Simply intelligent

Chromeleon goes MS
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The new 7.2 release of Thermo Scientific™ Dionex™ Chromeleon™ Chromatography Data System (CDS) software is the first CDS that combines separation (GC/IC/LC) and Mass Spectrometry (MS) in an enterprise (client/server) environment.

The Chromeleon CDS support for GC-MS uses native Thermo Scientific MS drivers for instrument control and extends the necessary MS-specific data views, data processing, and reporting capabilities. This merges the benefits of Chromeleon CDS with our leading GC-MS instrumentation and application expertise for a superior answer to the productivity challenges in the analytical laboratory.

Key Benefits

By extending Chromeleon CDS beyond chromatography into MS, you can now streamline your chromatography and MS quantitation workflows in one application.

- Reduced training effort for your lab staff – one single software package instead of several.
- Prevention from data loss during a network outage through secure XVault™ infrastructure.
- One set of methods, one set of reports and one central location for chromatography and MS data.
- Comprehensive suite of Chromeleon CDS productivity tools from dynamic data linking, instant processing, to SmartPeaks™ detection – now available for MS.
- Spreadsheet-based, easily customizable, flexible and powerful Chromeleon CDS reporting.

Ultimately this lets you use your MS like any other routine detector.

First CDS fully integrating MS into routine and quantitative workflows
Key Features

- Full control of the Thermo Scientific™ ISQ™ Single Quadrupole GC-MS system and Thermo Scientific™ TSQ™ 8000 Triple Quadrupole GC-MS/MS systems, including tuning and instrument calibration.
- MS-specific data views such as TIC, with Mass Spectra (Figure 1), quantitation channels, MS component traces, and XIC (Figure 2).
- NIST library searching including the direct import of a library search into your component tables (Figure 3).
- Seamless import of and central processing and reporting of Thermo Scientific™ Xcalibur™ raw data, which also enables data processing and reporting for all Thermo Scientific LC-MS/MS systems.
- New consolidated report tables catering to multiple traces and large data sets allow users to quickly and easily evaluate and report MS data.
- Enables architecture for MS including remote instrument access and data processing, full 21 CFR Part 11 GMP/GLP compliance, and fully scalable architecture.
- MS data processing on a component-by-component basis using MS-specific Genesis and ICIS detection algorithms, and all Chromeleon CDS quantitation tools and options.

Figure 1: Extraction and display of MS data in Chromeleon 7.2 CDS.

Figure 2: New component centric data view for MS data in Chromeleon 7.2 CDS.

Figure 3: NIST library search in Chromeleon 7.2 CDS.
Additional highlights in Chromeleon 7.2 CDS

Linking of Panes:
By linking the active Chromatography Studio panes to the chromatogram, data evaluation becomes simple. Calibration plots, interactive charts and reports are linked to the active chromatogram displaying only data relevant to the current zoom or selected peaks, providing the analyst with all the information needed for fast, easy data evaluation.

Intelligent Run Control (IRC):
Gets you from samples to results even quicker! IRC enables you to have the software automatically react to passed or failed user-defined conditions during the sequence run. IRC in Chromeleon CDS provides many different options including re-injections of the current injection, all injections, restarting from an earlier point in the sequence, or adding extra injections. It also includes built-in error handling, ensuring you get more right first time analyses.

eWorkflows:
The Chromeleon 7.2 CDS eWorkflow™ framework captures all the unique aspects of a chromatography workflow, and enables you to reduce the number of steps needed to perform your routine MS workflows while ensuring that procedural rules and guidelines are followed accurately. With just a few mouse clicks, any user can create and run analyses on all your chromatography instrumentation including MS.

Chromeleon 7.2 CDS gives superior data processing and automation capabilities, boosting your overall lab productivity.

For more information, please visit thermoscientific.com/chromeleon