

Lucie Delemotte

List of Publications by Year in descending order

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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	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
2	Molecular Dynamics Simulations of Lipid Membrane Electroporation. Journal of Membrane Biology, 2012, 245, 531-543.	2.1	158
3	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	2.1	157
4	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
5	Modeling Membranes under a Transmembrane Potential. Journal of Physical Chemistry B, 2008, 112, 5547-5550.	2.6	94
6	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
7	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
8	Conformational landscapes of membrane proteins delineated by enhanced sampling molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 909-926.	2.6	67
9	Molecular Insights from Conformational Ensembles via Machine Learning. Biophysical Journal, 2020, 118, 765-780.	0.5	67
10	The molecular basis for sugar import in malaria parasites. Nature, 2020, 578, 321-325.	27.8	65
11	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
12	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.	7.1	63
13	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
14	Conduction in a Biological Sodium Selective Channel. Journal of Physical Chemistry B, 2013, 117, 3782-3789.	2.6	59
15	Evolutionary imprint of activation: The design principles of VSDs. Journal of General Physiology, 2014, 143, 145-156.	1.9	57
16	Comparative sequence analysis suggests a conserved gating mechanism for TRP channels. Journal of General Physiology, 2015, 146, 37-50.	1.9	57
17	Helix breaking transition in the S4 of HCN channel is critical for hyperpolarization-dependent gating. ELife, 2019, 8, .	6.0	49
18	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

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19	Energy Landscapes Reveal Agonist Control of G Protein-Coupled Receptor Activation via Microswitches. <i>Biochemistry</i> , 2020, 59, 880-891.	2.5	45
20	Pulsed Electric Fields Can Create Pores in the Voltage Sensors of Voltage-Gated Ion Channels. <i>Biophysical Journal</i> , 2020, 119, 190-205.	0.5	43
21	Effect of Ca ²⁺ on the promiscuous target-protein binding of calmodulin. <i>PLoS Computational Biology</i> , 2018, 14, e1006072.	3.2	42
22	Identification of ligand-specific G protein-coupled receptor states and prediction of downstream efficacy via data-driven modeling. <i>ELife</i> , 2021, 10, .	6.0	40
23	Evidence of Conducting Hydrophobic Nanopores Across Membranes in Response to an Electric Field. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6752-6757.	3.1	38
24	Calmodulin acts as a state-dependent switch to control a cardiac potassium channel opening. <i>Science Advances</i> , 2020, 6, .	10.3	38
25	Cannabidiol inhibits the skeletal muscle Nav1.4 by blocking its pore and by altering membrane elasticity. <i>Journal of General Physiology</i> , 2021, 153, .	1.9	38
26	Dual Effect of Phosphatidyl (4,5)-Bisphosphate PIP ₂ on Shaker K ⁺ Channels. <i>Journal of Biological Chemistry</i> , 2012, 287, 36158-36167.	3.4	37
27	Molecular-Level Characterization of Lipid Membrane Electroporation using Linearly Rising Current. <i>Journal of Membrane Biology</i> , 2012, 245, 651-659.	2.1	36
28	InflCS: Clustering Free Energy Landscapes with Gaussian Mixtures. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6752-6759.	5.3	36
29	Does Proton Conduction in the Voltage-Gated H ⁺ Channel hHv1 Involve Grotthuss-Like Hopping via Acidic Residues?. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3340-3351.	2.6	34
30	On the role of water density fluctuations in the inhibition of a proton channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E8359-E8368.	7.1	33
31	Voltage-gated ion channel modulation by lipids: Insights from molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2014, 1838, 1322-1331.	2.6	32
32	Molecular Dynamics Simulations of Voltage-Gated Cation Channels: Insights on Voltage-Sensor Domain Function and Modulation. <i>Frontiers in Pharmacology</i> , 2012, 3, 97.	3.5	26
33	Sharing Data from Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4093-4099.	5.4	26
34	Inference of Calmodulin-Dependent Free Energy Landscapes via Gaussian Mixture Model Validation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 63-71.	5.3	23
35	Canine CNGA3 Gene Mutations Provide Novel Insights into Human Achromatopsia-Associated Channelopathies and Treatment. <i>PLoS ONE</i> , 2015, 10, e0138943.	2.5	21
36	Network analysis reveals how lipids and other cofactors influence membrane protein allostery. <i>Journal of Chemical Physics</i> , 2020, 153, 141103.	3.0	21

