Eugene I Shakhnovich

List of Publications by Citations

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	How does a protein fold?. *Nature*, **1994**, 369, 248-51	50.4	845
133	Kinetics of protein folding. A lattice model study of the requirements for folding to the native state. *Journal of Molecular Biology*, **1994**, 235, 1614-36	6.5	471
132	Theoretical studies of protein-folding thermodynamics and kinetics. *Current Opinion in Structural Biology*, **1997**, 7, 29-40	8.1	343
131	Universally conserved positions in protein folds: reading evolutionary signals about stability, folding kinetics and function. *Journal of Molecular Biology*, **1999**, 291, 177-96	6.5	334
130	Estimating the Entropic Cost of Self-Assembly of Multiparticle Hydrogen-Bonded Aggregates Based on the Cyanuric Acid·Melamine Lattice. *Journal of Organic Chemistry*, **1998**, 63, 3821-3830	4.2	320
129	Protein folding theory: from lattice to all-atom models. *Annual Review of Biophysics and Biomolecular Structure*, **2001**, 30, 361-96		301
128	Protein folding thermodynamics and dynamics: where physics, chemistry, and biology meet. *Chemical Reviews*, **2006**, 106, 1559-88	68.1	294
127	How to derive a protein folding potential? A new approach to an old problem. *Journal of Molecular Biology*, **1996**, 264, 1164-79	6.5	249
126	SMoG: de Novo Design Method Based on Simple, Fast, and Accurate Free Energy Estimates. 1. Methodology and Supporting Evidence. *Journal of the American Chemical Society*, **1996**, 118, 11733-11744	16.4	239
125	Enumeration of all compact conformations of copolymers with random sequence of links. *Journal of Chemical Physics*, **1990**, 93, 5967-5971	3.9	224
124	Physics and evolution of thermophilic adaptation. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 12742-7	11.5	207
123	Protein stability imposes limits on organism complexity and speed of molecular evolution. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 16152-7	11.5	188
122	Expanding protein universe and its origin from the biological Big Bang. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 14132-6	11.5	159
121	A biophysical protein folding model accounts for most mutational fitness effects in viruses. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 9916-21	11.5	144
120	Understanding hierarchical protein evolution from first principles. *Journal of Molecular Biology*, **2001**, 312, 289-307	6.5	144
119	The ensemble folding kinetics of protein G from an all-atom Monte Carlo simulation. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 11175-80	11.5	143
118	Direct molecular dynamics observation of protein folding transition state ensemble. *Biophysical Journal*, **2002**, 83, 3525-32	2.9	119

117	Common activation mechanism of class A GPCRs. *ELife*, **2019**, 8,	8.9	117
116	Using a Convenient, Quantitative Model for Torsional Entropy To Establish Qualitative Trends for Molecular Processes That Restrict Conformational Freedom. *Journal of Organic Chemistry*, **1998**, 63, 3168-3175	4.3	112
115	Protein quality control acts on folding intermediates to shape the effects of mutations on organismal fitness. *Molecular Cell*, **2013**, 49, 133-44	17.6	102
114	Universality and diversity of the protein folding scenarios: a comprehensive analysis with the aid of a lattice model. *Folding & Design*, **1996**, 1, 103-16		101
113	Structural determinant of protein designability. *Physical Review Letters*, **2003**, 90, 218101	7.4	87
112	Biophysical principles predict fitness landscapes of drug resistance. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E1470-8	11.5	83
111	Constraints imposed by non-functional protein-protein interactions on gene expression and proteome size. *Molecular Systems Biology*, **2008**, 4, 210	12.2	78
110	Topology of protein interaction network shapes protein abundances and strengths of their functional and nonspecific interactions. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 4258-63	11.5	77
109	Soluble oligomerization provides a beneficial fitness effect on destabilizing mutations. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 4857-62	11.5	75
108	Entropic stabilization of proteins and its proteomic consequences. *PLoS Computational Biology*, **2005**, 1, e47	5	72
107	Protein structure and evolutionary history determine sequence space topology. *Genome Research*, **2005**, 15, 385-92	9.7	71
106	Protein biophysics explains why highly abundant proteins evolve slowly. *Cell Reports*, **2012**, 2, 249-56	10.6	70
105	All-atom ab initio folding of a diverse set of proteins. *Structure*, **2007**, 15, 53-63	5.2	69
104	Commitment and nucleation in the protein G transition state. *Journal of Molecular Biology*, **2004**, 336, 745-61	6.5	69
103	A structure-based method for derivation of all-atom potentials for protein folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 5343-8	11.5	68
102	SMoG: de Novo Design Method Based on Simple, Fast, and Accurate Free Energy Estimates. 2. Case Studies in Molecular Design. *Journal of the American Chemical Society*, **1997**, 119, 4608-4617	16.4	64
101	Statistical mechanics of proteins with "evolutionary selected" sequences. *Physical Review E*, **1994**, 50, 1303-1312	2.4	64
100	Merging molecular mechanism and evolution: theory and computation at the interface of biophysics and evolutionary population genetics. *Current Opinion in Structural Biology*, **2014**, 26, 84-91	8.1	62

