Michael Nilges

List of Publications by Year
in descending order

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230 papers	32,553 citations	13099 68 h-index	4015 176 g-index
247 all docs	247 docs citations	247 times ranked	24646 citing authors

#	Article	IF	Citations
1	Crystallography & NMR System: A New Software Suite for Macromolecular Structure Determination. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 905-921.	2.5	14,711
2	Determination of three-dimensional structures of proteins from interproton distance data by hybrid distance geometry-dynamical simulated annealing calculations. FEBS Letters, 1988, 229, 317-324.	2.8	756
3	Refinement of protein structures in explicit solvent. Proteins: Structure, Function and Bioinformatics, 2003, 50, 496-506.	2.6	571
4	Determination of the three-dimensional solution structure of the C-terminal domain of cellobiohydrolase I from Trichoderma reesei. A study using nuclear magnetic resonance and hybrid distance geometry-dynamical simulated annealing. Biochemistry, 1989, 28, 7241-7257.	2.5	542
5	Determination of three-dimensional structures of proteins from interproton distance data by dynamical simulated annealing from a random array of atoms Circumventing problems associated with folding. FEBS Letters, 1988, 239, 129-136.	2.8	517
6	Determination of three-dimensional structures of proteins by simulated annealing with interproton distance restraints. Application to crambin, potato carboxypeptidase inhibitor and barley serine proteinase inhibitor 2. Protein Engineering, Design and Selection, 1988, 2, 27-38.	2.1	513
7	ARIA2: Automated NOE assignment and data integration in NMR structure calculation. Bioinformatics, 2007, 23, 381-382.	4.1	506
8	ARIA: automated NOE assignment and NMR structure calculation. Bioinformatics, 2003, 19, 315-316.	4.1	437
9	Automated NOESY interpretation with ambiguous distance restraints: the refined NMR solution structure of the pleckstrin homology domain from Î²-spectrin 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1997, 269, 408-422.	4.2	414
10	Architecture of the RNA polymerase IIâ€“TFIIF complex revealed by cross-linking and mass spectrometry. EMBO Journal, 2010, 29, 717-726.	7.8	355
11	Calculation of Protein Structures with Ambiguous Distance Restraints. Automated Assignment of Ambiguous NOE Crosspeaks and Disulphide Connectivities. Journal of Molecular Biology, 1995, 245, 645-660.	4.2	342
12	Inferential Structure Determination. Science, 2005, 309, 303-306.	12.6	333
13	A calculation strategy for the structure determination of symmetric demers by1H NMR. Proteins: Structure, Function and Bioinformatics, 1993, 17, 297-309.	2.6	323
14	RECOORD: A recalculated coordinate database of 500+ proteins from the PDB using restraints from the BioMagResBank. Proteins: Structure, Function and Bioinformatics, 2005, 59, 662-672.	2.6	323
15	Automated Assignment of Ambiguous Nuclear Overhauser Effects with ARIA. Methods in Enzymology, 2001, 339, 71-90.	1.0	319
16	Three-Dimensional Structure and Stability of the KH Domain: Molecular Insights into the Fragile X Syndrome. Cell, 1996, 85, 237-245.	28.9	283
17	Three-dimensional structure of potato carboxypeptidase inhibitor in solution. A study using nuclear magnetic resonance, distance geometry, and restrained molecular dynamics. Biochemistry, 1987, 26, 8012-8023.	2.5	279
18	ModBase, a database of annotated comparative protein structure models and associated resources. Nucleic Acids Research, 2014, 42, D336-D346.	14.5	275

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19	Structure of the pleckstrin homology domain from Î²-spectrin. Nature, 1994, 369, 675-677.	27.8	256
20	Influence of non-bonded parameters on the quality of NMR structures: a new force field for NMR structure calculation. , 1999, 13, 51-59.		246
21	The three-dimensional structure of Î±1-purothionin in solution: combined use of nuclear magnetic resonance, distance geometry and restrained molecular dynamics. EMBO Journal, 1986, 5, 2729-2735.	7.8	241
22	Bat coronaviruses related to SARS-CoV-2 and infectious for human cells. Nature, 2022, 604, 330-336.	27.8	238
