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	Protein structural ensembles by integrative computational-experimental approaches. Biophysical Journal, 2022, 121, 30a-31a.	0.5	0
2	An online database of RNA-small molecules complexes for rational drug design. Biophysical Journal, 2022, 121, 208a.	0.5	0
3	Bat coronaviruses related to SARS-CoV-2 and infectious for human cells. Nature, 2022, 604, 330-336.	27.8	238
4	Exploring the conformational diversity of proteins. ELife, 2022, 11, .	6.0	10
5	Multi-replica biased sampling for photoswitchable Ï€-conjugated polymers. Journal of Chemical Physics, 2021, 154, 174108.	3.0	6
6	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
7	Editorial: Experiments and Simulations: A Pas de Deux to Unravel Biological Function. Frontiers in Molecular Biosciences, 2021, 8, 799406.	3.5	0
8	Small-molecule sequestration of amyloid-Î² as a drug discovery strategy for Alzheimerâ€™s disease. Science Advances, 2020, 6, .	10.3	95
9	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
10	Biomolecular Simulations. Methods in Molecular Biology, 2019, , .	0.9	9
11	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
12	Simultaneous Determination of Protein Structure and Dynamics using Cryo-Electron Microscopy. Biophysical Journal, 2019, 116, 330a.	0.5	0
13	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
14	Probing Specificity in Disordered Protein Interactions with Small Molecules using Integrative Methods. Biophysical Journal, 2019, 116, 180a.	0.5	0
15	Determination of protein structural ensembles using cryo-electron microscopy. Current Opinion in Structural Biology, 2019, 56, 37-45.	5.7	67
16	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
17	Bayesian Weighing of Electron Cryo-Microscopy Data for Integrative Structural Modeling. Structure, 2019, 27, 175-188.e6.	3.3	50
18	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

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19	Simultaneous Determination of Protein Structure and Dynamics Using Cryo-Electron Microscopy. Biophysical Journal, 2018, 114, 1604-1613.	0.5	88
20	A Bayesian Integrative Structure Model of the Yeast Centrosome. Biophysical Journal, 2018, 114, 35a.	0.5	0
21	Structural Ensemble Modulation upon Small-Molecule Binding to Disordered Proteins. Journal of Molecular Biology, 2018, 430, 2288-2292.	4.2	53
22	Integrative structure modeling with the Integrative Modeling Platform. Protein Science, 2018, 27, 245-258.	7.6	92
23	Determination of Structural Ensembles of Proteins: Restraining vs Reweighting. Journal of Chemical Theory and Computation, 2018, 14, 6632-6641.	5.3	54
24	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
25	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
26	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
27	Principles of protein structural ensemble determination. Current Opinion in Structural Biology, 2017, 42, 106-116.	5.7	285
28	Simultaneous quantification of protein order and disorder. Nature Chemical Biology, 2017, 13, 339-342.	8.0	113
29	Integrative structural and dynamical biology with PLUMED-ISDB. Bioinformatics, 2017, 33, 3999-4000.	4.1	59
30	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
31	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
32	Metadynamic metainference: Enhanced sampling of the metainference ensemble using metadynamics. Scientific Reports, 2016, 6, 31232.	3.3	76
33	Metainference: A Bayesian inference method for heterogeneous systems. Science Advances, 2016, 2, e1501177.	10.3	180
34	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
35	The molecular architecture of the Dam1 kinetochore complex is defined by cross-linking based structural modelling. Nature Communications, 2015, 6, 8673.	12.8	51
36	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

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37	Structural Model of the Bilitranslocase Transmembrane Domain Supported by NMR and FRET Data. PLoS ONE, 2015, 10, e0135455.	2.5	8
38	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
39	Specific Ion Binding at Phospholipid Membrane Surfaces. Journal of Chemical Theory and Computation, 2015, 11, 4495-4499.	5.3	45
40	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
41	Tackling Sampling Challenges in Biomolecular Simulations. Methods in Molecular Biology, 2015, 1215, 151-171.	0.9	23
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	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
44	Elucidating the Mechanism of Substrate Recognition by the Bacterial Hsp90 Molecular Chaperone. Journal of Molecular Biology, 2014, 426, 2393-2404.	4.2	45
45	Modeling of Proteins and Their Assemblies with the Integrative Modeling Platform. Methods in Molecular Biology, 2014, 1091, 277-295.	0.9	40
46	PLUMED 2: New feathers for an old bird. Computer Physics Communications, 2014, 185, 604-613.	7.5	2,454
47	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
48	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
49	Crystal structure of a eukaryotic phosphate transporter. Nature, 2013, 496, 533-536.	27.8	202
50	Structural basis for alternating access of a eukaryotic calcium/proton exchanger. Nature, 2013, 499, 107-110.	27.8	87
51	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
52	Efficient Simulation of Explicitly Solvated Proteins in the Well-Tempered Ensemble. Journal of Chemical Theory and Computation, 2012, 8, 2189-2192.	5.3	127
53	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
54	Assessing the Quality of the OPEP Coarse-Grained Force Field. Journal of Chemical Theory and Computation, 2011, 7, 1928-1934.	5.3	28

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55	Metadynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 826-843.	14.6	971
56	A chiralityâ€based metrics for freeâ€energy calculations in biomolecular systems. Journal of Computational Chemistry, 2011, 32, 2627-2637.	3.3	25
57	Modeling of Proteins and Their Assemblies with the Integrative Modeling Platform. Methods in Molecular Biology, 2011, 781, 377-397.	0.9	18
58	Multiple Routes and Milestones in the Folding of HIVâ€“1 Protease Monomer. PLoS ONE, 2010, 5, e13208.	2.5	15
59	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
60	Linking Well-Tempered Metadynamics Simulations with Experiments. Biophysical Journal, 2010, 98, L44-L46.	0.5	56
61	Enhanced Sampling in the Well-Tempered Ensemble. Physical Review Letters, 2010, 104, 190601.	7.8	225
62	Multiple Routes and Milestones in the Folding of HIV-1 Protease Monomer. Biophysical Journal, 2010, 98, 199a.	0.5	0
63	Reconstructing the equilibrium Boltzmann distribution from wellâ€tempered metadynamics. Journal of Computational Chemistry, 2009, 30, 1615-1621.	3.3	297
64	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	7.5	1,448
65	Non-Native Structure in the Unfolded Ensemble of a Prototypical Î²-Hairpin. Biophysical Journal, 2009, 96, 78a-79a.	0.5	0
66	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
67	Insight into the Folding Inhibition of the HIV-1 Protease by a Small Peptide. Biophysical Journal, 2007, 93, 2813-2821.	0.5	40