Rafael BrÃ¼schweiler

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8928190/publications.pdf

Version: 2024-02-01

160 papers	8,455 citations	41344 49 h-index	56724 83 g-index
164 all docs	164 docs citations	164 times ranked	6708 citing authors

#	Article	IF	Citations
1	Cadaverine Is a Switch in the Lysine Degradation Pathway in Pseudomonas aeruginosa Biofilm Identified by Untargeted Metabolomics. Frontiers in Cellular and Infection Microbiology, 2022, 12, 833269.	3.9	9
2	Fundamental and practical aspects of machine learning for the peak picking of biomolecular NMR spectra. Journal of Biomolecular NMR, 2022, 76, 49-57.	2.8	5
3	COLMARq: A Web Server for 2D NMR Peak Picking and Quantitative Comparative Analysis of Cohorts of Metabolomics Samples. Analytical Chemistry, 2022, 94, 8674-8682.	6.5	8
4	Broadband Dynamics of Ubiquitin by Anionic and Cationic Nanoparticle Assisted NMR Spin Relaxation. Angewandte Chemie - International Edition, 2021, 60, 148-152.	13.8	14
5	Broadband Dynamics of Ubiquitin by Anionic and Cationic Nanoparticle Assisted NMR Spin Relaxation. Angewandte Chemie, 2021, 133, 150-154.	2.0	1
6	Systematic Differences between Current Molecular Dynamics Force Fields To Represent Local Properties of Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2021, 125, 798-804.	2.6	18
7	NMR Spin Relaxation Theory of Biomolecules Undergoing Highly Asymmetric Exchange with Large Interaction Partners. Journal of Chemical Theory and Computation, 2021, 17, 2374-2382.	5.3	3
8	2D NMR-Based Metabolomics with HSQC/TOCSY NOAH Supersequences. Analytical Chemistry, 2021, 93, 6112-6119.	6.5	28
9	Observation of Sub-Microsecond Protein Methyl-Side Chain Dynamics by Nanoparticle-Assisted NMR Spin Relaxation. Journal of the American Chemical Society, 2021, 143, 13593-13604.	13.7	10
10	DEEP picker is a deep neural network for accurate deconvolution of complex two-dimensional NMR spectra. Nature Communications, 2021, 12, 5229.	12.8	55
11	Balanced Amino-Acid-Specific Molecular Dynamics Force Field for the Realistic Simulation of Both Folded and Disordered Proteins. Journal of Chemical Theory and Computation, 2020, 16, 1311-1318.	5.3	43
12	Degree of N-Methylation of Nucleosides and Metabolites Controls Binding Affinity to Pristine Silica Surfaces. Journal of Physical Chemistry Letters, 2020, 11, 10401-10407.	4.6	3
13	Active Learning Approach for an Intuitive Understanding of the Boltzmann Distribution by Basic Computer Simulations. Journal of Chemical Education, 2020, 97, 3910-3913.	2.3	5
14	Quantitative Cooperative Binding Model for Intrinsically Disordered Proteins Interacting with Nanomaterials. Journal of the American Chemical Society, 2020, 142, 10730-10738.	13.7	22
15	COLMAR Lipids Web Server and Ultrahigh-Resolution Methods for Two-Dimensional Nuclear Magnetic Resonance- and Mass Spectrometry-Based Lipidomics. Journal of Proteome Research, 2020, 19, 1674-1683.	3.7	23
16	Accurate and Efficient Determination of Unknown Metabolites in Metabolomics by NMR-Based Molecular Motif Identification. Analytical Chemistry, 2019, 91, 15686-15693.	6.5	16
17	Functional protein dynamics on uncharted time scales detected by nanoparticle-assisted NMR spin relaxation. Science Advances, 2019, 5, eaax5560.	10.3	32
