

Jeffrey J Gray

List of Publications by Citations

Source: <https://exaly.com/author-pdf/660354/jeffrey-j-gray-publications-by-citations.pdf>

Version: 2024-04-25

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

148
papers

9,653
citations

47
h-index

97
g-index

191
ext. papers

12,004
ext. citations

5.9
avg. IF

6.42
L-index

#	Paper	IF	Citations
148	ROSETTA3: an object-oriented software suite for the simulation and design of macromolecules. <i>Methods in Enzymology</i> , 2011 , 487, 545-74	1.7	1216
147	Protein-protein docking with simultaneous optimization of rigid-body displacement and side-chain conformations. <i>Journal of Molecular Biology</i> , 2003 , 331, 281-99	6.5	858
146	The interaction of proteins with solid surfaces. <i>Current Opinion in Structural Biology</i> , 2004 , 14, 110-5	8.1	683
145	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3031-3048	6.4	486
144	The RosettaDock server for local protein-protein docking. <i>Nucleic Acids Research</i> , 2008 , 36, W233-8	20.1	389
143	PyRosetta: a script-based interface for implementing molecular modeling algorithms using Rosetta. <i>Bioinformatics</i> , 2010 , 26, 689-91	7.2	333
142	Serverification of molecular modeling applications: the Rosetta Online Server that Includes Everyone (ROSIE). <i>PLoS ONE</i> , 2013 , 8, e63906	3.7	230
141	A comprehensive, high-resolution map of a gene's fitness landscape. <i>Molecular Biology and Evolution</i> , 2014 , 31, 1581-92	8.3	190
140	Benchmarking and analysis of protein docking performance in Rosetta v3.2. <i>PLoS ONE</i> , 2011 , 6, e22477	3.7	190
139	Macromolecular modeling and design in Rosetta: recent methods and frameworks. <i>Nature Methods</i> , 2020 , 17, 665-680	21.6	165
138	Scientific benchmarks for guiding macromolecular energy function improvement. <i>Methods in Enzymology</i> , 2013 , 523, 109-43	1.7	164
137	Modeling and docking of antibody structures with Rosetta. <i>Nature Protocols</i> , 2017 , 12, 401-416	18.8	159
136	High-resolution protein-protein docking. <i>Current Opinion in Structural Biology</i> , 2006 , 16, 183-93	8.1	152
135	Toward high-resolution homology modeling of antibody Fv regions and application to antibody-antigen docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 74, 497-514	4.2	149
134	Conformer selection and induced fit in flexible backbone protein-protein docking using computational and NMR ensembles. <i>Journal of Molecular Biology</i> , 2008 , 381, 1068-87	6.5	128
133	Phosphorylation-dependent inhibition of mineralization by osteopontin ASARM peptides is regulated by PHEX cleavage. <i>Journal of Bone and Mineral Research</i> , 2010 , 25, 695-705	6.3	124
132	RosettaAntibody: antibody variable region homology modeling server. <i>Nucleic Acids Research</i> , 2009 , 37, W474-9	20.1	123

131	Large-scale sequence and structural comparisons of human naive and antigen-experienced antibody repertoires. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, E2636-45	11.5	118
130	Targeting the CoREST complex with dual histone deacetylase and demethylase inhibitors. <i>Nature Communications</i> , 2018 , 9, 53	17.4	116
129	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. <i>Journal of Molecular Biology</i> , 2011 , 414, 289-302	6.5	114
128	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 Suppl 1, 323-48	4.2	111
127	Structure-based design of supercharged, highly thermoresistant antibodies. <i>Chemistry and Biology</i> , 2012 , 19, 449-55		108
126	Structure prediction of protein-solid surface interactions reveals a molecular recognition motif of statherin for hydroxyapatite. <i>Journal of the American Chemical Society</i> , 2007 , 129, 13713-22	16.4	103
125	Chiral acidic amino acids induce chiral hierarchical structure in calcium carbonate. <i>Nature Communications</i> , 2017 , 8, 15066	17.4	99
124	Enzyme replacement therapy prevents dental defects in a model of hypophosphatasia. <i>Journal of Dental Research</i> , 2011 , 90, 470-6	8.1	96
123	SnugDock: paratope structural optimization during antibody-antigen docking compensates for errors in antibody homology models. <i>PLoS Computational Biology</i> , 2010 , 6, e1000644	5	95
122	Protein-protein docking predictions for the CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 52, 118-22	4.2	93
121	An Integrated Framework Advancing Membrane Protein Modeling and Design. <i>PLoS Computational Biology</i> , 2015 , 11, e1004398	5	92
120	Local motions in a benchmark of allosteric proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 67, 385-99	4.2	90
119	Functional loss of semaphorin 3C and/or semaphorin 3D and their epistatic interaction with ret are critical to Hirschsprung disease liability. <i>American Journal of Human Genetics</i> , 2015 , 96, 581-96	11	82
118	Allosteric communication occurs via networks of tertiary and quaternary motions in proteins. <i>PLoS Computational Biology</i> , 2009 , 5, e1000293	5	80
117	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 1980-7	4.2	78
116	Contact rearrangements form coupled networks from local motions in allosteric proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 71, 455-66	4.2	75
115	Blind prediction performance of RosettaAntibody 3.0: grafting, relaxation, kinematic loop modeling, and full CDR optimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 1611-23	4.2	72
114	Computational modeling of membrane proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015 , 83, 1-24	4.2	69

