Mikael Akke

List of Publications by Year
in descending order

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108 papers	7,653 citations	61984 43 h-index	53230 85 g-index
132 all docs	132 docs citations	132 times ranked	5910 citing authors

#	Article	IF	Citations
1	Structural characterization of the microbial enzyme urocanate reductase mediating imidazole propionate production. Nature Communications, 2021, 12, 1347.	12.8	9
2	Entropyâ€“Entropy Compensation between the Protein, Ligand, and Solvent Degrees of Freedom Fine-Tunes Affinity in Ligand Binding to Galectin-3C. Jacs Au, 2021, 1, 484-500.	7.9	17
3	Transition-State Compressibility and Activation Volume of Transient Protein Conformational Fluctuations. Jacs Au, 2021, 1, 833-842.	7.9	9
4	Rapid measurement of heteronuclear transverse relaxation rates using non-uniformly sampled <i>R</i>_{1<i>ï</i>} accordion experiments. Magnetic Resonance, 2021, 2, 571-587.	1.9	1
5	1H R1Ï•relaxation dispersion experiments in aromatic side chains. Journal of Biomolecular NMR, 2021, 75, 383-392.	2.8	3
6	Mapping the energy landscape of proteinâ€“ligand binding via linear free energy relationships determined by protein NMR relaxation dispersion. RSC Chemical Biology, 2021, 2, 259-265.	4.1	5
7	Dynamic allosteric communication pathway directing differential activation of the glucocorticoid receptor. Science Advances, 2020, 6, eabb5277.	10.3	32
8	Accurate Backbone ¹³C and ¹⁵N Chemical Shift Tensors in Galectinâ€3 Determined by MAS NMR and QM/MM: Details of Structure and Environment Matter. ChemPhysChem, 2020, 21, 1436-1443.	2.1	10
9	Ultrastructural evidence for self-replication of Alzheimer-associated AÎ²42 amyloid along the sides of fibrils. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11265-11273.	7.1	37
10	Minute Additions of DMSO Affect Protein Dynamics Measurements by NMR Relaxation Experiments through Significant Changes in Solvent Viscosity. ChemPhysChem, 2019, 20, 326-332.	2.1	9
11	Rotamer Jumps, Proton Exchange, and Amine Inversion Dynamics of Dimethylated Lysine Residues in Proteins Resolved by pH-Dependent ¹H and ¹³C NMR Relaxation Dispersion. Journal of Physical Chemistry B, 2019, 123, 9742-9750.	2.6	1
12	Revealing Well-Defined Soluble States during Amyloid Fibril Formation by Multilinear Analysis of NMR Diffusion Data. Journal of the American Chemical Society, 2019, 141, 18649-18652.	13.7	6
13	Adsorption of unfolded Cu/Zn superoxide dismutase onto hydrophobic surfaces catalyzes its formation of amyloid fibrils. Protein Engineering, Design and Selection, 2019, 32, 77-85.	2.1	1
14	Rapid NMR Relaxation Measurements Using Optimal Nonuniform Sampling of Multidimensional Accordion Data Analyzed by a Sparse Reconstruction Method. Journal of Physical Chemistry A, 2019, 123, 5718-5723.	2.5	9
15	Backbone 1H, 13C, and 15N resonance assignments of BoMan26A, a Î²-mannanase of the glycoside hydrolase family 26 from the human gut bacterium Bacteroides ovatus. Biomolecular NMR Assignments, 2019, 13, 213-218.	0.8	1
16	Stability and Local Unfolding of SOD1 in the Presence of Protein Crowders. Journal of Physical Chemistry B, 2019, 123, 1920-1930.	2.6	20
17	Interplay between Conformational Entropy and Solvation Entropy in Proteinâ€“Ligand Binding. Journal of the American Chemical Society, 2019, 141, 2012-2026.	13.7	89
18	Chemical Shifts of the Carbohydrate Binding Domain of Galectin-3 from Magic Angle Spinning NMR and Hybrid Quantum Mechanics/Molecular Mechanics Calculations. Journal of Physical Chemistry B, 2018, 122, 2931-2939.	2.6	9

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19	Elucidation of Hydrogen Bonding Patterns in Ligand-Free, Lactose- and Glycerol-Bound Galectin-3C by Neutron Crystallography to Guide Drug Design. Journal of Medicinal Chemistry, 2018, 61, 4412-4420.	6.4	32
