

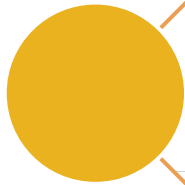


**ThermoFisher**  
S C I E N T I F I C

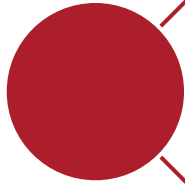
# Streamlining Your Chromatography Laboratory Operations Through End-to-End Workflows

Darren Barrington-Light  
Senior Manager - Product Marketing  
Informatics & Chromatography Software

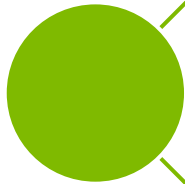
The world leader in serving science



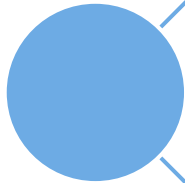
Introduction



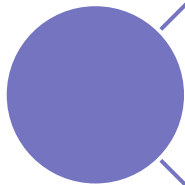
Sequence Creation



Data Analysis



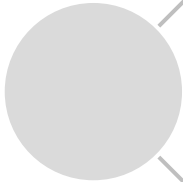
Result Retrieval



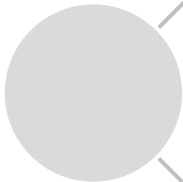
Summary



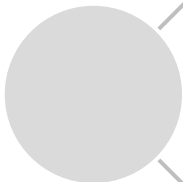
# Introduction



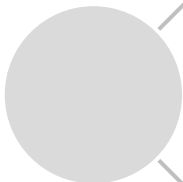
Sequence Creation



Data Analysis

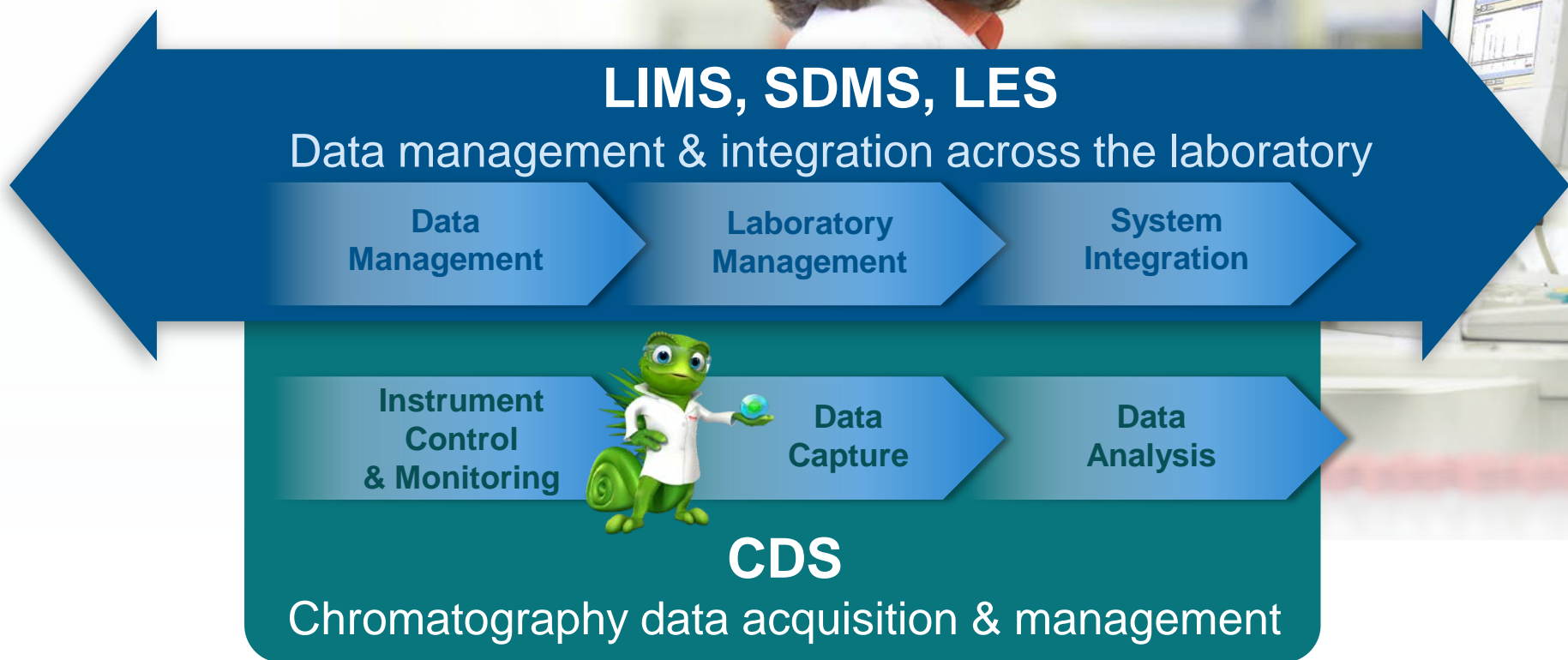


Result Retrieval



Summary

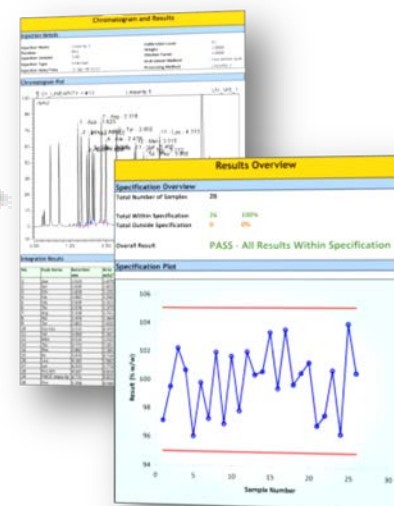
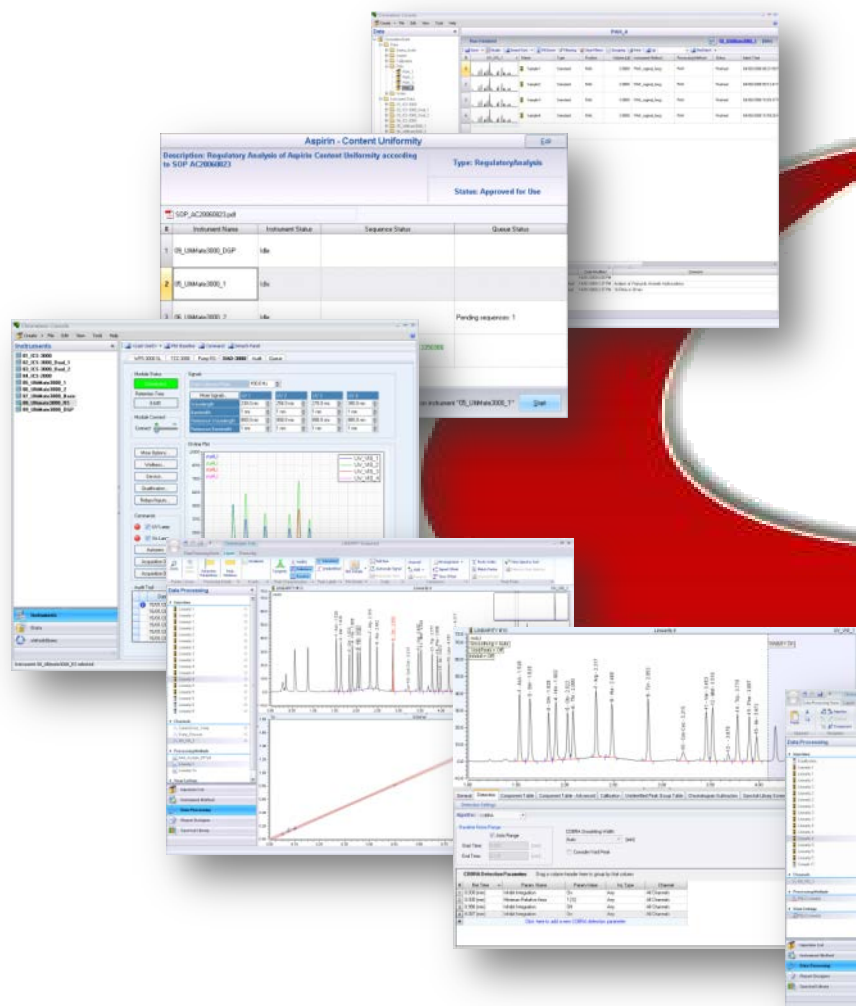
# Data Into Knowledge



# Streamlining Chromatography



From samples....



