

Sameer Velankar

List of Publications by Year in Descending Order

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Version: 2024-04-04

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

70 papers	4,714 citations	37 h-index	68 g-index
78 ext. papers	8,166 ext. citations	10.7 avg, IF	5.42 L-index

#	Paper	IF	Citations
70	PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology.. <i>Journal of Molecular Biology</i> , 2022 , 167599	6.5	1
69	AlphaFold Protein Structure Database: massively expanding the structural coverage of protein-sequence space with high-accuracy models. <i>Nucleic Acids Research</i> , 2021 ,	20.1	285
68	PDBe-KB: collaboratively defining the biological context of structural data. <i>Nucleic Acids Research</i> , 2021 ,	20.1	7
67	The impact of structural bioinformatics tools and resources on SARS-CoV-2 research and therapeutic strategies. <i>Briefings in Bioinformatics</i> , 2021 , 22, 742-768	13.4	16
66	Enhanced validation of small-molecule ligands and carbohydrates in the Protein Data Bank. <i>Structure</i> , 2021 , 29, 393-400.e1	5.2	7
65	Modernized uniform representation of carbohydrate molecules in the Protein Data Bank. <i>Glycobiology</i> , 2021 , 31, 1204-1218	5.8	5
64	Mol* Viewer: modern web app for 3D visualization and analysis of large biomolecular structures. <i>Nucleic Acids Research</i> , 2021 , 49, W431-W437	20.1	113
63	PDBe Aggregated API: Programmatic access to an integrative knowledge graph of molecular structure data. <i>Bioinformatics</i> , 2021 ,	7.2	2
62	The Protein Data Bank Archive. <i>Methods in Molecular Biology</i> , 2021 , 2305, 3-21	1.4	12
61	Highly accurate protein structure prediction for the human proteome. <i>Nature</i> , 2021 , 596, 590-596	50.4	399
60	PDBeCIF: an open-source mmCIF/CIF parsing and processing package. <i>BMC Bioinformatics</i> , 2021 , 22, 3833.6		
59	New restraints and validation approaches for nucleic acid structures in PDB-REDO. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021 , 77, 1127-1141	5.5	0
58	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
57	The ELIXIR Core Data Resources: fundamental infrastructure for the life sciences. <i>Bioinformatics</i> , 2020 , 36, 2636-2642	7.2	29
56	PDBe: improved findability of macromolecular structure data in the PDB. <i>Nucleic Acids Research</i> , 2020 , 48, D335-D343	20.1	50
55	High-performance macromolecular data delivery and visualization for the web. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020 , 76, 1167-1173	5.5	0
54	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo Community). <i>F1000Research</i> , 2020 , 9,	3.6	9

53	BinaryCIF and CIFTools-Lightweight, efficient and extensible macromolecular data management. <i>PLoS Computational Biology</i> , 2020 , 16, e1008247	5	5
52	Modeling protein-protein, protein-peptide, and protein-oligosaccharide complexes: CAPRI 7th edition. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020 , 88, 916-938	4.2	41
51	Genome3D: integrating a collaborative data pipeline to expand the depth and breadth of consensus protein structure annotation. <i>Nucleic Acids Research</i> , 2020 , 48, D314-D319	20.1	7
50	PDBe-KB: a community-driven resource for structural and functional annotations. <i>Nucleic Acids Research</i> , 2020 , 48, D344-D353	20.1	50
49	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019 , 87, 1200-1221	4.2	58
48	West-Life: A Virtual Research Environment for structural biology. <i>Journal of Structural Biology: X</i> , 2019 , 1, 100006	2.9	1
47	Finding enzyme cofactors in Protein Data Bank. <i>Bioinformatics</i> , 2019 , 35, 3510-3511	7.2	7
46	Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB). <i>Acta Crystallographica Section D: Structural Biology</i> , 2019 , 75, 451-454	5.5	32
45	Automatic annotation of protein residues in published papers. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2019 , 75, 665-672	1.1	2
44	Protein Data Bank: the single global archive for 3D macromolecular structure data. <i>Nucleic Acids Research</i> , 2019 , 47, D520-D528	20.1	308
43	SIFTS: updated Structure Integration with Function, Taxonomy and Sequences resource allows 40-fold increase in coverage of structure-based annotations for proteins. <i>Nucleic Acids Research</i> , 2019 , 47, D482-D489	20.1	69
42	Structural biology data archiving - where we are and what lies ahead. <i>FEBS Letters</i> , 2018 , 592, 2153-2167	3.8	8
41	Validation of ligands in macromolecular structures determined by X-ray crystallography. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018 , 74, 228-236	5.5	29
40	Worldwide Protein Data Bank validation information: usage and trends. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018 , 74, 237-244	5.5	11
39	The challenge of modeling protein assemblies: the CASP12-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018 , 86 Suppl 1, 257-273	4.2	56
38	Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. <i>Database: the Journal of Biological Databases and Curation</i> , 2018 , 2018,	5	31
37	PDBe: towards reusable data delivery infrastructure at protein data bank in Europe. <i>Nucleic Acids Research</i> , 2018 , 46, D486-D492	20.1	57
36	Cover Image, Volume 85, Issue 3. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017 , 85, C1-C1	4.2	

