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PUTATIVE G-PENTAPLEX IN DNA OF PATHOGENS IS PREDICTED WITH ALPHAFOLD 3 AI

Background. G-quadruplexes (G4s) are non-canonical secondary structures consisting of two or more planar G-tetrads formed by four guanidines and stabilized by Hoogsteen hydrogen bonds, stacking and coordination ion interactions. Currently, the formation of G-pentaplexes (G5s) has only been determined for structures in which guanidine is replaced by its isomer, isoguanidine [1]. **The aim** was the determination of putative G4s from two tetrads in the genome of bovine mycobacteria. **Methods.** QGRS Mapper software was used for search of G-rich motifs in DNA sense and antisense strands of *M. bovis* AF2122/97 reference strain [2]. 3D models G4s and G5 were generated by AlphaFold 3 AI (AF3) with 10 K⁺ ions [3]. **Results.** 4345 putative G4s in sense strand and 4649 G4s from two tetrads were identified in antisense DNA strand of the AF2122/97 *M. bovis* reference strain which were characterized by typical parameters for such G4s with loop from 1 to 3 nt, namely, a G-score was varied from 19 to 21, length from 11 to 17 nt. During the analysis of mentioned G4s, attention was drawn to a G-rich palindrome with length of 14 nt, for which 16 repeats in the sense and 6 repeats in the antisense strand were found. 3D model of this aptamer represents G5 which is formed by two planar G-pentads stabilized by 11 and 7 hydrogen bonds, respectively, as well as stacking and two coordination ions K⁺, unlike G4, in which one K⁺ ion is localized between two tetrads. Putative G5 was identified in the sense and antisense DNA strands of CDC1551 of *M. tuberculosis*, 1331 Danish *M. bovis* BCG applied for vaccination in Ukraine, PA14 *Pseudomonas aeruginosa* strains. **Conclusions.** Putative G5 formed by two pentads was identified in the sense and antisense strands of *M. bovis* and predicted by AF3 with high reliability (pLDDT>90). It is localized in the genes encoding *pe-pgrs* and *ppe* families proteins which are crucial for the host-pathogen interactions, immune modulation, suppression host's immune defense. **Grant.** 35.00.03.02 from NAAS of Ukraine.

Keywords: G-pentaplex, G-quadruplex, *Mycobacterium bovis*, AlphaFold 3, *Pseudomonas aeruginosa*, *Mycobacterium tuberculosis*.

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