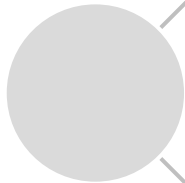
... to final results



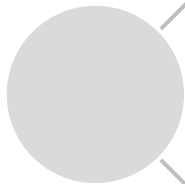
Introduction



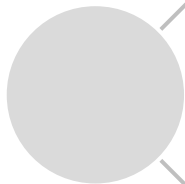
**Sequence Creation**



Data Analysis



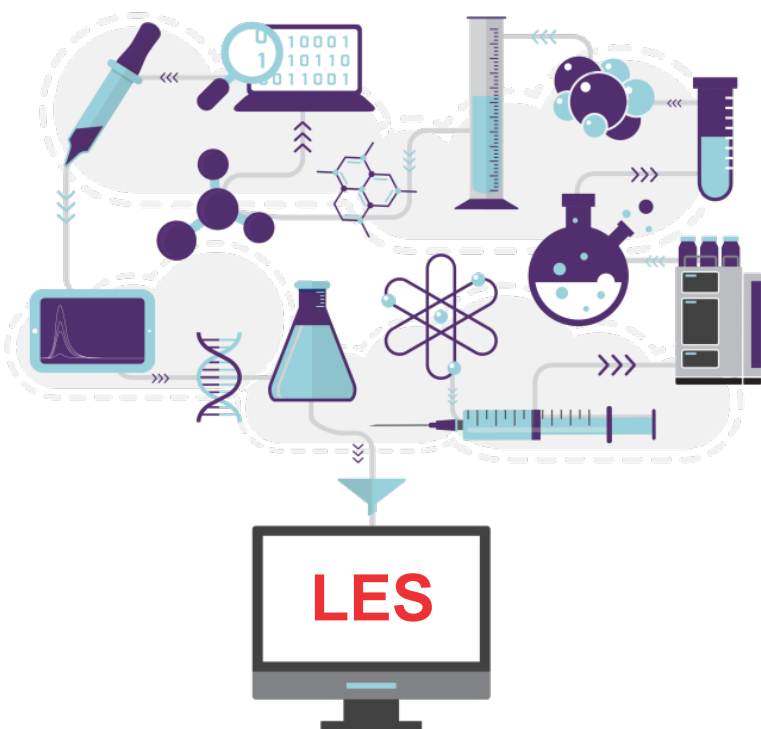
Result Retrieval



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

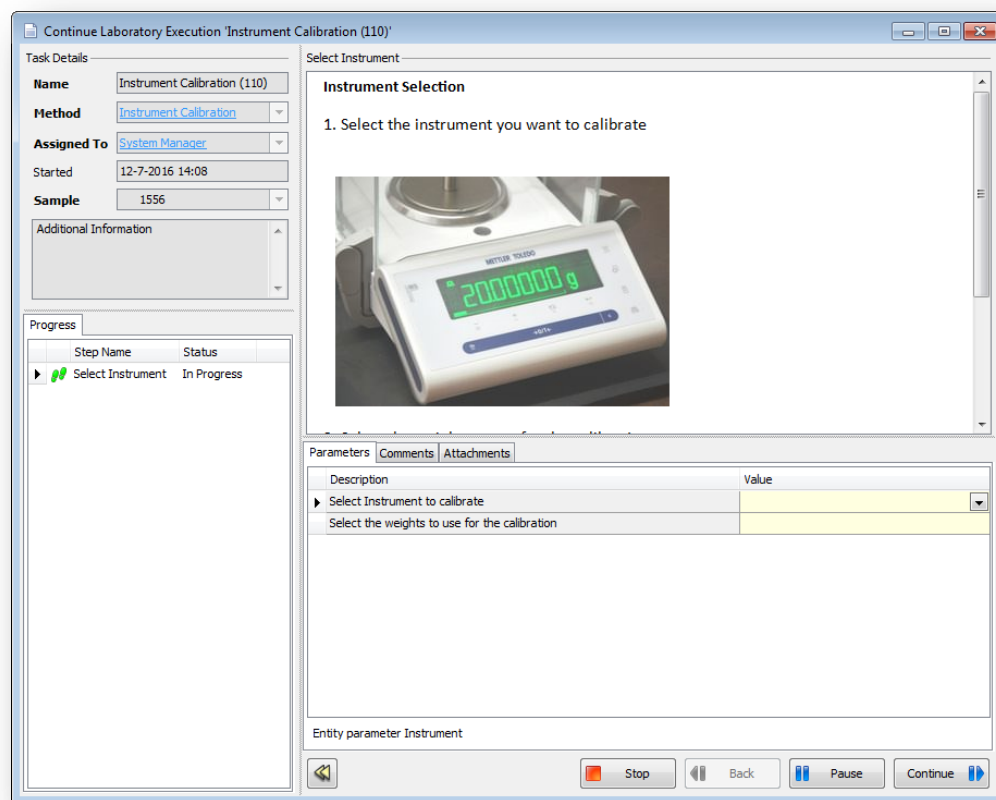


# Sequence Creation



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





# Sequence Creation



Create sequences from samples, tests, batches or LES

- Sequences can be reviewed & updated prior to creation in CDS

The screenshot displays the CDS software interface. On the left, a tree view shows a list of items with icons of vials and their status. A context menu is open over item 20, with 'Create Sequence' highlighted. The main window is titled 'Create Chromeleon Sequence from Samples'. It contains a table of 'Selected Samples' and fields for 'Required Analysis' and 'Instrument'. A 'Create Sequence' button is at the bottom right. A small dialog box in the foreground shows a success message: 'Sequence chrom://ukalt-3z3cyy1/ChromeleonLocal/Instrument Data/01\_ICS-3000 (25-MAR-2014 1636).seq created successfully.' with an 'OK' button.

ID Numeric	ID Text	Sample Name	Status	Product
20	SM-25-MAR-2014-000020		Available	
21	SM-25-MAR-2014-000021		Available	
22	SM-25-MAR-2014-000022		Available	

Required Analysis: **Analysis**  **Instrument**

Sequence chrom://ukalt-3z3cyy1/ChromeleonLocal/Instrument Data/01\_ICS-3000 (25-MAR-2014 1636).seq created successfully.

# Sequence Creation

- Information captured in LES can be passed into CDS sequence
  - Can also pass calibration standard concentrations

The screenshot illustrates the workflow of passing data from a 'Test Parameters' window to a sequence injection table. The 'Test Parameters' window contains a table with the following data:

Type	Name	Value	Units
Numeric	Dilution	1.234	
Numeric	Weight	4.321	
Numeric	Volume	0.122	
Numeric	Int Standard	1.543	
Text	Comment	Test Comment	

A green box highlights this table, and a green arrow points from it to the 'Weight', 'Dilution', and 'IntStd' columns of the injection table below. The injection table for '01\_ICS-3000 (26-JUL-2016 1642)' contains:

Method	Processing Method	Status	Inject Time	Lock Status	Weight	Dilution	IntStd	Replicate ID	Comment
One	ICS Processing	Idle			4.3210	1.2340	1.5430		Test Comment

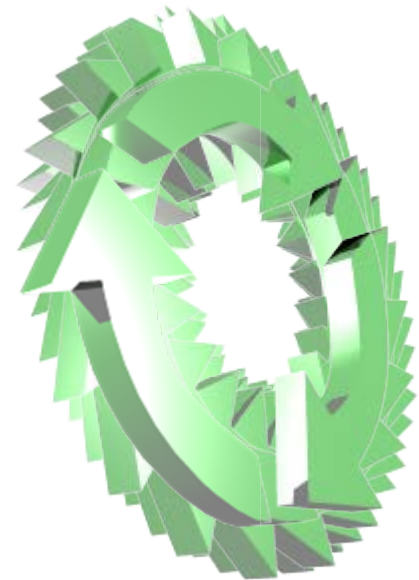
Another green box highlights the 'Weight', 'Dilution', and 'IntStd' columns in this table, with a green arrow pointing to the 'Standard Concentrations' table. The 'Standard Concentrations' table has an 'Update Standards' checkbox checked. The table data is:

Stand.Meth.	Cal.Type	Level "01"	Level "02"	Peak Type	Gr
External	Lin	1.001000	11.000000	Autodetect	
External	Lin	3.002000	33.000000	Autodetect	
External	Lin	2.003000	22.000000	Autodetect	

A green arrow points from the 'Update Standards' checkbox to the 'Standard Concentrations' table. A final green arrow points from the 'Level "01"' and 'Level "02"' columns of the 'Standard Concentrations' table to the 'Weight' and 'Dilution' columns of the injection table.

# 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

The screenshot shows the Chromeleon Console interface. The left sidebar lists various eWorkflows, with 'Dissolution Templates' selected. The main area displays the description for 'Dissolution Templates' and a table of instrument sequences. A 'Launch' button is visible above the table. Three callout boxes provide instructions: 1. Select eWorkflow, 2. Select Instrument, and 3. Click Launch.

**1. Select eWorkflow**

**2. Select Instrument**

**3. Click Launch**

#	Instrument Name	Instrument Status	Sequence St
1	01_ICS-5000+	Monitoring Baseline	Manual (Injection: 1 of 1)
2	02_ICS-5000_Dual_1	Idle	
3	03_ICS-5000_Dual_2	Idle	
4	UltiMate3000	Running	ICH Linearity 040214122838 (Injection: 1 of 15)
5	UltiMate3000_RS	Idle	

eWorkflow 'Dissolution Templates' selected

cmadmin: Full Access

# Sequence Creation

4. Input number of samples

5. Input position of first sample

Number of samples: 1

Sample location: RA1

Run sequence after creation

#	Chromatog	Name	Type	Level	Replicate ID	Position	Volume [μL]	Instrument
1	None	Blank	Unknown			RA1	10.0000	
2	None	SST Standard 1	Check Standard			RA2	10.0000	
3	None	SST Standard 2	Check Standard			RA3	10.0000	
4	None	SST Standard 3	Check Standard			RA4	10.0000	
5	None	SST Standard 4	Check Standard			RA5	10.0000	

Ca Finish

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



**Dissolution Experiment 21-Feb-2014 16-42**

New Start UltraMate3000\_RS (Idle)

Save Studio Print Up Insert Row Fill Down Lock Filtering Grouping

#	Chromatog	Name	Type	Level	Position	Volume [μl]	Instrument Method	Processing Method
1	None	Blank	Blank		R41	1.000	Dissolution_IM	Dissolution_PM
2	None	System Suitability	Check Standard		R42	1.000	Dissolution_IM	Dissolution_PM
		Suitability	Check Standard		R42	1.000	Dissolution_IM	Dissolution_PM
		Suitability	Check Standard		R42	1.000	Dissolution_IM	Dissolution_PM
		Suitability	Check Standard		R42	1.000	Dissolution_IM	Dissolution_PM
		Suitability	Check Standard		R42	1.000	Dissolution_IM	Dissolution_PM
		Suitability	Check Standard		R42	1.000	Dissolution_IM	Dissolution_PM
		on Standard	Calibration Standard	01	R43	1.000	Dissolution_IM	Dissolution_PM
9	None	Calibration Standard	Calibration Standard	02	R44	1.000	Dissolution_IM	Dissolution_PM
10	None	Calibration Standard	Calibration Standard	03	R45	1.000	Dissolution_IM	Dissolution_PM
11	None	Sample	Unknown		R46	1.000	Dissolution_IM	Dissolution_PM
12	None	Sample	Unknown		R47	1.000	Dissolution_IM	Dissolution_PM
13	None	Sample	Unknown		R48	1.000	Dissolution_IM	Dissolution_PM
14	None	Sample	Unknown		RB1	1.000	Dissolution_IM	Dissolution_PM
15	None	Sample	Unknown		RB2	1.000	Dissolution_IM	Dissolution_PM
16	None	Sample	Unknown		RB3	1.000	Dissolution_IM	Dissolution_PM
17	None	Calibration Standard	Calibration Standard	01	RB4	1.000	Dissolution_IM	Dissolution_PM
18	None	Calibration Standard	Calibration Standard	02	RB5	1.000	Dissolution_IM	Dissolution_PM
19	None	Calibration Standard	Calibration Standard	03	RB6	1.000	Dissolution_IM	Dissolution_PM

[Click here to add a new injection](#)

#	Name	Value	Description
1	Batch_No	<Enter Batch number>	Dissolution Batch Number
2	Disso_No	<Enter unique Dissolution Experiment number>	Dissolution Experiment Number
3	Initial_Volume	0	Dissolution Initial Volume in Vessel
4	Volume_Taken	0.00	Dissolution Volume Taken at Each Time Point

[Click here to add a custom sequence variable](#)

Associated Items Custom Sequence Variables (4) Custom Formulas

ChromleonLocal  
Chromleon\_Demonstration  
Chromleon7\_ExtensionPack  
Dissolution\_Tests  
Dissolution Experiment 21-Feb-2014 16-42

Injection Rack View

# Sequence Creation

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

**Create Chromeleon Sequence**

Sequence Properties

Name: 01\_ICS-3000 (25-MAR-2014 1644)

Folder: [Dropdown]

Start Position: 1 Instrument: 01\_ICS-3000

Sequence Entries

Name	Position	Type	Volume	Sample ID Text	Test Number
SM-25-MAR-2014-000014/1		Unknown	1.0000	SM-25-MAR-2014-000014	15
SM-25-MAR-2014-000015/1		Unknown	1.0000	SM-25-MAR-2014-000015	16
SM-25-MAR-2014-000016/1		Unknown	1.0000	SM-25-MAR-2014-000016	17

