

# Luca Maragliano

## List of Publications by Year in descending order

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45  
papers

2,507  
citations

331670

21  
h-index

254184

43  
g-index

50  
all docs

50  
docs citations

50  
times ranked

2993  
citing authors

#	ARTICLE	IF	CITATIONS
1	String method in collective variables: Minimum free energy paths and isocommittor surfaces. <i>Journal of Chemical Physics</i> , 2006, 125, 024106.	3.0	600
2	A temperature accelerated method for sampling free energy and determining reaction pathways in rare events simulations. <i>Chemical Physics Letters</i> , 2006, 426, 168-175.	2.6	428
3	On-the-fly string method for minimum free energy paths calculation. <i>Chemical Physics Letters</i> , 2007, 446, 182-190.	2.6	159
4	Single-sweep methods for free energy calculations. <i>Journal of Chemical Physics</i> , 2008, 128, 184110.	3.0	119
5	Interfacing Graphene-Based Materials With Neural Cells. <i>Frontiers in Systems Neuroscience</i> , 2018, 12, 12.	2.5	98
6	Mapping the Network of Pathways of CO Diffusion in Myoglobin. <i>Journal of the American Chemical Society</i> , 2010, 132, 1010-1017.	13.7	96
7	Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4672-4680.	5.3	89
8	Direct Imaging of DNA Fibers: The Visage of Double Helix. <i>Nano Letters</i> , 2012, 12, 6453-6458.	9.1	73
9	Neuronal firing modulation by a membrane-targeted photoswitch. <i>Nature Nanotechnology</i> , 2020, 15, 296-306.	31.5	71
10	De novo mutations of the ATP6V1A gene cause developmental encephalopathy with epilepsy. <i>Brain</i> , 2018, 141, 1703-1718.	7.6	69
11	Free Energy and Kinetics of Conformational Transitions from Voronoi Tessellated Milestoning with Restraining Potentials. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2589-2594.	5.3	62
12	A Novel Topology of Proline-rich Transmembrane Protein 2 (PRRT2). <i>Journal of Biological Chemistry</i> , 2016, 291, 6111-6123.	3.4	59
13	Intermediate state trapping of a voltage sensor. <i>Journal of General Physiology</i> , 2012, 140, 635-652.	1.9	50
14	â€œDFG-Flipâ€œ in the Insulin Receptor Kinase Is Facilitated by a Helical Intermediate State of the Activation Loop. <i>Biophysical Journal</i> , 2012, 102, 1979-1987.	0.5	50
15	Regulation of neural gene transcription by optogenetic inhibition of the RE1-silencing transcription factor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E91-100.	7.1	48
16	Molecular Dynamics Simulations of Ion Selectivity in a Claudin-15 Paracellular Channel. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10783-10792.	2.6	41
17	A refined model of claudin-15 tight junction paracellular architecture by molecular dynamics simulations. <i>PLoS ONE</i> , 2017, 12, e0184190.	2.5	41
18	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 524-533.	5.3	38

