Harold A Scheraga

List of Publications by Year in Descending Order

328 papers	22,455 citations	71 h-index	140 g-index
344 ext. papers	23,534 ext. citations	4.6 avg, IF	6.62 L-index

#	Paper	IF	Citations
328	Probing Protein Aggregation Using the Coarse-Grained UNRES Force Field.. *Methods in Molecular Biology*, **2022**, 2340, 79-104	1.4	
327	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	6.4	6
326	Curvature and Torsion of Protein Main Chain as Local Order Parameters of Protein Unfolding. *Journal of Physical Chemistry B*, **2020**, 124, 4391-4398	3.4	4
325	PMFF: Development of a Physics-Based Molecular Force Field for Protein Simulation and Ligand Docking. *Journal of Physical Chemistry B*, **2020**, 124, 974-989	3.4	0
324	Assessing the One-Bond C-H Spin-Spin Coupling Constants in Proteins: Pros and Cons of Different Approaches. *Journal of Physical Chemistry B*, **2020**, 124, 735-741	3.4	2
323	The structure of protein dynamic space. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 19938-19942	11.5	2
322	New Insights into Folding, Misfolding, and Nonfolding Dynamics of a WW Domain. *Journal of Physical Chemistry B*, **2020**, 124, 3855-3872	3.4	4
321	Outline of an experimental design aimed to detect a protein A mirror image in solution. *PeerJ Physical Chemistry*, **2019**, 1,		1
320	Statistical Model To Decipher Protein Folding/Unfolding at a Local Scale. *Journal of Physical Chemistry B*, **2018**, 122, 3540-3549	3.4	5
319	From a Highly Disordered to a Metastable State: Uncovering Insights of Synuclein. *ACS Chemical Neuroscience*, **2018**, 9, 1051-1065	5.7	17
318	Lysosomal enzyme tripeptidyl peptidase 1 destabilizes fibrillar A by multiple endoproteolytic cleavages within the sheet domain. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 1493-1498	11.5	21
317	Coupled molecular dynamics and continuum electrostatic method to compute the ionization pKa'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	3.6	8
316	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	3.6	2
315	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. *Scientific Reports*, **2018**, 8, 9939	4.9	16
314	A new protein nucleic-acid coarse-grained force field based on the UNRES and NARES-2P force fields. *Journal of Computational Chemistry*, **2018**, 39, 2360-2370	3.5	7
313	Dependence of the Formation of Tau and A Peptide Mixed Aggregates on the Secondary Structure of the N-Terminal Region of A *Journal of Physical Chemistry B*, **2018**, 122, 7049-7056	3.4	13
312	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	11.5	10

311	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	3.4	3
310	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino Acid Side Chains in Water. VII. Charged-Hydrophobic/Polar and Polar-Hydrophobic/Polar Side Chains. *Journal of Physical Chemistry B*, **2017**, 121, 379-390	3.4	16
309	Dynamics of Disulfide-Bond Disruption and Formation in the Thermal Unfolding of Ribonuclease A. *Journal of Chemical Theory and Computation*, **2017**, 13, 5721-5730	6.4	7
308	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	6.1	33
307	Elucidating Important Sites and the Mechanism for Amyloid Fibril Formation by Coarse-Grained Molecular Dynamics. *ACS Chemical Neuroscience*, **2017**, 8, 201-209	5.7	22
306	Eliminating a Protein Folding Intermediate by Tuning a Local Hydrophobic Contact. *Journal of Physical Chemistry B*, **2017**, 121, 3276-3284	3.4	4
305	George Hess: A scientific appreciation. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 1466-7	11.5	
304	Global informatics and physical property selection in protein sequences. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 1808-10	11.5	7
303	Detection of methylation, acetylation and glycosylation of protein residues by monitoring (13)C chemical-shift changes: A quantum-chemical study. *PeerJ*, **2016**, 4, e2253	3.1	3
302	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. *Bioinformatics*, **2016**, 32, 3270-3278	7.2	36
301	Molecular dynamics of protein A and a WW domain with a united-residue model including hydrodynamic interaction. *Journal of Chemical Physics*, **2016**, 144, 184110	3.9	8
300	Theoretical Studies of Interactions between O-Phosphorylated and Standard Amino-Acid Side-Chain Models in Water. *Journal of Physical Chemistry B*, **2015**, 119, 8526-34	3.4	4
299	My 65 years in protein chemistry. *Quarterly Reviews of Biophysics*, **2015**, 48, 117-77	7	7
298	New Insights into Protein (Un)Folding Dynamics. *Journal of Physical Chemistry Letters*, **2015**, 6, 1082-6	6.4	20
297	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, 5029-32	11.5	14
296	Preventing fibril formation of a protein by selective mutation. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 13549-54	11.5	16
295	Optimization of a Nucleic Acids united-RESidue 2-Point model (NARES-2P) with a maximum-likelihood approach. *Journal of Chemical Physics*, **2015**, 143, 243111	3.9	16
294	Molecular modeling of the binding modes of the iron-sulfur protein to the Jac1 co-chaperone from Saccharomyces cerevisiae by all-atom and coarse-grained approaches. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1414-26	4.2	29

