

Jos Nelson Onuchic

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

190 papers	17,444 citations	60 h-index	131 g-index
223 ext. papers	20,393 ext. citations	8 avg, IF	6.81 L-index

#	Paper	IF	Citations
190	Funnels, pathways, and the energy landscape of protein folding: a synthesis. <i>Proteins: Structure, Function and Bioinformatics</i> , 1995 , 21, 167-95	4.2	2175
189	Theory of protein folding: the energy landscape perspective. <i>Annual Review of Physical Chemistry</i> , 1997 , 48, 545-600	15.7	1719
188	Theory of protein folding. <i>Current Opinion in Structural Biology</i> , 2004 , 14, 70-5	8.1	992
187	Topological and energetic factors: what determines the structural details of the transition state ensemble and "en-route" intermediates for protein folding? An investigation for small globular proteins. <i>Journal of Molecular Biology</i> , 2000 , 298, 937-53	6.5	982
186	Direct-coupling analysis of residue coevolution captures native contacts across many protein families. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, E1293-301	11.5	837
185	Implications of the Hybrid Epithelial/Mesenchymal Phenotype in Metastasis. <i>Frontiers in Oncology</i> , 2015 , 5, 155	5.3	414
184	MicroRNA-based regulation of epithelial-hybrid-mesenchymal fate determination. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 18144-9	11.5	327
183	Protein topology determines binding mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004 , 101, 511-6	11.5	297
182	Folding kinetics of proteinlike heteropolymers. <i>Journal of Chemical Physics</i> , 1994 , 101, 1519-1528	3.9	296
181	Electron tunneling through covalent and noncovalent pathways in proteins. <i>Journal of Chemical Physics</i> , 1987 , 86, 4488-4498	3.9	281
180	Protein folding funnels: the nature of the transition state ensemble. <i>Folding & Design</i> , 1996 , 1, 441-50		277
179	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, 430-41	4.2	270
178	SMOG@ctbp: simplified deployment of structure-based models in GROMACS. <i>Nucleic Acids Research</i> , 2010 , 38, W657-61	20.1	256
177	Multiple-basin energy landscapes for large-amplitude conformational motions of proteins: Structure-based molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006 , 103, 11844-9	11.5	247
176	Conformational transitions of adenylate kinase: switching by cracking. <i>Journal of Molecular Biology</i> , 2007 , 366, 1661-71	6.5	242
175	The Energetics and Physiological Impact of Cohesin Extrusion. <i>Cell</i> , 2018 , 173, 1165-1178.e20	56.2	224
174	A predictive theoretical model for electron tunneling pathways in proteins. <i>Journal of Chemical Physics</i> , 1990 , 92, 722-733	3.9	202

173	Quantifying the roughness on the free energy landscape: entropic bottlenecks and protein folding rates. <i>Journal of the American Chemical Society</i> , 2004 , 126, 8426-32	16.4	194
172	The energy landscape theory of protein folding: insights into folding mechanisms and scenarios. <i>Advances in Protein Chemistry</i> , 2000 , 53, 87-152		192
171	A survey of flexible protein binding mechanisms and their transition states using native topology based energy landscapes. <i>Journal of Molecular Biology</i> , 2005 , 346, 1121-45	6.5	190
170	Kinetic and thermodynamic analysis of proteinlike heteropolymers: Monte Carlo histogram technique. <i>Journal of Chemical Physics</i> , 1995 , 103, 4732-4744	3.9	181
169	Transferable model for chromosome architecture. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 12168-12173	11.5	179
168	Protein folding mechanisms and the multidimensional folding funnel. <i>Proteins: Structure, Function and Bioinformatics</i> , 1998 , 32, 136-158	4.2	174
167	Fly-casting in protein-DNA binding: frustration between protein folding and electrostatics facilitates target recognition. <i>Journal of the American Chemical Society</i> , 2007 , 129, 738-9	16.4	168
166	Genomics-aided structure prediction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 10340-5	11.5	167
165	Interplay among tertiary contacts, secondary structure formation and side-chain packing in the protein folding mechanism: all-atom representation study of protein L. <i>Journal of Molecular Biology</i> , 2003 , 326, 933-54	6.5	153
164	Accommodation of aminoacyl-tRNA into the ribosome involves reversible excursions along multiple pathways. <i>Rna</i> , 2010 , 16, 1196-204	5.8	144
163	High-resolution protein complexes from integrating genomic information with molecular simulation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 22124-9	11.5	143
162	Statistical thermodynamics. Taking a walk on a landscape. <i>Science</i> , 2001 , 293, 612-3	33.3	143
161	Modeling the Genetic Regulation of Cancer Metabolism: Interplay between Glycolysis and Oxidative Phosphorylation. <i>Cancer Research</i> , 2017 , 77, 1564-1574	10.1	142
160	Elucidating cancer metabolic plasticity by coupling gene regulation with metabolic pathways. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 3909-3918	11.5	138
159	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. <i>PLoS Computational Biology</i> , 2016 , 12, e1004794	5	138
158	Walking along chromosomes with super-resolution imaging, contact maps, and integrative modeling. <i>PLoS Genetics</i> , 2018 , 14, e1007872	6	138
157	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, 8692-702	3.4	137
156	Toward understanding cancer stem cell heterogeneity in the tumor microenvironment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 148-157	11.5	137

