OpenLAB CDS ChemStation Edition C.01.06
Tips and Tricks for GC Users

Jennifer McCulley

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.

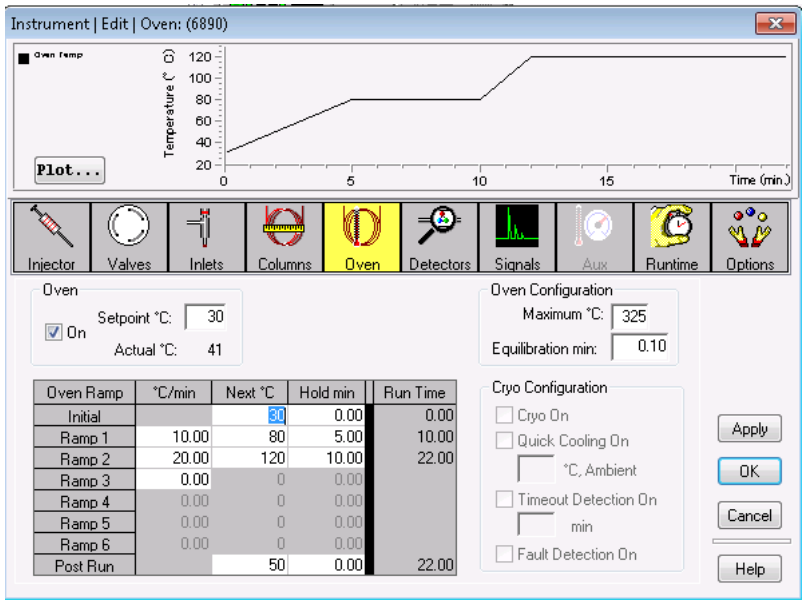
Solution:

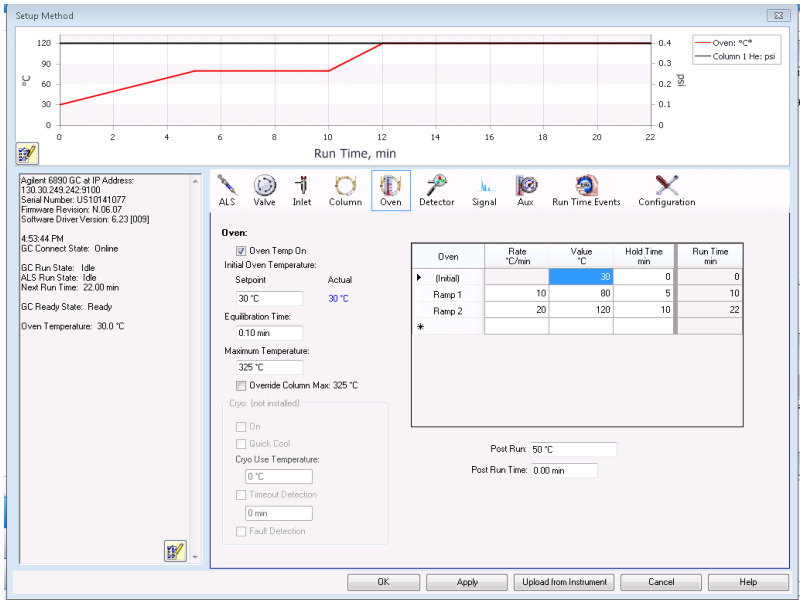
GC Acquisition Method Migration

Instrument Control Driver

Method Migration

OpenLAB CDS ChemStation-C.01.06





6890 GC Classic Method

6890 GC Enhanced Method

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

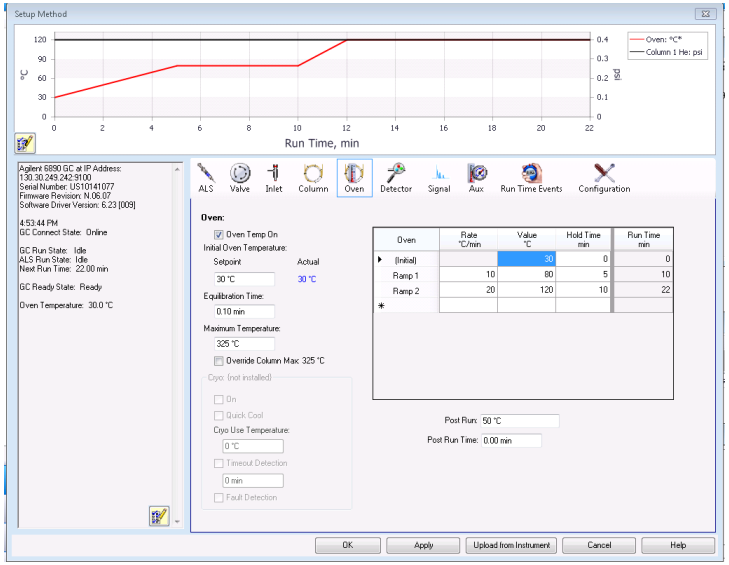
Instrument Control Driver

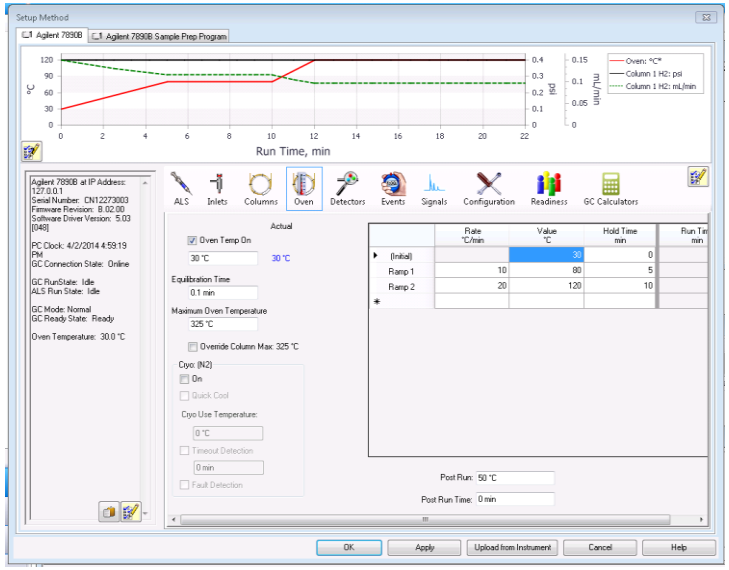
Method Migration

OpenLAB CDS ChemStation-C.01.06

6890 GC Method

Open Method in OpenLAB CDS C.01.06 and save

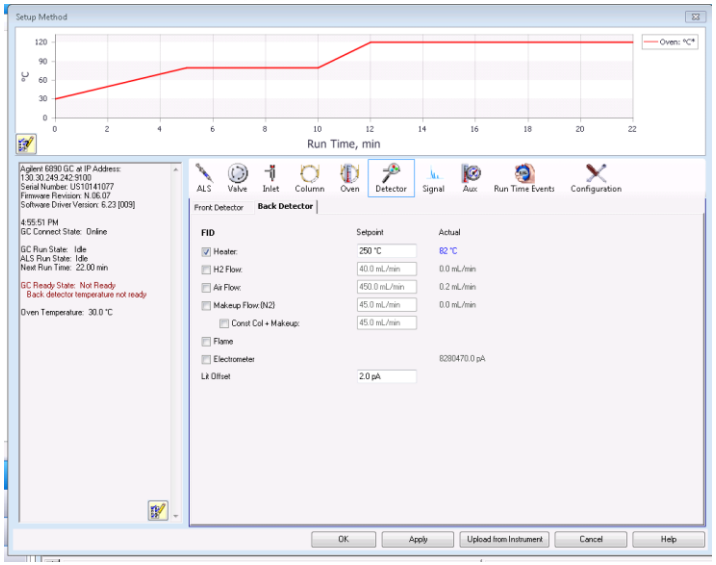


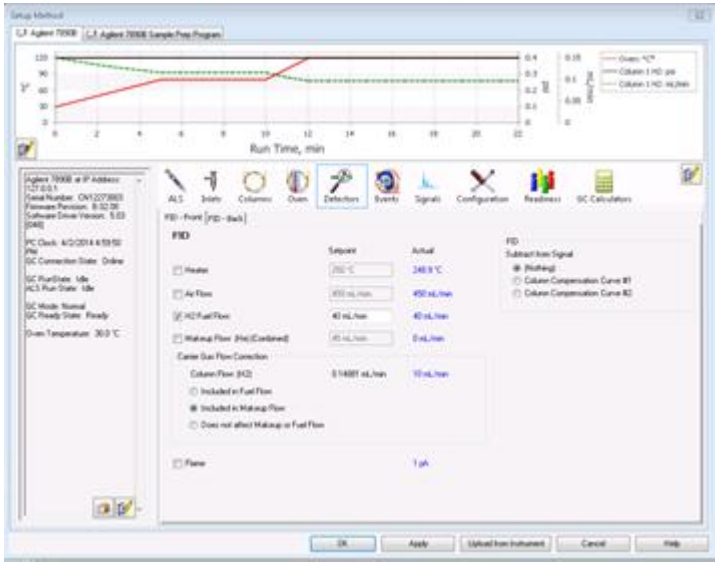


Instrument Control Driver

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

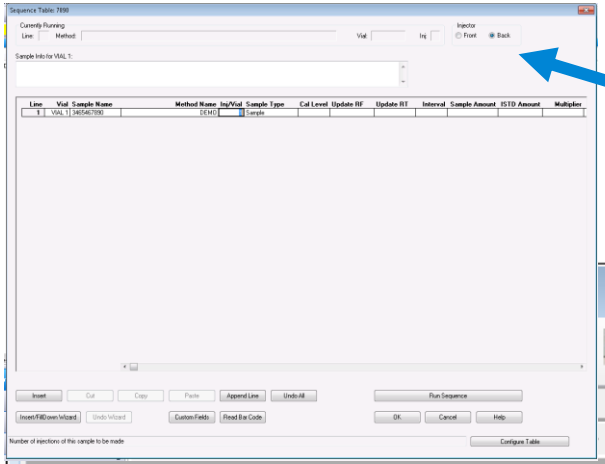
Problem:

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

Solution:

