MassHunter Profinder: Batch Processing Software for High Quality Feature Extraction of Mass Spectrometry Data

Technical Overview

Introduction

LC/MS metabolomics workflows typically involve the following steps: (1) data acquisition using high resolution accurate mass LC/MS, (2) feature extraction from raw data, (3) statistical analysis, (4) annotation and identification using database and library matching, and (5) increasingly, the use of pathway analysis.

The feature extraction step plays a critical role in differential analysis, as the quality of the feature extraction results impacts subsequent steps in the metabolomics workflow. Ultimately, it affects the effectiveness with which raw data is transformed into biologically relevant information.

Previously, a two-pass feature extraction[1] process was used to find compounds from complex accurate mass data. Compounds are comprised of neutral mass, retention time (RT), abundance and *m/z*. The first pass used Molecular Feature Extraction (MFE) in MassHunter Qualitative Analysis (Qual). Next the results were imported into Mass Profiler Professional (MPP) for binning, aligning, and creating a consensus for each compound. The second pass used the list of consensus compounds and the "Find by Ion (FbI)" algorithm in Qual for targeted feature extraction. This two-pass feature extraction approach improved the quality and accuracy of mass, retention time and abundance values for each candidate compound compared with the MFE only data mining. However, this workflow has some limitations such as low throughput, use of two separate software programs, as well as a lack of data visualization and curation tools.

MassHunter Profinder is a new software tool designed for batch processing of large, complex accurate mass LC/MS data. Profinder also integrates many software functions into one dedicated processing tool. As a result, this software reduces the complexity of raw data and improves the quality of extracted compounds. Most importantly, it improves user experience and increases the throughput using fully automated batch data processing.

Agilent Technologies

This Technical Overview describes the overall data processing workflow in Profinder, including a detailed review of the recursive algorithms, the simplified GUI design, as well as the benefits of grouping and batch analysis, which was not possible before. It also demonstrates the utility of Profinder using a relatively large batch of yeast metabolomics data that were acquired in a nontargeted LC/Q-TOF MS approach[2]. The improved results obtained by Profinder are illustrated through quality enhancement using statistical analyses.

Key Functionality and Benefits

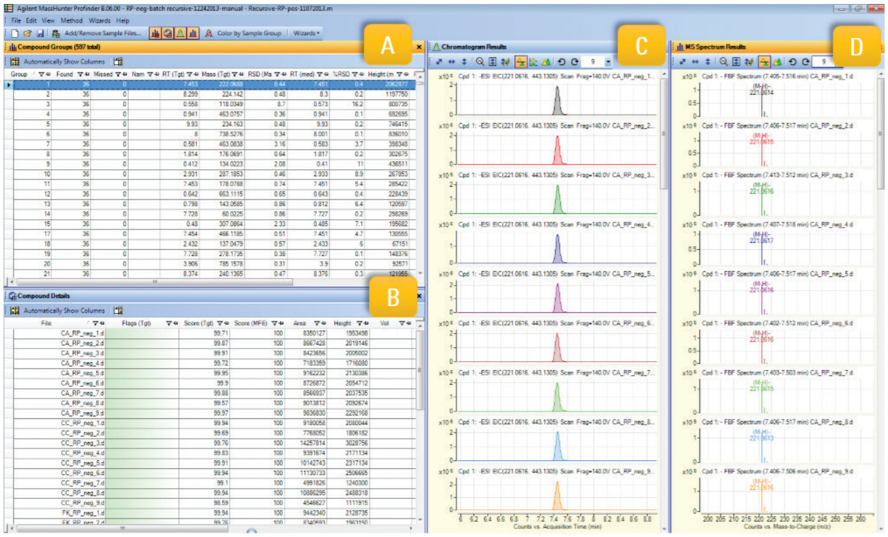
- Supports untargeted and targeted data mining of LC/TOF and LC/Q-TOF accurate mass data
- Integrates MFE and FbI in a single workflow, eliminating multiple import/export of results between Qual and MPP
- Increases data processing throughput using batch feature extraction
- Results in greater recovery of missing features by reducing false negatives through recursive feature extraction algorithm
- Offers compound-centric visualization across multiple sample files, enabling quick sorting and filtering of compound group results, visual review and identification of outliers for manual editing
- Extracted ion chromatograms and mass spectra are optionally overlaid and colored by sample group, enhancing visual inspection and comparison of two or more sample groups with or without replicates

Batch Feature Extraction Workflows

There are three feature extraction workflows.

Batch Recursive Feature Extraction is the primary untargeted feature extraction workflow in MassHunter Profinder. This workflow integrates the batch MFE and batch FbI two-pass feature extraction workflow into a single processing tool, eliminating the extra effort required before. A wizard guides the user through parameter setup. The data input and parameters settings take only a few minutes, and now the two-pass feature extraction process is automated and self-contained in Profinder.

Figure 1 shows the results of Profinder Batch Recursive Feature Extraction for yeast metabolomics data acquired on an Agilent Q-TOF LC/MS in positive ion mode. The main view consists of four linked navigation windows. The Compound Group Table (Figure 1A) displays the compound-level information grouped and summarized across multiple data files. The individual file details of a selected compound group are shown in the Compound Details Table (Figure 1B), Extracted Ion Chromatogram (Figure 1C), and MS Spectrum (Figure 1D) windows. This compound centric visualization allows a detailed inspection of feature extraction results. Users can quickly sort compound groups in multiple ways (i.e. neutral mass, RT, abundance, found, and missing) to identify spurious features for deletion. In the Chromatogram and MS Spectrum windows, the plots can be colored by individual sample file (Figure 2A), or by sample group (Figure 2B and 2C) for enhanced visualization. Furthermore, EICs can be stacked by individual sample file (Figure 2A and 2B), overlaid by sample groups (Figure 2C), or all the files can be overlaid (Figure 2D). This function is useful for quick comparison of a compound feature across sample files or sample groups, visualizing missing peaks, and manually editing EIC peak integration.