18	Extreme Nonuniform Sampling for Protein NMR Dynamics Studies in Minimal Time. Journal of the American Chemical Society, 2019, 141, 16829-16838.	13.7	12

#	Article	IF	Citations
19	Real-Time Pure Shift HSQC NMR for Untargeted Metabolomics. Analytical Chemistry, 2019, 91, 2304-2311.	6.5	25
20	Identification of Unknown Metabolomics Mixture Compounds by Combining NMR, MS, and Cheminformatics. Methods in Enzymology, 2019, 615, 407-422.	1.0	19
21	Reprogramming of Glucose Metabolism by Zerumbone Suppresses Hepatocarcinogenesis. Molecular Cancer Research, 2018, 16, 256-268.	3.4	33
22	Carbohydrate Background Removal in Metabolomics Samples. Analytical Chemistry, 2018, 90, 14100-14104.	6.5	6
23	Quantitative Binding Behavior of Intrinsically Disordered Proteins to Nanoparticle Surfaces at Individual Residue Level. Chemistry - A European Journal, 2018, 24, 16997-17001.	3.3	21
24	Time-Resolved Protein Side-Chain Motions Unraveled by High-Resolution Relaxometry and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2018, 140, 13456-13465.	13.7	40
25	Frontispiece: Nonâ€Uniform and Absolute Minimal Sampling for Highâ€Throughput Multidimensional NMR Applications. Chemistry - A European Journal, 2018, 24, .	3.3	0
26	Nonâ€Uniform and Absolute Minimal Sampling for Highâ€Throughput Multidimensional NMR Applications. Chemistry - A European Journal, 2018, 24, 11535-11544.	3.3	14
27	Nanoparticle-Assisted Metabolomics. Metabolites, 2018, 8, 21.	2.9	15
28	The Intracellular Loop of the Na+/Ca2+ Exchanger Contains an â€œAwareness Ribbonâ€•Shaped Two-Helix Bundle Domain. Biochemistry, 2018, 57, 5096-5104.	2.5	9
29	Improved Quantum Chemical NMR Chemical Shift Prediction of Metabolites in Aqueous Solution toward the Validation of Unknowns. Journal of Physical Chemistry A, 2017, 121, 3071-3078.	2.5	29
30	Elevated Î¼s-ms timescale backbone dynamics in the transition state analog form of arginine kinase. Journal of Structural Biology, 2017, 200, 258-266.	2.8	1
31	Statistical database analysis of the role of loop dynamics for proteinâ€“protein complex formation and allostery. Bioinformatics, 2017, 33, 1814-1819.	4.1	5
32	Differential Attenuation of NMR Signals by Complementary Ionâ€Exchange Resin Beads for De Novo Analysis of Complex Metabolomics Mixtures. Chemistry - A European Journal, 2017, 23, 9239-9243.	3.3	4
33	Absolute Minimal Sampling of Homonuclear 2D NMR TOCSY Spectra for Highâ€Throughput Applications of Complex Mixtures. Angewandte Chemie - International Edition, 2017, 56, 8149-8152.	13.8	16
34	Maximal clique method for the automated analysis of NMR TOCSY spectra of complex mixtures. Journal of Biomolecular NMR, 2017, 68, 195-202.	2.8	14
35	The Michaelis Complex of Arginine Kinase Samples the Transition State at a Frequency That Matches the Catalytic Rate. Journal of the American Chemical Society, 2017, 139, 4846-4853.	13.7	14
36	miRNA-122 Protects Mice and Human Hepatocytes from Acetaminophen Toxicity by Regulating Cytochrome P450 Family 1 Subfamily A Member 2 and Family 2 Subfamily E Member 1 Expression. American Journal of Pathology, 2017, 187, 2758-2774.	3.8	35

#	Article	IF	Citations
37	Accurate Identification of Unknown and Known Metabolic Mixture Components by Combining 3D NMR with Fourier Transform Ion Cyclotron Resonance Tandem Mass Spectrometry. Journal of Proteome Research, 2017, 16, 3774-3786.	3.7	26
