Streamlining Your Chromatography Laboratory Operations Through End-to-End Workflows

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Informatics & Chromatography Software
Introduction

- Sequence Creation
- Data Analysis
- Result Retrieval
- Summary
Introduction

Data Into Knowledge

LIMS, SDMS, LES
Data management & integration across the laboratory

Data Management
Laboratory Management
System Integration

Instrument Control & Monitoring
Data Capture
Data Analysis

CDS
Chromatography data acquisition & management
Introduction

Streamlining Chromatography

From samples…

… to final results
Introduction

Sequence Creation

Data Analysis

Result Retrieval

Summary
Beyond paper SOPs…
LES (Laboratory Execution System) provides a simple step-wise approach to executing laboratory processes

- Lab Execution
- Instrument Integration
- Lab Execution Reporting
- Lab Method Configuration
Sequence Creation

Transform your paper/digital SOPs into electronic methods for process execution

- Step-wise approach
- Workflow execution, such as Batch, Sequence, Stock Batch, Sample, …
- Instrument integration
- Review with auto-validate
- eSignatures/cross check
- Generate SOP report with execution outcomes
Sequences can be reviewed & updated prior to creation in CDS

Create sequences from samples, tests, batches or LES
• Information captured in LES can be passed into CDS sequence
• Can also pass calibration standard concentrations
Sequence Creation

- **eWorkflows™**
  - Fast, easy, accurate sequence creation
  - Assists user in creating an appropriate sequence for a suitable instrument with pre-defined associated files and a well-defined structure

- **Contain:**
  - Instruments on which the analysis can be run
  - **All** associated files:
    - Instrument methods
    - Processing methods
    - Reports
    - Spectral libraries
    - External documents (e.g. SOP)
  - Template for sequence name and storage location
  - Custom variables
  - Rules for sequence layout
Sequence Creation

1. Select eWorkflow
2. Select Instrument
3. Click Launch
Sequence Creation

4. Input number of samples

5. Input position of first sample

6. Click Finish
Sequence Creation

• Sequence created in 6 clicks with correct:
  • Name
  • Location
  • Methods
  • Report
  • Structure
  • Custom Variables
• Plus:
  • SOP attached
  • Can run immediately
Sequence Creation

- Thermo Scientific™ SampleManager LIMS™ can create sequences using eWorkflows™
Introduction

Sequence Creation

Data Analysis

Result Retrieval

Summary
Overview

Sequence Creation

Data Analysis

- Data Acquisition
- Data Processing
- Data Reporting

Result Retrieval

Summary
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Data Analysis
Data Acquisition
Data Processing
Data Reporting
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Summary
Thermo Scientific™ Chromeleon™ CDS controls over 450 different modules from 18 different manufacturers including:

- Thermo Fisher Scientific (LC, IC, GC, MS, Sample Prep)
- Agilent (LC, GC)
- Waters (LC)
- Shimadzu (LC, GC)
- Varian (LC, GC)
- Perkin Elmer (LC, GC)
- Gilson (LC)
- CTC PAL (Sample Prep)

LIMS can incorporate data from non-chromatographic e.g. AA, ICP, UV, FTIR, MS, etc.) & ‘simple’ instruments (balance, pH meter, etc.)
Overview

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Data Processing

• Batch review and reprocessing of chromatography data still most time consuming and error prone process

• Inefficient data visualization, tedious, repetitive integration, and multi-step batch reprocessing add significant time

• Operational Simplicity™ speeds up all operations including data review and processing

  ✓ Minimize steps needed to perform any task
  ✓ Make all steps easy to understand and easy-to-use
  ✓ Minimize the time it takes to perform any task

Tiziana Nardin, Fondazione Edmund Mach

“We found the software very easy to learn and to use day-to-day as it is extremely intuitive with a clean, user-friendly interface”
Translating Operational Simplicity into Lab Productivity

- Significant productivity gains reported by range of customers from different industries
- In addition, productivity gains have been verified by direct competitor comparison
  - Head-to-head comparison of the same tasks (prescribed by customer) in each CDS

Data Processing – Competitor Comparison

<table>
<thead>
<tr>
<th>Windows</th>
<th>Faster</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;50%</td>
<td>&gt;50%</td>
</tr>
</tbody>
</table>

Mouse Clicks

Rob Allen, Catalent Pharma

“After switching to Chromeleon we found we were saving on average 20 minutes per analyst per day on data processing and reporting.”
Data Processing

