Ali Rana Atilgan

List of Publications by Year
in descending order

85 papers	6,256 citations	201385 27 h-index	98622 67 g-index
91 all docs	91 docs citations	91 times ranked	3663 citing authors

#	Article	IF	Citations
1	Computational strategies for protein conformational ensemble detection. Current Opinion in Structural Biology, 2022, 72, 79-87.	2.6	6
2	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
3	Allosteric Communication in PDZ3 is Orchestrated by the Charged N-Terminus. Biophysical Journal, 2021, 120, 189a.	0.2	0
4	Dynamic Community Composition Unravels Allosteric Communication in PDZ3. Journal of Physical Chemistry B, 2021, 125, 2266-2276.	1.2	8
5	A trimethoprim derivative impedes antibiotic resistance evolution. Nature Communications, 2021, 12, 2949.	5.8	41
6	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
7	A Coarse-Grained Methodology Identifies Intrinsic Mechanisms That Dissociate Interacting Protein Pairs. Frontiers in Molecular Biosciences, 2020, 7, 210.	1.6	1
8	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
9	Unraveling the Motions behind Enterovirus 71ÂUncoating. Biophysical Journal, 2018, 114, 822-838.	0.2	19
10	MODE-TASK: large-scale protein motion tools. Bioinformatics, 2018, 34, 3759-3763.	1.8	45
11	FbpA iron storage and release are governed by periplasmic microenvironments. Physical Chemistry Chemical Physics, 2017, 19, 6064-6075.	1.3	16
12	Mechanisms by Which Salt Concentration Moderates the Dynamics of Human Serum Transferrin. Journal of Physical Chemistry B, 2017, 121, 4778-4789.	1.2	18
13	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
14	Computational approaches for deciphering the equilibrium and kinetic properties of iron transport proteins. Metallomics, 2017, 9, 1513-1533.	1.0	17
15	MD-TASK: a software suite for analyzing molecular dynamics trajectories. Bioinformatics, 2017, 33, 2768-2771.	1.8	142
16	Computational Assessment of Trimethoprim Resistance in Dihydrofolate Reductase. Biophysical Journal, 2016, 110, 47a-48a.	0.2	0
17	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
18	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

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19	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
20	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
21	Non-Equilibrium Fluctuation Theorems, Redundant Paths in Proteins, and Elucidating Conformational Changes by Single-Residue Perturbations. Biophysical Journal, 2013, 104, 70a.	0.2	0
22	Structural Basis of How Ferric Binding Proteins Utilize pH Differences for Controlled Release of Iron. Biophysical Journal, 2013, 104, 212a.	0.2	0
23	Designing Molecular Dynamics Simulations to Shift Populations of the Conformational States of Calmodulin. PLoS Computational Biology, 2013, 9, e1003366.	1.5	41
24	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
25	Driving Calmodulin Protein towards Conformational Shift by Changing Ionization States of Select Residues. Journal of Physics: Conference Series, 2012, 402, 012047.	0.3	2
26	Local motifs in proteins combine to generate global functional moves. Briefings in Functional Genomics, 2012, 11, 479-488.	1.3	17
27	On modifying properties of polymeric melts by nanoscopic particles. Journal of Polymer Science, Part B: Polymer Physics, 2012, 50, 1653-1662.	2.4	1
28	Exploring pH Dependent Landscape Shifts of Proteins. Biophysical Journal, 2012, 102, 450a.	0.2	0
29	Network-Based Models as Tools Hinting at Nonevident Protein Functionality. Annual Review of Biophysics, 2012, 41, 205-225.	4.5	54
30	Calmodulin Readily Switches Conformation upon Protonating High pK_a Acidic Residues. Journal of Physical Chemistry B, 2012, 116, 7145-7153.	1.2	9
31	Changes in Bond-Orientational Order of Residues are Associated with Shifts in Energy Landscapes. Biophysical Journal, 2012, 102, 445a.	0.2	0
32	Where do Proteins Fit in the Structural Classification of Condensed Matter?. Biophysical Journal, 2012, 102, 250a.	0.2	0
33	Molecular Recognition Mechanism of Calmodulin Examined by Perturbation-Response Scanning. Biophysical Journal, 2011, 100, 534a.	0.2	0
34	Subtle pH differences trigger single residue motions for moderating conformations of calmodulin. Journal of Chemical Physics, 2011, 135, 155102.	1.2	21
35	Molecular Recognition Mechanisms of Calmodulin Examined by Perturbation-Response Scanning. Materials Research Society Symposia Proceedings, 2011, 1301, 137.	0.1	0
36	Designed-in Molecular Interactions Lead to Superior Thermo-mechanical Properties in Nanocomposites. Materials Research Society Symposia Proceedings, 2011, 1304, 1.	0.1	3

