



Data integriteit met OpenLAB

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Topics voor vandaag

OpenLAB ECM

- Introductie

- Wat is het precies

- Integratie met andere systemen

- Voordelen

OpenLAB CDS

- Wat is het

- Hoe ziet het er uit

- Hoe is integriteit gewaarborgd

- Integratie met andere systemen

OpenLAB ELN

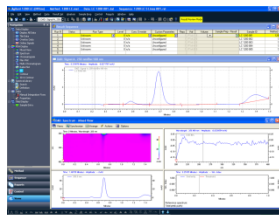
- Wat is nou een echt ELN????

OpenLAB - *The Operating System for the Laboratory*

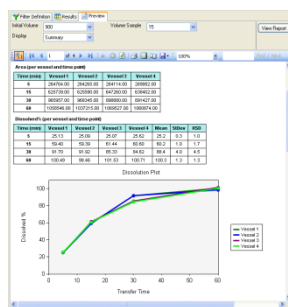
Agilent Solutions for the Lab Informatics



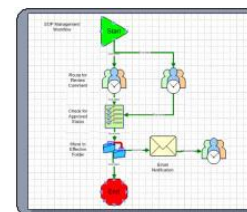
Enterprise
Content
Management
(ECM)



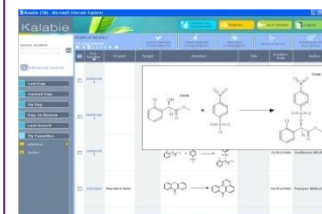
Multi-vendor
Instrument Control
Manager
(OL CDS)



Intelligent
Reporter



Business
Process
Management
(BPM)



Electronic Lab
Notebook
(ELN)

OpenLAB is a fully integrated laboratory system that links people, processes and data, providing all information needed for accelerated decision making.

Integrating framework for other applications and techniques
Web-based, n-tier architecture scalable from small lab to global implementation

OpenLAB manages instruments, people/process and content!



OpenLAB ECM

Data security and authenticity

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Product Specialist
Agilent Technologies



Challenges



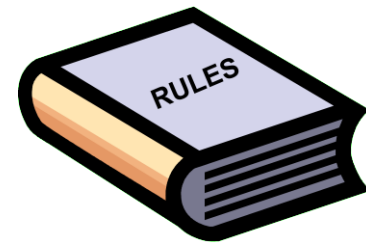
Laboratories are diverse environments

- Analytical raw data from all kind of instruments, often stand-alone
- Reports often to paper
- Lot of data control in place
- Many procedures to follow
- Lots of regulations (GxP, 21 CFR Part 11, etc.)
- Users need to be able to search and quickly find and retrieve the data, regardless of their storage location (online or in offline archive)

In order to get valuable information out of the data on these multiple systems:

- Data need to be stored on one central system
- Data need to be comparable and available for review in one common form.

Regulations and enforcements



Annex 11

- European Pharma Industry

Renewed 21 CFR Part 11

- FDA Pharma Industry

ISO 17025

- General for laboratories!



Data Integrity and authenticity



Common principles for all regulations apply

- Data security by central storage and controlled access
- Data authenticity by check sum controls
- Audit trail on activities done by users

Accountability

- Management responsible for implementing the new regulations
- Employees need to be trained accordingly
- Checks and balances need to be in place

This can all be supported by a technical solution.

Compliance by Design



Pressure is moving from customer to supplier

- Technical solution for compliance
 - Software build with compliance in mind, “Start with the end in mind”
- Facilitate audits for
 - Reviewing quality documentation
 - Life cycle approach
- Supplier should/must be aware of compliance regulations
 - Agilent has dedicated compliance officer in LI
- Support customer from cradle to cradle
 - That means provide customer a safe way of moving to the next version
- Documentation documentation documentation!

Key functionalities OpenLAB ECM is offering *designed with data integrity in mind*

- Advanced Data Archiving and Management
 - Secured storage
- Record Retention Policies
 - Automated and documented record management
- Scientific Data Management
 - Store *ANY* file from any source
- Document Management
 - Plug-in Office at no costs
- Workflow Management with BPM
 - Audited workflow inside ECM.



Agilent Systems with direct interface *achieving compliance with central control*

Masshunter ICP/MS

GC/MS Masshunter

LC/MS ChemStation

UV/Vis ChemStation

Dissolution OpenLAB ChemStation

OpenLAB EZChrom and ChemStation

All share a central repository and security.

