

Eugene I Shakhnovich

List of Publications by Year in Descending Order

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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.

134
papers

7,933
citations

44
h-index

88
g-index

165
ext. papers

9,164
ext. citations

7
avg. IF

6.39
L-index

#	Paper	IF	Citations
134	Effect of RNA on Morphology and Dynamics of Membraneless Organelles. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 5035-5044	3.4	1
133	Avoidance of protein unfolding constrains protein stability in long-term evolution. <i>Biophysical Journal</i> , 2021 , 120, 2413-2424	2.9	1
132	Metabolic response to point mutations reveals principles of modulation of in vivo enzyme activity and phenotype. <i>Molecular Systems Biology</i> , 2021 , 17, e10200	12.2	0
131	Accelerating high-throughput virtual screening through molecular pool-based active learning. <i>Chemical Science</i> , 2021 , 12, 7866-7881	9.4	25
130	Switching an active site helix in dihydrofolate reductase reveals limits to subdomain modularity. <i>Biophysical Journal</i> , 2021 , 120, 4738-4750	2.9	
129	Effects of Single Mutations on Protein Stability Are Gaussian Distributed. <i>Biophysical Journal</i> , 2020 , 118, 2872-2878	2.9	2
128	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. <i>PLoS Computational Biology</i> , 2020 , 16, e1008323	5	0
127	Dynamic metastable long-living droplets formed by sticker-spacer proteins. <i>ELife</i> , 2020 , 9,	8.9	42
126	Semi-rational design and molecular dynamics simulations study of the thermostability enhancement of cellobiose 2-epimerases. <i>International Journal of Biological Macromolecules</i> , 2020 , 154, 1356-1365	7.9	15
125	Cotranslational folding allows misfolding-prone proteins to circumvent deep kinetic traps. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 1485-1495	11.5	26
124	Effect of Protein Structure on Evolution of Cotranslational Folding. <i>Biophysical Journal</i> , 2020 , 119, 1123-1134	11.34	11
123	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins 2020 , 16, e1008323		
122	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins 2020 , 16, e1008323		
121	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins 2020 , 16, e1008323		
120	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins 2020 , 16, e1008323		
119	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins 2020 , 16, e1008323		
118	The Early Phase of α m Aggregation: An Integrative Computational Study Framed on the D76N Mutant and the Δ 6 Variant. <i>Biomolecules</i> , 2019 , 9,	5.9	6

117	Chimeric dihydrofolate reductases display properties of modularity and biophysical diversity. <i>Protein Science</i> , 2019 , 28, 1359-1367	6.3	2
116	Substrate inhibition imposes fitness penalty at high protein stability. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 11265-11274	11.5	9
115	Mutation rate variability as a driving force in adaptive evolution. <i>Physical Review E</i> , 2019 , 99, 022424	2.4	3
114	Common activation mechanism of class A GPCRs. <i>ELife</i> , 2019 , 8,	8.9	117
113	Adaptation to mutational inactivation of an essential gene converges to an accessible suboptimal fitness peak. <i>ELife</i> , 2019 , 8,	8.9	18
112	Simulation-guided enzyme discovery: A new microbial source of cellobiose 2-epimerase. <i>International Journal of Biological Macromolecules</i> , 2019 , 139, 1002-1008	7.9	10
111	Trade-offs between microbial growth phases lead to frequency-dependent and non-transitive selection. <i>Proceedings of the Royal Society B: Biological Sciences</i> , 2018 , 285,	4.4	15
110	Differential Enzyme Flexibility Probed Using Solid-State Nanopores. <i>ACS Nano</i> , 2018 , 12, 4494-4502	16.7	55
109	Stability of the Influenza Virus Hemagglutinin Protein Correlates with Evolutionary Dynamics. <i>MSphere</i> , 2018 , 3,	5	18
108	ProteomeVis: a web app for exploration of protein properties from structure to sequence evolution across organisms. <i>Bioinformatics</i> , 2018 , 34, 3557-3565	7.2	5
107	Accurate Protein-Folding Transition-Path Statistics from a Simple Free-Energy Landscape. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 11126-11136	3.4	10
106	Growth tradeoffs produce complex microbial communities on a single limiting resource. <i>Nature Communications</i> , 2018 , 9, 3214	17.4	17
105	Accessibility of the Shine-Dalgarno Sequence Dictates N-Terminal Codon Bias in E. coli. <i>Molecular Cell</i> , 2018 , 70, 894-905.e5	17.6	34
104	Dynamic disulfide exchange in a crystallin protein in the human eye lens promotes cataract-associated aggregation. <i>Journal of Biological Chemistry</i> , 2018 , 293, 17997-18009	5.4	30
103	Evolution on the Biophysical Fitness Landscape of an RNA Virus. <i>Molecular Biology and Evolution</i> , 2018 , 35, 2390-2400	8.3	13
102	Exploring the Mutational Robustness of Nucleic Acids by Searching Genotype Neighborhoods in Sequence Space. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 407-414	6.4	5
101	A Hybrid Knowledge-Based and Empirical Scoring Function for Protein-Ligand Interaction: SMOG2016. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 584-593	6.1	21
100	Graph Topology and Free Energy of a Spin Model on the Graph. <i>Physical Review Letters</i> , 2017 , 118, 088302	3.02	6