293	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, 817-31	6.4	34
292	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, 5225-9	11.5	12
291	DNA Duplex Formation with a Coarse-Grained Model. *Journal of Chemical Theory and Computation*, **2014**, 10, 5020-5035	6.4	27
290	Revised Backbone-Virtual-Bond-Angle Potentials to Treat the l- and d-Amino Acid Residues in the Coarse-Grained United Residue (UNRES) Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 2194-2203	6.4	16
289	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, 8458-63	11.5	17
288	Are accurate computations of the 13C' shielding feasible at the DFT level of theory?. *Journal of Computational Chemistry*, **2014**, 35, 309-12	3.5	2
287	Kinks, loops, and protein folding, with protein A as an example. *Journal of Chemical Physics*, **2014**, 140, 025101	3.9	17
286	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, 18243-8	11.5	27
285	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,	6.4	29
284	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	11.5	8
283	Local vs global motions in protein folding. *Journal of Chemical Theory and Computation*, **2013**, 9, 2907-2921	6.4	14
282	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, 14936-41	11.5	54
281	Extension of UNRES force field to treat polypeptide chains with D-amino-acid residues. *Journal of Chemical Theory and Computation*, **2012**, 8, 4746-4757	6.4	18
280	Effects of mutation, truncation, and temperature on the folding kinetics of a WW domain. *Journal of Molecular Biology*, **2012**, 420, 350-65	6.5	14
279	Coexistence of phases in a protein heterodimer. *Journal of Chemical Physics*, **2012**, 137, 035101	3.9	19
278	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, 10346-51	11.5	28
277	CheShift-2: graphic validation of protein structures. *Bioinformatics*, **2012**, 28, 1538-9	7.2	19
276	Respice, adspice, and prospice. *Annual Review of Biophysics*, **2011**, 40, 1-39	21.1	7

275	Ribonucleases as Models for Understanding Protein Folding. *Nucleic Acids and Molecular Biology*, **2011**, 367-397		3
274	Towards Temperature Dependent Coarse-grained Potential of Side-chain Interactions for Protein Folding Simulations **2010**,		3
273	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, 19844-9	11.5	27
272	Investigation of protein folding by coarse-grained molecular dynamics with the UNRES force field. *Journal of Physical Chemistry A*, **2010**, 114, 4471-85	2.8	79
271	Relation between free energy landscapes of proteins and dynamics. *Journal of Chemical Theory and Computation*, **2010**, 6, 583-595	6.4	85
270	Mechanism of fiber assembly: treatment of A peptide aggregation with a coarse-grained united-residue force field. *Journal of Molecular Biology*, **2010**, 404, 537-52	6.5	74
269	How adequate are one- and two-dimensional free energy landscapes for protein folding dynamics?. *Physical Review Letters*, **2009**, 102, 238102	7.4	45
268	CONFORMATIONALSTUDY OF [LEU5]-ENKEPHALIN BY LASER RAMAN SPECTROSCOPY. *International Journal of Peptide and Protein Research*, **2009**, 16, 173-182		31
267	Solution conformations of oligomers of aminoisobutyric acid *International Journal of Peptide and Protein Research*, **2009**, 20, 468-480		28
266	Exploring the parameter space of the coarse-grained UNRES force field by random search: selecting a transferable medium-resolution force field. *Journal of Computational Chemistry*, **2009**, 30, 2127-35	3.5	61
265	Application of Multiplexed Replica Exchange Molecular Dynamics to the UNRES Force Field: Tests with alpha and alpha+beta Proteins. *Journal of Chemical Theory and Computation*, **2009**, 5, 627-640	6.4	78
264	Principal component analysis for protein folding dynamics. *Journal of Molecular Biology*, **2009**, 385, 312-29	6.5	224
263	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, 19708-13	11.5	50
262	From helix-coil transitions to protein folding. *Biopolymers*, **2008**, 89, 479-85	2.2	10
261	Molecular dynamics with the United-residue force field: ab initio folding simulations of multichain proteins. *Journal of Physical Chemistry B*, **2007**, 111, 293-309	3.4	43
260	Predicting 13Calpha chemical shifts for validation of protein structures. *Journal of Biomolecular NMR*, **2007**, 38, 221-35	3	36
259	Predicting Three-Dimensional Structures of Oligopeptides. *Reviews in Computational Chemistry*, **2007**, 73-142		14
258	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, 260-85	3.4	160

