Multi-omics data and multiscale modelling in winemaking

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Introduction

Wine fermentation is a complicated ecological and biochemical process in which a wide variety of yeasts produce ethanol and contribute to the sensory attributes of the final product. The output of spontaneous fermentations depends on the amounts and variety of yeasts and bacteria available in must, grape variety and maturity and process conditions (e.g., temperature, aeration, etc.). However, the variability, mostly in the must flora and grape chemical properties, results in severe difficulties to predict and reproduce wine properties. The use of yeast starters has dramatically improved the reliability of the process and the quality of wines.

S. cerevisiae yeast starters are universally preferred to initiate fermentation processes. However, the new challenges faced by the wine industry such as those related to climate change, or the consumer's demands for lower-alcohol wines, call for the use of alternative starting strategies.

Multiscale modelling brings the potential of exploring the most relevant mechanisms and designing optimal processes more systematically.

In this workshop present an overview of what bioinformatics, omics technologies and systems biology approaches can bring to the winemaking industry.

The workshop is organised into four modules:

1. **<u>Primer on wine fermentation. Challenges.</u> Presenter: Amparo Querol**
   This module is intended to introduce basic concepts of wine fermentation and the current industrial challenges: the selection of yeast starters, non-conventional yeasts, stress conditions (nutrient limitation, ethanol, osmotic stress, low temperatures, etc), wine yeast improvement.
   This module will last around 30 min.

2. **Experimental methods**. **Presenter: Roberto Pérez-Torrado**
   This module is intended to describe usual experimental methods for the purpose of modelling wine fermentation. Here we will show the application of multi-omic techniques to lab scale simulations of the wine fermentation and how this information is essential to understand the yeast behaviour in these conditions alone or in competition between different species and the biochemical transformations that are implicated in winemaking as the generation of aromatic compounds.

   This module will last around 60 min.

3. **Genomic and Genetics tools.** **Presenter: Eladio Barrio**
   This module will cover genomic and genetic tools to understand the mechanisms involved in yeast adaptation and speciation and the acquisition of new gene functions of adaptive value through gene and genome duplication or interspecific hybridisation.

   This module will last around 60 min.

4. **Multiscale modelling of wine fermentation.** **Presenters: Eva Balsa-Canto & David Henriques**

   This module will present an overview of the state-of-the-art in the modelling of wine fermentation approaches with particular emphasis on current developments and the prospects of the Systems Biology approach. We will introduce kinetic modelling of single and mixed fermentations plus genome-scale dynamic modelling approaches with some tips on numerical methods to iteratively improve the quality of model predictions.

   This module will last around 60 min.

At the end of the session, we will enjoy a glass of wine.