Nicolae-Viorel Buchete

List of Publications by Year
in descending order

52 papers	3,213 citations	236833 25 h-index	197736 49 g-index
55 all docs	55 docs citations	55 times ranked	3843 citing authors

#	Article	IF	Citations
1	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	23.0	530
2	Coarse Master Equations for Peptide Folding Dynamics. Journal of Physical Chemistry B, 2008, 112, 6057-6069.	1.2	444
3	Are Current Molecular Dynamics Force Fields too Helical?. Biophysical Journal, 2008, 95, L07-L09.	0.2	419
4	Molecular Dynamics Simulations of Alzheimer's Î²-Amyloid Protofilaments. Journal of Molecular Biology, 2005, 353, 804-821.	2.0	250
5	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
6	Structure and Dynamics of Parallel Î²-Sheets, Hydrophobic Core, and Loops in Alzheimerâ€™s AÎ² Fibrils. Biophysical Journal, 2007, 92, 3032-3039.	0.2	126
7	Development of novel statistical potentials for protein fold recognition. Current Opinion in Structural Biology, 2004, 14, 225-232.	2.6	118
8	Peptide folding kinetics from replica exchange molecular dynamics. Physical Review E, 2008, 77, 030902.	0.8	104
9	Orientational potentials extracted from protein structures improve native fold recognition. Protein Science, 2004, 13, 862-874.	3.1	84
10	Thermostat Artifacts in Replica Exchange Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2009, 5, 1393-1399.	2.3	81
11	Nanoscale Piezoelectric Properties of Self-Assembled Fmocâ€“FF Peptide Fibrous Networks. ACS Applied Materials & Interfaces, 2015, 7, 12702-12707.	4.0	69
12	Molecular Interactions of Alzheimer's AÎ² Protofilaments with Lipid Membranes. Journal of Molecular Biology, 2012, 421, 572-586.	2.0	64
13	Alzheimer AÎ² peptide interactions with lipid membranes. Prion, 2012, 6, 339-345.	0.9	58
14	Modulation of Alzheimerâ€™s AÎ² Protofilament-Membrane Interactions by Lipid Headgroups. ACS Chemical Neuroscience, 2015, 6, 446-455.	1.7	55
15	Anisotropic coarse-grained statistical potentials improve the ability to identify nativelike protein structures. Journal of Chemical Physics, 2003, 118, 7658.	1.2	54
16	Dynamics of protein folding: Probing the kinetic network of foldingâ€“unfolding transitions with experiment and theory. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1001-1020.	1.1	51
17	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. Angewandte Chemie - International Edition, 2016, 55, 983-986.	7.2	43
18	Conformational dynamics and aggregation behavior of piezoelectric diphenylalanine peptides in an external electric field. Biophysical Chemistry, 2015, 196, 16-24.	1.5	41