Agilent MassHunter Profinder B.06.00 - RP-neg-batch recursive-12242013-manual - Recursive-RP-pos-11072013.m
File Edit View Method Wizards Help
Add/Remove Sample Files...
Color by Sample Group
Wizards
A
Compound Groups (597 total)
Automatically Show Columns
B
Compound Details
Automatically Show Columns
C
Chromatogram Results
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_1...
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_2...
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_3...
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_4...
x10^6
Counts vs. Acquisition Time (min)
D
MS Spectrum Results
Cpd 1: - FBF Spectrum (7.405-7.516 min) CA_RP_neg_1.d
(M-H)- 221.0614
Cpd 1: - FBF Spectrum (7.406-7.517 min) CA_RP_neg_2.d
(M-H)- 221.0615
Cpd 1: - FBF Spectrum (7.413-7.512 min) CA_RP_neg_3.d
(M-H)- 221.0616
Cpd 1: - FBF Spectrum (7.407-7.518 min) CA_RP_neg_4.d
(M-H)- 221.0617
x10^6
Counts vs. Mass-to-Charge (m/z)

Group	Found	Missed	Nam	RT (Tgt)	Mass (Tgt)	RSD (Ma	RT (med)	%RSD	Height (m
1	36	0		7.453	222.0688	0.44	7.451	0.4	2062877
2	36	0		8.299	224.142	0.48	8.3	0.2	1197750
3	36	0		0.558	118.0349	8.7	0.573	16.2	800735
4	36	0		0.941	463.0757	0.36	0.941	0.1	692695
5	36	0		9.93	234.163	0.48	9.93	0.2	746415
6	36	0		8	738.5276	0.34	8.001	0.1	836010
7	36	0		0.581	463.0838	3.16	0.583	3.7	398348
8	36	0		1.814	176.0691	0.64	1.817	0.2	302675
9	36	0		0.412	134.0223	2.08	0.41	11	436511
10	36	0		2.931	287.1853	0.46	2.933	8.9	267853
11	36	0		7.453	178.0788	0.74	7.451	5.4	285422
12	36	0		0.642	663.1115	0.65	0.643	0.4	228439
13	36	0		0.798	143.0585	0.86	0.812	6.4	120597
14	36	0		7.728	60.0225	0.86	7.727	0.2	298269
15	36	0		0.48	307.0864	2.33	0.485	7.1	195682
17	36	0		7.454	466.1185	0.51	7.451	4.7	130585
18	36	0		2.432	137.0479	0.57	2.433	6	67151
19	36	0		7.728	278.1736	0.38	7.727	0.1	148376
20	36	0		3.906	785.1578	0.31	3.9	0.2	92571
21	36	0		8.374	240.1365	0.47	8.376	0.3	121955

File	Flags (Tgt)	Score (Tgt)	Score (MFE)	Area	Height	Vol
CA_RP_neg_1.d		99.71	100	8350127	1953498	
CA_RP_neg_2.d		99.87	100	8667428	2019146	
CA_RP_neg_3.d		99.91	100	8423656	2005002	
CA_RP_neg_4.d		99.72	100	7183359	1716080	
CA_RP_neg_5.d		99.95	100	9162232	2130386	
CA_RP_neg_6.d		99.9	100	8726872	2054712	
CA_RP_neg_7.d		99.88	100	8566937	2037535	
CA_RP_neg_8.d		99.57	100	9013812	2092674	
CA_RP_neg_9.d		99.97	100	9836830	2292168	
CC_RP_neg_1.d		99.94	100	9180058	2080044	
CC_RP_neg_2.d		99.69	100	7768052	1806182	
CC_RP_neg_3.d		99.76	100	14257814	3028756	
CC_RP_neg_4.d		99.83	100	9391674	2171134	
CC_RP_neg_5.d		99.91	100	10142743	2317134	
CC_RP_neg_6.d		99.94	100	11130733	2506665	
CC_RP_neg_7.d		99.1	100	4991826	1240300	
CC_RP_neg_8.d		99.94	100	10886295	2488318	
CC_RP_neg_9.d		98.59	100	4546627	1111915	
FK_RP_neg_1.d		99.94	100	9442340	2128735	
FK_RP_neg_2.d		99.76	100	8340693	1963150	

Figure 1. MassHunter Profinder main view shows the results using Batch Recursive Feature Extraction. There are four windows: (A) Compound Group Table, (B) Compound Details Table, (C) Extracted Ion Chromatograms (EICs), and (D) Mass Spectra.