99	Robust protein protein interactions in crowded cellular environments. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 14952-7	11.5	60
98	Understanding protein evolution: from protein physics to Darwinian selection. *Annual Review of Physical Chemistry*, **2008**, 59, 105-27	15.7	59
97	Understanding ensemble protein folding at atomic detail. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 17747-52	11.5	59
96	Differential Enzyme Flexibility Probed Using Solid-State Nanopores. *ACS Nano*, **2018**, 12, 4494-4502	16.7	55
95	Protein Homeostasis Imposes a Barrier on Functional Integration of Horizontally Transferred Genes in Bacteria. *PLoS Genetics*, **2015**, 11, e1005612	6	55
94	Evidence of evolutionary selection for cotranslational folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 11434-11439	11.5	54
93	A first-principles model of early evolution: emergence of gene families, species, and preferred protein folds. *PLoS Computational Biology*, **2007**, 3, e139	5	50
92	Bridging the physical scales in evolutionary biology: from protein sequence space to fitness of organisms and populations. *Current Opinion in Structural Biology*, **2017**, 42, 31-40	8.1	45
91	Lethal mutagenesis in viruses and bacteria. *Genetics*, **2009**, 183, 639-50	4	44
90	Simulation study of the collapse of linear and ring homopolymers. *Journal of Chemical Physics*, **1995** , 103, 2615-2624	3.9	43
89	Dynamic metastable long-living droplets formed by sticker-spacer proteins. *ELife*, **2020**, 9,	8.9	42
88	Factors that affect the folding ability of proteins. *Proteins: Structure, Function and Bioinformatics*, **1999**, 35, 34-40	4.2	41
87	An Internal Disulfide Locks a Misfolded Aggregation-prone Intermediate in Cataract-linked Mutants of Human D-Crystallin. *Journal of Biological Chemistry*, **2016**, 291, 19172-83	5.4	39
86	Contribution of selection for protein folding stability in shaping the patterns of polymorphisms in coding regions. *Molecular Biology and Evolution*, **2014**, 31, 165-76	8.3	39
85	Development of a Knowledge-Based Potential for Crystals of Small Organic Molecules: Calculation of Energy Surfaces for C=0HN Hydrogen Bonds. *Journal of Physical Chemistry B*, **2000**, 104, 7293-7298	3.4	37
84	OpenGrowth: An Automated and Rational Algorithm for Finding New Protein Ligands. *Journal of Medicinal Chemistry*, **2016**, 59, 4171-88	8.3	35
83	Protein evolution within a structural space. *Biophysical Journal*, **2003**, 85, 2962-72	2.9	35
82	Accessibility of the Shine-Dalgarno Sequence Dictates N-Terminal Codon Bias in E.coli. *Molecular Cell*, **2018**, 70, 894-905.e5	17.6	34

