Thermo Scientific Orbitrap GC-MS Contaminants Library

Using the Thermo Scientific™ Orbitrap™ GC-MS systems for the analysis of pesticides and other food and environmental contaminants has unique advantages over alternative techniques. This technology allows analytical chemists to achieve comparable sensitivity, selectivity and dynamic range performance to GC triple quadrupole technology using an untargeted 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:

- A Thermo Scientific™ TraceFinder™ Compound Database of over 700 food and environmental contaminants
- A high-resolution, accurate-mass Spectral Library of over 700 food and environmental contaminants
- 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
- Additional common environmental contaminants

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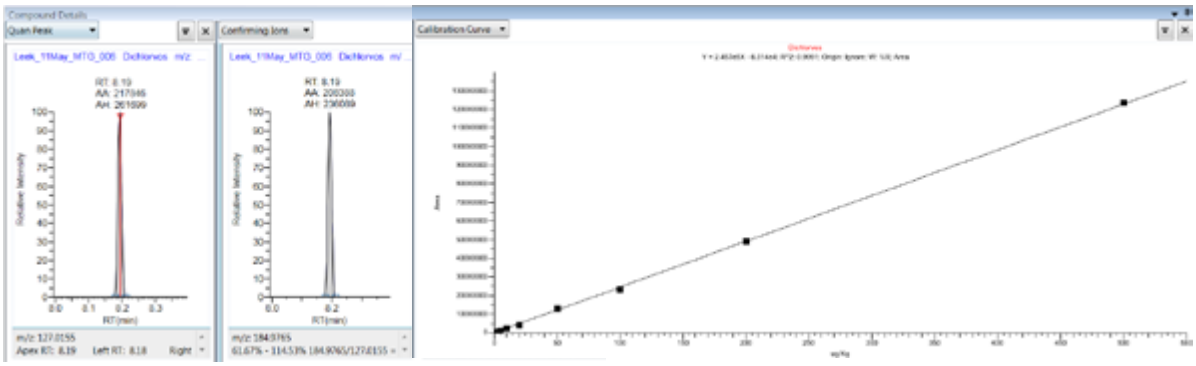
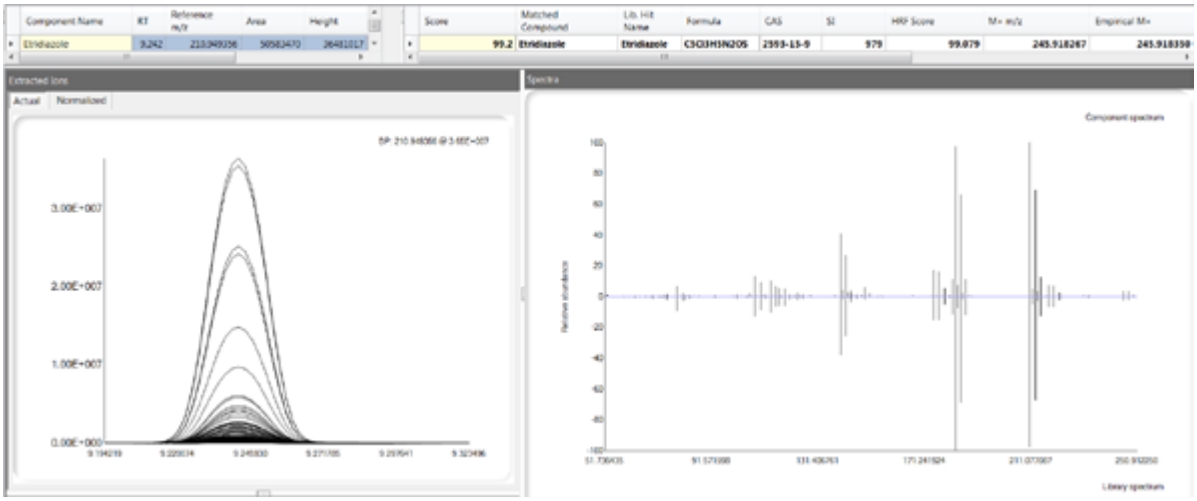
The Orbitrap GC-MS Contaminants Library has over 700 compounds, including 500 pesticides. For each compound in the library, the theoretical exact mass of major ions, determined from curated Orbitrap GC-MS data, is included. The Contaminants Library can be used to quickly pull the theoretical masses for each analyte into a TraceFinder full-scan targeted 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 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.



TraceFinder view of leek matrix matched calibration curve of dichlorvos (0.5-500 µg/Kg) including extracted quantifier and qualifier ions at 1 µg/Kg. Acquired using 60K resolution at *m/z* 200.



Etridiazole automatically detected and identified in a QuEChERS extracted apple matrix using TraceFinder through chromatographic deconvolution followed by library match against the Contaminants Library.

Find out more at **www.thermofisher.com/ExactiveGC**

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