

OpenLAB CDS ChemStation Edition C.01.06

Tips and Tricks for GC Users



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GC Software Product Manager

Problem / Solution

Problem:

I want to have the latest instrument control of the 6890 GC, but I need to seamless switch from the classic 6890 GC.

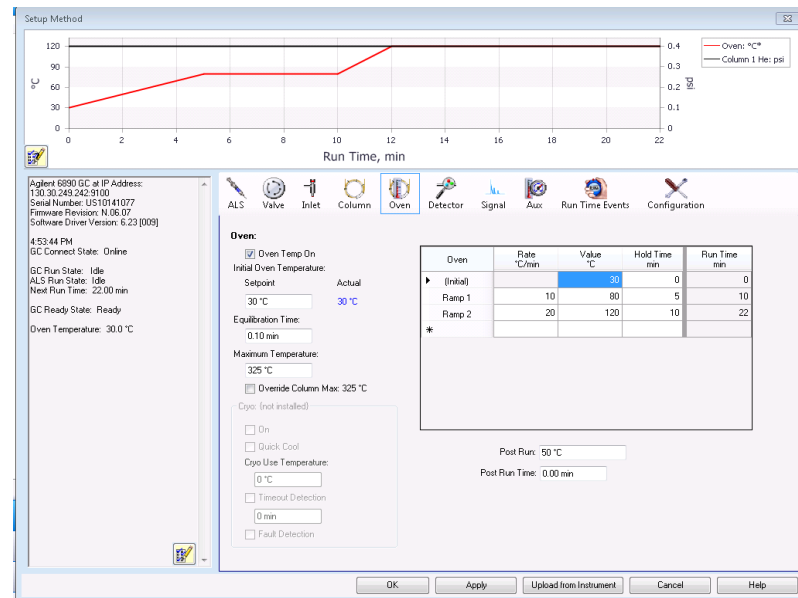
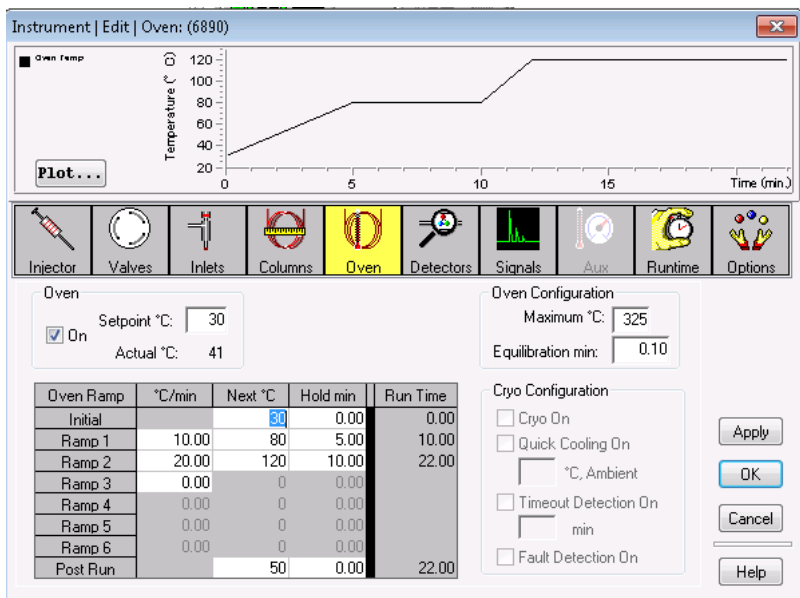
Solution:

GC Acquisition Method Migration

Instrument Control Driver

Method Migration

OpenLAB CDS ChemStation-C.01.06



6890 GC
Classic
Method



6890 GC
Enhanced
Method



Agilent Technologies

OpenLAB CDS ChemStation C.01.06 for GC Users

May 2014

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Problem / Solution

Problem:

I have purchase a new 7890B GC with OpenLAB CDS ChemStation C.01.06 replacing a 6890 GC. I want a seamless way to transfer method to the 7890B GC.

Solution:

GC Acquisition Method Migration

Instrument Control Driver

Method Migration

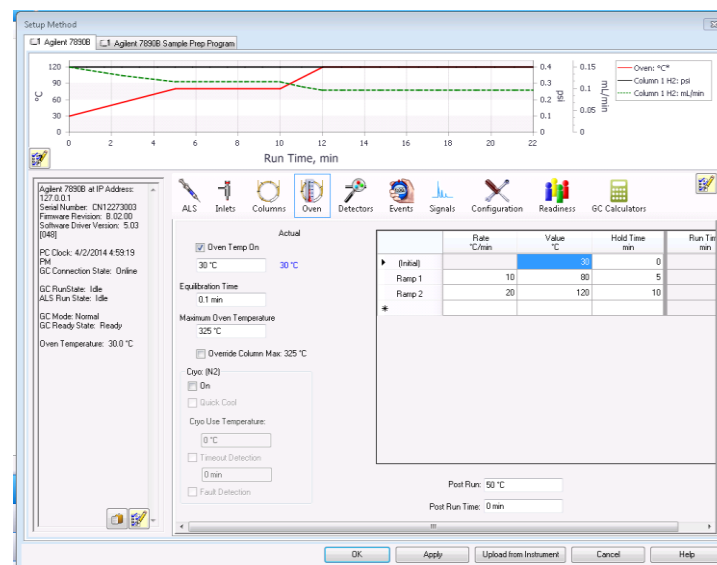
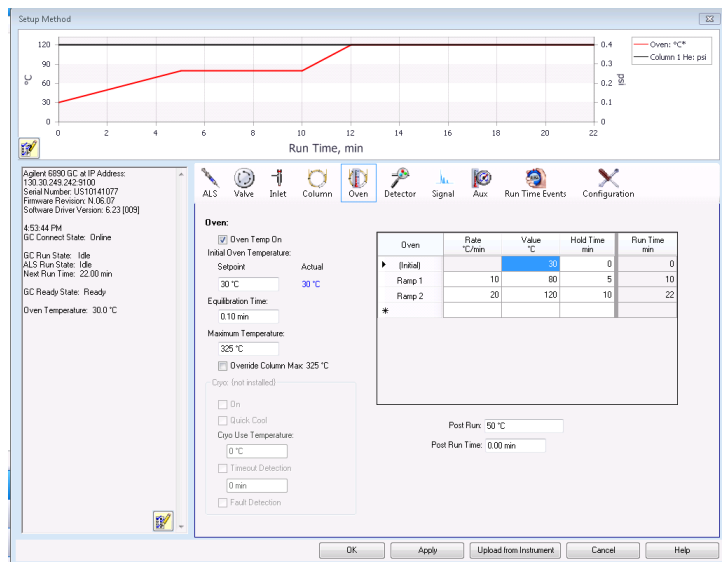
OpenLAB CDS ChemStation-C.01.06



6890 GC
Method



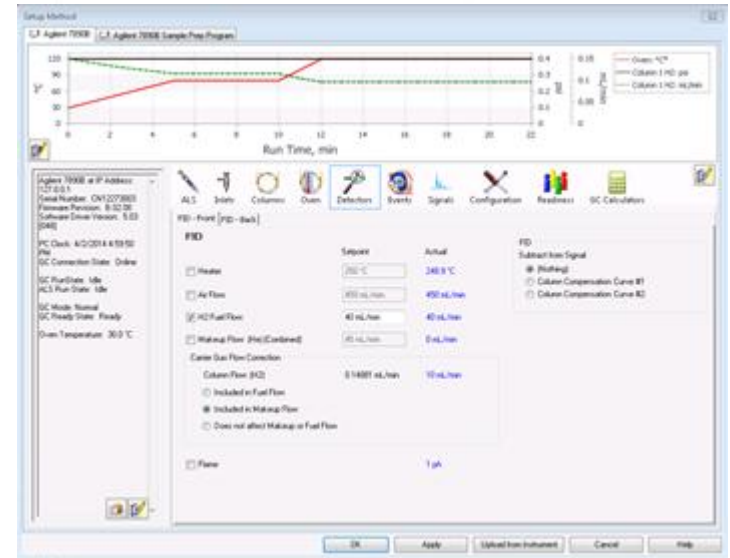
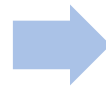
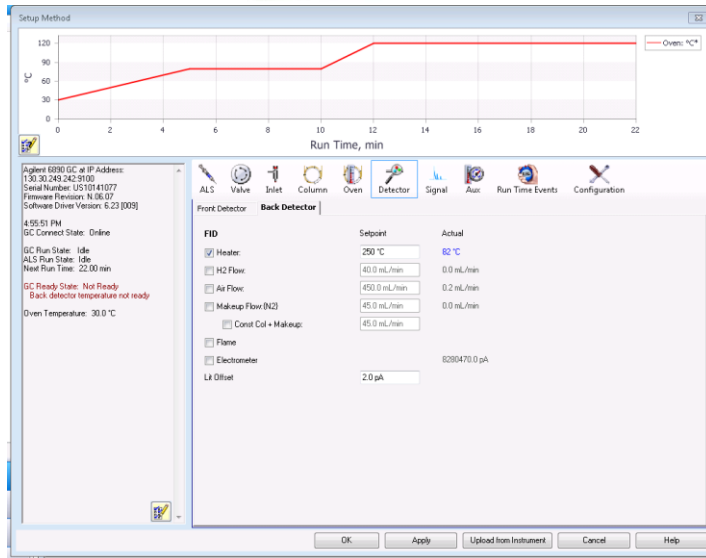
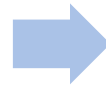
Open Method in
OpenLAB CDS
C.01.06 and
save