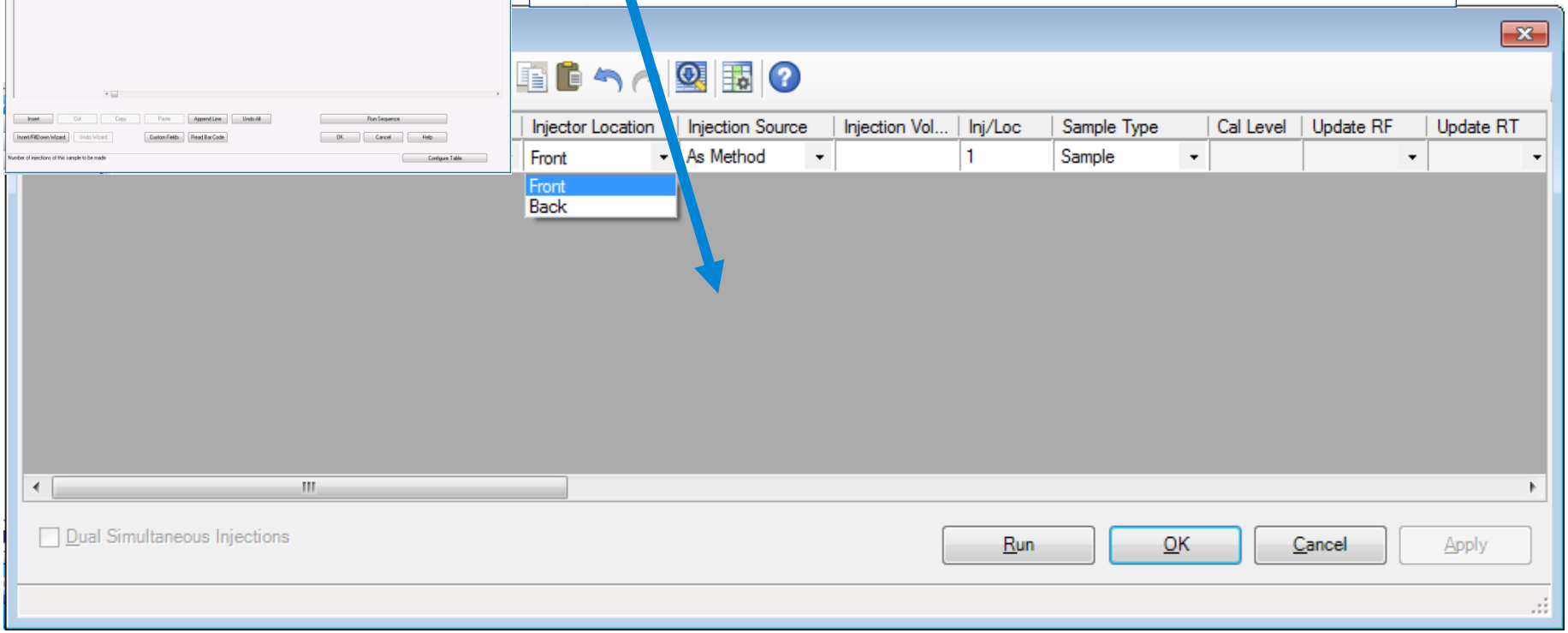
Improved Sequence Table

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:

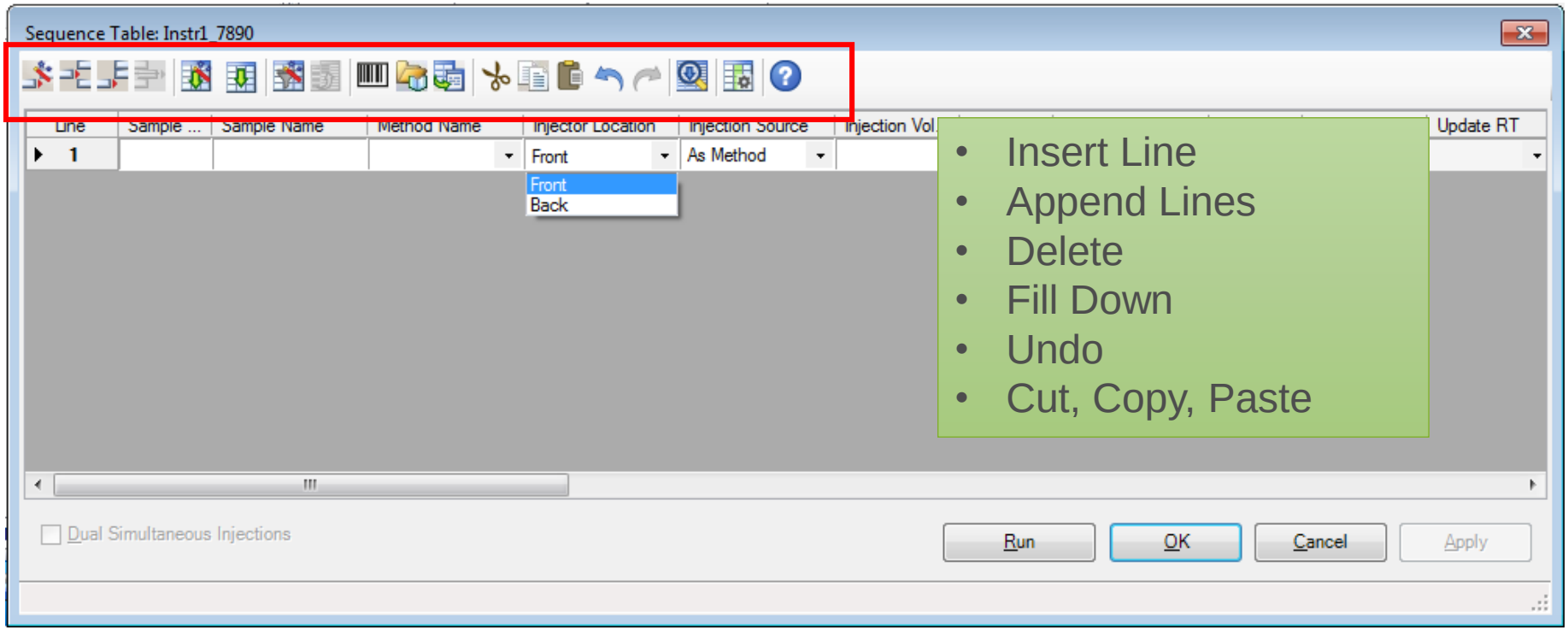
I need more flexibility with the sequence Table

- 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



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

Problem / Solution

Problem:

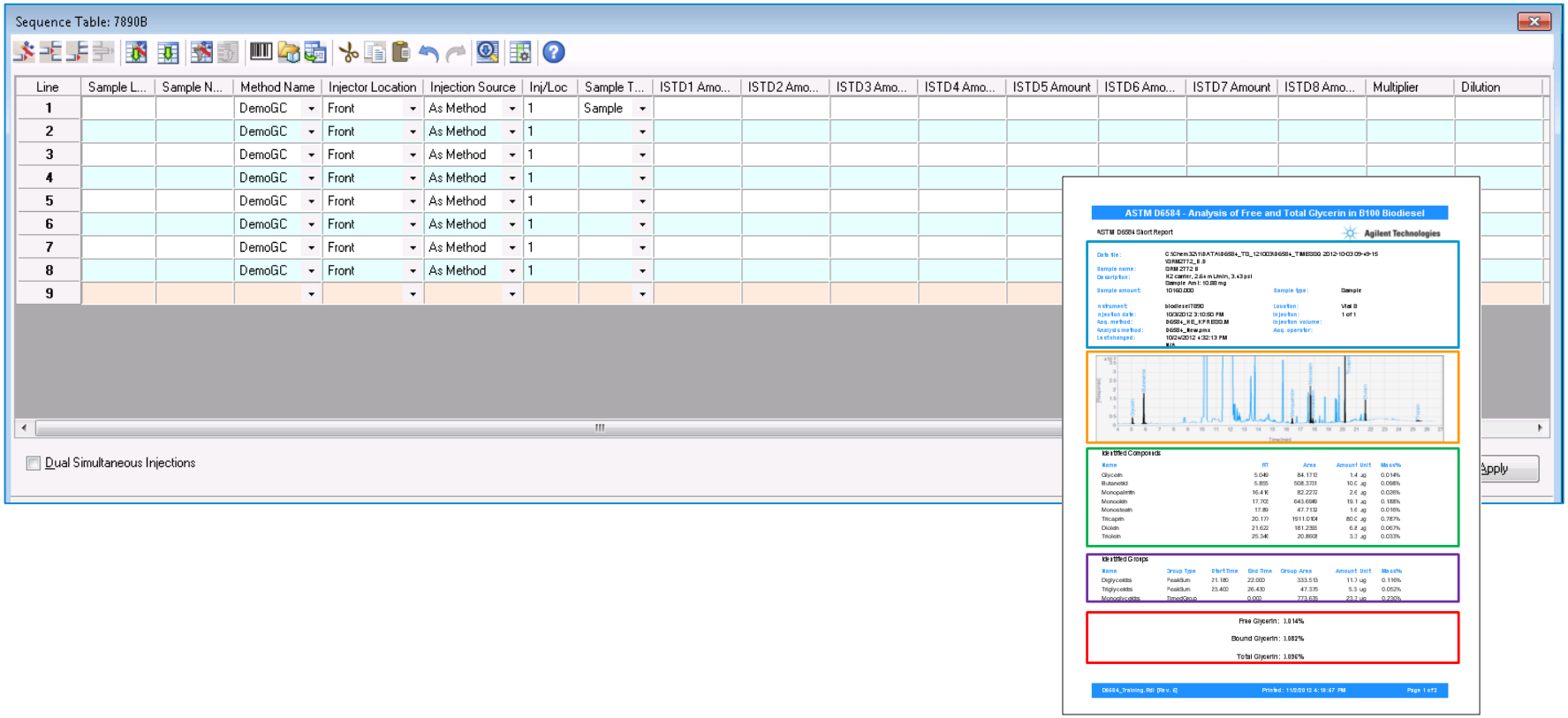
I need to add more than one ISTD to the sequence table.

