Waters
THE SCIENCE OF WHAT'S POSSIBLE.®

REIMS Research System with iKnife Sampling for Food and Agricultural Research

Convert scientific data into useful information

RAPID PROFILING OF FOODSTUFF – FROM RAW INGREDIENTS TO FINAL PRODUCT

With today's global food supply chain, the ability to rapidly profile food and agricultural produce is vitally important to ensure consumer safety, protect trade markets, maintain product quality, and preserve brand image.

Waters® Rapid Evaporative Ionization Mass Spectrometry (REIMS™) has removed many of the constraints associated with sample preparation and has opened new opportunities for point-of-control testing. REIMS offers possibilities for direct analysis of samples and can generate spectral profiles that are highly characteristic of the sample, making this approach excellent for rapid profiling analysis.

In REIMS analyses, the MS spectral information is used as a 'fingerprint' for the identification of critical attributes such as the authenticity, species, quality or phenotypic trait associated with the sample.

Waters REIMS Research System with the hand-held iKnife™ sampling device produces information-rich vapor directly from the surface of a sample, which when analyzed by a time-of- flight (Tof) MS, provides analysts with an accurate molecular profile in seconds.

Rapid Evaporative Ionization Mass Spectrometry (REIMS) Research System with the hand-held iKnife.

KEY BENEFITS

- No sample preparation or chromatography required.
- Quickly determine differences within and between samples.
- Identify molecular markers responsible for sample differences.
- Available with a choice of high performance Tof-MS systems.
- Potential to combine with other sampling techniques towards a holistic profiling approach.

FOOD FRAUD AND AUTHENTICITY

Food fraud has become a topic of major concern over the past few years mostly due to major incidences such as the 2008 Chinese melamine scandal and the 2013 European horsemeat scandal. Like many food commodities, fish has succumbed to food fraud on a global scale. A recent review identified that on average 30% of products sold are either misrepresented or mislabelled.[1]

There are many types of food fraud, including:

- Substitution of part or all of the food with a lower value commodity.
- Addition of a component to increase the value of the overall product.
- False claims on product labels that increase their value, such as organic, welfare friendly, fair trade, or country of origin.

The primary objective of authenticity testing is rapid verification, from raw ingredient testing through to finished (processed) product, to support verified traceability systems.

DNA-based methods are widely recognized as the "gold standard" of testing for the speciation of foods from animal origin as DNA is found in all organisms and can be analyzed in all types of food ranging from raw to processed and cooked samples. Some food processing methods, however, result in the degradation or modification of DNA and can reduce confidence in the results.

REIMS testing offers a number of benefits as a tool for food authenticity testing. As a direct analysis technique, REIMS can significantly reduce the timescales associated with traditional laboratory based testing. As immediate results are generated decisions can be reached quickly.

REIMS is a technique that provides information on stable small molecular weight analytes such as lipids and fatty acids enabling species classification or quality profiling in both raw and processed products.

LiveID™ is a web-based application platform that has been developed for use within a direct analysis workflow enabling the user to train and validate statistical models using characterized samples of known origin within a short timescale. In combination with REIMS, LiveID can address complex analytical challenges such as food authenticity, speciation and plant phenotyping – while providing answers in real time.

LiveID takes spectra acquired from a test sample and performs recognition to classify the sample as belonging to one of a number of user-defined sample types or groupings.

