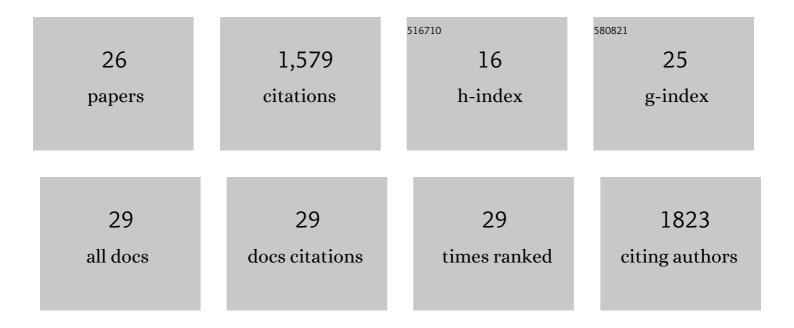
Samuela Pasquali

List of Publications by Year in descending order

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| # | Article | IF | CITATIONS |
|----|--|------|-----------|
| 1 | Amyloid β Protein and Alzheimer'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 5′ 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 | <i>Ab initio</i> RNA 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 |

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| # | Article | IF | CITATIONS |
|----|---|------|-----------|
| 19 | Structural transitions in the RNA 7SK 5′ 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 Kaposi'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 α2-macroglobulin neutralize heparin and direct oral anticoagulant effects. International Journal of Biological Macromolecules, 2021, 184, 209-217. | 7.5 | 4 |