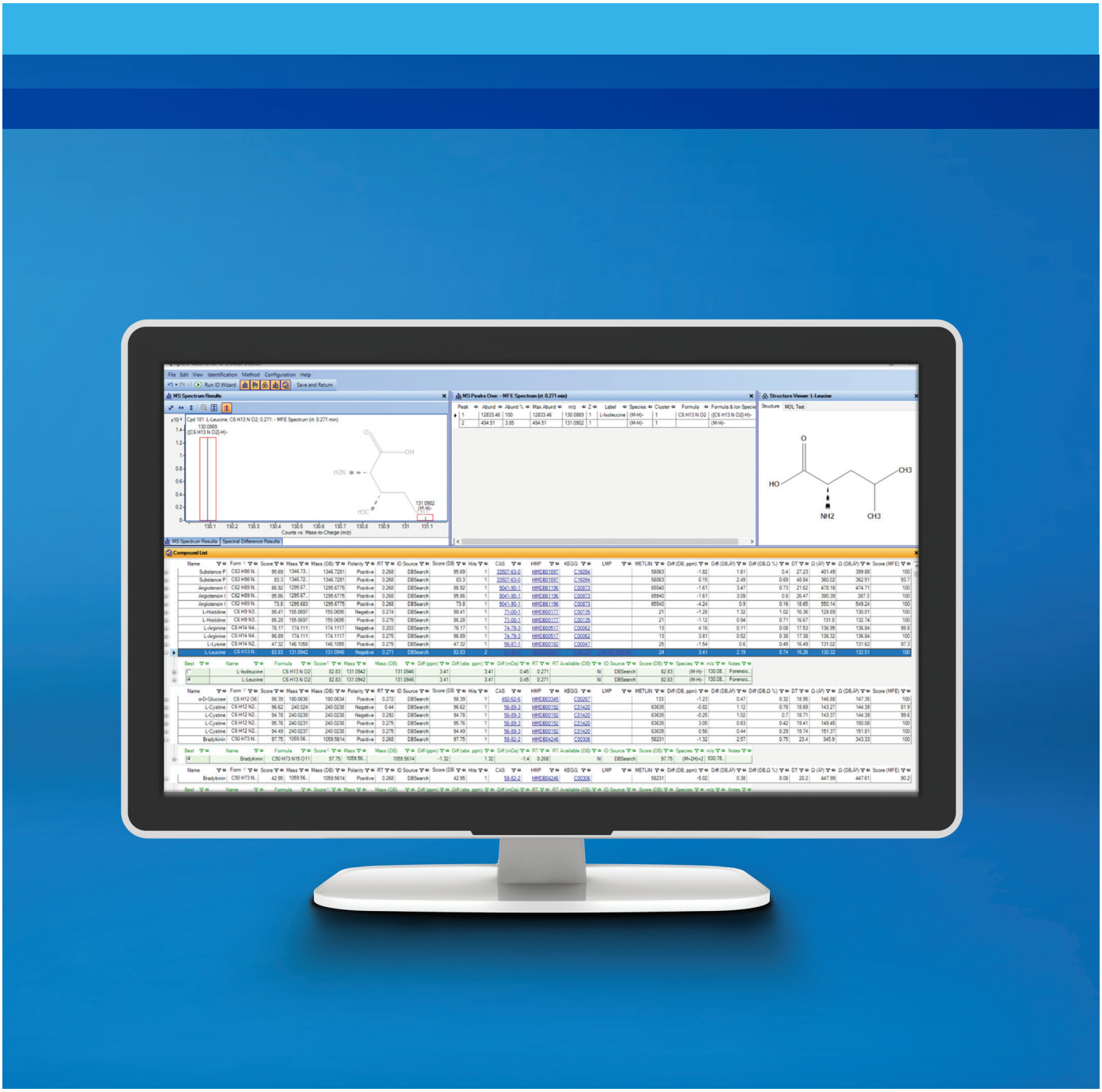
Agilent

Trusted Answers

Confident Metabolite Identification

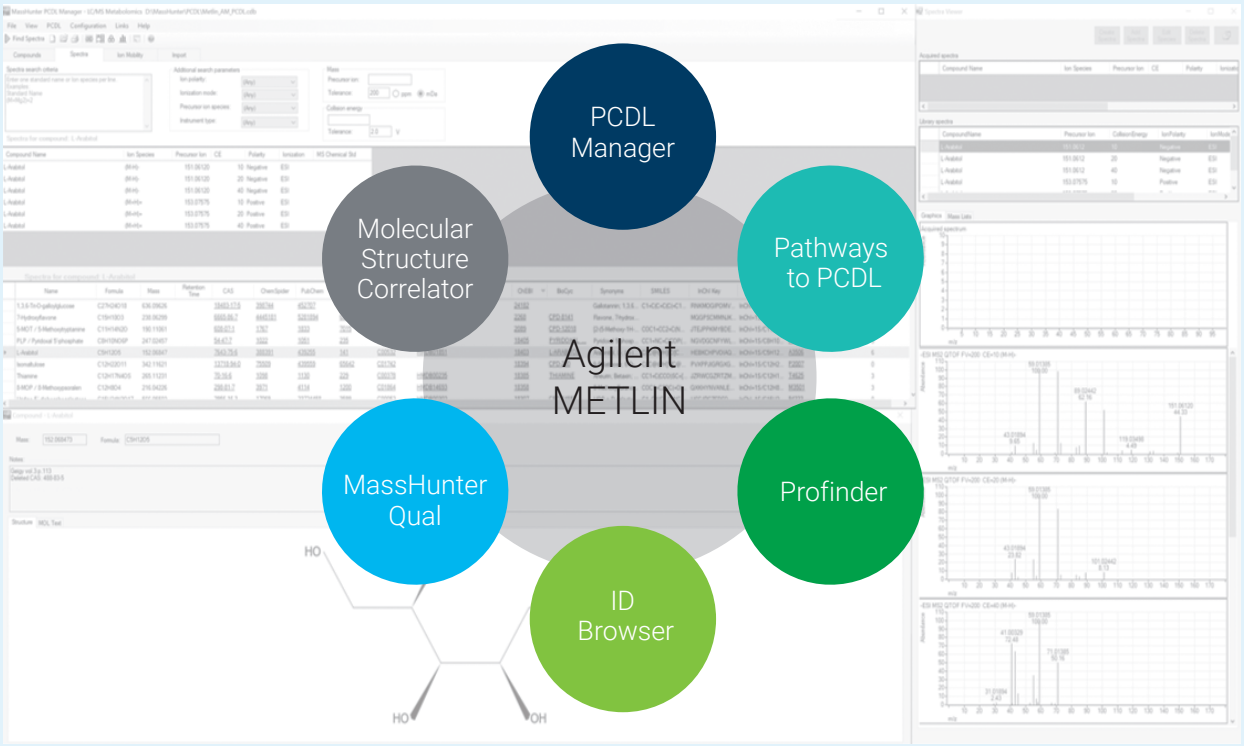
Agilent METLIN Metabolomics database and library



Agilent METLIN—developed for metabolomics research

Metabolite identification is a key element in discovery metabolomics experiments aimed at understanding the global metabolic changes that can occur in a biological system. Confidence in identification is directly dependent on the quality of the database used for metabolite identification. The Agilent METLIN Metabolomics database and library is highly curated to provide the greatest confidence and is one of the most and widely used metabolite databases. It is an integral part of Agilent's broad portfolio of software tools to address discovery metabolomics experiment needs.

Integrated workflows for metabolic identification



MassHunter MSC (Molecular Structure Correlator)—Correlate accurate mass MS/MS fragment ions with molecular structures

PCDL Manager—Personalize your database by adding retention times, metabolites, collision cross sections or MS/MS spectra

Agilent Pathways to PCDL—Create a pathway-specific database to target metabolic pathways of interest