Solution:

Improved Sequence Table

Sequence Table

- Improve customer experience
- Up to 8 ISTD input



Problem / Solution

Problem:

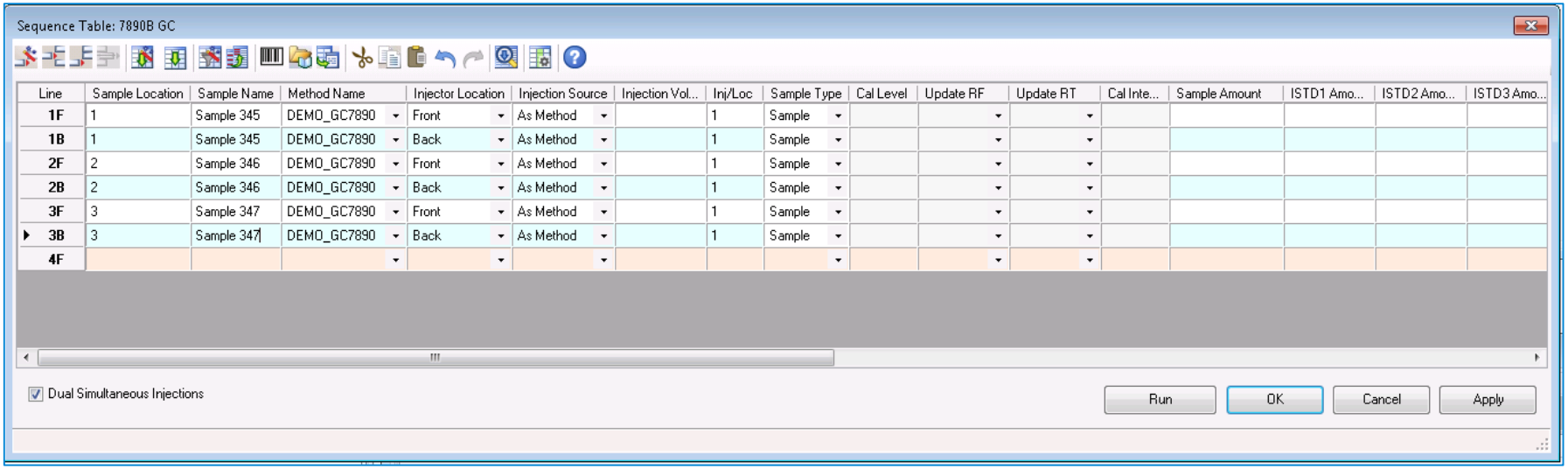
I want to be able to set up a dual simultaneous sequence to increase the throughput on the 6890/7890 series GC.

Solution:

Improved Sequence Table

Sequence Table

- Improve customer experience of ChemStation sequence table



Problem / Solution

Problem:

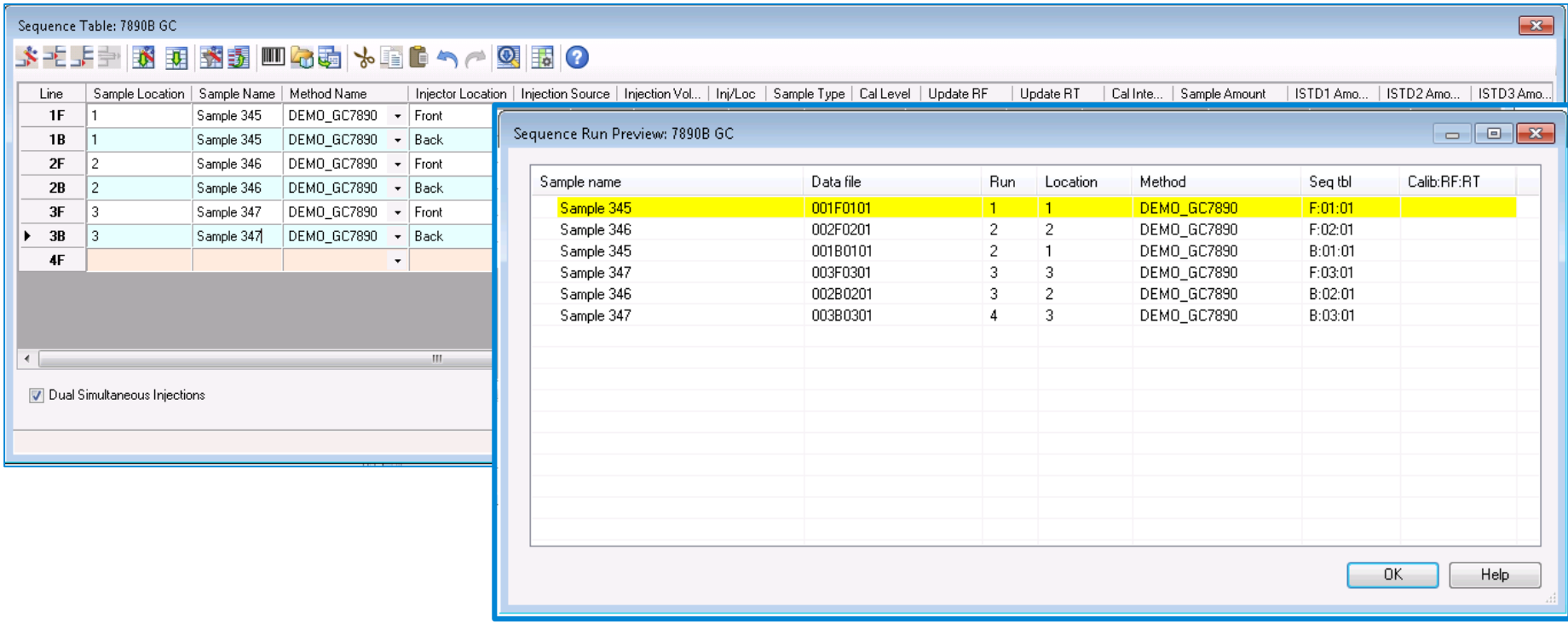
I want to see all the injections in the order in which they will run in the sequence, so there are no errors in the sequence table.

Solution:

Improved Sequence Table- Sequence Preview

Sequence Table

- Sequence Run Preview



Problem / Solution

Problem:

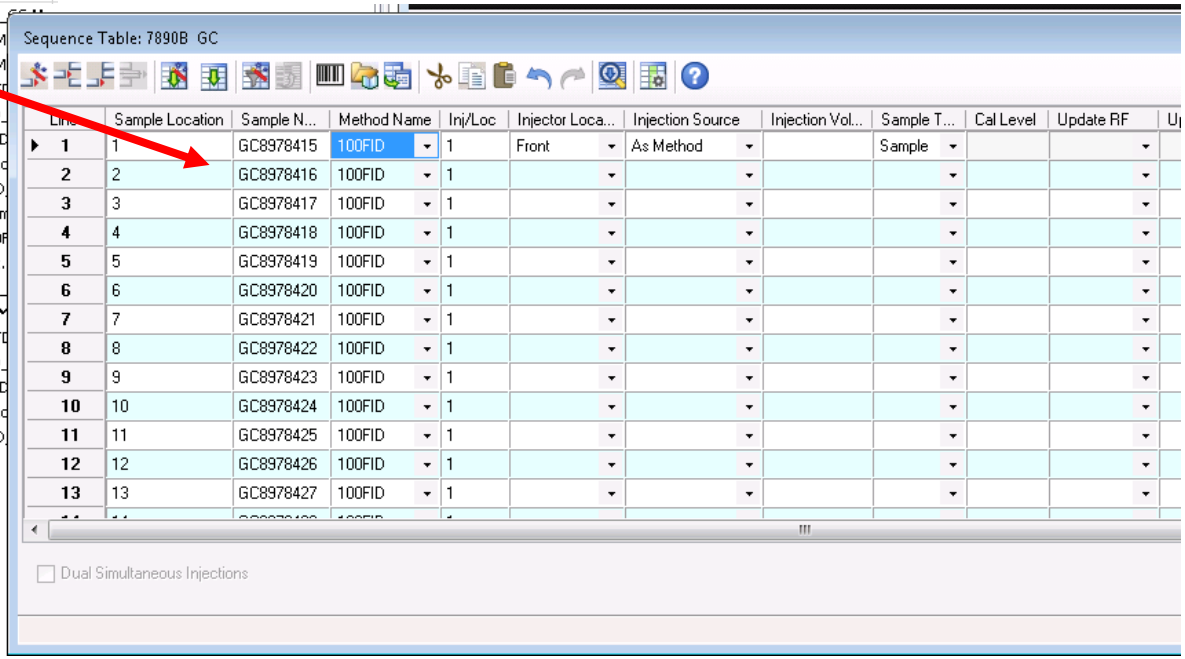
It is easier to obtain/edit the worklist of samples in excel, so I want an easy way to transfer it to the CDS sequence file.

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	
8	7	GC8978421	100FID	
9	8	GC8978422	100FID	
10	9	GC8978423	100FID	
11	10	GC8978424	100FID	
12	11	GC8978425	100FID	
13	12	GC8978426	100FID	
14	13	GC8978427	100FID	
15	14	GC8978428	100FID	
16	15	GC8978429	100FID	



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.