Masshunter integration

Secured storage for large volumes of files

Central login and security

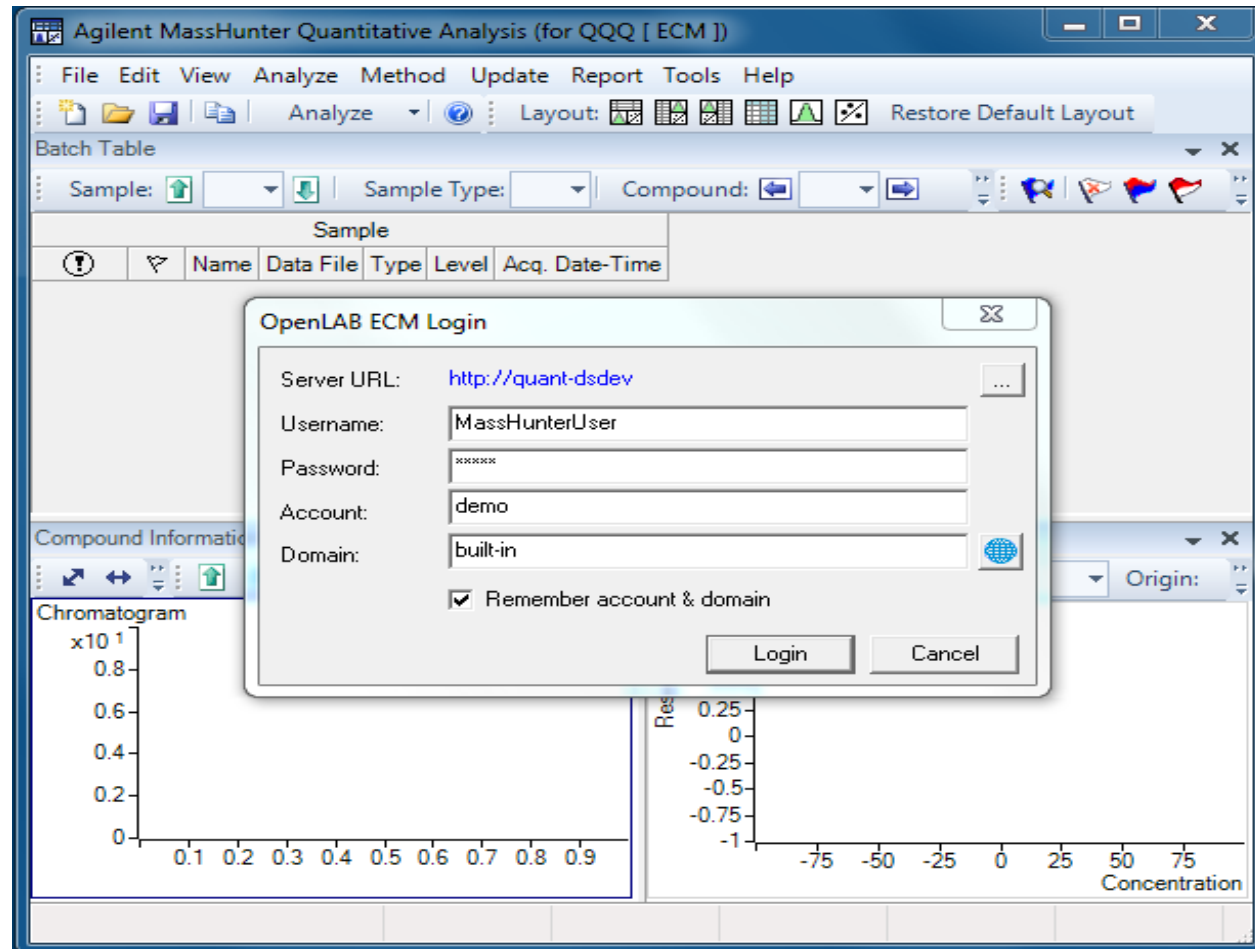
Central audit trail

Behaves just like a normal hard drive

