Michael Nilges

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3090407/publications.pdf

Version: 2024-02-01

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	Bat coronaviruses related to SARS-CoV-2 and infectious for human cells. Nature, 2022, 604, 330-336.	27.8	238
2	InDeep: 3D fully convolutional neural networks to assist in silico drug design on proteinâ€“protein interactions. Bioinformatics, 2022, 38, 1261-1268.	4.1	12
3	quicksom: Self-Organizing Maps on GPUs for clustering of molecular dynamics trajectories. Bioinformatics, 2021, 37, 2064-2065.	4.1	7
4	The iPPI-DB initiative: a community-centered database of proteinâ€“protein interaction modulators. Bioinformatics, 2021, 37, 89-96.	4.1	24
5	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
6	Automatic Bayesian Weighting for SAXS Data. Frontiers in Molecular Biosciences, 2021, 8, 671011.	3.5	4
7	Host-Pathogen Adhesion as the Basis of Innovative Diagnostics for Emerging Pathogens. Diagnostics, 2021, 11, 1259.	2.6	5
8	1H, 15ÂN and 13C resonance assignments of the C-terminal domain of PulL, a component of the Klebsiella oxytoca type II secretion system. Biomolecular NMR Assignments, 2021, 15, 455-459.	0.8	2
9	Computational and biochemical analysis of type IV pilus dynamics and stability. Structure, 2021, 29, 1397-1409.e6.	3.3	5
10	Quantitative Structural Interpretation of Protein Crosslinks. Structure, 2020, 28, 75-82.e4.	3.3	5
11	Structure and function of minor pilins of type IV pili. Medical Microbiology and Immunology, 2020, 209, 301-308.	4.8	40
12	ARIAweb: a server for automated NMR structure calculation. Nucleic Acids Research, 2020, 48, W41-W47.	14.5	14
13	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
14	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
15	Dynamics of a type 2 secretion system pseudopilus unraveled by complementary approaches. Journal of Biomolecular NMR, 2019, 73, 293-303.	2.8	9
16	Structure and Assembly of the Enterohemorrhagic Escherichia coli Type 4 Pilus. Structure, 2019, 27, 1082-1093.e5.	3.3	33
17	Bayesian Weighing of Electron Cryo-Microscopy Data for Integrative Structural Modeling. Structure, 2019, 27, 175-188.e6.	3.3	50
18	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

#	Article	IF	Citations
19	Minimal NMR distance information for rigidity of protein graphs. Discrete Applied Mathematics, 2019, 256, 91-104.	0.9	26
20	Quantitative Understanding of Distances from Cross Linking Mass Spectrometry. Biophysical Journal, 2018, 114, 45a.	0.5	0
21	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
22	Ordering Protein Contact Matrices. Computational and Structural Biotechnology Journal, 2018, 16, 140-156.	4.1	0
23	Tuning interval Branch-and-Prune for protein structure determination. Journal of Global Optimization, 2018, 72, 109-127.	1.8	19
24	Integrative Structural Biology of the Calcium Dependent Type 2 Secretion Pseudopilus. Biophysical Journal, 2018, 114, 229a.	0.5	0
25	Automatic Building of Protein Atomic Models from Cryo-EM Maps. Biophysical Journal, 2018, 114, 190a-191a.	0.5	2
26	Conformational sampling of CpxA: Connecting HAMP motions to the histidine kinase function. PLoS ONE, 2018, 13, e0207899.	2.5	1
27	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
28	Nicotine reverses hypofrontality in animal models of addiction and schizophrenia. Nature Medicine, 2017, 23, 347-354.	30.7	142
29	Integrative Structural Biology of a Type II Secretion Pseudopilus. Biophysical Journal, 2017, 112, 486a.	0.5	0
30	The Interval Branch-And-Prune Algorithm for the Protein Structure Determination. Biophysical Journal, 2017, 112, 56a.	0.5	0
31	Structural Characterization of Whirlin Reveals an Unexpected and Dynamic Supramodule Conformation of Its PDZ Tandem. Structure, 2017, 25, 1645-1656.e5.	3.3	22
32	Structure of the calcium-dependent type 2 secretion pseudopilus. Nature Microbiology, 2017, 2, 1686-1695.	13.3	68
33	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
34	SAS profile correlations reveal SAS hierarchical nature and information content. PLoS ONE, 2017, 12, e0177309.	2.5	6
35	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. Bioinformatics, 2016, 32, 85-95.	4.1	95
36	Modification in hydrophobic packing of HAMP domain induces a destabilization of the autoâ€phosphorylation site in the histidine kinase CpxA. Biopolymers, 2016, 105, 670-682.	2.4	2

