Jeffrey Skolnick

List of Publications by Year
in descending order

118 papers	10,346 citations	71061 41 h-index	37183 96 g-index
143 all docs	143 docs citations	143 times ranked	8498 citing authors

#	Article	IF	Citations
1	AF2Complex predicts direct physical interactions in multimeric proteins with deep learning. Nature Communications, 2022, 13, 1744.	5.8	128
2	The role of local versus nonlocal physicochemical restraints in determining protein native structure. Current Opinion in Structural Biology, 2021, 68, 1-8.	2.6	14
3	A novel sequence alignment algorithm based on deep learning of the protein folding code. Bioinformatics, 2021, 37, 490-496.	1.8	19
4	FRAGSITE: A Fragment-Based Approach for Virtual Ligand Screening. Journal of Chemical Information and Modeling, 2021, 61, 2074-2089.	2.5	20
5	Memories of Harold Scheraga. Journal of Chemical Theory and Computation, 2021, 17, 2011-2012.	2.3	0
6	A General Framework to Learn Tertiary Structure for Protein Sequence Characterization. Frontiers in Bioinformatics, 2021, 1, .	1.0	3
7	AlphaFold 2: Why It Works and Its Implications for Understanding the Relationships of Protein Sequence, Structure, and Function. Journal of Chemical Information and Modeling, 2021, 61, 4827-4831.	2.5	109
8	Prediction of severe adverse events, modes of action and drug treatments for COVID-19's complications. Scientific Reports, 2021, 11, 20864.	1.6	3
9	High-Performance Deep Learning Toolbox for Genome-Scale Prediction of Protein Structure and Function. , 2021, 2021, 46-57.		8
10	Tribute to Harold A. Scheraga. Journal of Physical Chemistry B, 2020, 124, 10301-10302.	1.2	0
11	Antimalarial Peptide and Polyketide Natural Products from the Fijian Marine Cyanobacterium Moorea producens. Marine Drugs, 2020, 18, 167.	2.2	29
12	MEDICASCY: A Machine Learning Approach for Predicting Small-Molecule Drug Side Effects, Indications, Efficacy, and Modes of Action. Molecular Pharmaceutics, 2020, 17, 1558-1574.	2.3	24
13	Differential kinase activity of ACVR1 G328V and R206H mutations with implications to possible TÎ²RI cross-talk in diffuse intrinsic pontine glioma. Scientific Reports, 2020, 10, 6140.	1.6	5
14	Time-resolved x-ray crystallography capture of a slow reaction tetrahydrofolate intermediate. Structural Dynamics, 2019, 6, 024701.	0.9	4
15	DESTINI: A deep-learning approach to contact-driven protein structure prediction. Scientific Reports, 2019, 9, 3514.	1.6	44
16	On the possible origin of protein homochirality, structure, and biochemical function. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26571-26579.	3.3	30
17	Chemical space of <i>Escherichia coli</i> dihydrofolate reductase inhibitors: New approaches for discovering novel drugs for old bugs. Medicinal Research Reviews, 2019, 39, 684-705.	5.0	29
18	The crystal structure of a tetrahydrofolate-bound dihydrofolate reductase reveals the origin of slow product release. Communications Biology, 2018, 1, 226.	2.0	23

