Guido Tiana

List of Publications by Year
in descending order

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114 papers	3,277 citations	185998 28 h-index	174990 52 g-index
117 all docs	117 docs citations	117 times ranked	3750 citing authors

#	Article	IF	Citations
1	Predictive Polymer Modeling Reveals Coupled Fluctuations in Chromosome Conformation and Transcription. Cell, 2014, 157, 950-963.	13.5	411
2	Reciprocal insulation analysis of Hi-C data shows that TADs represent a functionally but not structurally privileged scale in the hierarchical folding of chromosomes. Genome Research, 2017, 27, 479-490.	2.4	164
3	Kinetics of Different Processes in Human Insulin Amyloid Formation. Journal of Molecular Biology, 2007, 366, 258-274.	2.0	163
4	Noncooperative Interactions between Transcription Factors and Clustered DNA Binding Sites Enable Graded Transcriptional Responses to Environmental Inputs. Molecular Cell, 2010, 37, 418-428.	4.5	155
5	Sustained oscillations and time delays in gene expression of protein Hes1. FEBS Letters, 2003, 541, 176-177.	1.3	147
6	Urea and Guanidinium Chloride Denature Protein L in Different Ways in Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4654-4661.	0.2	141
7	Oscillations and temporal signalling in cells. Physical Biology, 2007, 4, R1-R17.	0.8	108
8	Time delay as a key to apoptosis induction in the p53 network. European Physical Journal B, 2002, 29, 135-140.	0.6	101
9	Î²-Hairpin conformation of fibrillogenic peptides: Structure and Î±-Î² transition mechanism revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 198-204.	1.5	85
10	Folding and aggregation of designed proteins. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 12930-12933.	3.3	81
11	Understanding the determinants of stability and folding of small globular proteins from their energetics. Protein Science, 2004, 13, 113-124.	3.1	78
12	HP1 drives de novo 3D genome reorganization in early Drosophila embryos. Nature, 2021, 593, 289-293.	13.7	76
13	DamC reveals principles of chromatin folding in vivo without crosslinking and ligation. Nature Structural and Molecular Biology, 2019, 26, 471-480.	3.6	71
14	Exploring the protein G helix freeâ€energy surface by solute tempering metadynamics. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1647-1654.	1.5	68
15	Folding and misfolding of designed proteinlike chains with mutations. Journal of Chemical Physics, 1998, 108, 757-761.	1.2	67
16	Structural Fluctuations of the Chromatin Fiber within Topologically Associating Domains. Biophysical Journal, 2016, 110, 1234-1245.	0.2	58
17	Imprint of evolution on protein structures. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 2846-2851.	3.3	55
18	Early Events in Insulin Fibrillization Studied by Time-Lapse Atomic Force Microscopy. Biophysical Journal, 2006, 90, 589-597.	0.2	54

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19	Hiking in the energy landscape in sequence space: A bumpy road to good folders. Proteins: Structure, Function and Bioinformatics, 2000, 39, 244-251.	1.5	46
20	Use of the Metropolis algorithm to simulate the dynamics of protein chains. Physica A: Statistical Mechanics and Its Applications, 2007, 380, 241-249.	1.2	45
21	Hierarchy of folding and unfolding events of protein G, ‹b›CI‹/b›2, and ACBP from explicit-solvent simulations. Journal of Chemical Physics, 2011, 134, 045105.	1.2	45
22	Insight into the Folding Inhibition of the HIV-1 Protease by a Small Peptide. Biophysical Journal, 2007, 93, 2813-2821.	0.2	40
23	HIV-1 protease folding and the design of drugs which do not create resistance. Current Opinion in Structural Biology, 2008, 18, 60-66.	2.6	39
24	Hierarchy of events in the folding of model proteins. Journal of Chemical Physics, 2001, 114, 7267-7273.	1.2	37
25	Statistical analysis of native contact formation in the folding of designed model proteins. Journal of Chemical Physics, 2001, 114, 2503-2510.	1.2	35
26	Design of HIV-1-PR inhibitors that do not create resistance: Blocking the folding of single monomers. Protein Science, 2005, 14, 2668-2681.	3.1	35
27	Sequence of events in folding mechanism: Beyond the Goì„ model. Protein Science, 2006, 15, 1638-1652.	3.1	34
28	The determinants of stability in the human prion protein: Insights into folding and misfolding from the analysis of the change in the stabilization energy distribution in different conditions. Proteins: Structure, Function and Bioinformatics, 2005, 62, 698-707.	1.5	33
29	The network of stabilizing contacts in proteins studied by coevolutionary data. Journal of Chemical Physics, 2013, 139, 155103.	1.2	33
30	A folding inhibitor of the HIV-1 protease. Proteins: Structure, Function and Bioinformatics, 2005, 62, 928-933.	1.5	29
31	A Highly Compliant Protein Native State with a Spontaneous-like Mechanical Unfolding Pathway. Journal of the American Chemical Society, 2012, 134, 17068-17075.	6.6	29
32	Stability of Designed Proteins against Mutations. Physical Review Letters, 1999, 82, 4727-4730.	2.9	28
33	Design and folding of dimeric proteins. Proteins: Structure, Function and Bioinformatics, 2002, 49, 82-94.	1.5	27
34	Thermodynamics of Î²-amyloid fibril formation. Journal of Chemical Physics, 2004, 120, 8307-8317.	1.2	27
35	Modeling the Î±-helix to Î²-hairpin transition mechanism and the formation of oligomeric aggregates of the fibrillogenic peptide A(12â€“28): insights from all-atom molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2004, 23, 263-273.	1.3	26
36	Hydrogen Bonds in Polymer Folding. Physical Review Letters, 2001, 86, 1031-1033.	2.9	24

