Harold A Scheraga

List of Publications by Year
in descending order

329 papers	25,183 citations	8755 75 h-index	8167 148 g-index
344 all docs	344 docs citations	344 times ranked	9667 citing authors

#	Article	IF	Citations
1	Energy parameters in polypeptides. VII. Geometric parameters, partial atomic charges, nonbonded interactions, hydrogen bond interactions, and intrinsic torsional potentials for the naturally occurring amino acids. The Journal of Physical Chemistry, 1975, 79, 2361-2381.	2.9	1,563
2	Structure of Water and Hydrophobic Bonding in Proteins. I. A Model for the Thermodynamic Properties of Liquid Water. Journal of Chemical Physics, 1962, 36, 3382-3400.	3.0	1,099
3	Global Optimization of Clusters, Crystals, and Biomolecules. Science, 1999, 285, 1368-1372.	12.6	995
4	Energy parameters in polypeptides. 9. Updating of geometrical parameters, nonbonded interactions, and hydrogen bond interactions for the naturally occurring amino acids. The Journal of Physical Chemistry, 1983, 87, 1883-1887.	2.9	961
5	THE STRUCTURE OF WATER AND HYDROPHOBIC BONDING IN PROTEINS. III. THE THERMODYNAMIC PROPERTIES OF HYDROPHOBIC BONDS IN PROTEINS1,2. The Journal of Physical Chemistry, 1962, 66, 1773-1789.	2.9	948
6	Energy parameters in polypeptides. 10. Improved geometrical parameters and nonbonded interactions for use in the ECEPP/3 algorithm, with application to proline-containing peptides. The Journal of Physical Chemistry, 1992, 96, 6472-6484.	2.9	664
7	Structure of Water and Hydrophobic Bonding in Proteins. II. Model for the Thermodynamic Properties of Aqueous Solutions of Hydrocarbons. Journal of Chemical Physics, 1962, 36, 3401-3417.	3.0	631
8	Disulfide Bonds and Protein Foldingâ€. Biochemistry, 2000, 39, 4207-4216.	2.5	556
9	Conformational Analysis of Macromolecules. III. Helical Structures of Polyglycine and Polyâ€Lâ€Alanine. Journal of Chemical Physics, 1966, 45, 2091-2101.	3.0	439
10	Structure of Water and Hydrophobic Bonding in Proteins. IV. The Thermodynamic Properties of Liquid Deuterium Oxide. Journal of Chemical Physics, 1964, 41, 680-689.	3.0	386
11	Intermolecular potentials from crystal data. 6. Determination of empirical potentials for O-H...O = C hydrogen bonds from packing configurations. The Journal of Physical Chemistry, 1984, 88, 6231-6233.	2.9	347
12	Method for Calculating Internal Rotation Barriers. Journal of Chemical Physics, 1965, 42, 2209-2215.	3.0	337
13	Conformational Analysis of Macromolecules. IV. Helical Structures of Polyâ€Lâ€Alanine, Polyâ€Lâ€Valine, Polyâ€Î²â€Methylâ€Lâ€Aspartate, Polyâ€Î³â€Methylâ€Lâ€Glutamate, and Polyâ€Lâ€Tyrosine. Journal of Chemical Physics, 1967, 46, 4410-4426.	3.0	332
14	Principal Component Analysis for Protein Folding Dynamics. Journal of Molecular Biology, 2009, 385, 312-329.	4.2	331
15	Protein-Folding Dynamics: Overview of Molecular Simulation Techniques. Annual Review of Physical Chemistry, 2007, 58, 57-83.	10.8	329
16	Protein folding. Quarterly Reviews of Biophysics, 1977, 10, 239-352.	5.7	276
17	Phase Transitions in One Dimension and the Helixâ€"Coil Transition in Polyamino Acids. Journal of Chemical Physics, 1966, 45, 1456-1463.	3.0	270
18	Influence of local interactions on protein structure. I. Conformational energy studies ofN-acetyl-N?-methylamides of pro-X and X-pro dipeptides. Biopolymers, 1977, 16, 811-843.	2.4	262

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19	Ab initio simulations of protein-folding pathways by molecular dynamics with the united-residue model of polypeptide chains. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 2362-2367.	7.1	256
20	Conformational Analysis of Macromolecules. II. The Rotational Isomeric States of the Normal Hydrocarbons. Journal of Chemical Physics, 1966, 44, 3054-3069.	3.0	254
21	Cumulant-based expressions for the multibody terms for the correlation between local and electrostatic interactions in the united-residue force field. Journal of Chemical Physics, 2001, 115, 2323-2347.	3.0	236
22	Statistical and energetic analysis of side‐chain conformations in oligopeptides. International Journal of Peptide and Protein Research, 1983, 22, 1-15.	0.1	232
23	Non‐Newtonian Viscosity of Solutions of Ellipsoidal Particles. Journal of Chemical Physics, 1955, 23, 1526-1532.	3.0	230
24	Analysis of the Contribution of Internal Vibrations to the Statistical Weights of Equilibrium Conformations of Macromolecules. Journal of Chemical Physics, 1969, 51, 4751-4767.	3.0	229
25	Occurrence of a Phase Transition in Nucleic Acid Models. Journal of Chemical Physics, 1966, 45, 1464-1469.	3.0	217
26	Oxidative Folding of Proteins. Accounts of Chemical Research, 2000, 33, 805-812.	15.6	209
27	Conformational energy studies of β-sheets of model silk fibroin peptides. I. Sheets of poly(Ala-Gly) chains. Biopolymers, 1991, 31, 1529-1541.	2.4	194
28	Modification and Optimization of the United-Residue (UNRES) Potential Energy Function for Canonical Simulations. I. Temperature Dependence of the Effective Energy Function and Tests of the Optimization Method with Single Training Proteins. Journal of Physical Chemistry B, 2007, 111, 260-285.	2.6	184
29	On the multiple-minima problem in the conformational analysis of polypeptides. II. An electrostatically driven Monte Carlo method?tests on poly(L-alanine). Biopolymers, 1988, 27, 1283-1303.	2.4	161
30	PREFERRED CONFORMATION OF THE <i>tert</i>‐BUTOXYCARBONYLAMINO GROUP IN PEPTIDES. International Journal of Peptide and Protein Research, 1980, 16, 156-172.	0.1	158
31	Influence of water structure and of hydrophobic interactions on the strength of side-chain hydrogen bonds in proteins. Biopolymers, 1963, 1, 43-69.	2.4	155
32	Computation of the sterically allowed conformations of peptides. Biopolymers, 1966, 4, 369-407.	2.4	155
33	A comparative study of the simulated-annealing and Monte Carlo-with-minimization approaches to the minimum-energy structures of polypeptides: [Met]-enkephalin. Journal of Computational Chemistry, 1991, 12, 594-605.	3.3	152
34	Theoretical determination of sterically allowed conformations of a polypeptide chain by a computer method. Biopolymers, 1965, 3, 155-184.	2.4	149
35	Conformational Analysis of Macromolecules. V. Helical Structures of Poly‐L‐aspartic Acid and Poly‐L‐glutamic Acid, and Related Compounds. Journal of Chemical Physics, 1968, 49, 2713-2726.	3.0	149
36	Regeneration of bovine pancreatic ribonuclease A. 1. Steady-state distribution. Biochemistry, 1993, 32, 2671-2679.	2.5	149

