

Thermo Scientific Pathfinder software enables results-driven analysis for routine qualitative screening experiments using the Thermo Scientific Exactive ultra-high resolution accurate mass LC-MS system.

## Thermo Scientific Pathfinder Software

Streamlined, results-driven analysis



- Simplified sample analysis for multiple users
- Ultra-high resolution and accurate mass capabilities ensure confident results
- Sophisticated elemental composition determination
- Automated summary reporting using pre-defined methods
- Compound library searching for high throughput analysis
- Method setup and configuration of results reporting is easy in administrator mode

Pathfinder™ software used with the Exactive™ LC-MS system provides confident, walk-up analysis of both simple and complex samples. Built-in basic and advanced workflows provide access to the ideal LC-MS platform for compound identification and high throughput screening. With flexible batch processing and automated display of elemental composition, Pathfinder creates a high productivity environment for multiple users with a range of mass spectrometry experience. All users become immediately productive without the need for extensive training or detailed knowledge of the instrument operation and control software. Users simply log in samples, select a pre-defined LC-MS method, and automatically receive their sample report.

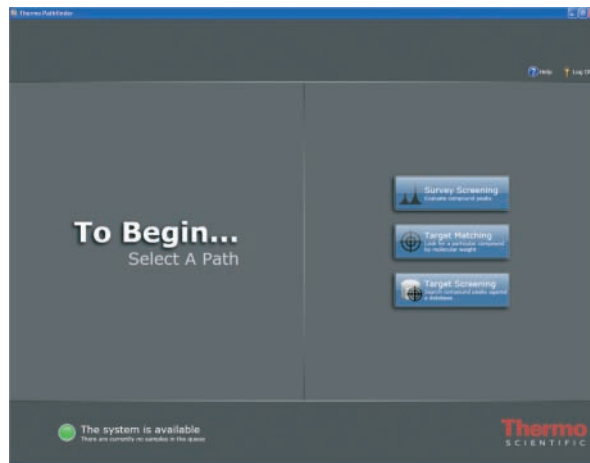
An open access LC-MS laboratory enables scientists to get answers quickly, without waiting for a remote laboratory to send back results. Routine analyses are performed efficiently, leaving mass spectrometry experts more time to focus on solving the most challenging analytical problems. Pathfinder software enables walk-up access to the unique and powerful capabilities of the Exactive instrument, which routinely delivers ultra-high resolution and accurate mass data for every scan without the need for data averaging. Operating at a 10 Hz scanning frequency, the Exactive is fully compatible with U-HPLC technologies and ensures exact mass measurement for fast chromatography applications. Rapid polarity switching enables the detection of the widest range of compound types.

### User Modes

#### Flexible Workflows Matching User Experience Levels and Requirements

Users have different levels of knowledge and requirements for sample analysis and Pathfinder's flexible interface provides the right workflow for every analysis. Pathfinder provides an intuitive interface for both the walk up and the experienced users. New users can easily follow developed methods to get analytical answers quickly and automatically. Pre-defined methods are used to produce automated reports for LC-MS analysis, limiting instrument set-up time. Experienced users can tune and optimize the system, develop methods, and perform a broad range of experiments.

#### Step 1 - Sample Login and Method Selection

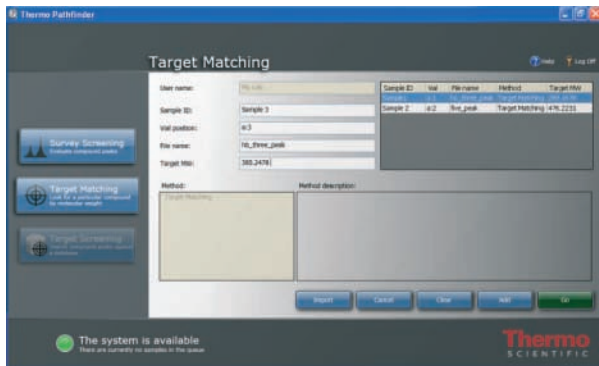


The user logs into Pathfinder and chooses from one of the following types of analyses:

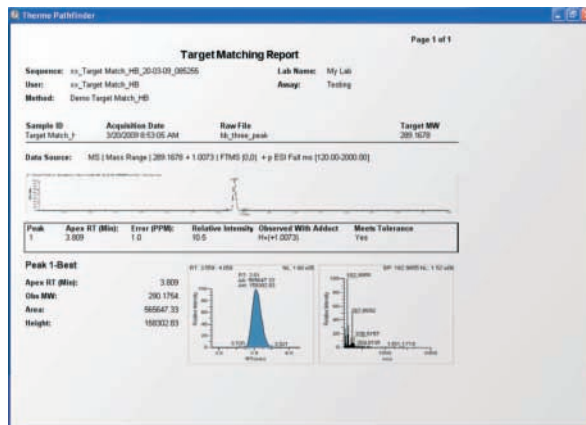
- Survey screening - performs overall peak processing and elemental composition for all peaks in a chromatogram.
- Target matching - searches the chromatogram for a peak of specified  $m/z$  value and perform an elemental composition if it is found within a specified mass tolerance.
- Target screening - searches for a targeted list of compounds from a database.



