List of Publications by Year in descending order

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Version: 2024-02-01

115 papers	44,572 citations	41344 49 h-index	22832 112 g-index
118 all docs	118 docs citations	118 times ranked	46227 citing authors

#	Article	IF	Citations
1	Evolution of the <scp>SARSâ€CoV</scp>â€2 proteome in three dimensions (3D) during the first 6 months of the <scp>COVID</scp>â€19 pandemic. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1054-1080.	2.6	31
2	<scp>RCSB</scp> Protein Data Bank: Celebrating 50â€‰years of the <scp>PDB</scp> with new tools for understanding and visualizing biological macromolecules in <scp>3D</scp>. Protein Science, 2022, 31, 187-208.	7.6	84
3	<scp>PDB</scp>â€101: Educational resources supporting molecular explorations through biology and medicine. Protein Science, 2022, 31, 129-140.	7.6	43
4	RCSB Protein Data Bank resources for structure-facilitated design of mRNA vaccines for existing and emerging viral pathogens. Structure, 2022, 30, 55-68.e2.	3.3	10
5	Building Structural Models of a Whole Mycoplasma Cell. Journal of Molecular Biology, 2022, 434, 167351.	4.2	40
6	Integrative illustration of a JCVI-syn3A minimal cell. Journal of Integrative Bioinformatics, 2022, 19, .	1.5	6
7	Exploring protein symmetry at the RCSB Protein Data Bank. Emerging Topics in Life Sciences, 2022, 6, 231-243.	2.6	7
8	Modeling in the Time of COVID-19: Statistical and Rule-based Mesoscale Models. IEEE Transactions on Visualization and Computer Graphics, 2021, 27, 722-732.	4.4	20
9	The <scp>AutoDock</scp> suite at 30. Protein Science, 2021, 30, 31-43.	7.6	85
10	Seeing the PDB. Journal of Biological Chemistry, 2021, 296, 100742.	3.4	13
11	CellPAINT: Turnkey Illustration of Molecular Cell Biology. Frontiers in Bioinformatics, 2021, 1, .	2.1	20
12	Molecular storytelling for online structural biology outreach and education. Structural Dynamics, 2021, 8, 020401.	2.3	7
13	Art as a tool for science. Nature Structural and Molecular Biology, 2021, 28, 402-403.	8.2	7
14	Moltemplate: A Tool for Coarse-Grained Modeling of Complex Biological Matter and Soft Condensed Matter Physics. Journal of Molecular Biology, 2021, 433, 166841.	4.2	189
15	RCSB Protein Data Bank: powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering and energy sciences. Nucleic Acids Research, 2021, 49, D437-D451.	14.5	918
16	RCSB Protein Data Bank: Enabling biomedical research and drug discovery. Protein Science, 2020, 29, 52-65.	7.6	223
17	RCSB Protein Data Bank tools for 3D structure-guided cancer research: human papillomavirus (HPV) case study. Oncogene, 2020, 39, 6623-6632.	5.9	6
18	Integrative illustration for coronavirus outreach. PLoS Biology, 2020, 18, e3000815.	5.6	18

