

Andrej Å ali

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7389172/publications.pdf>

Version: 2024-02-01

282
papers

68,875
citations

1994

101
h-index

751

250
g-index

309
all docs

309
docs citations

309
times ranked

72216
citing authors

#	ARTICLE	IF	CITATIONS
1	Comparative Protein Modelling by Satisfaction of Spatial Restraints. <i>Journal of Molecular Biology</i> , 1993, 234, 779-815.	4.2	11,892
2	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. <i>Nature</i> , 2020, 583, 459-468.	27.8	3,542
3	Comparative Protein Structure Modeling Using Modeller. <i>Current Protocols in Bioinformatics</i> , 2006, 15, Unit-5.6.	25.8	2,858
4	Comparative Protein Structure Modeling of Genes and Genomes. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 2000, 29, 291-325.	18.3	2,811
5	Comparative Protein Structure Modeling Using MODELLER. <i>Current Protocols in Bioinformatics</i> , 2016, 54, 5.6.1-5.6.37.	25.8	2,248
6	Statistical potential for assessment and prediction of protein structures. <i>Protein Science</i> , 2006, 15, 2507-2524.	7.6	2,104
7	Modeling of loops in protein structures. <i>Protein Science</i> , 2000, 9, 1753-1773.	7.6	1,895
8	Modeller: Generation and Refinement of Homology-Based Protein Structure Models. <i>Methods in Enzymology</i> , 2003, 374, 461-491.	1.0	1,469
9	Protein Structure Prediction and Structural Genomics. <i>Science</i> , 2001, 294, 93-96.	12.6	1,445
10	Protein Structure Modeling with MODELLER. <i>Methods in Molecular Biology</i> , 2008, 426, 145-159.	0.9	1,187
11	Comparative Protein Structure Modeling Using MODELLER. <i>Current Protocols in Protein Science</i> , 2007, 50, Unit 2.9.	2.8	1,056
12	Evaluation of comparative protein modeling by MODELLER. <i>Proteins: Structure, Function and Bioinformatics</i> , 1995, 23, 318-326.	2.6	1,035
13	The molecular architecture of the nuclear pore complex. <i>Nature</i> , 2007, 450, 695-701.	27.8	947
14	RCSB Protein Data Bank: powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering and energy sciences. <i>Nucleic Acids Research</i> , 2021, 49, D437-D451.	14.5	918
15	Comparative Protein Structure Modeling Using MODELLER. <i>Current Protocols in Bioinformatics</i> , 2014, 47, 5.6.1-32.	25.8	860
16	Insights into Secondary Metabolism from a Global Analysis of Prokaryotic Biosynthetic Gene Clusters. <i>Cell</i> , 2014, 158, 412-421.	28.9	801
17	Protein Folding: A Perspective from Theory and Experiment. <i>Angewandte Chemie - International Edition</i> , 1998, 37, 868-893.	13.8	778
18	ModLoop: automated modeling of loops in protein structures. <i>Bioinformatics</i> , 2003, 19, 2500-2501.	4.1	707

#	ARTICLE	IF	CITATIONS
19	Global landscape of HIVâ€‘human protein complexes. <i>Nature</i> , 2012, 481, 365-370.	27.8	651
20	Protein Structure Modeling with MODELLER. <i>Methods in Molecular Biology</i> , 2014, 1137, 1-15.	0.9	516
21	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. <i>Science</i> , 2020, 370, .	12.6	508
22	ModBase, a database of annotated comparative protein structure models, and associated resources. <i>Nucleic Acids Research</i> , 2011, 39, D465-D474.	14.5	506
23	UCSF Chimera, MODELLER, and IMP: An integrated modeling system. <i>Journal of Structural Biology</i> , 2012, 179, 269-278.	2.8	506
24	Determining the architectures of macromolecular assemblies. <i>Nature</i> , 2007, 450, 683-694.	27.8	499
25	The molecular sociology of the cell. <i>Nature</i> , 2007, 450, 973-982.	27.8	497
26	Accurate SAXS Profile Computation and its Assessment by Contrast Variation Experiments. <i>Biophysical Journal</i> , 2013, 105, 962-974.	0.5	489
27	FoXS: a web server for rapid computation and fitting of SAXS profiles. <i>Nucleic Acids Research</i> , 2010, 38, W540-W544.	14.5	474
28	From words to literature in structural proteomics. <i>Nature</i> , 2003, 422, 216-225.	27.8	473
29	Comparative Protein Structure Modeling Using MODELLER. <i>Current Protocols in Protein Science</i> , 2016, 86, 2.9.1-2.9.37.	2.8	471
30	Putting the Pieces Together: Integrative Modeling Platform Software for Structure Determination of Macromolecular Assemblies. <i>PLoS Biology</i> , 2012, 10, e1001244.	5.6	469
31	Structure of the 80S Ribosome from <i>Saccharomyces cerevisiae</i> â€‘trNA-Ribosome and Subunit-Subunit Interactions. <i>Cell</i> , 2001, 107, 373-386.	28.9	462
32	Integrative structure and functional anatomy of a nuclear pore complex. <i>Nature</i> , 2018, 555, 475-482.	27.8	435
33	FoXS, FoXSDock and MultiFoXS: Single-state and multi-state structural modeling of proteins and their complexes based on SAXS profiles. <i>Nucleic Acids Research</i> , 2016, 44, W424-W429.	14.5	427
34	Molecular architecture of the 26S proteasome holocomplex determined by an integrative approach. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 1380-1387.	7.1	422
35	Tools for comparative protein structure modeling and analysis. <i>Nucleic Acids Research</i> , 2003, 31, 3375-3380.	14.5	406
36	Protein Structure Modeling with MODELLER. <i>Methods in Molecular Biology</i> , 2017, 1654, 39-54.	0.9	376

