Sameer Velankar

List of Publications by Year
in descending order

70 papers	12,135 citations	76196 40 h-index	79541 73 g-index
78 all docs	78 docs citations	78 times ranked	10724 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.	6.5	3,692
2	PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542.	6.5	46
3	PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology. Journal of Molecular Biology, 2022, 434, 167599.	2.0	39
4	Characterizing and explaining the impact of disease-associated mutations in proteins without known structures or structural homologs. Briefings in Bioinformatics, 2022, 23, .	3.2	18
5	Whither structural biologists?. IUCrJ, 2022, 9, 399-400.	1.0	6
6	The Protein Data Bank Archive. Methods in Molecular Biology, 2021, 2305, 3-21.	0.4	49
7	Enhanced validation of small-molecule ligands and carbohydrates in the Protein Data Bank. Structure, 2021, 29, 393-400.e1.	1.6	28
8	Modernized uniform representation of carbohydrate molecules in the Protein Data Bank. Glycobiology, 2021, 31, 1204-1218.	1.3	17
9	Mol* Viewer: modern web app for 3D visualization and analysis of large biomolecular structures. Nucleic Acids Research, 2021, 49, W431-W437.	6.5	515
10	PDBe aggregated API: programmatic access to an integrative knowledge graph of molecular structure data. Bioinformatics, 2021, 37, 3950-3952.	1.8	12
11	Highly accurate protein structure prediction for the human proteome. Nature, 2021, 596, 590-596.	13.7	1,773
12	PDBeCIF: an open-source mmCIF/CIF parsing and processing package. BMC Bioinformatics, 2021, 22, 383.	1.2	2
13	New restraints and validation approaches for nucleic acid structures in PDB-REDO. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1127-1141.	1.1	6
14	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	1.5	73
15	The impact of structural bioinformatics tools and resources on SARS-CoV-2 research and therapeutic strategies. Briefings in Bioinformatics, 2021, 22, 742-768.	3.2	29
16	PDBe: improved findability of macromolecular structure data in the PDB. Nucleic Acids Research, 2020, 48, D335-D343.	6.5	86
17	PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Research, 2020, 48, D344-D353.	6.5	87
18	Modeling proteinâ€protein, proteinâ€peptide, and proteinâ€oligosaccharide complexes: CAPRI 7th edition. Proteins: Structure, Function and Bioinformatics, 2020, 88, 916-938.	1.5	96

#	Article	IF	Citations
19	Genome3D: integrating a collaborative data pipeline to expand the depth and breadth of consensus protein structure annotation. Nucleic Acids Research, 2020, 48, D314-D319.	6.5	13
20	The ELIXIR Core Data Resources: fundamental infrastructure for the life sciences. Bioinformatics, 2020, 36, 2636-2642.	1.8	47
21	High-performance macromolecular data delivery and visualization for the web. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1167-1173.	1.1	3
22	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 622 T	0.8	12
23	BinaryCIF and CIFTools–Lightweight, efficient and extensible macromolecular data management. PLoS Computational Biology, 2020, 16, e1008247.	1.5	15
24	Blind prediction of homo–and hetero–protein complexes: The CASP13–CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
25	West-Life: A Virtual Research Environment for structural biology. Journal of Structural Biology: X, 2019, 1, 100006.	0.7	2
26	Finding enzyme cofactors in Protein Data Bank. Bioinformatics, 2019, 35, 3510-3511.	1.8	20
27	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.	1.1	46
28	Automatic annotation of protein residues in published papers. Acta Crystallographica Section F, Structural Biology Communications, 2019, 75, 665-672.	0.4	2
29	Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.	6.5	671
30	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.	6.5	165
31	The challenge of modeling protein assemblies: the CASP12–CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2018, 86, 257-273.	1.5	85
32	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, .	1.4	45
33	PDBe: towards reusable data delivery infrastructure at protein data bank in Europe. Nucleic Acids Research, 2018, 46, D486-D492.	6.5	76
34	Structural biology data archiving –“ where we are and what lies ahead. FEBS Letters, 2018, 592, 2153-2167.	1.3	11
35	Validation of ligands in macromolecular structures determined by X-ray crystallography. Acta Crystallographica Section D: Structural Biology, 2018, 74, 228-236.	1.1	45
36	Worldwide Protein Data Bank validation information: usage and trends. Acta Crystallographica Section D: Structural Biology, 2018, 74, 237-244.	1.1	15

