Orbitrap GC-MS

Thermo Scientific Orbitrap GC-MS HRAM contaminants library

The Thermo Scientific™ Orbitrap™ GC-MS Contaminants Library is a high resolution accurate mass (HRAM) spectral library for electron ionization (EI) GC-MS. It contains more than > 1200 spectra. When used in combination with powerful Orbitrap technology and unique Thermo Scientific software data processing tools including Thermo Scientific Compound Discoverer™, the complex challenges of contaminant identification become fast and accurate.

Using the Thermo Scientific™ Orbitrap™ Exploris GC Mass Spectrometers for the analysis of food and environmental contaminants has unique advantages over alternative techniques. Orbitrap technology allows analytical chemists to gain data certainty, achieve unprecedented selectivity and dynamic range 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 to easily meet regulatory requirements governing full-scan accurate mass screening. The Thermo Scientific Orbitrap GC-MS Contaminants Library contains tools that support a rapid and customizable set-up of a contaminants screening method which allows users to quickly implement this powerful technology. Included in this Contaminants Library are:

- High-resolution, accurate-mass spectral Library acquired at 60,000 mass resolving power (FWHM *m/z* 200).
- >1200 spectra refined and curated with elemental composition of each EI fragment verified.
- Thermo Scientific™ TraceFinder™ Compound Database of 948 food and environmental contaminants.
- Kovats retention index entries
- Can be used in combination with existing unit mass libraries.
- A user guide detailing how to install and make custom enhancements to the library

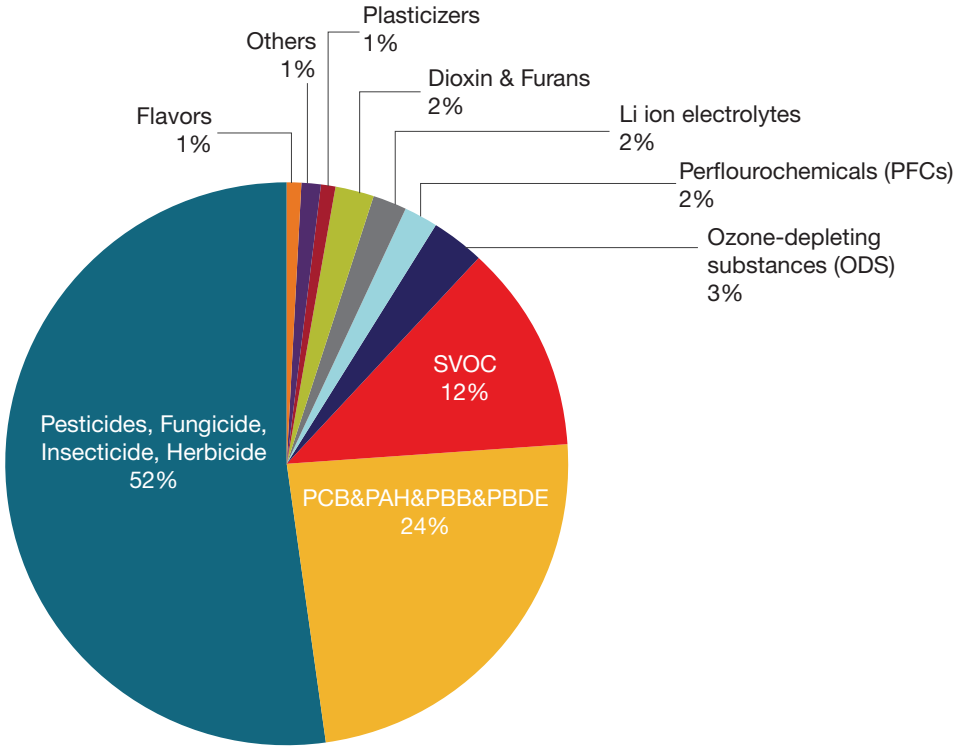
Compound classes included in the library are:

- Pesticides
- PAHs
- PCBs
- Dioxins and Furans
- Flame Retardants
- Plasticizers
- Lithium ion electrolytes
- Flavours
- Additional common environmental contaminants

The Orbitrap GC-MS Contaminants Library version 1.5 has over 1200 spectra, including over 500 pesticides. For each compound in the CDB, theoretical and observed masses are determined in the curated database, determined from curated Orbitrap GC-MS data, is included. The Contaminants Library can be used to quickly pull the theoretical masses for each analyte into a TraceFinder full-scan screening or quantitation processing method.

Also included for each compound is an accurate mass reference spectrum acquired on an Orbitrap GC-MS system. This spectral library can be used as a standalone reference or in conjunction with the unknowns screening functionality of Compound Discoverer or TraceFinder TraceFinder, which utilizes chromatographic deconvolution followed by accurate mass spectral library search to identify untargeted compounds.

Finally, a User Guide assists with the quick set-up of a customizable Compound Database and Spectral Library. It also details how the user can expand their library by uploading additional compounds acquired on their Orbitrap GC-MS system.



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