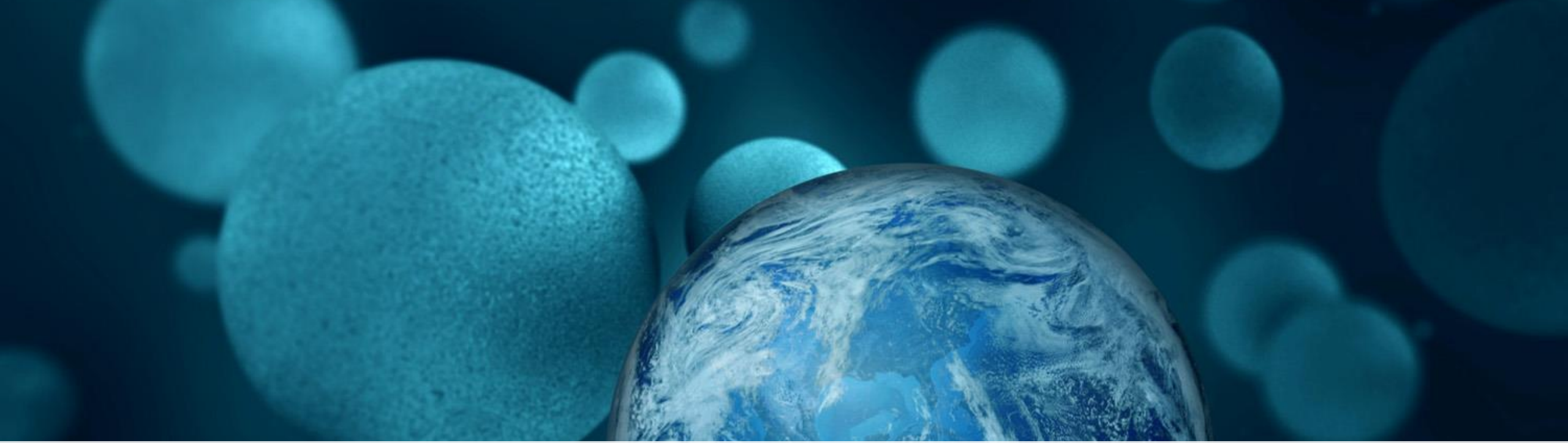

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What about the data management

26 November, 2015 **KVCV: Dataflows in the lab**

Topics

- Introducing Chromeleon 7
- User Interface
- eWorkflows™
- Data Processing and Reporting
- Samplemanager and Chromeleon
- Compliance
- Summary

Chromeleon CDS for your laboratory

Stand alone or for your entire Enterprise

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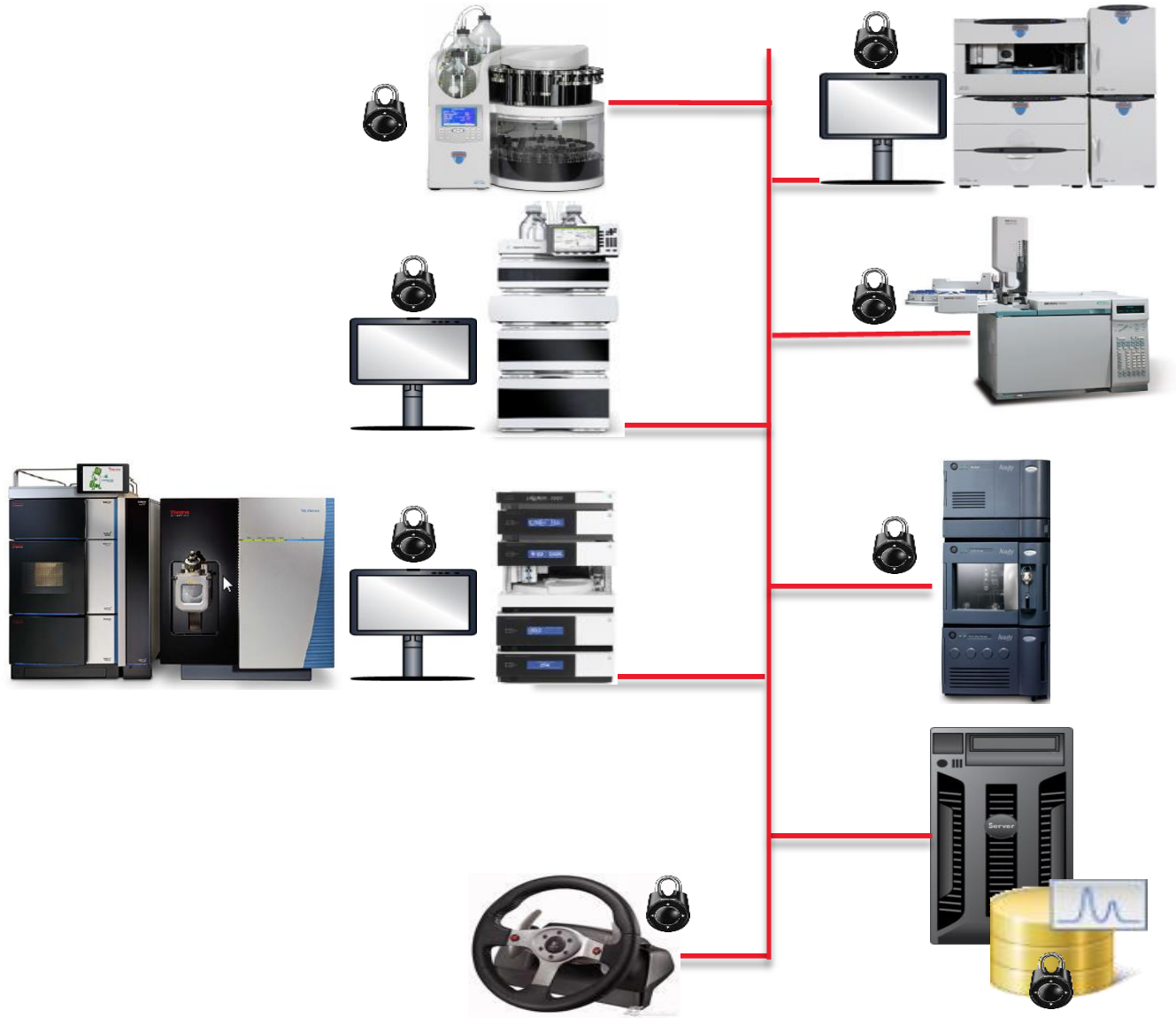
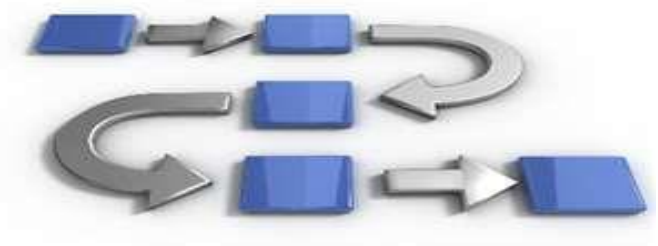
Key Features for an Enterprise Environment

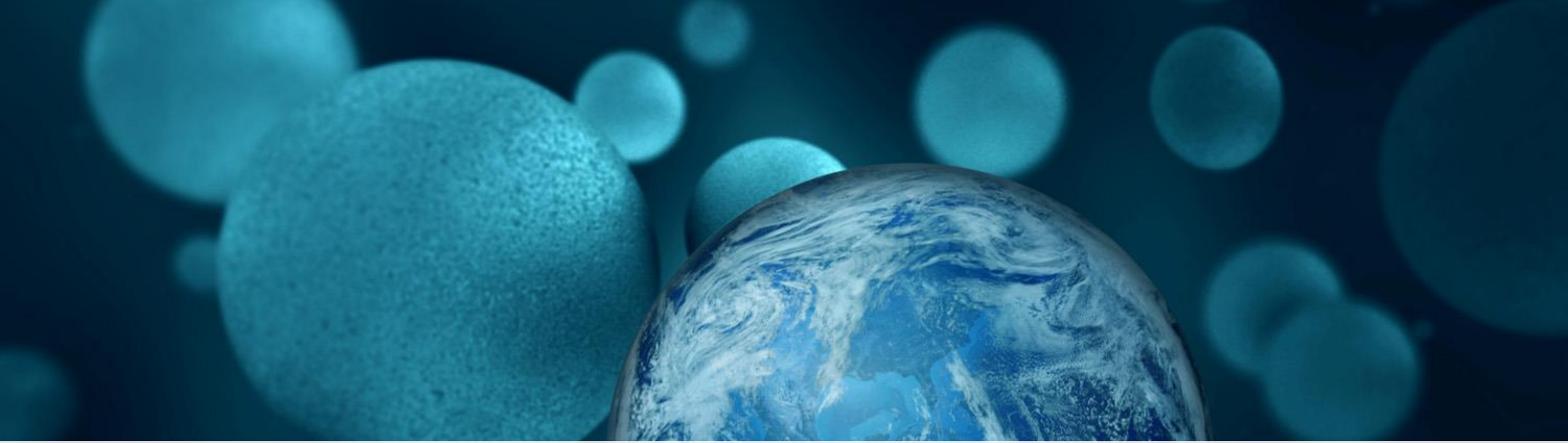
- Networking capabilities
  - Central data storage
    - Choice of database
  - Acquiring data to a central Data Vault
  - Network failure protection
- Multiple Instrument Control
  - Instruments from different vendors
- Centralized Administration
  - License management, license server
  - User management
- Security
  - User management, access control
  - Electronic signatures



Key Features for an Enterprise Environment

- Archiving
  - Transfer of data to a long term archive
- Backup
  - Securing installation and configuration data for emergency restore
- Qualification
  - Installation, Operational and Performance Qualification
  - Both Software and Instruments
- Integration
  - LIMS, ELN
  - Custom tools





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User Interface

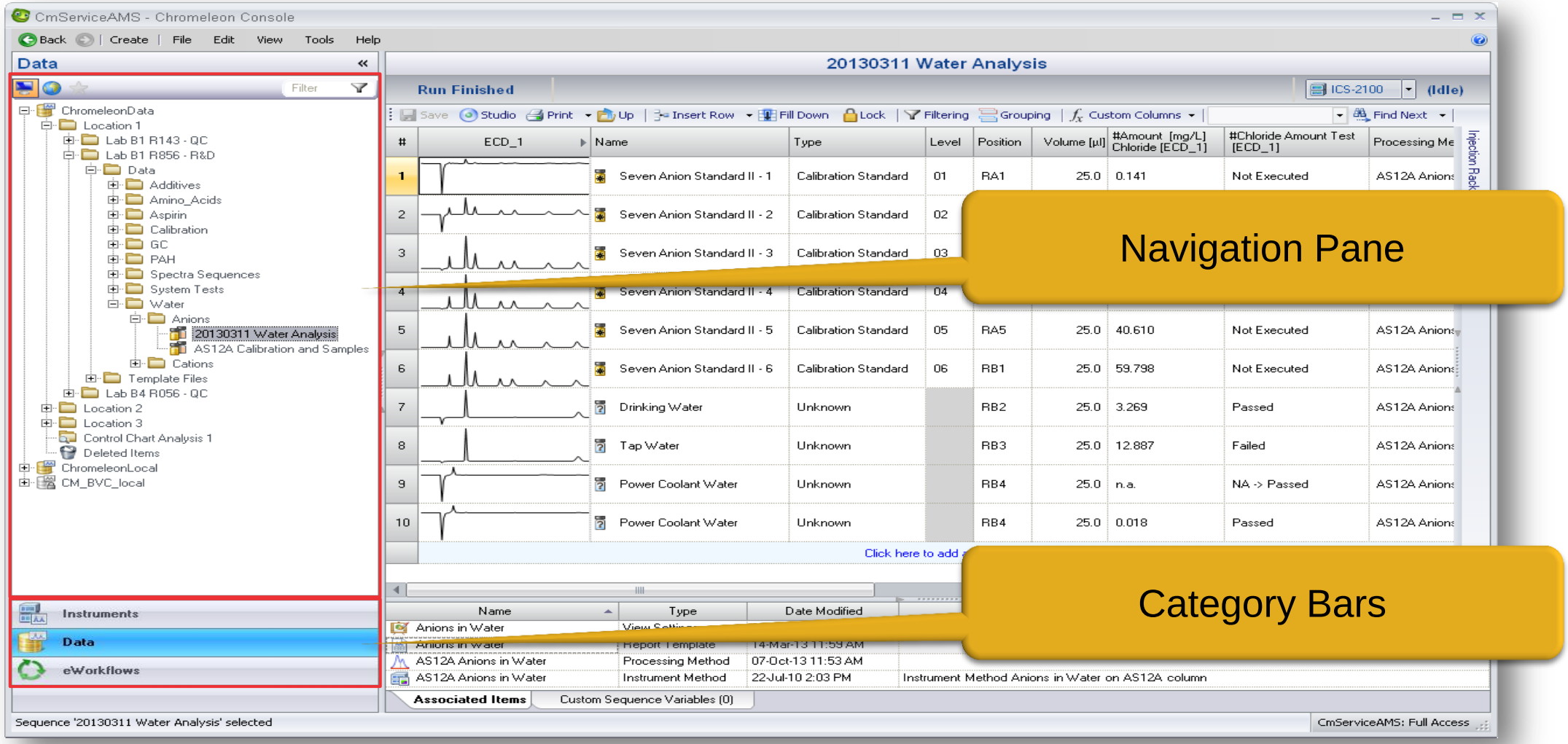
Intuitive - Simple

The Chromeleon User Interface consists of two major parts:

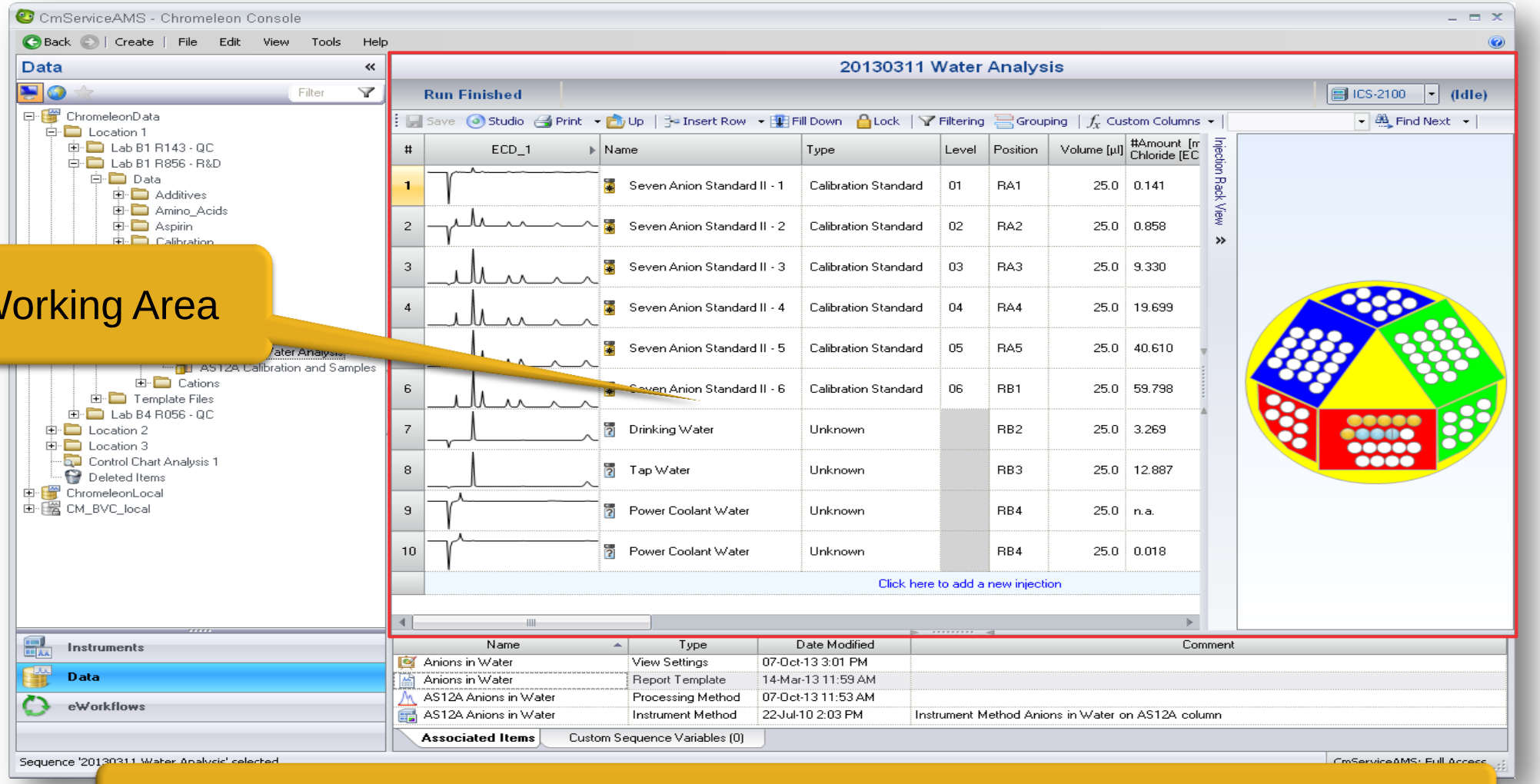
- Chromeleon **Console**
- Chromatography **Studio**

Chromeleon CDS Console

Chromeleon CDS Console



Integrated Sequence Editor



Working Area

Direct modification of Injection List

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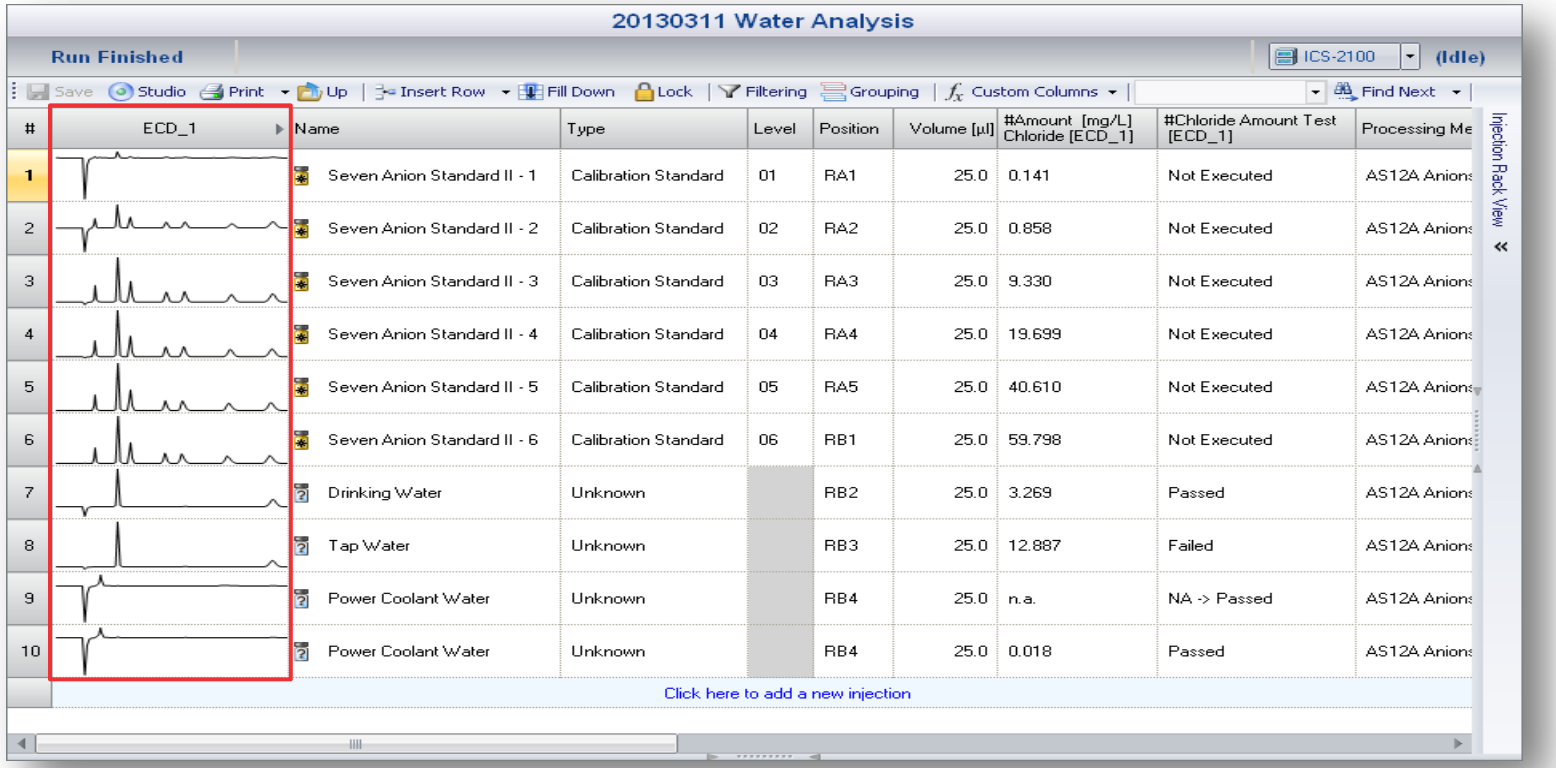
MiniPlots – Quick Access to Data



