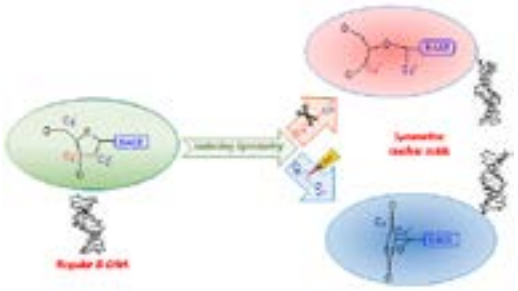
Pradeep Pant et al., J Proteomics Bioinform 2017, 10:8(Suppl)
DOI: 10.4172/0974-276X-C1-0101

Design and characterization of symmetric nucleic acids *via* molecular dynamics simulations

Pradeep Pant and **B Jayaram**
Indian Institute of Technology Delhi, India

Directionality (5'→3') is so fundamental to the nucleic acid architecture and is essential for replication and transcription. We observed that this asymmetry can be manipulated either by breaking (C3' to C2') or making (C5' to C2') chemical bond in each nucleotide unit leading to symmetric nucleic acids. Keeping their potential synthetic and therapeutic interest in mind, we designed a few novel symmetric nucleic acids. We investigated their conformational stability and flexibility *via* detailed all atom explicit solvent 100-ns long molecular dynamics simulations and compared the resulting structures with that of regular B-DNA. Quite interestingly, some of the symmetric nucleic acids retain the overall double helical structure indicating their potential for integration in physiological DNA without causing major structural perturbations.



Biography

Pradeep Pant has done his Master's in Chemistry from Indian Institute of Technology Delhi. He joined in the Department of Chemistry as a PhD scholar under the supervision of Prof. B. Jayaram in 2014. Currently, he is focusing on theoretical studies on the structure, dynamics and energetics of nucleic acid-protein/ligand interactions.

pradeep.pant25@gmail.com

Notes: