

# Kam Y J Zhang

## List of Publications by Year in descending order

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143  
papers

9,445  
citations

101384

36  
h-index

40881

93  
g-index

151  
all docs

151  
docs citations

151  
times ranked

12579  
citing authors

#	ARTICLE	IF	CITATIONS
1	Clinical efficacy of a RAF inhibitor needs broad target blockade in BRAF-mutant melanoma. <i>Nature</i> , 2010, 467, 596-599.	13.7	1,610
2	Discovery of a selective inhibitor of oncogenic B-Raf kinase with potent antimelanoma activity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 3041-3046.	3.3	1,206
3	Germline KRAS mutations cause Noonan syndrome. <i>Nature Genetics</i> , 2006, 38, 331-336.	9.4	670
4	Keynote review: Phosphodiesterase-4 as a therapeutic target. <i>Drug Discovery Today</i> , 2005, 10, 1503-1519.	3.2	604
5	Antimycin A mimics a cell-death-inducing Bcl-2 homology domain 3. <i>Nature Cell Biology</i> , 2001, 3, 183-191.	4.6	436
6	Structural Basis for the Activity of Drugs that Inhibit Phosphodiesterases. <i>Structure</i> , 2004, 12, 2233-2247.	1.6	360
7	A Glutamine Switch Mechanism for Nucleotide Selectivity by Phosphodiesterases. <i>Molecular Cell</i> , 2004, 15, 279-286.	4.5	271
8	Density modification for macromolecular phase improvement. <i>Progress in Biophysics and Molecular Biology</i> , 1999, 72, 245-270.	1.4	242
9	A family of phosphodiesterase inhibitors discovered by cocrystallography and scaffold-based drug design. <i>Nature Biotechnology</i> , 2005, 23, 201-207.	9.4	220
10	Design of a peptide-based subunit vaccine against novel coronavirus SARS-CoV-2. <i>Microbial Pathogenesis</i> , 2020, 145, 104236.	1.3	154
11	Crystal structure of <i>E. coli</i> $\hat{\Gamma}^2$ -carbonic anhydrase, an enzyme with an unusual pH-dependent activity. <i>Protein Science</i> , 2001, 10, 911-922.	3.1	151
12	Scaffold-based discovery of indeglitazar, a PPAR pan-active anti-diabetic agent. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 262-267.	3.3	134
13	Mcl-1 is required for Akata6 B-lymphoma cell survival and is converted to a cell death molecule by efficient caspase-mediated cleavage. <i>Oncogene</i> , 2004, 23, 4818-4827.	2.6	133
14	Computational design of a self-assembling symmetrical $\hat{\Gamma}^2$ -propeller protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 15102-15107.	3.3	122
15	Hierarchical virtual screening approaches in small molecule drug discovery. <i>Methods</i> , 2015, 71, 26-37.	1.9	121
16	[4] Combining constraints for electron-density modification. <i>Methods in Enzymology</i> , 1997, 277, 53-64.	0.4	109
17	The use of Sayre's equation with solvent flattening and histogram matching for phase extension and refinement of protein structures. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1990, 46, 377-381.	0.3	105
18	Advances in the Development of Shape Similarity Methods and Their Application in Drug Discovery. <i>Frontiers in Chemistry</i> , 2018, 6, 315.	1.8	105