## Step 2 - Sample Submission Information

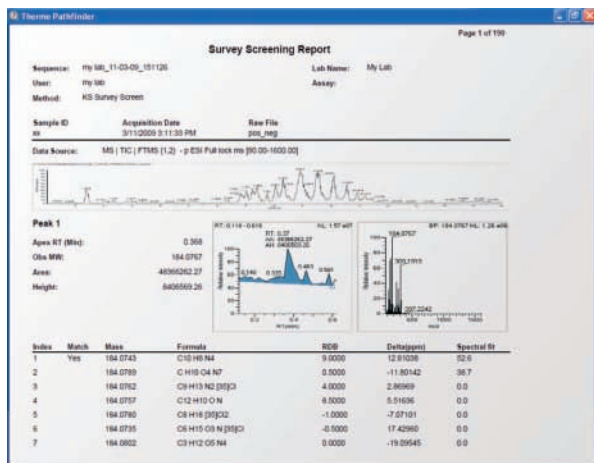


Pathfinder allows the user to select from a library of methods defined by the administrator. The user is prompted to enter a unique personal identifier in the User name box and for the sample identification in the Sample ID box. The autosampler vial position is entered and the sample data file name entered. If the Target Matching method is selected, the user enters the exact mass for the mono-isotopic molecular weight in the Target MW box. After that, a method is selected from the available list. Once the sample information has been entered, click "GO" to start the sample analysis.

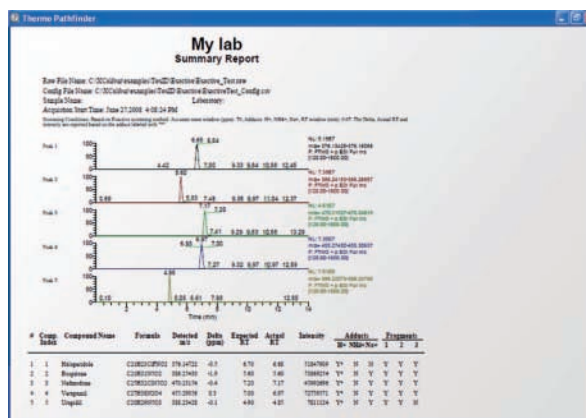


For the target matching workflow, Pathfinder searches for the presence of a specified molecular weight in a sample. Pathfinder checks for the  $MH^+$  adduct ion or other specified adducts for the target compound. Results reporting include a full scan mass spectrum, HPLC chromatogram, elemental composition confirmation and details of the target matching.

## Step 3 - Receive a Detailed Confirmation Report



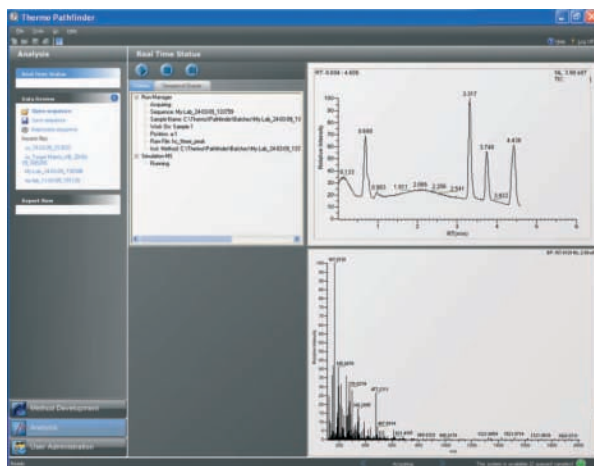
The administrator can configure the method to generate printed reports or electronic reports in pdf or other formats. For survey screening analysis, Pathfinder displays a chromatogram followed by a report summary for each peak detected. Peak information including the retention time, peak height and peak area are reported. There is also an enlarged view of the detected peak along with a mass spectrum from the peak apex. Elemental composition results are included as well.



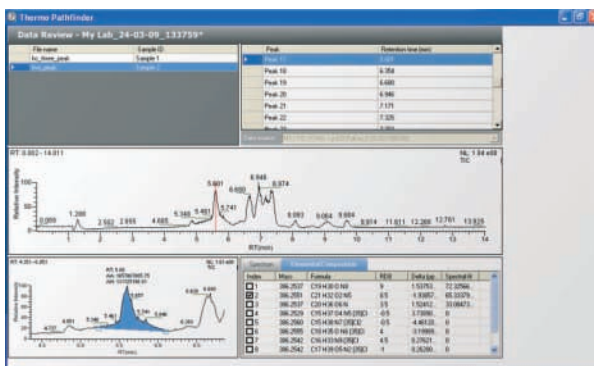
For the target screening workflow, Pathfinder screens the sample against a user defined library. Samples are identified by comparing observed mass spectra and retention times against the entries in the library. Additional adduct and fragment matching enhance confidence in the results. Reporting formats include a summary report for all compounds found in the sample and detailed reports for each compound found.



## Administrator Privileges and Data Review



Pathfinder allows the administrator to set up the system and monitor usage, either while in the laboratory or remotely. Using Pathfinder software, administrators have full access to the system to set up user access, sample processing, analytical method selection and results reporting. Administrators can also initiate an LC-MS analysis and track the status of the Exactive system.



Administrators have sophisticated data review capability within Pathfinder. Samples can be reprocessed, added and/or deleted. Mass spectra and chromatograms can be adjusted for detailed examination of the data. Peaks can be re-integrated manually in a point-and-drag fashion. Elemental composition is determined for masses of interest using intelligent software processing which reports confidence fit values.

## Summary

Samples submitted - thank you

Pathfinder provides results-driven analysis using the Exactive ultra-high resolution accurate mass LC-MS system.