# A Joshua Wand

## List of Publications by Citations



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|---|---|---|---|
| 123 papers | 7,527 citations | 45 h-index | 85 g-index |
| 129 ext. papers | 8,065 ext. citations | 9.4 avg, IF | 6.06 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 123 | Design and synthesis of multi-haem proteins. *Nature*, **1994**, 368, 425-32 | 50.4 | 535 |
| 122 | Conformational entropy in molecular recognition by proteins. *Nature*, **2007**, 448, 325-9 | 50.4 | 526 |
| 121 | Microscopic origins of entropy, heat capacity and the glass transition in proteins. *Nature*, **2001**, 411, 501-4 | 50.4 | 273 |
| 120 | Characterization of the fast dynamics of protein amino acid side chains using NMR relaxation in solution. *Chemical Reviews*, **2006**, 106, 1672-99 | 68.1 | 270 |
| 119 | Redistribution and loss of side chain entropy upon formation of a calmodulin-peptide complex. *Nature Structural Biology*, **2000**, 7, 72-7 | | 255 |
| 118 | Dynamic activation of protein function: a view emerging from NMR spectroscopy. *Nature Structural Biology*, **2001**, 8, 926-31 | | 253 |
| 117 | The Reorganization Energy of Cytochrome c Revisited. *Journal of Physical Chemistry B*, **1997**, 101, 825-836 | 3.4 | 213 |
| 116 | The role of conformational entropy in molecular recognition by calmodulin. *Nature Chemical Biology*, **2010**, 6, 352-8 | 11.7 | 209 |
| 115 | Insights into the local residual entropy of proteins provided by NMR relaxation. *Protein Science*, **1996**, 5, 2647-50 | 6.3 | 202 |
| 114 | Site-resolved measurement of water-protein interactions by solution NMR. *Nature Structural and Molecular Biology*, **2011**, 18, 245-9 | 17.6 | 178 |
| 113 | Fast internal main-chain dynamics of human ubiquitin. *Biochemistry*, **1992**, 31, 3645-52 | 3.2 | 167 |
| 112 | Internal dynamics of human ubiquitin revealed by 13C-relaxation studies of randomly fractionally labeled protein. *Biochemistry*, **1996**, 35, 6116-25 | 3.2 | 153 |
| 111 | The dark energy of proteins comes to light: conformational entropy and its role in protein function revealed by NMR relaxation. *Current Opinion in Structural Biology*, **2013**, 23, 75-81 | 8.1 | 133 |
| 110 | Self contained high pressure cell, apparatus and procedure for the preparation of encapsulated proteins dissolved in low viscosity fluids for NMR spectroscopy. *Review of Scientific Instruments*, **2005**, 76, 1-7 | 1.7 | 132 |
| 109 | Direct access to the cooperative substructure of proteins and the protein ensemble via cold denaturation. *Nature Structural and Molecular Biology*, **2004**, 11, 352-7 | 17.6 | 125 |
| 108 | Proton resonance assignments of horse ferricytochrome c. *Biochemistry*, **1989**, 28, 195-203 | 3.2 | 125 |
| 107 | Solution structure of horse heart ferricytochrome c and detection of redox-related structural changes by high-resolution 1H NMR. *Biochemistry*, **1996**, 35, 12275-86 | 3.2 | 123 |

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| 106 | Model-independent and model-dependent analysis of the global and internal dynamics of cyclosporin A. *Journal of the American Chemical Society*, **1989**, 111, 4571-4578 | 16.4 | 122 |
| 105 | Two-dimensional 1H NMR studies of cytochrome c: hydrogen exchange in the N-terminal helix. *Biochemistry*, **1986**, 25, 1107-14 | 3.2 | 122 |
