



METABOLOMICS GENOMICS INFORMATICS PROTEOMICS
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Agilent Software for Metabolomics

Software tools for each step in metabolomic data analysis

Metabolomics presents significant analytical challenges. Agilent Technologies offers powerful software tools to address the challenges of profiling, identification, quantitation, and statistical analysis. With two deconvolution programs designed for GC/MS and LC/MS metabolite extraction, the METLIN Personal database for metabolite searches, and an array of statistical analysis tools provided in the GeneSpring MS platform, Agilent provides a full range of software programs to turn raw metabolomics data into useful biological results.

Turning metabolomic data into results

Metabolomics is rapidly emerging as a logical complement to large-scale expression profiling and proteomics studies. However, metabolomics presents distinct challenges for obtaining results. Samples comprise a vast chemical diversity of metabolites that require specific analytical approaches.

In addition, studies involve large numbers of samples that require powerful data analysis capabilities.

Adding to these challenges, metabolomic data analysis involves several steps, each requiring a specific software tool. High-quality tools are needed for feature extraction and alignment, normalization, statistical analysis, and identification.



Metabolomic data analysis comprises several steps after data acquisition—feature extraction, alignment, data normalization, statistical analysis, and identification—that require software to process large amounts of data from complex samples.



Agilent Technologies offers effective software tools to address the challenges of profiling, identification, quantitation, and statistical analysis. With deconvolution programs designed for metabolite extraction, the METLIN Personal metabolite database for metabolite searches, and an array of statistical analysis tools provided in the GeneSpring MS platform, Agilent provides a full range of software programs to turn raw metabolomic data into useful biological results.

Optimal metabolite detection

To make the most of your time and resources, it is important to detect as many metabolites as possible within your MS data. Deconvolution programs address this challenge by finding ions whose individual abundances rise and fall together over time, indicating that they are from the same compound. The program then groups these ions to produce a reconstructed, single-component spectrum for each metabolite.

A single deconvolution program is not sufficient for all applications. This is why Agilent offers deconvolution programs designed specifically for the unique ionization and mass analysis characteristics of GC/MS and LC/MS.

For deconvolution of GC/MS data, Agilent offers Automated Mass Spectral Deconvolution and Identification

Software (AMDIS) as part of the NIST (National Institute of Standards and Technology) library search package. AMDIS extracts pure component spectra from complex GC/MS data and helps determine ion/peak associations. AMDIS produces library-searchable spectra and automatically exports a feature list ideal for statistical analysis by Agilent's GeneSpring MS software.

Agilent's MassHunter Workstation software for LC/MS includes a proprietary molecular feature extraction algorithm. Designed for LC/MS time-of-flight data, it identifies covariant ions associated with a single compound. In addition, it can identify and account for common electrospray artifacts such as sodium adduction or dimer formation. Identifying and grouping such ions improves the quantity estimate used for statistical analysis and removes spurious data from further analysis. The software uses isotope information in the reconstructed spectra to improve the accuracy of empirical formula determination.

Two software packages for powerful profiling studies

For simple differential analyses involving case-versus-control studies, Agilent MassHunter Profiling software is specifically designed for TOF and Q-TOF LC/MS expression profiling applications such as metabolite biomarker discovery. This software normalizes retention time

and abundance across data, provides visualization tools to identify statistically meaningful differences between samples, calculates abundance ratios, and clearly identifies differentially expressed features.

Agilent GeneSpring MS software supports complex experimental designs and enables the rapid discovery of metabolite biomarkers through the analysis of mass spectrometry data. Researchers can easily import, analyze, and visualize GC/MS data; TOF, Q-TOF, and triple quadrupole LC/MS data; as well as CE/MS data from large sample sets. Using an array of useful statistical analysis and visualization tools (including 1-way and 2-way ANOVA, PCA, and class prediction algorithms), GeneSpring MS can profile metabolites associated with changes in cellular function, enabling the rapid discovery of biomarkers that can detect disease or drug toxicity. GeneSpring MS can perform fold-change analyses similar to MassHunter Profiling software. In addition, GeneSpring MS supports meta data analysis to find relationships in complex experimental designs for a number of different applications.

