Eugene I Shakhnovich

List of Publications by Year
in descending order

140	10,038	46918 47	39575 94
papers	citations	h-index	g-index

165	165	165	7549
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	How does a protein fold?. Nature, 1994, 369, 248-251.	13.7	934
2	Kinetics of Protein Folding. Journal of Molecular Biology, 1994, 235, 1614-1636.	2.0	513
3	Estimating the Entropic Cost of Self-Assembly of Multiparticle Hydrogen-Bonded Aggregates Based on the Cyanuric AcidÂ·Melamine Lattice. Journal of Organic Chemistry, 1998, 63, 3821-3830.	1.7	403
4	Universally conserved positions in protein folds: reading evolutionary signals about stability, folding kinetics and function. Journal of Molecular Biology, 1999, 291, 177-196.	2.0	382
5	Theoretical studies of protein-folding thermodynamics and kinetics. Current Opinion in Structural Biology, 1997, 7, 29-40.	2.6	367
6	Common activation mechanism of class A GPCRs. ELife, 2019, 8, .	2.8	339
7	Protein Folding Thermodynamics and Dynamics:Â Where Physics, Chemistry, and Biology Meet. Chemical Reviews, 2006, 106, 1559-1588.	23.0	332
8	Protein Folding Theory: From Lattice to All-Atom Models. Annual Review of Biophysics and Biomolecular Structure, 2001, 30, 361-396.	18.3	326
9	How to Derive a Protein Folding Potential? A New Approach to an Old Problem. Journal of Molecular Biology, 1996, 264, 1164-1179.	2.0	268
10	SMoG:Â 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.	6.6	266
11	Physics and evolution of thermophilic adaptation. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 12742-12747.	3.3	242
12	Enumeration of all compact conformations of copolymers with random sequence of links. Journal of Chemical Physics, 1990, 93, 5967-5971.	1.2	240
13	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, 16152-16157.	3.3	236
14	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, 9916-9921.	3.3	194
15	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, 14132-14136.	3.3	174
16	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, 11175-11180.	3.3	167
17	Understanding hierarchical protein evolution from first principles 1 1Edited by J. Thornton. Journal of Molecular Biology, 2001, 312, 289-307.	2.0	158
18	Protein Quality Control Acts on Folding Intermediates to Shape the Effects of Mutations on Organismal Fitness. Molecular Cell, 2013, 49, 133-144.	4.5	145

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19	Direct Molecular Dynamics Observation of Protein Folding Transition State Ensemble. Biophysical Journal, 2002, 83, 3525-3532.	0.2	133
20	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.	3.3	132
21	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.	1.7	127
22	Accelerating high-throughput virtual screening through molecular pool-based active learning. Chemical Science, 2021, 12, 7866-7881.	3.7	115
23	Protein Biophysics Explains Why Highly Abundant Proteins Evolve Slowly. Cell Reports, 2012, 2, 249-256.	2.9	108
24	Structural Determinant of Protein Designability. Physical Review Letters, 2003, 90, 218101.	2.9	107
25	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, 4857-4862.	3.3	107
26	Dynamic metastable long-living droplets formed by sticker-spacer proteins. ELife, 2020, 9, .	2.8	107
27	Universality and diversity of the protein folding scenarios:a comprehensive analysis with the aid of a lattice model. Folding & Design, 1996, 1, 103-116.	4.5	106
28	Constraints imposed by nonâ€functional proteinâ€“protein interactions on gene expression and proteome size. Molecular Systems Biology, 2008, 4, 210.	3.2	99
29	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, 4258-4263.	3.3	94
30	Evidence of evolutionary selection for cotranslational folding. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11434-11439.	3.3	90
31	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.	2.6	88
32	Entropic Stabilization of Proteins and Its Proteomic Consequences. PLoS Computational Biology, 2005, 1, e47.	1.5	85
33	All-Atom Ab Initio Folding of a Diverse Set of Proteins. Structure, 2007, 15, 53-63.	1.6	85
34	Differential Enzyme Flexibility Probed Using Solid-State Nanopores. ACS Nano, 2018, 12, 4494-4502.	7.3	83
35	Protein structure and evolutionary history determine sequence space topology. Genome Research, 2005, 15, 385-392.	2.4	82
36	Protein Homeostasis Imposes a Barrier on Functional Integration of Horizontally Transferred Genes in Bacteria. PLoS Genetics, 2015, 11, e1005612.	1.5	79

