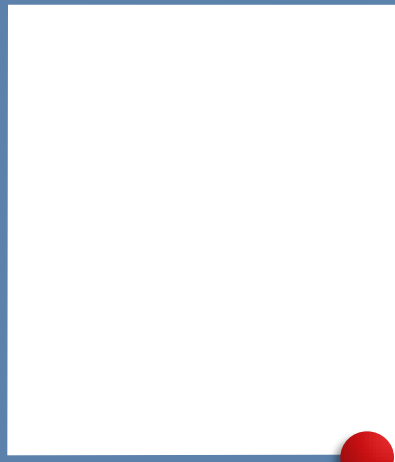




Taking the Pain Out of Chromatographic Peak Integration

Dan Kutscher

Eastern Analytical Symposium 2014

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Introduction

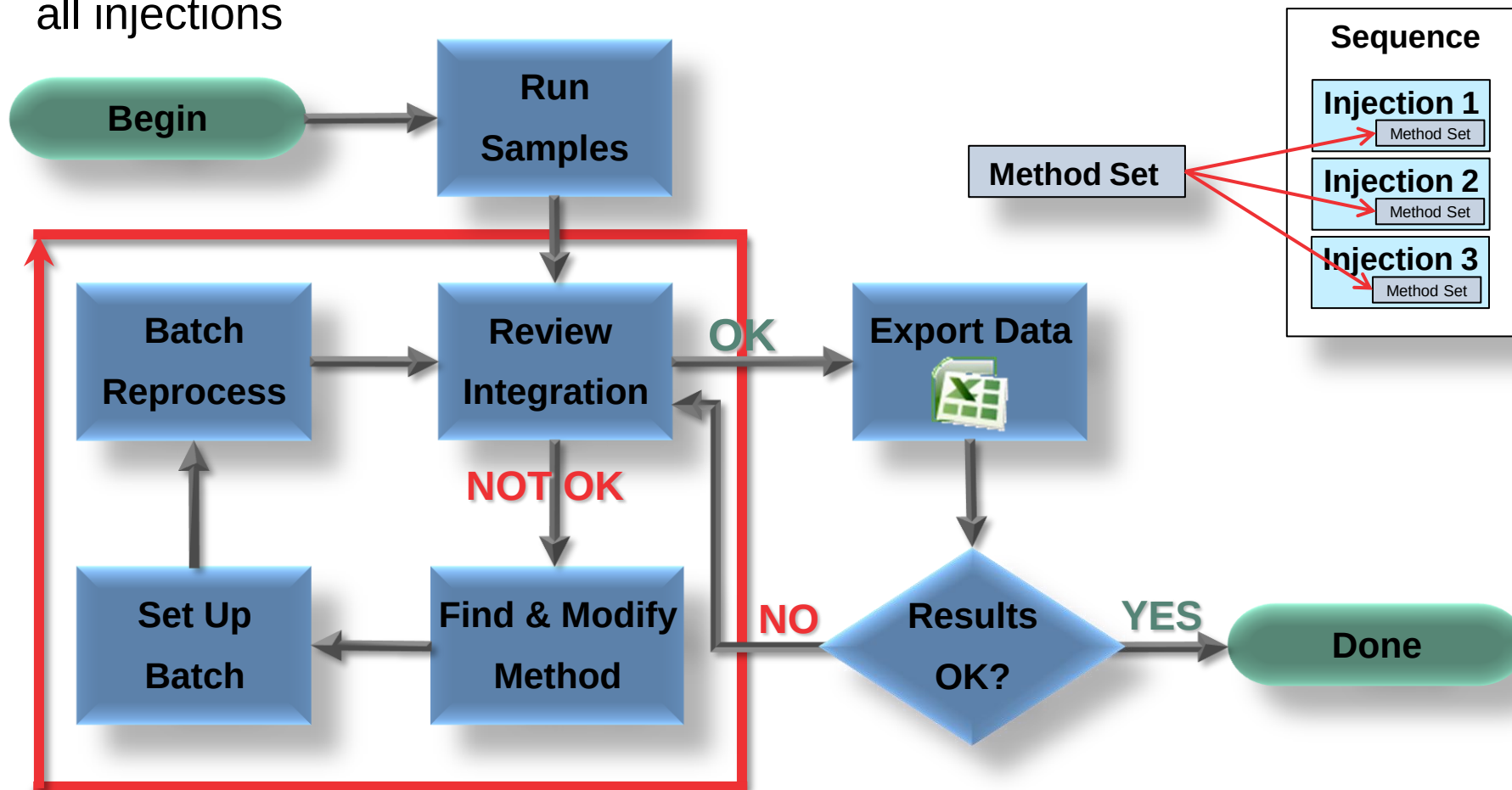
- In many laboratories, batch review and reprocessing of chromatography data is the most time consuming and error prone process.
- Inefficient data visualization together with tedious, repetitive integration and multi-step batch reprocessing can add significant amounts time to the process.
- Thermo Scientific™ 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

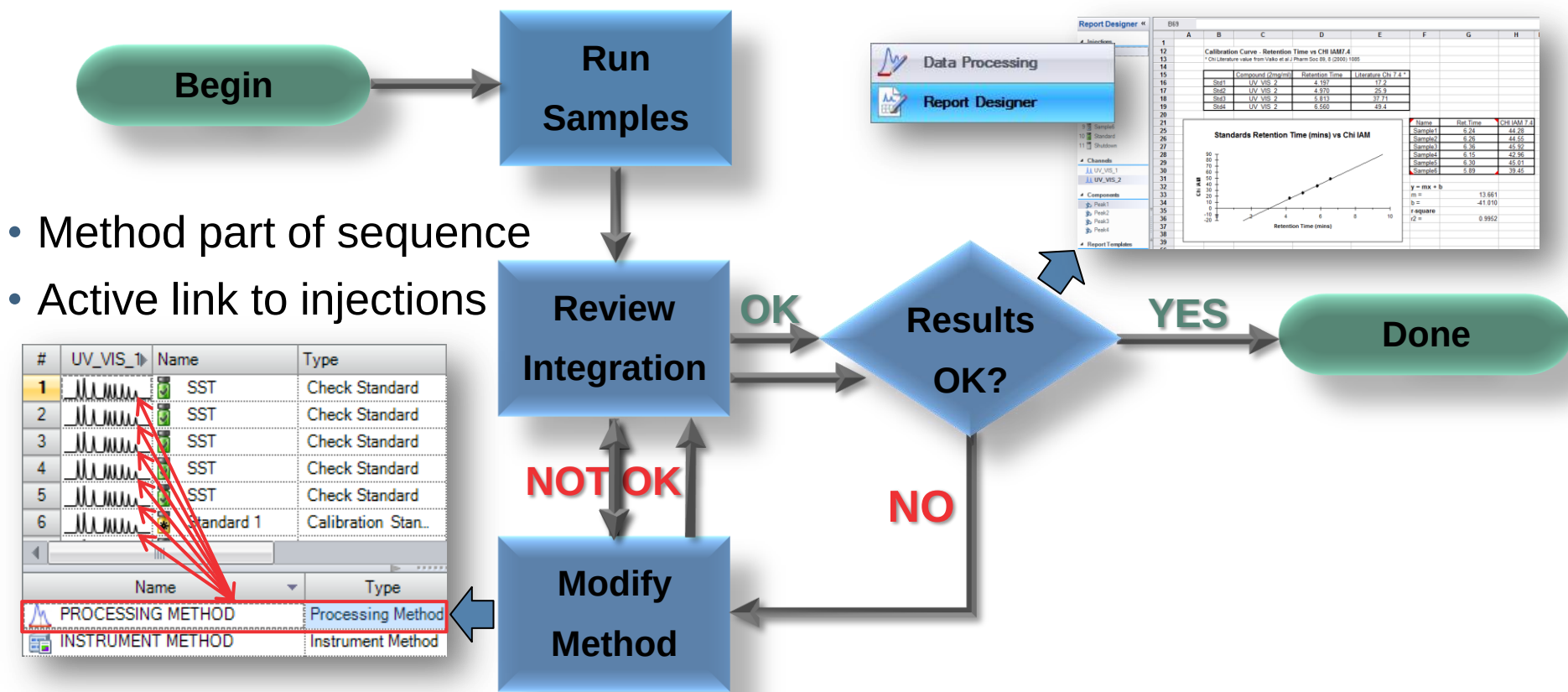
- Reprocessing of chromatography data is often the most time consuming and error prone post-run process.
- Re-integration can be a manual, unintuitive, multi-step process.
- You may need to repeatedly batch reprocess the entire sequence just to view the effect of changes made.
- In Chromeleon CDS, dynamic 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

