MassHunter Workstation B.04.00

METLIN Metabolite Personal Compound Database and Library for Accurate-Mass LC/MS

More confident identification of endogenous metabolites for metabolomics

METLIN PCD

- Includes masses, chemical formulas and structures for approximately 25,000 endogenous and exogenous metabolites, lipids, and di- and tri-peptides
- Many entries include CAS, HMP, LMP, or KEGG identifiers as well as web links to associated database entries
- Includes 679 compounds with retention times that have been determined using a standardized reversed-phase method providing more confident compound identification by using accurate mass and retention time (AMRT)

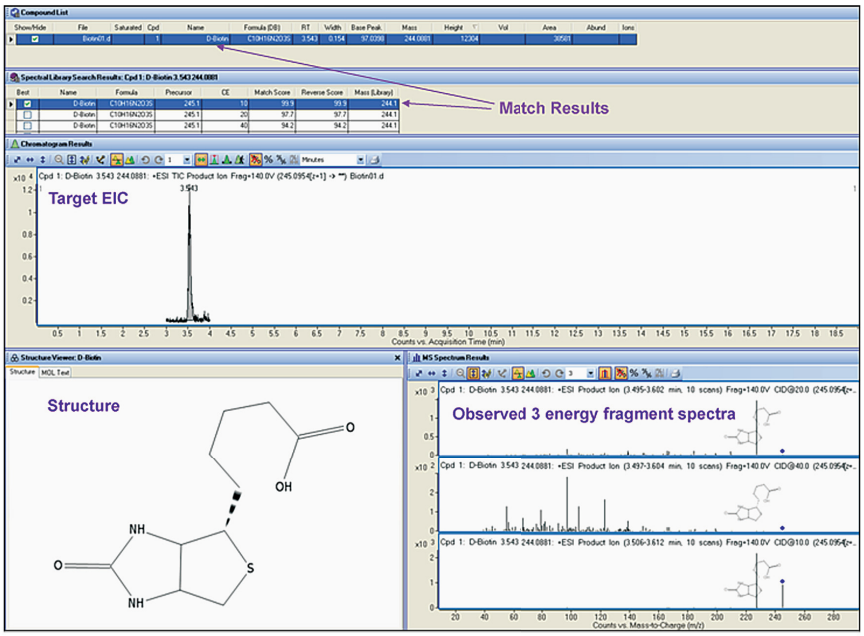
METLIN PCDL

- Includes all compounds contained in METLIN PCD, and additionally accurate mass Q-TOF MS/MS library reference spectra for 2278 compounds
- Generates higher confidence compound ID by matching unknown Q-TOF MS/MS spectra to the spectral library

Identify endogenous metabolites with confidence using METLIN Metabolite Personal Compound Database and Library

Compound identification is a key element in untargeted metabolomics experiments. The level of confidence in the identification is directly dependent on the quality of the database used to assign compound identity. The METLIN metabolite database, created by Gary Siuzdak, PhD, is one of the most comprehensive and widely used metabolite databases in the world today.

Agilent Technologies is the exclusive provider of the METLIN Personal Compound Database (PCD) and now the new accurate mass MS/MS Library (PCDL). The software resides on your local PC and facilitates faster, easier, compound identification for metabolomics research.



MS/MS Library match example – Biotin in positive ion mode

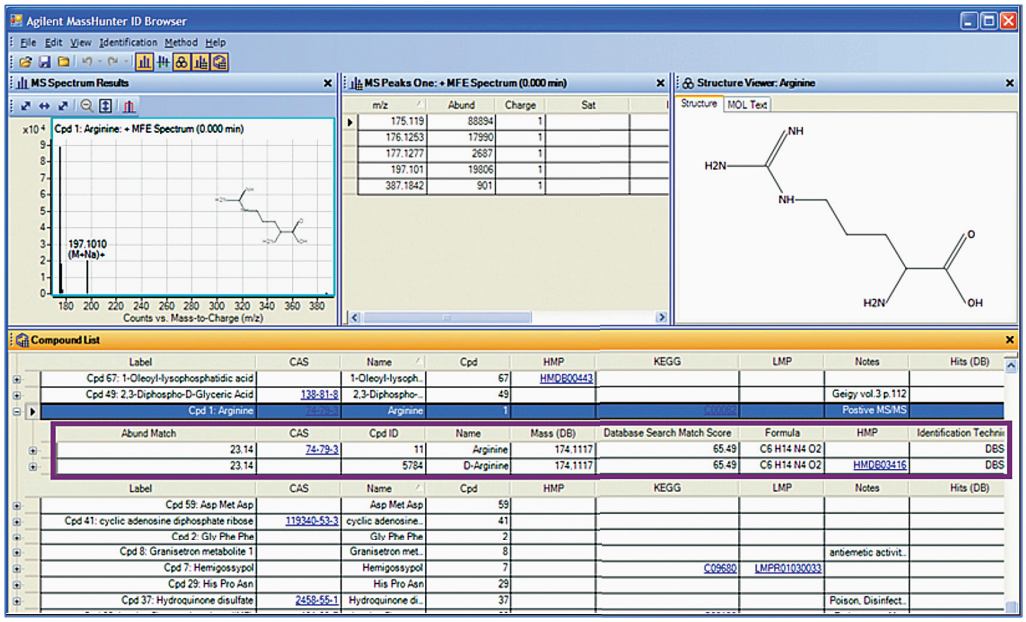
The Measure of Confidence

Agilent Technologies

Seamless Integration with Mass Profiler Professional (MPP)

Using a combination of advanced processing capabilities and powerful statistical and mathematical models to analyze complex MS data sets, MPP easily lets you classify, compare and analyze sample groups via differential analysis in metabolomics studies. MPP now runs in a Windows 7 as a native 64-bit application with capacity for faster processing and support for much larger sample sets.

MPP includes an integrated ID Browser that mirrors MassHunter's qualitative analysis functionality to allow identification using METLIN PCD for LC/MS TOF data and EI library for GC/MS data.



MassHunter ID Browser identifies compounds from an entity list generated by MPP. In this example, results for mass 174.1117 matched against the METLIN database reveals it to be arginine; molecular formula, database match score, name, KEGG and CASS ID are also shown.

Ordering information

G3849AA MassHunter Workstation for TOF/Q-TOF B.04.00 Upgrade
G3338AA MassHunter Workstation Offline Software B.04.00 Upgrade
G6825AA MassHunter METLIN Metabolite PCD
G3874AA MassHunter METLIN Metabolite PCDL
G3835AA MassHunter Mass Profiler Professional B.02.01
G1668AA High-End LC/MS PC Workstation (Windows 7, 64-bit)

www.agilent.com/chem/metlin

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