



Impact of Essential Oils of Lamiaceae Family Against *Tylenchulus semipenetrans*

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Abstract: The nematode of citrus *Tylenchulus semipenetrans* Cobb 1913, is an important parasitic nematode of plants, very widespread in citrus growing regions of the world, and it is responsible of slow decline of citrus fruits. The aim of the present study focuses on the molecular docking approach to inhibition of the “Acetyl CoA Carboxylase” enzyme responsible for fatty acid synthesis in *Tylenchulus semipenetrans* and alteration disrupting the synthesis of the surface layer, this inhibitory action is based on essential oils of aromatic plants, taking as an example the Lamiaceae family, using four species *Lavandula multifida*, *Lavandula stoechas*, *Rosmarinus officinalis*, and *Thymus ciliatus*. This study revealed that Carvacrol from *Lavandula multifida* gives the best docking scores compared to Biotine, the co-crystallized inhibitor of the Acetyl CoA Carboxylase, to spirotetramat as chemical insecticide already used against citrus nematode, and to the other complexes. Molecular Dynamics Simulation study showed a good result for the carvacrol- Acetyl CoA Carboxylase docked complex, for that can consider that carvacrol extracted from *Lavandula multifida*'s essential oil as a functional inhibitor of Acetyl CoA Carboxylase activities and it can be used as good Bio-nematicides against *Tylenchulus semipenetrans* for the protection of the human health and environment.

Keywords: Nematode, *Tylenchulus semipenetrans*, Molecular docking, Bio-nematicides, Lamiaceae, Molecular dynamics simulation
