

Paul Charles Whitford

List of Publications by Year in descending order

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72
papers

3,949
citations

147566
31
h-index

128067
60
g-index

87
all docs

87
docs citations

87
times ranked

2848
citing authors

#	ARTICLE	IF	CITATIONS
1	Head swivel on the ribosome facilitates translocation by means of intra-subunit tRNA hybrid sites. <i>Nature</i> , 2010, 468, 713-716.	13.7	336
2	An all-atom structure-based potential for proteins: Bridging minimal models with all-atom empirical forcefields. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 430-441.	1.5	327
3	SMOG@ctbp: simplified deployment of structure-based models in GROMACS. <i>Nucleic Acids Research</i> , 2010, 38, W657-W661.	6.5	291
4	Conformational Transitions of Adenylate Kinase: Switching by Cracking. <i>Journal of Molecular Biology</i> , 2007, 366, 1661-1671.	2.0	272
5	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. <i>PLoS Computational Biology</i> , 2016, 12, e1004794.	1.5	226
6	Nanopore-Based Measurements of Protein Size, Fluctuations, and Conformational Changes. <i>ACS Nano</i> , 2017, 11, 5706-5716.	7.3	219
7	The Shadow Map: A General Contact Definition for Capturing the Dynamics of Biomolecular Folding and Function. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8692-8702.	1.2	189
8	Accommodation of aminoacyl-tRNA into the ribosome involves reversible excursions along multiple pathways. <i>Rna</i> , 2010, 16, 1196-1204.	1.6	174
9	Biomolecular dynamics: order-to-disorder transitions and energy landscapes. <i>Reports on Progress in Physics</i> , 2012, 75, 076601.	8.1	105
10	Conformational Transitions in Adenylate Kinase. <i>Journal of Biological Chemistry</i> , 2008, 283, 2042-2048.	1.6	95
11	Nonlocal Helix Formation Is Key to Understanding S-Adenosylmethionine-1 Riboswitch Function. <i>Biophysical Journal</i> , 2009, 96, L7-L9.	0.2	95
12	Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. <i>Journal of the American Chemical Society</i> , 2012, 134, 12043-12053.	6.6	91
13	Excited states of ribosome translocation revealed through integrative molecular modeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 18943-18948.	3.3	89
14	Extracting function from a β^2 -trefoil folding motif. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 10384-10389.	3.3	79
15	Connecting the Kinetics and Energy Landscape of tRNA Translocation on the Ribosome. <i>PLoS Computational Biology</i> , 2013, 9, e1003003.	1.5	79
16	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. <i>Physical Review Letters</i> , 2015, 114, 258105.	2.9	69
17	Topography of funneled landscapes determines the thermodynamics and kinetics of protein folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 15763-15768.	3.3	62
18	Energy landscape along an enzymatic reaction trajectory: Hinges or cracks?. <i>HFSP Journal</i> , 2008, 2, 61-64.	2.5	60

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19	How EF-Tu can contribute to efficient proofreading of aa-tRNA by the ribosome. <i>Nature Communications</i> , 2016, 7, 13314.	5.8	57
20	Mutations as trapdoors to two competing native conformations of the Rop-dimer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 17674-17679.	3.3	53
21	A Novel Disulfide Bond in the SH2 Domain of the C-terminal Src Kinase Controls Catalytic Activity. <i>Journal of Molecular Biology</i> , 2007, 365, 1460-1468.	2.0	52
22	Steric interactions lead to collective tilting motion in the ribosome during mRNA-tRNA translocation. <i>Nature Communications</i> , 2016, 7, 10586.	5.8	52
23	Connecting Energy Landscapes with Experimental Rates for Aminoacyl-tRNA Accommodation in the Ribosome. <i>Journal of the American Chemical Society</i> , 2010, 132, 13170-13171.	6.6	48
24	Order and disorder control the functional rearrangement of influenza hemagglutinin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 12049-12054.	3.3	47
25	Reduced Model Captures Mg ²⁺ -RNA Interaction Free Energy of Riboswitches. <i>Biophysical Journal</i> , 2014, 106, 1508-1519.	0.2	46
26	Capturing Transition Paths and Transition States for Conformational Rearrangements in the Ribosome. <i>Biophysical Journal</i> , 2014, 107, 2881-2890.	0.2	44
27	Consensus among flexible fitting approaches improves the interpretation of cryo-EM data. <i>Journal of Structural Biology</i> , 2012, 177, 561-570.	1.3	38
28	Coordinate and time-dependent diffusion dynamics in protein folding. <i>Methods</i> , 2010, 52, 91-98.	1.9	36
29	Design and proof of concept for targeted phage-based COVID-19 vaccination strategies with a streamlined cold-free supply chain. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	35
30	The Origin of Nonmonotonic Complex Behavior and the Effects of Nonnative Interactions on the Diffusive Properties of Protein Folding. <i>Biophysical Journal</i> , 2010, 99, 600-608.	0.2	33
31	Proteins at Work. <i>Journal of Biological Chemistry</i> , 2010, 285, 36121-36128.	1.6	32
32	Diffusion of tRNA inside the ribosome is position-dependent. <i>Journal of Chemical Physics</i> , 2019, 151, 085102.	1.2	31
33	What protein folding teaches us about biological function and molecular machines. <i>Current Opinion in Structural Biology</i> , 2015, 30, 57-62.	2.6	30
34	Simulating movement of tRNA through the ribosome during hybrid-state formation. <i>Journal of Chemical Physics</i> , 2013, 139, 121919.	1.2	29
35	Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. <i>ELife</i> , 2021, 10, .	2.8	29
36	Structural insights into mRNA reading frame regulation by tRNA modification and slippery codon-anticodon pairing. <i>ELife</i> , 2020, 9, .	2.8	28

