Emanuele Paci

List of Publications by Year
in descending order

134 papers	13,367 citations	61984 43 h-index	22832 112 g-index
142 all docs	142 docs citations	142 times ranked	14445 citing authors

#	Article	IF	Citations
1	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
2	Three key residues form a critical contact network in a protein folding transition state. Nature, 2001, 409, 641-645.	27.8	423
3	Pulling geometry defines the mechanical resistance of a Î²-sheet protein. Nature Structural and Molecular Biology, 2003, 10, 731-737.	8.2	356
4	Small-world view of the amino acids that play a key role in protein folding. Physical Review E, 2002, 65, 061910.	2.1	336
5	Forced unfolding of fibronectin type 3 modules: an analysis by biased molecular dynamics simulations. Journal of Molecular Biology, 1999, 288, 441-459.	4.2	323
6	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	3.3	285
7	Unfolding proteins by external forces and temperature: The importance of topology and energetics. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 6521-6526.	7.1	282
8	Mechanical Unfolding of a Titin Ig Domain: Structure of Unfolding Intermediate Revealed by Combining AFM, Molecular Dynamics Simulations, NMR and Protein Engineering. Journal of Molecular Biology, 2002, 322, 841-849.	4.2	200
9	Mechanical Unfolding of a Titin Ig Domain: Structure of Transition State Revealed by Combining Atomic Force Microscopy, Protein Engineering and Molecular Dynamics Simulations. Journal of Molecular Biology, 2003, 330, 867-877.	4.2	168
10	Mechanically Unfolding the Small, Topologically Simple Protein L. Biophysical Journal, 2005, 89, 506-519.	0.5	154
11	Pulling Direction as a Reaction Coordinate for the Mechanical Unfolding of Single Molecules. Journal of Physical Chemistry B, 2008, 112, 5968-5976.	2.6	135
12	Rare Fluctuations of Native Proteins Sampled by Equilibrium Hydrogen Exchange. Journal of the American Chemical Society, 2003, 125, 15686-15687.	13.7	122
13	Mechanical Unfolding of TNfn3: The Unfolding Pathway of a fnIII Domain Probed by Protein Engineering, AFM and MD Simulation. Journal of Molecular Biology, 2005, 350, 776-789.	4.2	110
14	The Remarkable Mechanical Strength of Polycystin-1 Supports a Direct Role in Mechanotransduction. Journal of Molecular Biology, 2005, 349, 861-871.	4.2	108
15	Determination of a Transition State at Atomic Resolution from Protein Engineering Data. Journal of Molecular Biology, 2002, 324, 151-163.	4.2	107
16	Mechanical Resistance of Proteins Explained Using Simple Molecular Models. Biophysical Journal, 2006, 90, 287-297.	0.5	106
17	Protein folding and the organization of the protein topology universe. Trends in Biochemical Sciences, 2005, 30, 13-19.	7.5	101
18	Determination of an ensemble of structures representing the intermediate state of the bacterial immunity protein Im7. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 99-104.	7.1	90

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19	Transition states for protein folding have native topologies despite high structural variability. Nature Structural and Molecular Biology, 2004, 11, 443-449.	8.2	88
20	Title is missing!. Journal of Computational Chemistry, 1997, 18, 1848.	3.3	77
21	Structures and relative free energies of partially folded states of proteins. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 14817-14821.	7.1	71
22	Boxed Molecular Dynamics: A Simple and General Technique for Accelerating Rare Event Kinetics and Mapping Free Energy in Large Molecular Systems. Journal of Physical Chemistry B, 2009, 113, 16603-16611.	2.6	70
23	Intrinsic compressibility and volume compression in solvated proteins by molecular dynamics simulation at high pressure.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 11609-11614.	7.1	68
24	Activation energies by molecular dynamics with constraints. Chemical Physics Letters, 1991, 176, 581-587.	2.6	67
25	Molecular Dynamics Studies of the Process of Amyloid Aggregation of Peptide Fragments of Transthyretin. Journal of Molecular Biology, 2004, 340, 555-569.	4.2	65
26	Transition State Contact Orders Correlate with Protein Folding Rates. Journal of Molecular Biology, 2005, 352, 495-500.	4.2	64
27	Gating of TonB-dependent transporters by substrate-specific forced remodelling. Nature Communications, 2017, 8, 14804.	12.8	64
28	Exploration of partially unfolded states of human Î±-lactalbumin by molecular dynamics simulation11Edited by B. Honig. Journal of Molecular Biology, 2001, 306, 329-347.	4.2	61
29	Native and non-native interactions along protein folding and unfolding pathways. Proteins: Structure, Function and Bioinformatics, 2002, 47, 379-392.	2.6	61
30	Mechanical Unfolding of an Ankyrin Repeat Protein. Biophysical Journal, 2010, 98, 1294-1301.	0.5	56
31	Self-consistent determination of the transition state for protein folding: Application to a fibronectin type III domain. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 394-399.	7.1	55
32	Mechanical unfolding revisited through a simple but realistic model. Journal of Chemical Physics, 2006, 124, 154909.	3.0	55
33	Unraveling the molecular basis of subunit specificity in P pilus assembly by mass spectrometry. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12873-12878.	7.1	54
34	Stable Single Î±-Helices Are Constant Force Springs in Proteins. Journal of Biological Chemistry, 2014, 289, 27825-27835.	3.4	54
35	High pressure simulations of biomolecules. BBA - Proteins and Proteomics, 2002, 1595, 185-200.	2.1	53
36	Cooperative folding of intrinsically disordered domains drives assembly of a strong elongated protein. Nature Communications, 2015, 6, 7271.	12.8	52

