Vincenzo Carnevale

List of Publications by Year
in descending order

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70 papers	2,857 citations	159585 30 h-index	189892 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.	7.1	243
2	Hydration structure of salt solutions from ab initio molecular dynamics. Journal of Chemical Physics, 2013, 138, 014501.	3.0	158
3	Structure of Water at Charged Interfaces: A Molecular Dynamics Study. Langmuir, 2014, 30, 8056-8065.	3.5	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.	13.7	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.	7.1	127
6	Structural insights on TRPV5 gating by endogenous modulators. Nature Communications, 2018, 9, 4198.	12.8	118
7	Functional Studies and Modeling of Pore-Lining Residue Mutants of the Influenza A Virus M2 Ion Channel. Biochemistry, 2010, 49, 696-708.	2.5	107
8	TRPV1: A Target for Rational Drug Design. Pharmaceuticals, 2016, 9, 52.	3.8	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.	3.2	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.	7.1	65
11	Free-energy landscape of ion-channel voltage-sensorâ€“domain activation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 124-129.	7.1	63
12	Correspondences between lowâ€energy modes in enzymes: Dynamicsâ€based alignment of enzymatic functional families. Protein Science, 2008, 17, 918-929.	7.6	62
13	Convergent Dynamics in the Protease Enzymatic Superfamily. Journal of the American Chemical Society, 2006, 128, 9766-9772.	13.7	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.	4.6	59
15	Conduction in a Biological Sodium Selective Channel. Journal of Physical Chemistry B, 2013, 117, 3782-3789.	2.6	59
16	Modulation of a voltage-gated Na+ 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.	7.1	58
17	Evolutionary imprint of activation: The design principles of VSDs. Journal of General Physiology, 2014, 143, 145-156.	1.9	57
18	Comparative sequence analysis suggests a conserved gating mechanism for TRP channels. Journal of General Physiology, 2015, 146, 37-50.	1.9	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.	7.1	54
20	A Genetically Encoded Î²â€Lactamase Reporter for Ultrasensitive ¹²⁹Xe NMR in Mammalian Cells. Angewandte Chemie - International Edition, 2016, 55, 8984-8987.	13.8	50
21	Mechanistic Insights into the Modulation of Voltage-Gated Ion Channels by Inhalational Anesthetics. Biophysical Journal, 2015, 109, 2003-2011.	0.5	46
22	Microseconds Dynamics Simulations of the Outer-Membrane Protease T. Biophysical Journal, 2008, 94, 71-78.	0.5	43
23	Ion Channel Sensing: Are Fluctuations the Crux of the Matter?. Journal of Physical Chemistry Letters, 2018, 9, 1260-1264.	4.6	43
24	Hydration structure of Na⁺and K⁺fromab initiomolecular dynamics based on modern density functional theory. Molecular Physics, 2014, 112, 1448-1456.	1.7	37
25	Global and local mechanical properties control endonuclease reactivity of a DNA origami nanostructure. Nucleic Acids Research, 2020, 48, 4672-4680.	14.5	35
26	Asp44 Stabilizes the Trp41 Gate of the M2 Proton Channel of Influenza A Virus. Structure, 2013, 21, 2033-2041.	3.3	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.	7.1	34
28	Does Proton Conduction in the Voltage-Gated H⁺ Channel hHv1 Involve Grotthuss-Like Hopping via Acidic Residues?. Journal of Physical Chemistry B, 2017, 121, 3340-3351.	2.6	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.	2.6	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.	7.1	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.	7.1	33
32	SPECTRUS: A Dimensionality Reduction Approach for Identifying Dynamical Domains in Protein Complexes from Limited Structural Datasets. Structure, 2015, 23, 1516-1525.	3.3	32
33	Multiple Proton Confinement in the M2 Channel from the Influenza A Virus. Journal of Physical Chemistry C, 2010, 114, 20856-20863.	3.1	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.	2.6	31
35	Accurate Estimation of the Intrinsic Dimension Using Graph Distances: Unraveling the Geometric Complexity of Datasets. Scientific Reports, 2016, 6, 31377.	3.3	31
36	Arranging Small Molecules with Subnanometer Precision on DNA Origami Substrates for the Singleâ€Molecule Investigation of Proteinâ€“Ligand Interactions. Small Structures, 2020, 1, 2000038.	12.0	31

