Agilent's NEW MassHunter Profinder

The Most Advanced Batch Feature Extraction Software for Metabolomics

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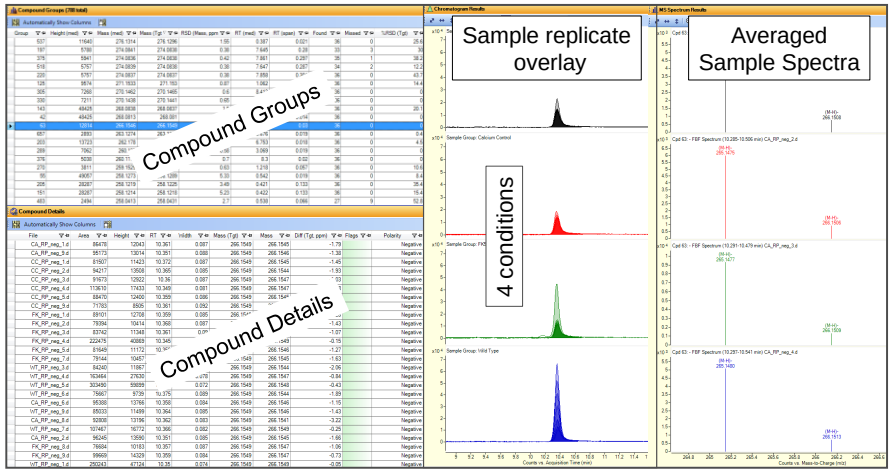
MassHunter Profinder

A Batch Feature Extraction and Review Tool



Which Metabolomics Customers can benefit from using MassHunter Profinder?

Biological Research

- Basic, clinical Research
- Drug Development

Food

- Food process development
- Food quality/ adulterants
- Nutrition

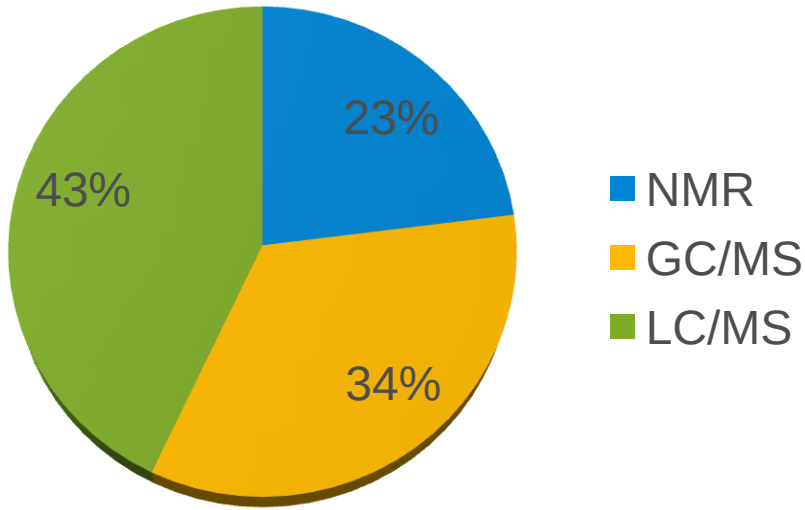
Ag Chem

- Crop development
- Pesticide / herbicide development

Synthetic Biology

- Biofuels

Toxicology



Metabolomics Workflow

Acquire Data
- Analyze metabolomics samples
- Use accurate mass LC/MS to analyze samples

Extract Data
- **Batch Feature Finding: MassHunter Profinder**

Analyze Data
- Differential Analysis in Mass Profiler Professional

Identify
- Annotate & Identify metabolites

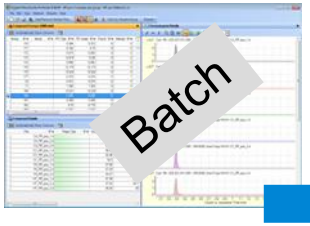
Pathway Analysis
- Map results onto pathways using Pathway Architect
- Export MS/MS inclusion list for next experiment

Agilent's *Comprehensive* Metabolomics Solution

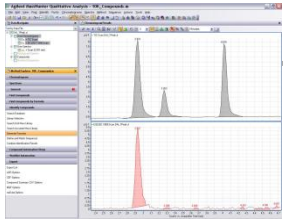
Agilent LCMS and GCMS

Separate & Detect	Feature Finding	Alignment & Statistics	Identify	Pathway Analysis

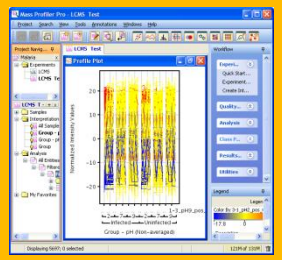
MassHunter Profinder (NEW)