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19	Identification of a Novel Noncatalytic Bicarbonate Binding Site in Eubacterial $\hat{\Gamma}^2$ -Carbonic Anhydrase. <i>Biochemistry</i> , 2006, 45, 4351-4361.	1.2	97
20	Design and pharmacology of a highly specific dual FMS and KIT kinase inhibitor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 5689-5694.	3.3	82
21	Biophysical Characterization of Recombinant Human Bcl-2 and Its Interactions with an Inhibitory Ligand, Antimycin A. <i>Biochemistry</i> , 2001, 40, 4911-4922.	1.2	81
22	Phosphodiesterase-4 as a potential drug target. <i>Expert Opinion on Therapeutic Targets</i> , 2005, 9, 1283-1305.	1.5	81
23	Spectomycin B1 as a Novel SUMOylation Inhibitor That Directly Binds to SUMO E2. <i>ACS Chemical Biology</i> , 2013, 8, 2635-2642.	1.6	80
24	Accurate computer-based design of a new backbone conformation in the second turn of protein L. <i>Journal of Molecular Biology</i> , 2002, 315, 471-477.	2.0	73
25	The Effect of F877L and T878A Mutations on Androgen Receptor Response to Enzalutamide. <i>Molecular Cancer Therapeutics</i> , 2016, 15, 1702-1712.	1.9	73
26	Conversion of monomeric protein L to an obligate dimer by computational protein design. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2001, 98, 10687-10691.	3.3	68
27	Bcl-XL Mutations Suppress Cellular Sensitivity to Antimycin A. <i>Journal of Biological Chemistry</i> , 2004, 279, 2159-2165.	1.6	68
28	Oncogene-dependent apoptosis in extracts from drug-resistant cells.. <i>Genes and Development</i> , 1997, 11, 1266-1276.	2.7	60
29	Structures of the B1 domain of protein L from <i>Peptostreptococcus magnus</i> with a tyrosine to tryptophan substitution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2001, 57, 480-487.	2.5	60
30	Advances in the development of SUMO specific protease (SENp) inhibitors. <i>Computational and Structural Biotechnology Journal</i> , 2015, 13, 204-211.	1.9	60
31	Single-Site Mutations Induce 3D Domain Swapping in the B1 Domain of Protein L from <i>Peptostreptococcus magnus</i> . <i>Structure</i> , 2001, 9, 1017-1027.	1.6	52
32	Pharmacophore modeling: advances, limitations, and current utility in drug discovery. <i>Journal of Receptor, Ligand and Channel Research</i> , 0, , 81.	0.7	48
33	Identification of 1,2,5-Oxadiazoles as a New Class of SENP2 Inhibitors Using Structure Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 870-880.	2.5	47
34	Investigation on the Effect of Key Water Molecules on Docking Performance in CSARdock Exercise. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1880-1892.	2.5	46
35	Synthesis, cholinesterase inhibition and molecular modelling studies of coumarin linked thiourea derivatives. <i>Bioorganic Chemistry</i> , 2015, 63, 58-63.	2.0	45
36	Post-translational modification of the N-terminal His tag interferes with the crystallization of the wild-type and mutant SH3 domains from chicken src tyrosine kinase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2001, 57, 759-762.	2.5	43

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37	EC359: A First-in-Class Small-Molecule Inhibitor for Targeting Oncogenic LIFR Signaling in Triple-Negative Breast Cancer. <i>Molecular Cancer Therapeutics</i> , 2019, 18, 1341-1354.	1.9	41
38	Identification of Sumoylation Activating Enzyme 1 Inhibitors by Structure-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 809-820.	2.5	40
39	A Probabilistic Fragment-Based Protein Structure Prediction Algorithm. <i>PLoS ONE</i> , 2012, 7, e38799.	1.1	40
40	Lean-Docking: Exploiting Ligands' Predicted Docking Scores to Accelerate Molecular Docking. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2341-2352.	2.5	38
41	SQUASH – combining constraints for macromolecular phase refinement and extension. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1993, 49, 213-222.	2.5	36
42	Biominalization of a Cadmium Chloride Nanocrystal by a Designed Symmetrical Protein. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9857-9860.	7.2	36
43	Targeting LIF/LIFR signaling in cancer. <i>Genes and Diseases</i> , 2022, 9, 973-980.	1.5	36
44	Protein Interface Pharmacophore Mapping Tools for Small Molecule Protein: Protein Interaction Inhibitor Discovery. <i>Current Topics in Medicinal Chemistry</i> , 2013, 13, 989-1001.	1.0	35
45	Computational design of a symmetrical $\beta$ -trefoil lectin with cancer cell binding activity. <i>Scientific Reports</i> , 2017, 7, 5943.	1.6	35
46	Identification of new SUMO activating enzyme 1 inhibitors using virtual screening and scaffold hopping. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016, 26, 1218-1223.	1.0	34
47	A variant in human AIOLOS impairs adaptive immunity by interfering with IKAROS. <i>Nature Immunology</i> , 2021, 22, 893-903.	7.0	33
48	Computational design of symmetrical eight-bladed $\beta$ -propeller proteins. <i>IUCr</i> , 2019, 6, 46-55.	1.0	33
49	Discovery of Fungal Denitrification Inhibitors by Targeting Copper Nitrite Reductase from <i>Fusarium oxysporum</i> . <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 203-213.	2.5	30
50	A Series of Compounds Bearing a Dipyrro-Pyrimidine Scaffold Acting as Novel Human and Insect Pest Chitinase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 987-1001.	2.9	29
51	The Discovery of Novel Human Androgen Receptor Antagonist Chemotypes Using a Combined Pharmacophore Screening Procedure. <i>ChemMedChem</i> , 2013, 8, 644-651.	1.6	27
52	A Novel Scaffold for Developing Specific or Broad-Spectrum Chitinase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2413-2420.	2.5	27
53	Pharmacophore Modelling as a Virtual Screening Tool for the Discovery of Small Molecule Protein-protein Interaction Inhibitors. <i>Current Pharmaceutical Design</i> , 2012, 18, 4586-4598.	0.9	25
54	Combining in silico and in cerebra approaches for virtual screening and pose prediction in SAMPL4. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 363-373.	1.3	25