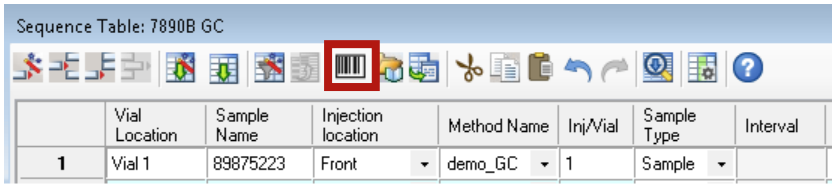
Solution:

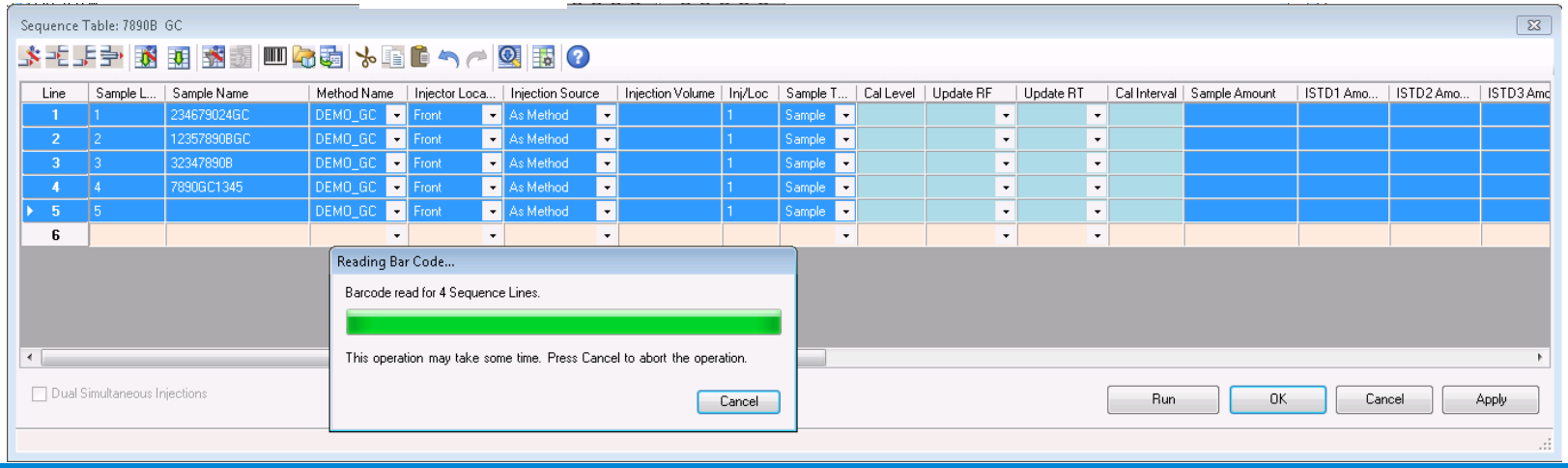
Barcode Reading in Sequence Table

Sequence Table

Barcode Reading

Print the barcode label → Sample on Instrument → Select the lines in the sequence table → Click on Read barcode icon → Barcode info - Sample Name





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:

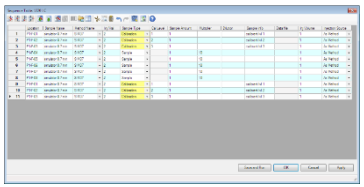
Barcode Reading-Chain of Custody

Barcode Reading

Chain of Custody Workflow

User labels the vials

Enter sample information including the sample ID into the sequence table



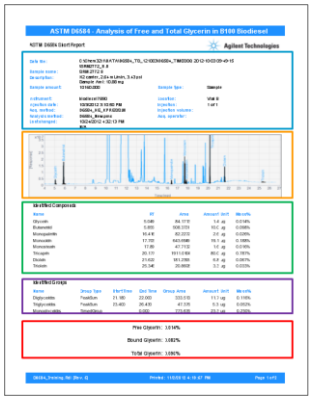
Instrument reads the barcode

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

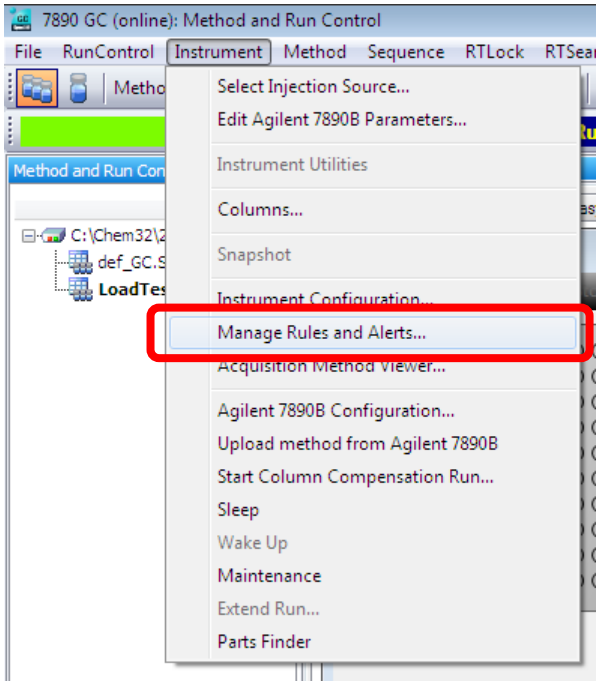
Problem:

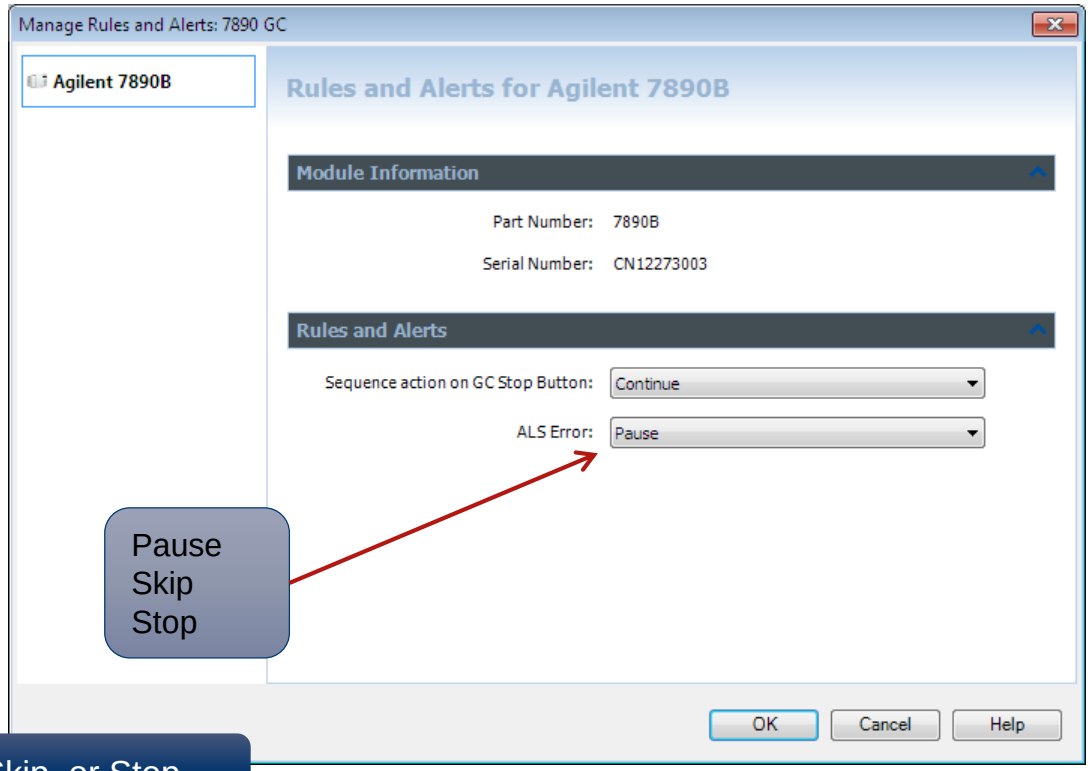
I missed putting a vial in the autosampler or miscounted the vials.

Solution:

Manage Rules and Alerts-Retry, Abort, or Skip

Manage Rules and Alerts





Pause
Skip
Stop

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.

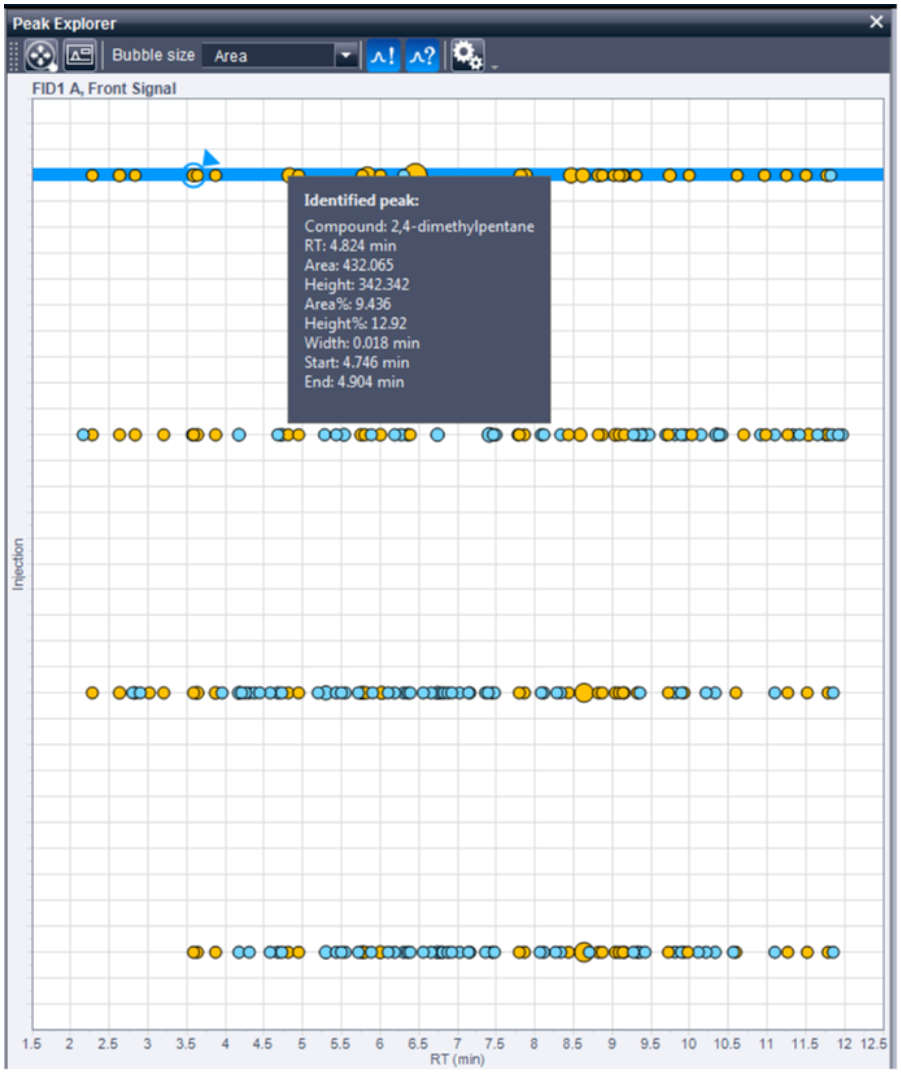
Solution:

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.

