Molecular biophysics: An integrative approach to investigate the bioherbicide effect of essential oils related to their interaction with plant plasma membrane

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Essential oils (EOs) are used in an increasingly number of sectors like medicine, cosmetics, food industry and more recently in agronomy. In agronomy, EOs are used as bio-pesticides for their insecticidal, antifungal or bactericidal effects but also as bio-herbicides. Owing to the current attraction for natural products, a better understanding of their mode of biological action for new and optimal applications is of importance. It has been shown that EOs antimicrobial activity, quite well described in the literature, is at least partly due to their interaction with the plasma membrane. They notably change the lipid composition, altering fluidity, leading to various effects which can induce cell lysis, apoptosis or necrosis. Citronellol, a major compound of lemongrass EO was notably shown to have antifungal activities by changing the membrane composition and inhibiting cell growth. Cinnamaldehyde (cinnamon EO) has been reported to have a broad spectrum of antibacterial activity, notably by affecting cell morphology, membrane integrity, permeability and composition.

We are currently working on the development of a bioherbicide made from *Cinnamomum zeylanicum* Blume (cinnamon) and *Cymbogognon winterianus* Jowitt (lemongrass) EOs. We have shown that the application of the whole EOs and their major individual compounds on the leaves and cotyledons of *A. thaliana* appears to be promising: when applied on cotyledons or leaves, EOs induce damages that are as important as those observed for commercial herbicides.

Since EOs are small amphiphilic molecules, they can cross the mesh of cell wall and interact directly with the plant plasma membrane (PPM). Modifying the lipid organization could lead to crucial cellular effects, notably on protein function.

We used a unique and original combination of *in silico* (molecular dynamics simulations) and *in vitro* (Langmuir monolayers, isothermal calorimetry, fluorescence and infrared spectroscopies) biophysical approaches, previously developed to study structure-function relationships of molecules of biological interest (pharmacological drugs , proteins, peptides, surfactants…) to investigate the interaction of EOs or their individual compounds with bio-mimetic plant plasma membranes to better understand the structure- activity relationships in the context of their bioherbicide activity.