Sameer Velankar

List of Publications by Year
in descending order

70	12,135	76326	79698
papers	citations	40 h-index	73 g-index

78	78	78	10724
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	AlphaFold Protein Structure Database: massively expanding the structural coverage of protein-sequence space with high-accuracy models. Nucleic Acids Research, 2022, 50, D439-D444.	14.5	3,692
2	Highly accurate protein structure prediction for the human proteome. Nature, 2021, 596, 590-596.	27.8	1,773
3	Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.	14.5	671
4	Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. Methods in Molecular Biology, 2017, 1607, 627-641.	0.9	592
5	Mol* Viewer: modern web app for 3D visualization and analysis of large biomolecular structures. Nucleic Acids Research, 2021, 49, W431-W437.	14.5	515
6	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. Nature Methods, 2011, 8, 528-529.	19.0	274
7	EMDataBank.org: unified data resource for CryoEM. Nucleic Acids Research, 2011, 39, D456-D464.	14.5	246
8	SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. Nucleic Acids Research, 2012, 41, D483-D489.	14.5	238
9	Validation of Structures in the Protein Data Bank. Structure, 2017, 25, 1916-1927.	3.3	210
10	Modeling proteinâ€“protein and proteinâ€“peptide complexes: CAPRI 6th edition. Proteins: Structure, Function and Bioinformatics, 2017, 85, 359-377.	2.6	198
11	SIFTS: updated Structure Integration with Function, Taxonomy and Sequences resource allows 40-fold increase in coverage of structure-based annotations for proteins. Nucleic Acids Research, 2019, 47, D482-D489.	14.5	165
12	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	3.3	159
13	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	2.6	148
14	LiteMol suite: interactive web-based visualization of large-scale macromolecular structure data. Nature Methods, 2017, 14, 1121-1122.	19.0	137
15	Remediation of the protein data bank archive. Nucleic Acids Research, 2007, 36, D426-D433.	14.5	136
16	UniChem: a unified chemical structure cross-referencing and identifier tracking system. Journal of Cheminformatics, 2013, 5, 3.	6.1	133
17	PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2014, 42, D285-D291.	14.5	133
18	PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. Nucleic Acids Research, 2016, 44, D385-D395.	14.5	131

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19	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. Structure, 2017, 25, 536-545.	3.3	130
20	BioJS: an open source JavaScript framework for biological data visualization. Bioinformatics, 2013, 29, 1103-1104.	4.1	110
21	The chemical component dictionary: complete descriptions of constituent molecules in experimentally determined 3D macromolecules in the Protein Data Bank. Bioinformatics, 2015, 31, 1274-1278.	4.1	110
22	PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2010, 38, D308-D317.	14.5	108
23	The complex portal - an encyclopaedia of macromolecular complexes. Nucleic Acids Research, 2015, 43, D479-D484.	14.5	100
24	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
25	Modeling proteinâ€protein, proteinâ€peptide, and proteinâ€oligosaccharide complexes: CAPRI 7th edition. Proteins: Structure, Function and Bioinformatics, 2020, 88, 916-938.	2.6	96
26	Implementing an X-ray validation pipeline for the Protein Data Bank. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 478-483.	2.5	88
27	PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Research, 2020, 48, D344-D353.	14.5	87
28	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	2.6	87
29	PDBe: improved findability of macromolecular structure data in the PDB. Nucleic Acids Research, 2020, 48, D335-D343.	14.5	86
30	The challenge of modeling protein assemblies: the CASP12â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2018, 86, 257-273.	2.6	85
31	PDB-Dev: a Prototype System for Depositing Integrative/Hybrid Structural Models. Structure, 2017, 25, 1317-1318.	3.3	84
32	PDBe: towards reusable data delivery infrastructure at protein data bank in Europe. Nucleic Acids Research, 2018, 46, D486-D492.	14.5	76
33	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	2.6	73
34	PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2011, 39, D402-D410.	14.5	64
35	Polymyxins and quinazolines are LSD1/KDM1A inhibitors with unusual structural features. Science Advances, 2016, 2, e1601017.	10.3	61
36	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. Nucleic Acids Research, 2012, 41, D499-D507.	14.5	53

