Harold A Scheraga

List of Publications by Year
in descending order

329 papers	25,183 citations	10070 75 h-index	9346 148 g-index
344 all docs	344 docs citations	344 times ranked	11053 citing authors

#	Article	IF	Citations
1	Probing Protein Aggregation Using the Coarse-Grained UNRES Force Field. Methods in Molecular Biology, 2022, 2340, 79-104.	0.4	1
2	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.	2.3	11
3	The structure of protein dynamic space. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 19938-19942.	3.3	10
4	Curvature and Torsion of Protein Main Chain as Local Order Parameters of Protein Unfolding. Journal of Physical Chemistry B, 2020, 124, 4391-4398.	1.2	9
5	PMFF: Development of a Physics-Based Molecular Force Field for Protein Simulation and Ligand Docking. Journal of Physical Chemistry B, 2020, 124, 974-989.	1.2	7
6	Assessing the One-Bond C_{Î±}â€“H Spinâ€“Spin Coupling Constants in Proteins: Pros and Cons of Different Approaches. Journal of Physical Chemistry B, 2020, 124, 735-741.	1.2	3
7	New Insights into Folding, Misfolding, and Nonfolding Dynamics of a WW Domain. Journal of Physical Chemistry B, 2020, 124, 3855-3872.	1.2	4
8	Outline of an experimental design aimed to detect protein A mirror image in solution. , 2019, 1, e2.		1
9	Statistical Model To Decipher Protein Folding/Unfolding at a Local Scale. Journal of Physical Chemistry B, 2018, 122, 3540-3549.	1.2	6
10	From a Highly Disordered to a Metastable State: Uncovering Insights of Î±-Synuclein. ACS Chemical Neuroscience, 2018, 9, 1051-1065.	1.7	22
11	Lysosomal enzyme tripeptidyl peptidase 1 destabilizes fibrillar AÎ² by multiple endoproteolytic cleavages within the Î²-sheet domain. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1493-1498.	3.3	33
12	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.	2.0	9
13	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.	2.0	2
14	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.	1.5	16
15	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.	1.2	22
16	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939.	1.6	19
17	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.	3.3	24
18	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.	1.8	6

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19	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.	1.2	19
20	Dynamics of Disulfide-Bond Disruption and Formation in the Thermal Unfolding of Ribonuclease A. Journal of Chemical Theory and Computation, 2017, 13, 5721-5730.	2.3	15
21	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.	2.5	38
22	Elucidating Important Sites and the Mechanism for Amyloid Fibril Formation by Coarse-Grained Molecular Dynamics. ACS Chemical Neuroscience, 2017, 8, 201-209.	1.7	32
23	Eliminating a Protein Folding Intermediate by Tuning a Local Hydrophobic Contact. Journal of Physical Chemistry B, 2017, 121, 3276-3284.	1.2	5
24	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	1.8	44
25	Molecular dynamics of protein A and a WW domain with a united-residue model including hydrodynamic interaction. Journal of Chemical Physics, 2016, 144, 184110.	1.2	10
26	George Hess: A scientific appreciation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1466-1467.	3.3	0
27	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.	3.3	8
28	Detection of methylation, acetylation and glycosylation of protein residues by monitoring¹³C chemical-shift changes: A quantum-chemical study. PeerJ, 2016, 4, e2253.	0.9	6
29	Optimization of a Nucleic Acids united-RESidue 2-Point model (NARES-2P) with a maximum-likelihood approach. Journal of Chemical Physics, 2015, 143, 243111.	1.2	25
30	Molecular modeling of the binding modes of the iron-sulfur protein to the Jac1 co-chaperone from S accharomyces cerevisiae by all-atom and coarse-grained approaches. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1414-1426.	1.5	32
31	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.	2.3	39
32	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.	1.2	4
33	My 65 years in protein chemistry. Quarterly Reviews of Biophysics, 2015, 48, 117-177.	2.4	9
34	New Insights into Protein (Un)Folding Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 1082-1086.	2.1	20
35	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.	3.3	23
36	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.	3.3	17

