinement at 7Å... Resolution. Structure, 2012, 20, 957-966.	1.6	37
106	Constructing side chains on near-native main chains for ab initio protein structure prediction. Protein Engineering, Design and Selection, 2000, 13, 453-457.	1.0	36
107	Probing Protein Fold Space with a Simplified Model. Journal of Molecular Biology, 2008, 375, 920-933.	2.0	36
108	Comparison of pandemic excess mortality in 2020-2021 across different empirical calculations. Environmental Research, 2022, 213, 113754.	3.7	36

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109	Protein folding. <i>Current Opinion in Structural Biology</i> , 1991, 1, 224-229.	2.6	35
110	The solution structure of monomeric α -CCL5 in complex with a doubly sulfated N-terminal segment of α -CCR5. <i>FEBS Journal</i> , 2018, 285, 1988-2003.	2.2	35
111	From Structure to Sequence and Back Again. <i>Journal of Molecular Biology</i> , 1996, 258, 201-209.	2.0	34
112	Funnel sculpting for in silico assembly of secondary structure elements of proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 10700-10705.	3.3	34
113	A COMBINED APPROACH FOR AB INITIO CONSTRUCTION OF LOW RESOLUTION PROTEIN TERTIARY STRUCTURES FROM SEQUENCE. , 1998, , 505-16.		34
114	Funnel-like organization in sequence space determines the distributions of protein stability and folding rate preferred by evolution. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 107-114.	1.5	33
115	Inhibition Mechanism of the Acetylcholine Receptor by α -Neurotoxins as Revealed by Normal-Mode Dynamics. <i>Biochemistry</i> , 2008, 47, 4065-4070.	1.2	33
116	Protein segment finder: an online search engine for segment motifs in the PDB. <i>Nucleic Acids Research</i> , 2009, 37, D224-D228.	6.5	33
117	The normal modes of a protein: Native bovine pancreatic trypsin inhibitor. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 181-199.	1.0	33
118	Multiscale natural moves refine macromolecules using single-particle electron microscopy projection images. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 9845-9850.	3.3	32
119	On the importance of accounting for nuclear quantum effects in ab initio calibrated force fields in biological simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 8878-8882.	3.3	32
120	Describing RNA Structure by Libraries of Clustered Nucleotide Doublets. <i>Journal of Molecular Biology</i> , 2005, 351, 26-38.	2.0	31
121	Simulations of RNA base pairs in a nanodroplet reveal solvation-dependent stability. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 12336-12340.	3.3	31
122	Proteomic analysis of monolayer-integrated proteins on lipid droplets identifies amphipathic interfacial α -helical membrane anchors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E8172-E8180.	3.3	31
123	A Novel Method for Sampling Alpha-helical Protein Backbones. <i>Journal of Molecular Biology</i> , 2001, 305, 191-201.	2.0	29
124	Deformable elastic network refinement for low-resolution macromolecular crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 2241-2255.	2.5	29
125	The language of the protein universe. <i>Current Opinion in Genetics and Development</i> , 2015, 35, 50-56.	1.5	27
126	Ab initio protein structure prediction using a combined hierarchical approach. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, Suppl 3, 194-8.	1.5	27

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127	Extracting knowledge-based energy functions from protein structures by error rate minimization: Comparison of methods using lattice model. <i>Journal of Chemical Physics</i> , 2000, 113, 9318-9330.	1.2	26
128	Application of DEN refinement and automated model building to a difficult case of molecular-replacement phasing: the structure of a putative succinyl-diaminopimelate desuccinylase from <i>Corynebacterium glutamicum</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 391-403.	2.5	26
129	Remarkable patterns of surface water ordering around polarized buckminsterfullerene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 14455-14460.	3.3	25
130	Clustering to identify RNA conformations constrained by secondary structure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 3590-3595.	3.3	25
131	Training-free atomistic prediction of nucleosome occupancy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 6293-6298.	3.3	25
132	Structural and kinetic studies of the Fab fragment of a monoclonal anti-spin label antibody by nuclear magnetic resonance. <i>Journal of Molecular Biology</i> , 1991, 221, 257-270.	2.0	24
133	A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution. <i>Chemical Physics</i> , 1991, 158, 501-512.	0.9	24
134	Design of an optimal Chebyshev-expanded discrimination function for globular proteins. <i>Protein Science</i> , 2002, 11, 2010-2021.	3.1	24
135	Conformational Optimization with Natural Degrees of Freedom: A Novel Stochastic Chain Closure Algorithm. <i>Journal of Computational Biology</i> , 2010, 17, 993-1010.	0.8	23
136	Sequential allosteric mechanism of ATP hydrolysis by the CCT/TRiC chaperone is revealed through Arrhenius analysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 5189-5194.	3.3	23
137	Real-time interactive frequency filtering of molecular dynamics trajectories. <i>Journal of Molecular Biology</i> , 1991, 220, 1-4.	2.0	22
138	Normal Modes of Prion Proteins: From Native to Infectious Particle. <i>Biochemistry</i> , 2011, 50, 2243-2248.	1.2	22
139	The Area Derivative of a Space-Filling Diagram. <i>Discrete and Computational Geometry</i> , 2004, 32, 293.	0.4	21
140	Integrating the equations of motion. <i>Journal of Molecular Biology</i> , 1983, 168, 617-620.	2.0	20
141	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. <i>Scientific Reports</i> , 2018, 8, 9939.	1.6	19
142	Improved recognition of native-like protein structures using a family of designed sequences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 691-696.	3.3	18
143	HYDROGEN BOND AND INTERNAL SOLVENT DYNAMICS OF BPTI PROTEIN. <i>Annals of the New York Academy of Sciences</i> , 1981, 367, 162-181.	1.8	14
144	Evolutionarily consistent families in SCOP: sequence, structure and function. <i>BMC Structural Biology</i> , 2012, 12, 27.	2.3	14