113	Efficient flexible backbone protein-protein docking for challenging targets. <i>Bioinformatics</i> , 2018 , 34, 3461-3469	7.2	57
112	The origin of CDR H3 structural diversity. <i>Structure</i> , 2015 , 23, 302-11	5.2	57
111	Analysis and modeling of the variable region of camelid single-domain antibodies. <i>Journal of Immunology</i> , 2011 , 186, 6357-67	5.3	57
110	Modulation of calcium oxalate dihydrate growth by selective crystal-face binding of phosphorylated osteopontin and polyaspartate peptide showing occlusion by sectoral (compositional) zoning. <i>Journal of Biological Chemistry</i> , 2009 , 284, 23491-501	5.4	53
109	Deep Learning in Protein Structural Modeling and Design. <i>Patterns</i> , 2020 , 1, 100142	5.1	52
108	Rapid calculation of protein pKa values using Rosetta. <i>Biophysical Journal</i> , 2012 , 103, 587-595	2.9	51
107	Alternative computational protocols for supercharging protein surfaces for reversible unfolding and retention of stability. <i>PLoS ONE</i> , 2013 , 8, e64363	3.7	50
106	Solution- and adsorbed-state structural ensembles predicted for the statherin-hydroxyapatite system. <i>Biophysical Journal</i> , 2009 , 96, 3082-91	2.9	49
105	CAPRI rounds 3-5 reveal promising successes and future challenges for RosettaDock. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 60, 181-6	4.2	49
104	Structural model of the mAb 806-EGFR complex using computational docking followed by computational and experimental mutagenesis. <i>Structure</i> , 2006 , 14, 401-14	5.2	48
103	Nanostructure, osteopontin, and mechanical properties of calcitic avian eggshell. <i>Science Advances</i> , 2018 , 4, eaar3219	14.3	47
102	Adding diverse noncanonical backbones to rosetta: enabling peptidomimetic design. <i>PLoS ONE</i> , 2013 , 8, e67051	3.7	47
101	Plasma Cells Are the Most Abundant Gluten Peptide MHC-expressing Cells in Inflamed Intestinal Tissues From Patients With Celiac Disease. <i>Gastroenterology</i> , 2019 , 156, 1428-1439.e10	13.3	45
100	Blind prediction of interfacial water positions in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 620-32	4.2	43
99	De novo design of peptide-calcite biomineralization systems. <i>Journal of the American Chemical Society</i> , 2010 , 132, 12252-62	16.4	43
98	Shape complementarity and hydrogen bond preferences in protein-protein interfaces: implications for antibody modeling and protein-protein docking. <i>Bioinformatics</i> , 2016 , 32, 2451-6	7.2	43
97	Acidic C-terminal domains autoregulate the RNA chaperone Hfq. <i>ELife</i> , 2017 , 6,	8.9	40
96	Enzymatic excision of uracil residues in nucleosomes depends on the local DNA structure and dynamics. <i>Biochemistry</i> , 2012 , 51, 6028-38	3.2	39

