Michael Nilges

List of Publications by Citations

220 papers	29,429 citations	65 h-index	171 g-index
247 ext. papers	30,893 ext. citations	6.9 avg, IF	6.47 L-index

#	Paper	IF	Citations
220	Crystallography & NMR system: A new software suite for macromolecular structure determination. *Acta Crystallographica Section D: Biological Crystallography*, **1998**, 54, 905-21		14106
219	Determination of three-dimensional structures of proteins from interproton distance data by hybrid distance geometry-dynamical simulated annealing calculations. *FEBS Letters*, **1988**, 229, 317-24	3.8	665
218	Refinement of protein structures in explicit solvent. *Proteins: Structure, Function and Bioinformatics*, **2003**, 50, 496-506	4.2	521
217	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, 7241-57	3.2	496
216	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	1.9	467
215	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, 129-36	3.8	466
214	ARIA2: automated NOE assignment and data integration in NMR structure calculation. *Bioinformatics*, **2007**, 23, 381-2	7.2	404
213	ARIA: automated NOE assignment and NMR structure calculation. *Bioinformatics*, **2003**, 19, 315-6	7.2	397
212	Automated NOESY interpretation with ambiguous distance restraints: the refined NMR solution structure of the pleckstrin homology domain from beta-spectrin. *Journal of Molecular Biology*, **1997**, 269, 408-22	6.5	395
211	Calculation of protein structures with ambiguous distance restraints. Automated assignment of ambiguous NOE crosspeaks and disulphide connectivities. *Journal of Molecular Biology*, **1995**, 245, 645-60	6.5	324
210	Architecture of the RNA polymerase II-TFIIF complex revealed by cross-linking and mass spectrometry. *EMBO Journal*, **2010**, 29, 717-26	13	322
209	A calculation strategy for the structure determination of symmetric dimers by 1H NMR. *Proteins: Structure, Function and Bioinformatics*, **1993**, 17, 297-309	4.2	301
208	Automated assignment of ambiguous nuclear overhauser effects with ARIA. *Methods in Enzymology*, **2001**, 339, 71-90	1.7	300
207	RECOORD: a recalculated coordinate database of 500+ proteins from the PDB using restraints from the BioMagResBank. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 662-72	4.2	285
206	Three-dimensional structure of potato carboxypeptidase inhibitor in solution. A study using nuclear magnetic resonance, distance geometry, and restrained molecular dynamics. *Biochemistry*, **1987**, 26, 8012-23	3.2	270
205	Inferential structure determination. *Science*, **2005**, 309, 303-6	33.3	268
204	Three-dimensional structure and stability of the KH domain: molecular insights into the fragile X syndrome. *Cell*, **1996**, 85, 237-45	56.2	258

