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	Domainâ€swapped dimeric Î³â€crystallin: the missing link in the evolution of oligomeric Î²â€crystallins. FASEB Journal, 2022, 36, .	0.2	1
2	Systematic Conformationâ€toâ€Phenotype Mapping via Limited Protein Sequencing. FASEB Journal, 2022, 36, .	0.2	0
3	The physics of liquid-to-solid transitions in multi-domain protein condensates. Biophysical Journal, 2022, 121, 2751-2766.	0.2	20
4	EMERGING BIOPHYSICAL MECHANISM AND EVOLUTION: SYNERGISTIC APPROACHES TO PREDICT EVOLUTIONARY DYNAMICS TO FIGHT DRUG RESISTANCE. , 2021, , .		0
5	Accelerating high-throughput virtual screening through molecular pool-based active learning. Chemical Science, 2021, 12, 7866-7881.	3.7	115
6	Metabolic response to point mutations reveals principles of modulation of in vivo enzyme activity and phenotype. FASEB Journal, 2021, 35, .	0.2	0
7	Effect of RNA on Morphology and Dynamics of Membraneless Organelles. Journal of Physical Chemistry B, 2021, 125, 5035-5044.	1.2	19
8	Avoidance of protein unfolding constrains protein stability in long-term evolution. Biophysical Journal, 2021, 120, 2413-2424.	0.2	7
9	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
10	Development of antibacterial compounds that constrain evolutionary pathways to resistance. ELife, 2021, 10, .	2.8	12
11	Switching an active site helix in dihydrofolate reductase reveals limits to subdomain modularity. Biophysical Journal, 2021, 120, 4738-4750.	0.2	0
12	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
13	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
14	Effect of Protein Structure on Evolution of Cotranslational Folding. Biophysical Journal, 2020, 119, 1123-1134.	0.2	19
15	Effects of Single Mutations on Protein Stability Are Gaussian Distributed. Biophysical Journal, 2020, 118, 2872-2878.	0.2	4
16	Dynamic metastable long-living droplets formed by sticker-spacer proteins. ELife, 2020, 9, .	2.8	107
17	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. PLoS Computational Biology, 2020, 16, e1008323.	1.5	11
18	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0

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19	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
20	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
21	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
22	Validation of DBFOLD: An efficient algorithm for computing folding pathways of complex proteins. , 2020, 16, e1008323.		0
23	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
24	Chimeric dihydrofolate reductases display properties of modularity and biophysical diversity. Protein Science, 2019, 28, 1359-1367.	3.1	3
25	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
26	Mutation rate variability as a driving force in adaptive evolution. Physical Review E, 2019, 99, 022424.	0.8	7
27	Simulation-guided enzyme discovery: A new microbial source of cellobiose 2-epimerase. International Journal of Biological Macromolecules, 2019, 139, 1002-1008.	3.6	16
28	Common activation mechanism of class A GPCRs. ELife, 2019, 8, .	2.8	339
29	Adaptation to mutational inactivation of an essential gene converges to an accessible suboptimal fitness peak. ELife, 2019, 8, .	2.8	36
30	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
31	Differential Enzyme Flexibility Probed Using Solid-State Nanopores. ACS Nano, 2018, 12, 4494-4502.	7.3	83
32	Stability of the Influenza Virus Hemagglutinin Protein Correlates with Evolutionary Dynamics. MSphere, 2018, 3, .	1.3	31
33	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
34	Evolution on the Biophysical Fitness Landscape of an RNA Virus. Molecular Biology and Evolution, 2018, 35, 2390-2400.	3.5	45
35	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
36	Accurate Protein-Folding Transition-Path Statistics from a Simple Free-Energy Landscape. Journal of Physical Chemistry B, 2018, 122, 11126-11136.	1.2	13

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37	Growth tradeoffs produce complex microbial communities on a single limiting resource. Nature Communications, 2018, 9, 3214.	5.8	30
38	Accessibility of the Shine-Dalgarno Sequence Dictates N-Terminal Codon Bias in E.Âcoli. Molecular Cell, 2018, 70, 894-905.e5.	4.5	58
39	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
40	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
41	Graphâ€™s Topology and Free Energy of a Spin Model on the Graph. Physical Review Letters, 2017, 118, 088302.	2.9	6
42	The Role of Evolutionary Selection in the Dynamics of Protein Structure Evolution. Biophysical Journal, 2017, 112, 1350-1365.	0.2	30
43	Optimization of lag phase shapes the evolution of a bacterial enzyme. Nature Ecology and Evolution, 2017, 1, 149.	3.4	51
44	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
45	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
46	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
47	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
48	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
49	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
50	Gene Dosage Experiments in Enterobacteriaceae Using Arabinose-regulated Promoters. Bio-protocol, 2017, 7, .	0.2	4
51	Benchmarking Inverse Statistical Approaches for Protein Structure and Design with Exactly Solvable Models. PLoS Computational Biology, 2016, 12, e1004889.	1.5	43
52	Virtual Screening of Human O-GlcNAc Transferase Inhibitors. Chinese Journal of Chemical Physics, 2016, 29, 374-380.	0.6	2
53	Evolutionary dynamics of viral escape under antibodies stress: A biophysical model. Protein Science, 2016, 25, 1332-1340.	3.1	12
54	Structure-Based Prediction of Protein-Folding Transition Paths. Biophysical Journal, 2016, 111, 925-936.	0.2	27