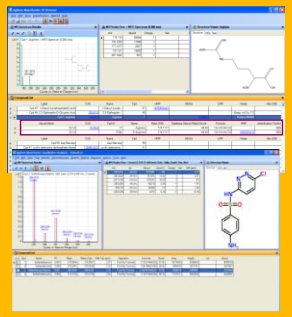


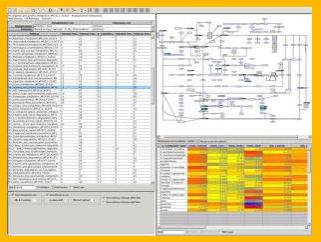
MassHunter Qual



Mass Profiler Professional







Statistics Visualization

Annotation & Identification

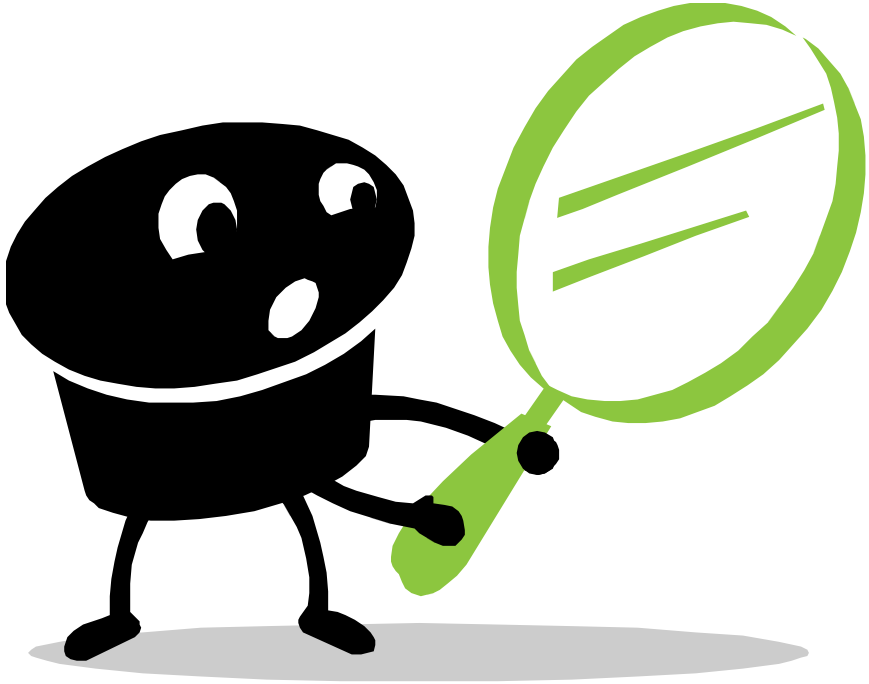
Pathway Analysis

LCMS and GCMS Data can be analyzed together in the same project

Customer Goal: Find and correctly extract all chromatographic peaks in a sample

Challenges:

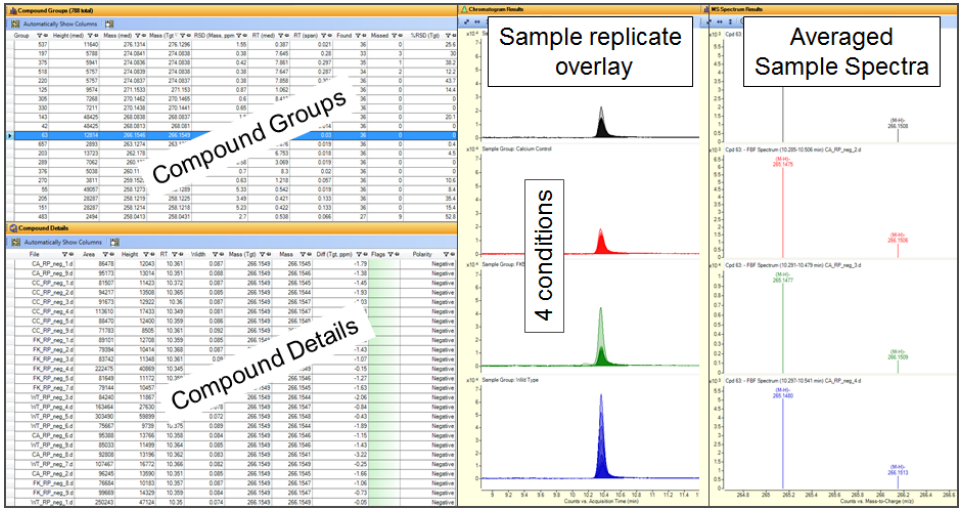
- Incomplete peak separation
- Unresolved peaks contribute to an increase in:
  - False peak detection, excessive missing values, incorrect identifications
  - Misdirected and wasted efforts
  - Missed or inaccurate biomarkers
  - Decreased productivity