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19	Selective and Effective: Current Progress in Computational Structure-Based Drug Discovery of Targeted Covalent Inhibitors. Trends in Pharmacological Sciences, 2020, 41, 1038-1049.	8.7	17
20	Art and Science of the Cellular Mesoscale. Trends in Biochemical Sciences, 2020, 45, 472-483.	7.5	36
21	Insights from 20â€‰years of the Molecule of the Month. Biochemistry and Molecular Biology Education, 2020, 48, 350-355.	1.2	16
22	Impact of the Protein Data Bank Across Scientific Disciplines. Data Science Journal, 2020, 19, 25.	1.3	17
23	Illustrate: Software for Biomolecular Illustration. Structure, 2019, 27, 1716-1720.e1.	3.3	87
24	Integrative modeling of the HIV-1 ribonucleoprotein complex. PLoS Computational Biology, 2019, 15, e1007150.	3.2	4
25	Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.	14.5	671
26	RCSB Protein Data Bank: biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. Nucleic Acids Research, 2019, 47, D464-D474.	14.5	918
27	Labels on Levels: Labeling of Multi-Scale Multi-Instance and Crowded 3D Biological Environments. IEEE Transactions on Visualization and Computer Graphics, 2019, 25, 977-986.	4.4	16
28	Symmetry at the Cellular Mesoscale. Symmetry, 2019, 11, 1170.	2.2	4
29	Instant Construction and Visualization of Crowded Biological Environments. IEEE Transactions on Visualization and Computer Graphics, 2018, 24, 862-872.	4.4	36
30	Lattice Models of Bacterial Nucleoids. Journal of Physical Chemistry B, 2018, 122, 5441-5447.	2.6	23
31	CellPAINT: Interactive Illustration of Dynamic Mesoscale Cellular Environments. IEEE Computer Graphics and Applications, 2018, 38, 51-66.	1.2	33
32	Molecular Illustration in Research and Education: Past, Present, and Future. Journal of Molecular Biology, 2018, 430, 3969-3981.	4.2	52
33	From Atoms to Cells: Using Mesoscale Landscapes to Construct Visual Narratives. Journal of Molecular Biology, 2018, 430, 3954-3968.	4.2	31
34	OUP accepted manuscript. Nucleic Acids Research, 2017, 45, D271-D281.	14.5	619
35	A visual review of the human pathogen Streptococcus pneumoniae. FEMS Microbiology Reviews, 2017, 41, 854-879.	8.6	72
36	Fragment-Based Analysis of Ligand Dockings Improves Classification of Actives. Journal of Chemical Information and Modeling, 2016, 56, 1597-1607.	5.4	4

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37	Covalent docking using autodock: Twoâ€point attractor and flexible side chain methods. Protein Science, 2016, 25, 295-301.	7.6	170
38	Computational proteinâ€“ligand docking and virtual drug screening with the AutoDock suite. Nature Protocols, 2016, 11, 905-919.	12.0	1,370
39	RCSB Protein Data Bank: A Resource for Chemical, Biochemical, and Structural Explorations of Large and Small Biomolecules. Journal of Chemical Education, 2016, 93, 569-575.	2.3	66
40	AutoDockFR: Advances in Protein-Ligand Docking with Explicitly Specified Binding Site Flexibility. PLoS Computational Biology, 2015, 11, e1004586.	3.2	287
41	Illustrations of the HIV Life Cycle. Current Topics in Microbiology and Immunology, 2015, 389, 243-252.	1.1	25
42	The RCSB PDB â€œMolecule of the Monthâ€: Inspiring a Molecular View of Biology. PLoS Biology, 2015, 13, e1002140.	5.6	88
43	The RCSB Protein Data Bank: views of structural biology for basic and applied research and education. Nucleic Acids Research, 2015, 43, D345-D356.	14.5	461
44	cellPACK: a virtual mesoscope to model and visualize structural systems biology. Nature Methods, 2015, 12, 85-91.	19.0	130
45	3D molecular models of whole HIV-1 virions generated with cellPACK. Faraday Discussions, 2014, 169, 23-44.	3.2	52
46	Protein structure in context: The molecular landscape of angiogenesis. Biochemistry and Molecular Biology Education, 2013, 41, 213-223.	1.2	6
47	The RCSB Protein Data Bank: new resources for research and education. Nucleic Acids Research, 2012, 41, D475-D482.	14.5	418
48	Protein Flexibility in Virtual Screening: The BACE-1 Case Study. Journal of Chemical Information and Modeling, 2012, 52, 2697-2704.	5.4	47
49	Illustrating the machinery of life: Viruses. Biochemistry and Molecular Biology Education, 2012, 40, 291-296.	1.2	8
50	Putting proteins in context. BioEssays, 2012, 34, 718-720.	2.5	4
51	ePMV Embeds Molecular Modeling into Professional Animation Software Environments. Structure, 2011, 19, 293-303.	3.3	82
52	The evolution of the RCSB Protein Data Bank website. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 782-789.	14.6	7
53	Redoxâ€Based Probes for Protein Tyrosine Phosphatases. Angewandte Chemie - International Edition, 2011, 50, 4423-4427.	13.8	48
54	Eukaryotic cell panorama. Biochemistry and Molecular Biology Education, 2011, 39, 91-101.	1.2	22

