Exploring the phytochemical space of land plants: insights of uniqueness from the Rosids and Superrosids metabolomes

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The specialized metabolome of plants represents the most complex chemical space in nature, characterized by immense structural and functional diversification that remains only partially uncovered. In relation to the evolution of biosynthetic traits and phylogenetic distance among land plants, species can synthesize metabolites (or metabolite classes) that are either shared across taxa or restricted to specific lineages. Investigating this diversity across selected clades provides key insights into metabolism evolution in land plants. While often addressed computationally at the genus or family level, large-scale metabolomics studies within a single experimental framework remain a pioneering research.

In this work, we exploited a collection of 700 Italian plant species established within the frame of Spoke 6 -Activity 2 of NBFC, designed to represent the phytochemical diversity of the Italian flora. We present here the results of an untargeted comparative LC-HR-MS analysis of 172 species belonging to the Rosids and Superrosids, two large clades that comprise approximately one quarter of flowering plants. The available methods for extracting relevant data from raw chromatographic analyses proved unsuitable for such a heterogeneous set of extracts, making it necessary to develop a new pipeline for dataset preparation. Analysis of the resulting dataset revealed, rather unexpectedly, that even metabolites belonging to ubiquitous chemical classes (*e.g.*, flavonols and flavones) display a remarkably high degree of uniqueness, *i.e.*, they are detected in a single species. Of approximately 2,000 identified metabolites, more than half were restricted to a single species, while only 4% were found in at least 20 species. This highlights an immense chemical biodiversity that requires thorough characterization and protection, also in view of its potential valorization.