

What about the data management

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

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



Chromeleon CDS for your laboratory



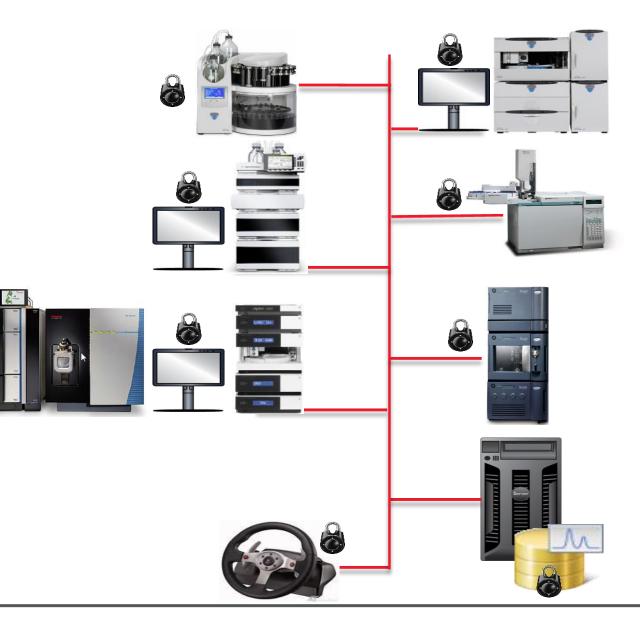


Chromeleon 7 CDS Streamlines Chromatography





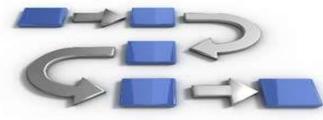
- Networking capabilities
 - Central data storage
 - Choice of database
 - Acquiring data to a central Data Vault
 - Network failure protection
- Multiple Instrument Control
 - Instruments from different vendors
- Centralized Administration
 - License management, license server
- User management
- Security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





- 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

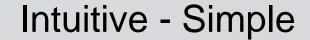








User Interface



The Chromeleon User Interface consists of two major parts:

- Chromeleon Console
- Chromatography Studio



Chromeleon CDS Console





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Proper and reproducible chromatography

Presence / absence of peaks

Quality of separation



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	Power Coolant Water	Unknown		RB4	25.0	n.a.	NA -> Passed	AS12A Anion
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View results without opening sequence data

Immediate SST result check



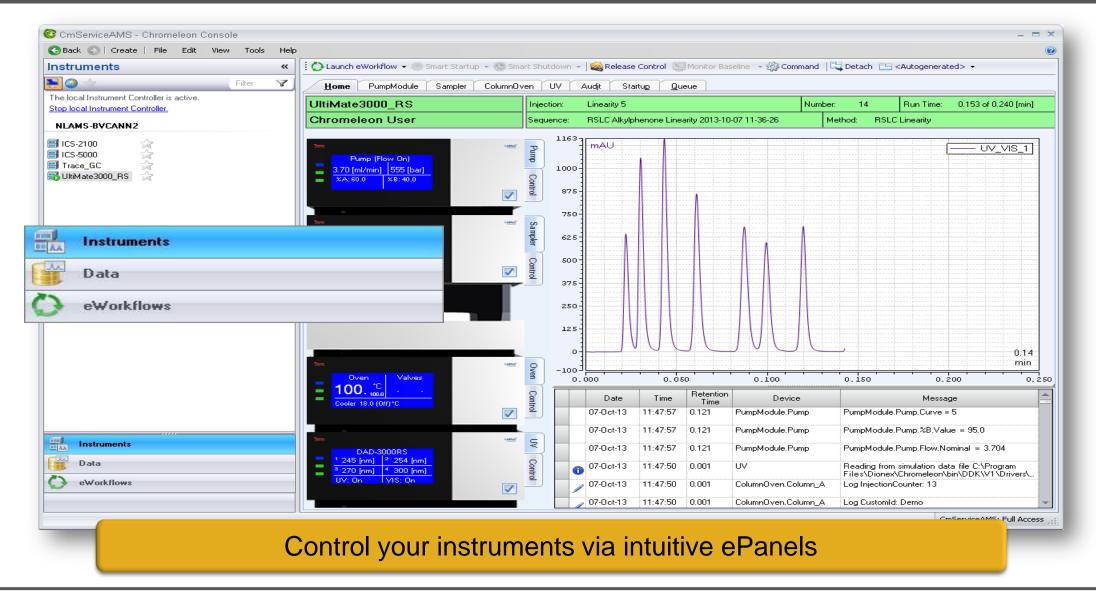
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		Associated Items Custom Sequence Variables (0)													





- Provide immediate access to:
 - Your instruments









• Provide immediate access to:

• Your data



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• Provide immediate access to:

Your eWorkflows



Category Bars – Easy Access

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- Used for All Data Evaluation
- Provides access to every object in the sequence:
 - Injection List

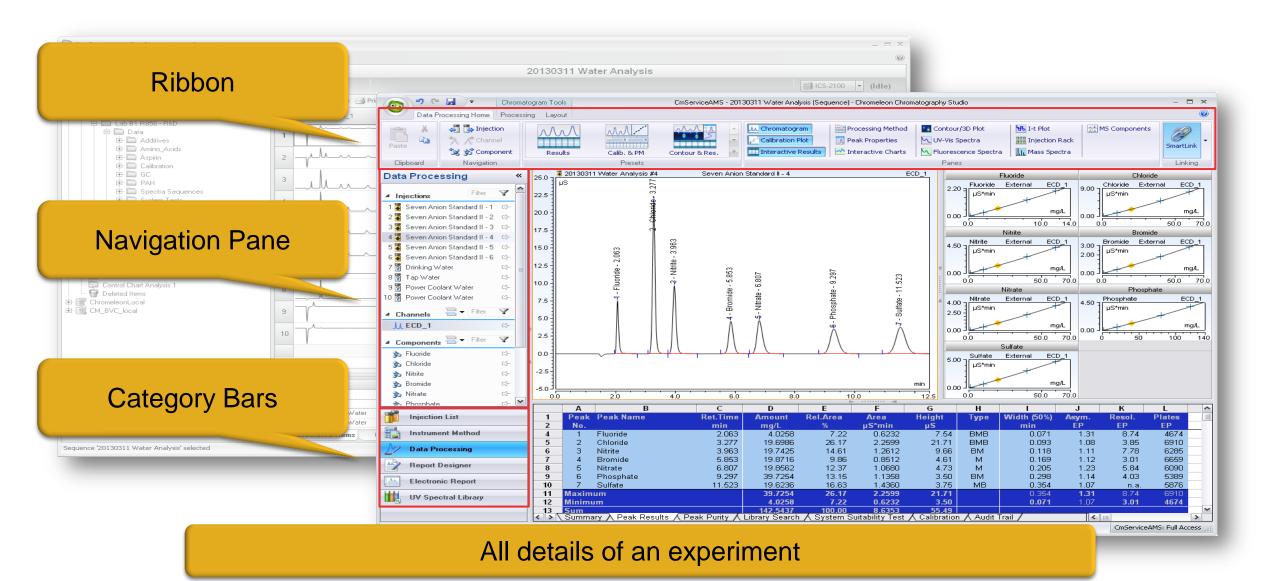
• Results

Report Template

- Instrument Method
- Processing Method

- 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





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eWorkflows[™]

The Ultimate in Operational Simplicity

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eWorkflows
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• 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



Help							JEUL	ノレーフィ		UCAI	zu ai	iu cali b	C			
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Uniformity of Dosage Units Report

General

Product Batch Number86315Peak NameAspirinCUT Number186781ChannelUV_VIS_1Dosage FormCommon Dosage FormsPharmacopeiaEP

Results

Mean Standard Deviation s Reference Value M Acceptance Value AV Test Result Correction Factor Max. Acceptance Value L1 Lower Amount Limit Torms Upper Amount Limit **n = 10** 110.5

110.5 2.5 102.0 14.4 **Test passed**

Target Content T

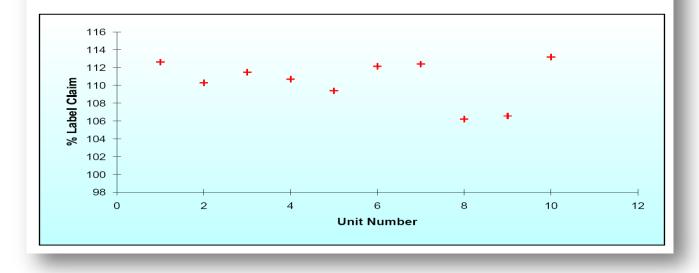
102.0

1.050

Not needed if n=10!

