Lucie Delemotte

List of Publications by Year
in descending order

72 papers	2,415 citations	201674 27 h-index	243625 44 g-index
103 all docs	103 docs citations	103 times ranked	2890 citing authors

#	Article	IF	Citations
1	TRP channels: branching out into the fungal kingdom. Structure, 2022, 30, 2-4.	3.3	1
2	An open state of a voltage-gated sodium channel involving a Ï€-helix and conserved pore-facing asparagine. Biophysical Journal, 2022, 121, 11-22.	0.5	8
3	Open state of bacterial sodium channel: insights from molecular dynamics simulations. Biophysical Journal, 2022, 121, 24a.	0.5	0
4	Identification of electroporation sites in the complex lipid organization of the plasma membrane. ELife, 2022, 11, .	6.0	11
5	Uniting diversity to create a more inclusive academic environment. Journal of Cell Science, 2022, 135, .	2.0	0
6	Cryo-EM structure of the human Kv3.1 channel reveals gating control by the cytoplasmic T1 domain. Nature Communications, 2022, 13, .	12.8	16
7	Molecular Dynamics of Cell Membrane Electroporation. Biophysical Journal, 2021, 120, 42a.	0.5	0
8	Resin-acid derivatives bind to multiple sites on the voltage-sensor domain of the Shaker potassium channel. Journal of General Physiology, 2021, 153, .	1.9	2
9	Informing NMR experiments with molecular dynamics simulations to characterize the dominant activated state of the KcsA ion channel. Journal of Chemical Physics, 2021, 154, 165102.	3.0	11
10	Cannabidiol inhibits the skeletal muscle Nav1.4 by blocking its pore and by altering membrane elasticity. Journal of General Physiology, 2021, 153, .	1.9	38
11	Molecular Dynamics Simulations of Ion Channels. Trends in Biochemical Sciences, 2021, 46, 621-622.	7.5	17
12	Ion Channels: Intersection of Structure, Function, and Pharmacology. Journal of Molecular Biology, 2021, 433, 167102.	4.2	2
13	Functional cross-talk between phosphorylation and disease-causing mutations in the cardiac sodium channel Na _v 1.5. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	15
14	Structure and Sequence-based Computational Approaches to Allosteric Signal Transduction: Application to Electromechanical Coupling in Voltage-gated Ion Channels. Journal of Molecular Biology, 2021, 433, 167095.	4.2	4
15	Identification of ligand-specific G protein-coupled receptor states and prediction of downstream efficacy via data-driven modeling. ELife, 2021, 10, .	6.0	40
16	Allosteric Effect of Nanobody Binding on Ligand-Specific Active States of the Î²2 Adrenergic Receptor. Journal of Chemical Information and Modeling, 2021, 61, 6024-6037.	5.4	14
17	Molecular Insights from Conformational Ensembles via Machine Learning. Biophysical Journal, 2020, 118, 765-780.	0.5	67
18	Pulsed Electric Fields Can Create Pores in the Voltage Sensors of Voltage-Gated Ion Channels. Biophysical Journal, 2020, 119, 190-205.	0.5	43

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19	Network analysis reveals how lipids and other cofactors influence membrane protein allostery. Journal of Chemical Physics, 2020, 153, 141103.	3.0	21
20	Energy Landscapes Reveal Agonist Control of G Protein-Coupled Receptor Activation via Microswitches. Biochemistry, 2020, 59, 880-891.	2.5	45
21	Tracking the motion of the K V 1.2 voltage sensor reveals the molecular perturbations caused by a de novo mutation in a case of epilepsy. Journal of Physiology, 2020, 598, 5245-5269.	2.9	7
22	Calmodulin acts as a state-dependent switch to control a cardiac potassium channel opening. Science Advances, 2020, 6, .	10.3	38
23	Biophysical Characterization of Epigallocatechin-3-Gallate Effect on the Cardiac Sodium Channel Nav1.5. Molecules, 2020, 25, 902.	3.8	3
24	The molecular basis for sugar import in malaria parasites. Nature, 2020, 578, 321-325.	27.8	65
25	InfleCS: Clustering Free Energy Landscapes with Gaussian Mixtures. Journal of Chemical Theory and Computation, 2019, 15, 6752-6759.	5.3	36
26	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	5.4	26
27	Outlining the proton-conduction pathway in otopetrin channels. Nature Structural and Molecular Biology, 2019, 26, 528-530.	8.2	1
28	A De Novo Mutation Associated with Epilepsy Enhances KV1.2 Voltage Dependence, Suppressing Neuronal Excitability. Biophysical Journal, 2019, 116, 247a.	0.5	1
29	Helix breaking transition in the S4 of HCN channel is critical for hyperpolarization-dependent gating. ELife, 2019, 8, .	6.0	49
30	Exploring the Viral Channel KcvPBCV-1 Function via Computation. Journal of Membrane Biology, 2018, 251, 419-430.	2.1	10
31	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
32	Gating interaction maps reveal a noncanonical electromechanical coupling mode in the Shaker K+ channel. Nature Structural and Molecular Biology, 2018, 25, 320-326.	8.2	61
33	Studying Kv Channels Function using Computational Methods. Methods in Molecular Biology, 2018, 1684, 321-341.	0.9	4
34	Conformational landscapes of membrane proteins delineated by enhanced sampling molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 909-926.	2.6	67
35	Inference of Calmodulinâ€™s Ca²⁺-Dependent Free Energy Landscapes via Gaussian Mixture Model Validation. Journal of Chemical Theory and Computation, 2018, 14, 63-71.	5.3	23
36	Opening leads to closing: Allosteric crosstalk between the activation and inactivation gates in KcsA. Journal of General Physiology, 2018, 150, 1356-1359.	1.9	7