23	The folding catalyst protein disulfide isomerase is constructed of active and inactive thioredoxin modules. Current Biology, 1997, 7, 239-245.	3.9	217
24	Sampling and efficiency of metric matrix distance geometry: A novel partial metrization algorithm. Journal of Biomolecular NMR, 1992, 2, 33-56.	2.8	210
25	Ambiguous NOEs and automated NOE assignment. Progress in Nuclear Magnetic Resonance Spectroscopy, 1998, 32, 107-139.	7.5	198
26	Internal repeats in the BRCA2 protein sequence. Nature Genetics, 1996, 13, 22-23.	21.4	189
27	Structure Determination of the N-Terminal Thioredoxin-like Domain of Protein Disulfide Isomerase Using Multidimensional Heteronuclear 13C/15N NMR Spectroscopy. Biochemistry, 1996, 35, 7684-7691.	2.5	185
28	Normal Mode Analysis Suggests a Quaternary Twist Model for the Nicotinic Receptor Gating Mechanism. Biophysical Journal, 2005, 88, 3954-3965.	0.5	178
29	The PH superfold: a structural scaffold for multiple functions. Trends in Biochemical Sciences, 1999, 24, 441-445.	7.5	175
30	Complementarity of Structure Ensembles in Protein-Protein Binding. Structure, 2004, 12, 2125-2136.	3.3	173
31	The structure of a novel insecticidal neurotoxin, Ï‰-atracotoxin-HV1, from the venom of an Australian funnel web spider. Nature Structural Biology, 1997, 4, 559-566.	9.7	172
32	Computational challenges for macromolecular structure determination by X-ray crystallography and solution NMRspectroscopy. Quarterly Reviews of Biophysics, 1993, 26, 49-125.	5.7	165
33	Relaxation matrix refinement of the solution structure of squash trypsin inhibitor. Journal of Molecular Biology, 1991, 219, 499-510.	4.2	162
34	Posttranslational Modification of Pili upon Cell Contact Triggers N. meningitidis Dissemination. Science, 2011, 331, 778-782.	12.6	162
35	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	3.3	159
36	SNARE Protein Mimicry by an Intracellular Bacterium. PLoS Pathogens, 2008, 4, e1000022.	4.7	156

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37	Assessing the quality of solution nuclear magnetic resonance structures by complete cross-validation. Science, 1993, 261, 328-331.	12.6	155
38	Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-1570.	3.3	151
39	Solution structure of the spectrin repeat: a left-handed antiparallel triple-helical coiled-coil 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1997, 273, 740-751.	4.2	143
40	Nicotine reverses hypofrontality in animal models of addiction and schizophrenia. Nature Medicine, 2017, 23, 347-354.	30.7	142
41	Visualization of macromolecular structures. Nature Methods, 2010, 7, S42-S55.	19.0	137
42	3D Structure Determination of the Crh Protein from Highly Ambiguous Solid-State NMR Restraints. Journal of the American Chemical Society, 2008, 130, 3579-3589.	13.7	135
43	Functional Analysis of Early Secreted Antigenic Target-6, the Dominant T-cell Antigen of Mycobacterium tuberculosis, Reveals Key Residues Involved in Secretion, Complex Formation, Virulence, and Immunogenicity. Journal of Biological Chemistry, 2005, 280, 33953-33959.	3.4	133
44	Flexibility and Conformational Entropy in Protein-Protein Binding. Structure, 2006, 14, 683-693.	3.3	132
45	The three-dimensional structure of the HRDC domain and implications for the Werner and Bloom syndrome proteins. Structure, 1999, 7, 1557-1566.	3.3	126
46	Structural Biology by NMR: Structure, Dynamics, and Interactions. PLoS Computational Biology, 2008, 4, e1000168.	3.2	120
47	Solution structure of the DNA-binding domain and model for the complex of multifunctiona hexameric arginine represser with DNA. Nature Structural Biology, 1997, 4, 819-826.	9.7	115
48	1H-Nmr stereospecific assignments by conformational data-base searches. Biopolymers, 1990, 29, 813-822.	2.4	108
49	Floating stereospecific assignment revisited: application to an 18 kDa protein and comparison with J-coupling data. Journal of Biomolecular NMR, 1997, 9, 245-258.	2.8	107
50	Toward a Unified Representation of Protein Structural Dynamics in Solution. Journal of the American Chemical Society, 2009, 131, 16968-16975.	13.7	105
