# *The effect of sequence on the conformation and dynamics of B-DNA and its bound cations*

Marco PASI [1], John MADDOCKS [2], Richard LAVERY [1]
[1] *IBCP, Université Claude Bernard - Lyon I (UCBL), CNRS, France*
[2] *Ecole Polytechnique Fédérale de Lausanne Département de Mathématiques, Lausanne, Switzerland*

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DNA carries out its function in the cell by interacting with proteins, which recognise their target sites in the genome both by "reading" the sequence and by probing the deformability of DNA; these interactions are fundamental in many important cellular processes, including DNA replication, genome organization and transcription regulation. The sequence dependence of the mechanical properties of DNA is at the basis of these "indirect recognition" processes. Understanding this second layer of genetic information requires extensive structural and dynamical knowledge of B-DNA, which is currently unavailable from experiment.
We analysed a large database of microsecond-scale MD simulations of a set of B-DNA oligomers with sequences designed to allow the comprehensive study of base-sequence effects, resulting from the collaborative effort of an international consortium of laboratories.
Statistical analysis of the trajectories allowed us to identify local B-DNA conformational substates, to exhaustively assess the sequence-dependent variations in the relative population of the substates and link these variations to the formation of specific interactions within the double helix.
Furthermore, thanks to the recently developed curvilinear helicoidal coordinate analysis of ion distributions around DNA, we were able to shed light on the sequence-dependent variability of cation densities, and how this variability couples to the conformational fluctuations of the double helix.