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List of Publications by Year
in descending order

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38 papers	2,608 citations	331259 21 h-index	315357 38 g-index
40 all docs	40 docs citations	40 times ranked	3582 citing authors

#	Article	IF	Citations
1	Parmbsc1: a refined force field for DNA simulations. Nature Methods, 2016, 13, 55-58.	9.0	790
2	Molecular dynamics simulations: advances and applications. Advances and Applications in Bioinformatics and Chemistry, 2015, 8, 37.	1.6	409
3	A consensus view of protein dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 796-801.	3.3	223
4	MDWeb and MDMoby: an integrated web-based platform for molecular dynamics simulations. Bioinformatics, 2012, 28, 1278-1279.	1.8	153
5	MoDEL (Molecular Dynamics Extended Library): AÂDatabase of Atomistic Molecular Dynamics Trajectories. Structure, 2010, 18, 1399-1409.	1.6	123
6	How accurate are accurate force-fields for B-DNA?. Nucleic Acids Research, 2017, 45, gkw1355.	6.5	107
7	Long-timescale dynamics of the Drewâ€“Dickerson dodecamer. Nucleic Acids Research, 2016, 44, 4052-4066.	6.5	86
8	FlexServ: an integrated tool for the analysis of protein flexibility. Bioinformatics, 2009, 25, 1709-1710.	1.8	72
9	BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. Nucleic Acids Research, 2016, 44, D272-D278.	6.5	57
10	Oncogenic mutations at the EGFR ectodomain structurally converge to remove a steric hindrance on a kinase-coupled cryptic epitope. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10009-10018.	3.3	46
11	NAFlex: a web server for the study of nucleic acid flexibility. Nucleic Acids Research, 2013, 41, W47-W55.	6.5	45
12	The static and dynamic structural heterogeneities of B-DNA: extending Calladineâ€“Dickerson rules. Nucleic Acids Research, 2019, 47, 11090-11102.	6.5	45
13	BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows. Scientific Data, 2019, 6, 169.	2.4	35
14	How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. Journal of Molecular Biology, 2019, 431, 3845-3859.	2.0	34
15	Coarse-grained Representation of Protein Flexibility. Foundations, Successes, and Shortcomings. Advances in Protein Chemistry and Structural Biology, 2011, 85, 183-215.	1.0	33
16	Modulation of the helical properties of DNA: next-to-nearest neighbour effects and beyond. Nucleic Acids Research, 2019, 47, 4418-4430.	6.5	32
17	Finding Conformational Transition Pathways from Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 4707-4718.	2.3	29
18	A multi-modal coarse grained model of DNA flexibility mappable to the atomistic level. Nucleic Acids Research, 2020, 48, e29-e29.	6.5	27

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19	Exploration of conformational transition pathways from coarse-grained simulations. Bioinformatics, 2013, 29, 1980-1986.	1.8	26
20	Mechanism of Structural Tuning of the Hepatitis C Virus Human Cellular Receptor CD81 Large Extracellular Loop. Structure, 2017, 25, 53-65.	1.6	25
21	Small Details Matter: The 2â€²-Hydroxyl as a Conformational Switch in RNA. Journal of the American Chemical Society, 2016, 138, 16355-16363.	6.6	23
22	DNA structure directs positioning of the mitochondrial genome packaging protein Abf2p. Nucleic Acids Research, 2017, 45, 951-967.	6.5	23
23	The Role of Unconventional Hydrogen Bonds in Determining BII Propensities in B-DNA. Journal of Physical Chemistry Letters, 2017, 8, 21-28.	2.1	18
24	The Multiple Roles of Waters in Protein Solvation. Journal of Physical Chemistry B, 2017, 121, 3636-3643.	1.2	17
25	Exploring the Conformational Landscape of Bioactive Small Molecules. Journal of Chemical Theory and Computation, 2020, 16, 6575-6585.	2.3	17
26	Surviving the deluge of biosimulation data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1449.	6.2	16
27	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. Angewandte Chemie - International Edition, 2019, 58, 3759-3763.	7.2	15
28	Sequence-dependent structural properties of B-DNA: what have we learned in 40Âyears?. Biophysical Reviews, 2021, 13, 995-1005.	1.5	13
29	Nucleosome Dynamics: a new tool for the dynamic analysis of nucleosome positioning. Nucleic Acids Research, 2019, 47, 9511-9523.	6.5	12
30	Bioactive Conformational Ensemble Server and Database. A Public Framework to Speed Up In Silico Drug Discovery. Journal of Chemical Theory and Computation, 2020, 16, 6586-6597.	2.3	10
31	Molecular Dynamics Study of Naturally Existing Cavity Couplings in Proteins. PLoS ONE, 2015, 10, e0119978.	1.1	10
32	BioExcel Building Blocks Workflows (BioBB-Wfs), an integrated web-based platform for biomolecular simulations. Nucleic Acids Research, 2022, 50, W99-W107.	6.5	7
33	Highâ€throughput molecular dynamics simulations: toward a dynamic view of macromolecular structure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 364-377.	6.2	6
34	3dRS, a Web-Based Tool to Share Interactive Representations of 3D Biomolecular Structures and Molecular Dynamics Trajectories. Frontiers in Molecular Biosciences, 2021, 8, 726232.	1.6	6
35	<scp>Preâ€exascale HPC</scp> approaches for molecular dynamics simulations. Covidâ€19 research: A use case. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	6
36	DFFR: A New Method for High-Throughput Recalibration of Automatic Force-Fields for Drugs. Journal of Chemical Theory and Computation, 2020, 16, 6598-6608.	2.3	5

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37	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. Angewandte Chemie, 2019, 131, 3799-3803.	1.6	4
38	A fast method for the determination of fractional contributions to solvation in proteins. Protein Science, 2006, 15, 2525-2533.	3.1	3