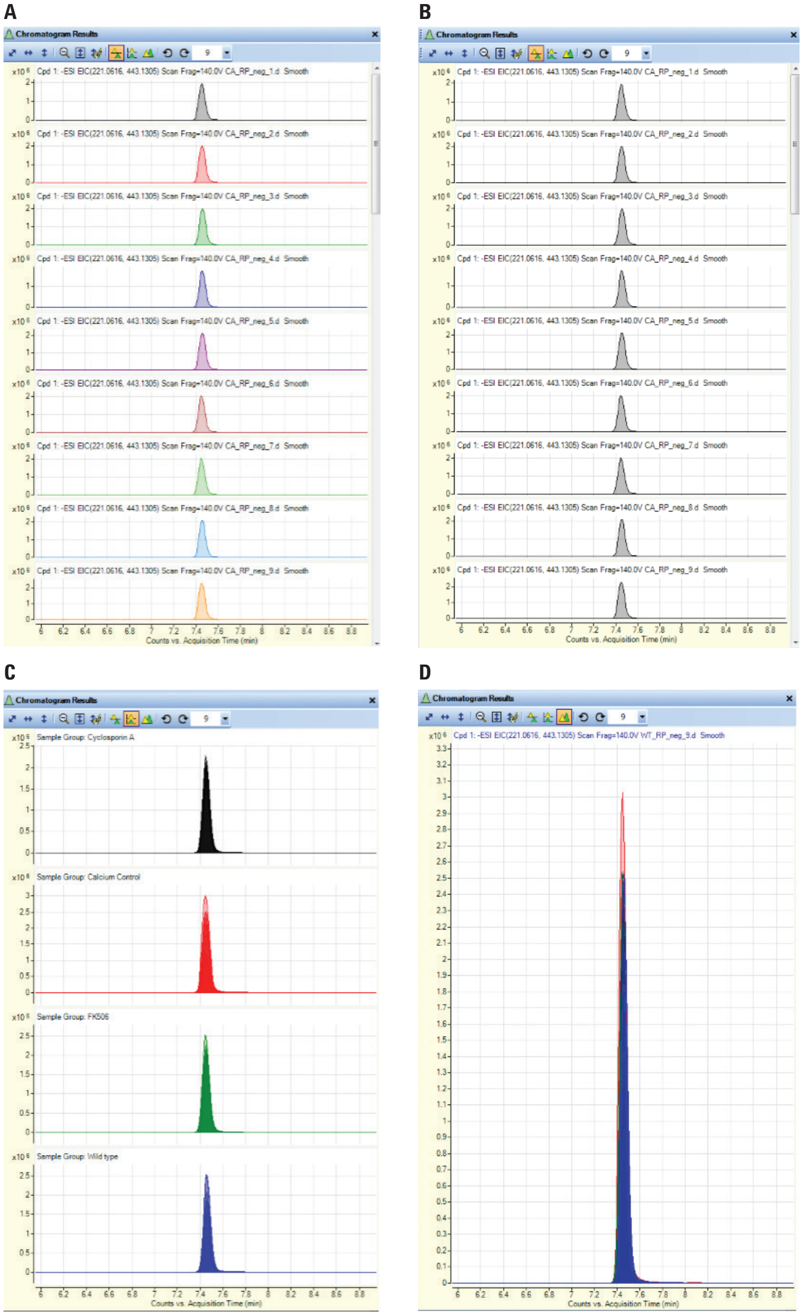

A
B
C
D
Chromatogram Results
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_1.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_2.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_3.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_4.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_5.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_6.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_7.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_8.d Smooth
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V CA_RP_neg_9.d Smooth
Sample Group: Cyclosporin A
Sample Group: Calcium Control
Sample Group: FK506
Sample Group: Wild type
Cpd 1: -ESI EIC(221.0616, 443.1305) Scan Frag=140.0V WT_RP_neg_9.d Smooth
x10^6
Counts vs. Acquisition Time (min)
6 6.2 6.4 6.6 6.8 7 7.2 7.4 7.6 7.8 8 8.2 8.4 8.6 8.8

Figure 2. EICs visualization modes (A) List mode, color by files, (B) List mode, color by sample group, (C) Sample group mode, color by sample group, and (D) Overlay mode.

Batch Recursive Feature Extraction provides greater missing feature recovery. This is achieved by binning and alignment of compound features in the first-pass MFE, after which a composite spectrum for all found ions is created for each consensus (summary) feature. The composite compound feature list is then used as a target list for the second-pass FbI feature extraction.

Batch Recursive Feature Extraction will sometimes report a zero abundance value for a compound. Figure 3 illustrates how a selected compound in one of four sample groups was curated. The EICs (Figure 3A, red traces) were extracted, however, their peak abundances were below the user-specified filter criteria and the peak abundances were reported as zero. Profinder provides raw data visualization and a manual integration tool, a very important feature of this software, which enables visual validation of the feature extraction results and manual editing of EIC peaks. As a result, the zero abundance values of this compound group were manually corrected for this sample group (Figure 3B, red traces).

