Sandro Bottaro

List of Publications by Citations

40 papers	1,494 citations	21 h-index	38 g-index
49 ext. papers	2,163 ext. citations	10.4 avg, IF	5.95 L-index

#	Paper	IF	Citations
40	Promoting transparency and reproducibility in enhanced molecular simulations. *Nature Methods*, **2019**, 16, 670-673	21.6	271
39	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. *Chemical Reviews*, **2018**, 118, 4177-4338	68.1	235
38	Biophysical experiments and biomolecular simulations: A perfect match?. *Science*, **2018**, 361, 355-360	33.3	110
37	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. *Journal of Chemical Theory and Computation*, **2016**, 12, 4534-48	6.4	77
36	The role of nucleobase interactions in RNA structure and dynamics. *Nucleic Acids Research*, **2014**, 42, 13306-14	20.1	75
35	Integrating Molecular Simulation and Experimental Data: A Bayesian/Maximum Entropy Reweighting Approach. *Methods in Molecular Biology*, **2020**, 2112, 219-240	1.4	60
34	Conformational ensembles of RNA oligonucleotides from integrating NMR and molecular simulations. *Science Advances*, **2018**, 4, eaar8521	14.3	59
33	Potentials of mean force for protein structure prediction vindicated, formalized and generalized. *PLoS ONE*, **2010**, 5, e13714	3.7	51
32	Free Energy Landscape of GAGA and UUCG RNA Tetraloops. *Journal of Physical Chemistry Letters*, **2016**, 7, 4032-4038	6.4	49
31	Empirical Corrections to the Amber RNA Force Field with Target Metadynamics. *Journal of Chemical Theory and Computation*, **2016**, 12, 2790-8	6.4	42
30	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution. *PLoS Computational Biology*, **2020**, 16, e1007870	5	39
29	Variational Optimization of an All-Atom Implicit Solvent Force Field to Match Explicit Solvent Simulation Data. *Journal of Chemical Theory and Computation*, **2013**, 9, 5641-5652	6.4	38
28	How to learn from inconsistencies: Integrating molecular simulations with experimental data. *Progress in Molecular Biology and Translational Science*, **2020**, 170, 123-176	4	35
27	Fitting Corrections to an RNA Force Field Using Experimental Data. *Journal of Chemical Theory and Computation*, **2019**, 15, 3425-3431	6.4	31
26	PHAISTOS: a framework for Markov chain Monte Carlo simulation and inference of protein structure. *Journal of Computational Chemistry*, **2013**, 34, 1697-705	3.5	31
25	RNA folding pathways in stop motion. *Nucleic Acids Research*, **2016**, 44, 5883-91	20.1	29
24	Elastic network models for RNA: a comparative assessment with molecular dynamics and SHAPE experiments. *Nucleic Acids Research*, **2015**, 43, 7260-9	20.1	28

23	Kissing loop interaction in adenine riboswitch: insights from umbrella sampling simulations. *BMC Bioinformatics*, **2015**, 16 Suppl 9, S6	3.6	26
22	Mapping the Universe of RNA Tetraloop Folds. *Biophysical Journal*, **2017**, 113, 257-267	2.9	24
21	Accuracy of the pseudopotential approximation in ab initio theoretical spectroscopies. *Physical Review B*, **2008**, 78,	3.3	23
20	Accurate multiple time step in biased molecular simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 139-46	6.4	21
19	Subtle Monte Carlo Updates in Dense Molecular Systems. *Journal of Chemical Theory and Computation*, **2012**, 8, 695-702	6.4	21
18	Barnaba: software for analysis of nucleic acid structures and trajectories. *Rna*, **2019**, 25, 219-231	5.8	21
17	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations. *ELife*, **2020**, 9,	8.9	20
16	A nucleobase-centered coarse-grained representation for structure prediction of RNA motifs. *Nucleic Acids Research*, **2018**, 46, 1674-1683	20.1	17
15	Generative probabilistic models extend the scope of inferential structure determination. *Journal of Magnetic Resonance*, **2011**, 213, 182-6	3	15
14	Integrating Molecular Simulation and Experimental Data: A Bayesian/Maximum Entropy reweighting approach		11
13	Formulation of probabilistic models of protein structure in atomic detail using the reference ratio method. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 288-99	4.2	8
12	An efficient null model for conformational fluctuations in proteins. *Structure*, **2012**, 20, 1028-39	5.2	7
11	Integrating NMR and simulations reveals motions in the UUCG tetraloop. *Nucleic Acids Research*, **2020**, 48, 5839-5848	20.1	5
10	Effects and limitations of a nucleobase-driven backmapping procedure for nucleic acids using steered molecular dynamics. *Biochemical and Biophysical Research Communications*, **2018**, 498, 352-358	3.4	4
9	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution		2
8	Conformational Ensemble of RNA Oligonucleotides from Reweighted Molecular Simulations		2
7	Conformational Ensembles of Noncoding Elements in the SARS-CoV-2 Genome from Molecular Dynamics Simulations. *Journal of the American Chemical Society*, **2021**, 143, 8333-8343	16.4	2
6	MEDTEC Students against Coronavirus: Investigating the Role of Hemostatic Genes in the Predisposition to COVID-19 Severity. *Journal of Personalized Medicine*, **2021**, 11,	3.6	1

5	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations	1
4	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution **2020**, 16, e1007870	
3	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution **2020**, 16, e1007870	
2	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution **2020**, 16, e1007870	
1	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution **2020**, 16, e1007870	