Not needed if n=10!

15.0



• This eWorkflow also:

• Processes all data

Calculates all results



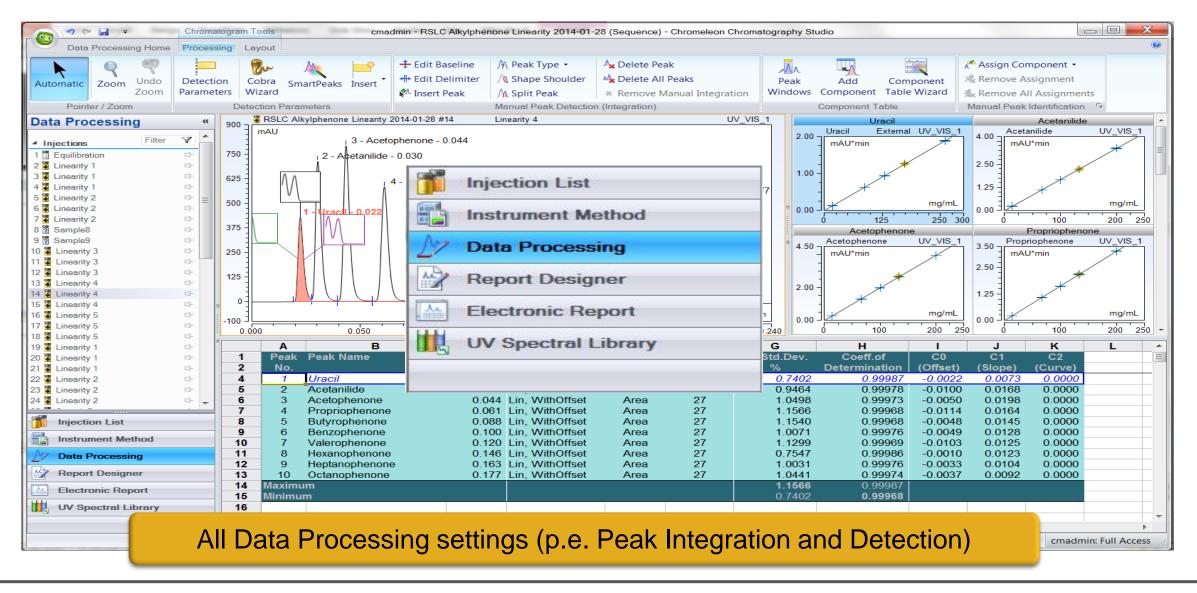
- eWorkflows take you from Sample to Results in the minimum number of steps
- Fully customizable for any application
- Minimum amount of training required
- Reduces errors and produces results faster
- A new framework for Operational Simplicity





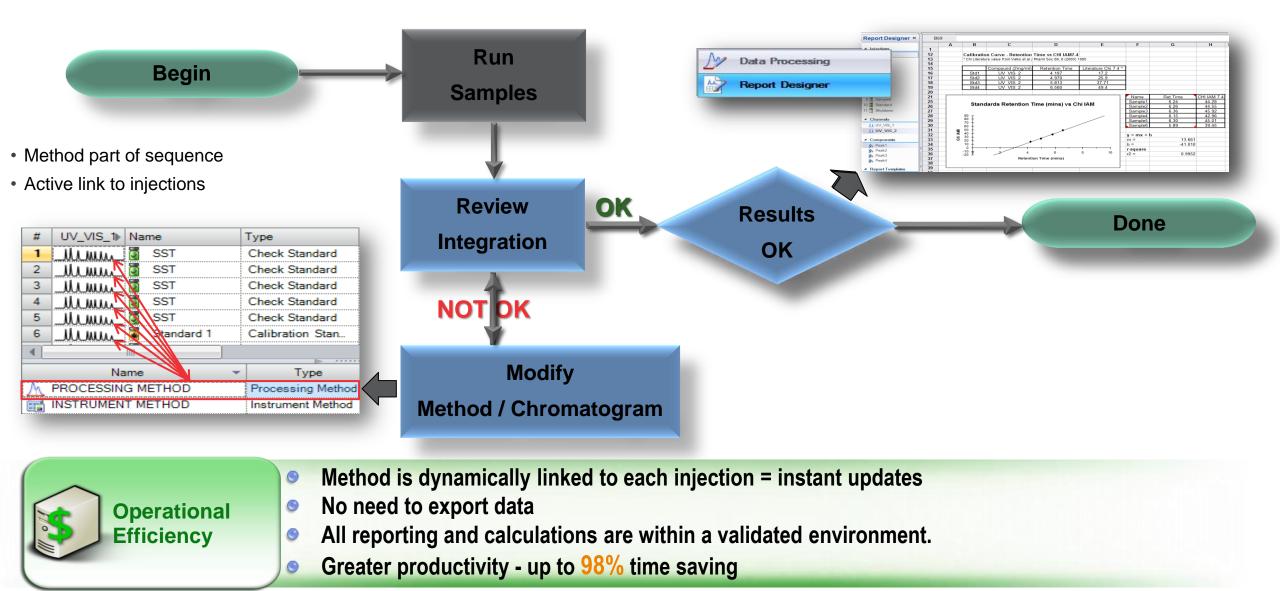
Data Processing and Reporting

COBRA[™] Detection Algorithm / SmartPeaks[™]





Chromeleon CDS Data Processing





Most time consuming and tedious task in chromatography process:

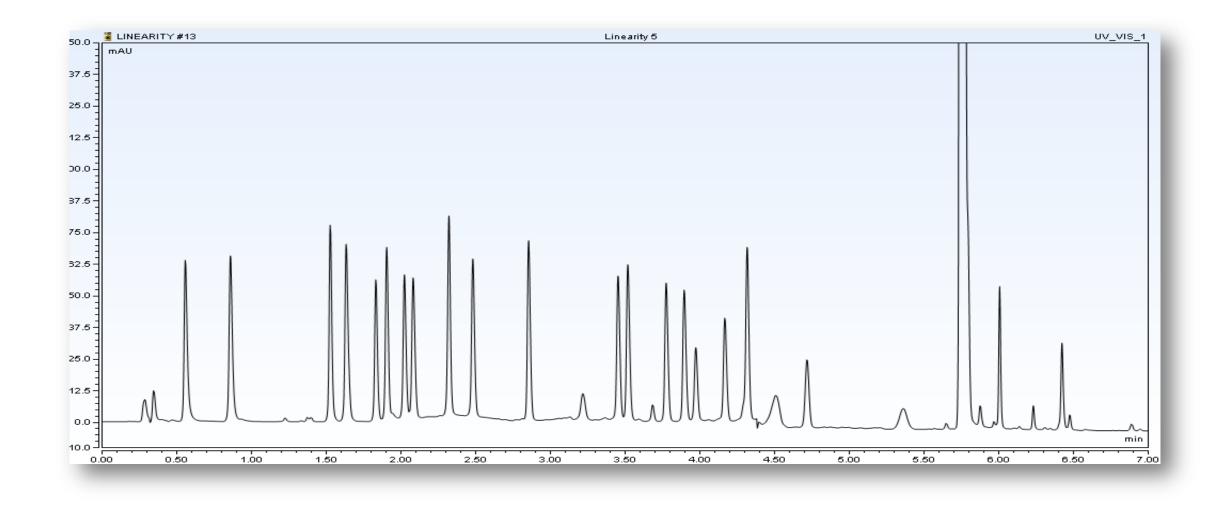
Chromatogram Integration

• Chromeleon 7 introduces two new tools to extremely simplify this process:

