
DNA and its environment: a close look at ion binding

Richard Lavery^{*1}, Marco Pasi , Pablo Dans , Modesto Orozco , Krystyna Zakrzewska ,
and John Maddocks

¹Bases Moléculaires et Structurales des Systèmes Infectieux (BMSI) – CNRS : UMR5086 – IBCP, 7
passage du Vercors, 69367 Lyon, France

Abstract

Molecular dynamics simulations of DNA now easily reach the microsecond timescale and reflect the fact that DNA undergoes very significant thermal fluctuations at room temperature. These fluctuations make it difficult to follow what is happening in solution close to the solute molecule. To overcome this problem, we have recently developed an analysis technique using the instantaneous helical axis of the nucleic acid to convert ion or water positions into curvilinear helicoidal coordinates. This approach enables us to calculate ion populations and local ion molarities in well defined regions around DNA. The results of this analysis show that monovalent ions bind very selectively to DNA, in some cases with surprisingly high occupancies and with sequence selectivity which extends beyond base pairs or base pair steps. We have used this technique to show that ions are capable of triggering conformational changes in DNA and it seems likely that they can play a significant role in recognition processes.

^{*}Speaker