# Rafael BrÃ¼schweiler

List of Publications by Year
in descending order

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|---|---|---|---|
| 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 | The future of NMR-based metabolomics. Current Opinion in Biotechnology, 2017, 43, 34-40. | 6.6 | 651 |
| 2 | 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 |
| 3 | Covariance nuclear magnetic resonance spectroscopy. Journal of Chemical Physics, 2004, 120, 5253-5260. | 3.0 | 232 |
| 4 | 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 |
| 5 | 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 |
| 6 | Model-Free Analysis of Protein Backbone Motion from Residual Dipolar Couplings. Journal of the American Chemical Society, 2002, 124, 5822-5833. | 13.7 | 200 |
| 7 | 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 |
| 8 | 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 |
| 9 | NMRâ€Based Protein Potentials. Angewandte Chemie - International Edition, 2010, 49, 6778-6780. | 13.8 | 173 |
| 10 | NMR in Metabolomics and Natural Products Research: Two Sides of the Same Coin. Accounts of Chemical Research, 2012, 45, 288-297. | 15.6 | 151 |
| 11 | Indirect Covariance NMR Spectroscopy. Journal of the American Chemical Society, 2004, 126, 13180-13181. | 13.7 | 136 |
| 12 | 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 |
| 13 | Collective protein dynamics and nuclear spin relaxation. Journal of Chemical Physics, 1995, 102, 3396-3403. | 3.0 | 115 |
| 14 | Multidimensional Approaches to NMR-Based Metabolomics. Analytical Chemistry, 2014, 86, 47-57. | 6.5 | 112 |
| 15 | 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 |
| 16 | Theory of covariance nuclear magnetic resonance spectroscopy. Journal of Chemical Physics, 2004, 121, 409. | 3.0 | 110 |
| 17 | Web Server Based Complex Mixture Analysis by NMR. Analytical Chemistry, 2008, 80, 3606-3611. | 6.5 | 110 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | Covariance NMR spectroscopy by singular value decomposition. Journal of Magnetic Resonance, 2004, 171, 277-283. | 2.1 | 99 |
| 21 | Quantitative Molecular Ensemble Interpretation of NMR Dipolar Couplings without Restraints. Journal of the American Chemical Society, 2007, 129, 4158-4159. | 13.7 | 98 |
| 22 | 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 |
| 23 | Customized Metabolomics Database for the Analysis of NMR <sup>1</sup>Hâ€“<sup>1</sup>H TOCSY and <sup>13</sup>Câ€“<sup>1</sup>H HSQC-TOCSY Spectra of Complex Mixtures. Analytical Chemistry, 2014, 86, 5494-5501. | 6.5 | 96 |
| 24 | Unified and Isomer-Specific NMR Metabolomics Database for the Accurate Analysis of <sup>13</sup>Câ€“<sup>1</sup>H HSQC Spectra. ACS Chemical Biology, 2015, 10, 452-459. | 3.4 | 96 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | Certification of Molecular Dynamics Trajectories with NMR Chemical Shifts. Journal of Physical Chemistry Letters, 2010, 1, 246-248. | 4.6 | 79 |
| 30 | Emerging new strategies for successful metabolite identification in metabolomics. Bioanalysis, 2016, 8, 557-573. | 1.5 | 79 |
| 31 | 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 |
| 32 | Characterization of biomolecular structure and dynamics by NMR cross relaxation. Progress in Nuclear Magnetic Resonance Spectroscopy, 1994, 26, 27-58. | 7.5 | 76 |
| 33 | 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 |
| 34 | TOCCATA: A Customized Carbon Total Correlation Spectroscopy NMR Metabolomics Database. Analytical Chemistry, 2012, 84, 9395-9401. | 6.5 | 72 |
| 35 | Dynamics of Lysine Side-Chain Amino Groups in a Protein Studied by Heteronuclear <sup>1</sup>Hâ€“<sup>15</sup>N NMR Spectroscopy. Journal of the American Chemical Society, 2011, 133, 909-919. | 13.7 | 71 |
| 36 | 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 |