#	ARTICLE	IF	CITATIONS
37	Structural genomics: beyond the Human Genome Project. <i>Nature Genetics</i> , 1999, 23, 151-157.	21.4	369
38	Architecture of the Protein-Conducting Channel Associated with the Translating 80S Ribosome. <i>Cell</i> , 2001, 107, 361-372.	28.9	368
39	Components of Coated Vesicles and Nuclear Pore Complexes Share a Common Molecular Architecture. <i>PLoS Biology</i> , 2004, 2, e380.	5.6	357
40	Simple rules for passive diffusion through the nuclear pore complex. <i>Journal of Cell Biology</i> , 2016, 215, 57-76.	5.2	337
41	Protein Structure Fitting and Refinement Guided by Cryo-EM Density. <i>Structure</i> , 2008, 16, 295-307.	3.3	334
42	Vif hijacks CBF- β to degrade APOBEC3G and promote HIV-1 infection. <i>Nature</i> , 2012, 481, 371-375.	27.8	312
43	Statistical potentials for fold assessment. <i>Protein Science</i> , 2002, 11, 430-448.	7.6	304
44	Advances in comparative protein-structure modelling. <i>Current Opinion in Structural Biology</i> , 1997, 7, 206-214.	5.7	289
45	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. <i>Nature Chemical Biology</i> , 2011, 7, 769-778.	8.0	285
46	Comparative protein structure modeling by iterative alignment, model building and model assessment. <i>Nucleic Acids Research</i> , 2003, 31, 3982-3992.	14.5	277
47	Derivation of rules for comparative protein modeling from a database of protein structure alignments. <i>Protein Science</i> , 1994, 3, 1582-1596.	7.6	275
48	ModBase, a database of annotated comparative protein structure models and associated resources. <i>Nucleic Acids Research</i> , 2014, 42, D336-D346.	14.5	275
49	Study of the Structural Dynamics of the E. coli 70S Ribosome Using Real-Space Refinement. <i>Cell</i> , 2003, 113, 789-801.	28.9	273
50	Crystal Structure of the β Subunit of the Clamp-Loader Complex of E. coli DNA Polymerase III. <i>Cell</i> , 1997, 91, 335-345.	28.9	268
51	MODBASE: a database of annotated comparative protein structure models and associated resources. <i>Nucleic Acids Research</i> , 2006, 34, D291-D295.	14.5	265
52	A structural perspective on protein-protein interactions. <i>Current Opinion in Structural Biology</i> , 2004, 14, 313-324.	5.7	260
53	MODBASE, a database of annotated comparative protein structure models, and associated resources. <i>Nucleic Acids Research</i> , 2004, 32, 217D-222.	14.5	256
54	Nuclear Import Receptor Inhibits Phase Separation of FUS through Binding to Multiple Sites. <i>Cell</i> , 2018, 173, 693-705.e22.	28.9	253

#	ARTICLE	IF	CITATIONS
55	Simple fold composition and modular architecture of the nuclear pore complex. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 2172-2177.	7.1	243
56	Integrative Structural Biology. Science, 2013, 339, 913-915.	12.6	216
57	Evaluation of comparative protein structure modeling by MODELLER-3. Proteins: Structure, Function and Bioinformatics, 1997, 29, 50-58.	2.6	207
58	2017 publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution: an update. Acta Crystallographica Section D: Structural Biology, 2017, 73, 710-728.	2.3	205
59	Integrating Diverse Data for Structure Determination of Macromolecular Assemblies. Annual Review of Biochemistry, 2008, 77, 443-477.	11.1	204
60	LS-SNP: large-scale annotation of coding non-synonymous SNPs based on multiple information sources. Bioinformatics, 2005, 21, 2814-2820.	4.1	202
61	Crystal structure of a eukaryotic phosphate transporter. Nature, 2013, 496, 533-536.	27.8	202
62	Principles for Integrative Structural Biology Studies. Cell, 2019, 177, 1384-1403.	28.9	201
63	Evidence for a Shared Nuclear Pore Complex Architecture That Is Conserved from the Last Common Eukaryotic Ancestor. Molecular and Cellular Proteomics, 2009, 8, 2119-2130.	3.8	200
64	Protein structure modeling for structural genomics. Nature Structural Biology, 2000, 7, 986-990.	9.7	199
65	Comparative Protein Structure Modeling: Introduction and Practical Examples with Modeller. , 2000, 143, 97-129.		193
66	Molecular Architecture of the 40Sâ€¦eIF1â€¦eIF3 Translation Initiation Complex. Cell, 2014, 158, 1123-1135.	28.9	193
67	CryptoSite: Expanding the Druggable Proteome by Characterization and Prediction of Cryptic Binding Sites. Journal of Molecular Biology, 2016, 428, 709-719.	4.2	190
68	Alignment of protein sequences by their profiles. Protein Science, 2004, 13, 1071-1087.	7.6	184
69	Opportunities and Challenges in Building a Spatiotemporal Multi-scale Model of the Human Pancreatic Î² Cell. Cell, 2018, 173, 11-19.	28.9	179
70	Function of human Rh based on structure of RhCG at 2.1Å. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9638-9643.	7.1	178
71	Role of organic cation transporter 3 (SLC22A3) and its missense variants in the pharmacologic action of metformin. Pharmacogenetics and Genomics, 2010, 20, 687-699.	1.5	175
72	Structure-based ligand discovery for the Large-neutral Amino Acid Transporter 1, LAT-1. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 5480-5485.	7.1	173