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55	Application of Shape Similarity in Pose Selection and Virtual Screening in CSARdock2014 Exercise. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 965-973.	2.5	24
56	A cross docking pipeline for improving pose prediction and virtual screening performance. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 163-173.	1.3	24
57	Human Chitinases: Structure, Function, and Inhibitor Discovery. <i>Advances in Experimental Medicine and Biology</i> , 2019, 1142, 221-251.	0.8	23
58	Crystal structure of human acetylcholinesterase in complex with tacrine: Implications for drug discovery. <i>International Journal of Biological Macromolecules</i> , 2022, 210, 172-181.	3.6	23
59	Entropy-accelerated exact clustering of protein decoys. <i>Bioinformatics</i> , 2011, 27, 939-945.	1.8	22
60	Efficient Sampling in Fragment-Based Protein Structure Prediction Using an Estimation of Distribution Algorithm. <i>PLoS ONE</i> , 2013, 8, e68954.	1.1	22
61	Electrostatic Similarities between Protein and Small Molecule Ligands Facilitate the Design of Protein-Protein Interaction Inhibitors. <i>PLoS ONE</i> , 2013, 8, e75762.	1.1	21
62	A rotation-translation invariant molecular descriptor of partial charges and its use in ligand-based virtual screening. <i>Journal of Cheminformatics</i> , 2014, 6, 23.	2.8	21
63	Human glutamyl cyclase: Structure, function, inhibitors and involvement in Alzheimer's disease. <i>Pharmacological Research</i> , 2019, 147, 104342.	3.1	21
64	Durandal: Fast exact clustering of protein decoys. <i>Journal of Computational Chemistry</i> , 2012, 33, 471-474.	1.5	20
65	Identification of quinazolinyloxy biaryl urea as a new class of SUMO activating enzyme 1 inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 5145-5149.	1.0	20
66	Balancing exploration and exploitation in population-based sampling improves fragment-based <i>de novo</i> protein structure prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 852-858.	1.5	20
67	A Novel Therapeutic Peptide Blocks SARS-CoV-2 Spike Protein Binding with Host Cell ACE2 Receptor. <i>Drugs in R and D</i> , 2021, 21, 273-283.	1.1	20
68	Evolutionary and codon usage preference insights into spike glycoprotein of SARS-CoV-2. <i>Briefings in Bioinformatics</i> , 2021, 22, 1006-1022.	3.2	20
69	Tumor Derived Extracellular Vesicles Drive T Cell Exhaustion in Tumor Microenvironment through Sphingosine Mediated Signaling and Impacting Immunotherapy Outcomes in Ovarian Cancer. <i>Advanced Science</i> , 2022, 9, e2104452.	5.6	20
70	Seven Amino Acid Types Suffice to Create the Core Fold of RNA Polymerase. <i>Journal of the American Chemical Society</i> , 2021, 143, 15998-16006.	6.6	18
71	Cloning, crystallization and preliminary characterization of a $\beta$ -carbonic anhydrase from <i>Escherichia coli</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 1176-1179.	2.5	17
72	Cryo-EM structure of the human ELMO1-DOCK5-Rac1 complex. <i>Science Advances</i> , 2021, 7, .	4.7	17