#	Article	IF	Citations
37	Deciphering the Binding Mode of Promising Antituberculosis Compounds with their Bacterial Membrane Target in Living Cells by NMR. Biophysical Journal, 2016, 110, 542a.	0.5	0
38	Building Graphs to Describe Dynamics, Kinetics and Energetics in the D-Ala:D-Lac Ligase Vana. Biophysical Journal, 2016, 110, 378a.	0.5	0
39	Automated Cross-Links-Based Conformational Sampling of Protein Assemblies: The Geometrical Challenge of Cross-Links. Biophysical Journal, 2016, 110, 539a.	0.5	0
40	Automated structure modeling of large protein assemblies using crosslinks as distance restraints. Nature Methods, 2016, 13, 515-520.	19.0	49
41	Building Graphs To Describe Dynamics, Kinetics, and Energetics in the <scp>d</scp>-ALa:<scp>d</scp>-Lac Ligase VanA. Journal of Chemical Information and Modeling, 2016, 56, 1762-1775.	5.4	9
42	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
43	Inferential Structure Determination of Chromosomes from Single-Cell Hi-C Data. PLoS Computational Biology, 2016, 12, e1005292.	3.2	52
44	SAS Profile Correlations Reveal the Hierarchical Nature of SAS Data and Suggest New Scoring Strategies. Biophysical Journal, 2015, 108, 45a.	0.5	0
45	Allosteric Communication within the Cytoplasmic Region of the Histidine Kinase CpxA, Revealed by Molecular Dynamics Simulations of the Wild-Type and M228V Proteins. Biophysical Journal, 2015, 108, 184a.	0.5	0
46	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
47	An automatic tool to analyze and cluster macromolecular conformations based on self-organizing maps. Bioinformatics, 2015, 31, 1490-1492.	4.1	28
48	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
49	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	3.3	159
50	Improved reliability, accuracy and quality in automated NMR structure calculation with ARIA. Journal of Biomolecular NMR, 2015, 62, 425-438.	2.8	34
51	An algorithm to enumerate all possible protein conformations verifying a set of distance constraints. BMC Bioinformatics, 2015, 16, 23.	2.6	42
52	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
53	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
54	Neisseria meningitidis Type IV Pili Composed of Sequence Invariable Pilins Are Masked by Multisite Glycosylation. PLoS Pathogens, 2015, 11, e1005162.	4.7	55

