

Pablo D Dans

List of Publications by Year in descending order

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43
papers

2,994
citations

257450

24
h-index

265206

42
g-index

47
all docs

47
docs citations

47
times ranked

3538
citing authors

#	ARTICLE	IF	CITATIONS
1	Parmbsc1: a refined force field for DNA simulations. <i>Nature Methods</i> , 2016, 13, 55-58.	19.0	790
2	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. <i>Nucleic Acids Research</i> , 2014, 42, 12272-12283.	14.5	186
3	Direct measurement of the dielectric polarization properties of DNA. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E3624-30.	7.1	160
4	A Coarse Grained Model for Atomic-Detailed DNA Simulations with Explicit Electrostatics. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1711-1725.	5.3	127
5	Multiscale simulation of DNA. <i>Current Opinion in Structural Biology</i> , 2016, 37, 29-45.	5.7	124
6	The structural impact of DNA mismatches. <i>Nucleic Acids Research</i> , 2015, 43, 4309-4321.	14.5	113
7	Connecting Proline and Î³-Aminobutyric Acid in Stressed Plants through Non-Enzymatic Reactions. <i>PLoS ONE</i> , 2015, 10, e0115349.	2.5	112
8	Another Coarse Grain Model for Aqueous Solvation: WAT FOUR?. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3793-3807.	5.3	111
9	How accurate are accurate force-fields for B-DNA?. <i>Nucleic Acids Research</i> , 2017, 45, gkw1355.	14.5	107
10	Epigenetic loss of RNA-methyltransferase NSUN5 in glioma targets ribosomes to drive a stress adaptive translational program. <i>Acta Neuropathologica</i> , 2019, 138, 1053-1074.	7.7	106
11	Glyceraldehyde-3-phosphate dehydrogenase is a chaperone that allocates labile heme in cells. <i>Journal of Biological Chemistry</i> , 2018, 293, 14557-14568.	3.4	93
12	Exploring polymorphisms in B-DNA helical conformations. <i>Nucleic Acids Research</i> , 2012, 40, 10668-10678.	14.5	89
13	Long-timescale dynamics of the Drewâ€Dickerson dodecamer. <i>Nucleic Acids Research</i> , 2016, 44, 4052-4066.	14.5	86
14	Switching Reversibility to Irreversibility in Glycogen Synthase Kinase 3 Inhibitors: Clues for Specific Design of New Compounds. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 4042-4056.	6.4	84
15	Unraveling the sequence-dependent polymorphic behavior of d(CpC) steps in B-DNA. <i>Nucleic Acids Research</i> , 2014, 42, 11304-11320.	14.5	81
16	Impact of DNA methylation on 3D genome structure. <i>Nature Communications</i> , 2021, 12, 3243.	12.8	61
17	BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data. <i>Nucleic Acids Research</i> , 2016, 44, D272-D278.	14.5	57
18	Saturation of recognition elements blocks evolution of new tRNA identities. <i>Science Advances</i> , 2016, 2, e1501860.	10.3	46

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19	The static and dynamic structural heterogeneities of B-DNA: extending Calladine's Dickerson rules. <i>Nucleic Acids Research</i> , 2019, 47, 11090-11102.	14.5	45
20	A hybrid all-atom/coarse grain model for multiscale simulations of DNA. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18134.	2.8	43
21	Breathing, bubbling, and bending: DNA flexibility from multimicrosecond simulations. <i>Physical Review E</i> , 2012, 86, 021903.	2.1	35
22	How B-DNA Dynamics Decipher Sequence-Selective Protein Recognition. <i>Journal of Molecular Biology</i> , 2019, 431, 3845-3859.	4.2	34
23	Modulation of the helical properties of DNA: next-to-nearest neighbour effects and beyond. <i>Nucleic Acids Research</i> , 2019, 47, 4418-4430.	14.5	32
24	Allosterism and signal transfer in DNA. <i>Nucleic Acids Research</i> , 2018, 46, 7554-7565.	14.5	30
25	A multi-modal coarse grained model of DNA flexibility mappable to the atomistic level. <i>Nucleic Acids Research</i> , 2020, 48, e29-e29.	14.5	27
26	Antimicrobial and structural insights of a new snakin-like peptide isolated from <i>Peltophorum dubium</i> (Fabaceae). <i>Amino Acids</i> , 2018, 50, 1245-1259.	2.7	25
27	Modeling, Simulations, and Bioinformatics at the Service of RNA Structure. <i>CheM</i> , 2019, 5, 51-73.	11.7	25
28	Small Details Matter: The 2'-OH as a Conformational Switch in RNA. <i>Journal of the American Chemical Society</i> , 2016, 138, 16355-16363.	13.7	23
29	Subcellular localization of the interaction between the human immunodeficiency virus transactivator Tat and the nucleosome assembly protein 1. <i>Amino Acids</i> , 2010, 38, 1583-1593.	2.7	20
30	Structural and Energetic Study of Cisplatin and Derivatives: Comparison of the Performance of Density Functional Theory Implementations. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 740-750.	5.3	18
31	The Role of Unconventional Hydrogen Bonds in Determining BII Propensities in B-DNA. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 21-28.	4.6	18
32	Assessing the Accuracy of the SIRAH Force Field to Model DNA at Coarse Grain Level. <i>Lecture Notes in Computer Science</i> , 2013, , 71-81.	1.3	18
33	Density Functional Theory Characterization and Descriptive Analysis of Cisplatin and Related Compounds. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1407-1419.	5.4	14
34	Sequence-dependent structural properties of B-DNA: what have we learned in 40 years?. <i>Biophysical Reviews</i> , 2021, 13, 995-1005.	3.2	13
35	An In-Depth Look at DNA Crystals through the Prism of Molecular Dynamics Simulations. <i>CheM</i> , 2019, 5, 649-663.	11.7	11
36	Isoform-specific determinants in the HP1 binding to histone 3: insights from molecular simulations. <i>Amino Acids</i> , 2010, 38, 1571-1581.	2.7	9

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37	The Impact of the HydroxyMethylCytosine epigenetic signature on DNA structure and function. PLoS Computational Biology, 2021, 17, e1009547.	3.2	6
38	Gene isolation and structural characterization of a legume tree defensin with a broad spectrum of antimicrobial activity. Planta, 2019, 250, 1757-1772.	3.2	5
39	VeriNA3d: an R package for nucleic acids data mining. Bioinformatics, 2019, 35, 5334-5336.	4.1	4
40	Antimicrobial peptides in the seedling transcriptome of the tree legume Peltophorum dubium. Biochimie, 2021, 180, 229-242.	2.6	2
41	Molecular Determinants for Nitric Oxide Regulation of the Murine Cationic Amino Acid Transporter CAT-2A. Biochemistry, 2020, 59, 4225-4237.	2.5	1
42	Molecular basis of Arginine and Lysine DNA sequence-dependent thermo-stability modulation. PLoS Computational Biology, 2022, 18, e1009749.	3.2	1
43	Chapter 7. Molecular Modelling of Nucleic Acids. Chemical Biology, 0, , 165-197.	0.2	0