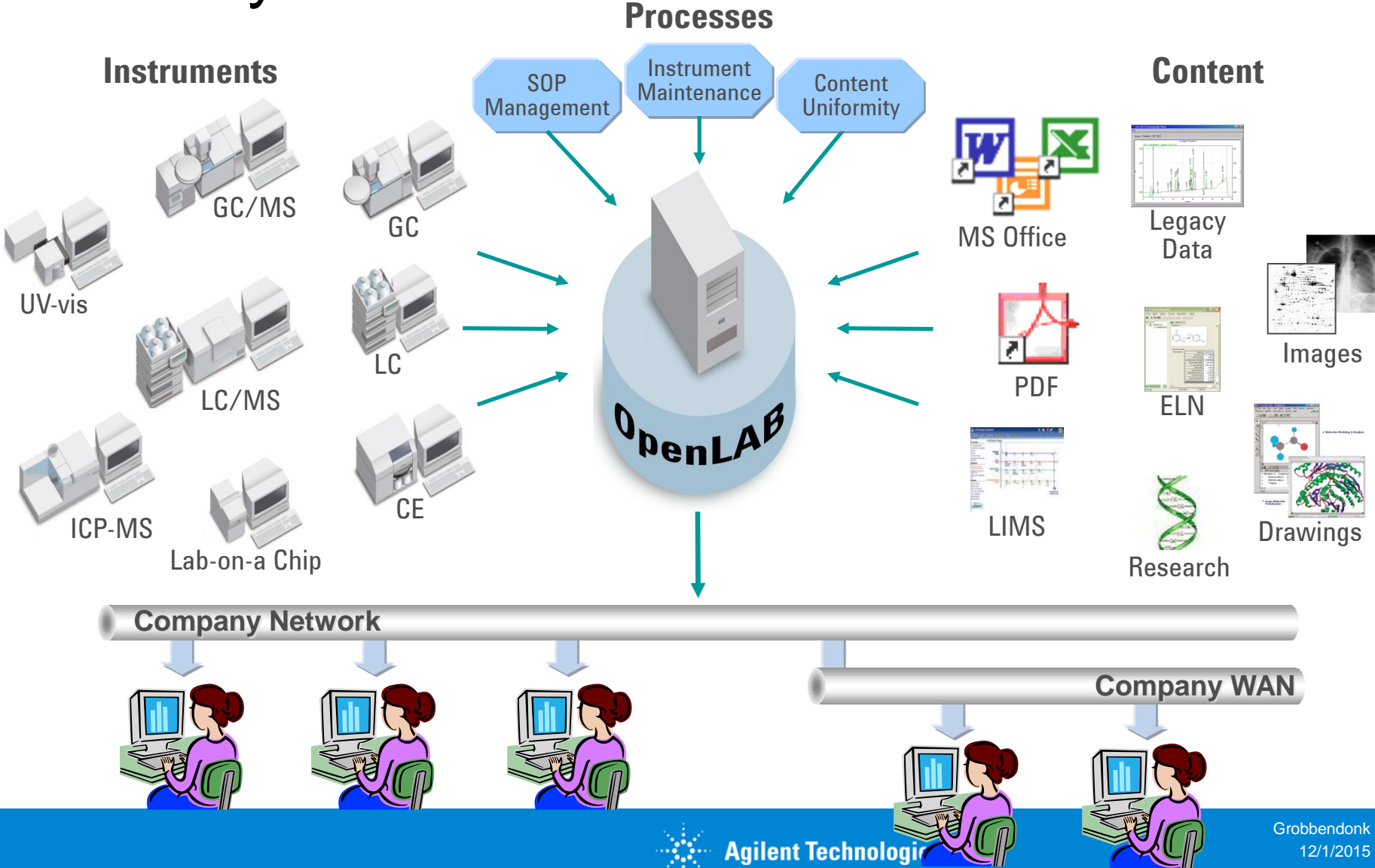
Easy to learn for users

Benefits

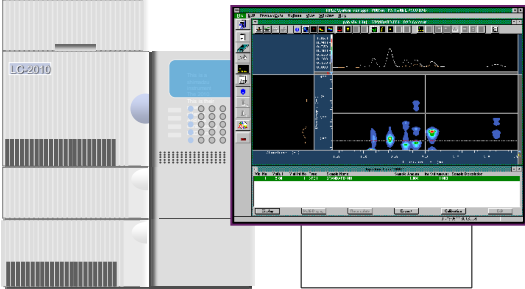
- No more manual back-ups
- No more data loss
- No more manual sharing
- Reprocessing made easy!



