Ioan Andricioaei

List of Publications by Year
in descending order

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83 papers	3,487 citations	212478 28 h-index	162838 57 g-index
87 all docs	87 docs citations	87 times ranked	4339 citing authors

#	Article	IF	Citations
1	Markovian Weighted Ensemble Milestoning (M-WEM): Long-Time Kinetics from Short Trajectories. Journal of Chemical Theory and Computation, 2022, 18, 79-95.	2.3	20
2	Point mutations in SARS-CoV-2 variants induce long-range dynamical perturbations in neutralizing antibodies. Chemical Science, 2022, 13, 7224-7239.	3.7	6
3	Kinetics and Free Energy of Protein Ligand Interaction using Weighted Ensemble Milestoning (WEM). Biophysical Journal, 2021, 120, 97a.	0.2	0
4	Distant residues modulate conformational opening in SARS-CoV-2 spike protein. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	69
5	Kinetics and free energy of ligand dissociation using weighted ensemble milestoning. Journal of Chemical Physics, 2020, 153, 154117.	1.2	10
6	Free Energy Landscape and Conformational Kinetics of Hoogsteen Base Pairing in DNA vs. RNA. Biophysical Journal, 2020, 119, 1568-1579.	0.2	10
7	Weighted ensemble milestoning (WEM): A combined approach for rare event simulations. Journal of Chemical Physics, 2020, 152, 234114.	1.2	22
8	Elastic continuum stiffness of contractile tail sheaths from molecular dynamics simulations. Journal of Chemical Physics, 2019, 151, 185103.	1.2	1
9	How the phage T4 injection machinery works including energetics, forces, and dynamic pathway. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 25097-25105.	3.3	23
10	Modulation of Hoogsteen dynamics on DNA recognition. Nature Communications, 2018, 9, 1473.	5.8	38
11	Advances in milestoning. I. Enhanced sampling via wind-assisted reweighted milestoning (WARM). Journal of Chemical Physics, 2018, 149, 084103.	1.2	17
12	Advances in milestoning. II. Calculating time-correlation functions from milestoning using stochastic path integrals. Journal of Chemical Physics, 2018, 149, 084104.	1.2	7
13	Electric-Field-Induced Protein Translocation via a Conformational Transition in SecDF: An MD Study. Biophysical Journal, 2017, 112, 2520-2528.	0.2	7
14	Automated placement of interfaces in conformational kinetics calculations using machine learning. Journal of Chemical Physics, 2017, 147, 152727.	1.2	4
15	Dynamic Model Exposes the Energetics and Dynamics of the Injection Machinery for Bacteriophage T4. Biophysical Journal, 2017, 113, 195-205.	0.2	8
16	A First Model of the Dynamics of the Bacteriophage T4 Injection Machinery. Journal of Computational and Nonlinear Dynamics, 2016, 11, .	0.7	7
17	Reaction Coordinate-Free Approach to Recovering Kinetics from Potential-Scaled Simulations: Application of Kramersâ€™ Rate Theory. Journal of Physical Chemistry B, 2016, 120, 8600-8605.	1.2	23
18	m1A and m1G disrupt A-RNA structure through the intrinsic instability of Hoogsteen base pairs. Nature Structural and Molecular Biology, 2016, 23, 803-810.	3.6	100

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19	Entropy Calculations of Hoogsteen and Watson-Crick Conformations. Biophysical Journal, 2016, 110, 405a.	0.2	0
20	The Role of Entropy in Explaining Tightly Bend DNA Propensity and Kinetic Barriers to Base Pair Unzipping. Biophysical Journal, 2016, 110, 566a.	0.2	0
21	Rate turnover in mechano-catalytic coupling: A model and its microscopic origin. Journal of Chemical Physics, 2015, 143, 045105.	1.2	7
22	Dendrimers in Nanoscale Confinement: The Interplay between Conformational Change and Nanopore Entrance. Nano Letters, 2015, 15, 4822-4828.	4.5	17
23	On the Possibility of Facilitated Diffusion of Dendrimers Along DNA. Journal of Physical Chemistry B, 2015, 119, 6894-6904.	1.2	6
24	Slowdown of Interhelical Motions Induces a Glass Transition in RNA. Biophysical Journal, 2015, 108, 2876-2885.	0.2	7
25	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
26	Free-Energy Landscape and Characteristic Forces for the Initiation of DNA Unzipping. Biophysical Journal, 2015, 108, 1727-1738.	0.2	8
27	Single-Walled Carbon Nanotubes Modulate the B- to A-DNA Transition. Journal of Physical Chemistry C, 2014, 118, 29441-29447.	1.5	5
28	Role of Microscopic Flexibility in Tightly Curved DNA. Journal of Physical Chemistry B, 2014, 118, 11028-11036.	1.2	11
29	Slowing down single-molecule trafficking through a protein nanopore reveals intermediates for peptide translocation. Scientific Reports, 2014, 4, 3885.	1.6	103
30	Structural Ensemble and Dynamics of Toroidal-like DNA Shapes in Bacteriophage Ï•29 Exit Cavity. Biophysical Journal, 2013, 104, 2058-2067.	0.2	10
31	Utility of 1H NMR Chemical Shifts in Determining RNA Structure and Dynamics. Journal of Physical Chemistry B, 2013, 117, 2045-2052.	1.2	31
32	Attractive Hydration Forces in DNAâ€“Dendrimer Interactions on the Nanometer Scale. Journal of Physical Chemistry B, 2013, 117, 973-981.	1.2	22
33	Conformational Transitions of Nucleic Acids under External Forces: Computer Simulations and a Stochastic Theory for their Kinetics. Biophysical Journal, 2013, 104, 16a.	0.2	0
34	Insights from simulations into the mechanism of human topoisomerase I: Explanation for a seeming controversy in experiments. Journal of Molecular Graphics and Modelling, 2013, 44, 286-296.	1.3	4
35	Reconstructing equilibrium entropy and enthalpy profiles from non-equilibrium pulling. Journal of Chemical Physics, 2013, 138, 114110.	1.2	7
36	A General Method for Constructing Atomic-Resolution RNA Ensembles using NMR Residual Dipolar Couplings: The Basis for Interhelical Motions Revealed. Journal of the American Chemical Society, 2013, 135, 5457-5466.	6.6	94