95	Partial high-resolution structure of phosphorylated and non-phosphorylated leucine-rich amelogenin protein adsorbed to hydroxyapatite. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 13775-13785 ^{3.8}	3.8	39
94	A generalized approach to sampling backbone conformations with RosettaDock for CAPRI rounds 13-19. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 3115-23	4.2	39
93	Adsorption of colloidal particles by Brownian dynamics simulation: Kinetics and surface structures. <i>Journal of Chemical Physics</i> , 2001 , 114, 1366-1381	3.9	39
92	Incorporating biochemical information and backbone flexibility in RosettaDock for CAPRI rounds 6-12. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 69, 793-800	4.2	37
91	Real-time PyMOL visualization for Rosetta and PyRosetta. <i>PLoS ONE</i> , 2011 , 6, e21931	3.7	35
90	Toward a structure determination method for biomineral-associated protein using combined solid-state NMR and computational structure prediction. <i>Structure</i> , 2010 , 18, 1678-87	5.2	35
89	Pushing the Backbone in Protein-Protein Docking. <i>Structure</i> , 2016 , 24, 1821-1829	5.2	33
88	Accurate Structure Prediction of CDR H3 Loops Enabled by a Novel Structure-Based C-Terminal Constraint. <i>Journal of Immunology</i> , 2017 , 198, 505-515	5.3	33
87	Web-accessible molecular modeling with Rosetta: The Rosetta Online Server that Includes Everyone (ROSIE). <i>Protein Science</i> , 2018 , 27, 259-268	6.3	32
86	Improved prediction of antibody VL-VH orientation. <i>Protein Engineering, Design and Selection</i> , 2016 , 29, 409-418	1.9	32
85	Residue-centric modeling and design of saccharide and glycoconjugate structures. <i>Journal of Computational Chemistry</i> , 2017 , 38, 276-287	3.5	31
84	Structural Diversity in the Type IV Pili of Multidrug-resistant <i>Acinetobacter</i> . <i>Journal of Biological Chemistry</i> , 2016 , 291, 22924-22935	5.4	31
83	Applying linear interaction energy method for rational design of noncompetitive allosteric inhibitors of the sarco- and endoplasmic reticulum calcium-ATPase. <i>Journal of Medicinal Chemistry</i> , 2005 , 48, 3005-14	8.3	29
82	Chiral switching in biomineral suprastructures induced by homochiral l-amino acid. <i>Science Advances</i> , 2018 , 4, eaas9819	14.3	28
81	Identification of structural mechanisms of HIV-1 protease specificity using computational peptide docking: implications for drug resistance. <i>Structure</i> , 2009 , 17, 1636-1648	5.2	28
80	Modeling the structure of mAb 14B7 bound to the anthrax protective antigen. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 70, 218-30	4.2	28
79	Protein Structure Prediction and Design in a Biologically Realistic Implicit Membrane. <i>Biophysical Journal</i> , 2020 , 118, 2042-2055	2.9	27
78	Targeted DNA methylation using an artificially bisected M.HhaI fused to zinc fingers. <i>PLoS ONE</i> , 2012 , 7, e44852	3.7	27

77	Rheology and dynamics of sheared arrays of colloidal particles. <i>Journal of Rheology</i> , 1998 , 42, 1121-1151.1	27
76	Repertoire Analysis of Antibody CDR-H3 Loops Suggests Affinity Maturation Does Not Typically Result in Rigidification. <i>Frontiers in Immunology</i> , 2018 , 9, 413	8.4 26
75	Neutron reflectometry studies of the adsorbed structure of the amelogenin, LRAP. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 3098-109	3.4 26
74	Microstructure Formation and Kinetics in the Random Sequential Adsorption of Polydisperse Tethered Nanoparticles Modeled as Hard Disks. <i>Langmuir</i> , 2001 , 17, 2317-2328	4 26
73	Structure-based cross-docking analysis of antibody-antigen interactions. <i>Scientific Reports</i> , 2017 , 7, 81454.9	24
72	Using the RosettaSurface algorithm to predict protein structure at mineral surfaces. <i>Methods in Enzymology</i> , 2013 , 532, 343-66	1.7 20
71	Extending RosettaDock with water, sugar, and pH for prediction of complex structures and affinities for CAPRI rounds 20-27. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 2201-9	4.2 20
70	Structurally distinct toxicity inhibitors bind at common loci on Amyloid fibril. <i>Protein Science</i> , 2010 , 19, 2291-304	6.3 20
69	Nonequilibrium phase behavior during the random sequential adsorption of tethered hard disks. <i>Physical Review Letters</i> , 2000 , 85, 4430-3	7.4 20
68	Structure-based non-canonical amino acid design to covalently crosslink an antibody-antigen complex. <i>Journal of Structural Biology</i> , 2014 , 185, 215-22	3.4 18
67	Interfacial Mineral Peptide Properties of a Mineral Binding Peptide from Osteonectin and Bone-like Apatite. <i>Chemistry of Materials</i> , 2015 , 27, 5562-5569	9.6 18
66	Structure prediction of domain insertion proteins from structures of individual domains. <i>Structure</i> , 2008 , 16, 513-27	5.2 17
65	Geometric potentials from deep learning improve prediction of CDR H3 loop structures. <i>Bioinformatics</i> , 2020 , 36, i268-i275	7.2 17
64	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021 , 89, 1800-1823	4.2 17
63	Analysis of protein kinase autophosphorylation using expressed protein ligation and computational modeling. <i>Journal of the American Chemical Society</i> , 2008 , 130, 5667-9	16.4 16
62	Origin of anomalous multibody interactions. <i>Nature</i> , 1999 , 402, 750-750	50.4 16
61	Antibody structure prediction using interpretable deep learning.. <i>Patterns</i> , 2022 , 3, 100406	5.1 16
60	Better together: Elements of successful scientific software development in a distributed collaborative community. <i>PLoS Computational Biology</i> , 2020 , 16, e1007507	5 15

