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	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
2	Computational methods to predict the mutational landscape of the spike protein.. Biophysical Journal, 2021, 120, 2763-2765.	0.5	0
3	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
4	Partial Opening of Cytochrome P450cam (CYP101A1) Is Driven by Allostery and Putidaredoxin Binding. Biochemistry, 2021, 60, 2932-2942.	2.5	6
5	Protein mechanics probed using simple molecular models. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129613.	2.4	5
6	Activation of PKA via asymmetric allosteric coupling of structurally conserved cyclic nucleotide binding domains. Nature Communications, 2019, 10, 3984.	12.8	18
7	Computational Modeling of Designed Ankyrin Repeat Protein Complexes with Their Targets. Journal of Molecular Biology, 2019, 431, 2852-2868.	4.2	6
8	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
9	Estimating Constraints for Protection Factors from HDX-MS Data. Biophysical Journal, 2019, 116, 1194-1203.	0.5	20
10	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
11	Can Hydrogen-Deuterium Exchange Rates at Single Residue Level Be Obtained from HDX-MS Data?. Biophysical Journal, 2019, 116, 288a-289a.	0.5	0
12	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	3.3	285
13	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
14	Dynamic ion pair behavior stabilizes single Î±-helices in proteins. Journal of Biological Chemistry, 2019, 294, 3219-3234.	3.4	12
15	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
16	Helical Polyampholyte Sequences Have Unique Thermodynamic Properties. Journal of Physical Chemistry B, 2018, 122, 11784-11791.	2.6	11
17	Assessment of ab initio models of protein complexes by molecular dynamics. PLoS Computational Biology, 2018, 14, e1006182.	3.2	33
18	Gating of TonB-dependent transporters by substrate-specific forced remodelling. Nature Communications, 2017, 8, 14804.	12.8	64

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19	Hydrogen-Deuterium Exchange Mass Spectroscopy to Determine Structure and Structural Dynamics of Protein Complexes. Biophysical Journal, 2017, 112, 469a.	0.5	0
20	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
21	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
22	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
23	Adaptive free energy sampling in multidimensional collective variable space using boxed molecular dynamics. Faraday Discussions, 2016, 195, 395-419.	3.2	17
24	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
25	Differential Effects of Hydrophobic Core Packing Residues for Thermodynamic and Mechanical Stability of a Hyperthermophilic Protein. Langmuir, 2016, 32, 7392-7402.	3.5	24
26	Tuning protein mechanics through an ionic cluster graft from an extremophilic protein. Soft Matter, 2016, 12, 2688-2699.	2.7	10
27	Prediction of stability changes upon mutation in an icosahedral capsid. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1733-1741.	2.6	2
28	Myosin tails and single Î±-helical domains. Biochemical Society Transactions, 2015, 43, 58-63.	3.4	9
29	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
30	Extraction of Accurate Biomolecular Parameters from Single-Molecule Force Spectroscopy Experiments. ACS Nano, 2015, 9, 1315-1324.	14.6	14
31	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
32	Cooperative folding of intrinsically disordered domains drives assembly of a strong elongated protein. Nature Communications, 2015, 6, 7271.	12.8	52
33	Effect of external pulling forces on the length distribution of peptides. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 903-910.	2.4	4
34	Optimal Reaction Coordinate as a Biomarker for the Dynamics of Recovery from Kidney Transplant. PLoS Computational Biology, 2014, 10, e1003685.	3.2	8
35	ALMOST: An all atom molecular simulation toolkit for protein structure determination. Journal of Computational Chemistry, 2014, 35, 1101-1105.	3.3	31
36	Functional Dynamics of Hexameric Helicase Probed by Hydrogen Exchange and Simulation. Biophysical Journal, 2014, 107, 983-990.	0.5	15