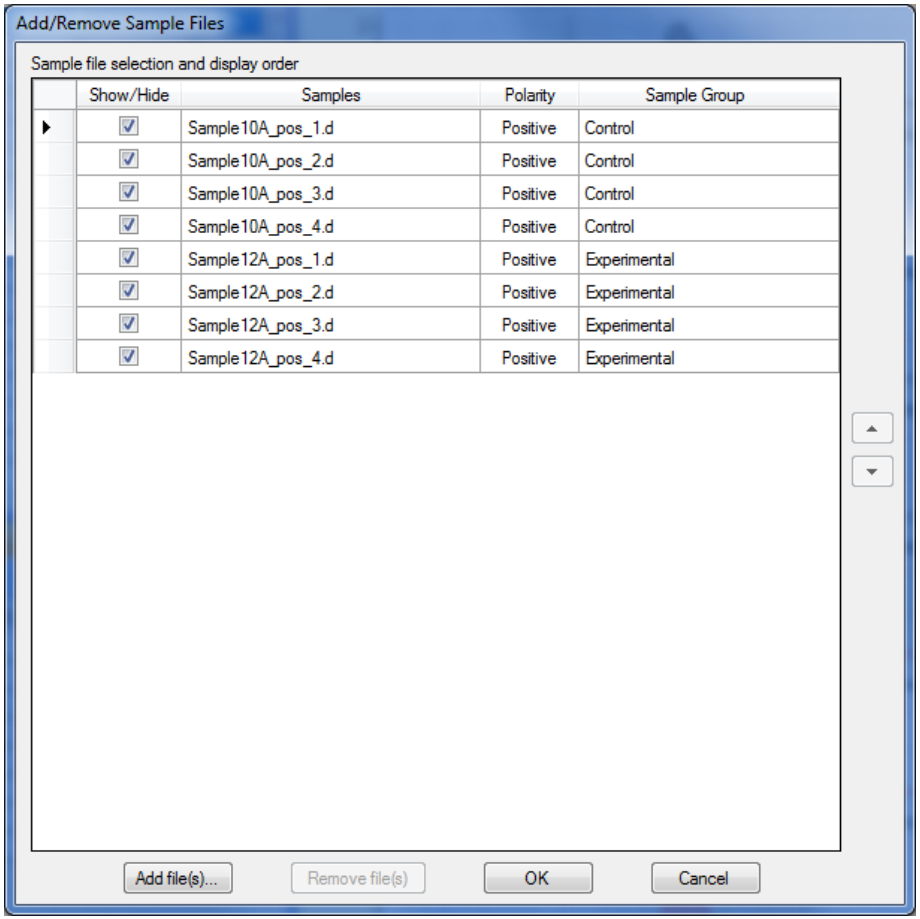
MassHunter Profinder Workflow solution:
So what's new?

- A one-shot process for untargeted and targeted feature extraction
- Designed specifically for the needs of the metabolomics user
- Processes many samples!
- Recursive analysis
- Compound Group Centric: new manual review and editing functionalities
- Major reduction in processing time
- It's FREE!!