**RSLC Alkylphenone Linearity 2014-03-25 16-45-06**

New [Start] [01\_ICS-3000]

Save Studio Print Up Insert Row Fill Down Lock Filtering Grouping Custom Columns Find Next

#	Chromatogram	Name	Type	Level	Position	Volume [μl]	Status	Inject Time	Instrument Method
12	None	Linearity 4	Calibration Standard	04	12	1.0	Idle		RSLC Linearity
13	None	Linearity 4	Calibration Standard	04	13	1.0	Idle		RSLC Linearity
14	None	Linearity 5	Calibration Standard	05	14	1.0	Idle		RSLC Linearity
15	None	Linearity 5	Calibration Standard	05	15	1.0	Idle		RSLC Linearity
16	None	Linearity 5	Calibration Standard	05	16	1.0	Idle		RSLC Linearity
17	None	SM-25-MAR-2014-000014/1	Unknown		17	1.0	Idle		RSLC Linearity
18	None	SM-25-MAR-2014-000015/1	Unknown		18	1.0	Idle		RSLC Linearity
19	None	SM-25-MAR-2014-000016/1	Unknown		19	1.0	Idle		RSLC Linearity



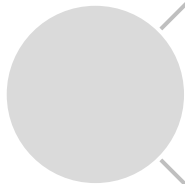
Introduction



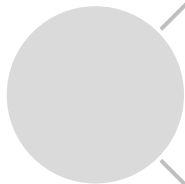
Sequence Creation



**Data Analysis**

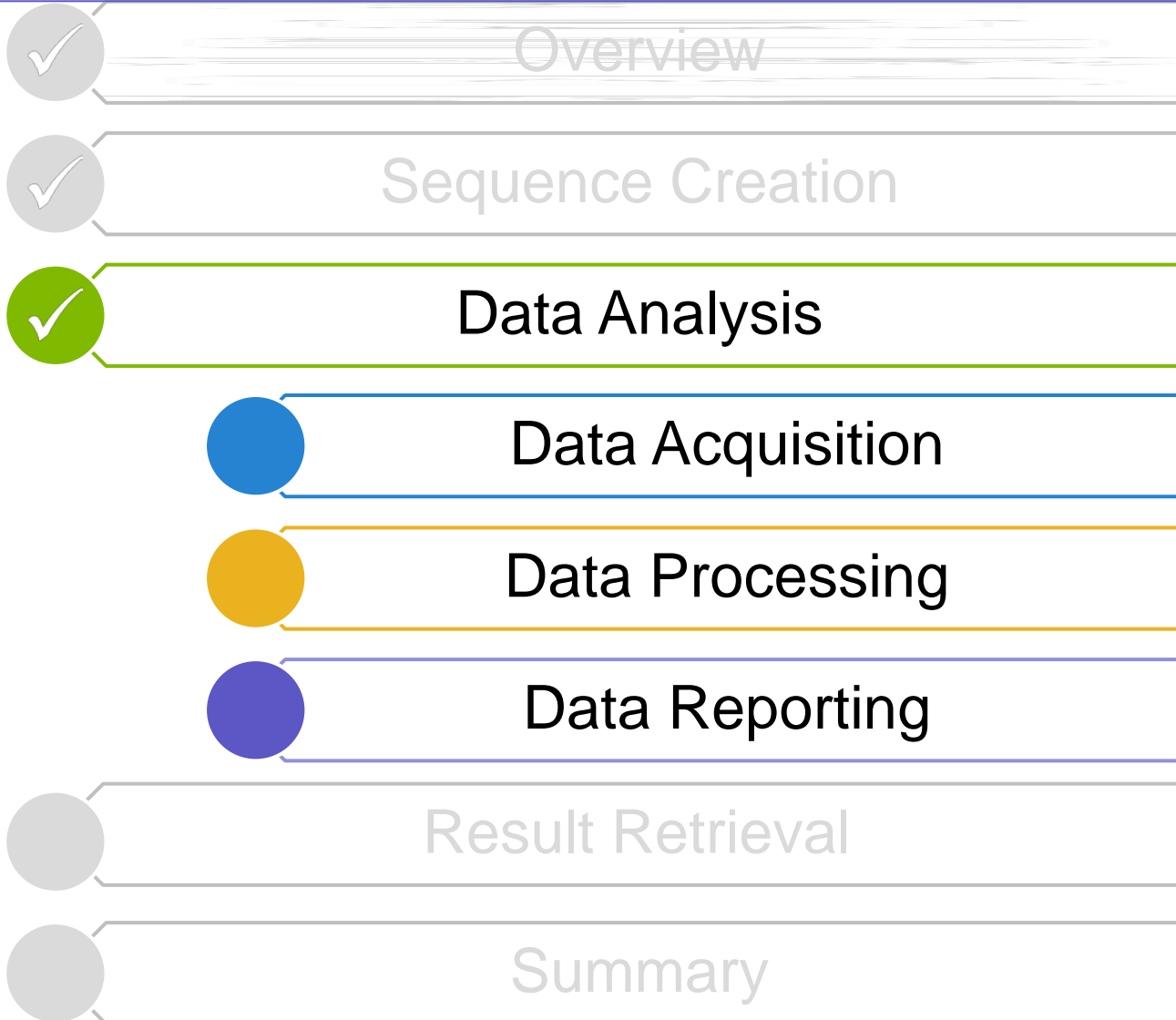


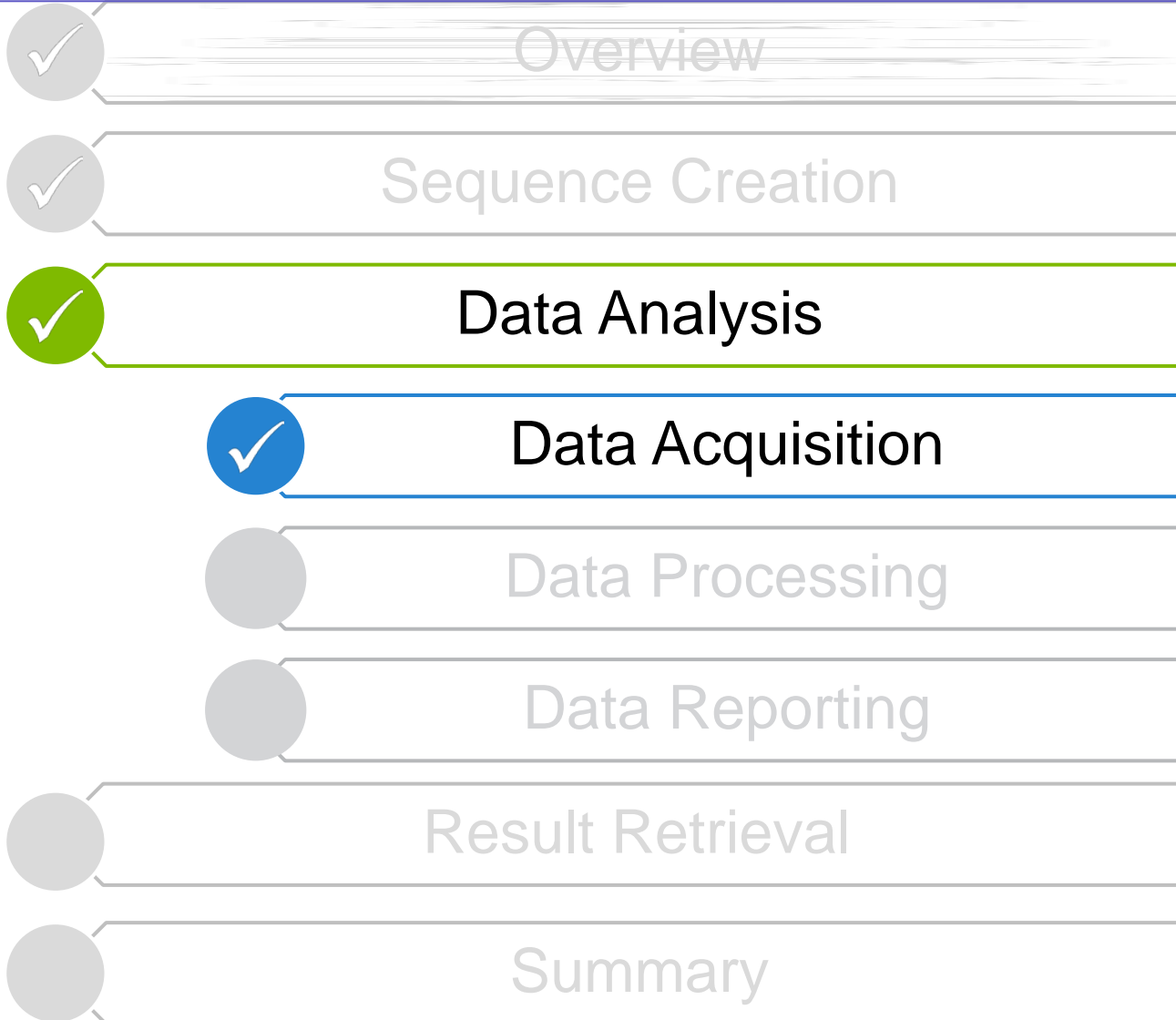
Result Retrieval



Summary



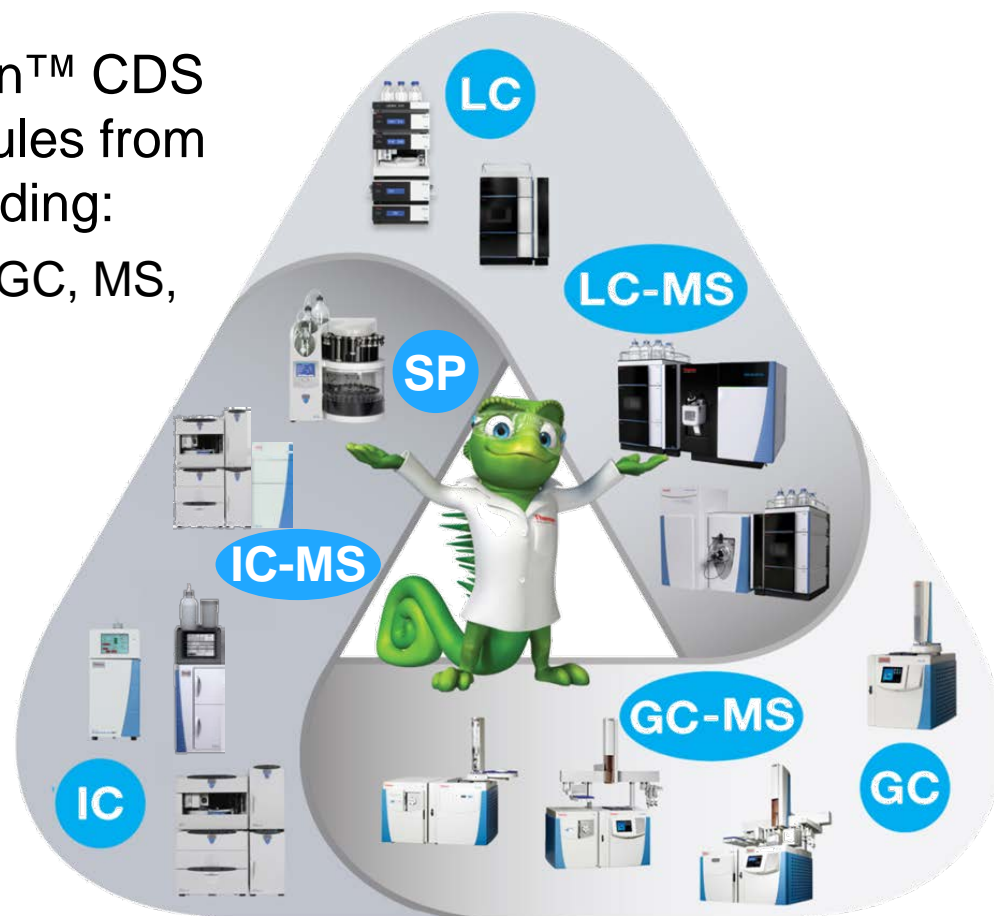




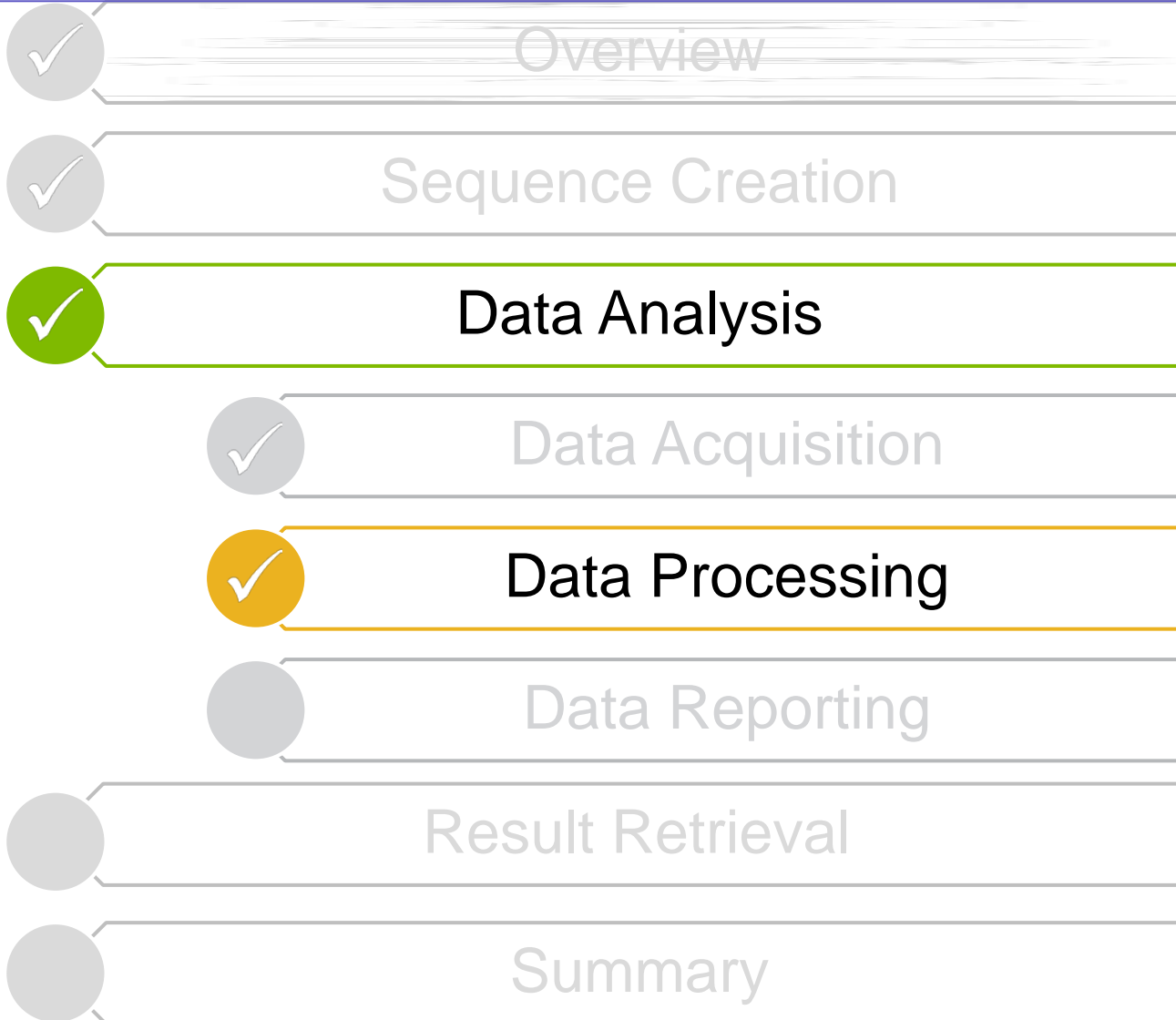
