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	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
2	Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields. Journal of Physical Chemistry B, 2021, 125, 5233-5242.	1.2	5
3	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
4	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
5	Computational Opportunities and Challenges in Finding Cyclic Peptide Modulators of Proteinâ€“Protein Interactions. Methods in Molecular Biology, 2019, 2001, 73-95.	0.4	7
6	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. Journal of Physical Chemistry B, 2018, 122, 5657-5665.	1.2	11
7	Amyloid Fibril Design: Limiting Structural Polymorphism in Alzheimerâ€™s AÎ² Protofilaments. Journal of Physical Chemistry B, 2018, 122, 11535-11545.	1.2	7
8	Conformational analysis of replica exchange MD: Temperature-dependent Markov networks for FF amyloid peptides. Journal of Chemical Physics, 2018, 149, 072323.	1.2	7
9	Thermal and aqueous stability improvement of graphene oxide enhanced diphenylalanine nanocomposites. Science and Technology of Advanced Materials, 2017, 18, 172-179.	2.8	18
10	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
11	Variational Identification of Markovian Transition States. Physical Review X, 2017, 7, .	2.8	28
12	Peptide dimerization-dissociation rates from replica exchange molecular dynamics. Journal of Chemical Physics, 2017, 147, 152725.	1.2	16
13	SARAH Domain-Mediated MST2-RASSF Dimeric Interactions. PLoS Computational Biology, 2016, 12, e1005051.	1.5	15
14	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. Angewandte Chemie, 2016, 128, 995-998.	1.6	0
15	Coarse Master Equations for Binding Kinetics of Amyloid Peptide Dimers. Journal of Physical Chemistry Letters, 2016, 7, 2676-2682.	2.1	25
16	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. Angewandte Chemie - International Edition, 2016, 55, 983-986.	7.2	43
17	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
18	MST2-RASSF proteinâ€“protein interactions through SARAH domains. Briefings in Bioinformatics, 2016, 17, 593-602.	3.2	13

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19	Structural Stability of Diabetes-Related Amylin Protofilaments: Applications to Fibril Design. Biophysical Journal, 2015, 108, 387a.	0.2	1
20	Nanoscale Piezoelectric Properties of Self-Assembled Fmocâ€“FF Peptide Fibrous Networks. ACS Applied Materials & Interfaces, 2015, 7, 12702-12707.	4.0	69
21	Modulation of Alzheimerâ€™s AÎ² Protofilament-Membrane Interactions by Lipid Headgroups. ACS Chemical Neuroscience, 2015, 6, 446-455.	1.7	55
22	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
23	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
24	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	23.0	530
25	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
26	Conformational dynamics and aggregation behavior of piezoelectric diphenylalanine peptides in an external electric field. Biophysical Chemistry, 2015, 196, 16-24.	1.5	41
27	Molecular mechanisms of asymmetric RAF dimer activation. Biochemical Society Transactions, 2014, 42, 784-790.	1.6	28
28	Conformational and Dynamic Properties of Extracellular Domains of Cell Adhesion Molecules. Biophysical Journal, 2014, 106, 51a-52a.	0.2	0
29	Molecular Interactions of Alzheimer's AÎ² Peptide Fibrils and Oligomers with Lipid Membranes. Biophysical Journal, 2013, 104, 592a.	0.2	0
30	Note: Network random walk model of two-state protein folding: Test of the theory. Journal of Chemical Physics, 2013, 138, 036101.	1.2	5
31	Alzheimer AÎ² peptide interactions with lipid membranes. Prion, 2012, 6, 339-345.	0.9	58
32	Molecular Interactions of Alzheimer's AÎ² Protofilaments with Lipid Membranes. Journal of Molecular Biology, 2012, 421, 572-586.	2.0	64
33	Unlocking the Atomic-Level Details of Amyloid Fibril Growth through Advanced Biomolecular Simulations. Biophysical Journal, 2012, 103, 1411-1413.	0.2	12
34	Conformational dynamics of human IAPP monomers. Biophysical Chemistry, 2012, 167, 1-7.	1.5	22
35	Are Peptides Good Two-State Folders?. Journal of Chemical Theory and Computation, 2011, 7, 2370-2375.	2.3	18
36	Probing the Kinetic Network of Folding-Unfolding Transitions in Proteins. Biophysical Journal, 2011, 100, 536a-537a.	0.2	0

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37	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
38	Thermostat Artifacts in Replica Exchange Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2009, 5, 1393-1399.	2.3	81
39	Dynamics of Intra- and Inter-Helix Contact Formation. Biophysical Journal, 2009, 96, 427a.	0.2	0
40	Dissecting contact potentials for proteins: Relative contributions of individual amino acids. Proteins: Structure, Function and Bioinformatics, 2008, 70, 119-130.	1.5	15
41	Are Current Molecular Dynamics Force Fields too Helical?. Biophysical Journal, 2008, 95, L07-L09.	0.2	419
42	Peptide folding kinetics from replica exchange molecular dynamics. Physical Review E, 2008, 77, 030902.	0.8	104
43	Coarse Master Equations for Peptide Folding Dynamics. Journal of Physical Chemistry B, 2008, 112, 6057-6069.	1.2	444
44	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
45	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
46	Molecular Dynamics Simulations of Alzheimer's Î²-Amyloid Protofilaments. Journal of Molecular Biology, 2005, 353, 804-821.	2.0	250
47	Development of novel statistical potentials for protein fold recognition. Current Opinion in Structural Biology, 2004, 14, 225-232.	2.6	118
48	Orientational potentials extracted from protein structures improve native fold recognition. Protein Science, 2004, 13, 862-874.	3.1	84
49	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
50	Orientation-dependent coarse-grained potentials derived by statistical analysis of molecular structural databases. Polymer, 2004, 45, 597-608.	1.8	25
51	Anisotropic coarse-grained statistical potentials improve the ability to identify nativelike protein structures. Journal of Chemical Physics, 2003, 118, 7658.	1.2	54
52	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