Agilent METLIN Personal Metabolite Database

Powerful database searching for easier metabolite identification

Identifying metabolites is a key step in untargeted metabolomic experiments. Metabolite database searches using accurate-mass MS information can greatly improve metabolite identification by significantly narrowing the list of possible identities. The METLIN metabolite database, compiled by the Center for Mass Spectrometry at The Scripps Research Institute, is one of the most-comprehensive metabolite databases in the world today. It includes masses, chemical formulas, and structures for over 15,000 endogenous and exogenous metabolites, and di- and tri-peptides. Agilent Technologies is the exclusive provider of the METLIN Personal metabolite database, which can reside on your local PC, facilitating faster, easier, multicom pound searching for high-volume research. Searches are private, and you can add proprietary compounds to the METLIN Personal database. The database software seamlessly integrates with Agilent’s other software tools for LC/MS metabolomics to expand your knowledge of your metabolomic samples.

A wealth of metabolite information

The METLIN metabolite database is one of the most comprehensive metabolite databases in the world today. It includes masses, chemical formulas, and structures for over 15,000 endogenous and exogenous metabolites, and di- and tripeptides. Most compounds are annotated with both a chemical formula and structure. Many compound entries also include CAS, HMD, or KEGG numbers and web links to the respective PubChem, Human Metabolome Database, and Kyoto Encyclopedia of Genes and Genomes database entries, making it easy for you to find additional information.

Greater power and security with your personal copy of the database

The METLIN metabolite database is available to the public online (http://metlin.scripps.edu), for metabolite searches, but installing the METLIN Personal metabolite database on your local PC provides many advantages. You can:

• Add proprietary compounds to the database
• Create entries for metabolites labeled with stable isotopes
• Add unmatched masses to the database and track these unknown metabolites across experiments
• Search more quickly
• Search an almost unlimited number of compounds at one time
• Add retention times to database entries and use retention times as a search criterion
Fast, powerful, and convenient searches

The METLIN Personal metabolite database software makes searching easy. You can search on a single compound or on a nearly unlimited number of compounds in batch mode. You can search by:

- Mass only
- Mass and retention time
- Retention time only

You can also perform informational searches based on:

- Keyword
- Molecular formula
- Compound name
- KEGG, CAS, HMP, or METLIN number

Flexible single-compound searches

Single-compound searching is commonly used to identify an ion observed during an analysis. Mass searches are most commonly used due to the specificity of accurate-mass measurements. A mass match with a metabolite in the database, however, does not necessarily provide a conclusive identification. The ability to add the LC retention times of standards to metabolite entries in the database and then searching using both parameters can provide you with a more confident identification.

Productive batch searching and summary

The METLIN Personal metabolite database gives you the power to automatically search an almost unlimited number of compounds at once. This vastly increases productivity compared to manual searching of individual masses, and is essential for fast, productive research.

Once a batch search is completed, an exportable batch summary report is created. It lists the best database match for each submitted mass. The results can be printed and/or saved for additional analyses such as pathway investigation. You can also update the database with retention times after compound assignment.
Customize your database for greater productivity

For maximum effectiveness, you can customize your METLIN Personal metabolite database to match your analytical needs. You can:

- Add proprietary compounds – including structures if a molfile exists for the compound
- Create custom entries for isotopically labeled metabolites by specifying the number and type of isotopes
- Generate subsets of the database to eliminate entries irrelevant to your research and make searches even faster
- Assign chromatographic retention times to metabolites for greater specificity and higher confidence

Additions you make to your METLIN database remain private, eliminating concerns related to proprietary compounds and intellectual property.

Integration with other software increases throughput and ease of use

Several Agilent software packages allow you to directly initiate single-compound or batch searches of the METLIN database. From the MassHunter qualitative analysis software, you can interactively or automatically execute searches and automatically integrate the search results with the rest of the sample data (see figure on page 4). You can also execute searches from MassHunter Profiling software and save, edit, and export the results. You can import results from Agilent’s GeneSpring MS statistical analysis software into the METLIN software for batch searching of compounds that have shown statistically significant variations. Results of METLIN database searches are readily exported to other data analysis packages such as pathway software.
For more information

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Searches of the METLIN Personal metabolite database can be initiated directly from MassHunter qualitative analysis software. As shown here, the search results can automatically be integrated with the other qualitative information such as chromatograms, mass spectra, and the results of molecular formula generation. This integration of results vastly simplifies data review.