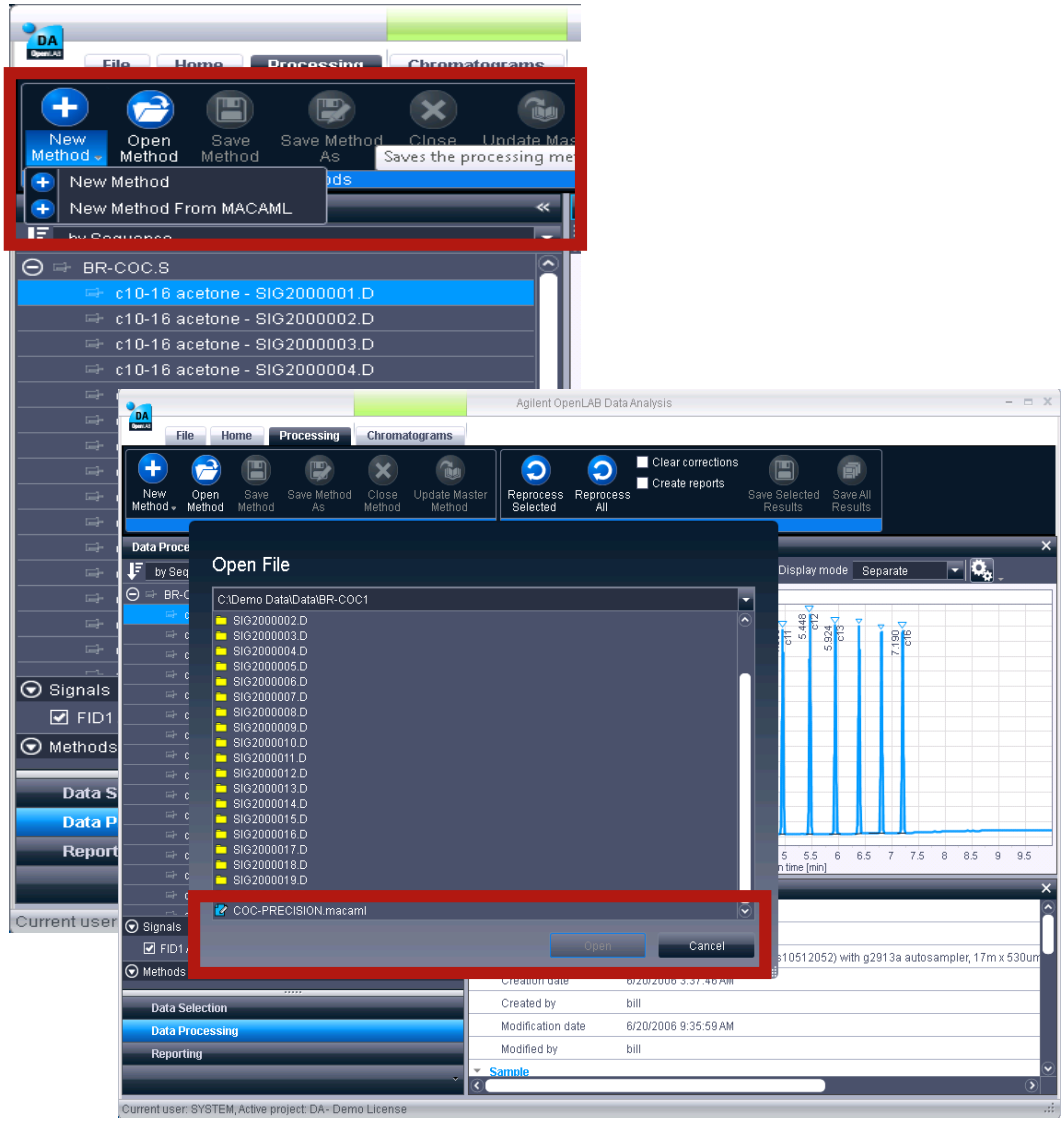
I previously used EzChrom or ChemStation and I want the same results when I reprocess the data.

Solution:

OpenLAB Data Analysis: Choice of integrators

Productivity

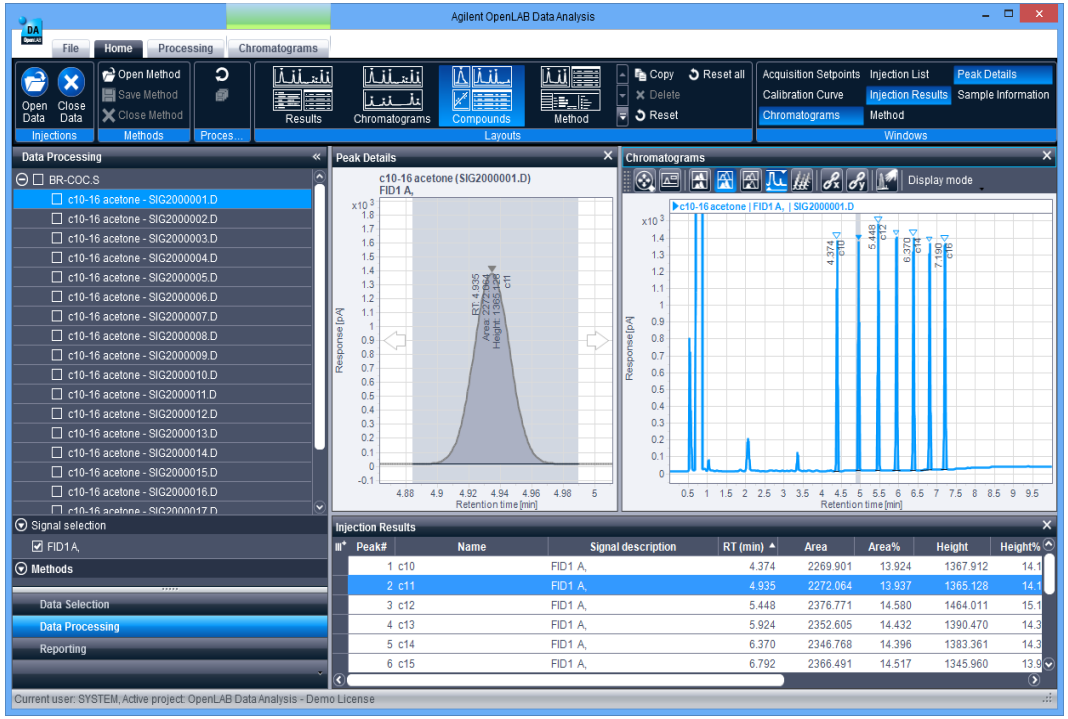
Import of compound ID table (Name, Expected RT, ISTD flag, RT Window) from EZChrom and ChemStation using MACAML files

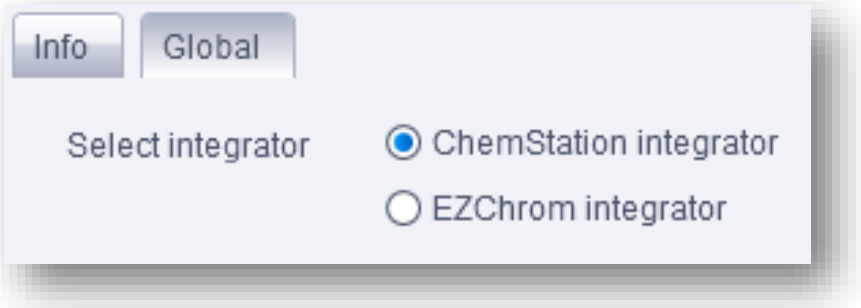


Productivity

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.

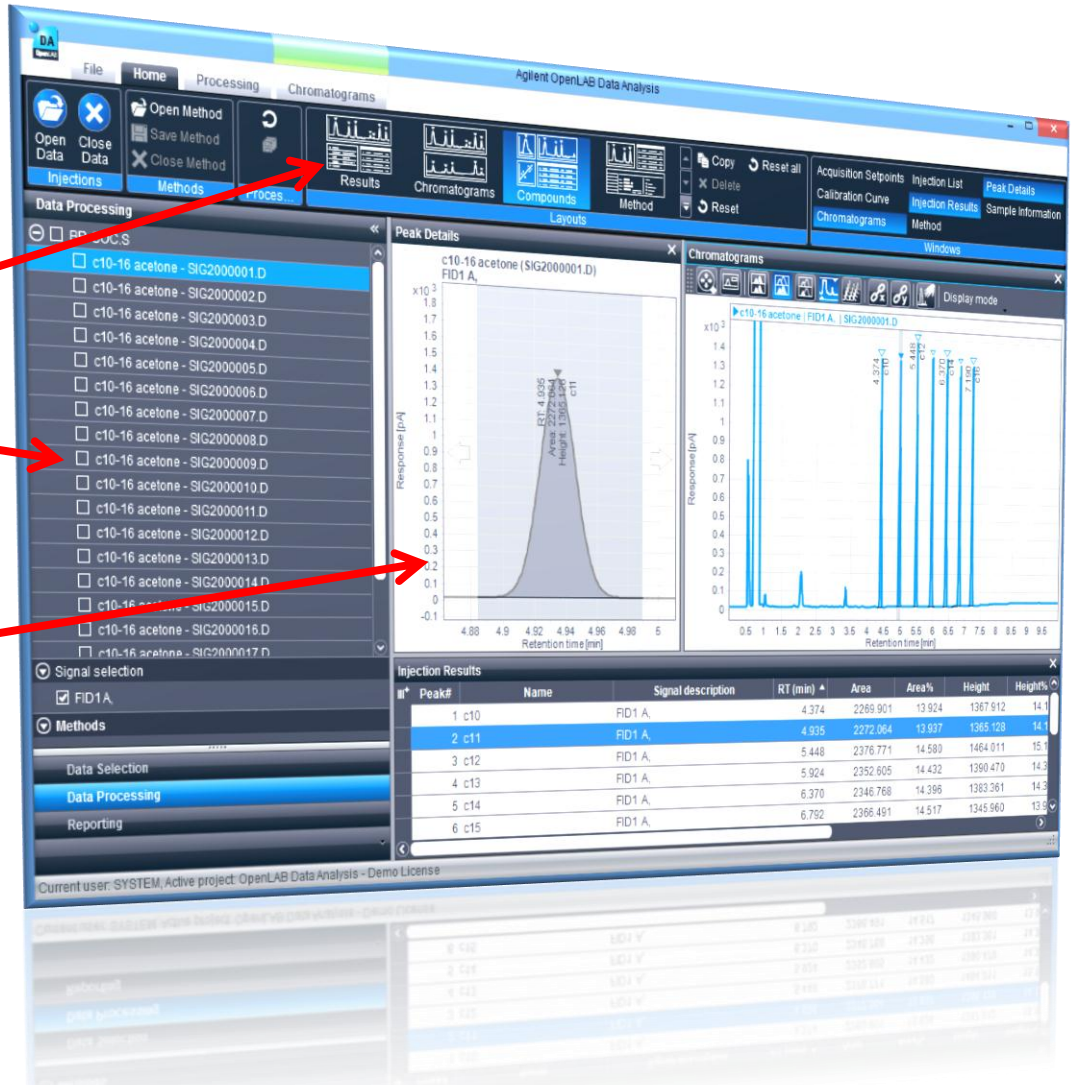
I want to view data in my personalized preferences while my colleagues have another preference.