Cobra Peak Detection Algorithm / Wizard

SmartPeaks Integration Assistant

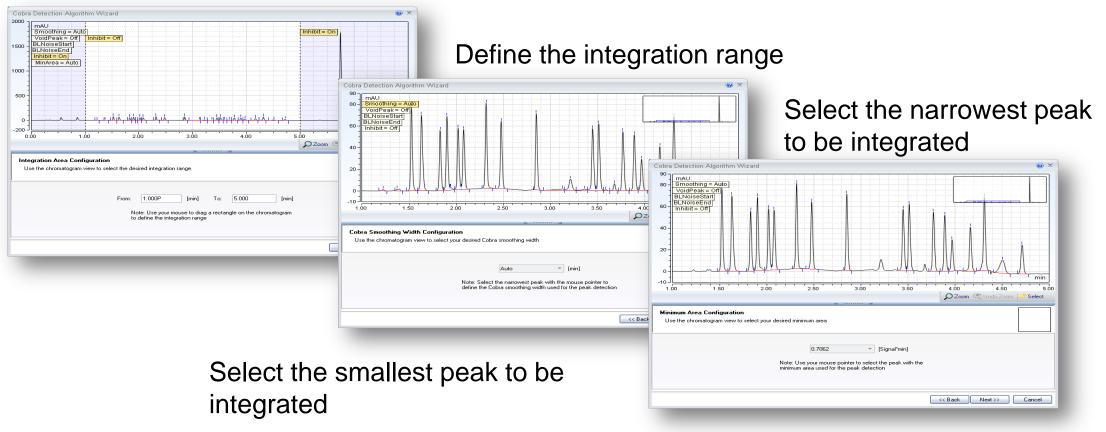




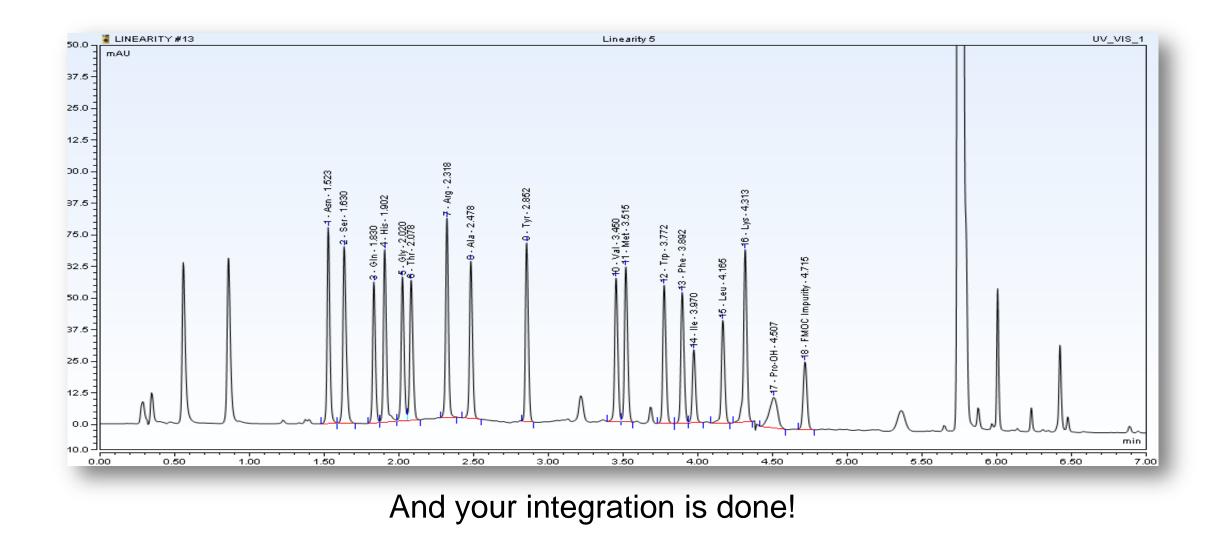




Start Cobra Wizard



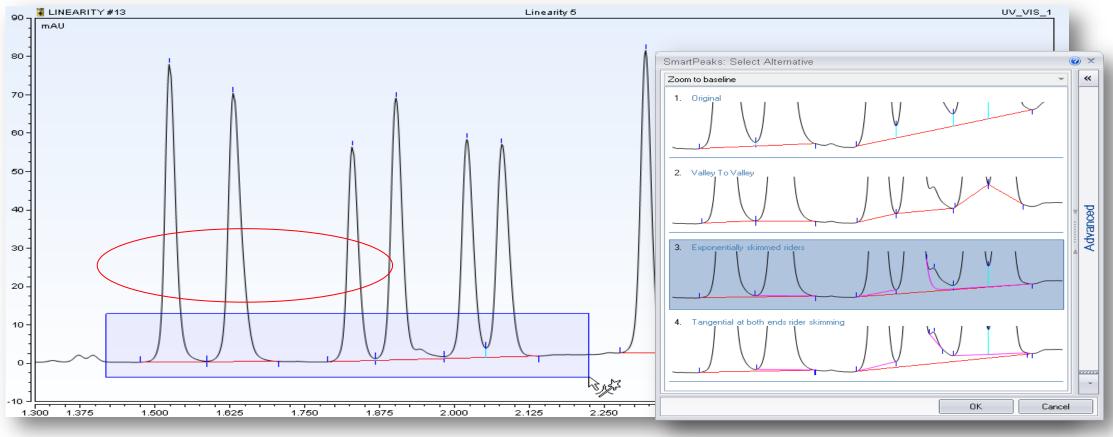






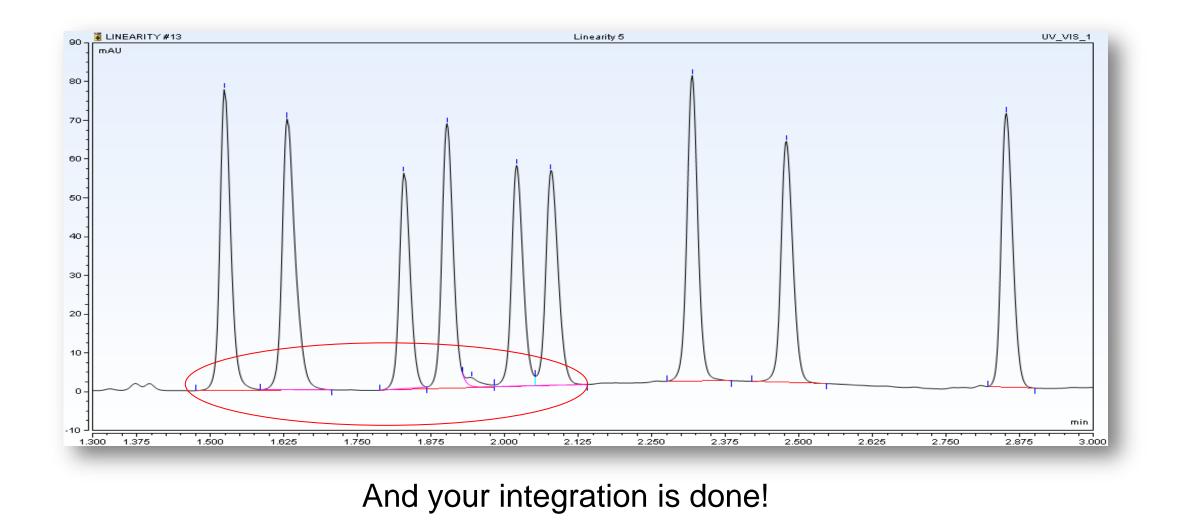


Activate SmartPeaks Wizard



Select the integration you want

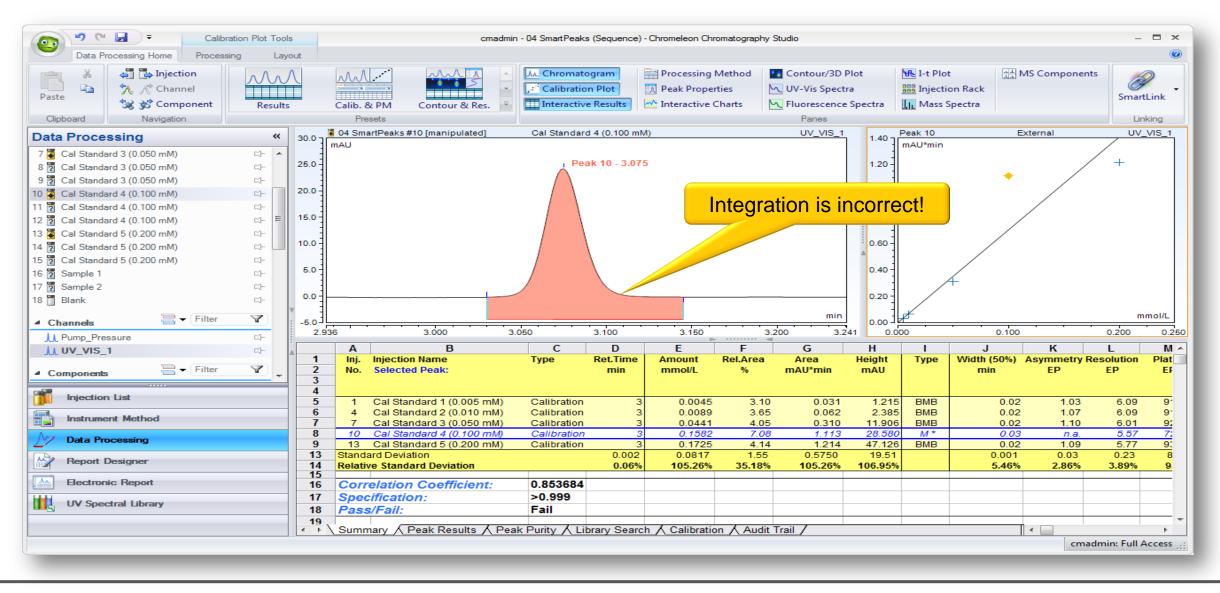






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		6		andard 2 (0.005 mM)	Calibration	3	0.0045	3.65	0.031	2.385	BMB	0.02	1.03	6.09 6.09	9.
Instrument Method		7		andard 3 (0.050 mM)	Calibration	3	0.0441	4.05	0.310	11.906	BMB	0.02	1.10	6.01	9:
		8		andard 4 (0.100 mM)	Calibration	3	0.1582	7.08	1.113	28.580	M *	0.03	n.a.	5.57	72
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Sample 2 Blank Channels Filter Pump_Pressure UV_VIS_1 Components Filter Injection List Instrument Method Data Processing	□ 0.0 □ -5.0 □ <t< td=""><td>A B Inj. Injection Name No. Selected Peak: Cal Standard 1 (0.005 mM 4 Cal Standard 2 (0.010 mM 7 Cal Standard 3 (0.050 mM 10 Cal Standard 4 (0.100 mM 13 Cal Standard 5 (0.200 mM Standard Deviation</td><td>C Type Re Calibration Calibration Calibration Calibration</td><td>D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0045 3 0.0045 3 0.0089 3 0.1725 0.002 0.0817</td><td>F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55</td><td>00 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750</td><td>41 0.20 0.00 z 0.00 H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51</td><td>I Widt</td><td>J h (50%) A nin 0.02 0.02 0.02 0.03 0.02 0.001</td><td>1.03 1.07 1.10 <u>n.a.</u> 1.09 0.03</td><td>0.200 L esolution EP 6.09 6.01 5.57 5.77 0.23</td><td>P</td></t<>	A B Inj. Injection Name No. Selected Peak: Cal Standard 1 (0.005 mM 4 Cal Standard 2 (0.010 mM 7 Cal Standard 3 (0.050 mM 10 Cal Standard 4 (0.100 mM 13 Cal Standard 5 (0.200 mM Standard Deviation	C Type Re Calibration Calibration Calibration Calibration	D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0045 3 0.0045 3 0.0089 3 0.1725 0.002 0.0817	F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55	00 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750	41 0.20 0.00 z 0.00 H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51	I Widt	J h (50%) A nin 0.02 0.02 0.02 0.03 0.02 0.001	1.03 1.07 1.10 <u>n.a.</u> 1.09 0.03	0.200 L esolution EP 6.09 6.01 5.57 5.77 0.23	P
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Sample 2 Blank Channels Filter Pump_Pressure UV_VIS_1 Components Filter Injection List Instrument Method Data Processing	□ 0.0 □ -5.0 □ <t< td=""><td>A B Inj. Injection Name No. Selected Peak: 1 Cal Standard 1 (0.005 mM 4 Cal Standard 2 (0.010 mM 7 Cal Standard 2 (0.010 mM 10 Cal Standard 3 (0.050 mM 10 Cal Standard 4 (0.100 mM 13 Cal Standard 5 (0.200 mM Standard Deviation Relative Standard Deviation</td><td>C Type Re Calibration Calibration Calibration Calibration Calibration Calibration</td><td>D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0045 3 0.0045 3 0.0089 3 0.1725 0.002 0.0817</td><td>F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55</td><td>00 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750</td><td>41 0.20 0.00 z 0.00 H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51</td><td>I Widt</td><td>J h (50%) A nin 0.02 0.02 0.02 0.03 0.02 0.001</td><td>1.03 1.07 1.10 <u>n.a.