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55	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
56	A Simple Model of Protein Domain Swapping in Crowded Cellular Environments. Biophysical Journal, 2016, 110, 2367-2376.	0.2	3
57	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
58	OpenGrowth: An Automated and Rational Algorithm for Finding New Protein Ligands. Journal of Medicinal Chemistry, 2016, 59, 4171-4188.	2.9	53
59	Transient protein-protein interactions perturb E. coli metabolome and cause gene dosage toxicity. ELife, 2016, 5, .	2.8	58
60	Isolation and Analysis of Rare Norovirus Recombinants from Coinfected Mice Using Drop-Based Microfluidics. Journal of Virology, 2015, 89, 7722-7734.	1.5	32
61	Minimalistic Predictor of Protein Binding Energy: Contribution of Solvation Factor to Protein Binding. Biophysical Journal, 2015, 108, 795-798.	0.2	17
62	Is Catalytic Activity of Chaperones a Selectable Trait for the Emergence of Heat Shock Response?. Biophysical Journal, 2015, 108, 438-448.	0.2	2
63	Thermal Stabilization of Dihydrofolate Reductase Using Monte Carlo Unfolding Simulations and Its Functional Consequences. PLoS Computational Biology, 2015, 11, e1004207.	1.5	32
64	Searching the Sequence Space for Potent Aptamers Using SELEX in Silico. Journal of Chemical Theory and Computation, 2015, 11, 5939-5946.	2.3	27
65	Systems-Level Response to Point Mutations in a Core Metabolic Enzyme Modulates Genotype-Phenotype Relationship. Cell Reports, 2015, 11, 645-656.	2.9	38
66	Mechanical Model of Globular Transition in Polymers. ChemPlusChem, 2015, 80, 37-41.	1.3	3
67	Protein Homeostasis Imposes a Barrier on Functional Integration of Horizontally Transferred Genes in Bacteria. PLoS Genetics, 2015, 11, e1005612.	1.5	79
68	Influenza A H1N1 Pandemic Strain Evolution â€“ Divergence and the Potential for Antigenic Drift Variants. PLoS ONE, 2014, 9, e93632.	1.1	45
69	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
70	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
71	The Influence of Selection for Protein Stability on dN/dS Estimations. Genome Biology and Evolution, 2014, 6, 2956-2967.	1.1	49
72	Evolution of Specificity in Protein-Protein Interactions. Biophysical Journal, 2014, 107, 1686-1696.	0.2	29

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73	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
74	A macroscopic device described by a Boltzmann-like distribution. Soft Matter, 2013, 9, 4480.	1.2	7
75	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
76	Highly Abundant Proteins Favor More Stable 3D Structures in Yeast. Biophysical Journal, 2013, 104, L1-L3.	0.2	33
77	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
78	Protein Biophysics Explains Why Highly Abundant Proteins Evolve Slowly. Cell Reports, 2012, 2, 249-256.	2.9	108
79	Soluble oligomerization provides a beneficial fitness effect on destabilizing mutations.. Nature Precedings, 2011, , .	0.1	0
80	Diversity Against Adversity: How Adaptive Immune System Evolves Potent Antibodies. Journal of Statistical Physics, 2011, 144, 241-267.	0.5	4
81	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
82	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
83	Lethal Mutagenesis in Viruses and Bacteria. Genetics, 2009, 183, 639-650.	1.2	55
84	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
85	Understanding Protein Evolution: From Protein Physics to Darwinian Selection. Annual Review of Physical Chemistry, 2008, 59, 105-127.	4.8	70
86	Constraints imposed by nonâ€functional proteinâ€“protein interactions on gene expression and proteome size. Molecular Systems Biology, 2008, 4, 210.	3.2	99
87	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
88	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
89	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
90	Divergent Evolution of a Structural Proteome: Phenomenological Models. Biophysical Journal, 2007, 92, 701-716.	0.2	7

