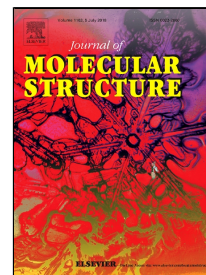


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Simplifying DNA NMR Spectroscopy by Silencing GH8 and AH8 Resonances

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Abstract

NMR studies of DNA oligonucleotides are limited by extensive resonance overlap and the availability of isotopically labeled samples. We have explored a nondestructive and economical method to simplify DNA NMR spectroscopy by exchanging the hydrogens of GH8 and AH8 with deuterons. Exchanging these hydrogens with deuterons results in spectral simplification and alleviates spectral overlap particularly for A and G rich sequences and is therefore uniquely suited for G-quadruplex sequences. The silencing of the GH8 and AH8 signals facilitates structural and ligand DNA binding studies.

1. Introduction

NMR spectroscopy is used for the structural characterization of a large range of samples, including biologically relevant macromolecules. Large molecules, however, present a challenge due to large number of resonances, resulting in extensive peak overlap within a limited chemical shift window. Labeling strategies and NMR experiments have therefore been developed to combat these challenges. RNA is generally labeled by *in vitro* transcription reactions using isotopically labeled triphosphates [1-4]. Isotopic labeling of DNA is less common; for a recent comprehensive review see Nelissen *et al* [5]. Although enzymatic methods for DNA labeling have been described, they have not yet been widely used [6-9]. Most DNA labeling is instead carried out using solid phase synthesis with commercially available phosphoramidites [1,5]. The high cost of the isotopically labeled phosphoramidites in conjunction with the large excess of reactants needed for solid phase conditions, have curtailed their use.

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