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| 37 | 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 |
| 38 | A Dictionary for Protein Side-Chain Entropies from NMR Order Parameters. Journal of the American Chemical Society, 2009, 131, 7226-7227. | 13.7 | 67 |
| 39 | Robust Deconvolution of Complex Mixtures by Covariance TOCSY Spectroscopy. Angewandte Chemie - International Edition, 2007, 46, 2639-2642. | 13.8 | 66 |
| 40 | 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 |
| 41 | Strategy for Automated Analysis of Dynamic Metabolic Mixtures by NMR. Application to an Insect Venom. Analytical Chemistry, 2007, 79, 7748-7752. | 6.5 | 60 |
| 42 | Two elephants in the room. Current Opinion in Clinical Nutrition and Metabolic Care, 2015, 18, 471-477. | 2.5 | 60 |
| 43 | Generalized Indirect Covariance NMR Formalism for Establishment of Multidimensional Spin Correlations. Journal of Physical Chemistry A, 2009, 113, 12898-12903. | 2.5 | 57 |
| 44 | 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 |
| 45 | Efficient RMSD measures for the comparison of two molecular ensembles. Proteins: Structure, Function and Bioinformatics, 2002, 50, 26-34. | 2.6 | 55 |
| 46 | Deconvolution of Chemical Mixtures with High Complexity by NMR Consensus Trace Clustering. Analytical Chemistry, 2011, 83, 7412-7417. | 6.5 | 55 |
| 47 | DEEP picker is a deep neural network for accurate deconvolution of complex two-dimensional NMR spectra. Nature Communications, 2021, 12, 5229. | 12.8 | 55 |
| 48 | 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 |
| 49 | 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 |
| 50 | 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 |
| 51 | 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 |
| 52 | Self-Consistency Analysis of Dipolar Couplings in Multiple Alignments of Ubiquitin. Journal of the American Chemical Society, 2003, 125, 5596-5597. | 13.7 | 53 |
| 53 | Orderâ€“Disorder Transitions Govern Kinetic Cooperativity and Allostery of Monomeric Human Glucokinase. PLoS Biology, 2012, 10, e1001452. | 5.6 | 51 |
| 54 | Collective NMR relaxation model applied to protein dynamics. Physical Review Letters, 1994, 72, 940-943. | 7.8 | 49 |

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| 55 | Entropy Localization in Proteins. Journal of Physical Chemistry B, 2010, 114, 16036-16044. | 2.6 | 49 |
| 56 | Assignment Strategy for Proteins with Known Structure. Journal of Magnetic Resonance, 2002, 157, 119-123. | 2.1 | 48 |
| 57 | Prediction of methyl-side Chain Dynamics in Proteins. Journal of Biomolecular NMR, 2004, 29, 363-368. | 2.8 | 48 |
| 58 | Quantitative Analysis of Metabolic Mixtures by Two-Dimensional <sup>13</sup>C Constant-Time TOCSY NMR Spectroscopy. Analytical Chemistry, 2013, 85, 6414-6420. | 6.5 | 47 |
| 59 | Atomistic Kinetic Model for Population Shift and Allostery in Biomolecules. Journal of the American Chemical Society, 2011, 133, 18999-19005. | 13.7 | 46 |
| 60 | 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 |
| 61 | In silicoRelationship between Configurational Entropy and Soft Degrees of Freedom in Proteins and Peptides. Physical Review Letters, 2009, 102, 118108. | 7.8 | 43 |
| 62 | 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 |
| 63 | 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 |
| 64 | In Silico Elucidation of the Recognition Dynamics of Ubiquitin. PLoS Computational Biology, 2011, 7, e1002035. | 3.2 | 41 |
| 65 | Spectral Deconvolution of Chemical Mixtures by Covariance NMR. ChemPhysChem, 2004, 5, 794-796. | 2.1 | 40 |
| 66 | Signature of Mobile Hydrogen Bonding of Lysine Side Chains from Long-Range <sup>15</sup>Nâ€“<sup>13</sup>C Scalar J-Couplings and Computation. Journal of the American Chemical Society, 2011, 133, 9192-9195. | 13.7 | 40 |
| 67 | PPM_One: a static protein structure based chemical shift predictor. Journal of Biomolecular NMR, 2015, 62, 403-409. | 2.8 | 40 |
| 68 | 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 |
| 69 | Decoding the Mobility and Time Scales of Protein Loops. Journal of Chemical Theory and Computation, 2015, 11, 1308-1314. | 5.3 | 39 |
| 70 | Dynamic and structural analysis of isotropically distributed molecular ensembles. Proteins: Structure, Function and Bioinformatics, 2002, 46, 177-189. | 2.6 | 38 |
| 71 | Web server suite for complex mixture analysis by covariance NMR. Magnetic Resonance in Chemistry, 2009, 47, S118-22. | 1.9 | 38 |
| 72 | Carbon Backbone Topology of the Metabolome of a Cell. Journal of the American Chemical Society, 2012, 134, 9006-9011. | 13.7 | 38 |