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19	Functional Role of ATP Binding to Synapsin I In Synaptic Vesicle Trafficking and Release Dynamics. <i>Journal of Neuroscience</i> , 2014, 34, 14752-14768.	3.6	27
20	Identification and Expression of Acetylcholinesterase in Octopus vulgaris Arm Development and Regeneration: a Conserved Role for ACHE?. <i>Molecular Neurobiology</i> , 2015, 52, 45-56.	4.0	25
21	Genotype-phenotype correlations in patients with de novo <i>KCNQ2</i> pathogenic variants. <i>Neurology: Genetics</i> , 2020, 6, e528.	1.9	24
22	Extended Phase-Space Methods for Enhanced Sampling in Molecular Simulations: A Review. <i>Frontiers in Bioengineering and Biotechnology</i> , 2015, 3, 125.	4.1	22
23	Optogenetic Modulation of Intracellular Signalling and Transcription: Focus on Neuronal Plasticity. <i>Journal of Experimental Neuroscience</i> , 2017, 11, 117906951770335.	2.3	21
24	Atomic Mean-Square Displacements in Proteins by Molecular Dynamics: A Case for Analysis of Variance. <i>Biophysical Journal</i> , 2004, 86, 2765-2772.	0.5	17
25	Conformational Changes in Acetylcholine Binding Protein Investigated by Temperature Accelerated Molecular Dynamics. <i>PLoS ONE</i> , 2014, 9, e88555.	2.5	16
26	A possible desensitized state conformation of the human $\alpha 7$ nicotinic receptor: A molecular dynamics study. <i>Biophysical Chemistry</i> , 2017, 229, 99-109.	2.8	14
27	Expanding the Nude SCID/CID Phenotype Associated with FOXP1 Homozygous, Compound Heterozygous, or Heterozygous Mutations. <i>Journal of Clinical Immunology</i> , 2021, 41, 756-768.	3.8	13
28	Temperature-accelerated molecular dynamics gives insights into globular conformations sampled in the free state of the AC catalytic domain. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2483-2496.	2.6	12
29	Temperature Accelerated Molecular Dynamics with Soft-Ratcheting Criterion Orients Enhanced Sampling by Low-Resolution Information. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3446-3454.	5.3	12
30	Thermodynamics and Kinetics of Ion Permeation in Wild-Type and Mutated Open Active Conformation of the Human $\alpha 7$ Nicotinic Receptor. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5045-5056.	5.4	12
31	Effective Binding Force Calculation in Dimeric Proteins. <i>Molecular Simulation</i> , 2004, 30, 807-816.	2.0	11
32	A Structural Model of the Human $\alpha 7$ Nicotinic Receptor in an Open Conformation. <i>PLoS ONE</i> , 2015, 10, e0133011.	2.5	11
33	Phenotypic and genetic spectrum of ATP6V1A encephalopathy: a disorder of lysosomal homeostasis. <i>Brain</i> , 2022, 145, 2687-2703.	7.6	11
34	Isobaric Labeling Proteomics Allows a High-Throughput Investigation of Protein Corona Orientation. <i>Analytical Chemistry</i> , 2021, 93, 784-791.	6.5	10
35	Computational Assessment of Different Structural Models for Claudin-5 Complexes in Blood-Brain Barrier Tight Junctions. <i>ACS Chemical Neuroscience</i> , 2022, 13, 2140-2153.	3.5	10
36	Computational study of ion permeation through claudin-4 paracellular channels. <i>Annals of the New York Academy of Sciences</i> , 2022, 1516, 162-174.	3.8	9

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37	Closed-Locked and Apo-Resting State Structures of the Human $\alpha 7$ Nicotinic Receptor: A Computational Study. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2278-2293.	5.4	6
38	Synapsins are expressed at neuronal and non-neuronal locations in <i>Octopus vulgaris</i> . <i>Scientific Reports</i> , 2019, 9, 15430.	3.3	6
39	Structural Mechanism of $\bar{I}$ -Currents in a Mutated Kv7.2 Voltage Sensor Domain from Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1354-1367.	5.4	6
40	Free energy and kinetics of cAMP permeation through connexin26 via applied voltage and milestoning. <i>Biophysical Journal</i> , 2021, 120, 2969-2983.	0.5	5
41	Effect of Intercalated Water on Potassium Ion Transport through Kv1.2 Channels Studied via On-the-Fly Free-Energy Parametrization. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2743-2750.	5.3	4
42	Engineering REST-Specific Synthetic PUF Proteins to Control Neuronal Gene Expression: A Combined Experimental and Computational Study. <i>ACS Synthetic Biology</i> , 2020, 9, 2039-2054.	3.8	4
43	Experimental and Simulative Dissociation of Dimeric Cu,Zn Superoxide Dismutase Doubly Mutated at the Intersubunit Surface. <i>Biophysical Journal</i> , 2005, 88, 2875-2882.	0.5	3
44	Interactions Between 2D Graphene-Based Materials and the Nervous tissue. , 2018, , 62-85.		2
45	Mapping Co Diffusion Paths in Myoglobin with the Single Sweep Method. <i>Biophysical Journal</i> , 2010, 98, 572a-573a.	0.5	0