Emiliano Brini

List of Publications by Year in descending order

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840776 839539 1,062 21 11 18 citations h-index g-index papers 21 21 21 1464 all docs docs citations times ranked citing authors

#	Article	IF	Citations
1	Accelerating Protein Folding Molecular Dynamics Using Inter-Residue Distances from Machine Learning Servers. Journal of Chemical Theory and Computation, 2022, 18, 1929-1935.	5.3	8
2	Accelerating Molecular Dynamics Enrichments of High-Affinity Ligands for Proteins. Journal of Chemical Theory and Computation, 2022, 18, 374-379.	5.3	2
3	Sampling and refinement protocols for template-based macrocycle docking: 2018 D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 179-189.	2.9	8
4	Modeling betaâ€sheet peptideâ€protein interactions: Rosetta FlexPepDock in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1037-1049.	2.6	10
5	Protein storytelling through physics. Science, 2020, 370, .	12.6	49
6	Computing Ligands Bound to Proteins Using MELD-Accelerated MD. Journal of Chemical Theory and Computation, 2020, 16, 6377-6382.	5.3	15
7	Determining Protein Structures using Accelerated MD Simulations and Noisy Data. Biophysical Journal, 2020, 118, 141a.	0.5	1
8	ClusPro in rounds 38 to 45 of CAPRI: Toward combining templateâ€based methods with free docking. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1082-1090.	2.6	5
9	Computing Poses of Ligands Bound to Proteins using MELD Accelerated Molecular Dynamics. Biophysical Journal, 2020, 118, 323a.	0.5	0
10	NMRâ€assisted protein structure prediction with MELDxMD. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1333-1340.	2.6	20
11	Predicting Protein Dimer Structures Using MELD × MD. Journal of Chemical Theory and Computation, 2019, 15, 3381-3389.	5.3	15
12	How Water's Properties Are Encoded in Its Molecular Structure and Energies. Chemical Reviews, 2017, 117, 12385-12414.	47.7	284
13	Adapting the semi-explicit assembly solvation model for estimating water-cyclohexane partitioning with the SAMPL5 molecules. Journal of Computer-Aided Molecular Design, 2016, 30, 1067-1077.	2.9	3
14	Blind protein structure prediction using accelerated free-energy simulations. Science Advances, 2016, 2, e1601274.	10.3	57
15	Combining Physics and Knowledge in Blind Protein Structure Prediction. Biophysical Journal, 2016, 110, 345a.	0.5	0
16	Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations. Journal of Chemical Theory and Computation, 2015, 11, 4770-4779.	5.3	76
17	Systematic coarse-graining methods for soft matter simulations – a review. Soft Matter, 2013, 9, 2108-2119.	2.7	301
18	Chemically transferable coarse-grained potentials from conditional reversible work calculations. Journal of Chemical Physics, 2012, 137, 154113.	3.0	58

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#	Article	IF	CITATIONS
19	Thermodynamic transferability of coarse-grained potentials for polymer–additive systems. Physical Chemistry Chemical Physics, 2012, 14, 11896.	2.8	26
20	Shape Governs the Motion of Chemically Propelled Janus Swimmers. Journal of Physical Chemistry C, 2012, 116, 592-598.	3.1	47
21	Conditional reversible work method for molecular coarse graining applications. Physical Chemistry Chemical Physics, 2011, 13, 10468.	2.8	77