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37	Are accurate computations of the ¹³Câ€² shielding feasible at the DFT level of theory?. Journal of Computational Chemistry, 2014, 35, 309-312.	1.5	2
38	Kinks, loops, and protein folding, with protein A as an example. Journal of Chemical Physics, 2014, 140, 025101.	1.2	18
39	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.	3.3	36
40	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.	3.3	17
41	DNA Duplex Formation with a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2014, 10, 5020-5035.	2.3	39
42	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.	2.3	16
43	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.	3.3	19
44	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.	2.3	30
45	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.	3.3	9
46	Local vs Global Motions in Protein Folding. Journal of Chemical Theory and Computation, 2013, 9, 2907-2921.	2.3	18
47	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.	3.3	62
48	CheShift-2: graphic validation of protein structures. Bioinformatics, 2012, 28, 1538-1539.	1.8	23
49	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.	2.3	20
50	Effects of Mutation, Truncation, and Temperature on the Folding Kinetics of a WW Domain. Journal of Molecular Biology, 2012, 420, 350-365.	2.0	17
51	Coexistence of Phases in a Protein Heterodimer. Journal of Chemical Physics, 2012, 137, 035101.	1.2	20
52	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.	3.3	29
53	Respice, Adspice, and Prospice. Annual Review of Biophysics, 2011, 40, 1-39.	4.5	8
54	Towards Temperature Dependent Coarse-grained Potential of Side-chain Interactions for Protein Folding Simulations. , 2010, , .		3

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55	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.	3.3	28
56	Investigation of Protein Folding by Coarse-Grained Molecular Dynamics with the UNRES Force Field. Journal of Physical Chemistry A, 2010, 114, 4471-4485.	1.1	91
57	Relation between Free Energy Landscapes of Proteins and Dynamics. Journal of Chemical Theory and Computation, 2010, 6, 583-595.	2.3	132
58	Mechanism of Fiber Assembly: Treatment of AÎ² Peptide Aggregation with a Coarse-Grained United-Residue Force Field. Journal of Molecular Biology, 2010, 404, 537-552.	2.0	87
59	How Adequate are One- and Two-Dimensional Free Energy Landscapes for Protein Folding Dynamics?. Physical Review Letters, 2009, 102, 238102.	2.9	48
60	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.	1.5	64
61	Application of Multiplexed Replica Exchange Molecular Dynamics to the UNRES Force Field: Tests with Î± and Î±+Î² Proteins. Journal of Chemical Theory and Computation, 2009, 5, 627-640.	2.3	93
62	Principal Component Analysis for Protein Folding Dynamics. Journal of Molecular Biology, 2009, 385, 312-329.	2.0	331
63	From helixâ€“coil transitions to protein folding. Biopolymers, 2008, 89, 479-485.	1.2	13
64	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.	3.3	52
65	Predicting Three-Dimensional Structures of Oligopeptides. Reviews in Computational Chemistry, 2007, , 73-142.	1.5	27
66	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.	1.2	184
67	Protein-Folding Dynamics: Overview of Molecular Simulation Techniques. Annual Review of Physical Chemistry, 2007, 58, 57-83.	4.8	329
68	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.	1.2	46
69	Predicting 13CÎ± chemical shifts for validation of protein structures. Journal of Biomolecular NMR, 2007, 38, 221-235.	1.6	39
70	A New Force Field (ECEPP-05) for Peptides, Proteins, and Organic Molecules. Journal of Physical Chemistry B, 2006, 110, 5025-5044.	1.2	111
71	A Localized Specific Interaction Alters the Unfolding Pathways of Structural Homologues. Journal of the American Chemical Society, 2006, 128, 1204-1213.	6.6	26
72	HELIX-RANDOM COIL TRANSFORMATIONS IN DEUTERATED MACROMOLECULES*. Annals of the New York Academy of Sciences, 2006, 84, 608-616.	1.8	38

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73	THROMBIN AND ITS INTERACTION WITH FIBRINOGEN*. Annals of the New York Academy of Sciences, 2006, 75, 189-194.	1.8	25
74	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.	1.8	43
75	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.	3.3	256
76	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.	0.8	18
77	Molecular Dynamics with the United-Residue Model of Polypeptide Chains. II. Langevin and Berendsen-Bath Dynamics and Tests on Model Î±-Helical Systems. Journal of Physical Chemistry B, 2005, 109, 13798-13810.	1.2	144
78	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.	1.2	114
79	The thrombinâ€“fibrinogen interaction. Biophysical Chemistry, 2004, 112, 117-130.	1.5	83
80	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.	1.2	68
81	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.	1.2	73
82	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.	1.2	19
83	Dissimilarity in the Reductive Unfolding Pathways of Two Ribonuclease Homologues. Journal of Molecular Biology, 2004, 338, 795-809.	2.0	31
84	Paul J Flory â€" The man who laid the foundations of modern polymer science. Resonance, 2003, 8, 2-5.	0.2	0
85	Amino Acid Residues at Proteinâ^'Protein Interfaces:Â Why Is Propensity so Different from Relative Abundance?. Journal of Physical Chemistry B, 2003, 107, 9929-9932.	1.2	13
86	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.	1.2	24
87	Adaptations of Metropolis Monte Carlo for Global Optimization in Treating Fluids, Crystals, and Structures of Peptides and Proteins. AIP Conference Proceedings, 2003, , .	0.3	0
88	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.	1.2	19
89	Formation of the Hydrophobic Core of Ribonuclease A through Sequential Coordinated Conformational Transitionsâ€. Biochemistry, 2002, 41, 14225-14231.	1.2	14
90	Evolution of physics-based methodology for exploring the conformational energy landscape of proteins. Journal of Computational Chemistry, 2002, 23, 28-34.	1.5	22