Experiment Parameters for GCMS_Diabetes_Study

Please select values for experimental parameters.
Warning: Modifying parameters may invalidate existing condition trees built from this experiment.

Parameter Name	Age	Sex	Weight (pounds)	Height (inches)	Condition
Parameter Units					
Numeric	yes	no	yes	yes	no
Logarithmic	no	no	no	no	no
1: Z09140602A.txt	51	male	180	68	diabetic
2: Z09140602B.txt	48	male	186	67	diabetic
3: Z09140602C.txt	65	male	191	72	non-diabetic
4: Z09140603A.txt	38	female	141	62	diabetic
5: Z09140603B.txt	39	female	139	68	non-diabetic
6: Z09140603C.txt	75	female	115	59	non-diabetic
7: Z09140604A.txt	48	male	274	73	diabetic
8: Z09140604B.txt	66	female	153	63	non-diabetic
9: Z09140604C.txt	32	female	146	61	diabetic
10: Z09140605A.txt	69	male	195	65	non-diabetic
11: Z09140605B.txt	47	female	165	64	non-diabetic
12: Z09140605C.txt	29	male	178	71	diabetic

Buttons: Save, Save As..., Cancel, Help

Right Panel Buttons: New Parameter..., Import Parameter..., Delete Parameter, Replace Text..., Extract Subvalues, Fill Down, Fill Sequence Down, Sort, Set Value Order..., Inspect...

GeneSpring MS is a powerful statistical analysis platform that supports meta data analysis to find relationships in complex experiments.

For future studies, GeneSpring MS enables subsequent MS/MS-based analyses such as metabolite identification and confirmation. And importantly, the GeneSpring platform can integrate metabolomic data with genomic and proteomic data, for understanding the biological relevance of the data in a systems context.

Agilent METLIN Personal database for secure, efficient metabolite searches

Agilent Technologies is the sole supplier of the METLIN Personal metabolite database for desktop metabolite searches based on LC/MS data. The METLIN database—an effort by the Center for Mass Spectrometry at The Scripps Research Institute—is probably

the best-known and most-comprehensive metabolite database in the world today. It currently includes annotated lists of over 15,000 endogenous and exogenous metabolites, as well as di- and tri-peptides; each entry includes mass, chemical formula, and structure information.

The METLIN database is available online to the public, but searches can only be performed on one compound at a time and in a nonsecure environment. In contrast, the Agilent METLIN Personal database enables you to:

- Save time by performing automated searches on multiple compounds
- Safeguard intellectual property by performing private, on-site searches
- Customize your database by adding proprietary compounds

Agilent is very pleased to offer this personal version of the METLIN database to metabolomics researchers, and is dedicated to seamlessly integrating this database with Agilent's other metabolomics software tools. To increase throughput and ease of use, future versions of MassHunter Workstation software and GeneSpring MS software will include links to the METLIN Personal metabolite database.

Additional information

- GeneSpring MS from Agilent.
Publication number 5989-5553EN.
- Introducing the New Agilent MassHunter Workstation Software for 6000 Series LC/MS Systems.
Publication number 5989-4895EN.
- MassHunter Profiling Software for the Agilent 6210 TOF LC/MS. Publication number 5989-5085EN.
- <http://www.amdis.net/>

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Agilent Technologies is a leading supplier of life science research systems that enable scientists to understand complex biological processes, determine disease mechanisms, and speed drug discovery. Engineered for sensitivity, reproducibility, and workflow productivity, Agilent's life science solutions include instrumentation, microfluidics, software, microarrays, consumables, and services for genomics, proteomics, and metabolomics applications.

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