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37	Stable Single Î±-Helices Are Constant Force Springs in Proteins. Journal of Biological Chemistry, 2014, 289, 27825-27835.	3.4	54
38	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
39	Functional Dynamics of the Packaging Motor P4 Probed by Hydrogen Exchange and Simulation. Biophysical Journal, 2014, 106, 457a.	0.5	0
40	Kinetic of Loop Formation in Polypeptides and Free Energy Landscapes. Biophysical Journal, 2014, 106, 260a-261a.	0.5	0
41	The Role of High-Dimensional Diffusive Search, Stabilization, and Frustration in Protein Folding. Biophysical Journal, 2014, 106, 1729-1740.	0.5	6
42	Using Time-Resolved Changes in Reflection Intensity to Test Mechanistic Hypotheses. Biophysical Journal, 2014, 106, 461a.	0.5	0
43	Unravelling the Properties of Single Î±-Helical Domains in Myosin and other Proteins. Biophysical Journal, 2014, 106, 626a.	0.5	0
44	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
45	Modulation of a Protein Free-Energy Landscape by Circular Permutation. Journal of Physical Chemistry B, 2013, 117, 13743-13747.	2.6	6
46	Single-Molecule Folding Mechanism of an EF-Hand Neuronal Calcium Sensor. Structure, 2013, 21, 1812-1821.	3.3	27
47	Effects of Ligand Binding on the Mechanical Properties of Ankyrin Repeat Protein Gankyrin. PLoS Computational Biology, 2013, 9, e1002864.	3.2	18
48	Terahertz time-domain spectroscopy of lysozyme and mouse urinary protein single crystals. , 2013, , .		1
49	Growth Kinetics of Bacterial Pili from Pairwise Pilin Association Rates. PLoS ONE, 2013, 8, e63065.	2.5	3
50	The Structure of Neuronal Calcium Sensor-1 in Solution Revealed by Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e74383.	2.5	12
51	Flexibility within the Rotor and Stators of the Vacuolar H+-ATPase. PLoS ONE, 2013, 8, e82207.	2.5	16
52	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
53	Using Models to Design New Bioinspired Materials. Biophysical Journal, 2012, 103, 1814-1815.	0.5	1
54	Modulation of a Protein Free Energy Landscape by Circular Permutation. Biophysical Journal, 2012, 102, 57a-58a.	0.5	0

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55	Prying Open Single GroES Ring Complexes by Force Reveals Cooperativity across Domains. Biophysical Journal, 2012, 102, 1961-1968.	0.5	1
56	Boxed Molecular Dynamics: Decorrelation Time Scales and the Kinetic Master Equation. Journal of Chemical Theory and Computation, 2011, 7, 1244-1252.	5.3	44
57	Communication: Conformation state diagram of polypeptides: A chain length induced Î±-Î² transition. Journal of Chemical Physics, 2011, 135, 061101.	3.0	8
58	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
59	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
60	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
61	Mechanical Unfolding of an Ankyrin Repeat Protein. Biophysical Journal, 2010, 98, 1294-1301.	0.5	56
62	Dynamics of the Coiled-Coil Unfolding Transition of Myosin Rod Probed byÂDissipation Force Spectrum. Biophysical Journal, 2010, 99, 257-262.	0.5	18
63	Complex Unfolding Kinetics of Single-Domain Proteins in the Presence of Force. Biophysical Journal, 2010, 99, 1620-1627.	0.5	25
64	Fluctuation power spectra reveal dynamical heterogeneity of peptides. Journal of Chemical Physics, 2010, 133, 015101.	3.0	4
65	Free-energy Landscapes of Proteins in the Presence of a Small Force. , 2009, , .		0
66	Orientational averaging of dye molecules attached to proteins in Foì`rster resonance energy transfer measurements: Insights from a simulation study. Journal of Chemical Physics, 2009, 131, 065101.	3.0	10
67	Analysis of the Free-Energy Surface of Proteins from Reversible Folding Simulations. PLoS Computational Biology, 2009, 5, e1000428.	3.2	22
68	Non-Native Interactions Are Critical for Mechanical Strength in PKD Domains. Structure, 2009, 17, 1582-1590.	3.3	28
69	Probing the free energy landscape of the FBP28WW domain using multiple techniques. Journal of Computational Chemistry, 2009, 30, 1059-1068.	3.3	6
70	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
71	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
72	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