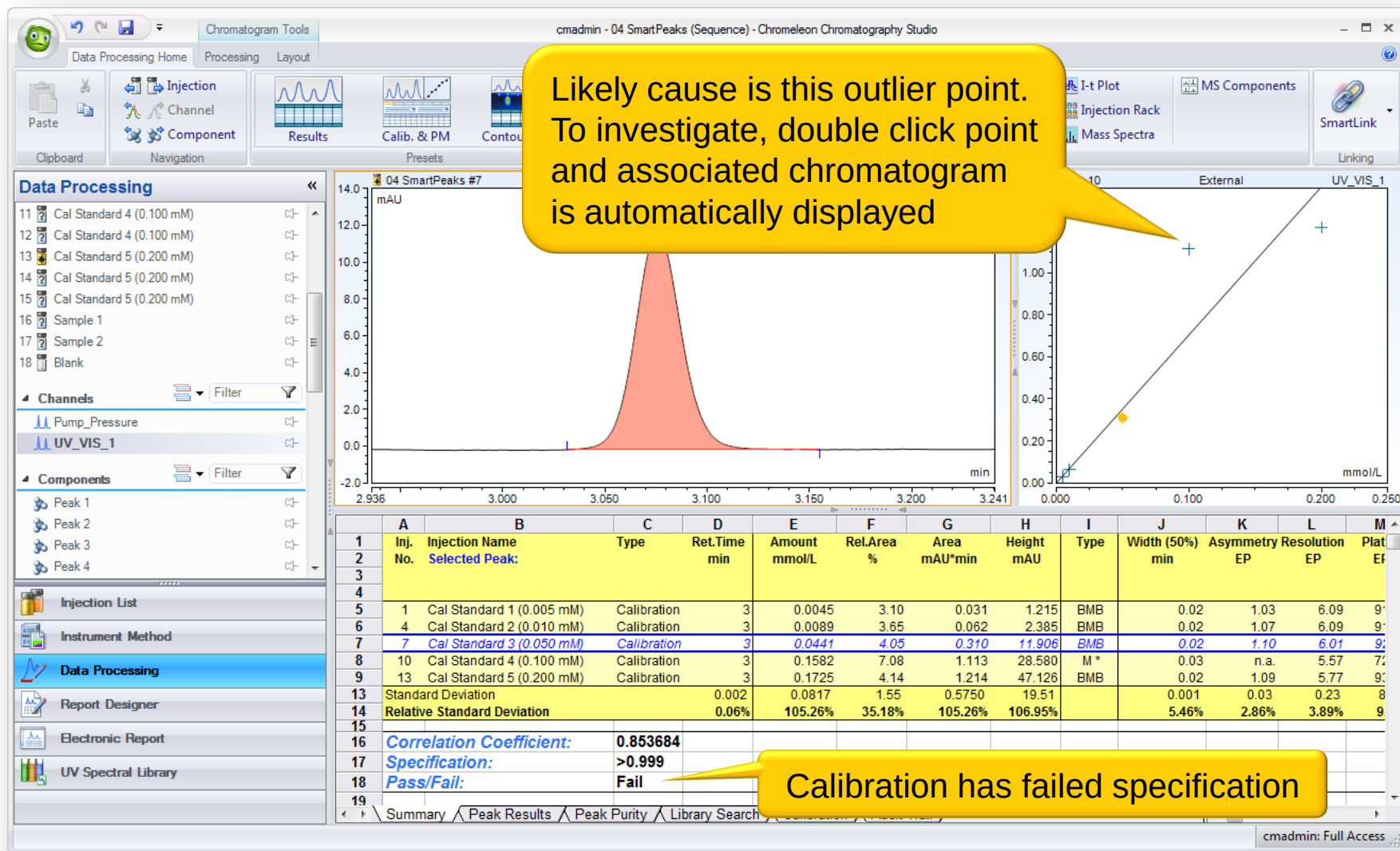


Chromeleon CDS Data Processing

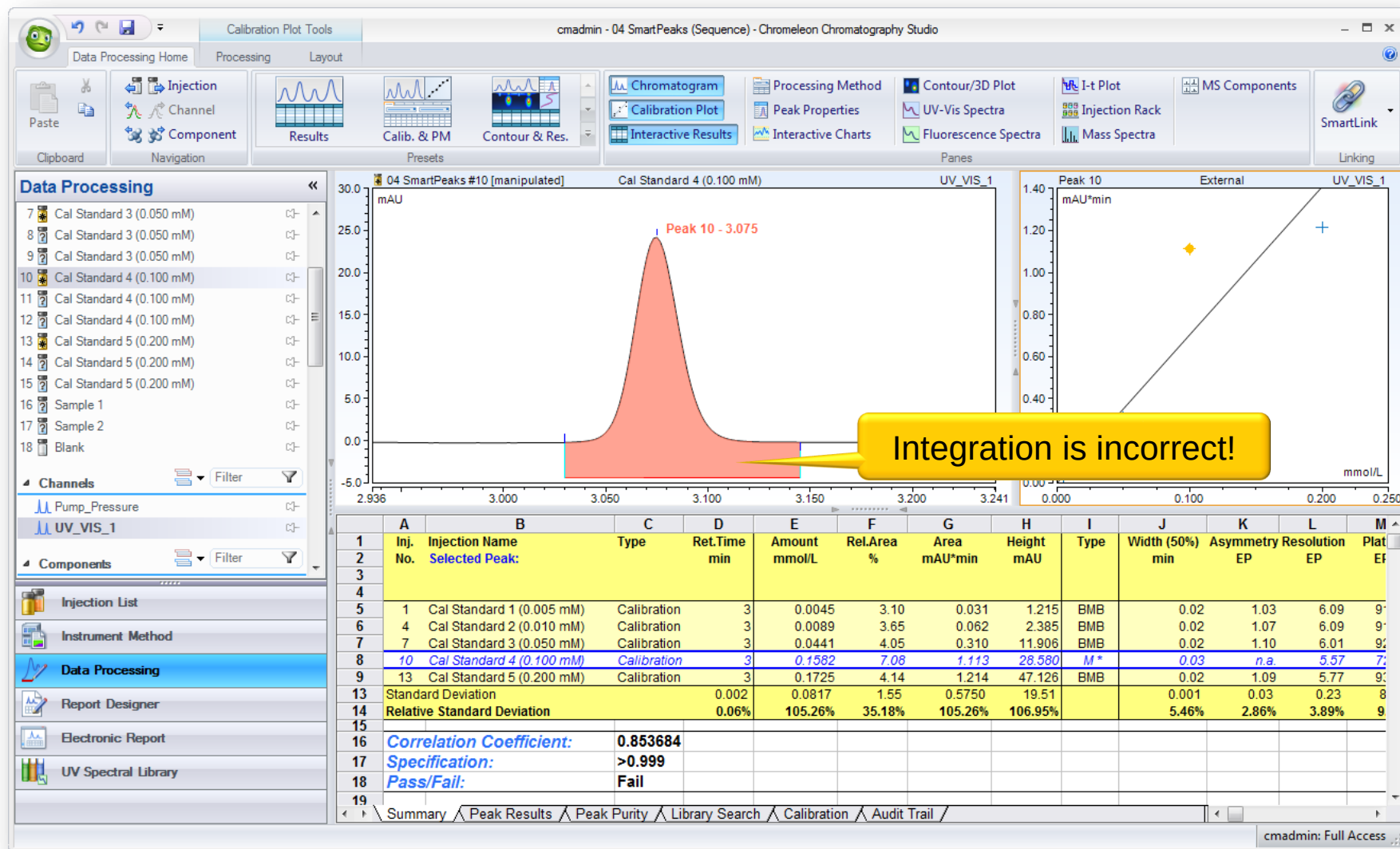


- Method is dynamically linked to each injection = instant updates
- No need to export data
- All reporting and calculations are within a validated environment.
- Greater productivity - up to **98%** time saving