#	Article	IF	Citations
55	Computational Design of Protein-Based Inhibitors of Plasmodium vivax Subtilisin-Like 1 Protease. PLoS ONE, 2014, 9, e109269.	2.5	4
56	ModBase, a database of annotated comparative protein structure models and associated resources. Nucleic Acids Research, 2014, 42, D336-D346.	14.5	275
57	Stabilization of the integraseâ€ÐNA 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
58	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
59	Functional Motions Modulating VanA Ligand Binding Unraveled by Self-Organizing Maps. Journal of Chemical Information and Modeling, 2014, 54, 289-301.	5.4	14
60	Convective Replica-Exchange in Ergodic Regimes. Journal of Chemical Theory and Computation, 2014, 10, 953-958.	5.3	3
61	Enhanced Sampling of the Catalytic Domain of the Adenyl Cyclase CyaA from Bordetella Pertussis. Biophysical Journal, 2014, 106, 610a.	0.5	0
62	Structural Basis of Conformational Transitions Involved in Pseudopilus Assembly and Stability. Biophysical Journal, 2014, 106, 26a.	0.5	0
63	SAXS Merge: an automated statistical method to merge SAXS profiles using Gaussian processes. Journal of Synchrotron Radiation, 2014, 21, 203-208.	2.4	15
64	Structures of Biomolecular Complexes from Heterogeneous Data and Bayesian Data Analysis. Biophysical Journal, 2013, 104, 376a.	0.5	0
65	Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-1570.	3.3	151
66	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
67	A convective replicaâ€exchange method for sampling new energy basins. Journal of Computational Chemistry, 2013, 34, 132-140.	3.3	18
68	Distance Geometry in Structural Biology: New Perspectives. , 2013, , 329-350.		16
69	Lobeline Docking on AChBP and Nicotinic Receptors: Discriminating Importance of the Pocket Geometry and of the Ligand Configuration. Letters in Drug Design and Discovery, 2012, 9, 54-62.	0.7	2
70	Efficient Modeling of Symmetric Protein Aggregates from NMR Data. Angewandte Chemie - International Edition, 2012, 51, 6916-6919.	13.8	7
71	Computational approaches to the interpretation of NMR data for studying protein dynamics. Chemical Physics, 2012, 396, 124-134.	1.9	9
72	Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data. Structure, 2012, 20, 227-236.	3.3	75

#	Article	IF	Citations
73	ARIA for Solution and Solid-State NMR. Methods in Molecular Biology, 2012, 831, 453-483.	0.9	54
74	Modeling pilus structures from sparse data. Journal of Structural Biology, 2011, 173, 436-444.	2.8	36
75	Combining computational modeling with sparse and low-resolution data. Journal of Structural Biology, 2011, 173, 419.	2.8	1
76	Posttranslational Modification of Pili upon Cell Contact Triggers N. meningitidis Dissemination. Science, 2011, 331, 778-782.	12.6	162
77	Computational Reverse-Engineering of a Spider-Venom Derived Peptide Active Against Plasmodium falciparum SUB1. PLoS ONE, 2011, 6, e21812.	2.5	35
78	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
79	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
80	The redundancy of NMR restraints can be used to accelerate the unfolding behavior of an SH3 domain during molecular dynamics simulations. BMC Structural Biology, 2011, 11, 46.	2.3	1
81	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
82	Grid computing for improving conformational sampling in NMR structurecalculation. Bioinformatics, 2011, 27, 1713-1714.	4.1	2
83	Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems. Lecture Notes in Computer Science, 2011, , 206-217.	1.3	12
84	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
85	Architecture of the RNA polymerase IIâ€“TFIIF complex revealed by cross-linking and mass spectrometry. EMBO Journal, 2010, 29, 717-726.	7.8	355
86	Visualization of macromolecular structures. Nature Methods, 2010, 7, S42-S55.	19.0	137
87	Simultaneous use of solution, solid-state NMR and X-ray crystallography to study the conformational landscape of the Crh protein during oligomerization and crystallization. Advances and Applications in Bioinformatics and Chemistry, 2010, 3, 25.	2.6	0
88	Structural Insights into Serine-rich Fimbriae from Gram-positive Bacteria. Journal of Biological Chemistry, 2010, 285, 32446-32457.	3.4	48
89	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
90	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