#	ECD_1	Name	Type	Level	Position	Volume [µl]	#Amount [mg/L] Chloride [ECD_1]	#Chloride Amount Test [ECD_1]	Processing Me
1		Seven Anion Standard II - 1	Calibration Standard	01	RA1	25.0	0.141	Not Executed	AS12A Anions
2		Seven Anion Standard II - 2	Calibration Standard	02	RA2	25.0	0.858	Not Executed	AS12A Anions
3		Seven Anion Standard II - 3	Calibration Standard	03	RA3	25.0	9.330	Not Executed	AS12A Anions
4		Seven Anion Standard II - 4	Calibration Standard	04	RA4	25.0	19.699	Not Executed	AS12A Anions
5		Seven Anion Standard II - 5	Calibration Standard	05	RA5	25.0	40.610	Not Executed	AS12A Anions
6		Seven Anion Standard II - 6	Calibration Standard	06	RB1	25.0	59.798	Not Executed	AS12A Anions
7		Drinking Water	Unknown		RB2	25.0	3.269	Passed	AS12A Anions
8		Tap Water	Unknown		RB3	25.0	12.887	Failed	AS12A Anions
9		Power Coolant Water	Unknown		RB4	25.0	n.a.	NA -> Passed	AS12A Anions
10		Power Coolant Water	Unknown		RB4	25.0	0.018	Passed	AS12A Anions

Proper and reproducible chromatography

Presence / absence of peaks

Quality of separation

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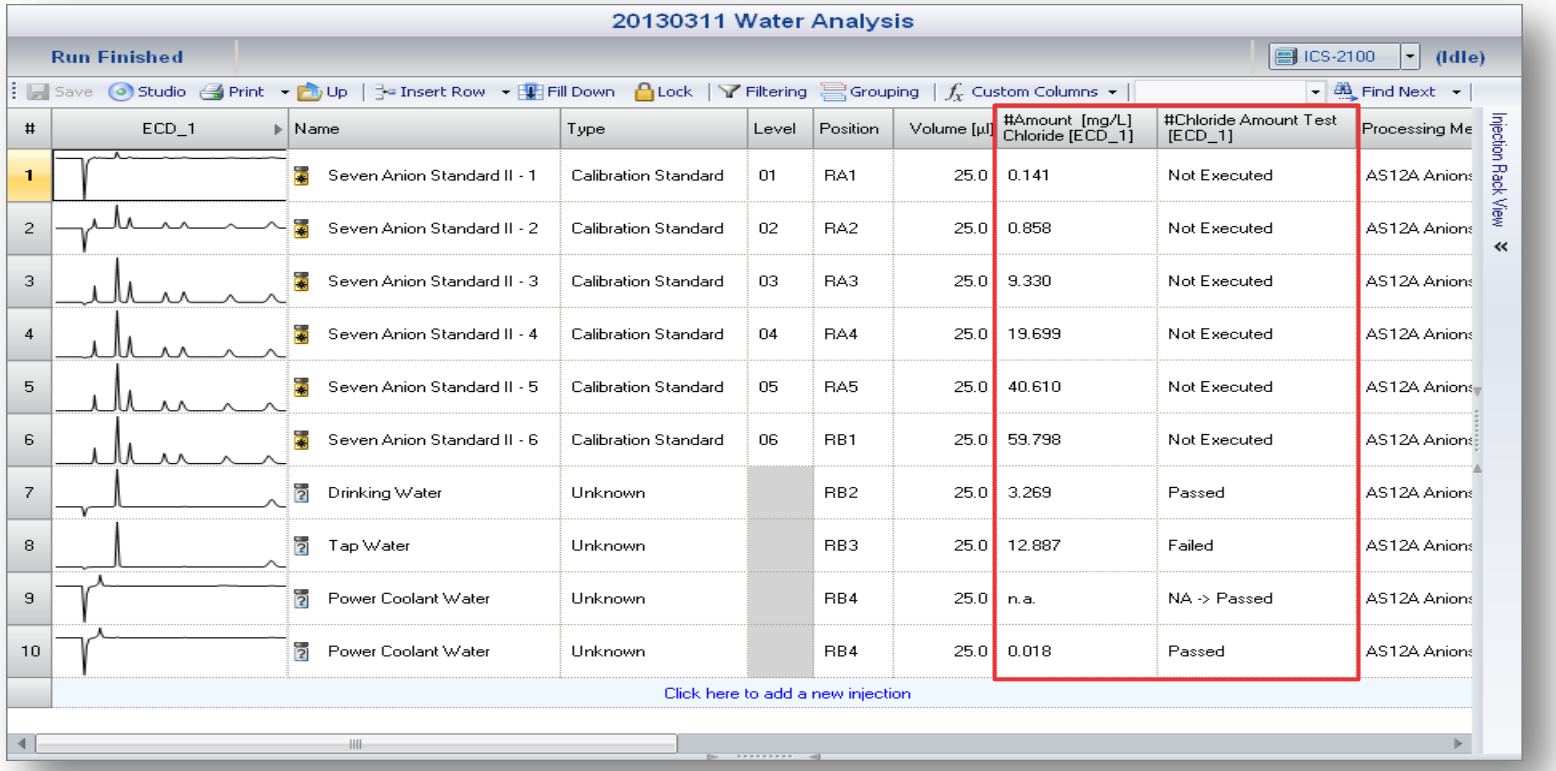
Result Formula Columns – Quick Access to Results



#	ECD_1	Name	Type	Level	Position	Volume [µl]	#Amount [mg/L] Chloride [ECD_1]	#Chloride Amount Test [ECD_1]	Processing Me
1		Seven Anion Standard II - 1	Calibration Standard	01	RA1	25.0	0.141	Not Executed	AS12A Anions
2		Seven Anion Standard II - 2	Calibration Standard	02	RA2	25.0	0.858	Not Executed	AS12A Anions
3		Seven Anion Standard II - 3	Calibration Standard	03	RA3	25.0	9.330	Not Executed	AS12A Anions
4		Seven Anion Standard II - 4	Calibration Standard	04	RA4	25.0	19.699	Not Executed	AS12A Anions
5		Seven Anion Standard II - 5	Calibration Standard	05	RA5	25.0	40.610	Not Executed	AS12A Anions
6		Seven Anion Standard II - 6	Calibration Standard	06	RB1	25.0	59.798	Not Executed	AS12A Anions
7		Drinking Water	Unknown		RB2	25.0	3.269	Passed	AS12A Anions
8		Tap Water	Unknown		RB3	25.0	12.887	Failed	AS12A Anions
9		Power Coolant Water	Unknown		RB4	25.0	n.a.	NA -> Passed	AS12A Anions
10		Power Coolant Water	Unknown		RB4	25.0	0.018	Passed	AS12A Anions

View results without opening sequence data

Immediate SST result check

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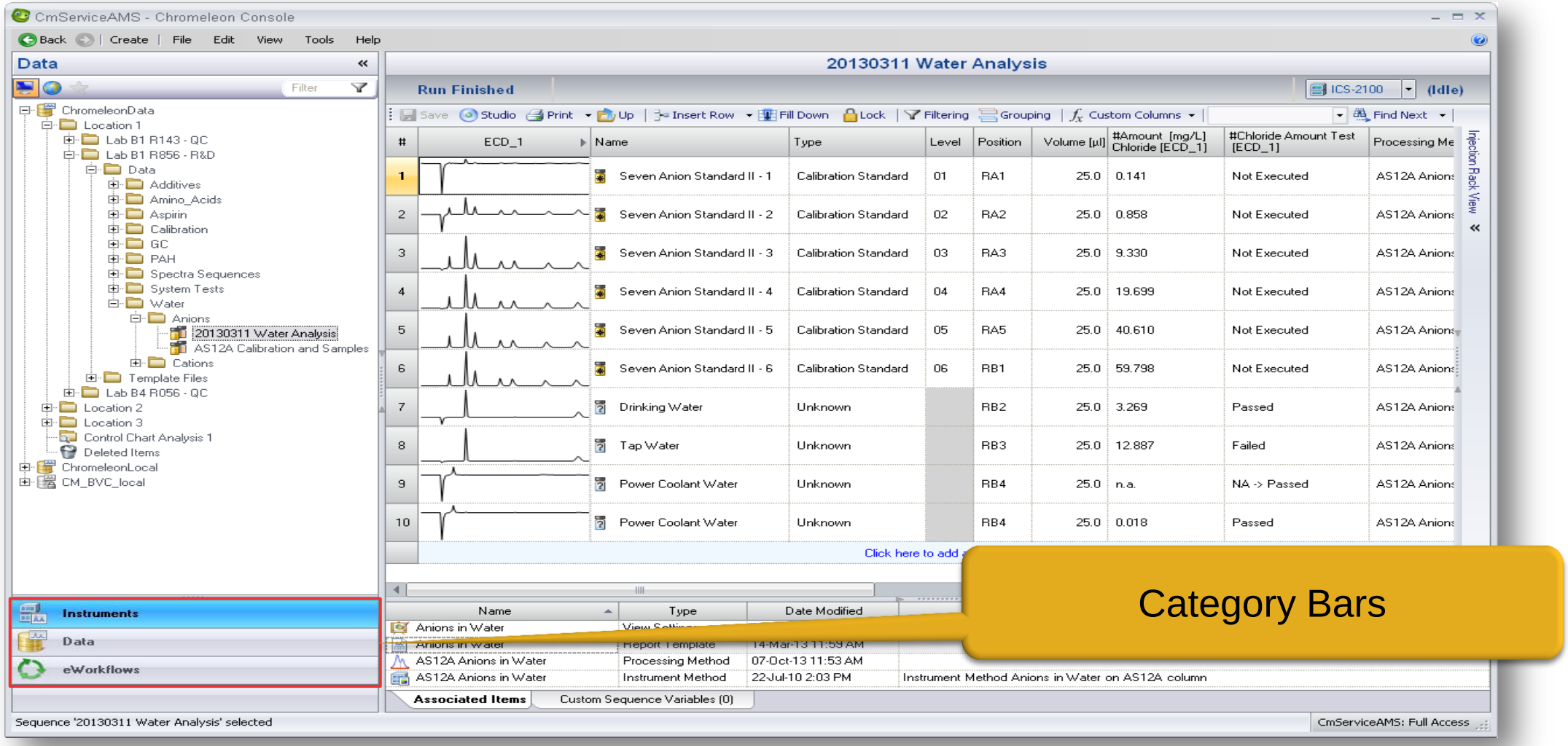
Chromeleon CDS Console



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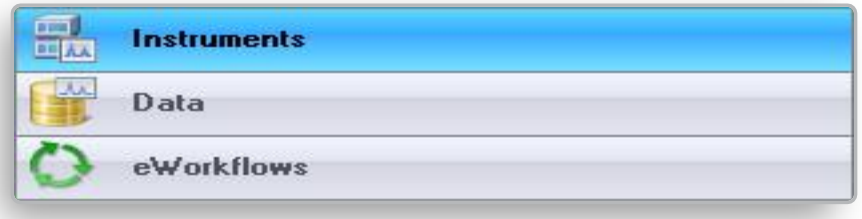
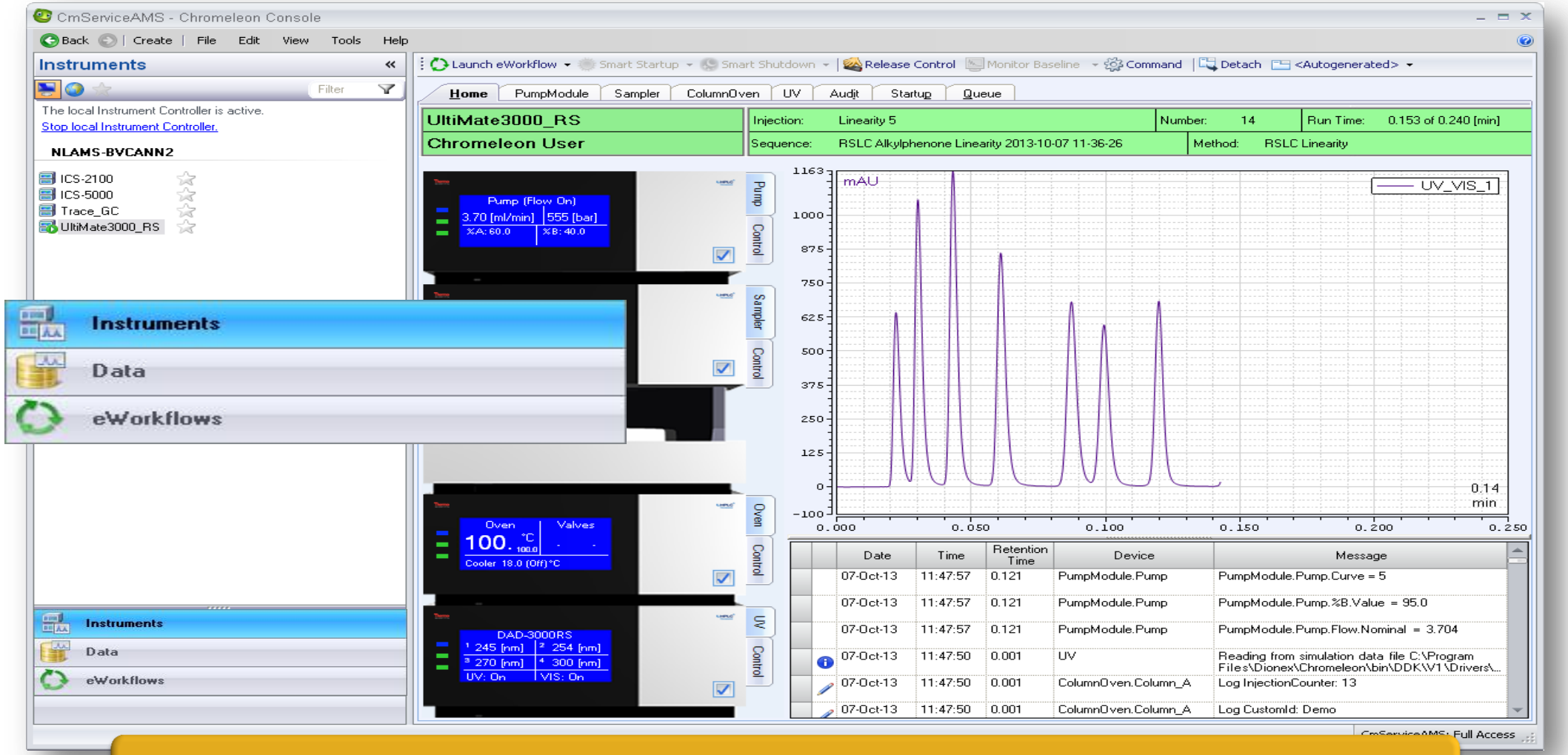
Category Bars – Easy Access



