Massimiliano Bonomi

List of Publications by Year
in descending order

67	10,159	87888 38	133252 59
papers	citations	h-index	g-index

78	78	78	10004
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	PLUMED 2: New feathers for an old bird. Computer Physics Communications, 2014, 185, 604-613.	7.5	2,454
2	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	7.5	1,448
3	Metadynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 826-843.	14.6	971
4	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
5	Funnel metadynamics as accurate binding free-energy method. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6358-6363.	7.1	337
6	Reconstructing the equilibrium Boltzmann distribution from wellâ€tempered metadynamics. Journal of Computational Chemistry, 2009, 30, 1615-1621.	3.3	297
7	Principles of protein structural ensemble determination. Current Opinion in Structural Biology, 2017, 42, 106-116.	5.7	285
8	Bat coronaviruses related to SARS-CoV-2 and infectious for human cells. Nature, 2022, 604, 330-336.	27.8	238
9	Enhanced Sampling in the Well-Tempered Ensemble. Physical Review Letters, 2010, 104, 190601.	7.8	225
10	Effects of Î±-tubulin acetylation on microtubule structure and stability. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10366-10371.	7.1	216
11	Crystal structure of a eukaryotic phosphate transporter. Nature, 2013, 496, 533-536.	27.8	202
12	Molecular basis of cyclooxygenase enzymes (COXs) selective inhibition. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5411-5416.	7.1	187
13	Efficient Sampling of High-Dimensional Free-Energy Landscapes with Parallel Bias Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 5062-5067.	5.3	182
14	Metainference: A Bayesian inference method for heterogeneous systems. Science Advances, 2016, 2, e1501177.	10.3	180
15	Efficient Simulation of Explicitly Solvated Proteins in the Well-Tempered Ensemble. Journal of Chemical Theory and Computation, 2012, 8, 2189-2192.	5.3	127
16	Simultaneous quantification of protein order and disorder. Nature Chemical Biology, 2017, 13, 339-342.	8.0	113
17	Accuracy of Current All-Atom Force-Fields in Modeling Protein Disordered States. Journal of Chemical Theory and Computation, 2015, 11, 2-7.	5.3	109
18	Cys-Scanning Disulfide Crosslinking and Bayesian Modeling Probe the Transmembrane Signaling Mechanism of the Histidine Kinase, PhoQ. Structure, 2014, 22, 1239-1251.	3.3	103

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19	The Unfolded Ensemble and Folding Mechanism of the C-Terminal GB1 Î²-Hairpin. Journal of the American Chemical Society, 2008, 130, 13938-13944.	13.7	97
20	Small-molecule sequestration of amyloid-Î² as a drug discovery strategy for Alzheimerâ€™s disease. Science Advances, 2020, 6, .	10.3	95
21	Integrative structure modeling with the Integrative Modeling Platform. Protein Science, 2018, 27, 245-258.	7.6	92
22	Simultaneous Determination of Protein Structure and Dynamics Using Cryo-Electron Microscopy. Biophysical Journal, 2018, 114, 1604-1613.	0.5	88
23	Structural basis for alternating access of a eukaryotic calcium/proton exchanger. Nature, 2013, 499, 107-110.	27.8	87
24	Free-energy landscape of protein oligomerization from atomistic simulations. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E4708-13.	7.1	79
25	Metadynamic metainference: Enhanced sampling of the metainference ensemble using metadynamics. Scientific Reports, 2016, 6, 31232.	3.3	76
26	Determination of protein structural ensembles using cryo-electron microscopy. Current Opinion in Structural Biology, 2019, 56, 37-45.	5.7	67
27	Ligand Discovery for the Alanine-Serine-Cysteine Transporter (ASCT2, SLC1A5) from Homology Modeling and Virtual Screening. PLoS Computational Biology, 2015, 11, e1004477.	3.2	62
28	Sequence Specificity in the Entropy-Driven Binding of a Small Molecule and a Disordered Peptide. Journal of Molecular Biology, 2017, 429, 2772-2779.	4.2	62
29	Integrative structural and dynamical biology with PLUMED-ISDB. Bioinformatics, 2017, 33, 3999-4000.	4.1	59
30	Linking Well-Tempered Metadynamics Simulations with Experiments. Biophysical Journal, 2010, 98, L44-L46.	0.5	56
31	Reversible inhibition of the ClpP protease via an N-terminal conformational switch. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E6447-E6456.	7.1	56
32	Determination of Structural Ensembles of Proteins: Restraining vs Reweighting. Journal of Chemical Theory and Computation, 2018, 14, 6632-6641.	5.3	54
33	Structural Ensemble Modulation upon Small-Molecule Binding to Disordered Proteins. Journal of Molecular Biology, 2018, 430, 2288-2292.	4.2	53
34	The molecular architecture of the Dam1 kinetochore complex is defined by cross-linking based structural modelling. Nature Communications, 2015, 6, 8673.	12.8	51
35	Bayesian Weighing of Electron Cryo-Microscopy Data for Integrative Structural Modeling. Structure, 2019, 27, 175-188.e6.	3.3	50
36	High Selectivity of the Î³-Aminobutyric Acid Transporter 2 (GAT-2, SLC6A13) Revealed by Structure-based Approach. Journal of Biological Chemistry, 2012, 287, 37745-37756.	3.4	49

