

STRUCTURAL CHARACTERIZATION OF A RECOMBINANT TN ANTIGEN-BINDING LECTIN FROM VATAIREA MACROCARPA

Sousa, B. L.¹; Silva Filho, J. C.¹; Pereira, R. I.¹; Rocha, B. A. M.¹; Delatorre, P.²; Bezerra, G. A.³; Nagano, C. S.¹; Gruber, K.⁴; Cavada, B.S.¹

Legume lectins represent the largest and most thoroughly studied lectin family, comprising a large group of homologous carbohydrate-binding proteins (Sharon & Lis, 1990). A few galactose/N-acetylgalactosamine (Gal/GalNAc) binding lectins isolated from legume plants have proven to be useful as markers in cancer histochemistry. Structural analysis of Tn-binding lectins is of considerable interest for elucidating the mechanism of specific protein-carbohydrate recognition as well as for engineering novel binding activities in legume lectins. Here we present the crystal structures of a single-chain recombinant legume lectin from *Vatairea macrocarpa* (VML), recombinatly expressed in *Escherichia coli*, in complex with lactose, N-acetyl-galactosamine and Tn antigen, respectively. The structural data is supported by isothermal titration calorimetry (ITC) and small-angle X-ray scattering assays. Molecular docking simulations were also performed to analyze the binding of this lectin to *O*-mucins. These findings provide a complete structural characterization of this new Tn-binding protein and strongly suggest recombinant VML as a new tool for cancer research.

¹Department of Biochemistry and Molecular Biology, Federal University of Ceará, Fortaleza, Brazil

²Department of Molecular Biology, Federal University of Paraíba, João Pessoa, Brazil

³Institute of Molecular Biosciences, University of Graz, Graz, Austria

⁴Department of Structural and Computational Biology, Max F. Perutz Laboratories, University of Vienna, Vienna, Austria

^{*}brunolopesdesousa@gmail.com