

Molecular dynamics of Frutalin isoforms

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INTRODUCTION: Frutalin is a lectin obtained from the seeds of *Artocarpus incisa*, popularly known as breadfruit. It is mainly α -D-galactose ligand, but also recognizes α -D-mannose. Several masses around 16 kDa was observed by Mass Spectrometry, which confirms the presence of isoforms. **OBJECTIVES:** The work aims to study the behavior of these isoforms using bioinformatics tools, and try to associate the affinity of each, the biological activity it performs at the maturation stages. **METHODS:** It was used the homology modeling from crystallographic data using the software Modeller (SALI; BLUNDELL, 1993). The Molecular Dynamics technique provided atomistic details of each isoform in a short timeline, and the program used was the GROMACS 5.0.1 (Abraham et al., 2015). **RESULTS:** The modeling establishes the differences between the isoforms from crystallographic data (Monteiro-Moreira et al, 2015), showing structural differences and allowing visualization of nuances and conformational interactions (Molecular and interatomic). Molecular Dynamics (MD) behaves as a simulated structure of frutalin isoforms when interacting with water and with different sugars, which local mutations and which key residues of the lectin activity. The 5 isoforms simulated against water and against monomeric binders shows promiscuity but also shows high affinity to D-galactose, with the exception of one of the isoforms (FTL4) that has a Lys residue capable of preventing this interaction. **CONCLUSIONS:** The molecular modeling and DM may be useful in characterizing proteins and based on what has been done, it can be concluded that frutalin isoforms may have different biological roles, since they have nuances and structural differences, further increasing the biotechnological potential of the molecule.

Key Words: Frutalin; Molecular modeling, Molecular dynamics; *Artocarpus incisa*.