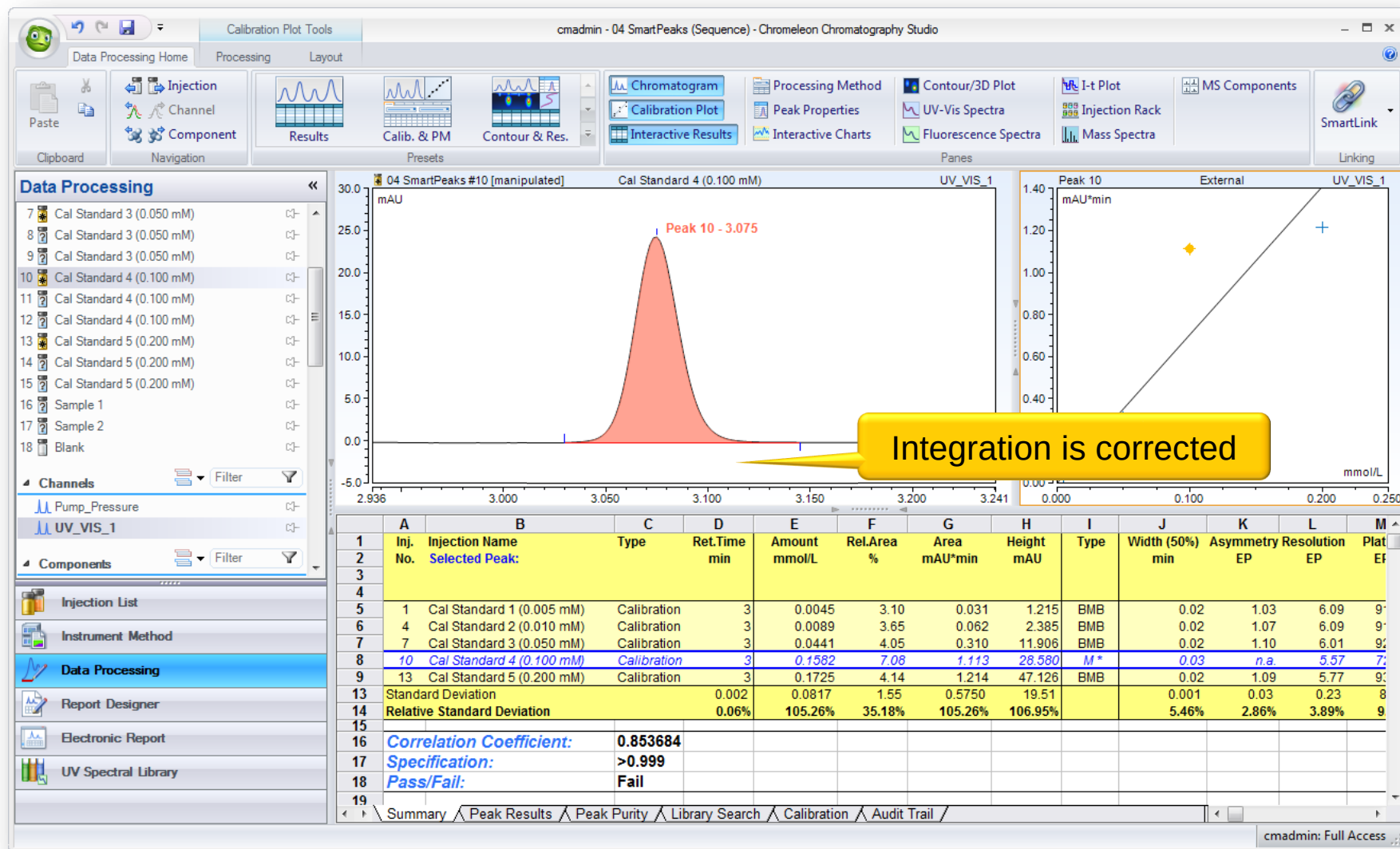
Data Dynamic Linking and Updating - 1



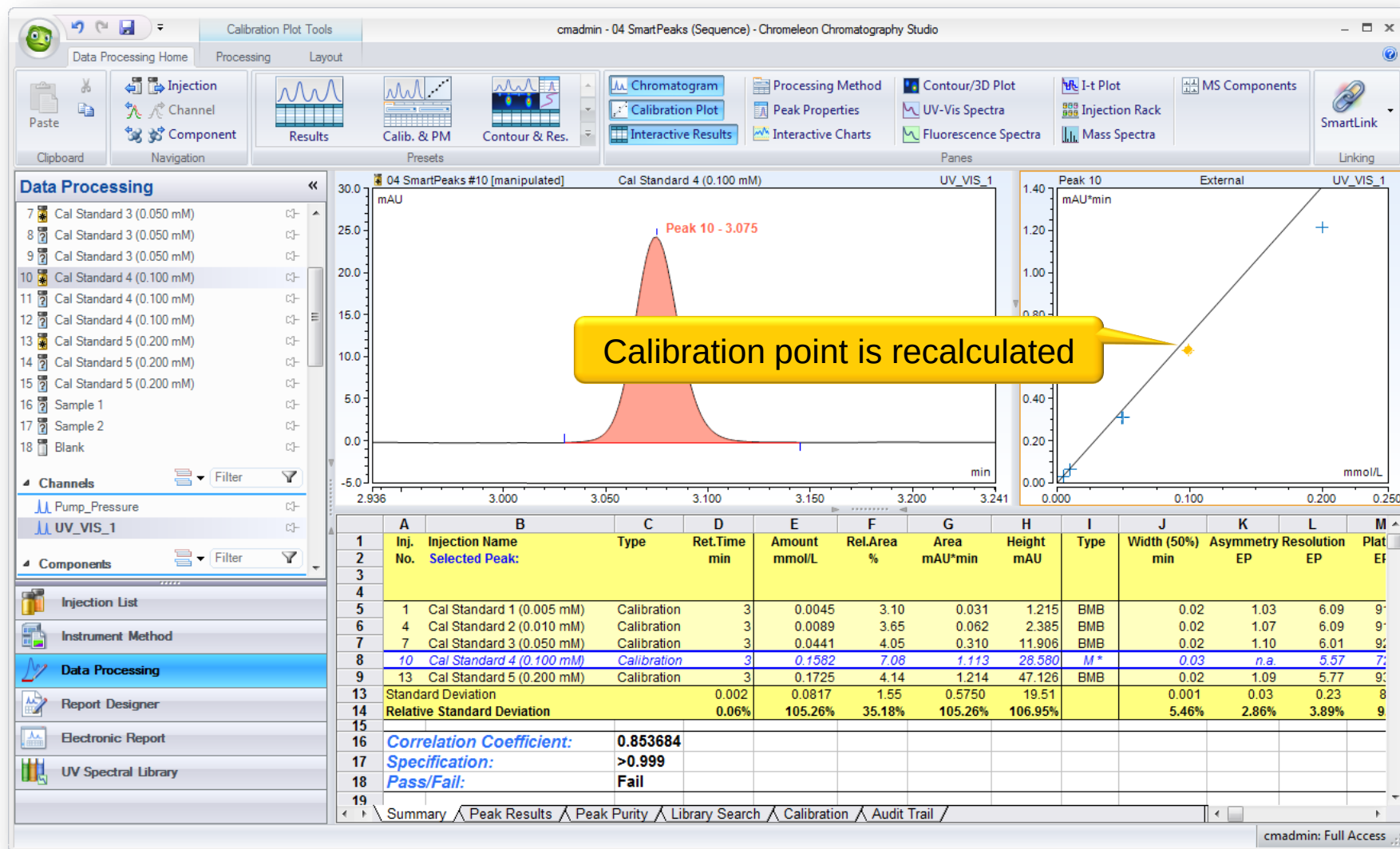
Data Dynamic Linking and Updating - 2



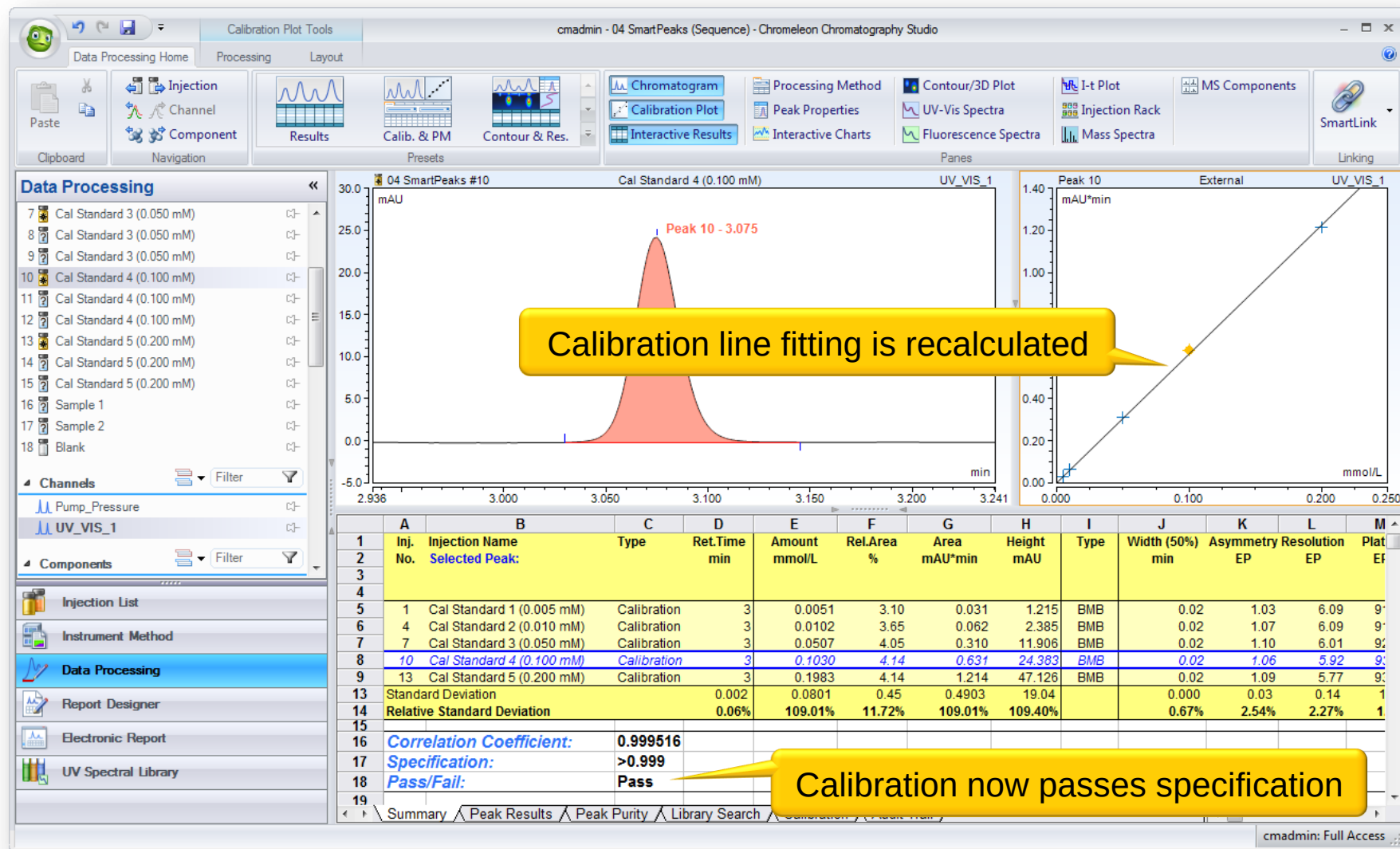
Data Dynamic Linking and Updating - 3



Data Dynamic Linking and Updating - 4



Data Dynamic Linking and Updating - 5



Faster Data Reviewing



Faster Data Reviewing

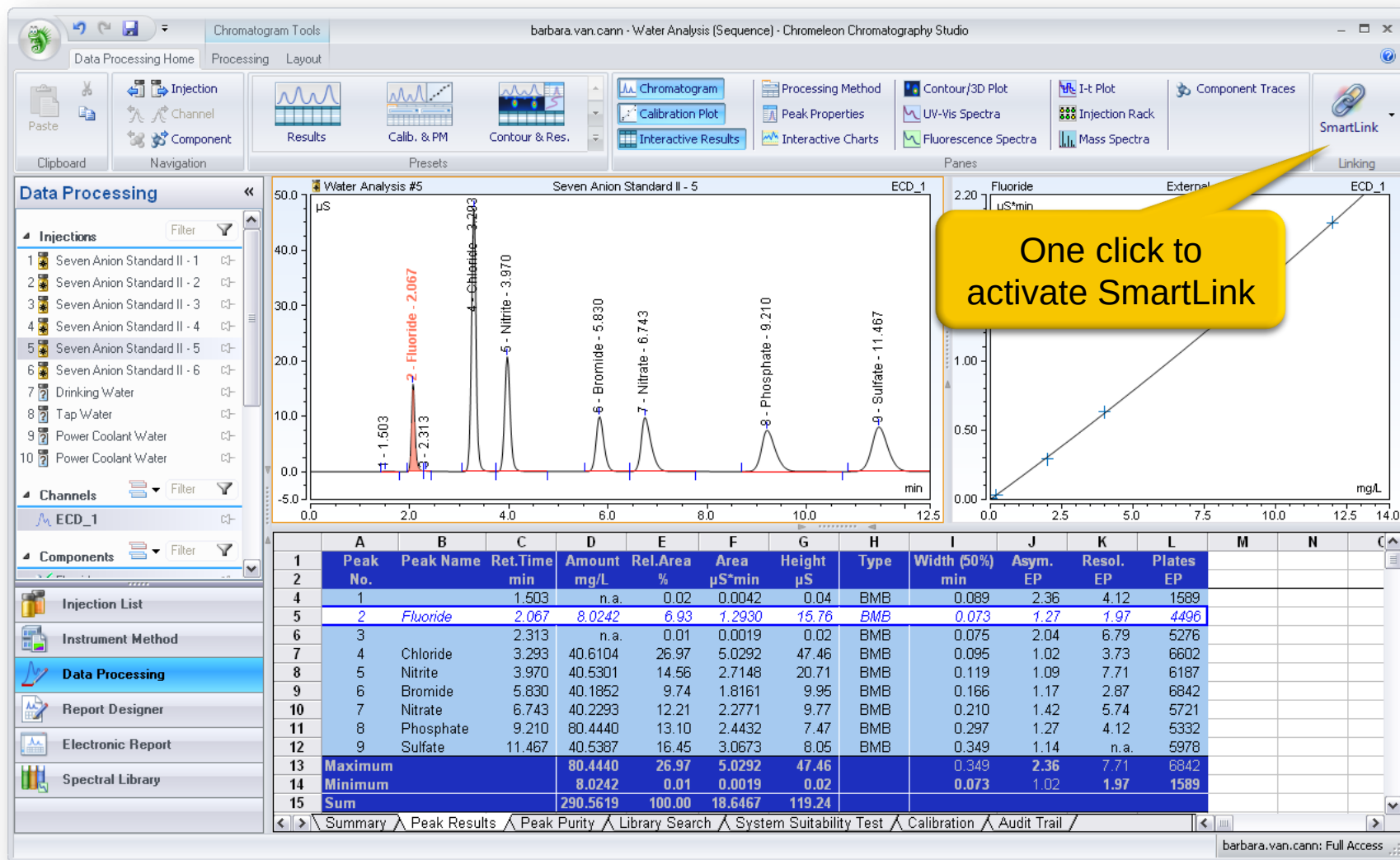
- When reviewing data you can waste a lot of effort and time moving between different views to display the results you want on the screen.
 - For example, you want to review the calibration plots of several components, or compare the results for only one type of injection e.g. only check standards or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