257	Protein-folding dynamics: overview of molecular simulation techniques. *Annual Review of Physical Chemistry*, **2007**, 58, 57-83	15.7	278
256	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	6.5	39
255	A new force field (ECEPP-05) for peptides, proteins, and organic molecules. *Journal of Physical Chemistry B*, **2006**, 110, 5025-44	3.4	96
254	A localized specific interaction alters the unfolding pathways of structural homologues. *Journal of the American Chemical Society*, **2006**, 128, 1204-13	16.4	25
253	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
252	Molecular dynamics with the united-residue model of polypeptide chains. II. Langevin and Berendsen-bath dynamics and tests on model alpha-helical systems. *Journal of Physical Chemistry B*, **2005**, 109, 13798-810	3.4	121
251	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, 13785-97	3.4	101
250	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, 2362-7	11.5	230
249	The thrombin-fibrinogen interaction. *Biophysical Chemistry*, **2004**, 112, 117-30	3.5	66
248	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	3.4	64
247	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	3.4	70
246	Derivation of a New Force Field for Crystal-Structure Prediction Using Global Optimization: Nonbonded Potential Parameters for Amines, Imidazoles, Amides, and Carboxylic Acids. *Journal of Physical Chemistry B*, **2004**, 108, 12181-12196	3.4	17
245	Dissimilarity in the reductive unfolding pathways of two ribonuclease homologues. *Journal of Molecular Biology*, **2004**, 338, 795-809	6.5	29
244	Paul J Flory The man who laid the foundations of modern polymer science **2003**, 8, 2-5		
243	Amino Acid Residues at Protein Protein Interfaces: Why Is Propensity so Different from Relative Abundance?. *Journal of Physical Chemistry B*, **2003**, 107, 9929-9932	3.4	12
242	Derivation of a New Force Field for Crystal-Structure Prediction Using Global Optimization: Nonbonded Potential Parameters for Hydrocarbons and Alcohols. *Journal of Physical Chemistry B*, **2003**, 107, 7143-7154	3.4	23
241	Evolution of physics-based methodology for exploring the conformational energy landscape of proteins. *Journal of Computational Chemistry*, **2002**, 23, 28-34	3.5	21
240	Helix-coil transitions re-visited. *Biophysical Chemistry*, **2002**, 101-102, 255-65	3.5	51

239	Can cooperativity in hydrophobic association be reproduced correctly by implicit solvation models?*. *International Journal of Quantum Chemistry*, **2002**, 88, 41-55	2.1	36
238	Exact solutions for chemical bond orientations from residual dipolar couplings. *Journal of Biomolecular NMR*, **2002**, 22, 137-51	3	28
237	Comment on "Anti-cooperativity in hydrophobic interactions: A simulation study of spatial dependence of three-body effects and beyond" [J. Chem. Phys. 115, 1414 (2001)]. *Journal of Chemical Physics*, **2002**, 116, 2665-2667	3.9	18
236	Formation of the hydrophobic core of ribonuclease A through sequential coordinated conformational transitions. *Biochemistry*, **2002**, 41, 14225-31	3.2	13
235	Influence of lysine content and pH on the stability of alanine-based copolypeptides. *Biopolymers*, **2001**, 58, 235-46	2.2	26
234	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	3.9	209
233	Effect of mutation of proline 93 on redox unfolding/folding of bovine pancreatic ribonuclease A. *Biochemistry*, **2001**, 40, 8536-41	3.2	12
232	Folding of a disulfide-bonded protein species with free thiol(s): competition between conformational folding and disulfide reshuffling in an intermediate of bovine pancreatic ribonuclease A. *Biochemistry*, **2001**, 40, 15002-8	3.2	22
231	Coupling of conformational folding and disulfide-bond reactions in oxidative folding of proteins. *Biochemistry*, **2001**, 40, 9059-64	3.2	95
230	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, 105-18	3.2	89
229	Influence of lysine content and PH on the stability of alanine-based copolypeptides **2001**, 58, 235		2
228	Solution NMR evidence for a cis Tyr-Ala peptide group in the structure of [Pro93Ala] bovine pancreatic ribonuclease A. *Protein Science*, **2000**, 9, 421-6	6.3	10
227	Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets. *International Journal of Quantum Chemistry*, **2000**, 77, 90-117	2.1	35
226	Molecular simulation study of cooperativity in hydrophobic association. *Protein Science*, **2000**, 9, 1235-45	6.3	87
225	Formation of native structure by intermolecular thiol-disulfide exchange reactions without oxidants in the folding of bovine pancreatic ribonuclease A. *FEBS Letters*, **2000**, 471, 177-81	3.8	12
224	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	3.8	11
223	Disulfide bonds and protein folding. *Biochemistry*, **2000**, 39, 4207-16	3.2	487
222	Reply to "Comment on "Crystal Structure Prediction by Global Optimization as a Tool for Evaluating Potentials: Role of the Dipole Moment Correction Term in Successful Predictions"" by B. P. van Eijck and J. Kroon. *Journal of Physical Chemistry B*, **2000**, 104, 8090-8092	3.4	7

