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Exploration of Ribosomal Exit Tunnel Heterogeneity Across All Domains of Life Using Molecular Dynamics Simulations

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Introduction:

Ribosomes translate genomic information into protein sequences. During this process, a nascent polypeptide chain travels through the long and narrow ribosomal exit tunnel that permits only limited secondary structure formation. Growing evidence suggests that the ribosome modulates nascent chain emergence and folding process, yet the extent and variability of this modulation across species remain largely unexplored.

Methods:

We use molecular dynamics (MD) simulations to examine in detail the geometric features of ribosomal exit tunnels across 68 distinct ribosome structures.

Results:

MD simulations reveal the main nascent chain path, its dynamic changes during biosynthesis, and potential alternative routes within the tunnel. We identify and characterise interaction sites along the tunnel surface, assessing their compositional and spatial diversity across ribosomes. Additionally, a genome-wide bioinformatics analysis of ribosomal proteins associated with the tunnel, complemented by AlphaFold models, uncovers significant variability and novel structural features.

Conclusion:

Our study uses computational methods to explore the structural and sequence heterogeneity of ribosomal tunnels across all domains of life, including those within mitochondria and chloroplasts and assesses its impact on protein co-translational folding.