Jonathan Barnoud

List of Publications by Year
in descending order

31	2,524	430754 18	526166 27
papers	citations	h-index	g-index

32	32	32	3210
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Martini 3 Coarseâ€Grained Force Field: Small Molecules. Advanced Theory and Simulations, 2022, 5, .	1.3	72
2	The emerging potential of interactive virtual reality in drug discovery. Expert Opinion on Drug Discovery, 2022, 17, 685-698.	2.5	11
3	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
4	Sex and Ontogenetic Variation in the Crest of Numida meleagris: Implications for Crested Vertebrates. Anatomical Record, 2020, 303, 1018-1034.	0.8	9
5	Piezo1 Forms Specific, Functionally Important Interactions with Phosphoinositides and Cholesterol. Biophysical Journal, 2020, 119, 1683-1697.	0.2	60
6	Titratable Martini model for constant pH simulations. Journal of Chemical Physics, 2020, 153, 024118.	1.2	57
7	Interactive Molecular Dynamics in Virtual Reality Is an Effective Tool for Flexible Substrate and Inhibitor Docking to the SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2020, 60, 5803-5814.	2.5	30
8	Resolving Donorâ€“Acceptor Interfaces and Charge Carrier Energy Levels of Organic Semiconductors with Polar Side Chains. Advanced Functional Materials, 2020, 30, 2004799.	7.8	28
9	Coupling Coarse-Grained to Fine-Grained Models via Hamiltonian Replica Exchange. Journal of Chemical Theory and Computation, 2020, 16, 5313-5322.	2.3	9
10	Capturing Cholineâ€“Aromatics Cationâˆ’Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	2.3	35
11	Dual Resolution Membrane Simulations Using Virtual Sites. Journal of Physical Chemistry B, 2020, 124, 3944-3953.	1.2	21
12	Size-dependent aggregation of hydrophobic nanoparticles in lipid membranes. Nanoscale, 2020, 12, 9452-9461.	2.8	13
13	Narupa iMD: A VR-Enabled Multiplayer Framework for Streaming Interactive Molecular Simulations. , 2020, , .		9
14	Gangliosides Destabilize Lipid Phase Separation in Multicomponent Membranes. Biophysical Journal, 2019, 117, 1215-1223.	0.2	9
15	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	2.5	26
16	Understanding Piezo1's Relationship with Lipids. Biophysical Journal, 2019, 116, 459a.	0.2	1
17	New Automated and High-throughput Tools for the Martini Forcefield. Biophysical Journal, 2018, 114, 676a-677a.	0.2	0
18	Alcohol Interactions with Lipid Bilayers. Molecules, 2017, 22, 2078.	1.7	28

#	Article	IF	Citations
19	Lipid phase separation in the presence of hydrocarbons in giant unilamellar vesicles. AIMS Biophysics, 2017, 4, 528-542.	0.3	5
20	PBxplore: a tool to analyze local protein structure and deformability with Protein Blocks. PeerJ, 2017, 5, e4013.	0.9	29
21	MDAnalysis: A Python Package for the Rapid Analysis of Molecular Dynamics Simulations. , 2016, , .		790
22	Protein flexibility in the light of structural alphabets. Frontiers in Molecular Biosciences, 2015, 2, 20.	1.6	71
23	C 60 fullerene promotes lung monolayer collapse. Journal of the Royal Society Interface, 2015, 12, 20140931.	1.5	31
24	Coarse-Grained Force Fields for Molecular Simulations. Methods in Molecular Biology, 2015, 1215, 125-149.	0.4	18
25	Hydrophobic Compounds Reshape Membrane Domains. PLoS Computational Biology, 2014, 10, e1003873.	1.5	58
26	Lipid Membranes as Solvents for Carbon Nanoparticles. Physical Review Letters, 2014, 112, 068102.	2.9	61
27	Polystyrene Nanoparticles Perturb Lipid Membranes. Journal of Physical Chemistry Letters, 2014, 5, 241-246.	2.1	266
28	Lipid Membranes as Solvent for Carbon Nanoparticles. Biophysical Journal, 2014, 106, 290a.	0.2	0
29	Free energy of WALP23 dimer association in DMPC, DPPC, and DOPC bilayers. Chemistry and Physics of Lipids, 2013, 169, 95-105.	1.5	111
30	Interaction of C70 fullerene with the Kv1.2 potassium channel. Physical Chemistry Chemical Physics, 2012, 14, 12526.	1.3	17
31	A Coarse-Grained MARTINI Model of Polyethylene Glycol and of Polyoxyethylene Alkyl Ether Surfactants. Journal of Physical Chemistry B, 2012, 116, 14353-14362.	1.2	90