#	Article	IF	Citations
19	FINDSITE^{comb2.0}: A New Approach for Virtual Ligand Screening of Proteins and Virtual Target Screening of Biomolecules. Journal of Chemical Information and Modeling, 2018, 58, 2343-2354.	2.5	35
20	ENTPRISE-X: Predicting disease-associated frameshift and nonsense mutations. PLoS ONE, 2018, 13, e0196849.	1.1	20
21	Rational Design of Novel Allosteric Dihydrofolate Reductase Inhibitors Showing Antibacterial Effects on Drug-Resistant <i>Escherichia coli</i> Escape Variants. ACS Chemical Biology, 2017, 12, 1848-1857.	1.6	22
22	DNA Internal Motion Likely Accelerates Protein Target Search in a Packed Nucleoid. Biophysical Journal, 2017, 112, 2261-2270.	0.2	21
23	Pocket detection and interaction-weighted ligand-similarity search yields novel high-affinity binders for Myocilin-OLF, a protein implicated in glaucoma. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4133-4139.	1.0	2
24	Why Is There a Glass Ceiling for Threading Based Protein Structure Prediction Methods?. Journal of Physical Chemistry B, 2017, 121, 3546-3554.	1.2	13
25	On the importance of composite protein multiple ligand interactions in protein pockets. Journal of Computational Chemistry, 2017, 38, 1252-1259.	1.5	10
26	Integrating the whole from the sum of the parts: vignettes in computational biology. Emerging Topics in Life Sciences, 2017, 1, 241-243.	1.1	0
27	Novel small molecule binders of human N-glycanase 1, a key player in the endoplasmic reticulum associated degradation pathway. Bioorganic and Medicinal Chemistry, 2016, 24, 4750-4758.	1.4	3
28	Repurposing FDA-approved drugs for anti-aging therapies. Biogerontology, 2016, 17, 907-920.	2.0	31
29	Catalytic and substrate promiscuity: distinct multiple chemistries catalysed by the phosphatase domain of receptor protein tyrosine phosphatase. Biochemical Journal, 2016, 473, 2165-2177.	1.7	8
30	Perspective: On the importance of hydrodynamic interactions in the subcellular dynamics of macromolecules. Journal of Chemical Physics, 2016, 145, 100901.	1.2	27
31	A knowledge-based approach for predicting gene–disease associations. Bioinformatics, 2016, 32, 2831-2838.	1.8	56
32	How special is the biochemical function of native proteins?. F1000Research, 2016, 5, 207.	0.8	9
33	ENTPRISE: An Algorithm for Predicting Human Disease-Associated Amino Acid Substitutions from Sequence Entropy and Predicted Protein Structures. PLoS ONE, 2016, 11, e0150965.	1.1	23
34	Are protein-protein interfaces special regions on a protein's surface?. Journal of Chemical Physics, 2015, 143, 243149.	1.2	18
35	Insights into the slow‐onset tight‐binding inhibition of <i>Escherichia coli</i> dihydrofolate reductase: detailed mechanistic characterization of pyrrolo[3,2‐<i>f</i>]quinazoline‐1,3‐diamine and its derivatives as novel tight‐binding inhibitors. FEBS Journal, 2015, 282, 1922-1938.	2.2	34
36	Insights into Disease-Associated Mutations in the Human Proteome through Protein Structural Analysis. Structure, 2015, 23, 1362-1369.	1.6	103

