Structural and dynamic properties of DNA : implications for forming nucleosome

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B-DNA flexibility, crucial for DNA-protein interaction, is sequence dependent. In principle, free DNA in solution is the best reference to uncover the relation between base sequence and the intrinsic flexibility of the molecule. This relationship was investigated by collecting a large dataset of NMR ^{31}P chemical shifts in solution, taking advantage of the DNA intrinsic mechanics that tightly associates the phosphate group motion to helicoidal descriptors of the curvature, winding and groove dimensions. Our approach provides an experimental scale, called TRX, free from dependence on any structural model, that quantifies the intrinsic flexibility of the ten complementary DNA dinucleotide steps in terms of Twist, Roll, and X-disp (base pair displacement).
The TRX scale enables, first, to rationalize the dinucleotide position frequencies found in both artificial or natural nucleosomal DNA sequences *in vitro*. Then, applying the TRX scale to DNA sequences optimized for nucleosome formation reveals that a 10 base-pair periodic alternation of stiff and flexible regions, each of minimal length of 4bp, characterizes the optimal nucleosomal sequences. Preliminary NMR studies of a series of oligomers related to the 601 sequence confirm that the DNA flexibility captured by the TRX scale is relevant to nucleosome formation. In sum, our results provide new insights on the properties of nucleosomal sequences, emphasizing the role the intrinsic, sequence dependent, flexibility of the DNA molecule in the histone core-DNA complex formation.

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