</u> 1.09 0.03</td><td>0.200 L esolution EP 6.09 6.01 5.57 5.77 0.23</td><td>PI</td></t<>	A B Inj. Injection Name No. Selected Peak: 1 Cal Standard 1 (0.005 mM 4 Cal Standard 2 (0.010 mM 7 Cal Standard 2 (0.010 mM 10 Cal Standard 3 (0.050 mM 10 Cal Standard 4 (0.100 mM 13 Cal Standard 5 (0.200 mM Standard Deviation Relative Standard Deviation	C Type Re Calibration Calibration Calibration Calibration Calibration Calibration	D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0045 3 0.0045 3 0.0089 3 0.1725 0.002 0.0817	F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55	00 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750	41 0.20 0.00 z 0.00 H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51	I Widt	J h (50%) A nin 0.02 0.02 0.02 0.03 0.02 0.001	1.03 1.07 1.10 <u>n.a.</u> 1.09 0.03	0.200 L esolution EP 6.09 6.01 5.57 5.77 0.23	PI
Sample 2 Blank Channels	□ 0.0 □ 0.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -7 □ -7 0 -7 0 -7 13 -7 13 -7 14 -5 16 -7 17 -7	A B Inj. Injection Name No. Selected Peak: 1 Cal Standard 1 (0.005 mM 4 Cal Standard 2 (0.010 mM 7 Cal Standard 2 (0.010 mM 10 Cal Standard 3 (0.050 mM 13 Cal Standard 4 (0.100 mM Standard Deviation Relative Standard Deviation Correlation Coefficient: Specification:	C Type Re Calibration Calibration Calibration Calibration Calibration Calibration 0.853684 >0.999	D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0045 3 0.0045 3 0.0089 3 0.1725 0.002 0.0817	F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55	00 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750	41 0.20 0.00 z 0.00 H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51	I Widt	J h (50%) A nin 0.02 0.02 0.02 0.03 0.02 0.001	1.03 1.07 1.10 <u>n.a.</u> 1.09 0.03	0.200 L esolution EP 6.09 6.01 5.57 5.77 0.23	PI
Sample 2 Blank Channels	□ 0.0 □ -5.0 □ -5.0 □ 2 □ 1	A B Inj. Injection Name No. Selected Peak: 1 Cal Standard 1 (0.005 mM 4 Cal Standard 2 (0.010 mM 7 Cal Standard 2 (0.010 mM 10 Cal Standard 3 (0.050 mM 10 Cal Standard 4 (0.100 mM 13 Cal Standard 5 (0.200 mM Standard Deviation Relative Standard Deviation Correlation Coefficient: Specification: Pass/Fail:	C Type Re Calibration Calibration Calibration Calibration Calibration Calibration	D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0045 3 0.0045 3 0.0089 3 0.1725 0.002 0.0817	F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55	00 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750	41 0.20 0.00 z 0.00 H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51	I Widt	J h (50%) A nin 0.02 0.02 0.02 0.03 0.02 0.001	1.03 1.07 1.10 <u>n.a.</u> 1.09 0.03	0.200 L esolution EP 6.09 6.01 5.57 5.77 0.23	PI
Pump_Pressure UV_VIS_1 Components Filter Injection List Instrument Method Data Processing Report Designer Electronic Report	□ 0.0 □ 0.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -5.0 □ -7 □ -7 0 -7 0 -7 13 -7 13 -7 14 -5 16 -7 17 -7	936 3.000 A B Inj. Injection Name No. Selected Peak: 1 Cal Standard 1 (0.005 mM 4 Cal Standard 2 (0.010 mM 7 Cal Standard 3 (0.050 mM 10 Cal Standard 4 (0.100 mM 13 Cal Standard 5 (0.200 mM Standard Deviation Relative Standard Deviation Correlation Coefficient: Specification: Pass/Fail: Pass/Fail:	C Type Re Type Re Calibration Calibration Calibration Calibration Calibration 0.853684 >0.999 Fail	D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0089 3 0.0441 3 0.1582 3 0.1725 0.002 0.0817 0.06% 105.26%	F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55 35.18%	00 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750 105.26%	41 0.20 0.00 z 0.00 H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51	I Widt	J h (50%) A nin 0.02 0.02 0.02 0.02 0.02 0.02 0.001 5.46%	1.03 1.07 1.10 <u>n.a.</u> 1.09 0.03	0.200 L esolution EP 6.09 6.01 5.57 5.77 0.23	Pl:



