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	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
2	Polymer Folding Simulations from Hi-C Data. Methods in Molecular Biology, 2022, 2301, 259-265.	0.4	0
3	Evolution of frustrated and stabilising contacts in reconstructed ancient proteins. European Biophysics Journal, 2021, 50, 699-712.	1.2	1
4	HP1 drives de novo 3D genome reorganization in early Drosophila embryos. Nature, 2021, 593, 289-293.	13.7	76
5	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
6	Native state of natural proteins optimizes local entropy. Physical Review E, 2021, 104, 064117.	0.8	2
7	Effective model of loop extrusion predicts chromosomal domains. Physical Review E, 2020, 102, 032414.	0.8	7
8	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
9	MicroRNA-222 Regulates Melanoma Plasticity. Journal of Clinical Medicine, 2020, 9, 2573.	1.0	10
10	Assessing the accuracy of direct-coupling analysis for RNA contact prediction. Rna, 2020, 26, 637-647.	1.6	20
11	Bifractal nature of chromosome contact maps. Physical Review Research, 2020, 2, .	1.3	4
12	DamC reveals principles of chromatin folding in vivo without crosslinking and ligation. Nature Structural and Molecular Biology, 2019, 26, 471-480.	3.6	71
13	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
14	Molecular mechanisms of heterogeneous oligomerization of huntingtin proteins. Scientific Reports, 2019, 9, 7615.	1.6	21
15	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
16	Coarse Graining of a Giant Molecular System: The Chromatin Fiber. Methods in Molecular Biology, 2019, 2022, 399-411.	0.4	2
17	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
18	An implementation of the maximum-caliber principle by replica-averaged time-resolved restrained simulations. Journal of Chemical Physics, 2018, 148, 184114.	1.2	16

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19	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
20	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
21	Spontaneous domain formation in disordered copolymers as a mechanism for chromosome structuring. Soft Matter, 2018, 14, 6128-6136.	1.2	3
22	Modelling genome-wide topological associating domains in mouse embryonic stem cells. Chromosome Research, 2017, 25, 5-14.	1.0	15
23	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
24	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
25	Cold Denaturation of the HIV-1 Protease Monomer. Biochemistry, 2017, 56, 1029-1032.	1.2	7
26	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
27	How likely are oscillations in a genetic feedback loop with delay?. European Physical Journal E, 2017, 40, 74.	0.7	0
28	From Chromosome Conformation Capture to Polymer Physics and Back. , 2017, , 203-224.		0
29	FRET studies of various conformational states adopted by transthyretin. Cellular and Molecular Life Sciences, 2017, 74, 3577-3598.	2.4	7
30	Complete coverage of space favors modularity of the grid system in the brain. Physical Review E, 2016, 94, 062409.	0.8	9
31	Properties of low-dimensional collective variables in the molecular dynamics of biopolymers. Physical Review E, 2016, 94, 052406.	0.8	4
32	Structural Fluctuations of the Chromatin Fiber within Topologically Associating Domains. Biophysical Journal, 2016, 110, 1234-1245.	0.2	58
33	Looping probability of random heteropolymers helps to understand the scaling properties of biopolymers. Physical Review E, 2016, 94, 032402.	0.8	5
34	Tools for the rational design of bivalent microtubule-targeting drugs. Biochemical and Biophysical Research Communications, 2016, 479, 48-53.	1.0	10
35	Thermodynamicallyâ€“Weighted Conformational Ensemble of Cyclic RGD Peptidomimetics from NOE Data. Journal of Physical Chemistry B, 2016, 120, 7098-7107.	1.2	15
36	Assessment of Mutational Effects on Peptide Stability through Confinement Simulations. Journal of Physical Chemistry Letters, 2016, 7, 126-130.	2.1	9

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37	Theory of feedback controlled brain stimulations for Parkinsonâ€™s disease. Physica A: Statistical Mechanics and Its Applications, 2016, 441, 121-130.	1.2	1
38	Effect of disorder on the contact probability of elongated conformations of biopolymers. Physical Review E, 2015, 92, 010702.	0.8	1
39	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
40	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
41	MonteGrappa: An iterative Monte Carlo program to optimize biomolecular potentials in simplified models. Computer Physics Communications, 2015, 186, 93-104.	3.0	12
42	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
43	The maturation of HIVâ€1 protease precursor studied by discrete molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 633-639.	1.5	10
44	Predictive Polymer Modeling Reveals Coupled Fluctuations in Chromosome Conformation and Transcription. Cell, 2014, 157, 950-963.	13.5	411
45	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
46	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
47	The network of stabilizing contacts in proteins studied by coevolutionary data. Journal of Chemical Physics, 2013, 139, 155103.	1.2	33
48	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
49	Ratcheted molecular-dynamics simulations identify efficiently the transition state of protein folding. Journal of Chemical Physics, 2012, 137, 235101.	1.2	24
50	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
51	Thermodynamics of strongly allosteric inhibition: a model study of HIV-1 protease. European Biophysics Journal, 2012, 41, 991-1001.	1.2	1
52	Hierarchy of folding and unfolding events of protein G, CI2, and ACBP from explicit-solvent simulations. Journal of Chemical Physics, 2011, 134, 045105.	1.2	45
53	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
54	Equilibrium properties of realistic random heteropolymers and their relevance for globular and naturally unfolded proteins. Physical Review E, 2011, 84, 061910.	0.8	10