51	An Efficient Protocol for NMRâ€Spectroscopyâ€Based Structure Determination of Protein Complexes in Solution. Angewandte Chemie - International Edition, 2010, 49, 1967-1970.	13.8	104
52	The conformations of hirudin in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. EMBO Journal, 1987, 6, 529-537.	7.8	97
53	Automated modeling of coiled coils: application to the GCN4 dimerization region. Protein Engineering, Design and Selection, 1991, 4, 649-659.	2.1	95
54	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. Bioinformatics, 2016, 32, 85-95.	4.1	95

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55	High Resolution NMR Solution Structure of the Leucine Zipper Domain of the c-Jun Homodimer. Journal of Biological Chemistry, 1996, 271, 13663-13667.	3.4	93
56	Structural and functional studies of titinâ€™s fn3 modules reveal conserved surface patterns and binding to myosin S1 - a possible role in the frank-starling mechanism of the heart. Journal of Molecular Biology, 2001, 313, 431-447.	4.2	91
57	A new approach for applying residual dipolar couplings as restraints in structure elucidation. Journal of Biomolecular NMR, 2000, 16, 245-252.	2.8	89
58	Classification of protein sequences by homology modeling and quantitative analysis of electrostatic similarity. , 1999, 37, 379-387.		87
59	Three-dimensional structure of acyl carrier protein in solution determined by nuclear magnetic resonance and the combined use of dynamical simulated annealing and distance geometry. FEBS Journal, 1988, 175, 9-15.	0.2	82
60	Conservation of the Biochemical Properties of IncA from Chlamydia trachomatis and Chlamydia caviae. Journal of Biological Chemistry, 2004, 279, 46896-46906.	3.4	82
61	Three-dimensional structure of phoratoxin in solution: combined use of nuclear magnetic resonance, distance geometry, and restrained molecular dynamics. Biochemistry, 1987, 26, 1732-1745.	2.5	81
62	Refinement of the solution structure of the DNA decamer 5'd(CTGGATCCAG)2: combined use of nuclear magnetic resonance and restrained molecular dynamics. Biochemistry, 1987, 26, 3734-3744.	2.5	80
63	The solution structure of the first KH domain of FMR1, the protein responsible for the fragile X syndrome. Nature Structural Biology, 1997, 4, 712-716.	9.7	80
64	CASD-NMR: critical assessment of automated structure determination by NMR. Nature Methods, 2009, 6, 625-626.	19.0	80
65	Pathways and Intermediates in Forced Unfolding of Spectrin Repeats. Structure, 2002, 10, 1085-1096.	3.3	75
66	Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data. Structure, 2012, 20, 227-236.	3.3	75
67	Refinement of the solution structure of the DNA hexamer 5'd(GCATGC)2: combined use of nuclear magnetic resonance and restrained molecular dynamics. Biochemistry, 1987, 26, 3718-3733.	2.5	74
68	Weighting of experimental evidence in macromolecular structure determination. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 1756-1761.	7.1	74
69	Successful prediction of the coiled coil geometry of the GCN4 leucine zipper domain by simulated annealing: Comparison to the X-ray structure. Proteins: Structure, Function and Bioinformatics, 1993, 15, 133-146.	2.6	73
70	Structure of the calcium-dependent type 2 secretion pseudopilus. Nature Microbiology, 2017, 2, 1686-1695.	13.3	68
71	The Solution Structure of the Tyr41â†'His Mutant of the Single-stranded DNA Binding Protein Encoded by Gene V of the Filamentous Bacteriophage M13. Journal of Molecular Biology, 1994, 236, 229-246.	4.2	66
72	Essential spaces defined by NMR structure ensembles and molecular dynamics simulation show significant overlap. Proteins: Structure, Function and Bioinformatics, 1998, 31, 370-382.	2.6	65

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73	Replica-Exchange Monte Carlo Scheme for Bayesian Data Analysis. Physical Review Letters, 2005, 94, 018105.	7.8	64
74	Detailed structural and assembly model of the type II secretion pilus from sparse data. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 13081-13086.	7.1	64