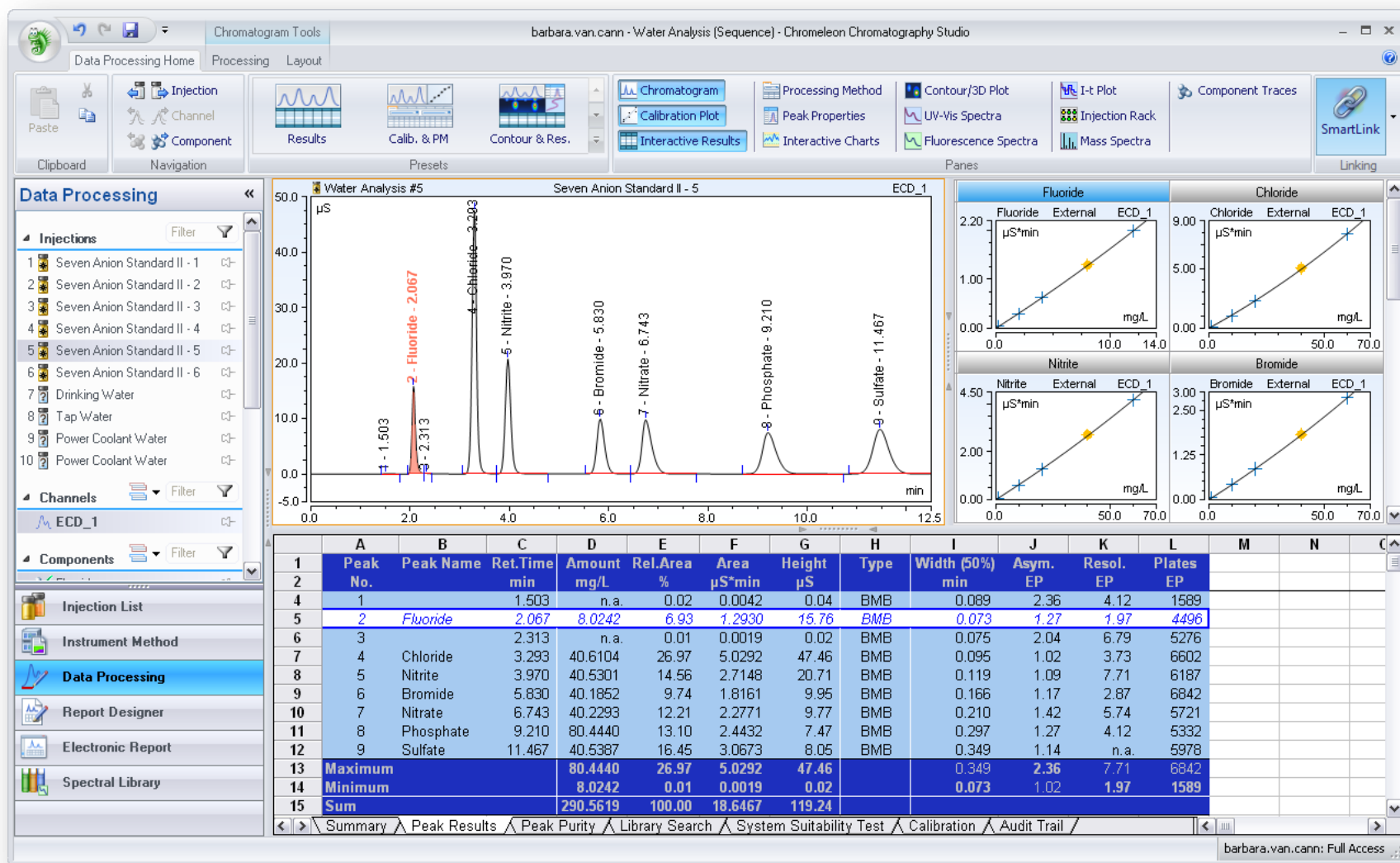
- Easy way to review required data, without setting advanced filters in the panes.
- Data is showed based on:
 - Zoom of chromatogram
 - Selection of peaks in the chromatogram
 - Selection of chromatograms in the sequence
- Link is created by a single click



