Jos Nelson Onuchic

List of Publications by Year in Descending Order

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	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,	11.5	2
189	Intrinsically disordered proteins: Ensembles at the limits of Anfinsen's dogma. *Biophysics Reviews*, **2022**, 3, 011306	2.6	1
188	Sergio Mascarenhas a Polymath in Physics. *Brazilian Journal of Physics*, **2022**, 52, 1	1.2	
187	Nrf2 Modulates the Hybrid Epithelial/Mesenchymal Phenotype and Notch Signaling During Collective Cancer Migration.. *Frontiers in Molecular Biosciences*, **2022**, 9, 807324	5.6	2
186	BAP1 forms a trimer with HMGB1 and HDAC1 that modulates gene environment interaction with asbestos. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	1
185	Expanding Direct Coupling Analysis to Identify Heterodimeric Interfaces from Limited Protein Sequence Data. *Journal of Physical Chemistry B*, **2021**, 125, 11408-11417	3.4	1
184	SMOG 2 and OpenSMOG: Extending the limits of structure-based models. *Protein Science*, **2021**,	6.3	3
183	The Nucleome Data Bank: web-based resources to simulate and analyze the three-dimensional genome. *Nucleic Acids Research*, **2021**, 49, D172-D182	20.1	12
182	Exploring Energy Landscapes of Intrinsically Disordered Proteins: Insights into Functional Mechanisms. *Journal of Chemical Theory and Computation*, **2021**, 17, 3178-3187	6.4	5
181	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
180	Improving the Thermostability of Xylanase A from by Combining Bioinformatics and Electrostatic Interactions Optimization. *Journal of Physical Chemistry B*, **2021**, 125, 4359-4367	3.4	4
179	Rapid assessment of T-cell receptor specificity of the immune repertoire. *Nature Computational Science*, **2021**, 1, 362-373		2
178	3D genomics across the tree of life reveals condensin II as a determinant of architecture type. *Science*, **2021**, 372, 984-989	33.3	33
177	Chelated Magnesium Logic Gate Regulates Riboswitch Pseudoknot Formation. *Journal of Physical Chemistry B*, **2021**, 125, 6479-6490	3.4	0
176	Chromosome Modeling on Downsampled Hi-C Maps Enhances the Compartmentalization Signal. *Journal of Physical Chemistry B*, **2021**, 125, 8757-8767	3.4	1
175	A Scalable Computational Approach for Simulating Complexes of Multiple Chromosomes. *Journal of Molecular Biology*, **2021**, 433, 166700	6.5	9
174	Mechanistic basis of propofol-induced disruption of kinesin processivity. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	2

173	Decoding leader cells in collective cancer invasion. *Nature Reviews Cancer*, **2021**, 21, 592-604	31.3	23
172	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
171	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
170	Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. *ELife*, **2021**, 10,	8.9	3
169	Examining the Ensembles of Amyloid-Monomer Variants and Their Propensities to Form Fibers Using an Energy Landscape Visualization Method.. *Journal of Physical Chemistry B*, **2021**,	3.4	4
168	Protein Structure Prediction in CASP13 Using AWSEM-Suite. *Journal of Chemical Theory and Computation*, **2020**, 16, 3977-3988	6.4	6
167	Tribute to David N. Beratan. *Journal of Physical Chemistry B*, **2020**, 124, 3437-3440	3.4	
166	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	6.5	2
165	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. *PLoS ONE*, **2020**, 15, e0222900	3.7	8
164	Exploring chromosomal structural heterogeneity across multiple cell lines. *ELife*, **2020**, 9,	8.9	15
163	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	11.5	10
162	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	4.1	4
161	Enhancing intracellular accumulation and target engagement of PROTACs with reversible covalent chemistry. *Nature Communications*, **2020**, 11, 4268	17.4	45
160	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
159	Drug-Tolerant Idling Melanoma Cells Exhibit Theory-Predicted Metabolic Low-Low Phenotype. *Frontiers in Oncology*, **2020**, 10, 1426	5.3	7
158	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro **2020**, 15, e0222900		
157	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro **2020**, 15, e0222900		
156	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro **2020**, 15, e0222900		