- Provide immediate access to:
  - **Your instruments**

Category Bars – Easy Access

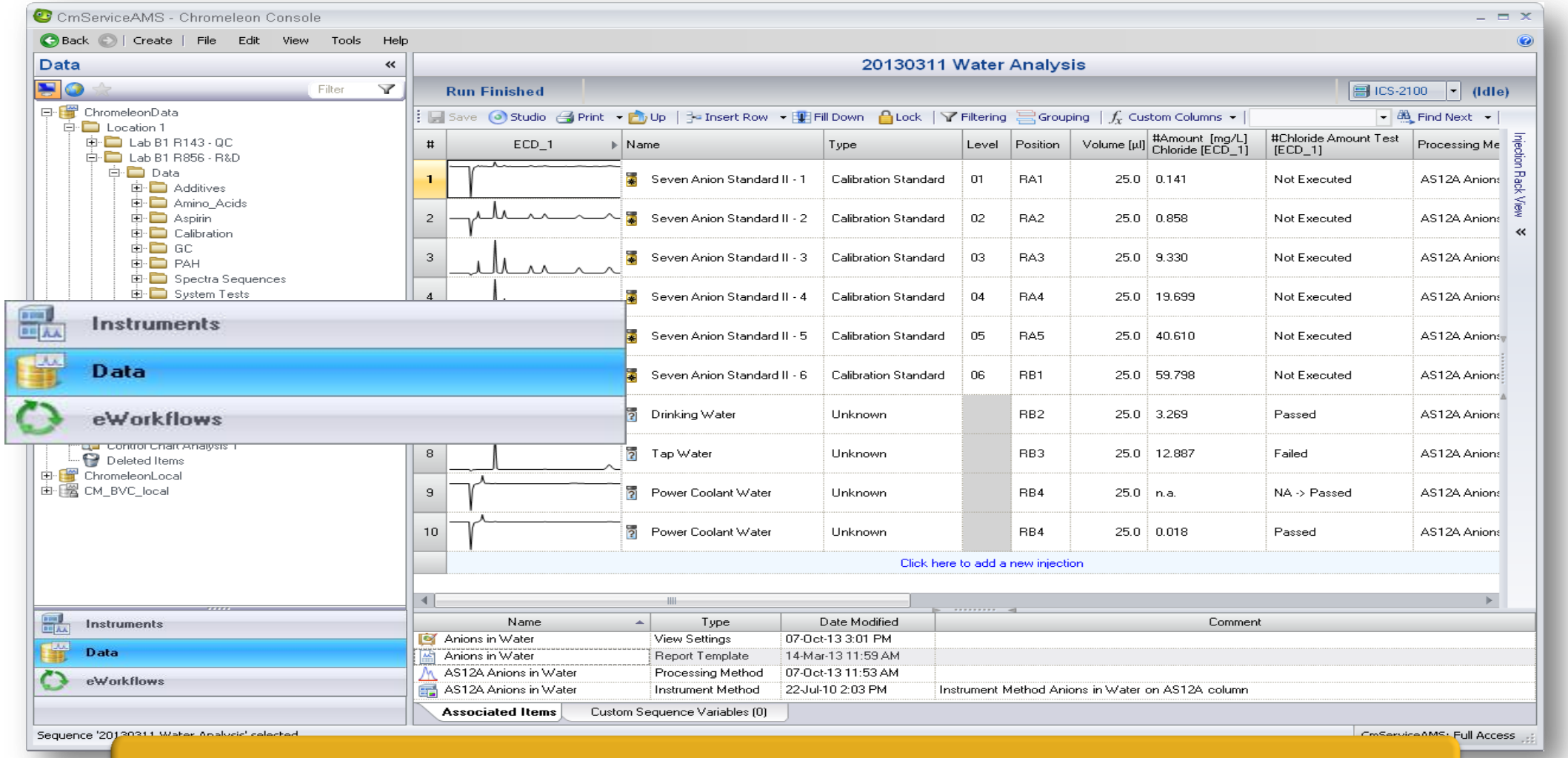


Control your instruments via intuitive ePanels

Category Bars – Easy Access

- Provide immediate access to:
  - **Your data**

Category Bars – Easy Access



Directly access your data and results

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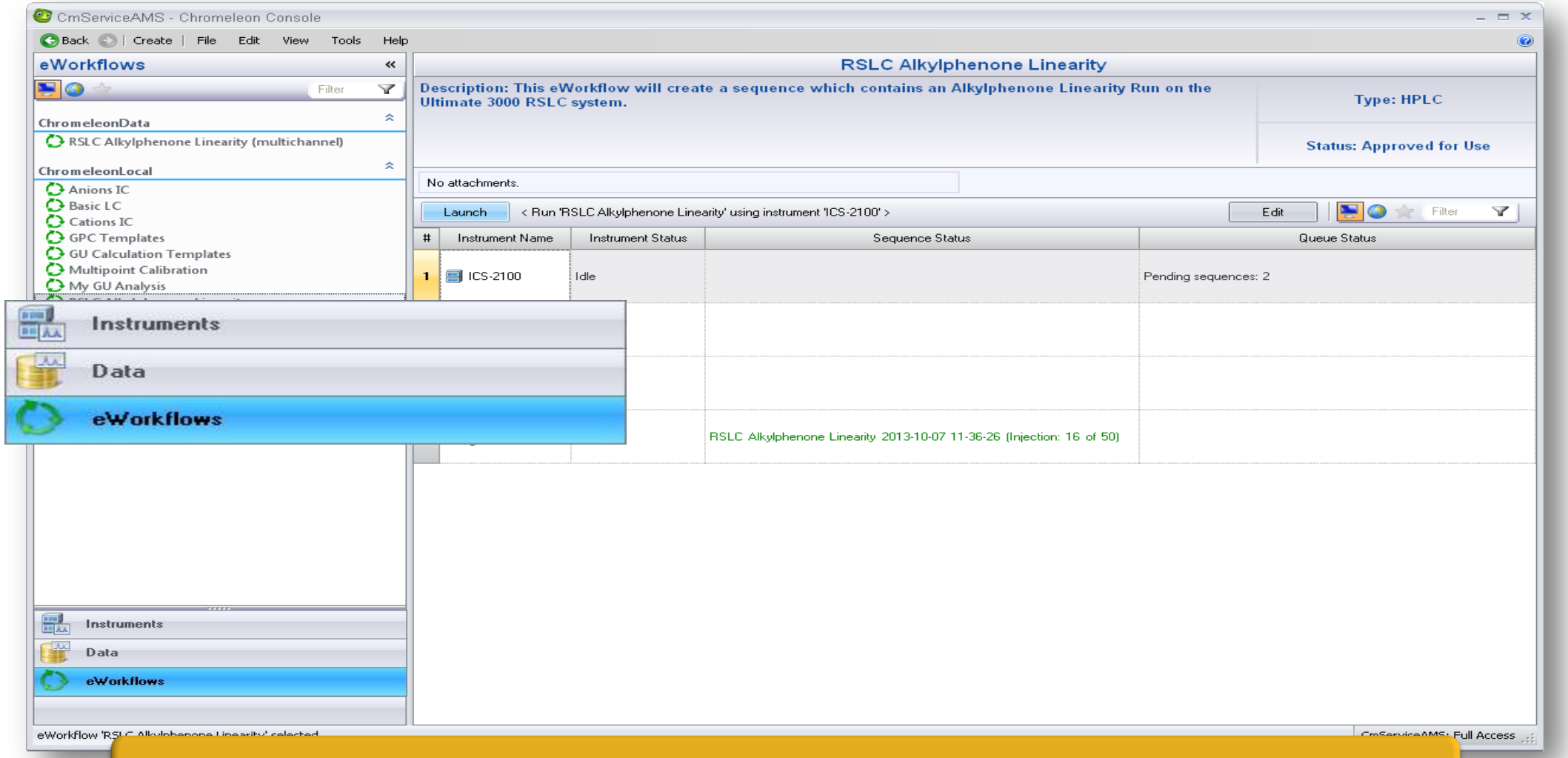
Category Bars – Easy Access

- Provide immediate access to:
  - **Your eWorkflows**

Category Bars – Easy Access



Start your runs via eWorkflows

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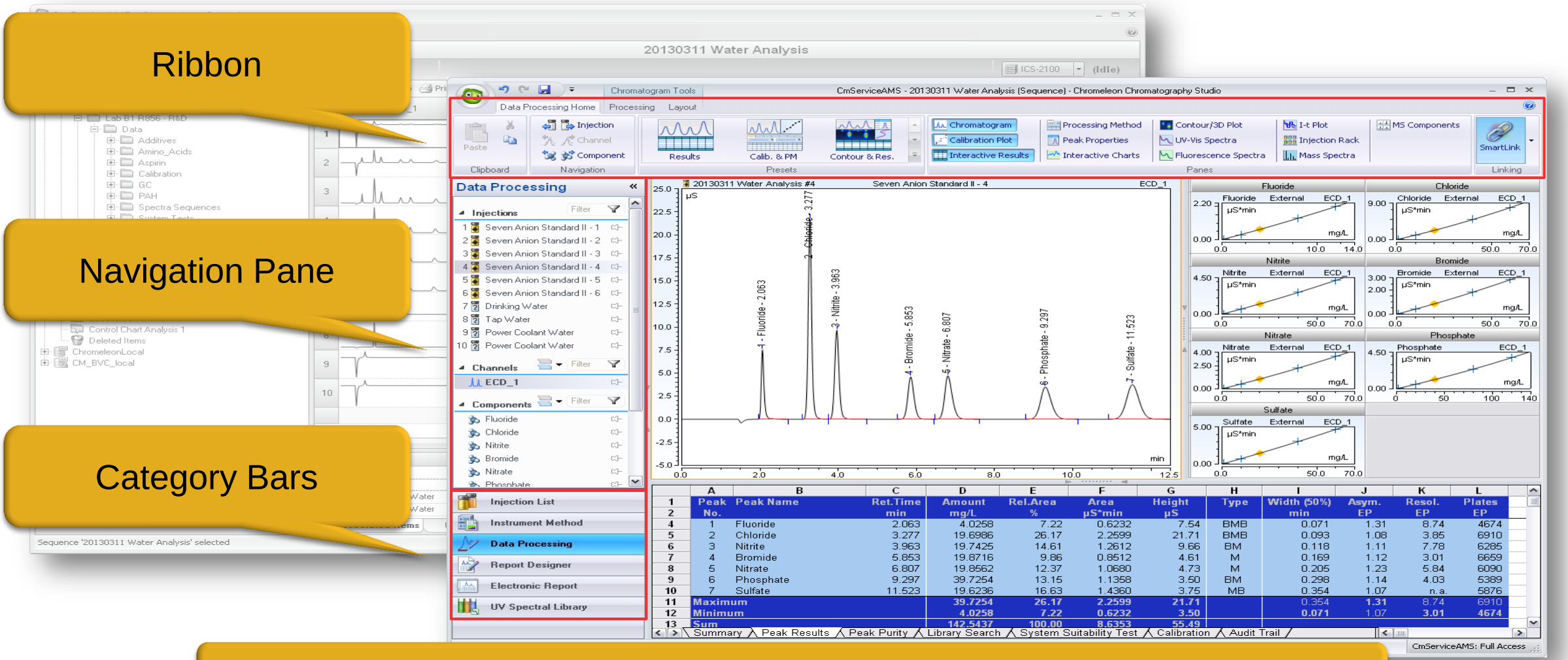
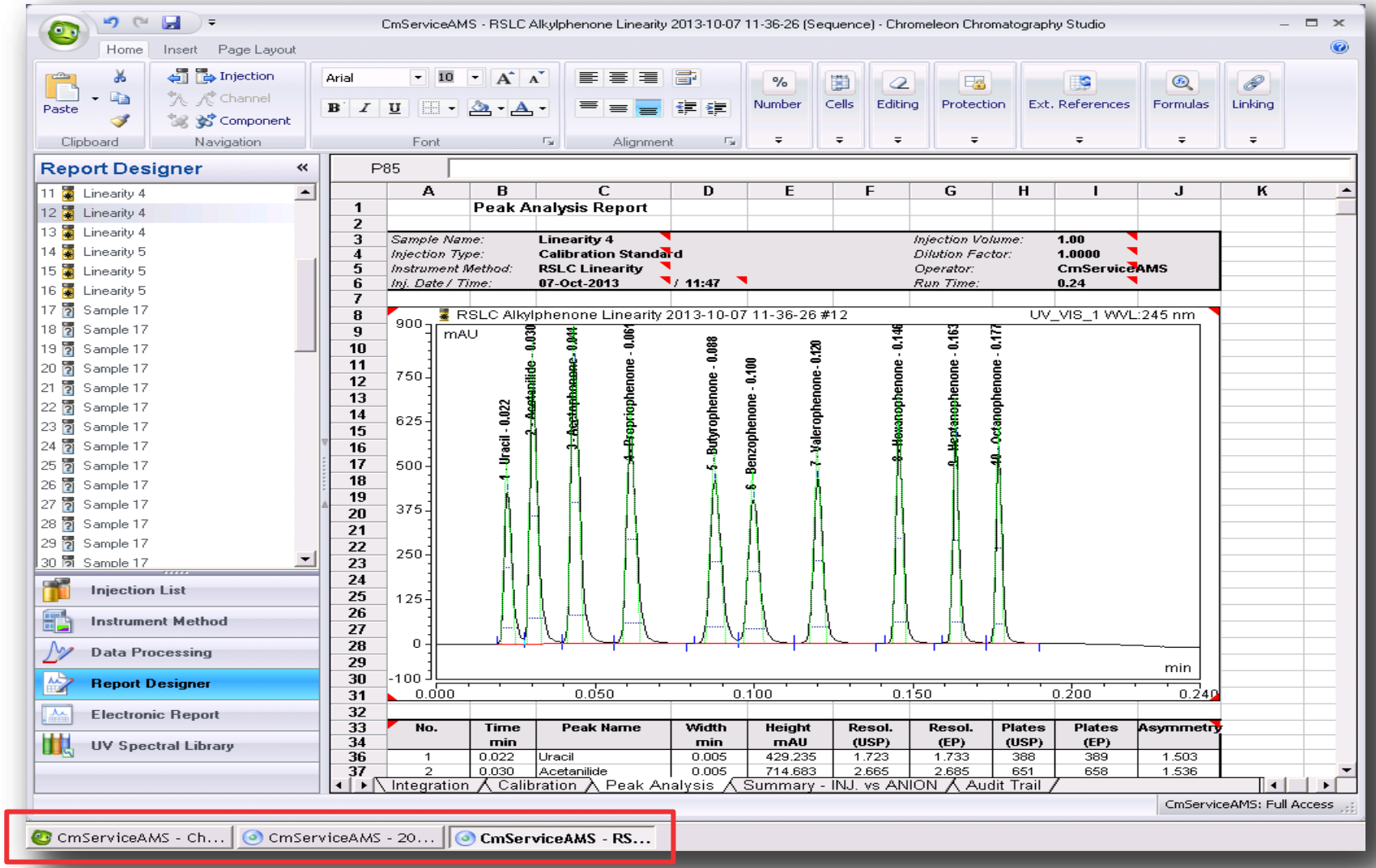
Chromatography Studio

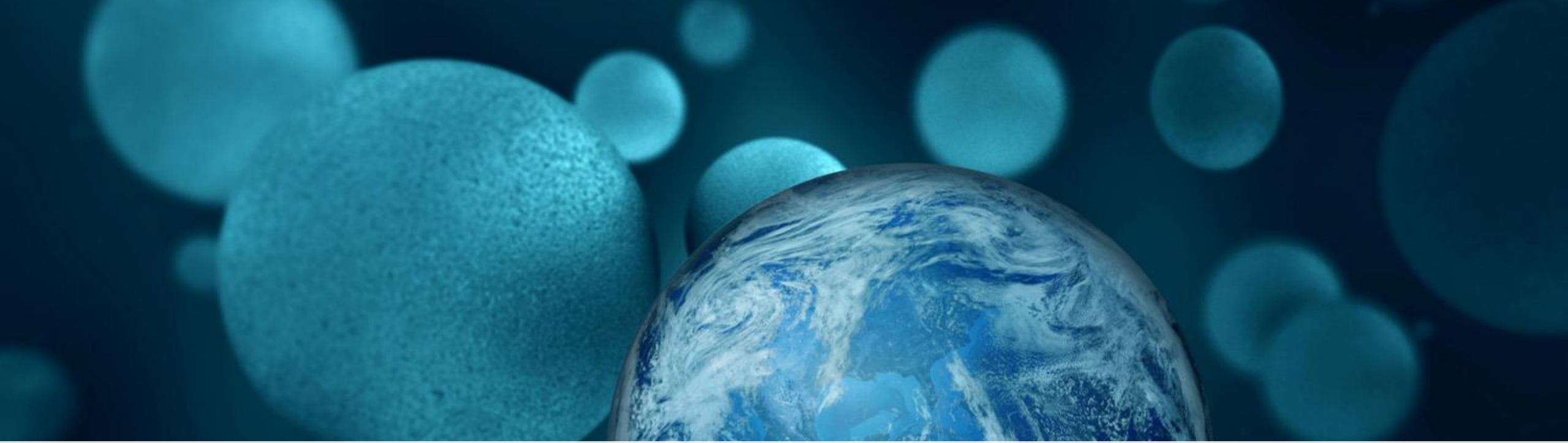
- Used for All Data Evaluation
- Provides access to every object in the sequence:
  - Injection List
  - Instrument Method
  - Processing Method
  - Results
  - Report Template
  - Electronic Report
  - Spectral Library
- Opens in separate window on task bar – makes working with multiple sequences easy
- Uses new “Ribbon” technology introduced in Microsoft Office 2007



No.	Peak Name	Ret.Time min	Amount mg/L	Rel.Area %	Area µS*min	Height µS	Type	Width (50%) min	Asym. EP	Resol. EP	Plates EP
1	Fluoride	2.063	4.0258	7.22	0.6232	7.54	BMB	0.071	1.31	8.74	4674
2	Chloride	3.277	19.6986	26.17	2.2599	21.71	BMB	0.093	1.08	3.85	6910
3	Nitrite	3.963	19.7425	14.61	1.2612	9.66	BM	0.118	1.11	7.78	6285
4	Bromide	5.853	19.8716	9.86	0.8512	4.61	M	0.169	1.12	3.01	6659
5	Nitrate	6.807	19.8562	12.37	1.0680	4.73	M	0.205	1.23	5.84	6090
6	Phosphate	9.297	39.7254	13.15	1.1358	3.50	BM	0.298	1.14	4.03	5389
7	Sulfate	11.523	19.6236	16.63	1.4360	3.75	MB	0.354	1.07	n.a.	5876
Maximum			39.7254	26.17	2.2599	21.71		0.354	1.31	8.74	6910
Minimum			4.0258	7.22	0.6232	3.50		0.071	1.07	3.01	4674
Sum			142.5437	100.00	8.6353	55.49					

Work with multiple objects at the same time





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eWorkflows™

The Ultimate in Operational Simplicity

Category Bars – Easy Access

- Provide immediate access to:
  - Your instruments
  - Your data
  - Your eWorkflows
- **Easily find functionality you need**
- **No training required to start run**

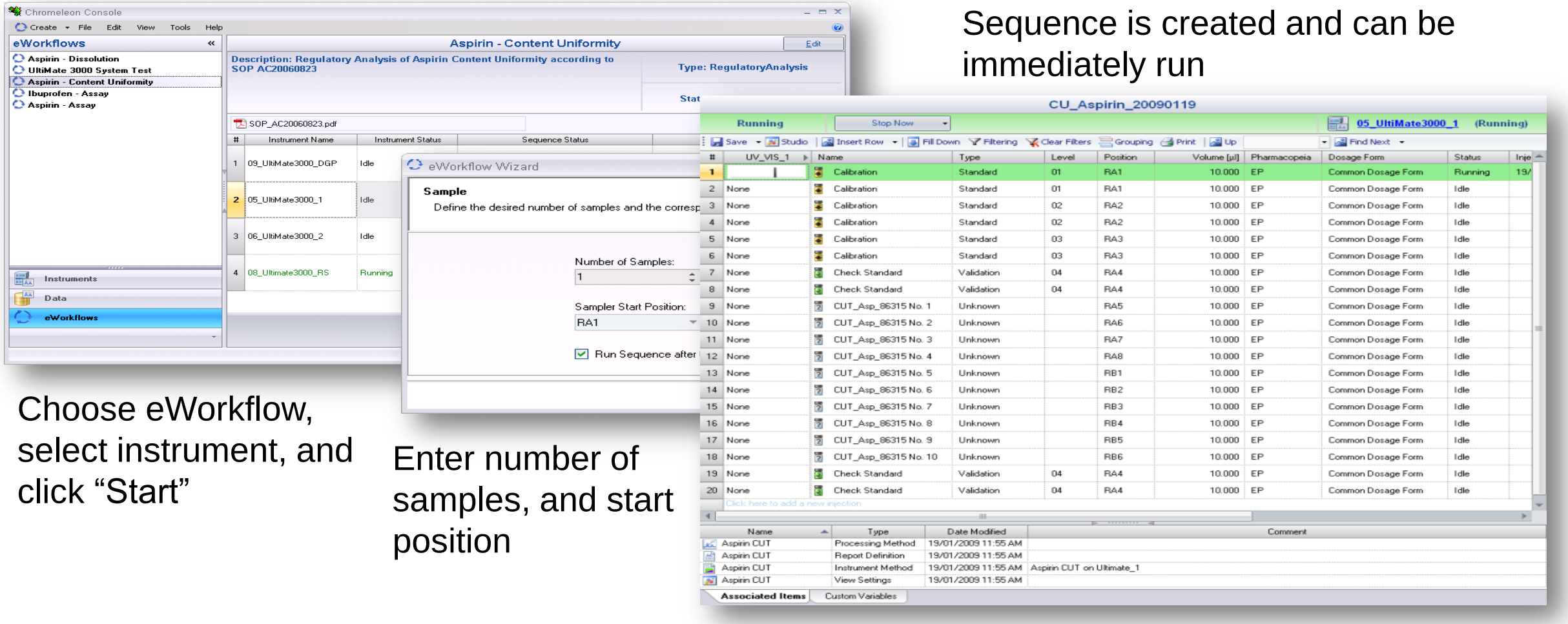
- eWorkflows automate all chromatography processes