Instrument Control Driver

Method Migration

OpenLAB CDS ChemStation-C.01.06



Problem / Solution

Problem:

I have purchase OpenLAB CDS ChemStation C.01.06. I want a seamless way to transfer method from a previous version of Multi-technique GC ChemStation B.04.03 SP2

Solution:

GC Acquisition Method Migration

Instrument Control Driver

Method Migration

OpenLAB CDS ChemStation-C.01.06



Methods from Multi-
Technique GC
ChemStation B.04.03 SP2
7890 or 6890 method
Transfer to C.01.06



Problem / Solution

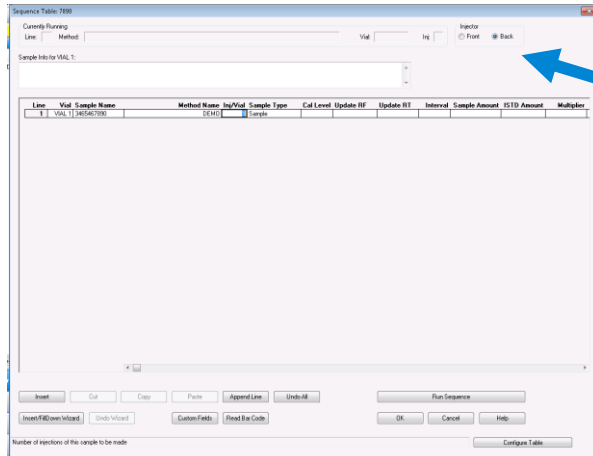
Problem:

I need more flexibility with scheduling back only injections and front and back mix injections in the same sequence.

Solution:

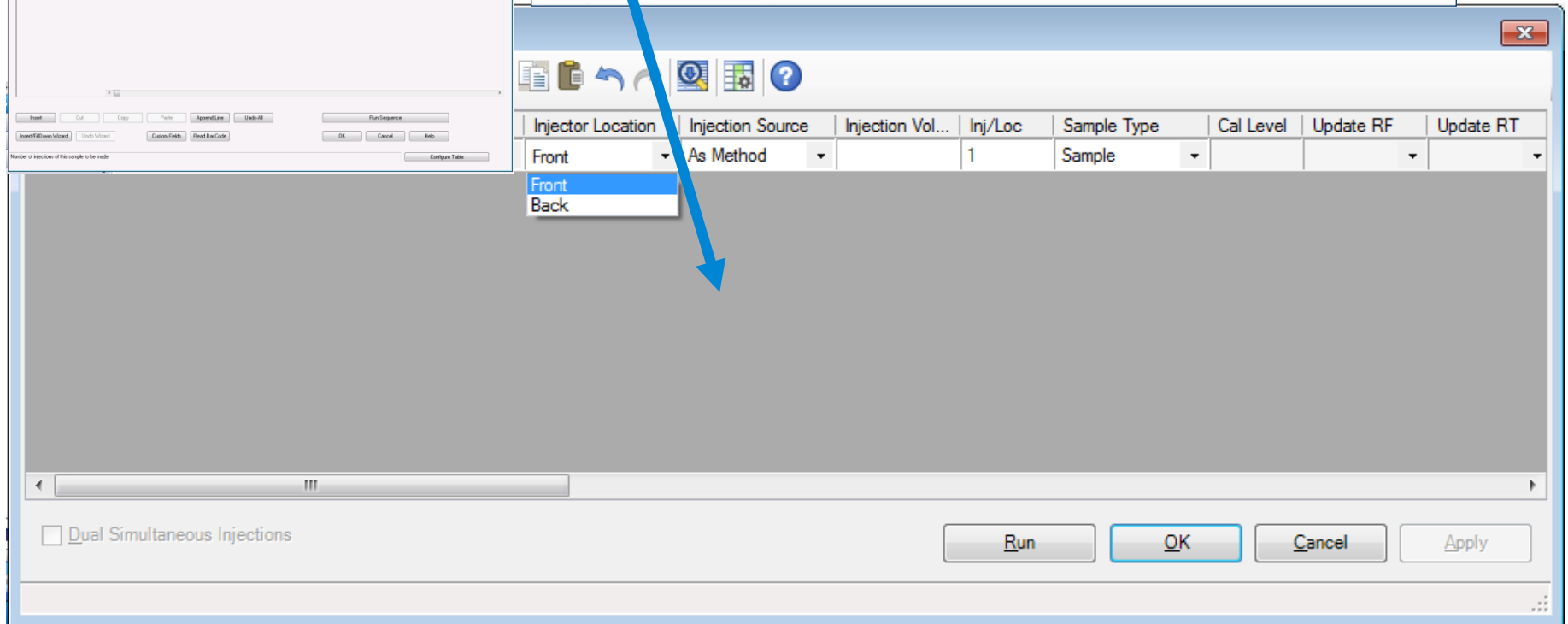
Improved Sequence Table

Sequence Table



Front and Back Injector Location

- Selection is no longer a different tab
- Just select the injector location in the table



Problem / Solution

Problem:

I need more flexibility with the sequence Table

- I want to copy and paste in the Sequence Table
- I have Front and back mix configurations
- I want to move the columns or delete columns

Solution:

Improved Sequence Table

Sequence Table

Sequence Table: Instr1_7890

Line	Sample ...	Sample Name	Method Name	Injector Location	Injection Source	Injection Vol.	Update RT
▶ 1				Front	As Method		

- Insert Line
- Append Lines
- Delete
- Fill Down
- Undo
- Cut, Copy, Paste

Dual Simultaneous Injections

Run OK Cancel Apply

Problem / Solution

Problem:

I need to add more than one ISTD to the sequence table.

Solution:

Improved Sequence Table

Sequence Table

- Improve customer experience
- Up to 8 ISTD input

Sequence Table: 7890B

Line	Sample L...	Sample N...	Method Name	Injector Location	Injection Source	Inj/Loc	Sample T...	ISTD1 Amo...	ISTD2 Amo...	ISTD3 Amo...	ISTD4 Amo...	ISTD5 Amount	ISTD6 Amo...	ISTD7 Amount	ISTD8 Amo...	Multiplier	Dilution
1			DemoGC	Front	As Method	1	Sample										
2			DemoGC	Front	As Method	1											
3			DemoGC	Front	As Method	1											
4			DemoGC	Front	As Method	1											
5			DemoGC	Front	As Method	1											
6			DemoGC	Front	As Method	1											
7			DemoGC	Front	As Method	1											
8			DemoGC	Front	As Method	1											
9																	

ASTM D6584 - Analysis of Free and Total Glycerin in B100 Biodiesel

ASTM D6584 Short Report

Client No: 0127493218ATM6584_TOL_G100049684_T185000 2012-10-03 09:49:15
 Sample name: 01862712_8
 On Sample: RZ center, 2.64 mL/min, 3.43 psi
 Sample amount: 10160.000 mg
 Inj Loc: Front
 Inj Volume: 10.000 µL
 Inj Rate: 10.000 µL/min
 Inj Pressure: 3.43 psi
 Inj Temp: 20.000 °C
 Inj Solvent: N/A

ISTD1 Components

Ret	Area	Amount	Unit	Mo. Wt.
5.040	84.1712	1.4	µg	0.014%
5.855	908.3331	10.0	µg	0.098%
16.418	82.2222	2.6	µg	0.026%
17.702	643.6960	16.1	µg	0.158%
17.706	47.7102	3.6	µg	0.035%
20.177	19119.054	80.0	µg	0.787%
21.622	181.2383	6.8	µg	0.067%
25.546	20.8608	3.3	µg	0.033%

ISTD2 Groups

Group	Start Time	End Time	Group Area	Amount	Unit	Mo. Wt.
Diglycerols	21.180	22.040	333.318	11.3	µg	0.11%
Triglycerols	23.460	26.430	47.376	5.9	µg	0.05%
Monoglycerols	TimeGroup	0.000	773.676	73.3	µg	0.73%

Free Glycerin: 3.014%

Bound Glycerin: 3.882%

Total Glycerin: 3.896%

Problem / Solution

Problem:

I want to be able to set up a dual simultaneous sequence to increase the throughput on the 6890/7890 series GC.

