

JosÃ© Nelson Onuchic

List of Publications by Year in descending order

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Version: 2024-02-01

190
papers

22,375
citations

17440

63
h-index

10158

140
g-index

223
all docs

223
docs citations

223
times ranked

15448
citing authors

#	ARTICLE	IF	CITATIONS
1	<scp>SMOG 2 and OpenSMOG: Extending the</scp> limits of structure-based models. Protein Science, 2022, 31, 158-172.	7.6	11
2	DNA supercoiling-mediated collective behavior of co-transcribing RNA polymerases. Nucleic Acids Research, 2022, 50, 1269-1279.	14.5	18
3	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, .	7.1	20
4	Intrinsically disordered proteins: Ensembles at the limits of Anfinsen's dogma. Biophysics Reviews, 2022, 3, .	2.7	15
5	Sergio Mascarenhas a Polymath in Physics. Brazilian Journal of Physics, 2022, 52, 1.	1.4	0
6	Nrf2 Modulates the Hybrid Epithelial/Mesenchymal Phenotype and Notch Signaling During Collective Cancer Migration. Frontiers in Molecular Biosciences, 2022, 9, 807324.	3.5	23
7	Examining the Ensembles of Amyloid-Î² Monomer Variants and Their Propensities to Form Fibers Using an Energy Landscape Visualization Method. Journal of Physical Chemistry B, 2022, 126, 93-99.	2.6	17
8	Shaping the genome via lengthwise compaction, phase separation, and lamina adhesion. Nucleic Acids Research, 2022, 50, 4258-4271.	14.5	25
9	Genetic and Structural Analysis of SARS-CoV-2 Spike Protein for Universal Epitope Selection. Molecular Biology and Evolution, 2022, 39, .	8.9	7
10	Biotin-painted proteins have thermodynamic stability switched by kinetic folding routes. Journal of Chemical Physics, 2022, 156, .	3.0	6
11	Uncovering the statistical physics of 3D chromosomal organization using data-driven modeling. Current Opinion in Structural Biology, 2022, 75, 102418.	5.7	8
12	A Scalable Computational Approach for Simulating Complexes of Multiple Chromosomes. Journal of Molecular Biology, 2021, 433, 166700.	4.2	28
13	Mechanistic basis of propofol-induced disruption of kinesin processivity. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	6
14	Exploring Energy Landscapes of Intrinsically Disordered Proteins: Insights into Functional Mechanisms. Journal of Chemical Theory and Computation, 2021, 17, 3178-3187.	5.3	21
15	Towards decoding the coupled decision-making of metabolism and epithelial-to-mesenchymal transition in cancer. British Journal of Cancer, 2021, 124, 1902-1911.	6.4	63
16	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.	2.6	9
17	Rapid assessment of T-cell receptor specificity of the immune repertoire. Nature Computational Science, 2021, 1, 362-373.	8.0	20
18	3D genomics across the tree of life reveals condensin II as a determinant of architecture type. Science, 2021, 372, 984-989.	12.6	132