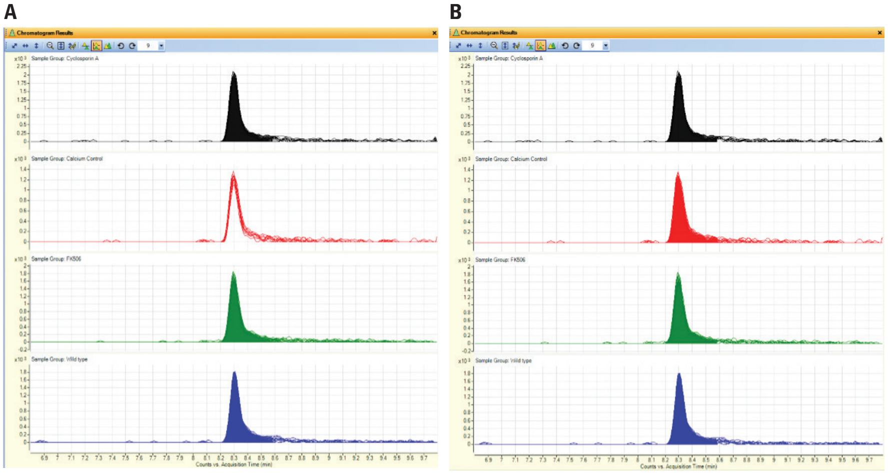
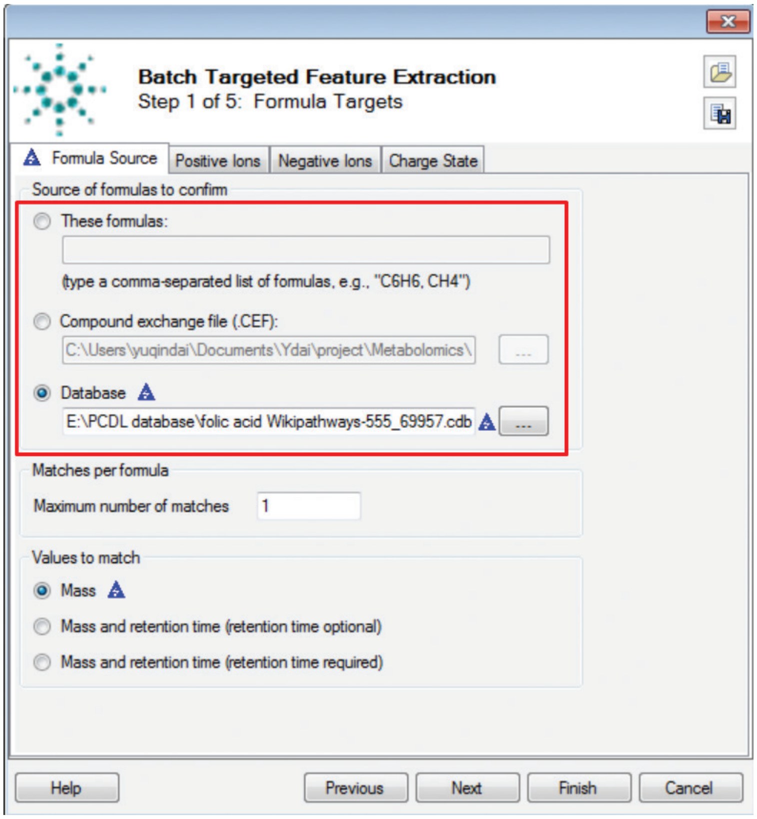

A
B
Chromatogram Results
x10 3 Sample Group: Cyclosporin A
x10 3 Sample Group: Calcium Control
x10 3 Sample Group: FK506
x10 3 Sample Group: Wild type
6.9 7 7.1 7.2 7.3 7.4 7.5 7.6 7.7 7.8 7.9 8 8.1 8.2 8.3 8.4 8.5 8.6 8.7 8.8 8.9 9 9.1 9.2 9.3 9.4 9.5 9.6 9.7
Counts vs. Acquisition Time (min)

Figure 3. Correcting a missing compound. EICs are overlaid by sample groups, before (A) and after (B) manual peak integration.

Batch MFE[3] uses a new proprietary algorithm to extract compounds from a batch of raw data files. Compounds from multiple files are aligned and binned using neutral mass and retention time. As a part of the alignment step, the software automatically reviews and regroups assigned compound ions using batch information. This workflow is highly beneficial for optimizing the settings for the primary Batch Recursive Feature Extraction workflow. This is because Batch MFE is a high speed untargeted feature extraction algorithm and is faster than Batch Recursive Feature Extraction.

Batch Targeted Feature Extraction allows the user to extract compounds of interest with known chemical formulas from large complex data sets. As shown in Figure 4, the user has several options, one can input formulas directly, supply a list of formulas by using a compound exchange file (.CEF), or use a chemical compound database (.CSV or Agilent .CDB format). This workflow offers advantages of high selectivity, fast data processing, and tentative compound annotation. It also provides a useful tool for biological pathway-driven data analysis through Targeted Feature Extraction using a database, for example, generated from Agilent MassHunter Pathways to PCDL software. The Pathways to PCDL software is designed to create an organism specific metabolite database by selecting pathways of interest from public sources BioCyc, KEGG, or WikiPathways. This software was used to create a folic acid biosynthesis pathway database based on the WikiPathways data source for *Saccharomyces cerevisiae*. Using the folic acid biosynthesis pathway database and Batch Targeted Feature Extraction workflow, five compounds (glutamate, ADP, GTP, L-serine, and phosphate) (Figure 5) were extracted and annotated from the yeast metabolomics data acquired on an Agilent Q-TOF LC/MS in negative ion mode.



Batch Targeted Feature Extraction
Step 1 of 5: Formula Targets

Source of formulas to confirm

○ These formulas:

(type a comma-separated list of formulas, e.g., "C6H6, CH4")

○ Compound exchange file (.CEF):
C:\Users\yuqindai\Documents\Ydai\project\Metabolomics\

● Database
E:\PCDL database\folic acid Wikipathways-555_69957.cdb

Matches per formula

Maximum number of matches: 1

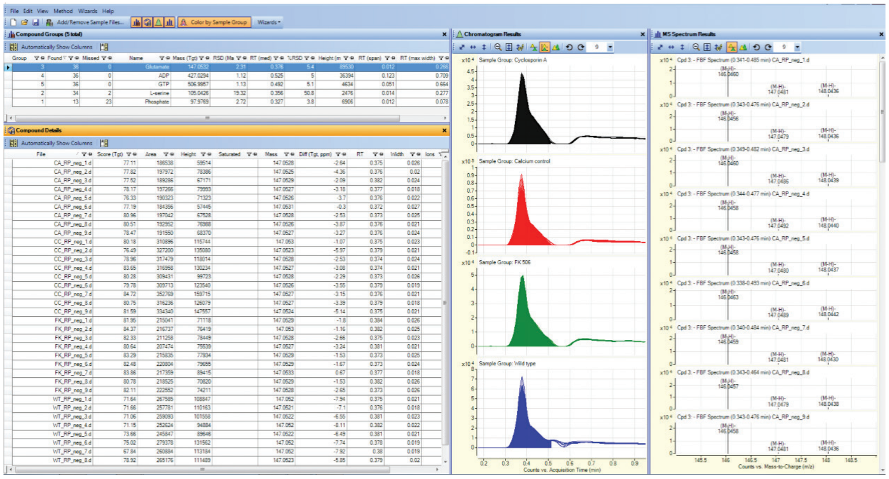
Values to match

● Mass

○ Mass and retention time (retention time optional)

