Fiehn GC/MS Metabolomics RTL Library

# IDENTIFY MORE METABOLITES

The Measure of Confidence

Agilent Technologies

## A Comprehensive GC/MS Solution for Metabolite Identification

To further facilitate identification of known metabolites through untargeted metabolomics, Agilent Technologies now offers the Fiehn GC/MS Metabolomics RTL Library (2013 Edition). This updated, retention time locked (RTL), metabolomics-specific library was developed in collaboration with the laboratory of Dr. Oliver Fiehn. It contains searchable GC/MS EI spectra and retention time indexes for 1,400 entries that is approximately 40% larger than the 2008 library.

### Key features of the Fiehn GC/MS library include:

**More robust identification**—includes an improved chromatographic methodology with an improved hardware configuration, enabling more compound identifications

**Expanded library**—contains searchable GC/MS EI spectra and retention time indexes for 900 common metabolites with over 1,400 entries

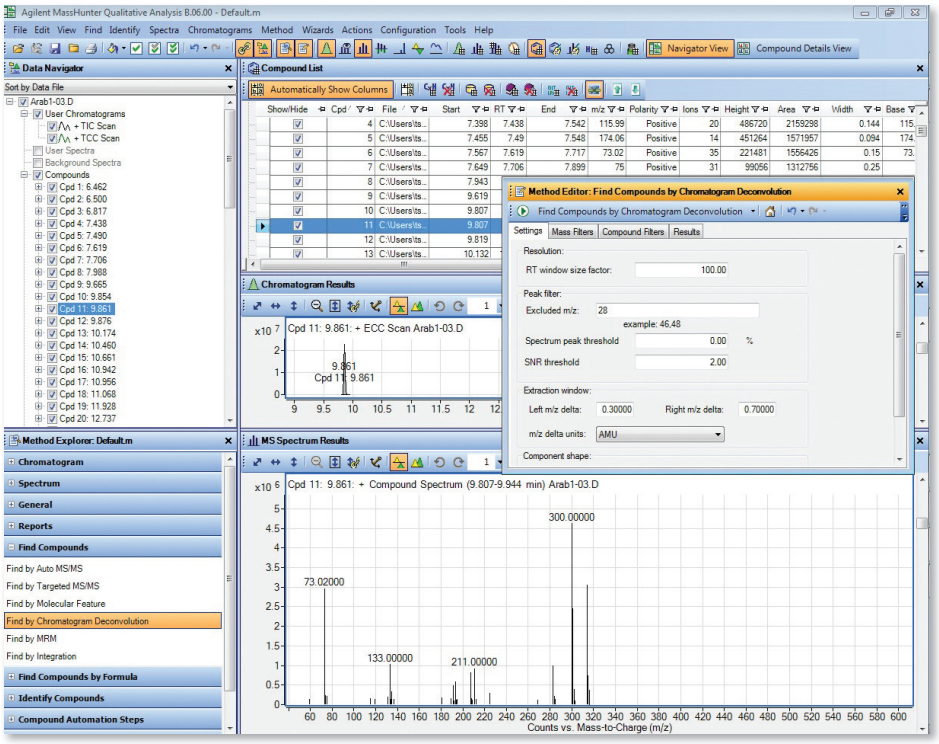
**Easy-to-use workflow**—comes with complete, preprogrammed GC/MS analytical methods with documentation to maximize research success

**Powerful software**—fully supported on MassHunter, ChemStation Data Analysis, and AMDIS software

# THE MOST COMPREHENSIVE METABOLOMICS GC/MS SPECTRAL LIBRARY

## Expanded library for more compound identifications

The Fiehn GC/MS Metabolomics RTL Library (2013 Edition) is the most comprehensive library of metabolite GC/MS spectra that is commercially available. This expanding library currently contains approximately 900 common metabolites with over 1,400 entries, including entries corresponding to partially derivatized metabolites for those metabolites that do not always derivatize completely. Each entry includes a searchable EI spectrum and retention index. It also includes the name and CAS number of the native molecule for easier compound recognition and subsequent literature or software searching.




Agilent MassHunter Qualitative Analysis software supports peak finding of GC/MS data files, and compound identification via library matching.

