Identifying vintage wines by their chemical signature

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Does every wine carry its own chemical signature and, if so, can this be used to identify its origin? Many specialists have tried to solve this mystery, without fully succeeding. By applying artificial intelligence

tools to existing data, a team from the University of Geneva (UNIGE), in collaboration with the Institute of Vine and Wine Science at the University of Bordeaux, has succeeded in identifying with 100% accuracy the chemical mark of red wines from seven major estates in the Bordeaux region.

These results, published in the journal *Communications Chemistry*, pave the way for potential new tools to combat counterfeiting and for predictive tools to guide decision-making in the wine sector.

Every wine is the result of fine, complex mixtures of thousands of molecules. Their concentrations fluctuate according to the composition of the grapes, which depends in particular on the nature and structure of the soil, the grape variety and the winegrower's practices.

These variations, even very small ones, can have a big impact on the taste of wine. This makes it very difficult to determine the precise origin of a wine based on this sensory criterion alone. With climate change, new consumer habits and an increase in counterfeiting, the need for effective tools to determine the identity of wines has become crucial.

Is there then a chemical signature, invariable and specific to each estate, that would make it possible to do this? "The wine sector has made numerous attempts to answer this question, with questionable or sometimes correct results but involving heavy techniques. This is due to the great complexity of the blends and the limitations of the methods used, which are a bit like looking for a needle in the middle of a haystack," explains Alexandre Pouget, full professor in the Department of Basic Neurosciences in the Faculty of Medicine at UNIGE.

One of the methods used is gas chromatography. This consists in separating the components of a mixture by affinity between two materials. The mixture passes through a very thin tube, 30 meters long.

The components that have the greatest affinity with the tube material gradually separate from the others.

Each separation is recorded by a mass spectrometer. A chromatogram is then produced, showing peaks that indicate the molecular separations. In the case of wine, because of the many molecules that make it up, these peaks are extremely numerous, making detailed and exhaustive analysis very difficult.

Data processed by machine learning

In collaboration with Stephanie Marchand's team from the Institute of Vine and Wine Science at the University of Bordeaux, Alexandre Pouget's team found the solution by combining chromatograms and artificial intelligence tools. These chromatograms came from 80 red wines from twelve vintages (1990–2007) and from seven estates in the Bordeaux region. This raw data was processed using machine learning, a field of artificial intelligence in which algorithms learn to identify recurring patterns in sets of information.

"Instead of extracting specific peaks and deducing concentrations, this method allowed us to take into account each wine's complete chromatograms—which can comprise up to 30,000 points—including background noise, and to summarize each chromatogram into two X and Y coordinates, after eliminating unnecessary variables. This process is called dimensionality reduction," explains Michael Schartner, a former postdoctoral scholar in the Department of Basic Neurosciences in the Faculty of Medicine at UNIGE, and first author of the study.

A 100% reliable model

By placing the new coordinates on a graph, the researchers were able to

see seven "clouds" of points. They found that each of these clouds grouped together vintages from the same estate on the basis of their chemical similarities.

"This allowed us to show that each estate does have its own chemical signature. We also observed that three wines were grouped together on the right and four on the left, which corresponds to the two banks of the Garonne on which these estates are located," explains Stéphanie Marchand, a professor at the Institute of Vine and Wine Science at the University of Bordeaux, and co-author of the study.

Throughout their analyses, the researchers found that the chemical identity of these wines was not defined by the concentration of a few specific molecules, but by a broad chemical spectrum. "Our results show that it is possible to identify the geographical origin of a wine with 100% accuracy, by applying dimensionality reduction techniques to gas chromatograms," says Alexandre Pouget, who led this research.

This research provides new insights into the components of a wine's identity and sensory properties. It also paves the way for the development of tools to support decision-making—to preserve the identity and expression of a terroir, for example—and to combat counterfeiting more effectively.

More information: Michael Schartner et al, Predicting Bordeaux red wine origins and vintages from raw gas chromatograms, *Communications Chemistry* (2023). DOI: 10.1038/s42004-023-01051-9

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