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.

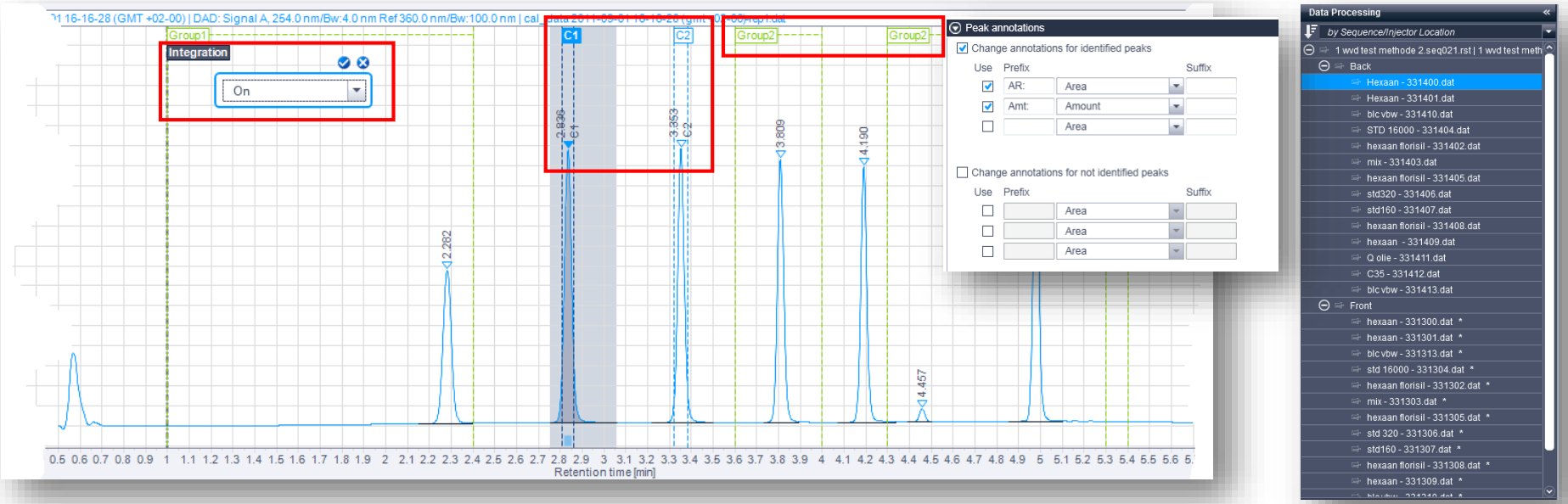
Solution:

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.

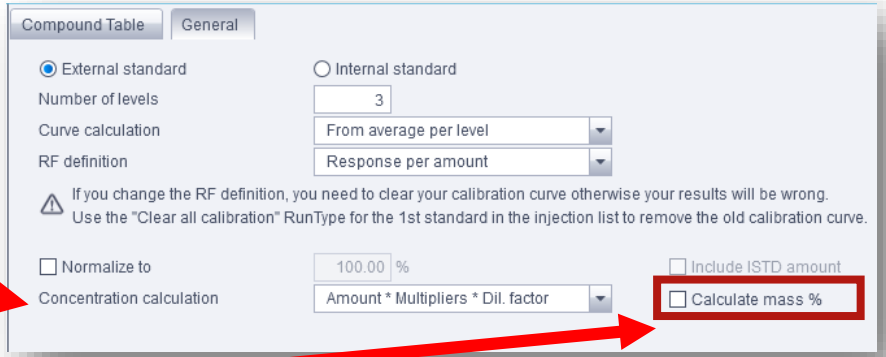
- I want to use published Relative Retention Times
- I need to report results in mass%.
- I need to add multipliers in the data analysis to obtain the result for my analysis.

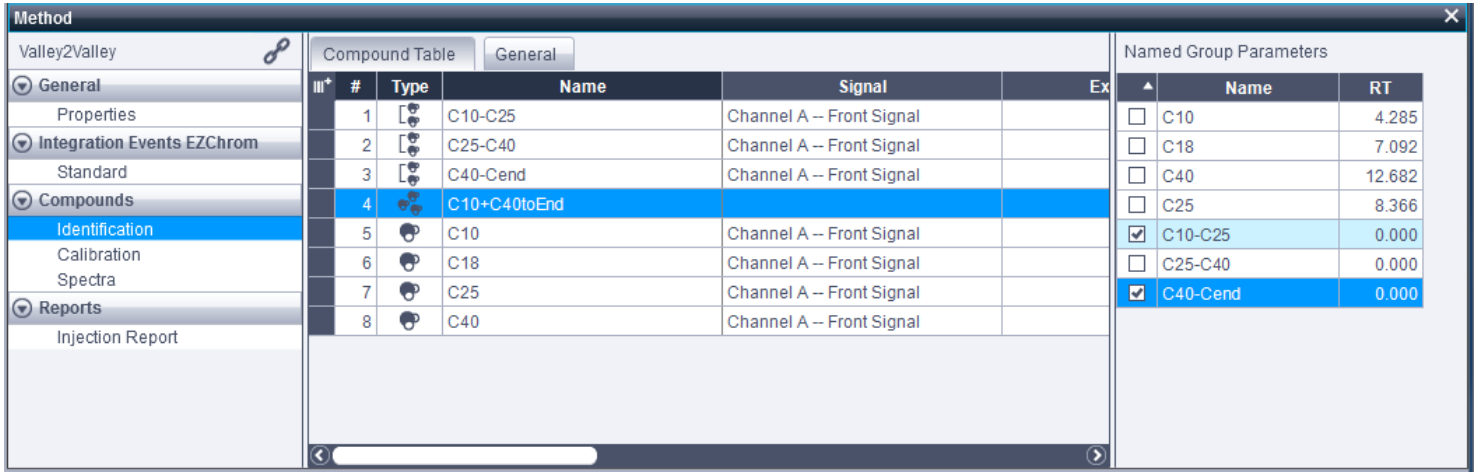
Solution:

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





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.

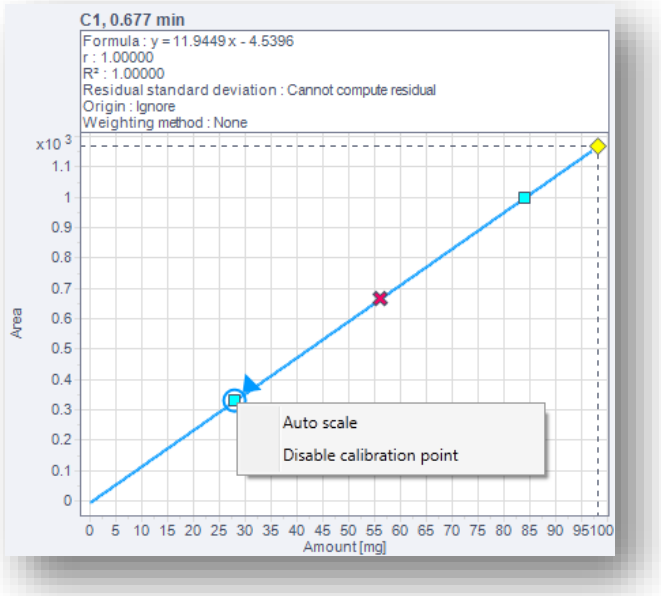
I need to use calibration curve functions.

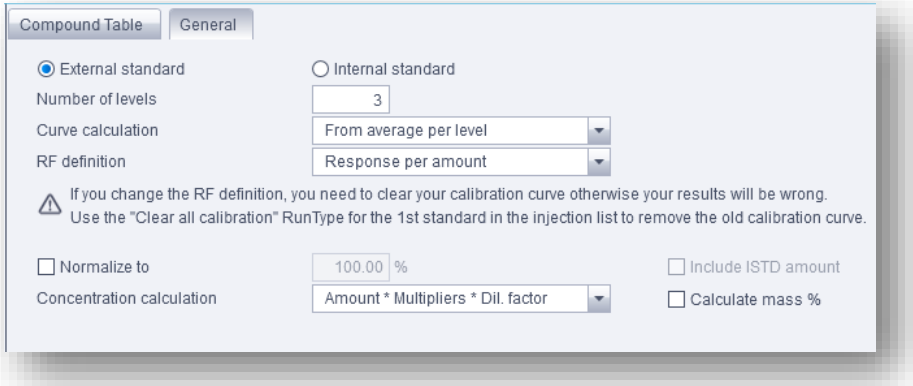
Solution:

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/Response^2 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





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.

