

Comparison of interproton distances in DNA models with nuclear Overhauser enhancement data

B. GOPALAKRISHNAN and MANJU BANSALS

Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560012, India

Abstract. The conformational flexibility inherent in the polynucleotide chain plays an important role in deciding its three-dimensional structure and enables it to undergo structural transitions in order to fulfil all its functions. Following certain stereochemical guidelines, both right and left handed double-helical models have been built in our laboratory and they are in reasonably good agreement with the fibre patterns for various polymorphous forms of DNA. Recently, nuclear magnetic resonance spectroscopy has become an important technique for studying the solution conformation and polymorphism of nucleic acids. Several workers have used ^1H nuclear magnetic resonance nuclear Overhauser enhancement measurements to estimate the interproton distances for the various DNA oligomers and compared them with the interproton distances for particular models of A and B form DNA. In some cases the solution conformation does not seem to fit either of these models. We have been studying various models for DNA with a view to exploring the full conformational space allowed for nucleic acid polymers. In this paper, the interproton distances calculated for the different stereochemically feasible models of DNA are presented and they are compared and correlated against those obtained from ^1H nuclear magnetic resonance nuclear Overhauser enhancement measurements of various nucleic acid oligomers.

Keywords. DNA models; interproton distances; nOe data.

Introduction

Based on theoretical conformational energy calculations and taking into account the experimentally observed values for the six backbone torsion angles as well as the glycosidic torsion angle, Sasisekharan *et al.* (1971) and Sundaralingam's group (Sakurai and Sundaralingam, 1971) had first examined the possible combinations which can lead to double helical structures with mononucleotide repeating units. Recent detailed calculations (Gupta *et al.*, 1982) reveal that there are only 8 distinctly different combinations which lead to the formation of duplex structures of both right and left handedness, designated as RU and LU helices. Of these 8 conformations 1 is sterically disallowed for a polynucleotide, 5 correspond to the *trans* conformation about both the O5'-C5' and C3'-O3' bonds while in the other 2 the torsion angle about the C3'-O3' bond is in the g^- conformation. In all the 7 sterically allowed helical domains, the glycosyl torsion angle χ falls in the anti region ($170^\circ < \chi < 260^\circ$) and hence both purines and pyrimidines can be accommodated in the RU and LU helices of these domains. Sasisekharan *et al.* (1981) have been able to obtain sterically acceptable models of both right and left handedness for the A, B and D forms of DNA. Recently Premilat and Albiser (1984), have proposed a left handed model for C-DNA which is very similar to the LU model for B-DNA, proposed in Sasisekharan *et al.* (1983). Models of both handedness give almost equally good agreement with the observed fibre diffraction pattern for their respective polymorphic forms and they have also been