75	A Model of the Complex between Single-stranded DNA and the Single-stranded DNA Binding Protein Encoded by Gene V of Filamentous Bacteriophage M13. Journal of Molecular Biology, 1994, 240, 341-357.	4.2	63
76	The structure in solution of the b domain of protein disulfide isomerase. Journal of Biomolecular NMR, 1999, 13, 357-368.	2.8	62
77	Biskit A software platform for structural bioinformatics. Bioinformatics, 2007, 23, 769-770.	4.1	61
78	Structure of Complement C3(H2O) Revealed By Quantitative Cross-Linking/Mass Spectrometry And Modeling. Molecular and Cellular Proteomics, 2016, 15, 2730-2743.	3.8	59
79	NOE Assignment With ARIA 2.0: The Nuts and Bolts. , 2004, 278, 379-402.		58
80	A structure refinement protocol combining NMR residual dipolar couplings and small angle scattering restraints. Journal of Biomolecular NMR, 2008, 41, 199-208.	2.8	58
81	Accurate NMR Structures Through Minimization of an Extended Hybrid Energy. Structure, 2008, 16, 1305-1312.	3.3	58
82	Correction of spin diffusion during iterative automated NOE assignment. Journal of Magnetic Resonance, 2004, 167, 334-342.	2.1	55
83	Neisseria meningitidis Type IV Pili Composed of Sequence Invariable Pilins Are Masked by Multisite Glycosylation. PLoS Pathogens, 2015, 11, e1005162.	4.7	55
84	ARIA for Solution and Solid-State NMR. Methods in Molecular Biology, 2012, 831, 453-483.	0.9	54
85	Improved strategies for the determination of protein structures from NMR data: The solution structure of acyl carrier protein. FEBS Letters, 1989, 242, 218-224.	2.8	53
86	Ambiguous distance data in the calculation of NMR structures. Folding & Design, 1997, 2, S53-S57.	4.5	53
87	Comparative Evaluation of 3D Virtual Ligand Screening Methods: Impact of the Molecular Alignment on Enrichment. Journal of Chemical Information and Modeling, 2010, 50, 992-1004.	5.4	52
88	Inferential Structure Determination of Chromosomes from Single-Cell Hi-C Data. PLoS Computational Biology, 2016, 12, e1005292.	3.2	52
89	Comparative Analysis of Structural and Dynamic Properties of the Loaded and Unloaded Hemophore HasA: Functional Implications. Journal of Molecular Biology, 2008, 376, 517-525.	4.2	50
90	Bayesian Weighing of Electron Cryo-Microscopy Data for Integrative Structural Modeling. Structure, 2019, 27, 175-188.e6.	3.3	50

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91	Automated structure modeling of large protein assemblies using crosslinks as distance restraints. Nature Methods, 2016, 13, 515-520.	19.0	49
92	Structure calculation from NMR data. Current Opinion in Structural Biology, 1996, 6, 617-623.	5.7	48
93	Structural Insights into Serine-rich Fimbriae from Gram-positive Bacteria. Journal of Biological Chemistry, 2010, 285, 32446-32457.	3.4	48
94	A role for specific collagen motifs during wound healing and inflammatory response of fibroblasts in the teleost fish gilthead seabream. Molecular Immunology, 2011, 48, 826-834.	2.2	48
95	Are there non-trivial dynamic cross-correlations in proteins?. Journal of Molecular Biology, 1998, 279, 911-920.	4.2	47
96	Distinct Docking and Stabilization Steps of the Pseudopilus Conformational Transition Path Suggest Rotational Assembly of Type IV Pilus-like Fibers. Structure, 2014, 22, 685-696.	3.3	47
97	Structure of the histone mRNA hairpin required for cell cycle regulation of histone gene expression. Rna, 2002, 8, 29-46.	3.5	45
98	Shelling the Voronoi interface of proteinâ€“protein complexes reveals patterns of residue conservation, dynamics, and composition. Proteins: Structure, Function and Bioinformatics, 2009, 76, 677-692.	2.6	45
99	A comparison of the restrained molecular dynamics and distance geometry methods for determining three-dimensional structures of proteins on the basis of interproton distances. FEBS Letters, 1987, 213, 269-277.	2.8	44
100	The three-dimensional structure of a type I module from titin: a prototype of intracellular fibronectin type III domains. Structure, 1998, 6, 1291-1302.	3.3	44
101	The impact of protein flexibility on protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2004, 58, 126-133.	2.6	42