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91	Helixâ€“coil transitions re-visited. Biophysical Chemistry, 2002, 101-102, 255-265.	1.5	52
92	Can cooperativity in hydrophobic association be reproduced correctly by implicit solvation models?. International Journal of Quantum Chemistry, 2002, 88, 41-55.	1.0	36
93	Exact solutions for chemical bond orientations from residual dipolar couplings. Journal of Biomolecular NMR, 2002, 22, 137-151.	1.6	31
94	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.	1.2	236
95	Effect of Mutation of Proline 93 on Redox Unfolding/Folding of Bovine Pancreatic Ribonuclease A. Biochemistry, 2001, 40, 8536-8541.	1.2	15
96	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.	1.2	22
97	Coupling of Conformational Folding and Disulfide-Bond Reactions in Oxidative Folding of Proteins. Biochemistry, 2001, 40, 9059-9064.	1.2	113
98	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.	1.2	93
99	Influence of lysine content and PH on the stability of alanine-based copolypeptides. Biopolymers, 2001, 58, 235-246.	1.2	28
100	Influence of lysine content and PH on the stability of alanineâ€based copolypeptides. Biopolymers, 2001, 58, 235-246.	1.2	2
101	Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets. International Journal of Quantum Chemistry, 2000, 77, 90-117.	1.0	36
102	Molecular simulation study of cooperativity in hydrophobic association. Protein Science, 2000, 9, 1235-1245.	3.1	90
103	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.	1.3	12
104	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.	1.3	12
105	Disulfide Bonds and Protein Foldingâ€. Biochemistry, 2000, 39, 4207-4216.	1.2	556
106	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.	1.2	8
107	Ion Pair Interactions in Aqueous Solution:Â Self-Consistent Reaction Field (SCRF) Calculations with Some Explicit Water Molecules. Journal of Physical Chemistry A, 2000, 104, 6505-6509.	1.1	37
108	Oxidative Folding of Proteins. Accounts of Chemical Research, 2000, 33, 805-812.	7.6	209

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109	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.	3.1	10
110	Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets. , 2000, 77, 90.		1
111	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.	0.5	25
112	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.	1.0	77
113	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.	1.5	23
114	Prodock: Software package for protein modeling and docking. Journal of Computational Chemistry, 1999, 20, 412-427.	1.5	98
115	Exact analytical loop closure in proteins using polynomial equations. Journal of Computational Chemistry, 1999, 20, 819-844.	1.5	94
116	Calculation of protein conformation by global optimization of a potential energy function. Proteins: Structure, Function and Bioinformatics, 1999, 37, 204-208.	1.5	96
117	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
118	Global Optimization of Clusters, Crystals, and Biomolecules. Science, 1999, 285, 1368-1372.	6.0	995
119	Effect of protein disulfide isomerase on the regeneration of bovine ribonuclease A with dithiothreitol. FEBS Letters, 1999, 456, 143-145.	1.3	10
120	Two new structured intermediates in the oxidative folding of RNase A. FEBS Letters, 1999, 460, 477-479.	1.3	45
121	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.	1.2	34
122	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:Â Identification of Specific Regions of Stable Structure along the Oxidative Folding Pathwayâ€. Biochemistry, 1999, 38, 16432-16442.	1.2	15
123	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.	1.2	52
124	Calculation of protein conformation by global optimization of a potential energy function. Proteins: Structure, Function and Bioinformatics, 1999, Suppl 3, 204-8.	1.5	23
125	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
126	Conformational analysis of the 20-residue membrane-bound portion of melittin by conformational space annealing. , 1998, 46, 103-115.		73