#	Article	IF	Citations
91	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
92	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
93	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
94	CASD-NMR: critical assessment of automated structure determination by NMR. Nature Methods, 2009, 6, 625-626.	19.0	80
95	Toward a Unified Representation of Protein Structural Dynamics in Solution. Journal of the American Chemical Society, 2009, 131, 16968-16975.	13.7	105
96	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
97	A unifying probabilistic framework for analyzing residual dipolar couplings. Journal of Biomolecular NMR, 2008, 40, 135-144.	2.8	16
98	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
99	Graphical analysis of NMR structural quality and interactive contact map of NOE assignments in ARIA. BMC Structural Biology, 2008, 8, 30.	2.3	5
100	Probabilistic structure calculation. Comptes Rendus Chimie, 2008, 11, 356-369.	0.5	6
101	Accurate NMR Structures Through Minimization of an Extended Hybrid Energy. Structure, 2008, 16, 1305-1312.	3.3	58
102	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
103	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
104	SNARE Protein Mimicry by an Intracellular Bacterium. PLoS Pathogens, 2008, 4, e1000022.	4.7	156
105	Structural Biology by NMR: Structure, Dynamics, and Interactions. PLoS Computational Biology, 2008, 4, e1000168.	3.2	120
106	ISD: a software package for Bayesian NMR structure calculation. Bioinformatics, 2008, 24, 1104-1105.	4.1	39
107	Shelling the Voronoi interface of protein-protein complexes predicts residue activity and conservation. Nature Precedings, 2008, , .	0.1	0
108	Shelling the Voronoi interface of protein-protein complexes predicts residue activity and conservation. Nature Precedings, 2008, , .	0.1	2

#	Article	IF	Citations
109	Structural Bioinformatics and NMR Structure Determination. Nucleic Acids and Molecular Biology, 2008, , 123-137.	0.2	1
110	ARIA2: Automated NOE assignment and data integration in NMR structure calculation. Bioinformatics, 2007, 23, 381-382.	4.1	506
111	Biskit A software platform for structural bioinformatics. Bioinformatics, 2007, 23, 769-770.	4.1	61
112	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
113	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
114	NMR in the SPINE Structural Proteomics project. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 1150-1161.	2.5	12
115	Error distribution derived NOE distance restraints. Proteins: Structure, Function and Bioinformatics, 2006, 64, 652-664.	2.6	12
116	Determination of dihedral Î¨ angles in large proteins by combining NHN/CÎ±HÎ± dipole/dipole cross-correlation and chemical shifts. Proteins: Structure, Function and Bioinformatics, 2006, 64, 931-939.	2.6	4
117	Comparison of Different Torsion Angle Approaches for NMR Structure Determination. Journal of Biomolecular NMR, 2006, 34, 153-166.	2.8	7
118	Flexibility and Conformational Entropy in Protein-Protein Binding. Structure, 2006, 14, 683-693.	3.3	132
119	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
120	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
121	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
122	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
123	Influence of chemical shift tolerances on NMR structure calculations using ARIA protocols for assigning NOE data. Journal of Biomolecular NMR, 2005, 31, 21-34.	2.8	9
124	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
125	Inferential Structure Determination. Science, 2005, 309, 303-306.	12.6	333
126	Replica-Exchange Monte Carlo Scheme for Bayesian Data Analysis. Physical Review Letters, 2005, 94, 018105.	7.8	64

#	Article	IF	Citations
127	Bayesian inference applied to macromolecular structure determination. Physical Review E, 2005, 72, 031912.	2.1	35
128	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
129	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
130	Normal Mode Analysis Suggests a Quaternary Twist Model for the Nicotinic Receptor Gating Mechanism. Biophysical Journal, 2005, 88, 3954-3965.	0.5	178
131	A new principle for macromolecular structure determination. AIP Conference Proceedings, 2004, , .	0.4	2
132	Estimation of proton configurations from NOESY spectra. AIP Conference Proceedings, 2004, , .	0.4	1
133	Conservation of the Biochemical Properties of IncA from Chlamydia trachomatis and Chlamydia caviae. Journal of Biological Chemistry, 2004, 279, 46896-46906.	3.4	82
134	Structure determination from heterogeneous NMR data. AIP Conference Proceedings, 2004, , .	0.4	0
135	Complementarity of Structure Ensembles in Protein-Protein Binding. Structure, 2004, 12, 2125-2136.	3.3	173
136	The impact of protein flexibility on protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2004, 58, 126-133.	2.6	42
137	Correction of spin diffusion during iterative automated NOE assignment. Journal of Magnetic Resonance, 2004, 167, 334-342.	2.1	55
138	Solution Structure of the 30 kDa Polysulfide-Sulfur Transferase Homodimer from Wolinella succinogenes,. Biochemistry, 2004, 43, 1418-1424.	2.5	23
139	NOE Assignment With ARIA 2.0: The Nuts and Bolts. , 2004, 278, 379-402.		58
140	Refinement of protein structures in explicit solvent. Proteins: Structure, Function and Bioinformatics, 2003, 50, 496-506.	2.6	571
141	ARIA: automated NOE assignment and NMR structure calculation. Bioinformatics, 2003, 19, 315-316.	4.1	437
142	Calculation of Symmetric Oligomer Structures from NMR Data. , 2002, , 131-161.		7
143	Structure of the histone mRNA hairpin required for cell cycle regulation of histone gene expression. Rna, 2002, 8, 29-46.	3.5	45
144	Pathways and Intermediates in Forced Unfolding of Spectrin Repeats. Structure, 2002, 10, 1085-1096.	3.3	75