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73	Neuroprotective derivatives of tacrine that target NMDA receptor and acetyl cholinesterase – Design, synthesis and biological evaluation. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 4517-4537.	1.9	17
74	Comprehensive Intrinsic Disorder Analysis of 6108 Viral Proteomes: From the Extent of Intrinsic Disorder Penetrance to Functional Annotation of Disordered Viral Proteins. <i>Journal of Proteome Research</i> , 2021, 20, 2704-2713.	1.8	16
75	Computational fragment-based screening using RosettaLigand: the SAMPL3 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 603-616.	1.3	15
76	A fragmentation and reassembly method for ab initio phasing. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 304-312.	2.5	15
77	A pose prediction approach based on ligand 3D shape similarity. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 457-469.	1.3	15
78	Evolutionary Signatures Governing the Codon Usage Bias in Coronaviruses and Their Implications for Viruses Infecting Various Bat Species. <i>Viruses</i> , 2021, 13, 1847.	1.5	15
79	Mutation and Modeling Analysis of the <i>Saccharomyces cerevisiae</i> Swi6 Ankyrin Repeats. <i>Biochemistry</i> , 1998, 37, 4437-4450.	1.2	13
80	Accelerating ab initio phasing with de novo models. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 804-812.	2.5	13
81	Quality Assessment of Predicted Protein Models Using Energies Calculated by the Fragment Molecular Orbital Method. <i>Molecular Informatics</i> , 2015, 34, 97-104.	1.4	13
82	Identification of Novel Cathepsin B Inhibitors with Implications in Alzheimer's Disease: Computational Refining and Biochemical Evaluation. <i>Cells</i> , 2021, 10, 1946.	1.8	13
83	Piperidine-4-carboxamide as a new scaffold for designing secretory glutamyl cyclase inhibitors. <i>International Journal of Biological Macromolecules</i> , 2021, 170, 415-423.	3.6	13
84	Identification of Sumoylation Inhibitors Targeting a Predicted Pocket in Ubc9. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2784-2793.	2.5	12
85	Prospective evaluation of shape similarity based pose prediction method in D3R Grand Challenge 2015. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 685-693.	1.3	12
86	Evolution-Inspired Computational Design of Symmetric Proteins. <i>Methods in Molecular Biology</i> , 2017, 1529, 309-322.	0.4	12
87	A protein sequence fitness function for identifying natural and nonnatural proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 1271-1284.	1.5	12
88	In-Silico Design of a Novel Tridecapeptide Targeting Spike Protein of SARS-CoV-2 Variants of Concern. <i>International Journal of Peptide Research and Therapeutics</i> , 2022, 28, 28.	0.9	12
89	An integrated fragment based screening approach for the discovery of small molecule modulators of the VWF-GPIIb/IIIa interaction. <i>Chemical Communications</i> , 2012, 48, 11349.	2.2	11
90	Glu-108 is essential for subunit assembly and dimer stability of d-phosphoglycerate dehydrogenase from <i>Entamoeba histolytica</i> . <i>Molecular and Biochemical Parasitology</i> , 2012, 181, 117-124.	0.5	11