Solution:

Improved Sequence Table

Sequence Table

- Improve customer experience of ChemStation sequence table

Sequence Table: 7890B GC

Line	Sample Location	Sample Name	Method Name	Injector Location	Injection Source	Injection Vol...	Inj/Loc	Sample Type	Cal Level	Update RF	Update RT	Cal Inte...	Sample Amount	ISTD1 Amo...	ISTD2 Amo...	ISTD3 Amo...
1F	1	Sample 345	DEMO_GC7890	Front	As Method		1	Sample								
1B	1	Sample 345	DEMO_GC7890	Back	As Method		1	Sample								
2F	2	Sample 346	DEMO_GC7890	Front	As Method		1	Sample								
2B	2	Sample 346	DEMO_GC7890	Back	As Method		1	Sample								
3F	3	Sample 347	DEMO_GC7890	Front	As Method		1	Sample								
3B	3	Sample 347	DEMO_GC7890	Back	As Method		1	Sample								
4F																

Dual Simultaneous Injections

Run OK Cancel Apply

Problem / Solution

Problem:

I want to see all the injections in the order in which they will run in the sequence, so there are no errors in the sequence table.

Solution:

Improved Sequence Table- Sequence Preview

Sequence Table

- Sequence Run Preview

Sequence Table: 7890B GC

Line	Sample Location	Sample Name	Method Name	Injector Location
1F	1	Sample 345	DEMO_GC7890	Front
1B	1	Sample 345	DEMO_GC7890	Back
2F	2	Sample 346	DEMO_GC7890	Front
2B	2	Sample 346	DEMO_GC7890	Back
3F	3	Sample 347	DEMO_GC7890	Front
3B	3	Sample 347	DEMO_GC7890	Back
4F				

Dual Simultaneous Injections

Sequence Run Preview: 7890B GC

Sample name	Data file	Run	Location	Method	Seq tbl	Calib:RF:RT
Sample 345	001F0101	1	1	DEMO_GC7890	F:01:01	
Sample 346	002F0201	2	2	DEMO_GC7890	F:02:01	
Sample 345	001B0101	2	1	DEMO_GC7890	B:01:01	
Sample 347	003F0301	3	3	DEMO_GC7890	F:03:01	
Sample 346	002B0201	3	2	DEMO_GC7890	B:02:01	
Sample 347	003B0301	4	3	DEMO_GC7890	B:03:01	

Problem / Solution

Problem:

It is easier to obtain/edit the worklist of samples in excel, so I want an easy way to transfer it to the CDS sequence file.

Solution:

Improved Sequence Table

Sequence Table

	A	B	C	D
1	Sample Location	Sample Name	Method Name	Inj/Loc
2		1 GC8978415	100FID	1
3		2 GC8978416	100FID	1
4		3 GC8978417	100FID	1
5		4 GC8978418	100FID	1
6		5 GC8978419	100FID	1
7		6 GC8978420	100FID	1
8		7 GC8978421	100FID	1
9		8 GC8978422	100FID	1
10		9 GC8978423	100FID	1
11		10 GC8978424	100FID	1
12		11 GC8978425	100FID	1
13		12 GC8978426	100FID	1
14		13 GC8978427	100FID	1
15		14 GC8978428	100FID	1
16		15 GC8978429	100FID	1

Sequence Table: 7890B GC

Line	Sample Location	Sample N...	Method Name	Inj/Loc	Injector Loca...	Injection Source	Injection Vol...	Sample T...	Cal Level	Update RF	Uj
1	1	GC8978415	100FID	1	Front	As Method		Sample			
2	2	GC8978416	100FID	1							
3	3	GC8978417	100FID	1							
4	4	GC8978418	100FID	1							
5	5	GC8978419	100FID	1							
6	6	GC8978420	100FID	1							
7	7	GC8978421	100FID	1							
8	8	GC8978422	100FID	1							
9	9	GC8978423	100FID	1							
10	10	GC8978424	100FID	1							
11	11	GC8978425	100FID	1							
12	12	GC8978426	100FID	1							
13	13	GC8978427	100FID	1							

Dual Simultaneous Injections

Copy and paste from Microsoft Excel into the sequence Table

Problem / Solution

Problem:

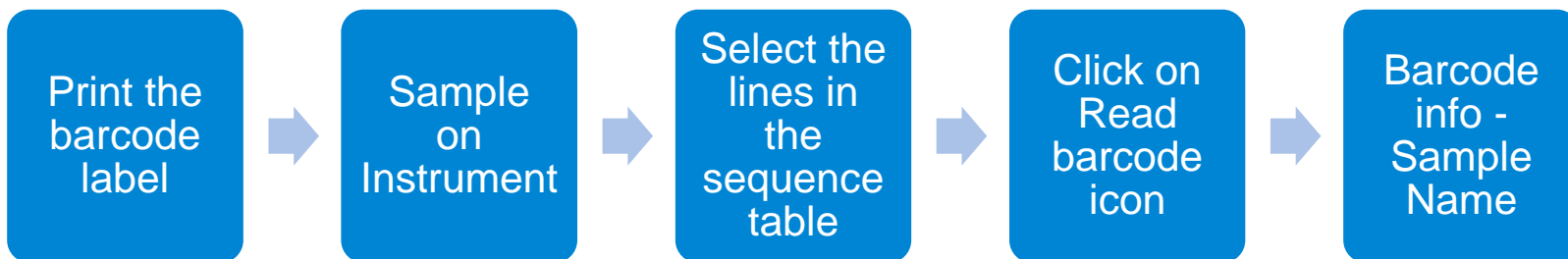
I want to minimize the typos of typing in a long digits sample ID in each line of the sequence.

Solution:

Barcode Reading in Sequence Table

Sequence Table

Barcode Reading



Sequence Table: 7890B GC

	Vial Location	Sample Name	Injection location	Method Name	Inj/Vial	Sample Type	Interval
1	Vial 1	89875223	Front	demo_GC	1	Sample	

Sequence Table: 7890B GC

Line	Sample L...	Sample Name	Method Name	Injector Loca...	Injection Source	Injection Volume	Inj/Loc	Sample T...	Cal Level	Update RF	Update RT	Cal Interval	Sample Amount	ISTD1 Amo...	ISTD2 Amo...	ISTD3 Amc
1	1	234679024GC	DEMO_GC	Front	As Method		1	Sample								
2	2	12357890BGC	DEMO_GC	Front	As Method		1	Sample								
3	3	32347890B	DEMO_GC	Front	As Method		1	Sample								
4	4	7890GC1345	DEMO_GC	Front	As Method		1	Sample								
5	5		DEMO_GC	Front	As Method		1	Sample								
6																

Reading Bar Code...

Barcode read for 4 Sequence Lines.

This operation may take some time. Press Cancel to abort the operation.

Cancel

Run OK Cancel Apply

Problem / Solution

Problem:

I am required to maintain the chain of custody of the samples throughout the laboratory including when the samples are being analyzed. Automatic tracking of the samples saves time and minimizing human error.

Solution:

Barcode Reading-Chain of Custody

Barcode Reading

Chain of Custody Workflow



User labels the vials

Enter sample information including the sample ID into the sequence table

Sample Name	Sample ID	Sample Type	Sample Location	Sample Volume	Sample Concentration	Sample Date	Sample Time	Sample Operator	Sample Status
Sample 1	101	100	100	100	100	100	100	100	100
Sample 2	102	100	100	100	100	100	100	100	100
Sample 3	103	100	100	100	100	100	100	100	100

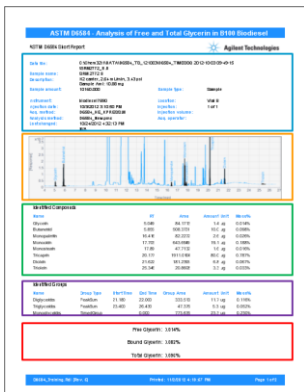
Instrument reads the barcode

Barcode is stored in the barcode field

CDS compares the Barcode field (Actual) to the sample field (Expected) and determines if it is mismatched

