List of Publications by Year in descending order

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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	AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of Computational Chemistry, 2009, 30, 2785-2791.	3.3	16,850
2	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
3	A semiempirical free energy force field with charge-based desolvation. Journal of Computational Chemistry, 2007, 28, 1145-1152.	3.3	1,854
4	Computational proteinâ€“ligand docking and virtual drug screening with the AutoDock suite. Nature Protocols, 2016, 11, 905-919.	12.0	1,370
5	Automated docking of flexible ligands: Applications of autodock. Journal of Molecular Recognition, 1996, 9, 1-5.	2.1	1,284
6	Automated docking of substrates to proteins by simulated annealing. Proteins: Structure, Function and Bioinformatics, 1990, 8, 195-202.	2.6	1,109
7	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
8	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
9	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
10	Structural Symmetry and Protein Function. Annual Review of Biophysics and Biomolecular Structure, 2000, 29, 105-153.	18.3	806
11	Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.	14.5	671
12	OUP accepted manuscript. Nucleic Acids Research, 2017, 45, D271-D281.	14.5	619
13	The RCSB Protein Data Bank: redesigned web site and web services. Nucleic Acids Research, 2011, 39, D392-D401.	14.5	549
14	Virtual screening with AutoDock: theory and practice. Expert Opinion on Drug Discovery, 2010, 5, 597-607.	5.0	462
15	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
16	The RCSB Protein Data Bank: new resources for research and education. Nucleic Acids Research, 2012, 41, D475-D482.	14.5	418
17	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
18	Inside a living cell. Trends in Biochemical Sciences, 1991, 16, 203-206.	7.5	315

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19	AutoDockFR: Advances in Protein-Ligand Docking with Explicitly Specified Binding Site Flexibility. PLoS Computational Biology, 2015, 11, e1004586.	3.2	287
20	Seeing the nanoscale. Nano Today, 2006, 1, 44-49.	11.9	285
21	Bending and curvature calculations in B-DNA. Nucleic Acids Research, 1994, 22, 5497-5503.	14.5	284
22	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
23	RCSB Protein Data Bank: Enabling biomedical research and drug discovery. Protein Science, 2020, 29, 52-65.	7.6	223
24	Morphology of proteinâ€“protein interfaces. Structure, 1998, 6, 421-427.	3.3	218
25	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
26	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
27	Covalent docking using autodock: Twoâ€point attractor and flexible side chain methods. Protein Science, 2016, 25, 295-301.	7.6	170
28	The Machinery of Life. , 2009, , .		156
29	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
30	Visualization of macromolecular structures. Nature Methods, 2010, 7, S42-S55.	19.0	137
31	Rapid Diversity-Oriented Synthesis in Microtiter Plates for In Situ Screening of HIV Protease Inhibitors. ChemBioChem, 2003, 4, 1246-1248.	2.6	134
32	Automated prediction of ligandâ€binding sites in proteins. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1506-1517.	2.6	134
33	cellPACK: a virtual mesoscope to model and visualize structural systems biology. Nature Methods, 2015, 12, 85-91.	19.0	130
34	The Effect of Crystal Packing on Oligonucleotide Double Helix Structure. Journal of Biomolecular Structure and Dynamics, 1987, 5, 557-579.	3.5	126
35	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
36	Visualizing biological dataâ€”now and in the future. Nature Methods, 2010, 7, S2-S4.	19.0	115