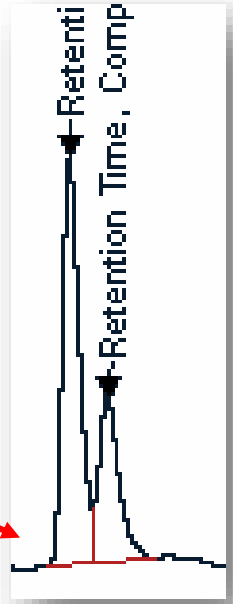
Solution:

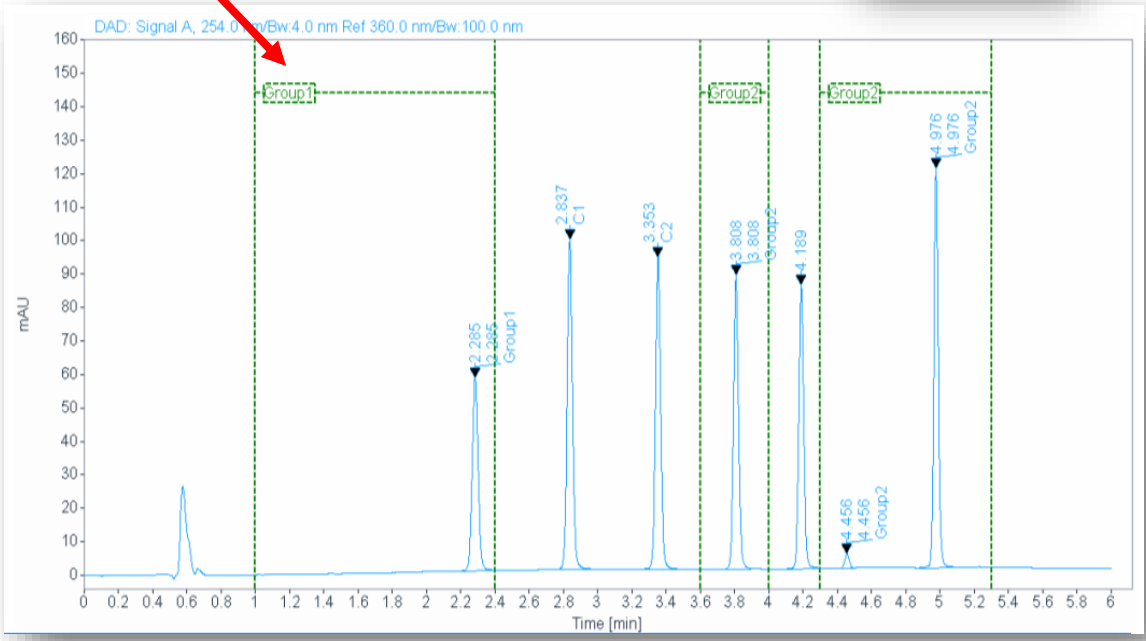
Intelligent Reporting

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:

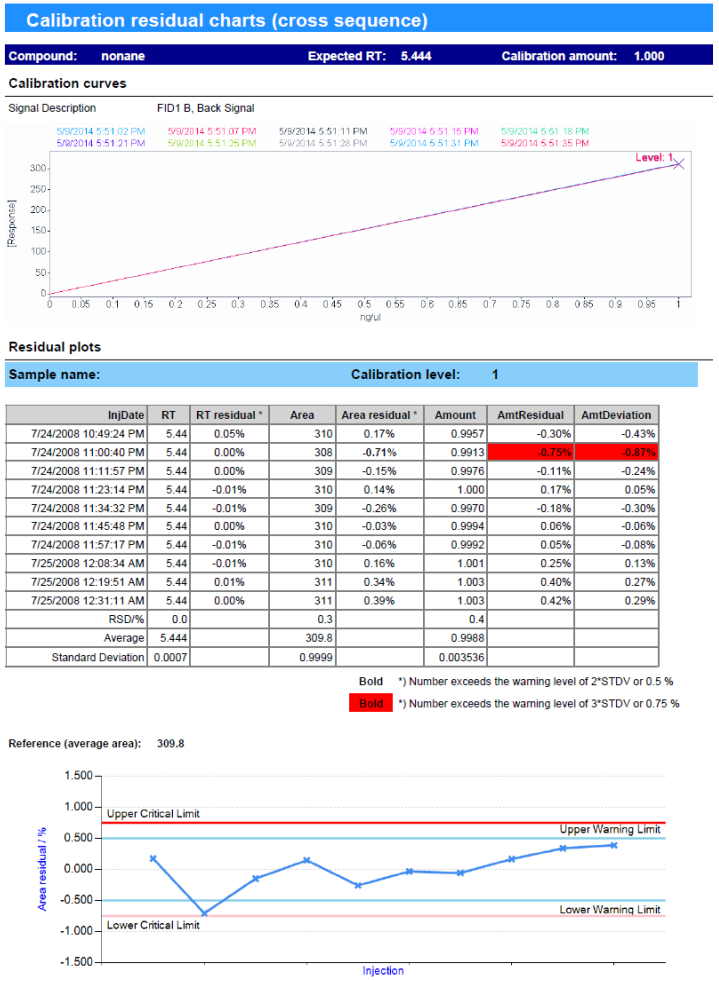
I need to see a trend chart of samples with upper and lower limits

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



Calibration residual charts (cross sequence)

Compound: nonane **Expected RT:** 5.444 **Calibration amount:** 1.000

Calibration curves

Signal Description FID1 B, Back Signal

5/9/2014 5:51:02 PM 5/9/2014 5:51:07 PM 5/9/2014 5:51:11 PM 5/9/2014 5:51:15 PM 5/9/2014 5:51:18 PM
5/9/2014 5:51:21 PM 5/9/2014 5:51:25 PM 5/9/2014 5:51:28 PM 5/9/2014 5:51:31 PM 5/9/2014 5:51:35 PM

Level: 1

[Response]

ng/ul

Residual plots

Sample name: **Calibration level:** 1

InjDate	RT	RT residual *	Area	Area residual *	Amount	AmtResidual	AmtDeviation
7/24/2008 10:49:24 PM	5.44	0.05%	310	0.17%	0.9957	-0.30%	-0.43%
7/24/2008 11:00:40 PM	5.44	0.00%	308	-0.71%	0.9913	-0.75%	-0.87%
7/24/2008 11:11:57 PM	5.44	0.00%	309	-0.15%	0.9976	-0.11%	-0.24%
7/24/2008 11:23:14 PM	5.44	-0.01%	310	0.14%	1.000	0.17%	0.05%
7/24/2008 11:34:32 PM	5.44	-0.01%	309	-0.26%	0.9970	-0.18%	-0.30%
7/24/2008 11:45:48 PM	5.44	0.00%	310	-0.03%	0.9994	0.06%	-0.06%
7/24/2008 11:57:17 PM	5.44	-0.01%	310	-0.06%	0.9992	0.05%	-0.08%
7/25/2008 12:08:34 AM	5.44	-0.01%	310	0.16%	1.001	0.25%	0.13%
7/25/2008 12:19:51 AM	5.44	0.01%	311	0.34%	1.003	0.40%	0.27%
7/25/2008 12:31:11 AM	5.44	0.00%	311	0.39%	1.003	0.42%	0.29%
RSD/%	0.0		0.3		0.4		
Average	5.444		309.8		0.9988		
Standard Deviation	0.0007		0.9999		0.003536		

Bold *) Number exceeds the warning level of 2*STDV or 0.5 %

Bold *) Number exceeds the warning level of 3*STDV or 0.75 %

Reference (average area): 309.8

Upper Critical Limit

Upper Warning Limit

Lower Warning Limit

Lower Critical Limit

Area residual / %

Injection

Problem / Solution

Problem:

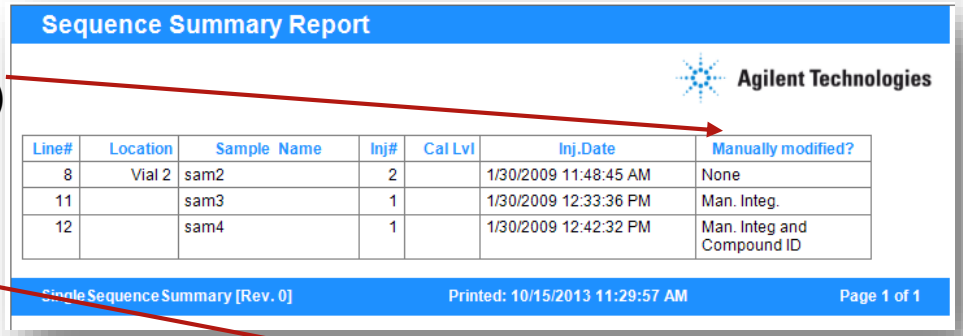
I need more flexibility in designing templates for the customized reports.

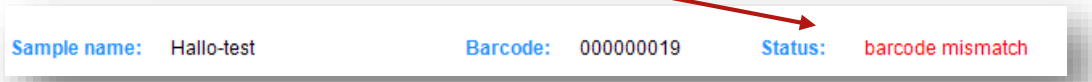
Solution:

