Paul Charles Whitford

List of Publications by Year
in descending order

72	3,949	147566 31	128067 60
papers	citations	h-index	g-index

87	87	87	2848
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>SMOG 2 and OpenSMOG: Extending the</scp> limits of structureâ€based models. Protein Science, 2022, 31, 158-172.	3.1	11
2	Quantifying biomolecular diffusion with a â€œspherical cowâ€•model. American Journal of Physics, 2022, 90, 225-238.	0.3	1
3	pH and the Breast Cancer Recurrent Mutation D538G Affect the Process of Activation of Estrogen Receptor Î±. Biochemistry, 2022, 61, 455-463.	1.2	5
4	Genetic and Structural Analysis of SARS-CoV-2 Spike Protein for Universal Epitope Selection. Molecular Biology and Evolution, 2022, 39, .	3.5	7
5	Diffuse Ions Coordinate Dynamics in a Ribonucleoprotein Assembly. Journal of the American Chemical Society, 2022, 144, 9510-9522.	6.6	10
6	The Dynamics of Subunit Rotation in a Eukaryotic Ribosome. Biophysica, 2021, 1, 204-221.	0.6	10
7	Design and proof of concept for targeted phage-based COVID-19 vaccination strategies with a streamlined cold-free supply chain. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	35
8	Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. ELife, 2021, 10, .	2.8	29
9	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. Biophysical Reviews, 2021, 13, 863-865.	1.5	1
10	The energetics of subunit rotation in the ribosome. Biophysical Reviews, 2021, 13, 1029-1037.	1.5	2
11	A steric gate controls P/E hybrid-state formation of tRNA on the ribosome. Nature Communications, 2020, 11, 5706.	5.8	13
12	Simulations of Phage T7 Capsid Expansion Reveal the Role of Molecular Sterics on Dynamics. Viruses, 2020, 12, 1273.	1.5	13
13	Probing remote residues important for catalysis in Escherichia coli ornithine transcarbamoylase. PLoS ONE, 2020, 15, e0228487.	1.1	4
14	How Nanopore Translocation Experiments Can Measure RNA Unfolding. Biophysical Journal, 2020, 118, 1612-1620.	0.2	13
15	Structural insights into mRNA reading frame regulation by tRNA modification and slippery codonâ€“anticodon pairing. ELife, 2020, 9, .	2.8	28
16	Distinguishing Biomolecular Pathways and Metastable States. Journal of Chemical Theory and Computation, 2019, 15, 6482-6490.	2.3	23
17	Diffusion of tRNA inside the ribosome is position-dependent. Journal of Chemical Physics, 2019, 151, 085102.	1.2	31
18	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

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19	Experimental and computational techniques for studying structural dynamics and function of RNA. Methods, 2019, 162-163, 1-2.	1.9	0
20	Dissecting the Energetics of Subunit Rotation in the Ribosome. Journal of Physical Chemistry B, 2019, 123, 2812-2823.	1.2	15
21	Studying ribosome dynamics with simplified models. Methods, 2019, 162-163, 128-140.	1.9	21
22	Using SMOG 2 to Simulate Complex Biomolecular Assemblies. Methods in Molecular Biology, 2019, 2022, 129-151.	0.4	3
23	Cover Image, Volume 86, Issue 10. Proteins: Structure, Function and Bioinformatics, 2018, 86, C1-C1.	1.5	0
24	Disorder guides domain rearrangement in elongation factor Tu. Proteins: Structure, Function and Bioinformatics, 2018, 86, 1037-1046.	1.5	16
25	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
26	Nanopore-Based Measurements of Protein Size, Fluctuations, and Conformational Changes. ACS Nano, 2017, 11, 5706-5716.	7.3	219
27	Challenges in describing ribosome dynamics. Physical Biology, 2017, 14, 023001.	0.8	4
28	Anisotropic Fluctuations in the Ribosome Determine tRNA Kinetics. Journal of Physical Chemistry B, 2017, 121, 10593-10601.	1.2	21
29	Quantifying the Relationship between Single-Molecule Probes and Subunit Rotation in the Ribosome. Biophysical Journal, 2017, 113, 2777-2786.	0.2	15
30	Capturing Transition States for tRNA Hybrid-State Formation in the Ribosome. Journal of Physical Chemistry B, 2016, 120, 8768-8775.	1.2	13
31	How EF-Tu can contribute to efficient proofreading of aa-tRNA by the ribosome. Nature Communications, 2016, 7, 13314.	5.8	57
32	Steric interactions lead to collective tilting motion in the ribosome during mRNAâ€“tRNA translocation. Nature Communications, 2016, 7, 10586.	5.8	52
33	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. PLoS Computational Biology, 2016, 12, e1004794.	1.5	226
34	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Physical Review Letters, 2015, 114, 258105.	2.9	69
35	What protein folding teaches us about biological function and molecular machines. Current Opinion in Structural Biology, 2015, 30, 57-62.	2.6	30
36	The ribosomeâ€™s energy landscape: Recent insights from computation. Biophysical Reviews, 2015, 7, 301-310.	1.5	6