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| 73 | Water self-diffusion model for protein-water NMR cross relaxation. Chemical Physics Letters, 1994, 229, 75-81. | 2.6 | 37 |
| 74 | 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 |
| 75 | 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 |
| 76 | Toward a Predictive Understanding of Slow Methyl Group Dynamics in Proteins. Biophysical Journal, 2011, 101, 910-915. | 0.5 | 37 |
| 77 | All-Atom Contact Model for Understanding Protein Dynamics from Crystallographic B-Factors. Biophysical Journal, 2009, 96, 3074-3081. | 0.5 | 36 |
| 78 | 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 |
| 79 | 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 |
| 80 | 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 |
| 81 | 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 |
| 82 | Enhanced Covariance Spectroscopy from Minimal Datasets. Journal of the American Chemical Society, 2006, 128, 15564-15565. | 13.7 | 34 |
| 83 | Self-Consistent Metabolic Mixture Analysis by Heteronuclear NMR. Application to a Human Cancer Cell Line. Analytical Chemistry, 2008, 80, 7549-7553. | 6.5 | 34 |
| 84 | Principal component method for assessing structural heterogeneity across multiple alignment media. Journal of Biomolecular NMR, 2002, 24, 123-132. | 2.8 | 33 |
| 85 | 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 |
| 86 | Bacterial Attraction and Quorum Sensing Inhibition in Caenorhabditis elegans Exudates. Journal of Chemical Ecology, 2009, 35, 878-892. | 1.8 | 33 |
| 87 | Reprogramming of Glucose Metabolism by Zerumbone Suppresses Hepatocarcinogenesis. Molecular Cancer Research, 2018, 16, 256-268. | 3.4 | 33 |
| 88 | Covariance NMR in higher dimensions: application to 4D NOESY spectroscopy of proteins. Journal of Biomolecular NMR, 2007, 39, 165-175. | 2.8 | 32 |
| 89 | Functional protein dynamics on uncharted time scales detected by nanoparticle-assisted NMR spin relaxation. Science Advances, 2019, 5, eaax5560. | 10.3 | 32 |
| 90 | 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 |

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| 91 | 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 |
| 92 | 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 |
| 93 | 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 |
| 94 | Direct Evidence of Conformational Heterogeneity in Human Pancreatic Glucokinase from High-Resolution Nuclear Magnetic Resonance. Biochemistry, 2010, 49, 7969-7971. | 2.5 | 29 |
| 95 | 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 |
| 96 | Use of Charged Nanoparticles in NMR-Based Metabolomics for Spectral Simplification and Improved Metabolite Identification. Analytical Chemistry, 2015, 87, 7211-7217. | 6.5 | 29 |
| 97 | 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 |
| 98 | 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 |
| 99 | 2D NMR-Based Metabolomics with HSQC/TOCSY NOAH Supersequences. Analytical Chemistry, 2021, 93, 6112-6119. | 6.5 | 28 |
| 100 | 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 |
| 101 | Initial Conformational Changes of Human Transthyretin under Partially Denaturing Conditions. Biophysical Journal, 2005, 89, 433-443. | 0.5 | 26 |
| 102 | Resolution-Enhanced 4D <sup>15</sup>N/<sup>13</sup>C NOESY Protein NMR Spectroscopy by Application of the Covariance Transform. Journal of the American Chemical Society, 2007, 129, 14126-14127. | 13.7 | 26 |
| 103 | Variation in Quadrupole Couplings of Î± Deuterons in Ubiquitin Suggests the Presence of C<sup>Î±</sup>â^'H<sup>Î±</sup>Â·Â·Â·Oâ•C Hydrogen Bonds. Journal of the American Chemical Society, 2010, 132, 7709-7719. | 13.7 | 26 |
| 104 | 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 |
| 105 | The structure of gramicidin A in dimethylsulfoxide/acetone. FEBS Journal, 1990, 194, 57-60. | 0.2 | 25 |
| 106 | Evaluation of Configurational Entropy Methods from Peptide Foldingâ^'Unfolding Simulation. Journal of Physical Chemistry B, 2007, 111, 13807-13813. | 2.6 | 25 |
| 107 | Competitive Binding between Dynamic p53 Transactivation Subdomains to Human MDM2 Protein. Journal of Biological Chemistry, 2012, 287, 30376-30384. | 3.4 | 25 |
| 108 | Real-Time Pure Shift HSQC NMR for Untargeted Metabolomics. Analytical Chemistry, 2019, 91, 2304-2311. | 6.5 | 25 |

