PS04.04.11 DAUNOMYCIN INDUCES DEGLYCOSYLATION OF DNA: STRUCTURE OF d(CG[glucose-T]ACG)-DAUNOMYCIN COMPLEX. YiGui Gao, Howard Robinson, +Jacques H. van Boom, Andrew H.-J. Wang, Biophysics Division & Dept. of Cell & Structural Biology, University of Illinois at Urbana-Champaign, Urbana, IL 61801 USA, +Leiden Institute of Chemistry, Gorlaeus Laboratory, 2300 RA Leiden, The Netherlands

DNA from certain organisms contains unusually-modified DNA bases. For example, glycosylated-T or C at C5 position of the base is found in *Trypanosoma Brucei*. The role of those modified bases remains largely unknown, although in trypanosome they are believed to be involved in the regulation of gene expression. Ethidium bromide, an intercalator, has been shown to have an cytotoxic effect towards trypanosomes.

We have undertaken a structural study in which intercalator anticancer drug daunomycin was added to the modified DNA hexamer d(CG[glucose-T]ACG). The solution structure of the hexamer was determined by NMR. In addition, the three-dimensional molecular and crystal structure of the complex of daunomycin and the hexamer was determined at 1.7Å by X-ray diffraction analyses. Crystal data: *P1*, $a = 18.63$ Å, $b = 20.01$ Å, $c = 26.54$ Å, $\alpha = 69.30°$, $\beta = 90.31°$, $\gamma = 108.16°$, R=17.9%, 3385 reflections at 2σ. Two daunomycin molecules bind to the DNA double helix. Unexpectedly we found that in the crystal structure one the glucose moieties is missing from the DNA. The biological implication of this will be addressed.

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PS04.04.12 SURVEYING AND CLASSIFYING NUCLEIC ACID STRUCTURES. Anke Gelbin, Les Clowney, Shu-Hsin Hsieh, Christine Zardecki, John Westbrook and Helen M. Berman, Department of Chemistry, Rutgers University, Piscataway NJ 08855.

Nucleic acids are highly flexible molecules that can assume a wide variety of shapes. A major challenge is to be able to relate the sequence and experimental conditions to the conformations. There are now over 400 structures of nucleic acid-containing crystals stored in the Nucleic Acid Database archive. The variety of ways in which these molecules can be classified yield different types of information that can be used to help relate the structures to their sequences and other properties. The tools that have been developed for classification and analysis, as well as some structure survey results, will be presented.

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PS04.04.13 POLYPURINE TRACT DNA SEQUENCE, CAAAGAAAAG CONTAINING 2 MOLECULES IN ASYMMETRIC UNIT. IS THE 2ND HELIX DISORDERED? Gye Won Han, Mary L. Kopka, David S. Goodsell and Richard E. Dickerson, Molecular Biology Institute, Department of Chemistry and Biochemistry, University of California at Los Angeles, CA 90095, USA

The DNA duplex decamer CAAAGAAAAG : CTTTTCTTTG was synthesized and crystallized to explore the structure of the polypurine tract of HIV-1. Although the polypurine tract consists of 16 purines, initially a 10-mer was used because of stacking considerations. A 15-mer also was synthesized for crystallization. This sequence is highly conserved in HIV, thus making an attractive target for drug design.

The native crystal is monoclinic in space group C2 with 2 helices (A and B) in asymmetric unit. Cell dimensions are a=59.82 Å, b=28.28 Å, c=72.49 Å and β=103.9°. X-ray data were collected using RAXIS-II at -180°C up to 1.85 Å resolution.

Using single isomorphous replacement methods with CAAAGAAAAG : $CTU_{Br}TTCTTTG$ gives only one Br site in difference Patterson map, and this is consistent with the molecular replacement result where a clear hydration spine appeared in helix A, but not in the 2nd helix.

Diffusion of cisplatin (cis-dichlorodiamino platinum (II)) into the native crystal once again gives only one Pt site in helix A in the Difference Fourier map using SIR_{Br} phases. We believe the 2nd helix may be disordered and in order to improve the phases, a second derivative CAAAGAAAAG : $CTTTTC_{Br}TTTG$ for MIR method will be used.

PS04.04.14 POTENTIALLY RIGHT HANDED SEQUENCE CRYSTALLIZES AS LEFT HANDED DNA: THE CRYSTAL STRUCTURE OF d(CCCGGG). P. Karthe[1], S. Krishnaswamy[2] & N. Gautham[1], [1]Department of Crystallography & Biophysics, University of Madras, Guindy Campus, Madras 600 025, India; [2]Bioinformatics Centre, School of Biotechnology, Madurai Kamaraj University, Madurai - 625 021, India

The DNA duplex d(CCCGGG).d(CCCGGG) has only one alternating pyrimidine- purine base step. Despite this, it crystallizes as a left handed helix and packs into a orthorhombic unit cell with a=17.76, b=30.92, c=43.92 Å, similar to the one observed previously for Z DNA hexamers. Moreover, the structure exhibits several remarkable features that are not hitherto observed in left handed Z DNA. The most stricking of these is that the successive base pairs with in the central tetranucleotide show uniform values of twist and rise, resulting in a novel uniform left handed DNA double helix. This structure thus demonstrates that DNA can take up a left handed conformation in the absence of stretches of alternating pyrimidine-purine sequences, and also that like right handed DNA, left handed DNA too can exist in polymorphic forms.

PS04.04.15 A NOVEL [G-(G.C)] BASE-TRIPLET: MODEL FOR BASE PAIR RECOGNITION DURING HOMOLOGOUS RECOMBINATION. Blaine H. M. Mooers & P. Shing Ho, Dept. of Biochemistry & Biophysics, Oregon State Univ., Corvallis, OR 97331

In the crystal structure of the nonamer d(GCGTACGCG), the 3'-terminal guanine forms a base-triplet in the minor groove of B-DNA that is consistent with recent biochemical evidence about the structure of RecA-DNA triplex complexes. During homologous recombination, RecA protein polymerizes on single-stranded DNA, and the resulting nucleoprotein filament incorporates a homologous region of double-stranded DNA into a RecA protein coated DNA triplex, otherwise known as "R-DNA". R-DNA has an extended and unwound conformation. The third strand in this enzymatically formed triplex is parallel to the homologous strand in the Watson-Crick duplex, and it has been generally thought to lie in the major groove of the DNA duplex. However, a recent study by Baliga et al., Proc. Natl. Acad. Sci., USA, 92, 10393-10397 (1995), indicates that the third DNA strand lies in the minor groove of the parent duplex. None of the available structures for DNA triplets, however, provide a model for how the third strand can recognize the homologous duplex in the minor groove. We present the 2.5 Angstrom structure of a base-triplet which has features common to R-DNA in that the third base sits in the minor groove parallel to the homologous strand in the Watson-Crick duplex. In the crystal lattice, the first eight nucleotides of the nonamer sequence form a standard B-DNA duplex with a complimentary strand. These duplexes stack end-to-end but fail to form continuous helices because the terminal base pairs of adjacent stacks are underwound with respect to each other. This underwinding places