155	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro **2020**, 15, e0222900		
154	A Biophysical Model Uncovers the Size Distribution of Migrating Cell Clusters across Cancer Types. *Cancer Research*, **2019**, 79, 5527-5535	10.1	23
153	The anti-apoptotic proteins NAF-1 and iASPP interact to drive apoptosis in cancer cells. *Chemical Science*, **2019**, 10, 665-673	9.4	7
152	Structure-Based Model of RNA Pseudoknot Captures Magnesium-Dependent Folding Thermodynamics. *Journal of Physical Chemistry B*, **2019**, 123, 1505-1511	3.4	4
151	Quantifying Cancer Epithelial-Mesenchymal Plasticity and its Association with Stemness and Immune Response. *Journal of Clinical Medicine*, **2019**, 8,	5.1	41
150	Forging tools for refining predicted protein structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 9400-9409	11.5	10
149	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
148	Structural and Dynamical Order of a Disordered Protein: Molecular Insights into Conformational Switching of PAGE4 at the Systems Level. *Biomolecules*, **2019**, 9,	5.9	11
147	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
146	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	11.5	138
145	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	3.7	67
144	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	11.5	23
143	Redox-dependent gating of VDAC by mitoNEET. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 19924-19929	11.5	35
142	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	11.5	137
141	Testing the gene expression classification of the EMT spectrum. *Physical Biology*, **2019**, 16, 025002	3	22
140	Quantitative Characteristic of ncRNA Regulation in Gene Regulatory Networks. *Methods in Molecular Biology*, **2019**, 1912, 341-366	1.4	2
139	Magnesium controls aptamer-expression platform switching in the SAM-I riboswitch. *Nucleic Acids Research*, **2019**, 47, 3158-3170	20.1	12
138	NEET Proteins: A New Link Between Iron Metabolism, Reactive Oxygen Species, and Cancer. *Antioxidants and Redox Signaling*, **2019**, 30, 1083-1095	8.4	70

137	The Energetics and Physiological Impact of Cohesin Extrusion. *Cell*, **2018**, 173, 1165-1178.e20	56.2	224
136	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	11.5	33
135	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. *Journal of the American Chemical Society*, **2018**, 140, 1203-1206	16.4	7
134	Rotation-Activated and Cooperative Zipping Characterize Class I Viral Fusion Protein Dynamics. *Biophysical Journal*, **2018**, 114, 1878-1888	2.9	4
133	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	11.5	11
132	RACIPE: a computational tool for modeling gene regulatory circuits using randomization. *BMC Systems Biology*, **2018**, 12, 74	3.5	15
131	Targeting CPT1A-mediated fatty acid oxidation sensitizes nasopharyngeal carcinoma to radiation therapy. *Theranostics*, **2018**, 8, 2329-2347	12.1	80
130	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	11.5	77
129	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	11.5	9
128	Designing bacterial signaling interactions with coevolutionary landscapes. *PLoS ONE*, **2018**, 13, e0201734	3.7	5
127	PAGE4 and Conformational Switching: Insights from Molecular Dynamics Simulations and Implications for Prostate Cancer. *Journal of Molecular Biology*, **2018**, 430, 2422-2438	6.5	24
126	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	3.3	49
125	Walking along chromosomes with super-resolution imaging, contact maps, and integrative modeling. *PLoS Genetics*, **2018**, 14, e1007872	6	138
124	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	11.5	8
123	Template-Guided Protein Structure Prediction and Refinement Using Optimized Folding Landscape Force Fields. *Journal of Chemical Theory and Computation*, **2018**, 14, 6102-6116	6.4	10
122	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	11.5	11
121	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	11.5	11
120	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