203	Structure of the pleckstrin homology domain from beta-spectrin. *Nature*, **1994**, 369, 675-7	50.4	239
202	Influence of non-bonded parameters on the quality of NMR structures: a new force field for NMR structure calculation. *Journal of Biomolecular NMR*, **1999**, 13, 51-9	3	231
201	The three-dimensional structure of α-purothionin in solution: combined use of nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO Journal*, **1986**, 5, 2729-2735	13	208
200	ModBase, a database of annotated comparative protein structure models and associated resources. *Nucleic Acids Research*, **2014**, 42, D336-46	20.1	207
199	Sampling and efficiency of metric matrix distance geometry: a novel partial metrization algorithm. *Journal of Biomolecular NMR*, **1992**, 2, 33-56	3	192
198	The folding catalyst protein disulfide isomerase is constructed of active and inactive thioredoxin modules. *Current Biology*, **1997**, 7, 239-45	6.3	185
197	Ambiguous NOEs and automated NOE assignment. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **1998**, 32, 107-139	10.4	185
196	Internal repeats in the BRCA2 protein sequence. *Nature Genetics*, **1996**, 13, 22-3	36.3	173
195	Structure determination of the N-terminal thioredoxin-like domain of protein disulfide isomerase using multidimensional heteronuclear 13C/15N NMR spectroscopy. *Biochemistry*, **1996**, 35, 7684-91	3.2	172
194	Normal mode analysis suggests a quaternary twist model for the nicotinic receptor gating mechanism. *Biophysical Journal*, **2005**, 88, 3954-65	2.9	165
193	Complementarity of structure ensembles in protein-protein binding. *Structure*, **2004**, 12, 2125-36	5.2	160
192	The PH superfold: a structural scaffold for multiple functions. *Trends in Biochemical Sciences*, **1999**, 24, 441-5	10.3	159
191	Posttranslational modification of pili upon cell contact triggers N. meningitidis dissemination. *Science*, **2011**, 331, 778-82	33.3	149
190	The structure of a novel insecticidal neurotoxin, omega-atracotoxin-HV1, from the venom of an Australian funnel web spider. *Nature Structural Biology*, **1997**, 4, 559-66		149
189	Relaxation matrix refinement of the solution structure of squash trypsin inhibitor. *Journal of Molecular Biology*, **1991**, 219, 499-510	6.5	148
188	Assessing the quality of solution nuclear magnetic resonance structures by complete cross-validation. *Science*, **1993**, 261, 328-31	33.3	146
187	Computational challenges for macromolecular structure determination by X-ray crystallography and solution NMR-spectroscopy. *Quarterly Reviews of Biophysics*, **1993**, 26, 49-125	7	143
186	Solution structure of the spectrin repeat: a left-handed antiparallel triple-helical coiled-coil. *Journal of Molecular Biology*, **1997**, 273, 740-51	6.5	135

185	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure*, **2015**, 23, 1156-67	5.2	131
184	3D structure determination of the Crh protein from highly ambiguous solid-state NMR restraints. *Journal of the American Chemical Society*, **2008**, 130, 3579-89	16.4	128
183	SNARE protein mimicry by an intracellular bacterium. *PLoS Pathogens*, **2008**, 4, e1000022	7.6	124
182	Recommendations of the wwPDB NMR Validation Task Force. *Structure*, **2013**, 21, 1563-70	5.2	117
181	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, 33953-9	5.4	117
180	Flexibility and conformational entropy in protein-protein binding. *Structure*, **2006**, 14, 683-93	5.2	113
179	The three-dimensional structure of the HRDC domain and implications for the Werner and Bloom syndrome proteins. *Structure*, **1999**, 7, 1557-66	5.2	110
178	Nicotine reverses hypofrontality in animal models of addiction and schizophrenia. *Nature Medicine*, **2017**, 23, 347-354	50.5	107
177	Visualization of macromolecular structures. *Nature Methods*, **2010**, 7, S42-55	21.6	107
176	Solution structure of the DNA-binding domain and model for the complex of multifunctional hexameric arginine repressor with DNA. *Nature Structural Biology*, **1997**, 4, 819-26		104
175	Floating stereospecific assignment revisited: application to an 18 kDa protein and comparison with J-coupling data. *Journal of Biomolecular NMR*, **1997**, 9, 245-58	3	100
174	Toward a unified representation of protein structural dynamics in solution. *Journal of the American Chemical Society*, **2009**, 131, 16968-75	16.4	98
173	1H-NMR stereospecific assignments by conformational data-base searches. *Biopolymers*, **1990**, 29, 813-22	2.2	97
172	Structural biology by NMR: structure, dynamics, and interactions. *PLoS Computational Biology*, **2008**, 4, e1000168	5	94
171	An efficient protocol for NMR-spectroscopy-based structure determination of protein complexes in solution. *Angewandte Chemie - International Edition*, **2010**, 49, 1967-70	16.4	88
170	High resolution NMR solution structure of the leucine zipper domain of the c-Jun homodimer. *Journal of Biological Chemistry*, **1996**, 271, 13663-7	5.4	85
169	Automated modeling of coiled coils: application to the GCN4 dimerization region. *Protein Engineering, Design and Selection*, **1991**, 4, 649-59	1.9	85
168	A new approach for applying residual dipolar couplings as restraints in structure elucidation. *Journal of Biomolecular NMR*, **2000**, 16, 245-52	3	83

