

Lorna J Smith

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69 papers	5,285 citations	27 h-index	71 g-index
71 ext. papers	5,686 ext. citations	5.7 avg, IF	5.05 L-index

#	Paper	IF	Citations
69	Hydrodynamic radii of native and denatured proteins measured by pulse field gradient NMR techniques. <i>Biochemistry</i> , 1999 , 38, 16424-31	3.2	786
68	Long-range interactions within a nonnative protein. <i>Science</i> , 2002 , 295, 1719-22	33.3	548
67	Defect-Rich Ultrathin ZnAl-Layered Double Hydroxide Nanosheets for Efficient Photoreduction of CO ₂ to CO with Water. <i>Advanced Materials</i> , 2015 , 27, 7824-31	24	445
66	Understanding protein folding via free-energy surfaces from theory and experiment. <i>Trends in Biochemical Sciences</i> , 2000 , 25, 331-9	10.3	413
65	Analysis of main chain torsion angles in proteins: prediction of NMR coupling constants for native and random coil conformations. <i>Journal of Molecular Biology</i> , 1996 , 255, 494-506	6.5	358
64	Structural and dynamical properties of a denatured protein. Heteronuclear 3D NMR experiments and theoretical simulations of lysozyme in 8 M urea. <i>Biochemistry</i> , 1997 , 36, 8977-91	3.2	271
63	The concept of a random coil. Residual structure in peptides and denatured proteins. <i>Folding & Design</i> , 1996 , 1, R95-106		252
62	Charge-state dependent compaction and dissociation of protein complexes: insights from ion mobility and molecular dynamics. <i>Journal of the American Chemical Society</i> , 2012 , 134, 3429-38	16.4	193
61	Characterisation of protein unfolding by NMR diffusion measurements. <i>Journal of Biomolecular NMR</i> , 1997 , 10, 199-203	3	181
60	Toward a Description of the Conformations of Denatured States of Proteins. Comparison of a Random Coil Model with NMR Measurements. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 2661-2666		148
59	A refined solution structure of hen lysozyme determined using residual dipolar coupling data. <i>Protein Science</i> , 2001 , 10, 677-88	6.3	141
58	Comparison of MD simulations and NMR experiments for hen lysozyme. Analysis of local fluctuations, cooperative motions, and global changes. <i>Biochemistry</i> , 1995 , 34, 10918-31	3.2	120
57	Heme proteins--diversity in structural characteristics, function, and folding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 2349-68	4.2	117
56	NMR analysis of main-chain conformational preferences in an unfolded fibronectin-binding protein. <i>Journal of Molecular Biology</i> , 1997 , 274, 152-9	6.5	114
55	Computer Simulation of Urea-Water Mixtures: A Test of Force Field Parameters for Use in Biomolecular Simulation. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 1065-1071	3.4	109
54	Amyloid fibril formation by a helical cytochrome. <i>FEBS Letters</i> , 2001 , 495, 184-6	3.8	107
53	Assessing equilibration and convergence in biomolecular simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002 , 48, 487-96	4.2	100