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91	Identification and structure-activity relationship of purine derivatives as novel MTH1 inhibitors. <i>Chemical Biology and Drug Design</i> , 2017, 89, 862-869.	1.5	11
92	A loss-of-function variant in SUV39H2 identified in autism-spectrum disorder causes altered H3K9 trimethylation and dysregulation of protocadherin $\beta$ -cluster genes in the developing brain. <i>Molecular Psychiatry</i> , 2021, 26, 7550-7559.	4.1	11
93	Improving fragment quality for de novo structure prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2240-2252.	1.5	10
94	Crystal Structure and Structure-Based Discovery of Inhibitors of the Nematode Chitinase <i>Ce</i> Cht1. <i>Journal of Agricultural and Food Chemistry</i> , 2021, 69, 3519-3526.	2.4	10
95	Role of conserved active site tryptophan-101 in functional activity and stability of phosphoserine aminotransferase from an enteric human parasite. <i>Amino Acids</i> , 2012, 43, 483-491.	1.2	9
96	Identification of small peptides inhibiting the integrase-LEDGF/p75 interaction through targeting the cellular cofactor. <i>Journal of Peptide Science</i> , 2013, 19, 651-658.	0.8	9
97	Discovery of small molecule inhibitors targeting the SUMO-SIM interaction using a protein interface consensus approach. <i>MedChemComm</i> , 2014, 5, 783-786.	3.5	9
98	Shape similarity guided pose prediction: lessons from D3R Grand Challenge 3. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 47-59.	1.3	9
99	Actin R256 Mono-methylation Is a Conserved Post-translational Modification Involved in Transcription. <i>Cell Reports</i> , 2020, 32, 108172.	2.9	9
100	EC330, a small-molecule compound, is a potential novel inhibitor of LIF signaling. <i>Journal of Molecular Cell Biology</i> , 2020, 12, 477-480.	1.5	9
101	Insights into the evolutionary forces that shape the codon usage in the viral genome segments encoding intrinsically disordered protein regions. <i>Briefings in Bioinformatics</i> , 2021, 22, .	3.2	9
102	The Two-Dimensional Histogram as a Constraint for Protein Phase Improvement. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 1230-1244.	2.5	8
103	Scaffold-Based Drug Discovery. , 2007, , 129-153.		8
104	Understanding the Assembly of an Artificial Protein Nanotube. <i>Advanced Materials Interfaces</i> , 2016, 3, 1600846.	1.9	8
105	Mechanistic insights into the loss-of-function mechanisms of rare human D-amino acid oxidase variants implicated in amyotrophic lateral sclerosis. <i>Scientific Reports</i> , 2020, 10, 17146.	1.6	8
106	Structure-based virtual screening of highly potent inhibitors of the nematode chitinase <i>Ce</i> Cht1. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 1198-1204.	2.5	8
107	Chemical similarity assisted search for acetylcholinesterase inhibitors: Molecular modeling and evaluation of their neuroprotective properties. <i>International Journal of Biological Macromolecules</i> , 2021, 174, 466-476.	3.6	8
108	TIRAP-mediated activation of p38 MAPK in inflammatory signaling. <i>Scientific Reports</i> , 2022, 12, 5601.	1.6	8



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109	Cell-Free Mutant Analysis Combined with Structure Prediction of a Lasso Peptide Biosynthetic Protease B2. <i>ACS Synthetic Biology</i> , 2022, 11, 2022-2028.	1.9	8
110	A two-dimensional histogram-matching method for protein phase refinement and extension. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1893-1900.	2.5	7
111	PAR: a PARallel and distributed job crusher. <i>Bioinformatics</i> , 2010, 26, 2918-2919.	1.8	7
112	Assay methods for small ubiquitin-like modifier (SUMO)â€™SUMO-interacting motif (SIM) interactions in vivo and in vitro using a split-luciferase complementation system. <i>Analytical Biochemistry</i> , 2014, 448, 92-94.	1.1	7
113	ProFitFun: a protein tertiary structure fitness function for quantifying the accuracies of model structures. <i>Bioinformatics</i> , 2022, 38, 369-376.	1.8	7
114	Novel proteinâ€™protein interactions between <i>Entamoeba histolytica</i> d-phosphoglycerate dehydrogenase and phosphoserine aminotransferase. <i>Biochimie</i> , 2012, 94, 1676-1686.	1.3	6
115	Error-estimation-guided rebuilding of <i>de novo</i> models increases the success rate of <i>ab initio</i> phasing. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1522-1534.	2.5	6
116	Population-Based Sampling and Fragment-Based De Novo Protein Structure Prediction. , 2019, , 774-784.		6
117	A structural homology approach for computational protein design with flexible backbone. <i>Bioinformatics</i> , 2019, 35, 2418-2426.	1.8	6
118	A novel structure-based approach for identification of vertebrate susceptibility to SARS-CoV-2: Implications for future surveillance programmes. <i>Environmental Research</i> , 2022, 212, 113303.	3.7	6
119	Computational Investigation of SENP:SUMO Proteinâ€™Protein Interaction for Structure Based Drug Design. <i>Molecular Informatics</i> , 2013, 32, 267-280.	1.4	5
120	CDC25A-inhibitory RE derivatives bind to pocket adjacent to the catalytic site. <i>Molecular BioSystems</i> , 2013, 9, 1026.	2.9	5
121	Chemoinformatics and structural bioinformatics in OCaml. <i>Journal of Cheminformatics</i> , 2019, 11, 10.	2.8	5
122	NbX: Machine Learning-Guided Re-Ranking of Nanobodyâ€™Antigen Binding Poses. <i>Pharmaceuticals</i> , 2021, 14, 968.	1.7	5
123	Molecular dynamics simulations: Principles, methods, and applications in protein conformational dynamics. , 2022, , 439-454.		5
124	Solid-state phase transition in the crystal structure of ribulose 1,5-bisphosphate carboxylase/oxygenase. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1994, 50, 258-262.	2.5	4
125	Crystallization and preliminary X-ray diffraction studies of mutants of B1 IgG-binding domain of protein L from <i>Peptostreptococcus magnus</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2000, 56, 506-508.	2.5	4
126	EC313-a tissue selective SPRM reduces the growth and proliferation of uterine fibroids in a human uterine fibroid tissue xenograft model. <i>Scientific Reports</i> , 2019, 9, 17279.	1.6	4



