

# Vincenzo Carnevale

## List of Publications by Year in descending order

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Version: 2024-02-01

70  
papers

2,857  
citations

159358

30  
h-index

189595

50  
g-index

82  
all docs

82  
docs citations

82  
times ranked

3317  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15075-15080.	3.3	243
2	Hydration structure of salt solutions from <i>ab initio</i> molecular dynamics. Journal of Chemical Physics, 2013, 138, 014501.	1.2	158
3	Structure of Water at Charged Interfaces: A Molecular Dynamics Study. Langmuir, 2014, 30, 8056-8065.	1.6	130
4	Molecular Dynamics Simulation Directed Rational Design of Inhibitors Targeting Drug-Resistant Mutants of Influenza A Virus M2. Journal of the American Chemical Society, 2011, 133, 12834-12841.	6.6	127
5	Understanding TRPV1 activation by ligands: Insights from the binding modes of capsaicin and resiniferatoxin. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E137-45.	3.3	127
6	Structural insights on TRPV5 gating by endogenous modulators. Nature Communications, 2018, 9, 4198.	5.8	118
7	Functional Studies and Modeling of Pore-Lining Residue Mutants of the Influenza A Virus M2 Ion Channel. Biochemistry, 2010, 49, 696-708.	1.2	107
8	TRPV1: A Target for Rational Drug Design. Pharmaceuticals, 2016, 9, 52.	1.7	85
9	Exploring Volatile General Anesthetic Binding to a Closed Membrane-Bound Bacterial Voltage-Gated Sodium Channel via Computation. PLoS Computational Biology, 2013, 9, e1003090.	1.5	71
10	Pore waters regulate ion permeation in a calcium release-activated calcium channel. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17332-17337.	3.3	65
11	Free-energy landscape of ion-channel voltage-sensor domain activation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 124-129.	3.3	63
12	Correspondences between low-energy modes in enzymes: Dynamics-based alignment of enzymatic functional families. Protein Science, 2008, 17, 918-929.	3.1	62
13	Convergent Dynamics in the Protease Enzymatic Superfamily. Journal of the American Chemical Society, 2006, 128, 9766-9772.	6.6	61
14	Sodium Ion Binding Sites and Hydration in the Lumen of a Bacterial Ion Channel from Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2011, 2, 2504-2508.	2.1	59
15	Conduction in a Biological Sodium Selective Channel. Journal of Physical Chemistry B, 2013, 117, 3782-3789.	1.2	59
16	Modulation of a voltage-gated Na <sup>+</sup> channel by sevoflurane involves multiple sites and distinct mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 6726-6731.	3.3	58
17	Evolutionary imprint of activation: The design principles of VSDs. Journal of General Physiology, 2014, 143, 145-156.	0.9	57
18	Comparative sequence analysis suggests a conserved gating mechanism for TRP channels. Journal of General Physiology, 2015, 146, 37-50.	0.9	57

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19	Exploring conformational states of the bacterial voltage-gated sodium channel NavAb via molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 21336-21341.	3.3	54
20	A Genetically Encoded $^{129}\text{Xe}$ -Lactamase Reporter for Ultrasensitive $^{129}\text{Xe}$ NMR in Mammalian Cells. Angewandte Chemie - International Edition, 2016, 55, 8984-8987.	7.2	50
21	Mechanistic Insights into the Modulation of Voltage-Gated Ion Channels by Inhalational Anesthetics. Biophysical Journal, 2015, 109, 2003-2011.	0.2	46
22	Microseconds Dynamics Simulations of the Outer-Membrane Protease T. Biophysical Journal, 2008, 94, 71-78.	0.2	43
23	Ion Channel Sensing: Are Fluctuations the Crux of the Matter?. Journal of Physical Chemistry Letters, 2018, 9, 1260-1264.	2.1	43
24	Hydration structure of $\text{Na}^+$ and $\text{K}^+$ from <i>ab initio</i> molecular dynamics based on modern density functional theory. Molecular Physics, 2014, 112, 1448-1456.	0.8	37
25	Global and local mechanical properties control endonuclease reactivity of a DNA origami nanostructure. Nucleic Acids Research, 2020, 48, 4672-4680.	6.5	35
26	Asp44 Stabilizes the Trp41 Gate of the M2 Proton Channel of Influenza A Virus. Structure, 2013, 21, 2033-2041.	1.6	34
27	Fluorine-19 NMR and computational quantification of isoflurane binding to the voltage-gated sodium channel NaChBac. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13762-13767.	3.3	34
28	Does Proton Conduction in the Voltage-Gated $\text{H}^+$ Channel hHv1 Involve Grothhuss-Like Hopping via Acidic Residues?. Journal of Physical Chemistry B, 2017, 121, 3340-3351.	1.2	34
29	Hydrogen-Bonded Water Molecules in the M2 Channel of the Influenza A Virus Guide the Binding Preferences of Ammonium-Based Inhibitors. Journal of Physical Chemistry B, 2015, 119, 1173-1183.	1.2	33
30	On the role of water density fluctuations in the inhibition of a proton channel. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8359-E8368.	3.3	33
31	Patterns of coevolving amino acids unveil structural and dynamical domains. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10612-E10621.	3.3	33
32	SPECTRUS: A Dimensionality Reduction Approach for Identifying Dynamical Domains in Protein Complexes from Limited Structural Datasets. Structure, 2015, 23, 1516-1525.	1.6	32
33	Multiple Proton Confinement in the M2 Channel from the Influenza A Virus. Journal of Physical Chemistry C, 2010, 114, 20856-20863.	1.5	31
34	Hinge-bending motions in the pore domain of a bacterial voltage-gated sodium channel. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2120-2125.	1.4	31
35	Accurate Estimation of the Intrinsic Dimension Using Graph Distances: Unraveling the Geometric Complexity of Datasets. Scientific Reports, 2016, 6, 31377.	1.6	31
36	Arranging Small Molecules with Subnanometer Precision on DNA Origami Substrates for the Single-Molecule Investigation of Protein-Ligand Interactions. Small Structures, 2020, 1, 2000038.	6.9	31