155	NAF-1 and mitoNEET are central to human breast cancer proliferation by maintaining mitochondrial homeostasis and promoting tumor growth. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 14676-81	11.5	126
154	Topological frustration and the folding of interleukin-1 beta. <i>Journal of Molecular Biology</i> , 2006 , 357, 986-96	6.5	125
153	De novo prediction of human chromosome structures: Epigenetic marking patterns encode genome architecture. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 12126-12131	11.5	122
152	Internal strain regulates the nucleotide binding site of the kinesin leading head. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 2175-80	11.5	122
151	Tunneling pathway and redox-state-dependent electronic couplings at nearly fixed distance in electron transfer proteins. <i>The Journal of Physical Chemistry</i> , 1992 , 96, 2852-2855		121
150	Coevolutionary signals across protein lineages help capture multiple protein conformations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 20533-8	11.5	120
149	Robustness and generalization of structure-based models for protein folding and function. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 77, 881-91	4.2	97
148	Biomolecular dynamics: order-disorder transitions and energy landscapes. <i>Reports on Progress in Physics</i> , 2012 , 75, 076601	14.4	91
147	Coevolutionary information, protein folding landscapes, and the thermodynamics of natural selection. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 12408-13	11.5	90
146	Nonlocal helix formation is key to understanding S-adenosylmethionine-1 riboswitch function. <i>Biophysical Journal</i> , 2009 , 96, L7-9	2.9	87
145	Nonlinear susceptibilities of finite conjugated organic polymers. <i>The Journal of Physical Chemistry</i> , 1987 , 91, 2696-2698		86
144	Interrogating the topological robustness of gene regulatory circuits by randomization. <i>PLoS Computational Biology</i> , 2017 , 13, e1005456	5	86
143	Toward rationally redesigning bacterial two-component signaling systems using coevolutionary information. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, E563-71	11.5	85
142	Molecular bridge effects on distant charge tunneling. <i>Journal of the American Chemical Society</i> , 1987 , 109, 6771-6778	16.4	81
141	Targeting CPT1A-mediated fatty acid oxidation sensitizes nasopharyngeal carcinoma to radiation therapy. <i>Theranostics</i> , 2018 , 8, 2329-2347	12.1	80
140	Numb prevents a complete epithelial-mesenchymal transition by modulating Notch signalling. <i>Journal of the Royal Society Interface</i> , 2017 , 14,	4.1	78
139	Jagged-Delta asymmetry in Notch signaling can give rise to a Sender/Receiver hybrid phenotype. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, E402-9	11.5	78
138	Anomalous diffusion, spatial coherence, and viscoelasticity from the energy landscape of human chromosomes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 7753-7758	11.5	77

