José Nelson Onuchic

List of Publications by Year
in descending order

190 papers	22,375 citations	17429 63 h-index	10152 140 g-index
223 all docs	223 docs citations	223 times ranked	15448 citing authors

#	Article	IF	Citations
1	Funnels, pathways, and the energy landscape of protein folding: A synthesis. Proteins: Structure, Function and Bioinformatics, 1995, 21, 167-195.	1.5	2,415
2	THEORY OF PROTEIN FOLDING: The Energy Landscape Perspective. Annual Review of Physical Chemistry, 1997, 48, 545-600.	4.8	1,936
3	Direct-coupling analysis of residue coevolution captures native contacts across many protein families. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, E1293-301.	3.3	1,231
4	Theory of protein folding. Current Opinion in Structural Biology, 2004, 14, 70-75.	2.6	1,140
5	Topological and energetic factors: what determines the structural details of the transition state ensemble and â€œen-routeâ€intermediates for protein folding? an investigation for small globular proteins. Journal of Molecular Biology, 2000, 298, 937-953.	2.0	1,136
6	Implications of the Hybrid Epithelial/Mesenchymal Phenotype in Metastasis. Frontiers in Oncology, 2015, 5, 155.	1.3	581
7	MicroRNA-based regulation of epithelialâ€"hybridâ€"mesenchymal fate determination. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 18144-18149.	3.3	442
8	The Energetics and Physiological Impact of Cohesin Extrusion. Cell, 2018, 173, 1165-1178.e20.	13.5	399
9	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
10	Protein topology determines binding mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 511-516.	3.3	318
11	Folding kinetics of proteinlike heteropolymers. Journal of Chemical Physics, 1994, 101, 1519-1528.	1.2	311
12	Electron tunneling through covalent and noncovalent pathways in proteins. Journal of Chemical Physics, 1987, 86, 4488-4498.	1.2	306
13	Protein folding funnels: the nature of the transition state ensemble. Folding & Design, 1996, 1, 441-450.	4.5	304
14	SMOG@ctbp: simplified deployment of structure-based models in GROMACS. Nucleic Acids Research, 2010, 38, W657-W661.	6.5	291
15	Transferable model for chromosome architecture. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12168-12173.	3.3	291
16	Multiple-basin energy landscapes for large-amplitude conformational motions of proteins: Structure-based molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 11844-11849.	3.3	286
17	Conformational Transitions of Adenylate Kinase: Switching by Cracking. Journal of Molecular Biology, 2007, 366, 1661-1671.	2.0	272
18	Toward understanding cancer stem cell heterogeneity in the tumor microenvironment. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 148-157.	3.3	238

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19	Elucidating cancer metabolic plasticity by coupling gene regulation with metabolic pathways. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3909-3918.	3.3	227
20	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. PLoS Computational Biology, 2016, 12, e1004794.	1.5	226
21	A predictive theoretical model for electron tunneling pathways in proteins. Journal of Chemical Physics, 1990, 92, 722-733.	1.2	220
22	The energy landscape theory of protein folding: Insights into folding mechanisms and scenarios. Advances in Protein Chemistry, 2000, 53, 87-152.	4.4	215
23	Quantifying the Roughness on the Free Energy Landscape:Â Entropic Bottlenecks and Protein Folding Rates. Journal of the American Chemical Society, 2004, 126, 8426-8432.	6.6	211
24	Genomics-aided structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10340-10345.	3.3	210
25	Walking along chromosomes with super-resolution imaging, contact maps, and integrative modeling. PLoS Genetics, 2018, 14, e1007872.	1.5	209
26	Modeling the Genetic Regulation of Cancer Metabolism: Interplay between Glycolysis and Oxidative Phosphorylation. Cancer Research, 2017, 77, 1564-1574.	0.4	207
27	A Survey of Flexible Protein Binding Mechanisms and their Transition States Using Native Topology Based Energy Landscapes. Journal of Molecular Biology, 2005, 346, 1121-1145.	2.0	205
28	Fly-Casting in Proteinâˆ’DNA Binding:Â Frustration between Protein Folding and Electrostatics Facilitates Target Recognition. Journal of the American Chemical Society, 2007, 129, 738-739.	6.6	199
29	De novo prediction of human chromosome structures: Epigenetic marking patterns encode genome architecture. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12126-12131.	3.3	193
30	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
31	Kinetic and thermodynamic analysis of proteinlike heteropolymers: Monte Carlo histogram technique. Journal of Chemical Physics, 1995, 103, 4732-4744.	1.2	187
32	Protein folding mechanisms and the multidimensional folding funnel. Proteins: Structure, Function and Bioinformatics, 1998, 32, 136-158.	1.5	181
33	High-resolution protein complexes from integrating genomic information with molecular simulation. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 22124-22129.	3.3	174
34	Accommodation of aminoacyl-tRNA into the ribosome involves reversible excursions along multiple pathways. Rna, 2010, 16, 1196-1204.	1.6	174
35	NAF-1 and mitoNEET are central to human breast cancer proliferation by maintaining mitochondrial homeostasis and promoting tumor growth. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 14676-14681.	3.3	171
36	Interplay Among Tertiary Contacts, Secondary Structure Formation and Side-chain Packing in the Protein Folding Mechanism: All-atom Representation Study of Protein L. Journal of Molecular Biology, 2003, 326, 933-954.	2.0	167