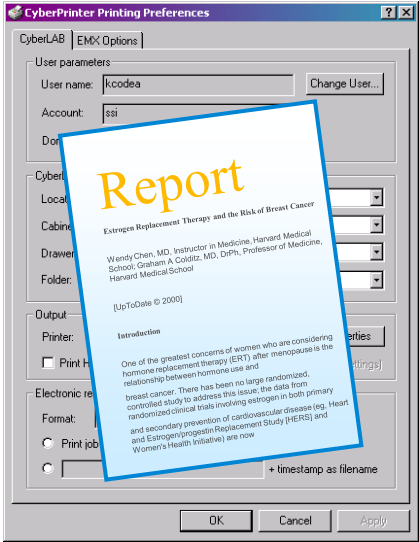
Agilent OpenLAB – linking data across the lab & beyond



There are multiple ways of uploading data into Agilent OpenLAB



Automatic using the Scheduler



Or printing from Instruments and PC's



Automatic meta-data capturing at the source *better safe than sorry!*

Meta-data is information extracted from records and stored in the database

- Automatic
- Manual

Uniquely identify each record to safe guard it

- Check-sums for protection

Search routines

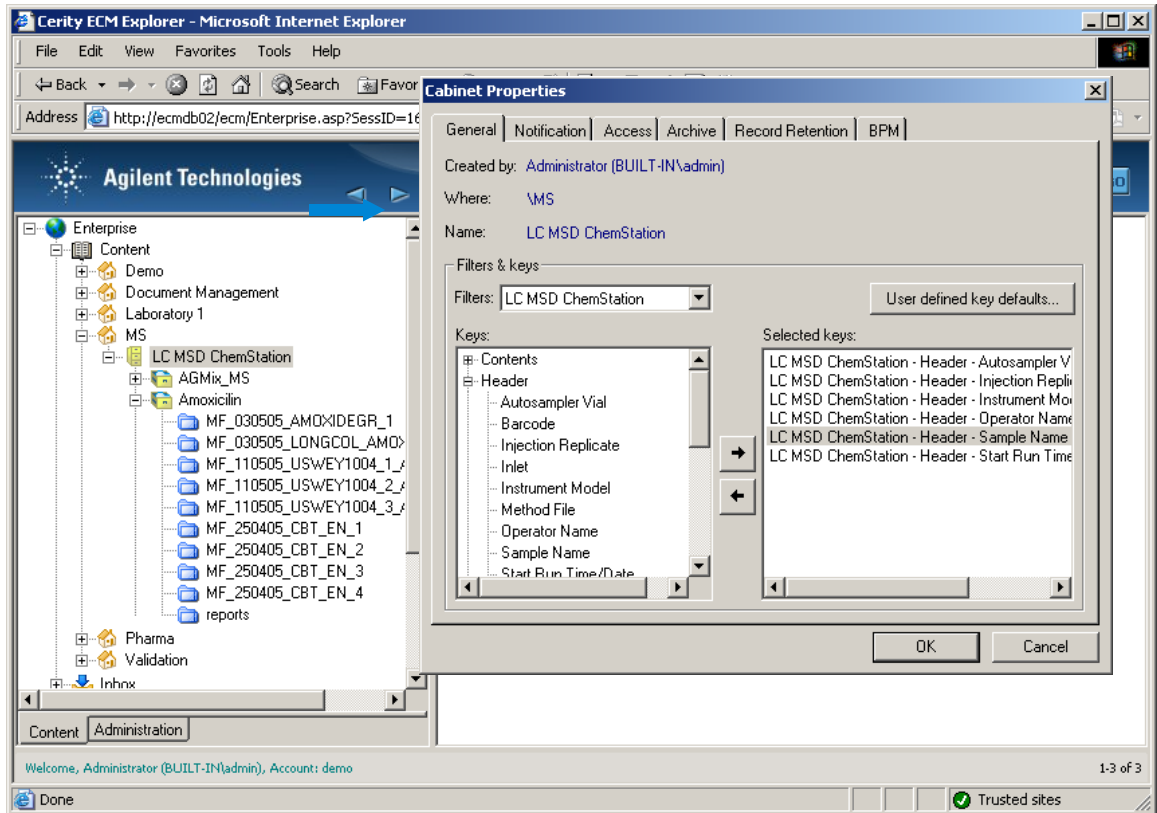
- Track and trace activities

PACA

- Pro-Active Corrective Actions based on audit trails and meta-data.