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37	Exploring the Balance between Folding and Functional Dynamics in Proteins and RNA. International Journal of Molecular Sciences, 2015, 16, 6868-6889.	1.8	20
38	Capturing Transition Paths and Transition States for Conformational Rearrangements in the Ribosome. Biophysical Journal, 2014, 107, 2881-2890.	0.2	44
39	Reduced Model Captures Mg2+-RNA Interaction Free Energy of Riboswitches. Biophysical Journal, 2014, 106, 1508-1519.	0.2	46
40	How Simulations Reveal Dynamics, Disorder, and the Energy Landscapes of Biomolecular Function. Israel Journal of Chemistry, 2014, 54, 1093-1107.	1.0	3
41	Order and disorder control the functional rearrangement of influenza hemagglutinin. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 12049-12054.	3.3	47
42	Simulating movement of tRNA through the ribosome during hybrid-state formation. Journal of Chemical Physics, 2013, 139, 121919.	1.2	29
43	Connecting the Kinetics and Energy Landscape of tRNA Translocation on the Ribosome. PLoS Computational Biology, 2013, 9, e1003003.	1.5	79
44	Disorder guides protein function. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 7114-7115.	3.3	14
45	Substrate-Specific Reorganization of the Conformational Ensemble of CSK Implicates Novel Modes of Kinase Function. PLoS Computational Biology, 2012, 8, e1002695.	1.5	14
46	The Shadow Map: A General Contact Definition for Capturing the Dynamics of Biomolecular Folding and Function. Journal of Physical Chemistry B, 2012, 116, 8692-8702.	1.2	189
47	Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. Journal of the American Chemical Society, 2012, 134, 12043-12053.	6.6	91
48	Topography of funneled landscapes determines the thermodynamics and kinetics of protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15763-15768.	3.3	62
49	Consensus among flexible fitting approaches improves the interpretation of cryo-EM data. Journal of Structural Biology, 2012, 177, 561-570.	1.3	38
50	Molecular Dynamics Simulations of the Ribosome. , 2012, , 51-68.		2
51	Massive conformation change in the prion protein: Using dualâ€basin structureâ€based models to find misfolding pathways. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1299-1307.	1.5	6
52	Biomolecular dynamics: orderâ€“disorder transitions and energy landscapes. Reports on Progress in Physics, 2012, 75, 076601.	8.1	105
53	Information Processing by Nanomachines: Decoding by the Ribosome. , 2011, , 67-86.		0
54	Excited states of ribosome translocation revealed through integrative molecular modeling. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 18943-18948.	3.3	89

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55	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
56	Head swivel on the ribosome facilitates translocation by means of intra-subunit tRNA hybrid sites. Nature, 2010, 468, 713-716.	13.7	336
57	SMOG@ctbp: simplified deployment of structure-based models in GROMACS. Nucleic Acids Research, 2010, 38, W657-W661.	6.5	291
58	Proteins at Work. Journal of Biological Chemistry, 2010, 285, 36121-36128.	1.6	32
59	Accommodation of aminoacyl-tRNA into the ribosome involves reversible excursions along multiple pathways. Rna, 2010, 16, 1196-1204.	1.6	174
60	The Origin of Nonmonotonic Complex Behavior and the Effects of Nonnative Interactions on the Diffusive Properties of Protein Folding. Biophysical Journal, 2010, 99, 600-608.	0.2	33
61	Connecting Energy Landscapes with Experimental Rates for Aminoacyl-tRNA Accommodation in the Ribosome. Journal of the American Chemical Society, 2010, 132, 13170-13171.	6.6	48
62	Coordinate and time-dependent diffusion dynamics in protein folding. Methods, 2010, 52, 91-98.	1.9	36
63	An allâ€atom structureâ€based potential for proteins: Bridging minimal models with allâ€atom empirical forcefields. Proteins: Structure, Function and Bioinformatics, 2009, 75, 430-441.	1.5	327
64	Nonlocal Helix Formation Is Key to Understanding S-Adenosylmethionine-1 Riboswitch Function. Biophysical Journal, 2009, 96, L7-L9.	0.2	95
65	Conformational Transitions in Adenylate Kinase. Journal of Biological Chemistry, 2008, 283, 2042-2048.	1.6	95
66	Extracting function from a Î²-trefoil folding motif. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 10384-10389.	3.3	79
67	Energy landscape along an enzymatic reaction trajectory: Hinges or cracks?. HFSP Journal, 2008, 2, 61-64.	2.5	60
68	Mutations as trapdoors to two competing native conformations of the Rop-dimer. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 17674-17679.	3.3	53
69	A Novel Disulfide Bond in the SH2 Domain of the C-terminal Src Kinase Controls Catalytic Activity. Journal of Molecular Biology, 2007, 365, 1460-1468.	2.0	52
70	Conformational Transitions of Adenylate Kinase: Switching by Cracking. Journal of Molecular Biology, 2007, 366, 1661-1671.	2.0	272
71	Enhanced septahedral ordering in cold Lennard-Jones fluids. Physical Review E, 2005, 72, 021203.	0.8	4
72	Extended-range order, diverging static length scales, and local structure formation in cold Lennard-Jones fluids. Journal of Chemical Physics, 2005, 122, 044508.	1.2	3