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| 109 | Quantitative covariance NMR by regularization. Journal of Biomolecular NMR, 2007, 38, 73-77. | 2.8 | 24 |
| 110 | Nanoparticle-Assisted Removal of Protein in Human Serum for Metabolomics Studies. Analytical Chemistry, 2016, 88, 1003-1007. | 6.5 | 24 |
| 111 | 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 |
| 112 | Quantitative Cooperative Binding Model for Intrinsically Disordered Proteins Interacting with Nanomaterials. Journal of the American Chemical Society, 2020, 142, 10730-10738. | 13.7 | 22 |
| 113 | Z-matrix formalism for quantitative noise assessment of covariance nuclear magnetic resonance spectra. Journal of Chemical Physics, 2008, 129, 104511. | 3.0 | 21 |
| 114 | Structural and Entropic Allosteric Signal Transduction Strength via Correlated Motions. Journal of Physical Chemistry Letters, 2012, 3, 1722-1726. | 4.6 | 21 |
| 115 | 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 |
| 116 | Absolute Minimal Sampling in Highâ€Dimensional NMR Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 14169-14172. | 13.8 | 19 |
| 117 | Identification of Unknown Metabolomics Mixture Compounds by Combining NMR, MS, and Cheminformatics. Methods in Enzymology, 2019, 615, 407-422. | 1.0 | 19 |
| 118 | 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 |
| 119 | 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 |
| 120 | Accurate and Efficient Determination of Unknown Metabolites in Metabolomics by NMR-Based Molecular Motif Identification. Analytical Chemistry, 2019, 91, 15686-15693. | 6.5 | 16 |
| 121 | Rapid Determination of Fast Protein Dynamics from NMR Chemical Exchange Saturation Transfer Data. Angewandte Chemie - International Edition, 2016, 55, 3117-3119. | 13.8 | 15 |
| 122 | Nanoparticle-Assisted Metabolomics. Metabolites, 2018, 8, 21. | 2.9 | 15 |
| 123 | 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 |
| 124 | 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 |
| 125 | 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 |
| 126 | Nonâ€Uniform and Absolute Minimal Sampling for Highâ€Throughput Multidimensional NMR Applications. Chemistry - A European Journal, 2018, 24, 11535-11544. | 3.3 | 14 |

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| 127 | Broadband Dynamics of Ubiquitin by Anionic and Cationic Nanoparticle Assisted NMR Spin Relaxation. Angewandte Chemie - International Edition, 2021, 60, 148-152. | 13.8 | 14 |
| 128 | Higher-Rank Correlation NMR Spectra with Spectral Moment Filtering. Journal of Physical Chemistry Letters, 2010, 1, 1086-1089. | 4.6 | 13 |
| 129 | Extreme Nonuniform Sampling for Protein NMR Dynamics Studies in Minimal Time. Journal of the American Chemical Society, 2019, 141, 16829-16838. | 13.7 | 12 |
| 130 | Model for the allosteric regulation of the <scp>N</scp>a<sup>+</sup>/<scp>C</scp>a<sup>2+</sup> exchanger <scp>NCX</scp>. Proteins: Structure, Function and Bioinformatics, 2016, 84, 580-590. | 2.6 | 11 |
| 131 | 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 |
| 132 | Whispering within. Nature Chemistry, 2011, 3, 665-666. | 13.6 | 10 |
| 133 | Conformational heterogeneity and intrinsic disorder in enzyme regulation: Glucokinase as a case study. Intrinsically Disordered Proteins, 2015, 3, e1011008. | 1.9 | 10 |
| 134 | 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 |
| 135 | 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 |
| 136 | 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 |
| 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 | 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 |
| 139 | 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 |
| 140 | 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 |
| 141 | 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 |
| 142 | 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 |
| 143 | Kinetic Cooperativity in Human Pancreatic Glucokinase Originates from Millisecond Dynamics of the Small Domain. Angewandte Chemie, 2015, 127, 8247-8250. | 2.0 | 7 |
| 144 | Carbohydrate Background Removal in Metabolomics Samples. Analytical Chemistry, 2018, 90, 14100-14104. | 6.5 | 6 |

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| 145 | 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 |
| 146 | Absolut minimales Sampling in der hochdimensionalen NMRâ€Spektroskopie. Angewandte Chemie, 2016, 128, 14376-14379. | 2.0 | 5 |
| 147 | Statistical database analysis of the role of loop dynamics for proteinâ€“protein complex formation and allostery. Bioinformatics, 2017, 33, 1814-1819. | 4.1 | 5 |
| 148 | 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 |
| 149 | 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 |
| 150 | Modulation and Functional Role of the Orientations of the N- and P-Domains of Cu<sup>+</sup>-Transporting ATPase along the Ion Transport Cycle. Biochemistry, 2015, 54, 5095-5102. | 2.5 | 4 |
| 151 | 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 |
| 152 | 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 |
| 153 | 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 |
| 154 | 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 |
| 155 | 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 |
| 156 | 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 |
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