

# Lorenzo Casalino

## List of Publications by Year in descending order

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Version: 2024-02-01

31  
papers

2,603  
citations

430874

18  
h-index

580821

25  
g-index

43  
all docs

43  
docs citations

43  
times ranked

4219  
citing authors

#	ARTICLE	IF	CITATIONS
1	Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. ACS Central Science, 2020, 6, 1722-1734.	11.3	727
2	A glycan gate controls opening of the SARS-CoV-2 spike protein. Nature Chemistry, 2021, 13, 963-968.	13.6	254
3	SARS-CoV-2 escape from a highly neutralizing COVID-19 convalescent plasma. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	251
4	A multiscale coarse-grained model of the SARS-CoV-2 virion. Biophysical Journal, 2021, 120, 1097-1104.	0.5	139
5	The flexibility of ACE2 in the context of SARS-CoV-2 infection. Biophysical Journal, 2021, 120, 1072-1084.	0.5	102
6	AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. International Journal of High Performance Computing Applications, 2021, 35, 432-451.	3.7	91
7	Mesoscale All-Atom Influenza Virus Simulations Suggest New Substrate Binding Mechanism. ACS Central Science, 2020, 6, 189-196.	11.3	86
8	Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns. Journal of the American Chemical Society, 2016, 138, 10374-10377.	13.7	79
9	Human Influenza A Virus Hemagglutinin Glycan Evolution Follows a Temporal Pattern to a Glycan Limit. MBio, 2019, 10, .	4.1	74
10	Catalytic Mechanism of Non-Target DNA Cleavage in CRISPR-Cas9 Revealed by <i>Ab Initio</i> Molecular Dynamics. ACS Catalysis, 2020, 10, 13596-13605.	11.2	63
11	All-atom simulations disentangle the functional dynamics underlying gene maturation in the intron lariat spliceosome. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6584-6589.	7.1	59
12	Development of Site-Specific Mg <sup>2+</sup> RNA Force Field Parameters: A Dream or Reality? Guidelines from Combined Molecular Dynamics and Quantum Mechanics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 340-352.	5.3	51
13	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. Biophysical Journal, 2021, 120, 983-993.	0.5	43
14	Understanding the mechanistic basis of non-coding RNA through molecular dynamics simulations. Journal of Structural Biology, 2019, 206, 267-279.	2.8	37
15	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. Journal of the American Chemical Society, 2020, 142, 8403-8411.	13.7	35
16	A Dehydrogenase Dual Hydrogen Abstraction Mechanism Promotes Estrogen Biosynthesis: Can We Expand the Functional Annotation of the Aromatase Enzyme?. Chemistry - A European Journal, 2018, 24, 10840-10849.	3.3	31
17	<i>GlycoGrip</i> : Cell Surface-Inspired Universal Sensor for Betacoronaviruses. ACS Central Science, 2022, 8, 22-42.	11.3	31
18	Atomic-Level Mechanism of Pre-mRNA Splicing in Health and Disease. Accounts of Chemical Research, 2021, 54, 144-154.	15.6	23

#	ARTICLE	IF	CITATIONS
19	Structural, dynamical and catalytic interplay between Mg <sup>2+</sup> ions and RNA. Vices and virtues of atomistic simulations. <i>Inorganica Chimica Acta</i> , 2016, 452, 73-81.	2.4	16
20	Decoding allosteric regulation by the acyl carrier protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	14
21	Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. <i>Biophysical Journal</i> , 2020, 119, 2275-2289.	0.5	13
22	Can multiscale simulations unravel the function of metallo-enzymes to improve knowledge-based drug discovery?. <i>Future Medicinal Chemistry</i> , 2019, 11, 771-791.	2.3	9
23	Unraveling the Molecular Mechanism of Pre-mRNA Splicing From Multi-Scale Simulations. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 62.	3.5	7
24	Two-Metal Ion Mechanism of DNA Cleavage in CRISPR-Cas9. <i>Biophysical Journal</i> , 2020, 118, 64a.	0.5	2
25	SARS-CoV-2 Glycosylated Spike Activation Mechanism - Simulations of the Full Unbiased Pathway. <i>Biophysical Journal</i> , 2021, 120, 276a.	0.5	1
26	Influenza Virulence and Transmissibility through the Computational Microscope. <i>Biophysical Journal</i> , 2019, 116, 342a.	0.5	0
27	Pre-mRNA Splicing: The Gene Maturation Symphony of the Intron Lariat Spliceosome Revealed by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2019, 116, 299a.	0.5	0
28	How does Glycosylation Affect Drug Binding on Influenza? The Roles of Electrostatics and Sterics Examined through Brownian Dynamics Simulations. <i>Biophysical Journal</i> , 2019, 116, 483a.	0.5	0
29	Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. <i>Biophysical Journal</i> , 2021, 120, 122a.	0.5	0
30	Critical Role of Conserved Histidine Residues in Genome Editing and Recombination. <i>Biophysical Journal</i> , 2021, 120, 137a-138a.	0.5	0
31	Vincent van Gogh's Autocatalysis. , 2020, , 114-115.		0