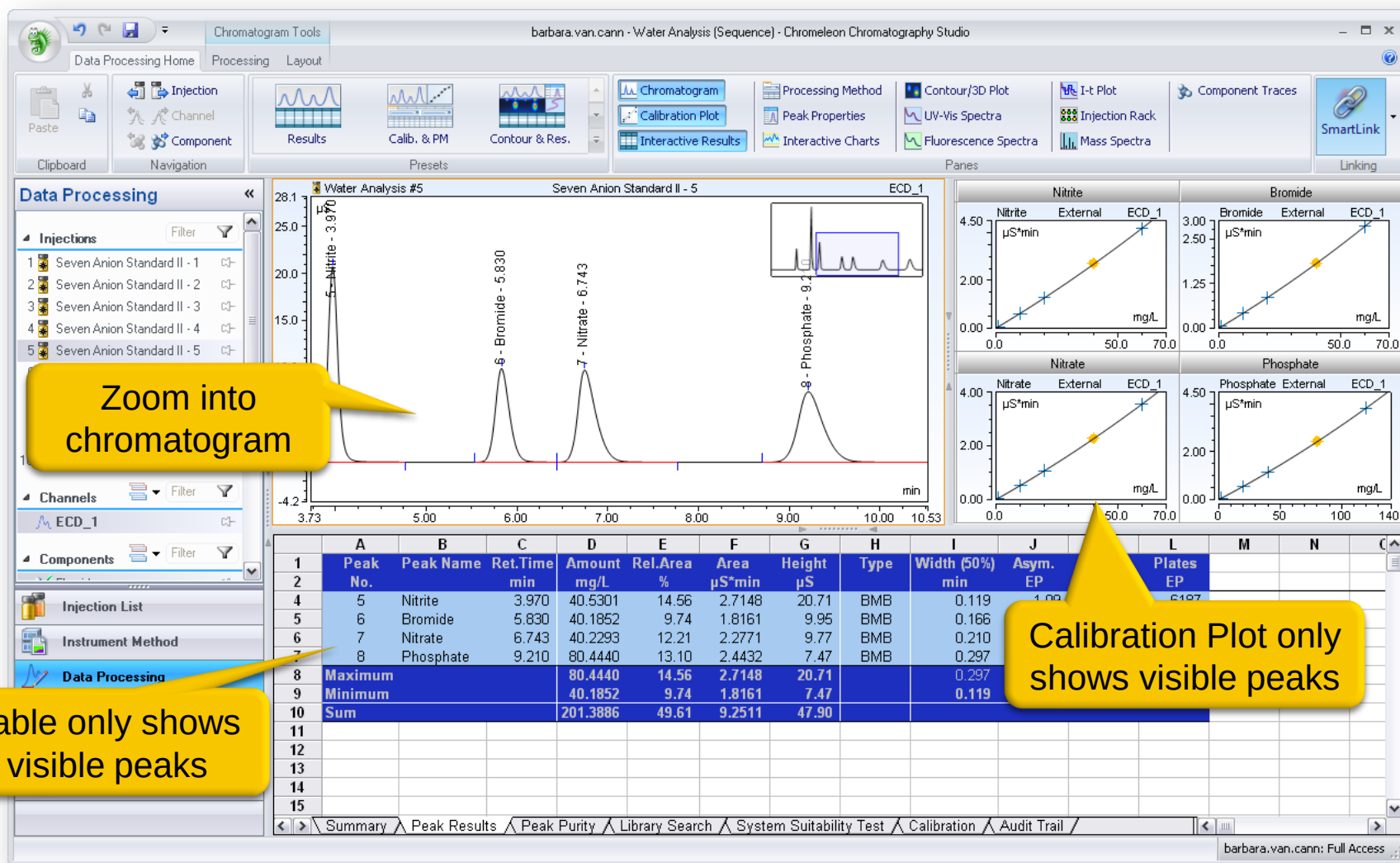
SmartLink of Panes to Chromatogram



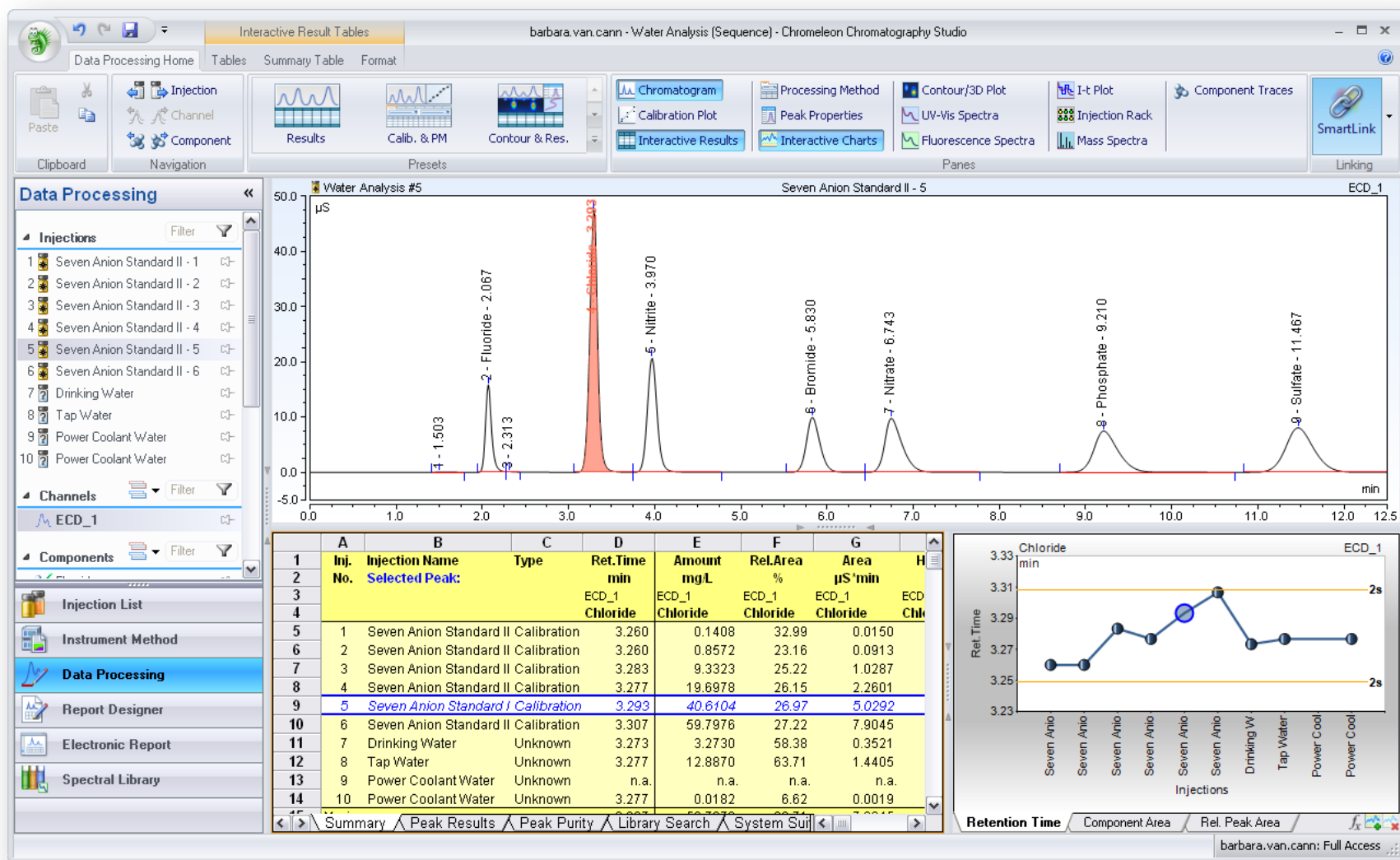
SmartLink of Panes to Chromatogram



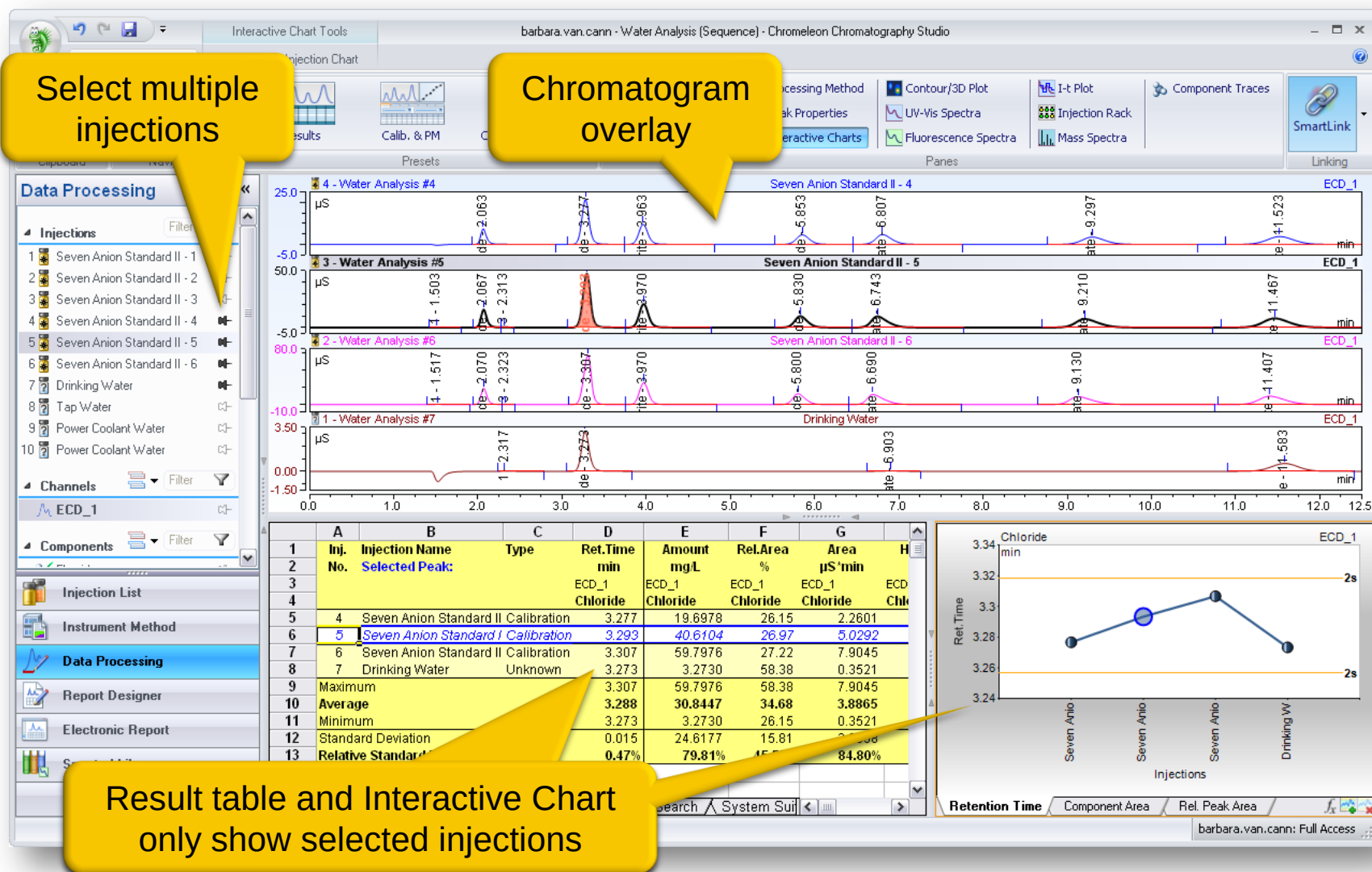
SmartLink of Panes to Chromatogram



SmartLink of Panes to Selected Injections



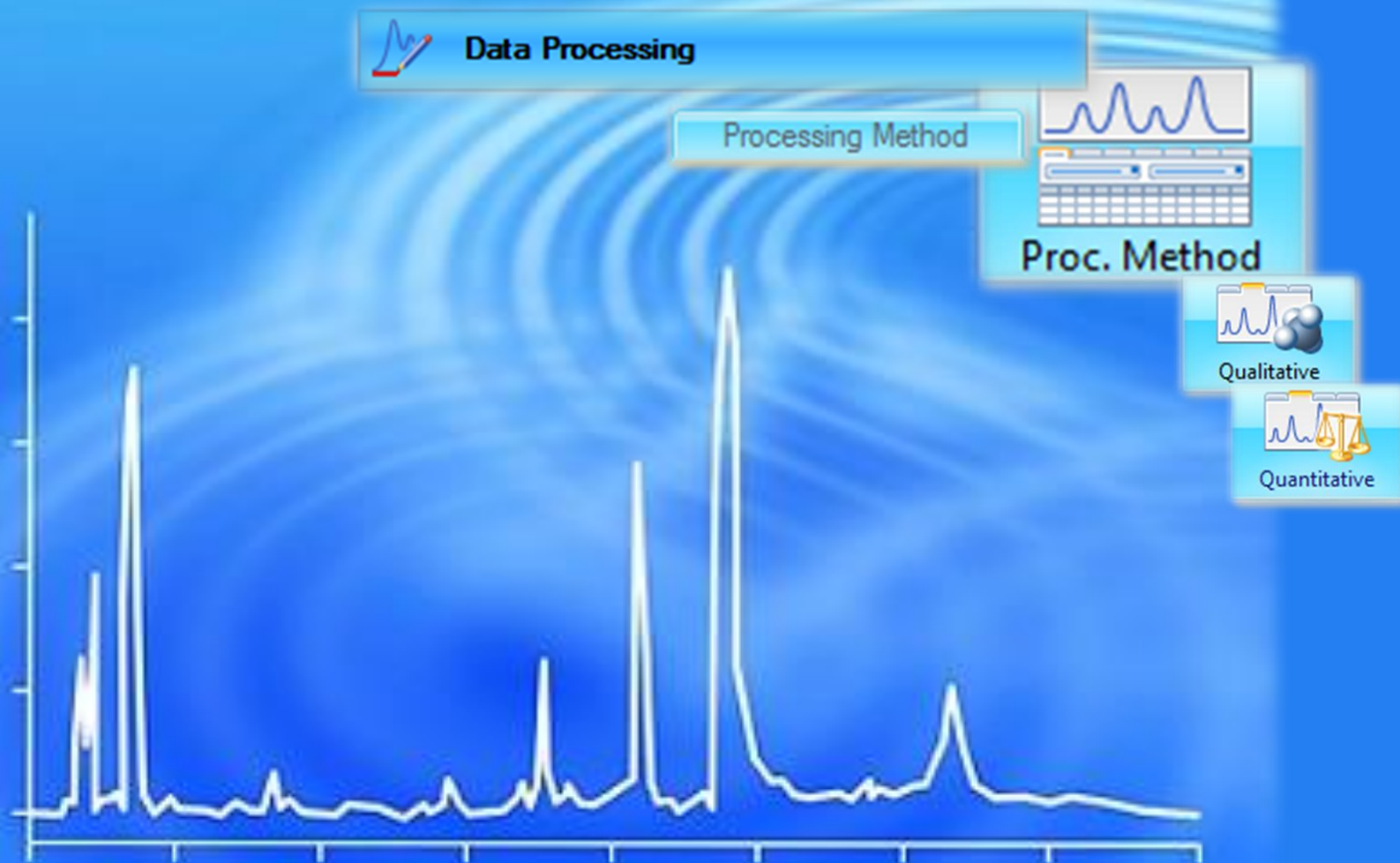
SmartLink of Panes to Selected Injections



