August 28, 2006

Publications of Harold A. Scheraga

1948

1. H. A. Scheraga and M. E. Hobbs - Kinetics of the thermal chlorination of benzal chloride, J. Am. Chem. Soc., 70, 3015-3019 (1948).

1949

2. M. Manes and H. A. Scheraga - Degassing low-boiling liquids by liquid-phase condensation, J. Am. Chem. Soc., 71, 2261 (1949).

3. H. A. Scheraga, M. E. Hobbs and P. M. Gross - On the relative measurement of Kerr constants, J. Opt. Soc. Am., 39, 410-411 (1949).

4. H. A. Scheraga and M. Manes - Apparatus for fractional crystallization in vacuum, Anal. Chem., 21, 1581-1582 (1949).

1951

5. E. W. Swegler, H. A. Scheraga and E. R. VanArtsdalen - Bromination of hydrocarbons. III. Photobromination of toluene, J. Chem. Phys., 19, 135-136 (1951).

6. J. T. Edsall, H. A. Scheraga and A. Rich - Double refraction of flow:-General relations and their application to nucleic acid solutions, ACS meeting abstracts p. 5J, April 1951.

7. H. A. Scheraga - Effect of a Gaussian distribution on flow birefringence, J. Chem. Phys., 19, 983-984 (1951).

8. H. A. Scheraga, J. T. Edsall and J. O. Gadd, Jr. - Double refraction of flow: Numerical evaluation of extinction angle and birefringence as a function of velocity gradient, J. Chem. Phys., 19, 1101-1108 (1951).

   Issued as AEC report, HUX-4, Sept. 1949, Contract No. AT(30-1)497 under title: Double refraction of flow and the dimensions of large asymmetrical molecules. See also Ann. Comp. Lab. Harv. Univ., 26, 219 (1951).

9. H. A. Scheraga - Relation between extinction angle and molecular size, Arch. Biochem. and Biophys., 33, 277-281 (1951).

10. H. A. Scheraga and J. K. Backus - Flow birefringence in solutions of n-hexadecyltrimethylammonium bromide, ACS meeting abstracts, p. 13G, April 1951, J. Am. Chem. Soc., 73, 5108-5112 (1951).

*11. J. K. Backus and H. A. Scheraga - Dynamo-optical properties of detergent micelles, J. Colloid Sci., 6, 508-521 (1951).

1952

*12. M. Laskowski, Jr., D. H. Rakowitz and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion, J. Am. Chem. Soc., 74, 280 (1952).

*13. C. S. Hocking, M. Laskowski, Jr. and H. A. Scheraga - Size and shape of bovine fibrinogen, J. Am. Chem. Soc., 74, 775-778 (1952).

*14. H. A. Scheraga and J. K. Backus - Flow birefringence in arrested clotting systems, ACS meeting abstracts, p. 39C, April 1952, J. Am. Chem. Soc., 74, 1979-1983 (1952).

*15. H. A. Scheraga and L. F. Nims - The action of X-rays on fibrinogen solutions, ACS meeting abstracts, p. 44C, Sept. 1950, Arch, Biochem. and Biophys., 36, 336-344 (1952).

*16. M. Laskowski, Jr., B. L. Schapiro, T. H. Donnelly and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion, Conference of the N.R.C., Division of Medical Sciences, Subcommittee on Blood Coagulation of the Committee on Surgery, May 21, 1952.

*17. L. Mandelkern, W. R. Krigbaum, H. A. Scheraga and P. J. Flory - Sedimentation behavior of flexible chain molecules: polyisobutylene, ACS meeting abstracts, p. 50, April 1952, J. Chem. Phys., 20, 1392-1397 (1952).

*18. R. Cerf and H. A. Scheraga - Flow birefringence in solutions of macromolecules. Chem. Revs., 51, 185-261 (1952).

*19. J. K. Backus, M. Laskowski, Jr., H. A. Scheraga and L. F. Nims - Distribution of intermediate polymers in the fibrinogen-fibrin conversion, Arch. Biochem. and Biophys., 41, 354-366 (1952).

1953

20. H. A. Scheraga and L. Mandelkern - Consideration of the hydrodynamic properties of proteins, ACS meeting abstracts, p. 39C, April 1952, J. Am. Chem. Soc., 75, 179-184 (1953).

*21. C. A. Streuli, H. A. Scheraga and M. L. Nichols - X-ray investigation of several contaminated barium sulfate precipitates, Anal. Chem., 25, 306-310 (1953).

*22. B. M. Siegel, J. P. Mernan and H. A. Scheraga - The configuration of native and partially polymerized fibrinogen, Biochim. Biophys. Acta, 11, 329-336 (1953).

Presented as Abstract No. 35 at meeting of Electron Microscope Society of America, Cleveland, Nov. 1952, under title: Correlation between Electron Microscope and Flow birefringence Observations on Native and Partially Polymerized Fibrinogen, J. Appl. Phys., 24, 116 (1953).

23. H. R. Anderson, Jr., H. A. Scheraga and E. R. VanArtsdalen - Bromination of Hydrocarbons. VI. Photochemical and thermal bromination of toluene. Bond dissociation energies, J. Chem. Phys., 21, 1258-1267 (1953).

24. H. A. Saroff, N. R. Rosenthal, E. R. Adamik, N. Hages and H. A. Scheraga - The methylation of bovine serum albumin, ACS meeting abstracts, p. 16C, Sept. 1952, J. Biol. Chem., 205, 255-270 (1953).

1954

25. B. H. Eckstein, H. A. Scheraga and E. R. VanArtsdalen - Bromination of hydrocarbons. VII. Bromination of isobutane. Bond dissociation energies from bromination kinetics, J. Chem. Phys., 22, 28-35 (1954).

*26. H. A. Scheraga - Fibrinogen and its polymerization, Baskerville Chemical Journal, 5, 16-18 (1954).

27. M. Laskowski, Jr. and H. A. Scheraga - Entropy changes in protein reactions, ACS meeting abstracts, p. 60C, Sept, 1954.

28. H. A. Scheraga - Book review: -Partington, An Advanced Treatise on Physical Chemistry, Vol. 4 Physico-Chemical Optics, J. Am. Chem. Soc., 76, 5576 (1954).

*29. H. A. Scheraga, W. R. Carroll, L. F. Nims, E. Sutton, J. K. Backus and J. M. Saunders - Hydrodynamic properties of urea-denatured fibrinogen, ACS meeting abstracts, p. 20C, Sept. 1952, Abstracts of the Symposium on Macromolecules of the XIIIth International Congress of Pure and Applied Chemistry, p. 281, Aug. 1953, J. Polymer Sci., 14, 427-442 (1954).

30. M. Laskowski, Jr. and H. A. Scheraga - Thermodynamic considerations of protein reactions. I. Modified reactivity of polar groups, ACS meeting abstracts, p. 36C, Sept. 1953, p. 60C, Sept 1954, J. Am. Chem. Soc., 76, 6305-6319 (1954).

1955

*31. J. T. Edsall, G. A. Gilbert and H. A. Scheraga - The Non-clotting component of the human plasma fraction I-1 ("Cold Insoluble Globulin"), ACS meeting abstracts, p. 33C, Sept. 1947, J. Am. Chem. Soc., 77, 157-161 (1955).

32. H. A. Scheraga - Rotary diffusion coefficients of proteins, Fed. Proc., 14, No. 894, p. 276, March 1955.

*33. E. V. Gouinlock, Jr., P. J. Flory and H. A. Scheraga - Molecular configuration of gelatin, J. Polymer Sci., 16, 383-395 (1955).

34. H. A. Saroff, G. I. Loeb and H. A. Scheraga - Low and high pH effects in serum albumin, J. Am. Chem. Soc., 77, 2908-2909 (1955).

*35. T. H. Donnelly, M. Laskowski, Jr., N. Notley and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. II. Reversibility of the polymerization steps, ACS meeting abstracts, p. 37C, Sept. 1953, Arch. Biochem. and Biophys., 56, 369-387 (1955).

36. H. A. Scheraga - Non-Newtonian viscosity of solutions of ellipsoidal particles, J. Chem. Phys., 23, 1526-1532 (1955).

37. J. M. Sturtevant, M. Laskowski, Jr., T. H. Donnelly and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. III. Heats of polymerization and clotting of fibrin monomer, J. Am. Chem. Soc., 77, 6168-6172 (1955).

1956

*38. H. A. Scheraga - Book Review:-Weissberger, Technique of Organic Chemistry, Vol. I., part III, J. Polymer Sci., 19, 593-594 (1956).

*39. M. Laskowski, Jr., J. M. Widom, M. L. McFadden and H. A. Scheraga - Differential ultraviolet spectra of insulin, ACS meeting abstracts, p. 24C, Sept. 1955, Biochim. Biophys. Acta, 19, 581-582 (1956).

40. H. A. Scheraga, G. I. Loeb and M. L. Wagner - Hydrodynamic properties, molecular configuration and reactivity of bovine serum albumin, Fed. Proc., 15, No. 1138, p. 348, March 1956.

*41. M. L. Wagner and H. A. Scheraga - Gouy diffusion studies of bovine serum albumin, J. Phys. Chem., 60, 1066-1076 (1956).

*42. M. L. Hunt, S. Newman, H. A. Scheraga and P. J. Flory - Dimensions and hydrodynamic properties of cellulose trinitrate molecules in dilute solutions, ACS meeting abstracts, p. 7R, April 1955, J. Phys. Chem., 60, 1278-1290 (1956).

43. M. Laskowski, Jr., T. H. Donnelly, B. A. Van Tijn and H. A. Scheraga - The Proteolytic Action of Thrombin on Fibrinogen, ACS meeting abstracts, p. 21C, Sept. 1952, J. Biol. Chem., 222, 815-821 (1956).

44. M. Laskowski, Jr. and H. A. Scheraga - Thermodynamic considerations of protein reactions. II. Modified reactivity of primary valence bonds. ACS meeting abstracts, p. 36C, Sept. 1953, J. Am. Chem. Soc., 78, 5793-5798 (1956).

45. G. I. Loeb and H. A. Scheraga - Hydrodynamic and thermo-dynamic properties of bovine serum albumin at low pH, J. Phys. Chem., 60, 1633-1644 (1956).

1957

*46. H. A. Scheraga - Tyrosyl-carboxylate ion hydrogen bonding in ribonuclease, Biochim. Biophys. Acta, 23, 196-197 (1957).

47. H. A. Scheraga - Some aspects of the gross and internal configurations of proteins. (Eli Lilly Award Address). ACS meeting abstracts, p. 55C, April 1957.

48. H. A. Scheraga - The role of tertiary structure in the reactions of several proteins, Gordon Conference, July 1957.

49. S. Ehrenpreis and H. A. Scheraga - Observations on the analysis for thrombin and the inactivation of fibrin monomer, ACS meeting abstracts, p. 71C, Sept. 1956, J. Biol. Chem., 227, 1043-1061 (1957).

50. S. Ehrenpreis, S. J. Leach and H. A. Scheraga - Action of thrombin on lysine substrates, J. Am. Chem. Soc., 79, 6086 (1957).

51. H. A. Scheraga and M. Laskowski, Jr. - The fibrinogen-fibrin conversion, Adv. Prot. Chem., 12, 1-131 (1957).

1958

52. S. J. Leach and H. A. Scheraga - Preparation, sedimentation, and deuterium exchange studies of the oxidized A and B chains of insulin, Compt. rend. Lab. Carlsberg, Ser. Chim., 30, 271-290 (1958).

53. H. A. Scheraga and L. Mandelkern - On the interpretation of hydrodynamic data for dilute protein solutions, J. Phys. Chem., 62, 370 (1958).

54. J. W. Donovan, M. Laskowski, Jr. and H. A. Scheraga - Influence of ionization of carboxyl groups on the ultraviolet absorption spectrum of lysozyme, ACS meeting abstracts, p. 48C, April 1957, Biochim. Biophys. Acta, 29, 455-456 (1958).

*55. H. A. Scheraga, S. Ehrenpreis and E. Sullivan - Comparative kinetic behavior of thrombin, plasmin and trypsin toward synthetic substrates, Nature, 182, 461-462 (1958).

56. S. Ehrenpreis, M. Laskowski, Jr., T. H. Donnelly and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. IV. Kinetics of the conversion of fibrinogen to fibrin monomer. ACS meeting abstracts, p. 49C, April 1957, J. Am. Chem. Soc., 80, 4255-4263 (1958).

57. H. A. Scheraga - Thrombin and its interaction with fibrinogen, Ann. New York Acad. Sci., 75, 189-194 (1958).

1959

58. S. Ehrenpreis and H. A. Scheraga - Kinetics of the conversion of fibrinogen to fibrin monomer at neutral pH, Arch. Biochem. and Biophys., 79, 27-43 (1959).

59. L. Gruen, M. Laskowski, Jr. and H. A. Scheraga - Preparation and characterization of a fully iodinated insulin derivative, ACS meeting abstracts, p. 48C, April 1957, J. Biol. Chem., 234, 2050-2053 (1959).

*60. L. Gruen, M. Laskowski, Jr. and H. A. Scheraga - Thermodynamics of the ionization of the lysyl residue of insulin, ACS meeting abstracts, p. 48C, April 1957, J. Am. Chem. Soc., 81, 3891-3901 (1959).

61. H. A. Scheraga - Proteins and synthetic polypeptides, Ann. Rev. Phys. Chem., 10, 191-218 (1959).

*62. H. A. Scheraga and S. Ehrenpreis - Kinetics of the fibrinogen-fibrin conversion, Proc. IVth International Congress of Biochemistry, Vienna, 1958, 10, 212-227 (1959).

*63. M. Calvin, J. Hermans, Jr. and H. A. Scheraga - Effect of deuterium on the strength of hydrogen bonds, J. Am. Chem. Soc., 81, 5048-5050 (1959).

64. J. W. Donovan, M. Laskowski, Jr. and H. A. Scheraga - Carboxyl group interactions in lysozyme, ACS meeting abstracts, p. 48C, April 1957, J. Molecular Biol., 1, 293-296 (1959).

*65. J. Hermans, Jr. and H. A. Scheraga - The thermallyinduced configurational change of ribonuclease in H_2O and D_2O, Biochim. Biophys. Acta, 36, 534-535 (1959).

1960

*66. C-Y. Cha and H. A. Scheraga - Structural studies of ribonuclease. I. Hydrogen ion equilibria in a denaturing solvent, ACS meeting abstracts, p. 43C, Sept. 1959, J. Am. Chem. Soc., 82, 54-58 (1960).

*67. C. L. Schildkraut and H. A. Scheraga - Structural Studies of Ribonuclease. II. Deuterium exchange studies of two crystalline forms of ribonuclease, ACS meeting abstracts, p. 43C, Sept. 1959, J. Am. Chem. Soc., 82, 58-62 (1960).

*68. J. Hermans, Jr., J. W. Donovan and H. A. Scheraga - Thermodynamic data from difference spectra. ACS meeting abstracts, p. 42C, Sept. 1958, J. Biol. Chem., 235, 91-93 (1960).

*69. M. Laskowski, Jr., S. J. Leach and H. A. Scheraga - Tyrosyl hydrogen bonds in insulin, ACS meeting abstracts, p. 48C, April 1957, J. Am. Chem. Soc., 82, 571-582 (1960).

70. M. Laskowski, Jr., S. Ehrenpreis, T. H. Donnelly and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. V. Reversibility and thermodynamics of the proteolytic action of thrombin on fibrinogen. ACS meeting abstracts, p. 23C, Sept. 1955, J. Am. Chem. Soc., 82, 1340-1348 (1960).

*71. H. A. Scheraga, C-Y. Cha, J. Hermans, Jr. and C. L. Schildkraut - Internal hydrogen bonding in ribonuclease. ACS meeting abstracts, p. 43C, Sept. 1959. Amino Acids, Proteins and Cancer Biochemistry, p. 31-41, Academic Press, NY (1960).

72. J. W. Donovan, M. Laskowski, Jr. and H. A. Scheraga - Abnormal ionizable groups in lysozyme, ACS meeting abstracts, p. 48C, April 1957, and p. 35C, Sept. 1959, J. Am. Chem. Soc., 82, 2154-2163 (1960).

73. H. A. Scheraga - Structural studies of ribonuclease. III. A model for the secondary and tertiary structure. ACS meeting abstracts, p. 43C, Sept. 1959, J. Am. Chem. Soc., 82, 3847-3852 (1960).

74. S. J. Leach and H. A. Scheraga - Effect of light scattering on ultraviolet difference spectra, J. Am. Chem. Soc., 82, 4790-4792 (1960).

*75. J. Hermans, Jr. and H. A. Scheraga - Structural studies of ribonuclease. IV. The near infrared absorption of the hydrogen-bonded peptide NH group. ACS meeting abstracts, p. 41C, Sept. 1960, J. Am. Chem. Soc., 82, 5156-5160 (1960).

76. H. A. Scheraga and R. Signer - Streaming birefringence, Ch. 35, p. 2387-2457, in Weissberger, Technique of Organic Chemistry, Vol. I, Part III, 3rd ed., New York (1960).

77. S. J. Leach and H. A. Scheraga - Ultraviolet difference spectra and the internal structure of proteins, J. Biol. Chem., 235, 2827-2829 (1960).

78. J. A. Rupley and H. A. Scheraga - Digestion of ribonuclease A with chymotrypsin and trypsin at high temperatures, Biochim. Biophys. Acta, 44, 191-193 (1960).

79. J. R. Sharpsteen, Jr., H. A. Scheraga and J. S. Butterworth - Method for analyzing materials, U.S. Patent 2,962,425, Nov. 29, 1960.

80. H. A. Scheraga - Deuterium exchange studies and protein structure, Brookhaven Symposia in Biology, 13, 71-88 (1960).

81. H. A. Scheraga - Helix-random coil transformations in deuterated macromolecules, Ann. N. Y. Acad. Sci., 84, 608-616 (1960).

82. H. A. Scheraga - Influence of side-chain hydrogen bonds on the elastic properties of protein fibers and on the configurations of proteins in solution. ACS meeting abstracts, p. 51C, Sept. 1958, J. Phys. Chem., 64, 1917-1926 (1960).

1961

83. M. Laskowski, Jr. and H. A. Scheraga - Thermodynamic considerations of protein reactions. III. Kinetics of protein denaturation. ACS meeting abstracts, p. 36C, Sept. 1953, J. Am. Chem. Soc., 83, 266-274 (1961).

84. C. A. Broomfield and H. A. Scheraga - Electrochemical analysis of protein mixtures on paper, Fed. Proc., 20, 380, March 1961.

85. A. Nakajima and H. A. Scheraga - Thermodynamic study of shrinkage and of phase equilibrium under stress in films made from ribonuclease. ACS meeting abstracts, p. 42C, Sept. 1960, J. Am. Chem. Soc., 83, 1575-1584 (1961).

86. A. Nakajima and H. A. Scheraga - Thermodynamic study of shrinkage in fibers made from insulin. ACS meeting abstracts, p. 32C, Sept. 1959, J. Am. Chem. Soc., 83, 1585-1589 (1961).

*87. H. A. Scheraga, R. A. Scott, G. I. Loeb, A. Nakajima and J. Hermans, Jr. - The sharpness of the transition in reversible protein denaturation, J. Phys. Chem., 65, 699 (1961).

88. C-Y. Cha and H. A. Scheraga - Differentiation of the tyrosyl groups of ribonuclease A by iodination, Biochem. Biophys. Res. Comm., 5, 67-70 (1961).

89. H. A. Scheraga - Effect of hydrophobic bonding on protein reactions, J. Phys. Chem., 65, 1071-1072 (1961).

90. H. A. Scheraga and M. A. Cohly - Physical chemical studies of thrombin, 9th Annual Symposium on Blood, Jan. 20-21, 1961, Thrombosis et Diathesis Haemorrhagica, 5, 609 (1961).

91. J. W. Donovan, M. Laskowski, Jr. and H. A. Scheraga - The effects of charged groups on the chromophores of lysozyme and of amino acids. ACS meeting abstracts, p. 48C, April 1957, J. Am. Chem. Soc., 83, 2686-2694 (1961).

*92. C. A. Broomfield and H. A. Scheraga - A method of scanning paper electrophoresis strips and its application to the study of plasma proteins, J. Biol. Chem., 236, 1960-1967 (1961).

93. H. A. Scheraga - "Protein Structure", Academic Press, N.Y. (1961).

*94. J. Hermans, Jr. and H. A. Scheraga - Structural studies of ribonuclease. V. Reversible change of configuration. ACS meeting abstracts, p. 42C, Sept. 1958, J. Am. Chem. Soc., 83, 3283-3292 (1961).

*95. J. Hermans, Jr. and H. A. Scheraga - Structural studies of ribonuclease. VI. Abnormal ionizable groups. ACS meeting abstracts, p. 42C, Sept. 1958, J. Am. Chem. Soc., 83, 3293-3300 (1961).

96. H. A. Scheraga - Protein denaturation, Proc. Vth International Congress of Biochemistry, Moscow, 1961, p. 59 of abstracts.

*97. M. A. Cohly and H. A. Scheraga - Aggregation of thrombin, Arch. Biochem. and Biophys., 95, 428-434 (1961).

*98. C-Y. Cha and H. A. Scheraga - Location of the three buried tyrosyl groups of ribonuclease A, Biochem. Biophys. Res. Comm., 6, 369-372 (1962).

1962

99. H. A. Scheraga - Configurational changes in protein fibers, Abstr. of 4th Delaware Valley Regional Meeting, ACS, p. 122, Jan. 25, 1962.

*100. G. Loeb and H. A. Scheraga - The thermally-induced transition in fibrin. ACS meeting abstracts, p. 16I, April, 1959, J. Am. Chem. Soc., 84, 134-142 (1962).

*101. L. M. Riddiford and H. A. Scheraga - Structural studies of paramyosin. I. Hydrogen ion equilibria. ACS meeting abstracts, p. 15C, Sept. 1961, Biochemistry, 1, 95-107 (1962).

*102. L. M. Riddiford and H. A. Scheraga - Structural studies of paramyosin. II. Conformational changes. ACS meeting abstracts, p. 15C, Sept. 1961, Biochemistry, 1, 108-114 (1962).

*103. G. Némethy and H. A. Scheraga - The structure of water and hydrophobic bonding in proteins. I. A model for the thermodynamic properties of liquid water. ACS meeting abstracts, p. 4C, Sept. 1960, J. Chem. Phys., 36, 3382-3400 (1962).

*104. G. Némethy and H. A. Scheraga - The structure of water and hydrophobic bonding in proteins. II. A model for the thermodynamic properties of aqueous solutions of hydrocarbons. ACS meeting abstracts, p. 4C, Sept. 1960, J. Chem. Phys., 36, 3401-3417 (1962).

*105. J. A. Rupley, T. Ooi and H. A. Scheraga - Limited proteolysis of ribonuclease-active components, Biochem. Biophys. Res. Comm., 8, 147-150 (1962).

*106. H. A. Scheraga - Effect of side-chain hydrogen bonds, hydrophobic bonds, and covalent cross-links on protein conformation in solution, in "Polyamino Acids, Polypeptides, and Proteins", Ed. M. A. Stahmann, p. 241-249, Univ. of Wisconsin Press, Madison (1962).

*107. Y. V. Wu and H. A. Scheraga - Studies of soybean trypsin inhibitor. I. Physicochemical properties, Biochemistry, 1, 698-705 (1962).

*108. I. Z. Steinberg and H. A. Scheraga - Chromatography on columns packed with a non-polar material, J. Am. Chem. Soc., 84, 2890-2892 (1962).

*109. H. A. Scheraga, G. Némethy and I. Z. Steinberg - The contribution of hydrophobic bonds to the thermal stability of protein conformations, J. Biol. Chem., 237, 2506-2508 (1962).

*110. H. A. Scheraga and J. A. Rupley - The structure and function of ribonuclease, Adv. in Enzymology, 24, 161-261 (1962).

111. E. E. Schrier, C. A. Broomfield and H. A. Scheraga - Molecular weight of bovine thrombin, Arch. Biochem. Biophys., Suppl. 1, 309-318 (1962).

*112. Y. V. Wu and H. A. Scheraga - Studies of soybean trypsin inhibitor. II. Conformational properties, Biochemistry, 1, 905-911 (1962).

113. G. Némethy and H. A. Scheraga - The structure of water and hydrophobic bonding in proteins. III. The thermodynamic properties of hydrophobic bonds in proteins. ACS meeting abstracts, p. 4C, Sept. 1960; Colloid Symp., June, 1962, J. Phys. Chem., 66, 1773-1789 (1962). Erratum:-J. Phys. Chem., 67, 2888 (1963).

*114. E. E. Schrier and H. A. Scheraga - The effect of aqueous alcohol solutions on the thermal transition of ribonuclease, Biochim. Biophys. Acta, 64, 406-408 (1962).

115. H. A. Scheraga - Purification of clotting factors from a physico-chemical viewpoint. "Progress in Coagulation", p. 186, Friedrich-Karl Schattauer-Verlag, Stuttgart, (1962).

1963

*116. I. Z. Steinberg and H. A. Scheraga - Entropy changes accompanying association reactions of proteins. ACS meeting abstracts, p. 59C, Sept. 1962, J. Biol. Chem., 238, 172-181 (1963).

117. G. Némethy, I. Z. Steinberg and H. A. Scheraga - The influence of water structure and of hydrophobic interactions on the strength of side-chain hydrogen bonds in proteins. ACS meeting abstracts, p. 58C, Sept. 1962, Biopolymers, 1, 43-69 (1963).

*118. J. A. Rupley and H. A. Scheraga - Structural studies of ribonuclease. VII. Chymotryptic hydrolysis of ribonuclease A at elevated temperatures. ACS meeting abstracts, p. 16C, Sept. 1961, Biochemistry, 2, 421-431 (1963).

*119. T. Ooi, J. A. Rupley and H. A. Scheraga - Structural studies of ribonuclease. VIII. Tryptic hydrolysis of ribonuclease A at elevated temperature. ACS meeting abstracts, p. 47C, Sept. 1962, Biochemistry, 2, 432-437 (1963).

*120. J. Hermans, Jr., S. J. Leach and H. A. Scheraga - Thermodynamic data from difference spectra. II. Hydrogen bonding in salicylic acid and its implications for proteins, ACS meeting abstracts, p. 42C, Sept. 1958, J. Am. Chem. Soc., 85, 1390-1395 (1963).

121. H. A. Scheraga - Reactions of proteins; denaturation. In "Comprehensive Biochemistry" (Ed. M. Florkin and E.H. Stotz), Vol. 7 Part 1, p. 148, Elsevier, Amsterdam (1963).

*122. C-Y. Cha and H. A. Scheraga - The buried tyrosyl residues of ribonuclease. I. Differential rates of iodination, J. Biol. Chem., 238, 2958-2964 (1963).

123. C-Y. Cha and H. A. Scheraga - The buried tyrosyl residues of ribonuclease. II. Positions in the amino acid sequence, J. Biol. Chem., 238, 2965-2975 (1963).

124. M. Bixon, H. A. Scheraga and S. Lifson - Effect of hydrophobic bonding on the stability of poly-L-alanine helices in water, Biopolymers, 1, 419-429 (1963).

125. D. J. Winzor and H. A. Scheraga - Studies of chemically reacting systems on sephadex. I. Chromatographic demonstration of the Gilbert theory, Biochemistry, 2, 1263-1267 (1963).

126. T. B. Paiva, A. C. M. Paiva and H. A. Scheraga - The conformation of angiotensin II in aqueous solution, Biochemistry, 2, 1327-1334 (1963).

127. R. A. Scott and H. A. Scheraga - Structural studies of ribonuclease. XI. Kinetics of denaturation. ACS meeting abstracts, p. 99C, Sept. 1963, J. Am. Chem. Soc., 85, 3866-3873 (1963).

128. H. A. Scheraga - Intramolecular bonds in proteins. II. Noncovalent bonds. In "The Proteins", 2nd Ed., (Ed. H. Neurath), Academic Press, New York, Vol. 1, Ch. 6, p. 477-594 (1963).

1964

*129. D. J. Winzor and H. A. Scheraga - Studies of chemically reacting systems on sephadex. II. Molecular weights of monomers in rapid association equilibrium, J. Phys. Chem., 68, 338-343 (1964).

130. D. J. Winzor and H. A. Scheraga - Titration behavior of bovine thrombin, Arch. Biochem. Biophys., 104, 202-207 (1964).

131. H. A. Scheraga, G. Némethy, E. E. Schrier, H. Schneider and G. C. Kresheck - Theoretical and experimental studies of hydrophobic bonding, Fed. Proc., 23, 215 (1964).

*132. T. Ooi and H. A. Scheraga - Structural studies of ribonuclease. XII. Enzymic hydrolysis of active tryptic modifications of ribonuclease, Biochemistry, 3, 641-647 (1964).

*133. T. Ooi and H. A. Scheraga - Structural studies of ribonuclease. XIII. Physicochemical properties of tryptic modifications of ribonuclease, Biochemistry, 3, 648-652 (1964).

*134. G. Némethy and H. A. Scheraga - Structure of water and hydrophobic bonding in proteins. IV. The thermodynamic properties of liquid deuterium oxide, J. Chem. Phys., 41, 680-689 (1964).

135. T. Ooi and H. A. Scheraga - Structural studies of ribonuclease. XIV. Tryptic hydrolysis of ribonuclease in propyl alcohol solution, Biochemistry, 3, 1209-1213 (1964).

*136. E. E. Schrier, M. Pottle and H. A. Scheraga - The influence of hydrogen and hydrophobic bonds on the stability of the carboxylic acid dimers in aqueous solution, J. Am. Chem. Soc., 86, 3444-3449 (1964).

137. H. A. Scheraga - Role of hydrophobic bonding in protein structure, Ber. d. Bunsengesellschaft f. phys. Chem.,68, 838-839 (1964).

1965

138. E. E. Schrier, R. T. Ingwall and H. A. Scheraga - The effect of aqueous alcohol solutions on the thermal transition of ribonuclease, J. Phys. Chem., 69, 298-303 (1965).

*139. H. A. Scheraga, G. Némethy, S. J. Leach, R. A. Scott and D. C. Poland - Theoretical calculations of protein structure and stability, Fed. Proc., 24, 413 (1965).

*140. R. A. Scott and H. A. Scheraga - A Method for calculating internal rotation barriers, J. Chem. Phys., 42, 2209-2215 (1965).

*141. C. A. Broomfield, J. P. Riehm and H. A. Scheraga - The abnormal carboxyl groups of ribonuclease. I. Preparation and properties of methylated ribonuclease, ACS meeting Abstracts, p. 15C, Sept. 1961, Biochemistry, 4, 751-759 (1965).

*142. J. P. Riehm, C. A. Broomfield and H. A. Scheraga - The abnormal carboxyl groups of ribonuclease. II. Positions in the amino acid sequence, ACS meeting abstracts, p.15C, Sept. 1961, Biochemistry, 4, 760-771 (1965).

*143. J. P. Riehm and H. A. Scheraga - Structural studies of ribonuclease. XVII. A reactive carboxyl group in ribonuclease, Biochemistry, 4, 772-782 (1965).

*144. H. Schneider, G. C. Kresheck and H. A. Scheraga - Thermodynamic parameters of hydrophobic bond formation in a model system, ACS meeting abstracts, p. 24A, Jan. 1964, J. Phys. Chem., 69, 1310-1324 (1965).

145. G. Némethy and H. A. Scheraga - Theoretical determination of sterically allowed conformations of a polypeptide chain by a computer method, Biopolymers, 3, 155-184 (1965).

146. G. C. Kresheck and H. A. Scheraga - The temperature dependence of the enthalpy of formation of the amide hydrogen bond; the urea model, J. Phys. Chem., 69, 1704-1706 (1965).

*147. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent bonds in polyamino acids. I. Hydrogen bonding of solutes in water, and the binding of water to polypeptides, Biopolymers, 3, 275-282 (1965); 3, 593 (1965).

*148. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent bonds in polyamino acids. II. Combinatorial formulation for short chains, including hydrophobic bonding in random coil, Biopolymers, 3, 283-304 (1965).

*149. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent bonds in polyamino acids. III. Interhelical hydrophobic bonds in short chains, Biopolymers, 3, 305-313 (1965).

*150. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent 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, 3, 315-334 (1965).

*151. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent 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, 3, 335-355 (1965).

*152. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent bonds in polyamino acids. VI. A simple model for side-chain hydrogen bonds between helices, Biopolymers, 3, 357-367 (1965).

*153. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent bonds in polyamino acids. VII. Fluorescence as an indication of conformation, Biopolymers, 3, 369-377 (1965).

*154. D. C. Poland and H. A. Scheraga - Statistical mechanics of noncovalent bonds in polyamino acids. VIII. Covalent loops in proteins, Biopolymers, 3, 379-399 (1965).

*155. D. C. Poland and H. A. Scheraga - Statistical mechanics of non-covalent bonds in polyamino acids. IX. The two-state theory of protein denaturation, Biopolymers, 3, 401-419 (1965).

*156. D. C. Poland and H. A. Scheraga - Hydrophobic bonding and micelle stability, J. Phys. Chem., 69, 2431-2442 (1965); 69, 4425 (1965).

157. H. A. Scheraga - Proc. Welch Found. Conf. on Chem. Res. VIII. Selected Topics in Modern Biochemistry, Nov.16-18, 1964; 149 (1965).

158. G. F. Endres, S. Ehrenpreis and H. A. Scheraga - Covalent bonding in the reversible polymerization of fibrin monomer, Biochim. Biophys. Acta, 104, 620-623 (1965).

*159. A. Y. Moon, D. C. Poland and H. A. Scheraga - Thermodynamic data from fluorescence spectra. I. The system phenol-acetate, J. Phys. Chem., 69, 2960-2966 (1965).

*160. G. C. Kresheck, H. Schneider and H. A. Scheraga - The effect of D_2O on the thermal stability of proteins. Thermodynamic parameters for the transfer of model compounds from H_2O to D_2O, J. Phys. Chem., 69, 3132-3144 (1965).

161. D. C. Poland and H. A. Scheraga - Comparison of theories of the helix-coil transition in polypeptides, J. Chem. Phys., 43, 2071-2074 (1965); Erratum:-J. Chem. Phys.,43, 3774 (1965).

*162. H. Fujioka and H. A. Scheraga - Structural studies of ribonuclease. XVIII. An investigation of the peptic digestion products of ribonuclease, Biochemistry, 4, 2197-2205 (1965).

*163. H. Fujioka and H. A. Scheraga - Structural studies of ribonuclease. XIX. Location of the buried tyrosylresidue in pepsin-inactivated ribonuclease, Biochemistry, 4, 2206-2218 (1965).

*164. H. A. Scheraga - The effect of solutes on the structure of water and its implications for protein structure, Ann. N. Y. Acad. Sci., 125, 253-276 (1965).