102	An algorithm to enumerate all possible protein conformations verifying a set of distance constraints. BMC Bioinformatics, 2015, 16, 23.	2.6	42
103	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434.	8.2	40
104	Principal Component Analysis reveals correlation of cavities evolution and functional motions in proteins. Journal of Molecular Graphics and Modelling, 2015, 55, 13-24.	2.4	40
105	Structure and function of minor pilins of type IV pili. Medical Microbiology and Immunology, 2020, 209, 301-308.	4.8	40
106	Modeling Errors in NOE Data with a Log-normal Distribution Improves the Quality of NMR Structures. Journal of the American Chemical Society, 2005, 127, 16026-16027.	13.7	39
107	ISD: a software package for Bayesian NMR structure calculation. Bioinformatics, 2008, 24, 1104-1105.	4.1	39
108	Calculation of symmetric multimer structures from NMR data using a priori knowledge of the monomer structure, co-monomer restraints, and interface mapping: The case of leucine zippers. Journal of Biomolecular NMR, 1996, 8, 193-206.	2.8	38

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109	Influence of internal dynamics on accuracy of protein NMR structures: derivation of realistic model distance data from a long molecular dynamics trajectory 1 1Edited by G. Von Heijne. Journal of Molecular Biology, 1999, 285, 727-740.	4.2	38
110	Determination of the backbone conformation of secretin by restrained molecular dynamics on the basis of interproton distance data. FEBS Journal, 1988, 171, 479-484.	0.2	37
111	Heteronuclear relaxation study of the PH domain of Î²-spectrin: restriction of loop motions upon binding inositol trisphosphate 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1998, 280, 879-896.	4.2	37
112	Unraveling the symmetry ambiguity in a hexamer: calculation of the R6 human insulin structure. Journal of Biomolecular NMR, 2000, 16, 93-108.	2.8	37
113	Modeling pilus structures from sparse data. Journal of Structural Biology, 2011, 173, 436-444.	2.8	36
114	Bayesian inference applied to macromolecular structure determination. Physical Review E, 2005, 72, 031912.	2.1	35
115	Computational Reverse-Engineering of a Spider-Venom Derived Peptide Active Against Plasmodium falciparum SUB1. PLoS ONE, 2011, 6, e21812.	2.5	35
116	Improved reliability, accuracy and quality in automated NMR structure calculation with ARIA. Journal of Biomolecular NMR, 2015, 62, 425-438.	2.8	34
117	Influence of different assignment conditions on the determination of symmetric homodimeric structures with ARIA. Proteins: Structure, Function and Bioinformatics, 2009, 75, 569-585.	2.6	33
118	Structure and Assembly of the Enterohemorrhagic Escherichia coli Type 4 Pilus. Structure, 2019, 27, 1082-1093.e5.	3.3	33
119	Functional diversity of PH domains: an exhaustive modelling study. Folding & Design, 1997, 2, 343-355.	4.5	32
120	A simple method for delineating well-defined and variable regions in protein structures determined from interproton distance data. FEBS Letters, 1987, 219, 11-16.	2.8	31
121	Sequential resonance assignment and secondary structure determination of the Ascaris trypsin inhibitor, a member of a novel class of proteinase inhibitors. Biochemistry, 1990, 29, 183-189.	2.5	31
122	Efficient sampling in collective coordinate space. , 2000, 39, 82-88.		31
123	Quantitative study of the effects of chemical shift tolerances and rates of SA cooling on structure calculation from automatically assigned NOE data. Journal of Magnetic Resonance, 2005, 175, 92-102.	2.1	31
124	SOLARIA: A Protocol for Automated Cross-Peak Assignment and Structure Calculation for Solid-State Magic-Angle Spinning NMR Spectroscopy. Angewandte Chemie - International Edition, 2005, 44, 6151-6154.	13.8	29
125	An automatic tool to analyze and cluster macromolecular conformations based on self-organizing maps. Bioinformatics, 2015, 31, 1490-1492.	4.1	28
126	Refinement of the solution structure of the ribonucleotide 5'r(GCAUGC)2: combined use of nuclear magnetic resonance and restrained molecular dynamics. Biochemistry, 1988, 27, 1735-1743.	2.5	27