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37	Validity of GÅ•Models: Comparison with a Solvent-Shielded Empirical Energy Decomposition. Biophysical Journal, 2002, 83, 3032-3038.	0.5	50
38	Protein folding: bringing theory and experiment closer together. Current Opinion in Structural Biology, 2003, 13, 82-87.	5.7	50
39	Analysis of the distributed computing approach applied to the folding of a small Î² peptide. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 8217-8222.	7.1	47
40	Forces and energetics of hapten-antibody dissociation: a biased molecular dynamics simulation study 1 1Edited by B. Honig. Journal of Molecular Biology, 2001, 314, 589-605.	4.2	46
41	On the volume of macromolecules. Biopolymers, 1997, 41, 785-797.	2.4	44
42	Comparison of the Transition States for Folding of Two Ig-like Proteins from Different Superfamilies. Journal of Molecular Biology, 2004, 343, 1111-1123.	4.2	44
43	Free energy for protein folding from nonequilibrium simulations using the Jarzynski equality. Journal of Chemical Physics, 2006, 125, 204910.	3.0	44
44	Boxed Molecular Dynamics: Decorrelation Time Scales and the Kinetic Master Equation. Journal of Chemical Theory and Computation, 2011, 7, 1244-1252.	5.3	44
45	Comparison of the transition state ensembles for folding of Im7 and Im9 determined using all-atom molecular dynamics simulations with Ï• value restraints. Proteins: Structure, Function and Bioinformatics, 2003, 54, 513-525.	2.6	41
46	The structure of a folding intermediate provides insight into differences in immunoglobulin amyloidogenicity. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13373-13378.	7.1	41
47	Direct evidence of the multidimensionality of the free-energy landscapes of proteins revealed by mechanical probes. Physical Review E, 2010, 81, 031923.	2.1	41
48	Fast protein folding on downhill energy landscape. Protein Science, 2003, 12, 1801-1803.	7.6	40
49	Characterization of long and stable de novo single alpha-helix domains provides novel insight into their stability. Scientific Reports, 2017, 7, 44341.	3.3	40
50	Constant-Pressure Molecular Dynamics Techniques Applied to Complex Molecular Systems and Solvated Proteins. The Journal of Physical Chemistry, 1996, 100, 4314-4322.	2.9	37
51	Prediction of the Translocation Kinetics of a Protein from Its Mechanical Properties. Biophysical Journal, 2006, 91, L51-L53.	0.5	34
52	Donor-Strand Exchange in Chaperone-Assisted Pilus Assembly Revealed in Atomic Detail by Molecular Dynamics. Journal of Molecular Biology, 2008, 375, 908-919.	4.2	34
53	Assessment of ab initio models of protein complexes by molecular dynamics. PLoS Computational Biology, 2018, 14, e1006182.	3.2	33
54	Sampling of molecular conformations by molecular dynamics techniques. Molecular Physics, 1993, 79, 515-522.	1.7	32