| 104 | Local stability and dynamics of apocytochrome b562 examined by the dependence of hydrogen exchange on hydrostatic pressure. *Biochemistry*, **1998**, 37, 9877-83 | 3.2 | 111 |
| 103 | Solution structure of apocytochrome b562. *Nature Structural and Molecular Biology*, **1994**, 1, 30-5 | 17.6 | 109 |
| 102 | Microscopic insights into the NMR relaxation-based protein conformational entropy meter. *Journal of the American Chemical Society*, **2013**, 135, 15092-100 | 16.4 | 105 |
| 101 | Elementary tetrahelical protein design for diverse oxidoreductase functions. *Nature Chemical Biology*, **2013**, 9, 826-833 | 11.7 | 104 |
| 100 | Proton resonance assignments of horse ferrocytochrome c. *Biochemistry*, **1989**, 28, 186-94 | 3.2 | 103 |
| 99 | Comparison of 2H and 13C NMR Relaxation Techniques for the Study of Protein Methyl Group Dynamics in Solution. *Journal of the American Chemical Society*, **1999**, 121, 2891-2902 | 16.4 | 97 |
| 98 | Entropy in molecular recognition by proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 6563-6568 | 11.5 | 96 |
| 97 | Mapping the hydration dynamics of ubiquitin. *Journal of the American Chemical Society*, **2011**, 133, 12326-9 | 16.4 | 96 |
| 96 | Local dynamics and stability of apocytochrome b562 examined by hydrogen exchange. *Biochemistry* , **1998**, 37, 3687-98 | 3.2 | 89 |
| 95 | Assignment of the backbone 1H and 15N NMR resonances of bacteriophage T4 lysozyme. *Biochemistry*, **1990**, 29, 6341-62 | 3.2 | 87 |
| 94 | Coupled motion in proteins revealed by pressure perturbation. *Journal of the American Chemical Society*, **2012**, 134, 8543-50 | 16.4 | 83 |
| 93 | Temperature dependence of the internal dynamics of a calmodulin-peptide complex. *Biochemistry*, **2002**, 41, 13814-25 | 3.2 | 83 |
| 92 | Improved side-chain prediction accuracy using an ab initio potential energy function and a very large rotamer library. *Protein Science*, **2004**, 13, 735-51 | 6.3 | 75 |
| 91 | Optimal Use of Cryogenic Probe Technology in NMR Studies of Proteins. *Journal of the American Chemical Society*, **2000**, 122, 4823-4824 | 16.4 | 74 |
| 90 | Validation of protein structure from preparations of encapsulated proteins dissolved in low viscosity fluids. *Journal of the American Chemical Society*, **2001**, 123, 2691-2 | 16.4 | 68 |
| 89 | Forced folding and structural analysis of metastable proteins. *Journal of the American Chemical Society*, **2004**, 126, 9498-9 | 16.4 | 64 |

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| 88 | Assessing potential bias in the determination of rotational correlation times of proteins by NMR relaxation. *Journal of Biomolecular NMR*, **1999**, 13, 101-12 | 3 | 64 |
| 87 | Calmodulin interacts with amphiphilic peptides composed of all D-amino acids. *Nature*, **1994**, 368, 651-3 | 50.4 | 61 |
| 86 | Dynamics and entropy of a calmodulin-peptide complex studied by NMR and molecular dynamics. *Biochemistry*, **2003**, 42, 562-70 | 3.2 | 59 |
| 85 | Role of cavities and hydration in the pressure unfolding of T4 lysozyme. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 13846-51 | 11.5 | 58 |
| 84 | High-Resolution Triple-Resonance NMR Spectroscopy of a Novel Calmodulin Peptide Complex at Kilobar Pressures. *Journal of the American Chemical Society*, **1996**, 118, 11329-11330 | 16.4 | 58 |