167	Structural and functional studies of titin'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, 431-47	6.5	82
166	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		77
165	Classification of protein sequences by homology modeling and quantitative analysis of electrostatic similarity. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 379-87	4.2	76
164	Three-dimensional structure of phoratoxin in solution: combined use of nuclear magnetic resonance, distance geometry, and restrained molecular dynamics. *Biochemistry*, **1987**, 26, 1732-1745	3.2	76
163	The conformations of hirudin in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO Journal*, **1987**, 6, 529-537	13	76
162	Conservation of the biochemical properties of IncA from Chlamydia trachomatis and Chlamydia caviae: oligomerization of IncA mediates interaction between facing membranes. *Journal of Biological Chemistry*, **2004**, 279, 46896-906	5.4	73
161	The solution structure of the first KH domain of FMR1, the protein responsible for the fragile X syndrome. *Nature Structural Biology*, **1997**, 4, 712-6		71
160	Pathways and intermediates in forced unfolding of spectrin repeats. *Structure*, **2002**, 10, 1085-96	5.2	71
159	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, 3718-33	3.2	71
158	Weighting of experimental evidence in macromolecular structure determination. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 1756-61	11.5	66
157	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, 133-46	4.2	66
156	Blind testing of routine, fully automated determination of protein structures from NMR data. *Structure*, **2012**, 20, 227-36	5.2	64
155	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, 3734-44	3.2	61
154	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. *Bioinformatics*, **2016**, 32, 85-95	7.2	60
153	The structure in solution of the b domain of protein disulfide isomerase. *Journal of Biomolecular NMR*, **1999**, 13, 357-68	3	60
152	The solution structure of the Tyr41-->His mutant of the single-stranded DNA binding protein encoded by gene V of the filamentous bacteriophage M13. *Journal of Molecular Biology*, **1994**, 236, 229-46	6.5	60
151	Essential spaces defined by NMR structure ensembles and molecular dynamics simulation show significant overlap. *Proteins: Structure, Function and Bioinformatics*, **1998**, 31, 370-382	4.2	58
150	Replica-exchange Monte Carlo scheme for bayesian data analysis. *Physical Review Letters*, **2005**, 94, 018105	7.4	56

149	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, 13081-6	11.5	54
148	A structure refinement protocol combining NMR residual dipolar couplings and small angle scattering restraints. *Journal of Biomolecular NMR*, **2008**, 41, 199-208	3	52
147	CASD-NMR: critical assessment of automated structure determination by NMR. *Nature Methods*, **2009**, 6, 625-6	21.6	51
146	Biskit--a software platform for structural bioinformatics. *Bioinformatics*, **2007**, 23, 769-70	7.2	51
145	Correction of spin diffusion during iterative automated NOE assignment. *Journal of Magnetic Resonance*, **2004**, 167, 334-42	3	51
144	NOE assignment with ARIA 2.0: the nuts and bolts. *Methods in Molecular Biology*, **2004**, 278, 379-402	1.4	50
143	Ambiguous distance data in the calculation of NMR structures. *Folding & Design*, **1997**, 2, S53-7		49
142	Improved strategies for the determination of protein structures from NMR data: the solution structure of acyl carrier protein. *FEBS Letters*, **1989**, 242, 218-24	3.8	49
141	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	6.1	47
140	Comparative analysis of structural and dynamic properties of the loaded and unloaded hemophore HasA: functional implications. *Journal of Molecular Biology*, **2008**, 376, 517-25	6.5	47
139	Structure of Complement C3(H2O) Revealed By Quantitative Cross-Linking/Mass Spectrometry And Modeling. *Molecular and Cellular Proteomics*, **2016**, 15, 2730-43	7.6	46
138	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, 341-57	6.5	46
137	Are there non-trivial dynamic cross-correlations in proteins?. *Journal of Molecular Biology*, **1998**, 279, 911-20	6.5	45
136	Automated structure modeling of large protein assemblies using crosslinks as distance restraints. *Nature Methods*, **2016**, 13, 515-20	21.6	44
135	Structural insights into serine-rich fimbriae from Gram-positive bacteria. *Journal of Biological Chemistry*, **2010**, 285, 32446-57	5.4	43
134	Accurate NMR structures through minimization of an extended hybrid energy. *Structure*, **2008**, 16, 1305-12	5.2	43
133	Neisseria meningitidis Type IV Pili Composed of Sequence Invariable Pilins Are Masked by Multisite Glycosylation. *PLoS Pathogens*, **2015**, 11, e1005162	7.6	42
132	Structure calculation from NMR data. *Current Opinion in Structural Biology*, **1996**, 6, 617-23	8.1	41