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73	Structural Determinants of Polymerization Reactivity of the P pilus Adaptor Subunit PapF. Structure, 2008, 16, 1724-1731.	3.3	22
74	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
75	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
76	Rate of Loop Formation in Peptides: A Simulation Study. Journal of Molecular Biology, 2008, 382, 556-565.	4.2	19
77	Free-Energy Landscapes of Proteins in the Presence and Absence of Force. Journal of Physical Chemistry B, 2008, 112, 16902-16907.	2.6	16
78	New Dynamical Window onto the Landscape for Forced Protein Unfolding. Physical Review Letters, 2008, 101, 248104.	7.8	8
79	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
80	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
81	Transition states for protein folding using molecular dynamics and experimental restraints. Journal of Physics Condensed Matter, 2007, 19, 285211.	1.8	8
82	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
83	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
84	Mechanical unfolding revisited through a simple but realistic model. Journal of Chemical Physics, 2006, 124, 154909.	3.0	55
85	Internal protein dynamics shifts the distance to the mechanical transition state. Physical Review E, 2006, 74, 061912.	2.1	15
86	Mechanical Resistance of Proteins Explained Using Simple Molecular Models. Biophysical Journal, 2006, 90, 287-297.	0.5	106
87	Structural Comparison of the Two Alternative Transition States for Folding of TI I27. Biophysical Journal, 2006, 91, 263-275.	0.5	21
88	Molecular Dynamics Simulation of Dextran Extension by Constant Force in Single Molecule AFM. Biophysical Journal, 2006, 91, 3579-3588.	0.5	31
89	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
90	Prediction of the Translocation Kinetics of a Protein from Its Mechanical Properties. Biophysical Journal, 2006, 91, L51-L53.	0.5	34

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91	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
92	Free energy for protein folding from nonequilibrium simulations using the Jarzynski equality. Journal of Chemical Physics, 2006, 125, 204910.	3.0	44
93	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
94	Protein folding and the organization of the protein topology universe. Trends in Biochemical Sciences, 2005, 30, 13-19.	7.5	101
95	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
96	Transition State Contact Orders Correlate with Protein Folding Rates. Journal of Molecular Biology, 2005, 352, 495-500.	4.2	64
97	The Remarkable Mechanical Strength of Polycystin-1 Supports a Direct Role in Mechanotransduction. Journal of Molecular Biology, 2005, 349, 861-871.	4.2	108
98	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
99	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
100	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
101	Mechanically Unfolding the Small, Topologically Simple Protein L. Biophysical Journal, 2005, 89, 506-519.	0.5	154
102	Transition states for protein folding have native topologies despite high structural variability. Nature Structural and Molecular Biology, 2004, 11, 443-449.	8.2	88
103	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
104	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
105	Protein folding: bringing theory and experiment closer together. Current Opinion in Structural Biology, 2003, 13, 82-87.	5.7	50
106	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
107	Pulling geometry defines the mechanical resistance of a Î²-sheet protein. Nature Structural and Molecular Biology, 2003, 10, 731-737.	8.2	356
108	Fast protein folding on downhill energy landscape. Protein Science, 2003, 12, 1801-1803.	7.6	40

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109	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
110	Calculation of Mutational Free Energy Changes in Transition States for Protein Folding. Biophysical Journal, 2003, 85, 1207-1214.	0.5	31
111	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
112	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
113	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
114	Rare Fluctuations of Native Proteins Sampled by Equilibrium Hydrogen Exchange. Journal of the American Chemical Society, 2003, 125, 15686-15687.	13.7	122
115	Small-world view of the amino acids that play a key role in protein folding. Physical Review E, 2002, 65, 061910.	2.1	336
116	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
117	Determination of a Transition State at Atomic Resolution from Protein Engineering Data. Journal of Molecular Biology, 2002, 324, 151-163.	4.2	107
118	Validity of GÅ•Models: Comparison with a Solvent-Shielded Empirical Energy Decomposition. Biophysical Journal, 2002, 83, 3032-3038.	0.5	50
119	High pressure simulations of biomolecules. BBA - Proteins and Proteomics, 2002, 1595, 185-200.	2.1	53
120	Native and non-native interactions along protein folding and unfolding pathways. Proteins: Structure, Function and Bioinformatics, 2002, 47, 379-392.	2.6	61
121	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
122	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
123	Three key residues form a critical contact network in a protein folding transition state. Nature, 2001, 409, 641-645.	27.8	423
124	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
125	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
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127	Title is missing!. Journal of Computational Chemistry, 1997, 18, 1848.	3.3	77
128	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
129	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
130	Dimer asymmetry in superoxide dismutase studied by molecular dynamics simulation. Journal of Computer-Aided Molecular Design, 1996, 10, 490-498.	2.9	20
131	Membrane Crossing by a Polar Molecule: A Molecular Dynamics Simulation. Molecular Simulation, 1994, 14, 1-10.	2.0	16
132	Sampling of molecular conformations by molecular dynamics techniques. Molecular Physics, 1993, 79, 515-522.	1.7	32
133	Vacancy migration rates by molecular dynamics with constraints. Journal of Physics Condensed Matter, 1992, 4, 2173-2184.	1.8	10
134	Activation energies by molecular dynamics with constraints. Chemical Physics Letters, 1991, 176, 581-587.	2.6	67