Canan Atilgan

List of Publications by Year
in descending order

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99 papers	2,244 citations	331259 21 h-index	264894 42 g-index
110 all docs	110 docs citations	110 times ranked	2061 citing authors

#	Article	IF	Citations
1	Small-World Communication of Residues and Significance for Protein Dynamics. Biophysical Journal, 2004, 86, 85-91.	0.2	295
2	Perturbation-Response Scanning Reveals Ligand Entry-Exit Mechanisms of Ferric Binding Protein. PLoS Computational Biology, 2009, 5, e1000544.	1.5	192
3	MD-TASK: a software suite for analyzing molecular dynamics trajectories. Bioinformatics, 2017, 33, 2768-2771.	1.8	142
4	Manipulation of Conformational Change in Proteins by Single-Residue Perturbations. Biophysical Journal, 2010, 99, 933-943.	0.2	139
5	Allosteric Modulation of Human Hsp90Î± Conformational Dynamics. Journal of Chemical Information and Modeling, 2018, 58, 383-404.	2.5	79
6	Perturbationâ€“Response Scanning Reveals Key Residues for Allosteric Control in Hsp70. Journal of Chemical Information and Modeling, 2017, 57, 1359-1374.	2.5	70
7	Noncovalent Intramolecular Interactions in the Monomers and Oligomers of the Acceptor and Donor Type of Low Band Gap Conducting Polymers. Journal of Physical Chemistry C, 2007, 111, 16362-16371.	1.5	69
8	Network-Based Models as Tools Hinting at Nonevident Protein Functionality. Annual Review of Biophysics, 2012, 41, 205-225.	4.5	54
9	Screened Nonbonded Interactions in Native Proteins Manipulate Optimal Paths for Robust Residue Communication. Biophysical Journal, 2007, 92, 3052-3062.	0.2	53
10	High-Order Epistasis in Catalytic Power of Dihydrofolate Reductase Gives Rise to a Rugged Fitness Landscape in the Presence of Trimethoprim Selection. Molecular Biology and Evolution, 2019, 36, 1533-1550.	3.5	52
11	Consistent Picture of the Reversible Thermal Unfolding of Hen Egg-White Lysozyme from Experiment and Molecular Dynamics. Biophysical Journal, 2010, 99, 2255-2263.	0.2	48
12	MODE-TASK: large-scale protein motion tools. Bioinformatics, 2018, 34, 3759-3763.	1.8	45
13	Designing Molecular Dynamics Simulations to Shift Populations of the Conformational States of Calmodulin. PLoS Computational Biology, 2013, 9, e1003366.	1.5	41
14	A trimethoprim derivative impedes antibiotic resistance evolution. Nature Communications, 2021, 12, 2949.	5.8	41
15	Mapping and Reverse-Mapping of the Morphologies for a Molecular Understanding of the Self-Assembly of Fluorinated Block Copolymers. Journal of Physical Chemistry C, 2010, 114, 370-382.	1.5	37
16	Elucidating the structural mechanisms for biological activity of the chemokine family. Proteins: Structure, Function and Bioinformatics, 2001, 43, 150-160.	1.5	33
17	Coordination topology and stability for the native and binding conformers of chymotrypsin inhibitor 2. Proteins: Structure, Function and Bioinformatics, 2001, 45, 62-70.	1.5	28
18	Relaxation Kinetics and the Glassiness of Proteins: The Case of Bovine Pancreatic Trypsin Inhibitor. Biophysical Journal, 2002, 83, 699-705.	0.2	28