38	Absolute Minimal Sampling of Homonuclear 2D NMR TOCSY Spectra for Highâ€Throughput Applications of Complex Mixtures. Angewandte Chemie, 2017, 129, 8261-8264.	2.0	8
39	Knowns and unknowns in metabolomics identified by multidimensional NMR and hybrid MS/NMR methods. Current Opinion in Biotechnology, 2017, 43, 17-24.	6.6	54
40	The future of NMR-based metabolomics. Current Opinion in Biotechnology, 2017, 43, 34-40.	6.6	651
41	Model for the allosteric regulation of the <scp>N</scp>a⁺/<scp>C</scp>a²⁺ exchanger <scp>NCX</scp>. Proteins: Structure, Function and Bioinformatics, 2016, 84, 580-590.	2.6	11
42	Residue-Specific Interactions of an Intrinsically Disordered Protein with Silica Nanoparticles and Their Quantitative Prediction. Journal of Physical Chemistry C, 2016, 120, 24463-24468.	3.1	28
43	Absolute Minimal Sampling in Highâ€Dimensional NMR Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 14169-14172.	13.8	19
44	Comprehensive Metabolite Identification Strategy Using Multiple Two-Dimensional NMR Spectra of a Complex Mixture Implemented in the COLMARm Web Server. Analytical Chemistry, 2016, 88, 12411-12418.	6.5	95
45	Absolut minimales Sampling in der hochdimensionalen NMRâ€Spektroskopie. Angewandte Chemie, 2016, 128, 14376-14379.	2.0	5
46	Rapid Determination of Fast Protein Dynamics from NMR Chemical Exchange Saturation Transfer Data. Angewandte Chemie, 2016, 128, 3169-3171.	2.0	1
47	Rapid Determination of Fast Protein Dynamics from NMR Chemical Exchange Saturation Transfer Data. Angewandte Chemie - International Edition, 2016, 55, 3117-3119.	13.8	15
48	Nanoparticle-Assisted Removal of Protein in Human Serum for Metabolomics Studies. Analytical Chemistry, 2016, 88, 1003-1007.	6.5	24
49	Emerging new strategies for successful metabolite identification in metabolomics. Bioanalysis, 2016, 8, 557-573.	1.5	79
50	Kinetic Cooperativity in Human Pancreatic Glucokinase Originates from Millisecond Dynamics of the Small Domain. Angewandte Chemie, 2015, 127, 8247-8250.	2.0	7
51	Kinetic Cooperativity in Human Pancreatic Glucokinase Originates from Millisecond Dynamics of the Small Domain. Angewandte Chemie - International Edition, 2015, 54, 8129-8132.	13.8	29
52	Two elephants in the room. Current Opinion in Clinical Nutrition and Metabolic Care, 2015, 18, 471-477.	2.5	60
53	Metabolomics Beyond Spectroscopic Databases: A Combined MS/NMR Strategy for the Rapid Identification of New Metabolites in Complex Mixtures. Analytical Chemistry, 2015, 87, 3864-3870.	6.5	111
54	Decoding the Mobility and Time Scales of Protein Loops. Journal of Chemical Theory and Computation, 2015, 11, 1308-1314.	5.3	39

#	Article	IF	Citations
55	Conformational heterogeneity and intrinsic disorder in enzyme regulation: Glucokinase as a case study. Intrinsically Disordered Proteins, 2015, 3, e1011008.	1.9	10
56	Modulation and Functional Role of the Orientations of the N- and P-Domains of Cu⁺-Transporting ATPase along the Ion Transport Cycle. Biochemistry, 2015, 54, 5095-5102.	2.5	4
57	PPM_One: a static protein structure based chemical shift predictor. Journal of Biomolecular NMR, 2015, 62, 403-409.	2.8	40
58	Use of Charged Nanoparticles in NMR-Based Metabolomics for Spectral Simplification and Improved Metabolite Identification. Analytical Chemistry, 2015, 87, 7211-7217.	6.5	29