20	Conformational Entropy of FK506 Binding to FKBP12 Determined by Nuclear Magnetic Resonance Relaxation and Molecular Dynamics Simulations. Biochemistry, 2018, 57, 1451-1461.	2.5	16
21	Systematic Tuning of Fluoro-galectin-3 Interactions Provides Thiodigalactoside Derivatives with Single-Digit nM Affinity and High Selectivity. Journal of Medicinal Chemistry, 2018, 61, 1164-1175.	6.4	76
22	Backbone 1H, 13C, and 15N resonance assignments of the ligand binding domain of the human wildtype glucocorticoid receptor and the F602S mutant variant. Biomolecular NMR Assignments, 2018, 12, 263-268.	0.8	3
23	Designing interactions by control of proteinâ€“ligand complex conformation: tuning arginineâ€“arene interaction geometry for enhanced electrostatic proteinâ€“ligand interactions. Chemical Science, 2018, 9, 1014-1021.	7.4	15
24	Conserved S/T Residues of the Human Chaperone DNAJB6 Are Required for Effective Inhibition of Aî²42 Amyloid Fibril Formation. Biochemistry, 2018, 57, 4891-4902.	2.5	52
25	Cu/Zn Superoxide Dismutase Forms Amyloid Fibrils under Near-Physiological Quiescent Conditions: The Roles of Disulfide Bonds and Effects of Denaturant. ACS Chemical Neuroscience, 2017, 8, 2019-2026.	3.5	25
26	The Dynameomics Entropy Dictionary: A Large-Scale Assessment of Conformational Entropy across Protein Fold Space. Journal of Physical Chemistry B, 2017, 121, 3933-3945.	2.6	21
27	Structural model of dodecameric heat-shock protein Hsp21: Flexible N-terminal arms interact with client proteins while C-terminal tails maintain the dodecamer and chaperone activity. Journal of Biological Chemistry, 2017, 292, 8103-8121.	3.4	24
28	Dynamics of Aromatic Side Chains in the Active Site of FKBP12. Biochemistry, 2017, 56, 334-343.	2.5	13
29	Molecular insights into substrate recognition and catalytic mechanism of the chaperone and FKBP peptidyl-prolyl isomerase SlyD. BMC Biology, 2016, 14, 82.	3.8	26
30	A De Novo Designed Coiled-Coil Peptide with a Reversible pH-Induced Oligomerization Switch. Structure, 2016, 24, 946-955.	3.3	36
31	Structural Analysis of a Complex between Small Ubiquitin-like Modifier 1 (SUMO1) and the ZZ Domain of CREB-binding Protein (CBP/p300) Reveals a New Interaction Surface on SUMO. Journal of Biological Chemistry, 2016, 291, 12658-12672.	3.4	23
32	Structural Insights into the Calcium-Mediated Allosteric Transition in the C-Terminal Domain of Calmodulin from Nuclear Magnetic Resonance Measurements. Biochemistry, 2016, 55, 19-28.	2.5	9
33	Site-Specific Protonation Kinetics of Acidic Side Chains in Proteins Determined by pH-Dependent Carboxyl ¹³C NMR Relaxation. Journal of the American Chemical Society, 2015, 137, 3093-3101.	13.7	31
34	Computational design of a leucine-rich repeat protein with a predefined geometry. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17875-17880.	7.1	53
35	Conformational Entropies and Order Parameters: Convergence, Reproducibility, and Transferability. Journal of Chemical Theory and Computation, 2014, 10, 432-438.	5.3	31
36	Ring Flips Revisited: ¹³C Relaxation Dispersion Measurements of Aromatic Side Chain Dynamics and Activation Barriers in Basic Pancreatic Trypsin Inhibitor. Biochemistry, 2014, 53, 4519-4525.	2.5	52

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37	Off-resonance rotating-frame relaxation dispersion experiment for 13C in aromatic side chains using L-optimized TROSY-selection. Journal of Biomolecular NMR, 2014, 59, 23-29.	2.8	24
38	Protein conformational exchange measured by 1H R1Ï•relaxation dispersion of methyl groups. Journal of Biomolecular NMR, 2013, 57, 47-55.	2.8	19
39	Slow Aromatic Ring Flips Detected Despite Near-Degenerate NMR Frequencies of the Exchanging Nuclei. Journal of Physical Chemistry B, 2013, 117, 9241-9247.	2.6	30
40	Local Unfolding and Aggregation Mechanisms of SOD1: A Monte Carlo Exploration. Journal of Physical Chemistry B, 2013, 117, 9194-9202.	2.6	20
