Luca Maragliano

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Phenotypic and genetic spectrum of ATP6V1A encephalopathy: a disorder of lysosomal homeostasis. Brain, 2022, 145, 2687-2703.	7.6	11
2	Computational study of ion permeation through claudinâ€4 paracellular channels. Annals of the New York Academy of Sciences, 2022, 1516, 162-174.	3.8	9
3	Computational Assessment of Different Structural Models for Claudin-5 Complexes in Blood–Brain Barrier Tight Junctions. ACS Chemical Neuroscience, 2022, 13, 2140-2153.	3.5	10
4	Structural Mechanism of ω-Currents in a Mutated Kv7.2 Voltage Sensor Domain from Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 1354-1367.	5.4	6
5	Free energy and kinetics of cAMP permeation through connexin26 via applied voltage and milestoning. Biophysical Journal, 2021, 120, 2969-2983.	0.5	5
6	Expanding the Nude SCID/CID Phenotype Associated with FOXN1 Homozygous, Compound Heterozygous, or Heterozygous Mutations. Journal of Clinical Immunology, 2021, 41, 756-768.	3.8	13
7	Isobaric Labeling Proteomics Allows a High-Throughput Investigation of Protein Corona Orientation. Analytical Chemistry, 2021, 93, 784-791.	6.5	10
8	Engineering REST-Specific Synthetic PUF Proteins to Control Neuronal Gene Expression: A Combined Experimental and Computational Study. ACS Synthetic Biology, 2020, 9, 2039-2054.	3.8	4
9	Thermodynamics and Kinetics of Ion Permeation in Wild-Type and Mutated Open Active Conformation of the Human α7 Nicotinic Receptor. Journal of Chemical Information and Modeling, 2020, 60, 5045-5056.	5.4	12
10	Neuronal firing modulation by a membrane-targeted photoswitch. Nature Nanotechnology, 2020, 15, 296-306.	31.5	71
11	Genotype-phenotype correlations in patients with de novo <i>KCNQ2</i> pathogenic variants. Neurology: Genetics, 2020, 6, e528.	1.9	24
12	Synapsins are expressed at neuronal and non-neuronal locations in Octopus vulgaris. Scientific Reports, 2019, 9, 15430.	3.3	6
13	De novo mutations of the ATP6V1A gene cause developmental encephalopathy with epilepsy. Brain, 2018, 141, 1703-1718.	7.6	69
14	Effect of Intercalated Water on Potassium Ion Transport through Kv1.2 Channels Studied via On-the-Fly Free-Energy Parametrization. Journal of Chemical Theory and Computation, 2018, 14, 2743-2750.	5.3	4
15	Closed-Locked and Apo-Resting State Structures of the Human α7 Nicotinic Receptor: A Computational Study. Journal of Chemical Information and Modeling, 2018, 58, 2278-2293.	5.4	6
16	Molecular Dynamics Simulations of Ion Selectivity in a Claudin-15 Paracellular Channel. Journal of Physical Chemistry B, 2018, 122, 10783-10792.	2.6	41
17	Interfacing Graphene-Based Materials With Neural Cells. Frontiers in Systems Neuroscience, 2018, 12, 12.	2.5	98

18 Interactions Between 2D Graphene-Based Materials and the Nervous tissue. , 2018, , 62-85.

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19	Optogenetic Modulation of Intracellular Signalling and Transcription: Focus on Neuronal Plasticity. Journal of Experimental Neuroscience, 2017, 11, 117906951770335.	2.3	21
20	A possible desensitized state conformation of the human α 7 nicotinic receptor: A molecular dynamics study. Biophysical Chemistry, 2017, 229, 99-109.	2.8	14
21	A refined model of claudin-15 tight junction paracellular architecture by molecular dynamics simulations. PLoS ONE, 2017, 12, e0184190.	2.5	41
22	A Novel Topology of Proline-rich Transmembrane Protein 2 (PRRT2). Journal of Biological Chemistry, 2016, 291, 6111-6123.	3.4	59
23	Regulation of neural gene transcription by optogenetic inhibition of the RE1-silencing transcription factor. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E91-100.	7.1	48
24	Extended Phase-Space Methods for Enhanced Sampling in Molecular Simulations: A Review. Frontiers in Bioengineering and Biotechnology, 2015, 3, 125.	4.1	22
25	Temperature Accelerated Molecular Dynamics with Soft-Ratcheting Criterion Orients Enhanced Sampling by Low-Resolution Information. Journal of Chemical Theory and Computation, 2015, 11, 3446-3454.	5.3	12
26	Identification and Expression of Acetylcholinesterase in Octopus vulgaris Arm Development and Regeneration: a Conserved Role for ACHE?. Molecular Neurobiology, 2015, 52, 45-56.	4.0	25
27	A Structural Model of the Human α7 Nicotinic Receptor in an Open Conformation. PLoS ONE, 2015, 10, e0133011.	2.5	11
28	Functional Role of ATP Binding to Synapsin I In Synaptic Vesicle Trafficking and Release Dynamics. Journal of Neuroscience, 2014, 34, 14752-14768.	3.6	27
29	Temperature-accelerated molecular dynamics gives insights into globular conformations sampled in the free state of the AC catalytic domain. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2483-2496.	2.6	12
30	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. Journal of Chemical Theory and Computation, 2014, 10, 524-533.	5.3	38
31	Conformational Changes in Acetylcholine Binding Protein Investigated by Temperature Accelerated Molecular Dynamics. PLoS ONE, 2014, 9, e88555.	2.5	16
32	Direct Imaging of DNA Fibers: The Visage of Double Helix. Nano Letters, 2012, 12, 6453-6458.	9.1	73
33	Intermediate state trapping of a voltage sensor. Journal of General Physiology, 2012, 140, 635-652.	1.9	50
34	"DFG-Flip―in the Insulin Receptor Kinase Is Facilitated by a Helical Intermediate State of the Activation Loop. Biophysical Journal, 2012, 102, 1979-1987.	0.5	50
35	Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer. Journal of Chemical Theory and Computation, 2012, 8, 4672-4680. 	5.3	89
36	Mapping Co Diffusion Paths in Myoglobin with the Single Sweep Method. Biophysical Journal, 2010, 98, 572a-573a.	0.5	0

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37	Mapping the Network of Pathways of CO Diffusion in Myoglobin. Journal of the American Chemical Society, 2010, 132, 1010-1017.	13.7	96
38	Free Energy and Kinetics of Conformational Transitions from Voronoi Tessellated Milestoning with Restraining Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2589-2594.	5.3	62
39	Single-sweep methods for free energy calculations. Journal of Chemical Physics, 2008, 128, 184110.	3.0	119
40	On-the-fly string method for minimum free energy paths calculation. Chemical Physics Letters, 2007, 446, 182-190.	2.6	159
41	A temperature accelerated method for sampling free energy and determining reaction pathways in rare events simulations. Chemical Physics Letters, 2006, 426, 168-175.	2.6	428
42	String method in collective variables: Minimum free energy paths and isocommittor surfaces. Journal of Chemical Physics, 2006, 125, 024106.	3.0	600
43	Experimental and Simulative Dissociation of Dimeric Cu,Zn Superoxide Dismutase Doubly Mutated at the Intersubunit Surface. Biophysical Journal, 2005, 88, 2875-2882.	0.5	3
44	Effective Binding Force Calculation in Dimeric Proteins. Molecular Simulation, 2004, 30, 807-816.	2.0	11
45	Atomic Mean-Square Displacements in Proteins by Molecular Dynamics: A Case for Analysis of Variance. Biophysical Journal, 2004, 86, 2765-2772.	0.5	17