MassHunter Profinder

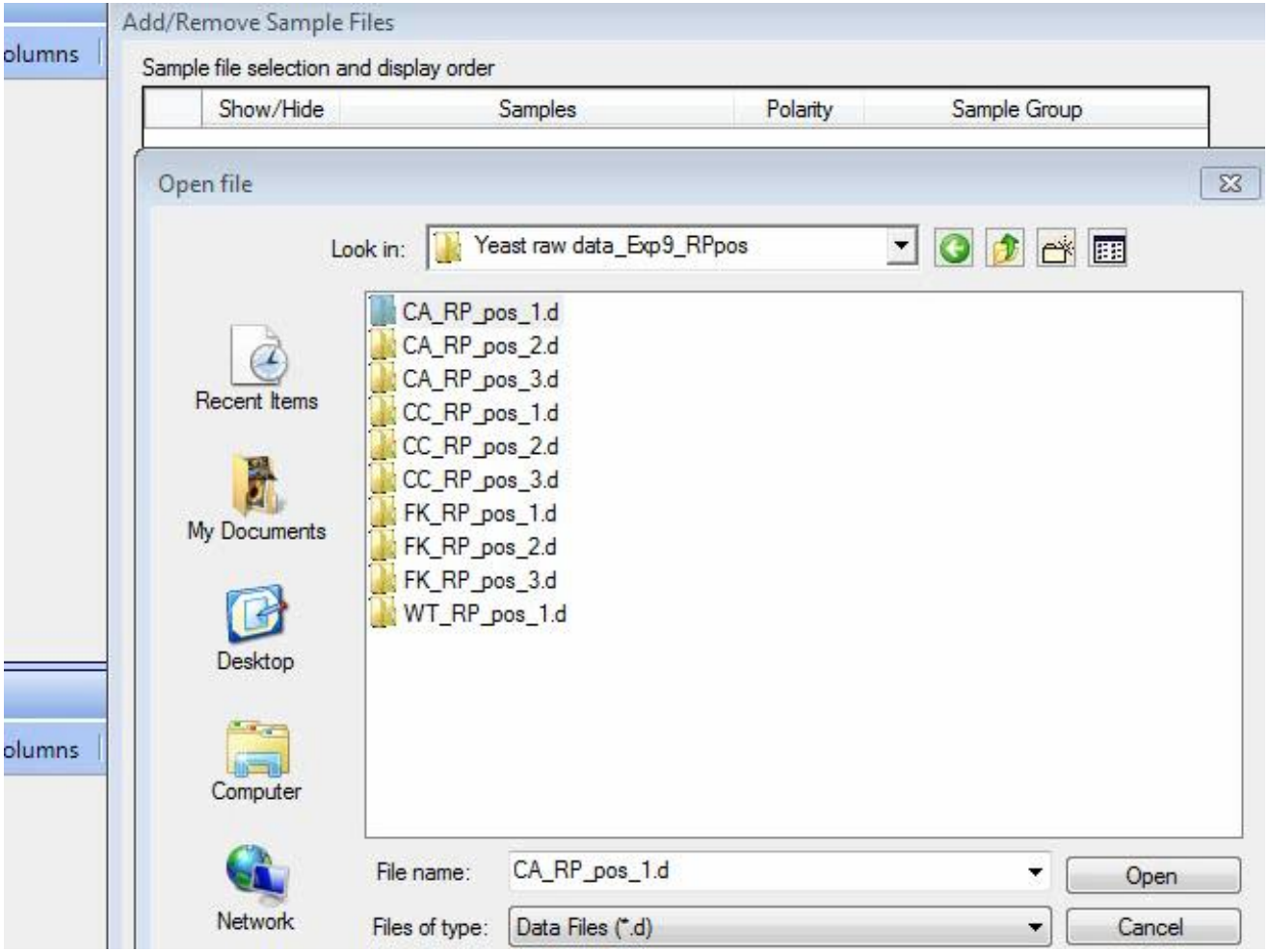


First step: Add/Remove Sample Files and Grouping



- Projects consist of multiple data (.d) files
- One sample group column, but multiple sample groups may be assigned
- This helps with filtering, and plot overlay of the results

Profinder software demo1: Add/Remove Sample Files and Grouping

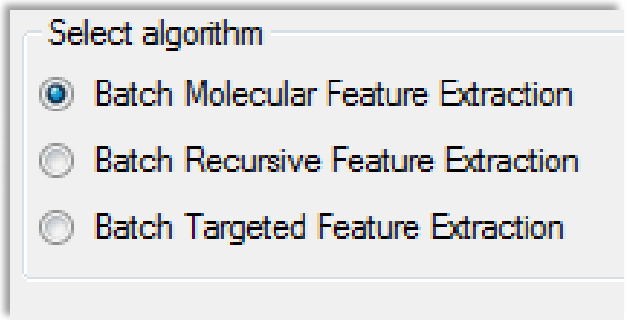


Profinder's **Three** Feature Extraction Algorithms

1. Batch Molecular Feature Extraction

MFE → rMFE

- Recursive MFE reduces false positives



2. Batch Recursive Feature Extraction

MFE → rMFE → Find by Ion

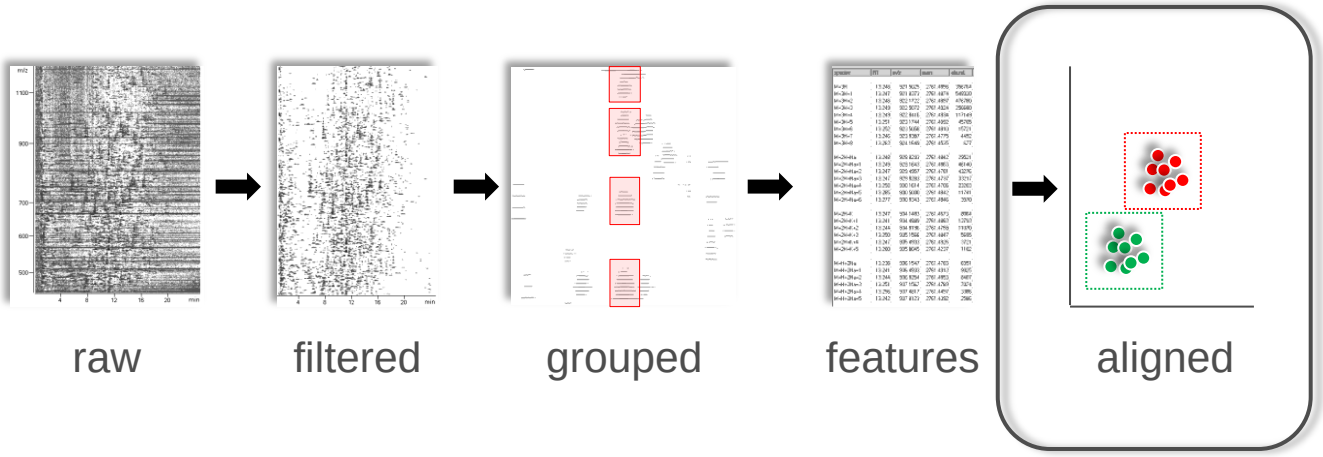
- Greater "missing feature" recovery
- Allows manual editing of compounds

3. Batch Targeted Feature Extraction

Find by Formula

- Also allows manual editing
- Data source

What is Batch Molecular Feature Extraction?



