Xavier Periole

List of Publications by Year
in descending order

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44 papers	8,289 citations	147801 31 h-index	254184 43 g-index
47 all docs	47 docs citations	47 times ranked	7652 citing authors

#	Article	IF	Citations
1	Effect of palmitoylation on the dimer formation of the human dopamine transporter. Scientific Reports, 2021, 11, 4164.	3.3	8
2	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
3	Molecular Modeling Investigation of the Interaction between Humicola insolens Cutinase and SDS Surfactant Suggests a Mechanism for Enzyme Inactivation. Journal of Chemical Information and Modeling, 2019, 59, 1977-1987.	5.4	14
4	Cholesterol binding to a conserved site modulates the conformation, pharmacology, and transport kinetics of the human serotonin transporter. Journal of Biological Chemistry, 2018, 293, 3510-3523.	3.4	55
5	Energetics Underlying Twist Polymorphisms in Amyloid Fibrils. Journal of Physical Chemistry B, 2018, 122, 1081-1091.	2.6	44
6	DNA-encircled lipid bilayers. Nanoscale, 2018, 10, 18463-18467.	5.6	35
7	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. Scientific Reports, 2018, 8, 5080.	3.3	32
8	Insight into the molecular mechanism behind PEG-mediated stabilization of biofluid lipases. Scientific Reports, 2018, 8, 12293.	3.3	15
9	A direct interaction of cholesterol with the dopamine transporter prevents its out-to-inward transition. PLoS Computational Biology, 2018, 14, e1005907.	3.2	81
10	Exchange pathways of plastoquinone and plastoquinol in the photosystem II complex. Nature Communications, 2017, 8, 15214.	12.8	71
11	Interplay of G Protein-Coupled Receptors with the Membrane: Insights from Supra-Atomic Coarse Grain Molecular Dynamics Simulations. Chemical Reviews, 2017, 117, 156-185.	47.7	50
12	Probing Self-Assembly of G Protein-Coupled Receptor Oligomers in Membranes Using Molecular Dynamics Modeling and Experimental Approaches. , 2017, , 385-414.		1
13	Molecular Dynamics of Photosystem II Embedded in the Thylakoid Membrane. Journal of Physical Chemistry B, 2017, 121, 3237-3249.	2.6	34
14	An Amphotericin B Derivative Equally Potent to Amphotericin B and with Increased Safety. PLoS ONE, 2016, 11, e0162171.	2.5	29
15	Computational â€˜microscopyâ€™ of cellular membranes. Journal of Cell Science, 2016, 129, 257-68.	2.0	119
16	From light-harvesting to photoprotection: structural basis of the dynamic switch of the major antenna complex of plants (LHCII). Scientific Reports, 2015, 5, 15661.	3.3	108
17	Atomistic and Coarse Grain Topologies for the Cofactors Associated with the Photosystem II Core Complex. Journal of Physical Chemistry B, 2015, 119, 7791-7803.	2.6	41
18	Dry Martini, a Coarse-Grained Force Field for Lipid Membrane Simulations with Implicit Solvent. Journal of Chemical Theory and Computation, 2015, 11, 260-275.	5.3	236

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19	The power of coarse graining in biomolecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 225-248.	14.6	423
20	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	13.7	734
21	Phytochemicals Perturb Membranes and Promiscuously Alter Protein Function. ACS Chemical Biology, 2014, 9, 1788-1798.	3.4	241
22	The Martini Coarse-Grained Force Field. Methods in Molecular Biology, 2013, 924, 533-565.	0.9	107
23	Improved Parameters for the Martini Coarse-Grained Protein Force Field. Journal of Chemical Theory and Computation, 2013, 9, 687-697.	5.3	1,181
24	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 3282-3292.	5.3	67
25	Evidence for Cardiolipin Binding Sites on the Membrane-Exposed Surface of the Cytochrome bc₁. Journal of the American Chemical Society, 2013, 135, 3112-3120.	13.7	146
26	Rhodopsin Forms a Dimer with Cytoplasmic Helix 8 Contacts in Native Membranes. Biochemistry, 2012, 51, 1819-1821.	2.5	65
27	Dimerization of Amino Acid Side Chains: Lessons from the Comparison of Different Force Fields. Journal of Chemical Theory and Computation, 2012, 8, 1003-1014.	5.3	54
28	Structural Determinants of the Supramolecular Organization of G Protein-Coupled Receptors in Bilayers. Journal of the American Chemical Society, 2012, 134, 10959-10965.	13.7	199
29	In Silico Design of Robust Bolalipid Membranes. Biomacromolecules, 2012, 13, 196-205.	5.4	38
30	Mimicking the action of folding chaperones by Hamiltonian replicaâ€exchange molecular dynamics simulations: Application in the refinement of de novo models. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1744-1754.	2.6	14
31	Protofibrillar Assembly Toward the Formation of Amyloid Fibrils. Journal of Physical Chemistry Letters, 2011, 2, 2385-2390.	4.6	39
32	A Structurally Flexible Protein Backbone for the MARTINI Coarse Grained Force Field. Biophysical Journal, 2011, 100, 613a.	0.5	1
33	Comment on â€œOn using a too large integration time step in molecular dynamics simulations of coarse-grained molecular modelsâ€• by M. Winger, D. Trzesniak, R. Baron and W. F. van Gunsteren, Phys. Chem. Chem. Phys., 2009, 11, 1934. Physical Chemistry Chemical Physics, 2010, 12, 2254.	2.8	66
34	Probing the free energy landscape of the FBP28WW domain using multiple techniques. Journal of Computational Chemistry, 2009, 30, 1059-1068.	3.3	6
35	Factors That Affect the Degree of Twist in Î²-Sheet Structures: A Molecular Dynamics Simulation Study of a Cross-Î² Filament of the GNNQQNY Peptide. Journal of Physical Chemistry B, 2009, 113, 1728-1737.	2.6	59
36	Combining an Elastic Network With a Coarse-Grained Molecular Force Field: Structure, Dynamics, and Intermolecular Recognition. Journal of Chemical Theory and Computation, 2009, 5, 2531-2543.	5.3	571

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37	Refining homology models by combining replicaâ€exchange molecular dynamics and statistical potentials. Proteins: Structure, Function and Bioinformatics, 2008, 72, 1171-1188.	2.6	75
38	The MARTINI Coarse-Grained Force Field: Extension to Proteins. Journal of Chemical Theory and Computation, 2008, 4, 819-834.	5.3	2,178
39	The MARTINI Force Field. , 2008, , 5-19.		3
40	Convergence and sampling efficiency in replica exchange simulations of peptide folding in explicit solvent. Journal of Chemical Physics, 2007, 126, 014903.	3.0	114
41	G Protein-Coupled Receptors Self-Assemble in Dynamics Simulations of Model Bilayers. Journal of the American Chemical Society, 2007, 129, 10126-10132.	13.7	298
42	Molecular dynamics simulations from putative transition states of Î±â€spectrin SH3 domain. Proteins: Structure, Function and Bioinformatics, 2007, 69, 536-550.	2.6	13
43	Acidâ^'Base Equilibria in Rhodopsin:Â Dependence of the Protonation State of Glu134 on Its Environmentâ€. Biochemistry, 2004, 43, 6858-6864.	2.5	25
44	Molecular Dynamics Simulations of Transducin: Interdomain and Front to Back Communication in Activation and Nucleotide Exchange. Journal of Molecular Biology, 2004, 338, 469-481.	4.2	41