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37	A Model for Highly Strained DNA Compressed Inside a Protein Cavity. Journal of Computational and Nonlinear Dynamics, 2013, 8, .	0.7	8
38	Probing Sequence-Specific DNA Flexibility in A-Tracts and Pyrimidine-Purine Steps by Nuclear Magnetic Resonance ¹³C Relaxation and Molecular Dynamics Simulations. Biochemistry, 2012, 51, 8654-8664.	1.2	44
39	A Multiscale Dynamic Model of DNA Supercoil Relaxation by Topoisomerase IB. Biophysical Journal, 2011, 100, 2016-2023.	0.2	24
40	Interfacial Orientation and Secondary Structure Change in Tachyplesin I: Molecular Dynamics and Sum Frequency Generation Spectroscopy Studies. Langmuir, 2011, 27, 14343-14351.	1.6	14
41	Investigating a Novel Toroid-Shaped DNA Structure Found in Mature Bacteriophage Ï†29. Biophysical Journal, 2011, 100, 401a.	0.2	0
42	Discovery of selective bioactive small molecules by targeting an RNA dynamic ensemble. Nature Chemical Biology, 2011, 7, 553-559.	3.9	232
43	Transient Hoogsteen base pairs in canonical duplex DNA. Nature, 2011, 470, 498-502.	13.7	291
44	A Comparative Study on the Ability of Two Implicit Solvent Lipid Models to Predict Transmembrane Helix Tilt Angles. Journal of Membrane Biology, 2011, 239, 57-62.	1.0	1
45	Microscopic Basis for the Mesoscopic Extensibility of Dendrimer-Compacted DNA. Biophysical Journal, 2010, 98, 834-842.	0.2	17
46	Free Energy Calculations Reveal Rotating-Ratchet Mechanism for DNA Supercoil Relaxation by Topoisomerase IB and its Inhibition. Biophysical Journal, 2010, 99, 869-878.	0.2	15
47	Referencing Strategy for the Direct Comparison of Nuclear Magnetic Resonance and Molecular Dynamics Motional Parameters in RNA. Journal of Physical Chemistry B, 2010, 114, 929-939.	1.2	18
48	Conformational and Solvent Entropy Contributions to the Thermal Response of Nucleic Acid-Based Nanothermometers. Journal of Physical Chemistry B, 2010, 114, 2076-2082.	1.2	10
49	Surface Orientation of Magainin 2: Molecular Dynamics Simulation and Sum Frequency Generation Vibrational Spectroscopic Studies. Langmuir, 2010, 26, 16031-16036.	1.6	25
50	Constructing RNA dynamical ensembles by combining MD and motionally decoupled NMR RDCs: new insights into RNA dynamics and adaptive ligand recognition. Nucleic Acids Research, 2009, 37, 3670-3679.	6.5	106
51	Constructing atomic-resolution RNA structural ensembles using MD and motionally decoupled NMR RDCs. Methods, 2009, 49, 167-173.	1.9	23
52	Energy Landscape for DNA Rotation and Sliding through a Phage Portal. Biophysical Journal, 2009, 96, L29-L31.	0.2	6
53	Simulated Single-Molecule FRET Trajectories: A Comparative Analysis Between Three Telomeric G-quadruplexes. Biophysical Journal, 2009, 96, 344a.	0.2	0
54	Characterizing Complex Dynamics in the Transactivation Response Element Apical Loop and Motional Correlations with the Bulge by NMR, Molecular Dynamics, and Mutagenesis. Biophysical Journal, 2008, 95, 3906-3915.	0.2	65