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19	Mean First-Passage Time Calculations for the Coil-to-Helix Transition:Â The Active Helix Ising Modelâ€. Journal of Physical Chemistry B, 2001, 105, 6684-6697.	1.2	29
20	Molecular mechanisms of asymmetric RAF dimer activation. Biochemical Society Transactions, 2014, 42, 784-790.	1.6	28
21	Variational Identification of Markovian Transition States. Physical Review X, 2017, 7, .	2.8	28
22	Continuous anisotropic representation of coarse-grained potentials for proteins by spherical harmonics synthesis. Journal of Molecular Graphics and Modelling, 2004, 22, 441-450.	1.3	27
23	Substrate-induced Conformational Changes and Dynamics of UDP-N-Acetylgalactosamine:Polypeptide N-Acetylgalactosaminyltransferase-2. Journal of Molecular Biology, 2007, 373, 439-451.	2.0	27
24	The transition between active and inactive conformations of Abl kinase studied by rock climbing and Milestoning. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129508.	1.1	26
25	Orientation-dependent coarse-grained potentials derived by statistical analysis of molecular structural databases. Polymer, 2004, 45, 597-608.	1.8	25
26	Exposure of chick embryos to cadmium changes the extra-embryonic vascular branching pattern and alters expression of VEGF-A and VEGF-R2. Toxicology and Applied Pharmacology, 2015, 289, 79-88.	1.3	25
27	Coarse Master Equations for Binding Kinetics of Amyloid Peptide Dimers. Journal of Physical Chemistry Letters, 2016, 7, 2676-2682.	2.1	25
28	Conformational dynamics of human IAPP monomers. Biophysical Chemistry, 2012, 167, 1-7.	1.5	22
29	Profiling of a panel of radioresistant prostate cancer cells identifies deregulation of key miRNAs. Clinical and Translational Radiation Oncology, 2017, 2, 63-68.	0.9	20
30	Computer Simulations of the Dissociation Mechanism of Gleevec from Abl Kinase with Milestoning. Journal of Physical Chemistry B, 2021, 125, 5706-5715.	1.2	20
31	Are Peptides Good Two-State Folders?. Journal of Chemical Theory and Computation, 2011, 7, 2370-2375.	2.3	18
32	Thermal and aqueous stability improvement of graphene oxide enhanced diphenylalanine nanocomposites. Science and Technology of Advanced Materials, 2017, 18, 172-179.	2.8	18
33	Peptide dimerization-dissociation rates from replica exchange molecular dynamics. Journal of Chemical Physics, 2017, 147, 152725.	1.2	16
34	Dissecting contact potentials for proteins: Relative contributions of individual amino acids. Proteins: Structure, Function and Bioinformatics, 2008, 70, 119-130.	1.5	15
35	SARAH Domain-Mediated MST2-RASSF Dimeric Interactions. PLoS Computational Biology, 2016, 12, e1005051.	1.5	15
36	MST2-RASSF proteinâ€“protein interactions through SARAH domains. Briefings in Bioinformatics, 2016, 17, 593-602.	3.2	13

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37	Unlocking the Atomic-Level Details of Amyloid Fibril Growth through Advanced Biomolecular Simulations. Biophysical Journal, 2012, 103, 1411-1413.	0.2	12
38	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. Journal of Physical Chemistry B, 2018, 122, 5657-5665.	1.2	11
39	Long-time methods for molecular dynamics simulations: Markov State Models and Milestoning. Progress in Molecular Biology and Translational Science, 2020, 170, 215-237.	0.9	8
40	Amyloid Fibril Design: Limiting Structural Polymorphism in Alzheimerâ€™s AÎ² Protofilaments. Journal of Physical Chemistry B, 2018, 122, 11535-11545.	1.2	7
41	Conformational analysis of replica exchange MD: Temperature-dependent Markov networks for FF amyloid peptides. Journal of Chemical Physics, 2018, 149, 072323.	1.2	7
42	Computational Opportunities and Challenges in Finding Cyclic Peptide Modulators of Proteinâ€“Protein Interactions. Methods in Molecular Biology, 2019, 2001, 73-95.	0.4	7
43	Note: Network random walk model of two-state protein folding: Test of the theory. Journal of Chemical Physics, 2013, 138, 036101.	1.2	5
44	Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields. Journal of Physical Chemistry B, 2021, 125, 5233-5242.	1.2	5
45	Structure and dynamics of the fibronectin-III domains of Aplysia californica cell adhesion molecules. Physical Chemistry Chemical Physics, 2015, 17, 9634-9643.	1.3	2
46	Structural Stability of Diabetes-Related Amylin Protofilaments: Applications to Fibril Design. Biophysical Journal, 2015, 108, 387a.	0.2	1
47	Coarse Master Equation-Based Analysis of N-Methylation and Temperature Effects on the Dynamics of Cyclic Peptides. Biophysical Journal, 2016, 110, 379a.	0.2	1
48	Dynamics of Intra- and Inter-Helix Contact Formation. Biophysical Journal, 2009, 96, 427a.	0.2	0
49	Probing the Kinetic Network of Folding-Unfolding Transitions in Proteins. Biophysical Journal, 2011, 100, 536a-537a.	0.2	0
50	Molecular Interactions of Alzheimer's AÎ² Peptide Fibrils and Oligomers with Lipid Membranes. Biophysical Journal, 2013, 104, 592a.	0.2	0
51	Conformational and Dynamic Properties of Extracellular Domains of Cell Adhesion Molecules. Biophysical Journal, 2014, 106, 51a-52a.	0.2	0
52	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. Angewandte Chemie, 2016, 128, 995-998.	1.6	0