# HIGHER QUALITY DATA WITH GC BACKFLUSHING

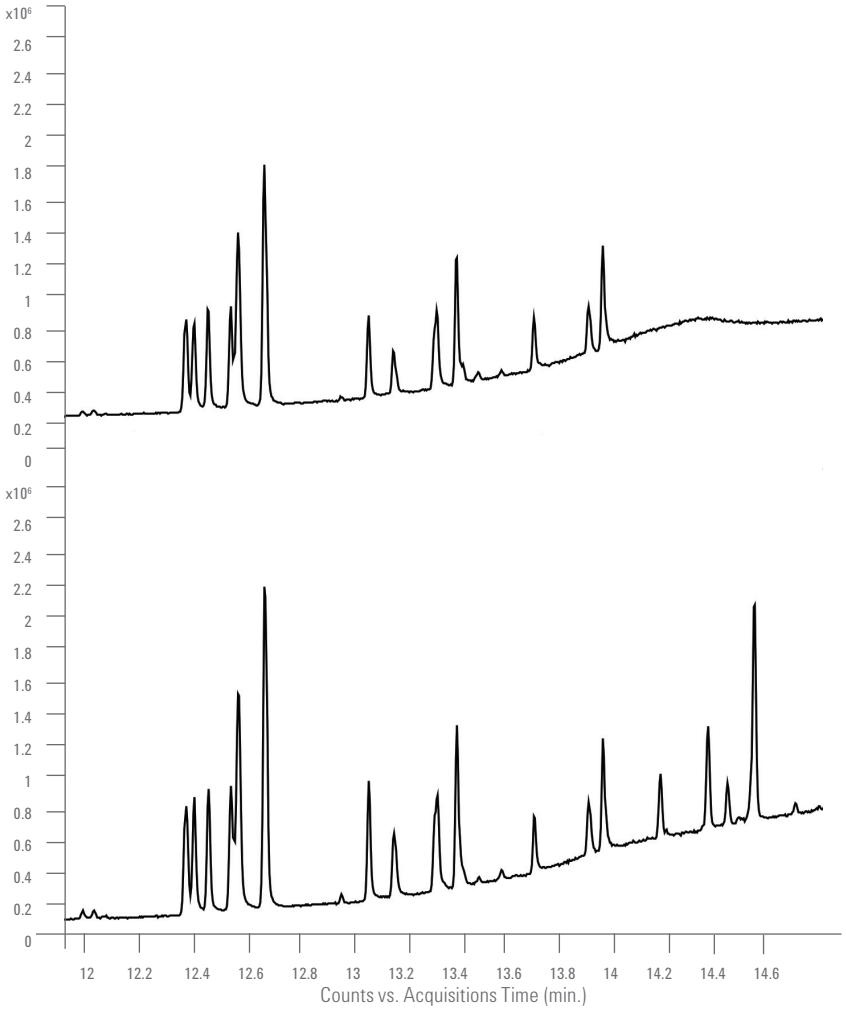
## Higher analytical integrity of data collection using "backflushing"

Installation of a Pressure Controlled-Tee (PCT) provides greater productivity, higher-quality data, simpler and faster servicing of critical GC components. For example, late eluting compounds, such as higher boiling components (e.g., triglycerides, cholesterols, larger lipids), are removed from the column by "backflushing" before they can compromise the MS source or the next analysis through carryover. This ensures higher analytical integrity of data collection as both the column phase and the MS source are protected.

- Stable retention times
- Easy maintenance; ventless point of inlet
- Reduction of run-to-run carryover

## Rugged and Robust Methods

The Fiehn GC/MS library takes advantage of retention time indexing and RTL to achieve higher confidence in search results. Retention indexing and the use of retention ladder compounds—internal standards with well-spaced retention times—allow for the use of chromatographic retention as an independent criteria even after making significant method changes. Inclusion of RTL in the method reduces run-to-run retention time variability, as well as the frequency of including a retention time ladder such as FAMES.