119	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	3.4	5
118	Uncovering the molecular mechanisms behind disease-associated leptin variants. *Journal of Biological Chemistry*, **2018**, 293, 12919-12933	5.4	7
117	Pierced Lasso Topology Controls Function in Leptin. *Journal of Physical Chemistry B*, **2017**, 121, 706-718	3.4	16
116	Modeling the Genetic Regulation of Cancer Metabolism: Interplay between Glycolysis and Oxidative Phosphorylation. *Cancer Research*, **2017**, 77, 1564-1574	10.1	142
115	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
114	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	11.5	122
113	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	11.5	22
112	Molecular Simulations Suggest a Force-Dependent Mechanism of Vinculin Activation. *Biophysical Journal*, **2017**, 113, 1697-1710	2.9	12
111	Cooperation between Magnesium and Metabolite Controls Collapse of the SAM-I Riboswitch. *Biophysical Journal*, **2017**, 113, 348-359	2.9	8
110	Numb prevents a complete epithelial-mesenchymal transition by modulating Notch signalling. *Journal of the Royal Society Interface*, **2017**, 14,	4.1	78
109	Protein Folding and Structure Prediction from the Ground Up II: AAWSEM for Proteins. *Journal of Physical Chemistry B*, **2017**, 121, 3473-3482	3.4	16
108	Distinguishing mechanisms underlying EMT tristability **2017**, 1, 2		47
107	A magnesium-induced triplex pre-organizes the SAM-II riboswitch. *PLoS Computational Biology*, **2017**, 13, e1005406	5	12
106	Interrogating the topological robustness of gene regulatory circuits by randomization. *PLoS Computational Biology*, **2017**, 13, e1005456	5	86
105	Activation of apoptosis in NAF-1-deficient human epithelial breast cancer cells. *Journal of Cell Science*, **2016**, 129, 155-65	5.3	35
104	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
103	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, 10890-5	11.5	49
102	Constructing sequence-dependent protein models using coevolutionary information. *Protein Science*, **2016**, 25, 111-22	6.3	12

101	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. *PLoS Computational Biology*, **2016**, 12, e1004794	5	138
100	Strain Mediated Adaptation Is Key for Myosin Mechanochemistry: Discovering General Rules for Motor Activity. *PLoS Computational Biology*, **2016**, 12, e1005035	5	12
99	Preface to Special Topic on Protein Dynamics: Beyond Static Snapshots in Structural Biology. *Structural Dynamics*, **2016**, 3, 011901	3.2	
98	Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. *F1000Research*, **2016**, 5,	3.6	11
97	Elucidating the druggable interface of protein-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	11.5	49
96	Periodic, Quasi-periodic and Chaotic Dynamics in Simple Gene Elements with Time Delays. *Scientific Reports*, **2016**, 6, 21037	4.9	38
95	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, 8557-65	3.4	22
94	Transferable model for chromosome architecture. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12168-12173	11.5	179
93	Gambogic acid identifies an isoform-specific druggable pocket in the middle domain of Hsp90 *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E4801-9	11.5	41
92	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	11.5	69
91	Integrating molecular dynamics simulations with chemical probing experiments using SHAPE-FIT. *Methods in Enzymology*, **2015**, 553, 215-34	1.7	13
90	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, 3698-703	11.5	56
89	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. *Physical Review Letters*, **2015**, 114, 258105	7.4	39
88	Constructing a folding model for protein S6 guided by native fluctuations deduced from NMR structures. *Journal of Chemical Physics*, **2015**, 143, 243141	3.9	6
87	Dimeric interactions and complex formation using direct coevolutionary couplings. *Scientific Reports*, **2015**, 5, 13652	4.9	56
86	Implications of the Hybrid Epithelial/Mesenchymal Phenotype in Metastasis. *Frontiers in Oncology*, **2015**, 5, 155	5.3	414
85	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	11.5	78
84	What protein folding teaches us about biological function and molecular machines. *Current Opinion in Structural Biology*, **2015**, 30, 57-62	8.1	24