#	ARTICLE	IF	CITATIONS
73	PIBASE: a comprehensive database of structurally defined protein interfaces. <i>Bioinformatics</i> , 2005, 21, 1901-1907.	4.1	169
74	The Enzyme Function Initiative. <i>Biochemistry</i> , 2011, 50, 9950-9962.	2.5	169
75	Structural genomics: A pipeline for providing structures for the biologist. <i>Protein Science</i> , 2002, 11, 723-738.	7.6	168
76	A Systematic Computational Analysis of Biosynthetic Gene Cluster Evolution: Lessons for Engineering Biosynthesis. <i>PLoS Computational Biology</i> , 2014, 10, e1004016.	3.2	164
77	A composite score for predicting errors in protein structure models. <i>Protein Science</i> , 2006, 15, 1653-1666.	7.6	160
78	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , 2015, 23, 1156-1167.	3.3	159
79	Multiple Conformations of <i>E. coli</i> Hsp90 in Solution: Insights into the Conformational Dynamics of Hsp90. <i>Structure</i> , 2008, 16, 755-765.	3.3	154
80	MODBASE, a database of annotated comparative protein structure models and associated resources. <i>Nucleic Acids Research</i> , 2009, 37, D347-D354.	14.5	154
81	Structure-based model of allostery predicts coupling between distant sites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 4875-4880.	7.1	153
82	Structural Characterization by Cross-linking Reveals the Detailed Architecture of a Coatomer-related Heptameric Module from the Nuclear Pore Complex. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 2927-2943.	3.8	152
83	Structural genomics of protein phosphatases. <i>Journal of Structural and Functional Genomics</i> , 2007, 8, 121-140.	1.2	148
84	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 323-348.	2.6	148
85	Structure and Function of the Nuclear Pore Complex Cytoplasmic mRNA Export Platform. <i>Cell</i> , 2016, 167, 1215-1228.e25.	28.9	148
86	Evolution of modular intraflagellar transport from a coatomer-like progenitor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 6943-6948.	7.1	144
87	Comprehensive Molecular Structure of the Eukaryotic Ribosome. <i>Structure</i> , 2009, 17, 1591-1604.	3.3	140
88	Integration of Small-Angle X-Ray Scattering Data into Structural Modeling of Proteins and Their Assemblies. <i>Journal of Molecular Biology</i> , 2008, 382, 1089-1106.	4.2	139
89	How well can the accuracy of comparative protein structure models be predicted?. <i>Protein Science</i> , 2008, 17, 1881-1893.	7.6	138
90	Host-pathogen protein interactions predicted by comparative modeling. <i>Protein Science</i> , 2007, 16, 2585-2596.	7.6	136

#	ARTICLE	IF	CITATIONS
91	Molecular architecture of the yeast Mediator complex. <i>ELife</i> , 2015, 4, .	6.0	136
92	Molecular Docking Screens Using Comparative Models of Proteins. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2512-2527.	5.4	132
93	Discovery of Potent, Selective Multidrug and Toxin Extrusion Transporter 1 (MATE1, SLC47A1) Inhibitors Through Prescription Drug Profiling and Computational Modeling. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 781-795.	6.4	131
94	Structure-based discovery of prescription drugs that interact with the norepinephrine transporter, NET. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 15810-15815.	7.1	120
95	Optimized atomic statistical potentials: assessment of protein interfaces and loops. <i>Bioinformatics</i> , 2013, 29, 3158-3166.	4.1	119
96	Inferential Optimization for Simultaneous Fitting of Multiple Components into a CryoEM Map of Their Assembly. <i>Journal of Molecular Biology</i> , 2009, 388, 180-194.	4.2	117
97	Packaging of Proteases and Proteoglycans in the Granules of Mast Cells and Other Hematopoietic Cells. <i>Journal of Biological Chemistry</i> , 1995, 270, 19524-19531.	3.4	116
98	A Conserved Coatmer-related Complex Containing Sec13 and Seh1 Dynamically Associates With the Vacuole in <i>Saccharomyces cerevisiae</i> . <i>Molecular and Cellular Proteomics</i> , 2011, 10, M110.006478.	3.8	115
99	Ring closure activates yeast $\hat{1}^3$ TuRC for species-specific microtubule nucleation. <i>Nature Structural and Molecular Biology</i> , 2015, 22, 132-137.	8.2	115
100	MODBASE, a database of annotated comparative protein structure models. <i>Nucleic Acids Research</i> , 2002, 30, 255-259.	14.5	114
101	A strategy for dissecting the architectures of native macromolecular assemblies. <i>Nature Methods</i> , 2015, 12, 1135-1138.	19.0	113
102	Structure- \hat{e} function mapping of a heptameric module in the nuclear pore complex. <i>Journal of Cell Biology</i> , 2012, 196, 419-434.	5.2	110
103	Subnanometer-resolution electron cryomicroscopy-based domain models for the cytoplasmic region of skeletal muscle RyR channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 9610-9615.	7.1	106
104	Recovering a Representative Conformational Ensemble from Underdetermined Macromolecular Structural Data. <i>Journal of the American Chemical Society</i> , 2013, 135, 16595-16609.	13.7	106
105	Refinement of Protein Structures by Iterative Comparative Modeling and CryoEM Density Fitting. <i>Journal of Molecular Biology</i> , 2006, 357, 1655-1668.	4.2	104
106	Evolution and Physics in Comparative Protein Structure Modeling. <i>Accounts of Chemical Research</i> , 2002, 35, 413-421.	15.6	103
107	Structure-Based Assessment of Missense Mutations in Human BRCA1. <i>Cancer Research</i> , 2004, 64, 3790-3797.	0.9	103
108	Cys-Scanning Disulfide Crosslinking and Bayesian Modeling Probe the Transmembrane Signaling Mechanism of the Histidine Kinase, PhoQ. <i>Structure</i> , 2014, 22, 1239-1251.	3.3	103