35	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. <i>Structure</i> , 2017 , 25, 536-545	5.2	86
34	Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. <i>Methods in Molecular Biology</i> , 2017 , 1607, 627-641	1.4	271
33	PDB-Dev: a Prototype System for Depositing Integrative/Hybrid Structural Models. <i>Structure</i> , 2017 , 25, 1317-1318	5.2	58
32	Validation of Structures in the Protein Data Bank. <i>Structure</i> , 2017 , 25, 1916-1927	5.2	130
31	LiteMol suite: interactive web-based visualization of large-scale macromolecular structure data. <i>Nature Methods</i> , 2017 , 14, 1121-1122	21.6	106
30	Modeling protein-protein and protein-peptide complexes: CAPRI 6th edition. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017 , 85, 359-377	4.2	148
29	Polymyxins and quinazolines are LSD1/KDM1A inhibitors with unusual structural features. <i>Science Advances</i> , 2016 , 2, e1601017	14.3	39
28	PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. <i>Nucleic Acids Research</i> , 2016 , 44, D385-95	20.1	111
27	Patterns of database citation in articles and patents indicate long-term scientific and industry value of biological data resources. <i>F1000Research</i> , 2016 , 5,	3.6	13
26	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
25	The archiving and dissemination of biological structure data. <i>Current Opinion in Structural Biology</i> , 2016 , 40, 17-22	8.1	23
24	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , 2015 , 23, 1156-67	5.2	131
23	The chemical component dictionary: complete descriptions of constituent molecules in experimentally determined 3D macromolecules in the Protein Data Bank. <i>Bioinformatics</i> , 2015 , 31, 1274-82	7.2	75
22	Assessing Structural Predictions of Protein-Protein Recognition: The CAPRI Experiment. <i>Reviews in Computational Chemistry</i> , 2015 , 137-173		3
21	The complex portal--an encyclopaedia of macromolecular complexes. <i>Nucleic Acids Research</i> , 2015 , 43, D479-84	20.1	68
20	Genome3D: exploiting structure to help users understand their sequences. <i>Nucleic Acids Research</i> , 2015 , 43, D382-6	20.1	33
19	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. <i>Nature Structural and Molecular Biology</i> , 2015 , 22, 433-4	17.6	26
18	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , 2014 , 42, D285-91	20.1	109

17	UniChem: a unified chemical structure cross-referencing and identifier tracking system. <i>Journal of Cheminformatics</i> , 2013 , 5, 3	8.6	90
16	BioJS: an open source JavaScript framework for biological data visualization. <i>Bioinformatics</i> , 2013 , 29, 1103-4	7.2	88
15	The role of structural bioinformatics resources in the era of integrative structural biology. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 710-21		14
14	The EBI enzyme portal. <i>Nucleic Acids Research</i> , 2013 , 41, D773-80	20.1	13
13	SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. <i>Nucleic Acids Research</i> , 2013 , 41, D483-9	20.1	181
12	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. <i>Nucleic Acids Research</i> , 2013 , 41, D499-507	20.1	48
11	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
10	Implementing an X-ray validation pipeline for the Protein Data Bank. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 478-83		73
9	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. <i>Nature Methods</i> , 2011 , 8, 528-9	21.6	227
8	The Protein Data Bank in Europe (PDBe): bringing structure to biology. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 324-30		25
7	EMDataBank.org: unified data resource for CryoEM. <i>Nucleic Acids Research</i> , 2011 , 39, D456-64	20.1	209
6	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , 2011 , 39, D402-10	20.1	48
5	PDBe: Protein Data Bank in Europe. <i>Nucleic Acids Research</i> , 2010 , 38, D308-17	20.1	86
4	Straightforward and complete deposition of NMR data to the PDBe. <i>Journal of Biomolecular NMR</i> , 2010 , 48, 85-92	3	7
3	Remediation of the protein data bank archive. <i>Nucleic Acids Research</i> , 2008 , 36, D426-33	20.1	124
2	Unconventional interactions between water and heterocyclic nitrogens in protein structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 57, 1-8	4.2	37
1	A structural biology community assessment of AlphaFold 2 applications		19