Inject Anyway

Skip Vial



Logic determines if the sample should be injected or not

Barcode and results of the comparison is printed on report

True= prints barcode

False= prints False

Problem / Solution

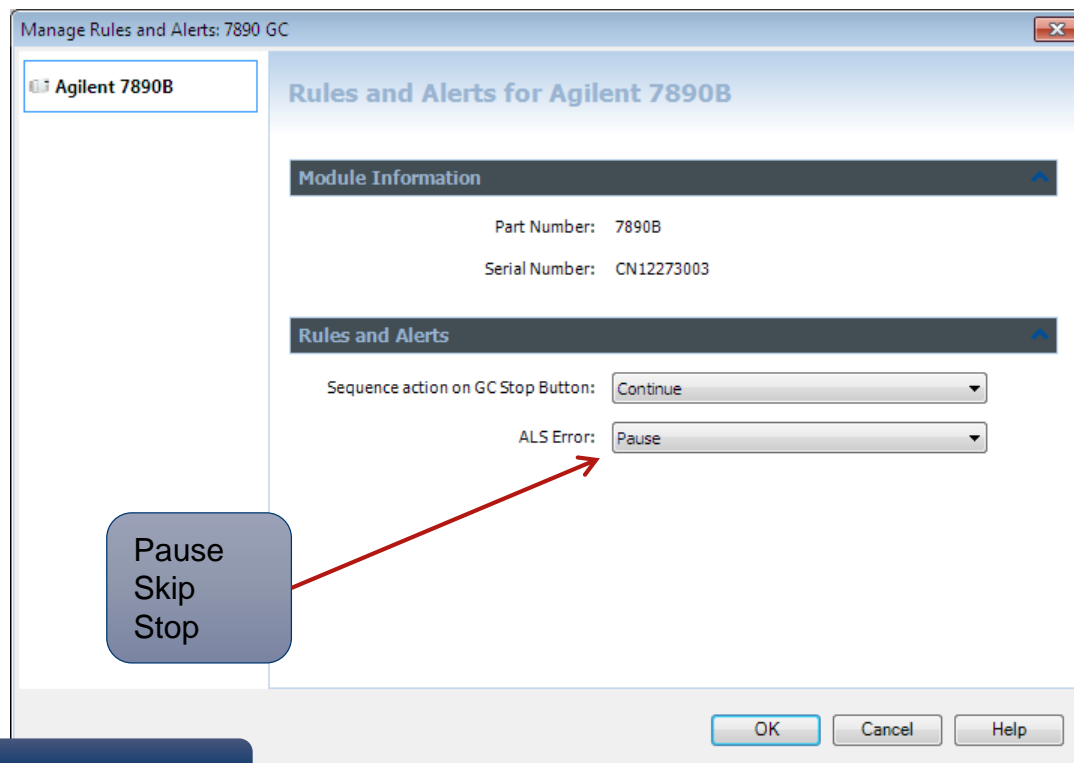
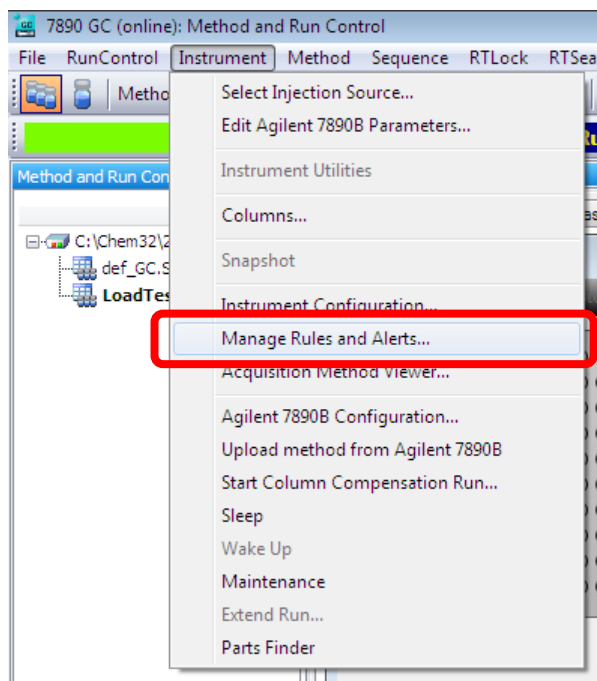
Problem:

I missed putting a vial in the autosampler or miscounted the vials.

Solution:

Manage Rules and Alerts-Retry, Abort, or Skip

Manage Rules and Alerts



The action can be preselected Pause, Skip, or Stop.

- Pause gives the options
- Abort: aborts the run; sequence stop
- Retry: Retries the current vial
- Skip: Skips the current vials and goes to the next line of the sequence

Also for the
7697A
Headspace
Sampler

Problem / Solution

Problem:

I need to get the final data/report before the shipment can go out.

I need to process more samples in a day.

Solution:

OpenLAB Data Analysis Package

Problem / Solution

Problem:

I need a faster way to determine integration problems, missing peaks, and retention time drifts.

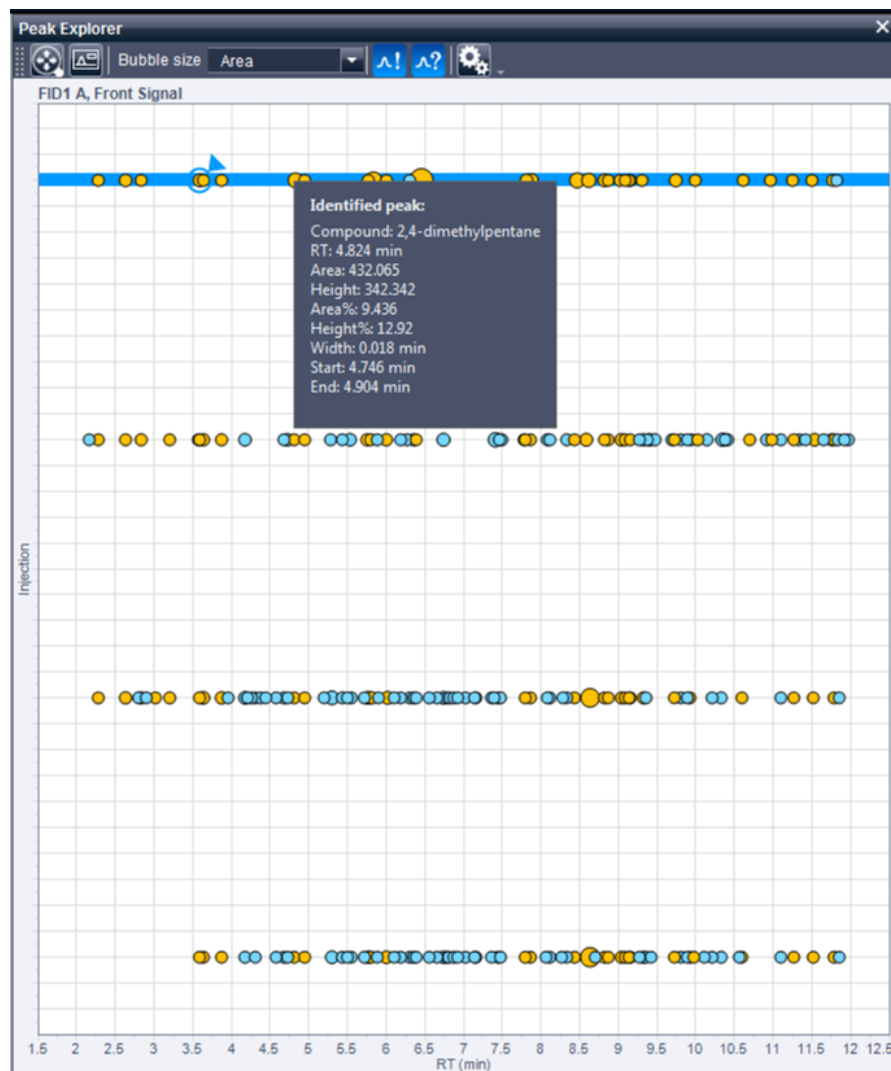
Solution:

OpenLAB Data Analysis: Peak Explorer

Productivity-new insights into the data

Peak Explorer

- Find artifacts (missing peaks, shift of RT's, additional peak, integration problems)
- Navigate through large sets of data with hundreds of peaks and compounds
- Ability to Zoom-in and out
- UI's synced to id and navigate injections.
- Tooltip displays more detailed information about the peak.



Problem / Solution

Problem:

I upgrade my software to the latest version and I don't want to type in the compound names and retention times for the data analysis methods.

I previously used EzChrom or ChemStation and I want the same results when I reprocess the data.

Solution:

OpenLAB Data Analysis: Choice of integrators

Productivity

Import of compound ID table
(Name, Expected RT, ISTD flag,
RT Window) from EZChrom and
ChemStation using MACAML files

The image displays two screenshots of the Agilent OpenLAB Data Analysis software interface. The top screenshot shows the 'New Method From MACAML' option highlighted in the 'New Method' dropdown menu. The bottom screenshot shows the 'Open File' dialog box with the file 'COC-PRECISION.macaml' selected. The background shows a chromatogram with several peaks labeled with retention times and compound names.

