Use of Computational Tools for Structural Studies of Human CDK11 and its Expression in *Escherichia coli*

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Introduction: The cyclin-dependent kinases (CDKs) are involved in cell cycle regulation, transcriptional and neuronal processes and they are relevant to cancer treatment studies. The cyclin-dependent kinase CDK11 is a kinase understudied, but it is described that is involved in RNA splicing and apoptosis processes. Objectives: Information about primary, secondary and tertiary structure of CDK11 by bioinformatics studies are targeted, and express the recombinant protein CDK11 in bacterial system (*Escherichia coli*). Material and Methods: The transformation of the recombinant pET28a-CDK11-M, which contains the DNA sequence referring to the kinase domain of human CDK11, was performed in strains of *E. coli* BL21(DE3) and Rosetta(DE3). After lysis and solubilization of the inclusion bodies, the samples were analyzed by SDS-PAGE 15%. Additionally, the secondary structure of the complete sequence of CDK11 was analyzed in PSIPRED program; to analyze the presence of rare codons in the sequence of the kinase domain was used RACC and the molecular modeling was performed using SWISS-MODEL. The molecular model was analysed using PyMOL tools. Results and Discussion: The expression of recombinant protein was possible only in Rosetta(DE3). The domain kinase was obtained as inclusion bodies and solubilization method used was inefficient. Analysis of the global secondary structure of CDK11 showed disordered regions in N- and C-terminus, and in the kinase domain was found many rare codons. For this, only the kinase domain was considered in this work. The model chosen for molecular modeling was CDK2 (PDB code 1oit.1.A). The identity between the two sequences was 44.36%, and the final model is structured in the kinase folding. Conclusions: It was possible to obtain expression of the kinase domain of a human protein in *E. coli*, and bioinformatics analysis were important to define the domain kinase and to find many rare codons in the DNA sequence, obtaining the heterologous expression anyway.

Keywords: CDK11, heterologous expression, molecular model
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