TITLE: TRANSCRIPTOMIC AND STRUCTURAL PROFILE OF THE *CORYNEBACTERIUM PSEUDOTUBERCULOSIS* PANTOTHENATE SYNTHETASE

AUTHORS: ARAÚJO, C.L.A.[1]; ALVES, J.T.C.[1]; DIAS, L.M.[1]; AZEVEDO, V.[2]; SILVA, A.[1]; FOLADOR, A.R.C.[1]

INSTITUTION: [1] LABORATÓRIO DE GENÔMICA E BIOINFORMÁTICA, UNIVERSIDADE FEDERAL DO PARÁ – UFPA (RUA AUGUSTO CORRÊA, 1 – GUAMÁ, BELÉM – PA, 66075-110); [2] LABORATÓRIO DE GENÉTICA CELULAR E MOLECULAR, UNIVERSIDADE FEDERAL DE MINAS GERAIS – UFMG (AV. PRES. ANTÔNIO CARLOS, 6627 – PAMPULHA, BELO HORIZONTE - MG, 31270-901)

ABSTRACT: Caseous lymphadenitis is a chronic infectious contagious disease prevalent in several countries, including Brazil, that causes damage to the world agribusiness. This illness is caused by the Gram-positive pathogen *Corynebacterium pseudotuberculosis*. Despite its zoonotic potential, there are still no fully effective methods of treatment, since antibiotic therapy and available vaccines have varying levels of action, and prophylactic measures are still needed to minimize the impact of infections. For this reason, efforts have been made to find molecules with potential for the development of new drugs and vaccines through the use of computational approaches, in order to found new therapeutic strategies against this bacterium. In this context, the enzyme pantothenate synthetase, involved in pantothenate and coenzyme A biosynthesis process, described as a suitable drug target against *Mycobacterium tuberculosis* has a homologous in the *C. pseudotuberculosis* genome. In this work, we aimed to characterize *in silico* the PanC protein through bioinformatics methods. Using RNA-Seq data of the strain 1002 (biovar *ovis*), available on the NCBI database, the differential expression profile of the *panC* gene under acid (pH 5) and osmotic (2M) stresses was analyzed by the TopHat and Cufflinks programs, considering it induced if the fold change value was ≥ 2 in relation to the control. Subsequently, the secondary structure was predicted through PSIPRED and the three-dimensional homology model was constructed by MODELLER and visualized in Chimera software. The model validation was performed through PROCHECK. The *panC* gene presented high levels of expression (fold change = 2,82 in acid and 2,25 in osmotic stress). In addition, the structural arrangement based on α-helices and β-sheets intercalated by loop regions is also present in the three-dimensional structure of its template. The Ramachandran plot showed that 87.2% of the amino acid residues are present in favorable regions, indicating that the generated structure has an excellent degree of reliability. This enzyme has no homologues in mammals, since they capture pantothenate from the diet using another metabolic pathway, what strongly suggests its potential for the development of drugs that will present no cytotoxic effects in the host. Thus, this study contributes to a better structural and functional understanding of this enzyme and it may serve as the basis for future *in silico* analysis for screening by PanC inhibitors.

Keywords: *Corynebacterium pseudotuberculosis*, RNA-Seq, protein structure homology-modelling, drug target.

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