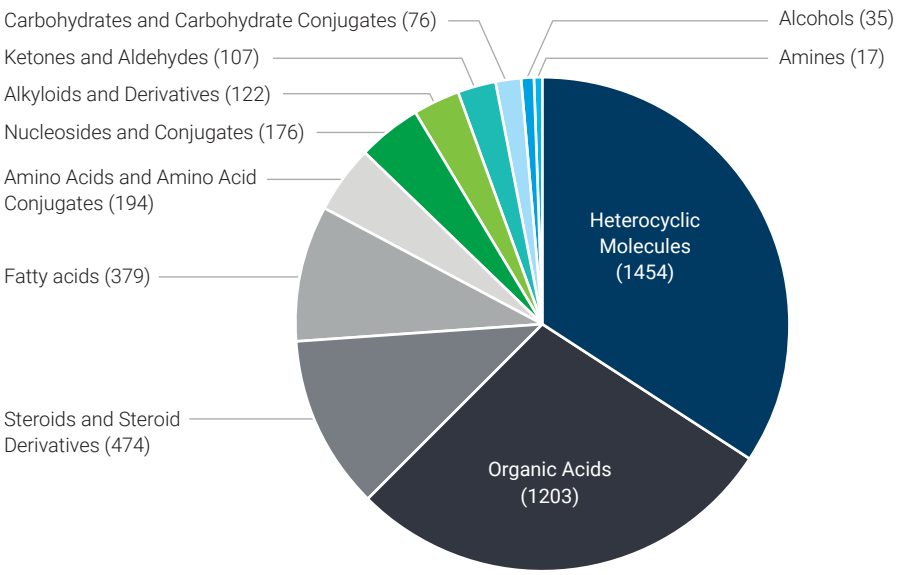
Profinder (including VistaFlux)—Extract metabolites of interest for targeted and flux analysis workflows

ID Browser—Identify metabolites after differential analysis by matching to the Agilent METLIN Metabolomics database and library using accurate mass, retention-time, isotope-pattern matching, collision cross section or MS/MS spectra

MassHunter Qualitative Analysis—Identify metabolites by matching to the Agilent METLIN Metabolomics database and library using accurate mass, retention-time, isotope-pattern matching or MS/MS spectra. Add custom MS/MS spectra to Agilent METLIN Metabolomics library from user-acquired data.

Confident results from high quality content

Agilent METLIN Metabolomics database and library is an integral part of the comprehensive MassHunter portfolio enabling confident identification of a range of metabolites relevant for your research.



The Agilent METLIN Metabolomics database and library contains a wide range of metabolites. The pie chart above shows the distribution of non-lipid metabolites contained in the database based on HMDB's classification scheme. This chart excludes the 38,000 lipids in the Agilent METLIN Metabolomics database and library.

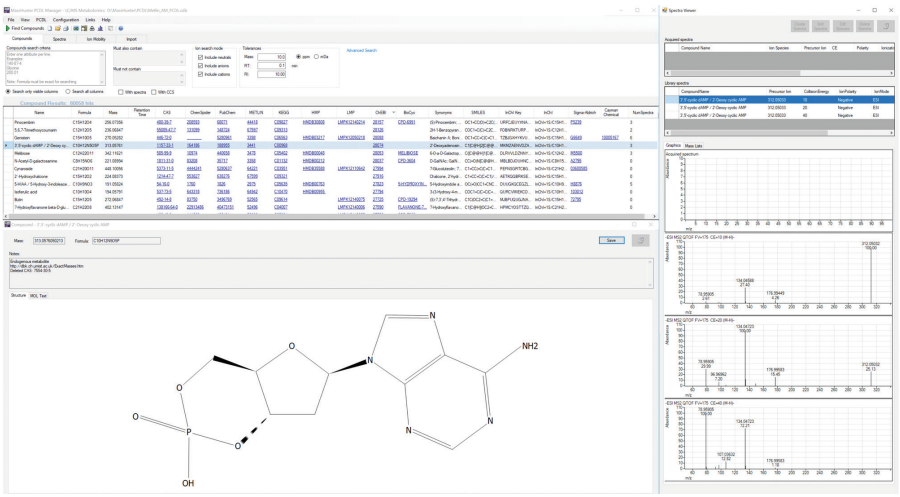
Confident identifications

Increasing confidence in compound identification data

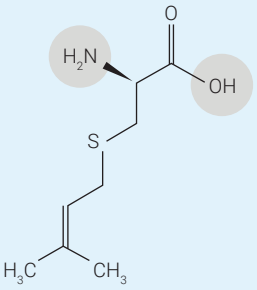
Accurate Mass (AM)	AM + Isotope Pattern (IP)	AM + Retention Time (AMRT) + IP	MS/MS	AMRT + MS/MS

The addition of orthogonal information increases confidence in compound identification.

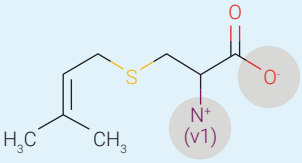
A quality database and library can be utilized to provide varying levels of identification confidence for your metabolite studies. Depending upon your needs, the Agilent METLIN Metabolomics database and library is available as a comprehensive database of metabolites (PCD) that optionally includes MS/MS spectra (PCDL). Higher confidence is achieved by combining MS/MS spectral matching with accurate mass, isotope pattern, and retention time.



