

MassHunter Profiling Software for the Agilent 6210 TOF LC/MS

PROTEOMICS METABOLOMICS GENOMICS INFORMATICS GLYILEVALCYSGLUGLNALASERLEUASPARG CYSVALLYSPROLYSPHETYRTHRLEUHISLYS

Turn highly accurate LC/MS mass data into putative biomarkers

The Agilent MassHunter Profiling software is specifically designed for expression profiling applications such as biomarker discovery. When used with the Agilent 6210 TOF LC/MS, the MassHunter Profiling software clearly identifies statistically meaningful differences between sample groups, allows selection of comparison criteria, and exports profile data for statistical analysis using Agilent's GeneSpring GX software, other database search programs, identification environments, or statistical analysis packages. MassHunter Profiling software also supports additional applications such as pharmaceutical impurity analysis, forensic analysis, environmental analysis, and pesticide analysis.

Mass profiling is widely used to compare the expression of peptides, proteins, or metabolites for biomarker discovery in a variety of comparative studies (e.g., healthy versus diseased or drug-treated samples, monitoring disease states). Mass profiling can also be used for other applications, including the detection of pharmaceutical impurities and targeted compounds such as pesticides or drugs of abuse.



MassHunter Profiling software

The Agilent MassHunter Profiling software is specifically designed for expression profiling applications such as biomarker discovery. Using data generated by the Agilent 6210 TOF LC/MS, MassHunter Profiling software provides retention time and *m/z* alignment for features across samples, response normalization, and t-test statistics for the identification of significant differences between samples. MassHunter Profiling software uses a unique feature identification algorithm that does a better job of locating all the components in even very complex peptide mixtures (Figure 1). The algorithm identifies all the components in a chromatogram, instead of just identifying chromatographic peaks, which may conceal multiple components. This facilitates very effective removal of chemical background data. The molecular feature extraction algorithm effectively removes noise (demonstrated as streaks in the contour plot, Figure 1a) and extracts even low-level peptides (Figure 1b). The extracted information for each sample is then combined and analyzed for differential features.

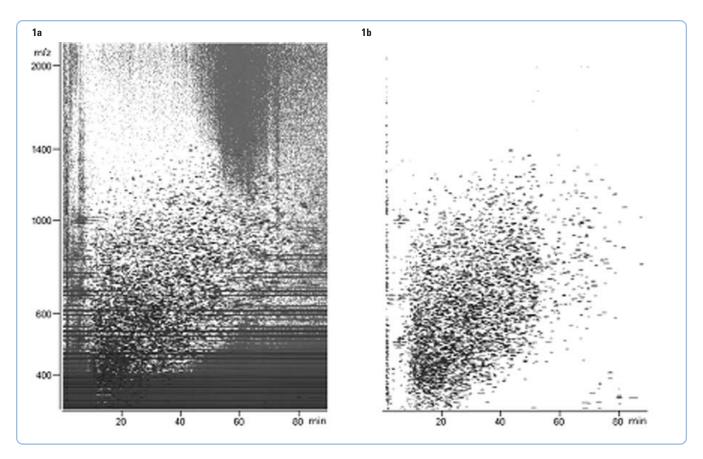


Figure 1. Contour plots showing the raw 6210 TOF LC/MS data (Figure 1a) and the feature-extracted data (Figure 1b) for subsequent expression profiling (*E. coli* cell lysate spiked with 2 bovine proteins, BSA and serotransferrin).

Flexible feature selection

MassHunter Profiling software provides the ability to easily choose, at a glance, the analysis tool that's required for your application (Figure 2).

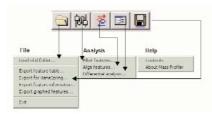


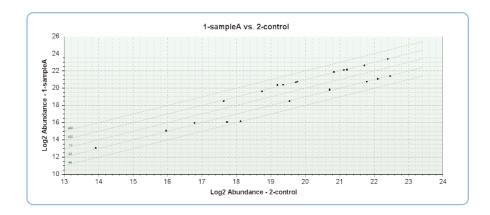
Figure 2. MassHunter Profiling menu options

The software provides visualization tools to allow the identification of statistically meaningful differences between sample groups (e.g. healthy versus disease). In addition, the profiling software calculates ratios of abundances of differentially-expressed features. The Differential Analysis parameters allow flexible user selection of the comparison criteria. Any selected feature may be inspected across all samples. With simple visual tools, you can quickly see and identify those differences between your groups of interest, yet the software is flexible enough to allow further detailed inspection of the data (Figure 3).

Export profile data

MassHunter Profiling data can be exported to a Microsoft Excel file or a text file for custom applications that suit your needs. Profiling data files may also be exported to Agilent's GeneSpring GX software to allow for easy comparison of molecular feature lists using principal component analysis (PCA), partial least square discriminant analysis (PLS-DA), various clustering analyses, ANOVA, and other statistical methods. The differential feature lists may also be exported to a database search program, other identification environments, or statistical analysis packages.

Powered by incredibly sophisticated algorithms, alignment and statistical tools, and a user-friendly interface, MassHunter Profiling software provides the utmost confidence in your results.



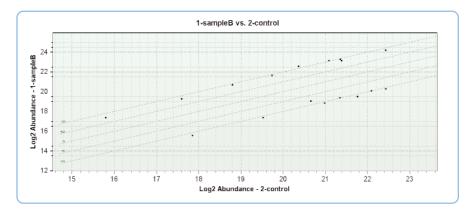


Figure 3

MassHunter Profiling software identifies features with relative 2-fold (Figure 3a) and relative 4-fold (Figure 3b) differences in abundance compared to control samples.

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