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A Cipboard Navigation	Results	Calib. & PM Cralib. & PM Presets	A Chromatog	Plot Peak Prope	rties 🗠	Contour/3D F UV-Vis Spectr Fluorescence Panes	a	맨 I-t Plot 555 Injection Rack Mass Spectra		Components	SmartL	Link
ata Processing	« 30.0	04 SmartPeaks #10 [manipulated]] Cal Standard	4 (0.100 mM)		UV_VIS_1	1.40 p F	Peak 10	Exter	rnal	UV_1	-
Cal Standard 3 (0.050 mM) Cal Standard 3 (0.050 mM) Cal Standard 3 (0.050 mM) Cal Standard 3 (0.050 mM) Cal Standard 4 (0.100 mM) Cal Standard 4 (0.100 mM)	は に に に に こ こ こ こ こ こ こ こ こ こ こ こ こ	mAU mAU	Peak	k 10 - 3.075			1.20	mAU*min	/		+	
 Cal Standard 4 (0.100 mM) Cal Standard 5 (0.200 mM) 	ଘ⊢ ≣ 15.0 ଘ⊢ ଘ⊢ 10.0 ଘ⊢		Ca	libration poin	t is rec	alculate	1					
Sample 1	ದ– 5.0	-					0.40 -					
2 Sample 2 Blank	ୟ⊢ ୟ⊢ 0.0						0.20	+				
Blank Channels 🗧 🗸 Filter	C⊢ 0.0 ▼ -5.0]	3,050	3 100 3 150				<u>+</u>	0.100	· · ·		mol/l
Blank Channels 등 ▼ Filter ↓ Pump_Pressure	C⊢ 0.0 ▼ -5.0 2	2.936 3.000			3.2	200 3.2	41 0.00		0.100	K	0.200	0
Blank Channels 🗧 🗸 Filter	□ □ 0.0 □ □ 0.0 <td>A B Inj. Injection Name No. Selected Peak:</td> <td>С</td> <td>3.100 3.150 D E Ret.Time Amount min mmol/L</td> <td>3.2 F Rel.Area %</td> <td></td> <td></td> <td>l . Type Width</td> <td>J</td> <td>K symmetry Re EP</td> <td>0.200</td> <td>Pl</td>	A B Inj. Injection Name No. Selected Peak:	С	3.100 3.150 D E Ret.Time Amount min mmol/L	3.2 F Rel.Area %			l . Type Width	J	K symmetry Re EP	0.200	Pl
Blank Channels → Filter ↓ Pump_Pressure ↓ UV_VIS_1 Components → Filter Injection List	□ 0.0 ▼ -5.0 □ 2 □ -4 1 2	A B Inj. Injection Name No. Selected Peak:	C Type mM) Calibration	D E Ret.Time Amount	F Rel.Area	200 3.2 G Area	41 0.00 2 41 0.00 H Height mAU 1.215	l . Type Width	J I (50%) As	ymmetry Re	0.200 L solution	(Pl
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Blank Channels	C→ 0.0 C→ 2 C→ 2 C→ 1 2 3 4 5 6 7 8 9 9 11 1	A B Inj. Injection Name No. Selected Peak: A Cal Standard 1 (0.005 r Cal Standard 2 (0.010 r Cal Standard 3 (0.050 r Cal Standard 3 (0.050 r Cal Standard 4 (0.100 r Cal Standard 5 (0.200 r Standard Deviation A Relative Standard Deviation	C Type MM) Calibration MM) Calibration mM) Calibration mM) Calibration	D E Ret.Time min 3 0.0045 3 0.0089 3 0.0441	Rel.Area % 3.10 3.65 4.05	G Area mAU*min 0.031 0.062 0.310	Height MAU 1.215 2.385 11.906	I Width m Type Width m BMB BMB BMB	J (50%) As hin 0.02 0.02 0.02	1.03 1.07 1.10	0.200 L solution EP 6.09 6.09 6.01	Pla
Blank Channels Filter Pump_Pressure UV_VIS_1 Components Filter Injection List Instrument Method Data Processing	CJ- 0.0 Image: Signal state sta	A B Inj. Injection Name No. Selected Peak: Inj. Injection Name Injection Coefficien Injection Coefficien	C Type MM) Calibration MM) Calibration mM) Calibration mM) Calibration	D E Ret.Time min Amount mmol/L 3 0.0045 3 0.0089 3 0.04541 3 0.1725 0.002 0.0817	F Rel.Area % 3.10 3.65 4.05 7.08 4.14 1.55	COO 3.2 G Area mAU*min 0.031 0.062 0.310 1.113 1.214 0.5750	H Height mAU 1.215 2.385 11.906 28.580 47.126 19.51	I Width m BMB BMB BMB M*	J (50%) As in 0.02 0.02 0.02 0.02 0.02 0.02 0.02 0.02 0.02	1.03 1.07 1.10 <i>n.a.</i> 1.09 0.03	0.200 L solution EP 6.09 6.09 6.01 5.57 5.77 0.23	_



Data Processing Home Proces	sing Lay	is vout		cma	dmin - 04 SmartPeak	s (Sequence)	- Chromeleon Chro	omatography	Studio					_	
A Cipboard Navigation	Result		Calib. 8		 Calibratio Interactive 	on Plot	Processing I	ties	Contour/3D F UV-Vis Spectr Fluorescence Panes	a	₩ I-t Plot Injectio	on Rack	IS Component	Smart	
ata Processing	**	30.0 -	🖥 04 Sma	ntPeaks #10	Cal Standar	d 4 (0.100 mN	A)		UV_VIS_1	1.40 p F	Peak 10	Ex	ternal	UV	_VIS_1
Cal Standard 3 (0.050 mM) Cal Standard 4 (0.100 mM) Cal Standard 4 (0.100 mM) Cal Standard 4 (0.100 mM)	* * * * * * *	25.0 20.0 15.0	mAU	_	Pe	ak 10 - 3.07	5			1.20	mAU*min			/	
Cal Standard 5 (0.200 mM)	¤- ¤-	10.0			Calibr	ation li	ine fitting	g is re	calculate	ed					
 Cal Standard 5 (0.200 mM) Cal Standard 5 (0.200 mM) Sample 1 Sample 2 Blank 	ಜ ಜ ಜ ಜ	5.0 0.0								0.40		*			
Channels Filter	Y	5.0	<u></u>	· · · · · · · · · · · · · · · · · · ·	· · · · · ·	· · · · ·	· · · · · · · · · · · · · · · · · · ·		min	0.00	¥				1mol/L
L Pump_Pressure	C)-	2.93		3.000	3.050	3.100	3.150	<	200 3.2			0.100		0.200	0
UV_VIS_1	C1-	▲ 1	A Inj.	B Injection Name	C Type	D Ret.Time	E Amount	F Rel.Area	G Area	H Height	I Type	J Width (50%)	K Asymmetry Re	L esolution	Pla
Components Filter	V ,	2	No.	Selected Peak:	.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	min	mmol/L	%	mAU*min	mAU		min	EP	ЕР	E
Injection List		4	1	Cal Standard 1 (0.005 mM) Calibration	3	0.0051	3.10	0.031	1.215	вмв	0.02	1.03	6.09	
Instrument Method		6	4	Cal Standard 2 (0.010 mM) Calibration	3	0.0102	3.65	0.062	2.385	BMB	0.02	1.07	6.09	9
instrument Method		7	7	Cal Standard 3 (0.050 mM Cal Standard 4 (0.100 mM			0.0507	4.05	0.310	11.906 24.383	BMB BMB	0.02	1.10 1.06	6.01 5.92	
Data Processing		9		Cal Standard 4 (0.100 mM Cal Standard 5 (0.200 mM			0.1030	4.14	1.214	47.126	BMB	0.02	1.06	5.77	
Report Designer		13	Standa	ard Deviation	,	0.002	0.0801	0.45	0.4903	19.04		0.000	0.03	0.14	
		14		e Standard Deviation		0.06%	109.01%	11.72%	109.01%	109.40%		0.67%	2.54%	2.27%	
Electronic Report		16		elation Coefficient:	0.999516										
UV Spectral Library		17		ification: /Fail:	>0.999 Pass			Cali	bration I	now pa	asses	s specific	cation		
		19	Summ	hary 🔨 Peak Results 🖌 F	Peak Purity 🖌 Li	brary Searc	h /					•	-		<u> </u>