# Data Acquisition

- 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.)



# 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

<50%

Mouse Clicks

<50%

Windows

>50%

Faster

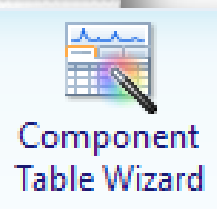
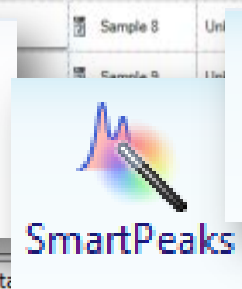
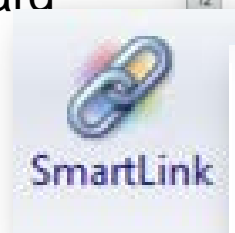
Rob Allen, Catalent Pharma

*“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

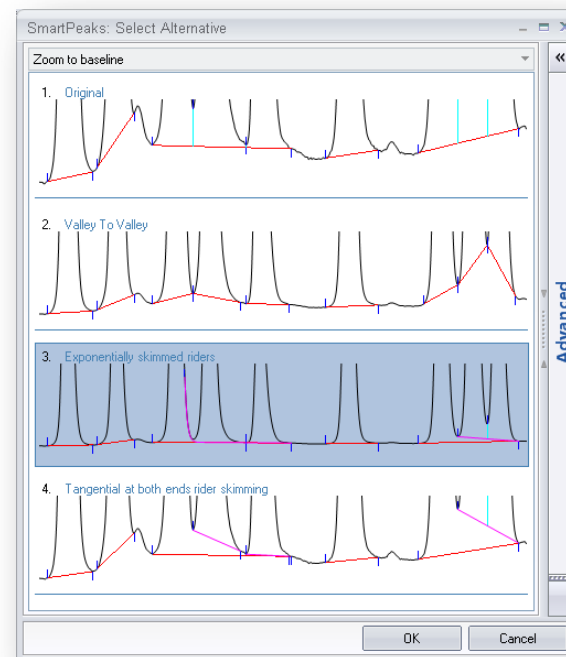
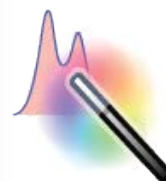
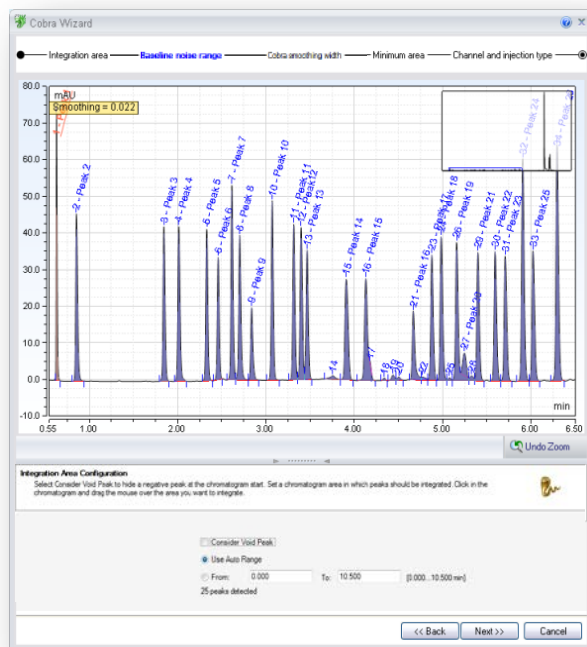
#	UV_VIS_1	Name	Type
1		Blank	Blank
2		Std 1	Calibration Standard
3		Std 2	Calibration Standard
4		Sample 1	Unknown
5		Sample 2	Unknown
6		Sample 3	Unknown
7		Check Std	Check Standard
8		Sample 4	Unknown
9		Sample 5	Unknown
10		Sample 6	Unknown
11		Std 2	Calibration Standard
12		Sample 7	Unknown



	A	B	C	D
1	<b>Sequence Details</b>			
2	Name:		01 Example Sequence	
3	Directory:		Demonstration Data	
4	Data Vault:		ChromelionLocal	
5	No. of Injections:		15	

# Data Processing

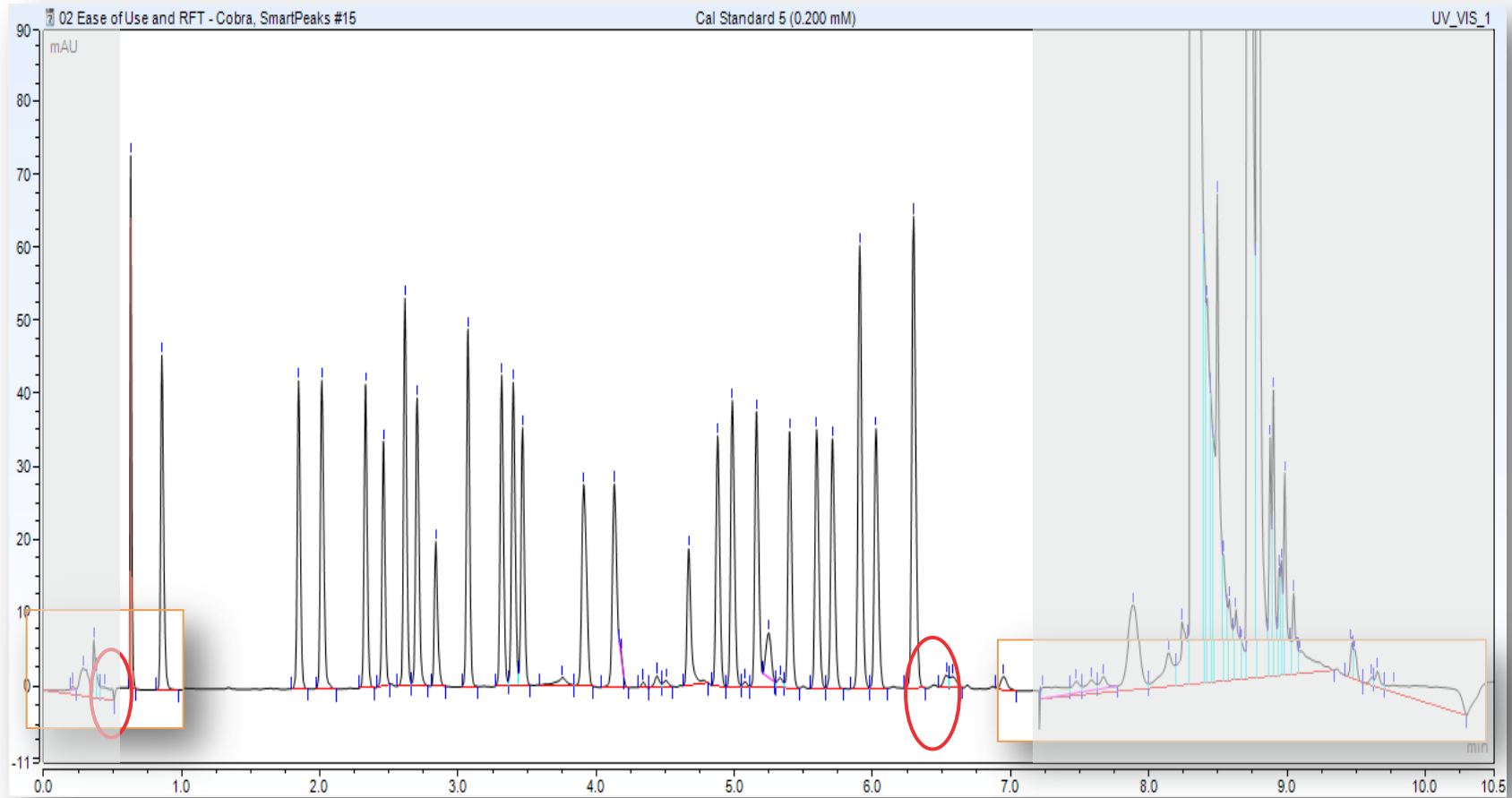
- Smart functions simplify and speed up data processing including:
  - Cobra peak detection algorithm and wizard
  - SmartPeaks Integration Assistant