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55	Identification of the folding inhibitors of hen-egg lysozyme: gathering the right tools. European Biophysics Journal, 2010, 39, 911-919.	1.2	2
56	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
57	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
58	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
59	The molecular evolution of HIVâ€1 protease simulated at atomic detail. Proteins: Structure, Function and Bioinformatics, 2009, 76, 895-910.	1.5	5
60	Exploring the protein G helix freeâ€energy surface by solute tempering metadynamics. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1647-1654.	1.5	68
61	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
62	Estimation of microscopic averages from metadynamics. European Physical Journal B, 2008, 63, 235-238.	0.6	15
63	Early events in protein folding: Is there something more than hydrophobic burst?. Protein Science, 2008, 17, 1424-1433.	3.1	14
64	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
65	Urea and Guanidinium Chloride Denature Protein L in Different Ways in Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4654-4661.	0.2	141
66	Atomistic Simulations of the HIV-1 Protease Folding Inhibition. Biophysical Journal, 2008, 95, 550-562.	0.2	12
67	Metadynamic sampling of the free-energy landscapes of proteins coupled with a Monte Carlo algorithm. Gene, 2008, 422, 37-40.	1.0	3
68	Dynamical Genetic Regulation. NATO Science for Peace and Security Series B: Physics and Biophysics, 2008, , 61-81.	0.2	0
69	Kinetics of Different Processes in Human Insulin Amyloid Formation. Journal of Molecular Biology, 2007, 366, 258-274.	2.0	163
70	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
71	Insight into the Folding Inhibition of the HIV-1 Protease by a Small Peptide. Biophysical Journal, 2007, 93, 2813-2821.	0.2	40
72	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

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73	Low-throughput model design of protein folding inhibitors. Proteins: Structure, Function and Bioinformatics, 2007, 67, 469-478.	1.5	7
74	Oscillations and temporal signalling in cells. Physical Biology, 2007, 4, R1-R17.	0.8	108
75	Early Events in Insulin Fibrillization Studied by Time-Lapse Atomic Force Microscopy. Biophysical Journal, 2006, 90, 589-597.	0.2	54
76	Similar folds with different stabilization mechanisms: the cases of Prion and Doppel proteins. BMC Structural Biology, 2006, 6, 17.	2.3	17
77	Sequence of events in folding mechanism: Beyond the Goì„ model. Protein Science, 2006, 15, 1638-1652.	3.1	34
78	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
79	THE PHYSICS OF PROTEIN FOLDING AND OF DRUG DESIGN. , 2005, , .		0
80	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
81	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
82	A folding inhibitor of the HIV-1 protease. Proteins: Structure, Function and Bioinformatics, 2005, 62, 928-933.	1.5	29
83	Design of amino acid sequences to fold into CÎ±-model proteins. Journal of Chemical Physics, 2005, 123, 054904.	1.2	4
84	Design of a folding inhibitor of the HIV-1 protease. Molecular Simulation, 2005, 31, 765-771.	0.9	2
85	Protein Folding and Aggregation. , 2005, , 414-418.		0
86	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
87	Protein folding and non-conventional drug design: a primer for nuclear structure physicists. AIP Conference Proceedings, 2004, , .	0.3	0
88	The evolution dynamics of model proteins. Journal of Chemical Physics, 2004, 121, 2381-2389.	1.2	8
89	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
90	Thermodynamics of Î²-amyloid fibril formation. Journal of Chemical Physics, 2004, 120, 8307-8317.	1.2	27

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91	Simple models of protein folding and of non-conventional drug design. Journal of Physics Condensed Matter, 2004, 16, R111-R144.	0.7	13
92	Understanding the determinants of stability and folding of small globular proteins from their energetics. Protein Science, 2004, 13, 113-124.	3.1	78
93	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
94	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
95	Oscillating Gene Expressions in Regulatory Networks. , 2004, , 195-202.		0
96	Sustained oscillations and time delays in gene expression of protein Hes1. FEBS Letters, 2003, 541, 176-177.	1.3	147
97	Resistance proof, folding-inhibitor drugs. Journal of Chemical Physics, 2003, 118, 4754-4758.	1.2	14
98	Role of bulk and of interface contacts in the behavior of lattice model dimeric proteins. Physical Review E, 2003, 67, 051909.	0.8	3
99	FROM ATOMIC NUCLEI TO DRUG DESIGN. , 2003, , .		0
100	Design and folding of dimeric proteins. Proteins: Structure, Function and Bioinformatics, 2002, 49, 82-94.	1.5	27
101	Time delay as a key to apoptosis induction in the p53 network. European Physical Journal B, 2002, 29, 135-140.	0.6	101
102	Statistical analysis of native contact formation in the folding of designed model proteins. Journal of Chemical Physics, 2001, 114, 2503-2510.	1.2	35
103	Hydrogen Bonds in Polymer Folding. Physical Review Letters, 2001, 86, 1031-1033.	2.9	24
104	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
105	Energy profile of the space of model protein sequences. Journal of Biological Physics, 2001, 27, 147-159.	0.7	2
106	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
107	Designability of lattice model heteropolymers. Physical Review E, 2001, 64, 011904.	0.8	11
108	Hierarchy of events in the folding of model proteins. Journal of Chemical Physics, 2001, 114, 7267-7273.	1.2	37

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109	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
110	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
111	Stability of Designed Proteins against Mutations. Physical Review Letters, 1999, 82, 4727-4730.	2.9	28
112	Folding and misfolding of designed proteinlike chains with mutations. Journal of Chemical Physics, 1998, 108, 757-761.	1.2	67
113	Mapping of mutation-sensitive sites in proteinlike chains. Physical Review E, 1998, 58, 3572-3577.	0.8	7
114	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