

**September 7, 2022 (14:45-15:30)**



**VENDOR SEMINAR:**

## **Developments in Food Safety and Trace of Origin Testing**

### **PART 1: FOOD SAFETY TESTING**

#### **From targeted to In Silico, the current state and future advancements of PFAS testing**

*Stephan Baumann, Academic Applied Segment Manager, Agilent Technologies, USA*

Greaseproof packaging often contains per and polyfluoroalkyl substances, (PFAS) and there are more than a hundred commercially available standards, and those tend to be expensive.

Tentatively identifying PFAS in food contact material (FCM) requires a screening instrument and annotation software. We introduced FluoroMatch software, which automates file conversion, chromatographic peak picking, blank feature filtering, PFAS annotation based on retention time, precursor masses and fragment masses, annotation ranking, and confidence assignment.

To aid interpretation by making homologous series more identifiable, we have added a Visualizer tool to the FluoroMatch suite of software utilizing Microsoft PowerBI.

This is the first application of FluoroMatch automated PFAS annotation using in-silico PFAS fragmentation to food packaging.

### **PART 2: TRACING ORIGIN**

#### **The metabolomics-based chemical fingerprint of foods: tracing origin and post-harvest operations of nuts and wine**

*Luigi Lucini, Università Cattolica del Sacro Cuore, Piacenza, Italy*

The phytochemical profile of foods determines specific and peculiar quality traits, a condition determined by the combination of cultivar and terroir effects. Under the latter, we include pedoclimatic conditions, as well as agronomic and post-harvest operations that arise from tradition and local practices.

The comprehensive nature of untargeted metabolomics through UHPLC-ESI/QTOF mass spectrometry, followed by appropriate multivariate statistics (both unsupervised for naïve patterns and supervised modelling) allows elucidating the effect of different pre- and post-harvest factors.

A representative case referring to hazelnuts from different geographic origins and different cultivars, following optimal and non-optimal post-harvest conditions, and following different shelf-life conditions, will be discussed. The work will elucidate specific effects and highlight as the outcome of shelf-life primarily depends on post-harvest storage.

A second case-study, dealing with the wine Amarone, will discuss the effect of berries drying conditions and yeast genotype on the distinct chemical signatures of the resulting wine.