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55	Atomic Evidence: The Foundations of Structural Molecular Biology. Science Progress, 2011, 94, 414-430.	1.9	1
56	The RCSB Protein Data Bank: redesigned web site and web services. Nucleic Acids Research, 2011, 39, D392-D401.	14.5	549
57	Promoting a structural view of biology for varied audiences: an overview of RCSB PDB resources and experiences. Journal of Applied Crystallography, 2010, 43, 1224-1229.	4.5	41
58	Visualization of macromolecular structures. Nature Methods, 2010, 7, S42-S55.	19.0	137
59	Visualizing biological dataâ€"now and in the future. Nature Methods, 2010, 7, S2-S4.	19.0	115
60	Artophagy: The Art of Autophagy-the Cvt pathway. Autophagy, 2010, 6, 3-6.	9.1	13
61	Virtual screening with AutoDock: theory and practice. Expert Opinion on Drug Discovery, 2010, 5, 597-607.	5.0	462
62	Fact and Fantasy in Nanotech Imagery. Leonardo, 2009, 42, 52-57.	0.3	9
63	AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of Computational Chemistry, 2009, 30, 2785-2791.	3.3	16,850
64	Neuromuscular synapse. Biochemistry and Molecular Biology Education, 2009, 37, 204-210.	1.2	11
65	Escherichia coli. Biochemistry and Molecular Biology Education, 2009, 37, 325-332.	1.2	28
66	The Machinery of Life. , 2009, , .		156
67	Computational Docking of Biomolecular Complexes with AutoDock. Cold Spring Harbor Protocols, 2009, 2009, pdb.prot5200.	0.3	33
68	Automated prediction of ligandâ€binding sites in proteins. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1506-1517.	2.6	134
69	Empirical entropic contributions in computational docking: Evaluation in APS reductase complexes. Journal of Computational Chemistry, 2008, 29, 1753-1761.	3.3	34
70	Structure-Based Virtual Screening and Biological Evaluation of Mycobacterium tuberculosis Adenosine 5â€²-Phosphosulfate Reductase Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 6627-6630.	6.4	32
71	Filling in the Gaps: Artistic License in Education and Outreach. PLoS Biology, 2007, 5, e308.	5.6	38
72	A semiempirical free energy force field with charge-based desolvation. Journal of Computational Chemistry, 2007, 28, 1145-1152.	3.3	1,854

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73	Making the step from chemistry to biology and back. Nature Chemical Biology, 2007, 3, 681-684.	8.0	4
74	Seeing the nanoscale. Nano Today, 2006, 1, 44-49.	11.9	285
75	Tactile teaching: Exploring protein structure/function using physical models. Biochemistry and Molecular Biology Education, 2006, 34, 247-254.	1.2	77
76	Representing Structural Information with RasMol. Current Protocols in Bioinformatics, 2005, 11, Unit 5.4.	25.8	23
77	Visual Methods from Atoms to Cells. Structure, 2005, 13, 347-354.	3.3	46
78	1,2,3-Triazole as a Peptide Surrogate in the Rapid Synthesis of HIV-1 Protease Inhibitors. ChemBioChem, 2005, 6, 1167-1169.	2.6	262
79	The cAMP binding domain: An ancient signaling module. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 45-50.	7.1	190
80	Automated docking of ligands to an artificial active site: augmenting crystallographic analysis with computer modeling. Journal of Computer-Aided Molecular Design, 2003, 17, 525-536.	2.9	81
81	Rapid Diversity-Oriented Synthesis in Microtiter Plates for In Situ Screening of HIV Protease Inhibitors. ChemBioChem, 2003, 4, 1246-1248.	2.6	134
82	Looking at Molecules-An Essay on Art and Science. ChemBioChem, 2003, 4, 1293-1297.	2.6	6
83	Automated docking to multiple target structures: Incorporation of protein mobility and structural water heterogeneity in AutoDock. Proteins: Structure, Function and Bioinformatics, 2002, 46, 34-40.	2.6	394
84	Recognition templates for predicting adenylate-binding sites in proteins. Journal of Molecular Biology, 2001, 314, 1245-1255.	4.2	16
85	Structural Symmetry and Protein Function. Annual Review of Biophysics and Biomolecular Structure, 2000, 29, 105-153.	18.3	806
86	The Molecular Perspective: DNA. Oncologist, 2000, 5, 81-82.	3.7	0
87	The Molecular Perspective: DNA. Stem Cells, 2000, 18, 148-149.	3.2	5
88	Atomistic vs. Continuous Representations in Molecular Biology. , 1999, , 146-155.		4
89	Morphology of proteinâ€“protein interfaces. Structure, 1998, 6, 421-427.	3.3	218
90	Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function. Journal of Computational Chemistry, 1998, 19, 1639-1662.	3.3	8,897