# Data Processing – Cobra Algorithm

- Parameter-less first pass Cobra integration



# Data Processing – Cobra Peak Detection Wizard



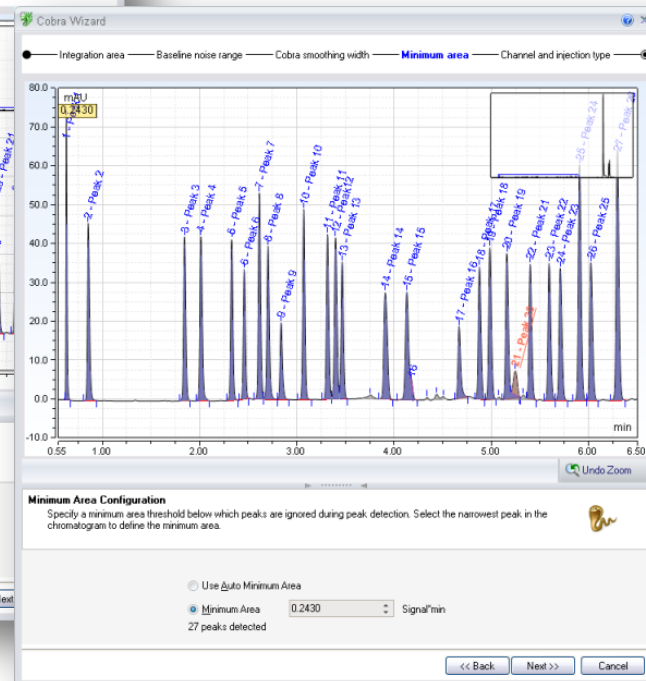
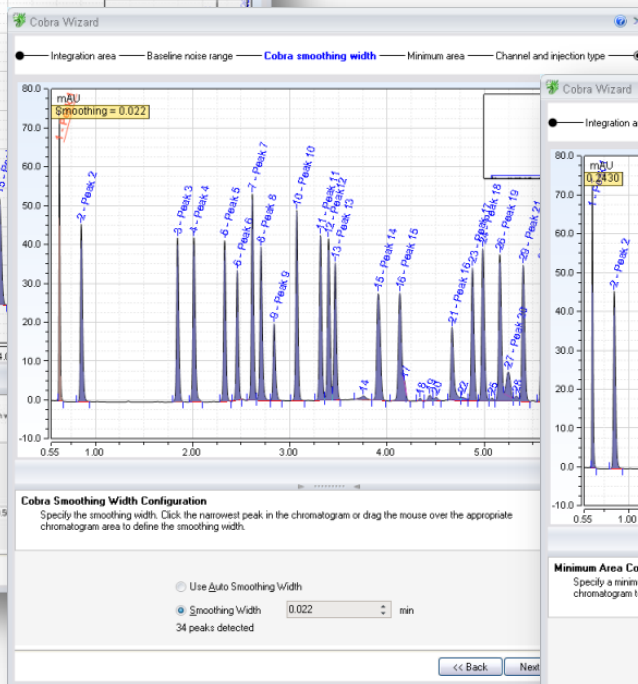
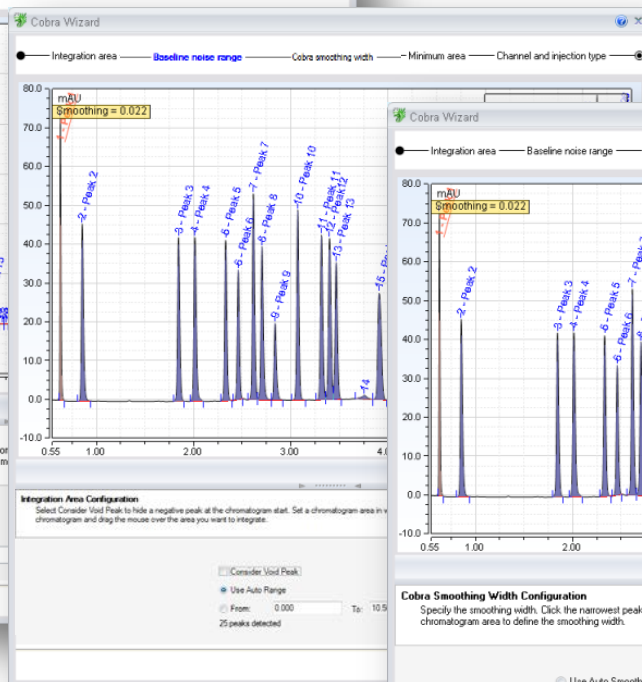
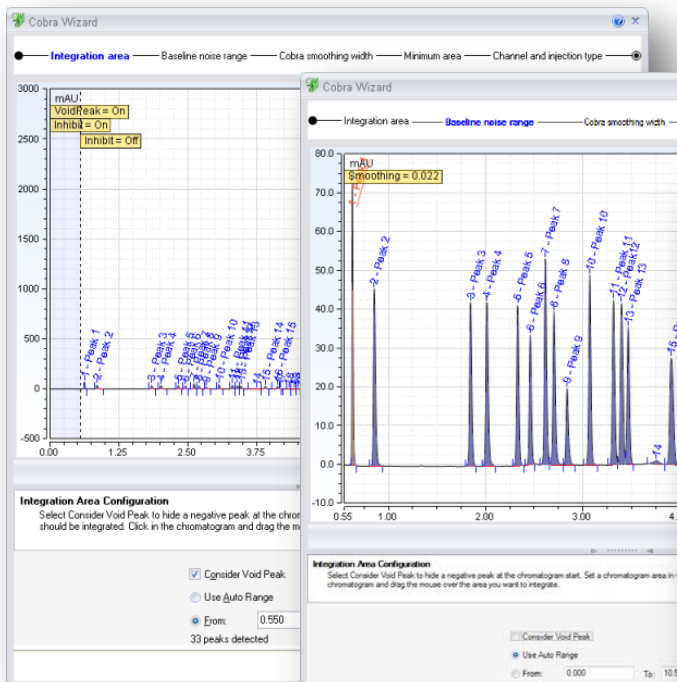
## 1. Start Cobra Wizard

## 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...

Detection Settings

Algorithm: Cobra [Run Cobra Wizard](#)

Baseline Noise Range

Auto Range

Start Time: 9.720 [min]

End Time: 9.980 [min]

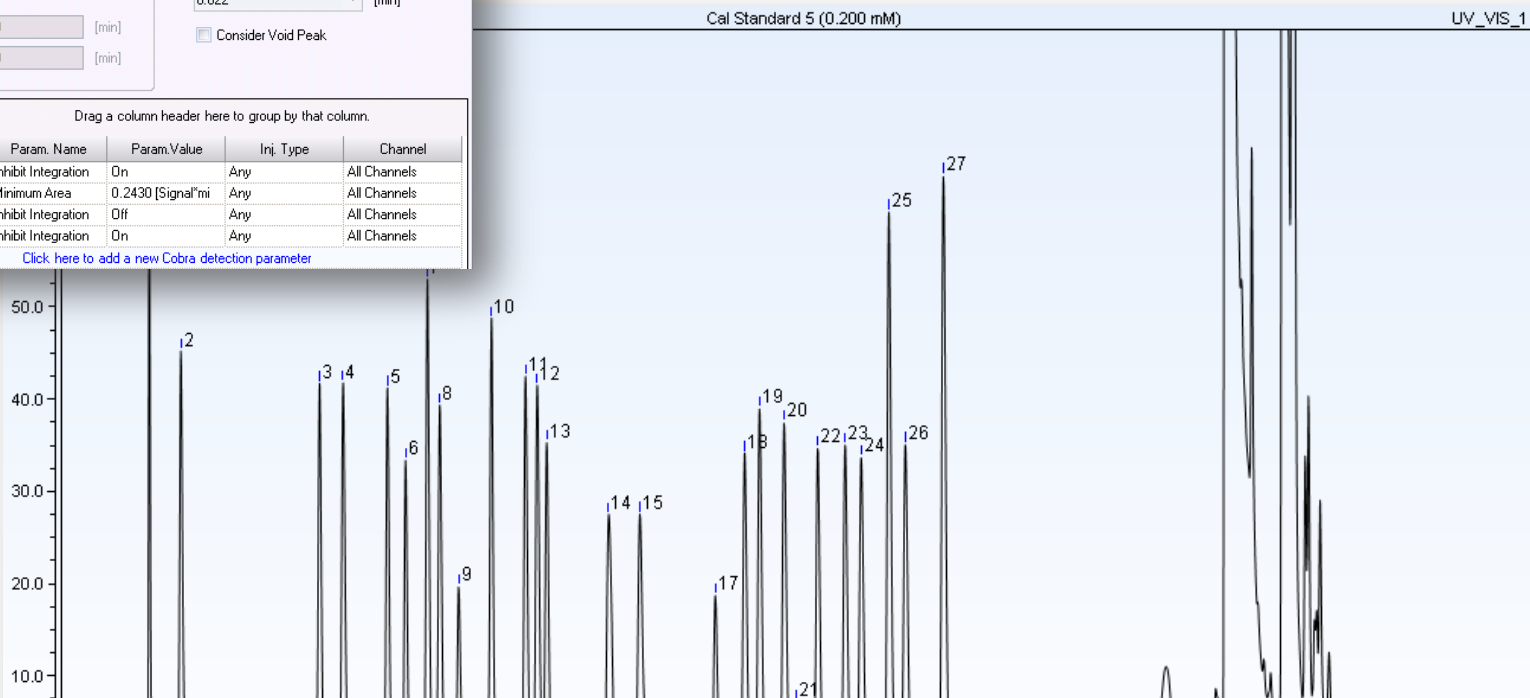
Cobra Smoothing Width: 0.022 [min]