41	13C relaxation experiments for aromatic side chains employing longitudinal- and transverse-relaxation optimized NMR spectroscopy. Journal of Biomolecular NMR, 2012, 53, 181-190.	2.8	26
42	Conformational exchange of aromatic side chains characterized by L-optimized TROSY-selected 13C CPMG relaxation dispersion. Journal of Biomolecular NMR, 2012, 54, 9-14.	2.8	40
43	The Carbohydrate-Binding Site in Galectin-3 Is Preorganized To Recognize a Sugarlike Framework of Oxygens: Ultra-High-Resolution Structures and Water Dynamics. Biochemistry, 2012, 51, 296-306.	2.5	137
44	Specific ¹²C^{Î²}D₂¹²C^{Î³}D₂S¹³C^{Îµ}HD<s Isotopomer Labeling of Methionine To Characterize Protein Dynamics by ¹H and ¹³C NMR Relaxation Dispersion. Journal of the American Chemical Society, 2012, 134, 18562-18565.	13.7	25
45	Conformational dynamics and thermodynamics of proteinâ€“ligand binding studied by NMR relaxation. Biochemical Society Transactions, 2012, 40, 419-423.	3.4	60
46	Protein loop compaction and the origin of the effect of arginine and glutamic acid mixtures on solubility, stability and transient oligomerization of proteins. European Biophysics Journal, 2011, 40, 1327-1338.	2.2	15
47	100% complete assignment of non-labile 1H, 13C, and 15N signals for calcium-loaded calbindin D9k P43G. Biomolecular NMR Assignments, 2011, 5, 79-84.	0.8	14
48	Protein Flexibility and Conformational Entropy in Ligand Design Targeting the Carbohydrate Recognition Domain of Galectin-3. Journal of the American Chemical Society, 2010, 132, 14577-14589.	13.7	209
49	Structure and Dynamics of Ribosomal Protein L12: An Ensemble Model Based on SAXS and NMR Relaxation. Biophysical Journal, 2010, 98, 2374-2382.	0.5	67
50	pKa Values for the Unfolded State under Native Conditions Explain the pH-Dependent Stability of PGB1. Biophysical Journal, 2010, 99, 3365-3373.	0.5	13
51	Local Cooperativity in an Amyloidogenic State of Human Lysozyme Observed at Atomic Resolution. Journal of the American Chemical Society, 2010, 132, 15580-15588.	13.7	55
52	Starting-Condition Dependence of Order Parameters Derived from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2010, 6, 2176-2190.	5.3	38
53	Transient structural distortion of metal-free Cu/Zn superoxide dismutase triggers aberrant oligomerization. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 18273-18278.	7.1	74
54	Conformational entropy changes upon lactose binding to the carbohydrate recognition domain of galectin-3. Journal of Biomolecular NMR, 2009, 45, 157-169.	2.8	75

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55	Differential Responses of the Backbone and Side-Chain Conformational Dynamics in FKBP12 upon Binding the Transition-State Analog FK506: Implications for Transition-State Stabilization and Target Protein Recognition. Journal of Molecular Biology, 2009, 387, 233-244.	4.2	35
56	Multiple-Timescale Dynamics of Side-Chain Carboxyl and Carbonyl Groups in Proteins by ¹³C Nuclear Spin Relaxation. Journal of the American Chemical Society, 2008, 130, 15805-15807.	13.7	37
57	Structural Characterization of the Ribosomal P1Aâ˜P2B Protein Dimer by Small-Angle X-ray Scattering and NMR Spectroscopy. Biochemistry, 2007, 46, 1988-1998.	2.5	25
58	The Ribosomal Stalk Binds to Translation Factors IF2, EF-Tu, EF-G and RF3 via a Conserved Region of the L12 C-terminal Domain. Journal of Molecular Biology, 2007, 365, 468-479.	4.2	114
59	Characterization of Chemical Exchange Using Residual Dipolar Coupling. Journal of the American Chemical Society, 2007, 129, 13396-13397.	13.7	67
60	Fractional 13C enrichment of isolated carbons using [1-13C]- or [2-13C]-glucose facilitates the accurate measurement of dynamics at backbone CÎ± and side-chain methyl positions in proteins. Journal of Biomolecular NMR, 2007, 38, 199-212.	2.8	160
61	Biosynthetic13C Labeling of Aromatic Side Chains in Proteins for NMR Relaxation Measurements. Journal of the American Chemical Society, 2006, 128, 2506-2507.	13.7	76