| 83 | Structural water in oxidized and reduced horse heart cytochrome c. *Nature Structural and Molecular Biology*, **1994**, 1, 378-82 | 17.6 | 53 |
| 82 | Improved labeling strategy for 13C relaxation measurements of methyl groups in proteins. *Journal of Biomolecular NMR*, **1997**, 9, 437-40 | 3 | 52 |
| 81 | Defining the Apoptotic Trigger: THE INTERACTION OF CYTOCHROME c AND CARDIOLIPIN. *Journal of Biological Chemistry*, **2015**, 290, 30879-87 | 5.4 | 48 |
| 80 | On the relationship between NMR-derived amide order parameters and protein backbone entropy changes. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 922-30 | 4.2 | 46 |
| 79 | Measuring Entropy in Molecular Recognition by Proteins. *Annual Review of Biophysics*, **2018**, 47, 41-61 | 21.1 | 45 |
| 78 | Optimized reverse micelle surfactant system for high-resolution NMR spectroscopy of encapsulated proteins and nucleic acids dissolved in low viscosity fluids. *Journal of the American Chemical Society*, **2014**, 136, 3465-74 | 16.4 | 45 |
| 77 | A direct test of the reductionist approach to structural studies of calmodulin activity: relevance of peptide models of target proteins. *Journal of Biological Chemistry*, **2002**, 277, 16351-4 | 5.4 | 43 |
| 76 | Structural characterization of the interactions between calmodulin and skeletal muscle myosin light chain kinase: effect of peptide (576-594)G binding on the Ca2+-binding domains. *Biochemistry*, **1989**, 28, 4011-20 | 3.2 | 43 |
| 75 | Dynamics of a de novo designed three-helix bundle protein studied by 15N, 13C, and 2H NMR relaxation methods. *Biochemistry*, **2001**, 40, 9560-9 | 3.2 | 42 |
| 74 | Reverse micelle encapsulation of membrane-anchored proteins for solution NMR studies. *Structure*, **2010**, 18, 9-16 | 5.2 | 41 |
| 73 | Hydrophobic modulation of heme properties in heme protein maquettes. *Biochemistry*, **2001**, 40, 10550-61 | 3.2 | 41 |
| 72 | Main chain and side chain dynamics of a heme protein: 15N and 2H NMR relaxation studies of R. capsulatus ferrocytochrome c2. *Biochemistry*, **2001**, 40, 6559-69 | 3.2 | 40 |
| 71 | A 13C labeling strategy reveals a range of aromatic side chain motion in calmodulin. *Journal of the American Chemical Society*, **2013**, 135, 9560-3 | 16.4 | 38 |

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| 70 | Changes in calmodulin main-chain dynamics upon ligand binding revealed by cross-correlated NMR relaxation measurements. *Journal of the American Chemical Society*, **2005**, 127, 828-9 | 16.4 | 37 |
| 69 | Cold denaturation of encapsulated ubiquitin. *Journal of the American Chemical Society*, **2006**, 128, 10652-3 | 16.4 | 37 |
| 68 | Dynamic activation and regulation of the mitogen-activated protein kinase p38. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 4655-4660 | 11.5 | 36 |
| 67 | Temperature dependence of fast dynamics in proteins. *Biophysical Journal*, **2007**, 92, L43-5 | 2.9 | 35 |
| 66 | Main chain and side chain dynamics of oxidized flavodoxin from Cyanobacterium anabaena. *Biochemistry*, **2001**, 40, 14744-53 | 3.2 | 35 |
| 65 | High-resolution NMR spectroscopy of encapsulated proteins dissolved in low-viscosity fluids. *Journal of Magnetic Resonance*, **2014**, 241, 137-47 | 3 | 34 |
| 64 | Reverse micelles in integral membrane protein structural biology by solution NMR spectroscopy. *Structure*, **2009**, 17, 345-51 | 5.2 | 33 |
