

## Food & Beverage Analysis

### Can LIMS profiling accelerate food and drink product quality testing?

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Quality testing is a crucial component of the food and drink industry, necessary to protect both consumer health and the organisation's reputation. But the process can be time-consuming, costly, and resource intensive. These drawbacks cause significant hinderance to workflows, eventually leading to loss of revenue.

Yet workflows in quality testing are rich with historical data that can be used to streamline testing - not only by directing the work but allowing products to 'fail early'. This removes the need to run redundant experiments, thereby saving costs, speeding up processes, and increasing test success rate. So, how can this data be collated and used?

Some lab information management systems (LIMS) come with profiling and machine learning (ML) capabilities, eliminating the need for particular tests and improving quality testing in the food and drink industry. Here we illustrate how this works by looking at 'failing early' in wine quality testing.

#### Wine testing complexity leaves a sour taste

Testing wine samples is notoriously complex. Many intertwined factors influence the quality, including pH, alcohol, residual sugars, and density – and all these complex relationships must be deciphered before the final quality test.

Traditionally, wine quality is assessed by sommeliers, but this approach is subjective, non-continuous, and expensive. Now, labs can now predict the outcome of this final quality test in advance with ML. Profiling capabilities analyse the complex relationships between variables and use this data to make predictions on which wines are unlikely to make the cut.

#### Using LIMS with profiling to 'fail early'

In a recent study, a wine laboratory applied LIMS profiling to wine samples, enabling them to use the model as a predictor for the final test. Here, the researchers trained an ML algorithm to model wine quality using 10 important chemical measurements and used it to predict the quality of new wines that have completed the same set of tests.

The team investigated variable importance to identify which tests have the strongest relationship to quality for 'failing early'. Breaking the tests into stages, the tests with the strongest relationship to quality for the first stage were picked: these were alcohol, density, and chlorides (Figure 1).

If the wine passed, it would be taken through to the next stage of tests, and a quality value predicted at the end. Any wine that failed early could be reprocessed or sold as cheaper products, saving considerable time and reducing costly assessments.

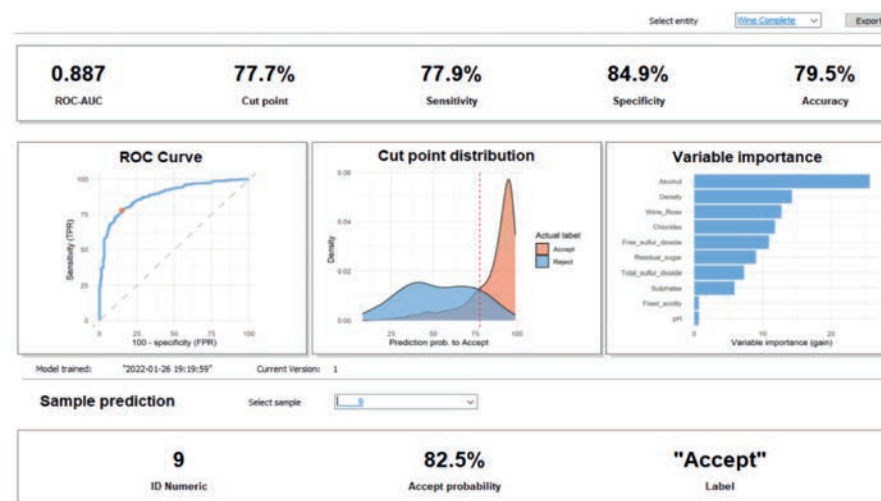


Figure 1. LIMS dashboard showing the receiver operating characteristic (ROC) curve (left), cut point distribution (centre) and the variable importance (right).

#### Fewer tests for faster processes

Product testing is vital for food and drink quality assessment but can be expensive and time-consuming. Failing early is critical to production processes, enabling labs to lower the number of required tests and consequently reducing both costs and consumable usage. LIMS software with profiling and ML capabilities lets users predict key test results without performing them, helping save resources and accelerate the quality processes.