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37	Coevolutionary signals across protein lineages help capture multiple protein conformations. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 20533-20538.	3.3	163
38	Interrogating the topological robustness of gene regulatory circuits by randomization. PLoS Computational Biology, 2017, 13, e1005456.	1.5	161
39	STATISTICAL THERMODYNAMICS: Taking a Walk on a Landscape. Science, 2001, 293, 612-613.	6.0	156
40	Targeting CPT1A-mediated fatty acid oxidation sensitizes nasopharyngeal carcinoma to radiation therapy. Theranostics, 2018, 8, 2329-2347.	4.6	155
41	Topological Frustration and the Folding of Interleukin-1β. Journal of Molecular Biology, 2006, 357, 986-996.	2.0	141
42	Internal strain regulates the nucleotide binding site of the kinesin leading head. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2175-2180.	3.3	133
43	Anomalous diffusion, spatial coherence, and viscoelasticity from the energy landscape of human chromosomes. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7753-7758.	3.3	133
44	3D genomics across the tree of life reveals condensin II as a determinant of architecture type. Science, 2021, 372, 984-989.	6.0	132
45	Tunneling pathway and redox-state-dependent electronic couplings at nearly fixed distance in electron transfer proteins. The Journal of Physical Chemistry, 1992, 96, 2852-2855.	2.9	131
46	NEET Proteins: A New Link Between Iron Metabolism, Reactive Oxygen Species, and Cancer. Antioxidants and Redox Signaling, 2019, 30, 1083-1095.	2.5	129
47	Jagged–Delta asymmetry in Notch signaling can give rise to a Sender/Receiver hybrid phenotype. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E402-9.	3.3	127
48	Coevolutionary information, protein folding landscapes, and the thermodynamics of natural selection. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 12408-12413.	3.3	126
49	Robustness and generalization of structure–based models for protein folding and function. Proteins: Structure, Function and Bioinformatics, 2009, 77, 881-891.	1.5	118
50	Toward rationally redesigning bacterial two-component signaling systems using coevolutionary information. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E563-71.	3.3	117
51	Enhancing intracellular accumulation and target engagement of PROTACs with reversible covalent chemistry. Nature Communications, 2020, 11, 4268.	5.8	112
52	Jagged mediates differences in normal and tumor angiogenesis by affecting tip-stalk fate decision. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3836-44.	3.3	107
53	Biomolecular dynamics: order–disorder transitions and energy landscapes. Reports on Progress in Physics, 2012, 75, 076601.	8.1	105
54	Numb prevents a complete epithelial–mesenchymal transition by modulating Notch signalling. Journal of the Royal Society Interface, 2017, 14, 20170512.	1.5	104