83	Cancer-Related NEET Proteins Transfer 2Fe-2S Clusters to Anamorsin, a Protein Required for Cytosolic Iron-Sulfur Cluster Biogenesis. *PLoS ONE*, **2015**, 10, e0139699	3.7	44
82	Geometrical Frustration in Interleukin-33 Decouples the Dynamics of the Functional Element from the Folding Transition State Ensemble. *PLoS ONE*, **2015**, 10, e0144067	3.7	8
81	Reduced model captures Mg(2+)-RNA interaction free energy of riboswitches. *Biophysical Journal*, **2014**, 106, 1508-19	2.9	32
80	From structure to function: the convergence of structure based models and co-evolutionary information. *Physical Chemistry Chemical Physics*, **2014**, 16, 6496-507	3.6	41
79	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, 12049-54	11.5	39
78	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, 12408-13	11.5	90
77	Intercellular stress reconstitution from traction force data. *Biophysical Journal*, **2014**, 107, 548-554	2.9	25
76	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, E4165-74	11.5	32
75	The three-way switch operation of Rac1/RhoA GTPase-based circuit controlling amoeboid-hybrid-mesenchymal transition. *Scientific Reports*, **2014**, 4, 6449	4.9	64
74	Pierced Lasso Bundles are a new class of knot-like motifs. *PLoS Computational Biology*, **2014**, 10, e1003613	3	32
73	Connecting thermal and mechanical protein (un)folding landscapes. *Biophysical Journal*, **2014**, 107, 2950-2961	2.9	25
72	Construction of an effective landscape for multistate genetic switches. *Physical Review Letters*, **2014**, 113, 078102	7.4	42
71	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	11.5	85
70	Physics transforming the life sciences. *Physical Biology*, **2014**, 11, 053006	3	2
69	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, 14676-81	11.5	126
68	MicroRNA-based regulation of epithelial-hybrid-mesenchymal fate determination. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 18144-9	11.5	327
67	Knotting a Protein in Explicit Solvent. *Journal of Physical Chemistry Letters*, **2013**, 4, 3570-3573	6.4	47
66	Learning from cancer how to defeat bacteria. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 3212-3	11.5	2

65	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, 4273-8	11.5	68
64	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, 20533-8	11.5	120
63	The shadow map: a general contact definition for capturing the dynamics of biomolecular folding and function. *Journal of Physical Chemistry B*, **2012**, 116, 8692-702	3.4	137
62	Magnesium fluctuations modulate RNA dynamics in the SAM-I riboswitch. *Journal of the American Chemical Society*, **2012**, 134, 12043-53	16.4	66
61	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, 15763-8	11.5	49
60	The Many Faces of Structure-Based Potentials: From Protein Folding Landscapes to Structural Characterization of Complex Biomolecules **2012**, 31-54		34
59	The unique cysteine knot regulates the pleotropic hormone leptin. *PLoS ONE*, **2012**, 7, e45654	3.7	32
58	Biomolecular dynamics: order-disorder transitions and energy landscapes. *Reports on Progress in Physics*, **2012**, 75, 076601	14.4	91
57	The origin of minus-end directionality and mechanochemistry of Ncd motors. *PLoS Computational Biology*, **2012**, 8, e1002783	5	25
56	Genomics-aided structure prediction. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 10340-5	11.5	167
55	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	11.5	837
54	SMOG@ctbp: simplified deployment of structure-based models in GROMACS. *Nucleic Acids Research*, **2010**, 38, W657-61	20.1	256
53	Accommodation of aminoacyl-tRNA into the ribosome involves reversible excursions along multiple pathways. *Rna*, **2010**, 16, 1196-204	5.8	144
52	The origin of nonmonotonic complex behavior and the effects of nonnative interactions on the diffusive properties of protein folding. *Biophysical Journal*, **2010**, 99, 600-8	2.9	27
51	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, 22124-9	11.5	143
50	An all-atom structure-based potential for proteins: bridging minimal models with all-atom empirical forcefields. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 430-41	4.2	270
49	Robustness and generalization of structure-based models for protein folding and function. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 881-91	4.2	97
48	Nonlocal helix formation is key to understanding S-adenosylmethionine-1 riboswitch function. *Biophysical Journal*, **2009**, 96, L7-9	2.9	87

