DNA-binding bacterial histone-like (HU) proteins are small (molecular weight of a single monomer is about 10 kDa) positively charged dimeric proteins that belong to the nucleoid-associated protein family and are involved in the maintenance of genomic DNA compaction of prokaryotes. HU proteins are present in all bacteria and regulate a variety of DNA-dependent processes, including replication, transcription, recombination, repair and adaptation. The principal possibility of using HU proteins as a target for pharmacological intervention for disorders of nucleoid structure and viability of pathogenic bacteria including mycoplasma M. tuberculosis are shown. In the present study we selected the bacterial expression conditions for two isotope-labeled recombinant HU proteins from mycoplasmas S. melliferum (HUSpm) and M. gallisepticum (HUMgal), as well as optimal experimental conditions for structural-dynamic studies of the free proteins and their complexes with DNA by nuclear magnetic resonance spectroscopy (NMR). As a result, using comparative modeling and MD simulations with distance and dihedral angle constraints derived from crystallography and triple-resonance NMR data for the 13C/15N-labelled recombinant proteins we obtained the all-atom models of HUMgal and HUSpm and described their backbone flexibility. It has been shown that with the addition of a DNA duplex JrA25/JrD22 conformation and dynamics of HU proteins undergo changes, indicating the formation of a functional complex. This work was supported by the Russian Science Foundation: Grant 15-14-00063.

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