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37	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
38	The RCSB PDB â€œMolecule of the Monthâ€• Inspiring a Molecular View of Biology. PLoS Biology, 2015, 13, e1002140.	5.6	88
39	Illustrate: Software for Biomolecular Illustration. Structure, 2019, 27, 1716-1720.e1.	3.3	87
40	Refinement of Netropsin Bound to DNA: Bias and Feedback in Electron Density Map Interpretation. Biochemistry, 1995, 34, 4983-4993.	2.5	86
41	The <scp>AutoDock</scp> suite at 30. Protein Science, 2021, 30, 31-43.	7.6	85
42	Automated docking in crystallography: Analysis of the substrates of aconitase. Proteins: Structure, Function and Bioinformatics, 1993, 17, 1-10.	2.6	84
43	<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
44	ePMV Embeds Molecular Modeling into Professional Animation Software Environments. Structure, 2011, 19, 293-303.	3.3	82
45	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
46	Tactile teaching: Exploring protein structure/function using physical models. Biochemistry and Molecular Biology Education, 2006, 34, 247-254.	1.2	77
47	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
48	A visual review of the human pathogen Streptococcus pneumoniae. FEMS Microbiology Reviews, 2017, 41, 854-879.	8.6	72
49	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
50	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
51	Rendering volumetric data in molecular systems. Journal of Molecular Graphics, 1989, 7, 41-47.	1.1	55
52	3D molecular models of whole HIV-1 virions generated with cellPACK. Faraday Discussions, 2014, 169, 23-44.	3.2	52
53	Molecular Illustration in Research and Education: Past, Present, and Future. Journal of Molecular Biology, 2018, 430, 3969-3981.	4.2	52
54	Redoxâ€Based Probes for Protein Tyrosine Phosphatases. Angewandte Chemie - International Edition, 2011, 50, 4423-4427.	13.8	48

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55	Protein Flexibility in Virtual Screening: The BACE-1 Case Study. Journal of Chemical Information and Modeling, 2012, 52, 2697-2704.	5.4	47
56	Visual Methods from Atoms to Cells. Structure, 2005, 13, 347-354.	3.3	46
57	<scp>PDB</scp>â€101: Educational resources supporting molecular explorations through biology and medicine. Protein Science, 2022, 31, 129-140.	7.6	43
58	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
59	Building Structural Models of a Whole Mycoplasma Cell. Journal of Molecular Biology, 2022, 434, 167351.	4.2	40
60	Filling in the Gaps: Artistic License in Education and Outreach. PLoS Biology, 2007, 5, e308.	5.6	38
61	Instant Construction and Visualization of Crowded Biological Environments. IEEE Transactions on Visualization and Computer Graphics, 2018, 24, 862-872.	4.4	36
62	Art and Science of the Cellular Mesoscale. Trends in Biochemical Sciences, 2020, 45, 472-483.	7.5	36
63	Empirical entropic contributions in computational docking: Evaluation in APS reductase complexes. Journal of Computational Chemistry, 2008, 29, 1753-1761.	3.3	34
64	Computational Docking of Biomolecular Complexes with AutoDock. Cold Spring Harbor Protocols, 2009, 2009, pdb.prot5200.	0.3	33
65	CellPAINT: Interactive Illustration of Dynamic Mesoscale Cellular Environments. IEEE Computer Graphics and Applications, 2018, 38, 51-66.	1.2	33
66	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
67	Visualizing Biological Molecules. Scientific American, 1992, 267, 76-81.	1.0	31
68	Structure of a dicationic monoimidazole lexitropsin bound to DNA. Biochemistry, 1995, 34, 16654-16661.	2.5	31
69	From Atoms to Cells: Using Mesoscale Landscapes to Construct Visual Narratives. Journal of Molecular Biology, 2018, 430, 3954-3968.	4.2	31
70	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
71	Progress in the design of DNA sequence-specific lexitropsins. , 1997, 44, 323-334.		28
72	Escherichia coli. Biochemistry and Molecular Biology Education, 2009, 37, 325-332.	1.2	28

