Assocâ€prof Jane R Allison

List of Publications by Year
in descending order

52 papers	1,574 citations	361045 20 h-index	315357 38 g-index
53 all docs	53 docs citations	53 times ranked	2145 citing authors

#	Article	IF	Citations
1	On developing coarse-grained models for biomolecular simulation: a review. Physical Chemistry Chemical Physics, 2012, 14, 12423.	1.3	216
2	Determination of the Free Energy Landscape of Î±-Synuclein Using Spin Label Nuclear Magnetic Resonance Measurements. Journal of the American Chemical Society, 2009, 131, 18314-18326.	6.6	187
3	GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. Journal of Chemical Theory and Computation, 2011, 7, 3379-3390.	2.3	180
4	New functionalities in the GROMOS biomolecular simulation software. Journal of Computational Chemistry, 2012, 33, 340-353.	1.5	98
5	On the Calculation of Acyl Chain Order Parameters from Lipid Simulations. Journal of Chemical Theory and Computation, 2017, 13, 5683-5696.	2.3	92
6	A Relationship between the Transient Structure in the Monomeric State and the Aggregation Propensities of Î±-Synuclein and Î²-Synuclein. Biochemistry, 2014, 53, 7170-7183.	1.2	50
7	Molecular Dynamics Simulation of Î²-Lactoglobulin at Different Oil/Water Interfaces. Biomacromolecules, 2016, 17, 1572-1581.	2.6	50
8	Molecular Dynamics Simulation of Proteins. Methods in Molecular Biology, 2020, 2073, 311-327.	0.4	47
9	Computational methods for exploring protein conformations. Biochemical Society Transactions, 2020, 48, 1707-1724.	1.6	43
10	Biomolecular structure refinement using the GROMOS simulation software. Journal of Biomolecular NMR, 2011, 51, 265-281.	1.6	41
11	Using simulation to interpret experimental data in terms of protein conformational ensembles. Current Opinion in Structural Biology, 2017, 43, 79-87.	2.6	38
12	Current Computer Modeling Cannot Explain Why Two Highly Similar Sequences Fold into Different Structures. Biochemistry, 2011, 50, 10965-10973.	1.2	33
13	Directed Evolution of a Model Primordial Enzyme Provides Insights into the Development of the Genetic Code. PLoS Genetics, 2013, 9, e1003187.	1.5	27
14	Chromosome conformation maps in fission yeast reveal cell cycle dependent sub nuclear structure. Nucleic Acids Research, 2014, 42, 12585-12599.	6.5	26
15	A Method to Explore Protein Side Chain Conformational Variability Using Experimental Data. ChemPhysChem, 2009, 10, 3213-3228.	1.0	25
16	Deciphering Î²-Lactoglobulin Interactions at an Oilâ€“Water Interface: A Molecular Dynamics Study. Biomacromolecules, 2015, 16, 1855-1861.	2.6	25
17	Deriving Structural Information from Experimentally Measured Data on Biomolecules. Angewandte Chemie - International Edition, 2016, 55, 15990-16010.	7.2	24
18	The Sodium Sialic Acid Symporter From Staphylococcus aureus Has Altered Substrate Specificity. Frontiers in Chemistry, 2018, 6, 233.	1.8	24