Agilent OpenLAB Data Analysis

File Home Processing Chromatograms

+ New Method - Open Method Save Method As Close Update Master Method

+ New Method From MACAML

by Sequence

BR-COC.S

c10-16 acetone - SIG2000001.D

c10-16 acetone - SIG2000002.D

c10-16 acetone - SIG2000003.D

c10-16 acetone - SIG2000004.D

Agilent OpenLAB Data Analysis

File Home Processing Chromatograms

+ New Method - Open Method Save Method As Close Update Master Method

Reprocess Selected Reprocess All Clear corrections Create reports Save Selected Results Save All Results

Data Processing

by Sequence

BR-COC.S

SIG2000002.D

SIG2000003.D

SIG2000004.D

SIG2000005.D

SIG2000006.D

SIG2000007.D

SIG2000008.D

SIG2000009.D

SIG2000010.D

SIG2000011.D

SIG2000012.D

SIG2000013.D

SIG2000014.D

SIG2000015.D

SIG2000016.D

SIG2000017.D

SIG2000018.D

SIG2000019.D

COC-PRECISION.macaml

Open Cancel

Display mode Separate

5 5.5 6 6.5 7 7.5 8 8.5 9 9.5

Retention time (min)

5.448

6.524

7.190

c12

c13

c16

Creation date 6/20/2006 3:37:46 AM

Created by bill

Modification date 6/20/2006 9:35:59 AM

Modified by bill

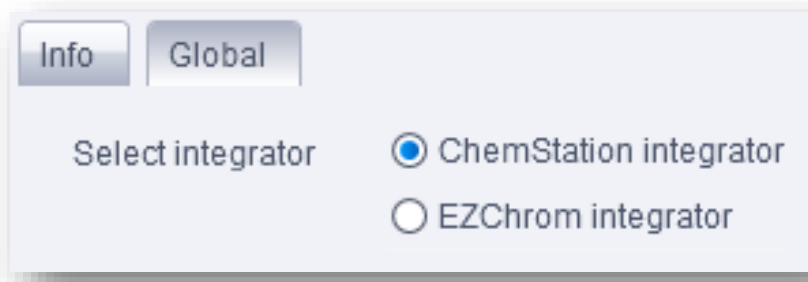
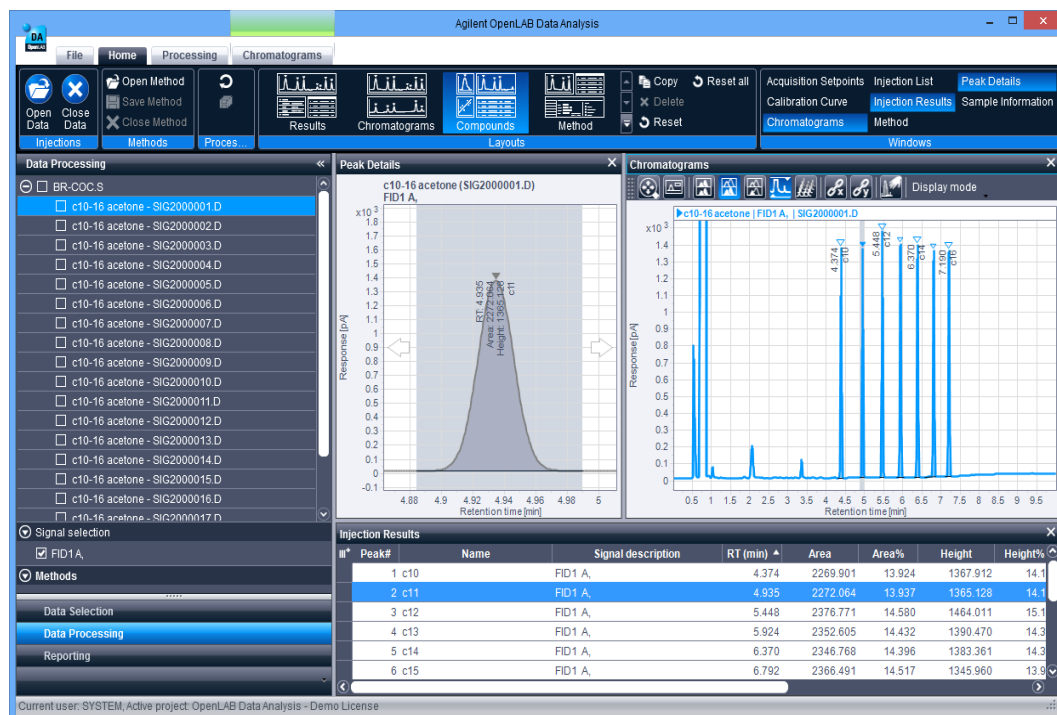
Sample

Current user: SYSTEM, Active project: DA - Demo License

Productivity

ChemStation and EZChrom integrator as a choice

- Get the same integration results as in EZChrom
- Use EZChrom integrator for ChemStation data as alternative to the ChemStation integrator



Problem / Solution

Problem:

I want to view data in a simple UI tailored to my needs without changing screen each time I start the software.

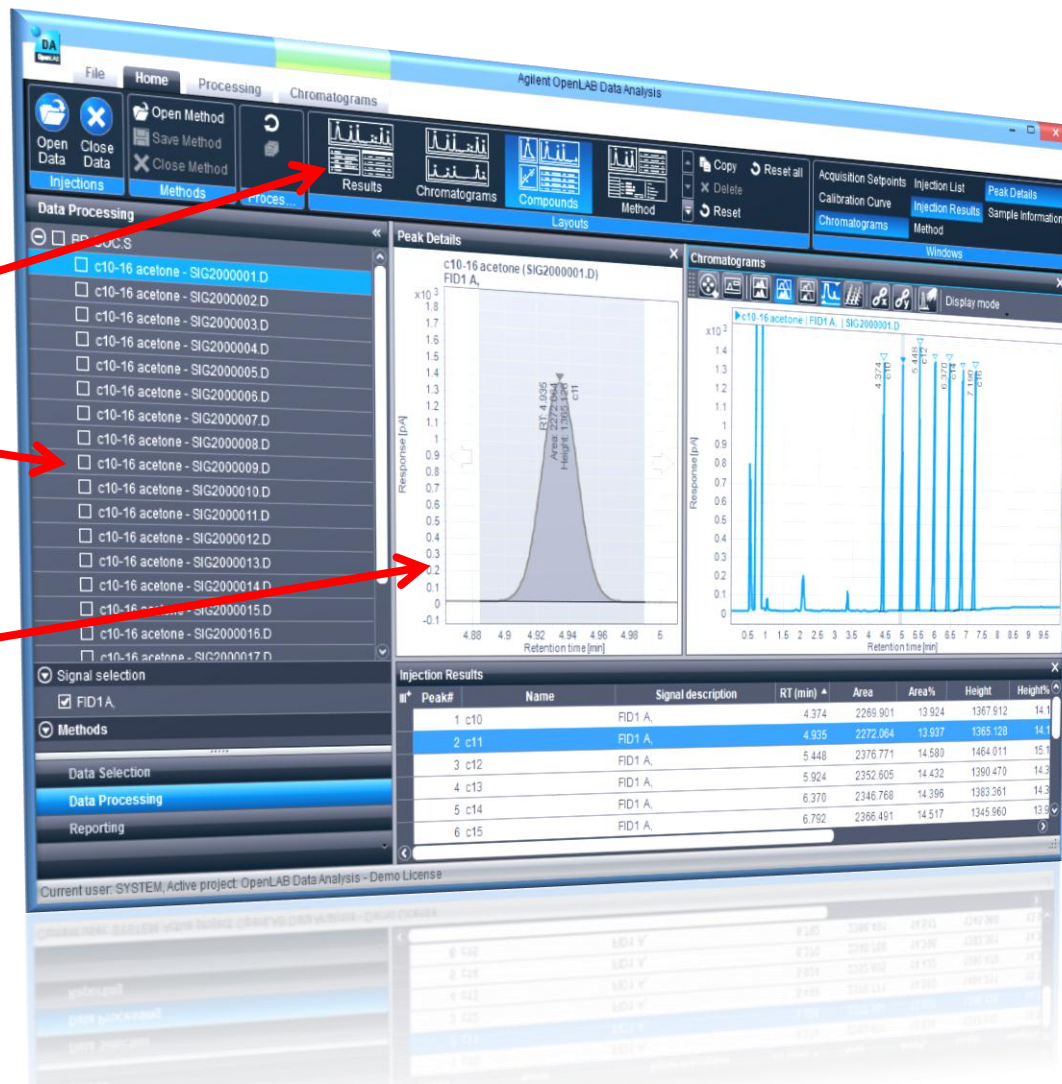
I want to view data in my personalized preferences while my colleagues have another preference.

