Thermo Scientific Orbitrap GC-MS HRAM Flavor and Fragrances Library

Flavors and fragrances analysis aims to give a comprehensive characterization of samples to determine their origin (natural or synthetic), assess their quality, ensure product consistency, and comply with regulatory standards. This analysis is crucial for industries such as food, beverages, cosmetics, and perfumery to develop and maintain consistent product formulations and control. With such a high number of possible compounds, a library is an essential tool to support compound identification within a fast time frame. The Thermo Scientific™ Orbitrap™ GC-MS Flavor and Fragrances Library is a high-resolution, accurate-mass (HRAM) spectral library for electron ionization (EI) GC-MS. It contains 411 compounds, which cover over eleven different chemical classes.

When used in combination with powerful Orbitrap technology and data processing tools such as Thermo Scientific™ Compound Discoverer™ software, accurate flavor and fragrance identification can be quickly achieved. The Thermo Scientific™ Orbitrap Exploris™ GC mass spectrometers provide unique advantages for flavor and flagrance analysis over alternative instrumental techniques. Orbitrap technology allows analytical chemists to gain data certainty and achieve unprecedented selectivity using a full-scan acquisition, enabling:

- The targeting of an unlimited number of analytes down to triple quadrupole level detection limits
- Identification of unknowns driven by spectral matching and sub-ppm mass accuracies
- Retrospective screening of compounds not known to be of interest at time of acquisition

Furthermore, the consistent sub-ppm mass accuracy delivered by the system, regardless of peak intensity, allows for confident targeting of compounds within narrow mass accuracy windows. The Thermo Scientific Orbitrap GC-MS Flavor and Fragrances Library enables a rapid and customizable set-up of a screening method, which allows users to quickly implement this powerful technology. Included in this Library are:

- High-resolution, accurate-mass spectral library acquired at 60,000 mass resolving power (FWHM *m/z* 200)
- Spectra for 411 flavor compounds across eleven categories refined and curated with elemental composition of each EI fragment verified (Figure 1)
- Compound information list showing chemical categories, odors, rendition index values, and GC column types used
- Kovats retention index entries
- Can be used in combination with existing unit mass libraries.

The Orbitrap GC-MS Flavor and Fragrances Library can be used to quickly apply the theoretical masses for each analyte into a Thermo Scientific™ TraceFinder™ software fullscan screening or quantitation processing method. Also included for each compound is an accurate mass reference spectrum acquired on an Orbitrap GC-MS system at 60,000 resolving power.

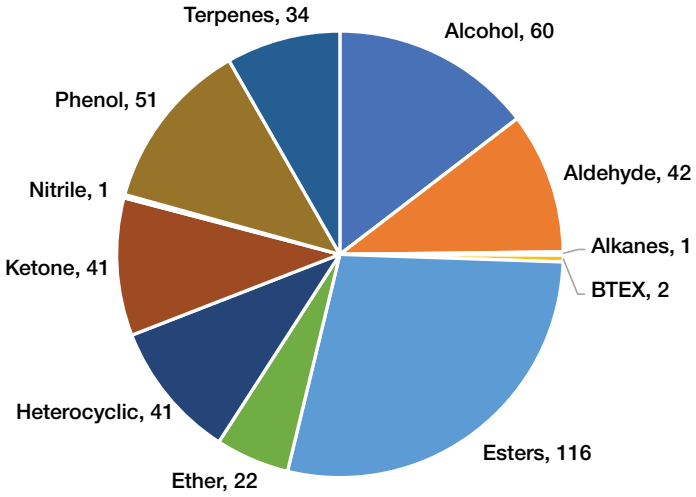

Figure 1. Pie chart of the eleven flavor and fragrance categories with the number of compounds in each labelled

This spectral library can be used as a standalone reference or in conjunction with the unknowns screening functionality of Compound Discoverer software (Figures 2 and 3) or TraceFinder software. Each software utilizes chromatographic deconvolution followed by accurate mass spectral library search to identify untargeted compounds.

