Taking the Pain Out of Chromatographic Peak Integration

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Eastern Analytical Symposium 2014
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Introduction

• In many laboratories, batch review and reprocessing of chromatography data is the most time consuming and error prone process.

• Inefficient data visualization together with tedious, repetitive integration and multi-step batch reprocessing can add significant amounts time to the process.

• Thermo Scientific™ Dionex™ Chromeleon™ Chromatography Data System (CDS) software applies Operational Simplicity™ to data processing and as a result, offers several unique tools to simplify and speed up data review and processing.
Faster Data Processing
Faster Data Processing

• Reprocessing of chromatography data is often the most time consuming and error prone post-run process.
• Re-integration can be a manual, unintuitive, multi-step process.
• You may need to repeatedly batch reprocess the entire sequence just to view the effect of changes made.
• In Chromeleon CDS, dynamic data processing ensures the selections and changes you make are instantly reflected in the data and results, for all injections in the sequence, saving huge amounts of data processing time.
Typical CDS Reprocessing

- Method is stored outside sequence
- Copy stored with each injection – need to reprocess sequence to update all injections
Method part of sequence
Active link to injections

Method is dynamically linked to each injection = instant updates
No need to export data
All reporting and calculations are within a validated environment.
Greater productivity - up to 98% time saving
Likely cause is this outlier point. To investigate, double click point and associated chromatogram is automatically displayed.

Calibration has failed specification.
Integration is incorrect!
Integration is corrected
Calibration point is recalculated.
Calibration line fitting is recalculated

Calibration now passes specification
Faster Data Reviewing
Faster Data Reviewing

• When reviewing data you can waste a lot of effort and time moving between different views to display the results you want on the screen.
  • For example, you want to review the calibration plots of several components, or compare the results for only one type of injection e.g. only check standards or calibration standards.

• SmartLink automatically displays only data relevant to the current zoom or selected components, providing the analyst with all the information needed for fast, easy data evaluation, saving valuable review time.
Faster Data Reviewing – SmartLink

• Easy way to review required data, without setting advanced filters in the panes.

• Data is showed based on:
  • Zoom of chromatogram
  • Selection of peaks in the chromatogram
  • Selection of chromatograms in the sequence

• Link is created by a single click
SmartLink of Panes to Chromatogram

One click to activate SmartLink
SmartLink of Panes to Chromatogram
SmartLink of Panes to Chromatogram

**Zoom into chromatogram**

**Calibration Plot only shows visible peaks**

**Table only shows visible peaks**
SmartLink of Panes to Selected Injections
SmartLink of Panes to Selected Injections

Select multiple injections

Chromatogram overlay

Result table and Interactive Chart only show selected injections
Faster Data Review – SmartLink

• SmartLink can drastically reduce the time and effort of data reviewing by displaying all the relevant data to enable you to perform fast, easy data evaluation.

• It also provides a simplified way of viewing large amounts of data, e.g. from long sequences or where there are large numbers of components.
  • Especially useful for GC and GC-MS users.

• Provides an easy way to review data and trends across specific injections or components within your sequence.

• Another unique implementation of Operational Simplicity!
Easier Processing Method Setup
Easier Processing Method Setup

- Creating your component table can be time consuming and error prone
  - Setting correct integration parameters can be a laborious trial and error process
  - Setting up calibration levels can be an unintuitive, complex procedure
  - Updating component retention times as peaks drift is often a lengthy, manual activity, especially when many peaks are present.

- Chromeleon CDS offers a suite of functionality to simplify and speed up processing method creation including:
  - A component table wizard
  - Cobra™ peak detection algorithm and wizard
  - SmartPeaks™ Integration Assistant
  - Fast, intuitive calibration level creation
  - One-click retention time updating
Easier Processing Method Setup – Component Table

- Component table wizard
  - Guides you to accurately create a table based on your chromatogram and/or UV spectral libraries.

- One click to use spectral library results
- 5 step wizard including naming of peaks

Component Table Wizard
Easier Processing Method Setup – Component Table

- Component table is quickly created with correct retention times, windows and names.