- Applies to all laboratories:
  - QA/QC laboratories
  - Pilot plant laboratories
  - Production plant laboratories
  - Method development laboratories
  - Research laboratories

- Takes you from Samples to Results in only a few steps

- An eWorkflow brings together all aspects of a chromatography run:
  - Instruments which are allowed to run this application
  - All associated files:
    - Instrument Methods
    - Processing Methods
    - Reports
    - Spectral Libraries
    - Documents with description of method
  - Template for sequence name and storage location
  - Custom Variables
  - Rules for sequence layout

eWorkflows – A Regulated USP/EP Method



Sequence is created and can be immediately run

Choose eWorkflow, select instrument, and click “Start”

Enter number of samples, and start position

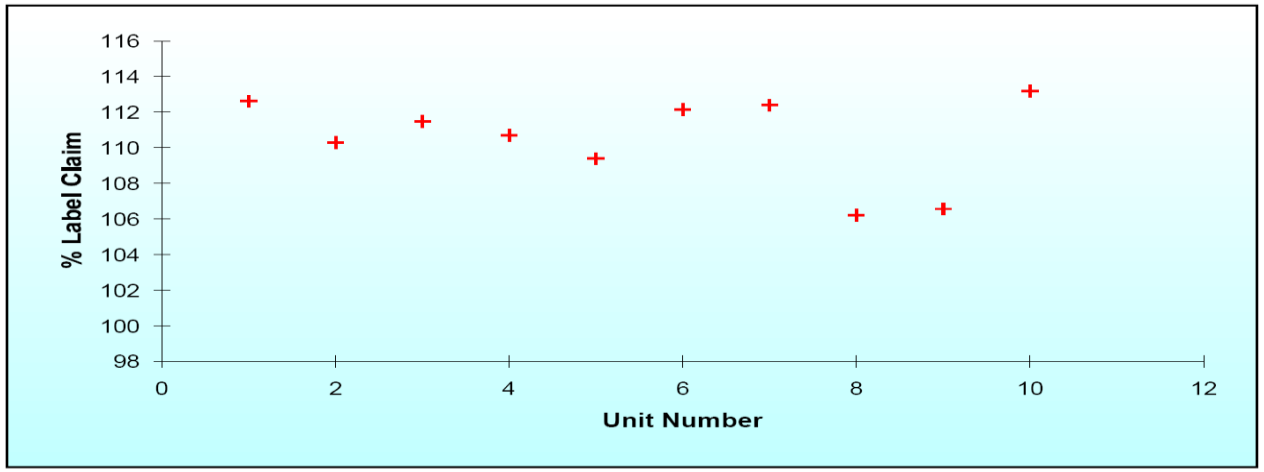
Uniformity of Dosage Units Report

General

Product Batch Number	**86315**	*Target Content T*	102.0
Peak Name	**Aspirin**	*Correction Factor*	1.050
CUT Number	186781	*Max. Acceptance Value L1*	15.0
Channel	UV_VIS_1	*Lower Amount Limit*	Not needed if n=10!
Dosage Form	Common Dosage Forms	*Upper Amount Limit*	Not needed if n=10!
Pharmacopeia	EP		

Results

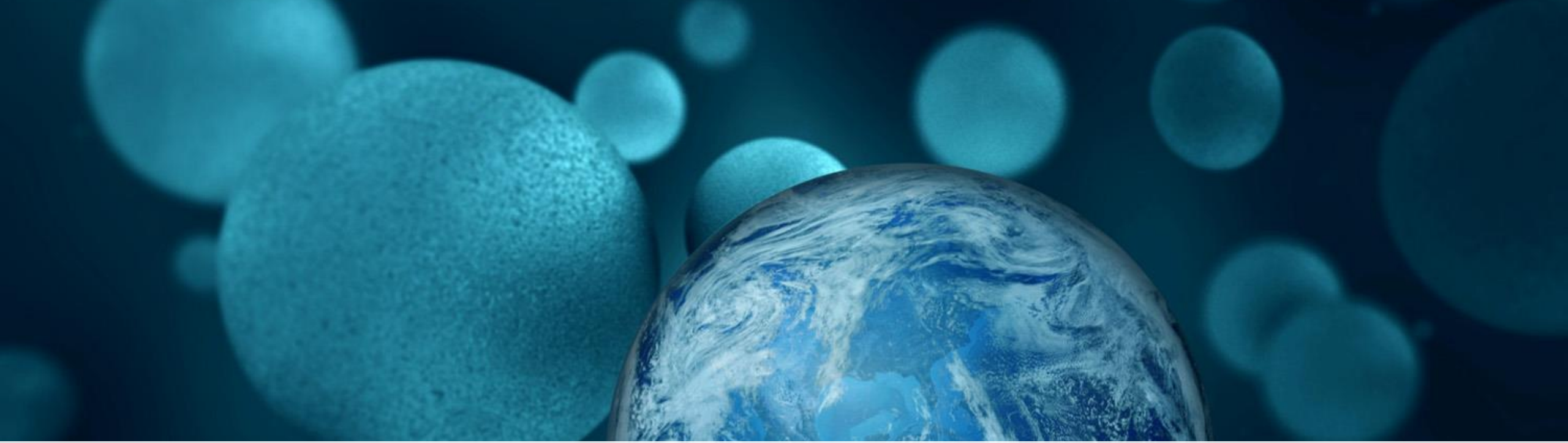
	n = 10
Mean	110.5
Standard Deviation s	2.5
Reference Value M	102.0
Acceptance Value AV	14.4
Test Result	**Test passed**



- This eWorkflow also:
  - Processes all data
  - Calculates all results

eWorkflows – From Samples to Results

- eWorkflows take you from Sample to Results in the minimum number of steps
- Fully customizable for any application
- Minimum amount of training required
- Reduces errors and produces results faster
- A new framework for Operational Simplicity



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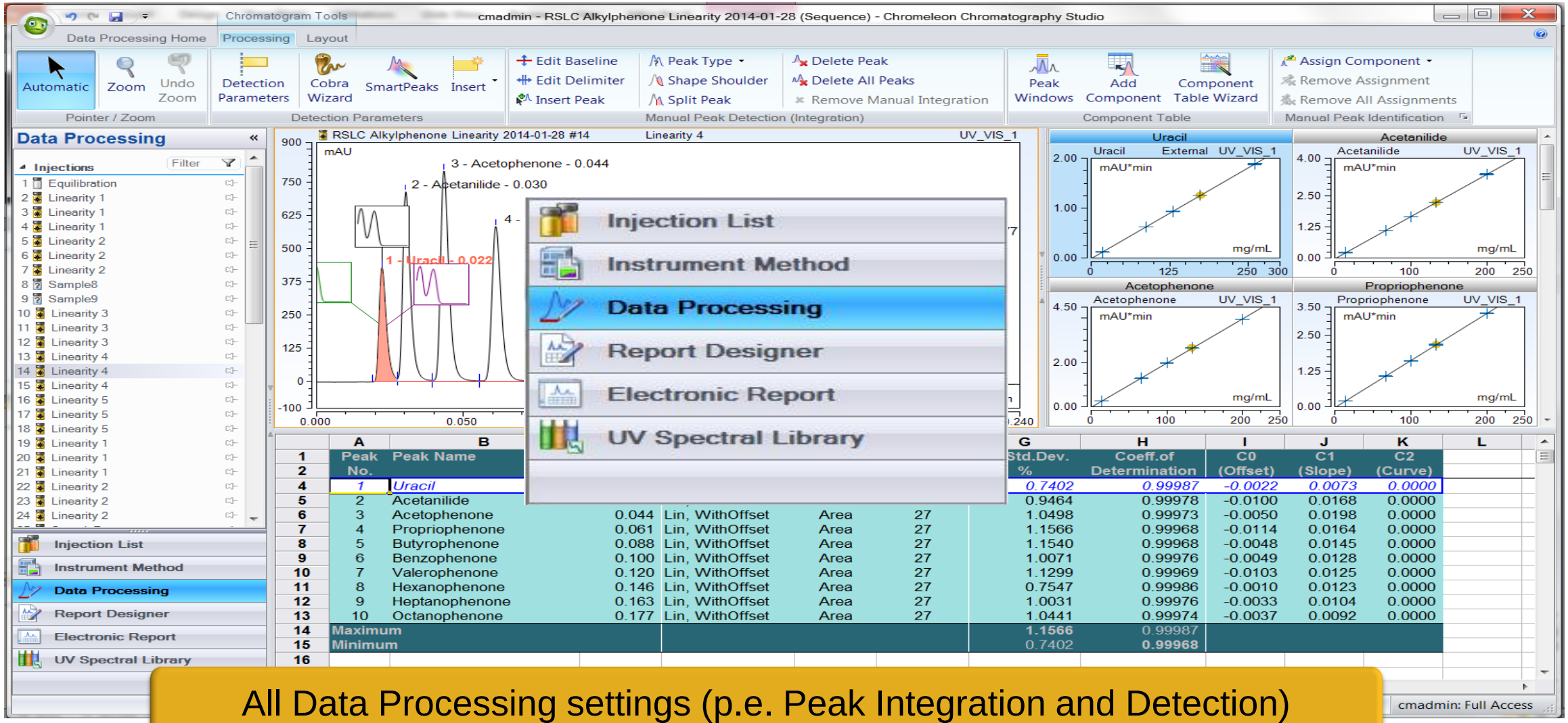
Data Processing and Reporting

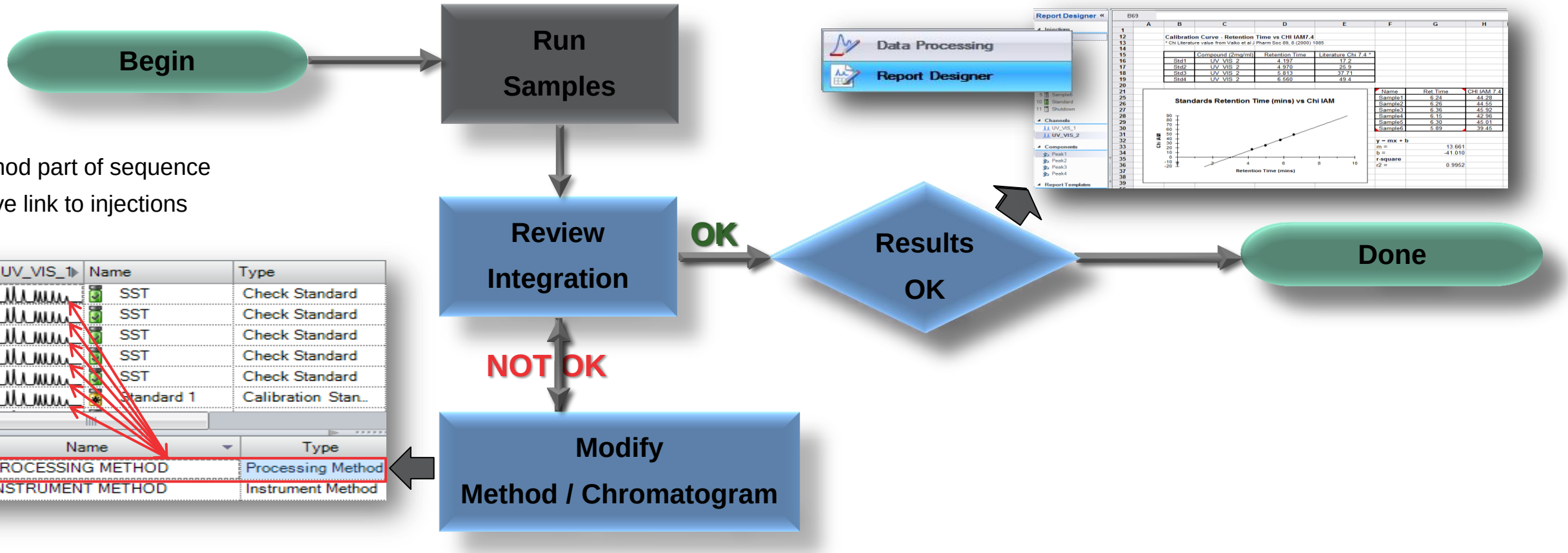
COBRA™ Detection Algorithm / SmartPeaks™

Category Bar – Data Processing



All Data Processing settings (p.e. Peak Integration and Detection)

Chromeleon CDS Data Processing



- Method part of sequence
- Active link to injections

Operational Efficiency

- 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

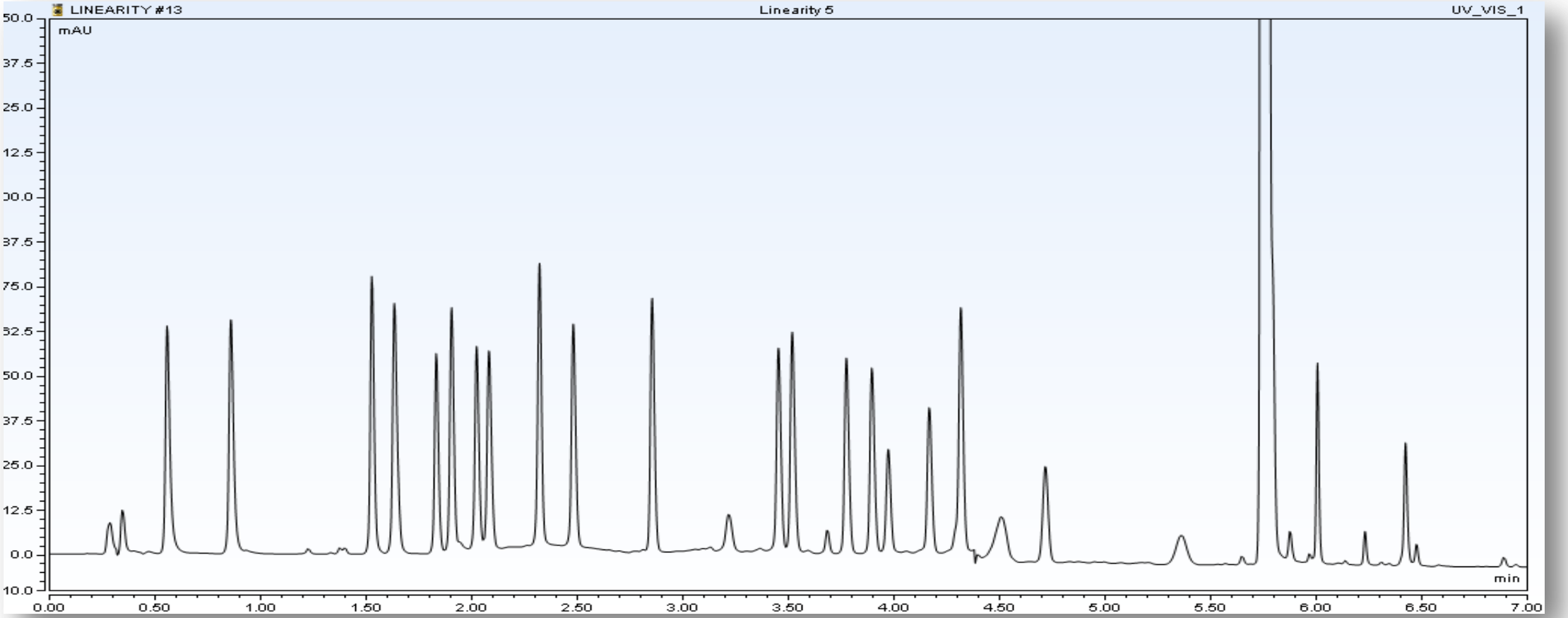
Peak Detection

- Most time consuming and tedious task in chromatography process:

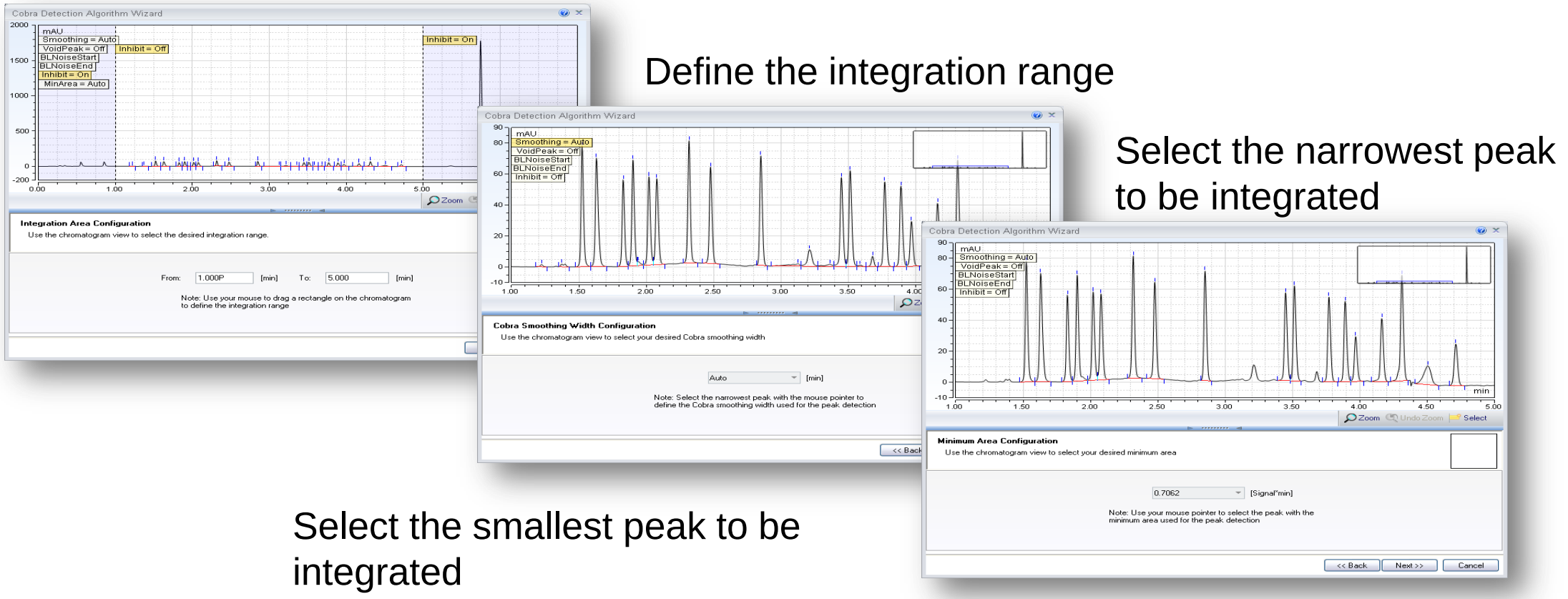
  Chromatogram Integration

- Chromeleon 7 introduces two new tools to extremely simplify this process:
  - Cobra Peak Detection Algorithm / Wizard
  - SmartPeaks Integration Assistant