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

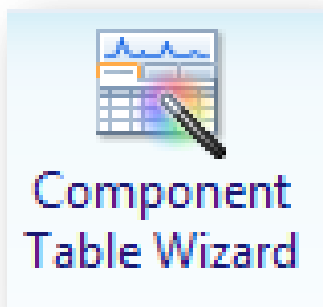


Easier Processing Method Setup

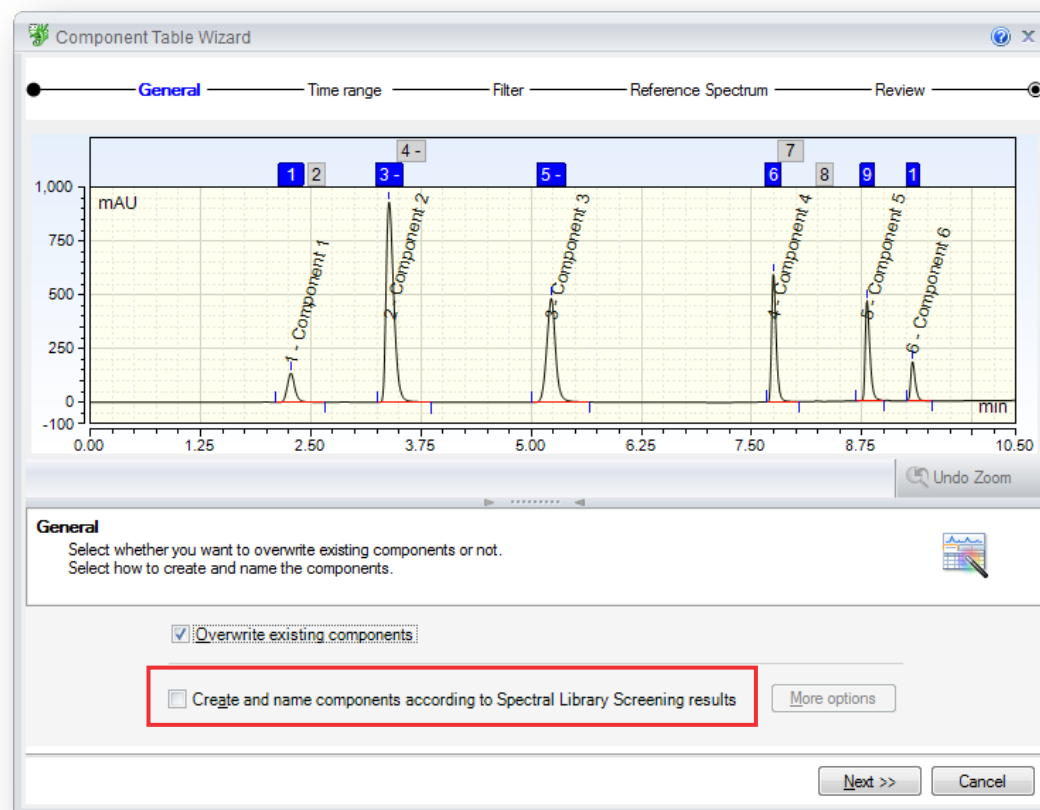
- Creating your component table can be time consuming and error prone
 - Setting correct integration parameters can be a laborious trial and error process
 - Setting up calibration levels can be an unintuitive, complex procedure
 - Updating component retention times as peaks drift is often a lengthy,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



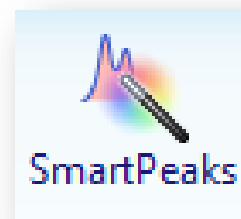
Easier Processing Method Setup – Component Table

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

Component Table						
Group Area						
Drag a column header here to group by that column.						
Run Component Table Wizard...						
#	Name	Ret.Time	Window	Channel	Eval.Type	Stand.Meth.
1	Thiamine	2.298	0.100 AG	All Channels	Area	External
2	Pyridoxine	3.445	0.165 AG	All Channels	Area	External
3	Niacinamid	5.250	0.100 AG	All Channels	Area	External
4	Pantothenic Acid	7.767	0.142 AG	All Channels	Area	External
5	Folic Acid	8.323	0.100 AG	All Channels	Area	External
6	Vitamin B12	8.819	0.100 AG	All Channels	Area	External
7	Riboflavin	9.360	0.100 AG	All Channels	Area	External
* Click here to add a new component						

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

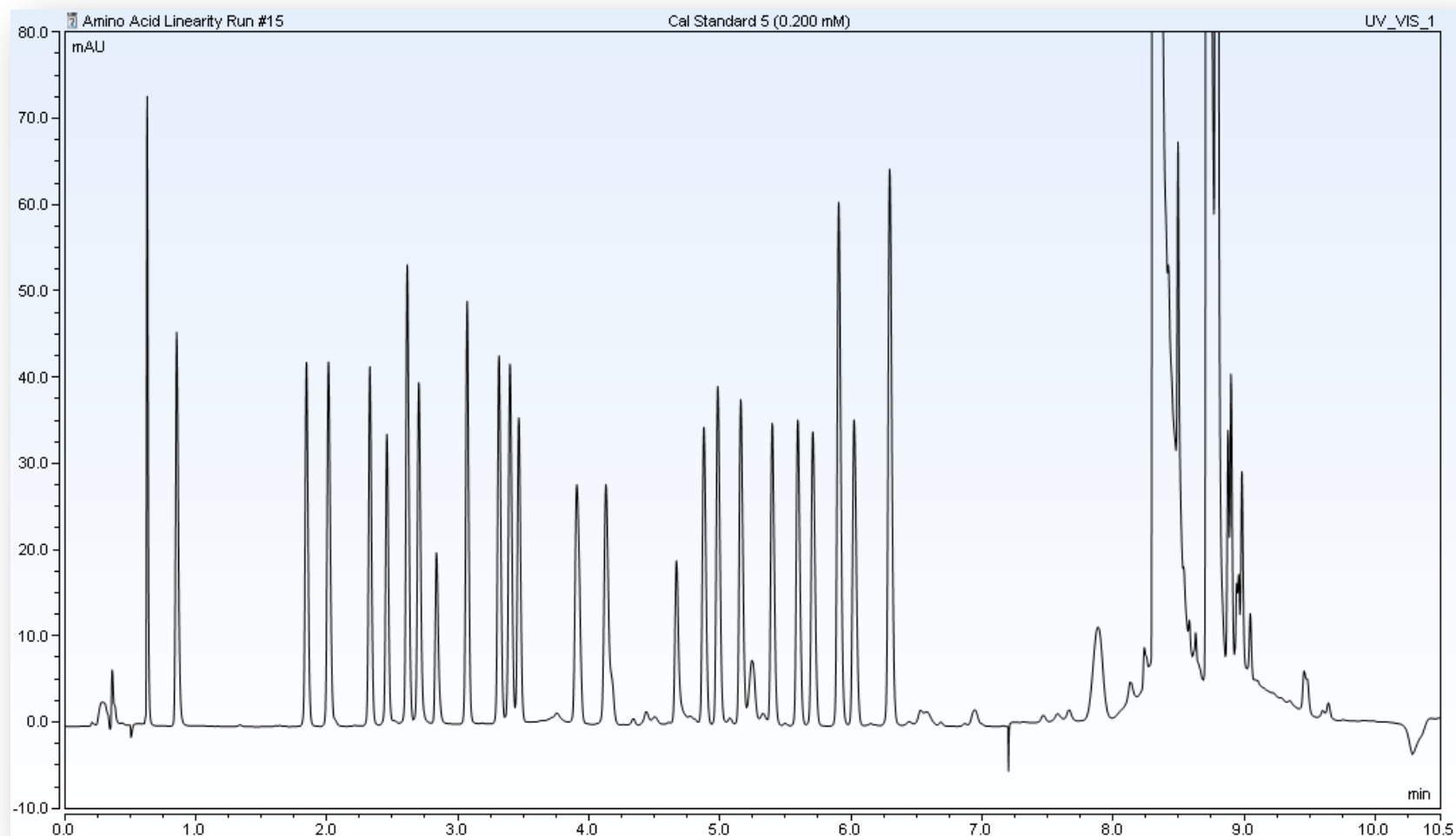


Cobra Peak Detection Algorithm / Wizard

- 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



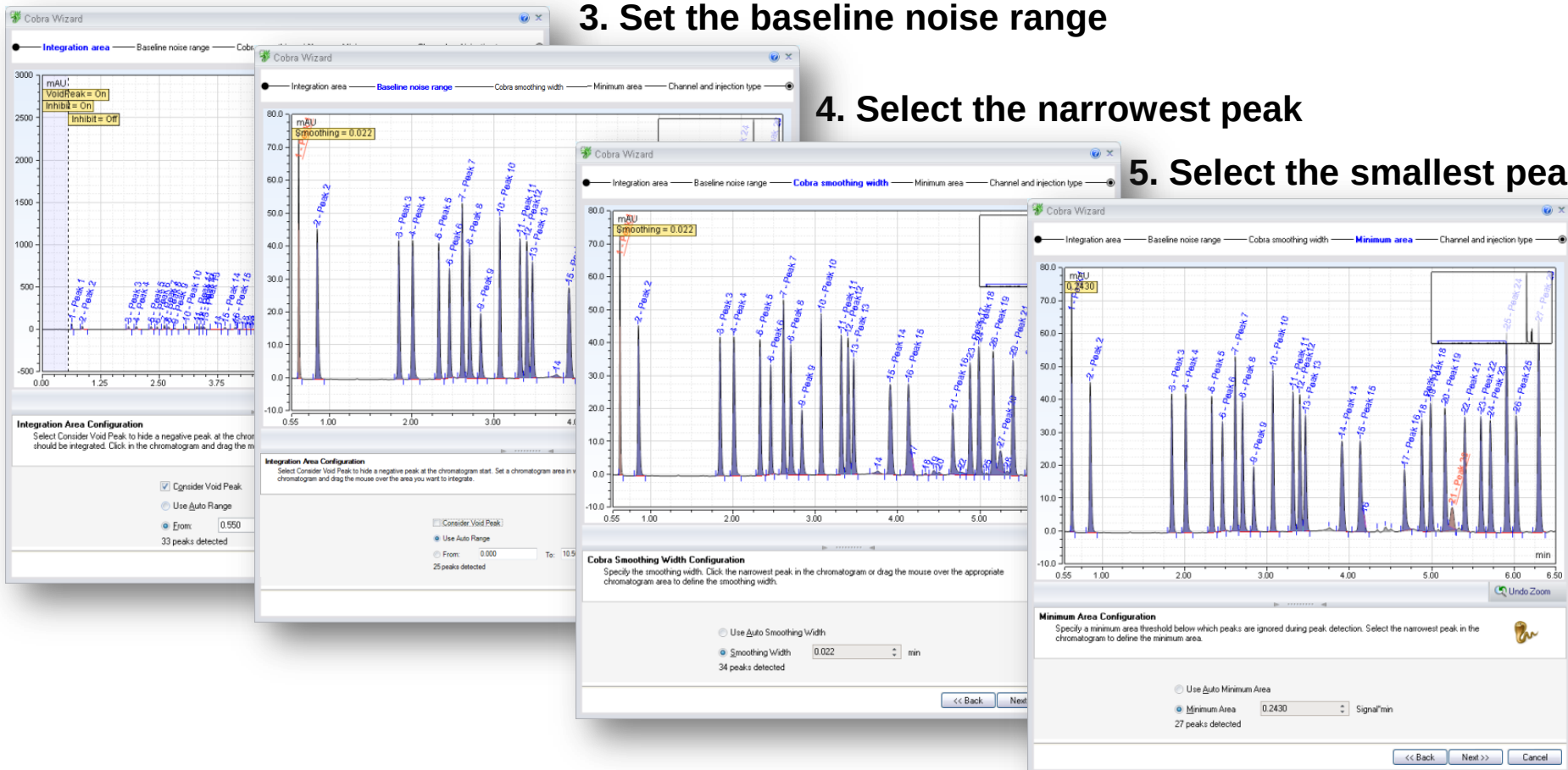
1. Start Cobra Wizard

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...

