Construction of a three-dimensional structural model for tRNA methyltransferase

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Three-dimensional structures of proteins are essential for understanding their functions. X-ray crystallography and NMR spectroscopy are widely used experimental methods for structure determination of proteins. However, there is a large gap between the overwhelming number of available protein sequences and experimentally determined protein structures. Homology modeling plays a central role in fulfilling the above gap by determining protein structures. Here, we modeled a three-dimensional structure of tRNA (guanine-N1-)-methyltransferase in *Mycobacterium tuberculosis* (tGN1Mtase). It consists of 230 amino acids. The function of this protein is processing of the primary tRNA transcript to yield a functional tRNA.

The computer programs such as BLAST, CLASTALW, O, SOD, MOLMAN, LSQMAN were used as tools. The crystal structure of putative tRNA (guanine-7-)-methyltransferase (trmD) was used as the template for modeling, which shows 45 % sequence identity with tGN1Mtase. Then the amino acid sequences of the target and the template were aligned using CLASTALW, thereby identified the insertions and deletions. Final structural model is built using the programs O, SOD, MOLMAN, LSQMAN from Uppsala Software Factory.

The modeled structure of tGN1Mtase mainly consists of two domains. The domain-I, the catalytic domain, contains five α-helices and four parallel β-strands forming a sheet. The α-helices are wrapped around in both sides of the beta sheet. The domain-II contains only two α-helices, which are linked by a

flexible loop. For the best of our knowledge, this is the first structural model of tGN1Mtase. This will be highly useful for biochemists for further studies of this protein.

Key words: *tGN1Mtase, tRNA (guanine-N1-)-methyltransferase, 3D-structural model*

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