*165. M. R. Thomas, H. A. Scheraga and E. E. Schrier - A near-infrared study of hydrogen bonding in water and deuterium oxide, J. Phys. Chem., 69, 3722-3726 (1965).

*166. M. E. Friedman and H. A. Scheraga - Volume changes in hydrocarbon-water systems. Partial molal volumes of alcohol-water solutions, J. Phys. Chem., 69, 3795-3800 (1965).

167. H. A. Scheraga - Calculation of protein conformation from amino acid sequence, Abstr. of Meeting of the British Biophysical Society, Dec. 1965, London.

*168. H. A. Scheraga, S. J. Leach, R. A. Scott and G. Némethy - Intramolecular forces and protein conformation, Disc. Faraday Soc., 40, 268-277 (1965).

1966

169. J.N. Vournakis, H.A. Scheraga, G.W. Rushizky and H.A. Sober - Neighbor-neighbor interactions in single-strand polynucleotides; optical rotatory dispersion studies of the ribonucleotide ApApCp, ACS meeting abstracts, p.65C, Sept. 1965, Biopolymers, 4, 33-41 (1966).

*170. J. P. Riehm and H. A. Scheraga - Structural studies of ribonuclease. XX. Acrylonitrile. A reagent for blocking the amino groups of lysine residues in ribonuclease, Biochemistry, 5, 93-99 (1966).

*171. J. P. Riehm and H. A. Scheraga - Structural studies of ribonuclease. XXI. The reaction between ribonuclease and a water-soluble carbodiimide, Biochemistry, 5, 99-115 (1966).

172. G.C. Kresheck, E. Hamori, G. Davenport and H.A. Scheraga - Determination of the dissociation rate of dodecylpyridinium iodide micelles by a temperature- jump technique, ACS meeting abstracts, p. 8V, Sept. 1965, J.Am. Chem. Soc., 88, 246-253 (1966).

173. G. Némethy, S. J. Leach and H. A. Scheraga - Peptide sequence and permitted conformations, Abstr. of First Middle Atlantic Regional Meeting, ACS, p. Feb. 3-4,1966.

*174. J. T. Edsall, P. J. Flory, J. C. Kendrew, A. M. Liquori, G. Némethy, G. N. Ramachandran and H. A. Scheraga - A proposal of standard conventions and nomenclature for the description of polypeptide conformations, Biopolymers, 4, 121-130 (1966), J. Biol. Chem., 241, 1004-1008 (1966), J. Molecular Biol., 15, 399-407(1966).

175. D. Poland, J. N. Vournakis and H. A. Scheraga - Cooperative interactions in single-strand oligomers of adenylic acid, Biopolymers, 4, 223-235 (1966).

176. R. A. Scott and H. A. Scheraga - Conformational analysis of macromolecules. I. Ethane, propane, n-butane, and n-pentane, Biopolymers, 4, 237-238 (1966).

177. N. Lotan, A. Berger, E. Katchalski, R. T. Ingwall and H. A. Scheraga - The thermal melting of poly-L-alanine helices in water, Biopolymers, 4, 239-241 (1966).

178. H. A. Scheraga, R. A. Scott and K. D. Gibson - Calculations of stable polypeptide conformations, Fed. Proc., 25, 345 (1966).

*179. D. C. Poland and H. A. Scheraga - Hydrophobic bonding and micelle stability; the influence of ionic head groups, J. Colloid and Interface Science, 21, 273-283 (1966).

*180. G. Némethy, S. J. Leach and H. A. Scheraga - The influence of amino acid side chains on the free energy of helix-coil transitions, J. Phys. Chem., 70, 998-1004 (1966).

*181. S. J. Leach, G. Némethy and H. A. Scheraga - Computation of the sterically allowed conformations of peptides, Biopolymers, 4, 369-407 (1966).

*182. R. A. Scott and H. A. Scheraga - Conformational analysis of macromolecules. II. The rotational isomeric states of the normal hydrocarbons, J. Chem. Phys., 44, 3054-3069 (1966).

183. G. F. Endres, S. Ehrenpreis and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. VI. Ionization changes in the reversible polymerization of fibrin monomer, ACS meeting abstracts, p. 26C, April 1958, Biochemistry, 5, 1561-1567 (1966).

184. G. F. Endres and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. VII. On the mechanism of the reversible polymerization of fibrin monomer, Biochemistry, 5, 1568-1577 (1966).

*185. R. W. Woody, M. E. Friedman and H. A. Scheraga - Structural studies of ribonuclease. XXII. Location of the third buried tyrosyl residue in ribonuclease, Biochemistry, 5, 2034-2042 (1966).

*186. L.-K. Li, J. P. Riehm and H. A. Scheraga - Structural studies of ribonuclease. XXIII. Pairing of the tyrosyl and carboxyl groups, Biochemistry, 5, 2043-2048 (1966).

187. K. D. Gibson and H. A. Scheraga - Influence of flexibility on the energy contours of dipeptide maps, Biopolymers, 4, 709-712 (1966).

*188. H. A. Scheraga - Principles of protein structure, in "Molecular Architecture in Cell Physiology" (Ed. by T. Hayashi and A. G. Szent-Györgyi), Prentice-Hall, Englewood Cliffs, N. J., p. 39-61 (1966).

189. S. J. Leach, G. Némethy and H. A. Scheraga - Intramolecular steric effects and hydrogen bonding in regular conformations of polyamino acids, Biopolymers, 4, 887-904 (1966).

*190. D. Poland and H. A. Scheraga - Phase transitions in one dimension, and the helix-coil transition in polyamino acids, ACS meeting abstracts, p. V41, Sept. 1966, J. Chem. Phys., 45, 1456-1463 (1966).

*191. D. Poland and H. A. Scheraga - Occurrence of a phase transition in nucleic acid models, ACS meeting abstracts, p. V41, Sept. 1966, J. Chem. Phys., 45, 1464-1469 (1966).

*192. G. Vanderkooi, S. J. Leach, G. Némethy, R. A. Scott and H. A. Scheraga - Initial attempts at a theoretical calculation of the conformation of gramicidin-S, Biochemistry, 5, 2991-2997 (1966).

*193. J. N. Vournakis and H. A. Scheraga - Optical rotatory dispersion studies of yeast alanine and tyrosine transfer ribonucleic acids. Evidence for intramolecular hydrogen bonding and discussion of conformational aspects, Biophys. Soc. meeting abstracts, p. 54, Feb. 1966, Biochemistry, 5, 2997-3006 (1966).

*194. J. H. Bradbury and H. A. Scheraga - Structural studies of ribonuclease. XXIV. The application of nuclear magnetic resonance spectroscopy to distinguish between the histidine residues of ribonuclease, meeting of the Australian Biochemical Society, p. 88, May 1966, J. Am. Chem. Soc., 88, 4240-4246 (1966).

195. D. Poland and H. A. Scheraga - Kinetics of the helix-coil transition in polyamino acids, J. Chem. Phys., 45, 2071-2090 (1966).

196. R. A. Scott and H. A. Scheraga - Conformational analysis of macromolecules. III. Helical structures of poly-glycine and poly-L-alanine, J. Chem. Phys., 45, 2091-2101 (1966).

197. G. C. Kresheck and H. A. Scheraga - Structural studies of ribonuclease. XXV. Enthalpy changes accompanying acid denaturation, J. Am. Chem. Soc., 88, 4588-4591 (1966).

198. H. H. Rüterjans and H. A. Scheraga - Chemical-shift data for water and aqueous solutions, J. Chem. Phys., 45, 3296-3298 (1966).

*199. G. G. Hammes and H. A. Scheraga - A model of ribonuclease based on chemical evidence, Biochemistry, 5, 3690-3693 (1966).

*200. T. Ooi, R. A. Scott, G. Vanderkooi, R. F. Epand and H. A. Scheraga - Stable conformations of polyamino acid helices, J. Am. Chem. Soc., 88, 5680 (1966).

*201. M. E. Friedman, H. A. Scheraga and R. F. Goldberger - Structural studies of ribonuclease. XXVI. The role of tyrosine 115 in the refolding of ribonuclease, ACS meeting abstracts, p. C221, Sept. 1966, Biochemistry, 5, 3770-3778 (1966).

202. M. E. Friedman and H. A. Scheraga - Iodination of ribonuclease in the presence of cytidine 3'-phosphate, Biochim. Biophys. Acta, 128, 576-578 (1966).

1967

203. H. A. Scheraga - Calculation of polypeptide conformation, Abstr. of Second Middle Atlantic Regional Meeting, ACS, p. 104, Feb. 6-7, 1967.

204. H. A. Scheraga - Calculation of polypeptide conformation from amino acid sequence, ACS meeting abstracts, p. 41S, April 1967.

205. H. A. Scheraga, G. Vanderkooi, K. D. Gibson, R. A. Scott, T. Ooi and D. Poland - Computation of polypeptide conformations of minimum energy, Fed. Proc., 26, 720 (1967).

206. G. Némethy, D. C. Phillips, S. J. Leach and H. A. Scheraga - A second right-handed helical structure with the parameters of the Pauling-Corey α-helix, Nature, 214, 363-365 (1967).

207. J. N. Vournakis, D. Poland and H. A. Scheraga - Anti-cooperative interactions in single-strand oligomers of deoxyriboadenylic acid, Biopolymers, 5, 403-422 (1967).

208. T. Ooi, R. A. Scott, G. Vanderkooi and H. A. Scheraga - Conformational analysis of macromolecules. IV. Helical structures of poly-L-alanine, poly-L-valine, poly-β-methyl-L-aspartate, poly-γ-methyl-L-glutamate, and poly-L-tyrosine, J. Chem. Phys., 46, 4410-4426 (1967).

*209. D. Poland and H. A. Scheraga - Theory of noncovalent structure in polyamino acids, in "Poly-α-Amino Acids", (G. D. Fasman, ed.), Marcel Dekker, Inc., New York, 1967, p. 391.

210. R. M. Epand and H. A. Scheraga - Enthalpy of stacking in single-stranded polyriboadenylic acid, ACS meeting abstracts, p. C65, Sept. 1966, J. Am. Chem. Soc., 89, 3888-3892 (1967).

*211. H. A. Scheraga - Contractility and conformation, J. General Physiology, 50, 5-27 (1967).

212. H. A. Scheraga, R. A. Scott, G. Vanderkooi, S. J. Leach, K. D. Gibson, T. Ooi and G. Némethy - Calculations of polypeptide structures from amino acid sequence, in "Conformation of Biopolymers" (G. N. Ramachandran, ed.), Academic Press, London, 1967, p. 43-60.

*213. K. D. Gibson and H. A. Scheraga - Minimization of polypeptide energy. I. Preliminary structures of bovine pancreatic ribonuclease S-peptide, Proc. Natl. Acad. Sci., U.S., 58, 420-427 (1967).

214. H. A. Scheraga - Calculation of polypeptide conformation, Proc. VIIth International Congress of Biochemistry, Tokyo, 1967, p. 171 of abstracts.

*215. H. A. Scheraga - Structural studies of pancreatic ribonuclease, Fed. Proc., 26, 1380-1387 (1967).

*216. C. A. Bush and H. A. Scheraga - Optical rotatory dispersion and RNA base pairing in ribosomes and in tobacco mosaic virus, ACS meeting abstracts, p. C117, Sept. 1967, Biochemistry, 6, 3036-3042 (1967).

*217. K. D. Gibson and H. A. Scheraga - Minimization of polypeptide energy. II. Preliminary structures of oxytocin, vasopressin and an octapeptide from ribonuclease, Proc. Natl. Acad. Sci., U.S., 58, 1317-1323 (1967).

218. E. Hamori and H. A. Scheraga - Calculation of the conformation change controlled ionization of polyamino acids from titration curves, J. Phys. Chem., 71, 4145-4 147 (1967).

*219. E. Hamori and H. A. Scheraga - pH jump measurements on the helix-coil transition of poly-L-tyrosine, Abstracts of Second Middle Atlantic Regional Meeting, ACS, p. 100, Feb. 6-7, 1967, J. Phys. Chem., 71, 4147-4150 (1967).

*220. R. A. Scott, G. Vanderkooi, R. W. Tuttle, P. M. Shames and H. A. Scheraga - Minimization of polypeptide energy, III. Application of a rapid energy minimization technique to the calculation of preliminary structures of gramicidin-S, Proc. Natl. Acad. Sci., 58, 2204-2211 (1967).

*221. D. Poland and H. A. Scheraga - Energy parameters in polypeptides. I. Charge distributions and the hydrogen bond, Biochemistry, 6, 3791-3800 (1967).

*222. H. A. Scheraga, R. A. Scott, T. Ooi and G. Vanderkooi - The relative stabilities of some polyamino acid helices, International Sypm. on Macromol. Chem., Tokyo-Kyoto, Sept. 1966, Pure and Applied Chem., 15, 503-506 (1967).

1968

223. D. K. Kunimitsu, A. Y. Woody, E. R. Stimson and H. A. Scheraga - Thermodynamic data from fluorescence spectra. II. Hydrophobic bond formation in binary complexes, J. Phys. Chem., 72, 856-866 (1968).

*224. R. T. Ingwall, H. A. Scheraga, N. Lotan, A. Berger and E. Katchalski - Conformational studies of poly-L-alanine in water, ACS meeting abstracts, p. C169, Sept. 1967, Biopolymers, 6, 331-368 (1968).

*225. N. Gō, M. Gō and H. A. Scheraga - Molecular theory of the helix-coil transition in polyamino acids. I. Formulation, Proc. Natl. Acad. Sci., U.S., 59, 1030-1037 (1968).

*226. H. A. Scheraga, K. D. Gibson, F. A. Momany, G. Vanderkooi and J. F. Yan - Potential energies, free energies and conformations of polypeptides, Fed. Proc., 27, 692 (1968).

227. G. Némethy, H. A. Scheraga and W. Kauzmann - Comments on the communication "A Criticism of the Term 'Hydrophobic Bond'" by Joel H. Hildebrand, J. Phys. Chem., 72, 1842 (1968).

228. D. H. Meadows, O. Jardetzky, R. M. Epand, H. H. Ruterjans and H. A. Scheraga - Assignment of the histidine peaks in the nuclear magnetic resonance spectrum of ribonuclease, Proc. Natl. Acad. Sci., U.S., 60, 766-772 (1968).

*229. H. A. Scheraga - Calculations of conformations of polypeptides, Adv. Phys. Org. Chem., 6, 103-184 (1968).

*230. R. M. Epand and H. A. Scheraga - The influence of long-range interactions on the structure of myoglobin, Biochemistry, 7, 2864-2872 (1968).

*231. R. F. Epand and H. A. Scheraga - The helix-coil transition of poly-L-lysine in methanol-water solvent mixtures, Biopolymers, 6, 1383-1386 (1968).

*232. J. F. Yan, G. Vanderkooi and H. A. Scheraga - Conformational analysis of macromolecules. V. Helical structures of poly-L-aspartic acid and poly-L-glutamic acid, and related compounds, J. Chem. Phys., 49, 2713-2726 (1968).

233. F. A. Momany, G. Vanderkooi and H. A. Scheraga - Determination of intermolecular potentials from crystal data. I. General theory and application to crystalline benzene at several temperatures, ACS meeting abstracts, p. Biol. 182, Sept. 1968, Proc. Natl. Acad. Sci., U.S., 61, 429-436 (1968).

234. J. N. Vournakis, J. F. Yan and H. A. Scheraga - Effect of side chains on the conformational energy and rotational strength of the nπ* transition for some α-helical poly- a-amino acids, Biopolymers, 6, 1531-1550 (1968).

235. R. F. Epand and H. A. Scheraga - Conformations of poly-L-valine in solution, Biopolymers, 6, 1551-1571 (1968).

236. G. F. Endres and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. VIII. Polymerization of acceptor-modified fibrin monomer, Biochemistry, 7, 4219-4226 (1968).

237. H. A. Scheraga - Calculations of polypeptide conformations, in "Recent Developments in Biochemistry" (H. W. Li, P.O.P. Ts'o, P. C. Huang, and T. T. Kuo, eds.), Academia Sinica, Taiwan, 1968, p. 82-103.

*238. D. Kotelchuck and H. A. Scheraga - The influence of short-range interactions on protein conformation. I. Side chain-backbone interactions within a single peptide unit, Proc. Natl. Acad. Sci., U.S., 61, 1163-1170 (1968).

1969

*239. H. A. Scheraga - Calculation of polypeptide conformation, Harvey Lectures, 63, 99-138 (1969).

*240. D. Kotelchuck and H. A. Scheraga - The influence of short-range interactions on protein conformation. II. A model for predicting the α-helical regions of proteins, Proc. Natl. Acad. Sci., U.S., 62, 14-21 (1969).

241. F. A. Momany, G. Vanderkooi, R. W. Tuttle and H. A. Scheraga - Minimization of polypeptide energy. IV. Further studies of gramicidin-S, Biochemistry, 8, 744-746 (1969).

242. H. A. Scheraga and D. Kotelchuck - Short-range interactions and helix formation in proteins, Fed. Proc., 28, 1189 (1969).

*243. C. A. Bush and H. A. Scheraga - Optical activity of single-stranded polydeoxyadenylic and polyriboadenylic acids; dependence of adenine chromophore Cotton effects on polymer conformation, Biopolymers, 7, 395-409 (1969).

244. K. D. Gibson and H. A. Scheraga - Minimization of polypeptide energy, V. Theoretical aspects, Physiol. Chem. and Phys., 1, 109-126 (1969).

*245. J. S. Ingwall and H. A. Scheraga - Purification and properties of bovine prothrombin, Biochemistry, 8, 1860-1869 (1969).

246. K. D. Gibson and H. A. Scheraga - Minimization of polypeptide energy. VI. Systematic searches for low-energy conformations of deca-L-alanine and the octapeptide loop of ribonuclease, Proc. Natl, Acad. Sci., U.S., 63, 9-15 (1969).

247. K. D. Gibson and H. A. Scheraga - Minimization of polypeptide energy. VII. Second derivatives and statistical weights of energy minima for deca-L-alanine, Proc. Nat. Acad. Sci., U.S., 63, 242-245 (1969).

248. E. H. Erenrich, R. H. Andreatta and H. A. Scheraga - Helix sense of poly-γ-p-chlorobenzyl L-glutamate, Biopolymers, 7, 805-808 (1969).

*249. T. C. Troxell and H. A. Scheraga - Use of electric dichroism to study polymer conformation, Biochem. Biophys. Res. Comm., 35, 913-919 (1969).

*250. H. A. Scheraga - Calculation of the three-dimensional structures of polypeptides, Baskerville Chemical Journal, 17, 5-8 (1969).

*251. D. Poland and H. A. Scheraga - The Lifson-Allegra theories of the helix-coil transition for random copolymers: comparison with exact results and extension, Biopolymers, 7, 887-908 (1969).

*252. H. A. Scheraga - Calculation of conformations of polypeptides from amino acid sequence, Nobel Symposium 11, on "Symmetry and Function of Biological Systems at the Macromolecular Level" (Ed. by A. Engstrom and B. Strandberg), Almqvist and Wiksell, Stockholm, p. 43-78 (1969).

253. N. Lotan, F. A. Momany, J. F. Yan, G. Vanderkooi and H. A. Scheraga - The Influence of temperature on the helix sense of several polyamino acids, Biopolymers, 8, 21-27 (1969).

*254. D. Kotelchuck, M. Dygert and H. A. Scheraga - The influence of short-range interactions on protein conformation. III. Dipeptide distributions in proteins of known sequence and structure, Proc. Natl. Acad. Sci., U.S., 63, 615-622 (1969).

255. F. J. Joubert, N. Lotan and H. A. Scheraga - A nuclear magnetic resonance study of the helix-coil transition of poly-L-lysine in methanol-water solvents, Physiol. Chem. and Phys., 1, 348-354 (1969).

256. G. M. Crippen and H. A. Scheraga - Minimization of polypeptide energy. VIII. Application of the deflation technique to a dipeptide, Proc. Natl, Acad. Sci., U.S., 64, 42-49 (1969).

257. D. Poland and H. A. Scheraga - The equilibrium unwinding in finite chains of DNA, Physiol. Chem. and Phys., 1, 389-446 (1969).

258. H. A. Scheraga, A. Katchalsky and Z. Alterman - Electrochemical properties of permeable multichain polyamino acids, J. Am. Chem. Soc., 91, 7242-7249 (1969).

259. N. Go and H. A. Scheraga - Analysis of the contribution of internal vibrations to the statistical weights of equilibrium conformations of macromolecules, J. Chem. Phys., 51, 4751-4767 (1969).

1970

*260. J. F. Yan, F. A. Momany, R. Hoffmann and H. A. Scheraga - Energy parameters in polypeptides. II. Semiempirical molecular orbital calculations for model peptides, ACS meeting abstracts, p. Biol. 172, Sept. 1969, J. Phys. Chem., 74, 420-433 (1970). Erratum:-J. Phys. Chem., 74, 4611 (1970).

261. D. Poland and H. A. Scheraga - "Theory of Helix-Coil Transitions in Biopolymers", Academic Press, N. Y. (1970).

262. M. Gō, N. Gō and H. A. Scheraga - Molecular theory of the helix-coil transition in polyamino acids. II. Numerical evaluation of s and σ for polyglycine and poly-L-alanine in the absence (for s and σ) and presence (for σ) of solvent, ACS meeting abstracts, p. Biol. 180, Sept. 1968, Abstracts of Third International Biophysics Congress, p. IG2, Sept. 1969, J. Chem. Phys., 52, 2060-2079 (1970).

*263. J. F. Yan, F. A. Momany and H. A. Scheraga - Conformational analysis of macromolecules. VI. Helical Structures of o-, m-, and p-chlorobenzyl Esters of Poly-L-Aspartic Acid, J. Am. Chem. Soc., 92, 1109-1115 (1970).

264. E. H. Erenrich, R. H. Andreatta and H. A. Scheraga - Experimental verification of predicted helix sense of two polyamino acids, J. Am. Chem. Soc., 92, 1116-1119 (1970).

265. N. Go and H. A. Scheraga - Ring closure and local conformational deformations of chain molecules, ACS meeting abstracts, p. Biol. 173, Sept. 1969, Macromolecules, 3, 178-187 (1970).

266. N. Go and H. A. Scheraga - Calculation of the conformation of the pentapeptide cyclo-(Glycylglycylglycylprolyl-prolyl). I. A complete energy map, ACS meeting abstra cts, p. Biol. 173, Sept. 1969, Macromolecules, 3, 188-194 (1970).

*267. P. N. Lewis, N. Go, M. Gō, D. Kotelchuck and H. A. Scheraga - Helix probability profiles of denatured proteins and their correlation with native structures, Proc. Natl. Acad. Sci., U.S., 65, 810-815 (1970).

*268. K. E. B. Platzer and H. A. Scheraga - The NH_2-terminal amino acid of bovine prothrombin, Biochim. Biophys. Acta, 207, 262-264 (1970).

*269. F. J. Joubert, N. Lotan and H. A. Scheraga - Nuclear resonance studies of intramolecular motions and side-chain interactions in water-soluble polyamino acids, Biochemistry, 9, 2197-2211 (1970).

*270. F. A. Momany, R. F. McGuire, J. F. Yan and H. A. Scheraga - Energy parameters in polypeptides. III. Semiempiric al molecular orbital calculations for hydrogen-bonded model peptides, J. Phys. Chem., 74, 2424-2438 (1970).

*271. S. E. Ostroy, N. Lotan, R. T. Ingwall and H. A. Scheraga -Effect of side-chain hydrophobic bonding on the stability of homopolyamino acid α-helices; conformational studies of poly-L-leucine in water, ACS meeting abstracts, p. C170, Sept. 1967, Biopolymers, 9, 749-764 (1970).

272. K. D. Gibson and H. A. Scheraga - Minimization of polypeptide energy. IX. A procedure for seeking the global minimum of functions with many minima, Computers and Biomedical Research, 3, 375-384 (1970).

273. R. K. H. Liem, D. Poland and H. A. Scheraga - Titration of α-helical poly-L-lysine in 95% methanol. A study of the range of the electrostatic potential in polypeptides, J. Am. Chem. Soc., 92, 5717-5724 (1970).

274. N. Go, P. N. Lewis and H. A. Scheraga - Calculation of the conformation of the pentapeptide cyclo(glycylglycylgly-cylprolylprolyl). II. Statistical weights, Macromolecules, 3, 628-634 (1970).

1971

*275. R. H. Andreatta, R. K. H. Liem and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. I. Synthesis of fibrinogen-like peptides, and their proteolysis by thrombin and trypsin, Proc. Natl. Acad. Sci., U.S., 68, 253-256 (1971).

276. R. F. McGuire, G. Vanderkooi, F. A. Momany, R. T. Ingwall, G. M. Crippen, N. Lotan, R. W. Tuttle, K. L. Kashuba and H. A. Scheraga - Determination of inter-molecular potentials from crystal data. II. Crystal packing with applications to polyamino acids, Macromolecules, 4, 112-124 (1971).

*277. H. A. Scheraga - Theoretical and experimental studies of conformations of polypeptides, Chem. Revs., 71, 195-217 (1971).

*278. D. N. Silverman and H. A. Scheraga - Nuclear magnetic resonance studies of side-chain interactions in polyamino acids with aromatic groups; comparison to conformational energy calculations, Biochemistry, 10, 1340-1346 (1971).

279. P. Y. Chou and H. A. Scheraga - Calorimetric measurement of enthalpy change in the isothermal helix-coil transition of poly-L-lysine in aqueous solution, Biopolymers, 10, 657-680 (1971).

280. P. H. Von Dreele, A. I. Brewster, H. A. Scheraga, M. F. Ferger and V. du Vigneaud - Nuclear magnetic resonance spectrum of lysine-vasopressin and its structural implications, Proc. Natl. Acad. Sci., U.S., 68, 1028-1031 (1971).

281. M. Gō, N. Gō and H. A. Scheraga - Molecular theory of the helix-coil transition in polyamino acids. III. Evaluation and analysis of s and σ for polyglycine and poly-L-alanine in water, J. Chem. Phys., 54, 4489-4503 (1971).

282. H. A. Scheraga, P. H. Von Dreele, D. Poland, V. S. Ananthanarayanan, N. Lotan, R. H. Andreatta, L. J. Hughes, K. E.B. Platzer, J. E. Alter, M. Dygert and P. N. Lewis - Helix-coil stability constants for the naturally-occurring amino acids in water, Fed. Proc., 30, 1107 (1971).

*283. R. H. Andreatta and H. A. Scheraga - The synthesis of [5-valine, 7-N-methylalanine]-angiotensin II, A hypertensive peptide, J. Med. Chem., 14, 489-492 (1971).

284. G. M. Crippen and H. A. Scheraga - Minimization of polypeptide energy. X. A global search algorithm, Arch. Biochem. Biophys., 144, 453-461 (1971).

285. G. M. Crippen and H. A. Scheraga - Minimization of polypeptide energy. XI. The method of gentlest ascent, Arch. Biochem. Biophys., 144, 462-466 (1971).

286. G. F. Endres and H. A. Scheraga - Molecular weight of bovine fibrinogen by sedimentation equilibrium, Arch. Biochem. Biophys., 144, 519-528 (1971).

287. P. N. Lewis and H. A. Scheraga - Predictions of structural homologies in cytochrome c proteins, Arch. Biochem. Biophys., 144, 576-583 (1971).

*288. P. N. Lewis and H. A. Scheraga - Prediction of structural homology between bovine α-lactalbumin and hen egg white lysozyme, Arch. Biochem. Biophys., 144, 584-588 (1971).

289. F. A. Momany, R. F. McGuire, J. F. Yan and H. A. Scheraga - Energy parameters in polypeptides. IV. Semiempirical molecular orbital calculations of conformational dependence of energy and partial charge in di- and tripeptides, J. Phys. Chem., 75, 2286-2297 (1971).

290. P. H. Von Dreele, D. Poland and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. I. Properties of copolymers and approximate theories, Macromolecules, 4, 396-407 (1971).

291. P. H. Von Dreele, N. Lotan, V. S. Ananthanarayanan, R. H. Andreatta, D. Poland and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. II. Characterization of the host polymers and application of the host-guest technique to random poly(hydroxypro- pylglutamine-co-hydroxybutyl-glutamine), Macromolecules, 4, 408-417 (1971).

292. V. S. Ananthanarayanan, R. H. Andreatta, D. Poland and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. III. Glycine parameters from random poly(hydroxybutylglutamine-co-glycine), Macromolecules, 4, 417-424 (1971).

*293. P. N. Lewis, F. A. Momany and H. A. Scheraga - Folding of polypeptide chains in proteins: A proposed mechanism for folding, Proc. Natl. Acad. Sci., U.S., 68, 2293-2297 (1971).

294. T. C. Troxell and H. A. Scheraga - Electric dichroism and polymer conformation. I. Theory of optical properties of anisotropic media, and method of measurement, Macromolecules, 4, 519-527 (1971).

295. T. C. Troxell and H. A. Scheraga - Electric dichroism and polymer conformation. II. Theory of electric dichroism, and measurements on poly(n-butyl isocyanate), Macromolecules, 4, 528-539 (1971).

296. A. Lewis and H. A. Scheraga - Laser Raman spectroscopy of polypeptides. I. Water-soluble block copolymers of L-alanine and D,L-lysine, Macromolecules, 4, 539-543 (1971).

*297. D. N. Silverman, G. T. Taylor and H. A. Scheraga - Nuclear magnetic resonance study of the side-chain conformation of α-helical poly-β- benzyl-L-aspartate, Arch. Biochem. Biophys., 146, 587-590 (1971).

*298. R. K. H. Liem, R. H. Andreatta and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. II. Kinetics of hydrolysis of fibrinogen-like peptides by thrombin and trypsin, Arch. Biochem. Biophys., 147, 201-213 (1971).

299. P. H. Von Dreele, A. I. Brewster, F. A. Bovey, H. A. Scheraga, M. F. Ferger and V. du Vigneaud - Nuclear magnetic resonance studies of lysine-vasopressin: structural constraints, Proc. Natl. Acad. Sci., U.S., 68, 3088-3091 (1971).

300. H. A. Scheraga - Factors affecting the folding of polypeptide chains in proteins, Pure and Applied Chem., Supplement 7, 273-279 (1971).

301. N. Gō, P. N. Lewis, M. Gō and H. A. Scheraga - A model for the helix-coil transition in specific-sequence copolymers of amino acids, Macromolecules, 4, 692-709 (1971). Erratum:-ibid, 5, 662 (1972).

1972

*302. R. F. McGuire, F. A. Momany and H. A. Scheraga - Energy parameters in polypeptides. V. An empirical hydrogen bond potential function based on molecular orbital calculations, J. Phys. Chem., 76, 375-393 (1972).

303. P. K. Warme, N. Go and H. A. Scheraga - Refinement of X-ray data on proteins. I. Adjustment of atomic coordinates to conform to a specified geometry, J. Computational Physics, 9, 303-317 (1972).

304. K. E. B. Platzer, V. S. Ananthanarayanan, R. H. Andreatta and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. IV. Alanine parameters from random poly(hydroxypropyl-glutamine-co-L-alanine), Macromolecules, 5, 177-187 (1972).

305. L. J. Hughes, R. H. Andreatta and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. V. Serine parameters from random poly(hydroxybutylglutamine-co-L-serine), Macromolecules, 5, 187-197 (1972).

306. J. C. Howard and H. A. Scheraga - Nuclear magnetic resonance study of hydrophobic bonding in $(D,L\text{-lysine})_m$-$(L\text{-alanine})_n$-$(D,L\text{-lysine})_m$, Macromolecules, 5, 328-329 (1972).

307. D. N. Silverman, D. Kotelchuck, G. T. Taylor and H. A. Scheraga - Nuclear magnetic resonance study of the N-terminal fragment of bovine pancreatic ribonuclease, Arch. Biochem. Biophys., 150, 757-766 (1972).

308. A. Lewis and H. A. Scheraga - Laser Raman spectroscopy of polypeptides. II. Spectra of random poly(hydroxy-butylglutamine-co-glycine) in the solid state, Macromolecules, 5, 450-455 (1972).

309. F. T. Hesselink and H. A. Scheraga - On the possible existence of α-helical structures of regular-sequence D,L-copolymers of amino acids; conformational energy calculations, Macromolecules, 5, 455-463 (1972).

310. P. H. Von Dreele, A. I. Brewster, J. Dadok, H. A. Scheraga, F. A. Bovey, M. F. Ferger and V. du Vigneaud - Nuclear magnetic resonance spectrum of lysine-vasopressin in aqueous solution and its structural implications, Proc. Natl. Acad. Sci., U.S., 69, 2169-2173 (1972).

*311. K. E. B. Platzer, F. A. Momany and H. A. Scheraga - Conformational energy calculations of enzyme-substrate interactions. I. Computation of preferred conformations of some substrates of α-chymotrypsin, Intntl. J. Peptide and Protein Research, 4, 187-200 (1972).

312. K. E. B. Platzer, F. A. Momany and H. A. Scheraga - Conformational energy calculations of enzyme-substrate interactions. II. Computation of the binding energy for substrates in the active site of α-chymotrypsin, Intntl. J. Peptide and Protein Research, 4, 201-219 (1972).

313. J. Dadok, P. H. Von Dreele and H. A. Scheraga - Decoupling proton magnetic resonance signals located under the H_2O peak, J.C.S. Chem. Commun., 1055-1056 (1972).

*314. A. T. Hagler, H. A. Scheraga and G. Némethy - Structure of liquid water. Statistical thermodynamic theory, ACS meeting abstracts, p. Coll 30, April 1969, J. Phys. Chem., 76, 3229-3243 (1972).

315. W. Krakow, G. F. Endres, B. M. Siegel and H. A. Scheraga -An electron microscopic investigation of the polymerization of bovine fibrin monomer, J. Mol. Biol., 71, 95-103 (1972).

316. P. K. Warme, R. W. Tuttle and H. A. Scheraga - Comparison of three-dimensional structures of macromolecules, Computer Programs in Biomedicine, 2, 248-256 (1972).

317. P. H. Von Dreele, H. A. Scheraga, D. F. Dyckes, M. F. Ferger and V. du Vigneaud - Nuclear magnetic resonance spectrum of deamino-lysine-vasopressin in aqueous solution and its structural implications, Proc. Natl. Acad. Sci., U.S., 69, 3322-3326 (1972).

318. G. F. Endres and H. A. Scheraga - Equilibria in the fibrinogen-fibrin conversion. IX. Effects of calcium ions on the reversible polymerization of fibrin monomer, Arch. Biochem. Biophys., 153, 266-278 (1972).

319. J. E. Alter, G. T. Taylor and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. VI. Leucine parameters from random poly(hydroxypropylglutamine-co-L-leucine) and poly-(hydroxybutylglutamine-co-L-leucine), Macromolecules, 5, 739-746 (1972).