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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	Assortative Mixing in Close-Packed Spatial Networks. PLoS ONE, 2010, 5, e15551.	1.1	13
39	Depth dependent dynamics in the hydration shell of a protein. Journal of Chemical Physics, 2010, 133, 085101.	1.2	7
40	Functional Pathways in Proteins Are Uncovered By Strong Disorder. Biophysical Journal, 2010, 98, 27a.	0.2	0
41	Manipulation of Conformational Change in Proteins by Single-Residue Perturbations. Biophysical Journal, 2010, 99, 933-943.	0.2	139
42	Perturbation-Response Scanning Reveals Ligand Entry-Exit Mechanisms of Ferric Binding Protein. PLoS Computational Biology, 2009, 5, e1000544.	1.5	192
43	Long-Range Structural Regularities and Collectivity of Folded Proteins. Materials Research Society Symposia Proceedings, 2009, 1227, 30601.	0.1	0
44	Multiple Channels of Structural Relaxations in Functional Proteins. Biophysical Journal, 2009, 96, 72a.	0.2	0
45	A Coarsened Network Model Reveals Allosteric Machinery. Biophysical Journal, 2009, 96, 5a-6a.	0.2	0
46	Nanosecond Motions in Proteins Impose Bounds on the Timescale Distributions of Local Dynamics. Biophysical Journal, 2009, 97, 2080-2088.	0.2	25
47	How a Vicinal Layer of Solvent Modulates the Dynamics of Proteins. Biophysical Journal, 2008, 94, 79-89.	0.2	11
48	COLLECTIVE BEHAVIOR OF EL FAROL ATTENDEES. International Journal of Modeling, Simulation, and Scientific Computing, 2008, 11, 629-639.	0.9	3
49	Screened Nonbonded Interactions in Native Proteins Manipulate Optimal Paths for Robust Residue Communication. Biophysical Journal, 2007, 92, 3052-3062.	0.2	53
50	El Farol revisited. Physica A: Statistical Mechanics and Its Applications, 2005, 346, 651-656.	1.2	7
51	Relaxation Kinetics and the Glassiness of Native Proteins: Coupling of Timescales. Biophysical Journal, 2005, 88, 1570-1576.	0.2	25
52	Small-World Communication of Residues and Significance for Protein Dynamics. Biophysical Journal, 2004, 86, 85-91.	0.2	295
53	Relaxation Kinetics and the Glassiness of Proteins: The Case of Bovine Pancreatic Trypsin Inhibitor. Biophysical Journal, 2002, 83, 699-705.	0.2	28
54	Anisotropy of Fluctuation Dynamics of Proteins with an Elastic Network Model. Biophysical Journal, 2001, 80, 505-515.	0.2	1,486

