A Theoretical Model to Predict Intrinsic and Induced Superstructures of DNAs and Some Relevant Thermodynamic Properties from the Sequence

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The substantial conformational homogeneity of DNA double helix has recently allowed a good progress in the knowledge of the molecular mechanisms which control the functional organization of the genome as well as in the prediction of some biologically relevant structural properties. We developed an analytical method to study the effects of the sequence on modeling the three-dimensional superstructure of DNA based on the theoretically evaluated slight conformational perturbations of the different dinucleotide steps along the sequence. Such a model is capable of predicting in striking agreement with the experimental data: the atomic force microscopy visualization of relevant DNA tracts and in particular the dynamics of a pBR322 plasmide after the mechanical cut of the cycle; the gel electrophoresis anomalies of a very large pull of DNA tracts; the thermodynamic constants of the sequence dependent circularization reactions of many DNAs ranging from 100 to 100000 bp and the sequence dependent writhing transitions from relaxed to supercoiled circular forms also in the presence of DNA binding proteins; and finally, the nucleosome positions and the corresponding thermodynamic stability of more than 50 DNA tracts whose the nucleosome competitive reconstitution experimental data are available. The thermodynamic properties were obtained using an original statistical mechanic approach based on the first order elasticity which allows an analytical solution in Fourier space.

Selected references

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