Solution:

OpenLAB Data Analysis-Customized layouts

OpenLAB Data Analysis

- Customized layouts: User selects which windows and items they want to view. They are persisted even if the software is closed.
- Use “up” and “down” arrows to review all the samples in the result set in a few minutes.
- Peak detail: View each peak in the sample in a zoom-in.



Problem / Solution

Problem:

I need to customized labeling the peaks to determine if a peak is present or missing.

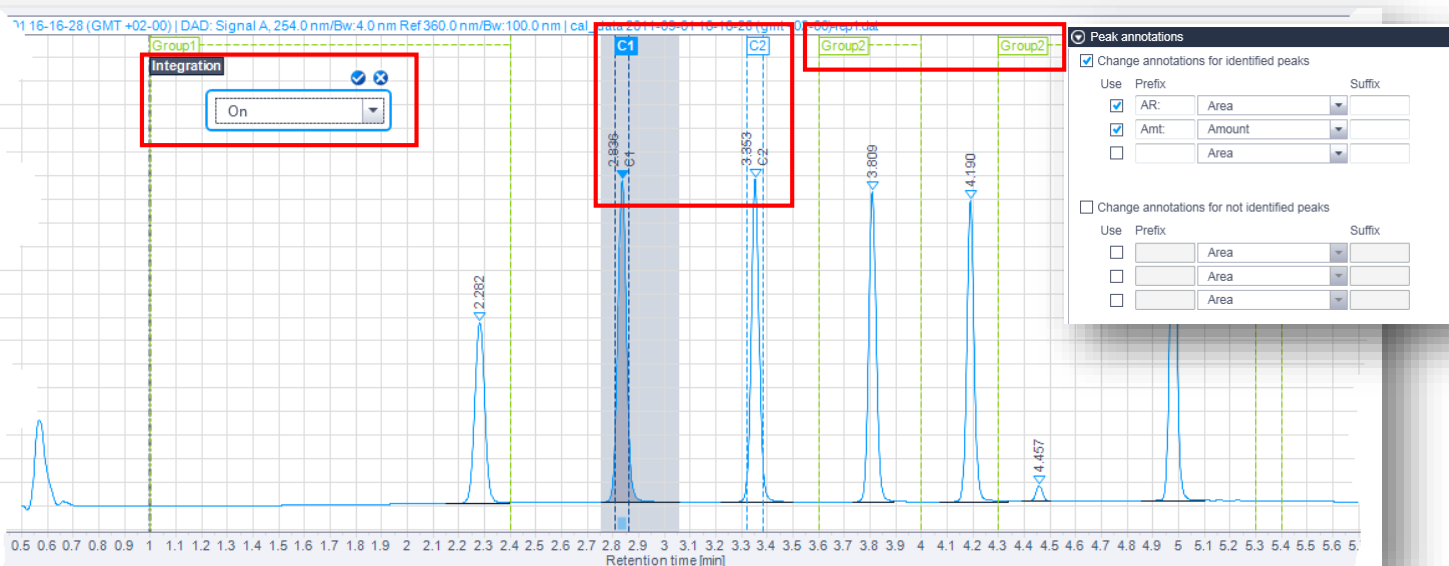
I need to view the groups sections within the chromatogram.

Solution:

OpenLAB Data Analysis-Groups Views

Enhanced UI for productive data review

- Display of compounds and groups in the chromatogram
- Display and editing of integration events in the chromatogram
- Customizable peak annotations
- Enhanced layout management
- Global shifting of expected RT's of all compounds
- Configuration of tables
 - Choose the columns you want to see
 - Define number precision to display
 - Re-order columns
 - Show identified and/or unidentified peaks in the injection results
- GC dual channel data review



Problem / Solution

Problem:

I need to use specific data analysis for my result calculation.

- I want to use published Relative Retention Times
- I need to report results in mass%.
- I need to add multipliers in the data analysis to obtain the result for my analysis.

Solution:

OpenLAB Data Analysis-Quantitation features

Compound ID & Quantitation features

- Compound identification by Relative Retention Time Groups of Groups
- Compound multipliers
 - Allows to correct for purity of standard compounds
- Mass% calculation
- Summarize amounts of timed groups and other compounds in a single named group

Compound Table General

External standard Internal standard

Number of levels: 3

Curve calculation: From average per level

RF definition: Response per amount

⚠ If you change the RF definition, you need to clear your calibration curve otherwise your results will be wrong. Use the "Clear all calibration" RunType for the 1st standard in the injection list to remove the old calibration curve.

Normalize to: 100.00 %

Concentration calculation: Amount * Multipliers * Dil. factor

Include ISTD amount

Calculate mass %

Ill*	#	Type	Name	Signal	Ex
	1	[Icon]	C10-C25	Channel A -- Front Signal	
	2	[Icon]	C25-C40	Channel A -- Front Signal	
	3	[Icon]	C40-Cend	Channel A -- Front Signal	
	4	[Icon]	C10+C40toEnd		
	5	[Icon]	C10	Channel A -- Front Signal	
	6	[Icon]	C18	Channel A -- Front Signal	
	7	[Icon]	C25	Channel A -- Front Signal	
	8	[Icon]	C40	Channel A -- Front Signal	

Named Group Parameters	Name	RT
<input type="checkbox"/>	C10	4.285
<input type="checkbox"/>	C18	7.092
<input type="checkbox"/>	C40	12.682
<input type="checkbox"/>	C25	8.366
<input checked="" type="checkbox"/>	C10-C25	0.000
<input type="checkbox"/>	C25-C40	0.000
<input checked="" type="checkbox"/>	C40-Cend	0.000

Problem / Solution

Problem:

I need to use specific data analysis for my result calculation.

I need to use a specific calibration curve and weighting types.

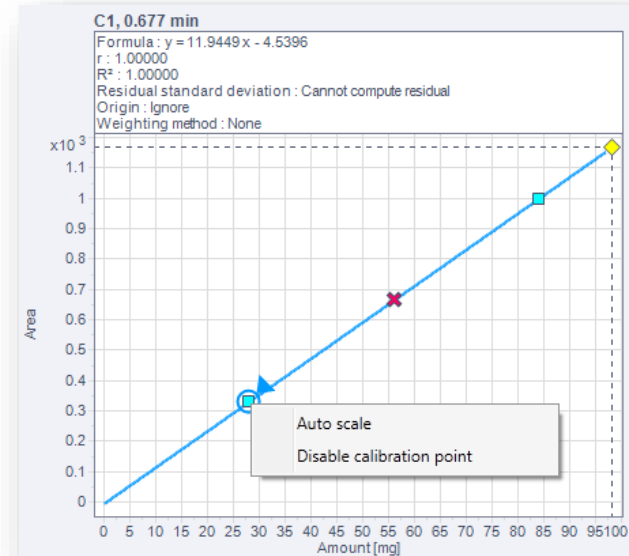
I need to use calibration curve functions.

Solution:

OpenLAB Data Analysis-Quantitation features

Calibration & Quantitation features

- New calibration curve and weighting types
 - quadratic, logarithmic, exponential, double-logarithmic - based on Area, Height, Area%, Height%
 - 1/Response and 1/Response² weighting
- Enhanced calibration curve functions
 - Enable/disable individual calibration points
 - display of last modification time of a calibration curve
 - display of last calibration time for a compound
 - curve calculation on average point per level or from all individual points



Compound Table | General

External standard Internal standard

Number of levels:

Curve calculation:

RF definition:

⚠ If you change the RF definition, you need to clear your calibration curve otherwise your results will be wrong.
Use the "Clear all calibration" RunType for the 1st standard in the injection list to remove the old calibration curve.

Normalize to: % Include ISTD amount

Concentration calculation: Calculate mass %

Problem / Solution

Problem:

I need to report the peaks in groups of certain compounds.

I need to report peaks in groups of groups.

I need to report the instrument parameters on my sample report.

