FONDAZIONE
EDMUND MACH
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SEMINAR

Decoding the chemical universe of plants

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Although plants are an incredibly rich source of pharmaceutically relevant specialized metabolites, biosynthetic pathway elucidation in non-model plant species has proven challenging. Unlike bacteria and many fungi that contain biosynthetic operons, the genes of a given plant typically scatter randomly across the genome, making pathway discovery via genome mining nearly impossible. My lab is developing generalized workflows for connecting biosynthetic gene sequences (obtained using RNAseq) to their downstream metabolites (detected in LC-MS data). To this end, we have developed EnzymeExplorer, a targeted machine learning pipeline for predicting the enzymatic functions of terpene synthases directly from their amino acid sequences (Samusevich et al, bioRxiv 2026) and DreaMS, a self-supervised foundation machine learning model for tandem mass spectrometry, which outperforms state-of-the-art methods in a range of different prediction tasks (Bushuiev et al., Nature Biotechnology 2025). We are further building on these foundations towards the final goal: a full computational characterization of the chemodiversity and biosynthetic potential of each plant species using easy-to-obtain experimental datasets.