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37	Ratcheted molecular-dynamics simulations identify efficiently the transition state of protein folding. Journal of Chemical Physics, 2012, 137, 235101.	1.2	24
38	Molecular mechanisms of heterogeneous oligomerization of huntingtin proteins. Scientific Reports, 2019, 9, 7615.	1.6	21
39	Assessing the accuracy of direct-coupling analysis for RNA contact prediction. Rna, 2020, 26, 637-647.	1.6	20
40	The complex folding behavior of HIV-1-protease monomer revealed by optical-tweezer single-molecule experiments and molecular dynamics simulations. Biophysical Chemistry, 2014, 195, 32-42.	1.5	19
41	Integrating experiment, theory and simulation to determine the structure and dynamics of mammalian chromosomes. Current Opinion in Structural Biology, 2018, 49, 11-17.	2.6	18
42	Similar folds with different stabilization mechanisms: the cases of Prion and Doppel proteins. BMC Structural Biology, 2006, 6, 17.	2.3	17
43	An implementation of the maximum-caliber principle by replica-averaged time-resolved restrained simulations. Journal of Chemical Physics, 2018, 148, 184114.	1.2	16
44	Estimation of microscopic averages from metadynamics. European Physical Journal B, 2008, 63, 235-238.	0.6	15
45	A many-body term improves the accuracy of effective potentials based on protein coevolutionary data. Journal of Chemical Physics, 2015, 143, 025103.	1.2	15
46	Thermodynamicallyâ€“Weighted Conformational Ensemble of Cyclic RGD Peptidomimetics from NOE Data. Journal of Physical Chemistry B, 2016, 120, 7098-7107.	1.2	15
47	Modelling genome-wide topological associating domains in mouse embryonic stem cells. Chromosome Research, 2017, 25, 5-14.	1.0	15
48	Reading the three-dimensional structure of lattice model-designed proteins from their amino acid sequence. Proteins: Structure, Function and Bioinformatics, 2001, 45, 421-427.	1.5	14
49	Resistance proof, folding-inhibitor drugs. Journal of Chemical Physics, 2003, 118, 4754-4758.	1.2	14
50	Early events in protein folding: Is there something more than hydrophobic burst?. Protein Science, 2008, 17, 1424-1433.	3.1	14
51	Hiking in the energy landscape in sequence space: a bumpy road to good folders. Proteins: Structure, Function and Bioinformatics, 2000, 39, 244-51.	1.5	14
52	Simple models of protein folding and of non-conventional drug design. Journal of Physics Condensed Matter, 2004, 16, R111-R144.	0.7	13
53	A Combined NMR-Computational Study of the Interaction between Influenza Virus Hemagglutinin and Sialic Derivatives from Human and Avian Receptors on the Surface of Transfected Cells. International Journal of Molecular Sciences, 2018, 19, 1267.	1.8	13
54	Atomistic Simulations of the HIV-1 Protease Folding Inhibition. Biophysical Journal, 2008, 95, 550-562.	0.2	12