- 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







- 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

2.665

2.405 2.205 2.0es

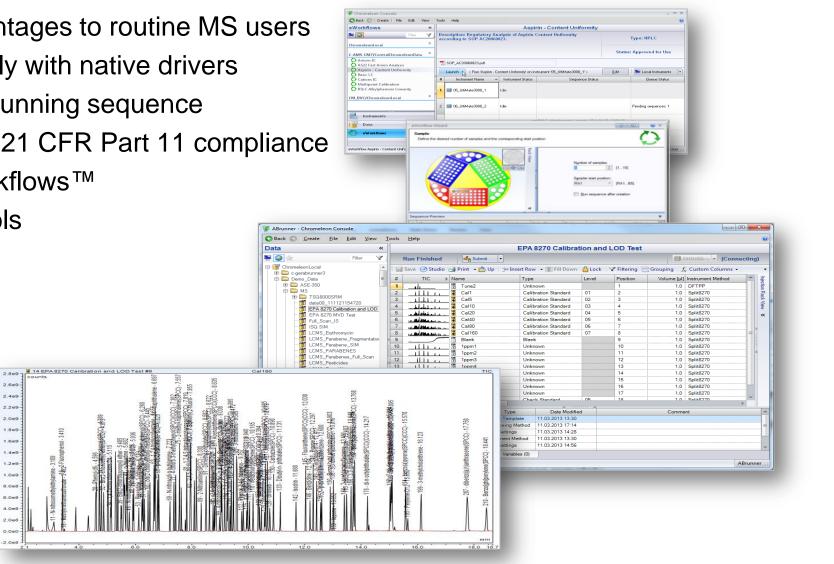
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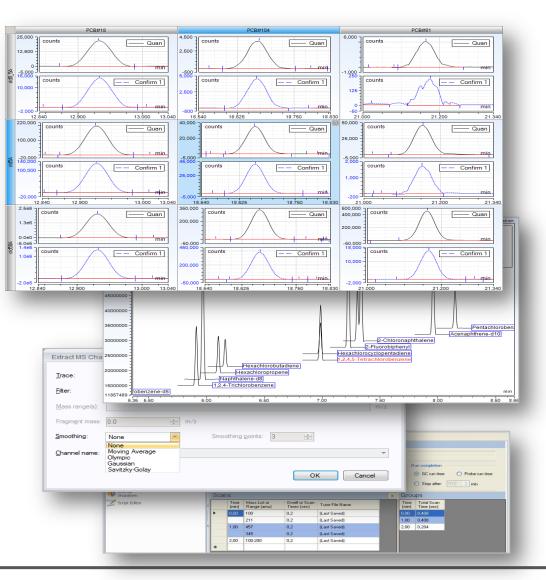
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- Easily start analyses with eWorkflows[™]
- Full suite of data processing tools



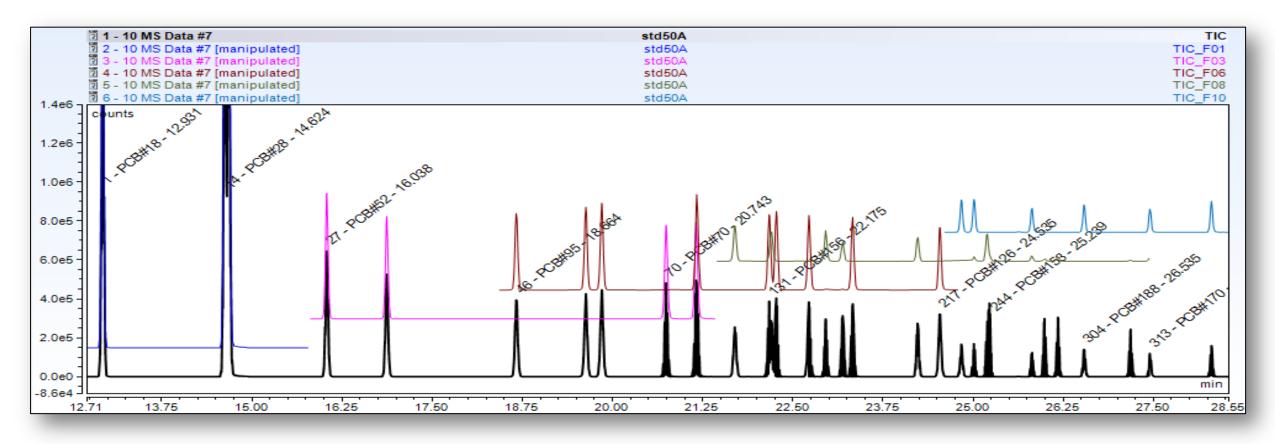


- Chromeleon 7.2 CDS provides:
 - MS-specific data organization at component level
 - Visualization of (large-volume) MS data
 - Channel-specific reporting of components
 - NIST format for MS Library searching, creation, and compound data import
- Key benefits:
 - Only need to install, validate and learn 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

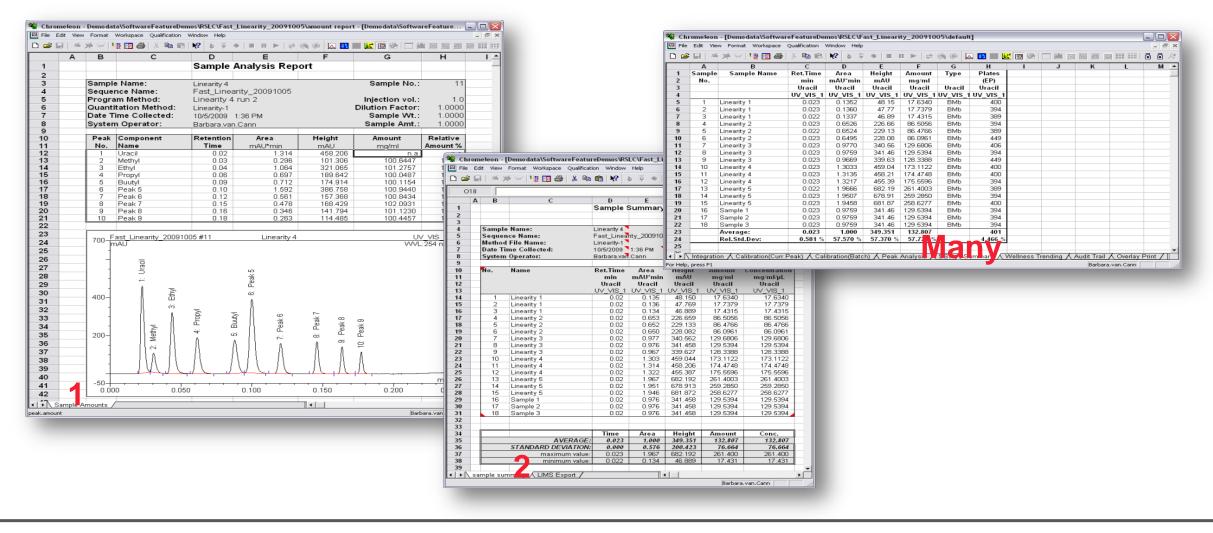
• Automatically report for the Channel with the highest response

No.	Peak Name	Area	Channel
		counts*min	
TIC	TIC	Highest Response	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