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145	Comparative modeling and protein-like features of hydrophobic-polar models on a two-dimensional lattice. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1683-1693.	1.5	14
146	Accurate determination of solvation free energies of neutral organic compounds from first principles. <i>Nature Communications</i> , 2022, 13, 414.	5.8	14
147	Spatial Regulation and the Rate of Signal Transduction Activation. <i>PLoS Computational Biology</i> , 2006, 2, e44.	1.5	12
148	Redundancy-weighting for better inference of protein structural features. <i>Bioinformatics</i> , 2014, 30, 2295-2301.	1.8	12
149	Simulation of protein-folding pathways: lost in (conformational) space?. <i>Trends in Biotechnology</i> , 1995, 13, 23-27.	4.9	11
150	Unique function words characterize genomic proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 6703-6708.	3.3	10
151	MOTIF-EM: an automated computational tool for identifying conserved regions in CryoEM structures. <i>Bioinformatics</i> , 2010, 26, i301-i309.	1.8	9
152	Orientation of double-helical segments in crystals of yeast phenylalanine transfer RNA. <i>Journal of Molecular Biology</i> , 1973, 80, 255-263.	2.0	8
153	Structural diversity in a conserved cholera toxin epitope involved in ganglioside binding. <i>Protein Science</i> , 1995, 4, 841-848.	3.1	8
154	Theory and simulation through the breach. <i>Current Opinion in Structural Biology</i> , 1996, 6, 193-194.	2.6	7
155	A unified sequence-structure classification of protein sequences. , 2000, , .		7
156	EVALUATING MIXTURE MODELS FOR BUILDING RNA KNOWLEDGE-BASED POTENTIALS. <i>Journal of Bioinformatics and Computational Biology</i> , 2012, 10, 1241010.	0.3	7
157	Theory and simulation. <i>Current Opinion in Structural Biology</i> , 2006, 16, 139-141.	2.6	5
158	Solving the structure of Lgl2, a difficult blind test of unsupervised structure determination. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 10819-10823.	3.3	5
159	Finite-difference solution of the Poisson-Boltzmann equation: Complete elimination of self-energy. , 1996, 17, 1344.		5
160	Probing Interplays between Human XBP1u Translational Arrest Peptide and 80S Ribosome. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1905-1914.	2.3	5
161	INSIGHTS INTO THE INTRA-RING SUBUNIT ORDER OF TRIC/CCT:. , 2009, , 252-259.		4
162	Unsupervised determination of protein crystal structures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 10813-10818.	3.3	4

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163	Simulating Protein Dynamics in Solution: Bovine Pancreatic Trypsin Inhibitor. , 1987, , 197-205.		4
164	Foreword by the Guest Editors of this Issue. Israel Journal of Chemistry, 1986, 27, 119-120.	1.0	3
165	Discussion of "Equi-energy sampler" by Kou, Zhou and Wong. Annals of Statistics, 2006, 34, .	1.4	3
166	Molecular Dynamics of the DNA Double Helix. , 1984, , 43-57.		1
167	Folding of Nucleic Acids. Novartis Foundation Symposium, 1972, 7, 147-171.	1.2	1
168	Probing structure-function relationships of the DNA polymerase alpha-associated zinc-finger protein using computational approaches. , 1999, , 179-90.		1
169	Geburt und Zukunft der Multiskalenmodellierung von makromolekularen Systemen (Nobel-Aufsatz). Angewandte Chemie, 2014, 126, 10168-10181.	1.6	0
170	Automatic Inference of Sequence from Low-Resolution Crystallographic Data. Structure, 2018, 26, 1546-1554.e2.	1.6	0
171	Computer Simulations in Service of Biology. Frontiers for Young Minds, 0, 8, .	0.8	0
172	Simulating the Dynamics of the DNA Double Helix in Solution. , 1996, , 173-191.		0