320. E. H. Erenrich and H. A. Scheraga - Dipole moments and the conformations of polypeptides. I. Some compounds related to poly(β-Benzyl-L-Aspartate), Macromolecules, 5, 746-754 (1972).

321. D. Kotelchuck, H. A. Scheraga and R. Walter - Conformational energy studies of oxytocin and its cyclic moiety, Proc. Natl. Acad. Sci., U.S., 69, 3629-3633 (1972).

322. D. N. Silverman and H. A. Scheraga - Hairpin bend and interhelical interactions in α-helical poly(L-alanine) in water, Arch. Biochem. Biophys., 153, 449-456 (1972).

1973

323. G. C.-C. Niu, N. Go and H. A. Scheraga - Calculation of the conformation of the pentapeptide cyclo(glycylglycyl-glycylprolylprolyl). III. Treatment of a flexible molecule, Macromolecules, 6, 91-99 (1973). Erratum: -ibid., 6, 796 (1973).

*324. A. T. Hagler, H. A. Scheraga and G. Némethy - Current status of the water-structure problem; application to proteins, Ann. N.Y. Acad. Sci., 204, 51-78 (1973).

325. H. A. Scheraga, P. N. Lewis, F. A. Momany, P. H. Von Dreele, A. W. Burgess and J. C. Howard - Hairpin bends in oligopeptides and proteins, Fed. Proc., 32, 495 (1973).

*326. P. K. Ponnuswamy, P. K. Warme and H. A. Scheraga - Role of medium-range interactions in proteins, Proc. Natl. Acad. Sci., U.S., 70, 830-833 (1973).

327. H. E. Van Wart, G. T. Taylor and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. VII. Phenylalanine parameters from random poly(hydroxypropylglutamine-co-phenylalanine). Macromolecules, 6, 266-273 (1973).

328. N. Go and H. A. Scheraga - Ring closure in chain molecules with C_n, I or S_{2n} symmetry, Macromolecules, 6, 273-281 (1973).

329. P. K. Ponnuswamy, R. F. McGuire and H. A. Scheraga - Refinement of the molecular structure of actinomycin D by energy minimization, Intntl. J. Peptide and Protein Research, 5, 73-84. (1973).

*330. P. N. Lewis, F. A. Momany and H. A. Scheraga - Chain reversals in proteins, Biochim. Biophys. Acta, 303, 211-229 (1973).

331. H. A. Scheraga - Interactions in polypeptides and proteins, Jerusalem Symp. Quantum Chem. and Biochem., Conformation of Biological Molecules and Polymers, Ed. E. D. Bergmann and B. Pullman, April 1972, 5, 51- 68 (1973).

332. P. K. Warme and H. A. Scheraga - Refinement of X-ray data on proteins. II. Adjustment of structure of specified geometry to relieve atomic overlaps, J. Comput. Phys., 12, 49-64 (1973).

*333. A. W. Burgess, F. A. Momany and H. A. Scheraga - Conformational analysis of thyrotropin releasing factor, Proc. Natl. Acad. Sci., U.S., 70, 1456-1460 (1973). Erratum: - ibid., 71, 4640 (1974).

334. N. Lotan, F. Th. Hesselink, H. Benderly, J. F. Yan, I. Schechter, A. Berger and H. A. Scheraga - Right- and left-handed α-helical structures in poly(L-alanyl-D-alanyl-L-alanyl-L-alanyl), Macromolecules, 6, 447-453 (1973).

*335. B. R. Lentz and H. A. Scheraga - Water molecule interactions. Stability of cyclic polymers, J. Chem. Phys., 58, 5296 (1973). Erratum: - ibid., 61, 3493 (1974).

336. N. Go and H. A. Scheraga - Calculation of the conformation of cyclo-hexaglycyl, Macromolecules, 6, 525-535 (1973). Erratum: - ibid., 7, 148 (1974).

*337. J. C. Howard, F. A. Momany, R. H. Andreatta and H. A. Scheraga - Investigation of the cis and trans isomers of sarcosylsarcosine by nuclear magnetic recsonance spectroscopy and conformational energy calculations, Macromolecules, 6, 535-541 (1973).

338. F. T. Hesselink, T. Ooi and H. A. Scheraga - Conformational energy calculations. Thermodynamic parameters of the helix-coil transition for poly(L-lysine) in aqueous salt solution, Macromolecules, 6, 541-552 (1973).

339. V. S. Ananthanarayanan, E. Leroy and H. A. Scheraga - Helix-coil transition in mixed solvents. I. Optical rotatory dispersion study of poly(γ-benzyl L-glutamate) in dichloroacetic acid-dichloroethane mixtures, Macromolecules, 6, 553-559 (1973).

340. V. S. Ananthanarayanan, G. Davenport, E. R. Stimson and H. A. Scheraga - Helix-coil transition in mixed solvents. II. Calorimetric study of poly(γ-benzyl L-glutamate) in dichloroacetic acid-dichloroethane mixtures, Macromolecules, 6, 559-563 (1973).

*341. J. E. Alter, R. H. Andreatta, G. T. Taylor and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. VIII. Valine parameters from random poly(hydroxypropylglutamine-co-L-valine) and poly(hydroxybutylglutamine-co-L-valine), Macromolecules, 6, 564-570 (1973).

342. P. N. Lewis, F. A. Momany and H. A. Scheraga - Energy parameters in polypeptides. VI. Conformational energy analysis of the N-acetyl N'-methyl amides of the twenty naturally occurring amino acids, Israel J. Chem., 11, 121-152 (1973).

343. G. M. Crippen and H. A. Scheraga - Minimization of polypeptide energy. XII. The methods of partial energies and cubic subdivision, J. Computational Phys., 12, 491-497 (1973).

344. A. W. Burgess and H. A. Scheraga - Stable conformations of dipeptides, Biopolymers, 12, 2177-2183 (1973).

345. H. A. Scheraga - On the dominance of short-range interactions in polypeptides and proteins, Prague Symp., Aug. 1972, Pure and Applied Chem., 36, 1-8 (1973).

*346. R. K. H. Liem and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. III. Partial mapping of the active sites of thrombin and trypsin, Arch. Biochem. Biophys., 158, 387-395 (1973).

*347. H. E. Van Wart, A. Lewis, H. A. Scheraga and F. D. Saeva -Disulfide bond dihedral angles from Raman spectroscopy, Proc. Natl. Acad. Sci., U.S., 70, 2619-2623 (1973).

*348. P. P. S. Saluja and H. A. Scheraga - Ion-water interactions in the gas phase, J. Phys. Chem., 77, 2736-2738 (1973).

1974

*349. R. K. H. Liem and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. IV. Further mapping of the active sites of thrombin and trypsin, Arch. Biochem. Biophys., 160, 333-339 (1974).

*350. P. K. Warme and H. A. Scheraga - Refinement of the X-ray structure of lysozyme by complete energy minimization, Biochemistry, 13, 757-767 (1974).

*351. P. K. Warme, F. A. Momany, S. V. Rumball, R. W. Tuttle and H. A. Scheraga - Computation of structures of homologous proteins; α-lactalbumin from lysozyme, Biochemistry, 13, 768-782 (1974).

*352. N. Gō, M. Gō and H. A. Scheraga - New method for calculating the conformational entropy of a regular helix, Macromolecules, 7, 137-139 (1974).

*353. H. A. Scheraga - Prediction of protein conformation, in "Current Topics in Biochemistry, 1973", ed. by C. B. Anfinsen and A. N. Schechter, Academic Press, New York, 1974, p. 1-42.

*354. L. L. Shipman and H. A. Scheraga - An empirical intermolecular potential energy function for water, J. Phys. Chem., 78, 909-916 (1974).

*355. B. R. Lentz, A. T. Hagler and H. A. Scheraga - Structure of liquid water. II. Improved statistical thermodynamic treatment and implications of a cluster model, J. Phys. Chem., 78, 1531-1550 (1974).

356. F. A. Momany, L. M. Carruthers, R. F. McGuire and H. A. Scheraga - Intermolecular potentials from crystal data. III. Determination of empirical potentials and application to the packing configurations and lattice energies in crystals of hydrocarbons, carboxylic acids, amines and amides, J. Phys. Chem., 78, 1595-1620 (1974).

357. F. A. Momany, L. M. Carruthers and H. A. Scheraga - Inter-molecular potentials from crystal data. IV. Application of empirical potentials to the packing configurations and lattice energies in crystals of amino acids, J. Phys. Chem., 78, 1621-1630 (1974).

358. M. Gō, F. T. Hesselink, N. Gō and H. A. Scheraga - Molecular theory of the helix-coil transition in poly(amino acids). IV. Evaluation and analysis of s for poly(L-valine) in the absence and presence of water, Macromolecules, 7, 459-467 (1974).

359. Y-C. Fu, R. F. McGuire and H. A. Scheraga - Intermolecular potentials from crystal data. V. Crystal packing of poly[β-(p-chlorobenzyl)-L-aspartate], Macromolecules, 7, 468-480 (1974).

360. R. R. Hantgan, G. G. Hammes and H. A. Scheraga - Pathways of folding of reduced bovine pancreatic ribonuclease, Biochemistry, 13, 3421-3431 (1974).

361. B. R. Lentz, A. T. Hagler and H. A. Scheraga - Vibrational frequencies of water clusters, J. Phys. Chem.. 78, 1844-1847 (1974).

362. H. E. Van Wart, L. L. Shipman and H. A. Scheraga - Variation of disulfide bond stretching frequencies with disulfide dihedral angle in dimethyl disulfide, J. Phys. Chem., 78, 1848-1853 (1974).

363. A. W. Burgess, P. K. Ponnuswamy and H. A. Scheraga - Analysis of conformations of amino acid residues and prediction of backbone topography in proteins, Israel J. Chem., 12, 239-286 (1974).

364. D. Rasse, P. K. Warme and H. A. Scheraga - Refinement of the X-ray structure of rubredoxin by conformational energy calculations, Proc. Natl. Acad. Sci., U.S., 71, 3736-3740 (1974).

*365. L. L. Shipman, J. C. Owicki and H. A. Scheraga - Structure, energetics, and dynamics of the water dimer, J. Phys. Chem., 78, 2055-2060 (1974).

366. S. Tanaka and H. A. Scheraga - Calculation of conformational properties of oligomers of L-proline, Macromolecules, 7, 698-705 (1974).

*367. T. C. Hageman and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. Reaction of the N-terminal CNBr fragment from the Aα chain of human fibrinogen with bovine thrombin, Arch. Biochem. Biophys., 164, 707-715 (1974).

*368. H. A. Scheraga - Poly(amino Acids), interatomic energies, and protein folding, in "Peptides, Polypeptides, and Proteins", ed. E. R. Blout, F. A. Bovey, M. Goodman and N. Lotan, John Wiley, New York, 1974, p. 49-70.

369. K. Nishikawa, F. A. Momany and H. A. Scheraga - Low-energy structures of two dipeptides and their relationship to bend conformations, Macromolecules, 7, 797-806 (1974).

*370. R. Arnon, E. Teicher and H. A. Scheraga - Correlation of conformation and biological activity in lysozyme "loop" homologs, J. Mol. Biol., 90, 403-407 (1974).

1975

*371. A. W. Burgess, L. I. Weinstein, D. Gabel and H. A. Scheraga - Immobilized carboxypeptidase A as a probe for studying the thermally induced unfolding of bovine pancreatic ribonuclease, Biochemistry, 14, 197-200 (1975).

372. L. L. Shipman and H. A. Scheraga - Computation of the intermolecular vibrational modes of a tetrahedral water pentamer at the core of an ice-like water cluster, J. Phys. Chem., 79, 380-383 (1975).

*373. L. L. Shipman, A. W. Burgess and H. A. Scheraga - A new approach to empirical intermolecular and conformational potential energy functions. I. Description of model and derivation of parameters, Proc. Natl. Acad. Sci., U.S., 72, 543-547 (1975).

374. A. W. Burgess, L. L. Shipman and H. A. Scheraga - A new approach to empirical intermolecular and conformational potential energy functions. II. Applications to crystal packing, rotational barriers and conformational analysis, Proc. Natl. Acad. Sci., U.S., 72, 854-858 (1975).

375. F. R. Maxfield, J. E. Alter, G. T. Taylor and H. A. Scheraga - Helix-coil stability constants for charged and uncharged glutamic acid, Fed. Proc., 34, 597 (1975).

*376. A. W. Burgess and H. A. Scheraga - Assessment of some problems associated with prediction of the three-dimensional structure of a protein from its amino-acid sequence, Proc. Natl. Acad. Sci., U.S., 72, 1221-1225 (1975).

377. G. F. Endres, M. K. Swenson and H. A. Scheraga - Structural aspects of thrombin specificity, Arch. Biochem. Biophys., 168, 180-187 (1975).

*378. C. B. Anfinsen and H. A. Scheraga - Experimental and theoretical aspects of protein folding, Adv. Protein Chem., 29, 205-300 (1975).

379. H. E. Van Wart, L. L. Shipman and H. A. Scheraga - The nature of the potential function for internal rotation about carbon-sulfur bonds in disulfides, J. Phys. Chem., 79, 1428-1435 (1975).

380. H. E. Van Wart, L. L. Shipman and H. A. Scheraga - Theoretical and experimental evidence for a Nonbonded 1,4 carbon-sulfur interaction in organosulfur compounds, J. Phys. Chem., 79, 1436-1447 (1975).

381. P. K. Warme and H. A. Scheraga - Conformational energy refinement of horse-heart ferricytochrome c, Biochemistry, 14, 3509-3517 (1975).

*382. J. C. Owicki, L. L. Shipman and H. A. Scheraga - Structure, energetics, and dynamics of small water clusters, ACS meeting abstracts, p. PHYS 137, April 1975, J. Phys. Chem., 79, 1794-1811 (1975). Erratum: - ibid., 79, 3081 (1975).

383. F. R. Maxfield, J. E. Alter, G. T. Taylor and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. IX. Glutamic acid parameters from random poly(hydroxybutylglutamine-co-L-glutamic acid), Macromolecules, 8, 479-491 (1975).

384. F. R. Maxfield and H. A. Scheraga - The effect of neighboring charges on the helix forming ability of charged amino acids in proteins, Macromolecules, 8, 491-493 (1975).

385. S. Tanaka and H. A. Scheraga - Theory of the cooperative transition between two ordered conformations of poly(L-proline). I. Phenomenological theory, Macromolecules, 8, 494-503 (1975).

386. S. Tanaka and H. A. Scheraga - Theory of the cooperative transition between two ordered conformations of poly(L-proline). II. Molecular theory in the absence of solvent, Macromolecules, 8, 504-516 (1975).

387. S. Tanaka and H. A. Scheraga - Theory of the cooperative transition between two ordered conformations of poly(L-proline). III. Molecular theory in the presence of solvent, Macromolecules, 8, 516-521 (1975).

*388. A. W. Burgess and H. A. Scheraga - A hypothesis for the pathway of the thermally-induced unfolding of bovine pancreatic ribonuclease, J. Theor. Biol., 53, 403-420 (1975).

389. J. C. Howard, A. Ali, H. A. Scheraga and F. A. Momany - Investigation of the conformations of four tetrapeptides by nuclear magnetic resonance and circular dichroism spectroscopy, and conformational energy calculations, Macromolecules, 8, 607-622 (1975).

390. S. Tanaka and H. A. Scheraga - Calculation of the characteristic ratio of randomly-coiled poly(L-proline), Macromolecules, 8, 623-631 (1975).

*391. J. C. Owicki, B. R. Lentz, A. T. Hagler and H. A. Scheraga - Structure of liquid water. III. Thermodynamic properties of liquid deuterium oxide, J. Phys. Chem., 79, 2352-2361 (1975).

392. F. A. Momany, R. F. McGuire, A. W. Burgess and H. A. Scheraga - 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, J. Phys. Chem., 79, 2361-2381 (1975).

393. S. Tanaka and H. A. Scheraga - Model of protein folding: inclusion of short-, medium-, and long-range interactions, Proc. Natl. Acad. Sci., U.S., 72, 3802-3806 (1975).

394. T. C. Hageman, G. F. Endres and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. On the role of the A chain of bovine thrombin in specificity and in differentiating between thrombin and trypsin, Arch. Biochem. Biophys., 171, 327-336 (1975).

395. M. Dygert, N. Go and H. A. Scheraga - Use of a symmetry condition to compute the conformation of gramicidin S, Macromolecules, 8, 750-761 (1975).

396. A. W. Burgess, F. A. Momany and H. A. Scheraga - On the structure of thyrotropin releasing factor, Biopolymers, 14, 2645-2647 (1975).

397. S. S. Zimmerman and H. A. Scheraga - The influence of short-range interactions in peptides and proteins, Peptides: Chemistry, Structure and Biology, ed. R. Walter and J. Meienhofer, Ann Arbor Science Publ., Ann Arbor (1975), p. 263-269.

1976

398. A. W. Burgess, L. L. Shipman, R. A. Nemenoff and H. A. Scheraga - A new approach to empirical intermolecular and conformational potential energy functions. III. Application of EPEN to the conformational analysis of 1,2-disubstituted ethanes, J. Am. Chem. Soc., 98, 23-29 (1976).

399. L. L. Shipman, A. W. Burgess and H. A. Scheraga - Lattice energies and heats of sublimation at 0 K for n-pentane, n-hexane, n-octane and ammonia, J. Phys. Chem., 80, 52-54 (1976).

400. R. K. Scheule, F. Cardinaux, G. T. Taylor and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. X. Tyrosine parameters from random poly(hydroxypropylglutamine-co-L-tyrosine), ACS meeting abstracts, p. PHYS 019, April 1975, Macromolecules, 9, 23-33 (1976).

*401. S. Tanaka and H. A. Scheraga - Statistical mechanical treatment of protein conformation. I. Conformational properties of amino acids in proteins, Macromolecules, 9, 142-159 (1976).

*402. S. Tanaka and H. A. Scheraga - Statistical mechanical treatment of protein conformation. II. A three-state model for specific-sequence copolymers of amino acids, Macromolecules, 9, 159-167 (1976).

*403. S. Tanaka and H. A. Scheraga - Statistical mechanical treatment of protein conformation. III. Prediction of protein conformation based on a three-state model, Macromolecules, 9, 168-182 (1976).

404. H. E. Van Wart, F. Cardinaux and H. A. Scheraga - Low frequency Raman spectra of dimethyl, methyl ethyl, and diethyl disulfides, and rotational isomerism about their carbon-sulfur bonds, J. Phys. Chem., 80, 625-630 (1976).

405. D. Gabel, D. Rasse and H. A. Scheraga - Search for low energy conformations of a neurotoxic protein by means of predictive rules, tests for hard-sphere overlaps, and energy minimization, Intntl. J. of Peptide and Protein Research, 8, 237-252 (1976).

*406. K. Nishikawa and H. A. Scheraga - Geometrical criteria for formation of coiled-coil structures of polypeptide chains, Macromolecules, 9, 395-407 (1976).

407. S. S. Zimmerman and H. A. Scheraga - Stability of cis, trans, and nonplanar peptide groups, Macromolecules, 9, 408-416 (1976).

408. H. E. Van Wart and H. A. Scheraga - Raman spectra of cystine-related disulfides. Effect of rotational isomerism about carbon-sulfur bonds on sulfur-sulfur stretching frequencies, J. Phys. Chem., 80, 1812-1823 (1976).

409. H. E. Van Wart and H. A. Scheraga - Raman spectra of strained disulfides. Effect of rotation about sulfur-sulfur bonds on sulfur-sulfur stretching frequencies, J. Phys. Chem., 80, 1823-1832 (1976).

410. H. E. Van Wart, H. A. Scheraga and R. B. Martin - Agreement concerning the nature of the variation of disulfide stretching frequencies with disulfide dihedral angles, J. Phys. Chem., 80, 1832 (1976).

411. N. Go and H. A. Scheraga - On the use of classical statistical mechanics in the treatment of polymer chain conformation, Macromolecules, 9, 535-542 (1976).

412. Y-C. Fu, H. E. Van Wart and H. A. Scheraga - Calorimetric measurement of enthalpy change in the isothermal helix-coil transition of poly(L-ornithine) in aqueous solution, Biopolymers, 15, 1795-1813 (1976).

*413. M. K. Dygert, G. T. Taylor, F. Cardinaux and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 11. Lysine parameters from random poly(hydroxybutylglutamine-co-L-lysine), Macromolecules, 9, 794-801 (1976).

*414. S. Tanaka and H. A. Scheraga - Statistical mechanical treatment of protein conformation. 4. A four-state model for specific-sequence copolymers of amino acids, Macromolecules, 9, 812-833 (1976).

*415. F. R. Maxfield and H. A. Scheraga - Status of empirical methods for the prediction of protein backbone topography, Biochemistry, 15, 5138-5153 (1976).

*416. S. Tanaka and H. A. Scheraga - Medium- and long-range interaction parameters between amino acids for predicting three-dimensional structures of proteins, Macromolecules, 9, 945-950 (1976).

*417. M. R. Pincus, A. W. Burgess and H. A. Scheraga -Conformational energy calculations of enzyme-substrate complexes of lysozyme. I. Energy minimization of mono- and oligosaccharide inhibitors and substrates of lysozyme, Biopolymers, 15, 2485-2521 (1976). Erratum: ibid., 16, 468 (1977).

*418. M. R. Pincus, S. S. Zimmerman and H. A. Scheraga - Prediction of the three-dimensional structures of enzyme-substrate and enzyme-inhibitor complexes of lysozyme, Proc. Natl. Acad. Sci., U.S., 73, 4261-4265 (1976).

419. M. H. Miller and H. A. Scheraga - Calculation of the structures of collagen models. Role of interchain interactions in determining the triple-helical coiled-coil conformation. I. Poly(glycyl-prolyl-prolyl), J. Polymer Sci.: Polymer Symposia,, No 54, p. 171-200 (1976).

1977

420. H. E. Van Wart and H. A. Scheraga - Stable conformations of aliphatic disulfides: The influence of 1,4 interactions involving sulfur atoms, Proc. Natl. Acad. Sci., U.S., 74, 13-17 (1977).

*421. S. S. Zimmerman, M. S. Pottle, G. Némethy and H. A. Scheraga - Conformational analysis of the twenty naturally occurring amino acid residues using ECEPP, Macromolecules, 10, 1-9 (1977).

422. S. Tanaka and H. A. Scheraga - Statistical mechanical treatment of protein conformation. 5. A multi-state model for specific-sequence copolymers of amino acids, Macromolecules, 10, 9-20 (1977).

*423. R. R. Matheson, Jr., H. E. Van Wart, A. W. Burgess, L. I. Weinstein and H. A. Scheraga - Study of protein topography with flash-photolytically-generated non-specific surface-labeling reagents: surface labeling of ribonuclease A, Biochemistry, 16, 396-403 (1977).

424. R. R. Matheson, Jr., H. Dugas and H. A. Scheraga - Electron paramagnetic resonance spectroscopy as a monitor of the pathway of the thermal unfolding of ribonuclease A, Biochem. Biophys. Res. Comm., 74, 869-876 (1977).

*425. Y. Isogai, G. Némethy and H. A. Scheraga - Enkephalin: conformational analysis by means of empirical energy calculations, Proc. Natl. Acad. Sci., U.S., 74, 414-418 (1977).

*426. S. J. Leach, G. Némethy and H. A. Scheraga - Use of proton nuclear Overhauser effects for the determination of the conformations of amino acid residues in oligopeptides, Biochem. Biophys. Res. Comm., 75, 207-215 (1977).

427. R. K. Scheule, H. E. Van Wart, B. L. Vallee and H. A. Scheraga - Resonance Raman studies of arsanilazo-carboxypeptidase A, Fed. Proc., 36, 697 (1977).

428. T. C. Hageman and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. Reaction of the N-terminal CNBr fragment from the Bβ chain of bovine fibrinogen with bovine thrombin, Arch. Biochem. Biophys., 179, 506-517 (1977).

429. S. Tanaka and H. A. Scheraga - Hypothesis about the mechanism of protein folding, Macromolecules, 10, 291-304 (1977).

430. S. Tanaka and H. A. Scheraga - Statistical mechanical treatment of protein conformation. 6. Elimination of empirical rules for prediction by use of a high-order probability. Correlation between the amino acid sequences and conformations for homologous neurotoxin proteins, Macromolecules, 10, 305-316 (1977).

*431. S. S. Zimmerman, L. L. Shipman and H. A. Scheraga - Bends in globular proteins. A statistical mechanical analysis of the conformational space of dipeptides and proteins, J. Phys. Chem., 81, 614-622 (1977).

432. S. S. Zimmerman and H. A. Scheraga - Influence of local interactions on protein structure. I. Conformational energy studies of N-acetyl-N'-methylamides of Pro-X and X-Pro dipeptides, Biopolymers, 16, 811-843 (1977). Erratum: ibid. 16, 1385 (1977).

*433. S. Tanaka and H. A. Scheraga - Model of protein folding: incorporation of a one-dimensional short-range (Ising) model into a three-dimensional model, Proc. Natl. Acad. Sci., U.S., 74, 1320-1323 (1977).

*434. J. C. Owicki and H. A. Scheraga - Preferential sampling near solutes in Monte Carlo calculations on dilute solutions, Chem. Phys. Letters, 47, 600-602 (1977).

*435. L. G. Chavez, Jr. and H. A. Scheraga - Immunological determination of the order of folding of portions of the molecule during air oxidation of reduced ribonuclease, Biochemistry, 16, 1849-1856 (1977).

*436. G. Némethy and H. A. Scheraga - Intermolecular potentials from crystal data. 5. Determination of empirical potentials for O-H…O hydrogen bonds from packing configurations and lattice energies of polyhydric alcohols, J. Phys. Chem., 80, 928-931 (1977).

437. R. R. Matheson, Jr., R. A. Nemenoff, F. Cardinaux and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. XII. Asparagine parameters from random poly(hydroxybutyl- glutamine-co-L-asparagine), Biopolymers, 16, 1567-1585 (1977).

438. J. W. van Nispen, D. J. Hill and H. A. Scheraga - Helix- coil stability constants for the naturally occurring amino acids in water. XIII. The presence of by-products in amino acid analysis of copolymers and their effect on the guest parameters; recomputed values of s and s for L-serine, Biopolymers, 16, 1587-1592 (1977).

*439. M. R. Pincus, S. S. Zimmerman and H. A. Scheraga - Structures of enzyme-substrate complexes of lysozyme, Proc. Natl. Acad. Sci., U.S., 74, 2629-2633 (1977).

440. I. D. Rae, E. R. Stimson and H. A. Scheraga - Nuclear Overhauser effects and the conformation of gramicidin S, Biochem. Biophys. Res. Commun., 77, 225-229 (1977).

*441. J. W. van Nispen, T. C. Hageman and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. The reaction of thrombin with fibrinogen-like peptides containing 11, 14 and 16 residues, Arch. Biochem. Biophys., 182, 227-243 (1977).

*442. R. K. Scheule, H. E. Van Wart, B. L. Vallee and H. A. Scheraga - Resonance Raman spectroscopy of arsanilazo-carboxypeptidase A: Determination of the nature of the AzoTyrosyl-248.Zinc complex, Proc. Natl. Acad. Sci., U.S., 74, 3273-3277 (1977).

*443. M. R. Pincus and H. A. Scheraga - An approximate treatment of long-range interactions in proteins, J. Phys. Chem., 81, 1579-1583 (1977).

444. G. Némethy and H. A. Scheraga - Protein folding, Quart. Rev. Biophys., 10, 239-352 (1977).

445. F. Cardinaux, J. C. Howard, G. T. Taylor and H. A. Scheraga - Block copolymers of amino acids. I. Synthesis and structure of copolymers of L-alanine or L-phenylalanine with D,L-lysine-d_7 or D,L-lysine, Biopolymers, 16, 2005-2028 (1977).

446. J. C. Howard, F. Cardinaux and H. A. Scheraga - Block copolymers of amino acids. II. Physicochemical data on copolymers containing L-alanine or L-phenylalanine, Biopolymers, 16, 2029-2051 (1977).

447. H. A. Scheraga - Active site mapping of thrombin, in "Chemistry and Biology of Thrombin", ed. R. L. Lundblad, J. W. Fenton II and K. G. Mann, Ann Arbor Science Publ., Ann Arbor (1977) p. 145-158.

448. E. R. Stimson, S. S. Zimmerman and H. A. Scheraga - Conformational studies of oligopeptides containing proline and glycine, Macromolecules, 10, 1049-1060 (1977).

*449. F. R. Maxfield and H. A. Scheraga - A Raman spectroscopic investigation of the disulfide conformation in oxytocin and lysine vasopressin, Biochemistry, 16, 4443-4449 (1977).

*450. S. S. Zimmerman and H. A. Scheraga - Local interactions in bends of proteins, Proc. Natl. Acad. Sci., U.S., 74, 4126-4129 (1977).

*451. J. C. Owicki and H. A. Scheraga - Monte Carlo calculations in the isothermal-isobaric ensemble. 1. Liquid water, J. Am. Chem. Soc., 99, 7403-7412 (1977).

*452. J. C. Owicki and H. A. Scheraga - Monte Carlo calculations in the isothermal-isobaric ensemble. 2. Dilute aqueous solution of methane, J. Am. Chem. Soc., 99, 7413-7418 (1977).

453. D. J. T. Hill, F. Cardinaux and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. XIV. Methionine parameters from random poly(hydroxypropylglutamine, L-methionine), Biopolymers, 16, 2447-2467 (1977).

454. D. J. T. Hill, F. Cardinaux and H. A. Scheraga - On the amino-acid-sequence distribution in benzylglutamate-methionine copolymers prepared from N-carboxyanhydrides, Biopolymers, 16, 2469-2480 (1977).

455. S. Sridhara, V. S. Ananthanarayanan, G. T. Taylor and H. A. Scheraga - Helix-coil stabilities of L-alanine and L-leucine in mixed organic solvents, Biopolymers, 16, 2565-2568 (1977).

456. Y. Konishi, J. W. van Nispen, G. Davenport and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 15. Arginine parameters from random poly(hydroxybutylglutamine-co-L-arginine), Macromolecules, 10, 1264-1271 (1977).

457. Y. Kobayashi, F. Cardinaux, B. O. Zweifel and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 16. Aspartic acid parameters from random poly(hydroxybutylglutamine-co-L-aspartic acid), Macromolecules, 10, 1271-1283 (1977).

*458. S. Rackovsky and H. A. Scheraga - Hydrophobicity, hydrophilicity and the radial and orientational distributions of residues in native proteins, Proc. Natl. Acad. Sci., U.S.A., 74, 5248-5251 (1977).

459. H. A. Scheraga - Conformational energy calculations on peptides, in "Proc. Fifth American Peptide Symposium", ed. M. Goodman and J. Meienhofer, John Wiley, New York, 1977, p. 246-256.

460. H. A. Scheraga - Intermolecular potential for water and the hydration of proteins, Ann. N. Y. Acad. Sci., 303, 2-9 (1977).

1978

461. S. Rackovsky and H. A. Scheraga - Influence of ordered backbone structure on protein folding. A study of some simple models, Macromolecules, 11, 1-8 (1978).

*462. D. H. Wertz and H. A. Scheraga - The influence of water on protein structure. An analysis of the preferences of amino acid residues for the inside or outside and for specific conformations in a protein molecule, Macromolecules, 11, 9-15 (1978).

463. P. H. Von Dreele, I. D. Rae and H. A. Scheraga - Nuclear magnetic resonance study of fibrinogen-like peptides and their structure in dimethyl sulfoxide and water, Biochemistry, 17, 956-962 (1978).

464. I. D. Rae and H. A. Scheraga - Shielding effects of the D-Phe aromatic ring in the ^{1}H NMR spectrum of gramicidin S, Biochem. Biophys. Res. Commun., 81, 481-485 (1978).

*465. H. E. Van Wart and H. A. Scheraga - Raman and resonance Raman spectroscopy, in "Enzyme Structure", part G of "Methods in Enzymology", Vol. 49, Ch. 5, eds. C. H. W. Hirs and S. N. Timasheff, Academic Press, New York, p. 67 (1978).

466. H. E. Van Wart and H. A. Scheraga - Resonance Raman probes of enzyme active sites, Fed. Proc., 37, 1484 (1978).

467. J. C. Owicki and H. A. Scheraga - Monte Carlo free energy calculations on dilute solutions in the isothermal-isobaric ensemble, J. Phys. Chem., 82, 1257-1264 (1978).

468. M. H. Hecht, B. O. Zweifel and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 17. Threonine parameters from random poly(hydroxybutylglutamine-co-L-threonine), Macromolecules, 11, 545-551 (1978).

469. N. Go and H. A. Scheraga - Calculation of the conformation of cyclo-hexaglycyl. 2. Application of a Monte Carlo method, Macromolecules, 11, 552-559 (1978).

470. H. A. Scheraga - Use of random copolymers to determine the helix-coil stability constants of the naturally occurring amino acids, Pure and Applied Chem., 50, 315-324 (1978).

471. S. S. Zimmerman and H. A. Scheraga - Influence of local interactions on protein structure. II. Conformational energy studies of N-acetyl-N'-methylamides of Ala-X and X-Ala dipeptides, Biopolymers, 17, 1849-1869 (1978).

*472. S. S. Zimmerman and H. A. Scheraga - Influence of local interactions on protein structure. III. Conformational energy studies of N-acetyl-N'- methylamides of Gly-X and X-Gly dipeptides, Biopolymers, 17, 1871-1884 (1978).

473. S. S. Zimmerman and H. A. Scheraga - Influence of local interactions on protein structure. IV. Conformational energy studies of N-acetyl-N'-methylamides of Ser-X and X-Ser dipeptides, Biopolymers, 17, 1885-1890 (1978).

474. I. Simon, G. Némethy and H. A. Scheraga - Conformational energy calculations of the effects of sequence variations on the conformations of two tetrapeptides, Macromolecules, 11, 797-804 (1978).

475. S. Fitzwater, Z. I. Hodes and H. A. Scheraga - Conformational energy study of tuftsin, Macromolecules, 11, 805-811 (1978).

476. J. S. Anderson and H. A. Scheraga - Conformational energy calculations on the contraceptive tetrapeptide H-Thr-Pro-Arg-Lys-OH, Macromolecules, 11, 812-819 (1978).

477. R. R. Matheson, Jr. and H. A. Scheraga - A method for predicting nucleation sites for protein folding based on hydrophobic contacts, Macromolecules, 11, 819-829 (1978).

478. J. Snir, R. A. Nemenoff and H. A. Scheraga - A revised empirical potential for conformational, intermolecular, and solvation studies. 1. Evaluation of problem and description of model, J. Phys. Chem., 82, 2497-2503 (1978).

479. R. A. Nemenoff, J. Snir and H. A. Scheraga - A revised empirical potential for conformational, intermolecular, and solvation studies. 2. Parameterization and testing for water and saturated organic molecules, J. Phys. Chem., 82, 2504-2512 (1978).