| 63 | High-resolution NMR studies of encapsulated proteins in liquid ethane. *Journal of the American Chemical Society*, **2005**, 127, 10176-7 | 16.4 | 32 |
| 62 | NMR spectroscopy of proteins encapsulated in a positively charged surfactant. *Journal of Magnetic Resonance*, **2005**, 175, 158-62 | 3 | 31 |
| 61 | Preparation of encapsulated proteins dissolved in low viscosity fluids. *Journal of Biomolecular NMR*, **1999**, 14, 75-8 | 3 | 30 |
| 60 | Preparation, characterization, and NMR spectroscopy of encapsulated proteins dissolved in low viscosity fluids. *Journal of Biomolecular NMR*, **2003**, 25, 313-23 | 3 | 28 |
| 59 | Backbone and side chain dynamics of mutant calmodulin-peptide complexes. *Biochemistry*, **2005**, 44, 12627-39 | 3.2 | 27 |
| 58 | Conformational dynamics of calmodulin in complex with the calmodulin-dependent kinase kinase alpha calmodulin-binding domain. *Biochemistry*, **2006**, 45, 8732-41 | 3.2 | 27 |
| 57 | Novel surfactant mixtures for NMR spectroscopy of encapsulated proteins dissolved in low-viscosity fluids. *Protein Science*, **2005**, 14, 2919-21 | 6.3 | 27 |
| 56 | Measurement and control of pH in the aqueous interior of reverse micelles. *Journal of Physical Chemistry B*, **2014**, 118, 2020-31 | 3.4 | 26 |
| 55 | A surprising role for conformational entropy in protein function. *Topics in Current Chemistry*, **2013**, 337, 69-94 | | 26 |
| 54 | A method for solution NMR structural studies of large integral membrane proteins: reverse micelle encapsulation. *Biochimica Et Biophysica Acta - Biomembranes*, **2010**, 1798, 150-60 | 3.8 | 26 |
| 53 | Characterization of the backbone and side chain dynamics of the CaM-CaMKIp complex reveals microscopic contributions to protein conformational entropy. *Biochemistry*, **2006**, 45, 9841-8 | 3.2 | 26 |

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| 52 | Backbone and side-chain heteronuclear resonance assignments and hyperfine NMR shifts in horse cytochrome c. *Protein Science*, **2003**, 12, 2104-8 | 6.3 | 25 |
| 51 | The dynamical response of hen egg white lysozyme to the binding of a carbohydrate ligand. *Protein Science*, **2012**, 21, 1066-73 | 6.3 | 24 |
| 50 | New reverse micelle surfactant systems optimized for high-resolution NMR spectroscopy of encapsulated proteins. *Langmuir*, **2005**, 21, 10632-7 | 4 | 24 |
| 49 | Practical aspects of high-pressure NMR spectroscopy and its applications in protein biophysics and structural biology. *Methods*, **2018**, 148, 67-80 | 4.6 | 23 |
| 48 | A simple and effective NMR cell for studies of encapsulated proteins dissolved in low viscosity solvents. *Journal of Biomolecular NMR*, **2002**, 23, 311-6 | 3 | 23 |
| 47 | A sharp thermal transition of fast aromatic-ring dynamics in ubiquitin. *Angewandte Chemie - International Edition*, **2015**, 54, 102-7 | 16.4 | 22 |
| 46 | On the ability of molecular dynamics force fields to recapitulate NMR derived protein side chain order parameters. *Protein Science*, **2016**, 25, 1156-60 | 6.3 | 20 |
| 45 | Characterization of Cetyltrimethylammonium Bromide/Hexanol Reverse Micelles by Experimentally Benchmarked Molecular Dynamics Simulations. *Langmuir*, **2016**, 32, 1674-84 | 4 | 20 |
| 44 | Re-evaluation of the model-free analysis of fast internal motion in proteins using NMR relaxation. *Journal of Physical Chemistry B*, **2008**, 112, 12095-103 | 3.4 | 20 |