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55	Calculation of Mutational Free Energy Changes in Transition States for Protein Folding. Biophysical Journal, 2003, 85, 1207-1214.	0.5	31
56	Molecular Dynamics Simulation of Dextran Extension by Constant Force in Single Molecule AFM. Biophysical Journal, 2006, 91, 3579-3588.	0.5	31
57	ALMOST: An all atom molecular simulation toolkit for protein structure determination. Journal of Computational Chemistry, 2014, 35, 1101-1105.	3.3	31
58	The Effect of Increasing the Stability of Non-native Interactions on the Folding Landscape of the Bacterial Immunity Protein Im9. Journal of Molecular Biology, 2007, 371, 554-568.	4.2	30
59	Non-Native Interactions Are Critical for Mechanical Strength in PKD Domains. Structure, 2009, 17, 1582-1590.	3.3	28
60	Tracking Local Conformational Changes of Ribonuclease A Using Picosecond Time-Resolved Fluorescence of the Six Tyrosine Residues. Biophysical Journal, 2007, 92, 4401-4414.	0.5	27
61	Fluorescence Lifetimes of Tyrosine Residues in Cytochrome câ€²â€² as Local Probes to Study Protein Unfolding. Journal of Physical Chemistry B, 2009, 113, 4466-4474.	2.6	27
62	Single-Molecule Folding Mechanism of an EF-Hand Neuronal Calcium Sensor. Structure, 2013, 21, 1812-1821.	3.3	27
63	The major determinant of exendinâ€4/glucagonâ€like peptide 1 differential affinity at the rat glucagonâ€like peptide 1 receptor Nâ€terminal domain is a hydrogen bond from SERâ€32 of exendinâ€4. British Journal of Pharmacology, 2010, 160, 1973-1984.	5.4	26
64	Nonexponential Kinetics of Loop Formation in Proteins and Peptides: A Signature of Rugged Free Energy Landscapes?. Journal of Physical Chemistry B, 2017, 121, 9518-9525.	2.6	26
65	Complex Unfolding Kinetics of Single-Domain Proteins in the Presence of Force. Biophysical Journal, 2010, 99, 1620-1627.	0.5	25
66	Disorder drives cooperative folding in a multidomain protein. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11841-11846.	7.1	24
67	Differential Effects of Hydrophobic Core Packing Residues for Thermodynamic and Mechanical Stability of a Hyperthermophilic Protein. Langmuir, 2016, 32, 7392-7402.	3.5	24
68	Structural Determinants of Polymerization Reactivity of the P pilus Adaptor Subunit PapF. Structure, 2008, 16, 1724-1731.	3.3	22
69	Analysis of the Free-Energy Surface of Proteins from Reversible Folding Simulations. PLoS Computational Biology, 2009, 5, e1000428.	3.2	22
70	Comparison of Sequence-Based and Structure-Based Energy Functions for the Reversible Folding of a Peptide. Biophysical Journal, 2005, 88, 3158-3166.	0.5	21
71	Structural Comparison of the Two Alternative Transition States for Folding of TI I27. Biophysical Journal, 2006, 91, 263-275.	0.5	21
72	Dimer asymmetry in superoxide dismutase studied by molecular dynamics simulation. Journal of Computer-Aided Molecular Design, 1996, 10, 490-498.	2.9	20