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19	Chelated Magnesium Logic Gate Regulates Riboswitch Pseudoknot Formation. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6479-6490.	2.6	9
20	Chromosome Modeling on Downsampled Hi-C Maps Enhances the Compartmentalization Signal. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8757-8767.	2.6	12
21	Decoding leader cells in collective cancer invasion. <i>Nature Reviews Cancer</i> , 2021, 21, 592-604.	28.4	80
22	Design and proof of concept for targeted phage-based COVID-19 vaccination strategies with a streamlined cold-free supply chain. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	35
23	Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. <i>ELife</i> , 2021, 10, .	6.0	29
24	The Nucleome Data Bank: web-based resources to simulate and analyze the three-dimensional genome. <i>Nucleic Acids Research</i> , 2021, 49, D172-D182.	14.5	25
25	Expanding Direct Coupling Analysis to Identify Heterodimeric Interfaces from Limited Protein Sequence Data. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11408-11417.	2.6	1
26	BAP1 forms a trimer with HMGB1 and HDAC1 that modulates gene–environment interaction with asbestos. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	14
27	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.	7.1	15
28	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.	3.4	19
29	Enhancing intracellular accumulation and target engagement of PROTACs with reversible covalent chemistry. <i>Nature Communications</i> , 2020, 11, 4268.	12.8	112
30	Understanding the Principles of Pattern Formation Driven by Notch Signaling by Integrating Experiments and Theoretical Models. <i>Frontiers in Physiology</i> , 2020, 11, 929.	2.8	68
31	Drug-Tolerant Idling Melanoma Cells Exhibit Theory-Predicted Metabolic Low-Low Phenotype. <i>Frontiers in Oncology</i> , 2020, 10, 1426.	2.8	24
32	Protein Structure Prediction in CASP13 Using AWSEM-Suite. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3977-3988.	5.3	15
33	Tribute to David N. Beratan. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3437-3440.	2.6	0
34	The Pierced Lasso Topology Leptin has a Bolt on Dynamic Domain Composed by the Disordered Loops I and III. <i>Journal of Molecular Biology</i> , 2020, 432, 3050-3063.	4.2	9
35	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. <i>PLoS ONE</i> , 2020, 15, e0222900.	2.5	12
36	Exploring chromosomal structural heterogeneity across multiple cell lines. <i>ELife</i> , 2020, 9, .	6.0	43

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37	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. , 2020, 15, e0222900.		0
38	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. , 2020, 15, e0222900.		0
39	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. , 2020, 15, e0222900.		0
40	Modeling Chikungunya control strategies and Mayaro potential outbreak in the city of Rio de Janeiro. , 2020, 15, e0222900.		0
41	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.	1.3	102
42	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.	7.1	49
43	A Biophysical Model Uncovers the Size Distribution of Migrating Cell Clusters across Cancer Types. Cancer Research, 2019, 79, 5527-5535.	0.9	40
44	The anti-apoptotic proteins NAF-1 and iASPP interact to drive apoptosis in cancer cells. Chemical Science, 2019, 10, 665-673.	7.4	11
45	Structure-Based Model of RNA Pseudoknot Captures Magnesium-Dependent Folding Thermodynamics. Journal of Physical Chemistry B, 2019, 123, 1505-1511.	2.6	6
46	Quantifying Cancer Epithelial-Mesenchymal Plasticity and its Association with Stemness and Immune Response. Journal of Clinical Medicine, 2019, 8, 725.	2.4	63
47	Forging tools for refining predicted protein structures. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9400-9409.	7.1	15
48	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.	5.7	18
49	Structural and Dynamical Order of a Disordered Protein: Molecular Insights into Conformational Switching of PAGE4 at the Systems Level. Biomolecules, 2019, 9, 77.	4.0	19
50	Deciphering the Dynamics of Epithelial-Mesenchymal Transition and Cancer Stem Cells in Tumor Progression. Current Stem Cell Reports, 2019, 5, 11-21.	1.6	27
51	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.	7.1	227
52	Redox-dependent gating of VDAC by mitoNEET. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19924-19929.	7.1	85
53	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.	7.1	238
54	Testing the gene expression classification of the EMT spectrum. Physical Biology, 2019, 16, 025002.	1.8	35