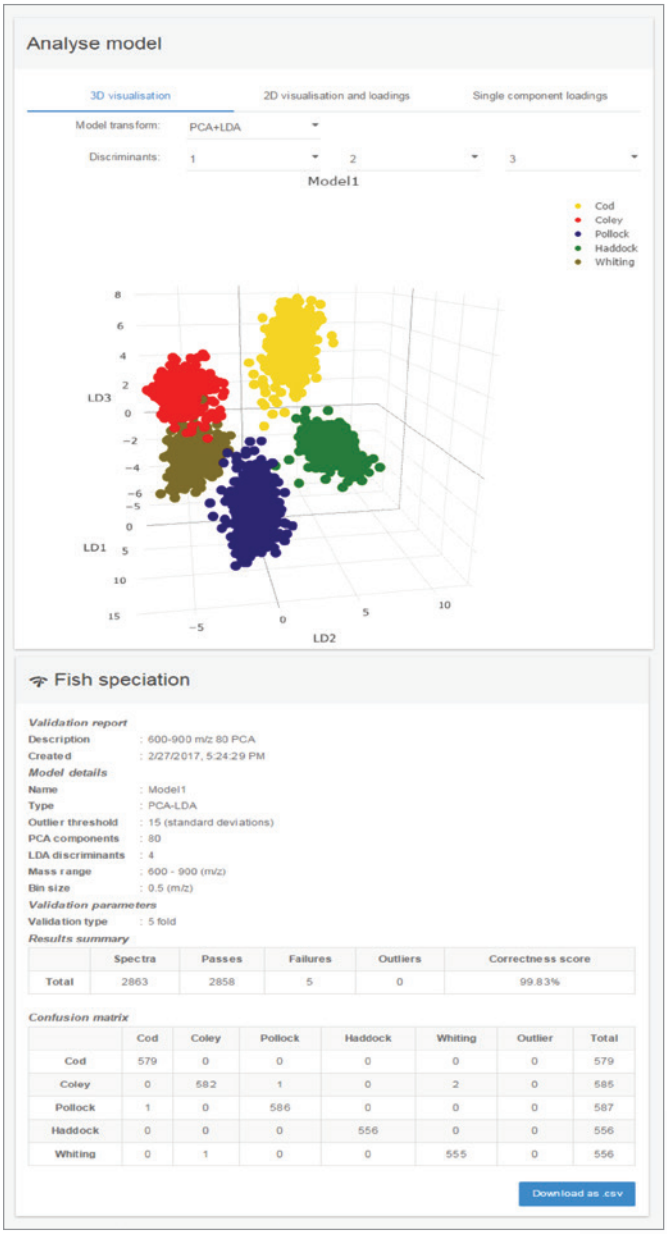

Figure 1. Model for the speciation of five of the most commonly consumed white sea fish in Northern Europe (cod, coley, pollock, haddock and whiting). The model was trained with over 400 biological replicates and over 2000 MS spectra. The predictive accuracy has been calculated as 99%.

Figure 2. Validation results when the LiveID fish speciation model was challenged with independent samples of "unknown" fish in recognition playback mode.

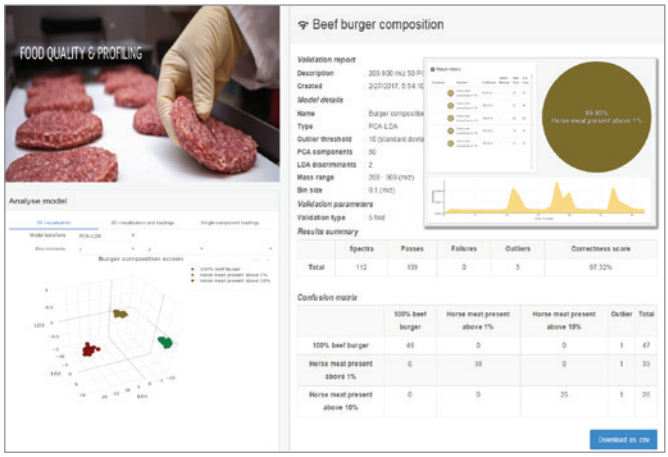

Figure 3. Processed product authenticity, burger composition. A. LiveID PCA/LDA model space created using REIMS acquired data of data burger compositions of beef and horse meat (n=20); B. model validation and C. real time recognition results from a sample known to contain horse meat above the screening detection limit of 1%.

MEAT SCIENCE

Carcass quality is a primary concern within the meat production industry and has warranted scientific research into better understanding the factors affecting the physical characteristics of meat. One example is “boar taint”, an off-odor caused by the release of androstenone (AEON), skatole (SK), and indole (IND) when the meat is processed and cooked. The boar taint odor is offensive to many consumers, de-valuing the meat and it is therefore desirable to rapidly identify contaminated carcasses at an early stage within the production process.