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

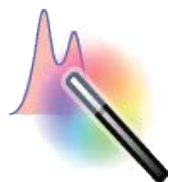
\* [Click here to add a new Cobra detection parameter](#)



Brian Alliston, Sterling Pharma Solutions

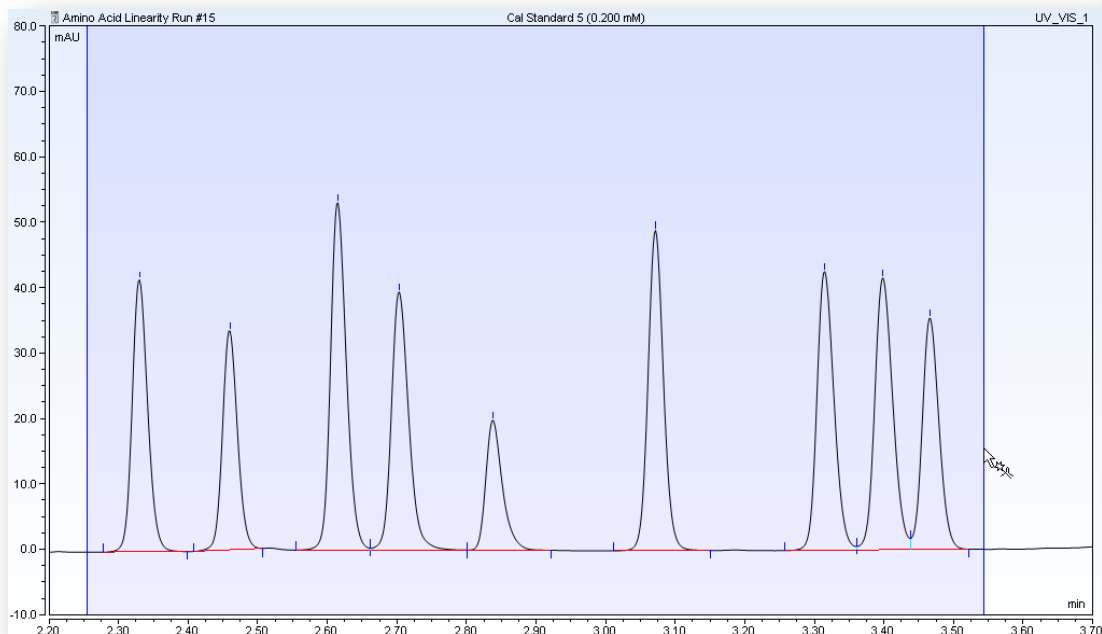
*“Chromeleon is **much quicker** in all activities. Use of the Cobra wizard allows for **quick setup** of optimum integration parameters giving us consistent integration **much faster** than either of our previous CDS.”*

# Data Processing – SmartPeaks Integration Assistant

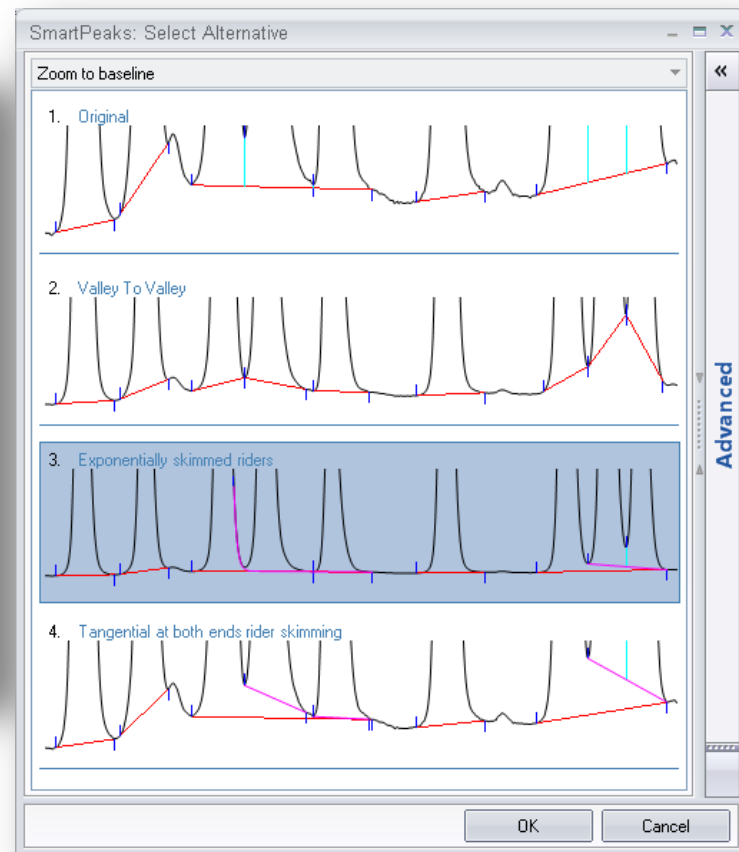


## 1. Activate SmartPeaks Wizard

## 2. Select Area of Interest

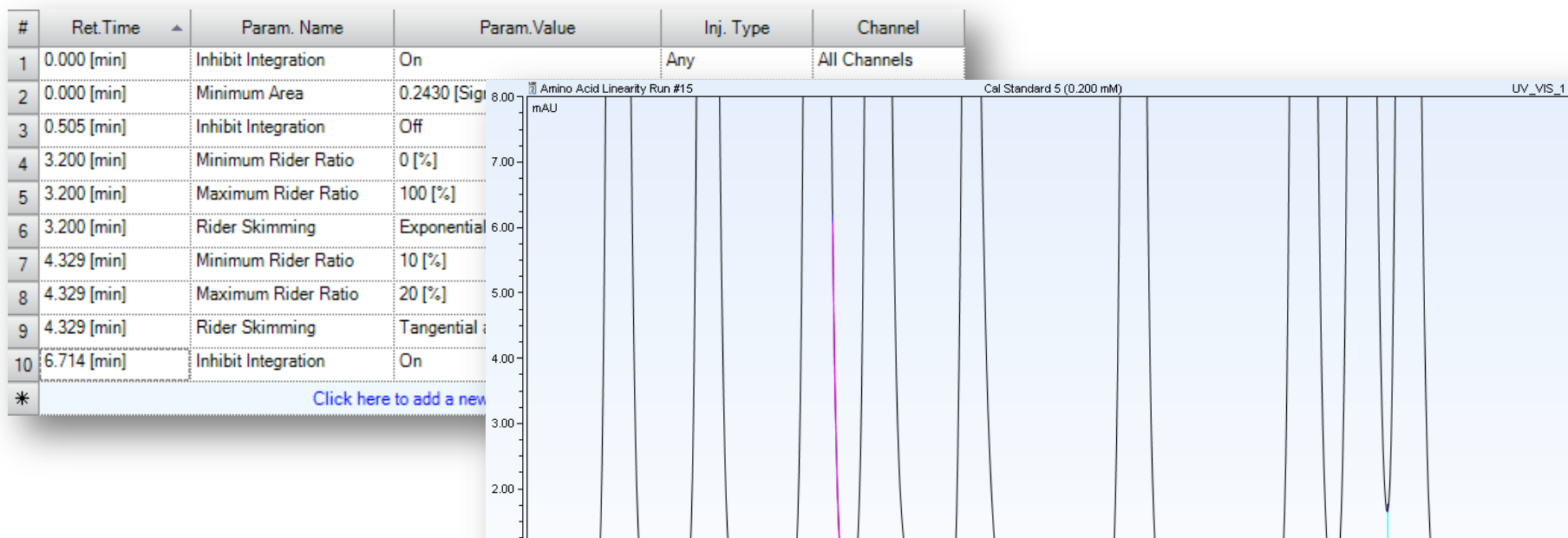


## 3. Select the Integration You Want



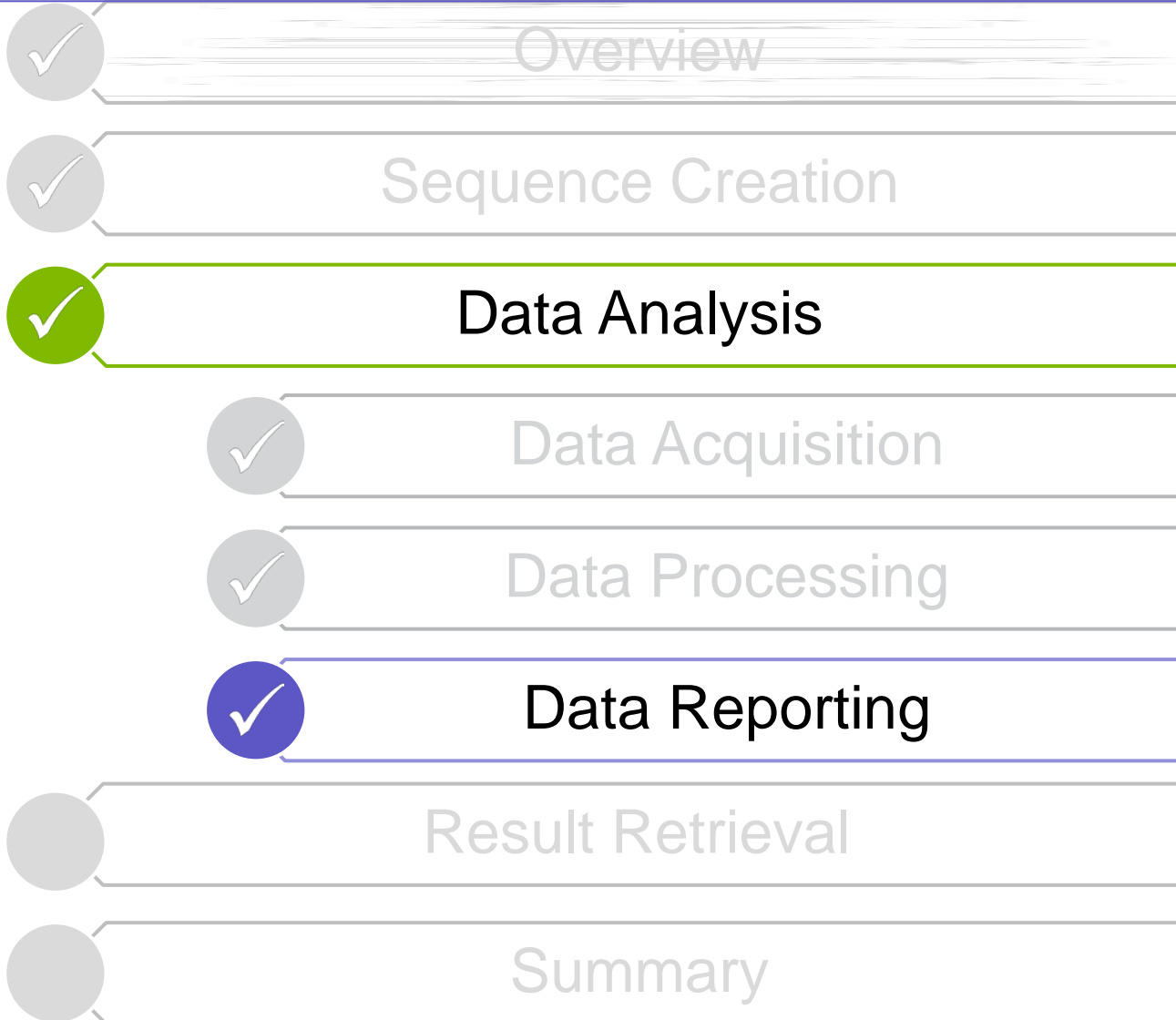
# Data Processing – SmartPeaks Integration Assistant