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55	Quantitative Characteristic of ncRNA Regulation in Gene Regulatory Networks. <i>Methods in Molecular Biology</i> , 2019, 1912, 341-366.	0.9	3
56	Magnesium controls aptamer-expression platform switching in the SAM-I riboswitch. <i>Nucleic Acids Research</i> , 2019, 47, 3158-3170.	14.5	26
57	NEET Proteins: A New Link Between Iron Metabolism, Reactive Oxygen Species, and Cancer. <i>Antioxidants and Redox Signaling</i> , 2019, 30, 1083-1095.	5.4	129
58	The Energetics and Physiological Impact of Cohesin Extrusion. <i>Cell</i> , 2018, 173, 1165-1178.e20.	28.9	399
59	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.	7.1	58
60	Fluorescent Proteins Detect Host Structural Rearrangements via Electrostatic Mechanism. <i>Journal of the American Chemical Society</i> , 2018, 140, 1203-1206.	13.7	12
61	Rotation-Activated and Cooperative Zipping Characterize Class I Viral Fusion Protein Dynamics. <i>Biophysical Journal</i> , 2018, 114, 1878-1888.	0.5	5
62	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.	7.1	20
63	Walking along chromosomes with super-resolution imaging, contact maps, and integrative modeling. <i>PLoS Genetics</i> , 2018, 14, e1007872.	3.5	209
64	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.	7.1	13
65	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.	5.3	15
66	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.	7.1	18
67	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.	7.1	15
68	Consensus report of the 8 and 9th Weinman Symposia on Gene x Environment Interaction in carcinogenesis: novel opportunities for precision medicine. <i>Cell Death and Differentiation</i> , 2018, 25, 1885-1904.	11.2	31
69	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.	2.6	11
70	Uncovering the molecular mechanisms behind disease-associated leptin variants. <i>Journal of Biological Chemistry</i> , 2018, 293, 12919-12933.	3.4	9
71	RACIPE: a computational tool for modeling gene regulatory circuits using randomization. <i>BMC Systems Biology</i> , 2018, 12, 74.	3.0	43
72	Targeting CPT1A-mediated fatty acid oxidation sensitizes nasopharyngeal carcinoma to radiation therapy. <i>Theranostics</i> , 2018, 8, 2329-2347.	10.0	155

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73	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.	7.1	133
74	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.	7.1	16
75	Designing bacterial signaling interactions with coevolutionary landscapes. <i>PLoS ONE</i> , 2018, 13, e0201734.	2.5	7
76	PAGE4 and Conformational Switching: Insights from Molecular Dynamics Simulations and Implications for Prostate Cancer. <i>Journal of Molecular Biology</i> , 2018, 430, 2422-2438.	4.2	36
77	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.	1.8	67
78	Pierced Lasso Topology Controls Function in Leptin. <i>Journal of Physical Chemistry B</i> , 2017, 121, 706-718.	2.6	20
79	Modeling the Genetic Regulation of Cancer Metabolism: Interplay between Glycolysis and Oxidative Phosphorylation. <i>Cancer Research</i> , 2017, 77, 1564-1574.	0.9	207
80	Modeling the response of a tumor-suppressive network to mitogenic and oncogenic signals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 5337-5342.	7.1	24
81	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.	7.1	193
82	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.	7.1	32
83	Molecular Simulations Suggest a Force-Dependent Mechanism of Vinculin Activation. <i>Biophysical Journal</i> , 2017, 113, 1697-1710.	0.5	19
84	Cooperation between Magnesium and Metabolite Controls Collapse of the SAM-I Riboswitch. <i>Biophysical Journal</i> , 2017, 113, 348-359.	0.5	20
85	Numb prevents a complete epithelial-to-mesenchymal transition by modulating Notch signalling. <i>Journal of the Royal Society Interface</i> , 2017, 14, 20170512.	3.4	104
86	Protein Folding and Structure Prediction from the Ground Up II: AAWSEM for \hat{I}_{\pm}/\hat{I}^2 Proteins. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3473-3482.	2.6	21
87	Distinguishing mechanisms underlying EMT tristability. <i>Cancer Convergence</i> , 2017, 1, 2.	8.0	69
88	A magnesium-induced triplex pre-organizes the SAM-II riboswitch. <i>PLoS Computational Biology</i> , 2017, 13, e1005406.	3.2	24
89	Interrogating the topological robustness of gene regulatory circuits by randomization. <i>PLoS Computational Biology</i> , 2017, 13, e1005456.	3.2	161
90	Activation of apoptosis in NAF-1-deficient human epithelial breast cancer cells. <i>Journal of Cell Science</i> , 2016, 129, 155-65.	2.0	44