480. R. A. Nemenoff, J. Snir and H. A. Scheraga - A revised empirical potential for conformational, intermolecular, and solvation studies. 3. Parameterization and testing for unsaturated hydrocarbons, J. Phys. Chem., 82, 2513-2520 (1978).

481. R. A. Nemenoff, J. Snir and H. A. Scheraga - A revised empirical potential for conformational, intermolecular, and solvation studies. 4. Development and testing of parameters for aldehydes, ketones and carboxylic acids, J. Phys. Chem., 82, 2521-2526 (1978).

482. J. Snir, R. A. Nemenoff and H. A. Scheraga - A revised empirical potential for conformational, intermolecular, and solvation studies. 5. Development and testing of parameters for amides, amino acids and peptides, J. Phys. Chem., 82, 2527-2530 (1978).

483. T. Ooi, K. Nishikawa, M. Oobatake and H. A. Scheraga - Flexibility of bovine pancreatic trypsin inhibitor, Biochim. Biophys. Acta, 536, 390-405 (1978).

484. L. G. Dunfield, A. W. Burgess and H. A. Scheraga - Energy parameters in polypeptides. 8. Empirical potential energy algorithm for the conformational analysis of large molecules, J. Phys. Chem., 82, 2609-2616 (1978).

485. S. Rackovsky and H. A. Scheraga - Differential geometry and polymer conformation. 1. Comparison of protein conformations, ACS meeting abstracts, p. BIOL 31, Sept. 1978, Macromolecules, 11, 1168-1174 (1978).

*486. G. Némethy, Z. I. Hodes and H. A. Scheraga - A model for hydration of peptides and its application to the conformational analysis of terminally blocked amino acids and dipeptides, Proc. Natl. Acad, Sci., U.S., 75, 5760-5764 (1978).

*487. H. A. Scheraga - An approximate model for protein folding: experimental and theoretical aspects, in "Versatility of Proteins", ed. C. H. Li, Academic Press, 1978, p. 119-132.

*488. M. K. Swenson, A. W. Burgess and H. A. Scheraga - Conformational analysis of polypeptides: Application to homologous proteins, in "Frontiers in Physicochemical Biology", ed. B. Pullman, Academic Press, 1978, p. 115-142.

1979

489. D. J. Sandman, A. J. Epstein, J. S. Chickos, J. Ketchum, J. S. Fu and H. A. Scheraga - Crystal lattice and polarization energy of tetrathiafulvalene, J. Chem. Phys., 70, 305-313 (1979).

*490. H. A. Scheraga - Interactions in aqueous solution, ACS meeting abstracts, p. Coll 45, March 1978, Accts. Chem. Res., 12, 7-14 (1979).

*491. R. A. Martinelli, A. S. Inglis, M. R. Rubira, T. C. Hageman, J. G. R. Hurrell, S. J. Leach and H. A. Scheraga - Amino acid sequences of portions of the α and β chains of bovine fibrinogen, Arch. Biochem. Biophys., 192, 27-32 (1979).

492. F. R. Maxfield and H. A. Scheraga - Improvements in the prediction of protein backbone topography by reduction of statistical errors, Biochemistry, 18, 697-704 (1979).

*493. I. D. Rae and H. A. Scheraga - ^{1}H and ^{13}C nuclear magnetic resonance spectra of some peptides with fibrinogen-like reactivity, Intntl. J. Peptide and Protein Res., 13, 304-314 (1979).

*494. E. R. Stimson, Y. C. Meinwald and H. A. Scheraga - Solution conformation of Enkephalin. A nuclear magnetic resonance study of ^{13}C-enriched carbonyl carbons in [Leu^{5}]-enkephalin, Biochemistry, 18, 1661-1671 (1979).

495. R. A. Martinelli and H. A. Scheraga - Assay of bovine fibrinopeptides by high performance liquid chromotography, Anal. Biochem., 96, 246-249 (1979).

*496. R. R. Matheson, Jr. and H. A. Scheraga - Steps in the pathway of the thermal unfolding of ribonuclease A. Anonspecific surface-labeling study, Biochemistry, 12, 2437-2445 (1979).

497. R. R. Matheson, Jr. and H. A. Scheraga - Steady-state kinetic study of action of ribonuclease A, involving a conformational change between 30 and 40 C, Biochemistry, 12, 2446-2450 (1979).

498. R. Deslauriers, S. J. Leach, F. R. Maxfield, E. Minasian, J. R. McQuie, Y. C. Meinwald, G. Némethy, M. S. Pottle, I. D. Rae, H. A. Scheraga, E. R. Stimson and J. W. van Nispen - Cyclized dipeptide model for a β-bend, Proc. Natl. Acad. Sci., U.S., 76, 2512-2514 (1979).

*499. Z. I. Hodes, G. Némethy and H. A. Scheraga - 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, 18, 1565-1610 (1979).

*500. Z. I. Hodes, G. Némethy and H. A. Scheraga - Influence of hydration on the conformational stability and formation of bends in terminally blocked dipeptides, Biopolymers, 18, 1611-1634 (1979).

501. M. R. Pincus and H. A. Scheraga - Conformational energy calculations of enzyme-substrate and enzyme-inhibitor complexes of lysozyme. 2. Calculation of the structures of complexes with a flexible enzyme, Macromolecules, 12, 633-644 (1979).

502. H. A. Scheraga - Experimental and theoretical aspects of protein folding, Hoppe-Seyler's Z. Physiol. Chem., 360, 1015-1016 (1979).

*503. L. G. Chavez, Jr. and H. A. Scheraga - Location of the antigenic determinants of bovine pancreatic ribonuclease, Biochemistry, 18, 4386-4395 (1979).

504. F. R. Maxfield, S. J. Leach, E. R. Stimson, S. P. Powers and H. A. Scheraga - Infrared spectra of the N-acetyl- N'-methylamides of Glycine, L-Alanine, and L-Leucine in dilute solutions of chloroform and carbon tetrachloride, Biopolymers, 18, 2507-2521 (1979).

505. R. K. Scheule, H. E. Van Wart, B. O. Zweifel, B. L. Vallee and H. A. Scheraga - Resonance Raman spectroscopy of Arsanilazocarboxypeptidase A: Assignment of the vibrations of Azotyrosyl-248, J. Inorganic Biochem., 11, 283 (1979).

*506. G. Némethy and H. A. Scheraga - A possible folding pathway of bovine pancreatic RNase, Proc. Natl. Acad. Sci., U.S., 76, 6050-6054 (1979).

1980

507. H. A. Scheraga - Protein folding; application to ribonuclease, in "Protein Folding", ed. R. Jaenicke, Elsevier, Amsterdam, 1980, p. 261-288.

508. R. K. Scheule, H. E. Van Wart, B. L. Vallee and H. A. Scheraga - Resonance Raman spectroscopy of Arsanilazocarboxypeptidase A: conformational equilibria in solution and crystal phases, Biochemistry, 19, 759-766 (1980).

*509. L. G. Chavez, Jr. and H. A. Scheraga - Folding of ribonuclease, S-protein, and Des(121-124)-ribonuclease during glutathione oxidation of the reduced proteins, Biochemistry, 19, 996-1004 (1980).

*510. L. G. Chavez, Jr. and H. A. Scheraga - Intrinsic stabilities of portions of the ribonuclease molecule, Biochemistry, 19, 1005-1012 (1980).

*511. C. Pottle, M. S. Pottle, R. W. Tuttle, R. J. Kinch and H. A. Scheraga - Conformational analysis of proteins: algorithms and data structures for array processing, J. Computational Chem., 1, 46-58 (1980).

512. S. Fitzwater and H. A. Scheraga - A model-building procedure with particular application to proteins, Acta Cryst., A36, 211-219 (1980).

513. Y. Konishi and H. A. Scheraga - Regeneration of ribonuclease A from the reduced protein. 1. Conformational analysis of the intermediates by measurements of enzymatic activity, optical density and optical rotation, Biochemistry, 19, 1308-1316 (1980).

514. Y. Konishi and H. A. Scheraga - Regeneration of ribonuclease A from the reduced protein. 2. Conformational analysis of the intermediates by nuclear magnetic resonance spectroscopy, Biochemistry, 19, 1316-1322 (1980).

515. J. N. Telford, J. A. Nagy, P. A. Hatcher and H. A. Scheraga - Location of peptide fragments in the fibrinogen molecule by immunoelectron microscopy, Proc. Natl. Acad. Sci., U.S., 77, 2372-2376 (1980).

516. R. A. Martinelli and H. A. Scheraga - Steady state kinetic study of the bovine thrombin-fibrinogen interaction, Biochemistry, 19, 2343-2350 (1980).

517. S-L. Han, J. E. Rivier and H. A. Scheraga - Conformational studies of somatostatin and selected analogues by Raman spectroscopy, Intntl. J. Peptide and Protein Res., 15, 355-364 (1980). Erratum: 16, 352 (1980).

518. Y. Isogai, G. Némethy, S. Rackovsky, S. J. Leach and H. A. Scheraga - Characterization of multiple bends in proteins, Biopolymers, 19, 1183-1210 (1980).

519. H. A. Scheraga - Paul J. Flory on His 70th Birthday, Macromolecules, 13, No. 3, p. 8A (1980).

*520. M. H. Miller, G. Némethy and H. A. Scheraga - Calculation of the structures of collagen models. Role of interchain interactions in determining the triple-helical coiled-coil conformation. 2. Poly(glycyl-prolyl-hydroxyprolyl), Macromolecules, 13, 470-478 (1980).

*521. G. Némethy and H. A. Scheraga - Stereochemical requirements for the existence of hydrogen bonds in β-bends, Biochem. Biophys. Res. Comm., 95, 320-327 (1980).

522. M. H. Miller, G. Némethy and H. A. Scheraga - Calculation of the structures of collagen models. Role of interchain interactions in determining the triple-helical coiled-coil conformation. 3. Poly(glycyl-prolyl-alanyl). Macromolecules, 13, 910-913 (1980).

523. G. Némethy, M. H. Miller and H. A. Scheraga - Calculation of the structures of collagen models. Role of interchain interactions in determining the triple-helical coiled-coil conformation. 4. Poly(glycyl-alanyl-prolyl). Macromolecules, 13, 914-919 (1980).

*524. Y. C. Meinwald, R. A. Martinelli, J. W. van Nispen and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. Size of the A fibrinogen-like peptide that contacts the active site of thrombin, Biochemistry, 19, 3820-3825 (1980).

525. E. Benedetti, C. Pedone, C. Toniolo, G. Némethy, M. S. Pottle and H. A. Scheraga - Preferred conformation of the tert-butoxycarbonyl-amino group in peptides, Intntl. J. Peptide and Protein Res., 16, 156-172 (1980).

526. S-L. Han, E. R. Stimson, F. R. Maxfield and H. A. Scheraga - Conformational Study of [Leu^5]-enkephalin by laser Raman spectroscopy, Intntl. J. Peptide and Protein Res., 16, 173-182 (1980).

527. S-L. Han, E. R. Stimson, F. R. Maxfield, S. J. Leach and H. A. Scheraga - Study of the state of ionization of [Leu^5]-enkephalin in the crystal and in solution, Intntl. J. Peptide and Protein Res., 16, 183-190 (1980).

*528. H. Meirovitch, S. Rackovsky and H. A. Scheraga - Empirical studies of hydrophobicity. 1. Effect of protein size on the hydrophobic behavior of amino acids, Macromolecules, 13, 1398-1405 (1980).

*529. H. Meirovitch and H. A. Scheraga - Empirical studies of hydrophobicity. 2. Distribution of the hydrophobic, hydrophilic, neutral and ambivalent amino acids in the interior and exterior layers of native proteins, Macromolecules, 13, 1406-1414 (1980).

*530. L. G. Dunfield and H. A. Scheraga - Ising model treatment of short-range interactions in polypeptides and its application to the structure of bovine pancreatic trypsin inhibitor, Macromolecules, 13, 1415-1428 (1980).

531. J. A. Nagy, S. P. Powers, B. O. Zweifel and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 18. Tryptophan parameters from random poly[(hydroxypropyl)glutamine-co-L-tryptophan], Macromolecules, 13, 1428-1440 (1980). Erratum: ibid., 14, 466 (1981).

532. S. Rackovsky and H. A. Scheraga - Differential geometry and polymer conformation. 2. Development of a conformational distance function, Macromolecules, 13, 1440-1453 (1980). Erratum: ibid., 14, 466 (1981).

533. S. Rackovsky and H. A. Scheraga - Intermolecular anti-parallel β-sheet: Comparison of predicted and observed conformations of gramicidin S, Proc. Natl. Acad. Sci., U.S.A., 77, 6965-6967 (1980).

534. H. A. Scheraga - Phase transitions in synthetic polymers of amino acids, and their relation to protein folding, Ferroelectrics, 30, 157-158 (1980).

1981

*535. G. Némethy and H. A. Scheraga - Strong interaction between disulfide derivatives and aromatic groups in peptides and proteins, Biochem. Biophys. Res. Comm., 98, 482-487 (1981).

536. S-L. Han, E. R. Stimson, F. R. Maxfield and H. A. Scheraga - Spectroscopic study of the conformations of proline-containing oligopeptides in the crystalline state and in solution, Intntl. J. Peptide and Protein Res., 17, 297-315 (1981).

537. R. K. Scheule, S-L. Han, H. E. Van Wart, B. L. Vallee and H. A. Scheraga - Resonance Raman spectroscopy of arsanilazocarboxypeptidase A: mode of inhibitor binding and active-site topography, Biochemistry, 20, 1778-1784 (1981).

*538. D. C. Rapaport and H. A. Scheraga - Structure and dynamics of the "Configuration Interaction" model of liquid water, Chem. Phys. Letters, 78, 491-494 (1981).

539. H. Meirovitch and H. A. Scheraga - Empirical studies of hydrophobicity. 3. Radial distribution of clusters of hydrophobic and hydrophilic amino acids, Macromolecules, 14, 340-345 (1981).

*540. Y. Paterson, G. Némethy and H. A. Scheraga - Hydration of amino acids, peptides and model compounds, Annals N. Y. Acad. Sci., 367, 132-150 (1981).

541. I. D. Rae, S. J. Leach, E. Minasian, J. A. Smith, S. S. Zimmerman, J. A. Weigold, Z. I. Hodes, G. Némethy, R. W. Woody and H. A. Scheraga - Conformational characteristics of the N-acetyl-N'-methylamides of the four (Lys,Tyr) dipeptides, Intntl. J. Peptide Protein Res., 17, 575-592 (1981). Erratum: ibid., 18, 220 (1981).

*542. G. Némethy, W. J. Peer and H. A. Scheraga - Effect of protein-solvent interactions on protein conformation, Ann. Rev. Biophys. Bioeng., 10, 459-497 (1981).

*543. Y. Paterson, S. M. Rumsey, E. Benedetti, G. Némethy and H. A. Scheraga - Sensitivity of polypeptide conformation to geometry. Theoretical conformational analysis of oligomers of α-aminoisobutyric acid, J. Am. Chem. Soc., 103, 2947-2955 (1981).

544. R. A. Fredrickson, M. C. Chang, S. P. Powers and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 19. Iso-leucine parameters from random poly[(hydroxypropyl)-glutamine-co-L-isoleucine], Macromolecules, 14, 625-632 (1981).

545. M. C. Chang, R. A. Fredrickson, S. P. Powers and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 20. Reinvestigation of valine parameters from random poly[(hydroxypropyl) glutamine-co-L-valine], Macromolecules, 14, 633-634 (1981).

546. H. A. Scheraga - Intersegment recognition in enzyme-substrate complexes and in fibrous and globular proteins, Proc. of the 7th Annual Katzir-Katchalsky Conference; Structural Aspects of Recognition and Assembly in Biological Macromolecules, ed. M. Balaban, J. L. Sussman, W. Traub and A. Yonath, Balaban ISS, Rehovot and Philadelphia, 1981, p. 87-98.

547. S. Sridhara, V. S. Ananthanarayanan, R. A. Fredrickson, B. O. Zweifel, G. T. Taylor and H. A. Scheraga - Helix-coil stability constants for amino acids in non-aqueous solvents. Studies of random poly(γ-benzyl-L-glutamate-co-L-alanine) and poly(γ-benzyl-L-glutamate-co-L-leucine) in a mixed solvent, Biopolymers, 20, 1435-1458 (1981).

548. Y. Konishi, T. Ooi and H. A. Scheraga - Regeneration of ribonuclease A from the reduced protein. Isolation and identification of intermediates, and equilibrium treatment, Biochemistry, 20, 3945-3955 (1981).

*549. M. R. Pincus and H. A. Scheraga - Prediction of the three-dimensional structures of complexes of lysozyme with cell wall substrates, Biochemistry, 20, 3960-3965 (1981).

*550. H. Wako and H. A. Scheraga - On the use of distance constraints to fold a protein, Macromolecules, 14, 961-969 (1981).

551. G. Némethy, J. R. McQuie, M. S. Pottle and H. A. Scheraga - Conformation of cyclo(L-alanylglycyl-E-aminocaproyl), a cyclized dipeptide model for a β-bend. 1. Conforma-tional energy calculations, Macromolecules, 14, 975-985 (1981).

552. R. Deslauriers, D. J. Evans, S. J. Leach, Y. C. Meinwald, E. Minasian, G. Némethy, I. D. Rae, H. A. Scheraga, R. L. Somorjai, E. R. Stimson, J. W. van Nispen and R. W. Woody - Conformation of cyclo(L-alanylglycyl-E-aminocaproyl), a cyclized dipeptide model for a -bend. 2. Synthesis, nuclear magnetic resonance, and circular dichroism measurements, Macromolecules, 14, 985-996 (1981).

553. F. R. Maxfield, J. Bandekar, S. Krimm, D. J. Evans, S. J. Leach, G. Némethy and H. A. Scheraga - Conformation of cyclo(L-alanylgylcyl-E-aminocaproyl), a cyclized dipeptide model for a β-bend. 3. Infrared and Raman spectroscopic studies, Macromolecules, 14, 997-1003 (1981).

*554. H. A. Scheraga - Influence of interatomic interactions on the structure and stability of polypeptides and proteins, Biopolymers, 20, 1877-1899 (1981).

555. D. C. Rapaport and H. A. Scheraga - Evolution and stability of polypeptide chain conformation: A simulation study, Macromolecules, 14, 1238-1246 (1981).

556. H. Meirovitch and H. A. Scheraga - An approach to the multiple-minimum problem in protein folding, involving a long-range geometrical restriction and short-, medium- and long-range interactions, Macromolecules, 14, 1250-1259 (1981).

557. S. Rackovsky and H. A. Scheraga - Differential geometry and polymer conformation. 3. Single-site and nearest- neighbor distributions, and nucleation of protein folding, Macromolecules, 14, 1259-1269 (1981).

*558. M. R. Pincus and H. A. Scheraga - Theoretical calculations on enzyme-substrate complexes: the basis of molecular recognition and catalysis, Accts. Chem. Res., 14, 299-306 (1981).

559. H. Meirovitch and H. A. Scheraga - Introduction of short-range restrictions in a protein-folding algorithm involving a long-range geometrical restriction and short-, medium- and long-range interactions, Proc. Natl. Acad. Sci., U.S.A., 78, 6584-6587 (1981).

560. H. E. Van Wart, B. L. Vallee, R. K. Scheule and H. A. Scheraga - Resonance Raman probes of enzyme active sites, Trends in Biochemical Sciences, 6, 316-318 (1981).

561. D. M. Rice, R. J. Wittebort, R. G. Griffin, E. Meirovitch, E. R. Stimson, Y. C. Meinwald, J. H. Freed and H. A. Scheraga - Rotational jumps of the tyrosine side chain in crystalline enkephalin. H NMR line shapes for aromatic ring motion in solids, J. Am. Chem. Soc., 103, 7707-7710 (1981).

*562. H. A. Scheraga - Simulations of protein folding, hydration and interaction with substrates, Proc. Workshop on "Computer Simulation of Organic and Biological Molecules", LBL-12979, NRCC Proc., Jan. 1981, p. 27-30.

1982

563. J. B. Denton, S. P. Powers, B. O. Zweifel and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. XXI. Glutamine parameters from random poly(hydroxypropyl-glutamine-co-L-glutamine) and poly(hydroxybutylglutamine-co-L-glutamine), Biopolymers, 21, 51-77 (1982).

564. S. S. Zimmerman, R. Baum and H. A. Scheraga - Conformational energy analysis of melanostatin, Intntl. J. Peptide and Protein Res., 19, 143-152 (1982).

565. J. Bandekar, D. J. Evans, S. Krimm, S. J. Leach, S. Lee, J. R. McQuie, E. Minasian, G. Némethy, M. S. Pottle, H. A. Scheraga, E. R. Stimson and R. W. Woody - Conformations of cyclo(L-alanyl-L-alanyl-E-aminocaproyl) and of cyclo(L-alanyl-D-alanyl-E-aminocaproyl); cyclized dipeptide models for specific types of β-bends, Intntl. J. Peptide and Protein Res., 19, 187-205 (1982).

*566. H. Wako and H. A. Scheraga - Visualization of the nature of protein folding by a study of a distance constraint approach in two-dimensional models, Biopolymers, 21, 611-632 (1982).

567. R. H. Kincaid and H. A. Scheraga - Revised empirical potential for conformational, intermolecular, and solvation studies. 6. Testing of parameters by application to liquid ammonia, J. Phys. Chem., 86, 833-838 (1982).

568. R. H. Kincaid and H. A. Scheraga - Revised empirical potential for conformational, intermolecular, and solvation studies. 7. Testing of parameters by application to liquid methane, J. Phys. Chem., 86, 838-841 (1982).

569. S. Fitzwater and H. A. Scheraga - Combined-information protein structure refinement: potential energy-constrained real-space method for refinement with limited diffraction data, Proc. Natl. Acad. Sci., U.S.A., 79, 2133-2137 (1982).

*570. D. C. Rapaport and H. A. Scheraga - Hydration of inert solutes. A molecular dynamics study, J. Phys. Chem., 86, 873-880 (1982).

571. J. A. Nagy, Y. C. Meinwald and H. A. Scheraga - Immuno-chemical determination of conformational equilibria for fragments of the Aα chain of fibrinogen, Biochemistry, 21, 1794-1806 (1982).

572. H. Wako and H. A. Scheraga - Distance-constraint approach to protein folding. I. Statistical analysis of protein conformations in terms of distances between residues, J. Protein Chem., 1, 5-45 (1982).

573. H. Wako and H. A. Scheraga - Distance-constraint approach to protein folding. II. Prediction of three-dimensional structure of bovine pancreatic trypsin inhibitor, J. Protein Chem., 1, 85-117 (1982).

574. H. A. Scheraga - Structure and thermodynamic properties of aqueous solutions of small molecules and proteins, Pure and Applied Chem., 54, 1495-1505 (1982).

575. M. R. Pincus, R. D. Klausner and H. A. Scheraga - Calculation of the three-dimensional structure of the membrane-bound portion of melittin from its amino acid sequence, Proc. Natl. Acad. Sci., U.S.A., 79, 5107-5110 (1982).

576. G. Némethy and H. A. Scheraga - Conformational preferences of amino acid side chains in collagen, Biopolymers, 21, 1535-1555 (1982).

577. H. A. Scheraga - Consideration of the hydrodynamic properties of proteins (Citation Classic), Current Contents (Physical Sciences), No. 35, p. 18 (August 30, 1982).

578. H. A. Scheraga - Interactions in biopolymers, Proc. 28th Macromolecular Symp., IUPAC, Amherst, Mass., July 1982, p. 525.

579. Y. Konishi, T. Ooi and H. A. Scheraga - Regeneration of ribonuclease A from the reduced protein. Rate-limiting steps, Biochemistry, 21, 4734-4740 (1982).

580. Y. Konishi, T. Ooi and H. A. Scheraga - Regeneration of ribonuclease A from the reduced protein. Energetic analysis, Biochemistry, 21, 4741-4748 (1982).

581. Y. Konishi, T. Ooi and H. A. Scheraga - Regeneration of RNase A from the reduced protein: models of regeneration pathways, Proc. Natl. Acad. Sci., U.S., 79, 5734-5738 (1982).

582. J. B. Denton, Y. Konishi and H. A. Scheraga - Folding of ribonuclease A from a partially disordered conformation. Kinetic study under folding conditions, Biochemistry, 21, 5155-5163 (1982).

583. E. R. Stimson, G. T. Montelione, Y. C. Meinwald, R. K. E. Rudolph and H. A. Scheraga - Equilibrium Ratios of cis- and trans-proline conformers in fragments of ribonuclease A from nuclear magnetic resonance spectra of adjacent tyrosine ring resonances, Biochemistry, 21, 5252-5262 (1982).

584. S. Rackovsky and H. A. Scheraga - Differential geometry and polymer conformation. 4. Conformational and nucleation properties of individual amino acids, Macromolecules, 15, 1340-1346 (1982).

585. Y. Paterson, E. R. Stimson, D. J. Evans, S. J. Leach and H. A. Scheraga - Solution conformations of oligomers of α-aminoisobutyric acid, Intntl. J. Peptide and Protein Res., 20, 468-480 (1982). Erratum: ibid., 22, 128a (1983).

586. T. Ooi and H. A. Scheraga - Self-organization of protein molecules, J. Protein Chem., 1, 157-162 (1982).

587. J. S. Anderson and H. A. Scheraga - Effect of short- and long-range interactions on protein folding, J. Protein Chem., 1, 281-304 (1982).

588. R. H. Kincaid and H. A. Scheraga - Acceleration of convergence in Monte Carlo simulations of aqueous solutions using the Metropolis algorithm. Hydrophobic hydration of methane, J. Computational Chem., 3, 525-547 (1982).

*589. K.-C. Chou, M. Pottle, G. Némethy, Y. Ueda and H. A. Scheraga - Structure of β-sheets. Origin of the right-handed twist and of the increased stability of antiparallel over parallel sheets, J. Mol. Biol., 162, 89-112 (1982).

590. K.-C. Chou and H. A. Scheraga - Origin of the right-handed twist of β-sheets of poly(L-Val) chains, Proc. Natl. Acad. Sci., U.S.A., 79, 7047-7051 (1982).

591. H. C. Marsh, Jr., Y. C. Meinwald, S. Lee and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. Direct evidence for the involvement of phenylalanine at position P_9, Biochemistry, 24, 6167-6171 (1982).

592. Y. Paterson, G. Némethy and H. A. Scheraga - An empirical potential function for the interaction between univalent ions in water, J. Solution Chem., 11, 831-856 (1982).

1983

593. H. A. Scheraga, M. R. Pincus and K. E. Burke - Calculations of structures of enzyme-substrate complexes, in "Structure of Complexes Between Biopolymers and Low Molecular Weight Molecules", eds. W. Bartmann and G. Snatzke, John Wiley, Chichester, p. 53-76 (1983).

594. H. A. Scheraga, K. C. Chou and G. Némethy - Interactions between the fundamental structures of polypeptide chains, in "Conformation in Biology", Ed. R. Srinivasan and R. H. Sarma, Adenine Press, p. 1-10 (1983).

595. H. A. Scheraga - Recent progress in the theoretical treatment of protein folding, Biopolymers, 22, 1-14 (1983). Also reprinted in "Structure and Dynamics: Nucleic Acids and Proteins", eds. E. Clementi and R. H. Sarma, Adenine Press, New York, p. 463 (1983).

596. G. Bolis, E. Clementi, D. H. Wertz, H. A. Scheraga and C. Tosi - Interaction of methane and methanol with water, J. Am. Chem. Soc., 105, 355-360 (1983).

597. D. J. Evans, I. D. Rae, E. Minasian, G. Némethy, H. A. Scheraga and S. J. Leach - A conformational study of the tetrapeptide CH CO-Ala-Asp-Gly-Lys-NHCH corresponding to a β-bend in staphylococcal nuclease, J. Protein Chem., 2, 77-99 (1983).

598. E. Benedetti, C. Pedone, C. Toniolo, M. Dudek, G. Némethy and H. A. Scheraga - Preferred conformation of the benzyloxycarbonyl-amino group in peptides, Intntl. J. Peptide and Protein Res., 21, 163-181 (1983).

599. A. Kidera, M. Mochizuki, R. Hasegawa, T. Hayashi, H. Sato, A. Nakajima, R. A. Fredrickson, S. P. Powers, S. Lee and H. A. Scheraga - Helix-coil transition in multicomponent random copolypeptides in water. 1. Theory, and application to random copolymers of (hydroxypropyl)-L-glutamine, L-alanine, and glycine, Macromolecules, 16, 162-172 (1983).

600. H. A. Scheraga - Theoretical and experimental aspects of protein folding, in "Supramolecular Structure and Function", ed. G. Pifat and J. N. Herak, Plenum Publ. Corp., New York, p. 45-58 (1983).

601. G. Némethy, M. S. Pottle and H. A. Scheraga - Energy parameters in polypeptides. 9. Updating of geometrical parameters, nonbonded interactions, and hydrogen bond interactions for the naturally occurring amino acids, J. Phys. Chem., 87, 1883-1887 (1983).

602. M. R. Pincus, F. Gerewitz, R. H. Schwartz and H. A. Scheraga - Correlation between the conformation of cytochrome c peptides and their stimulatory activity in a T-lymphocyte proliferation assay, Proc. Natl. Acad. Sci., U.S.A., 80, 3297-3300 (1983).

603. H. A. Scheraga - Interaction of thrombin and fibrinogen and the polymerization of fibrin monomer, Annals N.Y. Acad. Sci., 408, 330-343 (1983).

604. M. R. Pincus, F. Gerewitz, H. Wako and H. A. Scheraga - Cis-trans isomerization of proline in the peptide (His 105-Val 124) of ribonuclease A containing the primary nucleation site, J. Protein Chem., 2, 131-146 (1983).

605. E. Benedetti, G. Morelli, G. Némethy and H. A. Scheraga -Statistical and energetic analysis of side-chain conformations in oligopeptides, Intntl. J. Peptide and Protein Res., 22, 1-15 (1983).

606. R. R. Matheson, Jr. and H. A. Scheraga - Calculation of the Zimm-Bragg cooperativity parameter σ from a simple model of the nucleation process, Macromolecules, 16, 1037-1043 (1983).

607. M. Vasquez, G. Némethy and H. A. Scheraga - Computed conformational states of the 20 naturally occurring amino acid residues and of the prototype residue α-aminobutyric acid, Macromolecules, 16, 1043-1049 (1983).

608. K.-C. Chou, G. Némethy and H. A. Scheraga - Energetic Approach to the Packing of α-Helices. 1. Equivalent Helices, J. Phys. Chem., 87, 2869-2881 (1983). Erratum: ibid., 87, 4772 (1983).

609. K.-C. Chou, G. Némethy and H. A. Scheraga - Role of interchain interactions in the stabilization of the right-handed twist of β-sheets, J. Mol. Biol., 168, 389-407 (1983).

610. H. C. Marsh, Jr., Y. C. Meinwald, T. W. Thannhauser and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen. Kinetic evidence for involvement of aspartic acid at position P_{10}, Biochemistry, 22, 4170-4174 (1983).

611. H. Wako, N. Saito and H. A. Scheraga - Statistical mechanical treatment of α-helices and extended structures in proteins with inclusion of short- and medium-range interactions, J. Protein Chem., 2, 221-249 (1983).

612. K. C. Chou, G. Némethy and H. A. Scheraga - Effect of amino acid composition on the twist and the relative stability of parallel and antiparallel β-sheets, Biochemistry, 22, 6213-6221 (1983).

1984

613. G. Némethy and H. A. Scheraga - Hydrogen bonding involving the ornithine side chain of gramicidin S, Biochem. Biophys. Res. Commun., 118, 643-647 (1984).

*614. W. L. Mattice and H. A. Scheraga - Matrix formulation of the transition from a statistical coil to an antiparallel sheet, Biophys. J., 45, 259a (1984).

615. S. J. Smith-Gill, J. A. Rupley, M. R. Pincus, R. P. Carty and H. A. Scheraga - Experimental identification of a theoretically predicted "left-sided" binding mode for (GlcNAc) in the active site of lysozyme, Biochemistry, 23, 993-997 (1984).

616. M. Sueki, S. Lee, S. P. Powers, J. B. Denton, Y. Konishi and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. 22. Histidine parameters from random poly[(hydroxybutyl)glu-tamine-co- L-histidine], Macromolecules, 17, 148-155 (1984).

617. W. L. Mattice and H. A. Scheraga - Evaluation of intramolecular antiparallel sheet formation by matrix methods, ACS Polymer Preprints, 25, 276 (1984).

*618. H. A. Scheraga - Protein structure and function, from a colloidal to a molecular view (7th Linderstrøm-Lang Lecture, Copenhagen, May 10, 1983), Carlsberg Research Commun., 49, 1-55 (1984).

*619. T. W. Thannhauser, Y. Konishi and H. A. Scheraga - Sensitive quantitative analysis of disulfide bonds in polypeptides and proteins, Anal. Biochem., 138, 181-188 (1984).

620. R. M. Lynn, Y. Konishi and H. A. Scheraga - Folding of ribonuclease A from a partially disordered conformation. Kinetic study under transition conditions, Biochemistry, 23, 2470-2477 (1984).

621. K. C. Chou, G. Némethy and H. A. Scheraga - Energetic approach to the packing of α-helices. 2. General treatment of nonequivalent and nonregular helices, J. Am. Chem. Soc., 106, 3161-3170 (1984). Erratum: ibid., 107, 2199 (1985).

622. S. Rackovsky and H. A. Scheraga - Differential geometry and protein folding, Accts. Chem. Res., 17, 209-214 (1984).

623. E. Lee, G. Némethy, H. A. Scheraga and V. S. Ananthanarayanan - β-bend conformation of CH_3CO-Pro-Pro- Gly-Pro-$NHCH_3$: Implications for post-translational proline hydroxylation in collagen, Biopolymers, 23, 1193-1206 (1984).

624. E. O. Purisima and H. A. Scheraga - Conversion from a virtual-bond chain to a complete polypeptide backbone chain, Biopolymers, 23, 1207-1224 (1984).

625. J. K. Swadesh, G. T. Montelione, T. W. Thannhauser, and H. A. Scheraga - Local structure involving histidine-12 in reduced S-sulfonated ribonuclease A detected by proton NMR spectroscopy under folding conditions, Proc. Natl. Acad. Sci., U.S.A. 81, 4606-4610 (1984).

626. W. L. Mattice and H. A. Scheraga - Matrix formulation of the transition from a statistical coil to an intramolecular antiparallel β sheet, Biopolymers, 23, 1701-1724 (1984).

627. H. A. Scheraga - Theoretical studies of molecular recognition and catalysis by enzymes, Pont. Acad. Sci. Scr. Var., 55, 21-41 (1984). Also, in Proceedings of the XVIIIth Solvay Conference on Chemistry, ed. G. van Binst, Springer-Verlag, Berlin, p. 117 (1986).

