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Structural, enzymatic and pharmacological profiles of AplTX-II - A basic $sPLA_2$ (D49) isolated from the *Agkistrodon piscivorus leucostoma* snake venom

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Abstract

A basic $sPLA_2$ (D49) from the venom of snake *Agkistrodon piscivorus leucostoma* (AplTX-II) was isolated, purified and characterized. We determined the enzymatic and pharmacological profiles of this toxin. AplTX-II was isolated with a high level of purity through reverse phase chromatography and molecular exclusion. The enzyme showed pI 9.48 and molecular weight of 14,003 Da. The enzymatic activity of the AplTX-II depended on Ca^{2+} pH and temperature. The comparison of the primary structure with other $sPLA_2$s revealed that AplTX-II presented all the structural reasons expected for a basic $sPLA_2$s. Additionally, we have resolved its structure with the docked synthetic substrate NOBA (4-nitro-3-octanoyloxy benzoic acid) by homology modeling, and performed MD simulations with explicit solvent. Structural similarities were found between the enzyme's modeled structure and other snake $sPLA_2$ X-Ray structures, available in the PDB database. NOBA and active-site water molecules spontaneously adopted stable positions and established interactions in full agreement with the reaction mechanism, proposed for the physiological substrate, suggesting that NOBA hydrolysis is an excellent model to study phospholipid hydrolysis.

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Keywords

Basic sPLA$_2$ D49; *Agkistrodon piscivorus leuscostoma*; Molecular modeling; NOBA (4-nitro-3-octanoyloxy benzoic acid)

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