Structural Analysis of Alba Proteins of *Leishmania infantum*

Elvis Santos Leonardo[1], João Marcos Galúcio, Élcio Souza Leal, Kauê Santana da Costa[1] Jerônimo Lameira[2]

[1]Universidade Federal do Oeste do Pará – UFOPA [2]Universidade Federal do Pará - UFPA

The Alba are a superfamily of proteins involved in binding to the RNA/DNA that share a common domain. We modeled the structure of Alba13 and Alba20 proteins using the homology and threading approaches, respectively. In *Leishmania* species, the Alba20 and Alba13 are constitutively expressed in amastigote and promasigote forms of *Leishmania* life cycle, and previous studies showed that it is involved in the regulation of expression of δ-amastin gene. So considering it show to be interesting target for rational drug design against these parasites, we performed multiple structural analyses in these proteins, using protein prediction, mutational analysis and protein-protein docking. The amino acid sequences of Alba 13 and Alba20 were obtained in the TriTrypDB databank. We used the Modeller to predict the Alba13 structure using as template a hypothetical protein of *Arabidopsis thaliana* (PDB ID: 1VM0, chain A) which conserved the Alba domain and showed 36% of identity in the sequence alignment. The C-terminal region without homology was obtained by threading in I-TASSER server. The Alba20 structure was modeled only by *threading*, and all structures were refined in 3000 cycles of conjugated gradient algorithm and then validated by Ramachandram plot and ANOLEA energy profile. We docked the Alba20 and Alba13 in Rosie server. In order to analyze the stability effect of mutations in the structures, we also performed an alanine scanning in both proteins using FoldX. Our model showed a good energetic profile and a satisfactory stereochemical quality, with number residues in the favorable regions of Ramachadran plot. The residues of Alba domains interact in both proteins, stabilizing the interaction in the dimer complex. Our mutational analysis showed that most mutations in the C-termini region showed to be high destabilizing in Alba20 structure, and in that region is located the RGG box motif which interacts with the 3'UTR region of δ-amastin transcript.

Key-words: Alba, Prtozoa, Modeling