Lorna J Smith

List of Publications by Year in Descending Order

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	Molecular dynamics simulation or structure refinement of proteins: are solvent molecules required? A case study using hen lysozyme.. *European Biophysics Journal*, **2022**, 1	1.9	0
68	The UShape-ShifterUPeptide from the Disulphide Isomerase PmScsC Shows Context-Dependent Conformational Preferences. *Biomolecules*, **2021**, 11,	5.9	1
67	On the Use of Side-Chain NMR Relaxation Data to Derive Structural and Dynamical Information on Proteins: A Case Study Using Hen Lysozyme. *ChemBioChem*, **2021**, 22, 1049-1064	3.8	4
66	Backbone assignment of E. coli NfsB and the effects of addition of the cofactor analogue nicotinic acid. *Biomolecular NMR Assignments*, **2021**, 15, 143-151	0.7	0
65	On the use of J-coupling NMR data to derive structural information on proteins. *Journal of Biomolecular NMR*, **2021**, 75, 39-70	3	2
64	An NMR and MD study of complexes of bacteriophage lambda lysozyme with tetra- and hexa-N-acetylchitohexaose. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 82-93	4.2	3
63	Structural Aspects of the O-glycosylation Linkage in Glycopeptides via MD Simulations and Comparison with NMR Experiments. *ChemPhysChem*, **2019**, 20, 1527-1537	3.2	4
62	Structure of SPH (self-incompatibility protein homologue) proteins: a widespread family of small, highly stable, secreted proteins. *Biochemical Journal*, **2019**, 476, 809-826	3.8	1
61	H, C and N NMR assignments of self-incompatibility protein homologue 15 from Arabidopsis thaliana. *Biomolecular NMR Assignments*, **2019**, 13, 67-70	0.7	
60	Validierung von molekularen Simulationen: eine Übersicht verschiedener Aspekte. *Angewandte Chemie*, **2018**, 130, 894-915	3.6	3
59	Validation of Molecular Simulation: An Overview of Issues. *Angewandte Chemie - International Edition*, **2018**, 57, 884-902	16.4	74
58	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. *Chemistry - A European Journal*, **2017**, 23, 9585-9591	4.8	2
57	Using Complementary NMR Data Sets To Detect Inconsistencies and Model Flaws in the Structure Determination of Human Interleukin-4. *Journal of Physical Chemistry B*, **2017**, 121, 7055-7063	3.4	2
56	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. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4936-4948	3.4	2
55	Bestimmung von Strukturinformation aus experimentellen Messdaten fü Biomolekü. *Angewandte Chemie*, **2016**, 128, 16222-16244	3.6	7
54	On the use of time-averaging restraints when deriving biomolecular structure from -coupling values obtained from NMR experiments. *Journal of Biomolecular NMR*, **2016**, 66, 69-83	3	1
53	Deriving Structural Information from Experimentally Measured Data on Biomolecules. *Angewandte Chemie - International Edition*, **2016**, 55, 15990-16010	16.4	21