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127	New developments of the electrostatically driven monte carlo method: Test on the membrane-bound portion of melittin. , 1998, 46, 117-126.		49
128	B-spline method for energy minimization in grid-based molecular mechanics calculations. Journal of Computational Chemistry, 1998, 19, 71-85.	1.5	23
129	Crystal structures of two mutants that have implications for the folding of bovine pancreatic ribonuclease A. Protein Science, 1998, 7, 1255-1258.	3.1	39
130	Diffusion Equation and Distance Scaling Methods of Global Optimization:Â Applications to Crystal Structure Prediction. Journal of Physical Chemistry A, 1998, 102, 2904-2918.	1.1	46
131	Regeneration of Bovine Pancreatic Ribonuclease A:â€‰ Identification of Two Nativelike Three-Disulfide Intermediates Involved in Separate Pathways. Biochemistry, 1998, 37, 3760-3766.	1.2	100
132	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.	1.2	10
133	Regeneration of Three-Disulfide Mutants of Bovine Pancreatic Ribonuclease A Missing the 65â^'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.	1.2	54
134	Theory of Two-State Cooperative Folding of Proteins. Accounts of Chemical Research, 1998, 31, 433-440.	7.6	31
135	Characterization of Multiple Reduction Pathways of Proteins in the Presence of a Denaturant. Journal of the American Chemical Society, 1998, 120, 5806-5807.	6.6	6
136	Kinetic Folding Pathway of a Three-Disulfide Mutant of Bovine Pancreatic Ribonuclease A Missing the [40â^'95] Disulfide Bondâ€. Biochemistry, 1998, 37, 7561-7571.	1.2	46
137	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.	6.6	15
138	Regeneration of Bovine Pancreatic Ribonuclease A:â€‰ Detailed Kinetic Analysis of Two Independent Folding Pathways. Biochemistry, 1998, 37, 3767-3776.	1.2	83
139	Theory of Hydrophobic Interactions. Journal of Biomolecular Structure and Dynamics, 1998, 16, 447-460.	2.0	76
140	Macromolecular conformational dynamics in torsional angle space. Journal of Chemical Physics, 1998, 108, 271-286.	1.2	50
141	Brownian dynamics simulations of protein folding. Journal of Chemical Physics, 1998, 108, 287-300.	1.2	40
142	Use of sequence-specific tri-block copolymers to determine the helix-forming tendencies of amino acids. Biopolymers, 1998, 39, 531-536.	1.2	7
143	Characterization of foldable protein models: Thermodynamics, folding kinetics and force field. Journal of Chemical Physics, 1997, 107, 8089-8102.	1.2	21
144	Kinetic Studies of the Regeneration of Recombinant Hirudin Variant 1 with Oxidized and Reduced Dithiothreitolâ€. Biochemistry, 1997, 36, 2154-2165.	1.2	29

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145	Regeneration Studies of an Analog of Ribonuclease A Missing Disulfide Bonds 65â˜’72 and 40â˜’95. Biochemistry, 1997, 36, 13068-13076.	1.2	15
146	A fast adaptive multigrid boundary element method for macromolecular electrostatic computations in a solvent. Journal of Computational Chemistry, 1997, 18, 569-583.	1.5	118
147	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.	1.5	7
148	Role of Non-Native Aromatic and Hydrophobic Interactions in the Folding of Hen Egg White Lysozyme. Biochemistry, 1996, 35, 13797-13807.	1.2	101
149	Kinetic and Thermodynamic Studies of the Folding/Unfolding of a Tryptophan-Containing Mutant of Ribonuclease Aâ€. Biochemistry, 1996, 35, 12978-12992.	1.2	43
150	Structure of a Hydrophobically Collapsed Intermediate on the Conformational Folding Pathway of Ribonuclease A Probed by Hydrogenâ˜’Deuterium Exchangeâ€. Biochemistry, 1996, 35, 11734-11746.	1.2	63
151	Folding and Unfolding Kinetics of the Proline-to-Alanine Mutants of Bovine Pancreatic Ribonuclease A. Biochemistry, 1996, 35, 1548-1559.	1.2	99
152	The Role of the Insertion Loop around Tryptophan 148 in the Activity of Thrombinâ€,â€¡. Biochemistry, 1996, 35, 4427-4433.	1.2	27
153	Nature of the Unfolded State of Ribonuclease A:Â Effect of Cisâ˜’Trans Xâ˜’Pro Peptide Bond Isomerizationâ€. Biochemistry, 1996, 35, 11719-11733.	1.2	64
154	Circular Dichroism Evidence for the Presence of Burst-Phase Intermediates on the Conformational Folding Pathway of Ribonuclease Aâ€. Biochemistry, 1996, 35, 10125-10133.	1.2	49
155	Determination of Potential Parameters for Amino Acid Zwitterions. The Journal of Physical Chemistry, 1996, 100, 17670-17677.	2.9	14
156	Nonrandom Distribution of the One-Disulfide Intermediates in the Regeneration of Ribonuclease Aâ€. Biochemistry, 1996, 35, 6406-6417.	1.2	88
157	Effects on protein structure and function of replacing tryptophan with 5-hydroxytryptophan: Single-tryptophan mutants of the N-terminal domain of the bacteriophage Î» repressor. The Protein Journal, 1996, 15, 77-86.	1.1	2
158	State of aggregation of recombinant hirudin in solution under physiological conditions. The Protein Journal, 1996, 15, 751-753.	1.1	4
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