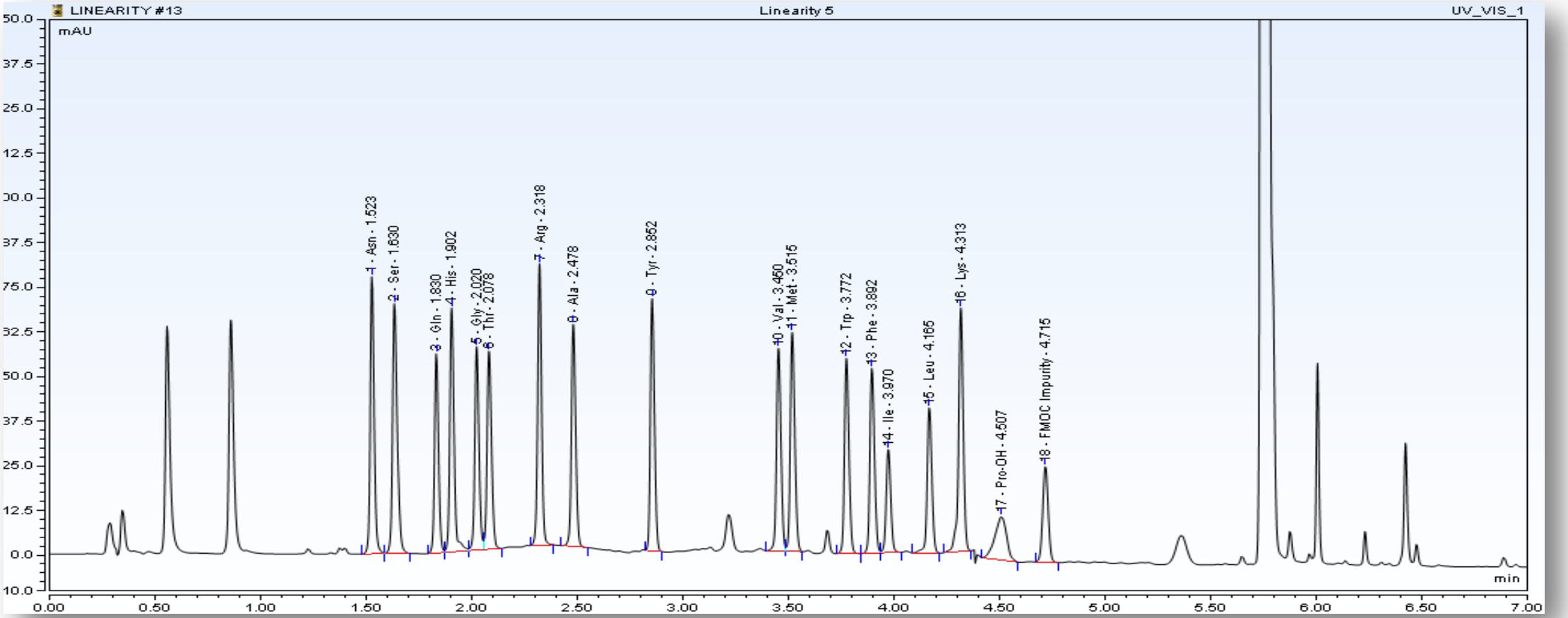
Peak Detection – Cobra Wizard



Start Cobra Wizard

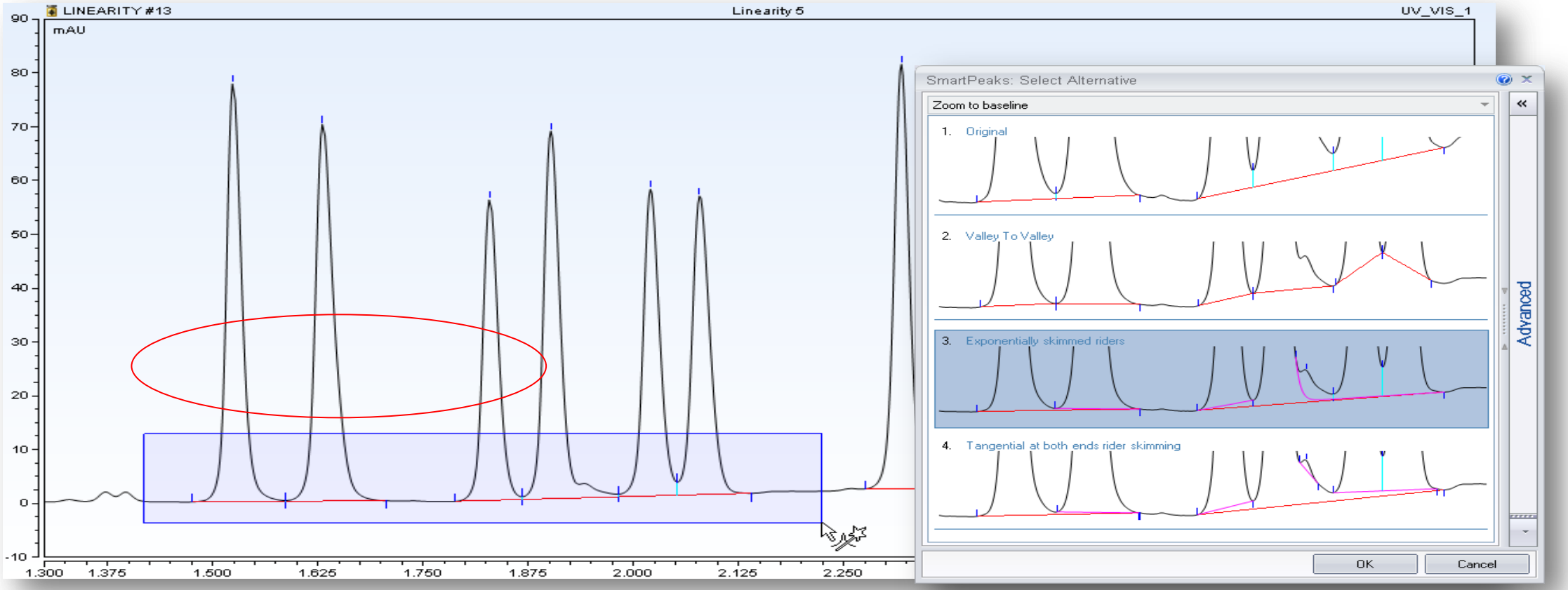


Peak Detection – Cobra Wizard



And your integration is done!

Activate SmartPeaks Wizard



Select the integration you want

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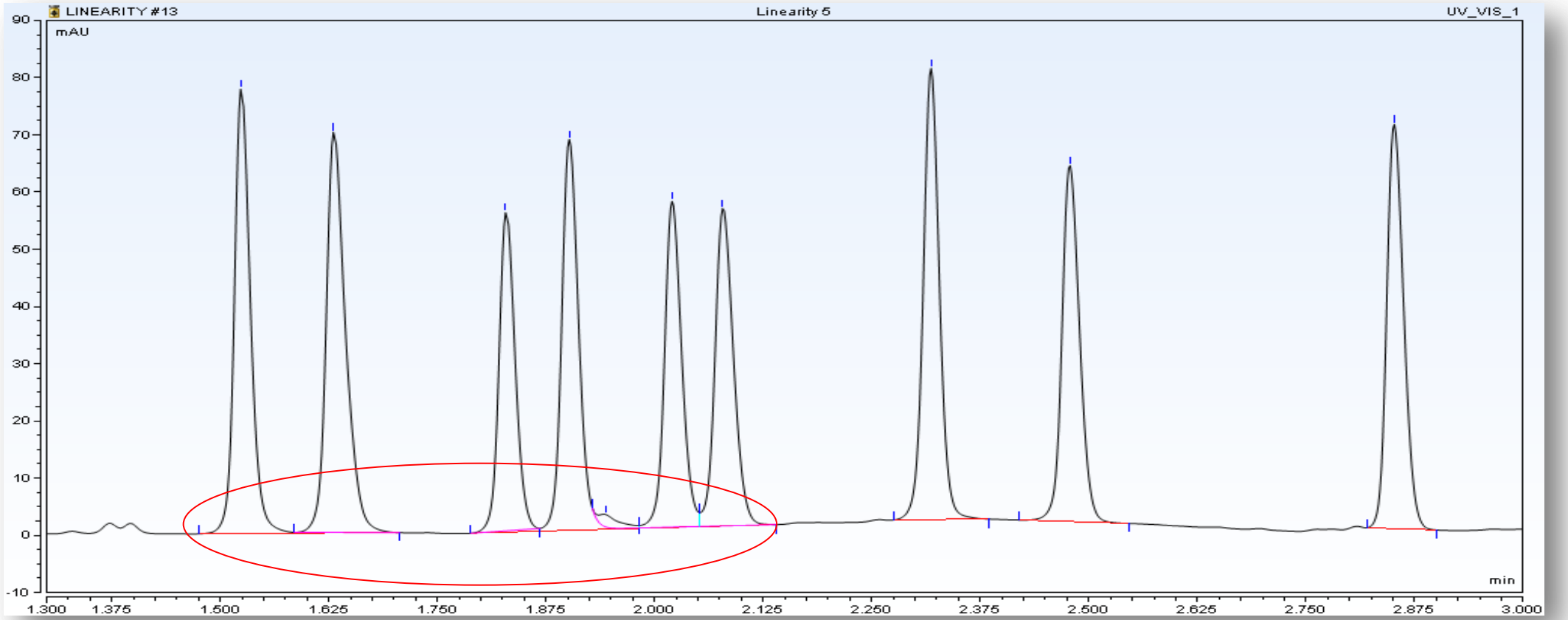
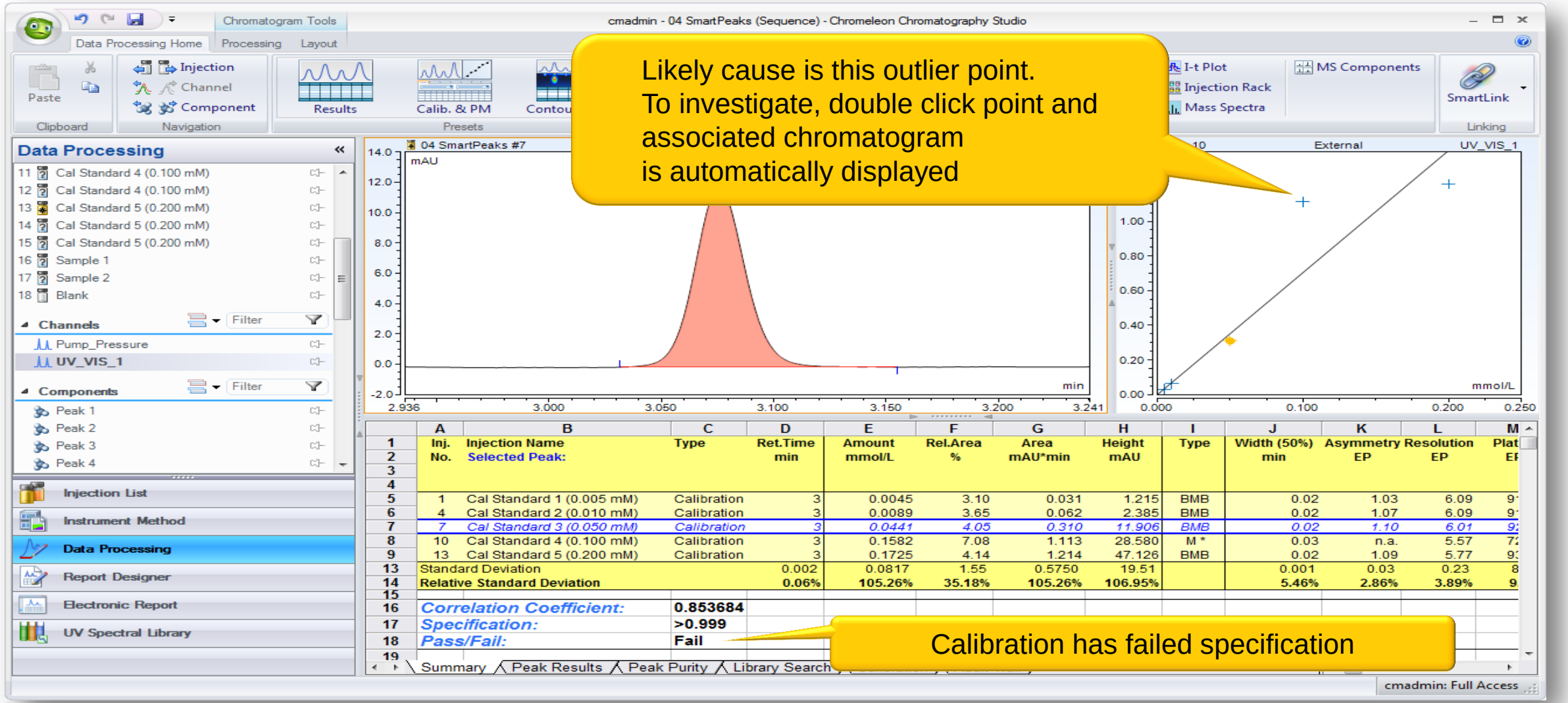
Peak Detection – SmartPeaks



And your integration is done!

Data Dynamic Linking and Updating - 1



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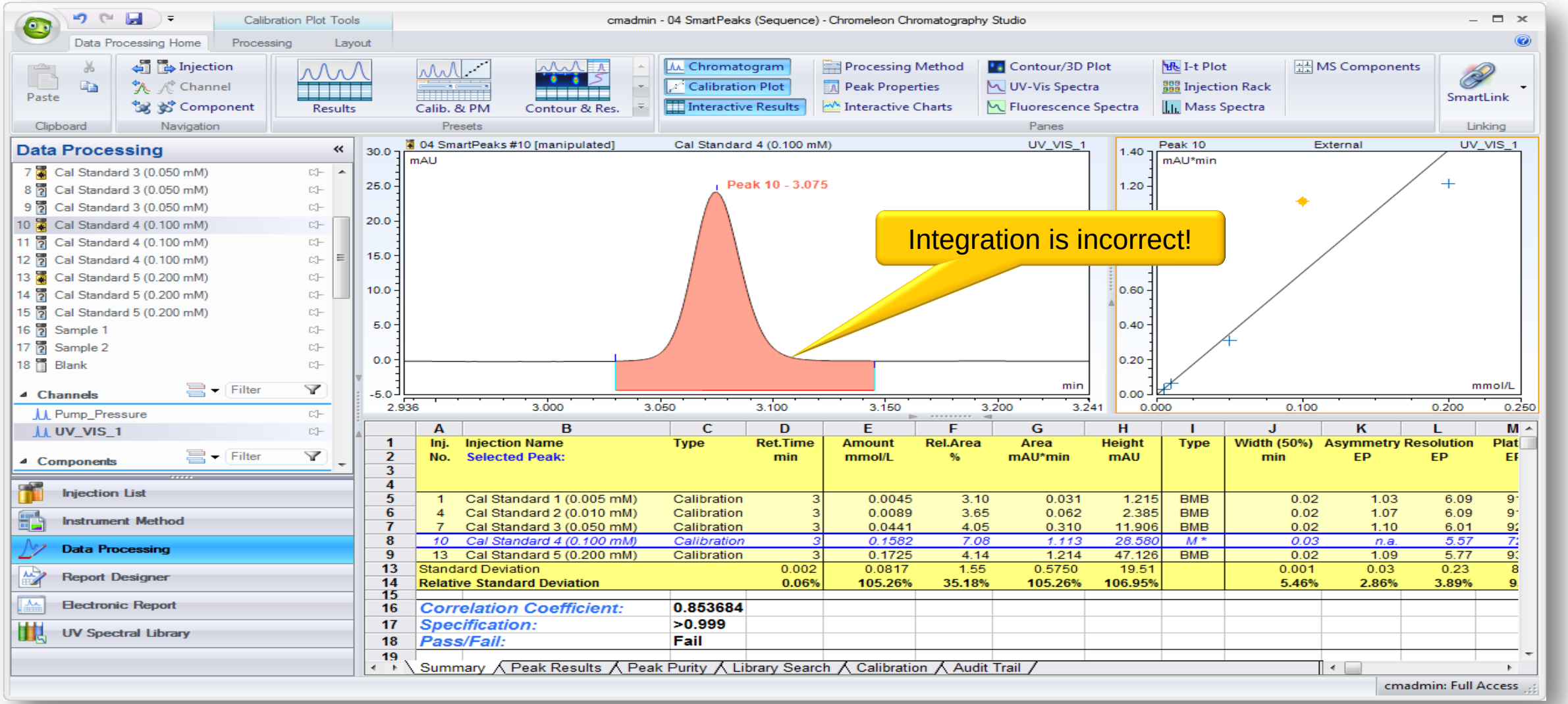
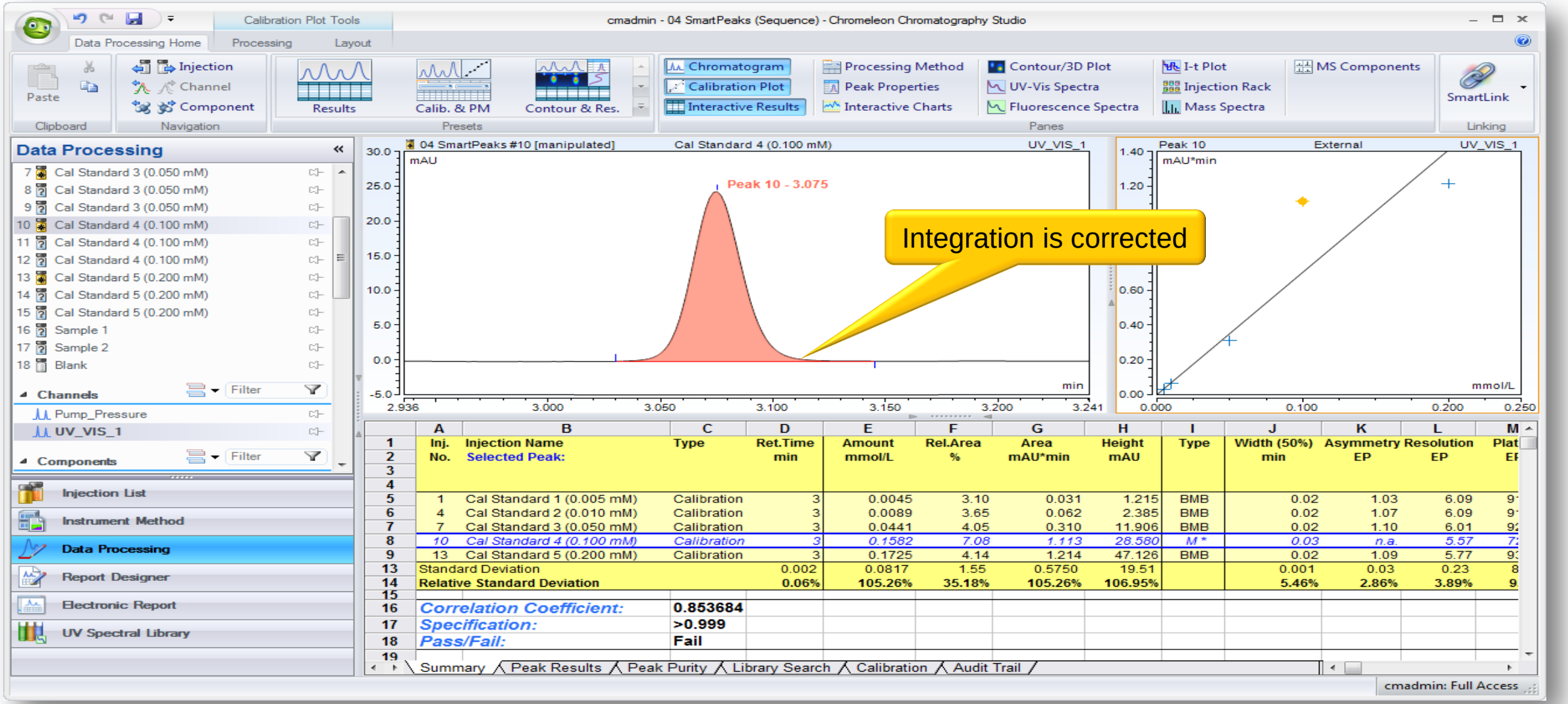
Data Dynamic Linking and Updating - 2