#	ARTICLE	IF	CITATIONS
109	Fold assessment for comparative protein structure modeling. <i>Protein Science</i> , 2007, 16, 2412-2426.	7.6	101
110	A phosphotyrosine switch regulates organic cation transporters. <i>Nature Communications</i> , 2016, 7, 10880.	12.8	100
111	Comparison of human solute carriers. <i>Protein Science</i> , 2010, 19, 412-428.	7.6	99
112	Atlas of the Radical SAM Superfamily: Divergent Evolution of Function Using a "Plug and Play" Domain. <i>Methods in Enzymology</i> , 2018, 606, 1-71.	1.0	99
113	Immunoglobulin motif DNA recognition and heterodimerization of the PEBP2/CBF Runt domain. <i>Nature Structural Biology</i> , 1999, 6, 615-619.	9.7	97
114	Macromolecular docking restrained by a small angle X-ray scattering profile. <i>Journal of Structural Biology</i> , 2011, 173, 461-471.	2.8	97
115	Reliability of Assessment of Protein Structure Prediction Methods. <i>Structure</i> , 2002, 10, 435-440.	3.3	95
116	Molecular Details Underlying Dynamic Structures and Regulation of the Human 26S Proteasome. <i>Molecular and Cellular Proteomics</i> , 2017, 16, 840-854.	3.8	93
117	Structural characterization of components of protein assemblies by comparative modeling and electron cryo-microscopy. <i>Journal of Structural Biology</i> , 2005, 149, 191-203.	2.8	92
118	Integrative structural modeling with small angle X-ray scattering profiles. <i>BMC Structural Biology</i> , 2012, 12, 17.	2.3	92
119	High-resolution network biology: connecting sequence with function. <i>Nature Reviews Genetics</i> , 2013, 14, 865-879.	16.3	92
120	Integrative structure modeling with the Integrative Modeling Platform. <i>Protein Science</i> , 2018, 27, 245-258.	7.6	92
121	Mechanism of lid closure in the eukaryotic chaperonin TRiC/CCT. <i>Nature Structural and Molecular Biology</i> , 2008, 15, 746-753.	8.2	91
122	Uncertainty in integrative structural modeling. <i>Current Opinion in Structural Biology</i> , 2014, 28, 96-104.	5.7	91
123	Architecture of the Human and Yeast General Transcription and DNA Repair Factor TFIH. <i>Molecular Cell</i> , 2015, 59, 794-806.	9.7	91
124	On a bender "BARs, ESCRTs, COPs, and finally getting your coat. <i>Journal of Cell Biology</i> , 2011, 193, 963-972.	5.2	88
125	Comprehensive structure and functional adaptations of the yeast nuclear pore complex. <i>Cell</i> , 2022, 185, 361-378.e25.	28.9	87
126	Slide-and-exchange mechanism for rapid and selective transport through the nuclear pore complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E2489-97.	7.1	85

#	ARTICLE	IF	CITATIONS
127	Molecular Modeling and Ligand Docking for Solute Carrier (SLC) Transporters. <i>Current Topics in Medicinal Chemistry</i> , 2013, 13, 843-856.	2.1	85
128	PDB-Dev: a Prototype System for Depositing Integrative/Hybrid Structural Models. <i>Structure</i> , 2017, 25, 1317-1318.	3.3	84
129	<scp>RCSB</scp> Protein Data Bank: Celebrating 50 years of the <scp>PDB</scp> with new tools for understanding and visualizing biological macromolecules in <scp>3D</scp>. <i>Protein Science</i> , 2022, 31, 187-208.	7.6	84
130	Finding Cures for Tropical Diseases: Is Open Source an Answer?. <i>PLoS Medicine</i> , 2004, 1, e56.	8.4	82
131	Alignment of multiple protein structures based on sequence and structure features. <i>Protein Engineering, Design and Selection</i> , 2009, 22, 569-574.	2.1	82
132	The proteasome-interacting Ecm29 protein disassembles the 26S proteasome in response to oxidative stress. <i>Journal of Biological Chemistry</i> , 2017, 292, 16310-16320.	3.4	82
133	Development of a Prototype System for Archiving Integrative/Hybrid Structure Models of Biological Macromolecules. <i>Structure</i> , 2018, 26, 894-904.e2.	3.3	81
134	Protein Structure Modeling with MODELLER. <i>Methods in Molecular Biology</i> , 2021, 2199, 239-255.	0.9	81
135	A method for integrative structure determination of protein-protein complexes. <i>Bioinformatics</i> , 2012, 28, 3282-3289.	4.1	78
136	Modeling mutations in protein structures. <i>Protein Science</i> , 2007, 16, 2030-2041.	7.6	77
137	Report of the wwPDB Small-Angle Scattering Task Force: Data Requirements for Biomolecular Modeling and the PDB. <i>Structure</i> , 2013, 21, 875-881.	3.3	77
138	LigBase: a database of families of aligned ligand binding sites in known protein sequences and structures. <i>Bioinformatics</i> , 2002, 18, 200-201.	4.1	76
139	The structural dynamics of macromolecular processes. <i>Current Opinion in Cell Biology</i> , 2009, 21, 97-108.	5.4	74
140	Combining electron microscopy and comparative protein structure modeling. <i>Current Opinion in Structural Biology</i> , 2005, 15, 578-585.	5.7	73
141	Statistical Potential for Modeling and Ranking of Protein-Ligand Interactions. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 3078-3092.	5.4	69
142	Comparative Protein Structure Modeling and its Applications to Drug Discovery. <i>Annual Reports in Medicinal Chemistry</i> , 2004, 39, 259-276.	0.9	68
143	Assessing Exhaustiveness of Stochastic Sampling for Integrative Modeling of Macromolecular Structures. <i>Biophysical Journal</i> , 2017, 113, 2344-2353.	0.5	68
144	Integrative Structure-Function Mapping of the Nucleoporin Nup133 Suggests a Conserved Mechanism for Membrane Anchoring of the Nuclear Pore Complex. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 2911-2926.	3.8	67