99	The Role of Evolutionary Selection in the Dynamics of Protein Structure Evolution. <i>Biophysical Journal</i> , 2017 , 112, 1350-1365	2.9	20
98	Optimization of lag phase shapes the evolution of a bacterial enzyme. <i>Nature Ecology and Evolution</i> , 2017 , 1, 149	12.3	33
97	Rational Design of Novel Allosteric Dihydrofolate Reductase Inhibitors Showing Antibacterial Effects on Drug-Resistant Escherichia coli Escape Variants. <i>ACS Chemical Biology</i> , 2017 , 12, 1848-1857	4.9	12
96	Effect of sampling on BACE-1 ligands binding free energy predictions via MM-PBSA calculations. <i>Journal of Computational Chemistry</i> , 2017 , 38, 1941-1951	3.5	8
95	Evidence of evolutionary selection for cotranslational folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 11434-11439	11.5	54
94	Absence of Selection for Quantum Coherence in the Fenna-Matthews-Olson Complex: A Combined Evolutionary and Excitonic Study. <i>ACS Central Science</i> , 2017 , 3, 1086-1095	16.8	7
93	A tale of two tails: The importance of unstructured termini in the aggregation pathway of α -microglobulin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017 , 85, 2045-2057	4.2	10
92	Bridging the physical scales in evolutionary biology: from protein sequence space to fitness of organisms and populations. <i>Current Opinion in Structural Biology</i> , 2017 , 42, 31-40	8.1	45
91	OpenGrowth: An Automated and Rational Algorithm for Finding New Protein Ligands. <i>Journal of Medicinal Chemistry</i> , 2016 , 59, 4171-88	8.3	35
90	An Internal Disulfide Locks a Misfolded Aggregation-prone Intermediate in Cataract-linked Mutants of Human D-Crystallin. <i>Journal of Biological Chemistry</i> , 2016 , 291, 19172-83	5.4	39
89	A Simple Model of Protein Domain Swapping in Crowded Cellular Environments. <i>Biophysical Journal</i> , 2016 , 110, 2367-2376	2.9	2
88	Biophysical principles predict fitness landscapes of drug resistance. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, E1470-8	11.5	83
87	Transient protein-protein interactions perturb metabolome and cause gene dosage toxicity. <i>ELife</i> , 2016 , 5,	8.9	34
86	Benchmarking Inverse Statistical Approaches for Protein Structure and Design with Exactly Solvable Models. <i>PLoS Computational Biology</i> , 2016 , 12, e1004889	5	27
85	Virtual Screening of Human O-GlcNAc Transferase Inhibitors. <i>Chinese Journal of Chemical Physics</i> , 2016 , 29, 374-380	0.9	2
84	Evolutionary dynamics of viral escape under antibodies stress: A biophysical model. <i>Protein Science</i> , 2016 , 25, 1332-40	6.3	9
83	Structure-Based Prediction of Protein-Folding Transition Paths. <i>Biophysical Journal</i> , 2016 , 111, 925-36	2.9	14
82	Is catalytic activity of chaperones a selectable trait for the emergence of heat shock response?. <i>Biophysical Journal</i> , 2015 , 108, 438-48	2.9	2