628. L. S. Hanna, H. A. Scheraga, C. W. Francis and V. J. Marder - Comparison of structures of various human fibrinogens and a derivative thereof by a study of the kinetics of release of fibrinopeptides, Biochemistry, 23, 4681-4687 (1984).

629. J. K. Swadesh, T. W. Thannhauser and H. A. Scheraga - Sodium sulfite as an antioxidant in the acid hydrolysis of bovine pancreatic ribonuclease A, Anal. Biochem., 141, 397-401 (1984).

630. C. A. McWherter, T. W. Thannhauser, R. A. Fredrickson, M. T. Zagotta and H. A. Scheraga - Peptide mapping of bovine pancreatic ribonuclease A by reverse-phase high-performance liquid chromatography. I. Application to the reduced and S-carboxymethylated protein, Anal. Biochem., 141, 523-537 (1984).

631. M. Gō and H. A. Scheraga - 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, 23, 1961-1977 (1984).

632. B. H. Horwitz, A. Varadi and H. A. Scheraga - Localization of a fibrin γ-chain polymerization site within segment Thr374-Glu396 of human fibrinogen, Proc. Natl. Acad. Sci., U.S.A., 81, 5980-5984 (1984).

633. S. H. Lin, Y. Konishi, M. E. Denton and H. A. Scheraga -Influence of an extrinsic cross-link on the folding pathway of ribonuclease A. Conformational and thermodynamic analysis of cross-linked ($Lysine^{7}$-$Lysine^{41}$) -ribonuclease A, Biochemistry, 23, 5504-5512 (1984).

634. V. G. Davenport, E. R. Stimson and H. A. Scheraga - Determination of molecular weights by differential cryoscopy on small volumes of dilute solutions of oligopeptides, Anal. Biochem., 142, 400-405 (1984).

635. G. Némethy and H. A. Scheraga - Role of proline ... proline interactions in the packing of collagen like poly-(tripeptide) triple helices, Biopolymers, 23, 2781-2799 (1984). Erratum: ibid., 24, 581 (1985).

636. W. L. Mattice and H. A. Scheraga - Suppression of the statistical coil state during the a- β transition in homopolypeptides, Biopolymers, 23, 2879-2890 (1984). Erratum: ibid., 24, 581 (1985).

637. G. T. Montelione, E. Arnold, Y. C. Meinwald, E. R. Stimson, J. B. Denton, S.-G. Huang, J. Clardy and H. A. Scheraga - Chain-folding initiation structures in ribonuclease A: Conformational analysis of trans-Ac-Asn-Pro-Tyr-NHMe and trans-Ac-Tyr-Pro-Asn-NHMe in water and in the solid state. J. Am. Chem. Soc., 106, 7946-7958 (1984). Erratum: ibid., 107, 1457 (1985).

638. M. Oka, G. T. Montelione and H. A. Scheraga - Chain-folding initiation structures in ribonuclease A: Conformational free energy calculations on Ac-Asn-Pro-Tyr-NHMe, Ac-Tyr-Pro-Asn-NHMe, and related peptides, J. Am. Chem. Soc., 106, 7959-7969 (1984). Erratum: ibid., 107, 1457 (1985).

639. M. J. Sippl, G. Némethy and H. A. Scheraga - Intermolecular potentials from crystal data. 6. Determination of empirical potentials for O-H···O=C hydrogen bonds from packing configurations, J. Phys. Chem., 88, 6231-6233 (1984).

640. Z. Li and H. A. Scheraga - Real-space renormalization group treatment of the helix-coil transition in a homopolyamino acid chain, J. Phys. Chem., 88, 6580-6586(1984).

641. V. M. Naik, S. Krimm, J. B. Denton, G. Némethy and H. A. Scheraga - Vibrational Analysis of peptides, polypeptides, and proteins. XXVII. Structure of gramicidin S from normal mode analyses of low-energy conformations, Intnl. J. Peptide and Protein Res., 24, 613-626 (1984).

642. W. L. Mattice and H. A. Scheraga - Practical estimates of the upper limit for the distribution function for strand lengths in large homopolymers containing intramolecular antiparallel sheets with tight bends, Macromolecules, 17, 2690-2696 (1984).

*643. H. A. Scheraga, Y. Konishi and T. Ooi - Multiple pathways for regenerating ribonuclease A, Adv. Biophys., 18, 21-41 (1984).

1985

644. E. R. Stimson, S. G. Huang, G. Némethy, S. J. Leach and H. A. Scheraga - Conformational analysis of cyclized dipeptide models for specific types of β-bends by two-dimensional nuclear Overhauser spectroscopy, Intntl. J. Peptide and Protein Res., 25, 89-98 (1985).

*645. W. L. Mattice and H. A. Scheraga - Long-range aspects of the formation of intramolecular antiparallel β sheets, in "Mathematics and Computers in Biomedical Applications", Proc. 2nd IMACS International Symposium on Biomedical Systems Modelling, eds. J. Eisenfeld and C. DeLisi, Elsevier, 1985, p. 13-17.

646. W. L. Mattice, E. Lee and H. A. Scheraga - Dominance of irregular structures in the formation of intramolecular antiparallel β sheets by homopolyamino acids, Can. J. Chem., 63, 140-146 (1985).

647. H. A. Scheraga - Calculations of the three-dimensional structures of proteins, Annals N.Y. Acad. Sci., 439, 170-194 (1985).

648. J. A. Nagy, Y. C. Meinwald and H. A. Scheraga - Immunochemical determination of conformational equilibria for fragments of the Bβ chain of fibrinogen, Biochemistry, 24, 882-887 (1985).

649. W. L. Mattice and H. A. Scheraga - Role of interstrand loops in the formation of intramolecular cross-β sheets by homopolyamino acids, Biopolymers, 24, 565-579 (1985).

650. P. C. Weber, F. R. Salemme, S. H. Lin, Y. Konishi and H. A. Scheraga - Preliminary crystallographic data for cross-linked (Lysine^{7}-Lysine^{41})- ribonuclease A, J. Mol. Biol., 181, 453 (1985).

651. M. J. Sippl and H. A. Scheraga - Solution of the embedding problem and decomposition of symmetric matrices, Proc. Natl. Acad. Sci., U.S.A, 82, 2197-2201 (1985).

652. S. H. Lin, Y. Konishi, B. T. Nall and H. A. Scheraga - Influence of an extrinsic cross-link on the folding pathway of ribonuclease A. Kinetics of folding/ unfolding, Biochemistry, 24, 2680-2686 (1985).

653. H. C. Marsh, Jr., Y. C. Meinwald, S. Lee, R. A. Martinelli and H. A. Scheraga - Mechanism of action of thrombin on fibrinogen: NMR evidence for a β-bend at or near fibrinogen A Gly(P_5)-Gly(P_4), Biochemistry, 24, 2806-2812 (1985).

654. T. Miki, A. Kidera, M. Oka, T. Hayashi, A. Nakajima, Y. C. Meinwald, T. W. Thannhauser and H. A. Scheraga - Helix-coil transition in multicomponent random copolypeptides in water. 2. Application to random copolymers of (Hydroxybutyl)-L-glutamine, L-phenylalanine, and L-lysine, Macromolecules, 18, 1069-1073 (1985).

655. M. Gerritsen, K. C. Chou, G. Némethy and H. A. Scheraga -Energetics of multihelix interactions in protein folding: Application to myoglobin, Biopolymers, 24, 1271-1291 (1985). Erratum: ibid., 24, 2177 (1985).

656. P. W. Mui, Y. Konishi and H. A. Scheraga - Kinetics and mechanism of the refolding of denatured ribonuclease A, Biochemistry, 24, 4481-4489 (1985).

657. G. H. Paine and H. A. Scheraga - Prediction of the native conformation of a polypeptide by a statistical-mechanical procedure. I. Backbone structure of enkephalin, Biopolymers, 24, 1391-1436 (1985).

658. M. Vasquez and H. A. Scheraga - Use of buildup and energy-minimization procedures to compute low-energy structures of the backbone of enkephalin, Biopolymers, 24, 1437-1447 (1985).

659. H. A. Scheraga - Effect of side chain - backbone electrostatic interactions on the stability of α-helices, Proc. Natl. Acad. Sci, U.S., 82, 5585-5587 (1985).

660. A. Kidera, Y. Konishi, M. Oka, T. Ooi and H. A. Scheraga -Statistical Analysis of the Physical Properties of the 20 Naturally Occurring Amino Acids, J. Protein Chem., 4, 23-55 (1985).

661. T. W. Thannhauser, C. A. McWherter and H. A. Scheraga - Peptide mapping of bovine pancreatic ribonuclease A by reverse-phase high-performance liquid chromatography. II. A two-dimensional technique for determination of disulfide pairings using a continuous-flow disulfide detection system, Anal. Biochem., 149, 322-330 (1985).

662. F. Ni and H. A. Scheraga - Resolution enhancement in spectroscopy by maximum entropy Fourier self-deconvolution, with applications to Raman spectra of peptides and proteins, J. Raman Spectr., 16, 337-349 (1985).

663. K.-C. Chou, G. Némethy, S. Rumsey, R. W. Tuttle and H. A. Scheraga - Interactions between an α-helix and a β-sheet. Energetics of α/β packing in proteins, J. Mol. Biol., 186, 591-609 (1985).

664. T. W. Thannhauser and H. A. Scheraga - Reversible blocking of half-cystine residues of proteins and an irreversible specific deamidation of Asparagine-67 of S-sulforibo-nuclease under mild conditions, Biochemistry, 24, 7681-7688 (1985).

665. K.-C. Chou, G. Némethy, M. S. Pottle and H. A. Scheraga -Folding of the twisted β-sheet in bovine pancreatic trypsin inhibitor, Biochemistry, 24, 7948-7953 (1985).

666. M. R. Pincus and H. A. Scheraga - Conformational analysis of biologically active polypeptides, with application to oncogenesis, Accts. Chem. Res., 18, 372-379 (1985).

667. A. Kidera, Y. Konishi, T. Ooi and H. A. Scheraga - Relation between sequence similarity and structural similarity in proteins. Role of important properties of amino acids, J. Protein Chem., 4, 265-297 (1985).

1986

668. F. Ni, G. C. Levy and H. A. Scheraga - Simultaneous resolution enhancement and noise suppression in NMR signal processing by combined use of maximum entropy and Fourier self-deconvolution methods, J. Magn. Resonance, 66, 385-390 (1986).

669. T. Kikuchi, G. Némethy and H. A. Scheraga - Spatial geometric arrangements of disulfide-crosslinked loops in proteins, J. Comput. Chem., 7, 67-88 (1986).

670. A. Varadi and H. A. Scheraga - Localization of segments essential for polymerization and for calcium binding in the γ-chain of human fibrinogen, Biochemistry, 25, 519-528 (1986).

671. K. A. Palmer, H. A. Scheraga, J. F. Riordan and B. L. Vallee - A preliminary three-dimensional structure of angiogenin, Proc. Natl. Acad. Sci., U.S.A., 83, 1965-1969 (1986).

672. M. J. Sippl and H. A. Scheraga - Cayley - Menger coordinates, Proc. Natl. Acad. Sci., U.S., 83, 2283-2287 (1986).

673. C. A. McWherter, E. Haas, A. R. Leed and H. A. Scheraga - Conformational unfolding in the N-terminal region of ribonuclease A detected by nonradiative energy transfer, Biochemistry, 25, 1951-1963 (1986).

674. E. O. Purisima and H. A. Scheraga - An approach to the multiple-minima problem by relaxing dimensionality, Proc. Natl. Acad. Sci., U.S.A., 83, 2782-2786 (1986).

675. K.-C. Chou, G. Némethy, S. Rumsey, R. W. Tuttle and H. A. Scheraga - Interactions between two β-sheets. Energetics of β/β packing in proteins, J. Mol. Biol., 188, 641-649 (1986).

676. H. E. Van Wart and H. A. Scheraga - Agreement with the disulfide stretching frequency-conformation correlation of Sugeta, Go and Miyazawa, Proc. Natl. Acad. Sci., U.S.A., 83, 3064-3067 (1986).

677. H. Meirovitch and H. A. Scheraga - Computer simulation of the entropy of continuum chain models: The two-dimensional freely jointed chain of hard disks, J. Chem. Phys., 84, 6369-6375 (1986).

678. G. Némethy and H. A. Scheraga - Stabilization of collagen fibrils by hydroxyproline, Biochemistry, 25, 3184-3188 (1986).

679. M. A. Eastman, L. G. Pedersen, R. G. Hiskey, M. Pique, K. A. Koehler, K. E. Gottschalk, G. Némethy and H. A. Scheraga - Conformation of the 18-23 loop region of bovine prothrombin in the absence and presence of a model Ca^{2+} ion: An energy minimization study, Intntl. J. Peptide Protein Res., 27, 530-553 (1986).

680. G. H. Paine and H. A. Scheraga - Prediction of the native conformation of a polypeptide by a statistical-mechanical procedure. II. Average backbone structure of enkephalin, Biopolymers, 25, 1547-1563 (1986).

681. K. D. Gibson and H. A. Scheraga - Predicted conformations for the immunodominant region of the circumsporozoite protein of the human malaria parasite Plasmodium falciparum, Proc. Natl. Acad. Sci., U.S.A., 83, 5649-5653 (1986).

682. E. R. Stimson, Y. C. Meinwald, G. T. Montelione and H. A. Scheraga - Conformational properties of trans Ac-Asn-Pro-Tyr-NHMe and trans Ac-Tyr-Pro-Asn-NHMe in dimethyl-sulfoxide and in water determined by multinuclear n.m.r. spectroscopy, Intntl. J. Peptide and Protein Res., 27, 569-582 (1986). Erratum: ibid., 28, 661 (1986).

683. Y. C. Meinwald, E. R. Stimson and H. A. Scheraga - Deamidation of the asparaginyl - glycyl sequence, Intntl. J. Peptide and Protein Res., 28, 79-84 (1986). Erratum: ibid., 28, 661 (1986).

684. P. W. Mui, Y. Konishi, and H. A. Scheraga - Comparison of intramolecular and intermolecular reactions in protein folding, J. Protein Chem., 5, 29-49 (1986).

685. G. T. Montelione, P. Hughes, J. Clardy and H. A. Scheraga - Conformational properties of 2,4-methanoproline (2-carboxy-2,4-methanopyrrolidine) in peptides: Determination of preferred peptide bond conformation in aqueous solution by proton Overhauser measurements, J. Am. Chem. Soc., 108, 6765-6773 (1986).

686. H. A. Scheraga - Conformational analysis of polypeptides and proteins, in "Protein Structure, Folding, and Design," ed. D. L. Oxender, UCLA Symposia on Molecular and Cellular Biology, New series, 39, 233-236 (1986), A. R. Liss, Inc., New York.

687. G. T. Montelione, K. Wüthrich, E. C. Nice, A. W. Burgess and H. A. Scheraga - Identification of two anti-parallel β-sheet conformations in the solution structure of murine epidermal growth factor by proton magnetic resonance, Proc. Natl. Acad.Sci., U.S.A., 83, 8594-8598 (1986).

688. F. Ni and H. A. Scheraga - Phase-sensitive spectral analysis by maximum entropy extrapolation, J. Magn. Reson., 70, 506-511 (1986).

689. K. D. Gibson, S. Chin, M. R. Pincus, E. Clementi and H. A. Scheraga - Parallelism in conformational energy calculations on proteins, in "Lecture Notes in Chemistry," Vol. 44, "Supercomputer Simulations in Chemistry," ed. M. Dupuis, Springer-Verlag, Berlin, 1986, p. 198-213.

690. H. A. Scheraga and G. H. Paine - Conformational energy calculations on polypeptides and proteins. Use of a statistical mechanical procedure for evaluating structure and properties, Annals N.Y. Acad. Sci., 482, 60-68 (1986).

691. H. A. Scheraga - Chemical basis of thrombin interactions with fibrinogen, Annals N.Y. Acad. Sci., 485, 124-133 (1986).

692. H. A. Scheraga - Conformational analysis of polypeptides and proteins for the study of protein folding, molecular recognition, and molecular design, Israel Journal of Chemistry, 27, 144-155 (1986); in "From Revolution to Evolution," Ed. V. Crescenzi, Euroma, Editrice Universitaria di Roma-La Goliardica, Rome, p. 159 (1986); Journal of Protein Chemistry, 6, 61-80 (1987); in "Structure and Dynamics of Nucleic Acids, Proteins, and Membranes", eds. E. Clementi and S. Chin, Plenum, New York, 1986, p. 1-20.

1987

693. L. Piela and H. A. Scheraga - On the multiple-minima problem in the conformational analysis of polypeptides. I. Backbone degrees of freedom for a perturbed α-helix, Biopolymers, 26, S33-S58 (1987).

694. T. W. Thannhauser, Y. Konishi and H. A. Scheraga - Analysis for disulfide bonds in peptides and proteins, Methods in Enzymology, 143, 115-119 (1987).

695. H. A. Scheraga and W. L. Mattice - Helix-coil transitions, in "Encyclopedia of Polymer Science and Engineering", ed. J. I. Kroschwitz, 2nd ed., Vol. 7, p. 685-698, John Wiley, New York (1987).

696. M. Vasquez, M. R. Pincus and H. A. Scheraga - Helix-coil transition theory including long-range electrostatic interactions: Application to globular proteins, Biopolymers, 26, 351-371 (1987).

697. M. Vasquez, M. R. Pincus and H. A. Scheraga - Correlation between computed conformational properties of cytochrome c peptides and their antigenicity in a T-lymphocyte proliferation assay, Biopolymers, 26, 373-386 (1987).

698. D. M. Rice, Y. C. Meinwald, H. A. Scheraga and R. G. Griffin - Tyrosyl motion in peptides: ^{2}H-NMR line shapes and spin-lattice relaxation, J. Am. Chem. Soc., 109, 1636-1640 (1987).

699. E. Haas, G. T. Montelione, C. A. McWherter and H. A. Scheraga - Local structure in a tryptic fragment of performic acid oxidized ribonuclease A corresponding to a proposed polypeptide chain-folding initiation site detected by Tyrosine fluorescence lifetime and proton magnetic resonance measurements, Biochemistry, 26, 1672-1683 (1987).

700. H. Meirovitch, M. Vasquez and H. A. Scheraga - Stability of polypeptide conformational states as determined by computer simulation of the free energy, Biopolymers, 26, 651-671 (1987).

701. R. R. Hantgan, C. W. Francis, H. A. Scheraga and V. J. Marder - Fibrinogen structure and physiology, in "Hemostasis and Thrombosis", eds. R.W. Colman, J. Hirsh, V.J. Marder and E.W. Salzman, 2nd ed., p. 269, J.B. Lippincott Co., Philadelphia (1987).

702. T. Ooi, M. Oobatake, G. Némethy and H. A. Scheraga - Accessible surface areas as a measure of the thermodynamic parameters of hydration of peptides, Proc. Natl. Acad. Sci., U.S.A., 84, 3086-3090 (1987). Erratum: ibid., 84, 6015 (1987).

703. G. H. Paine and H. A. Scheraga - Prediction of the native conformation of a polypeptide by a statistical-mechanical procedure. III. Probable and average conformations of enkephalin, Biopolymers, 26, 1125-1162 (1987).

704. M. R. Pincus, R. P. Carty, J. Chen, J. Lubowsky, M. Avitable, D. Shah, H. A. Scheraga, and R. B. Murphy - On the biologically active structures of cholecystokinin, little gastrin, and enkephalin in the gastrointestinal system, Proc. Natl. Acad. Sci., U.S.A., 84, 4821-4825 (1987).

705. S. Talluri, G. T. Montelione, G. van Duyne, L. Piela, J. Clardy and H. A. Scheraga - Conformational properties of 2,4-methanoproline (2-carboxy-2,4-methano-pyrrolidine) in peptides: Evidence for 2,4-methanopyrrolidine asymmetry based on solid-state x-ray crystallography, ^{1}H-NMR in aqueous solution, and CNDO/2 conformational energy calculations, J. Am. Chem. Soc., 109, 4473-4477 (1987).

706. L. Piela, G. Némethy and H. A. Scheraga - Conformational properties of 2,4-methanoproline (2-carboxy-2,4-methano-pyrrolidine) in peptides: Theoretical conformational energy analysis of restrictions of the polypeptide chain conformation, J. Am. Chem. Soc., 109, 4477-4485 (1987).

707. P. J. Milburn, Y. Konishi, Y. C. Meinwald and H. A. Scheraga - Chain reversals in model peptides: Studies of cystine-containing cyclic peptides. I. Conformational free energies of cyclization of hexapeptides of sequence Ac-Cys-X-Pro-Gly-Y-Cys-NHMe, J. Am. Chem. Soc., 109, 4486-4496 (1987). Erratum: ibid., 109, 8123 (1987).

708. L. Piela, G. Némethy and H. A. Scheraga - Conformational constraints of amino acid side chains in α-helices, Biopolymers, 26, 1273-1286 (1987).

709. Y. K. Kang, G. Némethy and H. A. Scheraga - Free energies of hydration of solute molecules. I. Improvement of the hydration shell model by exact computations of overlapping volumes, J. Phys. Chem., 91, 4105-4109 (1987). Erratum: ibid., 92, 1382 (1988).

710. Y. K. Kang, G. Némethy and H. A. Scheraga - Free energies of hydration of solute molecules. II. Application of the hydration shell model to nonionic organic molecules, J. Phys. Chem., 91, 4109-4117 (1987). Erratum: ibid., 91, 6568 (1987).

711. Y. K. Kang, G. Némethy and H. A. Scheraga - Free energies of hydration of solute molecules. III. Application of the hydration shell model to charged organic molecules, J. Phys. Chem., 91, 4118-4120 (1987). Erratum: ibid., 91, 6568 (1987).

712. K. D. Gibson and H. A. Scheraga - Volume of the intersection of three spheres of unequal size. A simplified formula, J. Phys. Chem., 91, 4121-4122 (1987). Erratum: ibid., 91, 6326 (1987).

713. G. T. Montelione, K. Wüthrich, E. C. Nice, A. W. Burgess and H. A. Scheraga - Solution structure of murine epidermal growth factor: Determination of the polypeptide backbone chain-fold by nuclear magnetic resonance and distance geometry, Proc. Natl. Acad. Sci., U.S.A., 84, 5226-5230 (1987).

714. K. D. Gibson and H. A. Scheraga - Revised algorithms for the build-up procedure for predicting protein conformations by energy minimization, J. Comput. Chem. 8, 826-834 (1987).

715. E. O. Purisima and H. A. Scheraga - An approach to the multiple-minima problem in protein folding by relaxing dimensionality. Tests on enkephalin, J. Mol. Biol., 196, 697-709 (1987).

716. H. A. Scheraga, Y. Konishi, D. M. Rothwarf and P. W. Mui -Toward an understanding of the folding of ribonuclease A, Proc. Natl. Acad. Sci., U.S.A., 84, 5740-5744 (1987).

717. L. Piela, G. Némethy and H. A. Scheraga - Proline-induced constraints in α-helices, Biopolymers 26, 1587-1600 (1987).

718. E. Meirovitch, E. T. Samulski, A. Leed, H. A. Scheraga, S. Rananavare, G. Némethy and J. H. Freed - Deuterium NMR study of the structure and dynamics of the side chains of several solid polyglutamates, J. Phys. Chem. 91, 4840-4851 (1987).

719. J. K. Swadesh, P. W. Mui and H. A. Scheraga - Thermodynamics of the quenching of tyrosyl fluorescence by dithiothreitol, Biochemistry, 26, 5761-5769 (1987). Erratum: ibid., 26, 8030 (1987).

*720. Z. Li and H. A. Scheraga - Monte Carlo-minimization approach to the multiple-minima problem in protein folding, Proc. Natl. Acad. Sci., U.S.A., 84, 6611-6615 (1987).

721. K. Takahashi, Y. K. Kang, G. Némethy, H. A. Scheraga and V. S. Ananthanarayanan - Low-energy conformations of two lysine-containing tetrapeptides of collagen: Implications for post-translational lysine hydroxylation, Biopolymers, 26, 1781-1788 (1987).

722. M. R. Pincus, P. W. Brandt-Rauf, R. P. Carty, J. Lubowsky, M. Avitable, K. D. Gibson and H. A. Scheraga - Conformational effects of substituting amino acids for glutamine-61 on the central transforming region of the P21 proteins, Proc. Natl. Acad. Sci., U.S.A., 84, 8375-8379 (1987).

723. G. Némethy, T. Ooi and H. A. Scheraga - Structural principles of protein architecture, J. Protein Chem., 6, 529-535 (1987).

724. K. D. Gibson and H. A. Scheraga - Exact calculation of the volume and surface area of fused hard-sphere molecules with unequal atomic radii, Molecular Physics, 62, 1247-1265 (1987).

1988

725. E. Haas, C. A. McWherter and H. A. Scheraga - Conformational unfolding in the N-terminal region of ribonuclease A detected by nonradiative energy transfer. Distribution of interresidue distances in the native, denatured and reduced-denatured states, Biopolymers, 27, 1-21 (1988).

726. M. Vasquez and H. A. Scheraga - Effect of sequence-specific interactions on the stability of helical conformations in polypeptides, Biopolymers, 27, 41-58 (1988).

727. T.-H. Lin, A. R. Leed, H. A. Scheraga and W. L. Mattice - Helix initiation and propagation by isolated arginine residues in aqueous sodium dodecyl sulfate, Macromolecules, 21, 131-136 (1988).

728. L. Glasser and H. A. Scheraga - Calculations on crystal packing of a flexible molecule, Leu-enkephalin, J. Mol. Biol., 199, 513-524 (1988).

729. M. Vasquez and H. A. Scheraga - Calculation of protein conformation by the build-up procedure. Application to bovine pancreatic trypsin inhibitor using limited simulated nuclear magnetic resonance data, J. Biomolecular Structure & Dynamics, 5, 705-755 (1988).

*730. M. Vasquez and H. A. Scheraga - 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, J. Biomolecular Structure & Dynamics, 5, 757-784 (1988).

731. K. D. Gibson and H. A. Scheraga - The multiple-minima problem in protein folding, in "Structure & Expression: Vol. 1: From Proteins to Ribosomes", Eds. R.H. Sarma & M.H. Sarma, Adenine Press, Guilderland, N.Y., p. 67-94 (1988).

732. M. R. Pincus, R. B. Murphy, R. P. Carty, J. Chen, D. Shah and H. A. Scheraga - Conformational analysis of possible biologically active (receptor-bound) conformations of peptides derived from cholecystokinin, cerulein and little gastrin and the opiate peptide, Met-enkephalin, Peptides, 9, Suppl. 1, 145-152 (1988).

733. P. J. Milburn, Y. C. Meinwald, S. Takahashi, T. Ooi and H. A. Scheraga - Chain reversals in model peptides: Studies of cystine-containing cyclic peptides. II. Effects of valyl residues and possible i-to-(i+3) attractive ionic interactions on cyclization of [Cys^1], [Cys^6] hexa-peptides, Intnl. J. Peptide and Protein Res., 31, 311-321 (1988). Erratum: ibid. 31, 587 (1988).

734. Z. Vali and H. A. Scheraga - Localization of the binding site on fibrin for the secondary binding site of thrombin, Biochemistry, 27, 1956-1963 (1988).

735. G. T. Montelione, K. Wüthrich and H. A. Scheraga -Sequence-specific ^{1}H NMR assignments and identification of slowly exchanging amide protons in murine epidermal growth factor, Biochemistry, 27, 2235-2243 (1988).

736. B-J. Yoon and H. A. Scheraga - Monte Carlo simulation of the hard-sphere fluid with quantum correction and estimate of its free energy, J. Chem. Phys., 88, 3923-3933 (1988).

737. M. Adler and H. A. Scheraga - Structural studies of a folding intermediate of bovine pancreatic ribonuclease A by continuous recycled flow, Biochemistry, 27, 2471-2480 (1988).

738. I. Simon, H. A. Scheraga and R. S. J. Manley - Structure of cellulose. 1. Low-energy conformations of single chains, Macromolecules, 21, 983-990 (1988).

739. I. Simon, L. Glasser, H. A. Scheraga and R. S. J. Manley - Structure of cellulose. 2. Low-energy crystalline arrangements, Macromolecules, 21, 990-998 (1988).

740. Z. Li and H. A. Scheraga - Monte Carlo recursion evaluation of free energy, J. Phys. Chem. 92, 2633-2636 (1988).

741. F. Ni, H. A. Scheraga and S. T. Lord - High-resolution NMR studies of fibrinogen-like peptides in solution: Resonance assignments and conformational analysis of residues 1-23 of the Aα chain of human fibrinogen, Biochemistry 27, 4481-4491 (1988).

742. K.-C. Chou, G. M. Maggiora, G. Némethy and H. A. Scheraga - Energetics of the structure of the four-α-helix bundle in proteins, Proc. Natl. Acad. Sci., U.S.A. 85, 4295-4299 (1988).

743. P. J. Milburn and H. A. Scheraga - Local interactions favor the native 8-residue disulfide loop in the oxidation of a fragment corresponding to the sequence Ser-50-Met-79 derived from bovine pancreatic ribonuclease A, J. Protein Chem. 7, 377-398 (1988).

*744. T. Kikuchi, G. Némethy and H. A. Scheraga - Prediction of the location of structural domains in globular proteins, J. Protein Chem. 7, 427-471 (1988).

745. T. Kikuchi, G. Némethy and H. A. Scheraga - Prediction of the packing arrangement of strands in β-sheets of globular proteins, J. Protein Chem. 7, 473-490 (1988).

*746. T. Kikuchi, G. Némethy and H. A. Scheraga - Prediction of probable pathways of folding in globular proteins, J. Protein Chem. 7, 491-507 (1988).

747. H. Meirovitch, M. Vasquez and H. A. Scheraga - 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 27, 1189-1204 (1988).

748. D. R. Ripoll and H. A. Scheraga - On the multiple-minima problem in the conformational analysis of polypeptides. II. An electrostatically driven Monte Carlo method-tests on poly(L-alanine), Biopolymers 27, 1283-1303 (1988).

749. K. D. Gibson and H. A. Scheraga - Surface area of the intersection of three spheres with unequal radii. A simplified analytical formula, Mol. Phys., 64, 641-644 (1988).

750. T.-H. Lin, A. R. Leed, H. A. Scheraga and W. L. Mattice - Helix destabilization caused by the interaction of unaggregated sodium dodecyl sulfate with isolated lysine residues, Macromolecules, 21, 2447-2452 (1988).

751. Y. K. Kang, K. D. Gibson, G. Némethy and H. A. Scheraga - Free energies of hydration of solute molecules. 4. Revised treatment of the hydration shell model, J. Phys. Chem., 92, 4739-4742 (1988).

752. W. L. Mattice, G. Némethy and H. A. Scheraga - Conformational entropy associated with the formation of internal loops in collagen, Macromolecules, 21, 2811-2818 (1988).

*753. M. P. Weiner, T. W. Thannhauser, J. H. Laity, M. E. Benning, D. P. Lee, and H. A. Scheraga - Plasmid purification using reverse-phase high performance liquid chromatography resin PRP-∞, Nucleic Acids Research, 16, 8185 (1988).

754. H. A. Scheraga - Approaches to the multiple-minima problem in conformational energy calculations on polypeptides and proteins, in "Biological and Artificial Intelligence Systems", Ed. E. Clementi and S. Chin, ESCOM Science Publ., Leiden, p. 1-14 (1988).

755. P. Ray, F. J. Moy, G. T. Montelione, J-F. Liu, S. A. Narang, H. A. Scheraga and R. Wu - Structure-function studies of murine epidermal growth factor: Expression and site-directed mutagenesis of epidermal growth factor gene, Biochemistry, 27, 7289-7295 (1988).

*756. Z. Li and H. A. Scheraga - Structure and free energy of complex thermodynamic systems, J. Molec. Str. (Theochem). 179, 333-352 (1988).

757. H. A. Scheraga - Calculations of conformations of polypeptides (Citation Classic), Current Contents (Physical Sciences), No. 49, p. 17 (Dec. 5, 1988).

758. S. Kim, M. S. Jhon and H. A. Scheraga - Analytic intermolecular potential functions from ab initio SCF calculations of interaction energies between CH_4, CH_3OH, CH_3COOH, and CH_3COO^- and water, J. Phys. Chem., 92, 7216-7223 (1988).

1989

759. H. A. Scheraga - Some computational problems in the conformational analysis of polypeptides and proteins, in "Computer-assisted modeling of receptor-ligand interactions: Theoretical aspects and applications to drug design", Eds. R. Rein and A. Golombek, Alan R. Liss, New York, p. 3-18 (1989).

760. G. T. Montelione and H. A. Scheraga - Formation of local structures in protein folding, Accts. Chem. Res. 22, 70-76 (1989).

761. K-C. Chou, G. Némethy, M. Pottle and H. A. Scheraga - Energy of stabilization of the right-handed crossover in proteins, J. Mol. Biol. 205, 241-249 (1989).

762. L. Piela, J. Kostrowicki and H. A. Scheraga - The multiple-minima problem in the conformational analysis of molecules. Deformation of the potential energy hypersurface by the diffusion equation method, J. Phys. Chem., 93, 3339-3346 (1989).

763. F. Ni, Y. Konishi, R. B. Frazier, H. A. Scheraga and S. T. Lord - High-resolution NMR studies of fibrinogen-like peptides in solution: Interaction of thrombin with residues 1-23 of the Aα chain of human fibrinogen, Biochemistry, 28, 3082-3094 (1989).

764. F. Ni, Y. C. Meinwald, M. Vasquez and H. A. Scheraga - High-resolution NMR studies of fibrinogen-like peptides in solution: Structure of a thrombin- bound peptide corresponding to residues 7-16 of the Aα chain of human fibrinogen, Biochemistry, 28, 3094-3105 (1989).

765. F. Ni, Y. Konishi, L. D. Bullock, M. N. Rivetna and H. A. Scheraga - High-resolution NMR studies of fibrinogen-like peptides in solution: Structural basis for the bleeding disorder caused by a single mutation of Gly(12) to Val(12) in the Aα chain of human fibrinogen Rouen, Biochemistry, 28, 3106-3119 (1989).

766. Z. Li and H. A. Scheraga - Computation of the free energy of liquid water by the Monte Carlo recursion method, Chem. Phys. Lett. 154, 516-520 (1989). Erratum: ibid., 157, 579 (1989).

767. F. Ni and H. A. Scheraga - Constrained iterative spectral deconvolution with applications in NMR spectroscopy, J. Magn. Reson., 82, 413-418 (1989).

768. T. Kikuchi, G. Némethy and H. A. Scheraga - Spatial geometric arrangements of disulfide-crosslinked loops in nonplanar proteins, J. Comput. Chem., 10, 287-294(1989).

769. D. R. Ripoll and H. A. Scheraga - The multiple-minima problem in the conformational analysis of polypeptides. III. An electrostatically driven Monte Carlo method; tests on enkephalin, J. Protein Chem., 8, 263-287 (1989).