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37	Allostery in the ferredoxin protein motif does not involve a conformational switch. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 2240-2245.	3.3	27
38	Distinguishing Biomolecular Pathways and Metastable States. Journal of Chemical Theory and Computation, 2019, 15, 6482-6490.	2.3	23
39	Anisotropic Fluctuations in the Ribosome Determine tRNA Kinetics. Journal of Physical Chemistry B, 2017, 121, 10593-10601.	1.2	21
40	Studying ribosome dynamics with simplified models. Methods, 2019, 162-163, 128-140.	1.9	21
41	Exploring the Balance between Folding and Functional Dynamics in Proteins and RNA. International Journal of Molecular Sciences, 2015, 16, 6868-6889.	1.8	20
42	How the Ribosomal A-Site Finger Can Lead to tRNA Species-Dependent Dynamics. Journal of Physical Chemistry B, 2017, 121, 2767-2775.	1.2	20
43	Disorder guides domain rearrangement in elongation factor Tu. Proteins: Structure, Function and Bioinformatics, 2018, 86, 1037-1046.	1.5	16
44	Quantifying the Relationship between Single-Molecule Probes and Subunit Rotation in the Ribosome. Biophysical Journal, 2017, 113, 2777-2786.	0.2	15
45	Dissecting the Energetics of Subunit Rotation in the Ribosome. Journal of Physical Chemistry B, 2019, 123, 2812-2823.	1.2	15
46	Substrate-Specific Reorganization of the Conformational Ensemble of CSK Implicates Novel Modes of Kinase Function. PLoS Computational Biology, 2012, 8, e1002695.	1.5	14
47	Disorder guides protein function. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 7114-7115.	3.3	14
48	Drift-diffusion (DrDiff) framework determines kinetics and thermodynamics of two-state folding trajectory and tunes diffusion models. Journal of Chemical Physics, 2019, 151, 114106.	1.2	14
49	Capturing Transition States for tRNA Hybrid-State Formation in the Ribosome. Journal of Physical Chemistry B, 2016, 120, 8768-8775.	1.2	13
50	A steric gate controls P/E hybrid-state formation of tRNA on the ribosome. Nature Communications, 2020, 11, 5706.	5.8	13
51	Simulations of Phage T7 Capsid Expansion Reveal the Role of Molecular Sterics on Dynamics. Viruses, 2020, 12, 1273.	1.5	13
52	How Nanopore Translocation Experiments Can Measure RNA Unfolding. Biophysical Journal, 2020, 118, 1612-1620.	0.2	13
53	<scp>SMOG 2 and OpenSMOG: Extending the</scp> limits of structure-based models. Protein Science, 2022, 31, 158-172.	3.1	11
54	The Dynamics of Subunit Rotation in a Eukaryotic Ribosome. Biophysica, 2021, 1, 204-221.	0.6	10

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55	Diffuse Ions Coordinate Dynamics in a Ribonucleoprotein Assembly. <i>Journal of the American Chemical Society</i> , 2022, 144, 9510-9522.	6.6	10
56	Genetic and Structural Analysis of SARS-CoV-2 Spike Protein for Universal Epitope Selection. <i>Molecular Biology and Evolution</i> , 2022, 39, .	3.5	7
57	Massive conformation change in the prion protein: Using dual-basin structure-based models to find misfolding pathways. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1299-1307.	1.5	6
58	The ribosome's energy landscape: Recent insights from computation. <i>Biophysical Reviews</i> , 2015, 7, 301-310.	1.5	6
59	pH and the Breast Cancer Recurrent Mutation D538G Affect the Process of Activation of Estrogen Receptor β . <i>Biochemistry</i> , 2022, 61, 455-463.	1.2	5
60	Enhanced septahedral ordering in cold Lennard-Jones fluids. <i>Physical Review E</i> , 2005, 72, 021203.	0.8	4
61	Challenges in describing ribosome dynamics. <i>Physical Biology</i> , 2017, 14, 023001.	0.8	4
62	Probing remote residues important for catalysis in Escherichia coli ornithine transcarbamoylase. <i>PLoS ONE</i> , 2020, 15, e0228487.	1.1	4
63	Extended-range order, diverging static length scales, and local structure formation in cold Lennard-Jones fluids. <i>Journal of Chemical Physics</i> , 2005, 122, 044508.	1.2	3
64	How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. <i>Israel Journal of Chemistry</i> , 2014, 54, 1093-1107.	1.0	3
65	Using SMOG 2 to Simulate Complex Biomolecular Assemblies. <i>Methods in Molecular Biology</i> , 2019, 2022, 129-151.	0.4	3
66	Molecular Dynamics Simulations of the Ribosome. , 2012, , 51-68.		2
67	The energetics of subunit rotation in the ribosome. <i>Biophysical Reviews</i> , 2021, 13, 1029-1037.	1.5	2
68	Overview of the Biomolecular Association and Dynamics session at the 20th IUPAB congress, 45th Brazilian congress of SBBF, and the 50th annual meeting of SBBq. <i>Biophysical Reviews</i> , 2021, 13, 863-865.	1.5	1
69	Quantifying biomolecular diffusion with a spherical cow-model. <i>American Journal of Physics</i> , 2022, 90, 225-238.	0.3	1
70	Information Processing by Nanomachines: Decoding by the Ribosome. , 2011, , 67-86.		0
71	Cover Image, Volume 86, Issue 10. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, C1-C1.	1.5	0
72	Experimental and computational techniques for studying structural dynamics and function of RNA. <i>Methods</i> , 2019, 162-163, 1-2.	1.9	0