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37	Energy Parameters in Polypeptides. VI. Conformational Energy Analysis of the N–Acetyl N'–Methyl Amides of the Twenty Naturally Occurring Amino Acids. Israel Journal of Chemistry, 1973, 11, 121-152.	2.3	145
38	Cooperative interactions in single-strand oligomers of adenylic acid. Biopolymers, 1966, 4, 223-235.	2.4	144
39	Molecular Dynamics with the United-Residue Model of Polypeptide Chains. II. Langevin and Berendsen-Bath Dynamics and Tests on Model α-Helical Systems. Journal of Physical Chemistry B, 2005, 109, 13798-13810.	2.6	144
40	Statistical mechanics of noncovalent bonds in polyamino acids. VIII. Covalent loops in proteins. Biopolymers, 1965, 3, 379-399.	2.4	140
41	Prediction of the native conformation of a polypeptide by a statistical-mechanical procedure. I. Backbone structure of enkephalin. Biopolymers, 1985, 24, 1391-1436.	2.4	137
42	Use of buildup and energy-minimization procedures to compute low-energy structures of the backbone of enkephalin. Biopolymers, 1985, 24, 1437-1447.	2.4	133
43	Relation between Free Energy Landscapes of Proteins and Dynamics. Journal of Chemical Theory and Computation, 2010, 6, 583-595.	5.3	132
44	A fast adaptive multigrid boundary element method for macromolecular electrostatic computations in a solvent. Journal of Computational Chemistry, 1997, 18, 569-583.	3.3	118
45	Deamidation of the asparaginyl–glycyl sequence. International Journal of Peptide and Protein Research, 1986, 28, 79-84.	0.1	116
46	Determination of net atomic charges using a modified partial equalization of orbital electronegativity method. 1. Application to neutral molecules as models for polypeptides. The Journal of Physical Chemistry, 1990, 94, 4732-4739.	2.9	115
47	Molecular Dynamics with the United-Residue Model of Polypeptide Chains. I. Lagrange Equations of Motion and Tests of Numerical Stability in the Microcanonical Mode. Journal of Physical Chemistry B, 2005, 109, 13785-13797.	2.6	114
48	Coupling of Conformational Folding and Disulfide-Bond Reactions in Oxidative Folding of Proteins. Biochemistry, 2001, 40, 9059-9064.	2.5	113
49	Calorimetric measurement of enthalpy change in the isothermal helix-coil transition of poly-L-lysine in aqueous solution. Biopolymers, 1971, 10, 657-680.	2.4	111
50	A New Force Field (ECEPP-05) for Peptides, Proteins, and Organic Molecules. Journal of Physical Chemistry B, 2006, 110, 5025-5044.	2.6	111
51	Proline-induced constraints in α-helices. Biopolymers, 1987, 26, 1587-1600.	2.4	110
52	Formation of local structures in protein folding. Accounts of Chemical Research, 1989, 22, 70-76.	15.6	105
53	Model for the conformational analysis of hydrated peptides. Effect of hydration on the conformational stability of the terminally blocked residues of the 20 naturally occurring amino acids. Biopolymers, 1979, 18, 1565-1610.	2.4	101
54	Role of Non-Native Aromatic and Hydrophobic Interactions in the Folding of Hen Egg White Lysozyme. Biochemistry, 1996, 35, 13797-13807.	2.5	101

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55	Regeneration of Bovine Pancreatic Ribonuclease A:â€‰ Identification of Two Nativelike Three-Disulfide Intermediates Involved in Separate Pathways. Biochemistry, 1998, 37, 3760-3766.	2.5	100
56	Folding and Unfolding Kinetics of the Proline-to-Alanine Mutants of Bovine Pancreatic Ribonuclease A. Biochemistry, 1996, 35, 1548-1559.	2.5	99
57	Prodock: Software package for protein modeling and docking. Journal of Computational Chemistry, 1999, 20, 412-427.	3.3	98
58	A Second Right-handed Helical Structure with the Parameters of the Paulingâ€"Corey α-helix. Nature, 1967, 214, 363-365.	27.8	97
59	Calculation of protein conformation by global optimization of a potential energy function. Proteins: Structure, Function and Bioinformatics, 1999, 37, 204-208.	2.6	96
60	Preferred conformation of the benzyloxycarbonylâ€‰amino group in peptides*. International Journal of Peptide and Protein Research, 1983, 21, 163-181.	0.1	96
61	Mechanism of reductive protein unfolding. Nature Structural and Molecular Biology, 1995, 2, 489-494.	8.2	95
62	Exact analytical loop closure in proteins using polynomial equations. Journal of Computational Chemistry, 1999, 20, 819-844.	3.3	94
63	Distributions of Intramolecular Distances in the Reduced and Denatured States of Bovine Pancreatic Ribonuclease A. Folding Initiation Structures in the C-Terminal Portions of the Reduced Protein. Biochemistry, 2001, 40, 105-118.	2.5	93
64	Application of Multiplexed Replica Exchange Molecular Dynamics to the UNRES Force Field: Tests with α and $\alpha+\beta$ Proteins. Journal of Chemical Theory and Computation, 2009, 5, 627-640.	5.3	93
65	Investigation of Protein Folding by Coarse-Grained Molecular Dynamics with the UNRES Force Field. Journal of Physical Chemistry A, 2010, 114, 4471-4485.	2.5	91
66	Molecular simulation study of cooperativity in hydrophobic association. Protein Science, 2000, 9, 1235-1245.	7.6	90
67	Recent progress in the theoretical treatment of protein folding. Biopolymers, 1983, 22, 1-14.	2.4	89
68	Nonrandom Distribution of the One-Disulfide Intermediates in the Regeneration of Ribonuclease Aâ€. Biochemistry, 1996, 35, 6406-6417.	2.5	88
69	Mechanism of Fiber Assembly: Treatment of Aβ Peptide Aggregation with a Coarse-Grained United-Residue Force Field. Journal of Molecular Biology, 2010, 404, 537-552.	4.2	87
70	Regeneration of Bovine Pancreatic Ribonuclease A:â€‰ Detailed Kinetic Analysis of Two Independent Folding Pathways. Biochemistry, 1998, 37, 3767-3776.	2.5	83
71	The thrombinâ€"fibrinogen interaction. Biophysical Chemistry, 2004, 112, 117-130.	2.8	83
72	Determination of net atomic charges using a modified partial equalization of orbital electronegativity method. 2. Application to ionic and aromatic molecules as models for polypeptides. The Journal of Physical Chemistry, 1990, 94, 4740-4746.	2.9	81