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127	Refined Structure, DNA Binding Studies, and Dynamics of the Bacteriophage Pf3 Encoded Single-Stranded DNA Binding Protein,. Biochemistry, 1997, 36, 9120-9135.	2.5	27
128	Refinement of the protein backbone angle psi in NMR structure calculations. Journal of Biomolecular NMR, 2000, 16, 47-58.	2.8	27
129	Minimal NMR distance information for rigidity of protein graphs. Discrete Applied Mathematics, 2019, 256, 91-104.	0.9	26
130	Sampling Properties of Simulated Annealing and Distance Geometry. , 1991, , 451-455.		26
131	Structure of a PH Domain from the C. elegans Muscle Protein UNC-89 Suggests a Novel Function. Structure, 2000, 8, 1079-1087.	3.3	25
132	Re-Face Stereospecificity of Methylenetetrahydromethanopterin and Methylenetetrahydrofolate Dehydrogenases is Predetermined by Intrinsic Properties of the Substrate. ChemBioChem, 2001, 2, 530-541.	2.6	25
133	Continuum solvent molecular dynamics study of flexibility in interleukin-8. Journal of Molecular Graphics and Modelling, 2001, 19, 136-145.	2.4	25
134	Bayesian estimation of Karplus parameters and torsion angles from three-bond scalar couplings constants. Journal of Magnetic Resonance, 2005, 177, 160-165.	2.1	25
135	The iPPI-DB initiative: a community-centered database of proteinâ€“protein interaction modulators. Bioinformatics, 2021, 37, 89-96.	4.1	24
136	Solution Structure of the 30 kDa Polysulfide-Sulfur Transferase Homodimer from Wolinella succinogenes,. Biochemistry, 2004, 43, 1418-1424.	2.5	23
137	Clinical and mutational investigations of tyrosinemia type II in Northern Tunisia: Identification and structural characterization of two novel TAT mutations. Molecular Genetics and Metabolism, 2006, 88, 184-191.	1.1	23
138	Bayesian estimation of NMR restraint potential and weight: A validation on a representative set of protein structures. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1525-1537.	2.6	23
139	Structural Characterization of Whirlin Reveals an Unexpected and Dynamic Supramodule Conformation of Its PDZ Tandem. Structure, 2017, 25, 1645-1656.e5.	3.3	22
140	Sequence-specific DNA binding activity of the cross-brace zinc finger motif of the piggyBac transposase. Nucleic Acids Research, 2018, 46, 2660-2677.	14.5	22
141	Functionally important correlated motions in the single-stranded DNA-binding protein encoded by filamentous phage Pf3. Journal of Molecular Biology, 1999, 287, 569-577.	4.2	21
142	Three Dimensional Structure and Implications for the Catalytic Mechanism of 6-Phosphogluconolactonase from Trypanosoma brucei. Journal of Molecular Biology, 2007, 366, 868-881.	4.2	21
143	In Silico Screening on the Three-dimensional Model of the Plasmodium vivax SUB1 Protease Leads to the Validation of a Novel Anti-parasite Compound. Journal of Biological Chemistry, 2013, 288, 18561-18573.	3.4	21
144	Identification of novel leishmanicidal molecules by virtual and biochemical screenings targeting Leishmania eukaryotic translation initiation factor 4A. PLoS Neglected Tropical Diseases, 2018, 12, e0006160.	3.0	21

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145	Molecular dynamics and accuracy of NMR structures: Effects of error bounds and data removal. Proteins: Structure, Function and Bioinformatics, 1999, 34, 453-463.	2.6	20
146	Stabilization of the integraseâ€ĐNA complex by Mg²⁺ ions and prediction of key residues for binding HIVâ€1 integrase inhibitors. Proteins: Structure, Function and Bioinformatics, 2014, 82, 466-478.	2.6	19
147	Tuning interval Branch-and-Prune for protein structure determination. Journal of Global Optimization, 2018, 72, 109-127.	1.8	19
148	Target Engagement and Binding Mode of an Antituberculosis Drug to Its Bacterial Target Deciphered in Whole Living Cells by NMR. Biochemistry, 2019, 58, 526-533.	2.5	19
149	Refined Solution Structure of the Tyr41His Mutant of the M13 Gene V Protein. A Comparison with the Crystal Structure. FEBS Journal, 1995, 232, 506-514.	0.2	18