59	Reliable resonance assignments of selected residues of proteins with known structure based on empirical NMR chemical shift prediction. Journal of Magnetic Resonance, 2015, 254, 93-97.	2.1	1
60	NMR/MS Translator for the Enhanced Simultaneous Analysis of Metabolomics Mixtures by NMR Spectroscopy and Mass Spectrometry: Application to Human Urine. Journal of Proteome Research, 2015, 14, 2642-2648.	3.7	54
61	Dual allosteric activation mechanisms in monomeric human glucokinase. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 11553-11558.	7.1	46
62	Unified and Isomer-Specific NMR Metabolomics Database for the Accurate Analysis of ¹³Câ€“¹H HSQC Spectra. ACS Chemical Biology, 2015, 10, 452-459.	3.4	96
63	NMR backbone resonance assignments of the N, P domains of CopA, a copper-transporting ATPase, in the apo and ligand bound states. Biomolecular NMR Assignments, 2015, 9, 129-133.	0.8	2
64	Backbone resonance assignments of the 42ÂkDa enzyme arginine kinase in the transition state analogue form. Biomolecular NMR Assignments, 2014, 8, 335-338.	0.8	3
65	Protocol To Make Protein NMR Structures Amenable to Stable Long Time Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 1781-1787.	5.3	8
66	Multidimensional Approaches to NMR-Based Metabolomics. Analytical Chemistry, 2014, 86, 47-57.	6.5	112
67	Customized Metabolomics Database for the Analysis of NMR ¹Hâ€“¹H TOCSY and ¹³Câ€“¹H HSQC-TOCSY Spectra of Complex Mixtures. Analytical Chemistry, 2014, 86, 5494-5501.	6.5	96
68	NMR Order Parameter Determination from Long Molecular Dynamics Trajectories for Objective Comparison with Experiment. Journal of Chemical Theory and Computation, 2014, 10, 2599-2607.	5.3	54
69	Quantitative Analysis of Metabolic Mixtures by Two-Dimensional ¹³C Constant-Time TOCSY NMR Spectroscopy. Analytical Chemistry, 2013, 85, 6414-6420.	6.5	47
70	Direct Observation of the Ion-Pair Dynamics at a Proteinâ€“DNA Interface by NMR Spectroscopy. Journal of the American Chemical Society, 2013, 135, 3613-3619.	13.7	57
71	Carbon Relaxation in 13CÎ±â€“HÎ± and 13CÎ±â€“DÎ± Spin Pairs as a Probe of Backbone Dynamics in Proteins. Journal of Physical Chemistry B, 2013, 117, 1308-1320.	2.6	5
72	Orderâ€“Disorder Transitions Govern Kinetic Cooperativity and Allostery of Monomeric Human Glucokinase. PLoS Biology, 2012, 10, e1001452.	5.6	51

#	Article	IF	Citations
73	PPM: a side-chain and backbone chemical shift predictor for the assessment of protein conformational ensembles. Journal of Biomolecular NMR, 2012, 54, 257-265.	2.8	75
74	Structural and Entropic Allosteric Signal Transduction Strength via Correlated Motions. Journal of Physical Chemistry Letters, 2012, 3, 1722-1726.	4.6	21
75	Carbon Backbone Topology of the Metabolome of a Cell. Journal of the American Chemical Society, 2012, 134, 9006-9011.	13.7	38
76	Probing Side-Chain Dynamics in Proteins by the Measurement of Nine Deuterium Relaxation Rates Per Methyl Group. Journal of Physical Chemistry B, 2012, 116, 606-620.	2.6	30
77	NMR in Metabolomics and Natural Products Research: Two Sides of the Same Coin. Accounts of Chemical Research, 2012, 45, 288-297.	15.6	151
78	Competitive Binding between Dynamic p53 Transactivation Subdomains to Human MDM2 Protein. Journal of Biological Chemistry, 2012, 287, 30376-30384.	3.4	25