○ Mass and retention time (retention time required)

Figure 4. Three different ways to supply formulas in Batch Targeted Feature Extraction.



File Edit View Method Wizards Help

Add/Remove Sample Files... | Color by Sample Group | Wizards

Compound Groups (5 total)

Automatically Show Columns

Group	Found	Missed	Name	Mass (Tgt)	RSD (Ma	RT (med)	%RSD	Height (m	RT (span)	RT (max width)
3	36	0	Glutamate	147.0532	2.31	0.376	5.4	89530	0.012	0.266
4	36	0	ADP	427.0294	1.12	0.525	5	36394	0.123	0.709
5	36	0	GTP	506.9957	1.13	0.492	5.1	4634	0.051	0.664
2	34	2	L-serine	105.0426	19.32	0.356	50.8	2476	0.014	0.277
1	13	23	Phosphate	97.9769	2.72	0.327	3.8	6906	0.012	0.078

Compound Details

Automatically Show Columns

File	Score (Tgt)	Area	Height	Saturated	Mass	Diff (Tgt, ppm)	RT	Width	Ions
CA_RP_neg_1.d	77.11	186538	59614		147.0528	-2.64	0.375	0.026	
CA_RP_neg_2.d	77.82	197972	78386		147.0525	-4.36	0.376	0.02	
CA_RP_neg_3.d	77.52	189286	67171		147.0529	-2.09	0.382	0.024	
CA_RP_neg_4.d	78.17	197266	79993		147.0527	-3.18	0.377	0.018	
CA_RP_neg_5.d	76.33	190323	71323		147.0526	-3.7	0.376	0.022	
CA_RP_neg_6.d	77.19	184356	57445		147.0531	-0.3	0.372	0.027	
CA_RP_neg_7.d	80.96	197042	67528		147.0528	-2.53	0.373	0.025	
CA_RP_neg_8.d	80.51	192952	76988		147.0526	-3.87	0.376	0.021	
CA_RP_neg_9.d	78.47	191550	68370		147.0527	-3.27	0.376	0.024	
CC_RP_neg_1.d	80.18	310896	115744		147.053	-1.07	0.375	0.023	
CC_RP_neg_2.d	76.49	327200	135080		147.0523	-5.97	0.379	0.021	
CC_RP_neg_3.d	78.96	317479	118014		147.0528	-2.53	0.374	0.024	
CC_RP_neg_4.d	83.65	316958	130234		147.0527	-3.08	0.374	0.021	
CC_RP_neg_5.d	80.28	309431	99723		147.0528	-2.29	0.373	0.026	
CC_RP_neg_6.d	79.78	309713	123540		147.0526	-3.55	0.379	0.019	
CC_RP_neg_7.d	84.72	352769	159715		147.0527	-3.15	0.376	0.021	
CC_RP_neg_8.d	80.75	316236	126079		147.0527	-3.39	0.379	0.018	
CC_RP_neg_9.d	81.59	334340	147557		147.0524	-5.14	0.375	0.021	
FK_RP_neg_1.d	81.95	215041	71118		147.0529	-1.8	0.384	0.026	
FK_RP_neg_2.d	84.37	216737	76419		147.053	-1.16	0.382	0.025	
FK_RP_neg_3.d	82.33	211258	78449		147.0528	-2.66	0.375	0.023	
FK_RP_neg_4.d	80.64	207474	75539		147.0527	-3.24	0.381	0.021	
FK_RP_neg_5.d	83.29	215835	77934		147.0529	-1.53	0.373	0.025	
FK_RP_neg_6.d	82.48	220804	79655		147.0529	-1.67	0.373	0.024	
FK_RP_neg_7.d	83.86	217359	89415		147.0533	0.67	0.377	0.018	
FK_RP_neg_8.d	80.78	218525	70820		147.0529	-1.53	0.382	0.026	
FK_RP_neg_9.d	82.11	222552	74211		147.0528	-2.65	0.373	0.026	
WT_RP_neg_1.d	71.64	267585	108847		147.052	-7.94	0.375	0.021	
WT_RP_neg_2.d	71.66	257781	110163		147.0521	-7.1	0.376	0.018	
WT_RP_neg_3.d	71.06	259093	101558		147.0522	-6.55	0.381	0.023	
WT_RP_neg_4.d	71.15	252624	94884		147.052	-8.11	0.382	0.022	
WT_RP_neg_5.d	73.66	245847	89646		147.0522	-6.49	0.381	0.021	
WT_RP_neg_6.d	75.02	279378	131562		147.052	-7.74	0.378	0.019	
WT_RP_neg_7.d	67.84	260884	113184		147.052	-7.92	0.38	0.019	
WT_RP_neg_8.d	78.92	265176	111489		147.0523	-5.85	0.379	0.02	

