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Nota di contenuto	NMR of Biomolecules: Towards Mechanistic Systems Biology; Contents; Preface; List of Contributors; List of Abbreviations; Part One: Introduction; 1 NMR and its Place in Mechanistic Systems Biology; 2 Structure of Biomolecules: Fundamentals; 2.1 Structural Features of Proteins; 2.1.1 Introduction: From Primary to Quaternary Structure; 2.1.2 Geometrical and Conformational Properties; 2.1.2.1 Backbone Dihedral Angles; 2.1.2.2 Side-Chain Dihedral Angles; 2.1.3 Secondary Structure Elements in Proteins; 2.1.4 Prediction of Secondary Structure 2.1.5 Structural Motifs and Structural Domains - Combination of

Secondary Structural Elements and Structural Motifs 2.1.6 Types of Folds and their Classification; 2.1.6.1 Folds of the Class; 2.1.6.2 Folds in the Class; 2.1.6.3 Folds in the / Class; 2.1.6.4 Folds in the + Class; 2.1.7 Tertiary Structure; 2.1.8 Quaternary Structure; 2.2 Nucleic Acids; 2.2.1 Introduction; 2.2.1.1 Conformations; 2.2.2 DNA Structure; 2.2.2.1 B-DNA and Derivatives; 2.2.2.2 A-DNA; 2.2.2.3 Z-DNA; 2.2.2.4 Nonstandard DNA Structures; 2.2.2.4.1 Circular DNA; 2.2.2.4.2 Helical Junction; 2.2.2.4.3 Triple Helix; 2.2.2.4.4 i-Motif; 2.2.2.4.5 Quadruplex DNA; 2.2.3 RNA Structure; 2.2.3.1 Regular RNA Structure - A-Form Helices; 2.2.3.2 Mismatches, Bulges, and Unusual Base Pairing; 2.2.3.3 Reversal and Alteration of Strand Direction: Commonly Observed Loop and Turn Motifs; 2.2.3.3.1 U-Turn; 2.2.3.3.2 K-Turn; 2.2.3.3.3 C-Loop; 2.2.3.3.4 E-Loop; 2.2.3.4 Tetraloops and Tetraloop-Receptor Contact; 2.2.3.5 Higher-Order RNA Tertiary Structure Elements: Coaxial Stacking Motifs; 2.2.3.6 DNA-RNA Hybrids; 3 What Can be Learned About the Structure and Dynamics of Biomolecules from NMR; 3.1 Proteins Studied by NMR; 3.1.1 Why NMR Structures? 3.1.2 NMR Bundle; 3.1.3 Protein Dynamics; 3.1.4 Intermolecular Interactions Involving Proteins; 3.2 Nucleic Acids Studied by NMR; 3.2.1 Structure, Mobility, and Function; Part Two: Role of NMR in the Study of the Structure and Dynamics of Biomolecules; 4 Determination of Protein Structure and Dynamics; 4.1 Determination of Protein Structures; 4.1.1 Resonance Assignment; 4.2 NMR Restraints; 4.2.1 Distance Restraints; 4.2.2 Dihedral Angles; 4.2.3 Residual Dipolar Couplings; 4.3 Structure Calculations; 4.3.1 Traditional; 4.3.2 Automated NOESY Assignment; 4.3.3 Energy Refinement of Protein Structures; 4.3.4 Chemical Shift-Based Approaches for Protein Structure Determination; 4.4 Validation of Protein Structures; 4.4.1 Experimental Data; 4.4.2 Geometric Quality; 4.5 Protein Dynamics and NMR Observables; 4.5.1 NMR Observables Affected by Dynamics; 4.5.2 NMR Experiments to Measure Dynamics and their Interpretation; 4.6 Protocols; 4.6.1 Sample Labeling; 4.6.2 NMR Assignment; 4.6.3 Manual Collection of Restraints; 4.6.4 Structure Calculations; 4.6.5 Structure Refinement; 4.6.6 Chemical Shift-Based Structure Calculations; 4.6.7 Structure Validation; 4.6.8 Protein Dynamics

## Sommario/riassunto

NMR is one of the most powerful methods for imaging of biomolecules. This book is the ultimate NMR guide for researchers in the biomedical community and gives not only background and practical tips but also a forward looking view on the future of NMR in systems biology.