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BOOK OF ABSTRACTS

Computational approaches for enzyme prediction and targeted strain selection, to degrade off-flavours and anti-nutritional factors in plant-based foods.

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The global food system is a major contributor to climate change, with animal-based products responsible for roughly twice the greenhouse gas emissions of plant-based alternatives. Transitioning toward plant-based diets is therefore essential to reducing our environmental impact. However, the acceptance of plant-based foods remains limited due to off-flavours and anti-nutritional factors (ANFs), which negatively affect both taste and nutritional value. Fermentation offers a promising natural strategy to address these challenges by degrading off-flavours and ANFs and producing beneficial compounds. Yet the enzymatic mechanisms underlying these conversions in microbial species remain poorly understood. Therefore, the metabolic screening of large numbers of microbial strains is required to select appropriate candidates to be used in starter cultures.

This project addresses this knowledge gap by developing computational approaches to predict enzymes involved in the biochemical conversion of off-flavours and ANFs. We apply two complementary strategies: (1) structure-based enzyme prediction using molecular docking and multiple structure alignments, and (2) enzyme-substrate prediction using transfer learning with pre-trained protein large language models.

The resulting enzyme predictions serve as markers to guide targeted strain selection for fermentation, enabling the rational design of microbial cultures and fermentation processes. A selected set of enzyme candidates will be experimentally validated in collaboration with partners within the FERMI consortium. Ultimately, this project contributes to the development of scalable, data-driven fermentation strategies that improve the sensory and nutritional properties of plant-based foods. In doing so, it supports broader efforts to promote climate-resilient, sustainable, and appealing food systems.

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