221	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	2.8	35
220	Oxidative folding of proteins. *Accounts of Chemical Research*, **2000**, 33, 805-12	24.3	174
219	Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets **2000**, 77, 90		1
218	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	1.9	21
217	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	2.1	69
216	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	3.5	20
215	Prodock: Software package for protein modeling and docking. *Journal of Computational Chemistry*, **1999**, 20, 412-427	3.5	91
214	Exact analytical loop closure in proteins using polynomial equations. *Journal of Computational Chemistry*, **1999**, 20, 819-844	3.5	81
213	Calculation of protein conformation by global optimization of a potential energy function. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 204-208	4.2	82
212	New general approach for determining the solution structure of a ligand bound weakly to a receptor: structure of a fibrinogen Aalpha-like peptide bound to thrombin (S195A) obtained using NOE distance constraints and an ECEPP/3 flexible docking program. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 29-48	4.2	19
211	Global optimization of clusters, crystals, and biomolecules. *Science*, **1999**, 285, 1368-72	33.3	881
210	Effect of protein disulfide isomerase on the regeneration of bovine ribonuclease A with dithiothreitol. *FEBS Letters*, **1999**, 456, 143-5	3.8	9
209	Two new structured intermediates in the oxidative folding of RNase A. *FEBS Letters*, **1999**, 460, 477-9	3.8	44
208	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, 2805-15	3.2	34
207	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 pathway. *Biochemistry*, **1999**, 38, 16432-42	3.2	14
206	Distribution of disulfide bonds in the two-disulfide intermediates in the regeneration of bovine pancreatic ribonuclease A: further insights into the folding process. *Biochemistry*, **1999**, 38, 7284-93	3.2	50
205	Calculation of protein conformation by global optimization of a potential energy function. *Proteins: Structure, Function and Bioinformatics*, **1999**, Suppl 3, 204-8	4.2	21
204	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		5

203	Conformational analysis of the 20-residue membrane-bound portion of melittin by conformational space annealing. *Biopolymers*, **1998**, 46, 103-16	2.2	66
202	New developments of the electrostatically driven Monte Carlo method: test on the membrane-bound portion of melittin. *Biopolymers*, **1998**, 46, 117-26	2.2	44
201	B-spline method for energy minimization in grid-based molecular mechanics calculations. *Journal of Computational Chemistry*, **1998**, 19, 71-85	3.5	22
200	Crystal structures of two mutants that have implications for the folding of bovine pancreatic ribonuclease A. *Protein Science*, **1998**, 7, 1255-8	6.3	36
199	Diffusion Equation and Distance Scaling Methods of Global Optimization:Applications to Crystal Structure Prediction. *Journal of Physical Chemistry A*, **1998**, 102, 2904-2918	2.8	40
198	Regeneration of bovine pancreatic ribonuclease A: identification of two nativelike three-disulfide intermediates involved in separate pathways. *Biochemistry*, **1998**, 37, 3760-6	3.2	96
197	Computation of the Structure-Dependent pKa Shifts in a Polypentapeptide of the Poly[fv(IPGVG), fE(IPGEG)] Family. *Journal of Physical Chemistry B*, **1998**, 102, 3065-3067	3.4	10
196	Regeneration of three-disulfide mutants of bovine pancreatic ribonuclease A missing the 65-72 disulfide bond: characterization of a minor folding pathway of ribonuclease A and kinetic roles of Cys65 and Cys72. *Biochemistry*, **1998**, 37, 4490-501	3.2	51
195	Theory of Two-State Cooperative Folding of Proteins. *Accounts of Chemical Research*, **1998**, 31, 433-440	24.3	28
194	Characterization of Multiple Reduction Pathways of Proteins in the Presence of a Denaturant. *Journal of the American Chemical Society*, **1998**, 120, 5806-5807	16.4	6
193	Kinetic folding pathway of a three-disulfide mutant of bovine pancreatic ribonuclease A missing the [40-95] disulfide bond. *Biochemistry*, **1998**, 37, 7561-71	3.2	44
192	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	16.4	14
191	Regeneration of bovine pancreatic ribonuclease A: detailed kinetic analysis of two independent folding pathways. *Biochemistry*, **1998**, 37, 3767-76	3.2	80
190	Theory of hydrophobic interactions. *Journal of Biomolecular Structure and Dynamics*, **1998**, 16, 447-60	3.6	68
189	Macromolecular conformational dynamics in torsional angle space. *Journal of Chemical Physics*, **1998**, 108, 271-286	3.9	43
188	Brownian dynamics simulations of protein folding. *Journal of Chemical Physics*, **1998**, 108, 287-300	3.9	37
187	Use of sequence-specific tri-block copolymers to determine the helix-forming tendencies of amino acids. *Biopolymers*, **1998**, 39, 531-536	2.2	6
186	Characterization of foldable protein models: Thermodynamics, folding kinetics and force field. *Journal of Chemical Physics*, **1997**, 107, 8089-8102	3.9	19

