Paul Robustelli

List of Publications by Citations

19 papers	1,975 citations	15 h-index	24 g-index
24 ext. papers	2,470 ext. citations	8.6 avg, IF	5.31 L-index

#	Paper	IF	Citations
19	Water dispersion interactions strongly influence simulated structural properties of disordered protein states. *Journal of Physical Chemistry B*, **2015**, 119, 5113-23	3.4	468
18	Developing a molecular dynamics force field for both folded and disordered protein states. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E4758-E4766	11.5	434
17	Structure of an intermediate state in protein folding and aggregation. *Science*, **2012**, 336, 362-6	33.3	292
16	Fast and accurate predictions of protein NMR chemical shifts from interatomic distances. *Journal of the American Chemical Society*, **2009**, 131, 13894-5	16.4	196
15	Using NMR chemical shifts as structural restraints in molecular dynamics simulations of proteins. *Structure*, **2010**, 18, 923-33	5.2	121
14	Interpreting protein structural dynamics from NMR chemical shifts. *Journal of the American Chemical Society*, **2012**, 134, 6365-74	16.4	88
13	Characterization of the conformational equilibrium between the two major substates of RNase A using NMR chemical shifts. *Journal of the American Chemical Society*, **2012**, 134, 3968-71	16.4	75
12	Molecular switch based on a biologically important redox reaction. *Journal of Physical Chemistry B*, **2005**, 109, 130-7	3.4	54
11	Development of a Force Field for the Simulation of Single-Chain Proteins and Protein-Protein Complexes. *Journal of Chemical Theory and Computation*, **2020**, 16, 2494-2507	6.4	46
10	Effects of the known pathogenic mutations on the aggregation pathway of the amyloidogenic peptide of apolipoprotein A-I. *Journal of Molecular Biology*, **2011**, 407, 465-76	6.5	42
9	Determination of protein structures in the solid state from NMR chemical shifts. *Structure*, **2008**, 16, 1764-9	5.2	38
8	Conformational Dynamics of the Partially Disordered Yeast Transcription Factor GCN4. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	29
7	Mechanism of Coupled Folding-upon-Binding of an Intrinsically Disordered Protein. *Journal of the American Chemical Society*, **2020**, 142, 11092-11101	16.4	26
6	Folding of small proteins by Monte Carlo simulations with chemical shift restraints without the use of molecular fragment replacement or structural homology. *Journal of Physical Chemistry B*, **2009**, 113, 7890-6	3.4	23
5	Thermal adaptation of conformational dynamics in ribonuclease H. *PLoS Computational Biology*, **2013**, 9, e1003218	5	19
4	Structure and conformational dynamics of trichothecene mycotoxins. *Journal of Natural Products*, **2008**, 71, 589-94	4.9	15
3	Functional implications of large backbone amplitude motions of the glycoprotein 130-binding epitope of interleukin-6. *FEBS Journal*, **2014**, 281, 2471-83	5.7	5

2	Molecular Basis of Small-Molecule Binding to Synuclein.. *Journal of the American Chemical Society*, **2022**,	16.4	2
1	Quantifying the Relationship between Conformational Dynamics and Enzymatic Activity in Ribonuclease HI Homologues. *Biochemistry*, **2020**, 59, 3201-3205	3.2	1