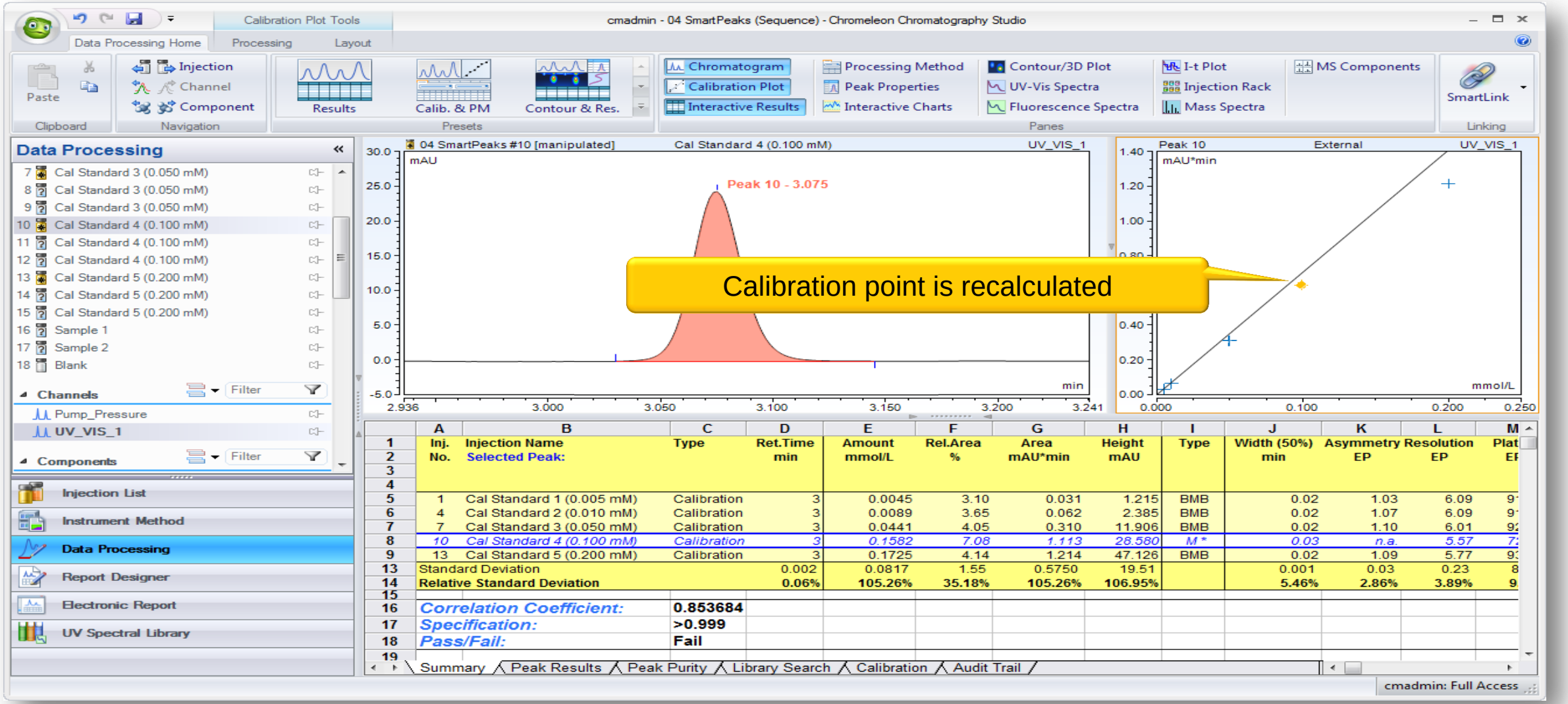


	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Inj.	Injection Name	Type	Ret.Time	Amount	Rel.Area	Area	Height	Type	Width (50%)	Asymmetry	Resolution	Plat
2	No.	Selected Peak:		min	mmol/L	%	mAU*min	mAU		min	EP	EP	EP
3													
4													
5	1	Cal Standard 1 (0.005 mM)	Calibration	3	0.0045	3.10	0.031	1.215	BMB	0.02	1.03	6.09	9
6	4	Cal Standard 2 (0.010 mM)	Calibration	3	0.0089	3.65	0.062	2.385	BMB	0.02	1.07	6.09	9
7	7	Cal Standard 3 (0.050 mM)	Calibration	3	0.0441	4.05	0.310	11.906	BMB	0.02	1.10	6.01	9
8	*10*	*Cal Standard 4 (0.100 mM)*	*Calibration*	*3*	*0.1582*	*7.08*	*1.113*	*28.580*	*M **	*0.03*	*n.a.*	*5.57*	*7*
9	13	Cal Standard 5 (0.200 mM)	Calibration	3	0.1725	4.14	1.214	47.126	BMB	0.02	1.09	5.77	9
13	Standard Deviation			0.002	0.0817	1.55	0.5750	19.51		0.001	0.03	0.23	8
14	**Relative Standard Deviation**			**0.06%**	**105.26%**	**35.18%**	**105.26%**	**106.95%**		**5.46%**	**2.86%**	**3.89%**	**9**
15													
16	***Correlation Coefficient:***		**0.853684**										
17	***Specification:***		**>0.999**										
18	***Pass/Fail:***		**Fail**										
19													

Data Dynamic Linking and Updating - 3

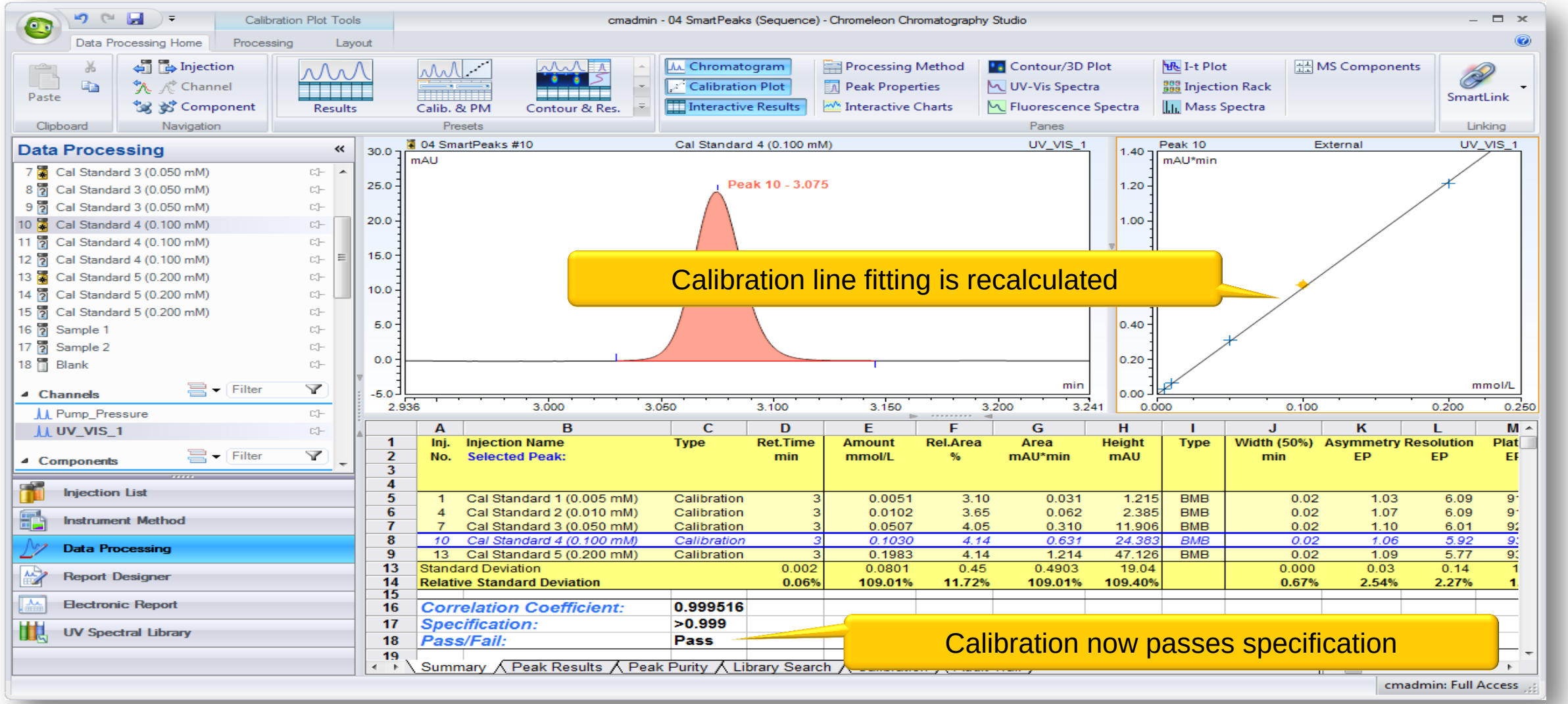


Data Dynamic Linking and Updating - 4



	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Inj.	Injection Name	Type	Ret.Time	Amount	Rel.Area	Area	Height	Type	Width (50%)	Asymmetry	Resolution	Plat
2	No.	Selected Peak:		min	mmol/L	%	mAU*min	mAU		min	EP	EP	EP
3													
4													
5	1	Cal Standard 1 (0.005 mM)	Calibration	3	0.0045	3.10	0.031	1.215	BMB	0.02	1.03	6.09	9
6	4	Cal Standard 2 (0.010 mM)	Calibration	3	0.0089	3.65	0.062	2.385	BMB	0.02	1.07	6.09	9
7	7	Cal Standard 3 (0.050 mM)	Calibration	3	0.0441	4.05	0.310	11.906	BMB	0.02	1.10	6.01	9
8	*10*	*Cal Standard 4 (0.100 mM)*	*Calibration*	*3*	*0.1582*	*7.08*	*1.113*	*28.580*	*M**	*0.03*	*n.a.*	*5.57*	*7*
9	13	Cal Standard 5 (0.200 mM)	Calibration	3	0.1725	4.14	1.214	47.126	BMB	0.02	1.09	5.77	9
13	Standard Deviation			0.002	0.0817	1.55	0.5750	19.51		0.001	0.03	0.23	8
14	**Relative Standard Deviation**			**0.06%**	**105.26%**	**35.18%**	**105.26%**	**106.95%**		**5.46%**	**2.86%**	**3.89%**	**9**
15													
16	***Correlation Coefficient:***		**0.853684**										
17	***Specification:***		**>0.999**										
18	***Pass/Fail:***		**Fail**										
19													

Data Dynamic Linking and Updating - 5



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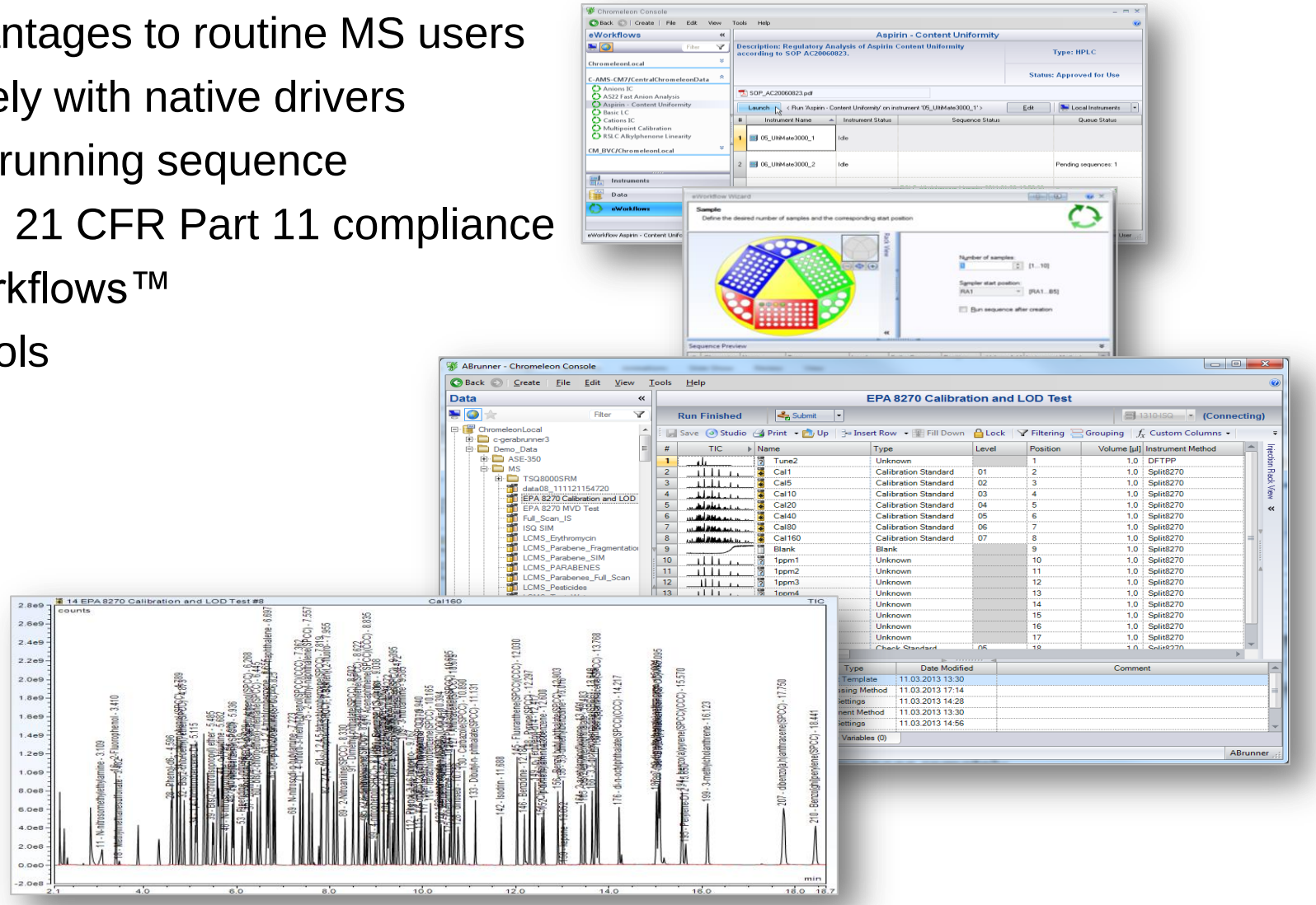
- How can you include MS in your laboratory CDS?
- Chromeleon™ 7.2 Chromatography Data System supports MS instrument control and data processing with all main front-end separation techniques (GC, LC, IC) in an enterprise environment

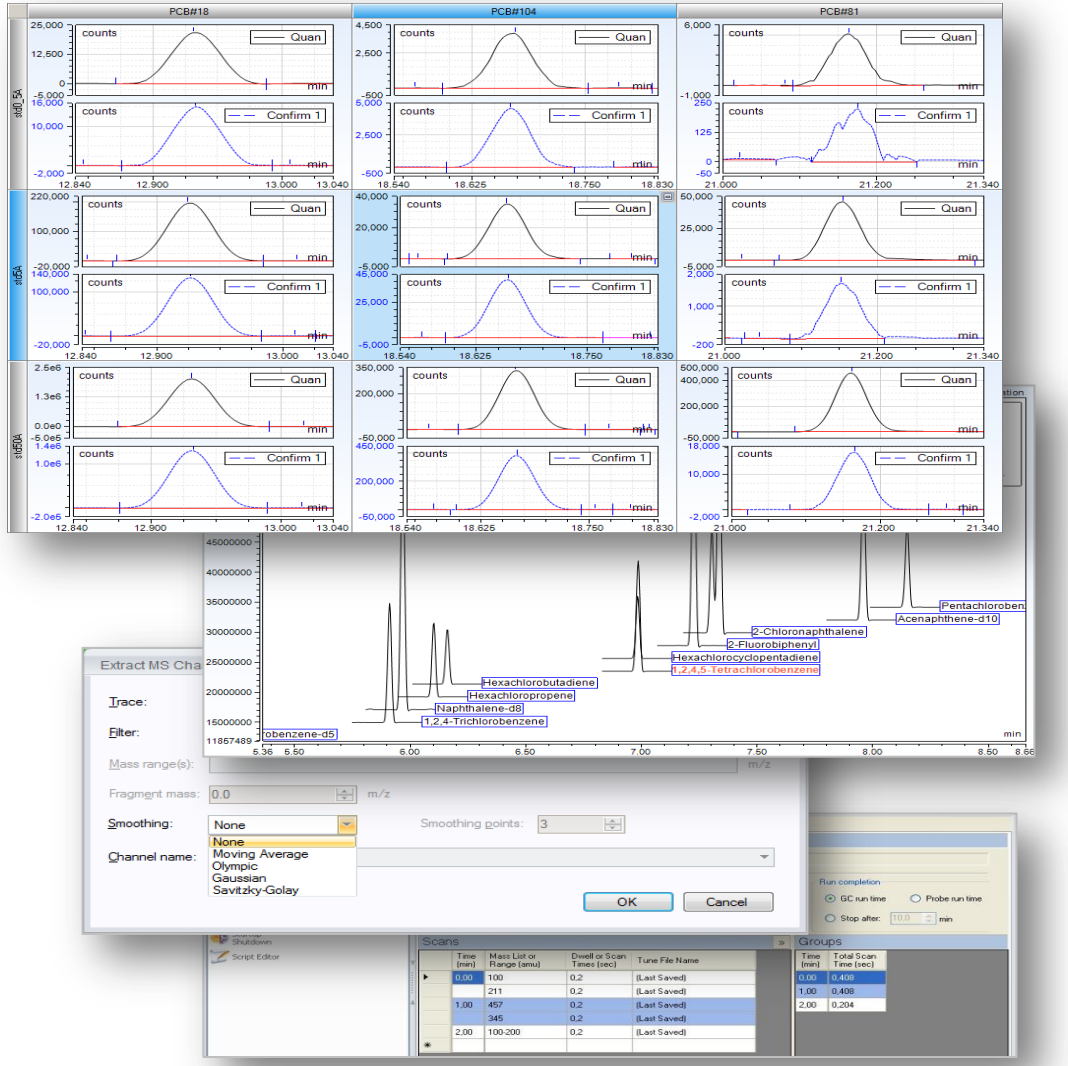
MS is Fully Integrated within Chromeleon CDS

- Extends Chromeleon CDS advantages to routine MS users
  - Control and monitor MS remotely with native drivers
  - View, edit, and manipulate the running sequence
  - Central storage of data with full 21 CFR Part 11 compliance
  - Easily start analyses with eWorkflows™
  - Full suite of data processing tools

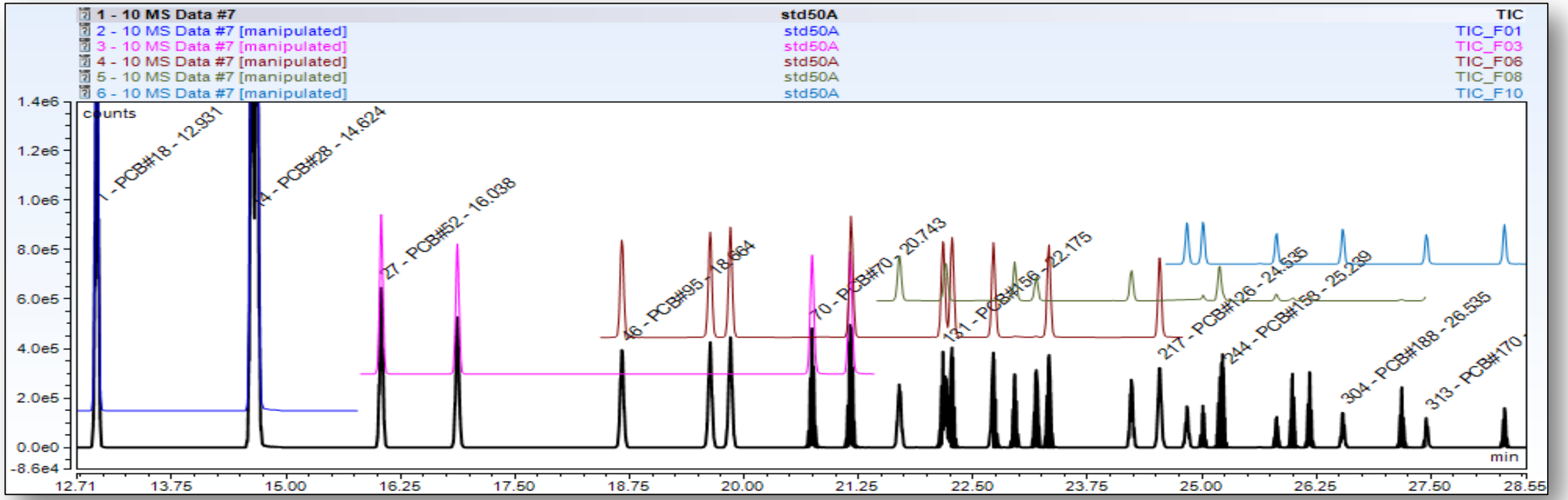


MS is Fully Integrated within Chromeleon CDS

- Chromeleon 7.2 CDS provides:
  - MS-specific data organization at component level
  - Visualization of (large-volume) MS data
  - Channel-specific reporting of components
  - NIST format for MS Library searching, creation, and compound data import
- Key benefits:
  - Only need to install, validate and learn one software package
  - Enhanced data security
  - Can use all compliance and processing features of Chromeleon CDS



MS peaks often only appear in certain detection channels (filters) – how do you create a report for your peaks of interest?