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91	Preface to Special Topic on Protein Dynamics: Beyond Static Snapshots in Structural Biology. Structural Dynamics, 2016, 3, 011901.	2.3	0
92	Sequence co-evolutionary information is a natural partner to minimally-frustrated models of biomolecular dynamics. F1000Research, 2016, 5, 106.	1.6	13
93	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.	7.1	65
94	Periodic, Quasi-periodic and Chaotic Dynamics in Simple Gene Elements with Time Delays. Scientific Reports, 2016, 6, 21037.	3.3	56
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, 8557-8565.	2.6	28
96	Transferable model for chromosome architecture. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12168-12173.	7.1	291
97	Gambogic acid identifies an isoform-specific druggable pocket in the middle domain of Hsp90 α 2. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4801-9.	7.1	52
98	Lowered pH Leads to Fusion Peptide Release and a Highly Dynamic Intermediate of Influenza Hemagglutinin. Journal of Physical Chemistry B, 2016, 120, 9654-9660.	2.6	13
99	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.	7.1	64
100	Constructing sequence-dependent protein models using coevolutionary information. Protein Science, 2016, 25, 111-122.	7.6	13
101	SMOG 2: A Versatile Software Package for Generating Structure-Based Models. PLoS Computational Biology, 2016, 12, e1004794.	3.2	226
102	Strain Mediated Adaptation Is Key for Myosin Mechanochemistry: Discovering General Rules for Motor Activity. PLoS Computational Biology, 2016, 12, e1005035.	3.2	15
103	Generalized Manning Condensation Model Captures the RNA Ion Atmosphere. Physical Review Letters, 2015, 114, 258105.	7.8	69
104	Constructing a folding model for protein S6 guided by native fluctuations deduced from NMR structures. Journal of Chemical Physics, 2015, 143, 243141.	3.0	7
105	Dimeric interactions and complex formation using direct coevolutionary couplings. Scientific Reports, 2015, 5, 13652.	3.3	75
106	Implications of the Hybrid Epithelial/Mesenchymal Phenotype in Metastasis. Frontiers in Oncology, 2015, 5, 155.	2.8	581
107	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.	7.1	127
108	What protein folding teaches us about biological function and molecular machines. Current Opinion in Structural Biology, 2015, 30, 57-62.	5.7	30

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109	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.	7.1	107
110	Integrating Molecular Dynamics Simulations with Chemical Probing Experiments Using SHAPE-FIT. Methods in Enzymology, 2015, 553, 215-234.	1.0	14
111	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.	7.1	64
112	Cancer-Related NEET Proteins Transfer 2Fe-2S Clusters to Anamorsin, a Protein Required for Cytosolic Iron-Sulfur Cluster Biogenesis. PLoS ONE, 2015, 10, e0139699.	2.5	59
113	Geometrical Frustration in Interleukin-33 Decouples the Dynamics of the Functional Element from the Folding Transition State Ensemble. PLoS ONE, 2015, 10, e0144067.	2.5	9
114	Pierced Lasso Bundles Are a New Class of Knot-like Motifs. PLoS Computational Biology, 2014, 10, e1003613.	3.2	41
115	Connecting Thermal and Mechanical Protein (Un)folding Landscapes. Biophysical Journal, 2014, 107, 2950-2961.	0.5	36
116	Construction of an Effective Landscape for Multistate Genetic Switches. Physical Review Letters, 2014, 113, 078102.	7.8	55
117	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.	7.1	117
118	Physics transforming the life sciences. Physical Biology, 2014, 11, 053006.	1.8	2
119	Reduced Model Captures Mg ²⁺ -RNA Interaction Free Energy of Riboswitches. Biophysical Journal, 2014, 106, 1508-1519.	0.5	46
120	From structure to function: the convergence of structure based models and co-evolutionary information. Physical Chemistry Chemical Physics, 2014, 16, 6496-6507.	2.8	47
121	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.	7.1	47
122	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.	7.1	126
123	Intercellular Stress Reconstitution from Traction Force Data. Biophysical Journal, 2014, 107, 548-554.	0.5	28
124	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.	7.1	39
125	The three-way switch operation of Rac1/RhoA GTPase-based circuit controlling amoeboid-hybrid-mesenchymal transition. Scientific Reports, 2014, 4, 6449.	3.3	88
126	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.	7.1	171