150	Tertiary structure prediction using mean-force potentials and internal energy functions: successful prediction for coiled-coil geometries. Folding & Design, 1997, 2, S47-S52.	4.5	18
151	A convective replicaâ€exchange method for sampling new energy basins. Journal of Computational Chemistry, 2013, 34, 132-140.	3.3	18
152	Discrimination of agonists versus antagonists of nicotinic ligands based on docking onto AChBP structures. Journal of Molecular Graphics and Modelling, 2011, 30, 100-109.	2.4	17
153	Molecular Replacement with NMR Models Using Distance-Derived PseudoBFactors. Acta Crystallographica Section D: Biological Crystallography, 1996, 52, 973-982.	2.5	16
154	A unifying probabilistic framework for analyzing residual dipolar couplings. Journal of Biomolecular NMR, 2008, 40, 135-144.	2.8	16
155	Insights Into the Enzymatic Mechanism of 6-Phosphogluconolactonase from Trypanosoma brucei Using Structural Data and Molecular Dynamics Simulation. Journal of Molecular Biology, 2009, 388, 1009-1021.	4.2	16
156	Identification of binding sites and favorable ligand binding moieties by virtual screening and self-organizing map analysis. BMC Bioinformatics, 2015, 16, 93.	2.6	16
157	In Silico prediction of the molecular basis of ClTx and AaCTx interaction with matrix metalloproteinase-2 (MMP-2) to inhibit glioma cell invasion. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2815-2829.	3.5	16
158	Distance Geometry in Structural Biology: New Perspectives. , 2013, , 329-350.		16
159	Conformation of secretin in dimethyl sulfoxide solution. NMR studies and restrained molecular dynamics. FEBS Journal, 1989, 186, 95-103.	0.2	15
160	mkgridXf: Consistent Identification of Plausible Binding Sites Despite the Elusive Nature of Cavities and Grooves in Protein Dynamics. Journal of Chemical Information and Modeling, 2019, 59, 3506-3518.	5.4	15
161	SAXS Merge: an automated statistical method to merge SAXS profiles using Gaussian processes. Journal of Synchrotron Radiation, 2014, 21, 203-208.	2.4	15
162	Functional Motions Modulating VanA Ligand Binding Unraveled by Self-Organizing Maps. Journal of Chemical Information and Modeling, 2014, 54, 289-301.	5.4	14

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163	ARIAweb: a server for automated NMR structure calculation. Nucleic Acids Research, 2020, 48, W41-W47.	14.5	14
164	Bayesian inference of chromatin structure ensembles from population-averaged contact data. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 7824-7830.	7.1	14
165	Exploring protein interiors: The role of a buried histidine in the KH module fold. Proteins: Structure, Function and Bioinformatics, 1999, 34, 484-496.	2.6	13
166	ATP conformations and ion binding modes in the active site of anthrax edema factor: A computational analysis. Proteins: Structure, Function and Bioinformatics, 2009, 77, 971-983.	2.6	13
167	NMR in the SPINE Structural Proteomics project. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 1150-1161.	2.5	12
168	Error distribution derived NOE distance restraints. Proteins: Structure, Function and Bioinformatics, 2006, 64, 652-664.	2.6	12
169	Temperature Accelerated Molecular Dynamics with Soft-Ratcheting Criterion Orients Enhanced Sampling by Low-Resolution Information. Journal of Chemical Theory and Computation, 2015, 11, 3446-3454.	5.3	12
170	Structural determination of Streptococcus pyogenes M1 protein interactions with human immunoglobulin G using integrative structural biology. PLoS Computational Biology, 2021, 17, e1008169.	3.2	12
171	Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems. Lecture Notes in Computer Science, 2011, , 206-217.	1.3	12
172	InDeep: 3D fully convolutional neural networks to assist in silico drug design on proteinâ€“protein interactions. Bioinformatics, 2022, 38, 1261-1268.	4.1	12
173	Solution structure of the coiled-coil trimerization domain from lung surfactant protein D. Journal of Biomolecular NMR, 2002, 24, 89-102.	2.8	11
174	1H and 15N NMR resonance assignments and secondary structure of titin type I domains. Journal of Biomolecular NMR, 1997, 9, 2-10.	2.8	10
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