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73	Optical activity of single-stranded polydeoxyadenylic and polyriboadenylic acids; dependence of adenine chromophore cotton effects on polymer conformation. Biopolymers, 1969, 7, 395-409.	2.4	79
74	Conformational space annealing by parallel computations: Extensive conformational search of Met-enkephalin and of the 20-residue membrane-bound portion of melittin. International Journal of Quantum Chemistry, 1999, 75, 255-265.	2.0	77
75	Theory of Hydrophobic Interactions. Journal of Biomolecular Structure and Dynamics, 1998, 16, 447-460.	3.5	76
76	Conformational analysis of the 20-residue membrane-bound portion of melittin by conformational space annealing. , 1998, 46, 103-115.		73
77	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 3. Use of Many Proteins in Optimization. Journal of Physical Chemistry B, 2004, 108, 16950-16959.	2.6	73
78	Improved genetic algorithm for the protein folding problem by use of a Cartesian combination operator. Protein Science, 1996, 5, 1800-1815.	7.6	72
79	Conformations of poly-L-valine in solution. Biopolymers, 1968, 6, 1551-1571.	2.4	71
80	The nature of the initial step in the conformational folding of disulphide-intact ribonuclease A. Nature Structural and Molecular Biology, 1995, 2, 495-503.	8.2	69
81	Regeneration of bovine pancreatic ribonuclease A. 2. Kinetics of regeneration. Biochemistry, 1993, 32, 2680-2689.	2.5	68
82	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 2. Off-Lattice Tests of the Method with Single Proteins. Journal of Physical Chemistry B, 2004, 108, 16934-16949.	2.6	68
83	An empirical method to calculate average molecular polarizabilities from the dependence of effective atomic polarizabilities on net atomic charge. Journal of the American Chemical Society, 1993, 115, 2005-2014.	13.7	67
84	Influence of flexibility on the energy contours of dipeptide maps. Biopolymers, 1966, 4, 709-712.	2.4	66
85	Protein structure prediction using a combination of sequence homology and global energy minimization I. Global energy minimization of surface loops. Journal of Computational Chemistry, 1990, 11, 121-151.	3.3	66
86	Analysis of the Structure of Ribonuclease A in Native and Partially Denatured States by Time-Resolved Nonradiative Dynamic Excitation Energy Transfer between Site-Specific Extrinsic Probes. Biochemistry, 1995, 34, 15965-15978.	2.5	64
87	Nature of the Unfolded State of Ribonuclease A:Â Effect of Cisâˆ'Trans Xâˆ'Pro Peptide Bond Isomerizationâ€. Biochemistry, 1996, 35, 11719-11733.	2.5	64
88	Exploring the parameter space of the coarseâ€grained UNRES force field by random search: Selecting a transferable mediumâ€resolution force field. Journal of Computational Chemistry, 2009, 30, 2127-2135.	3.3	64
89	On the multiple-minima problem in the conformational analysis of polypeptides. I. Backbone degrees of freedom for a perturbed Î±-helix. Biopolymers, 1987, 26, S33-S58.	2.4	63
90	Empirical solvation models in the context of conformational energy searches: Application to bovine pancreatic trypsin inhibitor. Proteins: Structure, Function and Bioinformatics, 1992, 14, 110-119.	2.6	63

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91	Structure of a Hydrophobically Collapsed Intermediate on the Conformational Folding Pathway of Ribonuclease A Probed by Hydrogenâˆ'Deuterium Exchangeâ€. Biochemistry, 1996, 35, 11734-11746.	2.5	63
92	Calculation of Protein Conformation by the Build-up Procedure. Application to Bovine Pancreatic Trypsin Inhibitor Using Limited Simulated Nuclear Magnetic Resonance Data. Journal of Biomolecular Structure and Dynamics, 1988, 5, 705-755.	3.5	62
93	Lessons from application of the UNRES force field to predictions of structures of CASP10 targets. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 14936-14941.	7.1	62
94	Effect of hydrophobic bonding on the stability of poly-L-alanine helices in water. Biopolymers, 1963, 1, 419-429.	2.4	61
95	Regeneration of bovine pancreatic ribonuclease A. 3. Dependence on the nature of the redox reagent. Biochemistry, 1993, 32, 2690-2697.	2.5	60
96	Molecular Theory of the Helixâ€Coil Transition in Polyamino Acids. II. Numerical Evaluation of s and σ for Polyglycine and Polyâ€‹â€‹alanine in the Absence (for s and σ) and Presence (for σ) of Solvent. Journal of Chemical Physics, 1970, 52, 2060-2079.	3.0	58
97	Molecular Theory of the Helixâ€"Coil Transition in Polyamino Acids. III. Evaluation and Analysis of s and σ for Polyglycine and Polyâ€‹â€‹alanine in Water. Journal of Chemical Physics, 1971, 54, 4489-4503.	3.0	58
98	Conformational energy calculations of enzyme-substrate complexes of lysozyme. I. Energy minimization of monosaccharide and oligosaccharide inhibitors and substrates of lysozyme. Biopolymers, 1976, 15, 2485-2521.	2.4	58
99	Kinetics of the Helixâ€"Coil Transition in Polyamino Acids. Journal of Chemical Physics, 1966, 45, 2071-2090.	3.0	57
100	Helix-coil transition theory including long-range electrostatic interactions: Application to globular proteins. Biopolymers, 1987, 26, 351-371.	2.4	57
101	Conformational constraints of amino acid side chains in Î±-helices. Biopolymers, 1987, 26, 1273-1286.	2.4	56
102	Pattern recognition in the prediction of protein structure. I. Tripeptide conformational probabilities calculated from the amino acid sequence. Journal of Computational Chemistry, 1989, 10, 770-797.	3.3	56
103	Statistical mechanics of noncovalent bonds in polyamino acids. IX. The two-state theory of protein denaturation. Biopolymers, 1965, 3, 401-419.	2.4	55
104	Variable step molecular dynamics: An exploratory technique for peptides with fixed geometry. Journal of Computational Chemistry, 1990, 11, 468-486.	3.3	55
105	Statistical thermodynamics of protein folding: Comparison of a meanâ€field theory with Monte Carlo simulations. Journal of Chemical Physics, 1995, 102, 1334-1348.	3.0	55
106	Conversion from a virtual-bond chain to a complete polypeptide backbone chain. Biopolymers, 1984, 23, 1207-1224.	2.4	54
107	Regeneration of Three-Disulfide Mutants of Bovine Pancreatic Ribonuclease A Missing the 65âˆ'72 Disulfide Bond:Â Characterization of a Minor Folding Pathway of Ribonuclease A and Kinetic Roles of Cys65 and Cys72â€. Biochemistry, 1998, 37, 4490-4501.	2.5	54
108	Prediction of the native conformation of a polypeptide by a statistical-mechanical procedure. III. Probable and average conformations of enkephalin. Biopolymers, 1987, 26, 1125-1162.	2.4	53

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109	Intramolecular steric effects and hydrogen bonding in regular conformations of polyamino acids. Biopolymers, 1966, 4, 887-904.	2.4	52
110	Effect of side chains on the conformational energy and rotational strength of then-?*transition for some ?-helical poly-?-amino acids. Biopolymers, 1968, 6, 1531-1550.	2.4	52
111	Standard-geometry chains fitted to X-ray derived structures: Validation of the rigid-geometry approximation. I. Chain closure through a limited search of ?loop? conformations. Journal of Computational Chemistry, 1991, 12, 505-526.	3.3	52
112	Distribution of Disulfide Bonds in the Two-Disulfide Intermediates in the Regeneration of Bovine Pancreatic Ribonuclease A:â€‰ Further Insights into the Folding Process. Biochemistry, 1999, 38, 7284-7293.	2.5	52
113	Helixâ€"coil transitions re-visited. Biophysical Chemistry, 2002, 101-102, 255-265.	2.8	52
114	How main-chains of proteins explore the free-energy landscape in native states. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19708-19713.	7.1	52
115	Regeneration of bovine pancreatic ribonuclease A. 4. Temperature dependence of the regeneration rate. Biochemistry, 1993, 32, 2698-2703.	2.5	51
116	Stable conformations of dipeptides. Biopolymers, 1973, 12, 2177-2183.	2.4	50
117	Structural Characterization of a Three-Disulfide Intermediate of Ribonuclease a Involved in both the Folding and Unfolding Pathways. Biochemistry, 1994, 33, 10437-10449.	2.5	50
118	Macromolecular conformational dynamics in torsional angle space. Journal of Chemical Physics, 1998, 108, 271-286.	3.0	50
119	Variable-Target-Function and Build-up Procedures for the Calculation of Protein Conformation. Application to Bovine Pancreatic Trypsin Inhibitor Using Limited Simulated Nuclear Magnetic Resonance Data. Journal of Biomolecular Structure and Dynamics, 1988, 5, 757-784.	3.5	49
120	Circular Dichroism Evidence for the Presence of Burst-Phase Intermediates on the Conformational Folding Pathway of Ribonuclease Aâ€. Biochemistry, 1996, 35, 10125-10133.	2.5	49
121	An efficient, differentiable hydration potential for peptides and proteins. Journal of Computational Chemistry, 1996, 17, 1549-1558.	3.3	49
122	New developments of the electrostatically driven monte carlo method: Test on the membrane-bound portion of melittin. , 1998, 46, 117-126.		49
123	Effect of side-chain hydrophobic bonding on the stability of homopolyamino acid ?-helices: Conformational studies of poly-L-leucine in water. Biopolymers, 1970, 9, 749-764.	2.4	48
124	The effect of theL-azetidine-2-carboxylic acid residue on protein conformation. I. Conformations of the residue and of dipeptides. Biopolymers, 1990, 30, 951-959.	2.4	48
125	How Adequate are One- and Two-Dimensional Free Energy Landscapes for Protein Folding Dynamics?. Physical Review Letters, 2009, 102, 238102.	7.8	48
126	Influence of interatomic interactions on the structure and stability of polypeptides and proteins. Biopolymers, 1981, 20, 1877-1899.	2.4	46