131	Distinct docking and stabilization steps of the Pseudopilus conformational transition path suggest rotational assembly of type IV pilus-like fibers. *Structure*, **2014**, 22, 685-96	5.2	40
130	Shelling the Voronoi interface of protein-protein complexes reveals patterns of residue conservation, dynamics, and composition. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 677-92	4.2	39
129	The three-dimensional structure of a type I module from titin: a prototype of intracellular fibronectin type III domains. *Structure*, **1998**, 6, 1291-302	5.2	39
128	Structure of the calcium-dependent type 2 secretion pseudopilus. *Nature Microbiology*, **2017**, 2, 1686-1695	25.6	38
127	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, 269-77	3.8	38
126	ARIA for solution and solid-state NMR. *Methods in Molecular Biology*, **2012**, 831, 453-83	1.4	38
125	A role for specific collagen motifs during wound healing and inflammatory response of fibroblasts in the teleost fish gilthead seabream. *Molecular Immunology*, **2011**, 48, 826-34	4.3	36
124	Inferential Structure Determination of Chromosomes from Single-Cell Hi-C Data. *PLoS Computational Biology*, **2016**, 12, e1005292	5	36
123	Bat coronaviruses related to SARS-CoV-2 and infectious for human cells.. *Nature*, **2022**,	50.4	36
122	The impact of protein flexibility on protein-protein docking. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 126-33	4.2	35
121	Modeling pilus structures from sparse data. *Journal of Structural Biology*, **2011**, 173, 436-44	3.4	34
120	Modeling errors in NOE data with a log-normal distribution improves the quality of NMR structures. *Journal of the American Chemical Society*, **2005**, 127, 16026-7	16.4	34
119	Structure of the histone mRNA hairpin required for cell cycle regulation of histone gene expression. *Rna*, **2002**, 8, 29-46	5.8	34
118	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	3	34
117	Heteronuclear relaxation study of the PH domain of beta-spectrin: restriction of loop motions upon binding inositol trisphosphate. *Journal of Molecular Biology*, **1998**, 280, 879-96	6.5	33
116	Influence of internal dynamics on accuracy of protein NMR structures: derivation of realistic model distance data from a long molecular dynamics trajectory. *Journal of Molecular Biology*, **1999**, 285, 727-40	6.5	33
115	Determination of the backbone conformation of secretin by restrained molecular dynamics on the basis of interproton distance data. *FEBS Journal*, **1988**, 171, 479-84		33
114	An algorithm to enumerate all possible protein conformations verifying a set of distance constraints. *BMC Bioinformatics*, **2015**, 16, 23	3.6	32