Using iKnife and REIMS, it is possible to identify biomarkers linked to the physical characteristics of meat without the need for laborious sample preparation and extraction. The REIMS approach significantly reduces the timescale for analysis in comparison to the conventional GC-MS methods with accurate results being generated in under 10 seconds.

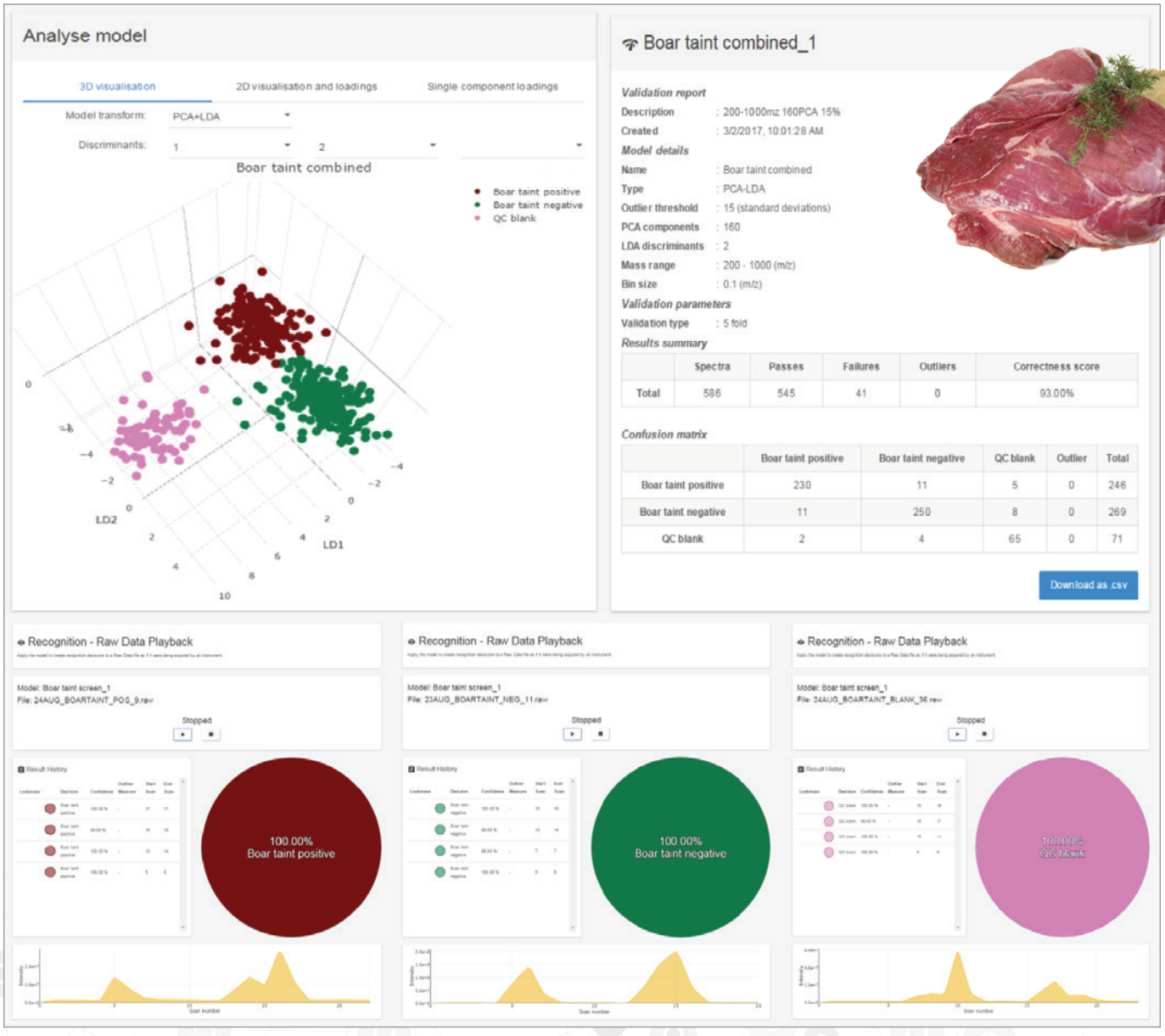

Figure 4. LiveID PCA/LDA model space generated for porcine fat populations screened positive for boar taint, negative for boar taint using ca.60 biological replicates and 250 spectra per class and fat from female animals using ca. 30 biological replicates and 70 spectra.