52	Stimulation and inhibition of fibril formation by a peptide in the presence of different concentrations of SDS. <i>FEBS Letters</i> , 2002 , 529, 193-7	3.8	78
51	Validation of Molecular Simulation: An Overview of Issues. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 884-902	16.4	74
50	Chemical shifts in denatured proteins: resonance assignments for denatured ubiquitin and comparisons with other denatured proteins. <i>Journal of Biomolecular NMR</i> , 2001 , 19, 153-65	3	62
49	Exploration of partially unfolded states of human alpha-lactalbumin by molecular dynamics simulation. <i>Journal of Molecular Biology</i> , 2001 , 306, 329-47	6.5	58
48	Response of native and denatured hen lysozyme to high pressure studied by ¹⁵ N/ ¹ H NMR spectroscopy. <i>FEBS Journal</i> , 2001 , 268, 1782-1793		53
47	The structural characteristics of nonspecific lipid transfer proteins explain their resistance to gastroduodenal proteolysis. <i>Biochemistry</i> , 2010 , 49, 2130-9	3.2	39
46	Comparison of four independently determined structures of human recombinant interleukin-4. <i>Nature Structural and Molecular Biology</i> , 1994 , 1, 301-10	17.6	39
45	Heat treatment of bovine alpha-lactalbumin results in partially folded, disulfide bond shuffled states with enhanced surface activity. <i>Biochemistry</i> , 2007 , 46, 9774-84	3.2	33
44	Side-chain conformational disorder in a molten globule: molecular dynamics simulations of the A-state of human alpha-lactalbumin. <i>Journal of Molecular Biology</i> , 1999 , 286, 1567-80	6.5	33
43	Characterization of the denaturation of human alpha-lactalbumin in urea by molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 58, 439-49	4.2	32
42	Molecular dynamics simulations of human alpha-lactalbumin: changes to the structural and dynamical properties of the protein at low pH. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 36, 77-86	4.2	27
41	Solution structure of a peptide fragment of human alpha-lactalbumin in trifluoroethanol: a model for local structure in the molten globule. <i>Structure</i> , 1994 , 2, 703-12	5.2	27
40	Photoreduction: Defect-Rich Ultrathin ZnAl-Layered Double Hydroxide Nanosheets for Efficient Photoreduction of CO ₂ to CO with Water (Adv. Mater. 47/2015). <i>Advanced Materials</i> , 2015 , 27, 7823-7823 ³⁴		25
39	Residual dipolar couplings: are multiple independent alignments always possible?. <i>Journal of Biomolecular NMR</i> , 2011 , 49, 53-60	3	25
38	The cytochrome c fold can be attained from a compact apo state by occupancy of a nascent heme binding site. <i>Journal of Biological Chemistry</i> , 2001 , 276, 45813-7	5.4	22
37	Deriving Structural Information from Experimentally Measured Data on Biomolecules. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 15990-16010	16.4	21
36	Asparagine and glutamine side-chain conformation in solution and crystal: a comparison for hen egg-white lysozyme using residual dipolar couplings. <i>Journal of Biomolecular NMR</i> , 2004 , 30, 327-46	3	20
35	The binding cavity of mouse major urinary protein is optimised for a variety of ligand binding modes. <i>Biochemical and Biophysical Research Communications</i> , 2009 , 390, 1266-71	3.4	19

34	Partially folded forms of barley lipid transfer protein are more surface active. <i>Biochemistry</i> , 2009 , 48, 12081-8	3.2	17
33	Computational methods for generating models of denatured and partially folded proteins. <i>Methods</i> , 2004 , 34, 144-50	4.6	16
32	NMR analysis shows that a b-type variant of <i>Hydrogenobacter thermophilus</i> cytochrome c552 retains its native structure. <i>Journal of Biological Chemistry</i> , 2004 , 279, 15177-82	5.4	15
31	Disulfide bond shuffling in bovine alpha-lactalbumin: MD simulation confirms experiment. <i>Biochemistry</i> , 2008 , 47, 12104-7	3.2	14
30	Native-like secondary structure in a peptide from the alpha-domain of hen lysozyme. <i>Folding & Design</i> , 1996 , 1, 473-84		14
29	Probing the Structure and Dynamics of Proteins by Combining Molecular Dynamics Simulations and Experimental NMR Data. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3430-44	6.4	11
28	Characterization of the molten globule state of retinol-binding protein using a molecular dynamics simulation approach. <i>FEBS Journal</i> , 2005 , 272, 4826-38	5.7	11
27	NMR and protein dynamics. <i>International Journal of Quantum Chemistry</i> , 1996 , 59, 315-332	2.1	9
26	Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12. <i>Protein Science</i> , 2013 , 22, 56-64	6.3	8
25	Probing the urea dependence of residual structure in denatured human alpha-lactalbumin. <i>Journal of Biomolecular NMR</i> , 2009 , 45, 121-31	3	8
24	Bestimmung von Strukturinformation aus experimentellen Messdaten für Biomoleküle. <i>Angewandte Chemie</i> , 2016 , 128, 16222-16244	3.6	7
23	Molecular dynamics simulations of <i>Hydrogenobacter thermophilus</i> cytochrome c552: comparisons of the wild-type protein, a b-type variant, and the apo state. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 65, 702-11	4.2	7
22	Post-translational modification of barley LTP1b: the lipid adduct lies in the hydrophobic cavity and alters the protein dynamics. <i>FEBS Letters</i> , 2007 , 581, 4557-61	3.8	6
21	Photo-CIDNP NMR spectroscopy of a heme-containing protein. <i>Journal of Magnetic Resonance</i> , 2005 , 175, 330-5	3	6
20	The dynamics of lysozyme from bacteriophage lambda in solution probed by NMR and MD simulations. <i>ChemBioChem</i> , 2013 , 14, 1780-8	3.8	5
19	Structural Aspects of the O-glycosylation Linkage in Glycopeptides via MD Simulations and Comparison with NMR Experiments. <i>ChemPhysChem</i> , 2019 , 20, 1527-1537	3.2	4
18	Molecular dynamics simulations of barley and maize lipid transfer proteins show different ligand binding preferences in agreement with experimental data. <i>Biochemistry</i> , 2013 , 52, 5029-38	3.2	4
17	Initial denaturing conditions influence the slow folding phase of acylphosphatase associated with proline isomerization. <i>Protein Science</i> , 2000 , 9, 1466-73	6.3	4