Chromeleon CDS Consolidated Report Tables

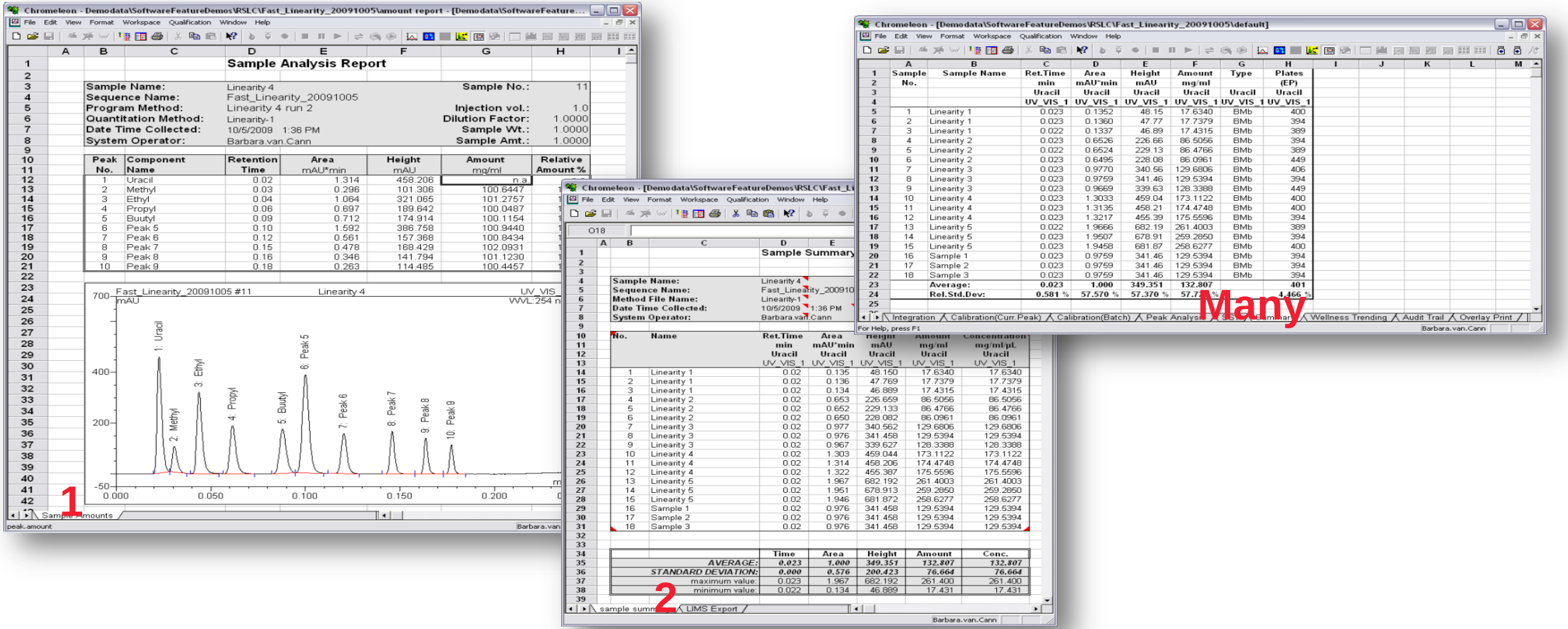
- Automatically report for the Channel with the highest response

No. TIC	Peak Name TIC	Area counts*min Highest Response	Channel Highest Response
3	PCB#18	15392	TIC_F01
10	PCB#28	19480	TIC_F01
11	PCB#33	17945	TIC_F01
25	PCB#52	5455	TIC_F03
34	PCB#95	3640	TIC_F06
50	PCB#70	2364	TIC
79	PCB#156	3650	TIC_F06
145	PCB#126	2757	TIC_F06
179	PCB#153	4781	TIC_F07
219	PCB#188	1100	TIC_F10
225	PCB#170	889	TIC_F10

- Useful for reporting large quantities of MS data in a generic, compact table

Chromeleon CDS Report Templates…

… can have as many worksheets as required



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Chromeleon CDS Report Templates…

… can include result tables

Peak No.	Component Name	Retention Time	Area mAU*min	Height mAU	Amount mg/ml	Relative Amount %
1	Uracil	0.02	1.303	459.044	n.a.	n.a.
2	Methyl	0.03	0.289	100.10	10.90	
3	Ethyl	0.04	1.057	318.78	11.16	
4	Propyl	0.06	0.693	187.379	99.4445	11.03
5	Buutyl	0.09	0.705	173.300	99.0898	10.99
6	Peak 5					
7	Peak 6					
8	Peak 7					
9	Peak 8					
10	Peak 9					

Peak Tables

No.	Name	Ret.Time min Benzophenone UV_VIS_1	Area mAU*min Benzophenone UV_VIS_1	Height mAU Benzophenone UV_VIS_1	Amou mg/ Benzoph UV_VI	
1	Linearity 1	0.10	0.161	40.625	13.581	
2	Linearity 1	0.10	0.161	40.073	13.630	
3	Linearity 1	0.10	0.162	39.759	13.675	
4	Linearity 2	0.10	0.776	191.967	65.613	
5	Linearity 2	0.10	0.779	192.297	65.907	
6	Linearity 2	0.10	0.784	192.225	66.317	
7	Linearity 3	0.10	1.182	289.564	99.965	
8	Linearity 3	0.10	1.186	289.292	100.29	
9	Linearity 3	0.10	1.179	285.307	99.706	
10	Linearity 4	0.10	1.587	382.335	134.13	
11	Linearity 4	0.10	1.592	386.758	134.58	
12	Linearity 4	0.10	1.572	381.628	132.90	
13	Linearity 5	0.10	2.361	566.797	199.6193	199.6193
14	Linearity 5	0.10	2.359	563.997	199.4263	199.4263
15	Linearity 5	0.10	2.373	567.937	200.5406	200.5406
16	Sample 1	0.10	1.186	289.292	100.2906	100.2906
17	Sample 2	0.10	1.186	289.292	100.2906	100.2906
18	Sample 3	0.10	1.186	289.292	100.2906	100.2906

Summary Tables

10	Linearity 4		Audit Trail	
Sample Name:	**Linearity 4**		*Injection Volume:*	**1.0**
Vial Number:	**RB2**		*Channel:*	**UV_VIS_1**
Sample Type:	**standard**		*Wavelength:*	**254.0**
Control Program:	**Linearity 4 run 1**		*Bandwidth:*	**1**
Quantif. Method:	**Linearity-1**		*Dilution Factor:*	**1.0000**
Recording Time:	**10/5/2009 13:35**		*Sample Weight:*	**1.0000**
Run Time (min):	**0.24**		*Sample Amount:*	**1.0000**

Day Time	Ret.Time	Command/Message
13:35:29		Audit trail of sample SMP::\Demodata\SoftwareFeatureDemos\RSLC\Fast_Linearity
13:35:29		Start of sample 10 "Linearity 4", using program "Linearity 4 run 1".
13:35:29	0.000	ColumnOven.Temperature.Nominal = 100.0
13:35:29	0.000	Cooler_Temperature.Nominal = 20.0
13:35:29	0.000	Pressure.LowerLimit = 0
13:35:29	0.000	Pressure.UpperLimit = 800
13:35:29	0.000	%A.Equate = "%A"
13:35:29	0.000	%B.Equate = "%B"
13:35:29	0.000	Data_Collection_Rate = 100.0
13:35:29	0.000	ResponseTime = 0.025
13:35:29	0.000	SlitWidth = Narrow
13:35:29	0.000	UV_VIS_1.Wavelength = 254.0
13:35:29	0.000	UV_VIS_1.Bandwidth = 1
13:35:29	0.000	UV_VIS_1.RefWavelength = 225.0
13:35:29	0.000	UV_VIS_1.RefBandwidth = 1
13:35:29	0.000	3DFIELD.RefWavelength = 800.0
13:35:29	0.000	3DFIELD.RefBandwidth = 1
13:35:29	0.000	Data_Collection_Rate = 100.0
13:35:29	0.000	ResponseTime = 0.025
13:35:29	0.000	SlitWidth = Narrow
13:35:29	0.000	UV_VIS_1.Wavelength = 254.0
13:35:29	0.000	UV_VIS_1.Bandwidth = 1
13:35:29	0.000	UV_VIS_1.RefWavelength = 225.0
13:35:29	0.000	UV_VIS_1.RefBandwidth = 1
13:35:29	0.000	3DFIELD.RefWavelength = 800.0
13:35:29	0.000	3DFIELD.RefBandwidth =
13:35:29	0.000	3DFIELD.MinWavelength = 190.0
13:35:29	0.000	3DFIELD.MaxWavelength = 800.0
13:35:29	0.000	3DFIELD.BunchWidth = 1
13:35:29	0.000	Autozero
13:35:29	0.000	Flow = 3.700

Audit Trails

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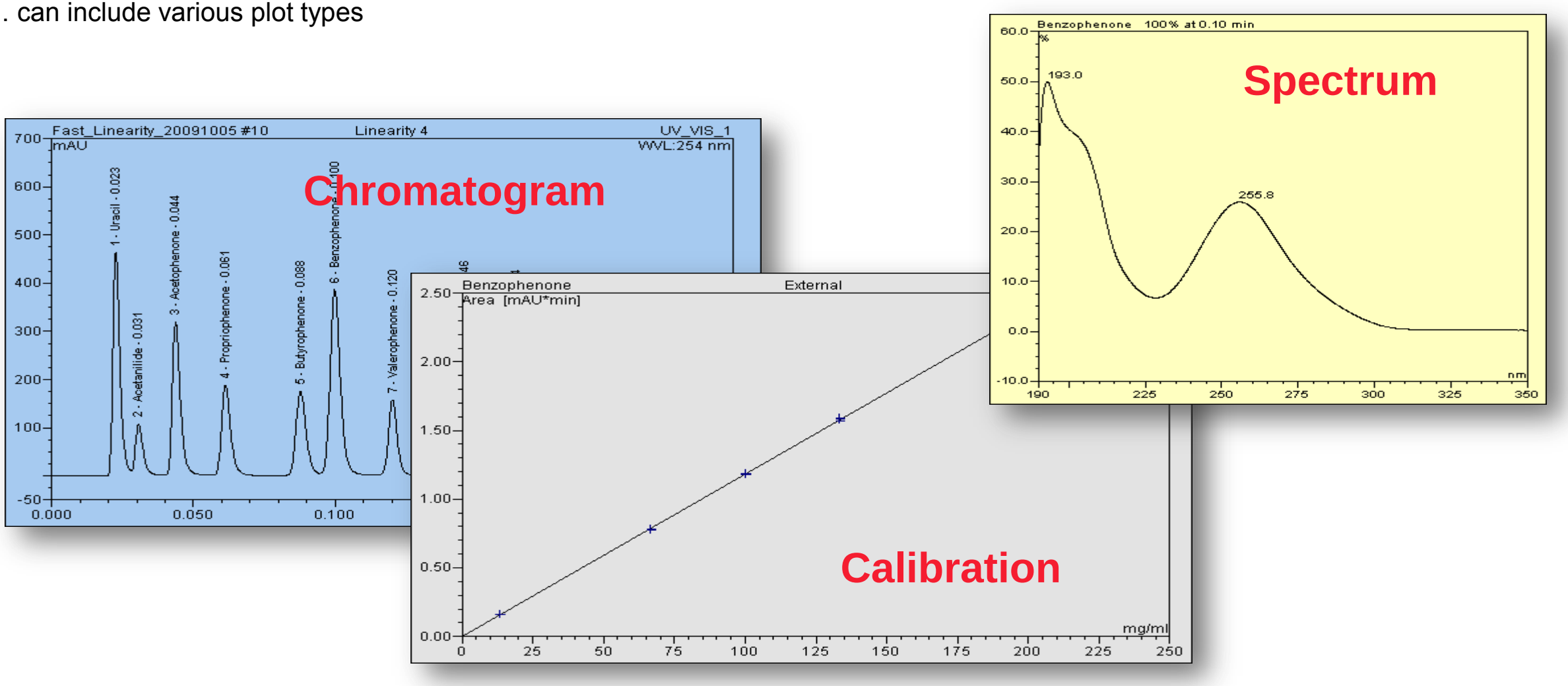
… can include various plot types



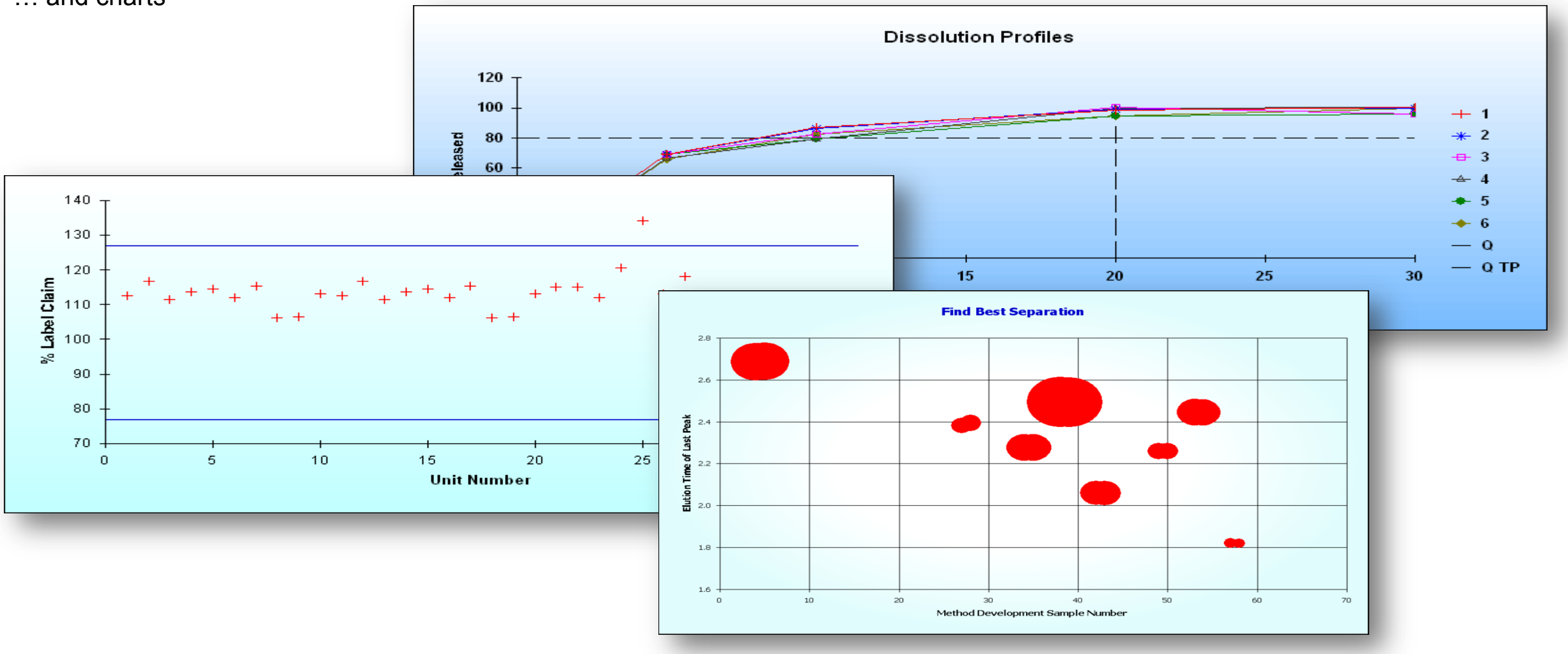
… and can even include custom equations…

	Time	Area	Height	Amount	Conc.
AVERAGE:	*0.023*	*1.000*	*349.351*	*132.807*	*132.807*
STANDARD DEVIATION:	*0.000*	*0.576*	*200.423*	*76.664*	*76.664*
maximum value:	0.023	1.967	682.192	261.400	261.400
minimum value:	0.022	0.134	46.889	17.431	17.431

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)

Chromeleon CDS Report Templates…

… and charts



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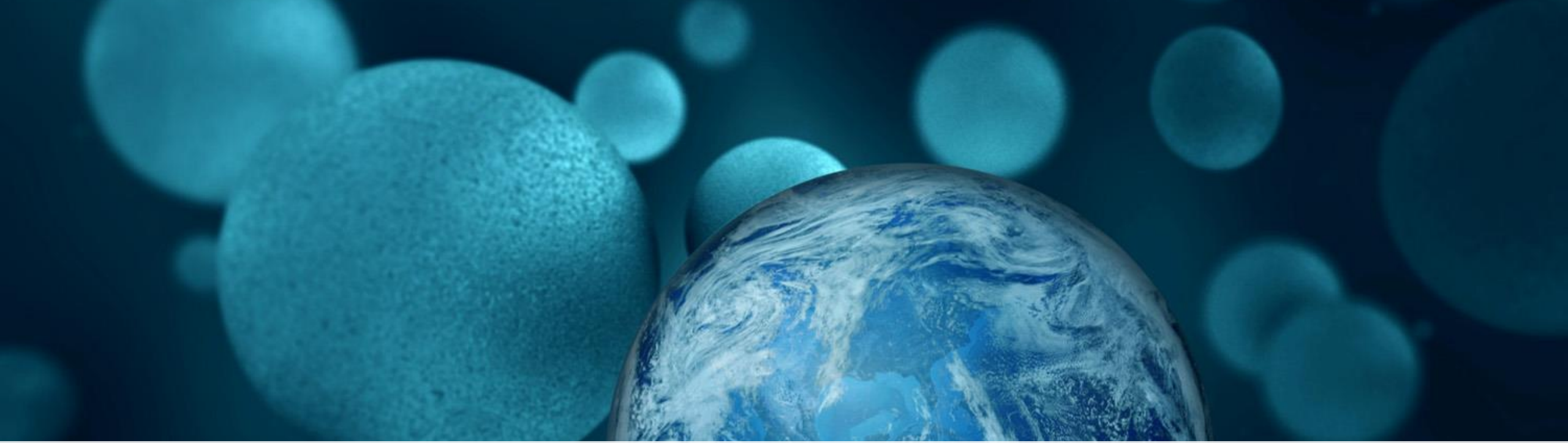