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19	Peppy: A virtual reality environment for exploring the principles of polypeptide structure. Protein Science, 2020, 29, 157-168.	3.1	23
20	On the calculation of 3 J Î±Î²-coupling constants for side chains in proteins. Journal of Biomolecular NMR, 2012, 53, 223-246.	1.6	22
21	Flexibility of the petunia strigolactone receptor DAD2 promotes its interaction with signaling partners. Journal of Biological Chemistry, 2020, 295, 4181-4193.	1.6	19
22	Molecular Dynamics Simulation of the Interaction of Two Linear Battacin Analogs with Model Gram-Positive and Gram-Negative Bacterial Cell Membranes. ACS Omega, 2021, 6, 388-400.	1.6	19
23	Implicit Solvation Parameters Derived from Explicit Water Forces in Large-Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 2391-2403.	2.3	18
24	Coarse-grained models for the solvents dimethyl sulfoxide, chloroform, and methanol. Journal of Chemical Physics, 2012, 136, 054505.	1.2	17
25	Site-specific glycation of AÎ²1â€“42 affects fibril formation and is neurotoxic. Journal of Biological Chemistry, 2019, 294, 8806-8818.	1.6	16
26	Investigation of Stability and Disulfide Bond Shuffling of Lipid Transfer Proteins by Molecular Dynamics Simulation. Biochemistry, 2010, 49, 6916-6927.	1.2	15
27	A diffusion model for the coordination of DNA replication in Schizosaccharomyces pombe. Scientific Reports, 2016, 6, 18757.	1.6	15
28	â€œCLipPâ€•ing on lipids to generate antibacterial lipopeptides. Chemical Science, 2020, 11, 5759-5765.	3.7	15
29	A Refined, Efficient Mean Solvation Force Model that Includes the Interior Volume Contribution. Journal of Physical Chemistry B, 2011, 115, 4547-4557.	1.2	14
30	A comparison of the different helices adopted by Î±â€•and Î²â€•peptides suggests different reasons for their stability. Protein Science, 2010, 19, 2186-2195.	3.1	13
31	Probing the Structure and Dynamics of Proteins by Combining Molecular Dynamics Simulations and Experimental NMR Data. Journal of Chemical Theory and Computation, 2012, 8, 3430-3444.	2.3	13
32	Inhibition of Arabidopsis growth by the allelopathic compound azetidineâ€2â€•carboxylate is due to the low amino acid specificity of cytosolic prolylâ€tRNA synthetase. Plant Journal, 2016, 88, 236-246.	2.8	11
33	Assessing and refining molecular dynamics simulations of proteins with nuclear magnetic resonance data. Biophysical Reviews, 2012, 4, 189-203.	1.5	9
34	Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline 12. Protein Science, 2013, 22, 56-64.	3.1	9
35	Positive Selection or Free to Vary? Assessing the Functional Significance of Sequence Change Using Molecular Dynamics. PLoS ONE, 2016, 11, e0147619.	1.1	9
36	Relative Free Enthalpies for Point Mutations in Two Proteins with Highly Similar Sequences but Different Folds. Biochemistry, 2013, 52, 4962-4970.	1.2	8

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37	Comment on â€œA Tensor-Free Method for the Structural and Dynamic Refinement of Proteins using Residual Dipolar Couplingsâ€. Journal of Physical Chemistry B, 2015, 119, 8223-8224.	1.2	8
38	Structural Phylogenetics with Confidence. Molecular Biology and Evolution, 2020, 37, 2711-2726.	3.5	8
39	Bestimmung von Strukturinformation aus experimentellen Messdaten fÃ¼r BiomolekÃ¼le. Angewandte Chemie, 2016, 128, 16222-16244.	1.6	7
40	Multiscale Modeling and Simulation Approaches to Lipidâ€“Protein Interactions. Methods in Molecular Biology, 2019, 2003, 1-30.	0.4	7
41	Automated simultaneous assignment of bond orders and formal charges. Journal of Cheminformatics, 2019, 11, 18.	2.8	7
42	Computational Prediction of Amino Acids Governing Protein-Membrane Interaction for the PIP3 Cell Signaling System. Structure, 2019, 27, 371-380.e3.	1.6	7
43	Reply to â€œComment on â€˜A Tensor-Free Method for the Structural and Dynamic Refinement of Proteins using Residual Dipolar Couplingsâ€™â€. Journal of Physical Chemistry B, 2015, 119, 8225-8226.	1.2	6
44	CherryPicker: An Algorithm for the Automated Parametrization of Large Biomolecules for Molecular Simulation. Frontiers in Chemistry, 2019, 7, 400.	1.8	6
45	Molecular Dynamics Simulations of Barley and Maize Lipid Transfer Proteins Show Different Ligand Binding Preferences in Agreement with Experimental Data. Biochemistry, 2013, 52, 5029-5038.	1.2	5
46	Fitting alignment tensor components to experimental RDCs, CSAs and RQCs. Journal of Biomolecular NMR, 2015, 62, 25-29.	1.6	5
47	Thermal adaptation in the honeybee (Apis mellifera) via changes to the structure of malate dehydrogenase. Journal of Experimental Biology, 2020, 223, .	0.8	5
48	The self-association and thermal denaturation of caprine and bovine Î²-lactoglobulin. European Biophysics Journal, 2018, 47, 739-750.	1.2	4
49	Illustration of a computational pipeline for evaluating cyclodextrin hostâ€“guest complex formation through conformational capture of bullvalene. Journal of Chemical Physics, 2021, 154, 154105.	1.2	3
50	Characterisation ofNâ€(Octadecyl)â€1,8â€naphthalimide Monolayer Compression Using Molecular Dynamics and Experimental Approaches. Chemistry - an Asian Journal, 2019, 14, 1221-1229.	1.7	2
51	Let the Powers Combine. Structure, 2016, 24, 5-6.	1.6	1
52	Block-restraining of residual dipolar couplings to allow fluctuating relative alignments of molecular subdomains. Progress in Biophysics and Molecular Biology, 2017, 128, 133-141.	1.4	0