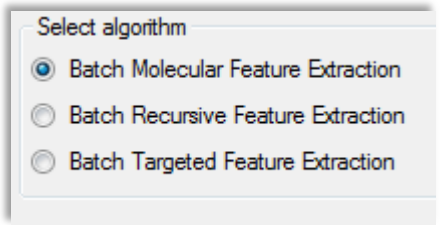
- Batch Molecular Feature Extraction begins with MFE on each data file:
  - From the raw data it finds co-eluting ions that are related:
    - isotopes, adducts (such as Na+ / K+), and dimers
  - Filters noise
  - Creates a compound chromatogram for the group of ions
  - Sums all ion signals into one value: one Feature = one compound

What is Batch Molecular Feature Extraction?

- In MassHunter Qualitative Analysis, features are extracted one file at a time
- However, in MassHunter Profinder Batch MFE aligns features across all sample files to build a consensus spectrum for each compound group, enabling recursive, re-extraction of the batch files

When should I use Batch MFE?

- Regular MFE doesn’t work across multiple data files
- Batch MFE is based on recursive analysis (rMFE) across multiple data files
- This results in a an averaged consensus spectrum, that is used for re-extracting all the data files
- Use Batch MFE to optimize settings first, prior to using Batch Recursive Feature Extraction



Profinder's "Batch Recursive Feature Extraction"

1. **Batch Molecular Feature Extraction**

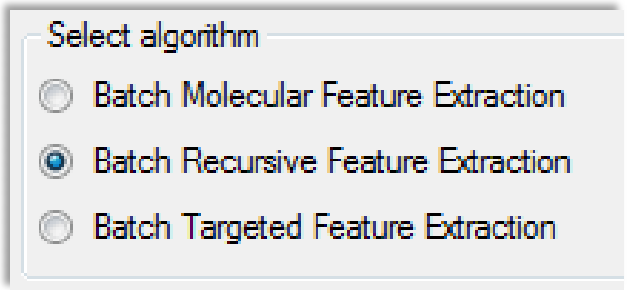
   MFE → rMFE

   - Recursive MFE reduces false positives

2. **Batch Recursive Feature Extraction**

   MFE → rMFE → Find by Ion

   - Find by Ion reduces false negatives
   - Allows manual editing of compounds



3. **Batch Targeted Feature Extraction**

   Find by Formula

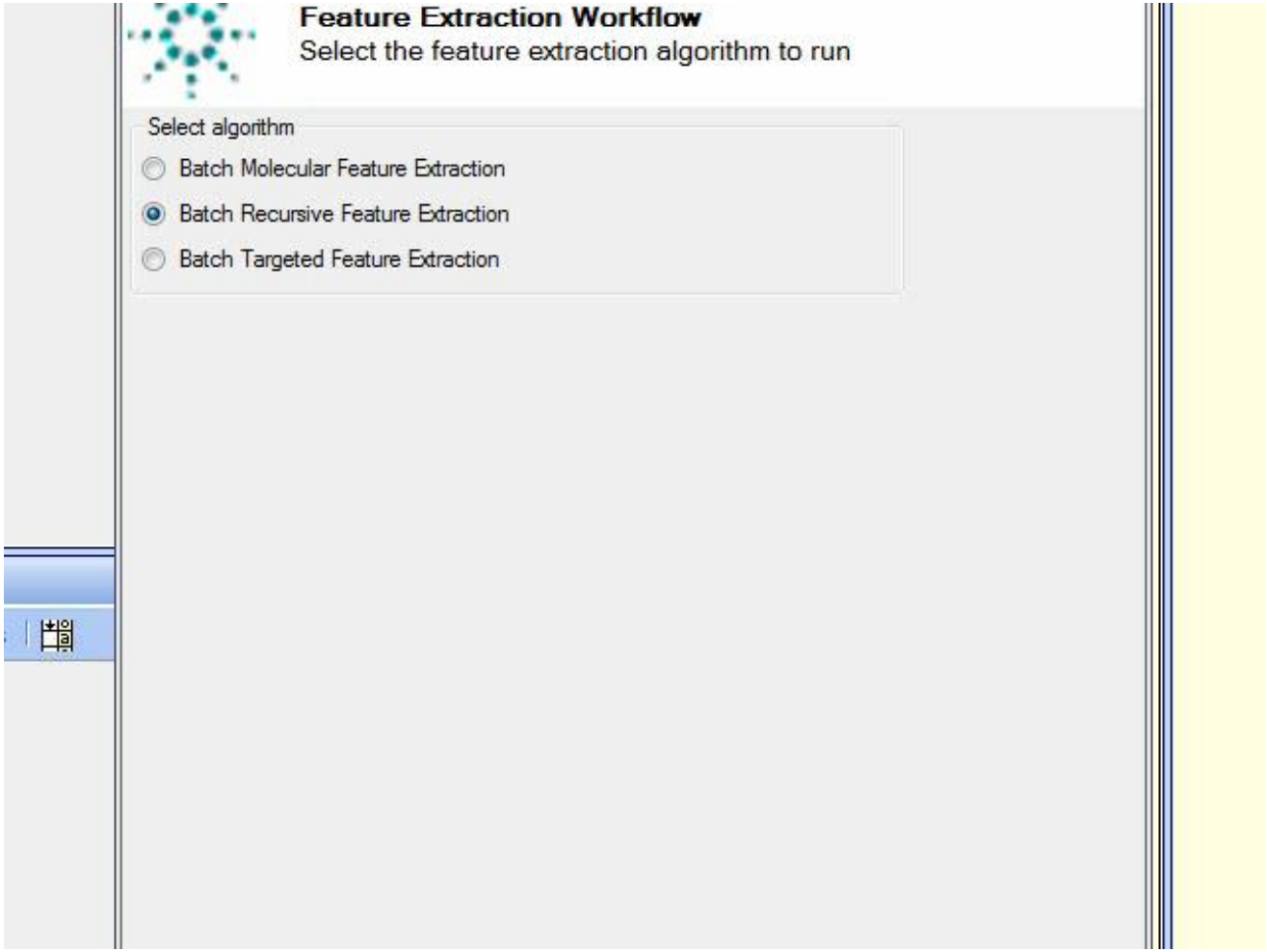
   - Also allows manual editing
   - Data source can be .CEF files, a .CSV file