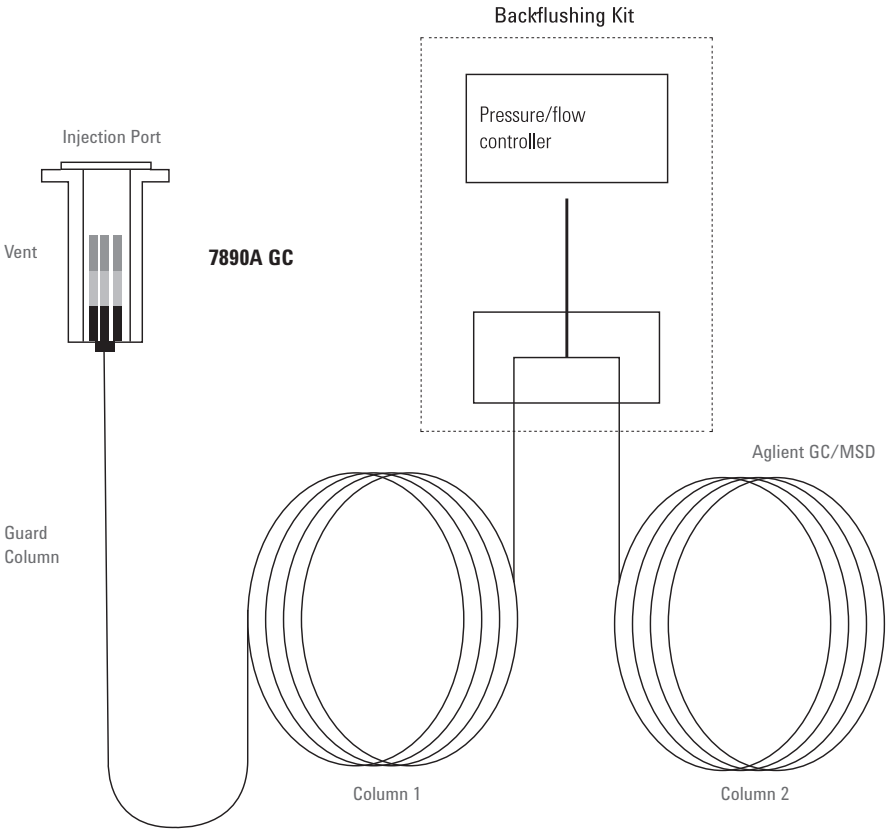



The new "Backflushing" method facilitates selective removal of late eluting compounds. The chromatograms show two runs that used this technique, where selective removal of cholesterols through parameter optimization is achieved in the top panel.

# AGILENT'S COMPREHENSIVE GC/MS METABOLOMICS SOLUTION PACKAGE

Agilent has created various kits, columns, and special connection parts to help you implement your metabolomics workflow efficiently and quickly:

- Rapid Universal GC/MS Backflushing Kit with pressure-controlled tee (Part Number G1472A)
- Guard column: Deactivated 0.32-mm id x ~ 1.5 m (Part Number 160-2325-10)
- Columns 1 & 2:  DB-5msUI 15-m x 0.25-mm id x 0.25-µm (Part Number 122-5512UI)
- Agilent Fiehn GC/MS Metabolomics Standards Kit (Part Number 400505)

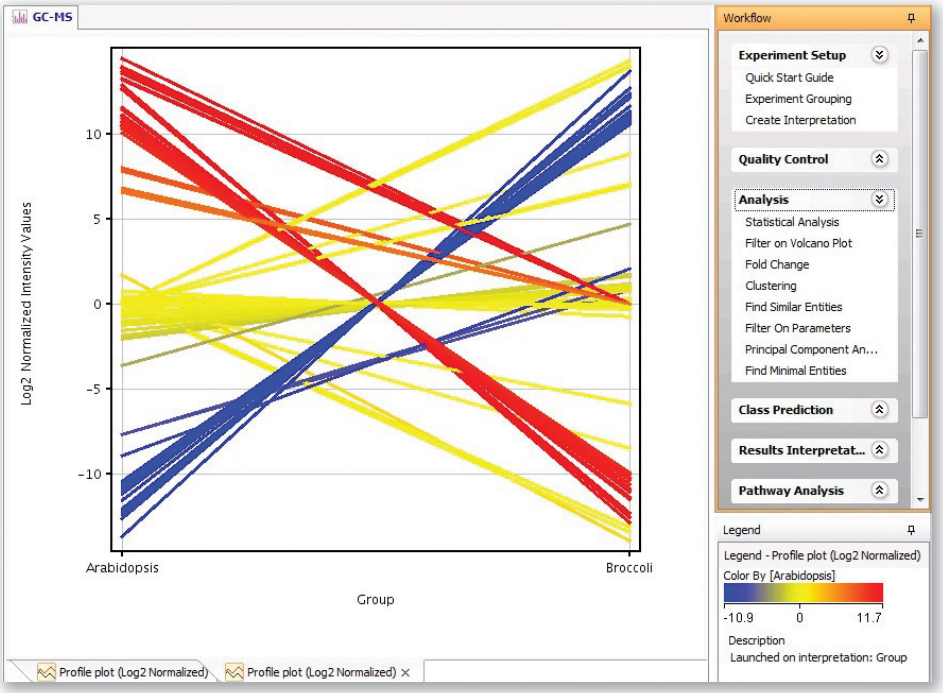



Backflushing control is achieved by interrupting two GC columns with a Pressure Controlled Tee (PCT).

# EASILY ANALYZE AND VISUALIZE GC/MS RESULTS IN MASS PROFILER PROFESSIONAL

## Complete workflow for more successful research

In addition to finding and identifying metabolites through library searching, the Fiehn GC/MS library includes extra features that help you through the entire workflow for untargeted metabolomic studies. Following feature finding in MassHunter Qualitative Analysis software, .xml formatted files can be saved and easily imported into MPP for differential analysis.




GC/MS results can be imported into MPP. A Profile plot shows clear differential abundances between Arabidopsis and Broccoli metabolites.

## Pathway Analysis facilitates biological interpretation

The Agilent Pathway Architect module, used together with MPP, allows the user to build a Single Experiment Analysis (SEA) or a Multi-Omic Analysis (MOA) workflow to find pathways enriched with compounds that match the list of entities in your experiment.