#	Article	IF	Citations
37	Comprehensive prediction of drug-protein interactions and side effects for the human proteome. Scientific Reports, 2015, 5, 11090.	1.6	90
38	GS-align for glycan structure alignment and similarity measurement. Bioinformatics, 2015, 31, 2653-2659.	1.8	11
39	Implications of the small number of distinct ligand binding pockets in proteins for drug discovery, evolution and biochemical function. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1163-1170.	1.0	27
40	*PoLi*: A Virtual Screening Pipeline Based on Template Pocket and Ligand Similarity. Journal of Chemical Information and Modeling, 2015, 55, 1757-1770.	2.5	36
41	Ligand binding studies, preliminary structure–activity relationship and detailed mechanistic characterization of 1-phenyl-6,6-dimethyl-1,3,5-triazine-2,4-diamine derivatives as inhibitors of Escherichia coli dihydrofolate reductase. European Journal of Medicinal Chemistry, 2015, 103, 600-614.	2.6	22
42	Hurt, tired and queasy: Specific variants in the ATPase domain of the TRAP1 mitochondrial chaperone are associated with common, chronic "functional" symptomatology including pain, fatigue and gastrointestinal dysmotility. Mitochondrion, 2015, 23, 64-70.	1.6	15
43	Effects of confinement on models of intracellular macromolecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14846-14851.	3.3	30
44	LIGSIFT: an open-source tool for ligand structural alignment and virtual screening. Bioinformatics, 2015, 31, 539-544.	1.8	40
45	Sliding of Proteins Non-specifically Bound to DNA: Brownian Dynamics Studies with Coarse-Grained Protein and DNA Models. PLoS Computational Biology, 2014, 10, e1003990.	1.5	43
46	On the Role of Physics and Evolution in Dictating Protein Structure and Function. Israel Journal of Chemistry, 2014, 54, 1176-1188.	1.0	10
47	Experimental validation of FINDSITEcomb virtual ligand screening results for eight proteins yields novel nanomolar and micromolar binders. Journal of Cheminformatics, 2014, 6, 16.	2.8	23
48	Are predicted protein structures of any value for binding site prediction and virtual ligand screening?. Current Opinion in Structural Biology, 2013, 23, 191-197.	2.6	29
49	APoc: large-scale identification of similar protein pockets. Bioinformatics, 2013, 29, 597-604.	1.8	109
50	FINDSITE^comb: A Threading/Structure-Based, Proteomic-Scale Virtual Ligand Screening Approach. Journal of Chemical Information and Modeling, 2013, 53, 230-240.	2.5	59
51	A Comprehensive Survey of Small-Molecule Binding Pockets in Proteins. PLoS Computational Biology, 2013, 9, e1003302.	1.5	103
52	Interplay of physics and evolution in the likely origin of protein biochemical function. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 9344-9349.	3.3	59
53	Further Evidence for the Likely Completeness of the Library of Solved Single Domain Protein Structures. Journal of Physical Chemistry B, 2012, 116, 6654-6664.	1.2	31
54	FINDSITE^X: A Structure-Based, Small Molecule Virtual Screening Approach with Application to All Identified Human GPCRs. Molecular Pharmaceutics, 2012, 9, 1775-1784.	2.3	34

#	ARTICLE	IF	CITATIONS
55	Template‐based protein structure modeling using TASSER^{VMT}. Proteins: Structure, Function and Bioinformatics, 2012, 80, 352-361.	1.5	38
56	Learning Protein Folding Energy Functions. , 2011, , 1062-1067.		4
57	New benchmark metrics for protein‐protein docking methods. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1623-1634.	1.5	31
58	Q‐Dock^{LHM}: Low‐resolution refinement for ligand comparative modeling. Journal of Computational Chemistry, 2010, 31, 1093-1105.	1.5	24
59	NOVEL COMPUTATIONAL APPROACHES TO DRUG DISCOVERY. , 2010, , .		0
60	iAlign: a method for the structural comparison of protein–protein interfaces. Bioinformatics, 2010, 26, 2259-2265.	1.8	81
61	Structural space of protein–protein interfaces is degenerate, close to complete, and highly connected. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 22517-22522.	3.3	133
62	Comprehensive Structural and Functional Characterization of the Human Kinome by Protein Structure Modeling and Ligand Virtual Screening. Journal of Chemical Information and Modeling, 2010, 50, 1839-1854.	2.5	37
63	Keynote I. , 2010, , .		0
64	The continuity of protein structure space is an intrinsic property of proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15690-15695.	3.3	72
65	FINDSITELHM: A Threading-Based Approach to Ligand Homology Modeling. PLoS Computational Biology, 2009, 5, e1000405.	1.5	69
66	FINDSITE: a combined evolution/structure-based approach to protein function prediction. Briefings in Bioinformatics, 2009, 10, 378-391.	3.2	92
67	Q‐Dock: Low‐resolution flexible ligand docking with pocket‐specific threading restraints. Journal of Computational Chemistry, 2008, 29, 1574-1588.	1.5	45
68	Aerobic uranium (VI) bioprecipitation by metal-resistant bacteria isolated from radionuclide- and metal-contaminated subsurface soils. Environmental Microbiology, 2008, 10, 1097-1097.	1.8	2
69	Fr-TM-align: a new protein structural alignment method based on fragment alignments and the TM-score. BMC Bioinformatics, 2008, 9, 531.	1.2	129
70	M-TASSER: An Algorithm for Protein Quaternary Structure Prediction. Biophysical Journal, 2008, 94, 918-928.	0.2	64
71	A threading-based method (FINDSITE) for ligand-binding site prediction and functional annotation. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 129-134.	3.3	287
72	Ab Initio Protein Structure Prediction Using Chunk-TASSER. Biophysical Journal, 2007, 93, 1510-1518.	0.2	84