Profinder's "Batch Recursive Feature Extraction":
Post-alignment filtering after rMFE and Find by Ion

There are two post-alignment filters:

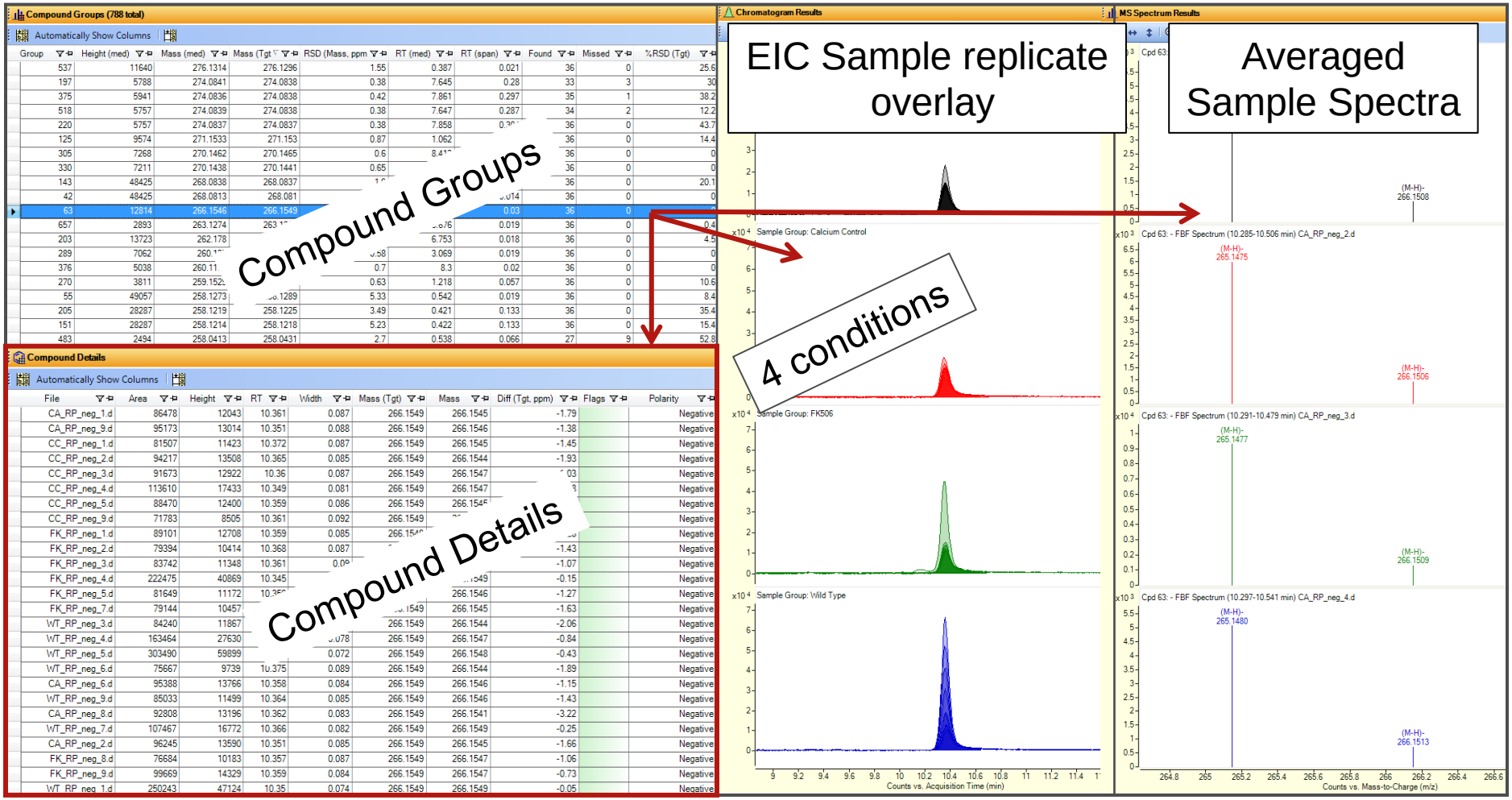
1. After rMFE → improves the quality of your target list for Find by Ion
2. After Find by Ion → improves the quality of your final compound group list, reducing the amount of manual cleanup

