Crystal structure of *Canavalia maritima* lectin (ConM) in complex with a dinucleotide and in complex with interleukin-1β primer

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Legume lectins are historically recognized as carbohydrate-binding proteins, and this property is roughly linked to the majority of their biological activities, such as pro- and antiinflammatory processes, apoptosis and mitogenic mechanisms. However, several studies have demonstrated the capability of these proteins to bind diverse other compounds, such as phytohormones and hydrophobic molecules. Although, the biological relevance of these interactions remains elusive. In the present work, we report two crystal structures of ConM, a lectin isolated from *Canavalia maritima* seeds, in complex with oligonucleotides. The ConM was purified and crystallized in complex with an interleukin-1β primer and a dinucleotide (2-AMP) soaked at 5 mM for 2 hours of incubation. X-ray diffraction was performed at the Brazilian Synchrotron Light Laboratory (LNLS - Brazil). The crystal from ConM/IL-1β and ConM/2-AMP belongs to the cubic space group F23 and orthorhombic space group I222, respectively. The final refinement resulted in an Rfactor/Rfree of 24.70/31.49% (ConM/IL-1β) and 21.62/26.71% (ConM/2-AMP). In one structure, an electron density map corresponding to two covalently linked adenine nucleotides was found in the polar central cavity of the lectin tetramer, while in the second one a fragment of four nucleotides from the interleukin-1β primer was fitted in an electron density map present in the interface of ConM non-canonical dimer. The oligonucleotides stabilization involves H-bonds and electrostatic forces with a specific histidine residue. Based on these crystallographic results and in a molecular docking simulation, it was hypothesized that the lectin may act as a transcription factor, which could help us to understand some of their biological activities.

Keywords: Lectins, dinucleotides, primer.

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