#	ARTICLE	IF	CITATIONS
145	Immunoproteasome functions explained by divergence in cleavage specificity and regulation. <i>ELife</i> , 2017, 6, .	6.0	66
146	Integrative Structure Modeling of Macromolecular Assemblies from Proteomics Data. <i>Molecular and Cellular Proteomics</i> , 2010, 9, 1689-1702.	3.8	64
147	Coordinating the impact of structural genomics on the human α -helical transmembrane proteome. <i>Nature Structural and Molecular Biology</i> , 2013, 20, 135-138.	8.2	64
148	Molecular Architecture and Function of the SEA Complex, a Modulator of the TORC1 Pathway. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 2855-2870.	3.8	64
149	Determining macromolecular assembly structures by molecular docking and fitting into an electron density map. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 3205-3211.	2.6	63
150	Prediction of protease substrates using sequence and structure features. <i>Bioinformatics</i> , 2010, 26, 1714-1722.	4.1	61
151	Molecular Architecture of the Major Membrane Ring Component of the Nuclear Pore Complex. <i>Structure</i> , 2017, 25, 434-445.	3.3	61
152	Functional links between proteins. <i>Nature</i> , 1999, 402, 23-26.	27.8	60
153	Outcome of a Workshop on Archiving Structural Models of Biological Macromolecules. <i>Structure</i> , 2006, 14, 1211-1217.	3.3	60
154	Cross-activating c-Met/ α 21 integrin complex drives metastasis and invasive resistance in cancer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E8685-E8694.	7.1	60
155	High-Throughput Computational and Experimental Techniques in Structural Genomics. <i>Genome Research</i> , 2004, 14, 2145-2154.	5.5	59
156	Structure of Complement C3(H2O) Revealed By Quantitative Cross-Linking/Mass Spectrometry And Modeling. <i>Molecular and Cellular Proteomics</i> , 2016, 15, 2730-2743.	3.8	59
157	Variable gap penalty for protein sequenceâ€“structure alignment. <i>Protein Engineering, Design and Selection</i> , 2006, 19, 129-133.	2.1	58
158	Evolutionary constraints on structural similarity in orthologs and paralogs. <i>Protein Science</i> , 2009, 18, 1306-1315.	7.6	58
159	Scoring Largeâ€“Scale Affinity Purification Mass Spectrometry Datasets with MiST. <i>Current Protocols in Bioinformatics</i> , 2015, 49, 8.19.1-8.19.16.	25.8	58
160	Discovery of Competitive and Noncompetitive Ligands of the Organic Cation Transporter 1 (OCT1); Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	6.4	58
161	Structural dynamics of the human COP9 signalosome revealed by cross-linking mass spectrometry and integrative modeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 4088-4098.	7.1	58
162	Functional Impact of Missense Variants in BRCA1 Predicted by Supervised Learning. <i>PLoS Computational Biology</i> , 2007, 3, e26.	3.2	57

#	ARTICLE	IF	CITATIONS
163	Protein complex compositions predicted by structural similarity. <i>Nucleic Acids Research</i> , 2006, 34, 2943-2952.	14.5	56
164	Selecting Optimum Eukaryotic Integral Membrane Proteins for Structure Determination by Rapid Expression and Solubilization Screening. <i>Journal of Molecular Biology</i> , 2009, 385, 820-830.	4.2	53
165	Structure, Dynamics, Evolution, and Function of a Major Scaffold Component in the Nuclear Pore Complex. <i>Structure</i> , 2013, 21, 560-571.	3.3	53
166	A Residue-Resolved Bayesian Approach to Quantitative Interpretation of Hydrogen-Deuterium Exchange from Mass Spectrometry: Application to Characterizing Protein-Ligand Interactions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3493-3501.	2.6	52
167	The optimal size of a globular protein domain: A simple sphere-packing model. <i>Chemical Physics Letters</i> , 2005, 405, 224-228.	2.6	51
168	Toward an Integrated Structural Model of the 26S Proteasome. <i>Molecular and Cellular Proteomics</i> , 2010, 9, 1666-1677.	3.8	50
169	Limits of Ligand Selectivity from Docking to Models: In Silico Screening for A1 Adenosine Receptor Antagonists. <i>PLoS ONE</i> , 2012, 7, e49910.	2.5	50
170	Bayesian Weighing of Electron Cryo-Microscopy Data for Integrative Structural Modeling. <i>Structure</i> , 2019, 27, 175-188.e6.	3.3	50
171	High Selectivity of the $\hat{3}$ -Aminobutyric Acid Transporter 2 (GAT-2, SLC6A13) Revealed by Structure-based Approach. <i>Journal of Biological Chemistry</i> , 2012, 287, 37745-37756.	3.4	49
172	New York-Structural GenomiX Research Consortium (NYSGXRC): A Large Scale Center for the Protein Structure Initiative. <i>Journal of Structural and Functional Genomics</i> , 2005, 6, 225-232.	1.2	48
173	Impact of Mutations on the Allosteric Conformational Equilibrium. <i>Journal of Molecular Biology</i> , 2013, 425, 647-661.	4.2	48
174	Importin-9 wraps around the H2A-H2B core to act as nuclear importer and histone chaperone. <i>ELife</i> , 2019, 8, .	6.0	47
175	Regulatory Elements within the Prodomain of Falcipain-2, a Cysteine Protease of the Malaria Parasite <i>Plasmodium falciparum</i> . <i>PLoS ONE</i> , 2009, 4, e5694.	2.5	46
176	Classifying Variants of Undetermined Significance in BRCA2 with Protein Likelihood Ratios. <i>Cancer Informatics</i> , 2008, 6, CIN.S618.	1.9	45
177	Elucidating the Mechanism of Substrate Recognition by the Bacterial Hsp90 Molecular Chaperone. <i>Journal of Molecular Biology</i> , 2014, 426, 2393-2404.	4.2	45
178	From integrative structural biology to cell biology. <i>Journal of Biological Chemistry</i> , 2021, 296, 100743.	3.4	45
179	Assembly of macromolecular complexes by satisfaction of spatial restraints from electron microscopy images. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 18821-18826.	7.1	44
180	The molecular architecture of the yeast spindle pole body core determined by Bayesian integrative modeling. <i>Molecular Biology of the Cell</i> , 2017, 28, 3298-3314.	2.1	44

