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Homology modeling of Homo sapiens Lipoic acid Synthase: substrate docking and insights on its binding mode

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Abstract:

Lipoic acid synthase (LIAS) is an iron-sulfur cluster mitochondrial enzyme which catalyzes the final step in the de novo pathway for the biosynthesis of lipoic acid, a potent antioxidant. Recently there has been significant interest in its role in metabolic diseases and its deficiency in LIAS expression has been linked to conditions such as diabetes, atherosclerosis and neonatal-onset epilepsy, suggesting a strong inverse correlation between LIAS reduction and disease status. In this study we use a bioinformatics approach to predict its structure, which would be helpful to understanding its role. A homology model for LIAS protein was generated using X – ray crystallographic structure of Thermosynechococcus elongatus BP-1

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