79	TOCCATA: A Customized Carbon Total Correlation Spectroscopy NMR Metabolomics Database. Analytical Chemistry, 2012, 84, 9395-9401.	6.5	72
80	Dynamic and Thermodynamic Signatures of Native and Non-Native Protein States with Application to the Improvement of Protein Structures. Journal of Chemical Theory and Computation, 2012, 8, 2531-2539.	5.3	7
81	Dynamics of Lysine Side-Chain Amino Groups in a Protein Studied by Heteronuclear ¹Hâ€™¹⁵N NMR Spectroscopy. Journal of the American Chemical Society, 2011, 133, 909-919.	13.7	71
82	Atomistic Kinetic Model for Population Shift and Allostery in Biomolecules. Journal of the American Chemical Society, 2011, 133, 18999-19005.	13.7	46
83	Signature of Mobile Hydrogen Bonding of Lysine Side Chains from Long-Range ¹⁵Nâ€“¹³C Scalar J-Couplings and Computation. Journal of the American Chemical Society, 2011, 133, 9192-9195.	13.7	40
84	Iterative Optimization of Molecular Mechanics Force Fields from NMR Data of Full-Length Proteins. Journal of Chemical Theory and Computation, 2011, 7, 1773-1782.	5.3	78
85	Toward a Predictive Understanding of Slow Methyl Group Dynamics in Proteins. Biophysical Journal, 2011, 101, 910-915.	0.5	37
86	Deconvolution of Chemical Mixtures with High Complexity by NMR Consensus Trace Clustering. Analytical Chemistry, 2011, 83, 7412-7417.	6.5	55
87	Whispering within. Nature Chemistry, 2011, 3, 665-666.	13.6	10
88	Arginine Kinase: Joint Crystallographic and NMR RDC Analyses Link Substrate-Associated Motions to Intrinsic Flexibility. Journal of Molecular Biology, 2011, 405, 479-496.	4.2	35
89	Ca2+ Binding Alters the Interdomain Flexibility between the Two Cytoplasmic Calcium-binding Domains in the Na+/Ca2+ Exchanger. Journal of Biological Chemistry, 2011, 286, 32123-32131.	3.4	35
90	In Silico Elucidation of the Recognition Dynamics of Ubiquitin. PLoS Computational Biology, 2011, 7, e1002035.	3.2	41

#	Article	IF	Citations
91	NMRâ€Based Protein Potentials. Angewandte Chemie - International Edition, 2010, 49, 6778-6780.	13.8	173
92	Higher-Rank Correlation NMR Spectra with Spectral Moment Filtering. Journal of Physical Chemistry Letters, 2010, 1, 1086-1089.	4.6	13
93	Entropy Localization in Proteins. Journal of Physical Chemistry B, 2010, 114, 16036-16044.	2.6	49
94	Simultaneous de Novo Identification of Molecules in Chemical Mixtures by Doubly Indirect Covariance NMR Spectroscopy. Journal of the American Chemical Society, 2010, 132, 16922-16927.	13.7	31
95	Variation in Quadrupole Couplings of Î± Deuterons in Ubiquitin Suggests the Presence of C^{Î±}â^'H^{Î±}Â·Â·Â·Oâ•C Hydrogen Bonds. Journal of the American Chemical Society, 2010, 132, 7709-7719.	13.7	26
96	Direct Evidence of Conformational Heterogeneity in Human Pancreatic Glucokinase from High-Resolution Nuclear Magnetic Resonance. Biochemistry, 2010, 49, 7969-7971.	2.5	29
97	Certification of Molecular Dynamics Trajectories with NMR Chemical Shifts. Journal of Physical Chemistry Letters, 2010, 1, 246-248.	4.6	79
98	In silicoRelationship between Configurational Entropy and Soft Degrees of Freedom in Proteins and Peptides. Physical Review Letters, 2009, 102, 118108.	7.8	43
99	Web server suite for complex mixture analysis by covariance NMR. Magnetic Resonance in Chemistry, 2009, 47, S118-22.	1.9	38