59	Advances to tackle backbone flexibility in protein docking. <i>Current Opinion in Structural Biology</i> , 2021 , 67, 178-186	8.1	15
58	Hfq structure reveals a conserved mechanism of RNA annealing regulation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 10978-10987	11.5	14
57	Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017 , 85, 479-486	4.2	14
56	Protein-protein docking with dynamic residue protonation states. <i>PLoS Computational Biology</i> , 2014 , 10, e1004018	5	14
55	Expanding the toolkit for membrane protein modeling in Rosetta. <i>Bioinformatics</i> , 2017 , 33, 754-756	7.2	14
54	An expanded benchmark for antibody-antigen docking and affinity prediction reveals insights into antibody recognition determinants. <i>Structure</i> , 2021 , 29, 606-621.e5	5.2	13
53	The structure of the colorectal cancer-associated enzyme GalNAc-T12 reveals how nonconserved residues dictate its function. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 20404-20410	11.5	12
52	Mechanism of polyubiquitin chain recognition by the human ubiquitin conjugating enzyme Ube2g2. <i>Journal of Biological Chemistry</i> , 2011 , 286, 3981-91	5.4	11
51	Adsorption of Charge-Bidisperse Mixtures of Colloidal Particles. <i>Langmuir</i> , 2001 , 17, 7935-7947	4	11
50	Truncation of the caspase-related subunit (Gpi8p) of <i>Saccharomyces cerevisiae</i> GPI transamidase: dimerization revealed. <i>Archives of Biochemistry and Biophysics</i> , 2007 , 462, 83-93	4.1	10
49	Effect of trisodium citrate treatment on hybridoma cell viability. <i>Biotechnology Letters</i> , 1991 , 5, 295-298		10
48	Modulation of calcium oxalate dihydrate growth by phosphorylated osteopontin peptides. <i>Journal of Structural Biology</i> , 2018 , 204, 131-144	3.4	9
47	Molecular Determinants for Protein Stabilization by Insertional Fusion to a Thermophilic Host Protein. <i>ChemBioChem</i> , 2015 , 16, 2392-402	3.8	9
46	Novel sampling strategies and a coarse-grained score function for docking homomers, flexible heteromers, and oligosaccharides using Rosetta in CAPRI rounds 37-45. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020 , 88, 973-985	4.2	9
45	A Benchmarking Study of PeptideBiomaterial Interactions. <i>Crystal Growth and Design</i> , 2018 , 18, 607-616	3.5	9
44	Glycoengineering of Esterase Activity through Metabolic Flux-Based Modulation of Sialic Acid. <i>ChemBioChem</i> , 2017 , 18, 1204-1215	3.8	8
43	Non-H3 CDR template selection in antibody modeling through machine learning. <i>PeerJ</i> , 2019 , 7, e6179	3.1	8
42	Flexible Backbone Assembly and Refinement of Symmetrical Homomeric Complexes. <i>Structure</i> , 2019 , 27, 1041-1051.e8	5.2	8