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127	Diffusion Equation and Distance Scaling Methods of Global Optimization:Â Applications to Crystal Structure Prediction. Journal of Physical Chemistry A, 1998, 102, 2904-2918.	2.5	46
128	Kinetic Folding Pathway of a Three-Disulfide Mutant of Bovine Pancreatic Ribonuclease A Missing the [40â˜95] Disulfide Bondâ€. Biochemistry, 1998, 37, 7561-7571.	2.5	46
129	Molecular Dynamics with the United-Residue Force Field:Â Ab Initio Folding Simulations of Multichain Proteins. Journal of Physical Chemistry B, 2007, 111, 293-309.	2.6	46
130	Two new structured intermediates in the oxidative folding of RNase A. FEBS Letters, 1999, 460, 477-479.	2.8	45
131	Prediction of the native conformation of a polypeptide by a statistical-mechanical procedure. II. average backbone structure of enkephalin. Biopolymers, 1986, 25, 1547-1563.	2.4	44
132	Optimizing Potential Functions for Protein Folding. The Journal of Physical Chemistry, 1996, 100, 14540-14548.	2.9	44
133	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	4.1	44
134	Matrix formulation of the transition from a statistical coil to an intramolecular antiparallel Î² sheet. Biopolymers, 1984, 23, 1701-1724.	2.4	43
135	Kinetic and Thermodynamic Studies of the Folding/Unfolding of a Tryptophan-Containing Mutant of Ribonuclease Aâ€. Biochemistry, 1996, 35, 12978-12992.	2.5	43
136	THE EFFECT OF SOLUTES ON THE STRUCTURE OF WATER AND ITS IMPLICATIONS FOR PROTEIN STRUCTURE*. Annals of the New York Academy of Sciences, 2006, 125, 253-276.	3.8	43
137	Influence of local interactions on protein structure. II. Conformational energy studies ofN-acetyl-N?-methylamides of Ala-X and X-Ala dipeptides. Biopolymers, 1978, 17, 1849-1869.	2.4	42
138	Effect of sequence-specific interactions on the stability of helical conformations in polypeptides. Biopolymers, 1988, 27, 41-58.	2.4	42
139	Anti-cooperative interactions in single-strand oligomers of deoxyriboadenylic acid. Biopolymers, 1967, 5, 403-422.	2.4	41
140	Acceleration of convergence in Monte Carlo simulations of aqueous solutions using the metropolis algorithm. Hydrophobic hydration of methane. Journal of Computational Chemistry, 1982, 3, 525-547.	3.3	41
141	Pattern recognition in the prediction of protein structure. II. Chain conformation from a probability-directed search procedure. Journal of Computational Chemistry, 1989, 10, 798-816.	3.3	40
142	Brownian dynamics simulations of protein folding. Journal of Chemical Physics, 1998, 108, 287-300.	3.0	40
143	Crystal structures of two mutants that have implications for the folding of bovine pancreatic ribonuclease A. Protein Science, 1998, 7, 1255-1258.	7.6	39
144	Predicting 13CÎ± chemical shifts for validation of protein structures. Journal of Biomolecular NMR, 2007, 38, 221-235.	2.8	39

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145	DNA Duplex Formation with a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2014, 10, 5020-5035.	5.3	39
146	Physics-Based Potentials for the Coupling between Backbone- and Side-Chain-Local Conformational States in the United Residue (UNRES) Force Field for Protein Simulations. Journal of Chemical Theory and Computation, 2015, 11, 817-831.	5.3	39
147	Comparison of Theories of the Helix–Coil Transition in Polypeptides. Journal of Chemical Physics, 1965, 43, 2071-2074.	3.0	38
148	HELIX-RANDOM COIL TRANSFORMATIONS IN DEUTERATED MACROMOLECULES*. Annals of the New York Academy of Sciences, 2006, 84, 608-616.	3.8	38
149	Maximum Likelihood Calibration of the UNRES Force Field for Simulation of Protein Structure and Dynamics. Journal of Chemical Information and Modeling, 2017, 57, 2364-2377.	5.4	38
150	Influence of local interactions on protein structure. III. Conformational energy studies ofN-acety-N?-methylamides of Gly-X and X-Gly dipeptides. Biopolymers, 1978, 17, 1871-1884.	2.4	37
151	Ion Pair Interactions in Aqueous Solution: Self-Consistent Reaction Field (SCRF) Calculations with Some Explicit Water Molecules. Journal of Physical Chemistry A, 2000, 104, 6505-6509.	2.5	37
152	CONFORMATIONALSTUDY OF [LEU⁵]–ENKEPHALIN BY LASER RAMAN SPECTROSCOPY. International Journal of Peptide and Protein Research, 1980, 16, 173-182.	0.1	37
153	Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets. International Journal of Quantum Chemistry, 2000, 77, 90-117.	2.0	36
154	Can cooperativity in hydrophobic association be reproduced correctly by implicit solvation models?. International Journal of Quantum Chemistry, 2002, 88, 41-55.	2.0	36
155	CONFORMATIONAL ENERGY CALCULATIONS OF ENZYME–SUBSTRATE INTERACTIONS. II. Computation of the Binding Energy for Substrates in the Active Site of α–Chymotrypsin. International Journal of Peptide and Protein Research, 1972, 4, 201-219.	0.1	36
156	Folding kinetics of WW domains with the united residue force field for bridging microscopic motions and experimental measurements. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 18243-18248.	7.1	36
157	Pattern recognition in the prediction of protein structure. III. An importance-sampling minimization procedure. Journal of Computational Chemistry, 1989, 10, 817-831.	3.3	35
158	Conformational Unfolding Studies of Three-Disulfide Mutants of Bovine Pancreatic Ribonuclease A and the Coupling of Proline Isomerization to Disulfide Redox Reactions. Biochemistry, 1999, 38, 2805-2815.	2.5	34
159	Spatial geometric arrangements of disulfide-crosslinked loops in proteins. Journal of Computational Chemistry, 1986, 7, 67-88.	3.3	33
160	On the multiple-minima problem in the conformational analysis of polypeptides. V. Application of the self-consistent electrostatic field and the electrostatically driven monte carlo methods to bovine pancreatic trypsin inhibitor. Proteins: Structure, Function and Bioinformatics, 1991, 10, 188-198.	2.6	33
161	Lysosomal enzyme tripeptidyl peptidase 1 destabilizes fibrillar Aβ by multiple endoproteolytic cleavages within the β-sheet domain. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1493-1498.	7.1	33
162	Monte Carlo simulation of the hard–sphere fluid with quantum correction and estimate of its free energy. Journal of Chemical Physics, 1988, 88, 3923-3933.	3.0	32

