CRYSTAL STRUCTURE OF BTHTX-II FROM BOTHROPS JARARACUSSU VENOM, A MYOTOXIC ASP49-PHOSPHOLIPASE A2 WITH LOW CATALYTIC ACTIVITY

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Phospholipases A₂ are components of bothropic venoms. They are enzymes that catalyze the hydrolysis of phospholipids. The structure of BthTX-II was solved by x-Ray diffraction experiments. A comparative analysis has been performed with PLA₂s from *B. jararacussu* venom: BthTX-II, BthTX-I (myotoxic Lys49PLA₂) and BthA-I (non-myotoxic and highly catalytic Asp49PLA₂). The comparison show the quaternary structure of BthTX-II resembles the Lys49-PLA₂s, although it does not present W77, an important residue in the dimeric contact. In contrast, it is totally different from BthA-I. In the superposition, we have noticed that the Cterminal region, involved with the myotoxicity, is similar between BthTX-I and BthTX-II, however is more open in BthA-I. This can be related to the absence of this effect in BthA-I. Additionally, several differences were found in the position of residues presents in the calcium binding loop and hydrophobic channel from BthA-I in comparison with BthTX-II. This can be the explanation of the low catalytic activity in BthTX-II.

Key-words: BthTX-II, Bothrops jararacussu venom, structure, comparative analysis.

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