#	ARTICLE	IF	CITATIONS
181	Structural basis of CD4 downregulation by HIV-1 Nef. <i>Nature Structural and Molecular Biology</i> , 2020, 27, 822-828.	8.2	44
182	The Overlap of Small Molecule and Protein Binding Sites within Families of Protein Structures. <i>PLoS Computational Biology</i> , 2010, 6, e1000668.	3.2	43
183	Insights into HIV-1 proviral transcription from integrative structure and dynamics of the Tat:AFF4:P-TEFb:TAR complex. <i>ELife</i> , 2016, 5, .	6.0	43
184	Regulation of Rvb1/Rvb2 by a Domain within the INO80 Chromatin Remodeling Complex Implicates the Yeast Rvbs as Protein Assembly Chaperones. <i>Cell Reports</i> , 2017, 19, 2033-2044.	6.4	43
185	Localization of protein-binding sites within families of proteins. <i>Protein Science</i> , 2005, 14, 2350-2360.	7.6	40
186	Minimalist Representations and the Importance of Nearest Neighbor Effects in Protein Folding Simulations. <i>Journal of Molecular Biology</i> , 2006, 363, 835-857.	4.2	40
187	Modeling of Proteins and Their Assemblies with the Integrative Modeling Platform. <i>Methods in Molecular Biology</i> , 2014, 1091, 277-295.	0.9	40
188	Structural Modeling of Protein Interactions by Analogy: Application to PSD-95. <i>PLoS Computational Biology</i> , 2006, 2, e153.	3.2	39
189	Topological Models of Heteromeric Protein Assemblies from Mass Spectrometry: Application to the Yeast eIF3:eIF5 Complex. <i>Chemistry and Biology</i> , 2015, 22, 117-128.	6.0	38
190	Crystallographic Conformers of Actin in a Biologically Active Bundle of Filaments. <i>Journal of Molecular Biology</i> , 2008, 375, 331-336.	4.2	37
191	Molecular Architecture of Photoreceptor Phosphodiesterase Elucidated by Chemical Cross-Linking and Integrative Modeling. <i>Journal of Molecular Biology</i> , 2014, 426, 3713-3728.	4.2	37
192	The AnnoLite and AnnoLyze programs for comparative annotation of protein structures. <i>BMC Bioinformatics</i> , 2007, 8, S4.	2.6	36
193	Visualizing subcellular rearrangements in intact $\hat{1}^2$ cells using soft x-ray tomography. <i>Science Advances</i> , 2020, 6, .	10.3	36
194	Highly synergistic combinations of nanobodies that target SARS-CoV-2 and are resistant to escape. <i>ELife</i> , 2021, 10, .	6.0	36
195	Detection of homologous proteins by an intermediate sequence search. <i>Protein Science</i> , 2004, 13, 54-62.	7.6	35
196	Integrative analysis reveals unique structural and functional features of the Smc5/6 complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	35
197	Modeling Biological Complexes Using Integrative Modeling Platform. <i>Methods in Molecular Biology</i> , 2019, 2022, 353-377.	0.9	34
198	Prion Protein- β Antibody Complexes Characterized by Chromatography-Coupled Small-Angle X-Ray Scattering. <i>Biophysical Journal</i> , 2015, 109, 793-805.	0.5	33

#	ARTICLE	IF	CITATIONS
199	Assignment of Pterin Deaminase Activity to an Enzyme of Unknown Function Guided by Homology Modeling and Docking. <i>Journal of the American Chemical Society</i> , 2013, 135, 795-803.	13.7	32
200	Small-Molecule Allosteric Modulators of the Protein Kinase PDK1 from Structure-Based Docking. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 8285-8291.	6.4	32
201	Predicting CD4 T-cell epitopes based on antigen cleavage, MHCII presentation, and TCR recognition. <i>PLoS ONE</i> , 2018, 13, e0206654.	2.5	31
202	Architecture of Pol II(G) and molecular mechanism of transcription regulation by Gdown1. <i>Nature Structural and Molecular Biology</i> , 2018, 25, 859-867.	8.2	31
203	Using <i>Integrative Modeling Platform</i> to compute, validate, and archive a model of a protein complex structure. <i>Protein Science</i> , 2021, 30, 250-261.	7.6	31
204	EpCAM homo-oligomerization is not the basis for its role in cell-cell adhesion. <i>Scientific Reports</i> , 2018, 8, 13269.	3.3	30
205	Prediction of enzymatic pathways by integrative pathway mapping. <i>ELife</i> , 2018, 7, .	6.0	30
206	Determining Protein Complex Structures Based on a Bayesian Model of in Vivo Förster Resonance Energy Transfer (FRET) Data. <i>Molecular and Cellular Proteomics</i> , 2014, 13, 2812-2823.	3.8	29
207	Integrative structure and function of the yeast exocyst complex. <i>Protein Science</i> , 2020, 29, 1486-1501.	7.6	29
208	Structural Characterization of Assemblies from Overall Shape and Subcomplex Compositions. <i>Structure</i> , 2005, 13, 435-445.	3.3	27
209	MultiFit: a web server for fitting multiple protein structures into their electron microscopy density map. <i>Nucleic Acids Research</i> , 2011, 39, W167-W170.	14.5	27
210	Detecting remotely related proteins by their interactions and sequence similarity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 7151-7156.	7.1	26
211	Target selection and annotation for the structural genomics of the amidohydrolase and enolase superfamilies. <i>Journal of Structural and Functional Genomics</i> , 2009, 10, 107-125.	1.2	25
212	Assembly and Molecular Architecture of the Phosphoinositide 3-Kinase p85 β Homodimer. <i>Journal of Biological Chemistry</i> , 2015, 290, 30390-30405.	3.4	25
213	Enzymatic Deamination of the Epigenetic Base N ⁶ -Methyladenine. <i>Journal of the American Chemical Society</i> , 2011, 133, 2080-2083.	13.7	24
214	Genetic interaction mapping informs integrative structure determination of protein complexes. <i>Science</i> , 2020, 370, .	12.6	24
215	A Kernel for Open Source Drug Discovery in Tropical Diseases. <i>PLoS Neglected Tropical Diseases</i> , 2009, 3, e418.	3.0	23
216	Structure of β -tubulin small complex based on a cryo-EM map, chemical cross-links, and a remotely related structure. <i>Journal of Structural Biology</i> , 2016, 194, 303-310.	2.8	23

