Higher productivity in trace analysis laboratories through faster method development and reporting

Due to the increasing amount of contamination being found in our food and environmental systems, today’s laboratories are under constant pressure to increase productivity. The need to balance productivity with high quality analytical data generation is critical. Thermo Scientific TraceFinder software provides an integrated workflow approach to meet these challenges.

TraceFinder™ software allows the analyst to develop high throughput screening and quantitative assays quickly and accurately, using Thermo Scientific mass spectrometer (MS) systems. TraceFinder is fully integrated with Thermo Scientific Xcalibur core software, and provides a comprehensive system incorporating built-in methods for commonly found contaminants, processing methods, library searching capabilities, data review, and reporting with built-in templates. It also includes a rights-based secure user login system to protect the integrity of analytical data.

Optimized Workflow for Trace Analysis Laboratories – A secure login procedure allows identification of the operator and performance of specific tasks necessary to start building the analytical workflow.
**TraceFinder Highlights**

**Built-in MS Methods and Compound Datastore**
TraceFinder software incorporates a comprehensive list of MS methods for a diverse group of contaminants: pesticides, antibiotics, veterinary products, and industrial chemicals such as melamine. The method development section incorporates an exhaustive list of SRM transitions and their associated parameters optimized for the Thermo Scientific TSQ Series mass spectrometers. This enables users to rapidly select and develop the method of their choice.

**Library Matching**
The unique QED-MS/MS scan function of the TSQ Series allows users to trigger data-dependent full scan MS/MS spectra from SRM transitions. The MS/MS spectra generated can be automatically searched against a built-in NIST format library for confirmation of the analyte structure.

**Method Forge**
Create processing methods automatically from raw data files using Method Forge. Peaks are filtered, labeled, and identified; qualifier ions are selected; and calibration settings are generated. This significantly reduces the analyst’s method development time.

**Easy Method Development**
Method development is simplified by using instrument-specific preconfigured MS methods. A wide range of methods are included for analysis of pesticides, antibiotics, and industrial chemicals like melamine. Newer methods are updated on the Thermo Scientific TraceFinder support Web site, and can be downloaded directly by licensed users.
**Reports**

TraceFinder includes many preconfigured reporting templates in both Crystal Reports® and Microsoft® Excel® format. These incorporate requirements of environmental and food safety regulations from laboratories globally.

**Rights-based user login for security**

TraceFinder allows five security levels for user logins. This enables different permission levels to be assigned for different users in large regulated laboratories, thus ensuring data security.

**Multiple languages**

TraceFinder software is available in English. Other languages, including Chinese, will be available in the future.

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**Data Processing and Review**

Data review is simplified with TraceFinder, and supports the analyst’s critical role in this key process. Inspect sample and reference mass spectra, evaluate peak integration, review different curve fits, and observe ion ratio values easily and fully interactively.

**Library Matching**

Following data acquisition and processing, mass spectra can be compared against built-in libraries. These can include NIST libraries, user-customized libraries, and instrument-specific libraries, such as the Quantitation-Enhanced Data-Dependent MS/MS library included with TSQ Series mass spectrometers.
TraceFinder Software

Thermo Scientific Nautilus LIMS
Software for Food and Beverage Laboratories

Nautilus LIMS™ is a Laboratory Information Management System designed for the unique requirements of food and beverage labs. Leveraging the power of TraceFinder, Thermo Scientific mass spectrometers, and Xcalibur™ software, this workflow solution will increase your lab’s ability to test more food samples in less time with greater accuracy. Along with the demands of increased throughput comes the growing burden of keeping track of all the samples, associated data, and raw results files. Nautilus LIMS helps laboratory managers control this ever-increasing information and data, and provides visibility into all aspects of your laboratory. Nautilus can help you oversee sample location, generate and track bar-codes, visualize sample progress through your testing regime, generate instrument run files, collect raw data, analyze results from instrumentation, render automated reports, monitor laboratory supplies, and more. For more information about Nautilus LIMS, go to www.thermo.com/nautilus.

Smart Reporting

With TraceFinder, the reporting process is an easy way to review the data. The Report View window is linked to the Data Review Page, allowing users to toggle between a specific spot in the processed data and a report. Changes made in the Data Review Page are reflected immediately in the report, without reprocessing or reanalyzing. Many predefined reporting templates – in both Crystal Reports and Excel formats – are included.