100	Protein Conformational Flexibility from Structureâ€Free Analysis of NMR Dipolar Couplings: Quantitative and Absolute Determination of Backbone Motion in Ubiquitin. Angewandte Chemie - International Edition, 2009, 48, 4154-4157.	13.8	87
101	Structural dynamics of protein backbone Ï† angles: extended molecular dynamics simulations versus experimental 3 J scalar couplings. Journal of Biomolecular NMR, 2009, 45, 17-21.	2.8	33
102	Bacterial Attraction and Quorum Sensing Inhibition in Caenorhabditis elegans Exudates. Journal of Chemical Ecology, 2009, 35, 878-892.	1.8	33
103	Deuterium Spin Probes of Backbone Order in Proteins: 2H NMR Relaxation Study of Deuterated Carbon Î± Sites. Journal of the American Chemical Society, 2009, 131, 15853-15865.	13.7	41
104	Generalized Indirect Covariance NMR Formalism for Establishment of Multidimensional Spin Correlations. Journal of Physical Chemistry A, 2009, 113, 12898-12903.	2.5	57
105	A Dictionary for Protein Side-Chain Entropies from NMR Order Parameters. Journal of the American Chemical Society, 2009, 131, 7226-7227.	13.7	67
106	Short-Range Coherence of Internal Protein Dynamics Revealed by High-Precision in Silico Study. Journal of the American Chemical Society, 2009, 131, 14610-14611.	13.7	61
107	All-Atom Contact Model for Understanding Protein Dynamics from Crystallographic B-Factors. Biophysical Journal, 2009, 96, 3074-3081.	0.5	36
108	Self-consistent residual dipolar coupling based model-free analysis for the robust determination of nanosecond to microsecond protein dynamics. Journal of Biomolecular NMR, 2008, 41, 139-155.	2.8	100

#	Article	IF	Citations
109	Structure and Dynamics of Ca2+-Binding Domain 1 of the Na+/Ca2+ Exchanger in the Presence and in the Absence of Ca2+. Journal of Molecular Biology, 2008, 377, 945-955.	4.2	30
110	A Multifaceted Approach to the Interpretation of NMR Order Parameters:â€‰ A Case Study of a Dynamic Î±-Helix. Journal of Physical Chemistry B, 2008, 112, 6203-6210.	2.6	14
111	Self-Consistent Metabolic Mixture Analysis by Heteronuclear NMR. Application to a Human Cancer Cell Line. Analytical Chemistry, 2008, 80, 7549-7553.	6.5	34
112	16-Fold Degeneracy of Peptide Plane Orientations from Residual Dipolar Couplings: Analytical Treatment and Implications for Protein Structure Determination. Journal of the American Chemical Society, 2008, 130, 15927-15937.	13.7	37
113	Web Server Based Complex Mixture Analysis by NMR. Analytical Chemistry, 2008, 80, 3606-3611.	6.5	110
114	Quantitative Lid Dynamics of MDM2 Reveals Differential Ligand Binding Modes of the p53-Binding Cleft. Journal of the American Chemical Society, 2008, 130, 6472-6478.	13.7	86
115	Z-matrix formalism for quantitative noise assessment of covariance nuclear magnetic resonance spectra. Journal of Chemical Physics, 2008, 129, 104511.	3.0	21
116	Validation of Molecular Dynamics Simulations of Biomolecules Using NMR Spin Relaxation as Benchmarks:â€‰ Application to the AMBER99SB Force Field. Journal of Chemical Theory and Computation, 2007, 3, 961-975.	5.3	231
117	Evaluation of Configurational Entropy Methods from Peptide Foldingâ^'Unfolding Simulation. Journal of Physical Chemistry B, 2007, 111, 13807-13813.	2.6	25
118	Toward Quantitative Interpretation of Methyl Side-Chain Dynamics from NMR by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2007, 129, 14146-14147.	13.7	67