Detection Settings

Algorithm: Cobra [Run Cobra Wizard](#)

Baseline Noise Range

☒ Auto Range

Start Time: 9.720 [min]

End Time: 9.980 [min]

Cobra Smoothing Width: 0.022 [min]

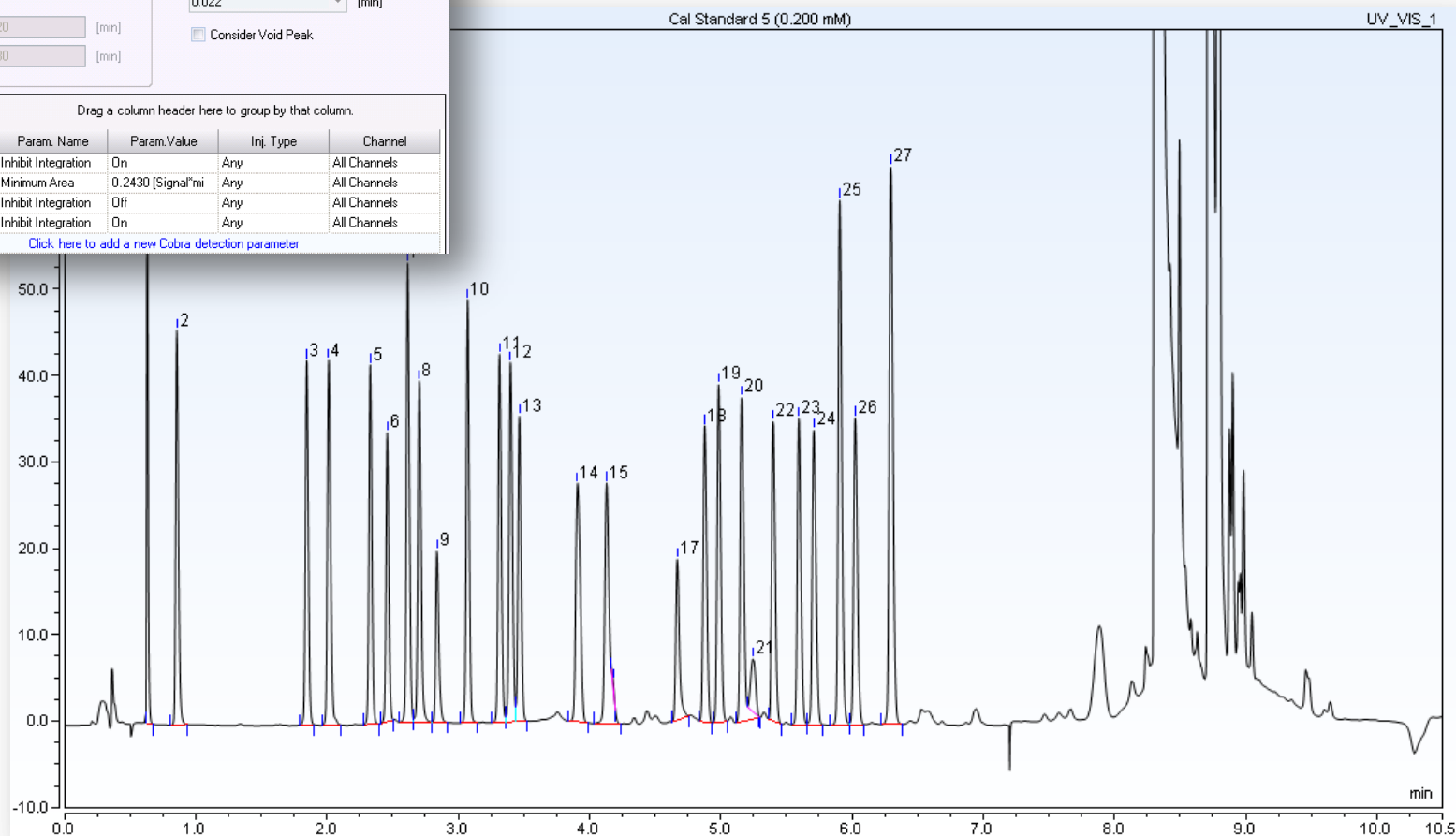
☐ Consider Void Peak

Group Area

Drag a column header here to group by that column.

#	Ret. Time	Param. Name	Param. Value	Inj. Type	Channel
1	0.000 [min]	Inhibit Integration	On	Any	All Channels
2	0.000 [min]	Minimum Area	0.2430 [Signal*mi]	Any	All Channels
3	0.550 [min]	Inhibit Integration	Off	Any	All Channels
4	6.500 [min]	Inhibit Integration	On	Any	All Channels

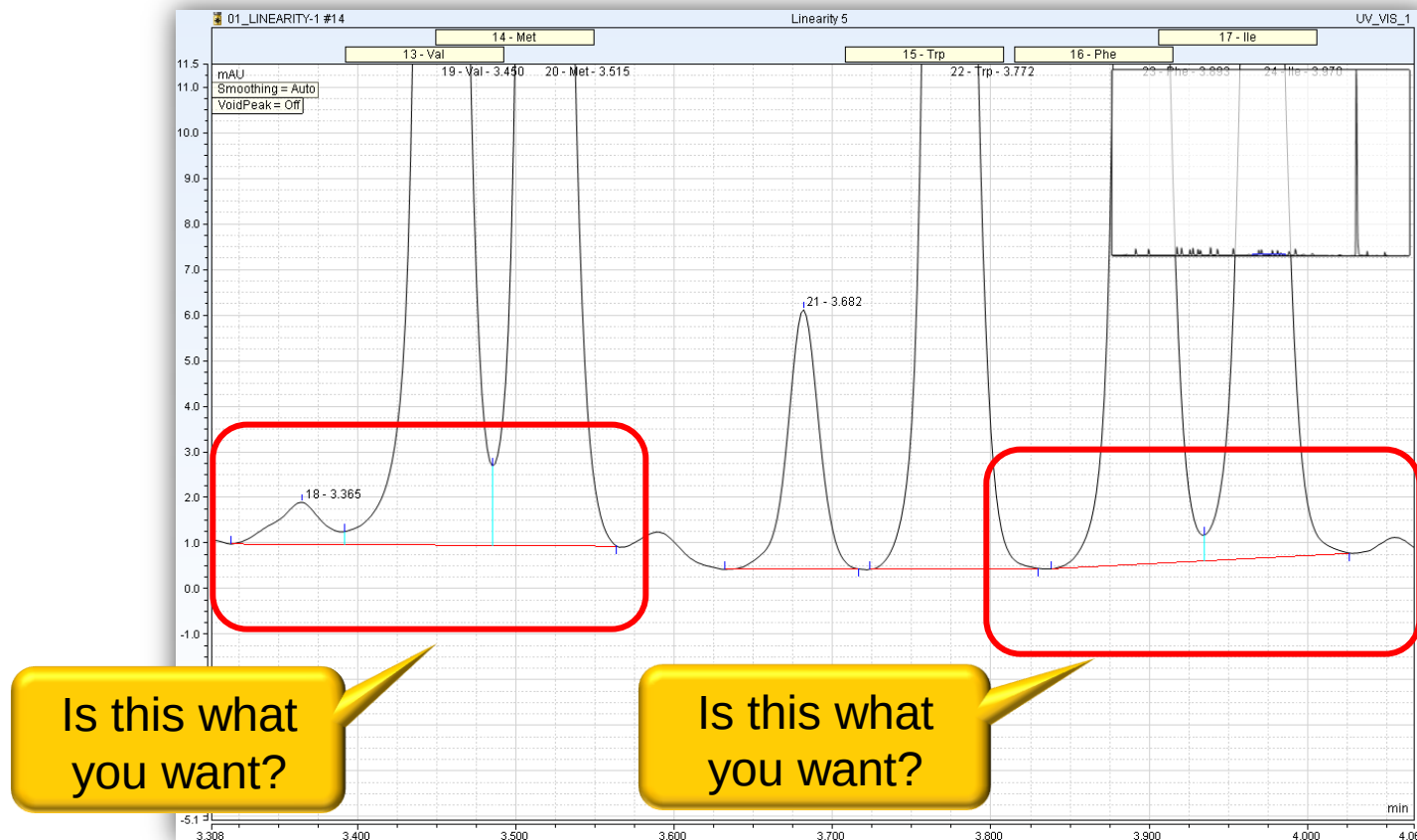
[Click here to add a new Cobra detection parameter](#)



... and your integration is done!

