Food Authenticity Testing Made Easy with MassHunter Classifier

Food fraud is a growing concern globally. Food fingerprinting is finding traction with labs tasked to develop tests for known issues or investigate new ones. Fingerprinting benefits from looking at foods and raw materials in a more holistic way than tests tuned only to a few compounds. Hence, it produces tests that are harder to be usurped by fraudsters. In the latest addition to the Agilent MassHunter suite, Agilent MassHunter Classifier, allows LC/MS and GC/MS users to transform fingerprinting strategies, developed through Agilent MassHunter Profinder and Mass Profiler Professional (MPP) into automated sample classification reports that present actionable results to an analyst or technician. Figure 1 shows the workflow for method development to automate the entire process.

Figure 1. Workflow for method development.

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Automated sample classification in Classifier

Automated sample classification processes the samples based on the chosen method in MPP such as linear discriminant analysis (LDA), partial least squares discriminant analysis (PLSDA), random forest, and soft independent modeling of class analogies (SIMCA), and provides the results in a simple view, allowing the user to determine if a sample is authentic.

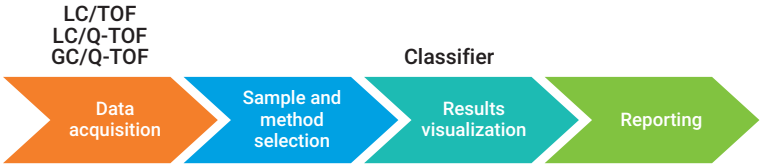

Figure 2. Automated sample classification in Classifier.

Results review and reporting

Principal component analysis (PCA) allows the user to see the position of the sample corresponding to the class from the existing model, indicating the similarity to a specific class (Figure 3). The results are exported as a report in the PDF format based on the template selected.

The simplified food authenticity workflow provides tools to perform method development and automated sample classification. It is easier than ever to add or enhance your capability to test for food authenticity or commodity origin.

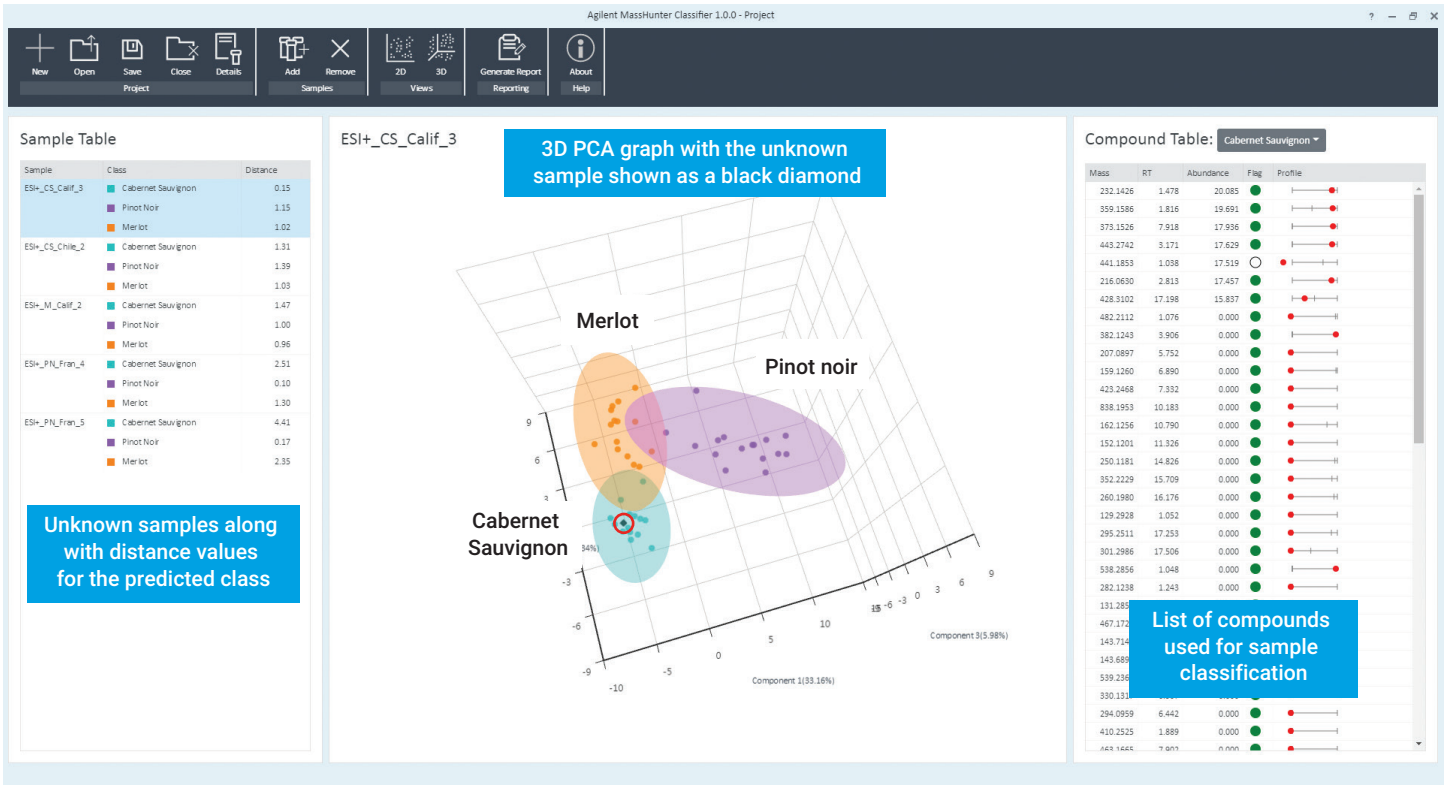

Figure 3. User interface of Classifier showing the Sample Table, PCA, and Compound Table. This 3D-PCA shows three classes of wine samples, Merlot, Pinot Noir, and Cabernet Sauvignon. The unknown sample is shown in a diamond shape (circled in red), indicating the class of the sample that it is closest to in the model. The colored dots are training samples used for model building, and confidence ellipses in the PCA are drawn for model training data used in MPP.

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