... can have as many worksheets as required





... can include result tables

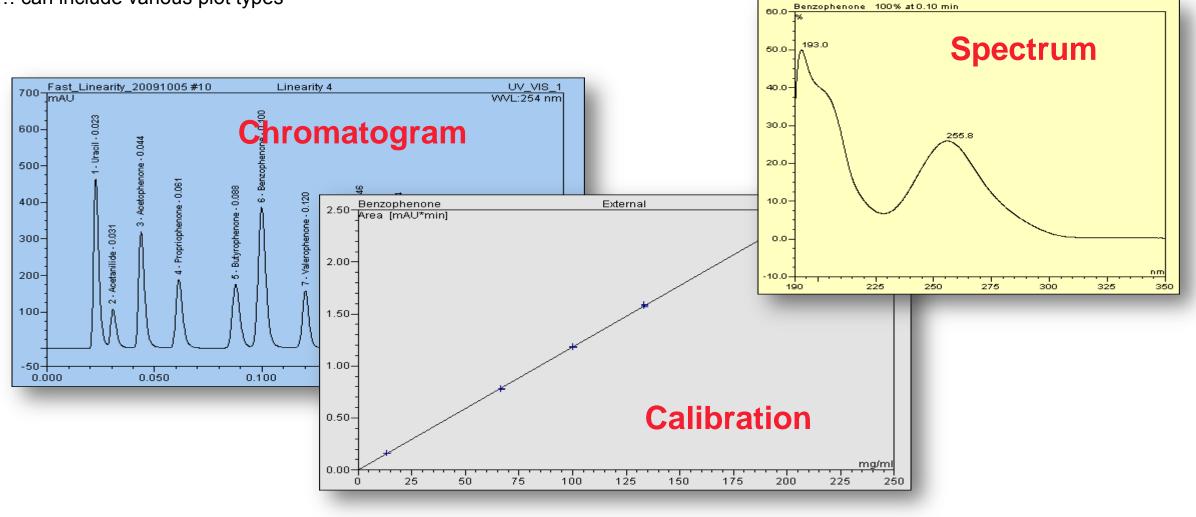
									Sample Na		Linearity 4	Injection Volume:	1.0
									Vial Numb		RB2	Channel:	
									Sample Ty		standard	Wavelength:	254.0
									Control Pro Quantif. M		Linearity 4 run 1 Linearity-1	Bandwidth: Dilution Factor:	1 1.0000
Peak	Componen	1t	Retention	Area	Heig	iht Amo	ount Re	elative	Recording		10/5/2009 13:35	Sample Weight:	1.0000
									Run Time		0.24	Sample Amount:	1.0000
No.	Name		Time	mAU*min	mA		g/ml Am	ount %					
1	Uracil		0.02	1.303	45	9.044	n.a.	n.a.	Day Time	Ret.Time	Command/Message		
2	Methyl		0.03	0.289	10	0.10	38,2799	10.90	13:35:29		Audit trail of sample SMP::\Demodata\Softw	areFeatureDemos\RSLC	C\Fast_Lin
3			0.04	1.057	.0	8.78 Peak	Tables	11.16	13:35:29		Start of sample 10 "Linearity 4", using progr	am "Linearity 4 run 1".	
-	Ethyl								13:35:29 13:35:29	0.000	ColumnOven.Temperature.Nominal = 100.0 Cooler Temperature.Nominal = 20.0		
4	Propyl		0.06	0.693	18	7.379	99.4445	11.03	13:35:29	0.000	Pressure.LowerLimit = 0		
5	Buutyl		0.09	0.705	17	3.300	99.0898	10.99	13:35:29	0.000	Pressure.UpperLimit = 800		
6	Peak 5		0.10	1 507				11 15	13:35:29	0.000	%A.Equate = "%A"		
		No.	Name		t.Time	Area	Height	Ame	13:35:29	0.000	%B.Equate = "%B"		
7	Peak 6				min	mAU*min	mAU		13:35:29 /n13:35:29	0.000	Data_Collection_Rate = 100.0 ResponseTime = 0.025		
8	Peak 7							D Ing	13:35:29	0.000	SlitWidth = Narrow		
9	Peak 8				ophenone	Benzophenone	Benzophenon		13:35:29	0.000	UV VIS 1.Wavelength = 254.0		
-				Uv	∕_VIS_1	UV_VIS_1	UV_VIS_1		<mark>/1</mark> :35:29		$UV_VIS_1.Bandwidth = 1$		
10	Peak 9	1	Linearity 1	(0.10	0.161	40.625	13.5	B113:35:29	0.000	$UV_VIS_1.RefWavelength = 225.0$		
		2	Linearity 1		D.10	0.161	40.073		13:35:29 3013:35:29	0.000	UV_VIS_1.RefBandwidth = 1 3DFIELD.RefWavelength = 800.0		
								10.0	76 13:35:29	0.000	3DFIELD.RefBandwidth = 1		
		3	Linearity 1		D.10	0.162	39.759	13.6	75 13:35:29 13:35:29	0.000	Data_Collection_Rate = 100.0		
		4	Linearity 2	(D.10	0.776	191.967	1 65.6	13:35:29	0.000	ResponseTime = 0.025		
		5	Linearity 2	(D.10	0.779	192.297	65.9	<u>13:35:29</u>	0.000	SlitWidth = Narrow		
		6	Linearity 2		D.10	0.784	192.225	66.3	07 13:35:29 13:35:29 17 13:35:29	0.000	UV_VIS_1.Wavelength = 254.0 UV_VIS_1.Bandwidth = 1		
		7			D.10	1.182	289.564	00.0	13:35:29		UV VIS 1.RefWavelength = 225.0		
		<u> </u>	Linearity 3					99.9	65 13:35:29 13:35:29	0.000	UV_VIS_1.RefBandwidth = 1		
		8	Linearity 3		D.10	1.186	289.292		29113:35:29	0.000	3DFIELD.RefWavelength = 200.0		
		9	Linearity 3	(0.10	1.179	285.307	99.7	DE 13:35:29 13:35:29	0.000	3DFIELD.RefWavelength = 00.0 3DFIELD.RefBandwidth = 0.0 3DFIELD.MinWavelength = 0.0	riraiis	
		10	Linearity 4	1	D.10	1.587	382.335	134.1	3.13:35:29	0.000	3DFIELD.Minwavelength = 800.0		
		11	Linearity 4		D.10	1.592	386.758	134 6	13:35:29 13:35:29	0.000	3DFIELD.BunchWidth = 1		
		12	Linearity 4		D.10	1.572	381.628	132 0	0.43:35:29	0.000	Autozero جسواے 2 700		
		13	Linearity 5		D.10	2.361	566.797	199.6			.6193		
		14	Linearity 5		D.10	2.359	563.997	199.4			.4263		
		15	Linearity 5			hlae	567.937	200.5			.5406		
		16	Sample 1	σπητιά		abl <mark>es</mark>	289.292	100.2			.2906		
		17	Sample 2		D. 10	1.186	289.292	100.2	2906	100	.2906		
		18	Sample 3	(D.10	1.186	289.292	100.2	2906	100	.2906		

10 Linearity 4



Audit Trail

... can include various plot types



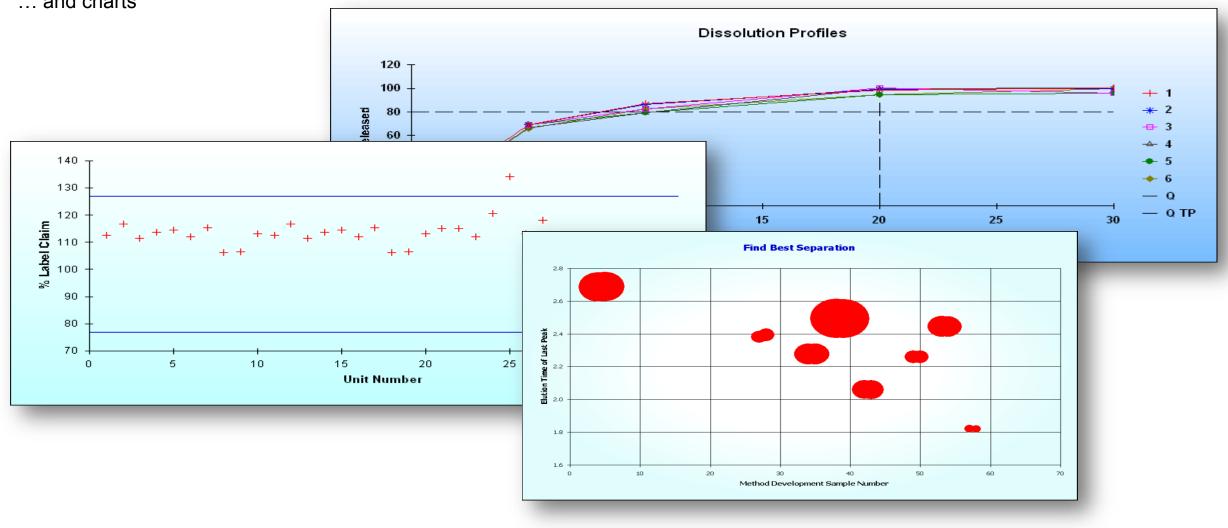


... and can even include custom equations...