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37	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, 5343-5348.	3.3	78
38	Commitment and Nucleation in the Protein G Transition State. Journal of Molecular Biology, 2004, 336, 745-761.	2.0	75
39	SMoG:Â 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.	6.6	73
40	Robust protein protein interactions in crowded cellular environments. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14952-14957.	3.3	70
41	Understanding Protein Evolution: From Protein Physics to Darwinian Selection. Annual Review of Physical Chemistry, 2008, 59, 105-127.	4.8	70
42	Statistical mechanics of proteins with â€˜â€˜evolutionary selectedâ€™â€™ sequences. Physical Review E, 1994, 50, 1303-1312.	0.8	69
43	Understanding ensemble protein folding at atomic detail. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 17747-17752.	3.3	64
44	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.	2.6	63
45	An Internal Disulfide Locks a Misfolded Aggregation-prone Intermediate in Cataract-linked Mutants of Human Î³D-Crystallin. Journal of Biological Chemistry, 2016, 291, 19172-19183.	1.6	59
46	Accessibility of the Shine-Dalgarno Sequence Dictates N-Terminal Codon Bias in E.Âcoli. Molecular Cell, 2018, 70, 894-905.e5.	4.5	58
47	Transient protein-protein interactions perturb E. coli metabolome and cause gene dosage toxicity. ELife, 2016, 5, .	2.8	58
48	A First-Principles Model of Early Evolution: Emergence of Gene Families, Species, and Preferred Protein Folds. PLoS Computational Biology, 2007, 3, e139.	1.5	55
49	Lethal Mutagenesis in Viruses and Bacteria. Genetics, 2009, 183, 639-650.	1.2	55
50	OpenGrowth: An Automated and Rational Algorithm for Finding New Protein Ligands. Journal of Medicinal Chemistry, 2016, 59, 4171-4188.	2.9	53
51	Simulation study of the collapse of linear and ring homopolymers. Journal of Chemical Physics, 1995, 103, 2615-2624.	1.2	51
52	Contribution of Selection for Protein Folding Stability in Shaping the Patterns of Polymorphisms in Coding Regions. Molecular Biology and Evolution, 2014, 31, 165-176.	3.5	51
53	Optimization of lag phase shapes the evolution of a bacterial enzyme. Nature Ecology and Evolution, 2017, 1, 149.	3.4	51
54	The Influence of Selection for Protein Stability on dN/dS Estimations. Genome Biology and Evolution, 2014, 6, 2956-2967.	1.1	49

