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List of Publications by Year in descending order

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Version: 2024-02-01

933447 1199594 12 499 10 12 citations h-index g-index papers 12 12 12 583 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Pressure control using stochastic cell rescaling. Journal of Chemical Physics, 2020, 153, 114107.	3.0	113
2	Kinetics of Drug Binding and Residence Time. Annual Review of Physical Chemistry, 2019, 70, 143-171.	10.8	105
3	Predicting Residence Time and Drug Unbinding Pathway through Scaled Molecular Dynamics. Journal of Chemical Information and Modeling, 2019, 59, 535-549.	5.4	64
4	Toward empirical force fields that match experimental observables. Journal of Chemical Physics, 2020, 152, 230902.	3.0	49
5	An Integrated Markov State Model and Path Metadynamics Approach To Characterize Drug Binding Processes. Journal of Chemical Theory and Computation, 2019, 15, 5689-5702.	5.3	45
6	Data-Driven Molecular Dynamics: A Multifaceted Challenge. Pharmaceuticals, 2020, 13, 253.	3.8	33
7	Reweighting of molecular simulations with explicit-solvent SAXS restraints elucidates ion-dependent RNA ensembles. Nucleic Acids Research, 2021, 49, e84-e84.	14.5	25
8	Structural and Kinetic Characterization of the Intrinsically Disordered Protein SeV N _{TAIL} through Enhanced Sampling Simulations. Journal of Physical Chemistry B, 2017, 121, 9572-9582.	2.6	23
9	Binding Residence Time through Scaled Molecular Dynamics: A Prospective Application to hDAAO Inhibitors. Journal of Chemical Information and Modeling, 2018, 58, 2255-2265.	5.4	21
10	Development of a multisite model for Ni(II) ion in solution from thermodynamic and kinetic data. Journal of Computational Chemistry, 2017, 38, 1834-1843.	3.3	11
11	Fully Flexible Docking via Reaction-Coordinate-Independent Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2018, 58, 490-500.	5.4	9
12	Molecular Dynamics of Solids at Constant Pressure and Stress Using Anisotropic Stochastic Cell Rescaling. Applied Sciences (Switzerland), 2022, 12, 1139.	2.5	1