#	Article	IF	Citations
163	Molecular modeling of the binding modes of the iron-sulfur protein to the Jac1 co-chaperone from <i>S</i> <i>accharomyces cerevisiae</i> by all-atom and coarse-grained approaches. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1414-1426.	2.6	32
164	Elucidating Important Sites and the Mechanism for Amyloid Fibril Formation by Coarse-Grained Molecular Dynamics. ACS Chemical Neuroscience, 2017, 8, 201-209.	3.5	32
165	Statistical mechanics of noncovalent bonds in polyamino acids. I. Hydrogen bonding of solutes in water, and the binding of water to polypeptides. Biopolymers, 1965, 3, 275-282.	2.4	31
166	Theory of Two-State Cooperative Folding of Proteins. Accounts of Chemical Research, 1998, 31, 433-440.	15.6	31
167	Exact solutions for chemical bond orientations from residual dipolar couplings. Journal of Biomolecular NMR, 2002, 22, 137-151.	2.8	31
168	Dissimilarity in the Reductive Unfolding Pathways of Two Ribonuclease Homologues. Journal of Molecular Biology, 2004, 338, 795-809.	4.2	31
169	Statistical mechanics of noncovalent bonds in polyamino acids. II. Combinatorial formulation for short chains, including hydrophobic bonding in random coil. Biopolymers, 1965, 3, 283-304.	2.4	30
170	Neighbor-neighbor interactions in single-strand polynucleotides: Optical rotatory dispersion studies of the ribonucleotide ApApCp. Biopolymers, 1966, 4, 33-41.	2.4	30
171	Resolution enhancement in spectroscopy by maximum entropy fourier self-deconvolution, with applications to Raman spectra of peptides and proteins. Journal of Raman Spectroscopy, 1985, 16, 337-349.	2.5	30
172	A Simple Functional Representation of Angular-Dependent Hydrogen-Bonded Systems. 1. Amide, Carboxylic Acid, and Amide-Carboxylic Acid Pairs. The Journal of Physical Chemistry, 1995, 99, 3478-3486.	2.9	30
173	Solution conformations of oligomers of Î± â€aminoisobutyric acidÂ°. International Journal of Peptide and Protein Research, 1982, 20, 468-480.	0.1	30
174	Improvement of the Treatment of Loop Structures in the UNRES Force Field by Inclusion of Coupling between Backbone- and Side-Chain-Local Conformational States. Journal of Chemical Theory and Computation, 2013, 9, 4620-4632.	5.3	30
175	Influence of hydration on the conformational stability and formation of bends in terminally blocked dipeptides. Biopolymers, 1979, 18, 1611-1634.	2.4	29
176	Determination of net atomic charges using a modified partial equalization of orbital electronegativity method. III. Application to halogenated and aromatic molecules. Journal of Computational Chemistry, 1993, 14, 1482-1490.	3.3	29
177	Kinetic Studies of the Regeneration of Recombinant Hirudin Variant 1 with Oxidized and Reduced Dithiothreitolâ€. Biochemistry, 1997, 36, 2154-2165.	2.5	29
178	Anomalous diffusion and dynamical correlation between the side chains and the main chain of proteins in their native state. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10346-10351.	7.1	29
179	Molecular theory of the helix-coil transition in polyamino acids. V. Explanation of the different conformational behavior of valine, isoleucine, and leucine in aqueous solution. Biopolymers, 1984, 23, 1961-1977.	2.4	28
180	Chemical Basis of Thrombin Interactions with Fibrinogen. Annals of the New York Academy of Sciences, 1986, 485, 124-133.	3.8	28

#	Article	IF	Citations
181	Some approaches to the multiple-minima problem in the calculation of polypeptide and protein structures. International Journal of Quantum Chemistry, 1992, 42, 1529-1536.	2.0	28
182	Standard-geometry chains fitted to X-ray derived structures: Validation of the rigid-geometry approximation. II. Systematic searches for short loops in proteins: Applications to bovine pancreatic ribonuclease A and human lysozyme. Journal of Computational Chemistry, 1992, 13, 329-350.	3.3	28
183	Influence of lysine content and PH on the stability of alanine-based copolypeptides. Biopolymers, 2001, 58, 235-246.	2.4	28
184	Nonexponential decay of internal rotational correlation functions of native proteins and self-similar structural fluctuations. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 19844-19849.	7.1	28
185	The Role of the Insertion Loop around Tryptophan 148 in the Activity of Thrombinâ€,â€¡. Biochemistry, 1996, 35, 4427-4433.	2.5	27
186	Predicting Three-Dimensional Structures of Oligopeptides. Reviews in Computational Chemistry, 2007, , 73-142.	1.5	27
187	The Lifson-Allegra theories of the helix-coil transition for random copolymers: Comparison with exact results and extension. Biopolymers, 1969, 7, 887-908.	2.4	26
188	Theoretical studies of protein conformation by means of energy computations. FASEB Journal, 1990, 4, 3189-3197.	0.5	26
189	A Localized Specific Interaction Alters the Unfolding Pathways of Structural Homologues. Journal of the American Chemical Society, 2006, 128, 1204-1213.	13.7	26
190	Determination of Nonbonded Potential Parameters for Peptides. The Journal of Physical Chemistry, 1995, 99, 13019-13027.	2.9	25
191	Prediction of protein structure using a knowledge-based off-lattice united-residue force field and global optimization methods. Theoretical Chemistry Accounts, 1999, 101, 16-20.	1.4	25
192	THROMBIN AND ITS INTERACTION WITH FIBRINOGEN*. Annals of the New York Academy of Sciences, 2006, 75, 189-194.	3.8	25
193	Optimization of a Nucleic Acids united-RESidue 2-Point model (NARES-2P) with a maximum-likelihood approach. Journal of Chemical Physics, 2015, 143, 243111.	3.0	25
194	Derivation of a New Force Field for Crystal-Structure Prediction Using Global Optimization:Â Nonbonded Potential Parameters for Hydrocarbons and Alcohols. Journal of Physical Chemistry B, 2003, 107, 7143-7154.	2.6	24
195	Sequence-, structure-, and dynamics-based comparisons of structurally homologous CheY-like proteins. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1578-1583.	7.1	24
196	Bromination of Hydrocarbons. VI. Photochemical and Thermal Bromination of Toluene. Bond Dissociation Energies. Journal of Chemical Physics, 1953, 21, 1258-1267.	3.0	23
197	Chemicalâ€Shift Data for Water and Aqueous Solutions. Journal of Chemical Physics, 1966, 45, 3296-3298.	3.0	23
198	Influence of local interactions on protein structure. IV. Conformational energy studies ofN-acetyl-N?-mehylamides of Ser-X- and X-Ser dipeptides. Biopolymers, 1978, 17, 1885-1890.	2.4	23

