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PUTATIVE G-QUADRUPLEXES IN GENES ENCODING HYDROGEN SULFIDE BIOSYNTHESIS ENZYMES OF MYCOBACTERIUM BOVIS

Background. Bacteria synthesize H₂S by enzymes of defense system orthologous to mammalian cystathionine-γ-lyase (CSE), cystathionine-β-synthase (CBS) or 3-mercaptopyruvate sulfurtransferase (3MST). Genetic disruption of H₂S biogenesis increases bacterial sensitivity to drugs, and enzymes of defense system may be targets for H₂S biosynthesis inhibition. **The aim** of the present study was the determining putative G-quadruplexes (G4s) formed by two G-tetrads in promoters and genes of *M. bovis* defense system encoding enzymes of H₂S biosynthesis. **Methods.** QGRS Mapper software was used for search of G4s motifs and determination of their G-scores in DNA sense and antisense strands of *M. bovis* AF2122/97 reference strain [1]. 3D models G4s were predicted with AlphaFold 3 AI (AF3) [2]. **Results.** A search of G4s in promoters and genes encoding H₂S biosynthesis enzymes of the reference strain *M. bovis* AF2122/97 with subsequent their estimation and confirmation by 3D modeling was performed. Promoter regions and genes (i) *cbs* encoding CBS, (ii) *cds1* (Rv3684) encoding cysteine desulfhydrase, (iii) *metB* (Rv1079) encoding cystathionine gamma-synthase, (iv) *sseA* encoding 3MST were analyzed for the G4s presence. In the *cbs* gene, four G4s with length of 11–14 nucleotides (nt) were found and characterized by a G-score from 19 to 21. Their 3D models were confirmed by AF3 with a parameter indicating the quality of the prediction: from 70> pLDDT>50 to pLDDT>90. In the *cds1* (Rv3684) gene, two G4s with length of 17 nt (G-score = 18, 90>pLDDT>70) and 11 nt (G-score = 21, pLDDT>90) were found. In the promoter of the *metB* gene (Rv1079), G4 with length of 14 nt was found (G-score = 19, 90>pLDDT>70 – pLDDT>90). In the promoter of the *sseA* gene, two G4s (15 nt, G-score = 20, pLDDT>90) were identified. **Conclusions.** Putative G-quadruplexes of two tetrads were identified in the genes and promoters of genes encoding enzymes of the *M. bovis* defense system of hydrogen sulfide synthesis. Their structures were confirmed by AF3 with high reliability (pLDDT>90). Determined G4s in the gene promoter regions may be targets for the H₂S synthesis inhibition. **Grants.** 35.00.03.02 from NAAS of Ukraine.

Keywords: G-quadruplex, hydrogen sulfide, *Mycobacterium bovis*, AlphaFold 3.

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