119	Quantitative Molecular Ensemble Interpretation of NMR Dipolar Couplings without Restraints. Journal of the American Chemical Society, 2007, 129, 4158-4159.	13.7	98
120	Resolution-Enhanced 4D ¹⁵N/¹³C NOESY Protein NMR Spectroscopy by Application of the Covariance Transform. Journal of the American Chemical Society, 2007, 129, 14126-14127.	13.7	26
121	Strategy for Automated Analysis of Dynamic Metabolic Mixtures by NMR. Application to an Insect Venom. Analytical Chemistry, 2007, 79, 7748-7752.	6.5	60
122	Robust Deconvolution of Complex Mixtures by Covariance TOCSY Spectroscopy. Angewandte Chemie - International Edition, 2007, 46, 2639-2642.	13.8	66
123	Quantitative covariance NMR by regularization. Journal of Biomolecular NMR, 2007, 38, 73-77.	2.8	24
124	Covariance NMR in higher dimensions: application to 4D NOESY spectroscopy of proteins. Journal of Biomolecular NMR, 2007, 39, 165-175.	2.8	32
125	Reorientational Contact-Weighted Elastic Network Model for the Prediction of Protein Dynamics: Comparison with NMR Relaxation. Biophysical Journal, 2006, 90, 3382-3388.	0.5	29
126	Enhanced Covariance Spectroscopy from Minimal Datasets. Journal of the American Chemical Society, 2006, 128, 15564-15565.	13.7	34

#	Article	IF	Citations
127	Simultaneous Determination of Protein Backbone Structure and Dynamics from Residual Dipolar Couplings. Journal of the American Chemical Society, 2006, 128, 15100-15101.	13.7	68
128	Identification of slow correlated motions in proteins using residual dipolar and hydrogen-bond scalar couplings. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13885-13890.	7.1	220
129	Initial Conformational Changes of Human Transthyretin under Partially Denaturing Conditions. Biophysical Journal, 2005, 89, 433-443.	0.5	26
130	Covariance nuclear magnetic resonance spectroscopy. Journal of Chemical Physics, 2004, 120, 5253-5260.	3.0	232
131	Theory of covariance nuclear magnetic resonance spectroscopy. Journal of Chemical Physics, 2004, 121, 409.	3.0	110
132	Prediction of methyl-side Chain Dynamics in Proteins. Journal of Biomolecular NMR, 2004, 29, 363-368.	2.8	48
133	Estimates of methyl 13C and 1H CSA values (??) in proteins from cross-correlated spin relaxation. Journal of Biomolecular NMR, 2004, 30, 397-406.	2.8	26
134	Spectral Deconvolution of Chemical Mixtures by Covariance NMR. ChemPhysChem, 2004, 5, 794-796.	2.1	40
135	Covariance NMR spectroscopy by singular value decomposition. Journal of Magnetic Resonance, 2004, 171, 277-283.	2.1	99
136	Indirect Covariance NMR Spectroscopy. Journal of the American Chemical Society, 2004, 126, 13180-13181.	13.7	136
137	Cross-correlation suppressed T1 and NOE experiments for protein side-chain 13CH2 groups. Journal of Biomolecular NMR, 2003, 26, 241-247.	2.8	8
138	New approaches to the dynamic interpretation and prediction of NMR relaxation data from proteins. Current Opinion in Structural Biology, 2003, 13, 175-183.	5.7	122
139	Self-Consistency Analysis of Dipolar Couplings in Multiple Alignments of Ubiquitin. Journal of the American Chemical Society, 2003, 125, 5596-5597.	13.7	53
140	Reconstruction of interatomic vectors by principle component analysis of nuclear magnetic resonance data in multiple alignments. Journal of Chemical Physics, 2002, 117, 1166-1172.	3.0	7
