Simulation Model of the Mitochondrial Ribosome

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Introduction

Mitochondrial Ribosomes

Mitochondrial ribosomes (mitoribosomes) are biomacromolecular complexes composed of mitochondrial rRNAs and proteins. As their name suggests, they are located within the mitochondrion and perform a function analogous to cytosolic ribosomes - facilitating mitochondrial translation, where mitochondrial mRNA is translated into proteins. These mitochondrial proteins are co-translationally integrated into the inner mitochondrial membrane, where they constitute essential components of the oxidative phosphorylation (OxPHOS) complexes. OxPHOS is a biochemical pathway crucial for ATP production.

Mitoribosomal Structure

Structurally, mitoribosomes differ significantly from cytosolic ribosomes. They are smaller and exhibit an inverted protein-to-rRNA ratio, with a higher proportion of proteins. Derived from bacterial ribosomes, mitoribosomes have evolved distinct structural adaptations absent in cytosolic ribosomes, for example including iron-sulfur (Fe₂S₂) clusters associated with proteins and the mL45 protein, which is essential for co-translational insertion of proteins into the inner mitochondrial membrane.

Project

Goals

- 1. Create complete all-atom simulation model
- 2. Describe dynamics of a chosen part of the mitoribosome

Process



Non-canonical residues

Mostly these are **modified amino acids** (in proteins) or **nucleotides** (in rRNA). Modifications are usually **small**, such as **methylation** or **acetylation**. Here are some examples.

n-acetylalanine N-acetylalanine RNA 1-methyladenosine

Missing inner sequences Missing sequences typically occur in proteins, as they often correspond

wissing sequences spirally occur in proteins, as they other corresponds to flexible peripheral loops that are difficult to resolve in cryo-EM experiments. However, the sequences of missing residues are known from experimental model and this allowed us to reconstruct these regions using AlphaFold 3.



Worth-to-remember

Mitoribosomes are biomacromolecular complexes of proteins and rRNAs within mitochondria. This project aims to create an all-atom simulation model to capture their dynamic behavior. That means we want to breathe life into them and see their moves:).

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Contact

If you have any further questions, feel free to contact me via email: kvasnovr@vscht.cz

proteins RNAs

mRNA

Iron-sulfur Fe₂S₂ cluster

protein mL45 tRNAs

protein + Fe₂S₂