52	Characterization of the flexible lip regions in bacteriophage lambda lysozyme using MD simulations. *European Biophysics Journal*, **2015**, 44, 235-47	1.9	3
51	Photoreduction: Defect-Rich Ultrathin ZnAl-Layered Double Hydroxide Nanosheets for Efficient Photoreduction of CO2 to CO with Water (Adv. Mater. 47/2015). *Advanced Materials*, **2015**, 27, 7823-7823	24	25
50	Defect-Rich Ultrathin ZnAl-Layered Double Hydroxide Nanosheets for Efficient Photoreduction of CO2 to CO with Water. *Advanced Materials*, **2015**, 27, 7824-31	24	445
49	Comparison of the backbone dynamics of wild-type Hydrogenobacter thermophilus cytochrome c(552) and its b-type variant. *Journal of Biomolecular NMR*, **2015**, 62, 221-31	3	1
48	Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12. *Protein Science*, **2013**, 22, 56-64	6.3	8
47	The dynamics of lysozyme from bacteriophage lambda in solution probed by NMR and MD simulations. *ChemBioChem*, **2013**, 14, 1780-8	3.8	5
46	Molecular dynamics simulations of barley and maize lipid transfer proteins show different ligand binding preferences in agreement with experimental data. *Biochemistry*, **2013**, 52, 5029-38	3.2	4
45	Probing the Structure and Dynamics of Proteins by Combining Molecular Dynamics Simulations and Experimental NMR Data. *Journal of Chemical Theory and Computation*, **2012**, 8, 3430-44	6.4	11
44	Charge-state dependent compaction and dissociation of protein complexes: insights from ion mobility and molecular dynamics. *Journal of the American Chemical Society*, **2012**, 134, 3429-38	16.4	193
43	Characterization of an alternative low energy fold for bovine α-lactalbumin formed by disulfide bond shuffling. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 913-9	4.2	3
42	Residual dipolar couplings: are multiple independent alignments always possible?. *Journal of Biomolecular NMR*, **2011**, 49, 53-60	3	25
41	The structural characteristics of nonspecific lipid transfer proteins explain their resistance to gastroduodenal proteolysis. *Biochemistry*, **2010**, 49, 2130-9	3.2	39
40	Heme proteins--diversity in structural characteristics, function, and folding. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2349-68	4.2	117
39	Probing the urea dependence of residual structure in denatured human alpha-lactalbumin. *Journal of Biomolecular NMR*, **2009**, 45, 121-31	3	8
38	The binding cavity of mouse major urinary protein is optimised for a variety of ligand binding modes. *Biochemical and Biophysical Research Communications*, **2009**, 390, 1266-71	3.4	19
37	Partially folded forms of barley lipid transfer protein are more surface active. *Biochemistry*, **2009**, 48, 12081-8	3.2	17
36	Disulfide bond shuffling in bovine alpha-lactalbumin: MD simulation confirms experiment. *Biochemistry*, **2008**, 47, 12104-7	3.2	14
35	Heat treatment of bovine alpha-lactalbumin results in partially folded, disulfide bond shuffled states with enhanced surface activity. *Biochemistry*, **2007**, 46, 9774-84	3.2	33

34	Post-translational modification of barley LTP1b: the lipid adduct lies in the hydrophobic cavity and alters the protein dynamics. *FEBS Letters*, **2007**, 581, 4557-61	3.8	6
33	Molecular dynamics simulations of Hydrogenobacter thermophilus cytochrome c552: comparisons of the wild-type protein, a b-type variant, and the apo state. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 702-11	4.2	7
32	Characterization of the denaturation of human alpha-lactalbumin in urea by molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 439-49	4.2	32
31	Characterization of the molten globule state of retinol-binding protein using a molecular dynamics simulation approach. *FEBS Journal*, **2005**, 272, 4826-38	5.7	11
30	Photo-CIDNP NMR spectroscopy of a heme-containing protein. *Journal of Magnetic Resonance*, **2005**, 175, 330-5	3	6
29	NMR analysis shows that a b-type variant of Hydrogenobacter thermophilus cytochrome c552 retains its native structure. *Journal of Biological Chemistry*, **2004**, 279, 15177-82	5.4	15
28	Asparagine and glutamine side-chain conformation in solution and crystal: a comparison for hen egg-white lysozyme using residual dipolar couplings. *Journal of Biomolecular NMR*, **2004**, 30, 327-46	3	20
27	Computational methods for generating models of denatured and partially folded proteins. *Methods* , **2004**, 34, 144-50	4.6	16
26	Computer Simulation of Urea Water Mixtures: A Test of Force Field Parameters for Use in Biomolecular Simulation. *Journal of Physical Chemistry B*, **2004**, 108, 1065-1071	3.4	109
25	Assessing equilibration and convergence in biomolecular simulations. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 487-96	4.2	100
24	Long-range interactions within a nonnative protein. *Science*, **2002**, 295, 1719-22	33.3	548
23	Stimulation and inhibition of fibril formation by a peptide in the presence of different concentrations of SDS. *FEBS Letters*, **2002**, 529, 193-7	3.8	78
22	Response of native and denatured hen lysozyme to high pressure studied by 15N/1H NMR spectroscopy. *FEBS Journal*, **2001**, 268, 1782-1793		53
21	A refined solution structure of hen lysozyme determined using residual dipolar coupling data. *Protein Science*, **2001**, 10, 677-88	6.3	141
20	Chemical shifts in denatured proteins: resonance assignments for denatured ubiquitin and comparisons with other denatured proteins. *Journal of Biomolecular NMR*, **2001**, 19, 153-65	3	62
19	The cytochrome c fold can be attained from a compact apo state by occupancy of a nascent heme binding site. *Journal of Biological Chemistry*, **2001**, 276, 45813-7	5.4	22
18	Exploration of partially unfolded states of human alpha-lactalbumin by molecular dynamics simulation. *Journal of Molecular Biology*, **2001**, 306, 329-47	6.5	58
17	Amyloid fibril formation by a helical cytochrome. *FEBS Letters*, **2001**, 495, 184-6	3.8	107

