CRYSTAL STRUCTURE OF FRUTALIN-D-GAL COMPLEX

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Lectin is a protein that can bind to carbohydrate with their carbohydrate recognition domains, allowing them to recognize and selectively and reversibly bind specific glycans. Frutalin is obtained from Artocarpus incisa (breadfruit) seeds, isolated by affinity chromatography on Agarose-D-Galactose matrix. Several masses, around 16 kDa, were observed in deconvoluted spectra in Mass Spectrometry, suggesting the presence of isoforms.

This work shows the crystallization and analysis of data obtained by x-ray diffraction to determine the three-dimensional structure of this lectin in the presence of ligand (D-galactose) and analyzing the molecular basis of interaction. Crystals of Frutalin-D-Galactose complex were grown primarily in wells of pH 8.5 containing PEG as precipitant and ethylene glycol and the best crystals appeared after two weeks of maturation being diffracted to a maximum resolution of 1.81 Å. The best solution, for the space group was obtained for the I2 space group, with an Rfactor of 38.6% and LLG = 19.9.

As results, the monomeric structure of frutalin presents a symmetrical β-prism with three groups of four beta strands each. The SRC involves the N-terminus of the α chain and the frutalin binding site cavity is formed by four key residues Gly25, Tyr146, Asp149, and Trp147. The interaction with the binder are related to the number of interactions occurring between the C1 hydroxyl and Tyr146 residue, C3 hydroxyl and Gly25 residue, C4 hydroxyl and Asp149/Gly25 residues, and C6 hydroxyl and Tyr146/Trp147/Asp149 residues.

In conclusion, the large number of interactions agrees with the high affinity that frutalin has with galactose, in addition to providing an analysis of the dimensions of the lectin in relation to the binder, which may justify the preference that frutalin tends to present by higher molecular weight glycoconjugates. Acknowledgements: FUNCAP, CNPq, CAPES, UFC, USP and UNIFOR. Keywords: frutalin; interaction; Galactose.