Back to the future: essential oils as remedies that never set. Acquisition of experimental chemical, (micro) biological data processed with machine learning algorithms to define predictive models and shed light on essential oils mechanism of action

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Essential oils (OE) are complex chemical mixtures that are industrially produced primarily by the techniques of hydrodistillation (HD) and steam distillation (SD). In the last decade, investigations on EOs have significantly increased in particularly in the case of innovative extraction techniques, in their chemical analysis and above all in their potential therapeutic use. However, there is still little information on the EOs mechanisms of action. At Rome Center for Molecular Design lab we have set-up new approaches on either extraction methods or data analysis. In particular a new 24 hours EOs extraction were achieved by means of either SD or HD. Fractionated or continued extractions allowed to produce a number of different EOs from the same plants. Routinely applied to several plants, the protocol led to a number of EOs samples that were chemically and microbiologically characterized. A first dataset compiled from 89 different EOs obtained from 3 different plants harvested in different seasons and assayed for their antibacterial and anti-biofilm activity against P. aeruginosa were subjected to machine learning algorithm to elaborate QCAR models (quantitative composition-activity relationships). The QCAR model aimed at identifying the chemical components most responsible for the observed biological effects and also for those compounds that have an anti-synergistic issue. In a second application, a different dataset was used to derive a predictive model for EOs evaluated against HSV. The model was used to select a number of microbiologically untested EOs revealing a high success rate.

A high level of interdisciplinarity among botanists, analytical chemists, pharmaceutical chemists and microbiologists all involved in a common interest have lead to interesting results whose details will be given during the presentation.