STRUCTURAL ANALYSIS OF A MODEL OF A LYS49-PHOSPHOLIPASE A_2 OF MYOTOXIN II FROM *BOTHROPS MOOJENI* COMPLEXED WITH STEARIC ACID USING MOLECULAR DYNAMICS METHODS

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Phospholipases A_2 (PLA_2 - E.C.3.1.1.4). are small stable calcium-dependent enzymes which belong to the superfamily of proteins which hydrolyzes the sn-2 ester bond of sn-3 membrane phospholipids to release arachidonic acid and lysophospholipids. They are components of *Bothrops* venoms responsible for disruption of cell membrane integrity via hydrolysis of its phospholipids. A class of PLA_2-like proteins has been described which, despite PLA_2 activity on artificial substrate, due to a D49K mutation, is still highly myonecrotic. These proteins are involved in several biochemical reactions and biological events being the study of chemical compounds that inhibit these molecules have a great relevance. The crystal structure of the dimeric Lys49-phospholipase A_2 myotoxin-II from *Bothrops moojeni* (MjTX-II) co-crystallized with stearic acid ($C_{18}H_{36}O_2$) has been determined at a resolution of 1.8 Å. The resulting model was submitted to 5 ns of molecular dynamics (MD) simulations using the software GROMACS (Groningen Machine for Chemical Simulations) with different force fields, temperatures, saline concentrations, and in the presence and absence of counter-ions and ligands. The models obtained by these simulations were analyzed in order to obtain structural insights into the structures under the proposed conditions. Support by FAPESP, CNPq, CAPES/PRODOC,FUNDUNESP.