| 43 | On the dynamic origins of allosteric activation. *Science*, **2001**, 293, 1395 | 33.3 | 19 |
| 42 | Reverse micelles as a platform for dynamic nuclear polarization in solution NMR of proteins. *Journal of the American Chemical Society*, **2014**, 136, 2800-7 | 16.4 | 18 |
| 41 | Optimization of NMR spectroscopy of encapsulated proteins dissolved in low viscosity fluids. *Journal of Biomolecular NMR*, **2011**, 50, 421-30 | 3 | 18 |
| 40 | High-resolution nuclear magnetic resonance of encapsulated proteins dissolved in low viscosity fluids. *Methods in Enzymology*, **2001**, 339, 54-70 | 1.7 | 15 |
| 39 | Fast structural dynamics in reduced and oxidized cytochrome c. *Protein Science*, **2009**, 18, 670-4 | 6.3 | 14 |
| 38 | Magnetic susceptibility-induced alignment of proteins in reverse micelles. *Journal of the American Chemical Society*, **2006**, 128, 15930-1 | 16.4 | 14 |
| 37 | Molecular recognition by calmodulin: pressure-induced reorganization of a novel calmodulin-peptide complex. *Biochemistry*, **1996**, 35, 1599-605 | 3.2 | 13 |
| 36 | Accurate determination of rates from non-uniformly sampled relaxation data. *Journal of Biomolecular NMR*, **2016**, 65, 157-170 | 3 | 13 |
| 35 | Characterization of Internal Protein Dynamics and Conformational Entropy by NMR Relaxation. *Methods in Enzymology*, **2019**, 615, 237-284 | 1.7 | 13 |

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| 34 | Banding of NMR-derived methyl order parameters: implications for protein dynamics. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2106-17 | 4.2 | 12 |
| 33 | Partial alignment and measurement of residual dipolar couplings of proteins under high hydrostatic pressure. *Journal of Biomolecular NMR*, **2013**, 56, 353-7 | 3 | 12 |
| 32 | Sequence-specific resonance assignments for a designed four-alpha-helix bundle protein. *Journal of Biomolecular NMR*, **1998**, 11, 227-8 | 3 | 12 |
| 31 | Improving yields of deuterated, methyl labeled protein by growing in HO. *Journal of Biomolecular NMR*, **2018**, 71, 263-273 | 3 | 11 |
| 30 | Modification of encapsulation pressure of reverse micelles in liquid ethane. *Journal of Magnetic Resonance*, **2011**, 212, 229-33 | 3 | 11 |
| 29 | Characterizing Protein Hydration Dynamics Using Solution NMR Spectroscopy. *Methods in Enzymology*, **2019**, 615, 77-101 | 1.7 | 10 |
| 28 | Water loading driven size, shape, and composition of cetyltrimethylammonium/hexanol/pentane reverse micelles. *Journal of Colloid and Interface Science*, **2019**, 540, 207-217 | 9.3 | 10 |
| 27 | Membrane Proteins Have Distinct Fast Internal Motion and Residual Conformational Entropy. *Angewandte Chemie - International Edition*, **2020**, 59, 11108-11114 | 16.4 | 9 |
| 26 | The Molecular Basis for Life in Extreme Environments. *Annual Review of Biophysics*, **2021**, 50, 343-372 | 21.1 | 9 |
| 25 | Design Principles for SuCESsFul Biosensors: Specific Fluorophore/Analyte Binding and Minimization of Fluorophore/Scaffold Interactions. *Journal of Molecular Biology*, **2016**, 428, 4228-4241 | 6.5 | 8 |
| 24 | Bringing disorder and dynamics in protein allostery into focus. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 4278-4280 | 11.5 | 7 |
