

Structural Studies with a BthTX-I a Lys49-PLA₂ from *Bothrops jararacussu* Snake
Venom Crystallized In Different Temperatures

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Phospholipases A₂ are among the main components of *Bothrops* venoms responsible for disruption of cell membrane integrity via hydrolysis of its phospholipids, culminating with cell death. Lys49PLA₂ are catalytically inactive on artificial substrates yet maintain cytolytic and myotoxic activities and retain the ability to disrupt the integrity of both plasma membranes and model lipid bilayers by a poorly understood Ca²⁺-independent mechanism. Botropstoxin-I or BthTX-I is the main protein of *Bothrops jararacussu* venom. BthTX-I is a basic myotoxic Lys49-PLA₂, which is catalytically inactive on artificial substrates, but promotes blockade of neuromuscular transmission. Here, we report the crystallization experiments in five different temperatures, X-ray diffraction data collection, structure elucidation and preliminary analysis studies. All crystals were obtained by hanging-drop vapour-diffusion method using similar crystallization conditions but with different temperatures (277K to 308K). X-ray diffraction data were collected at a wavelength of 1.425Å at LNLS (Campinas, Brazil) and processed using the HKL2000 program in the range of 1.5 to 2.8 Å resolution. The crystals belong to four different space groups and have two different oligomeric conformations: monomeric and dimeric. This systematic study may improve the knowledge about the oligomeric conformation changes suffer by PLA₂s and the influence of physico-chemical conditions in the crystallization process of this class of proteins.

Keywords: *Bothrops jararacussu*, Bothropstoxin-I, Phospholipase A₂ Homologue, Physico-Chemical Conditions and Snake Venom.

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