Easier Processing Method Setup – Peak Detection

- There are many ways to integrate unresolved peaks



Peak Detection – SmartPeaks Integration Assistant

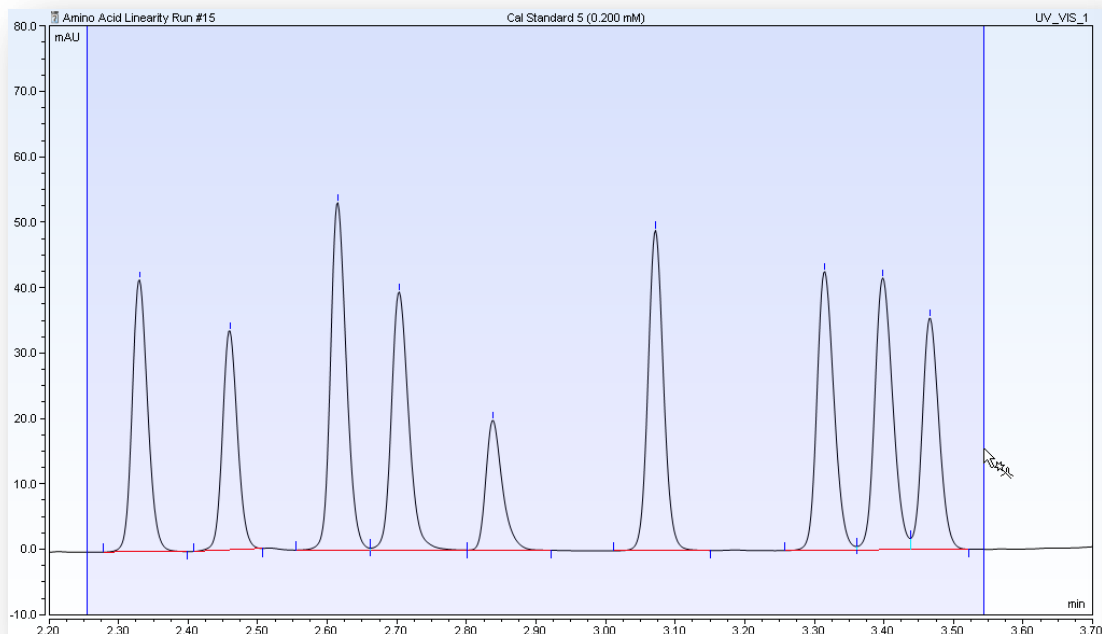
- Unique tool for easily reaching your integration goals for unresolved peaks
- Requires no training
- Great example of Operational Simplicity
 - Process is clear and understandable
 - Requires only a few steps
 - Correctly integrates all unresolved peaks in seconds

Peak Detection – SmartPeaks Integration Assistant

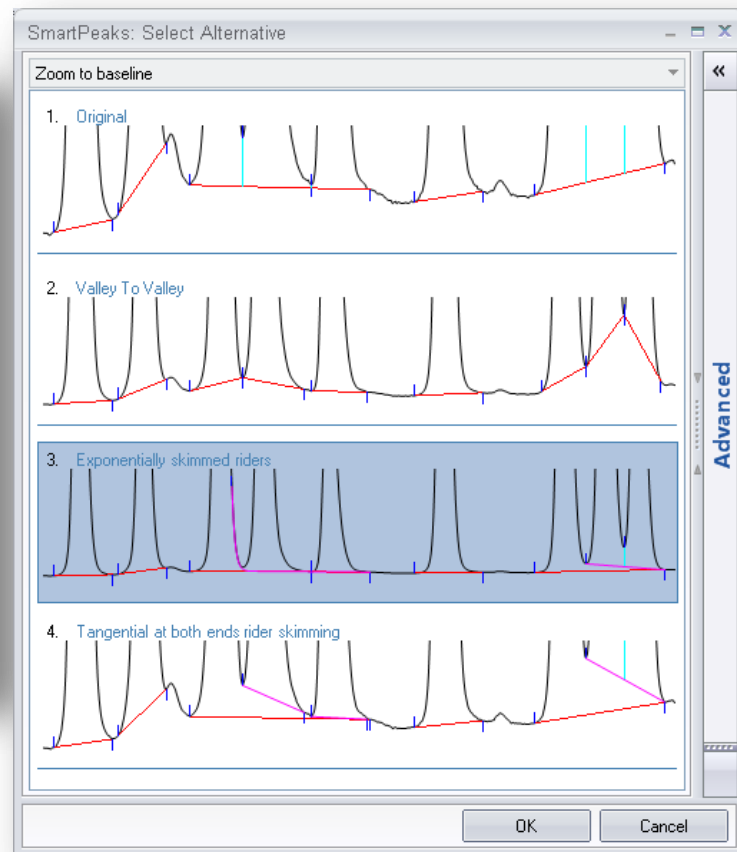


1. Activate SmartPeaks Wizard

2. Select Area of Interest

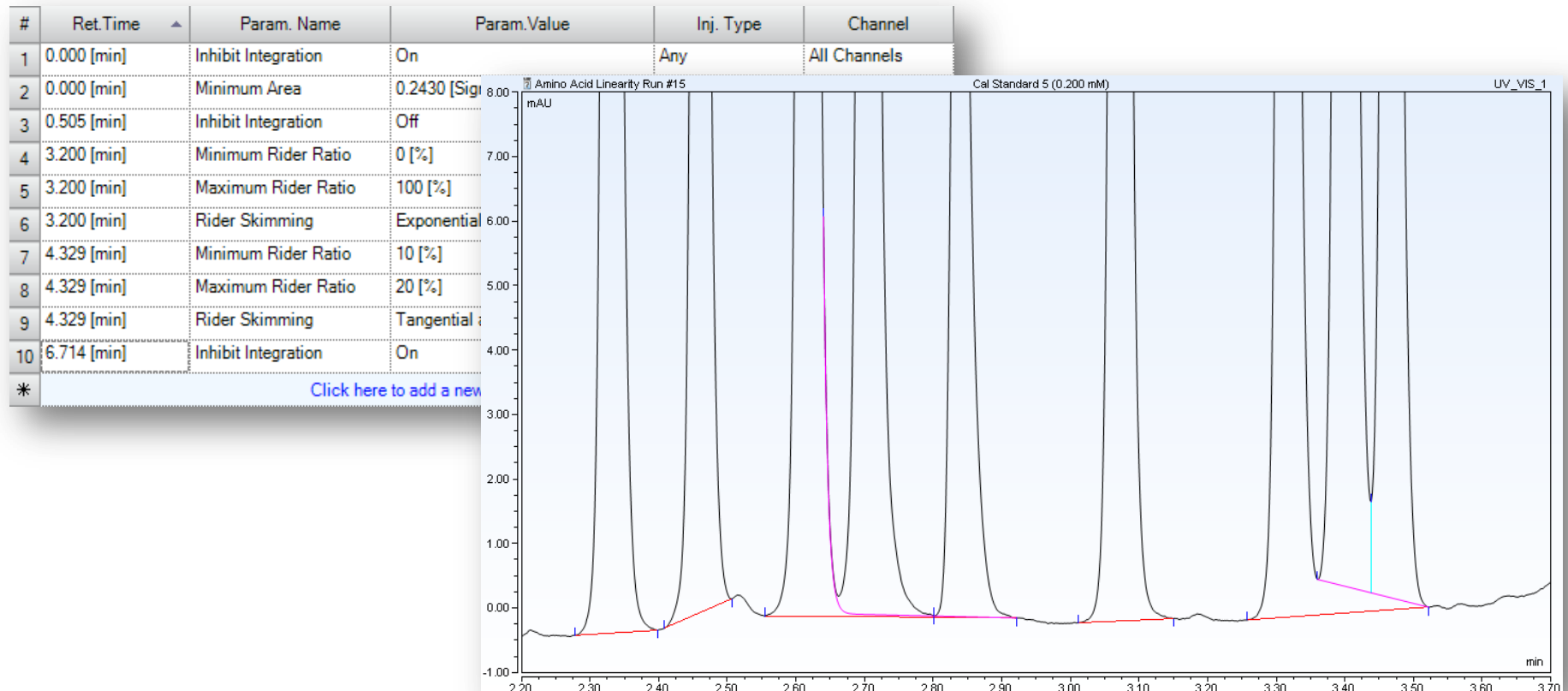


3. Select the Integration You Want



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.

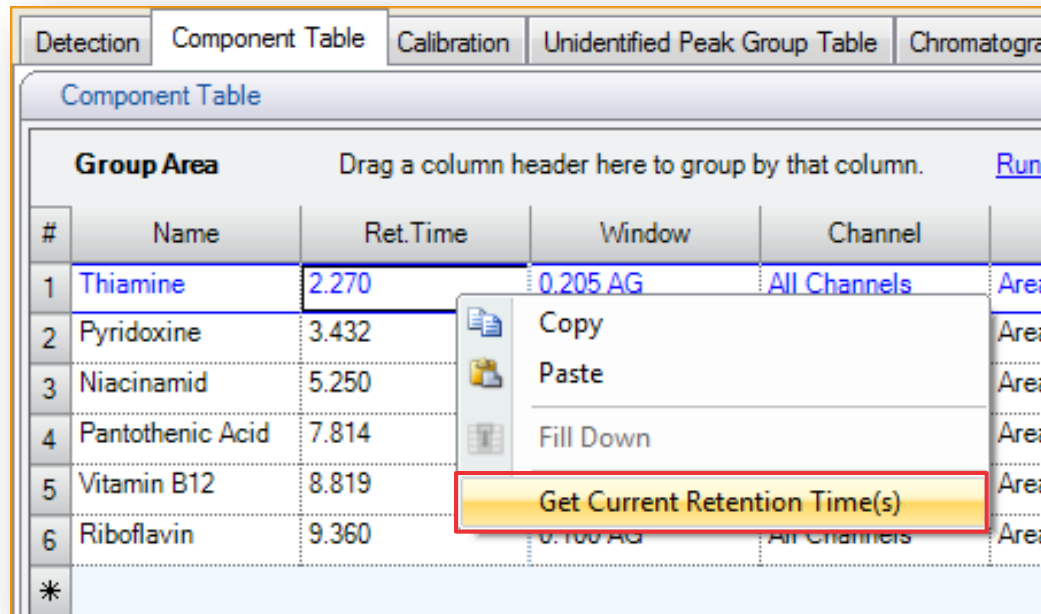
Type	Level	Position
Calibration Standard	01	RA1
Calibration Standard	01	
Calibration Standard	02	
Calibration Standard	03	
Calibration Standard	04	
Calibration Standard	05	
	Create new level...	
Calibration Standard		RA4



Component Table							
Group Area							
#	Name	Ret.Time	Level "01"	Level "02"	Level "03"	Level "04"	Le
1	Thiamine	2.270	20.000000	2.000000	0.800000	0.200000	1.000
2	Pyridoxine	3.432	20.000000	2.000000	0.800000	0.200000	1.000
3	Niacinamid	5.250	20.000000	2.000000	0.800000	0.200000	1.000
4	Pantothenic Acid	7.814	20.000000	2.000000	0.800000	0.200000	1.000
5	Vitamin B12	8.819	20.000000	2.000000	0.800000	0.200000	1.000
6	Riboflavin	9.360	20.000000	2.000000	0.800000	0.200000	1.000
*	Click here to add a new component						

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.



The screenshot shows the 'Component Table' window with a table of components. A context menu is open over the 'Ret.Time' column, with the 'Get Current Retention Time(s)' option highlighted in yellow.

#	Name	Ret.Time	Window	Channel	Area
1	Thiamine	2.270	0.205 AG	All Channels	Area
2	Pyridoxine	3.432			Area
3	Niacinamid	5.250			Area
4	Pantothenic Acid	7.814			Area
5	Vitamin B12	8.819			Area
6	Riboflavin	9.360	0.100 AG	All Channels	Area
*					

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?