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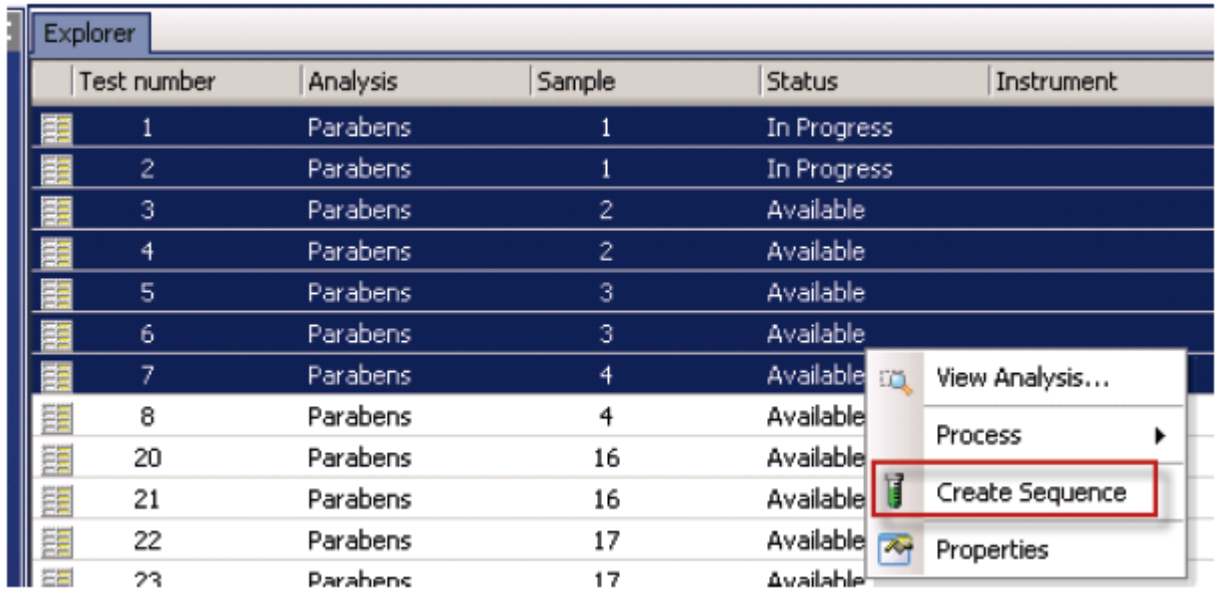
Chromeleon and Samplemanager

Interfacing

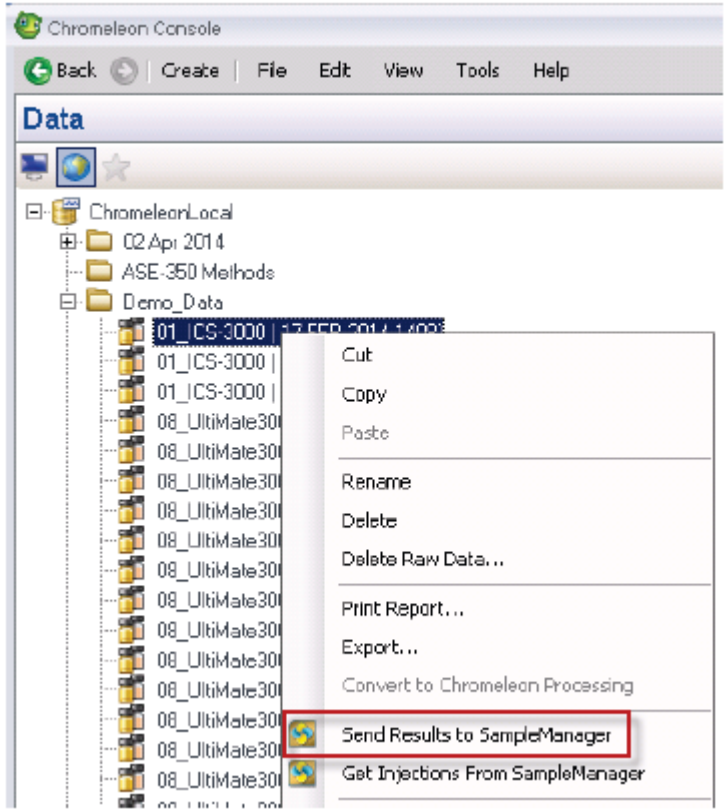
- Create a sequence from SampleManager

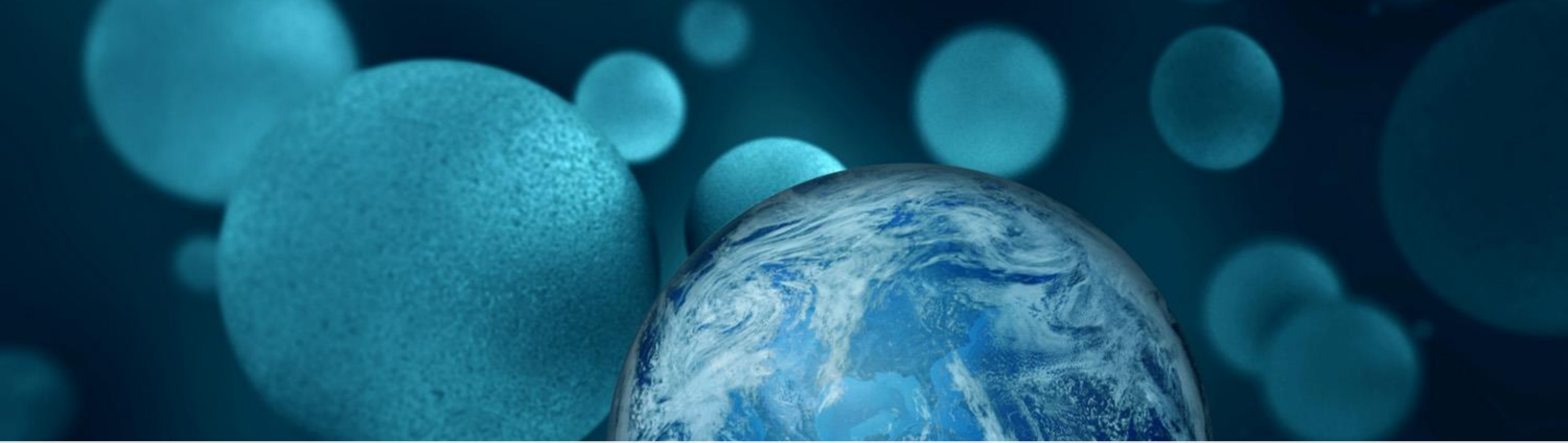
  - Select samples in SampleManager
  - In the context menu Create Sequence



SampleManager LIMS and Dionex Chromeleon CDS Link

- Upload results to SampleManager
  - Results ready in Chromeleon
  - Select sequence
  - Send Results to SampleManager





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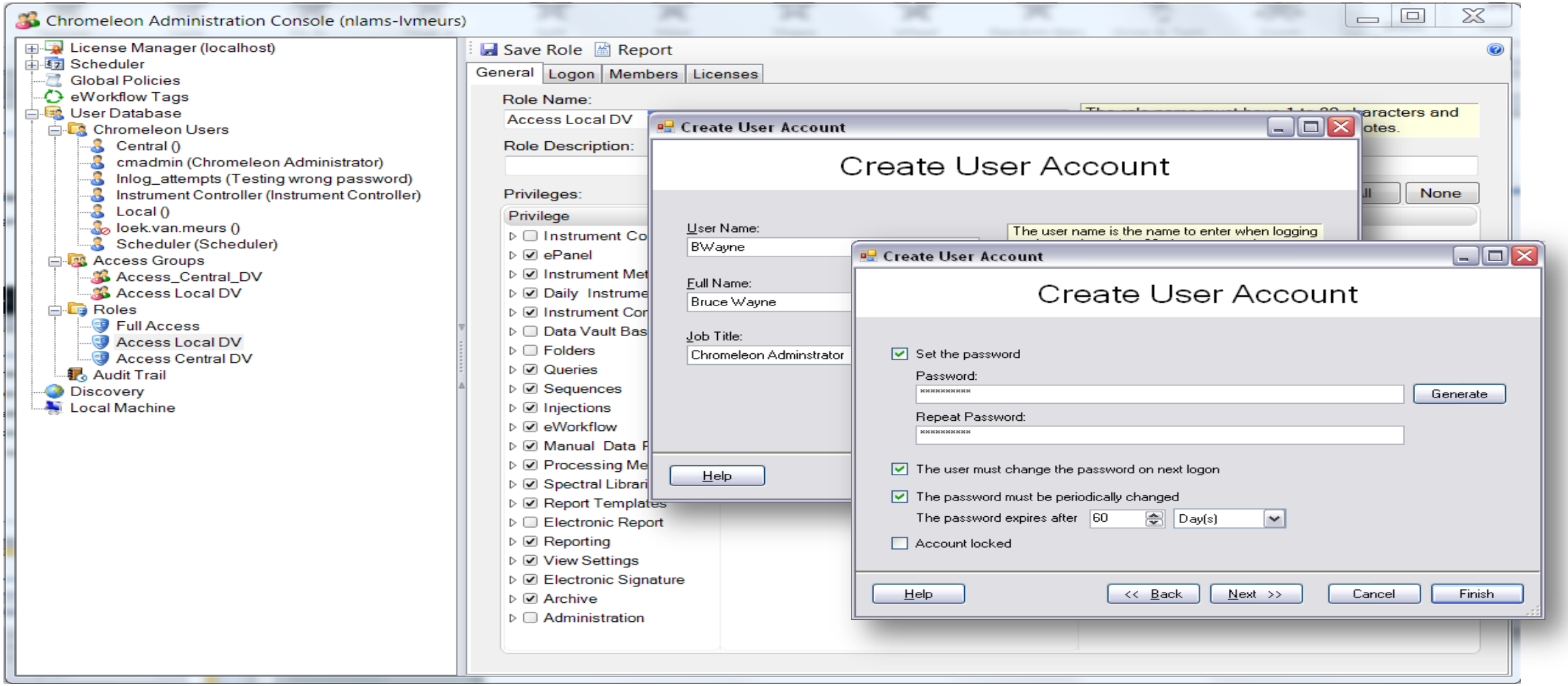
Compliance

User management and Audit Trails

Compliance

- Ensure Compliance in your laboratory using:
  - Comprehensive user management tools
  - Fully automated hardware and software validation
  - Audit Trails to trace all actions done in the software
  - History views of objects to track changes and easily revert to prior versions

User Management



Control what users can access and change

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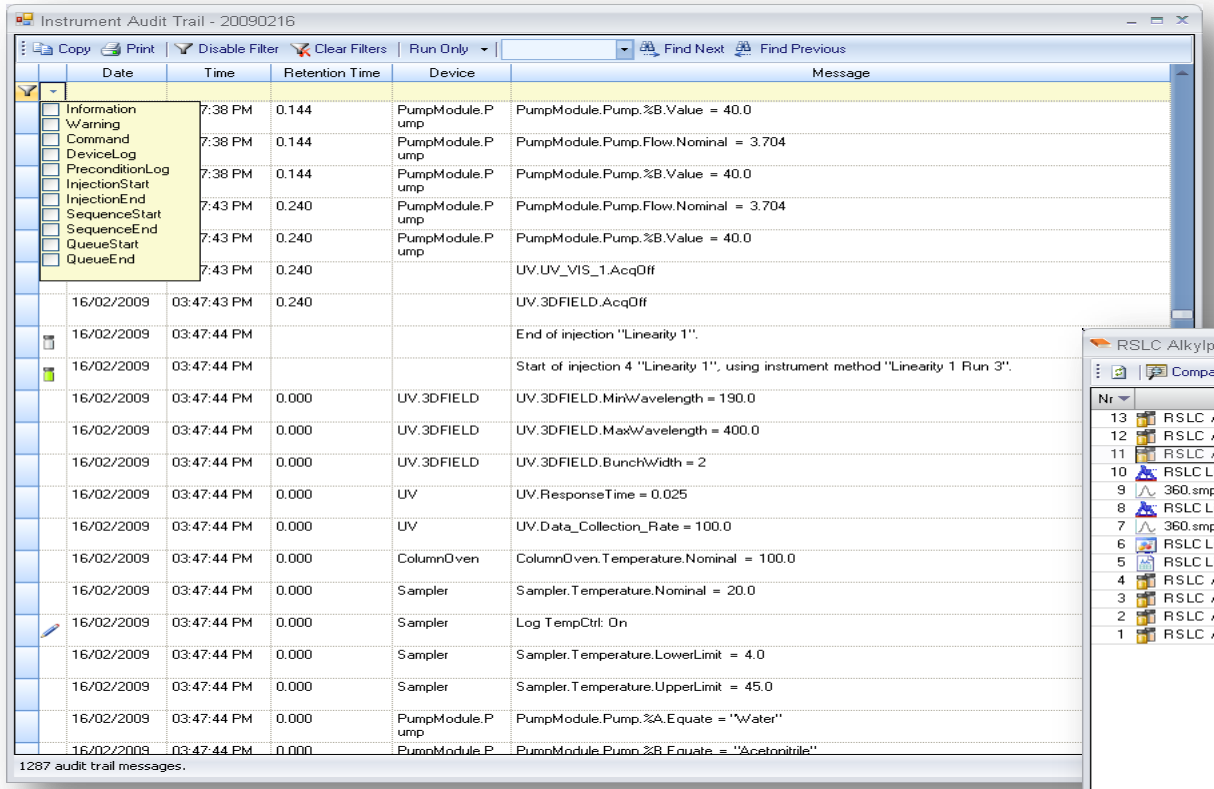
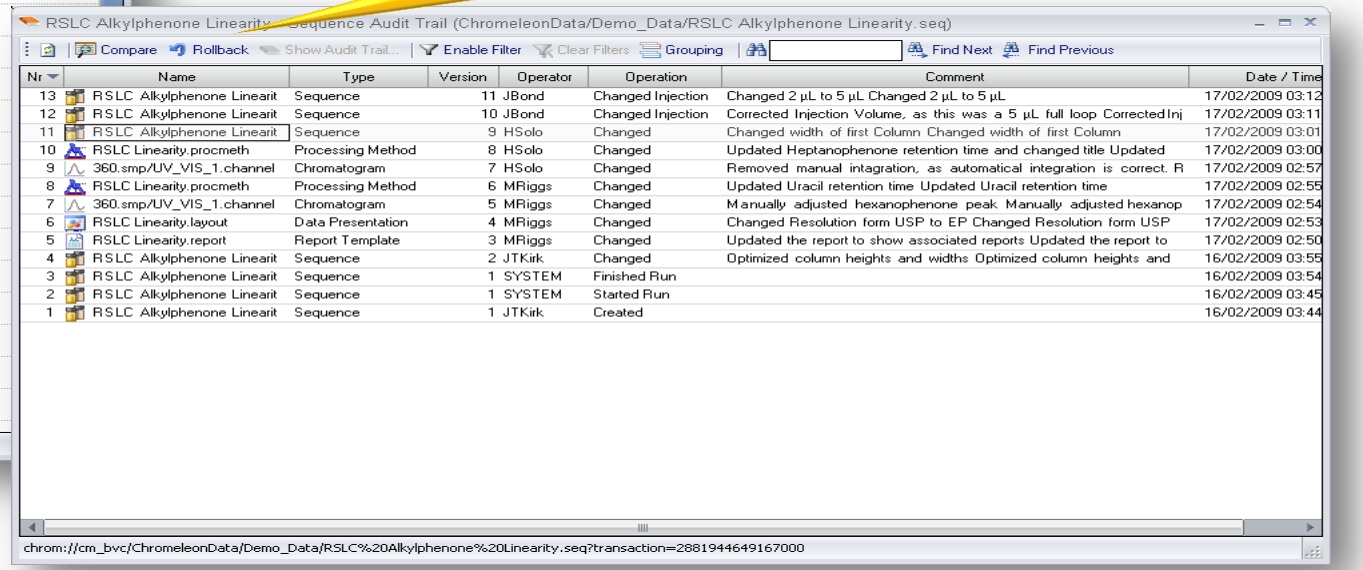
Audit Trails



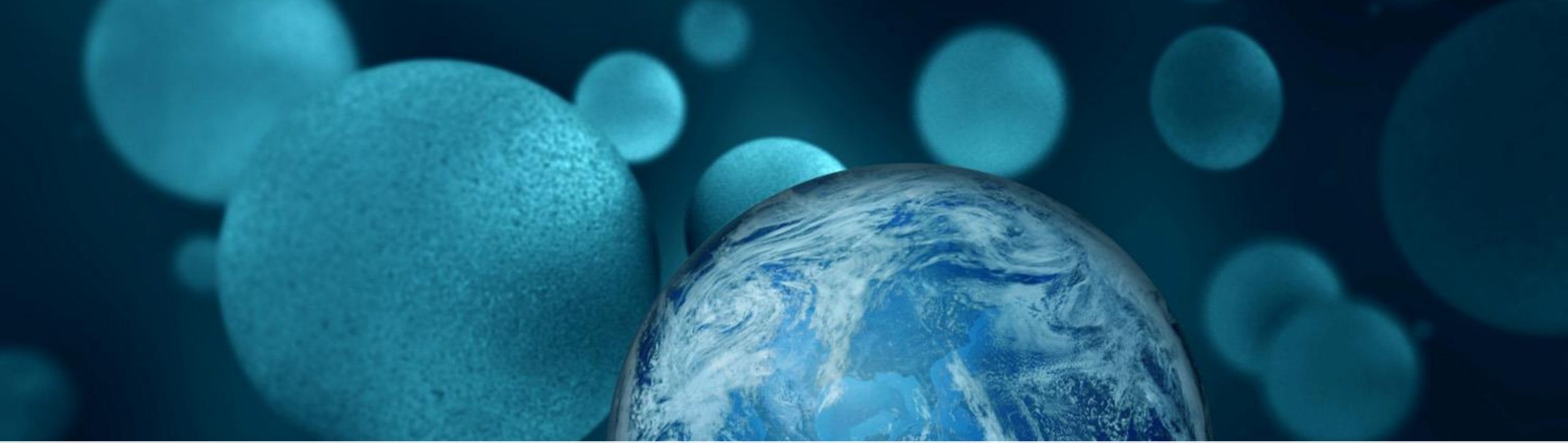
Instrument Audit Trails

Object Audit Trails:
Displays complete change history of object

Restore Previous Version



All Audit Trails can be searched, grouped and filtered



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Summary

- Uses Operational Simplicity™ to minimize the steps and time needed to generate the result!

- Offers state-of-the-art technology:
  - User Interface with “Ribbon”
  - Integration wizards
  - eWorkflows – THE framework for Operational Simplicity
  - MS integration
- Enhanced reporting functionality
- Advanced features to ensure compliance
- All data centralized in a secure environment

All chromatography data centralized in one software

Thank you