81	Thermal stabilization of dihydrofolate reductase using monte carlo unfolding simulations and its functional consequences. <i>PLoS Computational Biology</i> , 2015 , 11, e1004207	5	20
80	Searching the Sequence Space for Potent Aptamers Using SELEX in Silico. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5939-46	6.4	17
79	Systems-level response to point mutations in a core metabolic enzyme modulates genotype-phenotype relationship. <i>Cell Reports</i> , 2015 , 11, 645-56	10.6	25
78	Mechanical Model of Globular Transition in Polymers. <i>ChemPlusChem</i> , 2015 , 80, 37-41	2.8	3
77	Isolation and Analysis of Rare Norovirus Recombinants from Coinfected Mice Using Drop-Based Microfluidics. <i>Journal of Virology</i> , 2015 , 89, 7722-34	6.6	25
76	Minimalistic predictor of protein binding energy: contribution of solvation factor to protein binding. <i>Biophysical Journal</i> , 2015 , 108, 795-798	2.9	8
75	Protein Homeostasis Imposes a Barrier on Functional Integration of Horizontally Transferred Genes in Bacteria. <i>PLoS Genetics</i> , 2015 , 11, e1005612	6	55
74	Evolution of specificity in protein-protein interactions. <i>Biophysical Journal</i> , 2014 , 107, 1686-96	2.9	17
73	Merging molecular mechanism and evolution: theory and computation at the interface of biophysics and evolutionary population genetics. <i>Current Opinion in Structural Biology</i> , 2014 , 26, 84-91	8.1	62
72	Influenza A H1N1 pandemic strain evolution--divergence and the potential for antigenic drift variants. <i>PLoS ONE</i> , 2014 , 9, e93632	3.7	29
71	A simulated intermediate state for folding and aggregation provides insights into α 6 μ -microglobulin amyloidogenic behavior. <i>PLoS Computational Biology</i> , 2014 , 10, e1003606	5	28
70	Contribution of selection for protein folding stability in shaping the patterns of polymorphisms in coding regions. <i>Molecular Biology and Evolution</i> , 2014 , 31, 165-76	8.3	39
69	The influence of selection for protein stability on dN/dS estimations. <i>Genome Biology and Evolution</i> , 2014 , 6, 2956-67	3.9	33
68	Gene Dosage Experiments in Enterobacteriaceae Using Arabinose-regulated Promoters. <i>Bio-protocol</i> , 2014 , 7,	0.9	3
67	Construction of Drug-Like Compounds by Markov Chains 2013 , 311-323		
66	A macroscopic device described by a Boltzmann-like distribution. <i>Soft Matter</i> , 2013 , 9, 4480	3.6	5
65	Protein quality control acts on folding intermediates to shape the effects of mutations on organismal fitness. <i>Molecular Cell</i> , 2013 , 49, 133-44	17.6	102
64	Highly abundant proteins favor more stable 3D structures in yeast. <i>Biophysical Journal</i> , 2013 , 104, L1-3	2.9	23