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55	NRF2 activates a partial epithelial-mesenchymal transition and is maximally present in a hybrid epithelial/mesenchymal phenotype. Integrative Biology (United Kingdom), 2019, 11, 251-263.	0.6	102
56	Nonlinear susceptibilities of finite conjugated organic polymers. The Journal of Physical Chemistry, 1987, 91, 2696-2698.	2.9	96
57	Nonlocal Helix Formation Is Key to Understanding S-Adenosylmethionine-1 Riboswitch Function. Biophysical Journal, 2009, 96, L7-L9.	0.2	95
58	Molecular bridge effects on distant charge tunneling. Journal of the American Chemical Society, 1987, 109, 6771-6778.	6.6	91
59	Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. Journal of the American Chemical Society, 2012, 134, 12043-12053.	6.6	91
60	The three-way switch operation of Rac1/RhoA GTPase-based circuit controlling amoeboid-hybrid-mesenchymal transition. Scientific Reports, 2014, 4, 6449.	1.6	88
61	Redox-dependent gating of VDAC by mitoNEET. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19924-19929.	3.3	85
62	Statistics of Kinetic Pathways on Biased Rough Energy Landscapes with Applications to Protein Folding. Physical Review Letters, 1996, 76, 4861-4864.	2.9	81
63	Decoding leader cells in collective cancer invasion. Nature Reviews Cancer, 2021, 21, 592-604.	12.8	80
64	Free energy landscape for the binding process of Huperzine A to acetylcholinesterase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 4273-4278.	3.3	79
65	Dimeric interactions and complex formation using direct coevolutionary couplings. Scientific Reports, 2015, 5, 13652.	1.6	75
66	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Physical Review Letters, 2015, 114, 258105.	2.9	69
67	Distinguishing mechanisms underlying EMT tristability. Cancer Convergence, 2017, 1, 2.	8.0	69
68	Understanding the Principles of Pattern Formation Driven by Notch Signaling by Integrating Experiments and Theoretical Models. Frontiers in Physiology, 2020, 11, 929.	1.3	68
69	A mechanism-based computational model to capture the interconnections among epithelial-mesenchymal transition, cancer stem cells and Notch-Jagged signaling. Oncotarget, 2018, 9, 29906-29920.	0.8	67
70	Elucidating the druggable interface of proteinâˆ'protein interactions using fragment docking and coevolutionary analysis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8051-E8058.	3.3	65
71	The folding funnel landscape for the peptide met-enkephalin. , 1999, 34, 472-483.		64
72	The Fe-S cluster-containing NEET proteins mitoNEET and NAF-1 as chemotherapeutic targets in breast cancer. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3698-3703.	3.3	64

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73	Breast cancer tumorigenicity is dependent on high expression levels of NAF-1 and the lability of its Fe-S clusters. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10890-10895.	3.3	64
74	Quantifying Cancer Epithelial-Mesenchymal Plasticity and its Association with Stemness and Immune Response. Journal of Clinical Medicine, 2019, 8, 725.	1.0	63
75	Towards decoding the coupled decision-making of metabolism and epithelial-to-mesenchymal transition in cancer. British Journal of Cancer, 2021, 124, 1902-1911.	2.9	63
76	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
77	Knotting a Protein in Explicit Solvent. Journal of Physical Chemistry Letters, 2013, 4, 3570-3573.	2.1	61
78	Limiting forms of the tunneling matrix element in the long distance bridge mediated electron transfer problem. Journal of Chemical Physics, 1985, 83, 5325-5329.	1.2	60
79	Exploring the Interplay between Topology and Secondary Structural Formation in the Protein Folding Problem. Journal of Physical Chemistry B, 2003, 107, 11193-11200.	1.2	59
80	Cancer-Related NEET Proteins Transfer 2Fe-2S Clusters to Anamorsin, a Protein Required for Cytosolic Iron-Sulfur Cluster Biogenesis. PLoS ONE, 2015, 10, e0139699.	1.1	59
81	Kinetics of proteinlike models: The energy landscape factors that determine folding. Journal of Chemical Physics, 1995, 103, 773-787.	1.2	58
82	Structure of the human monomeric NEET protein MiNT and its role in regulating iron and reactive oxygen species in cancer cells. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 272-277.	3.3	58
83	Periodic, Quasi-periodic and Chaotic Dynamics in Simple Gene Elements with Time Delays. Scientific Reports, 2016, 6, 21037.	1.6	56
84	Construction of an Effective Landscape for Multistate Genetic Switches. Physical Review Letters, 2014, 113, 078102.	2.9	55
85	Gambogic acid identifies an isoform-specific druggable pocket in the middle domain of Hsp90Î². Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4801-9.	3.3	52
86	Pericytes enable effective angiogenesis in the presence of proinflammatory signals. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 23551-23561.	3.3	49
87	From structure to function: the convergence of structure based models and co-evolutionary information. Physical Chemistry Chemical Physics, 2014, 16, 6496-6507.	1.3	47
88	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
89	Reduced Model Captures Mg2+-RNA Interaction Free Energy of Riboswitches. Biophysical Journal, 2014, 106, 1508-1519.	0.2	46
90	The Many Faces of Structure-Based Potentials: From Protein Folding Landscapes to Structural Characterization of Complex Biomolecules. Biological and Medical Physics Series, 2012, , 31-54.	0.3	44