770. M. E. Denton and H. A. Scheraga - The folding of hen egg-white lysozyme: An immunochemical and spectroscopic study, in "The immune response to structurally defined proteins: The lysozyme model", Eds. S. Smith-Gill and E. Sercarz, Adenine Press, Guilderland, N.Y., p. 39-40 (1989).

771. R. Jernigan, D. Davies and H. A. Scheraga - Experimental and theoretical protein folding, J. Biomolecular Structure & Dynamics, 6, 1039-1043 (1989).

772. H. A. Scheraga - The multiple-minima problem in conformational energy calculations on polypeptides and proteins, in the Fourth European Symposium on "Computer-Aided Molecular Design", Helsingør, Denmark, October, 1987; in "Protein Recognition of Immobilized Ligands", ed. T. W. Hutchens, UCLA Symposia on Molecular and Cellular Biology, New Series, 80, 213-221 (1989), A. R. Liss, Inc., New York.

773. G. Némethy and H. A. Scheraga - Computational studies of the structure and assembly of triple-stranded models of collagen, Bull. Inst. Chem. Res., Kyoto Univ., 66, 398-408 (1989).

*774. A. D. Robertson, E. O. Purisima, M. A. Eastman and H. A. Scheraga - Proton NMR assignments and regular backbone structure of bovine pancreatic ribonuclease A in aqueous solution, Biochemistry, 28, 5930-5938 (1989).

775. G. Némethy and H. A. Scheraga - Free energy of hydration of collagen models and the enthalpy of the transition between the triple-helical coiled-coil and single- stranded conformations, Biopolymers, 28, 1573-1584 (1989).

776. M. H. Lambert and H. A. Scheraga - Pattern recognition in the prediction of protein structure. I. Tripeptide conformational probabilities calculated from the amino acid sequence, J. Comput. Chem., 10, 770-797 (1989).

777. M. H. Lambert and H. A. Scheraga - Pattern recognition in the prediction of protein structure. II. Chain conformation from a probability-directed search procedure, J. Comput. Chem., 10, 798-816 (1989).

778. M. H. Lambert and H. A. Scheraga - Pattern recognition in the prediction of protein structure. III. An importance-sampling minimization procedure, J. Comput. Chem., 10, 817-831 (1989).

779. B. J. Cherayil and H. A. Scheraga - On the equivalence between polymers in quenched disorder and randomly dilute n-vector models, Phys. Lett. A, 139, 175-182 (1989).

780. M. P. Weiner and H. A. Scheraga - A set of Macintosh computer programs for the design and analysis of synthetic genes, CABIOS, 5, 191-198 (1989).

781. H. A. Scheraga, F. Ni, S. T. Lord, Y. Konishi, Y. C. Meinwald, M. Vasquez, L. D. Bullock, R. B. Frazier and M. N. Rivetna - Conformational basis for the bleeding disorder caused by a single mutation of Gly(12) to Val(12) in the Aα chain of human fibrinogen Rouen, Thrombosis and Haemostasis, 62, 158 (1989).

782. M. P. Weiner and H. A. Scheraga - A method for the cloning of unpurified single-stranded oligonucleotides, Nucleic Acids Res., 17, 7113 (1989).

783. D. Shah, J. M. Chen, R. P. Carty, M. R. Pincus and H. A. Scheraga - Correlation of β-bend conformations of tetrapeptides with their activities in CD4-receptor binding assays, Intntl. J. Peptide Protein Res., 34, 325-332 (1989).

784. B-J. Yoon and H. A. Scheraga - Calculation of the entropy of a fluid by a Monte Carlo simulation based on free volume, J. Molec. Str. (Theochem.), 199, 33-54 (1989).

785. H. A. Scheraga - Calculations of stable conformations of polypeptides, proteins, and protein complexes, Chemica Scripta, 29A, 3-13 (1989).

786. I. K. Roterman, K. D. Gibson and H. A. Scheraga - A comparison of the CHARMM, AMBER and ECEPP potentials for peptides. I. Conformational predictions for the tandemly repeated peptide (Asn-Ala-Asn-Pro) 9, J. Biomolec. Structure & Dynamics, 7, 391-419 (1989).

787. I. K. Roterman, M. H. Lambert, K. D. Gibson and H. A. Scheraga - A comparison of the CHARMM, AMBER and ECEPP potentials for peptides. II. ø-φ maps for N-acetyl alanine N'-methyl amide: comparisons, contrasts and simple experimental tests, J. Biomolec. Structure & Dynamics, 7, 421-453 (1989).

788. F. J. Moy, H. A. Scheraga, J. F. Liu, R. Wu, and G. T. Montelione - Conformational characterization of a single-site mutant of murine epidermal growth factor (EGF) by ^{1}H-NMR provides evidence that Leu^{47} is involved in the interactions with the EGF receptor, Proc. Natl. Acad. Sci., U.S.A., 86, 9836-9840 (1989).

1990

789. S. Talluri and H. A. Scheraga - Cosy with in-phase cross peaks, J. Magn. Reson., 86, 1-10 (1990).

790. M. J. Dudek and H. A. Scheraga - Protein structure prediction using a combination of sequence homology and global energy minimization. I. Global energy minimization of surface loops, J. Comput. Chem., 11, 121-151 (1990).

791. S. S. Wee, S. Kim, M. S. Jhon and H. A. Scheraga -Analytical Intermolecular potential functions from ab initio SCF calculations for hydration of methylamine and methylammonium ion, J. Phys. Chem., 94, 1656-1660 (1990).

792. H. Meirovitch, M. Vasquez and H. A. Scheraga - Free energy and stability of macromolecules studied by the double scanning simulation procedure, J. Chem. Phys., 92, 1248-1257 (1990).

793. H. A. Scheraga - Determination of protein structure in aqueous solution with and without distance constraints, in "Frontiers of NMR in Molecular Biology", Eds. D. Live, I. M. Armitage and D. Patel, Wiley-Liss, New York, p. 189-194 (1990).

794. B. J. Yoon, M. S. Jhon and H. A. Scheraga - Vibrational quantum correction for the Lennard-Jones fluid; a formalism of effective intermolecular potentials depending on mass and temperature, J. Chem. Phys., 92, 3748-3755 (1990). Erratum: ibid. 93, 3728 (1990).

795. K. D. Gibson and H. A. Scheraga - Variable step molecular dynamics: An exploratory technique for peptides with fixed geometry, J. Comput. Chem., 11, 468-486 (1990).

796. K. D. Gibson and H. A. Scheraga - Dynamics of peptides with fixed geometry: Kinetic energy terms and potential energy derivatives as functions of dihedral angles, J. Comput. Chem., 11, 487-492 (1990).

797. K. C. Chou, G. Némethy and H. A. Scheraga - Energetics of interactions of regular structural elements in proteins, Accts. Chem. Res., 23, 134-141 (1990).

798. Z. Li and H. A. Scheraga - Monte Carlo recursion study of cluster formation from vapor, J. Chem. Phys., 92, 5499-5505 (1990).

799. F. Ni, Y. Konishi and H. A. Scheraga - Thrombin-bound conformation of the C-terminal fragments of hirudin determined by transferred nuclear Overhauser effects, Biochemistry, 29, 4479-4489 (1990).

800. K. H. Altmann and H. A. Scheraga - Local structure in ribonuclease A. Effect of amino acid substitutions on the preferential formation of the native disulfide loop in synthetic peptides corresponding to residues Cys^{58} -Cys^{72} of bovine pancreatic ribonuclease A, J. Am. Chem. Soc., 112, 4926-4931 (1990).

801. K. T. No, J. A. Grant and H. A. Scheraga - Determination of net atomic charges using a modified partial equalization of orbital electronegativity method. 1. Application to neutral molecules as models for polypeptides, J. Phys. Chem., 94, 4732-4739 (1990).

802. K. T. No, J. A. Grant, M. S. Jhon and H. A. Scheraga - 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, J. Phys. Chem., 94, 4740-4746 (1990).

803. J. Wojcik, A. Kidera, A. R. Leed, A. Nakajima and H. A. Scheraga - Helix-coil transition in multicomponent random copolypeptides in water. 3. Inclusion of nearest-neighbor interactions and application to random copolymers of (Hydroxybutyl)-L-glutamine, L-Alanine, L-Phenylalanine, L-Lysine and Glycine, Macromolecules, 23, 3655-3662 (1990).

804. K. C. Chou, A. Heckel, G. Némethy, S. Rumsey, L. Carlacci and H. A. Scheraga - Energetics of the structure and chain tilting of antiparallel β-barrels in proteins, Proteins: Structure, Function, and Genetics, 8, 14-22 (1990).

805. K. H. Altmann, J. Wojcik, M. Vasquez and H. A. Scheraga -Helix-coil stability constants for the naturally occurring amino acids in water. XXIII. Proline parameters from random poly(hydroxybutylglutamine-co-L-proline), Biopolymers, 30, 107-120 (1990).

806. J. Wojcik, K. H. Altmann and H. A. Scheraga - Helix-coil stability constants for the naturally occurring amino acids in water. XXIV. Half-cystine parameters from random Poly(hydroxybutylglutamine-co-S-methylthio-L-cysteine), Biopolymers, 30, 121-134 (1990).

807. D. R. Ripoll and H. A. Scheraga - On the multiple-minima problem in the conformational analysis of polypeptides. IV. Application of the electrostatically driven Monte Carlo method to the 20-residue membrane-bound portion of melittin, Biopolymers, 30, 165-176 (1990).

808. M. Adler and H. A. Scheraga - Nonnative isomers of proline-93 and -114 predominate in heat-unfolded ribonuclease A, Biochemistry, 29, 8211-8216 (1990).

809. J. M. Chen, G. Lee, P. W. Brandt-Rauf, R. B. Murphy, K. D. Gibson, H. A. Scheraga, S. Rackovsky and M. R. Pincus - Conformations of the central transforming region (Ile 55-Met 67) of the p21 protein and their relationship to activation of the protein, Intntl. J. Peptide Protein Res., 36, 247-254 (1990).

810. H. A. Scheraga - Current status of the protein structure problem, in "Frontiers in Drug Research. Crystallographic and computational methods", Eds. B. Jensen, F. S. Jørgensen, H. Kofod, Alfred Benzon Symposium 28, pp. 343-355, Munksgaard, Copenhagen (1990).

811. S. Talluri and H. A. Scheraga - Amide H/D exchange in the thermal transition of bovine pancreatic ribonuclease A, Biochem. Biophys. Res. Commun. 172, 800-803 (1990).

812. G. Némethy and H. A. Scheraga - Theoretical studies of protein conformation by means of energy computations, FASEB J. 4, 3189-3197 (1990).

813. F. Walker, E. Nice, L. Fabri, F. J. Moy, J. F. Liu, R. Wu, H. A. Scheraga and A. W. Burgess - Resistance to receptor-mediated degradation of a murine epidermal growth factor analogue (EGF-Val 47) potentiates its mitogenic activity, Biochemistry, 29, 10635-10640 (1990).

814. J. A. Grant, R. L. Williams and H. A. Scheraga - Ab initio self-consistent field and potential-dependent partial equalization of orbital electronegativity calculations of hydration properties of N-acetyl-N'-methyl-alanineamide, Biopolymers, 30, 929-949 (1990).

815. A. Zagari, G. Némethy and H. A. Scheraga - The effect of the L-azetidine-2-carboxylic acid residue on protein conformation. I. Conformations of the residue and of dipeptides, Biopolymers, 30, 951-959 (1990).

816. A. Zagari, G. Némethy and H. A. Scheraga - The effect of the L-azetidine-2-carboxylic acid residue on protein conformation. II. Homopolymers and copolymers, Biopolymers, 30, 961-966 (1990).

817. A. Zagari, G. Némethy and H. A. Scheraga - The effect of the L-azetidine-2-carboxylic acid residue on protein conformation. III. Collagen-like poly(tripeptide)s, Biopolymers, 30, 967-974 (1990).

818. K. R. Acharya, D. I. Stuart, D. C. Phillips and H. A. Scheraga - A critical evaluation of the predicted and X-ray structures of α-lactalbumin, J. Protein Chem. 9, 549-563 (1990).

819. M. Adler and H. A. Scheraga - Identification of a new site of conformational heterogeneity in unfolded ribonuclease A, J. Protein Chem., 9, 583-588 (1990).

1991

820. M. R. Witmer, C. M. Falcomer, M. P. Weiner, M. S. Kay, T. P. Begley, B. Ganem and H. A. Scheraga - U-3'-BCIP: a chromogenic substrate for the detection of RNase A in recombinant DNA expression systems, Nucleic Acids Research, 19, 1-4 (1991).

821. H. A. Scheraga - Experimental and theoretical aspects of protein conformation, in Theoretical Biochemistry and Molecular Biophysics, Vol. 2: Proteins, Ed. D. L. Beveridge and R. Lavery, Adenine Press, Guilderland, N.Y., p. 231-237 (1991).

822. K. A. Palmer and H. A. Scheraga - 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, J. Comput. Chem., 12, 505-526 (1991).

823. I. Simon, L. Glasser and H. A. Scheraga - Calculation of protein conformation as an assembly of stable overlapping segments: Application to bovine pancreatic trypsin inhibitor, Proc. Natl. Acad. Sci., U.S.A., 88, 3661-3665 (1991).

824. D. R. Ripoll, M. J. Vasquez and H. A. Scheraga - The electrostatically driven Monte Carlo method: Application to conformational analysis of decaglycine, Biopolymers, 31, 319-330 (1991).

825. A. Nayeem, J. Vila and H. A. Scheraga - A comparative study of the simulated-annealing and Monte Carlo-with-minimization approaches to the minimum-energy structures of polypeptides: [Met]-Enkephalin, J. Comput. Chem., 12, 594-605 (1991).

826. J. Kostrowicki, L. Piela, B. J. Cherayil and H. A. Scheraga - Performance of the diffusion equation method in searches for optimum structures of clusters of Lennard-Jones atoms, J. Phys. Chem., 95, 4113-4119 (1991).

827. M. E. Denton and H. A. Scheraga - Spectroscopic, immuno-chemical, and thermodynamic properties of carboxymethyl (Cys^{6}, Cys^{127})-hen egg white lysozyme, J. Protein Chem., 10, 213-232 (1991).

828. D. R. Ripoll, L. Piela, M. Vasquez and H. A. Scheraga - 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 Genetics, 10, 188-198 (1991).

829. J. Vila, R. L. Williams, M. Vasquez and H. A. Scheraga - Empirical solvation models can be used to differentiate native from near-native conformations of bovine pancreatic trypsin inhibitor, Proteins: Structure, Function, and Genetics, 10, 199-218 (1991).

830. K. D. Gibson and H. A. Scheraga - Decisions in force field development. Reply to Kollman and Dill, J. Biomolec. Structure & Dynamics, 8, 1109-1111 (1991).

831. B. J. Yoon, S. D. Hong, M. S. Jhon and H. A. Scheraga - Calculation of the entropy and the chemical potential of fluids and solids from the radial free-space distribution function, Chem. Phys. Lett., 181, 73-77 (1991).

832. L. Glasser and H. A. Scheraga - Investigation of a physical basis for conformational similarity in proteins, J. Protein Chem., 10, 273-285 (1991).

*833. D. M. Rothwarf and H. A. Scheraga - Regeneration and reduction of native bovine pancreatic ribonuclease A with oxidized and reduced dithiothreitol, J. Am. Chem. Soc., 113, 6293-6294 (1991).

834. J. M. Beals, E. Haas, S. Krausz and H. A. Scheraga - Conformational studies of a peptide corresponding to a region of the C-terminus of ribonuclease A: Implications as a potential chain-folding initiation site, Biochemistry, 30, 7680-7692 (1991).

835. A. B. Shapiro, K. D. Gibson, H. A. Scheraga and R. E. McCarty - Fluorescence resonance energy transfer mapping of the fourth of six nucleotide-binding sites of chloroplast coupling factor 1, J. Biol. Chem., 266, 17276-17285 (1991).

836. H. A. Scheraga - The multiple-minima problem in protein folding, in Adv. Biomolecular Simulation, AIP Conference Proceedings No. 239, Obernai, France, Eds. R. Lavery, J. L. Rivail, J. Smith, J. Metral, and C. Troyanowsky, 97-107 (1991).

837. G. Y. Kweon, H. A. Scheraga and M. S. Jhon - Monte Carlo treatment of hydration of models for side chains of proteins, J. Phys. Chem., 95, 8964-8968 (1991).

838. H. A. Scheraga and G. Némethy - Calculated structures and stabilities of fibrous macromolecules, in "Molecules in Natural Science and Medicine - an Encomium for Linus Pauling", Eds. Z. B. Maksic and M. E. Maksic, Ellis Horwood, Chichester, pp. 141-176 (1991).

839. D. J. Winzor, J. A. Nagy and H. A. Scheraga - Characterization of the immunochemical reactivity of fibrinogen fragments by competitive radioimmunoassay: An improved method of analysis, J. Protein Chem., 10, 629-635 (1991).

840. S. A. Fossey, G. Némethy, K. D. Gibson and H. A. Scheraga - Conformational energy studies of β-sheets of model silk fibroin peptides. I. Sheets of Poly(Ala- Gly) chains, Biopolymers, 31, 1529-1541 (1991).

1992

841. G. Perrot, B. Cheng, K. D. Gibson, J. Vila, K. A. Palmer, A. Nayeem, B. Maigret and H. A. Scheraga - MSEED: A program for the rapid analytical determination of accessible surface areas and their derivatives, J. Comput. Chem., 13, 1-11 (1992).

842. G. T. Montelione, K. Wüthrich, A. W. Burgess, E. C. Nice, G. Wagner, K. D. Gibson and H. A. Scheraga - Solution structure of murine epidermal growth factor determined by NMR spectroscopy and refined by energy minimization with restraints, Biochemistry, 31, 236-249 (1992). Erratum: ibid., 31, 10138 (1992).

843. R. M. Wolf, E. Francotte, L. Glasser, I. Simon and H. A. Scheraga - Computation of low-energy crystalline arrangements of cellulose triacetate, Macromolecules, 25, 709-720 (1992).

844. K. A. Palmer and H. A. Scheraga - Standard-geometry chains of the rigid-geometry approximation. II. Systematic searches for short loops in proteins; applications to bovine pancreatic ribonuclease A and human lysozyme, J. Comput. Chem., 13, 329-350 (1992).

845. H. A. Scheraga, J. M. Beals, D. R. Buckler, E. Haas and S. Krausz - Structure and dynamics of chain-folding-initiation sites in ribonuclease A, in "Time-resolved laser spectroscopy in Biochemistry III", ed. J. Lakowicz, SPIE Proceedings, 1640, 672-675 (1992).

846. H. A. Scheraga - Some approaches to the multiple-minima problem in the calculation of polypeptide and protein structures, Intntl. J. Quantum Chem. 42, 1529-1536 (1992).

847. Y. N. Vorobjev, J. A. Grant and H. A. Scheraga - A combined iterative and boundary-element approach for solution of the nonlinear Poisson-Boltzmann equation, J. Am. Chem. Soc., 114, 3189-3196 (1992).

848. B. J. Yoon, M. S. Jhon and H. A. Scheraga - Monte Carlo simulation of the hard-sphere fluid with a high-temperature quantum correction in the region of the fluid-solid phase transition, J. Chem. Phys., 96, 7005-7009 (1992).

849. C. M. Falcomer, Y. C. Meinwald, I. Choudhary, S. Talluri, P. J. Milburn, J. Clardy and H. A. Scheraga - Chain reversals in model peptides: Studies of cystine-containing cyclic peptides. 3. Conformational free energies of cyclization of tetrapeptides of sequence Ac-Cys-Pro-X-Cys-NHMe, J. Am. Chem. Soc. 114, 4036-4042 (1992).

850. Z. Zheng, R. W. Ashton, F. Ni and H. A. Scheraga - Thrombin hydrolysis of an N-terminal peptide from fibrinogen Lille: Kinetic and NMR studies, Biochemistry, 31, 4426-4431 (1992).

851. H. A. Scheraga - Contribution of physical chemistry to an understanding of protein structure and function, Protein Science, 1, 691-693 (1992).

852. K. A. Olszewski, L. Piela and H. A. Scheraga - Mean-field theory as a tool for intramolecular conformational optimization. 1. Tests on terminally-blocked alanine and Met-enkephalin, J. Phys. Chem., 96, 4672-4676 (1992).

853. R. J. Wawak, M. M. Wimmer and H. A. Scheraga - Application of the diffusion equation method of global optimization to water clusters, J. Phys. Chem., 96, 5138-5145 (1992).

854. H. A. Scheraga - Conformational energy calculations on polypeptides and proteins, in Molecular Aspects of Biotechnology; Computational Models and Theories, Ed. J. Bertran, Kluwer Academic Publ., Dordrecht, Netherlands, pp. 1-15 (1992).

855. F. J. Moy, H. A. Scheraga, S. L. Patt and G. T. Montelione - Application of frequency-shifted shaped pulses for overcoming solvent-saturation transfer and preirradiation-associated spin-diffusion effects in aqueous solutions of peptides and proteins, J. Mag. Reson., 98, 451-457 (1992).

856. M. H. Hao, S. Rackovsky, A. Liwo, M. R. Pincus and H. A. Scheraga - Effects of compact volume and chain stiffness on the conformations of native proteins, Proc. Natl. Acad. Sci., U.S.A., 89, 6614-6618 (1992).

857. G. Némethy, K. D. Gibson, K. A. Palmer, C. N. Yoon, G. Paterlini, A. Zagari, S. Rumsey and H. A. Scheraga - Energy parameters in polypeptides. 10. Improved geometrical parameters and nonbonded interactions for use in the ECEPP/3 algorithm, with application to proline-containing peptides, J. Phys. Chem., 96, 6472-6484 (1992).

858. K. C. Chou, G. M. Maggiora and H. A. Scheraga - The role of loop-helix interactions in stabilizing four-helix bundle proteins, Proc. Natl. Acad. Sci., U.S.A., 89, 7315-7319 (1992).

859. J. Vila, R. L. Williams, J. A. Grant, J. Wojcik and H. A. Scheraga - The intrinsic helix-forming tendency of L-alanine, Proc. Natl. Acad. Sci., U.S.A., 89, 7821-7825 (1992).

860. R. L. Williams, J. Vila, G. Perrot and H. A. Scheraga - Empirical solvation models in the context of conformational energy searches. Application to bovine pancreatic trypsin inhibitor, Proteins: Structure, Function, and Genetics, 14, 110-119 (1992).

861. D. M. Rothwarf and H. A. Scheraga - Equilibrium and kinetic constants for the thiol-disulfide interchange reaction between glutathione and dithiothreitol, Proc. Natl. Acad. Sci., U.S.A., 89, 7944-7948 (1992).

862. J. Kostrowicki and H. A. Scheraga - Application of the diffusion equation method for global optimization to oligopeptides, J. Phys. Chem., 96, 7442-7449 (1992).

863. F. Ni, K. D. Gibson and H. A. Scheraga - Nuclear magnetic resonance studies of thrombin-fibrinopeptide and thrombin-hirudin complexes, in "Thrombin: Structure and Function", ed. L. J. Berliner, Plenum Press, New York, pp. 63-85 (1992).

*864. H. A. Scheraga - Predicting three-dimensional structures of oligopeptides, in Reviews in Computational Chemistry, Vol. 3, Eds. K. B. Lipkowitz and D. B. Boyd, VCH Publ., New York, pp. 73-142 (1992).

865. C. Chipot, B. Maigret, J. L. Rivail and H. A. Scheraga - Modeling amino acid side chains: 1. Determination of net atomic charges from ab initio self-consistent-field molecular electrostatic properties, J. Phys. Chem. 96, 10276-10284 (1992). Erratum: ibid., 97, 3452 (1993).

1993

866. K. A. Olszewski, L. Piela and H. A. Scheraga - Mean Field Theory as a tool for intramolecular conformational optimization. 2. Tests on the homopolypeptides decaglycine and icosalanine, J. Phys. Chem., 97, 260-266 (1993).

867. K. A. Olszewski, L. Piela and H. A. Scheraga - Mean Field Theory as a tool for intramolecular conformational optimization. 3. Test on melittin, J. Phys. Chem., 97, 267-270 (1993).

868. J. H. Laity, S. Shimotakahara and H. A. Scheraga - Expression of wild-type and mutant bovine pancreatic ribonuclease A in Escherichia coli, Proc. Natl. Acad. Sci., U.S.A. 90, 615-619 (1993).

*869. D. R. Buckler, E. Haas and H. A. Scheraga - C-terminal labeling of ribonuclease A with an extrinsic fluorescent probe by carboxypeptide Y-catalyzed transpeptidation in the presence of urea, Anal. Biochem., 209, 20-31 (1993).

870. K. T. No, K. H. Cho, M. S. Jhon and H. A. Scheraga - An empirical method to calculate average molecular polarizabilities from the dependence of effective atomic polarizabilities on net atomic charge, J. Am. Chem. Soc., 115, 2005-2014 (1993).

871. D. M. Rothwarf and H. A. Scheraga - Regeneration of bovine pancreatic ribonuclease A. 1. Steady-state distribution, Biochemistry, 32, 2671-2679 (1993).

872. D. M. Rothwarf and H. A. Scheraga - Regeneration of bovine pancreatic ribonuclease A. 2. Kinetics of regeneration, Biochemistry, 32, 2680-2689 (1993).

873. D. M. Rothwarf and H. A. Scheraga - Regeneration of bovine pancreatic ribonuclease A. 3. Dependence on the nature of the redox reagent, Biochemistry, 32, 2690-2697 (1993). Erratum: ibid., 32 7064 (1993).

874. D. M. Rothwarf and H. A. Scheraga - Regeneration of bovine pancreatic ribonuclease A. 4. Temperature dependence of the regeneration rate, Biochemistry, 32, 2698-2703 (1993).

875. H. A. Scheraga - Theoretical Calculations of Protein Folding, in Computer Aided Innovation of New Materials II, Eds. M. Doyama, J. Kihara, M. Tanaka and R. Yamamoto, Elsevier Science Publ. B.V., Amsterdam, 1223-1227 (1993).

876. S. Talluri, C. M. Falcomer and H. A. Scheraga - Energetic and structural basis for the preferential formation of the native disulfide loop involving Cys-65 and Cys-72 in synthetic peptide fragments derived from the sequence of ribonuclease A, J. Am. Chem. Soc., 115 3041-3047 (1993).

877. Y. N. Vorobjev and H. A. Scheraga - Interaction of a biomolecule with mobile ions in aqueous solution. Comparison of three fast approximate methods with the direct solution of the nonlinear Poisson-Boltzmann equation, J. Phys. Chem., 97 4855-4864 (1993).

878. C. Chipot, J. G. Angyan, G. G. Ferenczy and H. A. Scheraga - Transferable net atomic charges from distributed multipole analysis for the description of electrostatic properties. A case study of saturated hydrocarbons, J. Phys. Chem., 97, 6628-6636 (1993).

*879. F. J. Moy, Y-C. Li, P. Rauenbuehler, M. E. Winkler, H. A. Scheraga and G. T. Montelione - Solution structure of human type-□ transforming growth factor determined by hetero-nuclear NMR spectroscopy and refined by energy minimization with restraints, Biochemistry, 32, 7334-7353 (1993).

*880. L. Vitagliano, G. Némethy, A. Zagari and H. A. Scheraga - Stabilization of the triple-helical structure of natural collagen by side-chain interactions, Biochemistry, 32, 7354-7359 (1993).

881. A. A. Rabow and H. A. Scheraga - Lattice neural network minimization-application of neural network optimization for locating the global-minimum conformation of proteins, J. Mol. Biol., 232, 1157-1168 (1993).

882. C. Chipot, J. G. Angyan, B. Maigret and H. A. Scheraga - Modeling amino acid side chains. 2. Determination of point charges from electrostatic properties: Toward transferable point charge models, J. Phys. Chem., 97, 9788-9796 (1993).

883. C. Chipot, J. G. Angyan, B. Maigret and H. A. Scheraga - Modeling amino acid side chains. 3. Influence of intra-and intermolecular environment on point charges, J. Phys. Chem., 97, 9797-9807 (1993). Erratum: ibid., 98, 1518 (1994).

884. M. H. Hao, M. R. Pincus, S. Rackovsky and H. A. Scheraga - Unfolding and refolding of the native structure of bovine pancreatic trypsin inhibitor studied by computer simulations, Biochemistry, 32, 9614-9631 (1993).

885. A. Liwo, M. R. Pincus, R. J. Wawak, S. Rackovsky and H. A. Scheraga - Calculation of protein backbone geometry from α-carbon coordinates based on peptide-group dipole alignment, Protein Science 2, 1697-1714 (1993).

886. A. Liwo, M. R. Pincus, R. J. Wawak, S. Rackovsky and H. A. Scheraga - Prediction of protein conformation on the basis of a search for compact structures; test on avian pancreatic polypeptide, Protein Science 2, 1715-1731 (1993).

887. J. M. Park, K. T. No, M. S. Jhon and H. A. Scheraga - Determination of net atomic charges using a modified partial equalization of orbital electronegativity method. III. Application to halogenated and aromatic molecules, J. Comput. Chem., 14, 1482-1490 (1993).

888. H. A. Scheraga - Foreward to "The Design of Synthetic Inhibitors of Thrombin", eds. G. Claeson, M. F. Scully, and V. V. Kakkar, and J. Deadman, Adv. Exptl. Med. and Biol. 340, v (1993).

889. H. A. Scheraga - Searching conformational space, in "Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications", Vol. 2, ed. W. F. van Gunsteren, P. K. Weiner and A. J. Wilkinson, ESCOM Science Publ., Leiden, pp. 231-248 (1993).

1994

890. A. Zagari, K. Palmer, K. D. Gibson, G. Némethy and H. A. Scheraga - The effect of the L-azetidine-2-carboxylic acid residue on protein conformation. IV. Local substitutions in the collagen triple helix, Biopolymers, 34, 51-60 (1994).

891. M. H. Hao and H. A. Scheraga - Analyzing the normal mode dynamics of macromolecules by the component synthesis method: Residue clustering and multiple-component approach, Biopolymers, 34, 321-335 (1994).

892. W. A. Houry, D. M. Rothwarf and H. A. Scheraga - A very fast phase in the refolding of disulfide-intact ribonuclease A: Implications for the refolding and unfolding pathways, Biochemistry, 33, 2516-2530 (1994).

*893. A. Magalhaes, B. Maigret, J. Hoflack, J. N. F. Gomes and H. A. Scheraga - Contribution of unusual Arginine-Arginine short-range interactions to stabilization and recognition in proteins, J. Protein Chem., 13, 195-215 (1994).

*894. A. Liwo, K. D. Gibson, H. A. Scheraga, P. W. Brandt-Rauf, R. Monaco, and M. R. Pincus - Comparison of the low energy conformations of an oncogenic and a non-oncogenic p21 protein, neither of which binds GTP or GDP, J. Protein Chem., 13, 237-251 (1994).

*895. H. A. Scheraga - The multiple-minima problem in protein folding, Polish J. Chem., 68, 889-891 (1994).

896. M. H. Hao and H. A. Scheraga - Monte Carlo simulation of a first-order transition for protein folding, J. Phys. Chem., 98, 4940-4948 (1994).

897. A. Nayeem and H. A. Scheraga - A statistical analysis of side-chain conformations in proteins: Comparison with ECEPP predictions, J. Protein Chem., 13, 283-296 (1994).

898. R. J. Wawak, K. D. Gibson and H. A. Scheraga - Gradient discontinuities in calculations involving molecular surface area, J. Math. Chem., 15, 207-232 (1994).

899. A. Liwo, S. Oldziej, J. Ciarkowski, G. Kupryszewski, M. R. Pincus, R. J. Wawak, S. Rackovsky and H. A. Scheraga - Prediction of conformation of rat galanin in the presence and absence of water with the use of Monte Carlo methods and the ECEPP/3 force field, J. Protein Chem., 13, 375-380 (1994).

900. R. W. Dodge, J. H. Laity, D. M. Rothwarf, S. Shimotakahara and H. A. Scheraga - Folding pathway of guanidine-denatured disulfide-intact wildtype and mutant bovine pancreatic ribonuclease A, J. Protein Chem., 13, 409-421 (1994).

*901. H. A. Scheraga - Toward a solution of the multiple-minima problem in protein folding, J. Protein Chem., 13, 468-469 (1994).

902. S. Talluri, D. M. Rothwarf and H. A. Scheraga - Structural characterization of a three-disulfide intermediate of ribonuclease A involved in both the folding and unfolding pathways, Biochemistry, 33, 10437-10449 (1994).

903. F. Ni and H. A. Scheraga - Use of the transferred nuclear Overhauser effect to determine the conformations of ligands bound to proteins, Acct. Chem. Res., 27, 257-264 (1994).

904. M. E. Denton, D. M. Rothwarf and H. A. Scheraga - Kinetics of folding of guanidine-denatured hen egg white lysozyme and carboxymethyl(Cys^{6}, Cys^{127})-lysozyme: A stopped-flow absorbance and fluorescence study, Biochemistry, 33, 11225-11236 (1994).

905. M. H. Hao and H. A. Scheraga - Statistical thermodynamics of protein folding: Sequence dependence, J. Phys. Chem., 98, 9882-9893 (1994).

906. H. A. Scheraga - Treatment of hydration in conformational energy calculations on polypeptides and proteins, in "Structure and Reactivity in Aqueous Solution", eds. C. J. Cramer and D. G. Truhlar, ACS Symposium Series 568, pp. 360-370 (1994).

907. K. T. No, K. H. Cho, O. Y. Kwon, M. S. Jhon and H. A. Scheraga - Determination of proton transfer energies and lattice energies of several amino acid zwitterions, J. Phys. Chem., 98, 10742-10749 (1994).

908. Y. N. Vorobjev, H. A. Scheraga, B. Hitz and B. Honig - Theoretical modeling of electrostatic effects of titratable side-chain groups on protein conformation in a polar ionic solution. 1. Potential of mean force between charged lysine residues and titration of poly-(L-lysine) in 95% methanol solution, J. Phys. Chem., 98, 10940-10948 (1994).

909. K. D. Gibson and H. A. Scheraga - A rapid and efficient algorithm for packing polypeptide chains by energy minimization, J. Comput. Chem., 15, 1403-1413 (1994).

910. K. D. Gibson and H. A. Scheraga - An algorithm for packing regular multistrand polypeptide structures by energy minimization, J. Comput. Chem., 15, 1414-1428 (1994).

911. S. C. Allen, K. R. Acharya, K. A. Palmer, R. Shapiro, B. L. Vallee and H. A. Scheraga - A comparison of the predicted and x-ray structures of angiogenin. Implications for further studies of model building of homologous proteins, J. Protein Chem., 13, 649-658 (1994).

912. M. Vásquez, G. Némethy and H. A. Scheraga - Conformational energy calculations on polypeptides and proteins, Chem. Revs., 94, 2183-2239 (1994).

