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Analysis of the interactions between thiocyanate dehydrogenase and thioredoxin like protein using bioinformatics methods

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Resently a novel copper-containing enzyme thiocyanate dehydrogenase (TcDH) was isolated from the periplasm of some thiocyanate converting haloalkaliphilic sulfur-oxidizing bacteria (SOB) [1]. TCDH catalyzes oxidative thiocyanate conversion into cyanate, elemental sulfur, and two re-

ducing equivalents without involvement of molecular oxygen. In the genomes of some SOB the gene of TcDH is adjacent to the gene of thioredoxin-like protein (TLP) [2]. According to our preliminary data TcDH forms a stable complex with TLP in the periplasm of bacterium *Thiohalobacter thiocyanaticus* HRh1. However, the details of the complex formation are unknown.

The aim of the research is analysis of possible interactive residues between the TCDH and TLP from *Thiohalobacter thiocyanaticus* using bioinformatics analysis. This problem is actual, because the structure of the TCDH and TLP complex is still unknown. TCDH and TLP sequences were found from BLAST searches against the NCBI's RefSeq database. The multiple alignment of TCDH and TLP sequences was constructed with MUSCLE [3] and visualized using GeneDoc and Jalview editing [4]. Bioinformatic analysis of TCDH and TLP sequences was made using pocketZebra, visualCMAT [6]. Thus, co-evolving residues and positions of probable binding sites were identified for TCDH: P171, S238, T253, Y315, E353, P355, D356, G465 (the numbering for TCDH is in accordance with WP_125181025 sequence) and TLP: D117, Q119, V147, L171, V185 (the numbering for TLP is in accordance with WP_125181026 sequence). These bioinformatic approach allow to characterize probable binding sites which could be useful for following molecular modelling of the TCDH and TLP complex.

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