137	Statistics of kinetic pathways on biased rough energy landscapes with applications to protein folding. <i>Physical Review Letters</i> , 1996 , 76, 4861-4864	7.4	76
136	NEET Proteins: A New Link Between Iron Metabolism, Reactive Oxygen Species, and Cancer. <i>Antioxidants and Redox Signaling</i> , 2019 , 30, 1083-1095	8.4	70
135	Jagged mediates differences in normal and tumor angiogenesis by affecting tip-stalk fate decision. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, E3836-44	11.5	69
134	Free energy landscape for the binding process of Huperzine A to acetylcholinesterase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 4273-8	11.5	68
133	NRF2 activates a partial epithelial-mesenchymal transition and is maximally present in a hybrid epithelial/mesenchymal phenotype. <i>Integrative Biology (United Kingdom)</i> , 2019 , 11, 251-263	3.7	67
132	Magnesium fluctuations modulate RNA dynamics in the SAM-I riboswitch. <i>Journal of the American Chemical Society</i> , 2012 , 134, 12043-53	16.4	66
131	The three-way switch operation of Rac1/RhoA GTPase-based circuit controlling amoeboid-hybrid-mesenchymal transition. <i>Scientific Reports</i> , 2014 , 4, 6449	4.9	64
130	The folding funnel landscape for the peptide Met-enkephalin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 34, 472-83	4.2	57
129	Limiting forms of the tunneling matrix element in the long distance bridge mediated electron transfer problem. <i>Journal of Chemical Physics</i> , 1985 , 83, 5325-5329	3.9	57
128	The Fe-S cluster-containing NEET proteins mitoNEET and NAF-1 as chemotherapeutic targets in breast cancer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 3698-703	11.5	56
127	Dimeric interactions and complex formation using direct coevolutionary couplings. <i>Scientific Reports</i> , 2015 , 5, 13652	4.9	56
126	Kinetics of proteinlike models: The energy landscape factors that determine folding. <i>Journal of Chemical Physics</i> , 1995 , 103, 773-787	3.9	54
125	Exploring the Interplay between Topology and Secondary Structural Formation in the Protein Folding Problem. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 11193-11200	3.4	53
124	Breast cancer tumorigenicity is dependent on high expression levels of NAF-1 and the lability of its Fe-S clusters. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 10890-5	11.5	49
123	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, 15763-8	11.5	49
122	A mechanism-based computational model to capture the interconnections among epithelial-mesenchymal transition, cancer stem cells and Notch-Jagged signaling. <i>Oncotarget</i> , 2018 , 9, 29906-29920	3.3	49
121	Elucidating the druggable interface of protein-protein interactions using fragment docking and coevolutionary analysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, E8051-E8058	11.5	49
120	Knotting a Protein in Explicit Solvent. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3570-3573	6.4	47

119	Distinguishing mechanisms underlying EMT tristability 2017 , 1, 2		47
118	Enhancing intracellular accumulation and target engagement of PROTACs with reversible covalent chemistry. <i>Nature Communications</i> , 2020 , 11, 4268	17.4	45
117	Cancer-Related NEET Proteins Transfer 2Fe-2S Clusters to Anamorsin, a Protein Required for Cytosolic Iron-Sulfur Cluster Biogenesis. <i>PLoS ONE</i> , 2015 , 10, e0139699	3.7	44
116	Construction of an effective landscape for multistate genetic switches. <i>Physical Review Letters</i> , 2014 , 113, 078102	7.4	42
115	Quantifying Cancer Epithelial-Mesenchymal Plasticity and its Association with Stemness and Immune Response. <i>Journal of Clinical Medicine</i> , 2019 , 8,	5.1	41
114	From structure to function: the convergence of structure based models and co-evolutionary information. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 6496-507	3.6	41
113	Gambogic acid identifies an isoform-specific druggable pocket in the middle domain of Hsp90 α . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, E4801-9	11.5	41
112	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, 12049-54	11.5	39
111	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. <i>Physical Review Letters</i> , 2015 , 114, 258105	7.4	39
110	Periodic, Quasi-periodic and Chaotic Dynamics in Simple Gene Elements with Time Delays. <i>Scientific Reports</i> , 2016 , 6, 21037	4.9	38
109	Activation of apoptosis in NAF-1-deficient human epithelial breast cancer cells. <i>Journal of Cell Science</i> , 2016 , 129, 155-65	5.3	35
108	Redox-dependent gating of VDAC by mitoNEET. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 19924-19929	11.5	35
107	The Many Faces of Structure-Based Potentials: From Protein Folding Landscapes to Structural Characterization of Complex Biomolecules 2012 , 31-54		34
106	Structure of the human monomeric NEET protein MiNT and its role in regulating iron and reactive oxygen species in cancer cells. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 272-277	11.5	33
105	3D genomics across the tree of life reveals condensin II as a determinant of architecture type. <i>Science</i> , 2021 , 372, 984-989	33.3	33
104	Reduced model captures Mg(2+)-RNA interaction free energy of riboswitches. <i>Biophysical Journal</i> , 2014 , 106, 1508-19	2.9	32
103	Modeling putative therapeutic implications of exosome exchange between tumor and immune cells. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, E4165-74	11.5	32
102	Pierced Lasso Bundles are a new class of knot-like motifs. <i>PLoS Computational Biology</i> , 2014 , 10, e1003633	3.3	32