CROP SCIENCE

Today, a primary concern for scientists in the field of agronomy and crop science is to enhance grain and seed nutrition. In addition, a considerable research effort is now focused on increasing the amount and quality of food via selective breeding and genetic modification techniques (e.g. producing crops resistant to abiotic stress factors such as drought, flooding and extreme temperatures).

The control of grass weeds represents a major challenge to sustainable intensification in arable agriculture. Consequently, there can be considerable variation in crop yield. As weed populations differ in their tolerance to herbicides, methods to discriminate between them using rapid phenotyping technologies are of increasing interest to scientists.

REIMS as a direct analysis technique allows rapid, *in situ* characterization of plant tissue. The example below shows the direct analysis of weed grass leaves for the identification of species, populations, and phenotypic traits based on profiling low molecular weight metabolites.

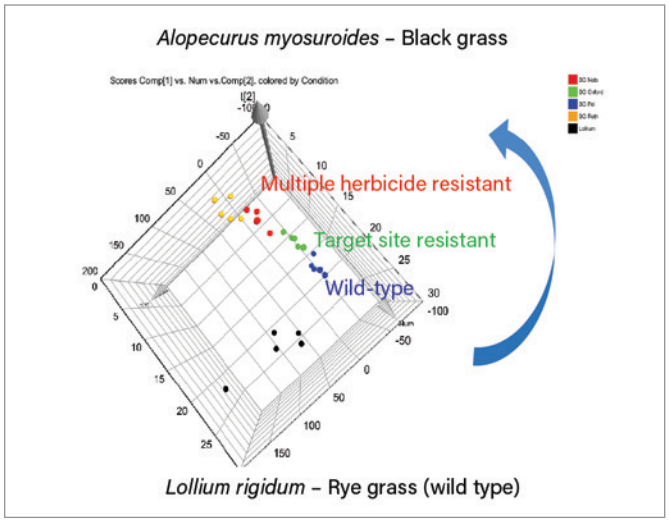

Figure 5. Progenesis QI 3D OPLS plot showing the different groups obtained following REIMS profiling of wild type rye grass, wild type, target site resistant and multi-herbicide resistant populations of black-grass populations.

WATERS LABORATORY INFORMATICS SOFTWARE

LiveID: Train and validate statistical models in real time

LiveID is a web-based application platform developed for a direct analysis workflow enabling users to train and validate statistical models using characterized samples of known origin within a short timescale. In combination with REIMS, LiveID can address complex analytical challenges such as food authenticity, speciation and plant phenotyping – while providing answers in real-time. LiveID takes high resolution mass spectra acquired from a test sample run on Waters SYNAPT or Xevo platform and performs recognition to classify the sample as belonging to one of a number of user-defined sample types or groupings.

Progenesis QI – Multi-variant software platform for metabolomics and lipidomics analysis

Progenesis QI is a powerful multi-variant software platform that allows scientists to rapidly, objectively, and reliably discover compounds of interest from samples using multi-group experimental design. With support for all common vendor data formats and a guided workflow, Progenesis QI Software helps you to overcome data analysis challenges, enabling you to rapidly, objectively, and reliably discover compounds of interest and export results for 'omics' research applications.

WATERS GLOBAL SERVICES

Delivering world renowned services and support

Waters Service and Support offerings are tailored to optimize your laboratory productivity while addressing your budget realities. Our offerings help maintain system peak performance, minimize down time, address scientific application challenges, and support stringent compliance requirements. As your services and support provider, we are committed to the success of your laboratory and business.

Waters quality support and consultative services ensure your success wherever your laboratory is located in the world.

Confirmit ACE AWARDS
Achievement in Customer Excellence

Waters has consecutively earned the ACE Award since 2001 for providing best-in-class technical knowledge, issue resolution, and process support.

Reference

1. *Pardo MÁ, Jiménez E, Pérez-Villarreal B. Misdescription incidents in seafood sector. Food control. 2016;62(1):277-283.*

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