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19	Determination of the Stable Microstates of a Peptide from NOE Distance Constraints and Optimization of Atomic Solvation Parameters. Journal of the American Chemical Society, 1998, 120, 800-812.	6.6	26
20	Perturbâ€“Scanâ€“Pull: A Novel Method Facilitating Conformational Transitions in Proteins. Journal of Chemical Theory and Computation, 2020, 16, 3825-3841.	2.3	26
21	Relaxation Kinetics and the Glassiness of Native Proteins: Coupling of Timescales. Biophysical Journal, 2005, 88, 1570-1576.	0.2	25
22	Nanosecond Motions in Proteins Impose Bounds on the Timescale Distributions of Local Dynamics. Biophysical Journal, 2009, 97, 2080-2088.	0.2	25
23	Complete mapping of the morphologies of some linear and graft fluorinated co-oligomers in an aprotic solvent by dissipative particle dynamics. Journal of Chemical Physics, 2006, 124, 064905.	1.2	24
24	Increased substrate affinity in the Escherichia coli L28R dihydrofolate reductase mutant causes trimethoprim resistance. Physical Chemistry Chemical Physics, 2017, 19, 11416-11428.	1.3	24
25	Detailed molecular dynamics simulations of human transferrin provide insights into iron release dynamics at serum and endosomal pH. Journal of Biological Inorganic Chemistry, 2015, 20, 705-718.	1.1	23
26	New conformational search method based on local torsional deformations for cyclic molecules, loops in proteins, and dense polymer systems. Journal of Chemical Physics, 1996, 105, 7868-7871.	1.2	22
27	Predicting long term cooperativity and specific modulators of receptor interactions in human transferrin from dynamics within a single microstate. Physical Chemistry Chemical Physics, 2016, 18, 7916-7926.	1.3	22
28	Efficiency of the Local Torsional Deformations Method for Identifying the Stable Structures of Cyclic Molecules. Journal of Physical Chemistry A, 1997, 101, 2185-2191.	1.1	21
29	Efficiency of simulated annealing for peptides with increasing geometrical restrictions. Journal of Computational Chemistry, 1999, 20, 1659-1670.	1.5	21
30	Subtle pH differences trigger single residue motions for moderating conformations of calmodulin. Journal of Chemical Physics, 2011, 135, 155102.	1.2	21
31	Surfactant formation efficiency of fluorocarbon-hydrocarbon oligomers in supercritical CO2. Journal of Chemical Physics, 2009, 131, 124701.	1.2	20
32	Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. Polymer, 2011, 52, 5503-5512.	1.8	20
33	Perturbation response scanning specifies key regions in subtilisin serine protease for both function and stability. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 867-873.	2.5	19
34	Unraveling the Motions behind Enterovirus 71ÂUncoating. Biophysical Journal, 2018, 114, 822-838.	0.2	19
35	Molecular Dynamics Analysis of Coupling between Librational Motions and Isomeric Jumps in Chain Molecules. Macromolecules, 1996, 29, 2510-2514.	2.2	18
36	Local Dynamics of Bulk Polybutadienes of Various Microstructures:Â Comparison of Theory with NMR Measurements. Macromolecules, 1997, 30, 2058-2066.	2.2	18

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37	How orientational order governs collectivity of folded proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3363-3375.	1.5	18
38	Multi-scale modelling of carbon nanotube reinforced crosslinked interfaces. Computational Materials Science, 2017, 129, 279-289.	1.4	18
39	Mechanisms by Which Salt Concentration Moderates the Dynamics of Human Serum Transferrin. Journal of Physical Chemistry B, 2017, 121, 4778-4789.	1.2	18
40	Local motifs in proteins combine to generate global functional moves. Briefings in Functional Genomics, 2012, 11, 479-488.	1.3	17
41	Computational approaches for deciphering the equilibrium and kinetic properties of iron transport proteins. Metallomics, 2017, 9, 1513-1533.	1.0	17
42	Conformational features of poly(1,1-dihydroperfluorooctyl acrylate) and poly(vinyl acetate) diblock oligomers in supercritical carbon dioxide. Journal of Chemical Physics, 2001, 114, 5444-5449.	1.2	16
43	FbpA iron storage and release are governed by periplasmic microenvironments. Physical Chemistry Chemical Physics, 2017, 19, 6064-6075.	1.3	16
44	Tuning Interaction Parameters of Thermoplastic Polyurethanes in a Binary Solvent To Achieve Precise Control over Microphase Separation. Journal of Chemical Information and Modeling, 2019, 59, 1946-1956.	2.5	15
45	Molecular basis for solvent dependent morphologies observed on electrosprayed surfaces. Physical Chemistry Chemical Physics, 2013, 15, 17862.	1.3	14
46	In silico mutational studies of <scp>H</scp>sp70 disclose sites with distinct functional attributes. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2077-2090.	1.5	14
47	Computational Methods for Efficient Sampling of Protein Landscapes and Disclosing Allosteric Regions. Advances in Protein Chemistry and Structural Biology, 2018, 113, 33-63.	1.0	14
48	Assortative Mixing in Close-Packed Spatial Networks. PLoS ONE, 2010, 5, e15551.	1.1	13
49	Novel Procedure for Developing Implicit Solvation Models for Peptides and Proteins. Journal of Physical Chemistry B, 1997, 101, 7368-7370.	1.2	12
50	Protonation States of Remote Residues Affect Bindingâ€“Release Dynamics of the Ligand but Not the Conformation of Apo Ferric Binding Protein. Journal of Physical Chemistry B, 2014, 118, 11677-11687.	1.2	12
51	Soft segment length controls morphology of poly(ethylene oxide) based segmented poly(urethane-urea) copolymers in a binary solvent. Computational Materials Science, 2017, 138, 58-69.	1.4	12
52	Multiscale modeling of poly(2-isopropyl-2-oxazoline) chains in aqueous solution. European Polymer Journal, 2017, 88, 594-604.	2.6	12
53	Collective deformations in proteins determined by a mode analysis of molecular dynamics trajectories. Polymer, 2002, 43, 431-439.	1.8	11
54	How a Vicinal Layer of Solvent Modulates the Dynamics of Proteins. Biophysical Journal, 2008, 94, 79-89.	0.2	11

