alberto Perez

List of Publications by Year
in descending order

66 papers	7,043 citations	109137 35 h-index	102304 66 g-index
91 all docs	91 docs citations	91 times ranked	6412 citing authors

#	ARTICLE	IF	CITATIONS
1	Searching for Low Probability Opening Events in a DNA Sliding Clamp. Life, 2022, 12, 261.	1.1	0
2	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	9.0	73
3	Computational Modeling as a Tool to Investigate PPI: From Drug Design to Tissue Engineering. Frontiers in Molecular Biosciences, 2021, 8, 681617.	1.6	25
4	Modeling SARSâ€CoVâ€2 proteins in the CASPâ€commons experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1987-1996.	1.5	24
5	Importance of Anionâ˜Ï€ Interactions in RNA GAAA and GGAG Tetraloops: A Combined MD and QM Study. Journal of Chemical Theory and Computation, 2021, 17, 6624-6633.	2.3	5
6	CryoFold: Determining protein structures and data-guided ensembles from cryo-EM density maps. Matter, 2021, 4, 3195-3216.	5.0	26
7	Binding Ensembles of p53-MDM2 Peptide Inhibitors by Combining Bayesian Inference and Atomistic Simulations. Molecules, 2021, 26, 198.	1.7	12
8	Sequence-dependent structural properties of B-DNA: what have we learned in 40Âyears?. Biophysical Reviews, 2021, 13, 995-1005.	1.5	13
9	Simultaneous Assignment and Structure Determination of Proteins From Sparsely Labeled NMR Datasets. Frontiers in Molecular Biosciences, 2021, 8, 774394.	1.6	7
10	Improving the analysis of biological ensembles through extended similarity measures. Physical Chemistry Chemical Physics, 2021, 24, 444-451.	1.3	6
11	Computing Ligands Bound to Proteins Using MELD-Accelerated MD. Journal of Chemical Theory and Computation, 2020, 16, 6377-6382.	2.3	15
12	NMRâ€assisted protein structure prediction with MELDxMD. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1333-1340.	1.5	20
13	High Accuracy Protein Structures from Minimal Sparse Paramagnetic Solidâ€State NMR Restraints. Angewandte Chemie - International Edition, 2019, 58, 6564-6568.	7.2	11
14	High Accuracy Protein Structures from Minimal Sparse Paramagnetic Solidâ€State NMR Restraints. Angewandte Chemie, 2019, 131, 6636-6640.	1.6	3
15	Monte Carlo on the manifold and MD refinement for binding pose prediction of proteinâ€“ligand complexes: 2017 D3R Grand Challenge. Journal of Computer-Aided Molecular Design, 2019, 33, 119-127.	1.3	12
16	MELD-Path Efficiently Computes Conformational Transitions, Including Multiple and Diverse Paths. Journal of Chemical Theory and Computation, 2018, 14, 2109-2116.	2.3	13
17	MELD Ã— MD Folds Nonthreadables, Giving Native Structures and Populations. Journal of Chemical Theory and Computation, 2018, 14, 6734-6740.	2.3	12
18	Allosterism and signal transfer in DNA. Nucleic Acids Research, 2018, 46, 7554-7565.	6.5	30

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19	Accelerating physical simulations of proteins by leveraging external knowledge. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1309.	6.2	16
20	Computed Binding of Peptides to Proteins with MELD-Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 870-876.	2.3	68
21	Molecular Simulations Identify Binding Poses and Approximate Affinities of Stapled Î±-Helical Peptides to MDM2 and MDMX. Journal of Chemical Theory and Computation, 2017, 13, 863-869.	2.3	49
22	Regulation of the activity of the promoter of RNAâ€induced silencing, C3PO. Protein Science, 2017, 26, 1807-1818.	3.1	12
23	Expanding the repertoire of DNA shape features for genome-scale studies of transcription factor binding. Nucleic Acids Research, 2017, 45, 12877-12887.	6.5	81
24	Blind protein structure prediction using accelerated free-energy simulations. Science Advances, 2016, 2, e1601274.	4.7	57
25	Advances in free-energy-based simulations of protein folding and ligand binding. Current Opinion in Structural Biology, 2016, 36, 25-31.	2.6	121
26	Parmbsc1: a refined force field for DNA simulations. Nature Methods, 2016, 13, 55-58.	9.0	790
27	Constraint methods that accelerate free-energy simulations of biomolecules. Journal of Chemical Physics, 2015, 143, 243143.	1.2	1
28	The lipid raft proteome ofBorrelia burgdorferi. Proteomics, 2015, 15, 3662-3675.	1.3	26
29	Refinement of Generalized Born Implicit Solvation Parameters for Nucleic Acids and Their Complexes with Proteins. Journal of Chemical Theory and Computation, 2015, 11, 3714-3728.	2.3	58
30	Determining protein structures by combining semireliable data with atomistic physical models by Bayesian inference. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6985-6990.	3.3	132
31	Accelerating molecular simulations of proteins using Bayesian inference on weak information. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 11846-11851.	3.3	88
32	Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations. Journal of Chemical Theory and Computation, 2015, 11, 4770-4779.	2.3	76
33	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283.	6.5	186
34	Extracting representative structures from protein conformational ensembles. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2671-2680.	1.5	5
35	Computing the Relative Stabilities and the Per-Residue Components in Protein Conformational Changes. Structure, 2014, 22, 168-175.	1.6	27
36	Structure, Stiffness and Substates of the Dickerson-Drew Dodecamer. Journal of Chemical Theory and Computation, 2013, 9, 707-721.	2.3	78

