Frutalin: structural and computational analysis of binding interaction

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INTRODUCTION: The frutalin is a plant lectin with various biotechnology activities reported. Was isolated (MOREIRA et al., 1998), characterized (MONTEIRO-MOREIRA, 2002), and had established their three-dimensional structure (MONTEIRO MOREIRA, et al, 2015). Modern techniques of bioinformatics proved useful for further investigation of the lectin. **OBJECTIVES:** Using Molecular Dynamics (MD) to model and understand how the structure behaves frutalin obtained by crystallography, as it interacts only with water and various sugars. **METHODS:** From the water simulation is intended to know more about the molecule and its ability to interact with ligands. The MD simulations were made from crystal structure deposited in PDB (4WOG) and was used GROMACS software. **RESULTS:** With the experiment it was possible to suggest change in specificity from allocation constraints in recognition site carbohydrate (SRC), and information about structural stability, which shows that almost any monomeric ligand can fit in place, although protein has been isolated on a column of Agarose-D-galactosis, different sugars can has different residence times at the SRC. Although it has been suggested that the site is promiscuous binding to monomeric sugar it should not occur for larger carbohydrates. The DM results corroborate the results of other experiments obtained above (Monteiro-Moreira, 2002), which realize the highest affinity binders larger as di-, tri- and oligosaccharides. **CONCLUSIONS:** The crystalline structure shows a protein associated with a monomeric linker, which in mutarotation is in the beta form, although the protein to be alfa-specific. DM shows that despite the higher saccharides alpha specificity for any monomeric sugar can compete with water for SRC.

Key Words: Frutalin; Molecular Dynamics; Simulation; *Artocarpus incisa*.