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91	All-Atom Ab Initio Folding of a Diverse Set of Proteins. Structure, 2007, 15, 53-63.	1.6	85
92	Protein Folding Thermodynamics and Dynamics:Â Where Physics, Chemistry, and Biology Meet. Chemical Reviews, 2006, 106, 1559-1588.	23.0	332
93	Physical Origins of Protein Superfamilies. Journal of Molecular Biology, 2006, 357, 1335-1343.	2.0	33
94	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
95	Physics and Evolution of Proteinâ€Protein Interactions. FASEB Journal, 2006, 20, A1473.	0.2	0
96	Entropic Stabilization of Proteins and Its Proteomic Consequences. PLoS Computational Biology, 2005, 1, e47.	1.5	85
97	Protein structure and evolutionary history determine sequence space topology. Genome Research, 2005, 15, 385-392.	2.4	82
98	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
99	Commitment and Nucleation in the Protein G Transition State. Journal of Molecular Biology, 2004, 336, 745-761.	2.0	75
100	Proteomic Traces of Speciation. Journal of Molecular Biology, 2004, 336, 695-706.	2.0	19
101	Structural Determinant of Protein Designability. Physical Review Letters, 2003, 90, 218101.	2.9	107
102	Protein Evolution within a Structural Space. Biophysical Journal, 2003, 85, 2962-2972.	0.2	37
103	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
104	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
105	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
106	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
107	Mechanical Response of Random Heteropolymers. Macromolecules, 2002, 35, 4429-4436.	2.2	18
108	Direct Molecular Dynamics Observation of Protein Folding Transition State Ensemble. Biophysical Journal, 2002, 83, 3525-3532.	0.2	133

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109	Exotic phase transitions in disordered globular networks. Journal of Chemical Physics, 2001, 114, 10968-10976.	1.2	2
110	Protein Folding Theory: From Lattice to All-Atom Models. Annual Review of Biophysics and Biomolecular Structure, 2001, 30, 361-396.	18.3	326
111	Understanding hierarchical protein evolution from first principles 1 1Edited by J. Thornton. Journal of Molecular Biology, 2001, 312, 289-307.	2.0	158
112	Dynamic charge-density correlation function in weakly charged polyampholyte globules. Physical Review E, 2001, 64, 041802.	0.8	0
113	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
114	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
115	Freezing in polyampholytes globules: Influence of the long-range nature of the interaction. Journal of Chemical Physics, 1999, 111, 772-785.	1.2	8
116	On the role of conformational geometry in protein folding. Journal of Chemical Physics, 1999, 111, 10375-10380.	1.2	28
117	Microphase Ordering in Melts of Randomly Grafted Copolymers. Physical Review Letters, 1999, 82, 2896-2899.	2.9	34
118	Folding by association. , 1999, 6, 99-102.		30
119	Factors that affect the folding ability of proteins. , 1999, 35, 34-40.		45
120	A Study on Local-Global Cooperativity in Protein Collapse. Journal of Physical Chemistry B, 1999, 103, 2535-2542.	1.2	10
121	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
122	SmoG: A Ligand Design Method Based on Knowledge-Based Parametrization of a Solvent Reorganization Model. ACS Symposium Series, 1999, , 70-86.	0.5	1
123	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
124	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
125	Phase diagram analysis of random heteropolymers with composition specific and quenched cross-links. Journal of Chemical Physics, 1998, 109, 2947-2958.	1.2	7
126	DISORDER IN PROTEIN STRUCTURE AND FUNCTION. , 1998, , .		1

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127	Cooperativity and stability in a Langevin model of proteinlike folding. Journal of Chemical Physics, 1997, 106, 9276-9285.	1.2	22
128	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
129	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
130	Theoretical studies of protein-folding thermodynamics and kinetics. Current Opinion in Structural Biology, 1997, 7, 29-40.	2.6	367
131	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
132	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
133	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
134	Protein dynamics: From the native to the unfolded state and back again. Molecular Engineering, 1995, 5, 55-70.	0.2	1
135	Simulation study of the collapse of linear and ring homopolymers. Journal of Chemical Physics, 1995, 103, 2615-2624.	1.2	51
136	How does a protein fold?. Nature, 1994, 369, 248-251.	13.7	934
137	Statistical mechanics of proteins with â€˜â€˜evolutionary selectedâ€™â€™ sequences. Physical Review E, 1994, 50, 1303-1312.	0.8	69
138	Kinetics of Protein Folding. Journal of Molecular Biology, 1994, 235, 1614-1636.	2.0	513
139	Enumeration of all compact conformations of copolymers with random sequence of links. Journal of Chemical Physics, 1990, 93, 5967-5971.	1.2	240
140	A native chemical chaperone in the human eye lens. ELife, 0, 11, .	2.8	8