Virtual Screening for *Citrus Tristeza* Disease Control

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Citrus tristeza virus (CTV) causes a most destructive citrus disease in many parts of the world and several approaches have been used to control damages like eradication programs, use of tolerant or resistant rootstock, use of transgenic *Citrus* and cross protection. The aim of this study is to identify, by a computational approach, molecules that interfere with CTV replication. Drug discovery is an extended process that can take as many as 15 years from the first compound synthesis in the laboratory until the therapeutic agent, or drug, is brought to market. GriDock is a molecular modeling software developed to identify potentially bioactive compounds (hit-compounds) in order to speed-up the drug discovery process. It's based on the virtual-screening approach in which the activity of a large set of molecules is predicted by multiple molecular docking calculations. With a view to verify its potentialities, the RdRp (RNA dependent RNA polymerase) enzyme was considered as potential therapeut target for citrus infected by CTV and its 3D structure was obtained through homology approaches. The screening of more than one million of molecules allowed the identification of some potential RdRp inhibitors. We chosen, to confirm experimental data, a sulfonic acid, a dithiocarbamate and a penicillin derivatives. The achieved results must be considered preliminary but they can be seen as a good starting point to develop a novel drug class against CTV infections.