101	The unique cysteine knot regulates the pleiotropic hormone leptin. <i>PLoS ONE</i> , 2012 , 7, e45654	3.7	32
100	Electron Transport in Disordered Polymeric and Biological Systems. <i>Physical Review Letters</i> , 1997 , 78, 146-149	7.4	32
99	Structural and energetic heterogeneity in protein folding. I. Theory. <i>Journal of Chemical Physics</i> , 2002 , 116, 5263	3.9	31
98	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, 600-8	2.9	27
97	Intercellular stress reconstitution from traction force data. <i>Biophysical Journal</i> , 2014 , 107, 548-554	2.9	25
96	Connecting thermal and mechanical protein (un)folding landscapes. <i>Biophysical Journal</i> , 2014 , 107, 2950-2961	2.9	25
95	The origin of minus-end directionality and mechanochemistry of Ncd motors. <i>PLoS Computational Biology</i> , 2012 , 8, e1002783	5	25
94	PAGE4 and Conformational Switching: Insights from Molecular Dynamics Simulations and Implications for Prostate Cancer. <i>Journal of Molecular Biology</i> , 2018 , 430, 2422-2438	6.5	24
93	What protein folding teaches us about biological function and molecular machines. <i>Current Opinion in Structural Biology</i> , 2015 , 30, 57-62	8.1	24
92	Exploring biomolecular machines: energy landscape control of biological reactions. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2006 , 361, 1439-43	5.8	24
91	Generalized pathway model to compute and analyze tunneling matrix elements in proteins. <i>Journal of Chemical Physics</i> , 1998 , 108, 4292-4298	3.9	24
90	A Biophysical Model Uncovers the Size Distribution of Migrating Cell Clusters across Cancer Types. <i>Cancer Research</i> , 2019 , 79, 5527-5535	10.1	23
89	Pericytes enable effective angiogenesis in the presence of proinflammatory signals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 23551-23561	11.5	23
88	Adiabaticity criteria for outer-sphere bimolecular electron-transfer reactions. <i>The Journal of Physical Chemistry</i> , 1988 , 92, 4817-4820		23
87	Decoding leader cells in collective cancer invasion. <i>Nature Reviews Cancer</i> , 2021 , 21, 592-604	31.3	23
86	Molecular origin of the weak susceptibility of kinesin velocity to loads and its relation to the collective behavior of kinesins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, E8611-E8617	11.5	22
85	Protein Folding and Structure Prediction from the Ground Up: The Atomistic Associative Memory, Water Mediated, Structure and Energy Model. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8557-65	3.4	22
84	Testing the gene expression classification of the EMT spectrum. <i>Physical Biology</i> , 2019 , 16, 025002	3	22

