

STRUCTURAL BASIS FOR α -AMYLASE INHIBITORY AND ALLERGENIC PROPERTIES OF 2S ALBUMIN ISOLATED FROM *Ricinus communis* SEEDS

Nascimento V.V.¹, Castro H.C.², Abreu P.A.², Santos, I.M.¹ and Machado O.L.T.¹

1 - LQFPP-CBB-UENF - Campos dos Goytacazes-RJ

2 - LABIOMOL- IB-UFF - Niterói-RJ

Ric c 1 and Ric c 3, isoforms of 2S albumins, are major allergenic proteins in castor bean. Some allergenic properties of these proteins as identification of IgE-epitopes and the elucidation of the critical amino acids involved in IgE-binding were previously described. Analyses of these protein sequences have been revealed that castor 2S albumin contains the trypsin/a-amylase inhibitor family domain, suggesting a role in insect resistance. In this work we have demonstrated that Ric c 1 and Ric c 3 inhibited the α -amylase activity of the insect larvae as *Zabrotes subfasciatus*, *Callosobruchus maculatus* and *Tenebrio molitor*. Ric c 1 and Ric c 3 present eight cysteine residues and have similarities in the secondary structure as determined by circular dichroism. We have predicted the tertiary structure of Ric c 1 utilizing Swiss model program, based in Ric c 3 structure that was determined by RMN and we also have modeled the three-dimensional structure of the *Tenebrio molitor* α -amylase in complex with Ric c 1 and Ric c 3. The major interactions between these inhibitors and alpha-amylase were determined. In order to discover a possible alpha amylase inhibitor with reduced allergenicity we introduced mutations in those residues that were involved in IgE binding and analyzed the modified proteins in complex with *T. molitor* alpha amylase. Our models indicated that to change glutamic acid residues, involved in IgE-binding, by leucine reduce the allergenic properties and preserve inhibition of insect alpha amylase. In principle, these modified proteins could be used in plant defense and allergy therapy.

Supported by: UENF, FAPERJ and CNPq