<table>
<thead>
<tr>
<th>#</th>
<th>Name</th>
<th>Ret.Time</th>
<th>Window</th>
<th>Channel</th>
<th>Eval.Type</th>
<th>Stand.Meth.</th>
<th>Eval.Time</th>
<th>Stand.Meth.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Thiamine</td>
<td>2.298</td>
<td>0.100 AG</td>
<td>All Channels</td>
<td>Area</td>
<td>External</td>
<td>Lin</td>
<td>Lin</td>
</tr>
<tr>
<td>2</td>
<td>Pyridoxine</td>
<td>3.445</td>
<td>0.165 AG</td>
<td>All Channels</td>
<td>Area</td>
<td>External</td>
<td>Lin</td>
<td>Lin</td>
</tr>
<tr>
<td>3</td>
<td>Niacinamid</td>
<td>5.250</td>
<td>0.100 AG</td>
<td>All Channels</td>
<td>Area</td>
<td>External</td>
<td>Lin</td>
<td>Lin</td>
</tr>
<tr>
<td>4</td>
<td>Pantothenic Acid</td>
<td>7.767</td>
<td>0.142 AG</td>
<td>All Channels</td>
<td>Area</td>
<td>External</td>
<td>Lin</td>
<td>Lin</td>
</tr>
<tr>
<td>5</td>
<td>Folic Acid</td>
<td>8.323</td>
<td>0.100 AG</td>
<td>All Channels</td>
<td>Area</td>
<td>External</td>
<td>Lin</td>
<td>Lin</td>
</tr>
<tr>
<td>6</td>
<td>Vitamin B12</td>
<td>8.819</td>
<td>0.100 AG</td>
<td>All Channels</td>
<td>Area</td>
<td>External</td>
<td>Lin</td>
<td>Lin</td>
</tr>
<tr>
<td>7</td>
<td>Riboflavin</td>
<td>9.360</td>
<td>0.100 AG</td>
<td>All Channels</td>
<td>Area</td>
<td>External</td>
<td>Lin</td>
<td>Lin</td>
</tr>
</tbody>
</table>
Easier Processing Method Setup – Peak Detection

• Most time consuming and tedious task in chromatography process:
  • Chromatogram Integration

• Chromeleon 7 CDS introduces two new tools that significantly simplify this process:
  • Cobra Peak Detection Algorithm / Wizard
  • SmartPeaks Integration Assistant
Cobra Peak Detection Algorithm / Wizard

• Cobra is an algorithm that:
  • Finds peak start/end times accurately and consistently
  • Accurately determines “true” underlying baseline
  • Requires minimum number of parameters to reach integration goal

• Cobra Wizard provides:
  • Fast, guided way to determine initial detection parameters
Cobra Peak Detection Wizard
Cobra Peak Detection Wizard

1. Start Cobra Wizard
2. Define the integration range
3. Set the baseline noise range
4. Select the narrowest peak
5. Select the smallest peak
Cobra Peak Detection Wizard

- Parameters added to component table...

... and your integration is done!
Easier Processing Method Setup – Peak Detection

• There are many ways to integrate unresolved peaks

Is this what you want?

Is this what you want?
Peak Detection – SmartPeaks Integration Assistant

- Unique tool for easily reaching your integration goals for unresolved peaks
- Requires no training
- Great example of Operational Simplicity
  - Process is clear and understandable
  - Requires only a few steps
  - Correctly integrates all unresolved peaks in seconds
Peak Detection – SmartPeaks Integration Assistant

1. Activate SmartPeaks Wizard

2. Select Area of Interest

3. Select the Integration You Want

[Graph and interface screenshot showing the selection of different integration methods]
Peak Detection – SmartPeaks Integration Assistant

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

Your integration is done!
Easier Processing Method Setup – Calibration Levels

- Creation and correct population of your calibration levels is often a manual multi-step process.
- Calibration levels are created directly in your injection list.
- Automatically synchronized to the component table.
- You only enter standard amounts.
Easier Processing Method Setup – Ret. Time Updating

- Updating component retention times as peaks drift can be time consuming, manual, error prone task, especially when many peaks are present.
- Automatically update with one click in the Processing Method, saving time and preventing errors.
Summary
Summary – Process Your Data

• Faster data processing
  • Dynamic data processing ensures selections and changes made are instantly reflected in data and results, for all injections in sequence.

• Faster data reviewing
  • SmartLink automatically displays only data relevant to current zoom or selected components, providing analyst with all information needed for fast, easy data evaluation

• Easier processing method setup
  • Chromeleon CDS offers a suite of functionality to simplify and speed up processing method setup including:
    • A component table wizard
    • Cobra peak detection algorithm and wizard
    • SmartPeaks Integration Assistant
    • Fast, intuitive calibration level creation
    • One-click retention time updating
Summary – Bringing It All Together

Chromeleon CDS has all the tools to help you process your data in the shortest time!
Thank You!

Any Questions?