Samuela Pasquali

List of Publications by Year
in descending order

26 papers	1,579 citations	516710 16 h-index	580821 25 g-index
29 all docs	29 docs citations	29 times ranked	1823 citing authors

#	Article	IF	Citations
1	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	47.7	530
2	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. Chemical Society Reviews, 2014, 43, 4871-4893.	38.1	147
3	Exploring the repertoire of RNA secondary motifs using graph theory; implications for RNA design. Nucleic Acids Research, 2003, 31, 2926-2943.	14.5	139
4	HiRE-RNA: A High Resolution Coarse-Grained Energy Model for RNA. Journal of Physical Chemistry B, 2010, 114, 11957-11966.	2.6	113
5	The Coarse-Grained OPEP Force Field for Non-Amyloid and Amyloid Proteins. Journal of Physical Chemistry B, 2012, 116, 8741-8752.	2.6	98
6	Coarse-Grained Simulations of RNA and DNA Duplexes. Journal of Physical Chemistry B, 2013, 117, 8047-8060.	2.6	77
7	Analysis of Protein Sequence/Structure Similarity Relationships. Biophysical Journal, 2002, 83, 2781-2791.	0.5	70
8	Coarse-Grained HiRE-RNA Model for ab Initio RNA Folding beyond Simple Molecules, Including Noncanonical and Multiple Base Pairings. Journal of Chemical Theory and Computation, 2015, 11, 3510-3522.	5.3	65
9	Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding and Unfolding of Human Telomeric G-Quadruplexes. Journal of Chemical Theory and Computation, 2016, 12, 6077-6097.	5.3	50
10	Electrostatics analysis of the mutational and pH effects of the N-terminal domain self-association of the major ampullate spidroin. Soft Matter, 2016, 12, 5600-5612.	2.7	38
11	Multifunctional energy landscape for a DNA G-quadruplex: An evolved molecular switch. Journal of Chemical Physics, 2017, 147, 152715.	3.0	32
12	Protein-RNA complexation driven by the charge regulation mechanism. Biochemical and Biophysical Research Communications, 2018, 498, 264-273.	2.1	29
13	Modular RNA architecture revealed by computational analysis of existing pseudoknots and ribosomal RNAs. Nucleic Acids Research, 2005, 33, 1384-1398.	14.5	26
14	The crystal structure of the 5â€² functional domain of the transcription riboregulator 7SK. Nucleic Acids Research, 2017, 45, gkw1351.	14.5	25
15	Impact of Thermostats on Folding and Aggregation Properties of Peptides Using the Optimized Potential for Efficient Structure Prediction Coarse-Grained Model. Journal of Chemical Theory and Computation, 2011, 7, 1502-1510.	5.3	20
16	Ten simple rules to create a serious game, illustrated with examples from structural biology. PLoS Computational Biology, 2018, 14, e1005955.	3.2	20
17	Ab initioRNA folding. Journal of Physics Condensed Matter, 2015, 27, 233102.	1.8	16
18	Coarse-grained dynamic RNA titration simulations. Interface Focus, 2019, 9, 20180066.	3.0	15

#	Article	IF	Citations
19	Structural transitions in the RNA 7SK 5â€² hairpin and their effect on HEXIM binding. Nucleic Acids Research, 2020, 48, 373-389.	14.5	15
20	Biasing RNA Coarse-Grained Folding Simulations with Small-Angle X-ray Scattering Data. Journal of Chemical Theory and Computation, 2021, 17, 6509-6521.	5.3	12
21	Molecular modelling as the spark for active learning approaches for interdisciplinary biology teaching. Interface Focus, 2019, 9, 20180065.	3.0	11
22	What Can Human-Guided Simulations Bring to RNA Folding?. Biophysical Journal, 2017, 113, 302-312.	0.5	8
23	Investigating the structural changes due to adenosine methylation of the Kaposiâ€™s sarcoma-associated herpes virus ORF50 transcript. PLoS Computational Biology, 2022, 18, e1010150.	3.2	8
24	UnityMol: interactive and ludic visual manipulation of coarse-grained RNA and other biomolecules. , 2015, , .		7
25	RNA Modeling with the Computational Energy Framework. Methods in Molecular Biology, 2021, 2323, 49-66.	0.9	4
26	Induced forms of Î±2-macroglobulin neutralize heparin and direct oral anticoagulant effects. International Journal of Biological Macromolecules, 2021, 184, 209-217.	7.5	4