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37	The Protein Data Bank Archive. Methods in Molecular Biology, 2021, 2305, 3-21.	0.9	49
38	The ELIXIR Core Data Resources: fundamental infrastructure for the life sciences. Bioinformatics, 2020, 36, 2636-2642.	4.1	47
39	Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB). Acta Crystallographica Section D: Structural Biology, 2019, 75, 451-454.	2.3	46
40	PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542.	14.5	46
41	Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	3.0	45
42	Validation of ligands in macromolecular structures determined by X-ray crystallography. Acta Crystallographica Section D: Structural Biology, 2018, 74, 228-236.	2.3	45
43	Genome3D: exploiting structure to help users understand their sequences. Nucleic Acids Research, 2015, 43, D382-D386.	14.5	42
44	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434.	8.2	40
45	PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology. Journal of Molecular Biology, 2022, 434, 167599.	4.2	39
46	Unconventional interactions between water and heterocyclic nitrogens in protein structures. Proteins: Structure, Function and Bioinformatics, 2004, 57, 1-8.	2.6	38
47	The impact of structural bioinformatics tools and resources on SARS-CoV-2 research and therapeutic strategies. Briefings in Bioinformatics, 2021, 22, 742-768.	6.5	29
48	The archiving and dissemination of biological structure data. Current Opinion in Structural Biology, 2016, 40, 17-22.	5.7	28
49	Enhanced validation of small-molecule ligands and carbohydrates in the Protein Data Bank. Structure, 2021, 29, 393-400.e1.	3.3	28
50	The Protein Data Bank in Europe (PDBe): bringing structure to biology. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 324-330.	2.5	27
51	Finding enzyme cofactors in Protein Data Bank. Bioinformatics, 2019, 35, 3510-3511.	4.1	20
52	The EBI enzyme portal. Nucleic Acids Research, 2013, 41, D773-D780.	14.5	19
53	Characterizing and explaining the impact of disease-associated mutations in proteins without known structures or structural homologs. Briefings in Bioinformatics, 2022, 23, .	6.5	18
54	The role of structural bioinformatics resources in the era of integrative structural biology. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 710-721.	2.5	17

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55	Modernized uniform representation of carbohydrate molecules in the Protein Data Bank. Glycobiology, 2021, 31, 1204-1218.	2.5	17
56	Patterns of database citation in articles and patents indicate long-term scientific and industry value of biological data resources. F1000Research, 2016, 5, 160.	1.6	16
57	Worldwide Protein Data Bank validation information: usage and trends. Acta Crystallographica Section D: Structural Biology, 2018, 74, 237-244.	2.3	15
58	BinaryCIF and CIFTools—Lightweight, efficient and extensible macromolecular data management. PLoS Computational Biology, 2020, 16, e1008247.	3.2	15
59	Genome3D: integrating a collaborative data pipeline to expand the depth and breadth of consensus protein structure annotation. Nucleic Acids Research, 2020, 48, D314-D319.	14.5	13
60	PDBe aggregated API: programmatic access to an integrative knowledge graph of molecular structure data. Bioinformatics, 2021, 37, 3950-3952.	4.1	12
61	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo) Tj ETQq1 1 0.784314 rgBT /Overlock 10	2.6	12
62	Structural biology data archiving â€“ where we are and what lies ahead. FEBS Letters, 2018, 592, 2153-2167.	2.8	11
63	Straightforward and complete deposition of NMR data to the PDBe. Journal of Biomolecular NMR, 2010, 48, 85-92.	2.8	7
64	New restraints and validation approaches for nucleic acid structures in PDB-REDO. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1127-1141.	2.3	6
65	Whither structural biologists?. IUCrJ, 2022, 9, 399-400.	2.2	6
66	High-performance macromolecular data delivery and visualization for the web. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1167-1173.	2.3	3
67	West-Life: A Virtual Research Environment for structural biology. Journal of Structural Biology: X, 2019, 1, 100006.	1.3	2
68	Automatic annotation of protein residues in published papers. Acta Crystallographica Section F, Structural Biology Communications, 2019, 75, 665-672.	0.8	2
69	PDBeCIF: an open-source mmCIF/CIF parsing and processing package. BMC Bioinformatics, 2021, 22, 383.	2.6	2
70	Cover Image, Volume 85, Issue 3. Proteins: Structure, Function and Bioinformatics, 2017, 85, C1.	2.6	0