16	On the Use of Side-Chain NMR Relaxation Data to Derive Structural and Dynamical Information on Proteins: A Case Study Using Hen Lysozyme. <i>ChemBioChem</i> , 2021 , 22, 1049-1064	3.8	4
15	Characterization of the flexible lip regions in bacteriophage lambda lysozyme using MD simulations. <i>European Biophysics Journal</i> , 2015 , 44, 235-47	1.9	3
14	Validierung von molekularen Simulationen: eine Übersicht verschiedener Aspekte. <i>Angewandte Chemie</i> , 2018 , 130, 894-915	3.6	3
13	Characterization of an alternative low energy fold for bovine α -lactalbumin formed by disulfide bond shuffling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 913-9	4.2	3
12	An NMR and MD study of complexes of bacteriophage lambda lysozyme with tetra- and hexa-N-acetylchitohexaose. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020 , 88, 82-93	4.2	3
11	Interpretation of Seemingly Contradictory Data: Low NMR S Order Parameters Observed in Helices and High NMR S Order Parameters in Disordered Loops of the Protein hGH at Low pH. <i>Chemistry - A European Journal</i> , 2017 , 23, 9585-9591	4.8	2
10	Using Complementary NMR Data Sets To Detect Inconsistencies and Model Flaws in the Structure Determination of Human Interleukin-4. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 7055-7063	3.4	2
9	A molecular dynamics simulation investigation of the relative stability of the cyclic peptide octreotide and its deprotonated and its (CF)-Trp substituted analogs in different solvents. <i>Bioorganic and Medicinal Chemistry</i> , 2016 , 24, 4936-4948	3.4	2
8	On the use of J-coupling NMR data to derive structural information on proteins. <i>Journal of Biomolecular NMR</i> , 2021 , 75, 39-70	3	2
7	Structure of SPH (self-incompatibility protein homologue) proteins: a widespread family of small, highly stable, secreted proteins. <i>Biochemical Journal</i> , 2019 , 476, 809-826	3.8	1
6	On the use of time-averaging restraints when deriving biomolecular structure from 3J -coupling values obtained from NMR experiments. <i>Journal of Biomolecular NMR</i> , 2016 , 66, 69-83	3	1
5	Comparison of the backbone dynamics of wild-type <i>Hydrogenobacter thermophilus</i> cytochrome c(552) and its b-type variant. <i>Journal of Biomolecular NMR</i> , 2015 , 62, 221-31	3	1
4	The β -Shape-Shifter α -Peptide from the Disulphide Isomerase PmScsC Shows Context-Dependent Conformational Preferences. <i>Biomolecules</i> , 2021 , 11,	5.9	1
3	Backbone assignment of E. coli NfsB and the effects of addition of the cofactor analogue nicotinic acid. <i>Biomolecular NMR Assignments</i> , 2021 , 15, 143-151	0.7	0
2	Molecular dynamics simulation or structure refinement of proteins: are solvent molecules required? A case study using hen lysozyme.. <i>European Biophysics Journal</i> , 2022 , 1	1.9	0
1	H, C and N NMR assignments of self-incompatibility protein homologue 15 from <i>Arabidopsis thaliana</i> . <i>Biomolecular NMR Assignments</i> , 2019 , 13, 67-70	0.7	