EuroSciCon

10th Edition of International Conference on

Structural Biology

March 15-16 2018
Barcelona, Spain

B. Montgomery Pettitt, Biochem Mol biol J, Volume 4
DOI: 10.21767/2471-8084-C1-007

DNA CONFINED: COMPARISON OF SIMULATION AND CRYO-EM

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The elastic properties of DNA molecules are sensitive to environment. DNA is often double stranded and occasionally knotted but must open to for replication, repair, transcription and recombination. On opening the elastic persistence length changes by over two orders of magnitude. The interface between surfaces or proteins and nucleic acids changes the properties of DNA. Interfaces offer large electrostatic fields and density gradients changing the local free energy surface and therefore form a challenging set of problems in current design issues. We consider examples of both DNA minicircles used as artificial vectors and phage packing. Our models describe aspects of sequence and target length dependence important in protein recognition.

Biography

B. Montgomery Pettitt is Robert A. Welch Distinguished University Chair of Chemistry at the University of Texas Medical Branch. He was a postdoctoral fellow at the University of Texas at Austin and an NIH Fellow at Harvard University. His research focuses on understanding molecular recognition of biopolymers in solution. Molecular recognition be it intermolecular between two species or intramolecular such as folding, underlies the mechanisms of biochemistry. This theoretical work relies on techniques in statistical mechanics and high performance scientific computing.

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