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55	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
56	Elucidating the structural mechanisms for biological activity of the chemokine family. Proteins: Structure, Function and Bioinformatics, 2001, 43, 150-160.	1.5	33
57	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to ?-amylase inhibitor. Proteins: Structure, Function and Bioinformatics, 2000, 40, 512-524.	1.5	260
58	Identifying the adaptive mechanism in globular proteins: Fluctuations in densely packed regions manipulate flexible parts. Journal of Chemical Physics, 2000, 113, 4454-4464.	1.2	32
59	Relating the Structure ofHIV-1 Reverse Transcriptaseto Its Processing Step. Journal of Biomolecular Structure and Dynamics, 2000, 17, 49-55.	2.0	10
60	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to Î±-amylase inhibitor. , 2000, 40, 512.		7
61	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: application to alpha-amylase inhibitor. Proteins: Structure, Function and Bioinformatics, 2000, 40, 512-24.	1.5	134
62	Collective Motions in HIV-1 Reverse Transcriptase: Examination of Flexibility and Enzyme Function. Journal of Molecular Biology, 1999, 285, 1023-1037.	2.0	199
63	A Nonlinear Model for the Kinking Behavior of Unidirectional Polymer Matrix Composites. ZAMM Zeitschrift Fur Angewandte Mathematik Und Mechanik, 1998, 78, 212-216.	0.9	0
64	Correlated fluctuations in polymer networks. Computational and Theoretical Polymer Science, 1998, 8, 55-59.	1.1	2
65	Identification of kinetically hot residues in proteins. Protein Science, 1998, 7, 2522-2532.	3.1	114
66	State-space prediction model for chaotic time series. Physical Review E, 1998, 58, 2640-2643.	0.8	14
67	Vibrational Dynamics of Folded Proteins: Significance of Slow and Fast Motions in Relation to Function and Stability. Physical Review Letters, 1998, 80, 2733-2736.	2.9	382
68	Statistical mechanics of Fermi-Pasta-Ulam chains with the canonical ensemble. Physical Review E, 1997, 55, 3727-3730.	0.8	1
69	Direct evaluation of thermal fluctuations in proteins using a single-parameter harmonic potential. Folding & Design, 1997, 2, 173-181.	4.5	1,243
70	Analogy between Dislocation Mechanics and Aerodynamics. ZAMM Zeitschrift Fur Angewandte Mathematik Und Mechanik, 1997, 77, 631-633.	0.9	1
71	Understanding the recognition of protein structural classes by amino acid composition. Proteins: Structure, Function and Bioinformatics, 1997, 29, 172-185.	1.5	120
72	DYNAMICS OF DISORDERED STRUCTURES: EFFECT OF NON-LINEARITY ON THE LOCALIZATION. Journal of Sound and Vibration, 1997, 205, 372-379.	2.1	7

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73	Understanding the recognition of protein structural classes by amino acid composition. Proteins: Structure, Function and Bioinformatics, 1997, 29, 172-85.	1.5	20
74	Molecular Dynamics Analysis of Coupling between Librational Motions and Isomeric Jumps in Chain Molecules. Macromolecules, 1996, 29, 2510-2514.	2.2	18
75	SPACE-TIME MIXED FINITE ELEMENTS FOR RODS. Journal of Sound and Vibration, 1996, 192, 731-739.	2.1	12
76	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
77	Some Remarks on the Stability of Laminated Composite Beams. ZAMM Zeitschrift Fur Angewandte Mathematik Und Mechanik, 1994, 74, 131-133.	0.9	1
78	Application of the variational-asymptotical method to laminated composite plates. AIAA Journal, 1993, 31, 1674-1683.	1.5	39
79	A Geometrically Nonlinear Theory of Elastic Plates. Journal of Applied Mechanics, Transactions ASME, 1993, 60, 109-116.	1.1	99
80	On a simplified strain energy function for geometrically nonlinear behaviour of anisotropic beams. Composites Part B: Engineering, 1992, 2, 513-526.	0.6	139
81	On the strain energy of laminated composite plates. International Journal of Solids and Structures, 1992, 29, 2527-2543.	1.3	41
82	Unified nonlinear analysis for nonhomogeneous anisotropic beams withclosed cross sections. AIAA Journal, 1991, 29, 1990-1999.	1.5	65
83	Freeâ€Vibration Analysis of Composite Beams. Journal of the American Helicopter Society, 1991, 36, 36-47.	0.5	141
84	Nonclassical Behavior of Thinâ€Walled Composite Beams with Closed Cross Sections. Journal of the American Helicopter Society, 1990, 35, 42-50.	0.5	171
85	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to Î±-amylase inhibitor. , 0, .		2