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91	The Unique Cysteine Knot Regulates the Pleotropic Hormone Leptin. PLoS ONE, 2012, 7, e45654.	1.1	44
92	Activation of apoptosis in NAF-1-deficient human epithelial breast cancer cells. Journal of Cell Science, 2016, 129, 155-65.	1.2	44
93	RACIPE: a computational tool for modeling gene regulatory circuits using randomization. BMC Systems Biology, 2018, 12, 74.	3.0	43
94	Exploring chromosomal structural heterogeneity across multiple cell lines. ELife, 2020, 9, .	2.8	43
95	Pierced Lasso Bundles Are a New Class of Knot-like Motifs. PLoS Computational Biology, 2014, 10, e1003613.	1.5	41
96	A Biophysical Model Uncovers the Size Distribution of Migrating Cell Clusters across Cancer Types. Cancer Research, 2019, 79, 5527-5535.	0.4	40
97	Modeling putative therapeutic implications of exosome exchange between tumor and immune cells. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E4165-E4174.	3.3	39
98	Connecting Thermal and Mechanical Protein (Un)folding Landscapes. Biophysical Journal, 2014, 107, 2950-2961.	0.2	36
99	PAGE4 and Conformational Switching: Insights from Molecular Dynamics Simulations and Implications for Prostate Cancer. Journal of Molecular Biology, 2018, 430, 2422-2438.	2.0	36
100	Testing the gene expression classification of the EMT spectrum. Physical Biology, 2019, 16, 025002.	0.8	35
101	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
102	Electron Transport in Disordered Polymeric and Biological Systems. Physical Review Letters, 1997, 78, 146-149.	2.9	33
103	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
104	Structural and energetic heterogeneity in protein folding. I. Theory. Journal of Chemical Physics, 2002, 116, 5263.	1.2	32
105	Molecular origin of the weak susceptibility of kinesin velocity to loads and its relation to the collective behavior of kinesins. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E8611-E8617.	3.3	32
106	Consensus report of the 8 and 9th Weinman Symposia on Gene x Environment Interaction in carcinogenesis: novel opportunities for precision medicine. Cell Death and Differentiation, 2018, 25, 1885-1904.	5.0	31
107	What protein folding teaches us about biological function and molecular machines. Current Opinion in Structural Biology, 2015, 30, 57-62.	2.6	30
108	Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. ELife, 2021, 10, .	2.8	29

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109	Intercellular Stress Reconstitution from Traction Force Data. Biophysical Journal, 2014, 107, 548-554.	0.2	28
110	Protein Folding and Structure Prediction from the Ground Up: The Atomistic Associative Memory, Water Mediated, Structure and Energy Model. Journal of Physical Chemistry B, 2016, 120, 8557-8565.	1.2	28
111	A Scalable Computational Approach for Simulating Complexes of Multiple Chromosomes. Journal of Molecular Biology, 2021, 433, 166700.	2.0	28
112	Deciphering the Dynamics of Epithelial-Mesenchymal Transition and Cancer Stem Cells in Tumor Progression. Current Stem Cell Reports, 2019, 5, 11-21.	0.7	27
113	The Origin of Minus-end Directionality and Mechanochemistry of Ncd Motors. PLoS Computational Biology, 2012, 8, e1002783.	1.5	26
114	Magnesium controls aptamer-expression platform switching in the SAM-I riboswitch. Nucleic Acids Research, 2019, 47, 3158-3170.	6.5	26
115	Adiabaticity criteria for outer-sphere bimolecular electron-transfer reactions. The Journal of Physical Chemistry, 1988, 92, 4817-4820.	2.9	25
116	Generalized pathway model to compute and analyze tunneling matrix elements in proteins. Journal of Chemical Physics, 1998, 108, 4292-4298.	1.2	25
117	Exploring biomolecular machines: energy landscape control of biological reactions. Philosophical Transactions of the Royal Society B: Biological Sciences, 2006, 361, 1439-1443.	1.8	25
118	The Nucleome Data Bank: web-based resources to simulate and analyze the three-dimensional genome. Nucleic Acids Research, 2021, 49, D172-D182.	6.5	25
119	Shaping the genome via lengthwise compaction, phase separation, and lamina adhesion. Nucleic Acids Research, 2022, 50, 4258-4271.	6.5	25
120	Modeling the response of a tumor-suppressive network to mitogenic and oncogenic signals. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 5337-5342.	3.3	24
121	Drug-Tolerant Idling Melanoma Cells Exhibit Theory-Predicted Metabolic Low-Low Phenotype. Frontiers in Oncology, 2020, 10, 1426.	1.3	24
122	A magnesium-induced triplex pre-organizes the SAM-II riboswitch. PLoS Computational Biology, 2017, 13, e1005406.	1.5	24
123	Nrf2 Modulates the Hybrid Epithelial/Mesenchymal Phenotype and Notch Signaling During Collective Cancer Migration. Frontiers in Molecular Biosciences, 2022, 9, 807324.	1.6	23
124	Energy Landscape Analysis of Protein Dimers. Israel Journal of Chemistry, 2004, 44, 281-297.	1.0	22
125	Protein Folding and Structure Prediction from the Ground Up II: AAWSEM for α/β Proteins. Journal of Physical Chemistry B, 2017, 121, 3473-3482.	1.2	21
126	Exploring Energy Landscapes of Intrinsically Disordered Proteins: Insights into Functional Mechanisms. Journal of Chemical Theory and Computation, 2021, 17, 3178-3187.	2.3	21