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37	Effect of Ca2+ on the promiscuous target-protein binding of calmodulin. PLoS Computational Biology, 2018, 14, e1006072.	3.2	42
38	Determining the molecular basis of voltage sensitivity in membrane proteins. Journal of General Physiology, 2018, 150, 1444-1458.	1.9	16
39	On the Selective Promiscuity of Calmodulin. Biophysical Journal, 2018, 114, 7a-8a.	0.5	0
40	Molecular simulations and free-energy calculations suggest conformation-dependent anion binding to a cytoplasmic site as a mechanism for Na+/K+-ATPase ion selectivity. Journal of Biological Chemistry, 2017, 292, 12412-12423.	3.4	12
41	Does Proton Conduction in the Voltage-Gated Proton Channel hH V 1 Involve Grotthus Hopping via Acidic Residues?. Biophysical Journal, 2017, 112, 163a-164a.	0.5	1
42	Gating Pore Currents in Sodium Channels. Handbook of Experimental Pharmacology, 2017, 246, 371-399.	1.8	10
43	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
44	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
45	In-Silico Electrophysiology: On the Activation of Voltage-Gated Ion Channels using Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 107a.	0.5	1
46	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
47	Characterization of the honeybee AmNaV1 channel and tools to assess the toxicity of insecticides. Scientific Reports, 2015, 5, 12475.	3.3	19
48	Canine CNGA3 Gene Mutations Provide Novel Insights into Human Achromatopsia-Associated Channelopathies and Treatment. PLoS ONE, 2015, 10, e0138943.	2.5	21
49	Understanding the Molecular Determinants of Capsaicin Mode of Action. Biophysical Journal, 2015, 108, 57a.	0.5	1
50	Gating pore currents are defects in common with two Nav1.5 mutations in patients with mixed arrhythmias and dilated cardiomyopathy. Journal of General Physiology, 2015, 145, 93-106.	1.9	64
51	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
52	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	2.1	157
53	Comparative sequence analysis suggests a conserved gating mechanism for TRP channels. Journal of General Physiology, 2015, 146, 37-50.	1.9	57
54	Voltage-gated ion channel modulation by lipids: Insights from molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1322-1331.	2.6	32

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55	Evidence of Conducting Hydrophobic Nanopores Across Membranes in Response to an Electric Field. Journal of Physical Chemistry C, 2014, 118, 6752-6757.	3.1	38
56	Evolutionary imprint of activation: The design principles of VSDs. Journal of General Physiology, 2014, 143, 145-156.	1.9	57
57	A Cyclic Nucleotide-Gated Channel Mutation Associated with Canine Daylight Blindness Provides Insight into a Role for the S2 Segment Tri-Asp motif in Channel Biogenesis. PLoS ONE, 2014, 9, e88768.	2.5	10
58	Dual Effect of PIP2 on Shaker K+ Channels. Biophysical Journal, 2013, 104, 464a.	0.5	1
59	Omega Currents in Voltage-Gated Ion Channels: What Can We Learn from Uncovering the Voltage-Sensing Mechanism Using MD Simulations?. Accounts of Chemical Research, 2013, 46, 2755-2762.	15.6	20
60	Conduction in a Biological Sodium Selective Channel. Journal of Physical Chemistry B, 2013, 117, 3782-3789.	2.6	59
61	Dual effect of phosphatidylinositol (4,5)-bisphosphate PIP2 on Shaker K+ channels.. Journal of Biological Chemistry, 2013, 288, 10951.	3.4	2
62	Gating pore currents and the resting state of Na _v 1.4 voltage sensor domains. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 19250-19255.	7.1	71
63	Dual Effect of Phosphatidyl (4,5)-Bisphosphate PIP2 on Shaker K+ Channels. Journal of Biological Chemistry, 2012, 287, 36158-36167.	3.4	37
64	Transport of siRNA through Lipid Membranes Driven by Nanosecond Electric Pulses: An Experimental and Computational Study. Journal of the American Chemical Society, 2012, 134, 13938-13941.	13.7	85
65	Molecular-Level Characterization of Lipid Membrane Electroporation using Linearly Rising Current. Journal of Membrane Biology, 2012, 245, 651-659.	2.1	36
66	Molecular Dynamics Simulations of Voltage-Gated Cation Channels: Insights on Voltage-Sensor Domain Function and Modulation. Frontiers in Pharmacology, 2012, 3, 97.	3.5	26
67	Molecular Dynamics Simulations of Lipid Membrane Electroporation. Journal of Membrane Biology, 2012, 245, 531-543.	2.1	158
68	Intermediate states of the Kv1.2 voltage sensor from atomistic molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6109-6114.	7.1	171
69	Effect of Sensor Domain Mutations on the Properties of Voltage-Gated Ion Channels: Molecular Dynamics Studies of the Potassium Channel Kv1.2. Biophysical Journal, 2010, 99, L72-L74.	0.5	48
70	The â€œhydrazinoturnâ€•hydrogen bonding network in hydrazinopeptides and aza-Î²3-peptides as probed by an AIM topological analysis of the electronic density. Computational and Theoretical Chemistry, 2008, 869, 41-46.	1.5	8
71	Modeling Membranes under a Transmembrane Potential. Journal of Physical Chemistry B, 2008, 112, 5547-5550.	2.6	94
72	Subtype-specific responses of hKv7.4 and hKv7.5 channels to polyunsaturated fatty acids reveal an unconventional modulatory site and mechanism. ELife, 0, 11, .	6.0	5