#	Article	IF	Citations
73	On the origin and highly likely completeness of single-domain protein structures. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 2605-2610.	3.3	182
74	The protein structure prediction problem could be solved using the current PDB library. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 1029-1034.	3.3	269
75	TM-align: a protein structure alignment algorithm based on the TM-score. Nucleic Acids Research, 2005, 33, 2302-2309.	6.5	2,634
76	Scoring function for automated assessment of protein structure template quality. Proteins: Structure, Function and Bioinformatics, 2004, 57, 702-710.	1.5	1,697
77	Computer simulations of the properties of the ?2, ?2C, and ?2D de novo designed helical proteins. , 2000, 38, 17-28.		7
78	Structure‐based functional motif identifies a potential disulfide oxidoreductase active site in the serine/threonine protein phosphatase‐1 subfamily. FASEB Journal, 1999, 13, 1866-1874.	0.2	81
79	De novo predictions of the quaternary structure of leucine zippers and other coiled coils. International Journal of Quantum Chemistry, 1999, 75, 165-176.	1.0	5
80	Ab initio folding of proteins using restraints derived from evolutionary information. Proteins: Structure, Function and Bioinformatics, 1999, 37, 177-185.	1.5	119
81	Averaging interaction energies over homologs improves protein fold recognition in gapless threading. Proteins: Structure, Function and Bioinformatics, 1999, 35, 353-359.	1.5	23
82	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. Proteins: Structure, Function and Bioinformatics, 1999, 35, 447-452.	1.5	30
83	Application of an artificial neural network to predict specific class I MHC binding peptide sequences. Nature Biotechnology, 1998, 16, 753-756.	9.4	75
84	Tertiary structure prediction of the KIX domain of CBP using Monte Carlo simulations driven by restraints derived from multiple sequence alignments. , 1998, 30, 287-294.		17
85	Assembly of protein structure from sparse experimental data: An efficient Monte Carlo model. Proteins: Structure, Function and Bioinformatics, 1998, 32, 475-494.	1.5	101
86	How do potentials derived from structural databases relate to "true" potentials?. Protein Science, 1998, 7, 112-122.	3.1	48
87	What should the Z‐score of native protein structures be?. Protein Science, 1998, 7, 1201-1207.	3.1	45
88	An Efficient Monte Carlo Model of Protein Chains. Modeling the Short-Range Correlations between Side Group Centers of Mass. Journal of Physical Chemistry B, 1998, 102, 4628-4637.	1.2	38
89	Monte Carlo studies of the thermodynamics and kinetics of reduced protein models: Application to small helical, β, and α/β proteins. Journal of Chemical Physics, 1998, 108, 2608-2617.	1.2	45
90	Reduced Protein Models and their Application to the Protein Folding Problem. Journal of Biomolecular Structure and Dynamics, 1998, 16, 381-396.	2.0	19