Chromatogram Results
x10 4 Sample Group: Cyclosporin A
x10 5 Sample Group: Calcium control
x10 4 Sample Group: FK 506
x10 4 Sample Group: Wild type
Counts vs. Acquisition Time (min)
MS Spectrum Results
x10 4 Cpd 3: - FBF Spectrum (0.341-0.485 min) CA_RP_neg_1.d
(M-H)- 146.0460
(M-H)- 147.0481
(M-H)- 148.0436
x10 4 Cpd 3: - FBF Spectrum (0.343-0.476 min) CA_RP_neg_2.d
(M-H)- 146.0456
(M-H)- 147.0479
(M-H)- 148.0436
x10 4 Cpd 3: - FBF Spectrum (0.349-0.482 min) CA_RP_neg_3.d
(M-H)- 146.0460
(M-H)- 147.0486
(M-H)- 148.0439
x10 4 Cpd 3: - FBF Spectrum (0.344-0.477 min) CA_RP_neg_4.d
(M-H)- 146.0458
(M-H)- 147.0492
(M-H)- 148.0440
x10 4 Cpd 3: - FBF Spectrum (0.343-0.476 min) CA_RP_neg_5.d
(M-H)- 146.0458
(M-H)- 147.0480
(M-H)- 148.0437
x10 4 Cpd 3: - FBF Spectrum (0.338-0.493 min) CA_RP_neg_6.d
(M-H)- 146.0463
(M-H)- 147.0489
(M-H)- 148.0442
x10 4 Cpd 3: - FBF Spectrum (0.340-0.484 min) CA_RP_neg_7.d
(M-H)- 146.0459
(M-H)- 147.0481
(M-H)- 148.0430
x10 4 Cpd 3: - FBF Spectrum (0.343-0.464 min) CA_RP_neg_8.d
(M-H)- 146.0457
(M-H)- 147.0479
(M-H)- 148.0438
x10 4 Cpd 3: - FBF Spectrum (0.343-0.476 min) CA_RP_neg_9.d
(M-H)- 146.0458
(M-H)- 147.0481
(M-H)- 148.0436
Counts vs. Mass-to-Charge (m/z)

Figure 5. Batch Targeted Feature Extraction results from the yeast metabolomics data.

Consistent peak integration across all files or sample groups is important for reliable downstream statistical analyses. When isobaric compounds in a complex matrix elute closely, it is sometimes difficult for peak integrators to establish the peak start/end. As illustrated in Figure 6, the EIC peaks were not consistently integrated across all data files (Figure 6A). Profinder allows the user to investigate EICs and perform manual integration consistently across all overlaid files. The curated peak abundances provide more reliable information for comparison between sample groups or sample files (Figure 6B).

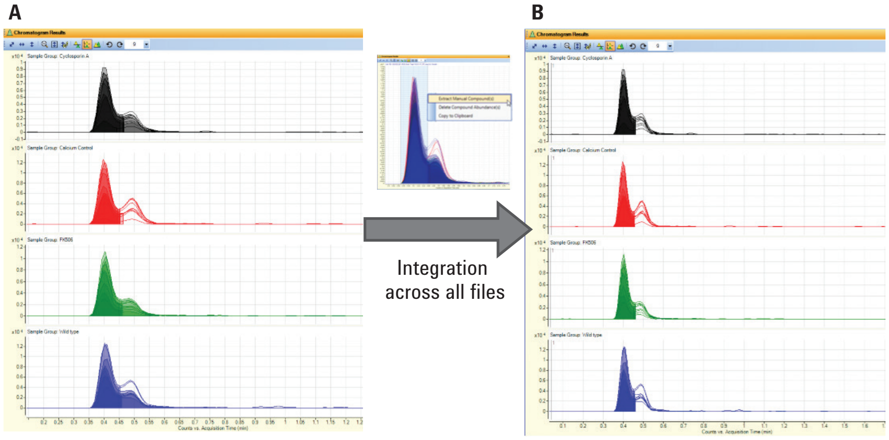


Figure 6. Reviewing for consistent peak integration across all overlaid files, before (A) and after (B) manual correction of peak integration.

Profinder Batch Recursive Feature Extraction Improves Quality of Statistics Analyses

Profinder has a significant impact on statistics from mass spectrometry data. By implementing two-pass batch feature extraction, data visualization, and a manual curation tool, Batch Recursive Feature Extraction reduces the number of false positives and false negatives, subsequently decreasing CVs within sample group replicates. To demonstrate this, we compared the results from Batch Recursive Feature Extraction with Batch MFE in MPP (Figures 7–9)

Figure 7 shows two histograms of CV % within compound groups (that is, the error in measured abundances for compounds aligned by mass and RT across multiple sample files) using Batch Recursive Feature Extraction (Figure 7A) and Batch MFE (Figure 7B). There were 36 samples across 4 sample groups. The lower CV % values suggest that the abundance measurements within a given compound group are of higher quality. The higher CV % values suggest that missing or incorrect peak integrations may be present within a given compound group. Two observations can be noted from the plots. First, the histograms are clearly shifted to lower CV % using Batch Recursive Feature Extraction as compared to Batch MFE. Second, the cumulative percentage of compound groups with low CV % values increased as the histogram distribution shifted to lower variance rates. These trends suggest an overall improvement in compound quality within those respective compound groups.