1995

913. E. E. DiBella, M. C. Maurer and H. A. Scheraga - Expression and folding of recombinant bovine prethrombin-2 and its activation to thrombin, J. Biol. Chem., 270, 163-169 (1995).

914. M. H. Hao and H. A. Scheraga - Statistical thermodynamics of protein folding: Comparison of a mean-field theory with Monte Carlo simulations, J. Chem. Phys., 102, 1334-1348 (1995).

915. M. H. Hao and H. A. Scheraga - Reply to "Comment on `Monte Carlo simulation of a first-order transition for protein folding'", J. Phys. Chem., 99, 2238 (1995).

916. J. D. Augspurger, V. A. Bindra, H. A. Scheraga and A. Kuki- Helical stability of de novo designed α-aminoisobutyric acid-rich peptides at high temperatures, Biochemistry, 34, 2566-2576 (1995).

917. K. T. No, O. Y. Kwon, S. Y. Kim, M. S. Jhon and H. A. Scheraga - A simple functional representation of angular-dependent hydrogen-bonded systems. 1. Amide, carboxylic acid, and amide-carboxylic acid pairs, J. Phys. Chem., 99, 3478-3486 (1995).

918. K. D. Gibson and H. A. Scheraga - Crystal packing without symmetry constraints. 1. Tests of a new algorithm for determining crystal structures by energy minimization, J. Phys. Chem., 99, 3752-3764 (1995).

919. K. D. Gibson and H. A. Scheraga - Crystal packing without symmetry constraints. 2. Possible crystal packings of benzene obtained by energy minimization from multiple starts, J. Phys. Chem., 99, 3765-3773 (1995).

*920. H. A. Scheraga - Molecular aggregates, Polymer Preprints (Amer. Chem. Soc.), 36, 633-634 (1995).

921. L. Vitagliano, G. Némethy, A. Zagari and H. A. Scheraga - Structure of the type I collagen molecule based on conformational energy computations: the triple-stranded helix and the N-terminal telopeptide, J. Mol. Biol., 247, 69-80 (1995).

*922. J. Kostrowicki and H. A. Scheraga - Simple global minimization algorithm for one-variable rational functions, J. Global Optimization, 6, 293-311 (1995).

923. Y. N. Vorobjev, H. A. Scheraga and B. Honig - Theoretical modeling of electrostatic effects of titratable side-chain groups on protein conformation in a polar ionic solution. 2. pH-induced helix-coil transition of poly-(L-lysine) in water and methanol ionic solutions, J. Phys. Chem., 99, 7180-7187 (1995).

924. M. G. Paterlini, G. Némethy and H. A. Scheraga - The energy of formation of internal loops in triple-helical collagen polypeptides, Biopolymers, 35, 607-619 (1995).

925. R. W. Ashton and H. A. Scheraga - Preparation and characterization of anhydrothrombin, Biochemistry, 34, 6454-6463 (1995).

926. Y.-J. Li, D. M. Rothwarf and H. A. Scheraga - Mechanism of reductive protein unfolding, Nature Struct. Biol., 2, 489-494 (1995).

927. W. A. Houry, D. M. Rothwarf and H. A. Scheraga - The nature of the initial step in the conformational folding of disulfide-intact ribonuclease A, Nature Struct. Biol., 2, 495-503 (1995).

*928. H. A. Scheraga - Conformational energy calculations on polypeptides and proteins, Society of Polymer Science, Japan, Polymer Preprints, 44, No. 1, 20-22 (1995).

929. J. M. Park, O. Y. Kwon, K. T. No, M. S. Jhon and H. A. Scheraga - Determination of net atomic charges using a modified partial equalization of orbital electro-negativity method. IV. Application to hypervalent sulfur and phosphorus containing molecules, J. Comput. Chem., 16, 1011-1026 (1995).

930. J. Kostrowicki and H. A. Scheraga - New method for calculation of the exact end-to-end distance distributions for the freely-rotating chain, Computational Polymer Science, 5, 47-55 (1995).

931. D. R. Ripoll, M. S. Pottle, K. D. Gibson, H. A. Scheraga and A. Liwo - Implementation of the ECEPP algorithm, the Monte Carlo minimization method, and the electrostatically driven Monte Carlo method on the Kendall Square Research KSR1 computer, J. Comput. Chem., 16, 1153-1163 (1995).

932. M. P. Joseph, B. Maigret, J. C. Bonnafous, J. Marie, and H. A. Scheraga - A computer modeling postulated mechanism for angiotensin II receptor activation, J. Protein Chem., 14, 381-398 (1995).

933. K. T. No, O. Y. Kwon, S. Y. Kim, K. H. Cho, C. N. Yoon, Y. K. Kang, K. D. Gibson, M. S. Jhon and H. A. Scheraga - Determination of nonbonded potential parameters for peptides, J. Phys. Chem., 99, 13019-13027 (1995).

934. F. Ni, Y. Zhu and H. A. Scheraga - Thrombin-bound structures of designed analogs of human fibrinopeptide A determined by quantitative transferred NOE spectroscopy: A new structural basis for thrombin specificity, J. Mol. Biol., 252, 656-671 (1995).

*935. M. P. Joseph, B. Maigret and H. A. Scheraga - Proposals for the angiotensin II receptor-bound conformation by comparative computer modeling of AII and cyclic analogs, Intl. J. Peptide Protein Res., 46, 514-526 (1995).

*936. M.- H. Hao and H. A. Scheraga - Computational approach to the statistical mechanics of protein folding, Proceedings of the 1995 ACM/IEEE Supercomputer conference, San Diego, CA, p. 57 (1995), available on CD-ROM.

937. C. C. Lester, B. Wang, R. Wu and H. A. Scheraga - Structure-function studies of mEGF: Probing the type-I β-turn between residues 25 and 26, J. Protein Chem., 14, 753-762 (1995).

938. D. R. Buckler, E. Haas and H. A. Scheraga - 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, 34, 15965-15978 (1995).

939. H. A. Scheraga, M. H. Hao and J. Kostrowicki - Theoretical studies of protein folding, in "Methods in Protein Structure Analysis", eds. M. Z. Atassi and E. Appella, Plenum, New York, 457-464 (1995).

1996

940. J. Kostrowicki and H. A. Scheraga - Some approaches to the multiple-minima problem in protein folding, in "Global minimization of nonconvex energy functions: Molecular conformation and protein folding", eds. P.M. Pardalos, D. Shalloway and G. Xue, DIMACS Series in Discrete Mathematics and Theoretical Computer Science (American Mathematical Society), 23, 123-132 (1996).

941. R. W. Dodge and H. A. Scheraga - Folding and unfolding kinetics of the proline-to-alanine mutants of bovine pancreatic ribonuclease A, Biochemistry, 35, 1548-1559 (1996).

942. D. C. Kombo, G. Némethy, K. D. Gibson, J. B. A. Ross, S. Rackovsky and H. A. Scheraga - 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, J. Protein Chem., 15, 77-86 (1996).

943. D. C. Kombo, G. Némethy, K. D. Gibson, S. Rackovsky and H. A. Scheraga - Computer-aided discrimination between active and inactive mutants of the N-terminal domain of the bacteriophage λ repressor, J. Mol. Biol., 256, 517-532 (1996).

944. R. J. Wawak, K. D. Gibson, A. Liwo and H. A. Scheraga - Theoretical prediction of a crystal structure, Proc. Natl. Acad. Sci., U.S.A., 93, 1743-1746 (1996).

945. E. E. DiBella and H. A. Scheraga - The role of the insertion loop around tryptophan 148 in the activity of thrombin, Biochemistry, 35., 4427-4433 (1996).

*946. T. J. O'Donnell, S. G. Hotovy, M. S. Pottle, D. R. Ripoll and H. A. Scheraga - Implementation of ECEPP-based programs on the IBM SP2 and the SGI power challenge computers, Lecture Notes in Computer Science, Vol. 1067: High Performance Computing and Networking, H. Liddell, A. Colbrook, B. Hertzberger and P. Sloot (Eds.); Springer-Verlag, Berlin, Heidelberg, New York, pp. 365-372 (1996).

947. M.-H. Hao and H. A. Scheraga - How optimization of potential functions affects protein folding, Proc. Natl. Acad. Sci., U.S.A., 93, 4984-4989 (1996).

*948. H. A. Scheraga - Recent developments in the theory of protein folding: searching for the global energy minimum, Biophys. Chem., 59, 329-339 (1996).

949. X. Xu, D. M. Rothwarf and H. A. Scheraga - Nonrandom distribution of the one-disulfide intermediates in the regeneration of ribonuclease A, Biochemistry, 35, 6406-6417 (1996).

*950. H. A. Scheraga - My experience with science in Korea, Center for Molecular Science Newsletter (Korea), 16, 4-5 (1996).

951. W. A. Houry, D. M. Rothwarf and H. A. Scheraga - Circular dichroism evidence for the presence of burst-phase intermediates on the conformational folding pathway of ribonuclease A, Biochemistry, 35, 10125-10133 (1996).

952. B. Cheng, A. Nayeem and H. A. Scheraga - From secondary structure to three-dimensional structure: Improved dihedral angle probability distribution function for use with energy searches for the native structures of polypeptides and proteins, J. Comput. Chem., 17, 1453-1480 (1996).

953. M.-H. Hao and H. A. Scheraga - Optimizing potential functions for protein folding, J. Phys. Chem., 100, 14540-14548 (1996).

954. W. A. Houry and H. A. Scheraga - The nature of the unfolded state of ribonuclease A: Effect of cis-trans X-Pro peptide bond isomerization, Biochemistry, 35, 11719-11733 (1996).

955. W. A. Houry and H. A. Scheraga - Structure of a hydrophobically collapsed intermediate on the conformational folding pathway of ribonuclease A probed by hydrogen-deuterium exchange, Biochemistry, 35, 11734-11746 (1996).

956. D. M. Rothwarf, V. G. Davenport, P.-T. Shi, J.-L. Peng and H. A. Scheraga - Use of sequence-specific tri-block copolymers to determine the helix-forming tendencies of amino acids, Biopolymers, 39, 531-536 (1996).

957. A. A. Rabow and H. A. Scheraga - Improved genetic algorithm for the protein folding problem by use of a Cartesian combination operator, Protein Science, 5, 1800-1815 (1996).

958. J. D. Augspurger and H. A. Scheraga - An efficient, differentiable hydration potential for peptides and proteins, J. Comput. Chem., 17, 1549-1558 (1996).

959. Y. K. Kang, K. T. No and H. A. Scheraga - Intrinsic torsional potential parameters for conformational analysis of peptides and proteins, J. Phys. Chem., 100, 15588-15598 (1996).

960. R. A. Sendak, D. M. Rothwarf, W. J. Wedemeyer, W. A. Houry, and H. A. Scheraga - Kinetic and thermodynamic studies of the folding/unfolding of a tryptophan-containing mutant of ribonuclease A, Biochemistry, 35, 12978-12992 (1996).

961. D. M. Rothwarf and H. A. Scheraga - The role of non-native aromatic and hydrophobic interactions in the folding of hen egg white lysozyme, Biochemistry, 35, 13797-13807 (1996).

962. O. Y. Kwon, S. Y. Kim, K. T. No, Y. K. Kang, M. S. Jhon, and H. A. Scheraga - Determination of potential parameters for amino acid zwitterions, J. Phys. Chem., 100, 17670-17677 (1996).

963. C. C. Lester, M. C. Maurer and H. A. Scheraga - Water suppression for TR-NOSEY with the DPFGSE technique, The NMR Newsletter, September 1996.

*964. H. A. Scheraga - Cyclic peptides and loops in proteins, in "Large Ring Molecules", ed. J. A. Semlyen, John Wiley & Sons Ltd., Chichester, pp. 99-111 (1996).

965. T. W. Thannhauser and H. A. Scheraga - State of aggregation of recombinant hirudin in solution under physiological conditions, J. Protein Chem., 15, 751-753 (1996).

966. D. R. Ripoll, Y. N. Vorobjev, A. Liwo, J. A. Vila and H. A. Scheraga - Coupling between folding and ionization equilibria: Effects of pH on the conformational preferences of polypeptides, J. Mol. Biol., 264, 770-783 (1996).

967. J. Lee, H. A. Scheraga and S. Rackovsky - Computational study of packing a collagen-like molecule: Quasi-hexagonal vs. "Smith" collagen microfibril model, Biopolymers, 40, 595-607 (1996).

1997

968. K. D. Gibson and H. A. Scheraga - Energy minimization of rigid-geometry polypeptides with exactly closed disulfide loops, J. Comput. Chem., 18, 403-415 (1997).

969. Y. N. Vorobjev and H. A. Scheraga - A fast adaptive multigrid boundary element method for macromolecular electrostatic computations in a solvent, J. Comput. Chem., 18, 569-583 (1997).

*970. G. Ashkenazi, D. R. Ripoll, N. Lotan and H. A. Scheraga - A molecular switch for biochemical logic gates: Conformational studies, Biosensors & Bioelectronics, 12, 85-95 (1997).

971. T. W. Thannhauser, D. M. Rothwarf and H. A. Scheraga - Kinetic studies of the regeneration of recombinant hirudin variant 1 with oxidized and reduced dithiothreitol, Biochemistry, 36, 2154-2165 (1997).

972. A. Liwo, S. Oldziej, M. R. Pincus, R. J. Wawak, S. Rackovsky and H. A. Scheraga - A united-residue force field for off-lattice protein-structure simulations. I. Functional forms and parameters of long-range side-chain interaction potentials from protein crystal data, J. Comput. Chem., 18, 849-873 (1997).

973. A. Liwo, M. R. Pincus, R. J. Wawak, S. Rackovsky, S. Oldziej and H. A. Scheraga - A united-residue force field for off-lattice protein-structure simulations. II. Parameterization of short-range interactions and determination of weights of energy terms by Z-score optimization, J. Comput. Chem., 18, 874-887 (1997).

974. W. J. Wedemeyer, R. W. Ashton and H. A. Scheraga - Kinetics of competitive binding with application to thrombin complexes, Anal. Biochem., 248, 130-140 (1997). Erratum: - Anal. Biochem. 248, 326 (1997).

975. S. Shimotakahara, C. B. Rios, J. H. Laity, D. E. Zimmerman, H. A. Scheraga and G. T. Montelione - NMR structural analysis of an analog of an intermediate formed in the rate-determining step of one pathway in the oxidative folding of bovine pancreatic ribonuclease A: Automated analysis of ^{1}H, ^{13}C, and ^{15}N resonance assignments for wild-type and [C65S, C72S] mutant forms, Biochemistry, 36, 6915-6929 (1997).

976. K. T. No, B. H. Chang, S. Y. Kim, M. S. Jhon and H. A. Scheraga - Description of the potential energy surface of the water dimer with an artificial neural network, Chem. Phys. Letters, 271, 152-156 (1997).

977. J. D. Augspurger and H. A. Scheraga - An assessment of the accuracy of the RRIGS hydration potential: Comparison to solutions of the Poisson-Boltzmann equation, J. Comput. Chem.,18, 1072-1078 (1997).

978. J. Lee, H. A. Scheraga and S. Rackovsky - New optimization method for conformational energy calculations on polypeptides: Conformational space annealing, J. Comput. Chem., 18, 1222-1232 (1997).

979. O. Collet, S. Prémilat, B. Maigret and H. A. Scheraga - Comparison of explicit and implicit treatments of solvation: Application to angiotensin II, Biopolymers 42, 363-371 (1997).

980. D. Juminaga, W. J. Wedemeyer, R. Garduño-Júarez, M. A. McDonald, and H. A. Scheraga - Tyrosyl interactions in the folding and unfolding of bovine pancreatic ribonuclease A: A study of tyrosine-to-phenylalanine mutants, Biochemistry, 36, 10131-10145 (1997).

981. M.-H. Hao and H. A. Scheraga - On foldable proteinlike models: A statistical-mechanical study with Monte Carlo simulations, Physica A, 244, 124-146 (1997).

982. J. H. Laity, C. C. Lester, S. Shimotakahara, D. E. Zimmerman, G. T. Montelione and H. A. Scheraga - Structural characterization of an analog of the major rate-determining disulfide folding intermediate of bovine pancreatic ribonuclease A, Biochemistry, 36, 12683-12699 (1997).

983. C. C. Lester, X. Xu, J. H. Laity, S. Shimotakahara and H. A. Scheraga - Regeneration studies of an analog of ribonuclease A missing disulfide bonds 65-72 and 40-95, Biochemistry, 36, 13068-13076 (1997).

984. M.-H. Hao and H.A. Scheraga - Characterization of foldable protein models: Thermodynamics, folding kinetics, and force field, J. Chem. Phys., 107, 8089-8102 (1997).

985. K. T. No, K.-Y. Nam and H. A.Scheraga - Stability of like and oppositely charged organic ion pairs in aqueous solution, J. Am. Chem. Soc., 119, 12917-12922 (1997).

1998

986. S. He and H. A. Scheraga - Macromolecular conformational dynamics in torsional angle space, J. Chem. Phys., 108, 271-286 (1998).

987. S. He and H. A. Scheraga - Brownian dynamics simulations of protein folding, J. Chem. Phys., 108, 287-300 (1998).

988. D. Oberlin Jr. and H. A. Scheraga - B-spline method for energy minimization in grid-based molecular mechanics calculations, J. Comput. Chem., 19, 71-85 (1998).

989. A. Liwo, R. Kazmierkiewicz, C. Czaplewski, M. Groth, S. Oldziej, R. J. Wawak, S. Rackovsky, M. R. Pincus, and H. A. Scheraga - United-residue force field for off-lattice protein-structure simulations; III. Origin of backbone hydrogen-bonding cooperativity in united-residue potentials, J. Comput. Chem., 19, 259-276 (1998).

990. T. W. Thannhauser, R. W. Sherwood and H. A. Scheraga - Determination of the cysteine and cystine content of proteins by amino acid analysis: Application to the characterization of disulfide-coupled folding intermediates, J. Protein Chem., 17, 37-43 (1998).

991. D. M. Rothwarf, Y.-J. Li and H. A. Scheraga - Regeneration of bovine pancreatic ribonuclease A. Identification of two nativelike three-disulfide intermediates involved in separate pathways, Biochemistry, 37, 3760-3766 (1998).

992. D. M. Rothwarf, Y.-J. Li and H. A. Scheraga - Regeneration of bovine pancreatic ribonuclease A. Detailed kinetic analysis of two independent folding pathways, Biochemistry, 37, 3767-3776 (1998).

993. Y.-J. Li, D. M. Rothwarf and H. A. Scheraga - An unusual adduct of dithiothreitol with a pair of cysteine residues of a protein as a stable folding intermediate, J. Am. Chem. Soc., 120, 2668-2669 (1998).

994. M. Iwaoka, D. Juminaga and H. A. Scheraga - 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, 37, 4490-4501 (1998).

995. M.-H. Hao and H.A. Scheraga - Molecular mechanisms for cooperative folding of proteins, J. Mol. Biol., 277, 973-983 (1998).

996. W. A. Houry, J. M. Sauder, H. Roder and H. A. Scheraga - Definition of amide protection factors for early kinetic intermediates in protein folding, Proc. Natl. Acad. Sci., U.S.A., 95, 4299-4302 (1998).

997. E. E. DiBella and H. A. Scheraga - Thrombin specificity: Further evidence for the importance of the β-insertion loop and Trp^{96}. Implications of the hydrophobic interaction between Trp^{96} and Pro^{60B} Pro^{60C} for the activity of thrombin, J. Protein. Chem., in 17, 197-208 (1998).

998. R. J. Wawak, J. Pillardy, A. Liwo, K.D. Gibson and H. A. Scheraga - Diffusion equation and distance scaling methods of global optimization: Applications to crystal structure prediction, J. Phys. Chem., 102, 2904-2918 (1998).

999. H. A. Scheraga - In Memory of Bernard Pullman (1919-1996), in "Structure, Motion, Interaction and Expression of Biological Macromolecules", Vol. I, Eds. R.H. Sarma and M. H. Sarma, Adenine Press, Guilderland, NY. pp. 13-15 (1998).

1000. M. C. Maurer, J.-L. Peng, S. S. An, J.-Y. Trosset, A. Henschen-Edman and H. A. Scheraga - Structural examination of the influence of phosphorylation on the binding of fibrinopeptide A to bovine thrombin, Biochemistry, 37, 5888-5902 (1998).

1001. M. A. Pearson, P. A. Karplus, R. W. Dodge, J. H. Laity and H. A. Scheraga - Crystal structures of two mutants that have implications for the folding of bovine pancreatic ribonuclease A, Protein Science, 7, 1255-1258 (1998).

1002. J. A. Vila, D. R. Ripoll, Y.N. Vorobjev and H A. Scheraga - Computation of the structure-dependent pK_a shifts in a polypentapeptide of the poly[f_V(IPGVG), f_E(IPGEG)] family, J. Phys. Chem. B, 102, 3065-3067 (1998).

1003. X. Xu and H. A. Scheraga - Kinetic folding pathway of a three-disulfide mutant of bovine pancreatic ribonuclease A missing the [40-95] disulfide bond, Biochemistry, 37, 7561-7571 (1998).

1004. M. Iwaoka and H. A. Scheraga - Characterization of multiple reduction pathways of proteins in the presence of a denaturant, J. Am. Chem. Soc., 120, 5806-5807 (1998).

1005. J. Lee, H. A. Scheraga and S. Rackovsky - Conformational analysis of the 20-residue membrane-bound portion of melittin by conformational space annealing, Biopolymers, 46, 103-115 (1998).

1006. D.R. Ripoll, A. Liwo, and H. A. Scheraga - New Developments of the electrostatically driven Monte Carlo method: Test on the membrane-bound portion of melittin, Biopolymers, 46, 117-126 (1998).

1007. J.-Y. Trosset and H. A. Scheraga - Reaching the global minimum in docking simulations: A Monte Carlo energy minimization approach using Bezier splines. Proc. Natl. Acad. Sci., U.S.A., 95, 8011-8015 (1998).

1008. D. Juminaga, W. J. Wedemeyer and H. A. Scheraga - Proline isomerization in bovine pancreatic ribonuclease A. I. Unfolding conditions, Biochemistry 37, 11614-11620 (1998).

1009. M.-H. Hao and H. A. Scheraga - Theory of two - state cooperative folding of proteins, Acct. Chem. Res., 31, 433-440 (1998).

1010. M.-H. Hao and H. A. Scheraga - Conformational sampling, in "The Encyclopedia of Computational Chemistry", Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R. (Eds.), John Wiley & Sons, Chichester, 1, 552-555 (1998).

1011. D. R. Ripoll and H. A. Scheraga - ECEPP: Empirical conformational energy program for peptides, in "The Encyclopedia of Computational Chemistry", Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R. (Eds.), John Wiley & Sons, Chichester, 2, 813-815 (1998).

1012. H. A. Scheraga - Theory of hydrophobic interactions, J. Biomolec. Structure and Dynamics, 16, 447-460 (1998).

1013. J. A. Vila, D. R. Ripoll, M. E. Villegas, Y. N. Vorobjev, and H. A. Scheraga - Role of hydrophobicity and solvent-mediated charge-charge interactions in stabilizing α-helices, Biophys. J., 75, 2637-2646 (1998).

1999

1014. H. A. Scheraga and M.-H. Hao - Entropy sampling Monte Carlo for polypeptides and proteins, Adv. in Chemical Physics, 105, 243-272 (1999).

1015. M. C. Maurer, J.-Y. Trosset, C. C. Lester, E. E. DiBella and H. A. Scheraga - New general approach for determining the solution structure of a ligand bound weakly to a receptor: Structure of a fibrinogen Aα-like peptide bound to thrombin (S195A) obtained using NOE distance constraints and an ECEPP/3 flexible docking program, Proteins, Struct., Funct. and Genet., 34, 29-48 (1999).

1016. E. Welker and H. A. Scheraga - Use of benzyl mercaptan for direct preparation of long polypeptide benzylthio esters as substrates of substiligase, Biochem. Biophys. Res. Commun., 254, 147-151 (1999).

1017. J.-Y. Trosset and H. A. Scheraga - Flexible docking simulations: Scaled collective variable Monte Carlo minimization approach using Bezier splines, and comparison with a standard Monte Carlo algorithm, J. Comput. Chem., 20, 244-252 (1999).

1018. J. Lee, A. Liwo and H. A. Scheraga - Energy-based *de novo* protein folding by conformational space annealing and an off-lattice united-residue force field: Application to the 10-55 fragment of staphylococcal protein A and to apo calbindin D9K, Proc. Natl. Acad. Sci., USA, 96, 2025-2030 (1999).

1019. M. Iwaoka, W. J. Wedemeyer and H. A. Scheraga - Conformational unfolding studies of three-disulfide mutants of bovine pancreatic ribonuclease A and the coupling of proline isomerization to disulfide redox reactions, Biochemistry, 38, 2805-2815 (1999).

1020. J.-Y. Trosset and H. A. Scheraga - PRODOCK: Software package for protein modeling and docking, J. Comput. Chem., 20, 412-427 (1999).

1021. A. Liwo, J. Pillardy, R. Kazmierkiewicz, R.J. Wawak, M. Groth, C. Czaplewski, S. Oldziej, and H.A. Scheraga - Prediction of protein structure using a knowledge -based off-lattice united-residue force field and global optimization methods, European Conference on "Computational Chemistry of the Living World--from Sequence to Function", Chambery, France, April 20-24, 1998, Abstracts, p. 52; Theor. Chem. Accounts, 101, 16-20 (1999).

1022. Y.-J. Li, C. C. Lester, D. M. Rothwarf, J.-L. Peng, T. W. Thannhauser, L. Zhang, J. Tam, and H. A. Scheraga - Retention of a cis-proline rotamer in a small fragment of RNase A containing a non-natural proline analog -- an NMR study, Peptides: Frontiers of Peptide Science, Eds., J. P. Tam and P. T. P. Kaumaya, Kluwer Academic Publ., Dordrecht (1999), pp. 422-423.

1023. Y.-J. Ye and H. A. Scheraga - Kinetics of protein folding, in "Slow Dynamics in Complex Systems: Eighth Tohwa University International Symposium", Eds. M. Tokuyama and I. Oppenheim. AIP Conference Proceedings 469, pp. 452-475, Amer. Inst. Phys. (1999).

1024. M. -H. Hao and H. A. Scheraga - Designing potential energy functions for protein folding, Current Opinion in Structural Biology, 9, 184-188 (1999).

1025. A. Liwo, J. Lee, D. R. Ripoll, J. Pillardy and H. A. Scheraga - Protein structure prediction by global optimization of a potential energy function, Proc. Natl. Acad. Sci., USA, 96, 5482-5485 (1999).

1026. K.T. No, S.G. Kim, K.-H. Cho, and H.A. Scheraga - Description of hydration free energy density as a function of molecular physical properties, Biophys. Chemistry, 78, 127-145 (1999).

1027. W.J. Wedemeyer and H.A. Scheraga - Exact analytical loop closure in proteins using polynomial equations, J. Comput. Chem.20, 819-844 (1999).

1028. M.J. Volles, X. Xu and H.A. Scheraga - Distribution of disulfide bonds in the two-disulfide

intermediates in the regeneration of bovine pancreatic ribonuclease A, Biochemistry, 38, 7284-7293 (1999).

1029. H.-C. Shin and H.A. Scheraga - Effect of protein disulfide isomerase on the regeneration of bovine ribonuclease A with dithiothreitol, FEBS LETT., 456, 143-145 (1999).

1030. J. Pillardy, A. Liwo, M. Groth and H.A. Scheraga - An efficient deformation-based global optimization method for off-lattice polymer chains; self-consistent basin-to-deformed-basin mapping (SCBDBM). Application to united-residue polypeptide chains, J. Phys. Chem., B103, 7353-7366 (1999).

1031. Y.-J. Ye, D.R. Ripoll and H.A. Scheraga - Kinetics of cooperative protein folding involving two separate conformational families, Comput. and Theor. Polymer Sci., 9, 359-370 (1999).

1032. D.J. Wales and H.A. Scheraga - Global optimization of clusters, crystals and biomolecules, Science, 285, 1368-1372 (1999).

1033. D.R. Ripoll, J.A. Vila, M.E. Villegas and H.A. Scheraga - On the pH-conformational dependence of the unblocked SYPYD peptide, J. Mol. Biol., 292, 431-440 (1999).

1034. J. Lee, A. Liwo, D.R. Ripoll, J. Pillardy and H.A. Scheraga - Calculation of protein conformation by global optimization of a potential energy function, Proteins: Structure, Function and Genetics, Suppl. 3, 204-208 (1999).

1035. J. Lee and H.A. Scheraga - Conformational space annealing by parallel computations: Extensive conformational search of Met-enkephalin and of the 20-residue membrane-bound portion of melittin, Intl. J. of Quantum Chem., 75, 255-265 (1999).

1036. A. Liwo, C. Czaplewski, J. Pillardy, J. Lee, D.R. Ripoll and H.A. Scheraga – Origin and role of cooperative terms coming from local and long-range interactions in united-residue protein potentials, 5th World Congress of Theoretically Oriented Chemists, WATOC '99, Imperial College, London, 1-6 August 1999, Abstract p. 556.

1037. H.A. Scheraga - The intrinsic tendency toward α-helix formation, in "Perspectives in Structural Biology", eds., M. Vijayan, N. Yathindra and A. S. Kolaskar, Indian Academy of Sciences, Universities Press, Hyderabad, India, pp. 275-292.

1038. E. Welker, M. Narayan, M.J. Volles, and H.A. Scheraga - Two new structured intermediates in the oxidative folding of RNase A, FEBS LETT., 460, 477-479 (1999).

1039. J. Pillardy, A. Liwo, and H.A. Scheraga - An efficient deformation-based global optimization method [self-consistent basin-to-deformed-basin mapping (SCBDBM)]. Application to Lennard-Jones atomic clusters, J. Phys. Chem., A103, 9370-9377 (1999).

1040. J.H. Laity, G.T. Montelione and H.A. Scheraga - Comparison of local and global stability of an analog 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, 38, 16432-16442 (1999).

1041. S.S.A. An, C.C. Lester, J.-L. Peng, Y.-J. Li, D. M. Rothwarf, E. Welker, T.W. Thannhauser, L.S. Zhang, J.P. Tam, and H.A. Scheraga – Retention of the cis proline conformation in tripeptide fragments of bovine pancreatic ribonuclease A containing a non-natural proline analog, 5,5-dimethylproline, J. Am. Chem. Soc., 121, 11558-11566 (1999).

1042. E. Locardi, J. Kwak, H.A. Scheraga, and M. Goodman - Thermodynamics of formation of the triple helix from free chains and from template-constrained chains of collagen-like monodisperse poly(Gly-Pro-Hyp) structures. J. Phys. Chem, A103, 10561-10566 (1999).

1043. H.A. Scheraga, J. Lee, J. Pillardy, Y.-J. Ye, A. Liwo, and D.R. Ripoll - Surmounting the multiple-minima problem in protein folding, J. Global Optimization, 15, 235-260 (1999).

2000

1044. J. Pillardy, R.J. Wawak, Y.A. Arnautova, C. Czaplewski, and H.A. Scheraga – Crystal structure prediction by global optimization as a tool for evaluating potentials: Role of the dipole moment correction term in successful predictions, J. Am. Chem. Soc., 122, 907-921 (2000).

1045. J. Lee, A. Liwo, D.R. Ripoll, J. Pillardy, J.A. Saunders, K.D. Gibson and H.A. Scheraga - Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets, Intl. J. Quantum Chem., 71, 90-117 (2000).

1046. Y. Xiong, D. Juminaga, G.V.T. Swapna, W.J. Wedemeyer, H.A. Scheraga, and G.T. Montelione - Solution NMR evidence for a cis Tyr-Ala peptide group in the structure of [Pro93Ala] bovine pancreatic ribonuclease A, Protein Science, 9, 421-426 (2000).

1047. M.-C. Song and H.A. Scheraga – Formation of native structure by intermoleculear thiol-disulfide exchange reactions without oxidants in the folding of bovine pancreatic ribonuclease A, FEBS LETT., 471, 177-181 (2000).

1048. W.J. Wedemeyer, E. Welker, M. Narayan, and H.A. Scheraga – Disulfide bonds and protein folding, Biochemistry, 39, 4207-4216 (2000); Erratum: Biochemistry, 39, 7032 (2000).

1049. A. Liwo, J. Pillardy, C. Czaplewski, J. Lee, D. R. Ripoll, M. Groth, S. Rodziewicz-Motowidło, R. Kaźmierkiewicz, R. J. Wawak, S. Ołdziej, and H. A. Scheraga – UNRES – a united-residue force field for energy-based prediction of protein structure - origin and significance of multibody terms, RECOMB 2000, Proceedings of the Fourth Annual International Conference on Computational Molecular Biology, R. Shamir, S. Miyano, S. Istrail, P. Pevzner and M. Waterman (Eds.), April 8-11, 2000, Tokyo, Japan, Publ. by ACM, New York, pp. 193-200.

1050. L. K. Low, H.-C. Shin, M. Narayan, W. J. Wedemeyer and H. A. Scheraga – Acceleration of oxidative folding of bovine pancreatic ribonuclease A by anion-induced stabilization and formation of structured native-like intermediates, FEBS LETT., 472, 67-72 (2000).

1051. C. Czaplewski, S. Rodziewicz-Motowidło, A. Liwo, D. R. Ripoll, R. J. Wawak and H.A. Scheraga – Molecular simulation study of cooperativity in hydrophobic association, Protein Science, 9, 1235-1245 (2000).

1052. J. Lee, J. Pillardy, C. Czaplewski, Y. Arnautova, D.R. Ripoll, A. Liwo, K.D. Gibson, R.J. Wawak, and H.A. Scheraga – Efficient parallel algorithms in global optimization of potential energy functions, Comput. Physics Commun., 128, 399-411 (2000).

1053. H.-C. Shin and H.A. Scheraga – Catalysis of the oxidative folding of bovine pancreatic ribonuclease A by protein disulfide isomerase, J. Mol. Biol., 300, 995-1003 (2000).

1054. K.-H. Cho, K.T. No, and H.A. Scheraga – Ion pair interactions in aqueous solution: self-consistent reaction field (SCRF) calculations with some explicit water molecules, J. Phys. Chem., A104, 6505-6509 (2000).

1055. W.J. Wedemeyer, Y.A. Arnautova, J. Pillardy, R.J. Wawak, C. Czaplewski, and H.A. Scheraga – 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, J. Phys. Chem. B104, 8090-8092 (2000).

1056. J. Pillardy, C. Czaplewski, W.J. Wedemeyer and H.A. Scheraga – Conformation-Family Monte Carlo (CFMC): An efficient computational method for identifying the low-energy states of a macromolecule, Helv. Chim. Acta, 83, 2214-2230 (2000).