#	Article	IF	Citations
199	Conformational preferences of amino acid side chains in collagen. Biopolymers, 1982, 21, 1535-1555.	2.4	23
200	Stability of polypeptide conformational states. II. Folding of a polypeptide chain by the scanning simulation method, and calculation of the free energy of the statistical coil. Biopolymers, 1988, 27, 1189-1204.	2.4	23
201	B-spline method for energy minimization in grid-based molecular mechanics calculations. Journal of Computational Chemistry, 1998, 19, 71-85.	3.3	23
202	Flexible docking simulations: Scaled collective variable Monte Carlo minimization approach using Bezier splines, and comparison with a standard Monte Carlo algorithm. Journal of Computational Chemistry, 1999, 20, 244-252.	3.3	23
203	<i>Che</i>Shift-2: graphic validation of protein structures. Bioinformatics, 2012, 28, 1538-1539.	4.1	23
204	Alternative approach to protein structure prediction based on sequential similarity of physical properties. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5029-5032.	7.1	23
205	Calculation of protein conformation by global optimization of a potential energy function. Proteins: Structure, Function and Bioinformatics, 1999, 37, 204-208.	2.6	23
206	Energetics of multihelix interactions in protein folding: Application to myoglobin. Biopolymers, 1985, 24, 1271-1291.	2.4	22
207	Energetics of the structure and chain tilting of antiparallel β-barrels in proteins. Proteins: Structure, Function and Bioinformatics, 1990, 8, 14-22.	2.6	22
208	The effect of theL-azetidine-2-carboxylic acid residue on protein conformation. III. Collagen-like poly(tripeptide)s. Biopolymers, 1990, 30, 967-974.	2.4	22
209	The effect of theL-azetidine-2-carboxylic acid residue on protein conformation. IV. Local substitutions in the collagen triple helix. Biopolymers, 1994, 34, 51-60.	2.4	22
210	Folding of a Disulfide-Bonded Protein Species with Free Thiol(s):Â Competition between Conformational Folding and Disulfide Reshuffling in an Intermediate of Bovine Pancreatic Ribonuclease Aâ€. Biochemistry, 2001, 40, 15002-15008.	2.5	22
211	Evolution of physics-based methodology for exploring the conformational energy landscape of proteins. Journal of Computational Chemistry, 2002, 23, 28-34.	3.3	22
212	CONFORMATIONAL ENERGY CALCULATIONS OF ENZYMEâ€SUBSTRATE INTERACTIONS. I. Computation of Preferred Conformations of Some Substrates of Î±â€Chymotrypsin. International Journal of Peptide and Protein Research, 1972, 4, 187-200.	0.1	22
213	From a Highly Disordered to a Metastable State: Uncovering Insights of Î±-Synuclein. ACS Chemical Neuroscience, 2018, 9, 1051-1065.	3.5	22
214	Dependence of the Formation of Tau and AÎ² Peptide Mixed Aggregates on the Secondary Structure of the N-Terminal Region of AÎ². Journal of Physical Chemistry B, 2018, 122, 7049-7056.	2.6	22
215	Characterization of foldable protein models: Thermodynamics, folding kinetics and force field. Journal of Chemical Physics, 1997, 107, 8089-8102.	3.0	21
216	New general approach for determining the solution structure of a ligand bound weakly to a receptor: structure of a fibrinogen A?-like peptide bound to thrombin(S195A) obtained using NOE distance constraints and an ECEPP/3 flexible docking program. , 1999, 34, 29-48.		21

#	Article	IF	Citations
217	Role of proline â€¦ï•proline interactions in the packing of collagenlike poly(tripeptide) triple helices. Biopolymers, 1984, 23, 2781-2799.	2.4	20
218	The Electrostatically Driven Monte Carlo method: Application to conformational analysis of decaglycine. Biopolymers, 1991, 31, 319-330.	2.4	20
219	Extension of UNRES Force Field to Treat Polypeptide Chains with <scp>d</scp>-Amino Acid Residues. Journal of Chemical Theory and Computation, 2012, 8, 4746-4757.	5.3	20
220	Coexistence of Phases in a Protein Heterodimer. Journal of Chemical Physics, 2012, 137, 035101.	3.0	20
221	New Insights into Protein (Un)Folding Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 1082-1086.	4.6	20
222	Statistical mechanics of noncovalent bonds in polyamino acids. IV. Matrix treatment of hydrophobic bonds in the random coil and of the helix-coil transition for chains of arbitrary length. Biopolymers, 1965, 3, 315-334.	2.4	19
223	Conformational analysis of macromolecules. I. Ethane, propane,n-butane, andn-pentane. Biopolymers, 1966, 4, 237-238.	2.4	19
224	Determination of net atomic charges using a modified partial equalization of orbital electronegativity method. IV. Application to hypervalent sulfur- and phosphorus-containing molecules. Journal of Computational Chemistry, 1995, 16, 1011-1026.	3.3	19
225	Comment on â€œAnti-cooperativity in hydrophobic interactions: A simulation study of spatial dependence of three-body effects and beyondâ€•[J. Chem. Phys. 115, 1414 (2001)]. Journal of Chemical Physics, 2002, 116, 2665-2667.	3.0	19
226	Derivation of a New Force Field for Crystal-Structure Prediction Using Global Optimization:â€‰ Nonbonded Potential Parameters for Amines, Imidazoles, Amides, and Carboxylic Acids. Journal of Physical Chemistry B, 2004, 108, 12181-12196.	2.6	19
227	Accounting for a mirror-image conformation as a subtle effect in protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 8458-8463.	7.1	19
228	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino Acid Side Chains in Water. VII. Chargedâ€“Hydrophobic/Polar and Polarâ€“Hydrophobic/Polar Side Chains. Journal of Physical Chemistry B, 2017, 121, 379-390.	2.6	19
229	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939.	3.3	19
230	Statistical mechanics of noncovalent bonds in polyamino acids. III. Interhelical hydrophobic bonds in short chains. Biopolymers, 1965, 3, 305-313.	2.4	18
231	Comparison of two approaches to potential of mean force calculations of hydrophobic association: particle insertion and weighted histogram analysis methods. Molecular Physics, 2005, 103, 3153-3167.	1.7	18
232	Local vs Global Motions in Protein Folding. Journal of Chemical Theory and Computation, 2013, 9, 2907-2921.	5.3	18
233	Kinks, loops, and protein folding, with protein A as an example. Journal of Chemical Physics, 2014, 140, 025101.	3.0	18
234	Statistical mechanics of noncovalent bonds in polyamino acids. V. Treatment of long chains by the method of sequence-generating functions: Hydrophobic bonding in random coil, and interactions between helical segments. Biopolymers, 1965, 3, 335-355.	2.4	17