Profinder software demo2: Batch Recursive Feature Extraction Wizard

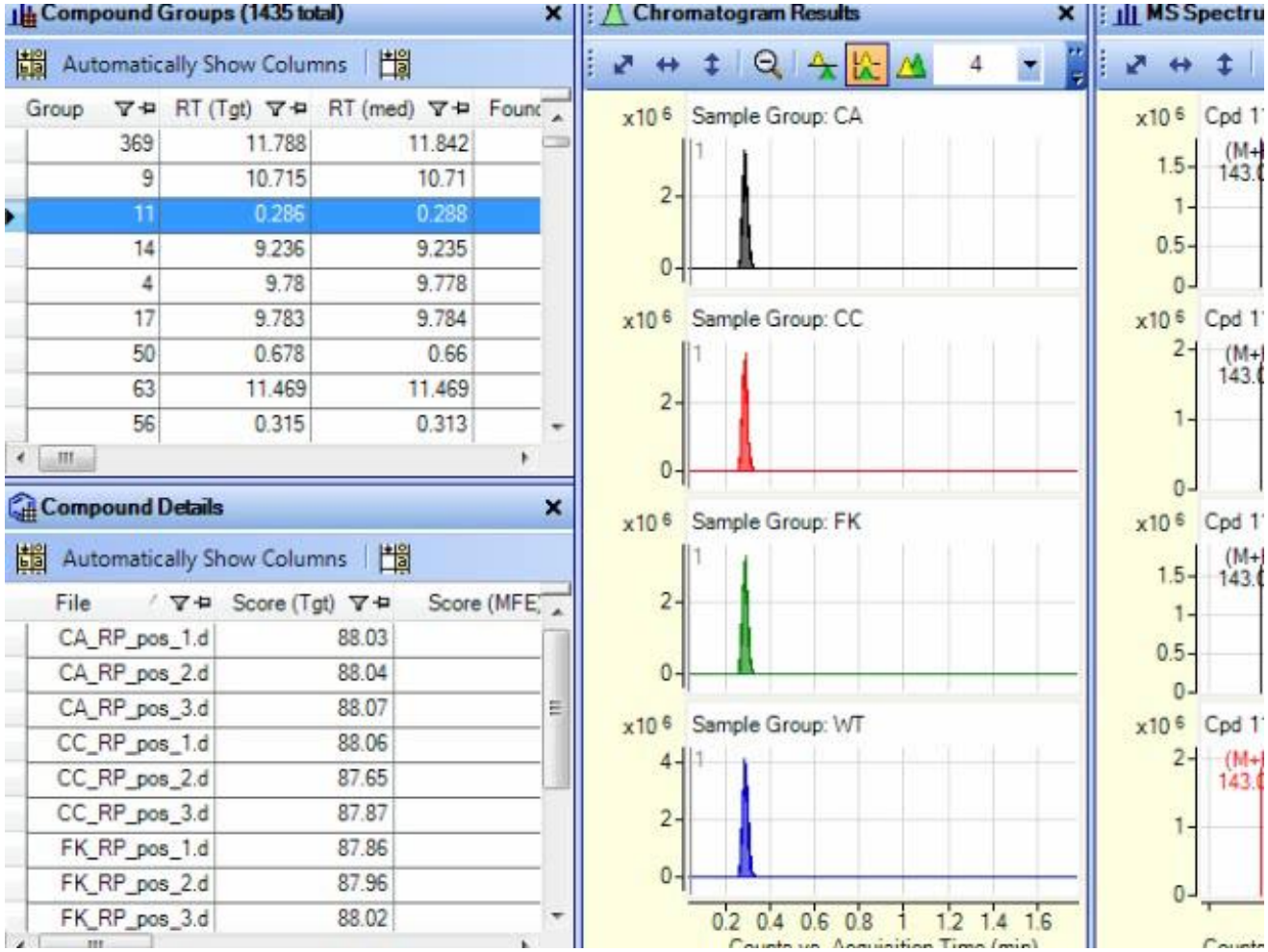


Four Profinder Windows:

Compound centric visualization and editing of results



Profinder software demo3: Batch Recursive Feature Extraction



Profinder's "Batch Targeted Feature Extraction"

