JÃ©rÃ´me HÃ©nin

List of Publications by Year
in descending order

40 papers	5,453 citations	270111 25 h-index	325983 40 g-index
48 all docs	48 docs citations	48 times ranked	7013 citing authors

#	Article	IF	Citations
1	Human Learning for Molecular Simulations: The Collective Variables Dashboard in VMD. Journal of Chemical Theory and Computation, 2022, 18, 1945-1956.	2.3	8
2	Symmetry-Adapted Restraints for Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2022, 18, 2494-2502.	2.3	6
3	Building intuition for binding free energy calculations: Bound state definition, restraints, and symmetry. Journal of Chemical Physics, 2021, 154, 204101.	1.2	22
4	Mechanistic Insights on Heme-to-Heme Transmembrane Electron Transfer Within NADPH Oxydases From Atomistic Simulations. Frontiers in Chemistry, 2021, 9, 650651.	1.8	3
5	Fast and Accurate Multidimensional Free Energy Integration. Journal of Chemical Theory and Computation, 2021, 17, 6789-6798.	2.3	10
6	Binding of divalent cations to acetate: molecular simulations guided by Raman spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 24014-24027.	1.3	28
7	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
8	Molecular Mechanics Parameterization of Anesthetic Molecules. Methods in Enzymology, 2018, 602, 61-76.	0.4	3
9	A Streamlined, General Approach for Computing Ligand Binding Free Energies and Its Application to GPCR-Bound Cholesterol. Journal of Chemical Theory and Computation, 2018, 14, 6560-6573.	2.3	42
10	Smoothed Biasing Forces Yield Unbiased Free Energies with the Extended-System Adaptive Biasing Force Method. Journal of Physical Chemistry B, 2017, 121, 3676-3685.	1.2	113
11	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 5173-5178.	2.3	49
12	A membrane-inserted structural model of the yeast mitofusin Fzo1. Scientific Reports, 2017, 7, 10217.	1.6	25
13	A Novel Bifunctional Alkylphenol Anesthetic Allows Characterization of Î³-Aminobutyric Acid, Type A (GABAA), Receptor Subunit Binding Selectivity in Synaptosomes. Journal of Biological Chemistry, 2016, 291, 20473-20486.	1.6	26
14	Evolution of Pentameric Ligand-Gated Ion Channels: Pro-Loop Receptors. PLoS ONE, 2016, 11, e0151934.	1.1	84
15	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
16	The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask. Journal of Physical Chemistry B, 2015, 119, 1129-1151.	1.2	351
17	Role of Internal Water on Protein Thermal Stability: The Case of Homologous G Domains. Journal of Physical Chemistry B, 2015, 119, 8939-8949.	1.2	21
18	Allosteric regulation of pentameric ligand-gated ion channels: An emerging mechanistic perspective. Channels, 2014, 8, 350-360.	1.5	31

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19	Type <scp>VI</scp> secretion and bacteriophage tail tubes share a common assembly pathway. EMBO Reports, 2014, 15, 315-321.	2.0	124
20	Lipid Concentration and Molar Ratio Boundaries for the Use of Isotropic Bicelles. Langmuir, 2014, 30, 6162-6170.	1.6	54
21	Foundations of Biomolecular Simulations: A Critical Introduction to Homology Modeling, Molecular Dynamics Simulations, and Free Energy Calculations of Membrane Proteins. , 2014, , 347-392.		0
22	CHARMM36 United Atom Chain Model for Lipids and Surfactants. Journal of Physical Chemistry B, 2014, 118, 547-556.	1.2	143
23	A Predicted Binding Site for Cholesterol on the GABAA Receptor. Biophysical Journal, 2014, 106, 1938-1949.	0.2	73
24	Using collective variables to drive molecular dynamics simulations. Molecular Physics, 2013, 111, 3345-3362.	0.8	750
25	General Anesthetics Predicted to Block the GLIC Pore with Micromolar Affinity. PLoS Computational Biology, 2012, 8, e1002532.	1.5	59
26	Multiple binding sites for the general anesthetic isoflurane identified in the nicotinic acetylcholine receptor transmembrane domain. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 14122-14127.	3.3	103
27	Single-spanning transmembrane domains in cell growth and cell-cell interactions. Cell Adhesion and Migration, 2010, 4, 313-324.	1.1	78
28	Exploring Multidimensional Free Energy Landscapes Using Time-Dependent Biases on Collective Variables. Journal of Chemical Theory and Computation, 2010, 6, 35-47.	2.3	366
29	An Atomistic Model for Simulations of the General Anesthetic Isoflurane. Journal of Physical Chemistry B, 2010, 114, 604-612.	1.2	24
30	Models for Phosphatidylglycerol Lipids Put to a Structural Test. Journal of Physical Chemistry B, 2009, 113, 6958-6963.	1.2	24
31	Diffusion of Glycerol through Escherichia coli Aquaglyceroporin GlpF. Biophysical Journal, 2008, 94, 832-839.	0.2	98
32	United-Atom Acyl Chains for CHARMM Phospholipids. Journal of Physical Chemistry B, 2008, 112, 7008-7015.	1.2	74
33	Embedded cholesterol in the nicotinic acetylcholine receptor. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14418-14423.	3.3	148
34	Conformational Equilibrium in Alanine-Rich Peptides Probed by Reversible Stretching Simulations. Journal of Physical Chemistry B, 2006, 110, 16718-16723.	1.2	17
35	Probing a Model of a GPCR/Ligand Complex in an Explicit Membrane Environment: The Human Cholecystokinin-1 Receptor. Biophysical Journal, 2006, 90, 1232-1240.	0.2	57
36	Hydrogen-bonding patterns of cholesterol in lipid membranes. Chemical Physics Letters, 2006, 425, 329-335.	1.2	45

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37	Exploring the free-energy landscape of a short peptide using an average force. Journal of Chemical Physics, 2005, 123, 244906.	1.2	113
38	Insights into the Recognition and Association of Transmembrane Î±-Helices. The Free Energy of Î±-Helix Dimerization in Glycophorin A. Journal of the American Chemical Society, 2005, 127, 8478-8484.	6.6	146
39	Overcoming free energy barriers using unconstrained molecular dynamics simulations. Journal of Chemical Physics, 2004, 121, 2904-2914.	1.2	423
40	Consistent Picture of Phosphateâ€“Divalent Cation Binding from Models with Implicit and Explicit Electronic Polarization. Journal of Physical Chemistry B, 0, , .	1.2	1