- 83 Thermodynamics and kinetics of folding of a small peptide. *Journal of Chemical Physics*, **2001**, 115, 1601-1606 20
- 82 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 11.5 18
- 81 Structure and Dynamics of Solvent Landscapes in Charge-Transfer Reactions. *The Journal of Physical Chemistry*, **1996**, 100, 7680-7690 18
- 80 Energy Landscape Analysis of Protein Dimers. *Israel Journal of Chemistry*, **2004**, 44, 281-297 3.4 18
- 79 Understanding the Principles of Pattern Formation Driven by Notch Signaling by Integrating Experiments and Theoretical Models. *Frontiers in Physiology*, **2020**, 11, 929 4.6 18
- 78 Electron Transfer. *Advances in Chemistry Series*, **1991**, 71-90 17
- 77 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 12.7 17
- 76 Pierced Lasso Topology Controls Function in Leptin. *Journal of Physical Chemistry B*, **2017**, 121, 706-718 3.4 16
- 75 Deciphering the Dynamics of Epithelial-Mesenchymal Transition and Cancer Stem Cells in Tumor Progression. *Current Stem Cell Reports*, **2019**, 5, 11-21 1.8 16
- 74 Protein Folding and Structure Prediction from the Ground Up II: AAWSEM for α Proteins. *Journal of Physical Chemistry B*, **2017**, 121, 3473-3482 3.4 16
- 73 RACIPE: a computational tool for modeling gene regulatory circuits using randomization. *BMC Systems Biology*, **2018**, 12, 74 3.5 15
- 72 Exploring chromosomal structural heterogeneity across multiple cell lines. *ELife*, **2020**, 9, 8.9 15
- 71 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 8.1 14
- 70 Towards decoding the coupled decision-making of metabolism and epithelial-to-mesenchymal transition in cancer. *British Journal of Cancer*, **2021**, 124, 1902-1911 8.7 14
- 69 Integrating molecular dynamics simulations with chemical probing experiments using SHAPE-FIT. *Methods in Enzymology*, **2015**, 553, 215-34 1.7 13
- 68 Lowered pH Leads to Fusion Peptide Release and a Highly Dynamic Intermediate of Influenza Hemagglutinin. *Journal of Physical Chemistry B*, **2016**, 120, 9654-60 3.4 13
- 67 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, 11.5 13
- 66 Molecular Simulations Suggest a Force-Dependent Mechanism of Vinculin Activation. *Biophysical Journal*, **2017**, 113, 1697-1710 2.9 12

65	Constructing sequence-dependent protein models using coevolutionary information. <i>Protein Science</i> , 2016 , 25, 111-22	6.3	12
64	Strain Mediated Adaptation Is Key for Myosin Mechanochemistry: Discovering General Rules for Motor Activity. <i>PLoS Computational Biology</i> , 2016 , 12, e1005035	5	12
63	A magnesium-induced triplex pre-organizes the SAM-II riboswitch. <i>PLoS Computational Biology</i> , 2017 , 13, e1005406	5	12
62	The Nucleome Data Bank: web-based resources to simulate and analyze the three-dimensional genome. <i>Nucleic Acids Research</i> , 2021 , 49, D172-D182	20.1	12
61	Magnesium controls aptamer-expression platform switching in the SAM-I riboswitch. <i>Nucleic Acids Research</i> , 2019 , 47, 3158-3170	20.1	12
60	Structural and Dynamical Order of a Disordered Protein: Molecular Insights into Conformational Switching of PAGE4 at the Systems Level. <i>Biomolecules</i> , 2019 , 9,	5.9	11
59	Role of metabolic spatiotemporal dynamics in regulating biofilm colony expansion. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 4288-4293	11.5	11
58	Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. <i>F1000Research</i> , 2016 , 5,	3.6	11
57	Structural consequences of hereditary spastic paraplegia disease-related mutations in kinesin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E10822-E10829	11.5	11
56	Deciphering the structure of the condensin protein complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 11911-11916	11.5	11
55	Forging tools for refining predicted protein structures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 9400-9409	11.5	10
54	Braiding topology and the energy landscape of chromosome organization proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 1468-1477	11.5	10
53	Template-Guided Protein Structure Prediction and Refinement Using Optimized Folding Landscape Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6102-6116	6.4	10
52	Atomistic simulations indicate the functional loop-to-coiled-coil transition in influenza hemagglutinin is not downhill. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E7905-E7913	11.5	9
51	A Scalable Computational Approach for Simulating Complexes of Multiple Chromosomes. <i>Journal of Molecular Biology</i> , 2021 , 433, 166700	6.5	9
50	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. <i>PLoS ONE</i> , 2020 , 15, e0222900	3.7	8
49	Cooperation between Magnesium and Metabolite Controls Collapse of the SAM-I Riboswitch. <i>Biophysical Journal</i> , 2017 , 113, 348-359	2.9	8
48	Geometrical Frustration in Interleukin-33 Decouples the Dynamics of the Functional Element from the Folding Transition State Ensemble. <i>PLoS ONE</i> , 2015 , 10, e0144067	3.7	8