#	Article	IF	Citations
235	Computer simulation of the entropy of continuum chain models: The twoâ€dimensional freely jointed chain of hard disks. Journal of Chemical Physics, 1986, 84, 6369-6375.	3.0	17
236	Correlation of β-bend conformations of tetrapeptides with their activities in CD4â€receptor binding assays. International Journal of Peptide and Protein Research, 1989, 34, 325-332.	0.1	17
237	Effects of Mutation, Truncation, and Temperature on the Folding Kinetics of a WW Domain. Journal of Molecular Biology, 2012, 420, 350-365.	4.2	17
238	Homolog detection using global sequence properties suggests an alternate view of structural encoding in protein sequences. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5225-5229.	7.1	17
239	Preventing fibril formation of a protein by selective mutation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13549-13554.	7.1	17
240	Role of interstrand loops in the formation of intramolecular cross-β-sheets by homopolymino acids. Biopolymers, 1985, 24, 565-579.	2.4	16
241	Revised Backbone-Virtual-Bond-Angle Potentials to Treat the <scp>l</scp>- and <scp>d</scp>-Amino Acid Residues in the Coarse-Grained United Residue (UNRES) Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2194-2203.	5.3	16
242	A new protein nucleicâ€acid coarseâ€grained force field based on the UNRES and NARESâ€2P force fields. Journal of Computational Chemistry, 2018, 39, 2360-2370.	3.3	16
243	Free energy of hydration of collagen models and the enthalpy of the transition between the triple-helical coiled-coil and single-stranded conformations. Biopolymers, 1989, 28, 1573-1584.	2.4	15
244	Regeneration Studies of an Analog of Ribonuclease A Missing Disulfide Bonds 65â~72 and 40â~95. Biochemistry, 1997, 36, 13068-13076.	2.5	15
245	An Unusual Adduct of Dithiothreitol with a Pair of Cysteine Residues of a Protein as a Stable Folding Intermediate. Journal of the American Chemical Society, 1998, 120, 2668-2669.	13.7	15
246	Comparison of Local and Global Stability of an Analogue of a Disulfide-Folding Intermediate with Those of the Wild-Type Protein in Bovine Pancreatic Ribonuclease A: Identification of Specific Regions of Stable Structure along the Oxidative Folding Pathwayâ€. Biochemistry, 1999, 38, 16432-16442.	2.5	15
247	Effect of Mutation of Proline 93 on Redox Unfolding/Folding of Bovine Pancreatic Ribonuclease A. Biochemistry, 2001, 40, 8536-8541.	2.5	15
248	Dynamics of Disulfide-Bond Disruption and Formation in the Thermal Unfolding of Ribonuclease A. Journal of Chemical Theory and Computation, 2017, 13, 5721-5730.	5.3	15
249	Visualization of the nature of protein folding by a study of a distance constraint approach in two-dimensional models. Biopolymers, 1982, 21, 611-632.	2.4	14
250	β-Bend conformation of CH3CO-Pro-Pro-Gly-Pro-NHCH3: Implications for posttranslational proline hydroxylation in collagen. Biopolymers, 1984, 23, 1193-1206.	2.4	14
251	Determination of Potential Parameters for Amino Acid Zwitterions. The Journal of Physical Chemistry, 1996, 100, 17670-17677.	2.9	14
252	Computational study of packing a collagen-like molecule: Quasi-hexagonal vs â€œSmithâ€collagen microfibril model. , 1996, 40, 595-607.		14

#	Article	IF	Citations
253	Formation of the Hydrophobic Core of Ribonuclease A through Sequential Coordinated Conformational Transitionsâ€. Biochemistry, 2002, 41, 14225-14231.	2.5	14
254	Effect of a Gaussian Distribution on Flow Birefringence. Journal of Chemical Physics, 1951, 19, 983-984.	3.0	13
255	Contribution of physical chemistry to an understanding of protein structure and function. Protein Science, 1992, 1, 691-693.	7.6	13
256	A rapid and efficient algorithm for packing polypeptide chains by energy minimization. Journal of Computational Chemistry, 1994, 15, 1403-1413.	3.3	13
257	Analyzing the normal mode dynamics of macromolecules by the component synthesis method: Residue clustering and multiple-component approach. Biopolymers, 1994, 34, 321-335.	2.4	13
258	Amino Acid Residues at Proteinâˆ'Protein Interfaces:Â Why Is Propensity so Different from Relative Abundance?. Journal of Physical Chemistry B, 2003, 107, 9929-9932.	2.6	13
259	From helixâ€"coil transitions to protein folding. Biopolymers, 2008, 89, 479-485.	2.4	13
260	Calorimetric measurement of enthalpy change in the isothermal helix-coil transition of poly(L-ornithine) in aqueous solution. Biopolymers, 1976, 15, 1795-1813.	2.4	12
261	Free energy and stability of macromolecules studied by the double scanning simulation procedure. Journal of Chemical Physics, 1990, 92, 1248-1257.	3.0	12
262	Formation of native structure by intermolecular thiol-disulfide exchange reactions without oxidants in the folding of bovine pancreatic ribonuclease A. FEBS Letters, 2000, 471, 177-181.	2.8	12
263	Acceleration of oxidative folding of bovine pancreatic ribonuclease A by anion-induced stabilization and formation of structured native-like intermediates. FEBS Letters, 2000, 472, 67-72.	2.8	12
264	SEARCH FOR LOWâ€ENERGY CONFORMATIONS OF A NEUROTOXIC PROTEIN BY MEANS OF PREDICTIVE RULES, TESTS FOR HARDâ€SPHERE OVERLAPS, AND ENERGY MINIMIZATION*. International Journal of Peptide and Protein Research, 1976, 8, 237-252.	0.1	11
265	CONFORMATIONAL STUDIES OF SOMATOSTATIN AND SELECTED ANALOGUES BY RAMAN SPECTROSCOPY. International Journal of Peptide and Protein Research, 1980, 15, 355-364.	0.1	11
266	Investigation of Phosphorylation-Induced Folding of an Intrinsically Disordered Protein by Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 3203-3220.	5.3	11
267	Spatial geometric arrangements of disulfide-crosslinked loops in nonplanar proteins. Journal of Computational Chemistry, 1989, 10, 287-294.	3.3	10
268	Computation of the Structure-Dependent pKaShifts in a Polypentapeptide of the Poly[fv(IPGVG),fE(IPGEG)] Family. Journal of Physical Chemistry B, 1998, 102, 3065-3067.	2.6	10
269	Effect of protein disulfide isomerase on the regeneration of bovine ribonuclease A with dithiothreitol. FEBS Letters, 1999, 456, 143-145.	2.8	10
270	Solution NMR evidence for a cis Tyrâ€Ala peptide group in the structure of [Pro93Ala] bovine pancreatic ribonuclease A. Protein Science, 2000, 9, 421-426.	7.6	10

#	Article	IF	Citations
271	Conformational energy analysis of melanostatin. International Journal of Peptide and Protein Research, 1982, 19, 143-152.	0.1	10
272	Molecular dynamics of protein A and a WW domain with a united-residue model including hydrodynamic interaction. Journal of Chemical Physics, 2016, 144, 184110.	3.0	10
273	The structure of protein dynamic space. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 19938-19942.	7.1	10
274	Monte Carlo recursion study of cluster formation from vapor. Journal of Chemical Physics, 1990, 92, 5499-5505.	3.0	9
275	Monte Carlo simulation of the hardâ€sphere fluid with a highâ€temperature quantum correction in the region of the fluidâ€"solid phase transition. Journal of Chemical Physics, 1992, 96, 7005-7009.	3.0	9
276	A generalized G-SFED continuum solvation free energy calculation model. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E662-7.	7.1	9
277	My 65 years in protein chemistry. Quarterly Reviews of Biophysics, 2015, 48, 117-177.	5.7	9
278	Coupled molecular dynamics and continuum electrostatic method to compute the ionization pKaâ€™s of proteins as a function of pH. Test on a large set of proteins. Journal of Biomolecular Structure and Dynamics, 2018, 36, 561-574.	3.5	9
279	Curvature and Torsion of Protein Main Chain as Local Order Parameters of Protein Unfolding. Journal of Physical Chemistry B, 2020, 124, 4391-4398.	2.6	9
280	Role of Hydrophobic Bonding in Protein Structure. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1964, 68, 838-839.	0.9	8
281	Suppression of the statistical coil state during the ? ? ? transition in homopolypeptides. Biopolymers, 1984, 23, 2879-2890.	2.4	8
282	Correlation between computed conformational properties of cytochromec peptides and their antigenicity in a T-lymphocyte proliferation assay. Biopolymers, 1987, 26, 373-386.	2.4	8
283	Dynamics of peptides with fixed geometry: Kinetic energy terms and potential energy derivatives as functions of dihedral angles. Journal of Computational Chemistry, 1990, 11, 487-492.	3.3	8
284	An algorithm for packing regular multistrand polypeptide structures by energy minimization. Journal of Computational Chemistry, 1994, 15, 1414-1428.	3.3	8
285	Reply to â€œComment on â€˜Crystal Structure Prediction by Global Optimization as a Tool for Evaluating Potentials:Â Role of the Dipole Moment Correction Term in Successful Predictions'â€•by B. P. van Eijck and J. Kroon. Journal of Physical Chemistry B, 2000, 104, 8090-8092.	2.6	8
286	SPECTROSCOPIC STUDY OF THE CONFORMATIONS OF PROLINEâ€CONTAINING OLIGOPEPTIDES IN THE CRYSTALLINE STATE AND IN SOLUTION. International Journal of Peptide and Protein Research, 1981, 17, 297-315.	0.1	8
287	Respice, Adspice, and Prospice. Annual Review of Biophysics, 2011, 40, 1-39.	10.0	8
288	Global informatics and physical property selection in protein sequences. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1808-1810.	7.1	8