141	Model-Free Analysis of Protein Backbone Motion from Residual Dipolar Couplings. Journal of the American Chemical Society, 2002, 124, 5822-5833.	13.7	200
142	Contact Model for the Prediction of NMR Nâ^'H Order Parameters in Globular Proteins. Journal of the American Chemical Society, 2002, 124, 12654-12655.	13.7	103
143	General Framework for Studying the Dynamics of Folded and Nonfolded Proteins by NMR Relaxation Spectroscopy and MD Simulation. Journal of the American Chemical Society, 2002, 124, 4522-4534.	13.7	193
144	Assignment Strategy for Proteins with Known Structure. Journal of Magnetic Resonance, 2002, 157, 119-123.	2.1	48

#	Article	IF	Citations
145	Dynamic and structural analysis of isotropically distributed molecular ensembles. Proteins: Structure, Function and Bioinformatics, 2002, 46, 177-189.	2.6	38
146	Efficient RMSD measures for the comparison of two molecular ensembles. Proteins: Structure, Function and Bioinformatics, 2002, 50, 26-34.	2.6	55
147	Principal component method for assessing structural heterogeneity across multiple alignment media. Journal of Biomolecular NMR, 2002, 24, 123-132.	2.8	33
148	Reorientational Eigenmode Dynamics:Â A Combined MD/NMR Relaxation Analysis Method for Flexible Parts in Globular Proteins. Journal of the American Chemical Society, 2001, 123, 7305-7313.	13.7	54
149	Model-Free Approach to the Dynamic Interpretation of Residual Dipolar Couplings in Globular Proteins. Journal of the American Chemical Society, 2001, 123, 6098-6107.	13.7	269
150	Geometric Dependence of3hJ(31Pâ^'15N) and2hJ(31Pâ^'1H) Scalar Couplings in Proteinâ^'Nucleotide Complexes. Journal of the American Chemical Society, 2001, 123, 11079-11080.	13.7	37
151	Static and Dynamic Effects on Vicinal ScalarJCouplings in Proteins and Peptides:Â A MD/DFT Analysis. Journal of the American Chemical Society, 2000, 122, 10390-10397.	13.7	97
152	Backbone Dynamics and Structural Characterization of the Partially Folded A State of Ubiquitin by 1H, 13C, and 15N Nuclear Magnetic Resonance Spectroscopy. Biochemistry, 1997, 36, 13043-13053.	2.5	181
153	Collective protein dynamics and nuclear spin relaxation. Journal of Chemical Physics, 1995, 102, 3396-3403.	3.0	115
154	Collective NMR relaxation model applied to protein dynamics. Physical Review Letters, 1994, 72, 940-943.	7.8	49
155	Water self-diffusion model for protein-water NMR cross relaxation. Chemical Physics Letters, 1994, 229, 75-81.	2.6	37
156	Characterization of biomolecular structure and dynamics by NMR cross relaxation. Progress in Nuclear Magnetic Resonance Spectroscopy, 1994, 26, 27-58.	7.5	76
157	Differential Side Chain Hydration in a Linear Peptide Containing a Type VI Turn. Journal of the American Chemical Society, 1994, 116, 12051-12052.	13.7	35
158	Determination of local ligand conformations in slowly tumbling proteins by homonuclear 2D and 3D NMR: application to heme propionates in leghemoglobin. Journal of the American Chemical Society, 1993, 115, 6238-6246.	13.7	10
159	Molecular dynamics monitored by crossâ€correlated cross relaxation of spins quantized along orthogonal axes. Journal of Chemical Physics, 1992, 96, 1758-1766.	3.0	94
160	The structure of gramicidin A in dimethylsulfoxide/acetone. FEBS Journal, 1990, 194, 57-60.	0.2	25