47	Molecular mechanisms of the interhead coordination by interhead tension in cytoplasmic dyneins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 10052-10057	11.5	8
46	The anti-apoptotic proteins NAF-1 and iASPP interact to drive apoptosis in cancer cells. <i>Chemical Science</i> , 2019 , 10, 665-673	9.4	7
45	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. <i>Journal of the American Chemical Society</i> , 2018 , 140, 1203-1206	16.4	7
44	Drug-Tolerant Idling Melanoma Cells Exhibit Theory-Predicted Metabolic Low-Low Phenotype. <i>Frontiers in Oncology</i> , 2020 , 10, 1426	5.3	7
43	Uncovering the molecular mechanisms behind disease-associated leptin variants. <i>Journal of Biological Chemistry</i> , 2018 , 293, 12919-12933	5.4	7
42	Protein Structure Prediction in CASP13 Using AWSEM-Suite. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3977-3988	6.4	6
41	Constructing a folding model for protein S6 guided by native fluctuations deduced from NMR structures. <i>Journal of Chemical Physics</i> , 2015 , 143, 243141	3.9	6
40	Designing bacterial signaling interactions with coevolutionary landscapes. <i>PLoS ONE</i> , 2018 , 13, e0201734	3.7	5
39	Donor-Acceptor Electronic Coupling in Ruthenium-Modified Heme Proteins. <i>Advances in Chemistry Series</i> , 1996 , 471-485		5
38	Exploring Energy Landscapes of Intrinsically Disordered Proteins: Insights into Functional Mechanisms. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3178-3187	6.4	5
37	RNA as a Complex Polymer with Coupled Dynamics of Ions and Water in the Outer Solvation Sphere. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 11218-11227	3.4	5
36	Structure-Based Model of RNA Pseudoknot Captures Magnesium-Dependent Folding Thermodynamics. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 1505-1511	3.4	4
35	Rotation-Activated and Cooperative Zipping Characterize Class I Viral Fusion Protein Dynamics. <i>Biophysical Journal</i> , 2018 , 114, 1878-1888	2.9	4
34	NRF2 activates a partial Epithelial-Mesenchymal Transition and is maximally present in a hybrid Epithelial/Mesenchymal phenotype		4
33	Decoding the mechanisms underlying cell-fate decision-making during stem cell differentiation by random circuit perturbation. <i>Journal of the Royal Society Interface</i> , 2020 , 17, 20200500	4.1	4
32	Improving the Thermostability of Xylanase A from by Combining Bioinformatics and Electrostatic Interactions Optimization. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 4359-4367	3.4	4
31	Examining the Ensembles of Amyloid- β Monomer Variants and Their Propensities to Form Fibers Using an Energy Landscape Visualization Method.. <i>Journal of Physical Chemistry B</i> , 2021 ,	3.4	4
30	SMOG 2 and OpenSMOG: Extending the limits of structure-based models. <i>Protein Science</i> , 2021 ,	6.3	3

29	Nrf2 modulates the hybrid epithelial/mesenchymal phenotype and Notch signaling during collective cancer migration		3
28	Apropos of Universal Epitope Discovery for COVID-19 Vaccines: A Framework for Targeted Phage Display-Based Delivery and Integration of New Evaluation Tools 2021 ,		3
27	Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. <i>ELife</i> , 2021 , 10,	8.9	3
26	Protein folding mechanisms and the multidimensional folding funnel 1998 , 32, 136		3
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