81	Transient protein-protein interactions perturb metabolome and cause gene dosage toxicity. *ELife*, **2016**, 5,	8.9	34
80	Optimization of lag phase shapes the evolution of a bacterial enzyme. *Nature Ecology and Evolution*, **2017**, 1, 149	12.3	33
79	The influence of selection for protein stability on dN/dS estimations. *Genome Biology and Evolution*, **2014**, 6, 2956-67	3.9	33
78	Comparison of two optimization methods to derive energy parameters for protein folding: Perceptron and Z score. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 192-201	4.2	32
77	Microphase Ordering in Melts of Randomly Grafted Copolymers. *Physical Review Letters*, **1999**, 82, 2896-2899	7.4	32
76	Dynamic disulfide exchange in a crystallin protein in the human eye lens promotes cataract-associated aggregation. *Journal of Biological Chemistry*, **2018**, 293, 17997-18009	5.4	30
75	Influenza A H1N1 pandemic strain evolution--divergence and the potential for antigenic drift variants. *PLoS ONE*, **2014**, 9, e93632	3.7	29
74	A simulated intermediate state for folding and aggregation provides insights into N6 2-microglobulin amyloidogenic behavior. *PLoS Computational Biology*, **2014**, 10, e1003606	5	28
73	Physical origins of protein superfamilies. *Journal of Molecular Biology*, **2006**, 357, 1335-43	6.5	28
72	Benchmarking Inverse Statistical Approaches for Protein Structure and Design with Exactly Solvable Models. *PLoS Computational Biology*, **2016**, 12, e1004889	5	27
71	On the role of conformational geometry in protein folding. *Journal of Chemical Physics*, **1999**, 111, 10375-10380	3.9	26
70	Cotranslational folding allows misfolding-prone proteins to circumvent deep kinetic traps. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 1485-1495	11.5	26
69	Systems-level response to point mutations in a core metabolic enzyme modulates genotype-phenotype relationship. *Cell Reports*, **2015**, 11, 645-56	10.6	25
68	Isolation and Analysis of Rare Norovirus Recombinants from Coinfected Mice Using Drop-Based Microfluidics. *Journal of Virology*, **2015**, 89, 7722-34	6.6	25
67	Accelerating high-throughput virtual screening through molecular pool-based active learning. *Chemical Science*, **2021**, 12, 7866-7881	9.4	25
66	Highly abundant proteins favor more stable 3D structures in yeast. *Biophysical Journal*, **2013**, 104, L1-3	2.9	23
65	A Hybrid Knowledge-Based and Empirical Scoring Function for Protein-Ligand Interaction: SMoG2016. *Journal of Chemical Information and Modeling*, **2017**, 57, 584-593	6.1	21
64	The Role of Evolutionary Selection in the Dynamics of Protein Structure Evolution. *Biophysical Journal*, **2017**, 112, 1350-1365	2.9	20