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55	Dynamic disulfide exchange in a crystallin protein in the human eye lens promotes cataract-associated aggregation. Journal of Biological Chemistry, 2018, 293, 17997-18009.	1.6	49
56	Factors that affect the folding ability of proteins. , 1999, 35, 34-40.		45
57	Influenza A H1N1 Pandemic Strain Evolution â€“ Divergence and the Potential for Antigenic Drift Variants. PLoS ONE, 2014, 9, e93632.	1.1	45
58	Evolution on the Biophysical Fitness Landscape of an RNA Virus. Molecular Biology and Evolution, 2018, 35, 2390-2400.	3.5	45
59	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.	3.3	44
60	Benchmarking Inverse Statistical Approaches for Protein Structure and Design with Exactly Solvable Models. PLoS Computational Biology, 2016, 12, e1004889.	1.5	43
61	Development of a Knowledge-Based Potential for Crystals of Small Organic Molecules:Â Calculation of Energy Surfaces for C=0Â·Â·Â·Hâ^'N Hydrogen Bonds. Journal of Physical Chemistry B, 2000, 104, 7293-7298.	1.2	39
62	Systems-Level Response to Point Mutations in a Core Metabolic Enzyme Modulates Genotype-Phenotype Relationship. Cell Reports, 2015, 11, 645-656.	2.9	38
63	Protein Evolution within a Structural Space. Biophysical Journal, 2003, 85, 2962-2972.	0.2	37
64	Adaptation to mutational inactivation of an essential gene converges to an accessible suboptimal fitness peak. ELife, 2019, 8, .	2.8	36
65	Microphase Ordering in Melts of Randomly Grafted Copolymers. Physical Review Letters, 1999, 82, 2896-2899.	2.9	34
66	Comparison of two optimization methods to derive energy parameters for protein folding: Perceptron andZ score. Proteins: Structure, Function and Bioinformatics, 2000, 41, 192-201.	1.5	34
67	A Simulated Intermediate State for Folding and Aggregation Provides Insights into Î”N6 Î²2-Microglobulin Amyloidogenic Behavior. PLoS Computational Biology, 2014, 10, e1003606.	1.5	34
68	Physical Origins of Protein Superfamilies. Journal of Molecular Biology, 2006, 357, 1335-1343.	2.0	33
69	Highly Abundant Proteins Favor More Stable 3D Structures in Yeast. Biophysical Journal, 2013, 104, L1-L3.	0.2	33
70	Isolation and Analysis of Rare Norovirus Recombinants from Coinfected Mice Using Drop-Based Microfluidics. Journal of Virology, 2015, 89, 7722-7734.	1.5	32
71	Thermal Stabilization of Dihydrofolate Reductase Using Monte Carlo Unfolding Simulations and Its Functional Consequences. PLoS Computational Biology, 2015, 11, e1004207.	1.5	32
72	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.	3.6	32

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73	Trade-offs between microbial growth phases lead to frequency-dependent and non-transitive selection. Proceedings of the Royal Society B: Biological Sciences, 2018, 285, 20172459.	1.2	31
74	Stability of the Influenza Virus Hemagglutinin Protein Correlates with Evolutionary Dynamics. MSphere, 2018, 3, .	1.3	31
75	Folding by association. , 1999, 6, 99-102.		30
76	The Role of Evolutionary Selection in the Dynamics of Protein Structure Evolution. Biophysical Journal, 2017, 112, 1350-1365.	0.2	30
77	Growth tradeoffs produce complex microbial communities on a single limiting resource. Nature Communications, 2018, 9, 3214.	5.8	30
78	Evolution of Specificity in Protein-Protein Interactions. Biophysical Journal, 2014, 107, 1686-1696.	0.2	29
79	A Hybrid Knowledge-Based and Empirical Scoring Function for Proteinâ€“Ligand Interaction: SMoG2016. Journal of Chemical Information and Modeling, 2017, 57, 584-593.	2.5	29
80	On the role of conformational geometry in protein folding. Journal of Chemical Physics, 1999, 111, 10375-10380.	1.2	28
81	Searching the Sequence Space for Potent Aptamers Using SELEX in Silico. Journal of Chemical Theory and Computation, 2015, 11, 5939-5946.	2.3	27
82	Structure-Based Prediction of Protein-Folding Transition Paths. Biophysical Journal, 2016, 111, 925-936.	0.2	27
83	Cooperativity and stability in a Langevin model of proteinlike folding. Journal of Chemical Physics, 1997, 106, 9276-9285.	1.2	22
84	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.	1.6	22
85	The physics of liquid-to-solid transitions in multi-domain protein condensates. Biophysical Journal, 2022, 121, 2751-2766.	0.2	20
86	Proteomic Traces of Speciation. Journal of Molecular Biology, 2004, 336, 695-706.	2.0	19
87	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.	3.3	19
88	Effect of Protein Structure on Evolution of Cotranslational Folding. Biophysical Journal, 2020, 119, 1123-1134.	0.2	19
89	Effect of RNA on Morphology and Dynamics of Membraneless Organelles. Journal of Physical Chemistry B, 2021, 125, 5035-5044.	1.2	19
90	Mechanical Response of Random Heteropolymers. Macromolecules, 2002, 35, 4429-4436.	2.2	18