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127	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.	7.1	442
128	Knotting a Protein in Explicit Solvent. Journal of Physical Chemistry Letters, 2013, 4, 3570-3573.	4.6	61
129	Learning from cancer how to defeat bacteria: Fig. 1.. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 3212-3213.	7.1	2
130	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.	7.1	79
131	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.	7.1	163
132	The Origin of Minus-end Directionality and Mechanochemistry of Ncd Motors. PLoS Computational Biology, 2012, 8, e1002783.	3.2	26
133	Genomics-aided structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10340-10345.	7.1	210
134	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.	2.6	189
135	Magnesium Fluctuations Modulate RNA Dynamics in the SAM-I Riboswitch. Journal of the American Chemical Society, 2012, 134, 12043-12053.	13.7	91
136	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.	7.1	62
137	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.	0.4	44
138	The Unique Cysteine Knot Regulates the Pleiotropic Hormone Leptin. PLoS ONE, 2012, 7, e45654.	2.5	44
139	Biomolecular dynamics: orderâ€“disorder transitions and energy landscapes. Reports on Progress in Physics, 2012, 75, 076601.	20.1	105
140	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.	7.1	1,231
141	SMOG@ctbp: simplified deployment of structure-based models in GROMACS. Nucleic Acids Research, 2010, 38, W657-W661.	14.5	291
142	Accommodation of aminoacyl-tRNA into the ribosome involves reversible excursions along multiple pathways. Rna, 2010, 16, 1196-1204.	3.5	174
143	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.	0.5	33
144	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.	7.1	174

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145	An all-atom structure-based potential for proteins: Bridging minimal models with all-atom empirical forcefields. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 430-441.	2.6	327
146	Robustness and generalization of structure-based models for protein folding and function. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 881-891.	2.6	118
147	Nonlocal Helix Formation Is Key to Understanding S-Adenosylmethionine-1 Riboswitch Function. <i>Biophysical Journal</i> , 2009, 96, L7-L9.	0.5	95
148	2P114 Analytical Model for Protein Folding(Proteins-stability, folding, and other physicochemical) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.1	0
149	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, 738-739.	13.7	199
150	Conformational Transitions of Adenylate Kinase: Switching by Cracking. <i>Journal of Molecular Biology</i> , 2007, 366, 1661-1671.	4.2	272
151	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, 2175-2180.	7.1	133
152	Topological Frustration and the Folding of Interleukin-1 β . <i>Journal of Molecular Biology</i> , 2006, 357, 986-996.	4.2	141
153	Exploring biomolecular machines: energy landscape control of biological reactions. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2006, 361, 1439-1443.	4.0	25
154	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, 11844-11849.	7.1	286
155	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, 1121-1145.	4.2	205
156	Dynamics of Electron Transfer Pathways in Redox Proteins. <i>ACS Symposium Series</i> , 2004, , 107-117.	0.5	0
157	Protein topology determines binding mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 511-516.	7.1	318
158	Theory of protein folding. <i>Current Opinion in Structural Biology</i> , 2004, 14, 70-75.	5.7	1,140
159	Quantifying the Roughness on the Free Energy Landscape: Entropic Bottlenecks and Protein Folding Rates. <i>Journal of the American Chemical Society</i> , 2004, 126, 8426-8432.	13.7	211
160	Energy Landscape Analysis of Protein Dimers. <i>Israel Journal of Chemistry</i> , 2004, 44, 281-297.	2.3	22
161	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.	2.6	59
162	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, 933-954.	4.2	167

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163	Structural and energetic heterogeneity in protein folding. I. Theory. Journal of Chemical Physics, 2002, 116, 5263.	3.0	32
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