| 23 | Dynamic and thermodynamic response of the Ras protein Cdc42Hs upon association with the effector domain of PAK3. *Journal of Molecular Biology*, **2014**, 426, 3520-38 | 6.5 | 7 |
| 22 | Al NMR: a novel NMR data processing program optimized for sparse sampling. *Journal of Biomolecular NMR*, **2012**, 52, 79-89 | 3 | 7 |
| 21 | AMORE-HX: a multidimensional optimization of radial enhanced NMR-sampled hydrogen exchange. *Journal of Biomolecular NMR*, **2009**, 45, 233-9 | 3 | 7 |
| 20 | Reverse Micelle Encapsulation of Proteins for NMR Spectroscopy. *Methods in Enzymology*, **2019**, 615, 43-75 | 1.7 | 7 |
| 19 | Solution NMR investigation of the response of the lactose repressor core domain dimer to hydrostatic pressure. *Biophysical Chemistry*, **2017**, 231, 39-44 | 3.5 | 6 |
| 18 | Optimized angle selection for radial sampled NMR experiments. *Journal of Magnetic Resonance*, **2008**, 195, 169-78 | 3 | 6 |
| 17 | Using biochemistry and biophysics to extinguish androgen receptor signaling in prostate cancer. *Journal of Biological Chemistry*, **2021**, 296, 100240 | 5.4 | 6 |

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| 16 | Extending the Detection Limit in Fragment Screening of Proteins Using Reverse Micelle Encapsulation. *ACS Chemical Biology*, **2019**, 14, 2224-2232 | 4.9 | 5 |
| 15 | Phasing arbitrarily sampled multidimensional NMR data. *Journal of Magnetic Resonance*, **2007**, 187, 363-370 | | 5 |
| 14 | Reply to Kitahara and Mulder: An ensemble view of protein stability best explains pressure effects in a T4 lysozyme cavity mutant. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E924 | 11.5 | 4 |
| 13 | Biophysics: Enzymes surf the heat wave. *Nature*, **2015**, 517, 149-50 | 50.4 | 4 |
| 12 | NMR Spectroscopy of Encapsulated Proteins Dissolved in Low Viscosity Fluids **2002**, 121-160 | | 4 |
| 11 | Optimized expression and purification of biophysical quantities of Lac repressor and Lac repressor regulatory domain. *Protein Expression and Purification*, **2016**, 123, 75-82 | 2 | 4 |
| 10 | The unusual internal motion of the villin headpiece subdomain. *Protein Science*, **2016**, 25, 423-32 | 6.3 | 4 |
| 9 | Membrane Proteins Have Distinct Fast Internal Motion and Residual Conformational Entropy. *Angewandte Chemie*, **2020**, 132, 11201-11207 | 3.6 | 3 |
| 8 | Site-Resolved and Quantitative Characterization of Very Weak Protein-Ligand Interactions. *ACS Chemical Biology*, **2019**, 14, 1398-1402 | 4.9 | 3 |
| 7 | Self-Masked Aldehyde Inhibitors: A Novel Strategy for Inhibiting Cysteine Proteases. *Journal of Medicinal Chemistry*, **2021**, 64, 11267-11287 | 8.3 | 3 |
| 6 | SEnD NMR: sensitivity enhanced n-dimensional NMR. *Journal of Magnetic Resonance*, **2010**, 202, 250-8 | 3 | 2 |
| 5 | Protein conformational entropy is not slaved to water. *Scientific Reports*, **2020**, 10, 17587 | 4.9 | 1 |
| 4 | A Sharp Thermal Transition of Fast Aromatic-Ring Dynamics in Ubiquitin. *Angewandte Chemie*, **2015**, 127, 104-109 | 3.6 | |
| 3 | Optimized linear prediction for radial sampled multidimensional NMR experiments. *Journal of Magnetic Resonance*, **2011**, 212, 240-4 | 3 | |
| 2 | Conformational entropy in molecular recognition by proteins. *FASEB Journal*, **2008**, 22, 528.3 | 0.9 | |
| 1 | NMR Structure of a Disulfide-Crosslinked □b□ Cytoplasmic Domain Heterodimer. *Blood*, **2008**, 112, 2866-2866 | 2.2 | |