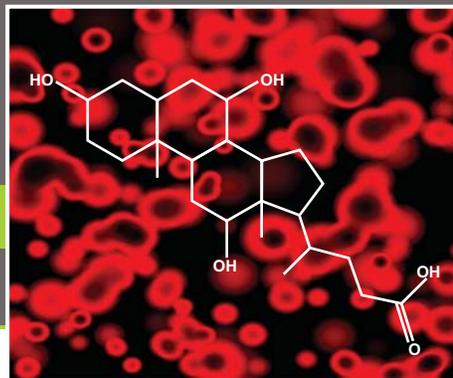


LECO/Fiehn Metabolomics Library



Fully integrated into ChromaTOF® brand software, it's the perfect tool for metabolite identification.

Over 1100 spectra of 700 unique metabolites are contained within the library, along with retention indices based on a series of fatty acid methyl esters (FAMES). The library identifies the underivatized name and structure of each metabolite while providing one or more spectra following derivatization. Developed through a unique partnership with Dr. Oliver Fiehn, this extensive and expandable library was obtained using a LECO Pegasus® HT GC-TOFMS in his laboratory at the University of California-Davis.

The sensitivity and robust data acquisition of the Pegasus HT GC-TOFMS make it ideal for the daily profiling of human, plant, or microbial metabolites. *ChromaTOF* features such as Automated Peak Find and True Signal Deconvolution® extract and process the large amounts of data that are obtained through time-of-flight mass spectrometry. The LECO/Fiehn Metabolomics Library assists the user in identifying the hundreds of metabolites that are detected through the deconvolution of coeluting peaks.

The Most Powerful Metabolomics Library Available

The LECO/Fiehn Metabolomics Library represents the largest GC-TOFMS Metabolomics Library currently on the market. Because of the amount of data acquired and utilized by the *Pegasus*, this library differs from those that have been developed using quadrupole GCMS.

"The Fiehn library empowers researchers for unambiguous identification of hundreds of metabolites by complementing mass spectral matching with a retention index that is based on FAME-RI markers," says Dr. Fiehn. "Since spectra of isomers are often hardly distinguishable by mass spectra alone, the information on retention indices is critical for truthfully reporting metabolite identities."

To order, or receive pricing information, contact your LECO sales representative, and refer to part number 359-008-100.

PubChem

The LECO/Fiehn Metabolomics Library also contains hyperlinks to the PubChem online database, providing an opportunity for the user to gain even more detailed information on structures of less familiar underivatized compounds. The PubChem database can also help users stay compliant within the reporting standards of the Metabolomics Society. In addition to requiring at least two independent parameters to authenticate a metabolite (such as RI or mass spectrum), the standards of the Metabolomics society also require annotation by a recognized standard, of which the PubChem number is an acceptable source.

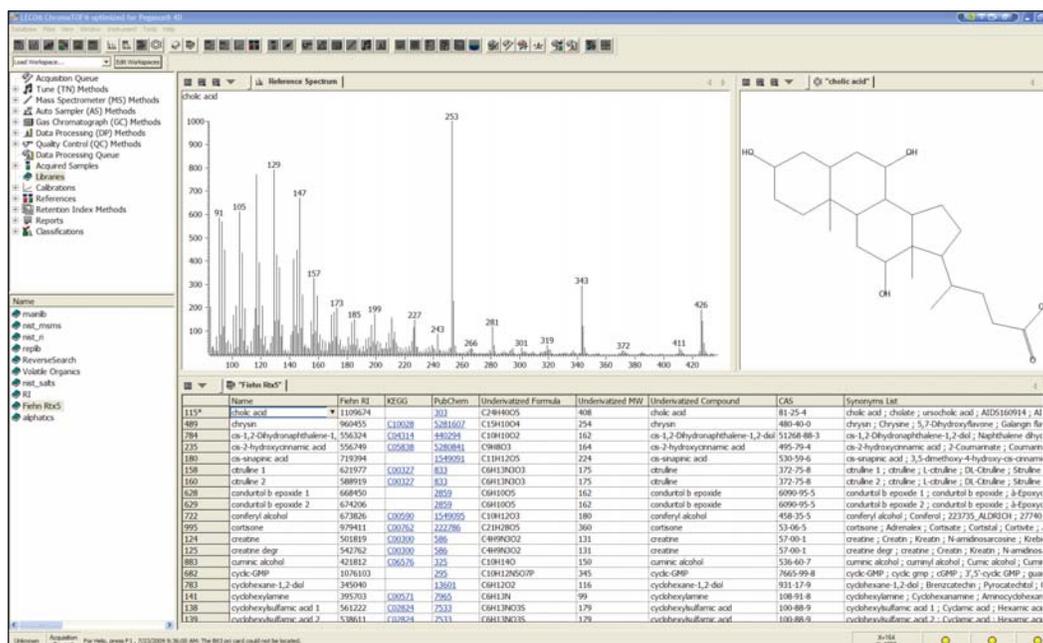
Visible Spectra

Spectra within the library are visually easy to identify thanks in part to a spectral cut within ChromaTOF that eliminates the abundant m/z 73 for the trimethylsilyl group, a product of derivatization. Since this group does not carry helpful information for identification, removing it allows only the more relevant information to be searched, resulting in improved library matches.

Continued Expansion

The LECO/Fiehn Metabolomics Library continues to be used in Dr. Fiehn's laboratory, and continues to expand in volume. Pegasus users also have the option of downloading BinBase, an open-source profiling database created by Dr. Fiehn's research team.

"This database runs all metabolomic studies in the Fiehn laboratory," says Dr. Fiehn, "and the GC-TOF Fiehn library is the most used underlying tool for metabolite identification."



Sample screen capture for Cholic Acid, one of 700 metabolites featured in the library. Data can be display in a variety of different ways according to user preference.

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