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91	Minimalistic Predictor of Protein Binding Energy: Contribution of Solvation Factor to Protein Binding. Biophysical Journal, 2015, 108, 795-798.	0.2	17
92	A tale of two tails: The importance of unstructured termini in the aggregation pathway of Î²2â€microglobulin. Proteins: Structure, Function and Bioinformatics, 2017, 85, 2045-2057.	1.5	17
93	Simulation-guided enzyme discovery: A new microbial source of cellobiose 2-epimerase. International Journal of Biological Macromolecules, 2019, 139, 1002-1008.	3.6	16
94	Effect of sampling on BACE-1 ligands binding free energy predictions via MM-PBSA calculations. Journal of Computational Chemistry, 2017, 38, 1941-1951.	1.5	14
95	Accurate Protein-Folding Transition-Path Statistics from a Simple Free-Energy Landscape. Journal of Physical Chemistry B, 2018, 122, 11126-11136.	1.2	13
96	Evolutionary dynamics of viral escape under antibodies stress: A biophysical model. Protein Science, 2016, 25, 1332-1340.	3.1	12
97	Development of antibacterial compounds that constrain evolutionary pathways to resistance. ELife, 2021, 10, .	2.8	12
98	Exploring the Mutational Robustness of Nucleic Acids by Searching Genotype Neighborhoods in Sequence Space. Journal of Physical Chemistry Letters, 2017, 8, 407-414.	2.1	11
99	Absence of Selection for Quantum Coherence in the Fennaâ€“Matthewsâ€“Olson Complex: A Combined Evolutionary and Excitonic Study. ACS Central Science, 2017, 3, 1086-1095.	5.3	11
100	The Early Phase of Î²2m Aggregation: An Integrative Computational Study Framed on the D76N Mutant and the Î”N6 Variant. Biomolecules, 2019, 9, 366.	1.8	11
101	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. PLoS Computational Biology, 2020, 16, e1008323.	1.5	11
102	A Study on Local-Global Cooperativity in Protein Collapse. Journal of Physical Chemistry B, 1999, 103, 2535-2542.	1.2	10
103	Metabolic response to point mutations reveals principles of modulation of in vivo enzyme activity and phenotype. Molecular Systems Biology, 2021, 17, e10200.	3.2	10
104	Freezing in polyampholytes globules: Influence of the long-range nature of the interaction. Journal of Chemical Physics, 1999, 111, 772-785.	1.2	8
105	A native chemical chaperone in the human eye lens. ELife, 0, 11, .	2.8	8
106	Frozen phases with re-entrant transition for random heteropolymers with composition specific and annealed cross-links. Journal of Chemical Physics, 1997, 107, 1247-1258.	1.2	7
107	Phase diagram analysis of random heteropolymers with composition specific and quenched cross-links. Journal of Chemical Physics, 1998, 109, 2947-2958.	1.2	7
108	Divergent Evolution of a Structural Proteome: Phenomenological Models. Biophysical Journal, 2007, 92, 701-716.	0.2	7