#	Article	IF	Citations
91	Assembly of protein structure from sparse experimental data: An efficient Monte Carlo model. Proteins: Structure, Function and Bioinformatics, 1998, 32, 475-494.	1.5	7
92	Protein Structure Prediction in the Post Genomic Era. , 1998, , .		0
93	Determinants of secondary structure of polypeptide chains: Interplay between short range and burial interactions. Journal of Chemical Physics, 1997, 107, 953-964.	1.2	17
94	MONSSTER: a method for folding globular proteins with a small number of distance restraints. Journal of Molecular Biology, 1997, 265, 217-241.	2.0	257
95	Derivation and testing of pair potentials for protein folding. When is the quasichemical approximation correct?. Protein Science, 1997, 6, 676-688.	3.1	182
96	Algorithm for rapid reconstruction of protein backbone from alpha carbon coordinates. Journal of Computational Chemistry, 1997, 18, 80-85.	1.5	35
97	A method for the prediction of surface â€œUâ€•turns and transglobular connections in small proteins. , 1997, 27, 290-308.		28
98	Improved method for prediction of protein backbone U-turn positions and major secondary structural elements between U-turns. , 1997, 29, 443-460.		8
99	Folding simulations and computer redesign of protein A three-helix bundle motifs. Proteins: Structure, Function and Bioinformatics, 1996, 25, 286-299.	1.5	16
100	On the origin of the cooperativity of protein folding: Implications from model simulations. Proteins: Structure, Function and Bioinformatics, 1996, 26, 271-287.	1.5	98
101	On the origin of the cooperativity of protein folding: Implications from model simulations. , 1996, 26, 271.		1
102	Are proteins ideal mixtures of amino acids? Analysis of energy parameter sets. Protein Science, 1995, 4, 2107-2117.	3.1	146
103	Computer design of idealized Î²â€•motifs. Journal of Chemical Physics, 1995, 103, 10286-10297.	1.2	33
104	A reduced model of short range interactions in polypeptide chains. Journal of Chemical Physics, 1995, 103, 4312-4323.	1.2	39
105	A simple technique to estimate partition functions and equilibrium constants from Monte Carlo simulations. Journal of Chemical Physics, 1995, 102, 6189-6193.	1.2	12
106	Neural network system for the evaluation of side-chain packing in protein structures. Protein Engineering, Design and Selection, 1995, 8, 225-236.	1.0	19
107	Monte carlo simulations of protein folding. I. Lattice model and interaction scheme. Proteins: Structure, Function and Bioinformatics, 1994, 18, 338-352.	1.5	282
108	Monte carlo simulations of protein folding. II. Application to protein A, ROP, and crambin. Proteins: Structure, Function and Bioinformatics, 1994, 18, 353-366.	1.5	148

#	ARTICLE	IF	CITATIONS
109	Dynamics of star branched polymers in a matrix of linear chains â€" a Monte Carlo study. Macromolecular Theory and Simulations, 1994, 3, 715-729.	0.6	21
110	Computer simulation of the folding of coiled coils. Journal of Chemical Physics, 1994, 100, 2267-2276.	1.2	16
111	Lattice representations of globular proteins: How good are they?. Journal of Computational Chemistry, 1993, 14, 1194-1202.	1.5	89
112	Insertion of peptide chains into lipid membranes: An off-lattice Monte Carlo dynamics model. Proteins: Structure, Function and Bioinformatics, 1993, 15, 10-25.	1.5	130
113	Computer modeling and folding of four-helix bundles. Proteins: Structure, Function and Bioinformatics, 1993, 16, 8-28.	1.5	39
114	A lattice dynamics study of a Langmuir monolayer of monounsaturated fatty acids. Journal of Chemical Physics, 1993, 98, 7581-7587.	1.2	23
115	A general method for the prediction of the three dimensional structure and folding pathway of globular proteins: Application to designed helical proteins. Journal of Chemical Physics, 1993, 98, 7420-7433.	1.2	192
116	Discretized model of proteins. I. Monte Carlo study of cooperativity in homopolypeptides. Journal of Chemical Physics, 1992, 97, 9412-9426.	1.2	118
117	Efficient algorithm for the reconstruction of a protein backbone from the ?-carbon coordinates. Journal of Computational Chemistry, 1992, 13, 443-456.	1.5	49
118	Monte Carlo Approaches to the Protein Folding Problem. Advances in Chemical Physics, 0, , 203-242.	0.3	5