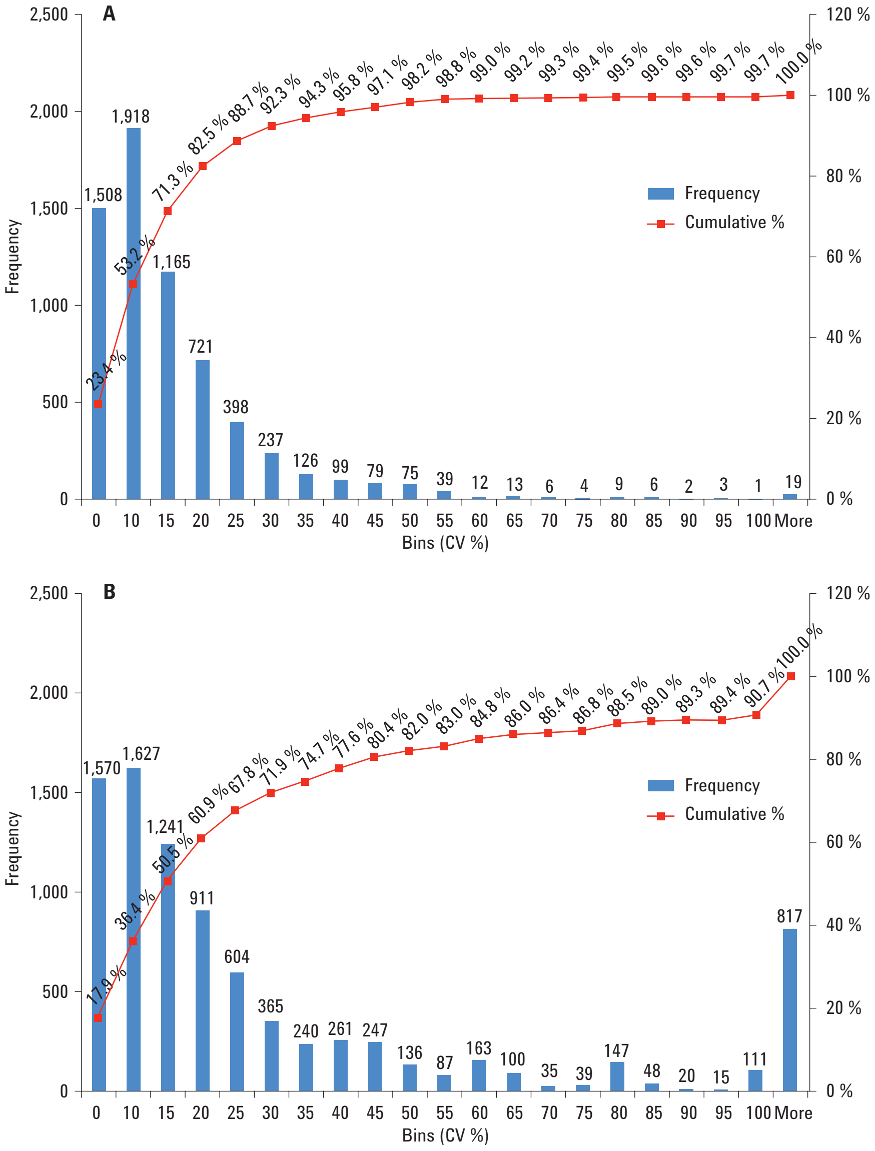


Figure 7. Distributions of binned compound CVs and their frequency (A) Batch Recursive Feature Extraction and (B) Batch MFE. The red line represents the cumulative percent of compounds at a given CV.

Figure 8 shows frequency histograms for 36 sample files extracted by Batch Recursive Feature Extraction (Figure 8A) and Batch MFE (Figure 8B). “Frequency” in MPP refers to the number of files in which a compound was found within a given compound group. The maximum frequency is, therefore, 36, given 36 sample files. If there are missing compounds as a result of the feature extractor not finding a compound within a given file, the frequency will be less than 36. Following Batch Recursive Feature Extraction, the compound groups have a full 36/36 compound representation (Figure 8A).

