Harold A Scheraga

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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	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		1453
327	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	3.9	949
326	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		902
325	Global optimization of clusters, crystals, and biomolecules. *Science*, **1999**, 285, 1368-72	33.3	881
324	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		830
323	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		619
322	The structure of water and the thermodynamic properties of aqueous solutions. *Journal of Chemical Physics*, **1970**, 6, Suppl:487-592	3.9	567
321	Disulfide bonds and protein folding. *Biochemistry*, **2000**, 39, 4207-16	3.2	487
320	Conformational Analysis of Macromolecules. III. Helical Structures of Polyglycine and Poly-L-Alanine. *Journal of Chemical Physics*, **1966**, 45, 2091-2101	3.9	391
319	Structure of Water and Hydrophobic Bonding in Proteins. IV. The Thermodynamic Properties of Liquid Deuterium Oxide. *Journal of Chemical Physics*, **1964**, 41, 680-689	3.9	351
318	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		332
317	METHOD FOR CALCULATION INTERNAL ROTATION BARRIERS. *Journal of Chemical Physics*, **1965**, 42, 2209-15	3.9	300
316	Conformation of analysis of macromolecules. IV. Helical structures of poly-L-alanine, poly-L-valine, poly-beta-methyl-L-aspartate, poly-gamma-methyl-L-glutamate, and poly-L-tyrosine. *Journal of Chemical Physics*, **1967**, 46, 4410-26	3.9	285
315	Protein-folding dynamics: overview of molecular simulation techniques. *Annual Review of Physical Chemistry*, **2007**, 58, 57-83	15.7	278
314	Protein folding. *Quarterly Reviews of Biophysics*, **1977**, 10, 239-52	7	261
313	Influence of local interactions on protein structure. I. Conformational energy studies of N-acetyl-N'-methylamides of Pro-X and X-Pro dipeptides. *Biopolymers*, **1977**, 16, 811-43	2.2	247
312	Phase transitions in one dimension and the helix-coil transition in polyamino acids. *Journal of Chemical Physics*, **1966**, 45, 1456-63	3.9	242

311	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
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309	Conformational Analysis of Macromolecules. II. The Rotational Isomeric States of the Normal Hydrocarbons. *Journal of Chemical Physics*, **1966**, 44, 3054-3069	3.9	219
308	Statistical and energetic analysis of side-chain conformations in oligopeptides. *International Journal of Peptide and Protein Research*, **1983**, 22, 1-15		214
307	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
306	Analysis of the Contribution of Internal Vibrations to the Statistical Weights of Equilibrium Conformations of Macromolecules. *Journal of Chemical Physics*, **1969**, 51, 4751-4767	3.9	208
305	Occurrence of a phase transition in nucleic acid models. *Journal of Chemical Physics*, **1966**, 45, 1464-9	3.9	196
304	Non-Newtonian Viscosity of Solutions of Ellipsoidal Particles. *Journal of Chemical Physics*, **1955**, 23, 1526-1532	3.9	189
303	Oxidative folding of proteins. *Accounts of Chemical Research*, **2000**, 33, 805-12	24.3	174
302	Conformational energy studies of beta-sheets of model silk fibroin peptides. I. Sheets of poly(Ala-Gly) chains. *Biopolymers*, **1991**, 31, 1529-41	2.2	169
301	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
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299	Preferred conformation of the tert-butoxycarbonyl-amino group in peptides. *International Journal of Peptide and Protein Research*, **1980**, 16, 156-72		146
298	Regeneration of bovine pancreatic ribonuclease A. 1. Steady-state distribution. *Biochemistry*, **1993**, 32, 2671-9	3.2	142
297	Computation of the sterically allowed conformations of peptides. *Biopolymers*, **1966**, 4, 369-407	2.2	140
296	Influence of water structure and of hydrophobic interactions on the strength of side-chain hydrogen bonds in proteins. *Biopolymers*, **1963**, 1, 43-69	2.2	136
295	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	3.5	135
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292	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, 2713-26	3.9	127
291	Theoretical determination of sterically allowed conformations of a polypeptide chain by a computer method. *Biopolymers*, **1965**, 3, 155-184	2.2	126
290	Statistical mechanics of noncovalent bonds in polyamino acids. VIII. Covalent loops in proteins. *Biopolymers*, **1965**, 3, 379-399	2.2	123
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285	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		109
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281	Proline-induced constraints in alpha-helices. *Biopolymers*, **1987**, 26, 1587-600	2.2	100
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