#	ARTICLE	IF	CITATIONS
217	Computational Discovery and Experimental Validation of Inhibitors of the Human Intestinal Transporter OATP2B1. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1402-1413.	5.4	23
218	CM1-driven assembly and activation of yeast $\hat{1}^3$ -tubulin small complex underlies microtubule nucleation. <i>ELife</i> , 2021, 10, .	6.0	23
219	Enhancer Reprogramming within Pre-existing Topologically Associated Domains Promotes TGF- $\hat{1}^2$ -Induced EMT and Cancer Metastasis. <i>Molecular Therapy</i> , 2020, 28, 2083-2095.	8.2	22
220	New system for archiving integrative structures. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 1486-1496.	2.3	22
221	Soft X-ray tomography to map and quantify organelle interactions at the mesoscale. <i>Structure</i> , 2022, 30, 510-521.e3.	3.3	22
222	Target practice. , 2001, 8, 482-484.		21
223	Localization of binding sites in protein structures by optimization of a composite scoring function. <i>Protein Science</i> , 2006, 15, 2366-2380.	7.6	21
224	Prediction of Substrates for Glutathione Transferases by Covalent Docking. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1687-1699.	5.4	20
225	Archiving and disseminating integrative structure models. <i>Journal of Biomolecular NMR</i> , 2019, 73, 385-398.	2.8	20
226	Crippling life support for SARS-CoV-2 and other viruses through synthetic lethality. <i>Journal of Cell Biology</i> , 2020, 219, .	5.2	20
227	Functional hot spots in human ATP- $\hat{1}$ binding cassette transporter nucleotide binding domains. <i>Protein Science</i> , 2010, 19, 2110-2121.	7.6	19
228	Bayesian metamodelling of complex biological systems across varying representations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	19
229	PharmGKB Submission Update: IV. PMT Submissions of Genetic Variations in ATP-Binding Cassette Transporters to the PharmGKB Network. <i>Pharmacological Reviews</i> , 2006, 58, 1-2.	16.0	18
230	Modeling of Proteins and Their Assemblies with the Integrative Modeling Platform. <i>Methods in Molecular Biology</i> , 2011, 781, 377-397.	0.9	18
231	Structure of the C- $\hat{1}$ terminal domain of <i>Saccharomyces cerevisiae</i> Nup133, a component of the nuclear pore complex. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 1672-1677.	2.6	16
232	Structure-Guided Discovery of New Deaminase Enzymes. <i>Journal of the American Chemical Society</i> , 2013, 135, 13927-13933.	13.7	16
233	Optimizing model representation for integrative structure determination of macromolecular assemblies. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 540-545.	7.1	16
234	^1H , ^{13}C , ^{15}N resonance assignments and fold verification of a circular permuted variant of the potent HIV-inactivating protein cyanovirin-N. <i>Journal of Biomolecular NMR</i> , 2001, 19, 289-290.	2.8	15

#	ARTICLE	IF	CITATIONS
235	Comparative Protein Structure Modeling. , 2005, , 831-860.		15
236	Discovery of a Cytokinin Deaminase. ACS Chemical Biology, 2011, 6, 1036-1040.	3.4	15
237	Human Concentrative Nucleoside Transporter 3 (hCNT3, SLC28A3) Forms a Cyclic Homotrimer. Biochemistry, 2017, 56, 3475-3483.	2.5	15
238	<i>SAXS Merge</i> : an automated statistical method to merge SAXS profiles using Gaussian processes. Journal of Synchrotron Radiation, 2014, 21, 203-208.	2.4	15
239	Prediction of Functionally Important Phospho-Regulatory Events in <i>Xenopus laevis</i> Oocytes. PLoS Computational Biology, 2015, 11, e1004362.	3.2	14
240	Reversible phosphorylation of cyclin T1 promotes assembly and stability of P-TEFb. ELife, 2021, 10, .	6.0	14
241	From systems to structure " using genetic data to model protein structures. Nature Reviews Genetics, 2022, 23, 342-354.	16.3	14
242	Soluble TREM2 inhibits secondary nucleation of A β 2 fibrillization and enhances cellular uptake of fibrillar A β 2. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	14
243	Structures of the autoproteolytic domain from the <i>Saccharomyces cerevisiae</i> nuclear pore complex component, Nup145. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1992-1998.	2.6	13
244	Glutamine Side Chain 13C α -18O as a Nonperturbative IR Probe of Amyloid Fibril Hydration and Assembly. Journal of the American Chemical Society, 2019, 141, 7320-7326.	13.7	13
245	A survey of integral α -helical membrane proteins. Journal of Structural and Functional Genomics, 2009, 10, 269-280.	1.2	12
246	Deamination of 6-Aminodeoxyfutasoline in Menaquinone Biosynthesis by Distantly Related Enzymes. Biochemistry, 2013, 52, 6525-6536.	2.5	12
247	Virtual Ligand Screening Against Comparative Protein Structure Models. Methods in Molecular Biology, 2012, 819, 105-126.	0.9	11
248	Reconstruction of 3D structures of MET antibodies from electron microscopy 2D class averages. PLoS ONE, 2017, 12, e0175758.	2.5	10
249	The Y β motif defines the structure-activity relationships of human 20S proteasome activators. Nature Communications, 2022, 13, 1226.	12.8	10
250	Clustering of disulfide-rich peptides provides scaffolds for hit discovery by phage display: application to interleukin-23. BMC Bioinformatics, 2016, 17, 481.	2.6	9
251	The active DNA-PK holoenzyme occupies a tensed state in a staggered synaptic complex. Structure, 2021, 29, 467-478.e6.	3.3	9
252	Structural Model of the Bilirubin Transmembrane Domain Supported by NMR and FRET Data. PLoS ONE, 2015, 10, e0135455.	2.5	8