113	Unraveling the symmetry ambiguity in a hexamer: calculation of the R6 human insulin structure. *Journal of Biomolecular NMR*, **2000**, 16, 93-108	3	32
112	Sequential resonance assignment and secondary structure determination of the Ascaris trypsin inhibitor, a member of a novel class of proteinase inhibitors. *Biochemistry*, **1990**, 29, 183-9	3.2	31
111	Functional diversity of PH domains: an exhaustive modelling study. *Folding & Design*, **1997**, 2, 343-55		30
110	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	3	30
109	Principal Component Analysis reveals correlation of cavities evolution and functional motions in proteins. *Journal of Molecular Graphics and Modelling*, **2015**, 55, 13-24	2.8	29
108	Influence of different assignment conditions on the determination of symmetric homodimeric structures with ARIA. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 569-85	4.2	29
107	Efficient sampling in collective coordinate space. *Proteins: Structure, Function and Bioinformatics*, **2000**, 39, 82-8	4.2	29
106	ISD: a software package for Bayesian NMR structure calculation. *Bioinformatics*, **2008**, 24, 1104-5	7.2	28
105	A simple method for delineating well-defined and variable regions in protein structures determined from interproton distance data. *FEBS Letters*, **1987**, 219, 11-16	3.8	28
104	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, 6151-4	16.4	27
103	Bayesian inference applied to macromolecular structure determination. *Physical Review E*, **2005**, 72, 031912	2.4	27
102	Refinement of the solution structure of the ribonucleotide 5P(GCAUGC)2: combined use of nuclear magnetic resonance and restrained molecular dynamics. *Biochemistry*, **1988**, 27, 1735-43	3.2	27
101	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. *Nature Structural and Molecular Biology*, **2015**, 22, 433-4	17.6	26
100	Computational reverse-engineering of a spider-venom derived peptide active against Plasmodium falciparum SUB1. *PLoS ONE*, **2011**, 6, e21812	3.7	26
99	Refined structure, DNA binding studies, and dynamics of the bacteriophage Pf3 encoded single-stranded DNA binding protein. *Biochemistry*, **1997**, 36, 9120-35	3.2	25
98	Structure of a PH domain from the C. elegans muscle protein UNC-89 suggests a novel function. *Structure*, **2000**, 8, 1079-87	5.2	25
97	Refinement of the protein backbone angle psi in NMR structure calculations. *Journal of Biomolecular NMR*, **2000**, 16, 47-58	3	25
96	Continuum solvent molecular dynamics study of flexibility in interleukin-8. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 136-45	2.8	24

95	Bayesian Weighing of Electron Cryo-Microscopy Data for Integrative Structural Modeling. *Structure*, **2019**, 27, 175-188.e6	5.2	24
94	Sampling Properties of Simulated Annealing and Distance Geometry **1991**, 451-455		24
93	Solution structure of the 30 kDa polysulfide-sulfur transferase homodimer from Wolinella succinogenes. *Biochemistry*, **2004**, 43, 1418-24	3.2	23
92	Re-face stereospecificity of methylenetetrahydromethanopterin and methylenetetrahydrofolate dehydrogenases is predetermined by intrinsic properties of the substrate. *ChemBioChem*, **2001**, 2, 530-41	3.8	22
91	Bayesian estimation of Karplus parameters and torsion angles from three-bond scalar couplings constants. *Journal of Magnetic Resonance*, **2005**, 177, 160-5	3	21
90	Coronaviruses with a SARS-CoV-2-like receptor-binding domain allowing ACE2-mediated entry into human cells isolated from bats of Indochinese peninsula		21
89	Bayesian estimation of NMR restraint potential and weight: a validation on a representative set of protein structures. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1525-37	4.2	20
88	Molecular dynamics and accuracy of NMR structures: Effects of error bounds and data removal. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 453-463	4.2	20
87	Structure and function of minor pilins of type IV pili. *Medical Microbiology and Immunology*, **2020**, 209, 301-308	4	20
86	An automatic tool to analyze and cluster macromolecular conformations based on self-organizing maps. *Bioinformatics*, **2015**, 31, 1490-2	7.2	19
85	Minimal NMR distance information for rigidity of protein graphs. *Discrete Applied Mathematics*, **2019**, 256, 91-104	1	19
84	Improved reliability, accuracy and quality in automated NMR structure calculation with ARIA. *Journal of Biomolecular NMR*, **2015**, 62, 425-38	3	18
83	Three dimensional structure and implications for the catalytic mechanism of 6-phosphogluconolactonase from Trypanosoma brucei. *Journal of Molecular Biology*, **2007**, 366, 868-81	6.5	18
82	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, 184-91	3.7	18
81	Functionally important correlated motions in the single-stranded DNA-binding protein encoded by filamentous phage Pf3. *Journal of Molecular Biology*, **1999**, 287, 569-77	6.5	18
80	Tertiary structure prediction using mean-force potentials and internal energy functions: successful prediction for coiled-coil geometries. *Folding & Design*, **1997**, 2, S47-52		17
79	Structural Characterization of Whirlin Reveals an Unexpected and Dynamic Supramodule Conformation of Its PDZ Tandem. *Structure*, **2017**, 25, 1645-1656.e5	5.2	16
78	A convective replica-exchange method for sampling new energy basins. *Journal of Computational Chemistry*, **2013**, 34, 132-40	3.5	16