41	Prediction of calcite morphology from computational and experimental studies of mutations of a de novo-designed peptide. <i>Langmuir</i> , 2011 , 27, 11520-7	4	8
40	Protein docking and steered molecular dynamics suggest alternative phospholamban-binding sites on the SERCA calcium transporter. <i>Journal of Biological Chemistry</i> , 2020 , 295, 11262-11274	5.4	7
39	A cyber-linked undergraduate research experience in computational biomolecular structure prediction and design. <i>PLoS Computational Biology</i> , 2017 , 13, e1005837	5	7
38	A high throughput mutagenic analysis of yeast sumo structure and function. <i>PLoS Genetics</i> , 2017 , 13, e1006612	6	7
37	A humanized yeast system to analyze cleavage of prelamins A by ZMPSTE24. <i>Methods</i> , 2019 , 157, 47-55	4.6	7
36	Robustification of RosettaAntibody and Rosetta SnugDock. <i>PLoS ONE</i> , 2021 , 16, e0234282	3.7	6
35	Antibody structure prediction using interpretable deep learning		6
34	Computed structures of point deletion mutants and their enzymatic activities. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 2844-60	4.2	5
33	Computational predictions of the mutant behavior of AraC. <i>Journal of Molecular Biology</i> , 2010 , 398, 462-469		5
32	The structural basis of PTEN regulation by multi-site phosphorylation. <i>Nature Structural and Molecular Biology</i> , 2021 , 28, 858-868	17.6	5
31	Solid-State NMR Studies of Biomineralization Peptides and Proteins. <i>ACS Symposium Series</i> , 2012 , 77-96	0.4	4
30	"How Do We Do This at a Distance?!" A Descriptive Study of Remote Undergraduate Research Programs during COVID-19.. <i>CBE Life Sciences Education</i> , 2022 , 21, ar1	3.4	4
29	Computer-based Engineering of Thermostabilized Antibody Fragments. <i>AICHE Journal</i> , 2020 , 66, e16864	3.6	4
28	Comparison of NMR and crystal structures of membrane proteins and computational refinement to improve model quality. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018 , 86, 57-74	4.2	3
27	Efficient Flexible Backbone Protein-Protein Docking for Challenging Targets		3
26	Development of a Broadly Accessible, Computationally Guided Biochemistry Course-Based Undergraduate Research Experience. <i>Journal of Chemical Education</i> , 2021 , 98, 400-409	2.4	3
25	The Rosetta all-atom energy function for macromolecular modeling and design		3
24	Geometric Potentials from Deep Learning Improve Prediction of CDR H3 Loop Structures		3

23	Development and Evaluation of GlycanDock: A Protein-Glycoligand Docking Refinement Algorithm in Rosetta. <i>Journal of Physical Chemistry B</i> , 2021 ,	3.4	3
22	Structural basis for peptide substrate specificities of glycosyltransferase GalNAc-T2. <i>ACS Catalysis</i> , 2021 , 11, 2977-2991	13.1	3
21	A high-affinity human TCR-like antibody detects celiac disease gluten peptide-MHC complexes and inhibits T cell activation. <i>Science Immunology</i> , 2021 , 6,	28	3
20	A Parametric Rosetta Energy Function Analysis with LK Peptides on SAM Surfaces. <i>Langmuir</i> , 2018 , 34, 5279-5289	4	2
19	Rosetta-MPDock: A Novel Computational Tool for Protein-Protein Docking within the Membrane Bilayer. <i>Biophysical Journal</i> , 2015 , 108, 250a	2.9	2
18	An Expanded Benchmark for Antibody-Antigen Docking and Affinity Prediction Reveals Insights into Antibody Recognition Determinants. <i>SSRN Electronic Journal</i> ,	1	2
17	Protein Docking and Steered Molecular Dynamics Reveal Alternative Regulatory Sites on the SERCA Calcium Transporter		2
16	Shotgun scanning glycomutagenesis: a simple and efficient strategy for constructing and characterizing neoglycoproteins		2
15	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks		2
14	Toward the computational design of protein crystals with improved resolution. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019 , 75, 1015-1027	5.5	2
13	Growing Glycans in Rosetta: Accurate de novo glycan modeling, density fitting, and rational sequon design		2
12	Novel sampling strategies and a coarse-grained score function for docking homomers, flexible heteromers, and oligosaccharides using Rosetta in CAPRI Rounds 37-45		1
11	Diverse scientific benchmarks for implicit membrane energy functions		1
10	Modeling and docking antibody structures with Rosetta		1
9	PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design.. <i>The Biophysicist</i> , 2021 , 2, 108-122	1	1
8	Membrane Protein Engineering with Rosetta. <i>Methods in Molecular Biology</i> , 2021 , 2315, 43-57	1.4	1
7	Diverse Scientific Benchmarks for Implicit Membrane Energy Functions. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5248-5261	6.4	1
6	Colicin-Mediated Transport of DNA through the Iron Transporter FepA. <i>MBio</i> , 2021 , 12, e0178721	7.8	1

5	Shotgun scanning glycomutagenesis: A simple and efficient strategy for constructing and characterizing neoglycoproteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	1
4	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. <i>Nature Communications</i> , 2021 , 12, 6947	17.4	0
3	Accurate positioning of functional residues with robotics-inspired computational protein design.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022 , 119, e2115480119	11.5	0
2	Cover Image, Volume 86, Issue 1. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018 , 86, C4-C4	4.2	
1	Induced fit with replica exchange improves protein complex structure prediction. <i>PLoS Computational Biology</i> , 2022 , 18, e1010124	5	