#	ARTICLE	IF	CITATIONS
253	SSEThread: Integrative threading of the DNA-PKcs sequence based on data from chemical cross-linking and hydrogen deuterium exchange. <i>Progress in Biophysics and Molecular Biology</i> , 2019, 147, 92-102.	2.9	8
254	Atomic structure of the nuclear pore complex targeting domain of a Nup116 homologue from the yeast, <i>Candida glabrata</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 2110-2116.	2.6	7
255	Integration of software tools for integrative modeling of biomolecular systems. <i>Journal of Structural Biology</i> , 2022, 214, 107841.	2.8	7
256	Doublecortin engages the microtubule lattice through a cooperative binding mode involving its C-terminal domain. <i>ELife</i> , 2022, 11, .	6.0	7
257	Modeling Protein Structure from its Sequence. <i>Current Protocols in Bioinformatics</i> , 2003, 3, 5.1.1.	25.8	6
258	Integrative Structure Determination of Protein Assemblies by Satisfaction of Spatial Restraints. <i>Computational Biology</i> , 2008, , 99-114.	0.2	6
259	IMProv: A Resource for Cross-link-Driven Structure Modeling that Accommodates Protein Dynamics. <i>Molecular and Cellular Proteomics</i> , 2021, 20, 100139.	3.8	6
260	Global Protease Activity Profiling Identifies HER2-Driven Proteolysis in Breast Cancer. <i>ACS Chemical Biology</i> , 2021, 16, 712-723.	3.4	6
261	Macromolecular Assemblies Highlighted. <i>Structure</i> , 2005, 13, 339-341.	3.3	5
262	Protein Structure Modeling. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2009, , 139-151.	0.5	5
263	Auto-segmentation and time-dependent systematic analysis of mesoscale cellular structure in $\hat{1}^2$ -cells during insulin secretion. <i>PLoS ONE</i> , 2022, 17, e0265567.	2.5	5
264	Macromolecular Assembly Structures by Comparative Modeling and Electron Microscopy. <i>Methods in Molecular Biology</i> , 2011, 857, 331-350.	0.9	4
265	Characterization of an A3G-VifHIV-1-CRL5-CBF $\hat{1}^2$ Structure Using a Cross-linking Mass Spectrometry Pipeline for Integrative Modeling of Host-Pathogen Complexes. <i>Molecular and Cellular Proteomics</i> , 2021, 20, 100132.	3.8	4
266	Protein interactions and disease phenotypes in the ABC transporter superfamily. <i>Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing</i> , 2007, , 51-63.	0.7	4
267	Response to Paoli. <i>Nature Structural Biology</i> , 2001, 8, 745-745.	9.7	3
268	Mapping Polymerization and Allostery of Hemoglobin S Using Point Mutations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13058-13068.	2.6	3
269	Guinea Pig Prion Protein Supports Rapid Propagation of Bovine Spongiform Encephalopathy and Variant Creutzfeldt-Jakob Disease Prions. <i>Journal of Virology</i> , 2016, 90, 9558-9569.	3.4	3
270	The <i>EBF1-PDGFRB</i> T681I mutation is highly resistant to imatinib and dasatinib <i>in vitro</i> and detectable in clinical samples prior to treatment. <i>Haematologica</i> , 2021, 106, 2242-2245.	3.5	3

#	ARTICLE	IF	CITATIONS
271	Protein dynamics: From the native to the unfolded state and back again. <i>Molecular Engineering</i> , 1995, 5, 55-70.	0.2	1
272	Integrative Structure Determination of Protein Complexes by Inferred Structural Equivalence. <i>Biophysical Journal</i> , 2018, 114, 61a.	0.5	1
273	Structure Determination of Macromolecular Complexes by Experiment and Computation. <i>Nucleic Acids and Molecular Biology</i> , 2008, , 73-96.	0.2	1
274	A structural perspective on protein-protein interactions. <i>Current Opinion in Structural Biology</i> , 2004, 14, 313-313.	5.7	0
275	Response to "Predictable difficulty or difficulty to predict". <i>Protein Science</i> , 2011, 20, 4-5.	7.6	0
276	Editorial overview: Biophysical and molecular biological methods. <i>Current Opinion in Structural Biology</i> , 2016, 40, ix-xi.	5.7	0
277	Characterization of Protein Hubs by Inferring Interacting Motifs from Protein Interactions. <i>PLoS Computational Biology</i> , 2005, preprint, e178.	3.2	0
278	Stereochemical Criteria for Prediction of the Effects of Proline Mutations on Protein Stability. <i>PLoS Computational Biology</i> , 2005, preprint, e241.	3.2	0
279	Large scale analysis of synaptic phosphorylation and O-GlcNAcylation reveals complex interplay between these post-translational modifications. <i>FASEB Journal</i> , 2012, 26, 978.2.	0.5	0
280	Structure of the 80S Ribosome from <i>Saccharomyces cerevisiae</i> tRNA-Ribosome and Subunit-Subunit Interactions. <i>Journal of Hand Surgery Asian-Pacific Volume</i> , The, 2018, , 286-299.	0.4	0
281	Architecture of the Protein-Conducting Channel Associated with the Translating 80S Ribosome. <i>Journal of Hand Surgery Asian-Pacific Volume</i> , The, 2018, , 274-285.	0.4	0
282	Integrative structure determination of histones H3 and H4 using genetic interactions. <i>FEBS Journal</i> , 2023, 290, 2565-2575.	4.7	0