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37	Cover Image, Volume 85, Issue 3. Proteins: Structure, Function and Bioinformatics, 2017, 85, C1.	1.5	0
38	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. Structure, 2017, 25, 536-545.	1.6	130
39	Protein Data Bank (PDB): The Single Global Macromolecular Structure Archive. Methods in Molecular Biology, 2017, 1607, 627-641.	0.4	592
40	PDB-Dev: a Prototype System for Depositing Integrative/Hybrid Structural Models. Structure, 2017, 25, 1317-1318.	1.6	84
41	Validation of Structures in the Protein Data Bank. Structure, 2017, 25, 1916-1927.	1.6	210
42	LiteMol suite: interactive web-based visualization of large-scale macromolecular structure data. Nature Methods, 2017, 14, 1121-1122.	9.0	137
43	Modeling proteinâ€“protein and proteinâ€“peptide complexes: CAPRI 6th edition. Proteins: Structure, Function and Bioinformatics, 2017, 85, 359-377.	1.5	198
44	Patterns of database citation in articles and patents indicate long-term scientific and industry value of biological data resources. F1000Research, 2016, 5, 160.	0.8	16
45	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.	1.5	148
46	The archiving and dissemination of biological structure data. Current Opinion in Structural Biology, 2016, 40, 17-22.	2.6	28
47	Polymyxins and quinazolines are LSD1/KDM1A inhibitors with unusual structural features. Science Advances, 2016, 2, e1601017.	4.7	61
48	PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. Nucleic Acids Research, 2016, 44, D385-D395.	6.5	131
49	The complex portal - an encyclopaedia of macromolecular complexes. Nucleic Acids Research, 2015, 43, D479-D484.	6.5	100
50	Genome3D: exploiting structure to help users understand their sequences. Nucleic Acids Research, 2015, 43, D382-D386.	6.5	42
51	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434.	3.6	40
52	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	1.6	159
53	The chemical component dictionary: complete descriptions of constituent molecules in experimentally determined 3D macromolecules in the Protein Data Bank. Bioinformatics, 2015, 31, 1274-1278.	1.8	110
54	PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2014, 42, D285-D291.	6.5	133

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55	UniChem: a unified chemical structure cross-referencing and identifier tracking system. Journal of Cheminformatics, 2013, 5, 3.	2.8	133
56	BioJS: an open source JavaScript framework for biological data visualization. Bioinformatics, 2013, 29, 1103-1104.	1.8	110
57	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
58	The EBI enzyme portal. Nucleic Acids Research, 2013, 41, D773-D780.	6.5	19
59	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	1.5	87
60	SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. Nucleic Acids Research, 2012, 41, D483-D489.	6.5	238
61	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.	6.5	53
62	Implementing an X-ray validation pipeline for the Protein Data Bank. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 478-483.	2.5	88
63	PSICQUIC and PSISCORE: accessing and scoring molecular interactions. Nature Methods, 2011, 8, 528-529.	9.0	274
64	The Protein Data Bank in Europe (PDBe): bringing structure to biology. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 324-330.	2.5	27
65	EMDataBank.org: unified data resource for CryoEM. Nucleic Acids Research, 2011, 39, D456-D464.	6.5	246
66	PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2011, 39, D402-D410.	6.5	64
67	Straightforward and complete deposition of NMR data to the PDBe. Journal of Biomolecular NMR, 2010, 48, 85-92.	1.6	7
68	PDBe: Protein Data Bank in Europe. Nucleic Acids Research, 2010, 38, D308-D317.	6.5	108
69	Remediation of the protein data bank archive. Nucleic Acids Research, 2007, 36, D426-D433.	6.5	136
70	Unconventional interactions between water and heterocyclic nitrogens in protein structures. Proteins: Structure, Function and Bioinformatics, 2004, 57, 1-8.	1.5	38