Homology model of 30S ribosomal subunit from *Mycobacteria tuberculosis*

University of Nairobi

Mathenge Peterson Gitonga

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Center for Biotechnology and Bioinformatics

University of Nairobi

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ABSTRACT

Mycobacterium tuberculosis, the causative agent of the tuberculosis, has infected more than a third of the world population to date. It has been known to be a very aggressive bacterium that is highly resistant to current drugs that target Tuberculosis. Antibiotics such as viomycin and capreomycin have been shown to bind to functionally important regions of the bacterial ribosome inhibiting protein synthesis process thereby affecting the bacterial cells viability. It is hypothesized that, a three dimensional structure of the 30S ribosomal subunit of the bacterium, will bring about a novel approach on drug target, and will be important in the development of a new class of anti-bacterial compounds. It will provide a structural scaffold on which structure based drug design studies can be performed. *In silico* screening of ligands can be carried out to identify compounds that show binding potential on ribosome, ribosomal RNA (16S rRNA) or the ribosomal proteins. Since current methods for obtaining three dimensional structures of the macromolecules are slow and tedious, we demonstrate a faster and inexpensive way of generating structural models *in silico* by employing both *de novo* and homology modeling methods

In this thesis, we report modeling of the three dimensional structure of the 30S ribosomal subunit from *Mycobacteria tuberculosis* through the structure prediction methods mentioned above. We report a high resolution ribosomal structure comparable in quality to experimentally determined crystal structures. It is hypothesized that, the structure will bring about a novel approach on drug target, and will be important in the development of a new class of anti-bacterial compounds. It will provide a structural scaffold on which structure based drug design studies can be performed. *In silico* screening of ligands can be carried out to identify compounds that show binding potential on ribosome, ribosomal RNA (16S rRNA) or the ribosomal proteins. Compounds identified this way can be further studied for antibacterial activity. We hypothesize that the generation of the 30S ribosomal subunit from *Mycobacteria Tuberculosis* will provide a structural scaffold that will allow *In-silico* structure based drug design