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Essential Dynamics of DNA-Antibody Complexes

Akberova N., Zhmurov A., Nevzorova T., Litvinov R.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2016, Springer Science+Business Media New York.Antibodies against double-stranded DNA play an important role in the pathogenesis of autoimmune diseases. Structural analysis of antibody-DNA complexes contributes to our understanding of the role of DNA-containing immune complexes in human pathologies and may help in designing novel treatments. In this paper, we study dynamics of the full-atomic structure of the molecular complexes formed by an antibody Fab fragment with double-stranded DNA, containing or not containing a thymine dimer. Molecular dynamics simulations are used in conjunction with the Principle Component Analysis technique. We found that removing a covalent bond from the thymine dimer results in changes of the structural dynamics of the light and heavy chains of Fab as well as in the DNA strands. A significant increase in mobility of the Fab light chain was observed throughout the entire simulation runs with a higher amplitude of fluctuations at the interface with DNA. Essential dynamics analysis of simulation trajectories of the antibody-dsDNA complexes shows that fluctuations in the low-frequency eigenvectors are localized at the ends of the DNA sequences, suggesting that these bending motions are important for the DNA-antibody interactions.

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Keywords

Anti-DNA antibody, dsDNA, Immune complex, Molecular dynamics simulation, Principal component analysis, Thymine dimer