- Faster data processing
  - Dynamic data updating

- Faster data reviewing
  - MiniPlots™
  - SmartLink

- Faster processing method setup
  - Cobra™ peak detection algorithm and wizard
  - SmartPeaks™ Integration Assistant
  - Component table wizard

- Advanced spreadsheet reporting
  - Eliminate external spreadsheets
  - Dynamic result updating
  - Controlled, compliant report generation
Data Processing

- Smart functions simplify and speed up data processing including:
  - Cobra peak detection algorithm and wizard
  - SmartPeaks Integration Assistant
Data Processing – Cobra Algorithm

- Parameter-less first pass Cobra integration
Data Processing – Cobra Peak Detection Wizard

1. Start Cobra Wizard

2. Define integration range

3. Set baseline noise range

4. Select narrowest peak

5. Select smallest peak
Data Processing – Cobra Peak Detection Wizard

- Parameters added to component table…

Brian Alliston, Sterling Pharma Solutions

“Chromeleon is much quicker in all activities. Use of the Cobra wizard allows for quick setup of optimum integration parameters giving us consistent integration much faster than either of our previous CDS.”
Data Processing – SmartPeaks Integration Assistant

1. Activate SmartPeaks Wizard

2. Select Area of Interest

3. Select the Integration You Want

[Diagram showing a graph with labeled areas and a window displaying integration options: 1. Original, 2. Valley To Valley, 3. Exponentially attenuated, 4. Tangential at both ends rider slippage.]
Data Processing – SmartPeaks Integration Assistant

- Parameters added to component table
- Changes apply to ALL chromatograms in sequence

Michael Faley, Sigma Aldrich

“After a brief familiarization it felt like you could just walk up to the system and accomplish what needed be done without jumping through an excessive number of hoops. You can tell that the software was built for the user’s ease.”
Overview

Sequence Creation

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Summary
• CDS Report Designer can contain:
  • Multiple worksheets
  • Text and variables
  • Various result tables
  • Various plot types
  • Custom equations
Data Reporting

... to create the report you need.
Data Reporting – Example Report in Microsoft Excel

Calibration Curve - Retention Time vs CHI IAM 7.4

* Chi Literature value from Valko et al. J Pharm Sci 89, 8 (2000) 1085

<table>
<thead>
<tr>
<th>Compound (2mg/ml)</th>
<th>Retention Time</th>
<th>Literature CHI IAM 7.4</th>
<th>CHI IAM 7.4</th>
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</thead>
<tbody>
<tr>
<td>Std 1 peak 1</td>
<td>4.197</td>
<td>17.2</td>
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</tr>
<tr>
<td>Std 2 peak 2</td>
<td>4.97</td>
<td>25.9</td>
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<tr>
<td>Std 3 peak 3</td>
<td>5.813</td>
<td>37.71</td>
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<tr>
<td>Std 4 peak 4</td>
<td>8.56</td>
<td>49.4</td>
<td></td>
</tr>
</tbody>
</table>

Samples Retention Time (mins) vs CHI IAM

\[ y = 13.663x - 41.023 \]
\[ R^2 = 0.9962 \]
Bernd Boscolo, Douglas Manufacturing Ltd.

“The Chromeleon Report Designer is a mighty tool to calculate and present data, and to our understanding is far better than any other software package. With the Chromeleon Reports, we are seeing time and cost savings equivalent to four to five full time employees depending on the workload in each month. These savings are higher than anticipated.”
Result Retrieval

- Results can be easily sent to any LIMS
- Thermo Scientific LIMS and CDS software tightly integrated
  - Data can be retrieved direct from variables or report sheets
  - Pull final calculated values from cells
Result Retrieval

- From SampleManager LIMS software
- Retrieve manually
- Automate retrieval via background schedule
Result Retrieval

- From Chromeleon chromatography data system (CDS)
  - Push to LIMS by sequence or individual injections
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Conclusions

SampleManager LIMS and Chromeleon CDS streamline your workflows getting you from samples to knowledge faster than ever.

LIMS, SDMS, LES
Data management & integration across the laboratory

CDS
Chromatography data acquisition & management

Streamlining Chromatography
Powerful software to drive efficiency for your entire lab
Thank you very much for your attention!

Questions?

Do you have additional questions or do you want to talk to an expert from Thermo Fisher Scientific?

Please send an E-Mail to analyze.eu@thermofisher.com and we will get back to you.