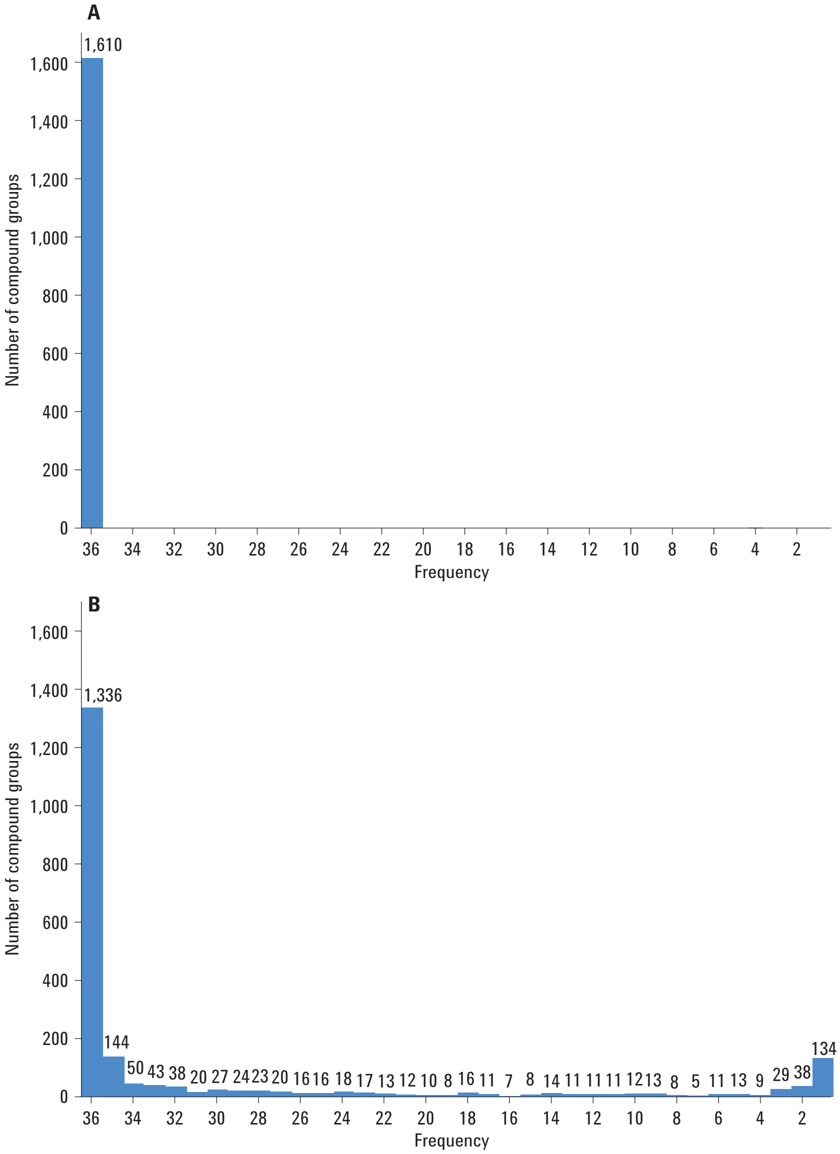


Figure 8. Frequency distribution of extracted compounds across all samples (A) Batch Recursive Feature Extraction and (B) Batch MFE.

Figure 9 shows 2D Principal Components Analysis (PCA) plots colored by sample group for 36 individual sample files representing four sample groups. It is clear that Batch Recursive Feature Extraction has improved the separation between sample groups and also tightened the clustering of the sample replicates. This suggests a marked reduction in noise within sample group replicates. In turn, there is greater visibility of the true sample group-dependent variance.

It is evident that, compared to the results from the Batch MFE only, Profinder Batch Recursive Feature Extraction significantly improves the quality of all subsequent statistical analyses, as evidenced by the higher frequency of lower CV % compound groups in the histograms (Figure 7), complete representation of compounds in each compound group (Figure 8), and better separation between the four biological groups in PCA plots (Figure 9).

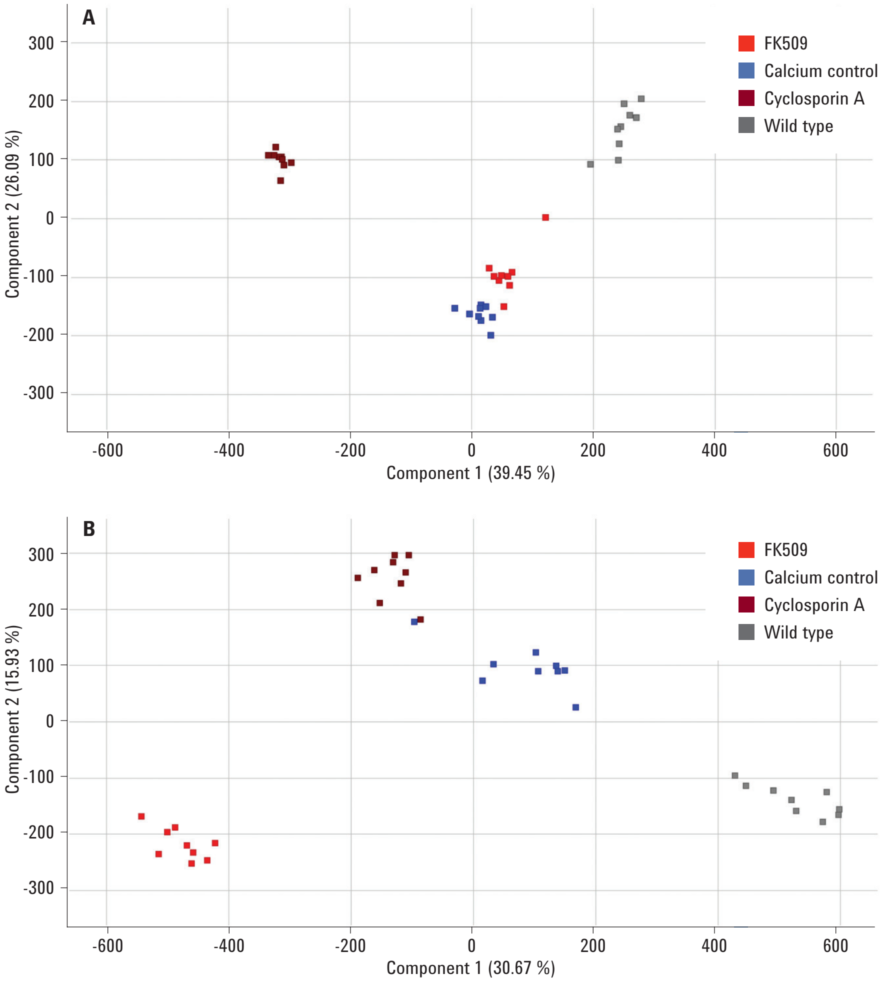


Figure 9. 2D PCA plots of 36 samples in four groups (A) Batch Recursive Feature Extraction and (B) Batch MFE.

Conclusions

MassHunter Profinder is a powerful feature finding software for high resolution accurate mass LC/MS data. It enables fully automated and self-contained two-pass batch feature extraction from large complex data sets. The intuitive and easy-to-use MassHunter Profinder software significantly improves the quality of data for reliable statistics analyses. This software can also be used to support applications beyond metabolomics, such as proteomics and food profiling.

References

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