62	Functional Dynamics of Human FKBP12 Revealed by Methyl13C Rotating Frame Relaxation Dispersion NMR Spectroscopy. Journal of the American Chemical Society, 2006, 128, 5718-5727.	13.7	58
63	The inverted chevron plot measured by NMR relaxation reveals a native-like unfolding intermediate in acyl-CoA binding protein. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 6877-6882.	7.1	22
64	Unfolding and inactivation of cutinases by AOT and guanidine hydrochloride. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1748, 74-83.	2.3	23
65	Microsecond Protein Dynamics Measured by 13CÎ± Rotating-Frame Spin Relaxation. ChemBioChem, 2005, 6, 1685-1692.	2.6	23
66	Off-resonance rotating-frame amide proton spin relaxation experiments measuring microsecond chemical exchange in proteins. Journal of Biomolecular NMR, 2005, 32, 163-173.	2.8	33
67	Correlated dynamics of consecutive residues reveal transient and cooperative unfolding of secondary structure in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 16984-16989.	7.1	47
68	Compact oleic acid in HAMLET. FEBS Letters, 2005, 579, 6095-6100.	2.8	34
69	Out of hot water. Nature Structural and Molecular Biology, 2004, 11, 912-913.	8.2	8
70	Letter to the Editor: Sequential1H,15N and13C NMR Assignment of Human Calbindin D28k. Journal of Biomolecular NMR, 2004, 28, 305-306.	2.8	3
71	Quantitative Analysis of Conformational Exchange Contributions to1Hâ˜15N Multiple-Quantum Relaxation Using Field-Dependent Measurements. Time Scale and Structural Characterization of Exchange in a Calmodulin C-Terminal Domain Mutant. Journal of the American Chemical Society, 2004, 126, 928-935.	13.7	23
72	Transient Aggregation and Stable Dimerization Induced by Introducing an Alzheimer Sequence into a Water-Soluble Proteinâ€. Biochemistry, 2004, 43, 12964-12978.	2.5	16

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73	Conformation and Dynamics of Ribosomal Stalk Protein L12 in Solution and on the Ribosomeâ€. Biochemistry, 2004, 43, 5930-5936.	2.5	71
74	Carbonyl13C transverse relaxation measurements to sample protein backbone dynamics. Magnetic Resonance in Chemistry, 2003, 41, 853-865.	1.9	39
75	A statistical analysis of NMR spectrometer noise. Journal of Magnetic Resonance, 2003, 162, 176-188.	2.1	20
76	Combined Use of NMR Relaxation Measurements and Hydrodynamic Calculations To Study Protein Association. Evidence for Tetramers of Low Molecular Weight Protein Tyrosine Phosphatase in Solution. Journal of the American Chemical Society, 2003, 125, 916-923.	13.7	38
77	Calbindin D28k Exhibits Properties Characteristic of a Ca2+ Sensor. Journal of Biological Chemistry, 2002, 277, 16662-16672.	3.4	113
78	Enzyme Dynamics During Catalysis. Science, 2002, 295, 1520-1523.	12.6	688
79	Intramolecular Dynamics of Low Molecular Weight Protein Tyrosine Phosphatase in Monomerâ€“Dimer Equilibrium Studied by NMR: A Model for Changes in Dynamics upon Target Binding. Journal of Molecular Biology, 2002, 322, 137-152.	4.2	49
80	NMR methods for characterizing microsecond to millisecond dynamics in recognition and catalysis. Current Opinion in Structural Biology, 2002, 12, 642-647.	5.7	120
81	An open and shut case. , 2001, 8, 910-912.		12
82	Dynamics of the Transition between Open and Closed Conformations in a Calmodulin C-Terminal Domain Mutant. Structure, 2001, 9, 185-195.	3.3	88
83	May the driving force be with you--whatever it is. , 2000, 7, 11-13.		41
84	From snapshot to movie: phi analysis of protein folding transition states taken one step further. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 14854-14859.	7.1	145
85	Backbone dynamics and energetics of a Calmodulin domain mutant exchanging between closed and open conformations. Journal of Molecular Biology, 1999, 289, 603-617.	4.2	122
86	Structural dynamics in the C-terminal domain of calmodulin at low calcium levels 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1999, 293, 883-899.	4.2	148