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55	Conformational Dependence of the Circular Dichroism Spectra of Single Amino Acids from Plane-Waves-Based Density Functional Theory Calculations. Journal of Physical Chemistry B, 2015, 119, 4803-4811.	1.2	12
56	MonteGrappa: An iterative Monte Carlo program to optimize biomolecular potentials in simplified models. Computer Physics Communications, 2015, 186, 93-104.	3.0	12
57	Designability of lattice model heteropolymers. Physical Review E, 2001, 64, 011904.	0.8	11
58	The dynamics of genetic control in the cell: the good and bad of being late. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20120469.	1.6	11
59	Deriving amino acid contact potentials from their frequencies of occurrence in proteins: a lattice model study. Journal of Physics Condensed Matter, 2004, 16, 2551-2564.	0.7	10
60	Equilibrium properties of realistic random heteropolymers and their relevance for globular and naturally unfolded proteins. Physical Review E, 2011, 84, 061910.	0.8	10
61	The maturation of HIVâ€1 protease precursor studied by discrete molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 633-639.	1.5	10
62	Tools for the rational design of bivalent microtubule-targeting drugs. Biochemical and Biophysical Research Communications, 2016, 479, 48-53.	1.0	10
63	SAGE: A Fast Computational Tool for Linear Epitope Grafting onto a Foreign Protein Scaffold. Journal of Chemical Information and Modeling, 2017, 57, 6-10.	2.5	10
64	MicroRNA-222 Regulates Melanoma Plasticity. Journal of Clinical Medicine, 2020, 9, 2573.	1.0	10
65	Managing Experimental 3D Structures in the Beyondâ€Ruleâ€ofâ€5 Chemical Space: The Case of Rifampicin. Chemistry - A European Journal, 2021, 27, 10394-10404.	1.7	10
66	Identification and characterization of folding inhibitors of hen egg lysozyme: An example of a new paradigm of drug design. Proteins: Structure, Function and Bioinformatics, 2009, 74, 390-399.	1.5	9
67	Complete coverage of space favors modularity of the grid system in the brain. Physical Review E, 2016, 94, 062409.	0.8	9
68	Assessment of Mutational Effects on Peptide Stability through Confinement Simulations. Journal of Physical Chemistry Letters, 2016, 7, 126-130.	2.1	9
69	The evolution dynamics of model proteins. Journal of Chemical Physics, 2004, 121, 2381-2389.	1.2	8
70	Mapping of mutation-sensitive sites in proteinlike chains. Physical Review E, 1998, 58, 3572-3577.	0.8	7
71	Low-throughput model design of protein folding inhibitors. Proteins: Structure, Function and Bioinformatics, 2007, 67, 469-478.	1.5	7
72	Cold Denaturation of the HIV-1 Protease Monomer. Biochemistry, 2017, 56, 1029-1032.	1.2	7

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73	Determination of Structural Ensembles of Flexible Molecules in Solution from NMR Data Undergoing Spin Diffusion. Journal of Chemical Information and Modeling, 2019, 59, 2973-2979.	2.5	7
74	Effective model of loop extrusion predicts chromosomal domains. Physical Review E, 2020, 102, 032414.	0.8	7
75	FRET studies of various conformational states adopted by transthyretin. Cellular and Molecular Life Sciences, 2017, 74, 3577-3598.	2.4	7
76	Iterative derivation of effective potentials to sample the conformational space of proteins at atomistic scale. Journal of Chemical Physics, 2014, 140, 195101.	1.2	6
77	Sampling the Denatured State of Polypeptides in Water, Urea, and Guanidine Chloride to Strict Equilibrium Conditions with the Help of Massively Parallel Computers. Journal of Chemical Theory and Computation, 2014, 10, 846-854.	2.3	6
78	Optical Absorption of a Green Fluorescent Protein Variant:â€‰Environment Effects in a Density Functional Study. Journal of Physical Chemistry B, 2007, 111, 10807-10812.	1.2	5
79	The molecular evolution of HIVâ€1 protease simulated at atomic detail. Proteins: Structure, Function and Bioinformatics, 2009, 76, 895-910.	1.5	5
80	Looping probability of random heteropolymers helps to understand the scaling properties of biopolymers. Physical Review E, 2016, 94, 032402.	0.8	5
81	A method for partitioning the information contained in a protein sequence between its structure and function. Proteins: Structure, Function and Bioinformatics, 2018, 86, 956-964.	1.5	5
82	Design of amino acid sequences to fold into CÎ±-model proteins. Journal of Chemical Physics, 2005, 123, 054904.	1.2	4
83	Thermodynamic features characterizing good and bad folding sequences obtained using a simplified off-lattice protein model. Physical Review E, 2006, 73, 061905.	0.8	4
84	Properties of low-dimensional collective variables in the molecular dynamics of biopolymers. Physical Review E, 2016, 94, 052406.	0.8	4
85	Statistical mechanical properties of sequence space determine the efficiency of the various algorithms to predict interaction energies and native contacts from protein coevolution.. Physical Biology, 2019, 16, 046007.	0.8	4
86	Bifractal nature of chromosome contact maps. Physical Review Research, 2020, 2, .	1.3	4
87	Role of bulk and of interface contacts in the behavior of lattice model dimeric proteins. Physical Review E, 2003, 67, 051909.	0.8	3
88	Denatured state is critical in determining the properties of model proteins designed on different folds. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1047-1055.	1.5	3
89	Metadynamic sampling of the free-energy landscapes of proteins coupled with a Monte Carlo algorithm. Gene, 2008, 422, 37-40.	1.0	3
90	Corrigendum to â€œKinetics of Different Processes in Human Insulin Amyloid Formationâ€•[J. Mol. Biol. 366/1 (2007) 258-274]. Journal of Molecular Biology, 2011, 406, 354.	2.0	3