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73	Illustrations of the HIV Life Cycle. Current Topics in Microbiology and Immunology, 2015, 389, 243-252.	1.1	25
74	Representing Structural Information with RasMol. Current Protocols in Bioinformatics, 2005, 11, Unit 5.4.	25.8	23
75	Lattice Models of Bacterial Nucleoids. Journal of Physical Chemistry B, 2018, 122, 5441-5447.	2.6	23
76	Eukaryotic cell panorama. Biochemistry and Molecular Biology Education, 2011, 39, 91-101.	1.2	22
77	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
78	CellPAINT: Turnkey Illustration of Molecular Cell Biology. Frontiers in Bioinformatics, 2021, 1, .	2.1	20
79	Integrative illustration for coronavirus outreach. PLoS Biology, 2020, 18, e3000815.	5.6	18
80	Molecular illustration in black and white. Journal of Molecular Graphics, 1992, 10, 235-240.	1.1	17
81	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
82	Impact of the Protein Data Bank Across Scientific Disciplines. Data Science Journal, 2020, 19, 25.	1.3	17
83	Recognition templates for predicting adenylate-binding sites in proteins. Journal of Molecular Biology, 2001, 314, 1245-1255.	4.2	16
84	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
85	Insights from 20â€‰years of the Molecule of the Month. Biochemistry and Molecular Biology Education, 2020, 48, 350-355.	1.2	16
86	Design of B-DNA cross-linking and sequence-reading molecules. Biopolymers, 1995, 35, 543-553.	2.4	15
87	Artophagy: The Art of Autophagy-the Cvt pathway. Autophagy, 2010, 6, 3-6.	9.1	13
88	Seeing the PDB. Journal of Biological Chemistry, 2021, 296, 100742.	3.4	13
89	Neuromuscular synapse. Biochemistry and Molecular Biology Education, 2009, 37, 204-210.	1.2	11
90	RMS: programs for generating raster molecular surfaces. Journal of Molecular Graphics, 1988, 6, 41-44.	1.1	10

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91	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
92	Macromolecular graphics. Current Opinion in Structural Biology, 1992, 2, 193-201.	5.7	9
93	Fact and Fantasy in Nanotech Imagery. Leonardo, 2009, 42, 52-57.	0.3	9
94	Illustrating the machinery of life: Viruses. Biochemistry and Molecular Biology Education, 2012, 40, 291-296.	1.2	8
95	Interactive modeling of supramolecular assemblies. Journal of Molecular Graphics and Modelling, 1998, 16, 115-120.	2.4	7
96	The evolution of the RCSB Protein Data Bank website. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 782-789.	14.6	7
97	Molecular storytelling for online structural biology outreach and education. Structural Dynamics, 2021, 8, 020401.	2.3	7
98	Art as a tool for science. Nature Structural and Molecular Biology, 2021, 28, 402-403.	8.2	7
99	Exploring protein symmetry at the RCSB Protein Data Bank. Emerging Topics in Life Sciences, 2022, 6, 231-243.	2.6	7
100	Looking at Molecules-An Essay on Art and Science. ChemBioChem, 2003, 4, 1293-1297.	2.6	6
101	Protein structure in context: The molecular landscape of angiogenesis. Biochemistry and Molecular Biology Education, 2013, 41, 213-223.	1.2	6
102	RCSB Protein Data Bank tools for 3D structure-guided cancer research: human papillomavirus (HPV) case study. Oncogene, 2020, 39, 6623-6632.	5.9	6
103	Integrative illustration of a JCVI-syn3A minimal cell. Journal of Integrative Bioinformatics, 2022, 19, .	1.5	6
104	The Molecular Perspective: DNA. Stem Cells, 2000, 18, 148-149.	3.2	5
105	Making the step from chemistry to biology and back. Nature Chemical Biology, 2007, 3, 681-684.	8.0	4
106	Putting proteins in context. BioEssays, 2012, 34, 718-720.	2.5	4
107	Fragment-Based Analysis of Ligand Dockings Improves Classification of Actives. Journal of Chemical Information and Modeling, 2016, 56, 1597-1607.	5.4	4
108	Integrative modeling of the HIV-1 ribonucleoprotein complex. PLoS Computational Biology, 2019, 15, e1007150.	3.2	4

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109	Atomistic vs. Continuous Representations in Molecular Biology. , 1999, , 146-155.		4
110	Symmetry at the Cellular Mesoscale. Symmetry, 2019, 11, 1170.	2.2	4
111	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
112	An Analysis of a Class of DNA Sequence Reading Molecules. Journal of Computational Biology, 1998, 5, 571-583.	1.6	1
113	Atomic Evidence: The Foundations of Structural Molecular Biology. Science Progress, 2011, 94, 414-430.	1.9	1
114	Chapter 7 Molecules in living cells. Principles of Medical Biology, 1996, , 173-180.	0.1	0
115	The Molecular Perspective: DNA. Oncologist, 2000, 5, 81-82.	3.7	0