Attribute Extraction Services

- ✦ Agilent OpenLAB provides over 40 Attribute Extraction Services for different file and document types.
- ✦ To apply an AES to a set of files, simply select the keys and apply them e.g. to a Cabinet in the LCDF hierarchy.
- ✦ All files entered into the Cabinet are automatically indexed with the selected keys.
- ✦ Modify the selection of keys at any time and re-index the files/ documents.



PDF Templates make reports searchable

- ✦ Reports can be printed to Agilent OpenLAB ECM in a PDF format using ECM Printer.
- ✦ PDF Extraction
Templates allow the extraction of metadata (text, graphics, or tables) from the PDF reports.

The screenshot shows the Adobe Acrobat Professional interface. The main window displays a PDF report with the following text:

```
Data File C:\HPCHEM\2\DATA\AMOXICILIN\MF_110505_USWEY1004_1_AMOXI\AMOXIDEGR_3.D
Sample Name: AmoxiDegr
-----
Operator Operator : MF                               Seq. Line : 2
                                           Location : Vial 2
                                           Inj : 3
                                           Inj Volume : 1 µl
Inj Date Inj Date : 5/11/2005 1:15:53 PM
Acq Method Method : C:\CHEM32\1\METHODS\LCMS_CBT_STARL_2-40
Last changed : 5/11/2005 1:15:10 PM by MF
              (modified after loading)
Analysis Method : C:\HPCHEM\2\METHODS\DA_AGMIX.M
Last changed : 2/8/2006 3:49:56 PM
              (modified after load
Method Info : LC Demo method, Pos
-----
MS Signal: MSD1 TIC, MS File, API-ES,
Spectra averaged over upper half c
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.
-----
MS Signal MSD1 TIC
Retention Time (MS) MS Area Mol. Weight or Ion
0.093 38303 183.00 I
0.093 38303 151.25 I
0.163 56884 335.00 I
0.163 56884 297.25 I
0.163 56884 297.00 I
0.163 56884 217.25 I
0.163 56884 189.25 I
```

The 'Template Preview Results' dialog box is overlaid on the right side of the PDF, showing the following table:

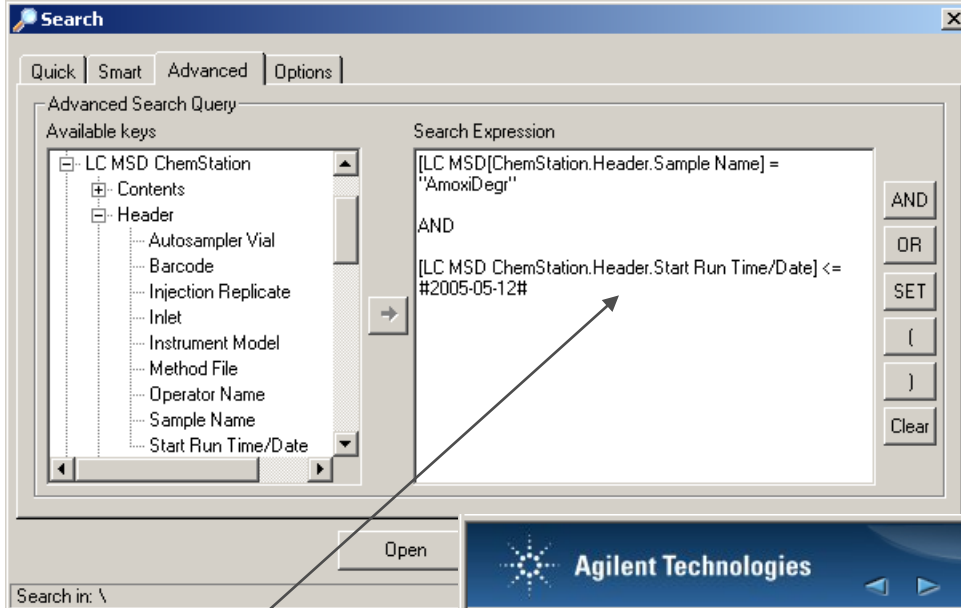
Key	Key Value
MW (or Ion)	183.00
MW (or Ion)	151.25
MS Signal MSD1 TIC	0.093
MS Signal MSD1 TIC	0.093
Operator	MF
Inj Date	5/11/2005 1:15:53 PM
Acq Method	C:\CHEM32\1\METHODS\LCMS_CBT_S...