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37	A hypothetical molecular mechanism for TRPV1 activation that invokes rotation of an S6 asparagine. Journal of General Physiology, 2018, 150, 1554-1566.	1.9	30
38	The generative capacity of probabilistic protein sequence models. Nature Communications, 2021, 12, 6302.	12.8	28
39	A molecular determinant of phosphoinositide affinity in mammalian TRPV channels. Scientific Reports, 2016, 6, 27652.	3.3	26
40	Sites Contributing to TRPA1 Activation by the Anesthetic Propofol Identified by Photoaffinity Labeling. Biophysical Journal, 2017, 113, 2168-2172.	0.5	26
41	Conformational dynamics in TRPV1 channels reported by an encoded coumarin amino acid. ELife, 2017, 6, .	6.0	25
42	Structural and dynamical alignment of enzymes with partial structural similarity. Journal of Physics Condensed Matter, 2007, 19, 285206.	1.8	22
43	Propofol inhibits the voltage-gated sodium channel NaChBac at multiple sites. Journal of General Physiology, 2018, 150, 1317-1331.	1.9	22
44	Investigations of water/oxide interfaces by molecular dynamics simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1537.	14.6	21
45	Sodium Halide Adsorption and Water Structure at the Î±-Alumina(0001)/Water Interface. Journal of Physical Chemistry C, 2019, 123, 15618-15628.	3.1	19
46	First-Principles Calculation of Water pK_a Using the Newly Developed SCAN Functional. Journal of Physical Chemistry Letters, 2020, 11, 54-59.	4.6	19
47	TRPA1 modulation by piperidine carboxamides suggests an evolutionarily conserved binding site and gating mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26008-26019.	7.1	18
48	Propofol inhibits prokaryotic voltage-gated Na+ channels by promoting activation-coupled inactivation. Journal of General Physiology, 2018, 150, 1299-1316.	1.9	17
49	A Structural Basis for ¹²⁹Xe Hyperâ€CEST Signal in TEMâ€1 Î²â€Lactamase. ChemPhysChem, 2019, 20, 260-267.	2.1	17
50	Molecular Dynamics Simulations of Ion Channels. Trends in Biochemical Sciences, 2021, 46, 621-622.	7.5	17
51	Dual regulation of TRPV1 channels by phosphatidylinositol via functionally distinct binding sites. Journal of Biological Chemistry, 2021, 296, 100573.	3.4	16
52	Molecular dynamics simulations of outer-membrane protease T fromE. colibased on a hybrid coarse-grained/atomistic potential. Journal of Physics Condensed Matter, 2006, 18, S347-S355.	1.8	14
53	Proton affinity of the histidine-tryptophan cluster motif from the influenza A virus from ab initio molecular dynamics. Chemical Physics, 2013, 422, 156-164.	1.9	12
54	Combined computational and experimental analysis of a complex of ribonuclease III and the regulatory macrodomain protein, YmdB. Proteins: Structure, Function and Bioinformatics, 2015, 83, 459-472.	2.6	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, .	7.1	12
56	The Flu's Proton Escort. Science, 2010, 330, 456-458.	12.6	11
57	Cross-kingdom auxiliary subunit modulation of a voltage-gated sodium channel. Journal of Biological Chemistry, 2018, 293, 4981-4992.	3.4	11
58	Small molecule modulation of voltage gated sodium channels. Current Opinion in Structural Biology, 2017, 43, 156-162.	5.7	10
59	Polyamine blockade and binding energetics in the MthK potassium channel. Journal of General Physiology, 2020, 152, .	1.9	10
60	Evolutionarily Conserved Interactions within the Pore Domain of Acid-Sensing Ion Channels. Biophysical Journal, 2020, 118, 861-872.	0.5	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.	2.6	8
62	Sequence and structural conservation reveal fingerprint residues in TRP channels. ELife, 0, 11, .	6.0	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.	7.1	6
65	Computational Approaches to Studying Voltage-Gated Ion Channel Modulation by General Anesthetics. Methods in Enzymology, 2018, 602, 25-59.	1.0	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.	3.5	3
67	Microcanonical coarse-graining of the kinetic Ising model. Journal of Chemical Physics, 2020, 152, 084104.	3.0	2
68	Particle-based Ising model. Physical Review E, 2021, 103, 012125.	2.1	2
69	Epistasis Creates Invariant Sites and Modulates the Rate of Molecular Evolution. Molecular Biology and Evolution, 2022, 39, .	8.9	2
70	AlphaFold2 Workflow Optimization for High Throughput Predictions in HPC Environment. , 2022, , .		1