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Nota di contenuto	BioNMR in Drug Research; Contents; Preface; Foreword; List of Authors; List of Abbreviations; Part I: Basic Techniques; 1 Modern Methods for the Expression of Proteins in Isotopically Enriched Form; 1.1 Introduction; 1.2 Isotope-Labeled Proteins from Hydrolyzates of the

Green Alga Scenedesmus obliquus; 1.2.1 Production of Isotope-Labeled Algal Hydrolyzates; 1.2.2 Adaptation of the Protein Overproducer to the Algal Medium; 1.2.3 Preparation of Homogenously Isotope-Labeled Protein by Fermentation on Algal Media; 1.2.4 Amino Acid-Type Specific Labeling
1.2.5 Mass Spectrometric Analysis of the Labeled Amino Acids1.3 Selective Labeling Schemes; 1.3.1 Reverse-Labeling Schemes; 1.3.1.1 Selective Protonation of Methyl Groups in (2)H-Labeled Proteins; 1.3.1.2 Structure Determination of Selectively Methyl Protonated Proteins; 1.3.1.3 Introducting (1)H,(12)C Aromatic Residues into Otherwise (13)C Uniformly Labeled Proteins; 1.3.1.4 Backbone-Labeled Proteins; 1.3.2 Selective (13)C Methyl Group Labeling; 1.4 Intein-Based Protein Engineering for NMR Spectroscopy; 1.4.1 Segmental Labeling of Proteins
1.4.1.1 Intein-Mediated Protein Ligation (IPL)/Expressed Protein Ligation (EPL) using the IMPACT System1.4.1.2 Reconstitution of Split Inteins; 1.4.2 Stabilizing Proteins by Intein-Mediated Backbone Cyclization; 1.4.2.1 In vitro Cyclization of Proteins; 1.4.2.2 In vivo Cyclization; 1.4.2.3 Stability Enhancement by Backbone Cyclization; 1.5 Alternatives to E. coli Expression Systems; 1.5.1 Expression Vectors; 1.5.1.1 Halobacterium salinarum; 1.5.1.2 Saccharomyces cerevisiae; 1.5.1.3 Schizosaccharomyces pombe; 1.5.1.4 Pichia pastoris; 1.5.1.5 Baculovirus; 1.5.1.6 Transient Mammalian Expression
1.5.1.7 Stable Mammalian Expression1.5.1.8 Viral Vectors; 1.5.2 Comparison of Expression Systems; 1.5.3 Isotope Labeling and NMR; 1.5.4 Target Proteins; 1.6 The Use of Cell-Free Protein Expression for NMR Analysis; 1.6.1 The Cell-Free Protein Expression Systems RTS; 1.6.2 From PCR Product to (15)N-Labeled Protein; 1.6.3 Discussion and Outlook; 1.7 References; 2 Structure Calculation Using Automated Techniques; 2.1 Introduction; 2.2 Conformational Constraints for NMR Structure Calculations; 2.2.1 Constraints from Covalent Structure; 2.2.2 Steric Repulsion
2.2.3 Distance Constraints from Nuclear Overhauser Effects2.2.4 Hydrogen Bond Distance Constraints; 2.2.5 Torsion Angle Constraints from Chemical Shifts; 2.2.6 Torsion Angle Constraints from Scalar Coupling Constants; 2.2.7 Orientation Constraints; 2.3 Structure Calculation Algorithms; 2.3.1 Simulated Annealing by Molecular Dynamics Simulation in Cartesian Space; 2.3.2 Torsion Angle Dynamics; 2.4 Automated NOESY Assignment; 2.4.1 The NOESY Assignment Problem; 2.4.2 Semi-Automatic Methods; 2.4.3 General Principles of Automatic NOESY Assignment; 2.4.4 Requirements on Input Data
2.4.5 Overview of Algorithms

Sommario/riassunto

The vast progress made in the investigation of biomolecules using NMR has only recently been rewarded with the Nobel Prize for Kurt W?thrich. Edited by a former coworker of W?thrich, this book presents the theoretical background on NMR of biomolecules, plus the use of NMR techniques in determining the structures of proteins and nucleic acids. BioNMR spectroscopy offers a universal tool for examining the binding of an active substance to its target protein. Its use thereby benefits the rational development of drugs. This interaction can now be investigated in a hitherto unparalleled precisi