- 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.**”*



# Data Reporting

- CDS Report Designer can contain:
  - Multiple worksheets
  - Text and variables
  - Various result tables
  - Various plot types
  - Custom equations

The screenshot displays the Chromeleon Chromatography Studio interface. The main window shows a chromatogram plot with several peaks labeled: 1 - Fluoride - 2.063, 2 - Chloride - 3.277, 3 - Nitrite - 3.963, 4 - Bromide - 5.853, 5 - Nitrate - 6.807, 6 - Phosphate - 9.297, and 7 - Sulfate. Below the plot is an 'Integration Results' table.

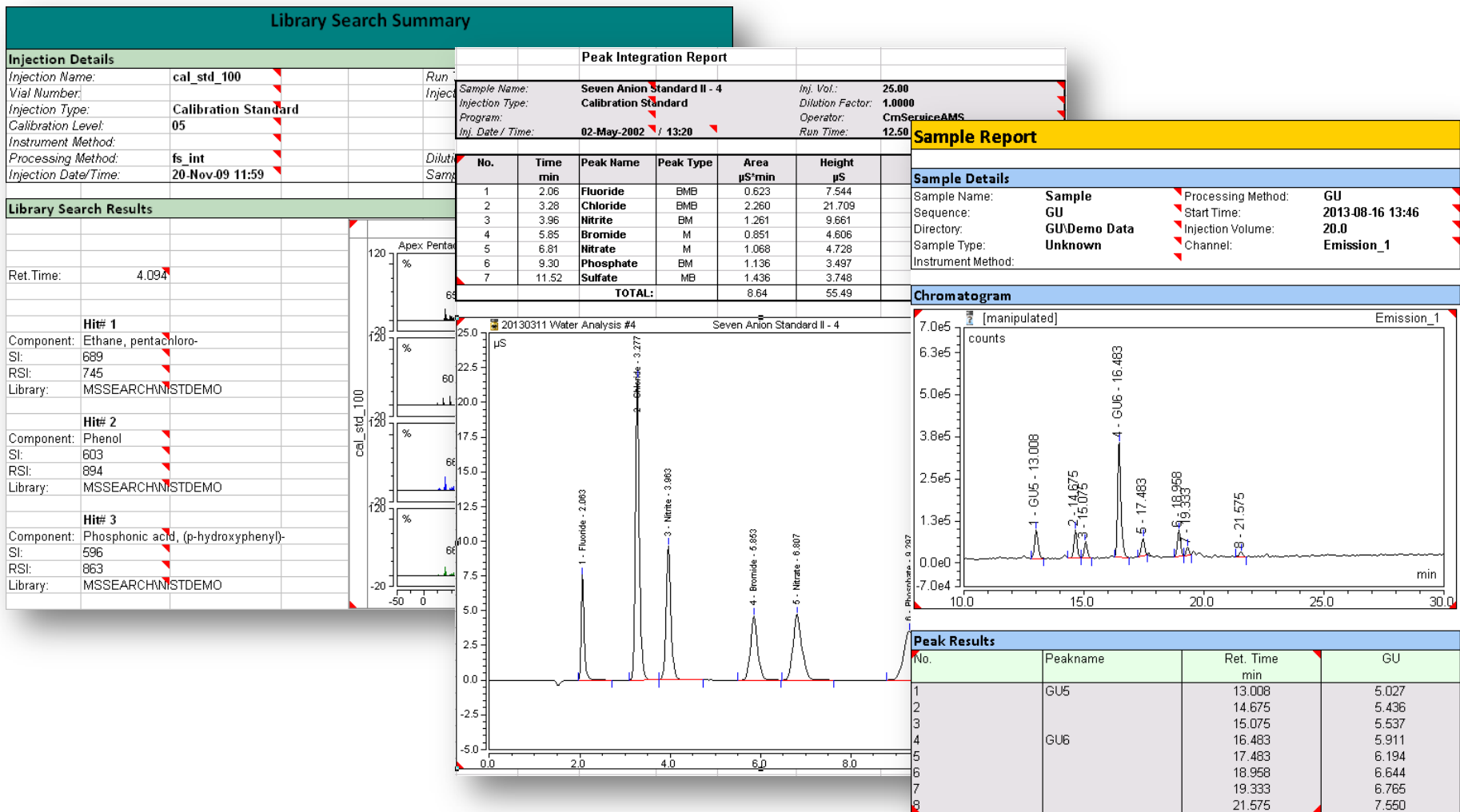
No.	Peak Name	Retention Time min	Area $\mu\text{S}^*\text{min}$	Height $\mu\text{S}$	Relative Area %	Relative Height %	Amount mg/L
1	Fluoride	2.063	0.623	7.544	7.22	13.59	4.0258
2	Chloride	3.277	2.260	21.709	26.17	39.12	19.6966
3	Nitrite	3.963	1.261	9.661	14.61	17.41	19.7425
35	Bromide	5.853	0.851	4.606	9.86	8.30	19.8716
36	Nitrate	6.807	1.068	4.728	12.37	8.52	19.8662
37	Phosphate	9.297	1.136	3.497	13.15	6.30	39.7254
	Sulfate						19.6236

Below the table, a formula bar contains the following text:

```
Area
=IF(ISERROR(AVERAGE(E14:E31)), "n.a.", AVERAGE(E14:E31))
=IF(ISERROR(STDEV(E14:E31)), "n.a.", STDEV(E14:E31))
=MAX(E14:E31)
=MIN(E14:E31)
```

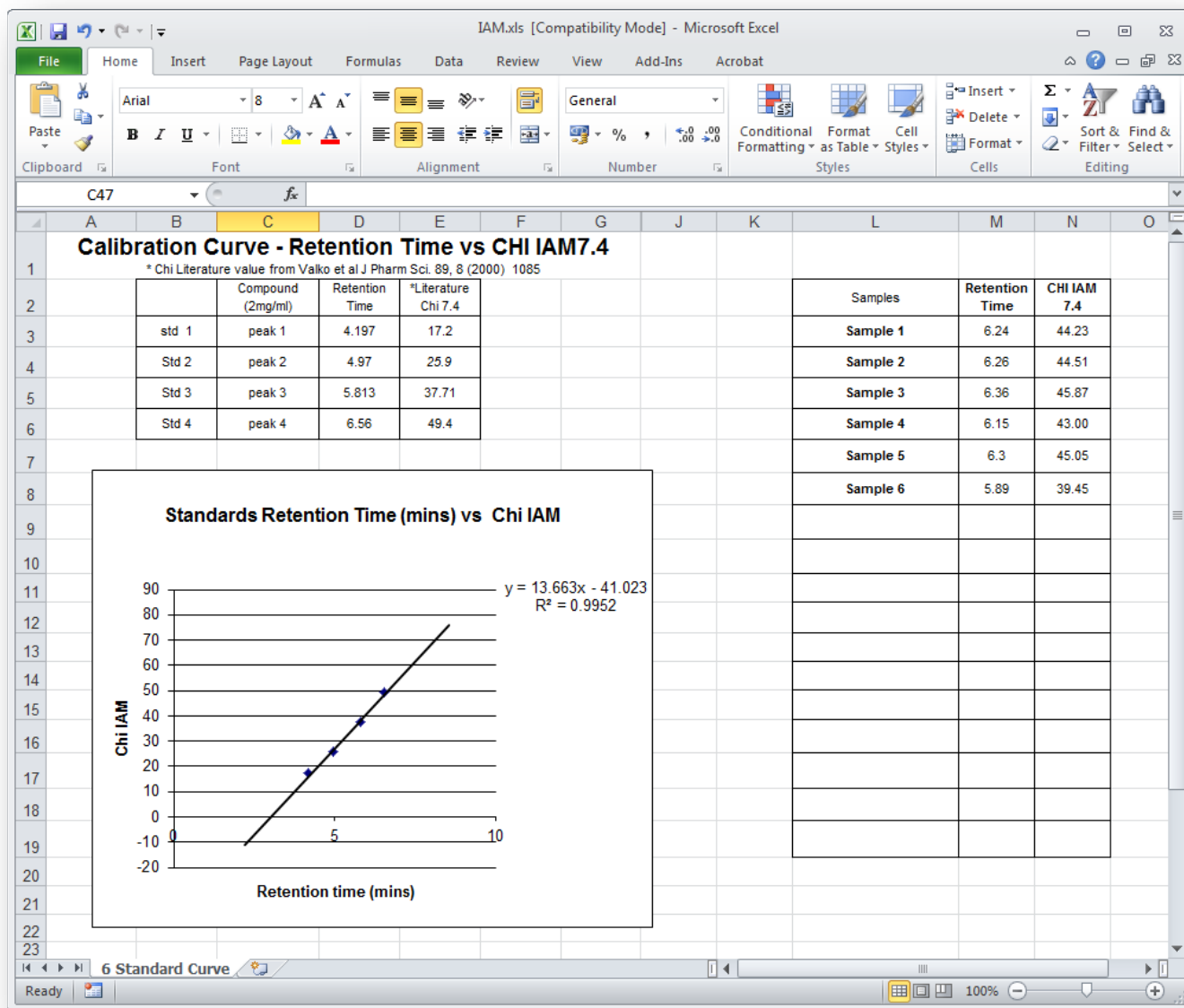
# Data Reporting

... to create the report you need.





# Data Reporting – Example Report in Microsoft Excel



# Data Reporting – Example Report in Chromeleon CDS

The screenshot displays the Chromeleon Chromatography Studio interface. The main window is titled "cmadmin - 06 Report Example 2 (Sequence) - Chromeleon Chromatography Studio". The "Report Designer" pane on the left shows a list of injections, including "Standard" and "Sample1" through "Sample6". The main report area shows a table with columns A through K. The table contains a calibration curve and a standards retention time table.