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55	Poly(amidoamine) Dendrimers on Lipid Bilayers II: Effects of Bilayer Phase and Dendrimer Termination. Journal of Physical Chemistry B, 2008, 112, 9346-9353.	1.2	90
56	Poly(amidoamine) Dendrimers on Lipid Bilayers I: Free Energy and Conformation of Binding. Journal of Physical Chemistry B, 2008, 112, 9337-9345.	1.2	74
57	Entropy-energy decomposition from nonequilibrium work trajectories. Journal of Chemical Physics, 2008, 128, 024104.	1.2	10
58	An experimentally guided umbrella sampling protocol for biomolecules. Journal of Chemical Physics, 2008, 129, 114101.	1.2	23
59	Directionally negative friction: A method for enhanced sampling of rare event kinetics. Journal of Chemical Physics, 2008, 128, 114112.	1.2	16
60	iRED Analysis of TAR RNA Reveals Motional Coupling, Long-Range Correlations, and a Dynamical Hinge. Biophysical Journal, 2007, 93, 411-422.	0.2	31
61	Exact Low-Force Kinetics from High-Force Single-Molecule Unfolding Events. Biophysical Journal, 2007, 93, 3373-3381.	0.2	22
62	Parameterization of Peptide13C Carbonyl Chemical Shielding Anisotropy in Molecular Dynamics Simulations. ChemPhysChem, 2007, 8, 1375-1385.	1.0	6
63	Size, Motion, and Function of the SecY Translocon Revealed by Molecular Dynamics Simulations with Virtual Probes. Biophysical Journal, 2006, 90, 2718-2730.	0.2	48
64	Dynamic Distance Disorder in Proteins Is Caused by Trapping. Journal of Physical Chemistry B, 2006, 110, 9363-9367.	1.2	88
65	Impact of static and dynamic A-form heterogeneity on the determination of RNA global structural dynamics using NMR residual dipolar couplings. Journal of Biomolecular NMR, 2006, 36, 235-249.	1.6	54
66	On the calculation of time correlation functions by potential scaling. Journal of Chemical Physics, 2006, 124, 034110.	1.2	29
67	On structural transitions, thermodynamic equilibrium, and the phase diagram of DNA and RNA duplexes under torque and tension. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 16200-16205.	3.3	42
68	Rotation of DNA around intact strand in human topoisomerase I implies distinct mechanisms for positive and negative supercoil relaxation. Nucleic Acids Research, 2005, 33, 6621-6634.	6.5	27
69	A skewed-momenta method to efficiently generate conformational-transition trajectories. Journal of Chemical Physics, 2005, 123, 074107.	1.2	32
70	Repetitive Pulling Catalyzes Co-translocational Unfolding of Barnase During Import Through a Mitochondrial Pore. Journal of Molecular Biology, 2005, 350, 1017-1034.	2.0	53
71	Conversion between Three Conformational States of Integrin I Domains with a C-Terminal Pull Spring Studied with Molecular Dynamics. Structure, 2004, 12, 2137-2147.	1.6	94
72	Dependence of DNA Polymerase Replication Rate on External Forces: A Model Based on Molecular Dynamics Simulations. Biophysical Journal, 2004, 87, 1478-1497.	0.2	30

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73	An improved method for nonbonded list generation: Rapid determination of near-neighbor pairs. Journal of Computational Chemistry, 2003, 24, 222-231.	1.5	20
74	Self-guided enhanced sampling methods for thermodynamic averages. Journal of Chemical Physics, 2003, 118, 1074-1084.	1.2	55
75	On the calculation of entropy from covariance matrices of the atomic fluctuations. Journal of Chemical Physics, 2001, 115, 6289-6292.	1.2	472
76	Smart Darting Monte Carlo. Journal of Chemical Physics, 2001, 114, 6994-7000.	1.2	60
77	Simulation of quantum systems using path integrals in a generalized ensemble. Chemical Physics Letters, 2001, 346, 274-282.	1.2	5
78	Computational methods inspired by Tsallis statistics: Monte Carlo and molecular dynamics algorithms for the simulation of classical and quantum systems. Brazilian Journal of Physics, 1999, 29, 179-186.	0.7	14
79	Global optimization using bad derivatives: Derivative-free method for molecular energy minimization. Journal of Computational Chemistry, 1998, 19, 1445-1455.	1.5	22
80	On Monte Carlo and molecular dynamics methods inspired by Tsallis statistics: Methodology, optimization, and application to atomic clusters. Journal of Chemical Physics, 1997, 107, 9117-9124.	1.2	112
81	An efficient Monte Carlo algorithm for overcoming broken ergodicity in the simulation of spin systems. Physica A: Statistical Mechanics and Its Applications, 1997, 247, 553-558.	1.2	11
82	Finding the needle in the haystack: Algorithms for conformational optimization. Computers in Physics, 1996, 10, 449.	0.6	22
83	Generalized simulated annealing algorithms using Tsallis statistics: Application to conformational optimization of a tetrapeptide. Physical Review E, 1996, 53, R3055-R3058.	0.8	149