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Researchers Create the First Large-Scale Chemical Atlas of Grapevines

The map draws on 462 samples from 126 accessions across four seasons to trace molecular differences among varieties.

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An international team of researchers has built what it describes as the first large-scale chemical atlas of grapevine diversity, using liquid chromatography-mass spectrometry to compare hundreds of grape samples across multiple harvests and varieties. The

work, published in the Journal of Agricultural and Food Chemistry, offers a new reference for understanding how grape varieties differ at the molecular level and how those differences may be used in classification, authentication, breeding, and winemaking research.

The project, called the Grape Metabolome Project, analyzed 462 samples from 126 grapevine accessions collected over four growing seasons. According to the study, the researchers used LC-MS profiling, quality controls, data correction methods, and pattern analysis tools to organize the samples into major chemical groups while also detecting finer differences among individual varieties.

Those differences were linked to families of compounds that play a central role in grape and wine characteristics, including anthocyanins, which help determine red and purple color, flavonols, aroma-related molecules, and tannins, which contribute to structure and astringency. The researchers reported that the resulting map did more than separate broad groups. It also identified smaller subgroups, including particularly aromatic grape types, and connected those patterns to underlying biological processes in the fruit.

The study addresses a gap that researchers say has persisted despite the economic and scientific importance of grapevines. Grapes include thousands of cultivated varieties, along with rootstocks and wild relatives, and they are important not only to agriculture and food production but also to plant science. Even so, the authors said there had been no systematic and publicly available effort to capture grape chemical diversity on this scale across cultivated varieties.

That gap is partly explained by the complexity of grape chemistry. Grapes contain a large and still incompletely described set of compounds produced through many biological pathways, including those linked to pigments, flavor and aroma molecules, amino acids, defense compounds, lipids, sugars, and acids. The authors said that while grapevine has become a model species in research on plant secondary metabolism, stress biology, and food chemistry, most previous studies have focused on narrower parts of that chemistry or on other plant tissues, such as grape canes and wood biomass, rather than on berry composition at this breadth.

By assembling a broader dataset, the researchers said they created a practical framework for exploring grapevine biodiversity through chemistry. In the paper, they described the atlas as an expandable resource that can support several uses at once: classifying grape varieties, checking authenticity and origin, identifying compounds associated with biodiversity, and finding traits that may be useful in breeding programs.

That could have direct relevance for the beverage sector. A more detailed chemical reference for grapes could help wineries and researchers improve varietal selection, support authenticity testing, and guide precision viticulture and enology work. Those applications remain potential uses rather than confirmed commercial outcomes, but they point to how a research tool like this could be used beyond basic plant science.

The work may also help address practical questions in a wine market where grape identity, geographic origin, and production methods can carry financial and regulatory weight. A chemical atlas cannot replace all other forms of verification, but a standardized metabolomic reference may add another layer of evidence when producers, regulators, or researchers need to distinguish between varieties or investigate whether a sample matches a claimed origin or profile.

The researchers said one of the strengths of the project is that it bridges broad chemical fingerprinting with more specific metabolite families. In other words, the atlas does not just show that one grape differs from another. It also begins to explain which groups of molecules are driving those differences and how they relate to known features such as color, aroma, and mouthfeel.

The authors also suggested that the resource could become more useful if it is combined with genetic data in future work. Linking metabolomic patterns with genomic information could help researchers understand how certain traits are inherited and expressed, and it could improve efforts to breed grapes with desired sensory, agronomic, or climate-related characteristics. That could be important as growers and winemakers adapt to shifting weather patterns, disease pressure, and changing market demand.

The study does not claim to capture the full chemical diversity of all grapevines. Instead, it presents a large reference framework that can be expanded as more varieties and compounds are added. Even so, the scale of the dataset marks a step forward compared with earlier targeted studies, which were more limited in scope and often focused on a narrower set of compounds.

In the paper, the researchers said the atlas establishes a comprehensive LC-MS-based grape metabolome resource and a practical framework for studying grapevine biodiversity through chemistry. For grape science, the significance is the dataset itself: a structured, reusable map of berry chemistry across many varieties and seasons. For wine and other grape-based beverage research, the value may lie in how that map can be applied to questions of selection, traceability, and product character as the industry seeks more precise tools to understand the raw material at its source.