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127	Thermodynamics and kinetics of folding of a small peptide. Journal of Chemical Physics, 2001, 115, 1601-1606.	1.2	20
128	Pierced Lasso Topology Controls Function in Leptin. Journal of Physical Chemistry B, 2017, 121, 706-718.	1.2	20
129	Cooperation between Magnesium and Metabolite Controls Collapse of the SAM-I Riboswitch. Biophysical Journal, 2017, 113, 348-359.	0.2	20
130	Role of metabolic spatiotemporal dynamics in regulating biofilm colony expansion. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 4288-4293.	3.3	20
131	Rapid assessment of T-cell receptor specificity of the immune repertoire. Nature Computational Science, 2021, 1, 362-373.	3.8	20
132	A VDAC1-mediated NEET protein chain transfers [2Fe-2S] clusters between the mitochondria and the cytosol and impacts mitochondrial dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	20
133	Molecular Simulations Suggest a Force-Dependent Mechanism of Vinculin Activation. Biophysical Journal, 2017, 113, 1697-1710.	0.2	19
134	Structural and Dynamical Order of a Disordered Protein: Molecular Insights into Conformational Switching of PAGE4 at the Systems Level. Biomolecules, 2019, 9, 77.	1.8	19
135	Decoding the mechanisms underlying cell-fate decision-making during stem cell differentiation by random circuit perturbation. Journal of the Royal Society Interface, 2020, 17, 20200500.	1.5	19
136	Structure and Dynamics of Solvent Landscapes in Charge-Transfer Reactions. The Journal of Physical Chemistry, 1996, 100, 7680-7690.	2.9	18
137	Structural consequences of hereditary spastic paraplegia disease-related mutations in kinesin. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10822-E10829.	3.3	18
138	The role of coevolutionary signatures in protein interaction dynamics, complex inference, molecular recognition, and mutational landscapes. Current Opinion in Structural Biology, 2019, 56, 179-186.	2.6	18
139	DNA supercoiling-mediated collective behavior of co-transcribing RNA polymerases. Nucleic Acids Research, 2022, 50, 1269-1279.	6.5	18
140	Electron Transfer. Advances in Chemistry Series, 1991, , 71-90.	0.6	17
141	Examining the Ensembles of Amyloid-β Monomer Variants and Their Propensities to Form Fibers Using an Energy Landscape Visualization Method. Journal of Physical Chemistry B, 2022, 126, 93-99.	1.2	17
142	Atomistic simulations indicate the functional loop-to-coiled-coil transition in influenza hemagglutinin is not downhill. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7905-E7913.	3.3	16
143	Template-Guided Protein Structure Prediction and Refinement Using Optimized Folding Landscape Force Fields. Journal of Chemical Theory and Computation, 2018, 14, 6102-6116.	2.3	15
144	Deciphering the structure of the condensin protein complex. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 11911-11916.	3.3	15