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37	Exploring Early Stages of the Chemical Unfolding of Proteins at the Proteome Scale. PLoS Computational Biology, 2013, 9, e1003393.	1.5	14
38	FlexE: Using Elastic Network Models to Compare Models of Protein Structure. Journal of Chemical Theory and Computation, 2012, 8, 3985-3991.	2.3	20
39	Frontiers in Molecular Dynamics Simulations of DNA. Accounts of Chemical Research, 2012, 45, 196-205.	7.6	194
40	Exploring polymorphisms in B-DNA helical conformations. Nucleic Acids Research, 2012, 40, 10668-10678.	6.5	89
41	Impact of Methylation on the Physical Properties of DNA. Biophysical Journal, 2012, 102, 2140-2148.	0.2	118
42	Physical properties of naked DNA influence nucleosome positioning and correlate with transcription start and termination sites in yeast. BMC Genomics, 2011, 12, 489.	1.2	31
43	Assessment of protein structure refinement in CASP9. Proteins: Structure, Function and Bioinformatics, 2011, 79, 74-90.	1.5	87
44	MoDEL (Molecular Dynamics Extended Library): AÂDatabase of Atomistic Molecular Dynamics Trajectories. Structure, 2010, 18, 1399-1409.	1.6	123
45	Realâ€Time Atomistic Description of DNA Unfolding. Angewandte Chemie - International Edition, 2010, 49, 4805-4808.	7.2	30
46	Toward a Consensus View of Duplex RNA Flexibility. Biophysical Journal, 2010, 99, 1876-1885.	0.2	54
47	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. Nucleic Acids Research, 2010, 38, 299-313.	6.5	349
48	Towards a molecular dynamics consensus view of B-DNA flexibility. Nucleic Acids Research, 2008, 36, 2379-2394.	6.5	147
49	Recent advances in the study of nucleic acid flexibility by molecular dynamics. Current Opinion in Structural Biology, 2008, 18, 185-193.	2.6	113
50	Geometrical and Electronic Structure Variability of the Sugarâ^'phosphate Backbone in Nucleic Acids. Journal of Physical Chemistry B, 2008, 112, 8188-8197.	1.2	52
51	8-Amino guanine accelerates tetramolecular G-quadruplex formation. Chemical Communications, 2008, , 2926.	2.2	32
52	DNAlive: a tool for the physical analysis of DNA at the genomic scale. Bioinformatics, 2008, 24, 1731-1732.	1.8	28
53	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
54	Refinement of the AMBER Force Field for Nucleic Acids: Improving the Description of Î±/Î³ Conformers. Biophysical Journal, 2007, 92, 3817-3829.	0.2	2,036

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55	Theoretical study of large conformational transitions in DNA: the Bâ†"A conformational change in water and ethanol/water. Nucleic Acids Research, 2007, 35, 3330-3338.	6.5	71
56	Dynamics of B-DNA on the Microsecond Time Scale. Journal of the American Chemical Society, 2007, 129, 14739-14745.	6.6	250
57	Determining promoter location based on DNA structure first-principles calculations. Genome Biology, 2007, 8, R263.	13.9	121
58	Essential Dynamics:â€‰ A Tool for Efficient Trajectory Compression and Management. Journal of Chemical Theory and Computation, 2006, 2, 251-258.	2.3	98
59	Data Mining of Molecular Dynamics Trajectories of Nucleic Acids. Journal of Biomolecular Structure and Dynamics, 2006, 23, 447-455.	2.0	12
60	Are the Hydrogen Bonds of RNA (Aâ‹…U) Stronger Than those of DNA (Aâ‹…T)? A Quantum Mechanics Study. Chemistry - A European Journal, 2005, 11, 5062-5066.	1.7	42
61	Structure, Recognition Properties, and Flexibility of the DNAÂ·RNA Hybrid. Journal of the American Chemical Society, 2005, 127, 4910-4920.	6.6	64
62	Exploring the Essential Dynamics of B-DNA. Journal of Chemical Theory and Computation, 2005, 1, 790-800.	2.3	61
63	The relative flexibility of B-DNA and A-RNA duplexes: database analysis. Nucleic Acids Research, 2004, 32, 6144-6151.	6.5	119
64	Theoretical Methods for the Simulation of Nucleic Acids. ChemInform, 2004, 35, no.	0.1	0
65	Relative Flexibility of DNA and RNA: a Molecular Dynamics Study. Journal of Molecular Biology, 2004, 343, 627-638.	2.0	94
66	Theoretical methods for the simulation of nucleic acids. Chemical Society Reviews, 2003, 32, 350-364.	18.7	150