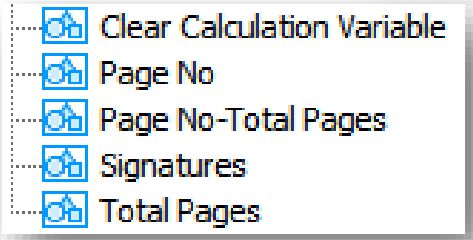
OpenLAB CDS-Intelligent Reporting

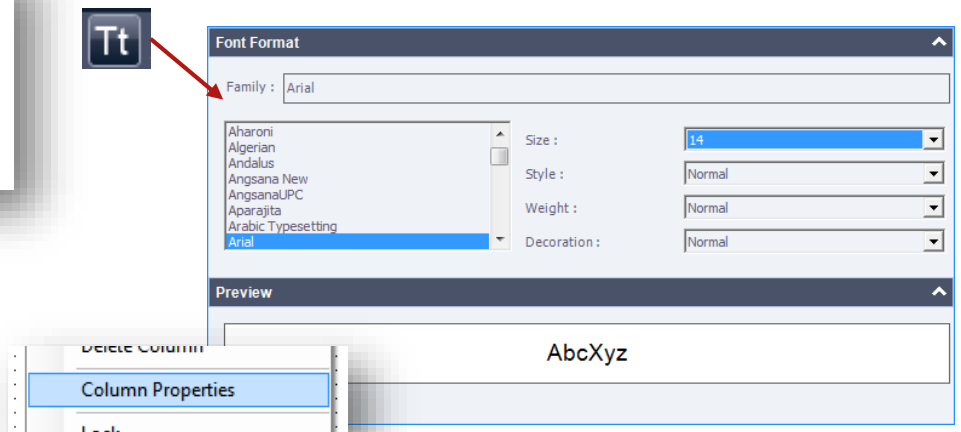
OpenLAB CDS-Intelligent Reporting

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



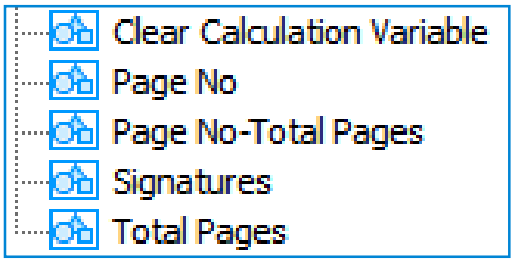


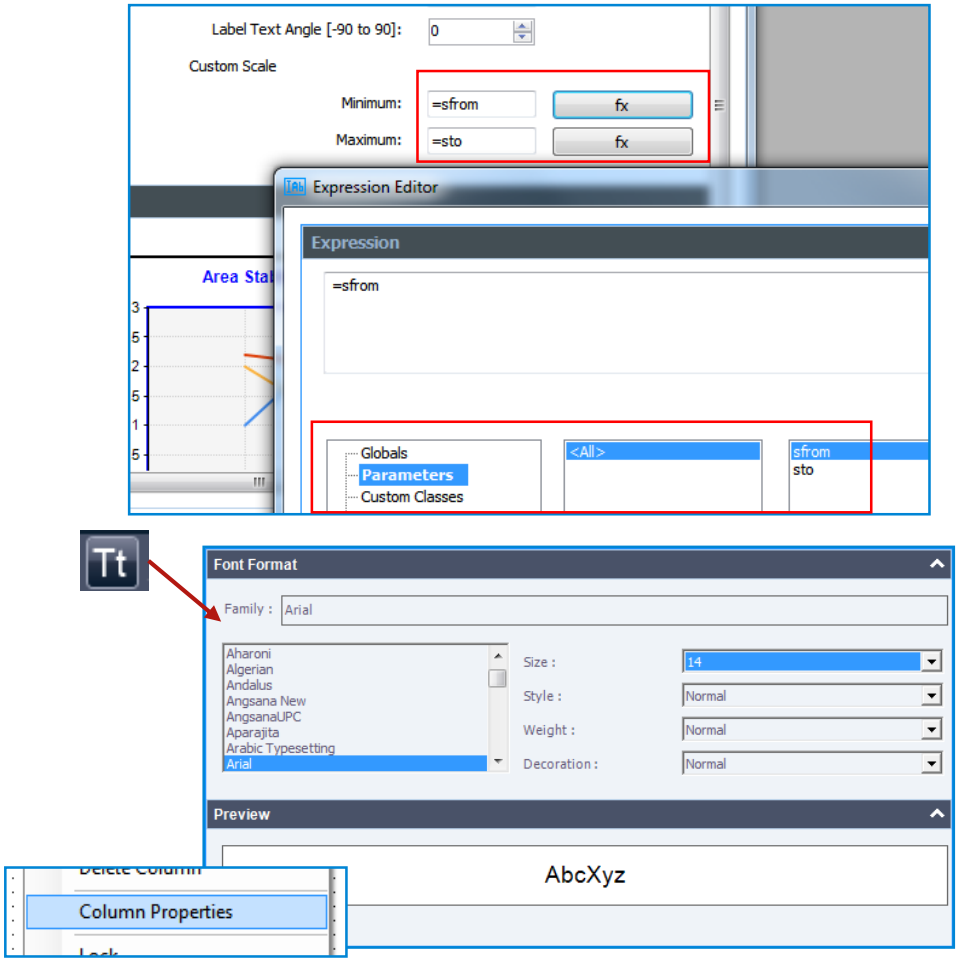




Charts and Customization

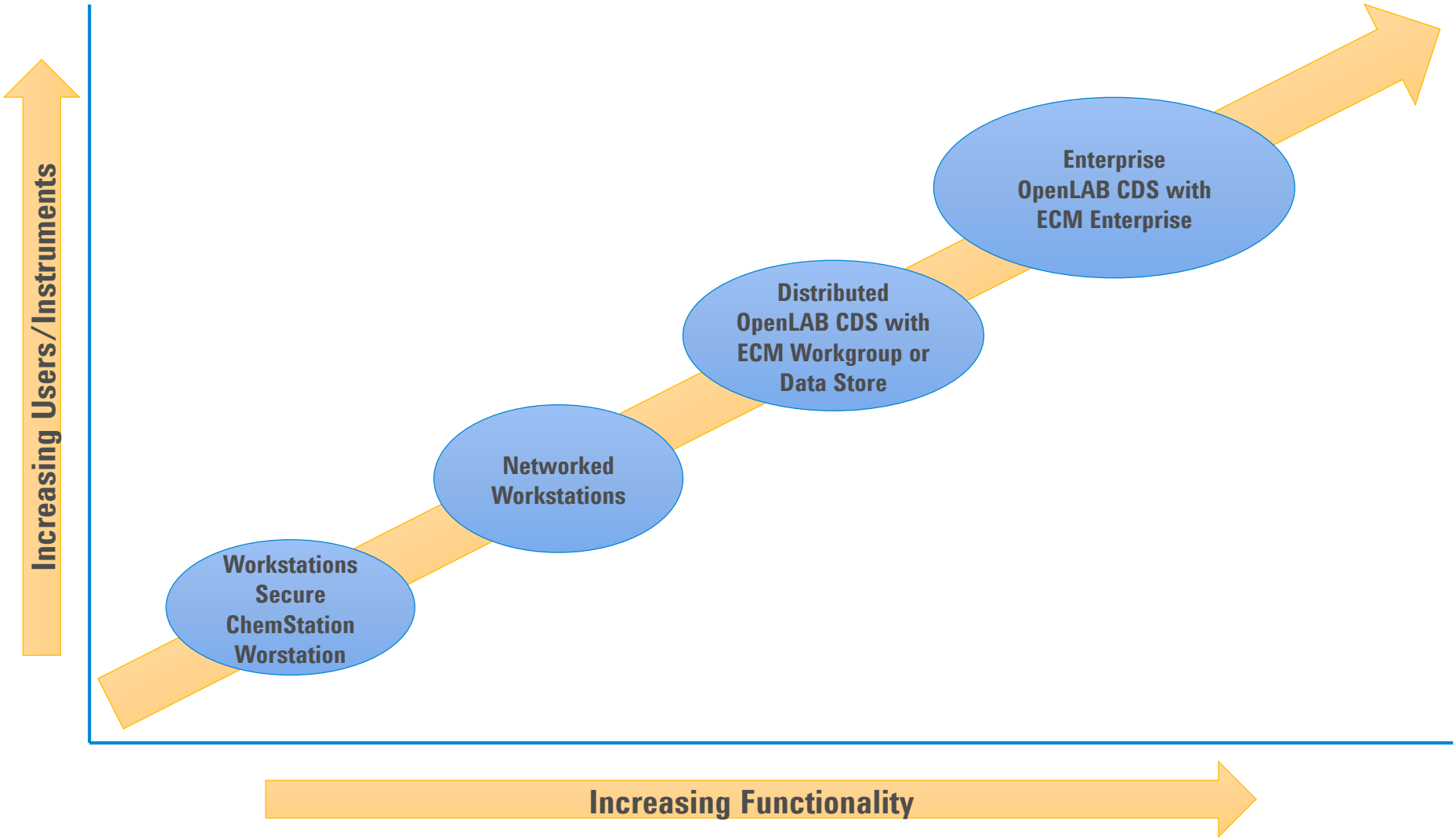
- Expression support for chart axis scaling
- Simple peak filter settings for chart control (like table/matrix)
- Snippets to insert page numbers into header or footer





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.

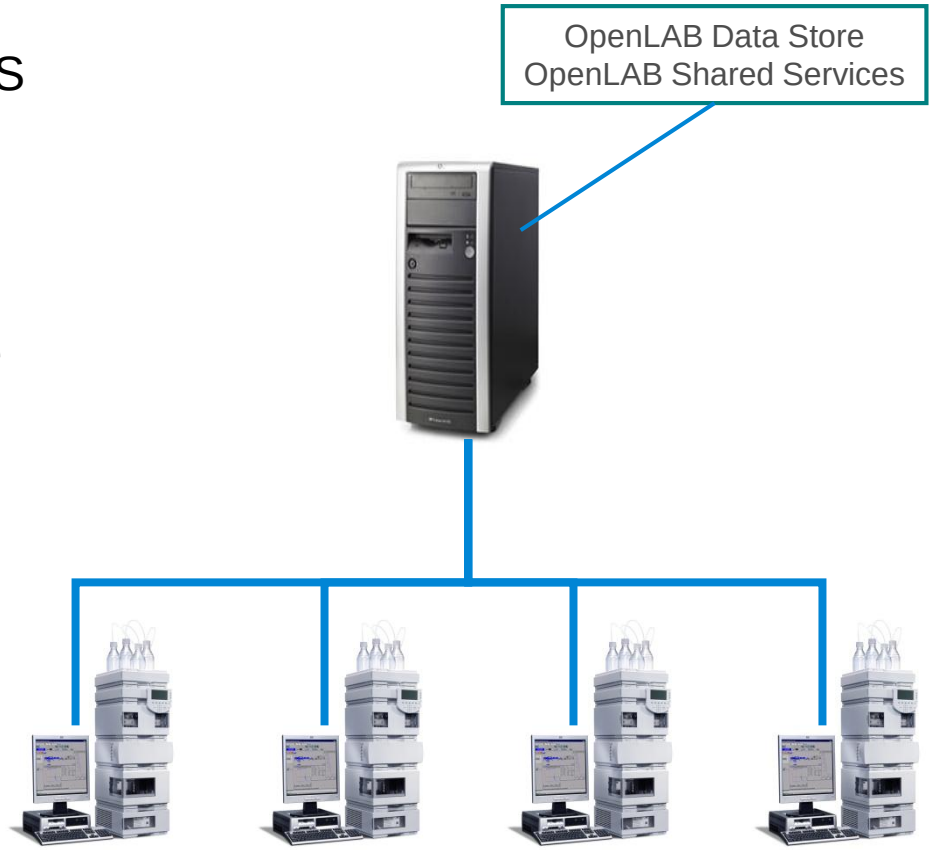
OpenLAB Data Store – Central Data Storage for OpenLAB CDS

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.