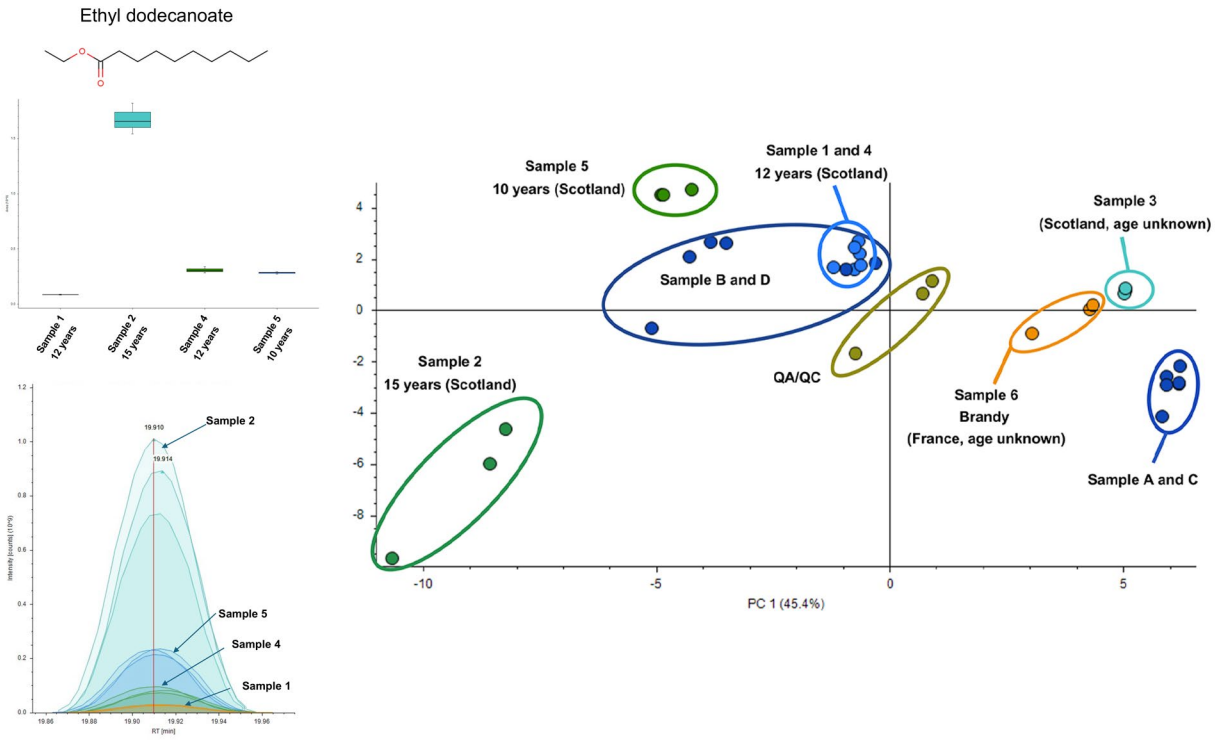

Figure 2. Compound Discoverer software provides extensive functionality for peak deconvolution, statistical analysis (PCA, boxplot shown for a whisky profiling study), and library matching using both nominal mass libraries such as NIST or high-resolution, accurate-mass libraries such as the Orbitrap GC-MS Flavor and Fragrances Library

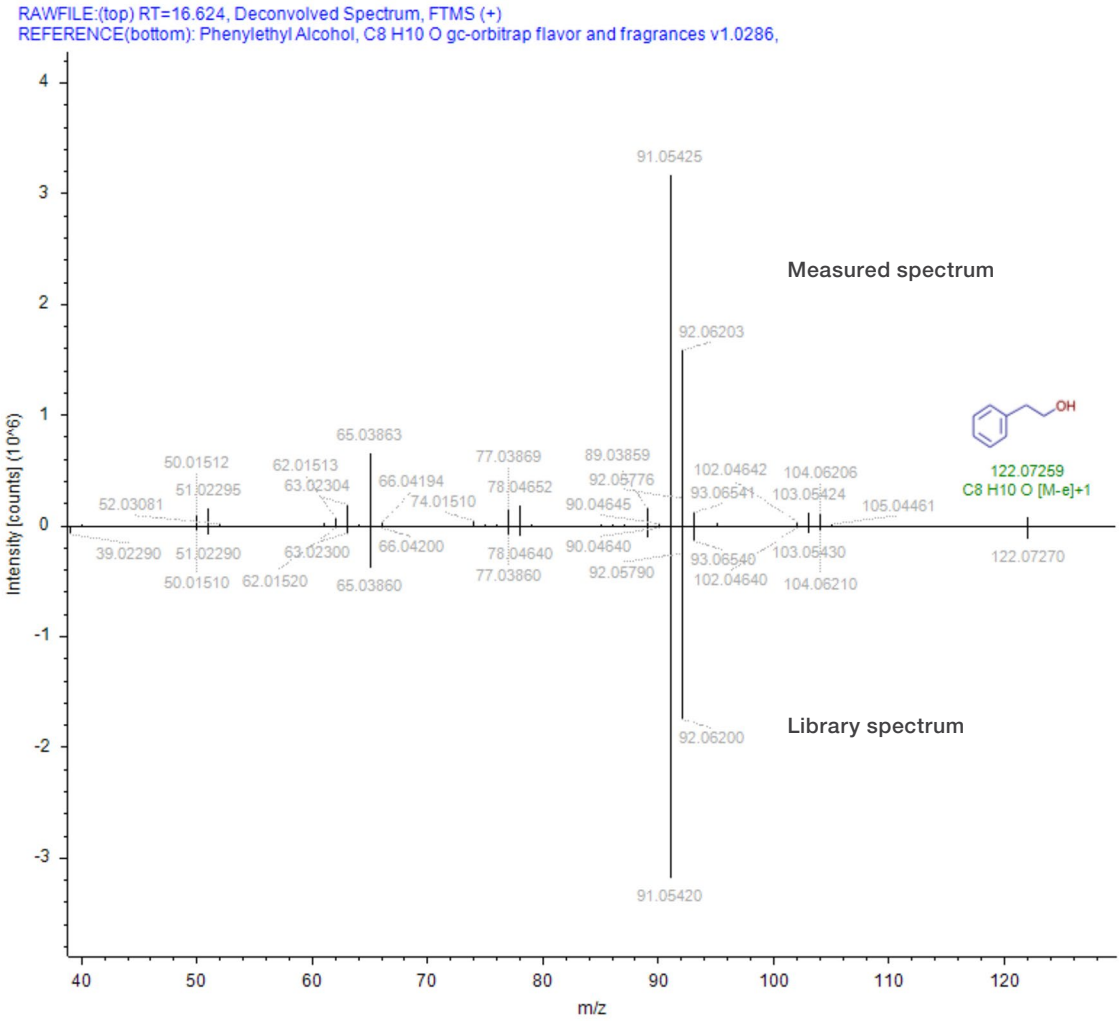

Figure 3. Phenylethyl alcohol in whisky extract library match in Compound Discoverer software to the Orbitrap GC-MS Flavor and Fragrances Library. The upper spectrum is the measured and lower spectrum is the library entry.

Acknowledgement

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