63	Thermal stabilization of dihydrofolate reductase using monte carlo unfolding simulations and its functional consequences. *PLoS Computational Biology*, **2015**, 11, e1004207	5	20
62	Cooperativity and stability in a Langevin model of proteinlike folding. *Journal of Chemical Physics*, **1997**, 106, 9276-9285	3.9	20
61	Stability of the Influenza Virus Hemagglutinin Protein Correlates with Evolutionary Dynamics. *MSphere*, **2018**, 3,	5	18
60	Adaptation to mutational inactivation of an essential gene converges to an accessible suboptimal fitness peak. *ELife*, **2019**, 8,	8.9	18
59	Searching the Sequence Space for Potent Aptamers Using SELEX in Silico. *Journal of Chemical Theory and Computation*, **2015**, 11, 5939-46	6.4	17
58	Growth tradeoffs produce complex microbial communities on a single limiting resource. *Nature Communications*, **2018**, 9, 3214	17.4	17
57	Evolution of specificity in protein-protein interactions. *Biophysical Journal*, **2014**, 107, 1686-96	2.9	17
56	Proteomic traces of speciation. *Journal of Molecular Biology*, **2004**, 336, 695-706	6.5	17
55	Mechanical Response of Random Heteropolymers. *Macromolecules*, **2002**, 35, 4429-4436	5.5	16
54	Trade-offs between microbial growth phases lead to frequency-dependent and non-transitive selection. *Proceedings of the Royal Society B: Biological Sciences*, **2018**, 285,	4.4	15
53	Semi-rational design and molecular dynamics simulations study of the thermostability enhancement of cellobiose 2-epimerases. *International Journal of Biological Macromolecules*, **2020**, 154, 1356-1365	7.9	15
52	Structure-Based Prediction of Protein-Folding Transition Paths. *Biophysical Journal*, **2016**, 111, 925-36	2.9	14
51	Evolution on the Biophysical Fitness Landscape of an RNA Virus. *Molecular Biology and Evolution*, **2018**, 35, 2390-2400	8.3	13
50	Rational Design of Novel Allosteric Dihydrofolate Reductase Inhibitors Showing Antibacterial Effects on Drug-Resistant Escherichia coli Escape Variants. *ACS Chemical Biology*, **2017**, 12, 1848-1857	4.9	12
49	Effect of Protein Structure on Evolution of Cotranslational Folding. *Biophysical Journal*, **2020**, 119, 1123-1134	3.9	11
48	Accurate Protein-Folding Transition-Path Statistics from a Simple Free-Energy Landscape. *Journal of Physical Chemistry B*, **2018**, 122, 11126-11136	3.4	10
47	A tale of two tails: The importance of unstructured termini in the aggregation pathway of 2-microglobulin. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 2045-2057	4.2	10
46	Simulation-guided enzyme discovery: A new microbial source of cellobiose 2-epimerase. *International Journal of Biological Macromolecules*, **2019**, 139, 1002-1008	7.9	10

45	Substrate inhibition imposes fitness penalty at high protein stability. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 11265-11274	11.5	9
44	A Study on Local-Global Cooperativity in Protein Collapse. *Journal of Physical Chemistry B*, **1999**, 103, 2535-2542	3.4	9
43	Evolutionary dynamics of viral escape under antibodies stress: A biophysical model. *Protein Science*, **2016**, 25, 1332-40	6.3	9
42	Effect of sampling on BACE-1 ligands binding free energy predictions via MM-PBSA calculations. *Journal of Computational Chemistry*, **2017**, 38, 1941-1951	3.5	8
41	Minimalistic predictor of protein binding energy: contribution of solvation factor to protein binding. *Biophysical Journal*, **2015**, 108, 795-798	2.9	8
40	Freezing in polyampholytes globules: Influence of the long-range nature of the interaction. *Journal of Chemical Physics*, **1999**, 111, 772-785	3.9	8
39	Absence of Selection for Quantum Coherence in the Fenna-Matthews-Olson Complex: A Combined Evolutionary and Excitonic Study. *ACS Central Science*, **2017**, 3, 1086-1095	16.8	7
38	Frozen phases with re-entrant transition for random heteropolymers with composition specific and annealed cross-links. *Journal of Chemical Physics*, **1997**, 107, 1247-1258	3.9	7
37	Phase diagram analysis of random heteropolymers with composition specific and quenched cross-links. *Journal of Chemical Physics*, **1998**, 109, 2947-2958	3.9	7
36	Graph Ts Topology and Free Energy of a Spin Model on the Graph. *Physical Review Letters*, **2017**, 118, 088302	7.4	6
35	The Early Phase of 2m Aggregation: An Integrative Computational Study Framed on the D76N Mutant and the N6 Variant. *Biomolecules*, **2019**, 9,	5.9	6
34	Divergent evolution of a structural proteome: phenomenological models. *Biophysical Journal*, **2007**, 92, 701-16	2.9	6
33	Exploring the Mutational Robustness of Nucleic Acids by Searching Genotype Neighborhoods in Sequence Space. *Journal of Physical Chemistry Letters*, **2017**, 8, 407-414	6.4	5
32	ProteomeVis: a web app for exploration of protein properties from structure to sequence evolution across organismsTproteomes. *Bioinformatics*, **2018**, 34, 3557-3565	7.2	5
31	A macroscopic device described by a Boltzmann-like distribution. *Soft Matter*, **2013**, 9, 4480	3.6	5
30	Diversity Against Adversity: How Adaptive Immune System Evolves Potent Antibodies. *Journal of Statistical Physics*, **2011**, 144, 241-267	1.5	4
29	Protein folding roller coaster, one molecule at a time. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 11823-4	11.5	4
28	Mutation rate variability as a driving force in adaptive evolution. *Physical Review E*, **2019**, 99, 022424	2.4	3