63	Protein biophysics explains why highly abundant proteins evolve slowly. <i>Cell Reports</i> , 2012 , 2, 249-56	10.6	70
62	Soluble oligomerization provides a beneficial fitness effect on destabilizing mutations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 4857-62	11.5	75
61	Diversity Against Adversity: How Adaptive Immune System Evolves Potent Antibodies. <i>Journal of Statistical Physics</i> , 2011 , 144, 241-267	1.5	4
60	A biophysical protein folding model accounts for most mutational fitness effects in viruses. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 9916-21	11.5	144
59	Topology of protein interaction network shapes protein abundances and strengths of their functional and nonspecific interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 4258-63	11.5	77
58	Lethal mutagenesis in viruses and bacteria. <i>Genetics</i> , 2009 , 183, 639-50	4	44
57	Protein folding roller coaster, one molecule at a time. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 11823-4	11.5	4
56	Understanding protein evolution: from protein physics to Darwinian selection. <i>Annual Review of Physical Chemistry</i> , 2008 , 59, 105-27	15.7	59
55	Constraints imposed by non-functional protein-protein interactions on gene expression and proteome size. <i>Molecular Systems Biology</i> , 2008 , 4, 210	12.2	78
54	Divergent evolution of a structural proteome: phenomenological models. <i>Biophysical Journal</i> , 2007 , 92, 701-16	2.9	6
53	All-atom ab initio folding of a diverse set of proteins. <i>Structure</i> , 2007 , 15, 53-63	5.2	69
52	Protein stability imposes limits on organism complexity and speed of molecular evolution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 16152-7	11.5	188
51	A first-principles model of early evolution: emergence of gene families, species, and preferred protein folds. <i>PLoS Computational Biology</i> , 2007 , 3, e139	5	50
50	Robust protein protein interactions in crowded cellular environments. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 14952-7	11.5	60
49	Understanding ensemble protein folding at atomic detail. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006 , 103, 17747-52	11.5	59
48	Protein folding thermodynamics and dynamics: where physics, chemistry, and biology meet. <i>Chemical Reviews</i> , 2006 , 106, 1559-88	68.1	294
47	Physical origins of protein superfamilies. <i>Journal of Molecular Biology</i> , 2006 , 357, 1335-43	6.5	28
46	Physics and Evolution of Protein-Protein Interactions. <i>FASEB Journal</i> , 2006 , 20, A1473	0.9	

45	Physics and evolution of thermophilic adaptation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 12742-7	11.5	207
44	Entropic stabilization of proteins and its proteomic consequences. <i>PLoS Computational Biology</i> , 2005 , 1, e47	5	72
43	Protein structure and evolutionary history determine sequence space topology. <i>Genome Research</i> , 2005 , 15, 385-92	9.7	71
42	Commitment and nucleation in the protein G transition state. <i>Journal of Molecular Biology</i> , 2004 , 336, 745-61	6.5	69
41	Proteomic traces of speciation. <i>Journal of Molecular Biology</i> , 2004 , 336, 695-706	6.5	17
40	Structural determinant of protein designability. <i>Physical Review Letters</i> , 2003 , 90, 218101	7.4	87
39	Protein evolution within a structural space. <i>Biophysical Journal</i> , 2003 , 85, 2962-72	2.9	35
38	Expanding protein universe and its origin from the biological Big Bang. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 14132-6	11.5	159
37	Field theory and segmental alignment analysis for a solution of sequence disordered liquid crystalline polymers. <i>Journal of Chemical Physics</i> , 2002 , 116, 3134-3140	3.9	1
36	A structure-based method for derivation of all-atom potentials for protein folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 5343-8	11.5	68
35	The ensemble folding kinetics of protein G from an all-atom Monte Carlo simulation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 11175-80	11.5	143
34	Mechanical Response of Random Heteropolymers. <i>Macromolecules</i> , 2002 , 35, 4429-4436	5.5	16
33	Direct molecular dynamics observation of protein folding transition state ensemble. <i>Biophysical Journal</i> , 2002 , 83, 3525-32	2.9	119
32	Dynamic charge-density correlation function in weakly charged polyampholyte globules. <i>Physical Review E</i> , 2001 , 64, 041802	2.4	
31	Exotic phase transitions in disordered globular networks. <i>Journal of Chemical Physics</i> , 2001 , 114, 10968-10976	3.9	2
30	Protein folding theory: from lattice to all-atom models. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 2001 , 30, 361-96		301
29	Understanding hierarchical protein evolution from first principles. <i>Journal of Molecular Biology</i> , 2001 , 312, 289-307	6.5	144
28	Comparison of two optimization methods to derive energy parameters for protein folding: Perceptron and Z score. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000 , 41, 192-201	4.2	32