1057. J. A. Vila, D.R. Ripoll and H.A. Scheraga – Physical reasons for the unusual α-helix stabilization afforded by charged or neutral polar residues in alanine-rich peptides, Proc. Natl. Acad. Sci., U.S.A., 97, 13075-13079 (2000).

1058. M. Narayan, E. Welker, W.J. Wedemeyer, and H.A. Scheraga – Oxidative folding of proteins, Accts. Chem. Res., 33, 805-812 (2000).

2001

1059. A. Navon, V. Ittah, J.H. Laity, H.A. Scheraga, E. Haas and E.E. Gussakovsky – Local and long-range interactions in the thermal unfolding transition of bovine pancreatic ribonuclease A, Biochemistry, 40, 93-104 (2001).

1060. A. Navon, V. Ittah, P. Landsman, H.A. Scheraga and E. Haas – 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, 40, 105-118 (2001).

1061. J.A. Vila, D.R. Ripoll and H.A. Scheraga – Influence of lysine content and pH on the stability of alanine-based co-polypeptides, Biopolymers, 58, 235-246 (2001).

1062. E. Welker, M. Narayan, W. J. Wedemeyer and H.A. Scheraga – Structural determinants of oxidative folding in proteins, Proc. Natl. Acad. Sci., U.S.A., 98, 2312-2316 (2001).

1063. J. Pillardy, C. Czaplewski, A. Liwo, J. Lee, D.R. Ripoll, R. Kazmierkiewicz, S. Oldziej, W. J. Wedemeyer, K.D. Gibson, Y.A. Arnautova, J. Saunders, Y.-J. Ye and H.A. Scheraga – Recent improvements in prediction of protein structure by global optimization of a potential energy function, Proc. Natl. Acad. Sci., U.S.A., 98, 2329-2333 (2001).

1064. M. Narayan, E. Welker, and H.A. Scheraga – Development of a novel method to study the rate-determining step during protein regeneration: Application to the oxidative folding of RNase A at low temperature reveals BPTI-like kinetic traps, J. Am. Chem. Soc., 123, 2909-2910 (2001).

1065. E. Welker, W.J. Wedemeyer and H.A. Scheraga – A role for intermolecular disulfide bonds in prion diseases?, Proc. Natl. Acad. Sci., U.S.A., 98, 4334-4336 (2001).

1066. K.-H. Cho, Y.K. Kang, K.T. No and H.A. Scheraga – A fast method for calculating geometry-dependent net atomic charges, J. Phys. Chem., B105, 3624-3634 (2001).

1067. A. Cao, E. Welker and H.A. Scheraga – Effect of mutation of proline 93 on redox unfolding/folding of bovine pancreatic ribonuclease A, Biochemistry, 40, 8536-8541 (2001).

1068. A. Liwo, C. Czaplewski, J. Pillardy and H. A. Scheraga – Cumulant-based expressions for the multibody terms for the correlation between local and electrostatic interactions in the united-residue force field, J. Chem. Phys., 115, 2323-2347 (2001).

1069. J. Lee, D.R. Ripoll, C. Czaplewski, J. Pillardy, W.J. Wedemeyer and H.A. Scheraga – Optimization of parameters in macromolecular potential energy functions by conformational space annealing, J. Phys. Chem. B., 105, 7291-7298 (2001).

1070. J. Pillardy, C. Czaplewski, A. Liwo, W.J. Wedemeyer, J. Lee, D.R. Ripoll, P. Arłukowicz, S. Ołdziej, Y.A. Arnautova and H.A. Scheraga – Development of physics-based energy functions that predict medium-resolution structures for proteins of the α, β and α/β structural classes, J. Phys. Chem. B, 105, 7299-7311 (2001).

1071. E. Welker, W.J. Wedemeyer, M. Narayan and H.A. Scheraga – Coupling of conformational folding and disulfide-bond reactions in oxidative folding of proteins, Biochemistry, 40, 9059-9064 (2001).

1072. D.R. Ripoll and H.A. Scheraga – Global optimization in protein folding, Encyclopedia of Optimization, II, 310-325 (2001). Kluwer Academic Publishers.

1073. H.A. Scheraga, W.J. Wedemeyer and E. Welker – Bovine pancreatic ribonuclease A: Oxidative and conformational folding studies, Methods in Enzymology, Ed. A.W. Nicholson, Academic Press, San Diego, 341, 189-221 (2001).

1074. J. Pillardy, Y.A. Arnautova, C. Czaplewski, K.D. Gibson, and H.A. Scheraga – Conformation-family Monte Carlo: A new method for crystal structure prediction, Proc. Natl. Acad. Sci., U.S.A., 98, 12351-12356 (2001).

1075. L.C. Roisman, J. Piehler, J.-Y. Trosset, H.A. Scheraga and G. Schreiber – Structure of the interferon-receptor complex determined by distance constraints from double-mutant cycles and flexible docking, Proc. Natl. Acad. Sci., U.S.A., 98, 13231-13236 (2001).

1076. K. Saito, E. Welker and H.A. Scheraga – 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, 40, 15002-15008 (2001).

2002

1077. W.J. Wedemeyer and H.A. Scheraga – Protein folding: overview of pathways, Encyclopedia of Life Sciences, 15, 334-342 (2002), http://www.els.net. London: Nature Publishing Group. Also published as "Protein folding pathways", Encyclopedia of the Human Genome, 817-826 (2003).

1078. H.A. Scheraga, J. Pillardy, A. Liwo, J. Lee, C. Czaplewski, D.R. Ripoll, W.J. Wedemeyer and Y.A. Arnautova – Evolution of physics-based methodology for exploring the conformational energy landscape of proteins, J. Comput. Chem., 23, 28-34 (2002).

1079. J.A. Saunders, K.D. Gibson and H.A. Scheraga – Ab initio folding of multiple-chain proteins, Proc. Pacific Symposium on Biocomputing, 2002, Eds. R.B. Altman, A.K. Dunker, L. Hunter, K. Lauderdale and T.E. Klein, World Scientific Publ. Co., Singapore, (2002) pp. 601-612.

1080. L. K. Low, H.-C. Shin and H.A. Scheraga – Oxidative folding of bovine pancreatic ribonuclease A: Insight into the overall catalysis of the refolding pathway by phosphate, J. Protein Chem., 21, 19-27 (2002).

1081. C. Czaplewski, S. Rodziewicz,-Motowidło, A. Liwo, D.R. Ripoll, R.J. Wawak and H.A. Scheraga – Comment on "Anti-cooperativity in hydrophobic interactions: A simulation study of spatial dependence of three-body effects and beyond" by S. Shimizu and H.S. Chan, J. Chem. Phys., 116, 2665-2667 (2002).

1082. W.J. Wedemeyer, X. Xu, E. Welker and H.A. Scheraga – Conformational propensities of protein folding intermediates: Distribution of species in the 1S, 2S and 3S ensembles of the [C40A, C95A] mutant of bovine pancreatic ribonuclease A, Biochemistry, 41, 1483-1491 (2002).

1083. A. Liwo, P. Arlukowicz, C. Czaplewski, S. Ołdziej, J. Pillardy and H.A. Scheraga – A method for optimizing potential-energy functions by a hierarchical design of the potential-energy landscape: Application to the UNRES force field, Proc. Natl. Acad. Sci., U.S.A., 99, 1937-1942 (2002).

1084. W.J. Wedemeyer, C.A. Rohl and H.A. Scheraga – Exact solutions for chemical bond orientations from residual dipolar couplings, J. Biomolecular NMR, 22, 137-151 (2002).

1085. C. Czaplewski, D.R. Ripoll, A. Liwo, S. Rodziewicz-Motowidło, R.J. Wawak and H.A. Scheraga – Can cooperativity in hydrophobic association be reproduced correctly by implicit solvation models?, Intl. J. of Quantum Chem., 88, 41-55 (2002).

1086. R. Kazmierkiewicz, A. Liwo and H.A. Scheraga – Energy-based reconstruction of a protein backbone from its α-carbon trace by a Monte-Carlo method, J. Comput. Chem., 23, 715-723 (2002).

1087. B.P. English, E. Welker, M. Narayan and H.A. Scheraga – Development of a novel method to populate native disulfide-bonded intermediates for structural characterization of proteins: Implications for the mechanism of oxidative folding of RNase A, J. Am. Chem. Soc., 124, 4995-4999 (2002).

1088. H.-C. Shin, M.-C. Song and H.A. Scheraga – Effect of protein disulfide isomerase on the rate-determining steps of the folding of bovine pancreatic ribonuclease A, FEBS Letters, 521, 77-80 (2002).

1089. A. Ghosh, R. Elber and H.A. Scheraga – An atomically detailed study of the folding pathways of protein A with the stochastic difference equation, Proc. Natl. Acad. Sci., U.S.A., 99, 10394-10398 (2002).

1090. W.D.S. Motherwell, H.L. Ammon, J.D. Dunitz, A. Dzyabchenko, P. Erk, A. Gavezzotti, D.W.M. Hofmann, F.J.J. Leusen, J.P.M. Lommerse, W.T.M. Mooij, S.L. Price, H. Scheraga, B.Schweizer, M.U. Schmidt, B.P. van Eijck, P. Verwer, and D.E. Williams – Crystal structure prediction of small organic molecules: a second blind test, Acta Cryst. B58, 647-661 (2002).

1091. K.-H. Cho, K.T. No and H.A. Scheraga – A polarizable force field for water using an artificial neural network, J. Molec. Struc., 641, 77-91 (2002).

1092. E. Welker, L.D. Raymond, H.A. Scheraga and B. Caughey – Intramolecular versus intermolecular disulfide bonds in prion proteins, J. Biol. Chem., 277, 33477-33481 (2002).

1093. A. Navon, V. Ittah, H.A. Scheraga and E. Haas – Formation of the hydrophobic core of ribonuclease A through sequential coordinated conformational transitions, Biochemistry, 41, 14225-14231 (2002).

1094. W.J. Wedemeyer, E. Welker and H.A. Scheraga – Proline cis-trans isomerization and protein folding, Biochemistry, 41, 14637-14644 (2002).

1095. R.P. Carty, M.R. Pincus and H.A. Scheraga – Interactions that favor the native over the non-native disulfide bond among residues 58-72 in the oxidative folding of bovine pancreatic ribonuclease A, Biochemistry, 41, 14815-14819 (2002).

1096. J.A. Vila, D.R. Ripoll, H.A. Baldoni and H.A. Scheraga – Unblocked statistical-coil tetrapeptides and pentapeptides in aqueous solution: A theoretical study, J. Biomolecular NMR, 24, 245-262 (2002); Erratum, J. Biomolecular NMR, 25, 171 (2003).

1097. H.A. Scheraga, J.A. Vila and D.R. Ripoll – Helix-coil transitions re-visited, Biophys., Chem., 101-102, 255-265 (2002).

2003

1098. R. Kazmierkiewicz, A. Liwo and H.A. Scheraga – Addition of side chains to a known backbone with defined side-chain centroids, Biophys. Chem., 100, 261-280 (2003). Erratum: Biophys. Chem., 106, 91 (2003).

1099. A. Fernández and H.A. Scheraga – Insufficiently dehydrated hydrogen bonds as determinants for protein interactions, Proc. Natl. Acad. Sci., U.S.A., 100, 113-118 (2003).

1100. Y.A. Arnautova, J. Pillardy, C. Czaplewski and H.A. Scheraga – Global optimization-based method for deriving intermolecular potential parameters for crystals, J. Phys. Chem. B., 107, 712-723 (2003).

1101. V. Čeřovský, E. Welker and H.A. Scheraga – A convenient incorporation of conformationally constrained 5,5-dimethylproline into the ribonuclease A 89-124 sequence by condensation of synthetic peptide fragments, J. Peptide Res., 61, 140-151 (2003).

1102. J.A. Saunders and H.A. Scheraga – Ab initio structure prediction of two α-helical oligomers with a multiple-chain united residue force field and global search, Biopolymers, 68, 300-317 (2003).

1103. J.A. Saunders and H.A. Scheraga – Challenges in structure prediction of oligomeric proteins at the united-residue level: searching the multiple-chain energy landscape with CSA and CFMC, Biopolymers, 68, 318-332 (2003).

1104. M. Narayan, E. Welker and H.A. Scheraga – Native conformational tendencies in unfolded polypeptides: Development of a novel method to assess native conformational tendencies in the reduced form of multiple disulfide-bonded proteins, J. Am. Chem. Soc., 125, 2036-2037 (2003).

1105. M. Nanias, M. Chinchio, J. Pillardy, D.R. Ripoll and H.A. Scheraga – Packing helices in proteins by global optimization of a potential energy function, Proc. Natl. Acad. Sci., U.S.A., 100, 1706-1710 (2003).

1106. J.A. Vila, H.A. Baldoni, D.R. Ripoll and H.A. Scheraga – Unblocked statistical-coil tetrapeptides in aqueous solution: Quantum-chemical computation of the carbon-13 NMR chemical shifts, J. Biomolecular NMR, 26, 113-130 (2003).

1107. R. Bhat, W.J. Wedemeyer and H.A. Scheraga – Proline isomerization in bovine pancreatic ribonuclease A. 2. Folding conditions, Biochemistry, 42, 5722-5728 (2003).

1108. M. Narayan, E. Welker and H.A. Scheraga - Characterizing the Unstructured Intermediates in Oxidative Folding, Biochemistry, 42, 6947-6955 (2003).

1109. H.A. Scheraga – Paul J. Flory: The man who laid the foundations of modern polymer science, Resonance, 8, 2-5 (2003).

1110. Y.A. Arnautova, A. Jagielska, J. Pillardy and H.A. Scheraga – Derivation of a new force field for crystal-structure prediction using global optimization: nonbonded potential parameters for hydrocarbons and alcohols, J. Phys. Chem. B, 107, 7143-7154 (2003).

1111. A. Fernández, L.R. Scott and H.A. Scheraga – Amino-acid residues at protein-protein interfaces: Why is propensity so different from relative abundance?, J. Phys. Chem. B, 107, 9929-9932 (2003).

1112. M. Narayan, E. Welker, C. Wanjalla, G. Xu and H.A. Scheraga – Shifting the competition between the intramolecular reshuffling reaction and the direct oxidation reaction during the oxidative folding of kinetically trapped disulfide-insecure intermediates, Biochemistry, 42, 10783-10789 (2003).

1113. C. Czaplewski, S. Rodziewicz-Motowidło, M. Dabal, A. Liwo, D.R. Ripoll and H.A. Scheraga – Molecular simulation study of cooperativity in hydrophobic association: clusters of four hydrophobic particles, Biophys. Chem., 105, 339-359 (2003). Erratum: - Biophys. Chem., 111, 267- 271 (2004). Erratum: 111, 267-271 (2004).

1114. S. Ołdziej, U. Kozłowska, A. Liwo and H.A. Scheraga – Determination of the potentials of mean force for rotation about C^{α}-C^{α} virtual bonds in polypeptides from the ab initio energy surfaces of terminally-blocked glycine, alanine, and proline, J. Phys. Chem., A, 107, 8035-8046 (2003).

1115. H.-C. Shin, M. Narayan, M.-C. Song and H.A. Scheraga – Role of the [65-72] disulfide bond in oxidative folding of bovine pancreatic ribonuclease A, Biochemistry, 42, 11514-11519 (2003).

1116. G. Xu, M. Narayan, E. Welker and H. A. Scheraga – A novel method to determine thermal transition curves of disulfide-containing proteins and their structured folding intermediates, Biochem. Biophys. Res. Commun., 311, 514-517 (2003).

1117. H.A. Scheraga – Adaptations of Metropolis Monte Carlo for global optimization in treating fluids, crystals, and structures of peptides and proteins, in "The Monte Carlo Method in the Physical Sciences", Ed. J. E. Gubernatis, AIP Conference Proceedings, vol. 690, 309-317 (2003).

1118. K. Maksimiak, S. Rodziewicz-Motowidło, C. Czaplewski, A. Liwo and H.A. Scheraga – Molecular simulation study of the potentials of mean force for the interactions between models of like-charged and between charged and nonpolar amino acid side chains in water, J. Phys. Chem. B, 107, 13496-13504 (2003).

1119. M. Narayan, G. Xu, S.K. Schultz and H.A. Schreaga – Assessing the magnitude of folding forces along the oxidative folding pathway of multi-disulfide-containing proteins, J. Am. Chem. Soc., 125, 16184-16185 (2003).

1120. J.A. Vila, D.R. Ripoll and H.A. Scheraga – Atomically detailed folding simulation of the B domain of staphylococcal protein A from random structures, Proc. Natl. Acad. Sci., U.S.A., 100, 14812-14816 (2003).

2004

1121. C. Czaplewski, A. Liwo, J. Pillardy, S. Ołdziej and H.A. Scheraga – Improved conformational space annealing method to treat β-structure with the UNRES force-field and to enhance scalability of parallel implementation, Polymer, 45, 677-686 (2004).

1122. J.A. Vila, H.A. Baldoni, D.R. Ripoll, A. Ghosh and H.A. Scheraga – Polyproline II helix conformation in a proline-rich environment: A theoretical study, Biophys. J., 86, 731-742 (2004).

1123. C. Czaplewski, S. Ołdziej, A. Liwo and H.A. Scheraga – Prediction of the structures of proteins with the UNRES force field, including dynamic formation and breaking of disulfide bonds, Protein Engineering, Design & Selection, 17, 29-36 (2004).

1124. A. Dzyabchenko and H. A. Scheraga – Model for the crystal packing and conformational changes of biphenyl in incommensurate phase transitions, Acta Cryst. B, 60, 228-237 (2004).

1125. G.Xu, M. Narayan, E. Welker and H. A. Scheraga – Characterization of the fast – forming intermediate, des [30-75], in the reductive unfolding of onconase, Biochemistry, 43, 3246-3254 (2004).

1126. E. Welker, L. Hathaway and H. A. Scheraga – A new method for rapid characterization of the folding pathways of multidisulfide – containing proteins, J. Am. Chem. Soc., 126, 3720-3721 (2004).

1127. G. Xu, H. Zhai, M. Narayan, F.W. McLafferty and H.A. Scheraga – Simultaneous characterization of the reductive unfolding pathways of RNase B isoforms by top-down mass spectrometry, Chemistry & Biology, 11, 517-524 (2004).

1128. M. Narayan, G. Xu, D. R. Ripoll, H. Zhai, K. Breuker, C. Wanjalla, H. J. Leung, A. Navon, E. Welker, E. W. McLafferty and H. A. Scheraga – Dissimilarity in the reductive unfolding pathways of two ribonuclease homologues, J. Mol. Biol., 338, 795-809 (2004).

1129. Y. Kamikubo, R. De Guzman, G. Kroon, S. Curriden, J.G. Neels, M.J. Churchill, P. Dawson, S. Ołdiej, A. Jagielska, H. A. Scheraga, D.J. Loskutoff and H.J. Dyson – Disulfide bond arrangements in active forms of the somatomedin B domain of Human vitronectin, Biochemistry, 43, 6519-6534 (2004).

1130. D.R. Ripoll, J.A. Vila and H.A. Scheraga – Folding of the villin headpiece subdomain from random structures. Analysis of the charge distribution as a function of pH, J. Mol. Biol., 339, 915-925 (2004).

1131. A. Liwo, S. Ołdziej, C. Czaplewski, U. Kosłowska and H.A. Scheraga – Parameterization of backbone-electrostatic and multibody contributions to the UNRES force field for protein-structure prediction from *ab initio* energy surfaces of model systems, J. Phys. Chem., B108, 9421-9438 (2004).

1132. A Fernández, K. Rogale, R. Scott and H. A. Scheraga – Inhibitor design by wrapping packing defects in HIV-1 proteins, Proc. Natl. Acad. Sci., U.S.A., 101, 11640-11645 (2004).

1133. A. Jagielska, Y.A. Arnautova and H. A. Scheraga – Derivation of a new force field for crystal – structure prediction using global optimization: nonbonded potential parameters for amines, imidazoles, amides and carboxylic acids, J. Phys. Chem. B, 108, 12181-12196 (2004).

1134. J.H. Griffith and H.A. Scheraga – Statistical thermodynamics of aqueous solutions. I. Water structure, solutions with non-polar solutes, and hydrophobic interactions, J. Molec. Str., 682, 97-113 (2004).

1135. J.H. Griffith and H.A. Scheraga – Statistical thermodynamics of aqueous solutions. II. Alkali halides at infinite dilution, J. Molec. Str., 711, 33-48 (2004).

1136. M. Khalili, J.A. Saunders, A. Liwo, S. Ołdziej and H.A. Scheraga – A united residue force-field for calcium-protein interactions, Protein Science, 13, 2725-2735 (2004).

1137. J. A. Vila, H. A. Baldoni, D. R. Ripoll and H. A. Scheraga – Fast and accurate computation of the ^{13}C chemical shifts for an alanine-rich peptide, Proteins: Struct., Funct. & Bioinf., 57, 87-98 (2004).

1138. J.D. Dunitz and H.A. Scheraga – Exercises in prognostication: Crystal structures and protein folding, Proc. Natl. Acad. Sci., U.S.A., 101, 14309-14311 (2004).

1139. A. Liwo, P. Arłukowicz, S. Ołdziej, C. Czaplewski, M. Makowski, and H.A. Scheraga – Optimization of the UNRES force field by hierarchical design of the potential-energy landscape. 1. Tests of the approach using simple lattice protein models, J. Phys. Chem. B., 108, 16918-16933 (2004).

1140. S. Ołdziej, A. Liwo, C. Czaplewski, J. Pillardy, and H.A. Scheraga – Optimization of the UNRES force field by hierarchical design of the potential-energy landscape. 2. Off-lattice tests of the method with single proteins, J. Phys. Chem. B, 108, 16934-16949 (2004).

1141. S. Ołdziej, J. Lagiewka, A. Liwo, C Czaplewski, M. Chinchio, M. Nanias, and H.A. Scheraga – Optimization of the UNRES force field by hierarchical design of the potential-energy landscape. 3. Use of many proteins in optimization, J. Phys. Chem. B, 108, 16950-16959 (2004).

1142. S.-H. Jang, D.-K. Kang, S.-I. Chang, H.A. Scheraga and H.-C. Shin – High level production of bovine angiogenin in E. coli by an efficient refolding procedure, Biotechnology Letters, 26, 1501-1504 (2004).

1143. J.A. Vila, H.A. Baldoni and H.A. Scheraga – Position dependence of the ^{13}C chemical shifts of α-helical model peptides. Fingerprint of the 20 naturally occurring amino acids, Protein Science, 13, 2939-2948 (2004).

1144. H.A. Scheraga, A. Liwo, S. Ołdziej, C Czaplewski, J. Pillardy, D.R. Ripoll, J.A. Vila, R. Kazmierkiewicz, J.A. Saunders, Y.A. Arnautova, A. Jagielski, M. Chinchio and M. Nanias – The protein folding problem: Global optimization of force fields, Frontiers in Bioscience, 9, 3296-3323 (2004).

1145. R.F. Gahl, M. Narayan, G. Xu and H.A. Scheraga – Trimethylamine N-oxide modulates the reductive unfolding of onconase, Biochem. Biophys. Res. Commun., 325, 707-710 (2004).

1146. H.A. Scheraga – The thrombin-fibrinogen interaction, Biophys. Chem., 112, 117-130 (2004).

1147. E. Welker, K. Maki, M.C. Ramachandra Shastry, D. Juminaga, R. Bhat, H.A. Scheraga and H. Roder – Ultrarapid mixing experiments shed new light on the characteristics of the initial conformational ensemble during the folding of ribonuclease A, Proc. Natl. Acad. Sci., U.S.A., 101, 17681-17686 (2004).

2005

1148. H.J. Leung, G. Xu, M. Narayan and H.A. Scheraga – Impact of an easily reducible disulfide bond on the oxidative folding rate of multi-disulfide-containing proteins, J. Peptide Res., 65, 47-54 (2005).

1149. A. Liwo, M. Khalili and H.A. Scheraga – Ab initio simulations of protein-folding pathways by molecular dynamics with the united-residue model of polypeptide chains, Proc. Natl. Acad. Sci., U.S.A., 102, 2362-2367 (2005).

1150. J. Makowska, K. Bagińska, F. Kasprzykowski, J.A. Vila, A. Jagielska, A. Liwo, L. Chmurzyński and H.A. Scheraga – Interplay of charge distribution and conformation in peptides: Comparison of theory and experiment, Biopolymers, (Peptide Science), 80, 214-224 (2005).

1151. C. Czaplewski, A. Liwo, D.R. Ripoll and H.A. Scheraga – Molecular origin of anticooperativity in hydrophobic association, J. Phys. Chem. B, 109, 8108-8119 (2005).

1152. S. Ołdziej, C. Czaplewski, A. Liwo, M. Chinchio, M. Nanias, J.A. Vila, M. Khalili, Y.A. Arnautova, A. Jagielska, M. Makowski, H.D. Schafroth, R. Kaźmierkiewicz, D.R. Ripoll, J. Pillardy, J.A. Saunders, Y.K. Kang, K.D. Gibson and H.A. Scheraga – Physics-based protein-structure prediction using a hierarchical protocol based on the UNRES force field: assessment in two blind tests, Proc. Natl. Acad. Sci., U.S.A., 102, 7547-7552 (2005).

1153. D.R. Ripoll, J.A. Vila and H.A. Scheraga – On the orientation of the backbone dipoles in native folds, Proc. Natl. Acad. Sci., U.S.A., 102, 7559-7564 (2005).

1154. V. Čeřovský and H.A. Scheraga – Combined solid-phase/solution synthesis of large ribonuclease A C-terminal peptides containing a non-natural proline analog, J. Peptide Res., 65, 518-528 (2005).

1155. M. Khalili, A. Liwo, F. Rakowski, P. Grochowski and H.A. Scheraga – Molecular dynamics with the united-residue model of polypeptide chains. I. Lagrange equations of motion and tests of numerical stability in the microcanonical mode, J. Phys. Chem. B., 109, 13785-13797 (2005).

1156. M. Khalili, A. Liwo, A. Jagielska and H.A. Scheraga – Molecular dynamics with the united-residue model of polypeptide chains. II. Langevin and Berendsen-bath dynamics and tests on model α-helical systems, J. Phys. Chem. B, 109, 13798-13810 (2005).

1157. G. Xu, M. Narayan and H.A. Scheraga – The oxidative folding rate of bovine pancreatic ribonuclease is enhanced by a convalently attached oligosaccharide, Biochemistry, 44, 9817-9823 (2005).

1158. M. Nanias, M. Chinchio, S. Ołdziej, C. Czaplewski and H.A. Scheraga – Protein structure prediction with the UNRES force-field using Replica-Exchange Monte Carlo-with-Minimization; Comparison with MCM, CSA and CFMC, J. Comput. Chem., 26, 1472-1486 (2005).

1159. J.A. Vila, D.R. Ripoll, Y.A. Arnautova, Y.N. Vorobjev and H.A. Scheraga – Coupling between conformation and proton binding in proteins, Proteins: Structure, Function, and Bioinformatics, 61, 56-68 (2005).

1160. G.M. Day, W.D.S. Motherwell, H.L. Ammon, S.X.M. Boerrigter, R.G. Della Valle, E. Venuti, A. Dzyabchenko, J.D. Dunitz, B. Schweizer, B.P. van Eijck, P. Erk, J.C. Facelli, V.E. Bazterra, M.B. Ferrero, D.W.M. Hofmann, F.J.J. Leusen, C. Liang, C.C. Pantelides, P.G. Karamertzanis, S.L. Price, T.C. Lewis, H. Nowell, A. Torrisi, H.A. Scheraga, Y.A. Arnautova, M.U. Schmidt and P. Verwer – A third blind test of crystal structure prediction, Acta Cryst., B61, 511-527 (2005).

1161. C. Czaplewski, S. Kalinowski, A. Liwo and H. A. Scheraga – Comparison of two approaches to potential of mean force calculations of hydrophobic association: particle insertion and weighted histogram analysis method, Molecular Physics, 103, 3153-3167 (2005).

1162. C. Czaplewski, S. Kalinowski, A. Liwo, D.R. Ripoll and H.A. Scheraga – Reply to "Comment on 'Molecular origin of anticooperativity in hydrophobic association'", J. Phys. Chem. B, 109, 21222-21224 (2005).

2006

1163. M. Khalili, A. Liwo and H.A. Scheraga – Kinetic studies of folding of the B-domain of staphylococcal protein A with molecular dynamics and a united-residue (UNRES) model of polypeptide chains, J. Mol. Biol., 355, 536-547 (2006).

1164. H.A. Scheraga, A. Liwo, S. Ołdziej, C. Czaplewski, J. Pillardy, J. Lee, D.R. Ripoll, J.A. Vila, R. Kaźmierkiewicz, J.A. Saunders, Y.A. Arnautova, K.D. Gibson, A. Jagielska, M. Khalili, M. Chinchio, M. Nanias, Y.K. Kang, H.D. Schafroth, A. Ghosh, R. Elber and M. Makowski – The protein folding problem, in "New Algorithms for Macromolecular Simulation", Eds. B. Leimkuhler, C. Chipot, R. Elber, A. Laaksonen, A. Mark, T. Schlick, C. Schütte, R. Skeel, Lecture Notes in Computational Science and Engineering, Springer-Verlag, Berlin, 49, 89-100 (2006).

1165. G. Xu, M. Narayan, I. Kurinov, D.R. Ripoll, E. Welker, M. Khalili, S.E. Ealick and H.A. Scheraga – A localized specific interaction alters the unfolding pathways of structural homologues, J. Am. Chem. Soc., 128, 1204-1213 (2006). Presented at ASBMB meeting, San Francisco, April 2006.

1166. V. Zabrouskov, X. Han, E. Welker, H. Zhai, C. Lin, K. van Wijk, H.A. Scheraga and F.W. McLafferty – Stepwise deamidation of ribonuclease A at five sites determined by top down mass spectrometry, Biochemistry, 45, 987-992 (2006).

1167. J. Makowska, S. Rodziewicz-Motowidło, K. Baginska, J.A. Vila, A. Liwo, L. Chmurzynski and H.A. Scheraga – Polyproline II conformation is one of many local conformational states and is not an overall conformation of unfolded peptides and proteins, Proc. Natl. Acad. Sci., U.S.A., 103, 1744-1749 (2006).

1168. J. Makowska, K. Bagińska, M. Makowski, A. Jagielska, A. Liwo, F. Kasprzykowski, L. Chmurzyński and H.A. Scheraga – Assessment of two theoretical methods to estimate potentiometric-titration curves of peptides: comparison with experiment, J. Phys. Chem. B, 110, 4451-4458 (2006).

1169. Y.A. Arnautova, A. Jagielska and H.A. Scheraga – A new force field (ECEPP-05) for peptides, proteins and organic molecules, J. Phys. Chem. B., 110, 5025-5044 (2006).

1170. M. Nanias, C. Czaplewski and H.A. Scheraga – Replica exchange and multicanonical algorithms with the coarse-grained united-residue (UNRES) force field, J. Chem. and Theor. Comput., 2, 513-528 (2006).

1171. E. Welker, M. Narayan and H.A. Scheraga – Protein disulfide bonds, Encyclopedia Reference of Genomics and Proteomics in Molecular Medicine, 2, 1487-1490 (2006).

1172. H.J. Dyson, P.E. Wright and H.A. Scheraga – The role of hydrophobic interactions in initiation and propagation of protein folding, Proc. Natl. Acad. Sci., U.S.A., 103, 13057-13061 (2006).

1173. L. Pradeep, H.-C. Shin and H.A. Scheraga – Folding kinetics of a family of three structurally homologous proteins: A direct correlation with the number and isomerization states of their proline residues, FEBS LETT., in press.

1174. M. Chinchio, C. Czaplewski, S. Ołdziej and H.A. Scheraga – A hierarchical multiscale approach to protein structure prediction: Production of low-resolution packing arrangements of helices, and refinement of the best models with a united-residue force field, in "Multiscale Modeling and Simulation", eds. K. Dill and T. Schlick, in press.

1175. H.A. Scheraga, M. Khalili and A. Liwo – Protein folding dynamics: overview of molecular simulation techniques, Annual Rev. Phys. Chem., in press.

1176. A. Jagielska and H.A. Scheraga – Influence of temperature, friction, and random forces on folding of the B-domain of Staphylococcal Protein A. All-atom molecular dynamics in implicit solvent, J. Comput. Chem., submitted.

1177. M.E. Villegas, J.A. Vila and H.A. Scheraga – Effects of side-chain orientation on the ^{13}C chemical shifts of antiparallel β-sheet model peptides, J. Biomolec. NMR, submitted.

1178. H.A. Scheraga, A. Liwo, S. Ołdziej, C. Czaplewski, M. Khalili, J.A. Vila and D.R. Ripoll – The two aspects of the protein folding problem, Proc. of Conf. on Computational Biophysics to Systems Biology, in press.

1179. A. Liwo, M. Khalili, C. Czaplewski, S. Kalinowski, S. Ołdziej and H.A. Scheraga – Optimization of the united-residue UNRES force field for Langevin dynamics, Proc. of Conf. on Computational Biophysics to Systems Biology, in press.

1180. C. Czaplewski, S. Kalinowski, S. Ołdziej, A. Liwo and H.A. Scheraga – Multiplexed-replica exchange molecular dynamics with the UNRES force-field as an effective method for exploring the conformational energy landscape of proteins, Proc. of Conf. on Computational Biophysics to Systems Biology, in press.

1181. F. Rakowski, F. Grochowski, B. Lesyng, A. Liwo and H.A. Scheraga – Symplectic algorithms of molecular dynamics. An application to the united-residue model, Proc. of Conf. on Computational Biophysics to Systems Biology, in press.

1182. M. Makowski, A. Liwo, K. Maksimiak, J. Makowska, L. Chmurzyński and H.A. Scheraga – Simple physics-based analytical formulas for the potentials of mean force for the interaction of amino-acid side chains in water. Tests with simple spherical systems, Proc. of Conf. on Computational Biophysics to Systems Biology, in press.

1183. U. Kozlowska, K. Wachucik, A. Liwo and H.A. Scheraga – Determination of short-range potentials for physics-based protein-structure predictions, Proc. of Conf. on Computational Biophysics to Systems Biology, in press.

1184. J.A. Vila, ME. Villegas, H.A. Baldoni and H.A. Scheraga – Predicting $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ chemical shifts from protein structure, J. Am. Chem. Soc, submitted.

1185. A. Liwo, M. Khalili, C. Czaplewski, S. Kalinowski, S. Ołdziej, K. Wachucik and H.A. Scheraga – 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, J. Phys. Chem. B., submitted.

1186. F. Rakowski, P. Grochowski, B. Lesyng, A. Liwo and H.A. Scheraga – Implementation of a symplectic multiple-time-step molecular dynamics algorithm, based on the united-residue (UNRES) mesoscopic potential-energy function, J. Chem. Phys., submitted.

D:\back\backup\Publication list\PUBS - 08 28 06.doc