87	Pervasive conformational fluctuations on microsecond time scales in a fibronectin type III domain. Nature Structural Biology, 1998, 5, 55-59.	9.7	105
88	Sequence and Context Dependence of EF-Hand Loop Dynamics. An15N Relaxation Study of a Calcium-Binding Site Mutant of Calbindin D9kâ€. Biochemistry, 1998, 37, 2586-2595.	2.5	41
89	Base dynamics in a UUCG tetraloop RNA hairpin characterized by 15N spin relaxation: correlations with structure and stability. Rna, 1997, 3, 702-9.	3.5	70
90	Monitoring Macromolecular Motions on Microsecond to Millisecond Time Scales by R1Ïâ^'R1 Constant Relaxation Time NMR Spectroscopy. Journal of the American Chemical Society, 1996, 118, 911-912.	13.7	273

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91	Dynamics of Ribonuclease H:Â Temperature Dependence of Motions on Multiple Time Scalesâ€. Biochemistry, 1996, 35, 16009-16023.	2.5	195
92	The structure of calcyclin reveals a novel homodimeric fold for S100 Ca2+-binding proteins. Nature Structural and Molecular Biology, 1995, 2, 790-796.	8.2	180
93	Backbone Dynamics ofEscherichia coliRibonuclease HI: Correlations with Structure and Function in an Active Enzyme. Journal of Molecular Biology, 1995, 246, 144-163.	4.2	948
94	Solution Structure of (Cd2+)1-calbindin D9kReveals Details of the Stepwise Structural Changes along the Apo*rarr;(Ca2+)1II*rarr;(Ca2+)2I,IIBinding Pathway. Journal of Molecular Biology, 1995, 252, 102-121.	4.2	68
95	Heteronuclear-Correlation NMR Spectroscopy with Simultaneous Isotope Filtration, Quadrature Detection, and Sensitivity Enhancement Using z Rotations. Journal of Magnetic Resonance Series B, 1994, 104, 298-302.	1.6	27
96	Signal transduction versus buffering activity in Ca2+â€“binding proteins. Nature Structural and Molecular Biology, 1994, 1, 239-245.	8.2	152
97	Practical Aspects of Two-Dimensional Proton-Detected 15N Spin Relaxation Measurements. Journal of Magnetic Resonance Series B, 1993, 102, 253-264.	1.6	162
98	15N NMR assignments of (Cd2+,)2-calbindin D9k and comparison with (Ca2+)2-calbindin D9k. Cadmium as a substitute for calcium in calcium-binding proteins. Magnetic Resonance in Chemistry, 1993, 31, S128-S132.	1.9	6
99	High-resolution Solution Structure of Calcium-loaded Calbindin D9k. Journal of Molecular Biology, 1993, 231, 711-734.	4.2	112
100	NMR order parameters and free energy: an analytical approach and its application to cooperative calcium(2+) binding by calbindin D9k. Journal of the American Chemical Society, 1993, 115, 9832-9833.	13.7	347
101	Effects of ion binding on the backbone dynamics of calbindin D9k determined by nitrogen-15 NMR relaxation. Biochemistry, 1993, 32, 9832-9844.	2.5	184
102	Backbone dynamics of calcium-loaded calbindin D9k studied by two-dimensional proton-detected nitrogen-15 NMR spectroscopy. Biochemistry, 1992, 31, 4856-4866.	2.5	210
103	Three-dimensional solution structure of calcium-loaded porcine calbindin D9k determined by nuclear magnetic resonance spectroscopy. Biochemistry, 1992, 31, 1011-1020.	2.5	54
104	15N NMR assignments and chemical shift analysis of uniformly labeled15N calbindin D9kin the apo, (Cd2+)1and (Ca2+)2states. FEBS Letters, 1992, 303, 136-140.	2.8	25
105	Nuclear magnetic resonance studies of the internal dynamics in apo, (Cd2+)1 and (Ca2+)2 Calbindin D9k. Journal of Molecular Biology, 1992, 227, 1100-1117.	4.2	67
106	Molecular basis for co-operativity in Ca2+ binding to calbindin D9k. Journal of Molecular Biology, 1991, 220, 173-189.	4.2	75
107	Ca ²⁺ Binding in Proteins of the Calmodulin Superfamily: Cooperativity, Electrostatic Contributions and Molecular Mechanisms. Novartis Foundation Symposium, 1991, 161, 222-236.	1.1	6
108	Protein stability and electrostatic interactions between solvent exposed charged side chains. Proteins: Structure, Function and Bioinformatics, 1990, 8, 23-29.	2.6	98