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145	Forging tools for refining predicted protein structures. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9400-9409.	3.3	15
146	Braiding topology and the energy landscape of chromosome organization proteins. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 1468-1477.	3.3	15
147	Protein Structure Prediction in CASP13 Using AWSEM-Suite. Journal of Chemical Theory and Computation, 2020, 16, 3977-3988.	2.3	15
148	Strain Mediated Adaptation Is Key for Myosin Mechanochemistry: Discovering General Rules for Motor Activity. PLoS Computational Biology, 2016, 12, e1005035.	1.5	15
149	Intrinsically disordered proteins: Ensembles at the limits of Anfinsen's dogma. Biophysics Reviews, 2022, 3, .	1.0	15
150	Integrating Molecular Dynamics Simulations with Chemical Probing Experiments Using SHAPE-FIT. Methods in Enzymology, 2015, 553, 215-234.	0.4	14
151	BAP1 forms a trimer with HMGB1 and HDAC1 that modulates gene Ã— environment interaction with asbestos. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	14
152	Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. F1000Research, 2016, 5, 106.	0.8	13
153	Lowered pH Leads to Fusion Peptide Release and a Highly Dynamic Intermediate of Influenza Hemagglutinin. Journal of Physical Chemistry B, 2016, 120, 9654-9660.	1.2	13
154	Constructing sequenceâ€dependent protein models using coevolutionary information. Protein Science, 2016, 25, 111-122.	3.1	13
155	Molecular mechanisms of the interhead coordination by interhead tension in cytoplasmic dyneins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10052-10057.	3.3	13
156	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. Journal of the American Chemical Society, 2018, 140, 1203-1206.	6.6	12
157	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. PLoS ONE, 2020, 15, e0222900.	1.1	12
158	Chromosome Modeling on Downsampled Hi-C Maps Enhances the Compartmentalization Signal. Journal of Physical Chemistry B, 2021, 125, 8757-8767.	1.2	12
159	RNA as a Complex Polymer with Coupled Dynamics of Ions and Water in the Outer Solvation Sphere. Journal of Physical Chemistry B, 2018, 122, 11218-11227.	1.2	11
160	The anti-apoptotic proteins NAF-1 and iASPP interact to drive apoptosis in cancer cells. Chemical Science, 2019, 10, 665-673.	3.7	11
161	<scp>SMOG 2 and OpenSMOG: Extending the</scp> limits of structureâ€based models. Protein Science, 2022, 31, 158-172.	3.1	11
162	Uncovering the molecular mechanisms behind disease-associated leptin variants. Journal of Biological Chemistry, 2018, 293, 12919-12933.	1.6	9

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163	The Pierced Lasso Topology Leptin has a Bolt on Dynamic Domain Composed by the Disordered Loops I and III. Journal of Molecular Biology, 2020, 432, 3050-3063.	2.0	9
164	Improving the Thermostability of Xylanase A from <i>Bacillus subtilis</i> by Combining Bioinformatics and Electrostatic Interactions Optimization. Journal of Physical Chemistry B, 2021, 125, 4359-4367.	1.2	9
165	Chelated Magnesium Logic Gate Regulates Riboswitch Pseudoknot Formation. Journal of Physical Chemistry B, 2021, 125, 6479-6490.	1.2	9
166	Geometrical Frustration in Interleukin-33 Decouples the Dynamics of the Functional Element from the Folding Transition State Ensemble. PLoS ONE, 2015, 10, e0144067.	1.1	9
167	Uncovering the statistical physics of 3D chromosomal organization using data-driven modeling. Current Opinion in Structural Biology, 2022, 75, 102418.	2.6	8
168	Constructing a folding model for protein S6 guided by native fluctuations deduced from NMR structures. Journal of Chemical Physics, 2015, 143, 243141.	1.2	7
169	Designing bacterial signaling interactions with coevolutionary landscapes. PLoS ONE, 2018, 13, e0201734.	1.1	7
170	Genetic and Structural Analysis of SARS-CoV-2 Spike Protein for Universal Epitope Selection. Molecular Biology and Evolution, 2022, 39, .	3.5	7
171	Structure-Based Model of RNA Pseudoknot Captures Magnesium-Dependent Folding Thermodynamics. Journal of Physical Chemistry B, 2019, 123, 1505-1511.	1.2	6
172	Mechanistic basis of propofol-induced disruption of kinesin processivity. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	6
173	Biotin-painted proteins have thermodynamic stability switched by kinetic folding routes. Journal of Chemical Physics, 2022, 156, .	1.2	6
174	Donor—Acceptor Electronic Coupling in Ruthenium-Modified Heme Proteins. Advances in Chemistry Series, 1996, , 471-485.	0.6	5
175	Rotation-Activated and Cooperative Zipping Characterize Class I Viral Fusion Protein Dynamics. Biophysical Journal, 2018, 114, 1878-1888.	0.2	5
176	Quantitative Characteristic of ncRNA Regulation in Gene Regulatory Networks. Methods in Molecular Biology, 2019, 1912, 341-366.	0.4	3
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