#	Article	IF	Citations
145	Protein folding in mode space: A collective coordinate approach to structure prediction. Proteins: Structure, Function and Bioinformatics, 2002, 49, 365-377.	2.6	2
146	Solution structure of the coiled-coil trimerization domain from lung surfactant protein D. Journal of Biomolecular NMR, 2002, 24, 89-102.	2.8	11
147	Automated Assignment of Ambiguous Nuclear Overhauser Effects with ARIA. Methods in Enzymology, 2001, 339, 71-90.	1.0	319
148	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
149	Re-Face Stereospecificity of Methylenetetrahydromethanopterin and Methylenetetrahydrofolate Dehydrogenases is Predetermined by Intrinsic Properties of the Substrate. ChemBioChem, 2001, 2, 530-541.	2.6	25
150	NMR studies of the sporulation protein SpoIIAA: implications for the regulation of the transcription factor sigmaF in Bacillus subtilis. Journal of Biomolecular NMR, 2001, 19, 293-304.	2.8	9
151	Continuum solvent molecular dynamics study of flexibility in interleukin-8. Journal of Molecular Graphics and Modelling, 2001, 19, 136-145.	2.4	25
152	Re-Face Stereospecificity of Methylenetetrahydromethanopterin and Methylenetetrahydrofolate Dehydrogenases is Predetermined by Intrinsic Properties of the Substrate. ChemBioChem, 2001, 2, 530-541.	2.6	1
153	Applications of Molecular Modeling in NMR Structure Determination. , 2001, , .		0
154	Efficient sampling in collective coordinate space. , 2000, 39, 82-88.		31
155	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
156	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
157	Refinement of the protein backbone angle psi in NMR structure calculations. Journal of Biomolecular NMR, 2000, 16, 47-58.	2.8	27
158	A new approach for applying residual dipolar couplings as restraints in structure elucidation. Journal of Biomolecular NMR, 2000, 16, 245-252.	2.8	89
159	1H, 15N, and 13C resonance assignment of the PH domain from C. elegans UNC-89. Journal of Biomolecular NMR, 1999, 15, 269-270.	2.8	7
160	The structure in solution of the b domain of protein disulfide isomerase. Journal of Biomolecular NMR, 1999, 13, 357-368.	2.8	62
161	StarDOM: from STAR format to XML. Journal of Biomolecular NMR, 1999, 15, 169-172.	2.8	2
162	Influence of non-bonded parameters on the quality of NMR structures: a new force field for NMR structure calculation. , 1999, 13, 51-59.		246