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37	Omega Currents in Voltage-Gated Ion Channels: What Can We Learn from Uncovering the Voltage-Sensing Mechanism Using MD Simulations?. <i>Accounts of Chemical Research</i> , 2013, 46, 2755-2762.	15.6	20
38	Characterization of the honeybee AmNaV1 channel and tools to assess the toxicity of insecticides. <i>Scientific Reports</i> , 2015, 5, 12475.	3.3	19
39	Molecular Dynamics Simulations of Ion Channels. <i>Trends in Biochemical Sciences</i> , 2021, 46, 621-622.	7.5	17
40	Determining the molecular basis of voltage sensitivity in membrane proteins. <i>Journal of General Physiology</i> , 2018, 150, 1444-1458.	1.9	16
41	Cryo-EM structure of the human Kv3.1 channel reveals gating control by the cytoplasmic T1 domain. <i>Nature Communications</i> , 2022, 13, .	12.8	16
42	Functional cross-talk between phosphorylation and disease-causing mutations in the cardiac sodium channel Na ^v 1.5. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	15
43	Allosteric Effect of Nanobody Binding on Ligand-Specific Active States of the β_2 Adrenergic Receptor. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 6024-6037.	5.4	14
44	Molecular simulations and free-energy calculations suggest conformation-dependent anion binding to a cytoplasmic site as a mechanism for Na ⁺ /K ⁺ -ATPase ion selectivity. <i>Journal of Biological Chemistry</i> , 2017, 292, 12412-12423.	3.4	12
45	Informing NMR experiments with molecular dynamics simulations to characterize the dominant activated state of the KcsA ion channel. <i>Journal of Chemical Physics</i> , 2021, 154, 165102.	3.0	11
46	Identification of electroporation sites in the complex lipid organization of the plasma membrane. <i>ELife</i> , 2022, 11, .	6.0	11
47	Gating Pore Currents in Sodium Channels. <i>Handbook of Experimental Pharmacology</i> , 2017, 246, 371-399.	1.8	10
48	Exploring the Viral Channel KcvPBCV-1 Function via Computation. <i>Journal of Membrane Biology</i> , 2018, 251, 419-430.	2.1	10
49	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. <i>PLoS ONE</i> , 2014, 9, e88768.	2.5	10
50	The ϵ -hydrazinoturn ϵ -hydrogen bonding network in hydrazinopeptides and aza- β -peptides as probed by an AIM topological analysis of the electronic density. <i>Computational and Theoretical Chemistry</i> , 2008, 869, 41-46.	1.5	8
51	Permeating disciplines: Overcoming barriers between molecular simulations and classical structure-function approaches in biological ion transport. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 927-942.	2.6	8
52	An open state of a voltage-gated sodium channel involving a β -helix and conserved pore-facing asparagine. <i>Biophysical Journal</i> , 2022, 121, 11-22.	0.5	8
53	Opening leads to closing: Allosteric crosstalk between the activation and inactivation gates in KcsA. <i>Journal of General Physiology</i> , 2018, 150, 1356-1359.	1.9	7
54	Tracking the motion of the KV 1.2 voltage sensor reveals the molecular perturbations caused by a de novo mutation in a case of epilepsy. <i>Journal of Physiology</i> , 2020, 598, 5245-5269.	2.9	7

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55	Subtype-specific responses of hKv7.4 and hKv7.5 channels to polyunsaturated fatty acids reveal an unconventional modulatory site and mechanism. <i>ELife</i> , 0, 11, .	6.0	5
56	Studying Kv Channels Function using Computational Methods. <i>Methods in Molecular Biology</i> , 2018, 1684, 321-341.	0.9	4
57	Structure and Sequence-based Computational Approaches to Allosteric Signal Transduction: Application to Electromechanical Coupling in Voltage-gated Ion Channels. <i>Journal of Molecular Biology</i> , 2021, 433, 167095.	4.2	4
58	Biophysical Characterization of Epigallocatechin-3-Gallate Effect on the Cardiac Sodium Channel Nav1.5. <i>Molecules</i> , 2020, 25, 902.	3.8	3
59	Dual effect of phosphatidylinositol (4,5)-bisphosphate PIP2 on Shaker K+ channels.. <i>Journal of Biological Chemistry</i> , 2013, 288, 10951.	3.4	2
60	Resin-acid derivatives bind to multiple sites on the voltage-sensor domain of the Shaker potassium channel. <i>Journal of General Physiology</i> , 2021, 153, .	1.9	2
61	Ion Channels: Intersection of Structure, Function, and Pharmacology. <i>Journal of Molecular Biology</i> , 2021, 433, 167102.	4.2	2
62	Dual Effect of PIP2 on Shaker K+ Channels. <i>Biophysical Journal</i> , 2013, 104, 464a.	0.5	1
63	Understanding the Molecular Determinants of Capsaicin Mode of Action. <i>Biophysical Journal</i> , 2015, 108, 57a.	0.5	1
64	In-Silico Electrophysiology: On the Activation of Voltage-Gated Ion Channels using Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2016, 110, 107a.	0.5	1
65	Does Proton Conduction in the Voltage-Gated Proton Channel hH V 1 Involve Grotthus Hopping via Acidic Residues?. <i>Biophysical Journal</i> , 2017, 112, 163a-164a.	0.5	1
66	Outlining the proton-conduction pathway in otopetrin channels. <i>Nature Structural and Molecular Biology</i> , 2019, 26, 528-530.	8.2	1
67	A De Novo Mutation Associated with Epilepsy Enhances KV1.2 Voltage Dependence, Suppressing Neuronal Excitability. <i>Biophysical Journal</i> , 2019, 116, 247a.	0.5	1
68	TRP channels: branching out into the fungal kingdom. <i>Structure</i> , 2022, 30, 2-4.	3.3	1
69	On the Selective Promiscuity of Calmodulin. <i>Biophysical Journal</i> , 2018, 114, 7a-8a.	0.5	0
70	Molecular Dynamics of Cell Membrane Electroporation. <i>Biophysical Journal</i> , 2021, 120, 42a.	0.5	0
71	Open state of bacterial sodium channel: insights from molecular dynamics simulations. <i>Biophysical Journal</i> , 2022, 121, 24a.	0.5	0
72	Uniting diversity to create a more inclusive academic environment. <i>Journal of Cell Science</i> , 2022, 135, .	2.0	0