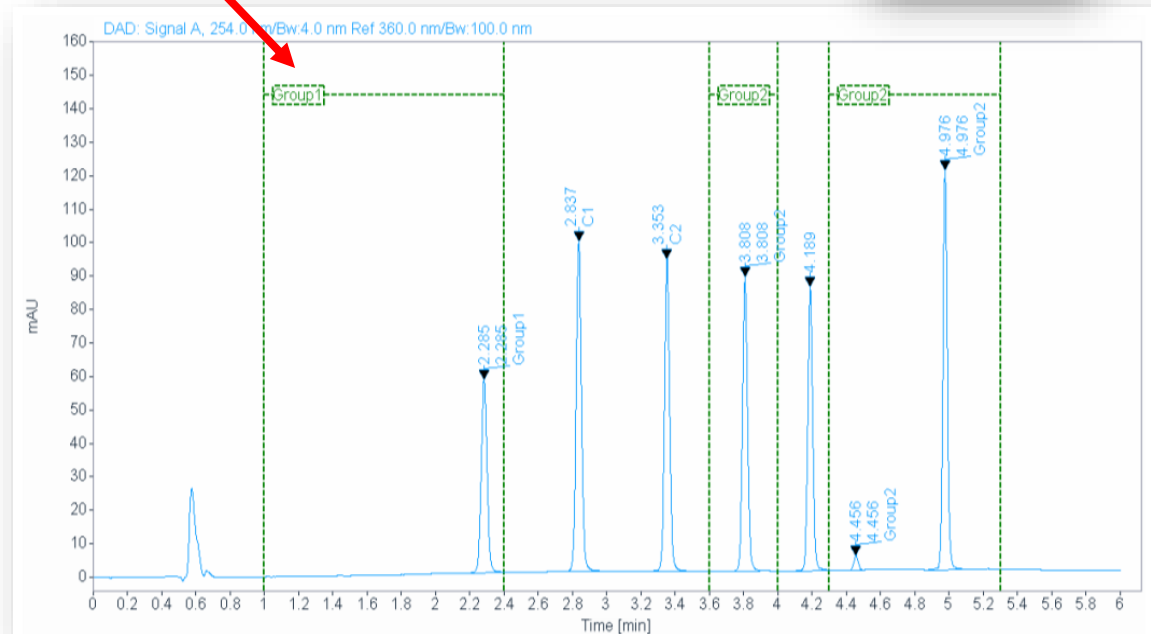
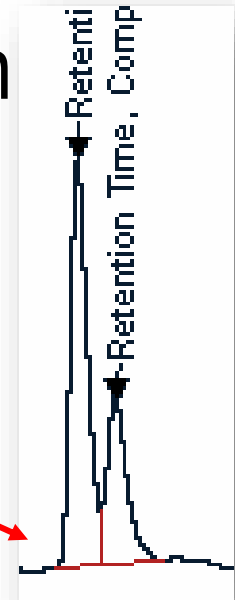
Solution:

Intelligent Reporting

Calibration curves / Chromatogram annotation

- Define color of the peak baseline
- Timed group annotation
 - Supports multiple regions
- Allow to define fixed marker intervals for the time axis of a chromatogram

Baseline is red



Problem / Solution

Problem:

I need to see a trend chart of samples with upper and lower limits

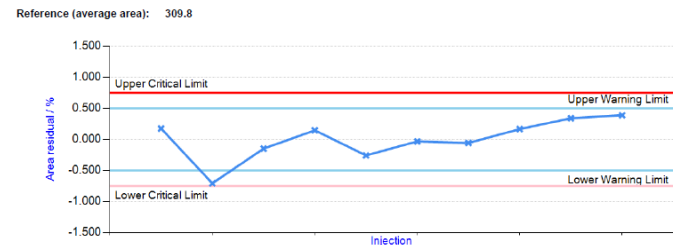
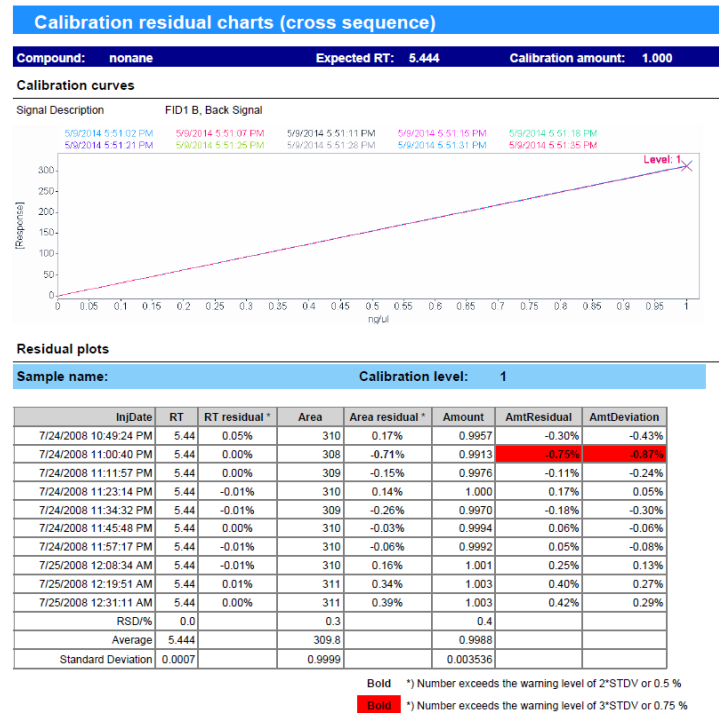
Solution:

OpenLAB Data Analysis-Intelligent Reporting

OpenLAB Data Analysis-Intelligent Reporting

Trend Charting

- Upper and Lower control limits can be entered interactively
- Outliers can be flagged automatically
 - 2- Sigma limits & 3- Sigma limits
- Applying Shewart- or Westgard- rules are possible
 - x points above or below average
 - x points showing up- or down-trend



Problem / Solution

Problem:


I need more flexibility in designing templates for the customized reports.

Solution:

OpenLAB CDS-Intelligent Reporting

OpenLAB CDS-Intelligent Reporting






- New “modified injection” flag (new DA) such as manually modified
- Barcode mismatch status


Sequence Summary Report  **Agilent Technologies**

Line#	Location	Sample Name	Inj#	Cal Lvl	Inj.Date	Manually modified?
8	Vial 2	sam2	2		1/30/2009 11:48:45 AM	None
11		sam3	1		1/30/2009 12:33:36 PM	Man. Integ.
12		sam4	1		1/30/2009 12:42:32 PM	Man. Integ and Compound ID

Single Sequence Summary [Rev. 0] Printed: 10/15/2013 11:29:57 AM Page 1 of 1

Sample name: Hallo-test Barcode: 000000019 Status: **barcode mismatch**

-  Clear Calculation Variable
-  Page No
-  Page No-Total Pages
-  Signatures
-  Total Pages

 **Font Format**

Family: Arial

Aharoni
Algerian
Andalus
Angsana New
AngsanaUPC
Aparajita
Arabic Typesetting
Arial

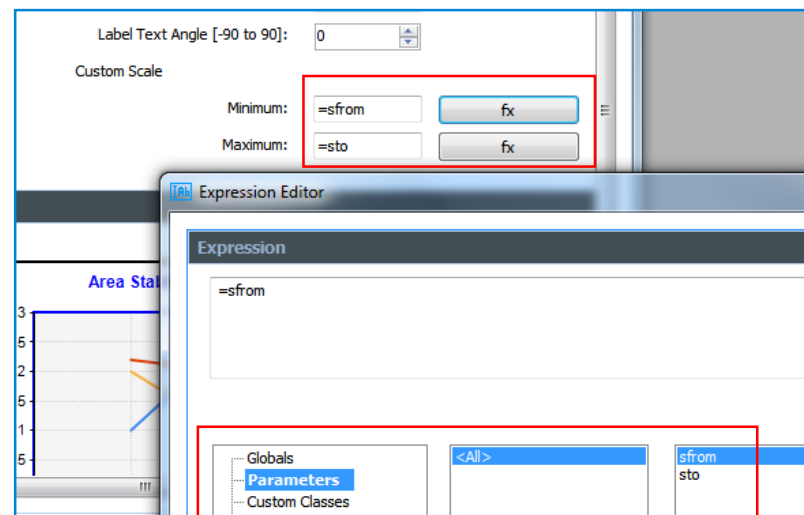
Size: 14
Style: Normal
Weight: Normal
Decoration: Normal

Preview
AbcXyz

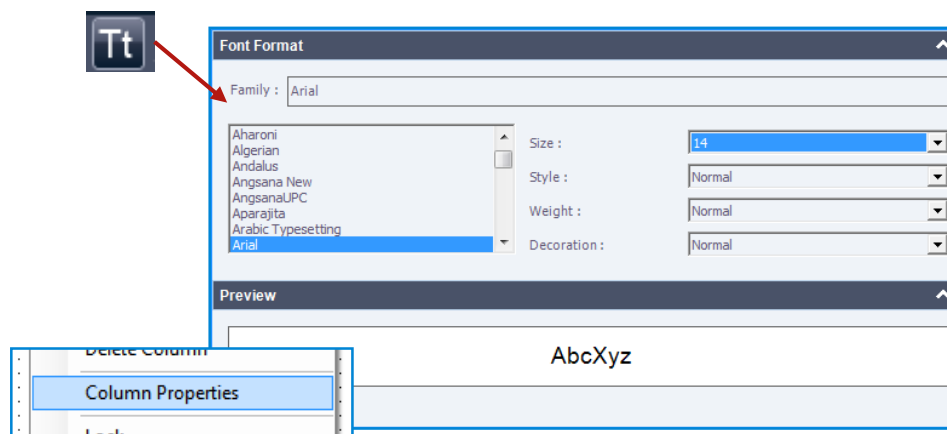
Delete Column
Column Properties
Lock

Charts and Customization

- Expression support for chart axis scaling
- Simple peak filter settings for chart control (like table/matrix)
- Snippets to insert page numbers into header or footer