185	Kinetic studies of the regeneration of recombinant hirudin variant 1 with oxidized and reduced dithiothreitol. *Biochemistry*, **1997**, 36, 2154-65	3.2	28
184	Regeneration studies of an analog of ribonuclease A missing disulfide bonds 65-72 and 40-95. *Biochemistry*, **1997**, 36, 13068-76	3.2	14
183	A fast adaptive multigrid boundary element method for macromolecular electrostatic computations in a solvent. *Journal of Computational Chemistry*, **1997**, 18, 569-583	3.5	113
182	An assessment of the accuracy of the RRIGS hydration potential: Comparison to solutions of the PoissonBoltzmann equation. *Journal of Computational Chemistry*, **1997**, 18, 1072-1078	3.5	7
181	Optimizing Potential Functions for Protein Folding. *The Journal of Physical Chemistry*, **1996**, 100, 14540-14548		41
180	Role of non-native aromatic and hydrophobic interactions in the folding of hen egg white lysozyme. *Biochemistry*, **1996**, 35, 13797-807	3.2	93
179	Kinetic and thermodynamic studies of the folding/unfolding of a tryptophan-containing mutant of ribonuclease A. *Biochemistry*, **1996**, 35, 12978-92	3.2	42
178	Structure of a hydrophobically collapsed intermediate on the conformational folding pathway of ribonuclease A probed by hydrogen-deuterium exchange. *Biochemistry*, **1996**, 35, 11734-46	3.2	56
177	Folding and unfolding kinetics of the proline-to-alanine mutants of bovine pancreatic ribonuclease A. *Biochemistry*, **1996**, 35, 1548-59	3.2	94
176	The role of the insertion loop around tryptophan 148 in tthe activity of thrombin. *Biochemistry*, **1996**, 35, 4427-33	3.2	21
175	Nature of the unfolded state of ribonuclease A: effect of cis-trans X-Pro peptide bond isomerization. *Biochemistry*, **1996**, 35, 11719-33	3.2	59
174	Circular dichroism evidence for the presence of burst-phase intermediates on the conformational folding pathway of ribonuclease A. *Biochemistry*, **1996**, 35, 10125-33	3.2	45
173	Determination of Potential Parameters for Amino Acid Zwitterions. *The Journal of Physical Chemistry*, **1996**, 100, 17670-17677		12
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171	Effects on protein structure and function of replacing tryptophan with 5-hydroxytryptophan: single-tryptophan mutants of the N-terminal domain of the bacteriophage lambda repressor. *The Protein Journal*, **1996**, 15, 77-86		2
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169	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	3.5	2
168	An efficient, differentiable hydration potential for peptides and proteins. *Journal of Computational Chemistry*, **1996**, 17, 1549-1558	3.5	42

167	Computational study of packing a collagen-like molecule: quasi-hexagonal vs "Smith" collagen microfibril model. *Biopolymers*, **1996**, 40, 595-607	2.2	11
166	Improved genetic algorithm for the protein folding problem by use of a Cartesian combination operator. *Protein Science*, **1996**, 5, 1800-15	6.3	63
165	Simple global minimization algorithm for one-variable rational functions. *Journal of Global Optimization*, **1995**, 6, 293-311	1.5	5
164	Mechanism of reductive protein unfolding. *Nature Structural and Molecular Biology*, **1995**, 2, 489-94	17.6	93
163	The nature of the initial step in the conformational folding of disulphide-intact ribonuclease A. *Nature Structural and Molecular Biology*, **1995**, 2, 495-503	17.6	65
162	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		28
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