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55	Kinematics of Polymer Chains in Dense Medium. 4. Effect of Backbone Geometry and Application to Polybutadiene. Macromolecules, 1996, 29, 2980-2988.	2.2	10
56	New surfactants design for CO2 applications: Molecular dynamics simulations of fluorocarbonâ€“hydrocarbon oligomers. Journal of Chemical Physics, 2003, 119, 4953-4961.	1.2	9
57	Calmodulin Readily Switches Conformation upon Protonating High pK_a Acidic Residues. Journal of Physical Chemistry B, 2012, 116, 7145-7153.	1.2	9
58	Performance of efficient minimization algorithms as applied to models of peptides and proteins. Journal of Computational Chemistry, 1999, 20, 354-364.	1.5	8
59	Blends of highly branched and linear poly(arylene ether sulfone)s: Multiscale effect of the degree of branching on the morphology and mechanical properties. Polymer, 2020, 188, 122114.	1.8	8
60	Dynamic Community Composition Unravels Allosteric Communication in PDZ3. Journal of Physical Chemistry B, 2021, 125, 2266-2276.	1.2	8
61	Contribution of Short-Range Intramolecular Interactions to Local Chain Dynamics. Macromolecules, 1994, 27, 3650-3657.	2.2	7
62	Solvent effect on the synthesis of clarithromycin: A molecular dynamics study. Journal of Computer-Aided Molecular Design, 2004, 18, 145-154.	1.3	7
63	Synthesis of fluorinated oligomers for supercritical carbon dioxide applications. Journal of Polymer Science Part A, 2005, 43, 5312-5322.	2.5	7
64	Depth dependent dynamics in the hydration shell of a protein. Journal of Chemical Physics, 2010, 133, 085101.	1.2	7
65	Coupling between different modes in local chain dynamics: a modal correlation analysis. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 2483.	1.7	6
66	Employment of Iron-Binding Protein from Haemophilus influenzae in Functional Nanopipettes for Iron Monitoring. ACS Chemical Neuroscience, 2019, 10, 1970-1977.	1.7	6
67	Computational strategies for protein conformational ensemble detection. Current Opinion in Structural Biology, 2022, 72, 79-87.	2.6	6
68	Modeling the selective methylation in the synthesis of clarithromycin. Perkin Transactions II RSC, 2002, , 670-675.	1.1	5
69	Structural analysis of the PATZ1 BTB domain homodimer. Acta Crystallographica Section D: Structural Biology, 2020, 76, 581-593.	1.1	5
70	Conformational Properties of the Bacterial Polyester Poly(3-hydroxy-5,8-decadienoate). Macromolecules, 2003, 36, 1132-1137.	2.2	4
71	Hybrid Usage of Computational Tools in Drug Synthesis. Current Computer-Aided Drug Design, 2007, 3, 149-159.	0.8	4
72	Understanding the mode of action of ThDP in benzoylformate decarboxylase. Biopolymers, 2010, 93, 32-46.	1.2	4