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127	Understanding the molecular interactions of inhibitors against Bla1 beta-lactamase towards unraveling the mechanism of antimicrobial resistance. <i>International Journal of Biological Macromolecules</i> , 2021, 177, 337-350.	3.6	4
128	An integrated computational pipeline for designing high-affinity nanobodies with expanded genetic codes. <i>Briefings in Bioinformatics</i> , 2021, 22, .	3.2	4
129	A Glutamine Switch Mechanism for Nucleotide Selectivity by Phosphodiesterases. <i>Molecular Cell</i> , 2004, 15, 659.	4.5	3
130	Improving ligand 3D shape similarity-based pose prediction with a continuum solvent model. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 1045-1055.	1.3	3
131	ATP7A Clinical Genetics Resource – A comprehensive clinically annotated database and resource for genetic variants in ATP7A gene. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 2347-2356.	1.9	3
132	Identification of a Selective RelA Inhibitor Based on DSE-FRET Screening Methods. <i>International Journal of Molecular Sciences</i> , 2020, 21, 9150.	1.8	3
133	The symmetric designer protein Pizza as a scaffold for metal coordination. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 945-951.	1.5	3
134	Ambiguities in Ab Initio Phasing. <i>Science</i> , 1993, 259, 1771-1772.	6.0	2
135	Crystal Structure of Phosphodiesterase Families and the Potential for Rational Drug Design. , 2006, , .		2
136	Fragger: a protein fragment picker for structural queries. <i>F1000Research</i> , 2017, 6, 1722.	0.8	2
137	Fragger: a protein fragment picker for structural queries. <i>F1000Research</i> , 2017, 6, 1722.	0.8	2
138	Characterization of pH-induced transitions of <i>Entamoeba histolytica</i> d-phosphoglycerate dehydrogenase. <i>International Journal of Biological Macromolecules</i> , 2015, 79, 284-289.	3.6	1
139	The crystal and solution structure of YdiE from <i>Escherichia coli</i> . <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2015, 71, 919-924.	0.4	1
140	A multidimensional computational exploration of congenital myasthenic syndrome causing mutations in human choline acetyltransferase. <i>Journal of Cellular Biochemistry</i> , 2021, 122, 787-800.	1.2	1
141	<scp>FPredX</scp>: Interpretable models for the prediction of spectral maxima, brightness, and oligomeric states of fluorescent proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 732-746.	1.5	1
142	Multidimensional Histograms for Density Modification. <i>Methods in Enzymology</i> , 2003, 374, 188-203.	0.4	0
143	Identification of 1,2,4-Triazolylthioethanone Scaffold for the Design of New Acetylcholinesterase Inhibitors. <i>Molecular Informatics</i> , 2021, 40, 2100020.	1.4	0