27	Development of a Knowledge-Based Potential for Crystals of Small Organic Molecules: Calculation of Energy Surfaces for C=O⋯H⋯N Hydrogen Bonds. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 7293-7298	3.4	37
26	Freezing in polyampholytes globules: Influence of the long-range nature of the interaction. <i>Journal of Chemical Physics</i> , 1999 , 111, 772-785	3.9	8
25	On the role of conformational geometry in protein folding. <i>Journal of Chemical Physics</i> , 1999 , 111, 10375-10380	3.1	6
24	Microphase Ordering in Melts of Randomly Grafted Copolymers. <i>Physical Review Letters</i> , 1999 , 82, 2896-2899	7.1	32
23	Factors that affect the folding ability of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 35, 34-40	4.2	41
22	A Study on Local-Global Cooperativity in Protein Collapse. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 2535-2542	3.4	9
21	Universally conserved positions in protein folds: reading evolutionary signals about stability, folding kinetics and function. <i>Journal of Molecular Biology</i> , 1999 , 291, 177-96	6.5	334
20	SmoG: A Ligand Design Method Based on Knowledge-Based Parametrization of a Solvent Reorganization Model. <i>ACS Symposium Series</i> , 1999 , 70-86	0.4	1
19	Using a Convenient, Quantitative Model for Torsional Entropy To Establish Qualitative Trends for Molecular Processes That Restrict Conformational Freedom. <i>Journal of Organic Chemistry</i> , 1998 , 63, 3168-3175	4.2	112
18	Estimating the Entropic Cost of Self-Assembly of Multiparticle Hydrogen-Bonded Aggregates Based on the Cyanuric Acid-Melamine Lattice. <i>Journal of Organic Chemistry</i> , 1998 , 63, 3821-3830	4.2	320
17	Phase diagram analysis of random heteropolymers with composition specific and quenched cross-links. <i>Journal of Chemical Physics</i> , 1998 , 109, 2947-2958	3.9	7
16	Cooperativity and stability in a Langevin model of proteinlike folding. <i>Journal of Chemical Physics</i> , 1997 , 106, 9276-9285	3.9	20
15	Frozen phases with re-entrant transition for random heteropolymers with composition specific and annealed cross-links. <i>Journal of Chemical Physics</i> , 1997 , 107, 1247-1258	3.9	7
14	SMoG: de Novo Design Method Based on Simple, Fast, and Accurate Free Energy Estimates. 2. Case Studies in Molecular Design. <i>Journal of the American Chemical Society</i> , 1997 , 119, 4608-4617	16.4	64
13	Theoretical studies of protein-folding thermodynamics and kinetics. <i>Current Opinion in Structural Biology</i> , 1997 , 7, 29-40	8.1	343
12	How to derive a protein folding potential? A new approach to an old problem. <i>Journal of Molecular Biology</i> , 1996 , 264, 1164-79	6.5	249
11	SMoG: de Novo Design Method Based on Simple, Fast, and Accurate Free Energy Estimates. 1. Methodology and Supporting Evidence. <i>Journal of the American Chemical Society</i> , 1996 , 118, 11733-11744	16.4	239
10	Universality and diversity of the protein folding scenarios: a comprehensive analysis with the aid of a lattice model. <i>Folding & Design</i> , 1996 , 1, 103-16		101

9	Protein dynamics: From the native to the unfolded state and back again. <i>Molecular Engineering</i> , 1995 , 5, 55-70		1
8	Simulation study of the collapse of linear and ring homopolymers. <i>Journal of Chemical Physics</i> , 1995 , 103, 2615-2624	3.9	43
7	How does a protein fold?. <i>Nature</i> , 1994 , 369, 248-51	50.4	845
6	Statistical mechanics of proteins with "evolutionary selected" sequences. <i>Physical Review E</i> , 1994 , 50, 1303-1312	2.4	64
5	Kinetics of protein folding. A lattice model study of the requirements for folding to the native state. <i>Journal of Molecular Biology</i> , 1994 , 235, 1614-36	6.5	471
4	Enumeration of all compact conformations of copolymers with random sequence of links. <i>Journal of Chemical Physics</i> , 1990 , 93, 5967-5971	3.9	224
3	The role of evolutionary selection in the dynamics of protein structure evolution		1
2	Tradeoffs between microbial growth phases lead to frequency-dependent and non-transitive selection		1
1	Growth tradeoffs produce complex microbial communities on a single limiting resource		1