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73	A computational approach to the synthesis of dirithromycin. Journal of Molecular Modeling, 2004, 10, 94-101.	0.8	3
74	COLLECTIVE BEHAVIOR OF EL FAROL ATTENDEES. International Journal of Modeling, Simulation, and Scientific Computing, 2008, 11, 629-639.	0.9	3
75	Designed-in Molecular Interactions Lead to Superior Thermo-mechanical Properties in Nanocomposites. Materials Research Society Symposia Proceedings, 2011, 1304, 1.	0.1	3
76	Theoretical study of selective methylation in the synthesis of azithromycin. Journal of Computer-Aided Molecular Design, 2004, 18, 1-11.	1.3	2
77	Driving Calmodulin Protein towards Conformational Shift by Changing Ionization States of Select Residues. Journal of Physics: Conference Series, 2012, 402, 012047.	0.3	2
78	N-Terminus of the Third PDZ Domain of PSD-95 Orchestrates Allosteric Communication for Selective Ligand Binding. Journal of Chemical Information and Modeling, 2021, 61, 347-357.	2.5	2
79	On modifying properties of polymeric melts by nanoscopic particles. Journal of Polymer Science, Part B: Polymer Physics, 2012, 50, 1653-1662.	2.4	1
80	A Coarse-Grained Methodology Identifies Intrinsic Mechanisms That Dissociate Interacting Protein Pairs. Frontiers in Molecular Biosciences, 2020, 7, 210.	1.6	1
81	Long-Range Structural Regularities and Collectivity of Folded Proteins. Materials Research Society Symposia Proceedings, 2009, 1227, 30601.	0.1	0
82	Multiple Channels of Structural Relaxations in Functional Proteins. Biophysical Journal, 2009, 96, 72a.	0.2	0
83	A Coarsened Network Model Reveals Allosteric Machinery. Biophysical Journal, 2009, 96, 5a-6a.	0.2	0
84	An Electrohydrodynamic Model and Extensive MD Simulations Agree on the Positional and Intra-Residual Relaxations Up to Sub-Microsecond Dynamics. Biophysical Journal, 2010, 98, 236a.	0.2	0
85	Functional Pathways in Proteins Are Uncovered By Strong Disorder. Biophysical Journal, 2010, 98, 27a.	0.2	0
86	Molecular Recognition Mechanism of Calmodulin Examined by Perturbation-Response Scanning. Biophysical Journal, 2011, 100, 534a.	0.2	0
87	Orchestrating Population Shifts of Native Proteins in Different Environments. Biophysical Journal, 2011, 100, 372a.	0.2	0
88	Molecular Recognition Mechanisms of Calmodulin Examined by Perturbation-Response Scanning. Materials Research Society Symposia Proceedings, 2011, 1301, 137.	0.1	0
89	Effect of van der Waals Interaction Strength and Nanocluster Size on the Dynamical and Mechanical Properties of 1,4-cis-polybutadiene Melts. Materials Research Society Symposia Proceedings, 2012, 1424, 121.	0.1	0
90	Exploring pH Dependent Landscape Shifts of Proteins. Biophysical Journal, 2012, 102, 450a.	0.2	0

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91	Changes in Bond-Orientational Order of Residues are Associated with Shifts in Energy Landscapes. Biophysical Journal, 2012, 102, 445a.	0.2	0
92	Where do Proteins Fit in the Structural Classification of Condensed Matter?. Biophysical Journal, 2012, 102, 250a.	0.2	0
93	Non-Equilibrium Fluctuation Theorems, Redundant Paths in Proteins, and Elucidating Conformational Changes by Single-Residue Perturbations. Biophysical Journal, 2013, 104, 70a.	0.2	0
94	Structural Basis of How Ferric Binding Proteins Utilize pH Differences for Controlled Release of Iron. Biophysical Journal, 2013, 104, 212a.	0.2	0
95	Computational Assessment of Trimethoprim Resistance in Dihydrofolate Reductase. Biophysical Journal, 2016, 110, 47a-48a.	0.2	0
96	Characterization and Iron Binding Dynamics of Haemophilus Influenzae Ferric Binding Protein. Biophysical Journal, 2019, 116, 182a.	0.2	0
97	Structure-Function Investigation of Haemophilus Influenzae Ferric Binding Protein under Changing Environmental Conditions. Biophysical Journal, 2020, 118, 335a.	0.2	0
98	Allosteric Communication in PDZ3 is Orchestrated by the Charged N-Terminus. Biophysical Journal, 2021, 120, 189a.	0.2	0
99	Could network structures generated with simple rules imposed on a cubic lattice reproduce the structural descriptors of globular proteins?. Journal of Complex Networks, 2021, 10, .	1.1	0