Brownian Dynamics Simulations of Linker Histone - Nucleosome Binding

Mehmet Ali Öztürk [1,2] , Rebecca C. Wade[1]

1- Molecular and Cellular Modeling Group, Heidelberg Institute for Theoretical Studies (HITS), Heidelberg, 69118, Germany

2- The Hartmut Hoffmann-Berling International Graduate School of Molecular and Cellular Biology (HBIGS), Heidelberg University, Heidelberg, 69120, Germany

Abstract:

The binding of linker histone (LH) proteins to nucleosomes plays an important role in chromatin compaction and regulation of transcription. Currently, the sequence determinants of the binding site, orientation and dynamics of different LHs to nucleosomes are not well understood. In this study, Brownian dynamics (BD) simulations were performed to simulate the association of the globular domains of H1 and H5 LH wild-type and mutant proteins with a 167 bp nucleosome, including two flanking 10 bp long linker-DNAs. Diffusional encounter complexes were obtained and the results were compared for the LHs and their mutants. The results give insights into important interactions that determine LH-nucleosome binding.