#	Article	IF	Citations
289	Entropy Sampling Monte Carlo for Polypeptides and Proteins. Advances in Chemical Physics, 0, , 243-272.	0.3	8
290	Statistical mechanics of noncovalent bonds in polyamino acids. VII. Fluorescence as an indication of conformation. Biopolymers, 1965, 3, 369-377.	2.4	7
291	An assessment of the accuracy of the RRIGS hydration potential: Comparison to solutions of the Poisson-Boltzmann equation. Journal of Computational Chemistry, 1997, 18, 1072-1078.	3.3	7
292	Use of sequence-specific tri-block copolymers to determine the helix-forming tendencies of amino acids. Biopolymers, 1998, 39, 531-536.	2.4	7
293	PMFF: Development of a Physics-Based Molecular Force Field for Protein Simulation and Ligand Docking. Journal of Physical Chemistry B, 2020, 124, 974-989.	2.6	7
294	Contractility and Conformation. Journal of General Physiology, 1967, 50, 5-27.	1.9	6
295	Low-energy conformations of two lysine-containing tetrapeptides of collagen: Implications for posttranslational lysine hydroxylation. Biopolymers, 1987, 26, 1781-1788.	2.4	6
296	Vibrational quantum correction for the Lennard–Jones fluid: A formalism of effective intermolecular potentials depending on mass and temperature. Journal of Chemical Physics, 1990, 92, 3748-3755.	3.0	6
297	Simple global minimization algorithm for one-variable rational functions. Journal of Global Optimization, 1995, 6, 293-311.	1.8	6
298	Characterization of Multiple Reduction Pathways of Proteins in the Presence of a Denaturant. Journal of the American Chemical Society, 1998, 120, 5806-5807.	13.7	6
299	Conformations of the central transforming region (Ile 55–Met 67) of the p21 protein and their relationship to activation of the protein. International Journal of Peptide and Protein Research, 1990, 36, 247-254.	0.1	6
300	Limiting values of the one-bond C H spin-spin coupling constants of the imidazole ring of histidine at high-pH. Journal of Molecular Structure, 2017, 1134, 576-581.	3.6	6
301	Statistical Model To Decipher Protein Folding/Unfolding at a Local Scale. Journal of Physical Chemistry B, 2018, 122, 3540-3549.	2.6	6
302	Detection of methylation, acetylation and glycosylation of protein residues by monitoring ^{13}C chemical-shift changes: A quantum-chemical study. PeerJ, 2016, 4, e2253.	2.0	6
303	Statistical mechanics of noncovalent bonds in polyamino acids. VI. A simple model for side-chain hydrogen bonds between helices. Biopolymers, 1965, 3, 357-367.	2.4	5
304	Thrombin specificity: further evidence for the importance of the beta-insertion loop and Trp96. Implications of the hydrophobic interaction between Trp96 and Pro60B Pro60C for the activity of thrombin. The Protein Journal, 1998, 17, 197-208.	1.1	5
305	Eliminating a Protein Folding Intermediate by Tuning a Local Hydrophobic Contact. Journal of Physical Chemistry B, 2017, 121, 3276-3284.	2.6	5
306	Helix sense of poly-Î³-p-chlorobenzylL-glutamate. Biopolymers, 1969, 7, 805-808.	2.4	4

#	Article	IF	Citations
307	Treatment of Hydration in Conformational Energy Calculations on Polypeptides and Proteins. ACS Symposium Series, 1994, , 360-370.	0.5	4
308	State of aggregation of recombinant hirudin in solution under physiological conditions. The Protein Journal, 1996, 15, 751-753.	1.1	4
309	From secondary structure to three-dimensional structure: Improved dihedral angle probability distribution function for use with energy searches for native structures of polypeptides and proteins. Journal of Computational Chemistry, 1996, 17, 1453-1480.	3.3	4
310	Theoretical Studies of Interactions between O-Phosphorylated and Standard Amino-Acid Side-Chain Models in Water. Journal of Physical Chemistry B, 2015, 119, 8526-8534.	2.6	4
311	New Insights into Folding, Misfolding, and Nonfolding Dynamics of a WW Domain. Journal of Physical Chemistry B, 2020, 124, 3855-3872.	2.6	4
312	Comparison of intramolecular and intermolecular reactions in protein folding. The Protein Journal, 1986, 5, 29-49.	1.1	3
313	Towards Temperature Dependent Coarse-grained Potential of Side-chain Interactions for Protein Folding Simulations. , 2010, , .		3
314	Assessing the One-Bond C_α–H Spin–Spin Coupling Constants in Proteins: Pros and Cons of Different Approaches. Journal of Physical Chemistry B, 2020, 124, 735-741.	2.6	3
315	Conformational Analysis of Polypeptides and Proteins for the Study of Protein Folding, Molecular Recognition, and Molecular Design. Israel Journal of Chemistry, 1986, 27, 144-155.	2.3	2
316	Effects on protein structure and function of replacing tryptophan with 5-hydroxytryptophan: Single-tryptophan mutants of the N-terminal domain of the bacteriophage λ repressor. The Protein Journal, 1996, 15, 77-86.	1.1	2
317	Are accurate computations of the $^{13}C_\beta$ shielding feasible at the DFT level of theory?. Journal of Computational Chemistry, 2014, 35, 309-312.	3.3	2
318	A comprehensive analysis of the computed tautomer fractions of the imidazole ring of histidines in *Loligo vulgaris*. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3094-3105.	3.5	2
319	Influence of lysine content and PH on the stability of alanine‐based copolypeptides. Biopolymers, 2001, 58, 235-246.	2.4	2
320	Phase transitions in synthetic polymers of amino acids, and their relation to protein folding. Ferroelectrics, 1980, 30, 157-158.	0.6	1
321	The Multiple-Minima Problem in Protein Folding. AIP Conference Proceedings, 1991, , .	0.4	1
322	Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets. International Journal of Quantum Chemistry, 2000, 77, 90.	2.0	1
323	Outline of an experimental design aimed to detect protein A mirror image in solution. , 2019, 1, e2.		1
324	Probing Protein Aggregation Using the Coarse-Grained UNRES Force Field. Methods in Molecular Biology, 2022, 2340, 79-104.	0.9	1

#	Article	IF	Citations
325	Monte Carlo studies of oligopeptide conformation. Ferroelectrics, 1980, 30, 159-159.	0.6	0
326	Experimental and Theoretical Protein Folding. Journal of Biomolecular Structure and Dynamics, 1989, 6, 1039-1043.	3.5	0
327	Paul J Flory â€" The man who laid the foundations of modern polymer science. Resonance, 2003, 8, 2-5.	0.3	0
328	Adaptations of Metropolis Monte Carlo for Global Optimization in Treating Fluids, Crystals, and Structures of Peptides and Proteins. AIP Conference Proceedings, 2003, , .	0.4	0
329	George Hess: A scientific appreciation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1466-1467.	7.1	0