77	A unifying probabilistic framework for analyzing residual dipolar couplings. *Journal of Biomolecular NMR*, **2008**, 40, 135-44	3	16
76	Refined Solution Structure of the Tyr41->His Mutant of the M13 Gene V Protein. *FEBS Journal*, **1995**, 232, 506-514		16
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74	Discrimination of agonists versus antagonists of nicotinic ligands based on docking onto AChBP structures. *Journal of Molecular Graphics and Modelling*, **2011**, 30, 100-9	2.8	15
73	Sequence-specific DNA binding activity of the cross-brace zinc finger motif of the piggyBac transposase. *Nucleic Acids Research*, **2018**, 46, 2660-2677	20.1	14
72	Molecular replacement with NMR models using distance-derived pseudo B factors. *Acta Crystallographica Section D: Biological Crystallography*, **1996**, 52, 973-82		14
71	Structure and Assembly of the Enterohemorrhagic Escherichia coli Type 4 Pilus. *Structure*, **2019**, 27, 1082-1093.e5	5.1	13
70	Identification of novel leishmanicidal molecules by virtual and biochemical screenings targeting Leishmania eukaryotic translation initiation factor 4A. *PLoS Neglected Tropical Diseases*, **2018**, 12, e0006160	4.8	13
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66	Stabilization of the integrase-DNA complex by Mg2+ ions and prediction of key residues for binding HIV-1 integrase inhibitors. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 466-78	4.2	12
65	Insights into the enzymatic mechanism of 6-phosphogluconolactonase from Trypanosoma brucei using structural data and molecular dynamics simulation. *Journal of Molecular Biology*, **2009**, 388, 1009-21	6.5	12
64	Exploring protein interiors: the role of a buried histidine in the KH module fold. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 484-96	4.2	12
63	SAXS Merge: an automated statistical method to merge SAXS profiles using Gaussian processes. *Journal of Synchrotron Radiation*, **2014**, 21, 203-8	2.4	12
62	Temperature Accelerated Molecular Dynamics with Soft-Ratcheting Criterion Orients Enhanced Sampling by Low-Resolution Information. *Journal of Chemical Theory and Computation*, **2015**, 11, 3446-54	6.4	11
61	Identification of binding sites and favorable ligand binding moieties by virtual screening and self-organizing map analysis. *BMC Bioinformatics*, **2015**, 16, 93	3.6	11
60	Functional motions modulating VanA ligand binding unraveled by self-organizing maps. *Journal of Chemical Information and Modeling*, **2014**, 54, 289-301	6.1	11

59	Error distribution derived NOE distance restraints. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 652-64	4.2	11
58	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	3.2	11
57	ATP conformations and ion binding modes in the active site of anthrax edema factor: a computational analysis. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 971-83	4.2	10
56	NMR in the SPINE Structural Proteomics project. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1150-61		10
55	Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems. *Lecture Notes in Computer Science*, **2011**, 206-217	0.9	10
54	Distance Geometry in Structural Biology: New Perspectives **2013**, 329-350		10
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52	Solution structure of the coiled-coil trimerization domain from lung surfactant protein D. *Journal of Biomolecular NMR*, **2002**, 24, 89-102	3	9
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49	Influence of chemical shift tolerances on NMR structure calculations using ARIA protocols for assigning NOE data. *Journal of Biomolecular NMR*, **2005**, 31, 21-34	3	8
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47	Efficient modeling of symmetric protein aggregates from NMR data. *Angewandte Chemie - International Edition*, **2012**, 51, 6916-9	16.4	7
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45	Comparison of different torsion angle approaches for NMR structure determination. *Journal of Biomolecular NMR*, **2006**, 34, 153-66	3	6
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