# POWERFUL DATA ANALYSIS AND FAST, FLEXIBLE, HIGH-THROUGHPUT SEARCHING

## Intuitive and powerful data analysis

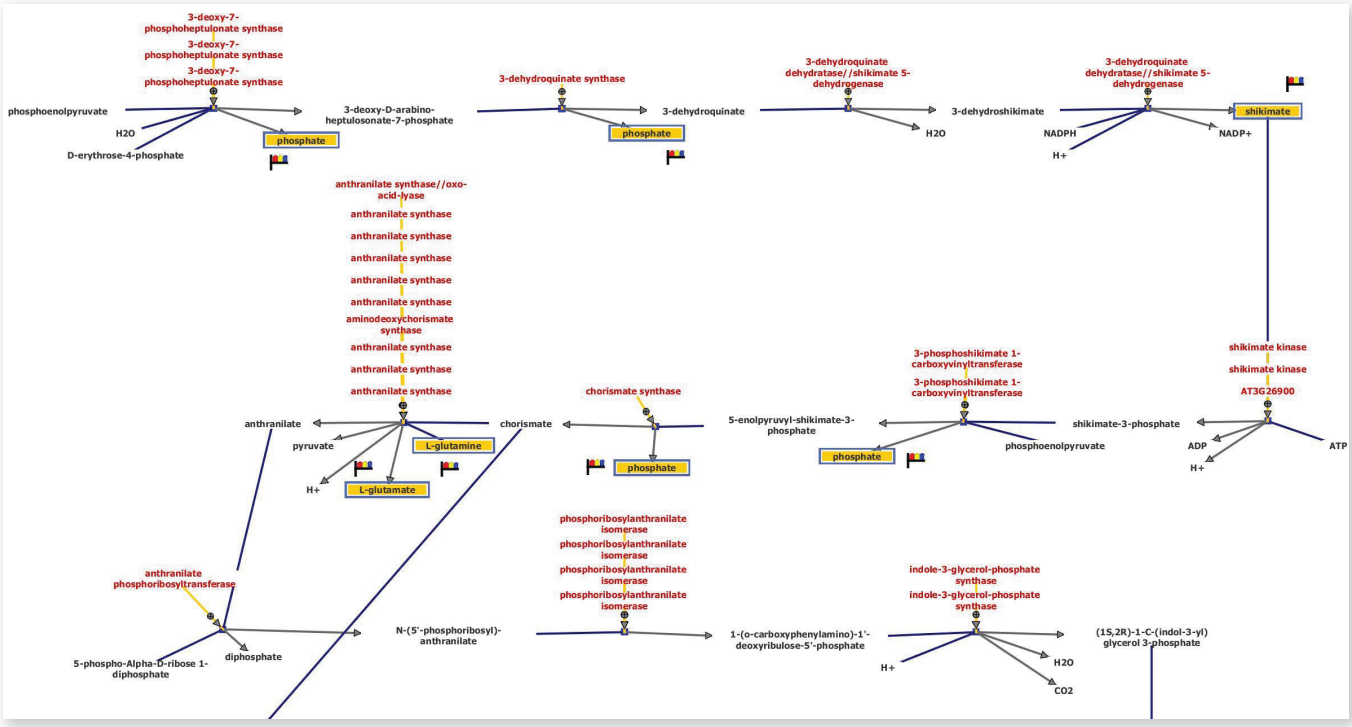
The Fiehn GC/MS Metabolite RTL Library (2013 Edition) is supported in the latest version of Agilent MassHunter Qualitative Analysis software. A proprietary algorithm, "Find by Chromatographic Deconvolution" is routinely used for peak finding. All the found features can subsequently be identified by loading and matching to the latest Fiehn GC/MS Metabolite RTL Library.

The new 2013 library comes with the well-known AMDIS—an automated GC/MS identification program from the U.S. National Institute of Standards and Technology. GC/MS data analysis methods are provided, which automatically invoke AMDIS to deconvolute merged chromatographic components and identify metabolites.

AMDIS results can also be imported into Agilent's MassHunter Mass Profiler Professional (MPP) software to take advantage of its powerful statistical analysis and data visualization capabilities.

## Easier Data Analysis Screening and Library Searches

The new 2013 library can also be searched using the native probability-based matching capabilities of the Agilent MSD Productivity ChemStation software. ChemStation methods for quantitative data analysis and qualitative screening are also provided.




The Pathway Architect module in MPP shows the results for projecting several metabolite abundance profiles onto organism specific biological pathways from MetaCyc.

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U.S. and Canada
**1-800-227-9770**
**agilent_inquiries@agilent.com**

Europe
**info_agilent@agilent.com**

Asia Pacific
**inquiry_lsca@agilent.com**


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