Molecular modelling, docking simulations and substrate specificity of the protein alcohol acyltransferase from *Vasconcellea pubescens*

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The Aroma in fruits is an important attribute of quality that influences the consumer’s acceptance, which is a complex carácter, determined by a set of low molecular weight volatile compounds. In *Vasconcellea pubescens* the aroma is formed mainly by esters, which are produced through an esterification reaction between alcohols and acyl-CoAs catalyzed by the enzyme acyl alcohol transferase (VpAAT1). For the purpose of increasing our understanding about the production of aroma during the process of fruit maturation of *V. pubescens*, a study of the molecular mechanisms of the VpAAT1 was carried out. The comparative modeling methodology was used to build the enzyme structure, which was validated and refined with molecular dynamics simulation. The resulting model showed that the protein structure is composed of 15 β sheets and 14 α helix, the protein’s active site is the segment HTMSD and located in a loop between the sheet 7 and the helix 5. The molecular dynamic simulation of 2 ns showed that the residue H166 and D170 it part of active site and exposed to the solvent channel, allowing the interaction with the substrates. Additionally, the conformational interaction between the protein and several ligands was explored by molecular docking simulations, and the predictions obtained were tested through kinetic analysis. Kinetic results showed that the lowest $K_M$ values were obtained for acetyl-CoA and benzyl alcohol. In addition, the most favourable predicted substrate orientation was observed for benzyl alcohol and acetyl CoA, showing a perfect coincidence between kinetic studies and molecular docking analysis.