	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(AVEF	RAGE(E1	4:E31)),"r	n.a.",AVE	RAGE(E1	4:E31))
=IF(ISERROR(STDE	:V(E14:E	31)),"n.a."	',STDEV(I	E14:E31))	
=MAX(E14:E31)					
=MIN(E14:E31)					



... and charts







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Chromeleon and Samplemanager

Interfacing

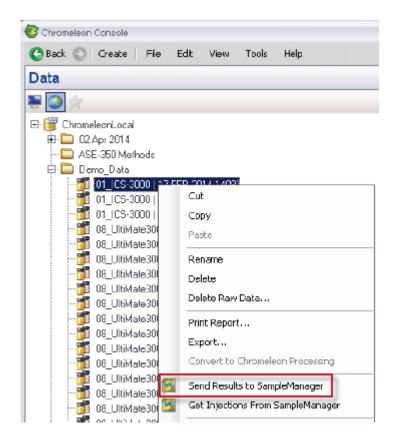
The world leader in serving science

- Create a sequence from SampleManager
- Select samples in SampleManager
- In the context menu Create Sequence

Test number	Analysis	Sample	Status	Instrument
1	Parabens	1	In Progress	
2	Parabens	1	In Progress	
3	Parabens	2	Available	
4	Parabens	2	Available	
5	Parabens	3	Available	
6	Parabens	3	Available	
7	Parabens	4	Available 🚌	View Analysis
8	Parabens	4	Available	Process
20	Parabens	16	Available	Process
21	Parabens	16	Available 🔋	Create Sequence
22	Parabens	17	Available 🛜	Properties
23	Parahens	17	Available	



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







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Compliance

User management and Audit Trails

- 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

S Chromeleon Administration Console (nlams-lvmeurs	
License Manager (localhost) Scheduler Global Policies Workflow Tags User Database	Save Role Report General Logon Members Licenses Role Name: The share the state of the share term and
Chromeleon Users Central () Caddmin (Chromeleon Administrator) Sinstrument Controller (Instrument Controller) Local () Scheduler (Scheduler) Scheduler (Scheduler)	Access Local DV Role Description: Privileges: Privilege Privil
Access Groups Access Local DV Construction Access Local DV Access Local DV Access Central DV Audit Trail Construction Local Machine	 Instrument Met ✓ Instrument Met ✓ Daity Instrument Cor ○ Data Vault Bas ○ Folders ✓ Queries ✓ Queries ✓ Sequences ✓ Injections ✓ Report Templates ○ Electronic Report ○ Seport Templates ○ Electronic Signature ✓ View Settings ✓ Electronic Signature ✓ Archive ○ Administration

Control what users can access and change



	Copy 🆂 Print	🛛 🍸 Disable Fil	ter - 🦹 Clear Filters	🛛 Run Only 👻	🝷 🤐 Find Next 🌺 Find Previous			1
	Date	Time	Retention Time	Device	Message			
	Information	7:38 PM	0.144	PumpModule.P	PumpModule.Pump.%B.Value = 40.0			
	Warning	7:30 FM	0.144	ump	rumpModule.rump.%b.value = 40.0			
	Command DeviceLog	7:38 PM	0.144	PumpModule.P ump	PumpModule.Pump.Flow.Nominal = 3.704			
	PreconditionLo InjectionStart	9 7:38 PM	0.144	PumpModule.P ump	PumpModule.Pump.%B.Value = 40.0			
	InjectionEnd SequenceStart	7:43 PM	0.240	PumpModule.P ump	PumpModule.Pump.Flow.Nominal = 3.704			
	SequenceEnd QueueStart	7:43 PM	0.240	PumpModule.P ump	PumpModule.Pump.%B.Value = 40.0			
Ľ	QueueEnd	7:43 PM	0.240		UV.UV_VIS_1.AcqOff			
	16/02/2009	03:47:43 PM	0.240		UV.3DFIELD.AcqOff			
ĩ	16/02/2009	03:47:44 PM			End of injection "Linearity 1".	R	SLC Alkylpher	none
1	16/02/2009	03:47:44 PM			Start of injection 4 "Linearity 1", using instrument method "Linearity 1 Run 3".	: 🖻	Dompare	9
	16/02/2009	03:47:44 PM	0.000	UV.3DFIELD	UV.3DFIELD.MinWavelength = 190.0	Nr 🕶		lame
	16/02/2009	03:47:44 PM	0.000	UV.3DFIELD	UV.3DFIELD.MaxWavelength = 400.0	12	📅 RSLC Alky	, Iphe
	16/02/2009	03:47:44 PM	0.000	UV.3DFIELD	UV.3DFIELD.BunchWidth = 2		RSLC Alky	
	16/02/2009	03:47:44 PM	0.000	UV	UV.ResponseTime = 0.025		A 360.smp/UV	
	16/02/2009	03:47:44 PM	0.000	UV	UV.Data_Collection_Rate = 100.0	7	∧ 360.smp/U\	v_vi
	16/02/2009	03:47:44 PM	0.000	ColumnOven	ColumnOven.Temperature.Nominal = 100.0		· · · · · · · · · · · · · · · · · · ·	
	16/02/2009	03:47:44 PM	0.000	Sampler	Sampler.Temperature.Nominal = 20.0		· · · · · · · · · · · · · · · · ·	
1	16/02/2009	03:47:44 PM	0.000	Sampler	Log TempCtrl: On	2	🗂 RSLC Alky	lphe
	16/02/2009	03:47:44 PM	0.000	Sampler	Sampler.Temperature.LowerLimit = 4.0		🎁 RSLC Alky	ipne
	16/02/2009	03:47:44 PM	0.000	Sampler	Sampler.Temperature.UpperLimit = 45.0			
	16/02/2009	03:47:44 PM	0.000	PumpModule.P	PumpModule.Pump.%A.Equate = ''Water''			
				ump				

Object Audit Trails: Displays complete change history of object

Restore Previous Version

lr 🕶	Name	Туре	Version	Operator	Operation	Comment	Date / T
13	TRSLC Alkylphenone Linearit	Sequence		JBond	Changed Injection	Changed 2 µL to 5 µL Changed 2 µL to 5 µL	17/02/2009 03
12	RSLC Alkylphenone Linearit	Sequence	10	JBond	Changed Injection	Corrected Injection Volume, as this was a 5 µL full loop Corrected Inj	17/02/2009 0
11	RSLC Alkylphenone Linearit	Sequence	9	HSolo	Changed	Changed width of first Column Changed width of first Column	17/02/2009 0
10	RSLC Linearity.procmeth	Processing Method	8	HSolo	Changed	Updated Heptanophenone retention time and changed title Updated	17/02/2009 0
9	∧ 360.smp/UV_VIS_1.channel	Chromatogram	7	HSolo	Changed	Removed manual intagration, as automatical integration is correct. R	17/02/2009 0
8	RSLC Linearity.procmeth	Processing Method	6	MRiggs	Changed	Updated Uracil retention time Updated Uracil retention time	17/02/2009 0
7	∧ 360.smp/UV_VIS_1.channel	Chromatogram	5	MRiggs	Changed	Manually adjusted hexanophenone peak Manually adjusted hexanop	17/02/2009 0
6	RSLC Linearity.layout	Data Presentation	4	MRiggs	Changed	Changed Resolution form USP to EP Changed Resolution form USP	17/02/2009 0
5	RSLC Linearity.report	Report Template	3	MRiggs	Changed	Updated the report to show associated reports Updated the report to	17/02/2009 0
4	TRSLC Alkylphenone Linearit	Sequence	2	JTKirk	Changed	Optimized column heights and widths Optimized column heights and	16/02/2009 (
3	RSLC Alkylphenone Linearit	Sequence	1	SYSTEM	Finished Run		16/02/2009 0
2	RSLC Alkylphenone Linearit	Sequence	1	SYSTEM	Started Run		16/02/2009 0
1	RSLC Alkylphenone Linearit	Sequence	1	JTKirk	Created		16/02/2009 0

Instrument Audit Trails

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