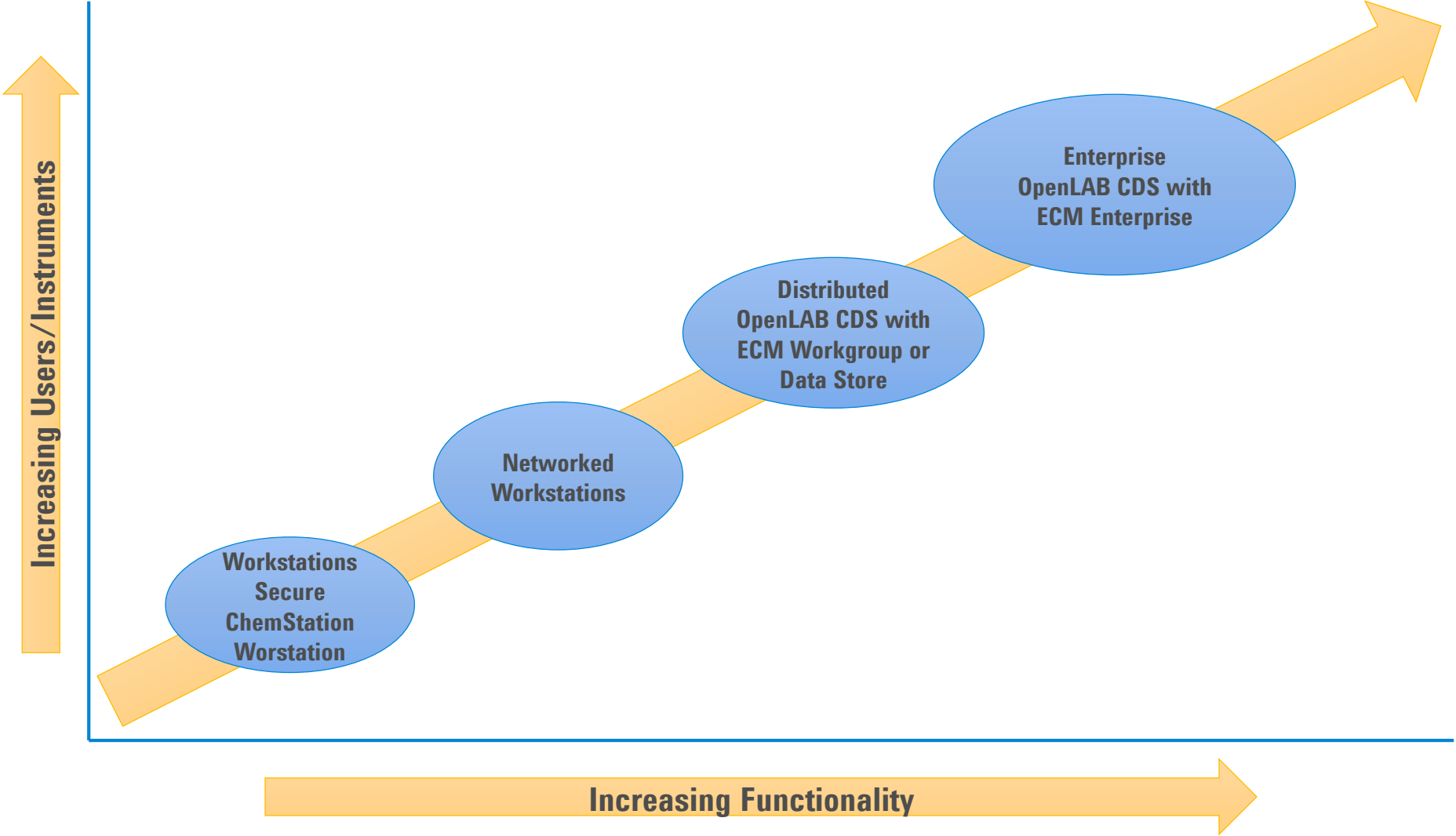


- Clear Calculation Variable
- Page No
- Page No-Total Pages
- Signatures
- Total Pages



In addition.....

OpenLAB CDS: Scalable in Storage, Lab Management and Administration



OpenLAB CDS: Networked Workstation Configuration

OpenLAB CDS Configurations: Networked workstation



- **Instrument Control:** Local on each workstation
- **Administration:** Central in OpenLAB Core Server Software
- **Storage:** Local on each workstation
- **Benefits:**
 - Central administration for all users, licenses and all user privileges
 - Status information in lab-at-a-glance view from all instruments connected

Fits well with:

- Laboratories with many instruments and few users, budget-controlled
- Laboratories looking for central lab monitoring without putting their instruments on the network

OpenLAB CDS Networked Workstation with Central Storage

OpenLAB CDS Configurations: Networked workstation with OpenLAB ECM



- **Instrument Control:** Local
- **Administration:** Central
- **Storage:** Central (OpenLAB ECM)
- **Benefits:**
 - Central administration (users, licenses, user privileges)
 - Instrument status information (lab-at-a-glance view)
 - Result data available from anywhere
 - Storage in central OpenLAB ECM with database storage

Fits well with:

- Laboratories who need GLP/GMP compliance and central storage
- Laboratories looking for central lab monitoring without putting their instruments on the network and have a need of database storage

Problem / Solution

Problem:

I cannot afford to duplicate work one of my colleagues has already done.

I need to securely store my data for a set period of time.

Solution:

OpenLAB Data Store allows you to centrally store your data, share it with colleagues, backup and archive.

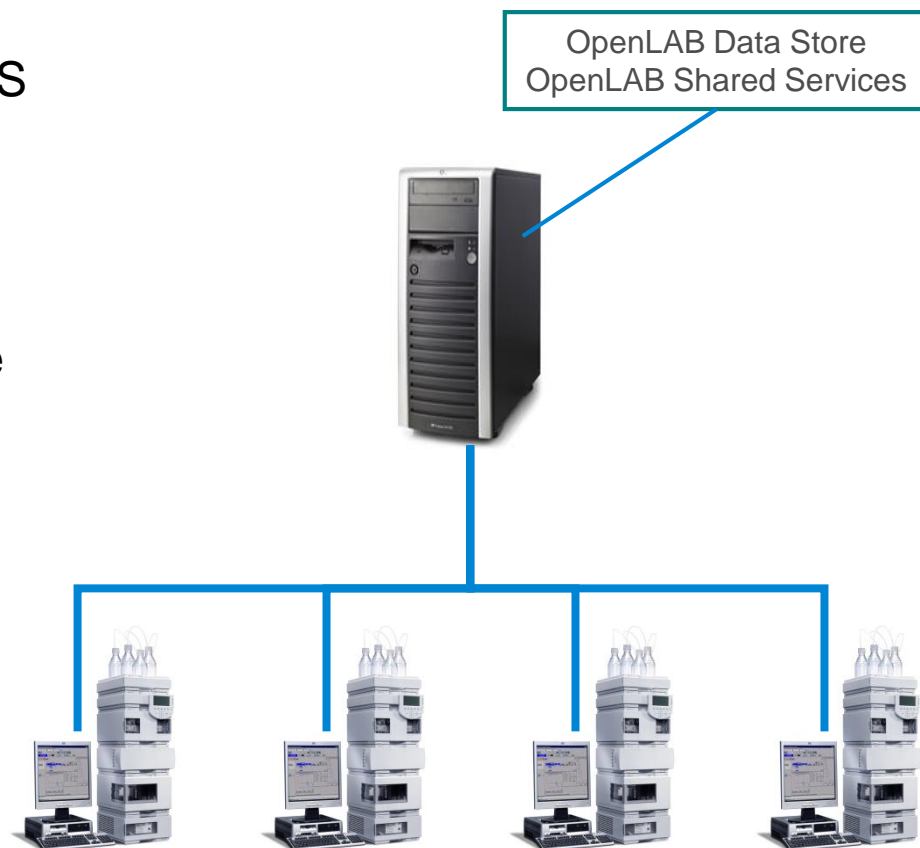
OpenLAB Data Store – Central Data Storage for OpenLAB CDS

Efficient Data Storage and Retrieval

- ✓ Centralized Storage for OpenLAB CDS
- ✓ Efficient search and retrieval of files
- ✓ Local Language Support (Chinese & Japanese)
- ✓ Free of Charge PostgreSQL database

21 CFR Part 11 Compliant

- ✓ Built to support FDA regulations
 - ✓ Data Integrity and Traceability
 - ✓ Electronic Signatures
 - ✓ Archival Capabilities



For More Information ...



For more information, check the Agilent web site
or contact your Agilent sales representative.