1. **Batch Molecular Feature Extraction**

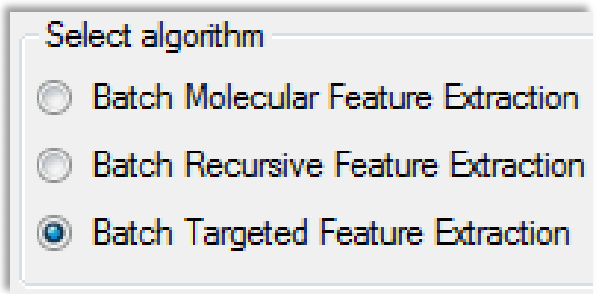
   MFE → rMFE

   - Recursive MFE reduces false positives

2. **Batch Recursive Feature Extraction**

   MFE → rMFE → Find by Ion

   - Find by Ion reduces false negatives
   - Allows manual editing of compounds

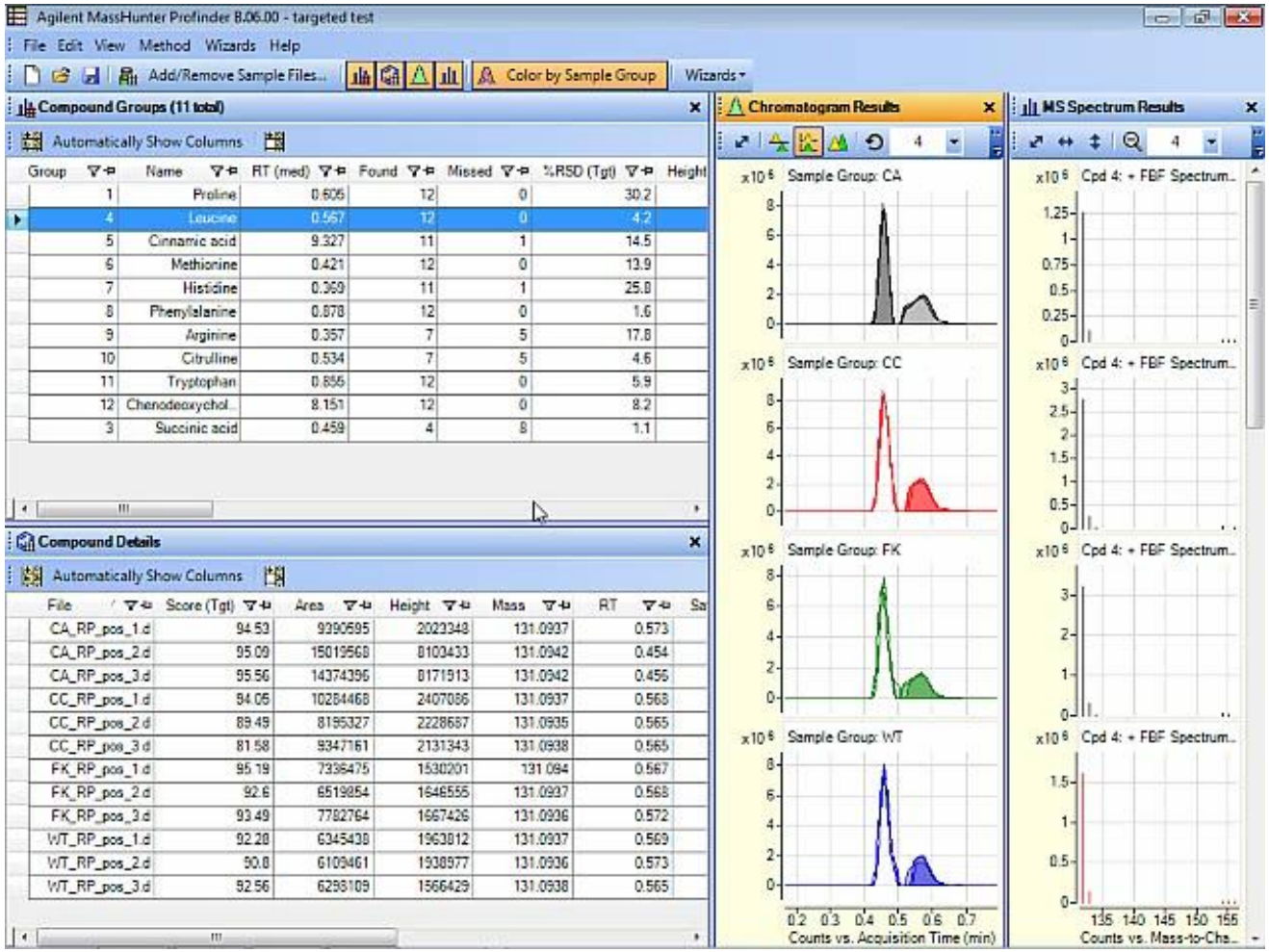


3. **Batch Targeted Feature Extraction**

   Find by Formula

   - Also allows manual editing
   - Formula source can be .CEF files, a .CSV file or a PCD/L database

Profinder software demo4: Batch Targeted Feature Extraction



The Profinder Advantage:
A Complete Solution

Features	Agilent Profinder	Customer Benefits
Supported instruments	LC/TOF, and LC/Q-TOF GC/MS planned	Load raw accurate mass LC/MS data without any conversion
Feature finding	Untargeted and targeted	Maximum flexibility for discovery profiling
Ion grouping	Compound-centric	Let's the software determine which ions are related
Recursive analysis	Yes	Higher quality results
Feature quality score	Q-score	Helps in ranking which compound groups to review
Feature visualization and editing	Yes	Quickly re-integrate or remove compounds
Peak alignment	Yes, by compound	Takes advantage of two separate peak alignment steps

How Can You Obtain a copy of MassHunter Profinder?

- MassHunter Profinder is FREE for MPP customers
- It will be placed on the MPP Supplemental DVD
- It will also be available on Agilent SubscribeNet in the near future to update existing customers
- Please contact your local product specialist for further information