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37	A hypothetical molecular mechanism for TRPV1 activation that invokes rotation of an S6 asparagine. <i>Journal of General Physiology</i> , 2018, 150, 1554-1566.	0.9	30
38	The generative capacity of probabilistic protein sequence models. <i>Nature Communications</i> , 2021, 12, 6302.	5.8	28
39	A molecular determinant of phosphoinositide affinity in mammalian TRPV channels. <i>Scientific Reports</i> , 2016, 6, 27652.	1.6	26
40	Sites Contributing to TRPA1 Activation by the Anesthetic Propofol Identified by Photoaffinity Labeling. <i>Biophysical Journal</i> , 2017, 113, 2168-2172.	0.2	26
41	Conformational dynamics in TRPV1 channels reported by an encoded coumarin amino acid. <i>ELife</i> , 2017, 6, .	2.8	25
42	Structural and dynamical alignment of enzymes with partial structural similarity. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 285206.	0.7	22
43	Propofol inhibits the voltage-gated sodium channel NaChBac at multiple sites. <i>Journal of General Physiology</i> , 2018, 150, 1317-1331.	0.9	22
44	Investigations of water/oxide interfaces by molecular dynamics simulations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1537.	6.2	21
45	Sodium Halide Adsorption and Water Structure at the $\gamma$ -Alumina(0001)/Water Interface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15618-15628.	1.5	19
46	First-Principles Calculation of Water $pK_a$ Using the Newly Developed SCAN Functional. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 54-59.	2.1	19
47	TRPA1 modulation by piperidine carboxamides suggests an evolutionarily conserved binding site and gating mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 26008-26019.	3.3	18
48	Propofol inhibits prokaryotic voltage-gated Na <sup>+</sup> channels by promoting activation-coupled inactivation. <i>Journal of General Physiology</i> , 2018, 150, 1299-1316.	0.9	17
49	A Structural Basis for <sup>129</sup> Xe Hyperâ€CEST Signal in TEMâ€1 $\beta$ -Lactamase. <i>ChemPhysChem</i> , 2019, 20, 260-267.	1.0	17
50	Molecular Dynamics Simulations of Ion Channels. <i>Trends in Biochemical Sciences</i> , 2021, 46, 621-622.	3.7	17
51	Dual regulation of TRPV1 channels by phosphatidylinositol via functionally distinct binding sites. <i>Journal of Biological Chemistry</i> , 2021, 296, 100573.	1.6	16
52	Molecular dynamics simulations of outer-membrane protease T from <i>E. coli</i> based on a hybrid coarse-grained/atomistic potential. <i>Journal of Physics Condensed Matter</i> , 2006, 18, S347-S355.	0.7	14
53	Proton affinity of the histidine-tryptophan cluster motif from the influenza A virus from ab initio molecular dynamics. <i>Chemical Physics</i> , 2013, 422, 156-164.	0.9	12
54	Combined computational and experimental analysis of a complex of ribonuclease III and the regulatory macrodomain protein, Ymdb. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 459-472.	1.5	12

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55	Regulation and drug modulation of a voltage-gated sodium channel: Pivotal role of the S4â€“S5 linker in activation and slow inactivation. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	12
56	The Flu's Proton Escort. Science, 2010, 330, 456-458.	6.0	11
57	Cross-kingdom auxiliary subunit modulation of a voltage-gated sodium channel. Journal of Biological Chemistry, 2018, 293, 4981-4992.	1.6	11
58	Small molecule modulation of voltage gated sodium channels. Current Opinion in Structural Biology, 2017, 43, 156-162.	2.6	10
59	Polyamine blockade and binding energetics in the MthK potassium channel. Journal of General Physiology, 2020, 152, .	0.9	10
60	Evolutionarily Conserved Interactions within the Pore Domain of Acid-Sensing Ion Channels. Biophysical Journal, 2020, 118, 861-872.	0.2	9
61	Permeating disciplines: Overcoming barriers between molecular simulations and classical structure-function approaches in biological ion transport. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 927-942.	1.4	8
62	Sequence and structural conservation reveal fingerprint residues in TRP channels. ELife, 0, 11, .	2.8	7
63	Multi-scale modeling of HIV-1 proteins. Computational and Theoretical Chemistry, 2009, 898, 97-105.	1.5	6
64	Protonation underlies tonic vs. use-dependent block. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3512-3514.	3.3	6
65	Computational Approaches to Studying Voltage-Gated Ion Channel Modulation by General Anesthetics. Methods in Enzymology, 2018, 602, 25-59.	0.4	3
66	Binding Sites and the Mechanism of Action of Propofol and a Photoreactive Analogue in Prokaryotic Voltage-Gated Sodium Channels. ACS Chemical Neuroscience, 2021, 12, 3898-3914.	1.7	3
67	Microcanonical coarse-graining of the kinetic Ising model. Journal of Chemical Physics, 2020, 152, 084104.	1.2	2
68	Particle-based Ising model. Physical Review E, 2021, 103, 012125.	0.8	2
69	Epistasis Creates Invariant Sites and Modulates the Rate of Molecular Evolution. Molecular Biology and Evolution, 2022, 39, .	3.5	2
70	AlphaFold2 Workflow Optimization for High Throughput Predictions in HPC Environment. , 2022, , .		1