Agilent MassHunter Qualitative Analysis workflows, showing compound identifications from a database search against Agilent METLIN Metabolomics database and library including structures, metabolite identifiers, CAS, and notes. Equally high quality can be obtained using Agilent METLIN Metabolomics database and library with ID Browser as well.



Agilent METLIN PCDL
METLIN ID: 62914
Mass 189.082349
Formula: $C_8H_{15}NO_2S$
HMDB12286



Public database entry
METLIN ID: 62914
Mass 186.058874323
Formula: $C_8H_{12}NO_2S$
HMDB12286

Incorrect formula in public database would fail to identify correct metabolite.

Accurate, high-quality metabolite database

The success of your study depends on correctly identifying metabolites and the Agilent METLIN Metabolite database is highly curated to avoid these issues. As part of the curation process, database formula entries are corrected to match observed ESI data.

Curated MS/MS spectral library

Metabolite identification through MS/MS spectral matching requires first comparing observed masses to the database and then comparing MS/MS fragmentation patters. Spectra in the Agilent METLIN Metabolomics library are corrected to their theoretical accurate mass allowing the use of smaller mass tolerance windows. Smaller mass tolerance windows limit superfluous identification making the user more successful.

Agilent METLIN*	Public Database	Error in Public Database (ppm)
41.00329	41.0017	**38.74**
43.01894	43.0190	-1.43
71.01385	missing	
89.02442	89.0205	**44.01**

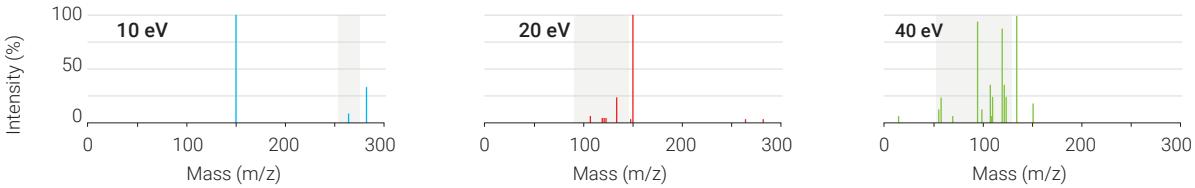
**Agilent METLIN has 0 mass error*

The Agilent curation process also qualifies MS/MS spectra by requiring sufficient intensity of the primary fragment ion to ensure that low abundance fragment ions are included in the MS/MS spectra. Given that many metabolites produce only a few fragment ions, it is critical to include reliable low intensity fragment ions. As shown above for D-lactic acid, a public database entry not only has large mass errors but is missing 1 of the 3 fragment ions (89.02442 is the precursor ion).

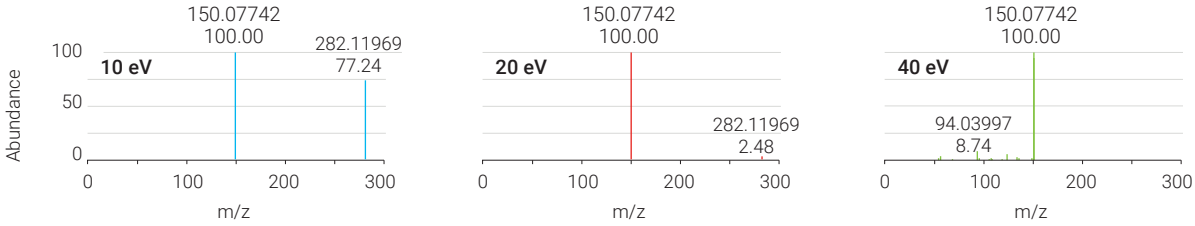
Authentic MS/MS spectra for more confident identification

Agilent METLIN Metabolomics library includes high quality authentic MS/MS spectra and therefore produces more confident identifications when compared to a library which relies on in silico MS/MS spectra. Nuances in the relative abundance of fragment ions can result in significant differences between the predicted and observed spectra.

***in silico* MS/MS** 1-Methyladensine MID: 6888 Insilico predicted spectra



Agilent METLIN – Authentic MS/MS Library spectrum



Comparison of authentic MS/MS spectra for 1-methyladenosine from the Agilent METLIN database compared to the predicted MS/MS from a popular public database. The shaded areas in the in silico MS/MS spectra highlight regions where there are significant differences between the predicted and observed spectra.

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