16	Understanding protein folding via free-energy surfaces from theory and experiment. *Trends in Biochemical Sciences*, **2000**, 25, 331-9	10.3	413
15	Initial denaturing conditions influence the slow folding phase of acylphosphatase associated with proline isomerization. *Protein Science*, **2000**, 9, 1466-73	6.3	4
14	Molecular dynamics simulations of human alpha-lactalbumin: changes to the structural and dynamical properties of the protein at low pH. *Proteins: Structure, Function and Bioinformatics*, **1999** , 36, 77-86	4.2	27
13	Hydrodynamic radii of native and denatured proteins measured by pulse field gradient NMR techniques. *Biochemistry*, **1999**, 38, 16424-31	3.2	786
12	Side-chain conformational disorder in a molten globule: molecular dynamics simulations of the A-state of human alpha-lactalbumin. *Journal of Molecular Biology*, **1999**, 286, 1567-80	6.5	33
11	Structural and dynamical properties of a denatured protein. Heteronuclear 3D NMR experiments and theoretical simulations of lysozyme in 8 M urea. *Biochemistry*, **1997**, 36, 8977-91	3.2	271
10	NMR analysis of main-chain conformational preferences in an unfolded fibronectin-binding protein. *Journal of Molecular Biology*, **1997**, 274, 152-9	6.5	114
9	Characterisation of protein unfolding by NMR diffusion measurements. *Journal of Biomolecular NMR*, **1997**, 10, 199-203	3	181
8	Analysis of main chain torsion angles in proteins: prediction of NMR coupling constants for native and random coil conformations. *Journal of Molecular Biology*, **1996**, 255, 494-506	6.5	358
7	Toward a Description of the Conformations of Denatured States of Proteins. Comparison of a Random Coil Model with NMR Measurements. *The Journal of Physical Chemistry*, **1996**, 100, 2661-2666		148
6	The concept of a random coil. Residual structure in peptides and denatured proteins. *Folding & Design*, **1996**, 1, R95-106		252
5	Native-like secondary structure in a peptide from the alpha-domain of hen lysozyme. *Folding & Design*, **1996**, 1, 473-84		14
4	NMR and protein dynamics. *International Journal of Quantum Chemistry*, **1996**, 59, 315-332	2.1	9
3	Comparison of MD simulations and NMR experiments for hen lysozyme. Analysis of local fluctuations, cooperative motions, and global changes. *Biochemistry*, **1995**, 34, 10918-31	3.2	120
2	Comparison of four independently determined structures of human recombinant interleukin-4. *Nature Structural and Molecular Biology*, **1994**, 1, 301-10	17.6	39
1	Solution structure of a peptide fragment of human alpha-lactalbumin in trifluoroethanol: a model for local structure in the molten globule. *Structure*, **1994**, 2, 703-12	5.2	27