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37	Elucidating the Mechanism of Substrate Recognition by the Bacterial Hsp90 Molecular Chaperone. Journal of Molecular Biology, 2014, 426, 2393-2404.	4.2	45
38	Specific Ion Binding at Phospholipid Membrane Surfaces. Journal of Chemical Theory and Computation, 2015, 11, 4495-4499.	5.3	45
39	The molecular architecture of the yeast spindle pole body core determined by Bayesian integrative modeling. Molecular Biology of the Cell, 2017, 28, 3298-3314.	2.1	44
40	Insight into the Folding Inhibition of the HIV-1 Protease by a Small Peptide. Biophysical Journal, 2007, 93, 2813-2821.	0.5	40
41	Modeling of Proteins and Their Assemblies with the Integrative Modeling Platform. Methods in Molecular Biology, 2014, 1091, 277-295.	0.9	40
42	The Free Energy Profile of Tubulin Straight-Bent Conformational Changes, with Implications for Microtubule Assembly and Drug Discovery. PLoS Computational Biology, 2014, 10, e1003464.	3.2	35
43	Rational design of ASCT2 inhibitors using an integrated experimental-computational approach. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	35
44	Determining Protein Complex Structures Based on a Bayesian Model of in Vivo FÃ¶rster Resonance Energy Transfer (FRET) Data. Molecular and Cellular Proteomics, 2014, 13, 2812-2823.	3.8	29
45	Assessing the Quality of the OPEP Coarse-Grained Force Field. Journal of Chemical Theory and Computation, 2011, 7, 1928-1934.	5.3	28
46	A chiralityâ€based metrics for freeâ€energy calculations in biomolecular systems. Journal of Computational Chemistry, 2011, 32, 2627-2637.	3.3	25
47	Biasing Smarter, Not Harder, by Partitioning Collective Variables into Families in Parallel Bias Metadynamics. Journal of Chemical Theory and Computation, 2018, 14, 4985-4990.	5.3	23
48	Tackling Sampling Challenges in Biomolecular Simulations. Methods in Molecular Biology, 2015, 1215, 151-171.	0.9	23
49	Modeling of Proteins and Their Assemblies with the Integrative Modeling Platform. Methods in Molecular Biology, 2011, 781, 377-397.	0.9	18
50	Multiple Routes and Milestones in the Folding of HIVâ€“1 Protease Monomer. PLoS ONE, 2010, 5, e13208.	2.5	15
51	Solid-State NMR and MD Study of the Structure of the Statherin Mutant SNa15 on Mineral Surfaces. Journal of the American Chemical Society, 2019, 141, 1998-2011.	13.7	15
52	What Will Computational Modeling Approaches Have to Say in the Era of Atomistic Cryo-EM Data?. Journal of Chemical Information and Modeling, 2020, 60, 2410-2412.	5.4	15
53	A Versatile Computational Strategy To Characterize the Free-Energy Landscape of Excited States in Oligofluorenes. Journal of Chemical Theory and Computation, 2018, 14, 5441-5445.	5.3	12
54	Exploring the conformational diversity of proteins. ELife, 2022, 11, .	6.0	10

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55	Biomolecular Simulations. Methods in Molecular Biology, 2019, , .	0.9	9
56	Structural Model of the Bilitranslocase Transmembrane Domain Supported by NMR and FRET Data. PLoS ONE, 2015, 10, e0135455.	2.5	8
57	Multi-replica biased sampling for photoswitchable Ï€-conjugated polymers. Journal of Chemical Physics, 2021, 154, 174108.	3.0	6
58	Free energy landscapes of sodium ions bound to DMPCâ€“cholesterol membrane surfaces at infinite dilution. Physical Chemistry Chemical Physics, 2016, 18, 9036-9041.	2.8	5
59	A Practical Guide to the Simultaneous Determination of Protein Structure and Dynamics Using Metainference. Methods in Molecular Biology, 2019, 2022, 313-340.	0.9	3
60	Non-Native Structure in the Unfolded Ensemble of a Prototypical Î²-Hairpin. Biophysical Journal, 2009, 96, 78a-79a.	0.5	0
61	Multiple Routes and Milestones in the Folding of HIV-1 Protease Monomer. Biophysical Journal, 2010, 98, 199a.	0.5	0
62	A Bayesian Integrative Structure Model of the Yeast Centrosome. Biophysical Journal, 2018, 114, 35a.	0.5	0
63	Simultaneous Determination of Protein Structure and Dynamics using Cryo-Electron Microscopy. Biophysical Journal, 2019, 116, 330a.	0.5	0
64	Probing Specificity in Disordered Protein Interactions with Small Molecules using Integrative Methods. Biophysical Journal, 2019, 116, 180a.	0.5	0
65	Editorial: Experiments and Simulations: A Pas de Deux to Unravel Biological Function. Frontiers in Molecular Biosciences, 2021, 8, 799406.	3.5	0
66	Protein structural ensembles by integrative computational-experimental approaches. Biophysical Journal, 2022, 121, 30a-31a.	0.5	0
67	An online database of RNA-small molecules complexes for rational drug design. Biophysical Journal, 2022, 121, 208a.	0.5	0