Compound (2mg/ml)	Retention Time	Literature Chi 7.4 *
Std1	Peak1	4.197
Std2	Peak2	4.970
Std3	Peak3	5.813
Std4	Peak4	6.560

Name	Ret.Time	CHI IAM 7.4
Sample1	6.24	44.28
Sample2	6.26	44.55
Sample3	6.36	45.92
Sample4	6.15	42.96

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.**”*



Introduction



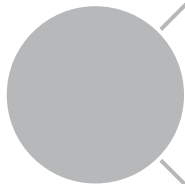
Sequence Creation



Data Analysis



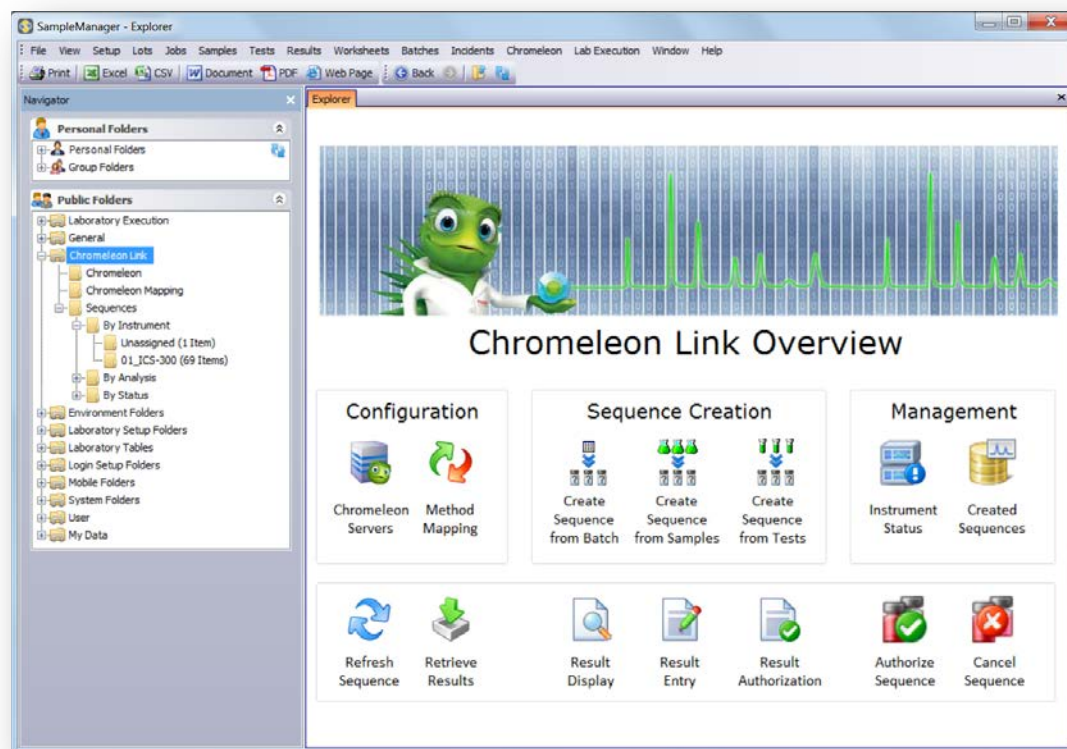
**Result Retrieval**



Summary

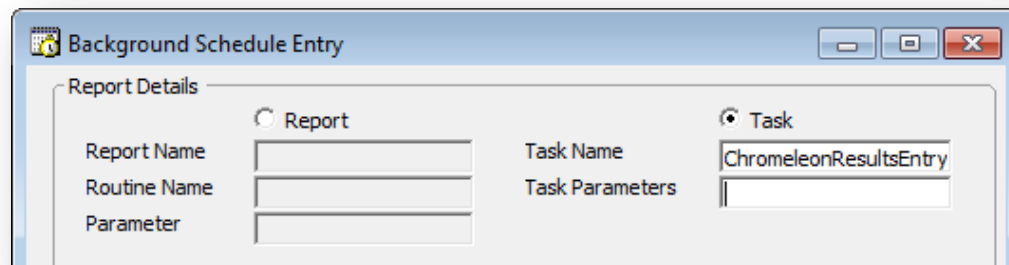
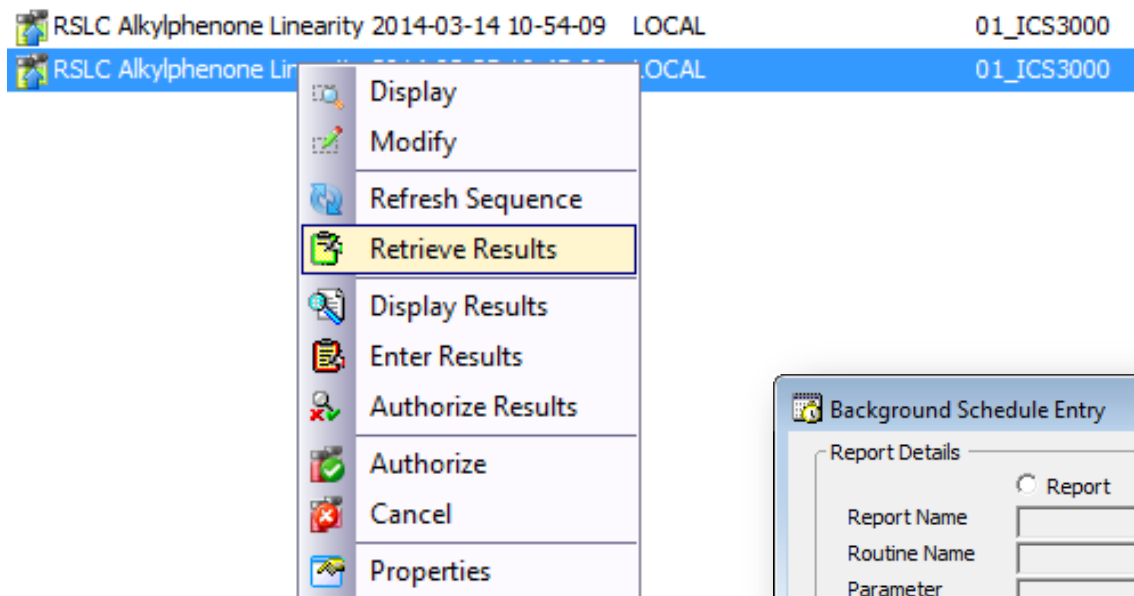
# Result Retrieval

- 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

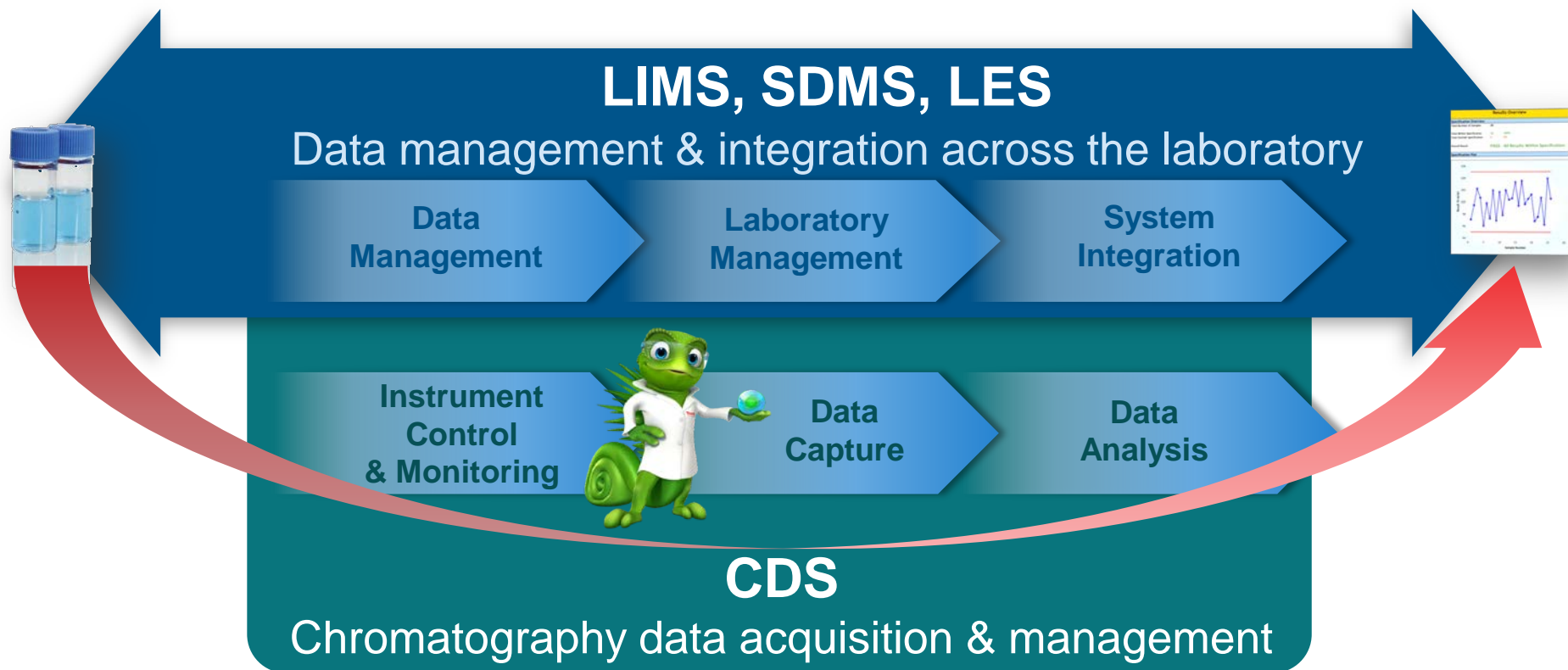
The screenshot displays the Chromeleon software interface. In the background, a file explorer window shows a directory structure under 'ChromeleonLocal', with 'RSLC Alkylphenone Linearity Sample Pull Test' selected. In the foreground, the 'Data Processing' window is open, showing a list of samples. A context menu is overlaid on the 'Data Processing' window, with 'Send Results to SampleManager' highlighted. Another context menu is overlaid on the file explorer window, also with 'Send Results to SampleManager' highlighted. The 'Data Processing' window shows a list of samples with columns for 'Component' and 'Results'. The 'Data Processing' window also shows a chromatogram plot with a y-axis ranging from 0.0 to 50.0. The 'Data Processing' window has tabs for 'Clipboard', 'Navigation', and 'Results'. The 'Data Processing' window also shows a 'Component' tab and a 'Results' tab. The 'Data Processing' window also shows a 'Clipboard' tab and a 'Navigation' tab. The 'Data Processing' window also shows a 'Clipboard' tab and a 'Navigation' tab.

#	UV_VIS
1	
2	

- ✓ Overview
- ✓ Sequence Creation
- ✓ Data Analysis
- ✓ Result Retrieval
- ✓ Summary

# Conclusions

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



# Streamlining Chromatography



Thank You!



**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](mailto:analyze.eu@thermofisher.com)  
and we will get back to you.