47	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, 2175-80	11.5	122
46	2P114 Analytical Model for Protein Folding(Proteins-stability, folding, and other physicochemical properties,Poster Presentations). *Seibutsu Butsuri*, **2007**, 47, S141	0	
45	Fly-casting in protein-DNA binding: frustration between protein folding and electrostatics facilitates target recognition. *Journal of the American Chemical Society*, **2007**, 129, 738-9	16.4	168
44	Conformational transitions of adenylate kinase: switching by cracking. *Journal of Molecular Biology*, **2007**, 366, 1661-71	6.5	242
43	Exploring biomolecular machines: energy landscape control of biological reactions. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2006**, 361, 1439-43	5.8	24
42	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, 11844-9	11.5	247
41	Topological frustration and the folding of interleukin-1 beta. *Journal of Molecular Biology*, **2006**, 357, 986-96	6.5	125
40	A survey of flexible protein binding mechanisms and their transition states using native topology based energy landscapes. *Journal of Molecular Biology*, **2005**, 346, 1121-45	6.5	190
39	Dynamics of Electron Transfer Pathways in Redox Proteins. *ACS Symposium Series*, **2004**, 107-117	0.4	
38	Protein topology determines binding mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 511-6	11.5	297
37	Theory of protein folding. *Current Opinion in Structural Biology*, **2004**, 14, 70-5	8.1	992
36	Quantifying the roughness on the free energy landscape: entropic bottlenecks and protein folding rates. *Journal of the American Chemical Society*, **2004**, 126, 8426-32	16.4	194
35	Energy Landscape Analysis of Protein Dimers. *Israel Journal of Chemistry*, **2004**, 44, 281-297	3.4	18
34	Exploring the Interplay between Topology and Secondary Structural Formation in the Protein Folding Problem. *Journal of Physical Chemistry B*, **2003**, 107, 11193-11200	3.4	53
33	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, 933-54	6.5	153
32	Structural and energetic heterogeneity in protein folding. I. Theory. *Journal of Chemical Physics*, **2002**, 116, 5263	3.9	31
31	Thermodynamics and kinetics of folding of a small peptide. *Journal of Chemical Physics*, **2001**, 115, 1601-1606	3.9	20
30	Statistical thermodynamics. Taking a walk on a landscape. *Science*, **2001**, 293, 612-3	33.3	143

29	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. *Journal of Molecular Biology*, **2000**, 298, 937-53	6.5	982
28	The energy landscape theory of protein folding: insights into folding mechanisms and scenarios. *Advances in Protein Chemistry*, **2000**, 53, 87-152		192
27	The folding funnel landscape for the peptide Met-enkephalin. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 472-83	4.2	57
26	Protein folding mechanisms and the multidimensional folding funnel. *Proteins: Structure, Function and Bioinformatics*, **1998**, 32, 136-158	4.2	174
25	Generalized pathway model to compute and analyze tunneling matrix elements in proteins. *Journal of Chemical Physics*, **1998**, 108, 4292-4298	3.9	24
24	Protein folding mechanisms and the multidimensional folding funnel **1998**, 32, 136		2
23	Protein folding mechanisms and the multidimensional folding funnel **1998**, 32, 136		3
22	Electron Transport in Disordered Polymeric and Biological Systems. *Physical Review Letters*, **1997**, 78, 146-149	7.4	32
21	Theory of protein folding: the energy landscape perspective. *Annual Review of Physical Chemistry*, **1997**, 48, 545-600	15.7	1719
20	Structure and Dynamics of Solvent Landscapes in Charge-Transfer Reactions. *The Journal of Physical Chemistry*, **1996**, 100, 7680-7690		18
19	Donor–Acceptor Electronic Coupling in Ruthenium-Modified Heme Proteins. *Advances in Chemistry Series*, **1996**, 471-485		5
18	Protein folding funnels: the nature of the transition state ensemble. *Folding & Design*, **1996**, 1, 441-50		277
17	Statistics of kinetic pathways on biased rough energy landscapes with applications to protein folding. *Physical Review Letters*, **1996**, 76, 4861-4864	7.4	76
16	Funnels, pathways, and the energy landscape of protein folding: a synthesis. *Proteins: Structure, Function and Bioinformatics*, **1995**, 21, 167-95	4.2	2175
15	Kinetic and thermodynamic analysis of proteinlike heteropolymers: Monte Carlo histogram technique. *Journal of Chemical Physics*, **1995**, 103, 4732-4744	3.9	181
14	Kinetics of proteinlike models: The energy landscape factors that determine folding. *Journal of Chemical Physics*, **1995**, 103, 773-787	3.9	54
13	Folding kinetics of proteinlike heteropolymers. *Journal of Chemical Physics*, **1994**, 101, 1519-1528	3.9	296
12	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		121

11	Electron Transfer. *Advances in Chemistry Series*, **1991**, 71-90		17
10	A predictive theoretical model for electron tunneling pathways in proteins. *Journal of Chemical Physics*, **1990**, 92, 722-733	3.9	202
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4	Exploring Chromosomal Structural Heterogeneity Across Multiple Cell Lines		2
3	The Nucleome Data Bank: Web-based Resources to Simulate and Analyze the Three-Dimensional Genome		2
2	NRF2 activates a partial Epithelial-Mesenchymal Transition and is maximally present in a hybrid Epithelial/Mesenchymal phenotype		4
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