27	Mechanical Model of Globular Transition in Polymers. *ChemPlusChem*, **2015**, 80, 37-41	2.8	3
26	Gene Dosage Experiments in Enterobacteriaceae Using Arabinose-regulated Promoters. *Bio-protocol*, **2014**, 7,	0.9	3
25	Chimeric dihydrofolate reductases display properties of modularity and biophysical diversity. *Protein Science*, **2019**, 28, 1359-1367	6.3	2
24	Is catalytic activity of chaperones a selectable trait for the emergence of heat shock response?. *Biophysical Journal*, **2015**, 108, 438-48	2.9	2
23	Effects of Single Mutations on Protein Stability Are Gaussian Distributed. *Biophysical Journal*, **2020**, 118, 2872-2878	2.9	2
22	A Simple Model of Protein Domain Swapping in Crowded Cellular Environments. *Biophysical Journal* , **2016**, 110, 2367-2376	2.9	2
21	Exotic phase transitions in disordered globular networks. *Journal of Chemical Physics*, **2001**, 114, 10968-10976	3.9	2
20	Virtual Screening of Human O-GlcNAc Transferase Inhibitors. *Chinese Journal of Chemical Physics*, **2016**, 29, 374-380	0.9	2
19	Field theory and segmental alignment analysis for a solution of sequence disordered liquid crystalline polymers. *Journal of Chemical Physics*, **2002**, 116, 3134-3140	3.9	1
18	SmoG: A Ligand Design Method Based on Knowledge-Based Parametrization of a Solvent Reorganization Model. *ACS Symposium Series*, **1999**, 70-86	0.4	1
17	Protein dynamics: From the native to the unfolded state and back again. *Molecular Engineering*, **1995**, 5, 55-70		1
16	The role of evolutionary selection in the dynamics of protein structure evolution		1
15	Tradeoffs between microbial growth phases lead to frequency-dependent and non-transitive selection		1
14	Growth tradeoffs produce complex microbial communities on a single limiting resource		1
13	Effect of RNA on Morphology and Dynamics of Membraneless Organelles. *Journal of Physical Chemistry B*, **2021**, 125, 5035-5044	3.4	1
12	Avoidance of protein unfolding constrains protein stability in long-term evolution. *Biophysical Journal*, **2021**, 120, 2413-2424	2.9	1
11	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. *PLoS Computational Biology*, **2020**, 16, e1008323	5	0
10	Metabolic response to point mutations reveals principles of modulation of in vivo enzyme activity and phenotype. *Molecular Systems Biology*, **2021**, 17, e10200	12.2	0

List of Publications

9	Construction of Drug-Like Compounds by Markov Chains **2013**, 311-323	
8	Dynamic charge-density correlation function in weakly charged polyampholyte globules. *Physical Review E*, **2001**, 64, 041802	2.4
7	Physics and Evolution of Protein-Protein Interactions. *FASEB Journal*, **2006**, 20, A1473	0.9
6	Switching an active site helix in dihydrofolate reductase reveals limits to subdomain modularity. *Biophysical Journal*, **2021**, 120, 4738-4750	2.9
5	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins **2020**, 16, e1008323	
4	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins **2020**, 16, e1008323	
3	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins **2020**, 16, e1008323	
2	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins **2020**, 16, e1008323	
1	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins **2020**, 16, e1008323	