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73	Peptide kinetics from picoseconds to microseconds using boxed molecular dynamics: Power law rate coefficients in cyclisation reactions. Journal of Chemical Physics, 2012, 137, 165102.	3.0	20
74	Estimating Constraints for Protection Factors from HDX-MS Data. Biophysical Journal, 2019, 116, 1194-1203.	0.5	20
75	Change of the unbinding mechanism upon a mutation: A molecular dynamics study of an antibody-hapten complex. Protein Science, 2005, 14, 2499-2514.	7.6	19
76	Rate of Loop Formation in Peptides: A Simulation Study. Journal of Molecular Biology, 2008, 382, 556-565.	4.2	19
77	Dynamics of the Coiled-Coil Unfolding Transition of Myosin Rod Probed byÂDissipation Force Spectrum. Biophysical Journal, 2010, 99, 257-262.	0.5	18
78	Effects of Ligand Binding on the Mechanical Properties of Ankyrin Repeat Protein Gankyrin. PLoS Computational Biology, 2013, 9, e1002864.	3.2	18
79	Activation of PKA via asymmetric allosteric coupling of structurally conserved cyclic nucleotide binding domains. Nature Communications, 2019, 10, 3984.	12.8	18
80	Directed Assembly of Homopentameric Cholera Toxin B-Subunit Proteins into Higher-Order Structures Using Coiled-Coil Appendages. Journal of the American Chemical Society, 2019, 141, 5211-5219.	13.7	18
81	Adaptive free energy sampling in multidimensional collective variable space using boxed molecular dynamics. Faraday Discussions, 2016, 195, 395-419.	3.2	17
82	Membrane Crossing by a Polar Molecule: A Molecular Dynamics Simulation. Molecular Simulation, 1994, 14, 1-10.	2.0	16
83	Free-Energy Landscapes of Proteins in the Presence and Absence of Force. Journal of Physical Chemistry B, 2008, 112, 16902-16907.	2.6	16
84	Flexibility within the Rotor and Stators of the Vacuolar H+-ATPase. PLoS ONE, 2013, 8, e82207.	2.5	16
85	Internal protein dynamics shifts the distance to the mechanical transition state. Physical Review E, 2006, 74, 061912.	2.1	15
86	Functional Dynamics of Hexameric Helicase Probed by Hydrogen Exchange and Simulation. Biophysical Journal, 2014, 107, 983-990.	0.5	15
87	Defining the remarkable structural malleability of a bacterial surface protein Rib domain implicated in infection. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 26540-26548.	7.1	15
88	Periscope Proteins are variable-length regulators of bacterial cell surface interactions. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	15
89	Understanding the apparent statorâ€rotor connections in the rotary <scp>ATP</scp>ase family using coarseâ€grained computer modeling. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3298-3311.	2.6	14
90	Extraction of Accurate Biomolecular Parameters from Single-Molecule Force Spectroscopy Experiments. ACS Nano, 2015, 9, 1315-1324.	14.6	14

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91	Characterization of the molten globule state of retinol-binding protein using a molecular dynamics simulation approach. FEBS Journal, 2005, 272, 4826-4838.	4.7	13
92	Sequential Unfolding of Individual Helices of Bacterioopsin Observed in Molecular Dynamics Simulations of Extraction from the Purple Membrane. Biophysical Journal, 2006, 91, 3276-3284.	0.5	13
93	The Structure of Neuronal Calcium Sensor-1 in Solution Revealed by Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e74383.	2.5	12
94	Dynamic ion pair behavior stabilizes single Î±-helices in proteins. Journal of Biological Chemistry, 2019, 294, 3219-3234.	3.4	12
95	Helical Polyampholyte Sequences Have Unique Thermodynamic Properties. Journal of Physical Chemistry B, 2018, 122, 11784-11791.	2.6	11
96	Vacancy migration rates by molecular dynamics with constraints. Journal of Physics Condensed Matter, 1992, 4, 2173-2184.	1.8	10
97	Orientational averaging of dye molecules attached to proteins in FoÌˆrster resonance energy transfer measurements: Insights from a simulation study. Journal of Chemical Physics, 2009, 131, 065101.	3.0	10
98	Tuning protein mechanics through an ionic cluster graft from an extremophilic protein. Soft Matter, 2016, 12, 2688-2699.	2.7	10
99	A mechanism for agonist activation of the glucagon-like peptide-1 (GLP-1) receptor through modelling & molecular dynamics. Biochemical and Biophysical Research Communications, 2018, 498, 359-365.	2.1	10
100	Myosin tails and single Î±-helical domains. Biochemical Society Transactions, 2015, 43, 58-63.	3.4	9
101	Transition states for protein folding using molecular dynamics and experimental restraints. Journal of Physics Condensed Matter, 2007, 19, 285211.	1.8	8
102	New Dynamical Window onto the Landscape for Forced Protein Unfolding. Physical Review Letters, 2008, 101, 248104.	7.8	8
103	Communication: Conformation state diagram of polypeptides: A chain length induced Î±-Î² transition. Journal of Chemical Physics, 2011, 135, 061101.	3.0	8
104	Optimal Reaction Coordinate as a Biomarker for the Dynamics of Recovery from Kidney Transplant. PLoS Computational Biology, 2014, 10, e1003685.	3.2	8
105	Detection of non-native hydrophobic interactions in the denatured state of lysozyme by molecular dynamics simulations. Journal of Physics Condensed Matter, 2005, 17, S1617-S1626.	1.8	6
106	Probing the free energy landscape of the FBP28WW domain using multiple techniques. Journal of Computational Chemistry, 2009, 30, 1059-1068.	3.3	6
107	Simulation of fluorescence resonance energy transfer experiments: effect of the dyes on protein folding. Journal of Physics Condensed Matter, 2010, 22, 235103.	1.8	6
108	Modulation of a Protein Free-Energy Landscape by Circular Permutation. Journal of Physical Chemistry B, 2013, 117, 13743-13747.	2.6	6