#	Article	IF	Citations
163	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	0
164	The PH superfold: a structural scaffold for multiple functions. Trends in Biochemical Sciences, 1999, 24, 441-445.	7.5	175
165	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
166	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
167	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
168	Classification of protein sequences by homology modeling and quantitative analysis of electrostatic similarity. , 1999, 37, 379-387.		87
169	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
170	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
171	Ambiguous NOEs and automated NOE assignment. Progress in Nuclear Magnetic Resonance Spectroscopy, 1998, 32, 107-139.	7.5	198
172	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
173	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
174	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
175	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
176	Are there non-trivial dynamic cross-correlations in proteins?. Journal of Molecular Biology, 1998, 279, 911-920.	4.2	47
177	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
178	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
179	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
180	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

#	Article	IF	Citations
181	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
182	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
183	The folding catalyst protein disulfide isomerase is constructed of active and inactive thioredoxin modules. Current Biology, 1997, 7, 239-245.	3.9	217
184	Functional diversity of PH domains: an exhaustive modelling study. Folding & Design, 1997, 2, 343-355.	4.5	32
185	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
186	Ambiguous distance data in the calculation of NMR structures. Folding & Design, 1997, 2, S53-S57.	4.5	53
187	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
188	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
189	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
190	Three-Dimensional Structure and Stability of the KH Domain: Molecular Insights into the Fragile X Syndrome. Cell, 1996, 85, 237-245.	28.9	283
191	Structure calculation from NMR data. Current Opinion in Structural Biology, 1996, 6, 617-623.	5.7	48
192	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
193	Molecular Replacement with NMR Models Using Distance-Derived PseudoBFactors. Acta Crystallographica Section D: Biological Crystallography, 1996, 52, 973-982.	2.5	16
194	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
195	Internal repeats in the BRCA2 protein sequence. Nature Genetics, 1996, 13, 22-23.	21.4	189
196	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
197	Three-dimensional structure of the single-stranded DNA-binding protein encoded by gene V of the filamentous bacteriophage M13 and a model of its complex with single-stranded DNA. FEMS Microbiology Reviews, 1995, 17, 57-72.	8.6	8
198	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

#	Article	IF	Citations
199	Structure of the pleckstrin homology domain from Î²-spectrin. Nature, 1994, 369, 675-677.	27.8	256
200	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
201	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
202	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
203	A calculation strategy for the structure determination of symmetric demers by1H NMR. Proteins: Structure, Function and Bioinformatics, 1993, 17, 297-309.	2.6	323
204	Assessing the quality of solution nuclear magnetic resonance structures by complete cross-validation. Science, 1993, 261, 328-331.	12.6	155
205	Computational challenges for macromolecular structure determination by X-ray crystallography and solution NMRspectroscopy. Quarterly Reviews of Biophysics, 1993, 26, 49-125.	5.7	165
206	NMR Relaxation Matrix Refinement of a DNA Octamer Solution Structure.. Acta Chemica Scandinavica, 1993, 47, 43-56.	0.7	7
207	Sampling and efficiency of metric matrix distance geometry: A novel partial metrization algorithm. Journal of Biomolecular NMR, 1992, 2, 33-56.	2.8	210
208	Relaxation matrix refinement of the solution structure of squash trypsin inhibitor. Journal of Molecular Biology, 1991, 219, 499-510.	4.2	162
209	Automated modeling of coiled coils: application to the GCN4 dimerization region. Protein Engineering, Design and Selection, 1991, 4, 649-659.	2.1	95
210	Sampling Properties of Simulated Annealing and Distance Geometry. , 1991, , 451-455.		26
211	1H-Nmr stereospecific assignments by conformational data-base searches. Biopolymers, 1990, 29, 813-822.	2.4	108
212	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
213	Conformation of secretin in dimethyl sulfoxide solution. NMR studies and restrained molecular dynamics. FEBS Journal, 1989, 186, 95-103.	0.2	15
214	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
215	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
216	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

#	Article	IF	Citations
217	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
218	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
219	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
220	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
221	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
222	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
223	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
224	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
225	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
226	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
227	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
228	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
229	Application of the z-COSY technique with a modified pulse sequence to measurement of coupling constants in macromolecules. Journal of Magnetic Resonance, 1987, 75, 534-539.	0.5	8
230	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