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109	A macroscopic device described by a Boltzmann-like distribution. Soft Matter, 2013, 9, 4480.	1.2	7
110	ProteomeVis: a web app for exploration of protein properties from structure to sequence evolution across organismsâ€™ proteomes. Bioinformatics, 2018, 34, 3557-3565.	1.8	7
111	Mutation rate variability as a driving force in adaptive evolution. Physical Review E, 2019, 99, 022424.	0.8	7
112	Avoidance of protein unfolding constrains protein stability in long-term evolution. Biophysical Journal, 2021, 120, 2413-2424.	0.2	7
113	Graphâ€™s Topology and Free Energy of a Spin Model on the Graph. Physical Review Letters, 2017, 118, 088302.	2.9	6
114	Protein folding roller coaster, one molecule at a time. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11823-11824.	3.3	4
115	Diversity Against Adversity: How Adaptive Immune System Evolves Potent Antibodies. Journal of Statistical Physics, 2011, 144, 241-267.	0.5	4
116	Effects of Single Mutations on Protein Stability Are Gaussian Distributed. Biophysical Journal, 2020, 118, 2872-2878.	0.2	4
117	Gene Dosage Experiments in Enterobacteriaceae Using Arabinose-regulated Promoters. Bio-protocol, 2017, 7, .	0.2	4
118	Mechanical Model of Globular Transition in Polymers. ChemPlusChem, 2015, 80, 37-41.	1.3	3
119	A Simple Model of Protein Domain Swapping in Crowded Cellular Environments. Biophysical Journal, 2016, 110, 2367-2376.	0.2	3
120	Chimeric dihydrofolate reductases display properties of modularity and biophysical diversity. Protein Science, 2019, 28, 1359-1367.	3.1	3
121	Exotic phase transitions in disordered globular networks. Journal of Chemical Physics, 2001, 114, 10968-10976.	1.2	2
122	Is Catalytic Activity of Chaperones a Selectable Trait for the Emergence of Heat Shock Response?. Biophysical Journal, 2015, 108, 438-448.	0.2	2
123	Virtual Screening of Human O-GlcNAc Transferase Inhibitors. Chinese Journal of Chemical Physics, 2016, 29, 374-380.	0.6	2
124	Protein dynamics: From the native to the unfolded state and back again. Molecular Engineering, 1995, 5, 55-70.	0.2	1
125	SmoG: A Ligand Design Method Based on Knowledge-Based Parametrization of a Solvent Reorganization Model. ACS Symposium Series, 1999, , 70-86.	0.5	1
126	Field theory and segmental alignment analysis for a solution of sequence disordered liquid crystalline polymers. Journal of Chemical Physics, 2002, 116, 3134-3140.	1.2	1

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127	DISORDER IN PROTEIN STRUCTURE AND FUNCTION. , 1998, , .		1
128	Domainâ€swapped dimeric Î³â€crystallin: the missing link in the evolution of oligomeric Î²â€crystallins. FASEB Journal, 2022, 36, .	0.2	1
129	Dynamic charge-density correlation function in weakly charged polyampholyte globules. Physical Review E, 2001, 64, 041802.	0.8	0
130	Soluble oligomerization provides a beneficial fitness effect on destabilizing mutations.. Nature Precedings, 2011, , .	0.1	0
131	EMERGING BIOPHYSICAL MECHANISM AND EVOLUTION: SYNERGISTIC APPROACHES TO PREDICT EVOLUTIONARY DYNAMICS TO FIGHT DRUG RESISTANCE. , 2021, , .		0
132	Metabolic response to point mutations reveals principles of modulation of in vivo enzyme activity and phenotype. FASEB Journal, 2021, 35, .	0.2	0
133	Switching an active site helix in dihydrofolate reductase reveals limits to subdomain modularity. Biophysical Journal, 2021, 120, 4738-4750.	0.2	0
134	Physics and Evolution of Proteinâ€Protein Interactions. FASEB Journal, 2006, 20, A1473.	0.2	0
135	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
136	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
137	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
138	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
139	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
140	Systematic Conformationâ€toâ€Phenotype Mapping via Limited Protein Sequencing. FASEB Journal, 2022, 36, .	0.2	0