Adam Hospital Gasch

List of Publications by Year
in descending order

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Version: 2024-02-01

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	<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
2	BioExcel Building Blocks Workflows (BioBB-Wfs), an integrated web-based platform for biomolecular simulations. Nucleic Acids Research, 2022, 50, W99-W107.	6.5	7
3	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
4	Sequence-dependent structural properties of B-DNA: what have we learned in 40Âyears?. Biophysical Reviews, 2021, 13, 995-1005.	1.5	13
5	Surviving the deluge of biosimulation data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1449.	6.2	16
6	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
7	Exploring the Conformational Landscape of Bioactive Small Molecules. Journal of Chemical Theory and Computation, 2020, 16, 6575-6585.	2.3	17
8	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
9	A multi-modal coarse grained model of DNA flexibility mappable to the atomistic level. Nucleic Acids Research, 2020, 48, e29-e29.	6.5	27
10	How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. Journal of Molecular Biology, 2019, 431, 3845-3859.	2.0	34
11	The static and dynamic structural heterogeneities of B-DNA: extending Calladineâ€“Dickerson rules. Nucleic Acids Research, 2019, 47, 11090-11102.	6.5	45
12	BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows. Scientific Data, 2019, 6, 169.	2.4	35
13	Nucleosome Dynamics: a new tool for the dynamic analysis of nucleosome positioning. Nucleic Acids Research, 2019, 47, 9511-9523.	6.5	12
14	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. Angewandte Chemie - International Edition, 2019, 58, 3759-3763.	7.2	15
15	Predicting the Limit of Intramolecular Hydrogen Bonding with Classical Molecular Dynamics. Angewandte Chemie, 2019, 131, 3799-3803.	1.6	4
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	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
18	The Multiple Roles of Waters in Protein Solvation. Journal of Physical Chemistry B, 2017, 121, 3636-3643.	1.2	17

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19	How accurate are accurate force-fields for B-DNA?. Nucleic Acids Research, 2017, 45, gkw1355.	6.5	107
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	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
22	DNA structure directs positioning of the mitochondrial genome packaging protein Abf2p. Nucleic Acids Research, 2017, 45, 951-967.	6.5	23
23	Long-timescale dynamics of the Drewâ€“Dickerson dodecamer. Nucleic Acids Research, 2016, 44, 4052-4066.	6.5	86
24	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
25	Parmbsc1: a refined force field for DNA simulations. Nature Methods, 2016, 13, 55-58.	9.0	790
26	BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. Nucleic Acids Research, 2016, 44, D272-D278.	6.5	57
27	Molecular dynamics simulations: advances and applications. Advances and Applications in Bioinformatics and Chemistry, 2015, 8, 37.	1.6	409
28	Molecular Dynamics Study of Naturally Existing Cavity Couplings in Proteins. PLoS ONE, 2015, 10, e0119978.	1.1	10
29	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
30	NAFlex: a web server for the study of nucleic acid flexibility. Nucleic Acids Research, 2013, 41, W47-W55.	6.5	45
31	Exploration of conformational transition pathways from coarse-grained simulations. Bioinformatics, 2013, 29, 1980-1986.	1.8	26
32	MDWeb and MDMoby: an integrated web-based platform for molecular dynamics simulations. Bioinformatics, 2012, 28, 1278-1279.	1.8	153
33	Finding Conformational Transition Pathways from Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 4707-4718.	2.3	29
34	Coarse-grained Representation of Protein Flexibility. Foundations, Successes, and Shortcomings. Advances in Protein Chemistry and Structural Biology, 2011, 85, 183-215.	1.0	33
35	MoDEL (Molecular Dynamics Extended Library): AÂDatabase of Atomistic Molecular Dynamics Trajectories. Structure, 2010, 18, 1399-1409.	1.6	123
36	FlexServ: an integrated tool for the analysis of protein flexibility. Bioinformatics, 2009, 25, 1709-1710.	1.8	72

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37	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
38	A fast method for the determination of fractional contributions to solvation in proteins. Protein Science, 2006, 15, 2525-2533.	3.1	3