Agilent MassHunter Profinder Software

ATTAIN SUPERIOR FEATURE EXTRACTION

Agilent Technologies

ACHIEVE HIGHER QUALITY RESULTS

Agilent MassHunter Profinder software provides targeted and untargeted molecular feature extraction (MFE) for batches of mass-spec data—not just one file at a time—and is designed to accelerate your differential analysis workflow.

Profinder's MFE algorithm extracts data based on mass spectral and chromatographic characteristics to generate a complete list of compounds, which includes molecular weight, retention time, *m/z*, and abundance—and it has a recursive mode to address missing features. This batch-recursive mode first bins and aligns compound features found in a first-pass MFE, then uses those results to create a list for a targeted second pass.

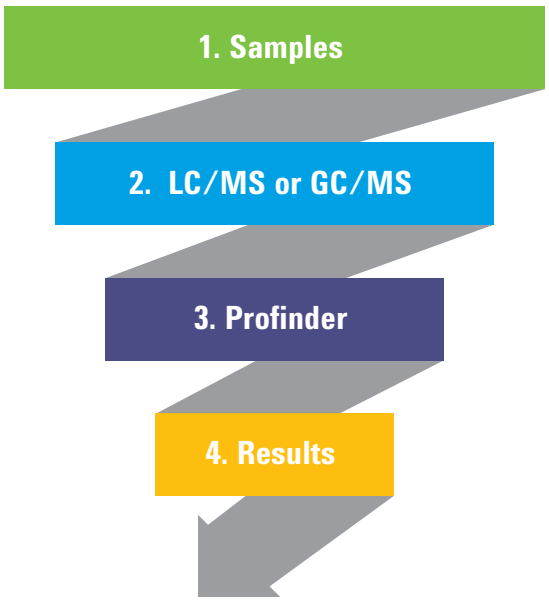
If you know your compounds of interest, Profinder's targeted feature finding algorithm will extract compounds of interest with known chemical formulas from large complex data sets. This workflow offers higher selectivity, faster data processing, and tentative compound annotation.

Intuitive and easy to use, Profinder offers an array of useful features:

- Grouping of replicate data files
- Binning and alignment
- Chromatogram overlay
- Manual re-integration of compounds
- Export of results

Profinder supports MS-only data from Agilent's broad portfolio of mass spectrometers including TOF-based instruments (with GC, LC, CE or SFC) as well as nominal mass GC/MS systems.

Agilent MassHunter Profinder Workflow



Extra performance for fast results

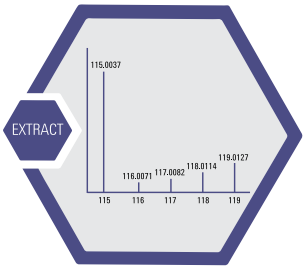
Even with an advanced algorithm, sometimes user intervention is required. Profinder provides data visualization across all files and a manual integration tool that enables visual validation of the feature extraction results.

Profiling experiments can be quite large, presenting a computational challenge for any feature extraction software. Profinder's feature-finding algorithms are multithreaded to take advantage of common multicore Intel processor configurations—and its memory management optimized to run large datasets in the Microsoft's 64-bit Windows operating systems.

Profinder simplifies connecting results for downstream analysis by offering multiple export options. A common format (.CSV) is supported to allow you to interface to any software package. In addition, Agilent created a richer single data file format (.CEF) to support enhanced information exchange with other Agilent-supported software applications. Profinder also offers a rich multiple data file format (.PFA) for transferring results to batch-oriented software applications such as Omix Premium.

Workflow solutions

Profinder provides workflow solutions for small molecule profiling, intact protein profiling, and isotopologue profiling. Small molecule profiling is useful for a wide range of applications including the analysis of foods, beverages, wastewater, polymers, and metabolites. Profinder includes a special algorithm for intact protein profiling designed for multiply-charged protein spectra. Protein profiling can be of use in food analysis as well as basic protein research.



Profinder supports qualitative flux analysis based on data acquired on Agilent high-resolution, accurate-mass, time-of-flight LC/MS systems. The algorithm mines for stable isotope-labeled ions (isotopologues) and supports ^{13}C, ^{15}N, or ^{2}H stable isotope labeling. Profinder provides a batch format result output (.PFA) for Agilent MassHunter VistaFlux software.

"In my lab, MassHunter Profinder is already our tool of choice for untargeted analysis of TOF and Q-TOF data. Profinder's powerful algorithms sit behind a biologist-friendly interface that lets students, post-docs, and visiting scientists focus on sample collection and interpretation. I'm particularly excited by the addition of isotopologue analysis to the latest version. It's been great to see individual members of the lab empowered to analyze their own kinetic flux profiling data."

ADAM ROSEBROCK, PHD, UNIVERSITY OF TORONTO

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