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91	Interactive modeling of supramolecular assemblies. Journal of Molecular Graphics and Modelling, 1998, 16, 115-120.	2.4	7
92	An Analysis of a Class of DNA Sequence Reading Molecules. Journal of Computational Biology, 1998, 5, 571-583.	1.6	1
93	Defining GC-specificity in the minor groove: side-by-side binding of the di-imidazole lexitropsin to C-A-T-G-G-C-C-A-T-G. Structure, 1997, 5, 1033-1046.	3.3	109
94	Design of stapled DNA-minor-groove-binding molecules with a mutable atom simulated annealing method. Journal of Computer-Aided Molecular Design, 1997, 11, 539-546.	2.9	3
95	Progress in the design of DNA sequence-specific lexitropsins. , 1997, 44, 323-334.		28
96	Chapter 7 Molecules in living cells. Principles of Medical Biology, 1996, , 173-180.	0.1	0
97	Automated docking of flexible ligands: Applications of autodock. Journal of Molecular Recognition, 1996, 9, 1-5.	2.1	1,284
98	Distributed automated docking of flexible ligands to proteins: Parallel applications of AutoDock 2.4. Journal of Computer-Aided Molecular Design, 1996, 10, 293-304.	2.9	907
99	Design of B-DNA cross-linking and sequence-reading molecules. Biopolymers, 1995, 35, 543-553.	2.4	15
100	Crystal Structure of C-T-C-T-C-G-A-G-A-G. Implications for the Structure of the Holliday Junction. Biochemistry, 1995, 34, 1022-1029.	2.5	62
101	Structure of a dicationic monoimidazole lexitropsin bound to DNA. Biochemistry, 1995, 34, 16654-16661.	2.5	31
102	Refinement of Netropsin Bound to DNA: Bias and Feedback in Electron Density Map Interpretation. Biochemistry, 1995, 34, 4983-4993.	2.5	86
103	Crystal Structure of a Covalent DNA-Drug Adduct: Anthramycin Bound to C-C-A-A-C-G-T-T-G-G and a Molecular Explanation of Specificity. Biochemistry, 1994, 33, 13593-13610.	2.5	115
104	The Crystal Structure of C-C-A-T-T-A-A-T-G-G. Journal of Molecular Biology, 1994, 239, 79-96.	4.2	149
105	Bending and curvature calculations in B-DNA. Nucleic Acids Research, 1994, 22, 5497-5503.	14.5	284
106	Automated docking in crystallography: Analysis of the substrates of aconitase. Proteins: Structure, Function and Bioinformatics, 1993, 17, 1-10.	2.6	84
107	Crystallographic analysis of C-C-A-A-G-C-T-T-G-G and its implications for bending in B-DNA. Biochemistry, 1993, 32, 8923-8931.	2.5	76
108	Macromolecular graphics. Current Opinion in Structural Biology, 1992, 2, 193-201.	5.7	9

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109	Visualizing Biological Molecules. Scientific American, 1992, 267, 76-81.	1.0	31
110	Molecular illustration in black and white. Journal of Molecular Graphics, 1992, 10, 235-240.	1.1	17
111	Inside a living cell. Trends in Biochemical Sciences, 1991, 16, 203-206.	7.5	315
112	Automated docking of substrates to proteins by simulated annealing. Proteins: Structure, Function and Bioinformatics, 1990, 8, 195-202.	2.6	1,109
113	Rendering volumetric data in molecular systems. Journal of Molecular Graphics, 1989, 7, 41-47.	1.1	55
114	RMS: programs for generating raster molecular surfaces. Journal of Molecular Graphics, 1988, 6, 41-44.	1.1	10
115	The Effect of Crystal Packing on Oligonucleotide Double Helix Structure. Journal of Biomolecular Structure and Dynamics, 1987, 5, 557-579.	3.5	126