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91	Spontaneous domain formation in disordered copolymers as a mechanism for chromosome structuring. Soft Matter, 2018, 14, 6128-6136.	1.2	3
92	Energy profile of the space of model protein sequences. Journal of Biological Physics, 2001, 27, 147-159.	0.7	2
93	Design of a folding inhibitor of the HIV-1 protease. Molecular Simulation, 2005, 31, 765-771.	0.9	2
94	Identification of the folding inhibitors of hen-egg lysozyme: gathering the right tools. European Biophysics Journal, 2010, 39, 911-919.	1.2	2
95	Coarse Graining of a Giant Molecular System: The Chromatin Fiber. Methods in Molecular Biology, 2019, 2022, 399-411.	0.4	2
96	Native state of natural proteins optimizes local entropy. Physical Review E, 2021, 104, 064117.	0.8	2
97	Predicting the tertiary structure of a lattice designed model protein from its primary structure. Journal of Biological Physics, 2001, 27, 161-168.	0.7	1
98	Thermodynamics of strongly allosteric inhibition: a model study of HIV-1 protease. European Biophysics Journal, 2012, 41, 991-1001.	1.2	1
99	Effect of disorder on the contact probability of elongated conformations of biopolymers. Physical Review E, 2015, 92, 010702.	0.8	1
100	Theory of feedback controlled brain stimulations for Parkinsonâ€™s disease. Physica A: Statistical Mechanics and Its Applications, 2016, 441, 121-130.	1.2	1
101	Thermodynamic and structural effect of urea and guanidine chloride on the helical and on a hairpin fragment of GB1 from molecular simulations. Proteins: Structure, Function and Bioinformatics, 2017, 85, 753-763.	1.5	1
102	Evolution of frustrated and stabilising contacts in reconstructed ancient proteins. European Biophysics Journal, 2021, 50, 699-712.	1.2	1
103	The denatured state of <scp>HIV</scp>â€1 protease under native conditions. Proteins: Structure, Function and Bioinformatics, 2022, 90, 96-109.	1.5	1
104	Protein folding and non-conventional drug design: a primer for nuclear structure physicists. AIP Conference Proceedings, 2004, , .	0.3	0
105	THE PHYSICS OF PROTEIN FOLDING AND OF DRUG DESIGN. , 2005, , .		0
106	Non-Cooperative Interactions Between Transcription Factors and Clustered DNA Binding Sites Enable Graded Transcriptional Responses To Environmental Inputs. Biophysical Journal, 2010, 98, 68a.	0.2	0
107	How likely are oscillations in a genetic feedback loop with delay?. European Physical Journal E, 2017, 40, 74.	0.7	0
108	From Chromosome Conformation Capture to Polymer Physics and Back. , 2017, , 203-224.		0

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109	Molecular Recognition between Cadherins Studied by a Coarse-Grained Model Interacting with a Coevolutionary Potential. Journal of Physical Chemistry B, 2020, 124, 4079-4088.	1.2	0
110	Polymer Folding Simulations from Hi-C Data. Methods in Molecular Biology, 2022, 2301, 259-265.	0.4	0
111	FROM ATOMIC NUCLEI TO DRUG DESIGN. , 2003, , .		0
112	Protein Folding and Aggregation. , 2005, , 414-418.		0
113	Oscillating Gene Expressions in Regulatory Networks. , 2004, , 195-202.		0
114	Dynamical Genetic Regulation. NATO Science for Peace and Security Series B: Physics and Biophysics, 2008, , 61-81.	0.2	0