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109	The Role of High-Dimensional Diffusive Search, Stabilization, and Frustration in Protein Folding. Biophysical Journal, 2014, 106, 1729-1740.	0.5	6
110	Computational Modeling of Designed Ankyrin Repeat Protein Complexes with Their Targets. Journal of Molecular Biology, 2019, 431, 2852-2868.	4.2	6
111	Induction of rare conformation of oligosaccharide by binding to calcium-dependent bacterial lectin: X-ray crystallography and modelling study. European Journal of Medicinal Chemistry, 2019, 177, 212-220.	5.5	6
112	Partial Opening of Cytochrome P450cam (CYP101A1) Is Driven by Allostery and Putidaredoxin Binding. Biochemistry, 2021, 60, 2932-2942.	2.5	6
113	Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. Journal of Physical Chemistry C, 2014, 118, 10159-10169.	3.1	5
114	Protein mechanics probed using simple molecular models. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129613.	2.4	5
115	Fluctuation power spectra reveal dynamical heterogeneity of peptides. Journal of Chemical Physics, 2010, 133, 015101.	3.0	4
116	Effect of external pulling forces on the length distribution of peptides. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 903-910.	2.4	4
117	High-Resolution Hydrogenâ€“Deuterium Protection Factors from Sparse Mass Spectrometry Data Validated by Nuclear Magnetic Resonance Measurements. Journal of the American Society for Mass Spectrometry, 2022, 33, 813-822.	2.8	4
118	Growth Kinetics of Bacterial Pili from Pairwise Pilin Association Rates. PLoS ONE, 2013, 8, e63065.	2.5	3
119	Prediction of stability changes upon mutation in an icosahedral capsid. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1733-1741.	2.6	2
120	Characterization of the flexibility of the peripheral stalk of prokaryotic rotary A-ATPases by atomistic simulations. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1203-1212.	2.6	2
121	Using Models to Design New Bioinspired Materials. Biophysical Journal, 2012, 103, 1814-1815.	0.5	1
122	Prying Open Single GroES Ring Complexes by Force Reveals Cooperativity across Domains. Biophysical Journal, 2012, 102, 1961-1968.	0.5	1
123	Terahertz time-domain spectroscopy of lysozyme and mouse urinary protein single crystals. , 2013, , .		1
124	Free-energy Landscapes of Proteins in the Presence of a Small Force. , 2009, , .		0
125	Modulation of a Protein Free Energy Landscape by Circular Permutation. Biophysical Journal, 2012, 102, 57a-58a.	0.5	0
126	Functional Dynamics of the Packaging Motor P4 Probed by Hydrogen Exchange and Simulation. Biophysical Journal, 2014, 106, 457a.	0.5	0

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127	Kinetic of Loop Formation in Polypeptides and Free Energy Landscapes. Biophysical Journal, 2014, 106, 260a-261a.	0.5	0
128	Using Time-Resolved Changes in Reflection Intensity to Test Mechanistic Hypotheses. Biophysical Journal, 2014, 106, 461a.	0.5	0
129	Unravelling the Properties of Single Î±-Helical Domains in Myosin and other Proteins. Biophysical Journal, 2014, 106, 626a.	0.5	0
130	Determining How Many Ionic Interactions are Needed for the High Stability of Single Alpha Helical (SAH) Domains. Biophysical Journal, 2015, 108, 16a.	0.5	0
131	The Folding of SasG: A Long and Remarkably Strong Monomeric Protein Responsible for Biofilm Formation is a Highly Cooperative System. Biophysical Journal, 2015, 108, 346a.	0.5	0
132	Hydrogen-Deuterium Exchange Mass Spectroscopy to Determine Structure and Structural Dynamics of Protein Complexes. Biophysical Journal, 2017, 112, 469a.	0.5	0
133	Can Hydrogen-Deuterium Exchange Rates at Single Residue Level Be Obtained from HDX-MS Data?. Biophysical Journal, 2019, 116, 288a-289a.	0.5	0
134	Computational methods to predict the mutational landscape of the spike protein.. Biophysical Journal, 2021, 120, 2763-2765.	0.5	0