Agilent OpenLAB: Powerful searches save hours

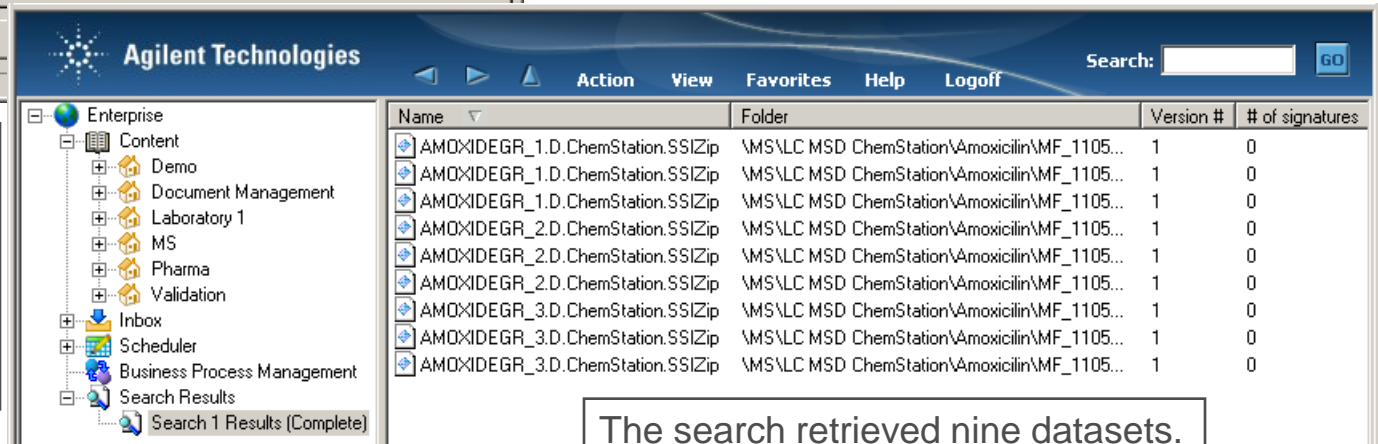


Find exactly what you need – *fast!!*

- Quick searches
- Smart searches
- Advanced searches with multiple criteria



Example: Search for LC/MSD ChemStation data files with the sample name “AmoxiDegr” acquired on or before 5-12-2005.



The search retrieved nine datasets.

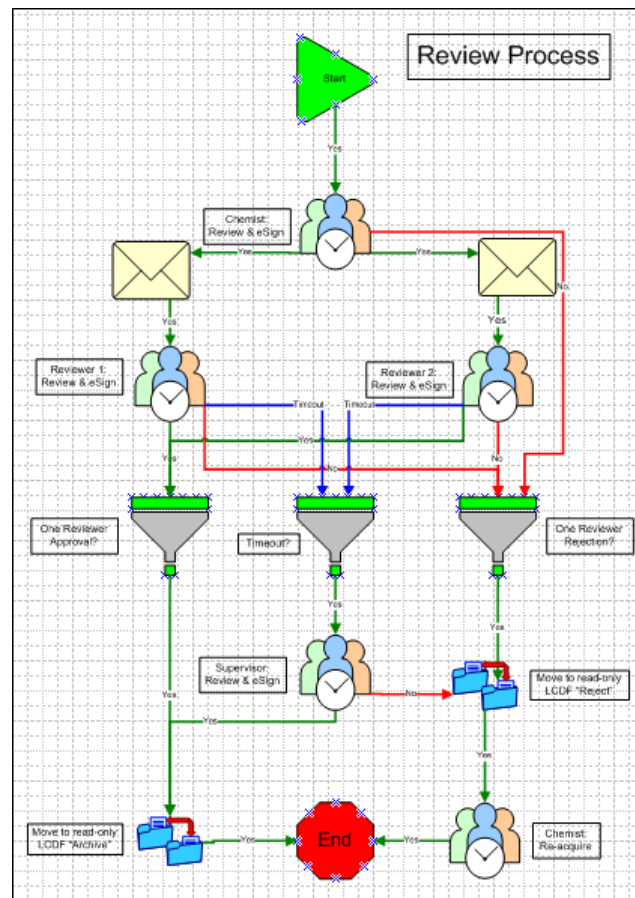
OL ECM Business Process Management

Workflow Automation of report review and approvals

A BPM review process automates document and report review and approval.

This speeds up review and approval by:

- ⇒ Automated email notification for new review activities
- ⇒ Automated or manual delegation of activities
 - ⇒ Based on timeout
 - ⇒ Manual transfer of approval ownership
- ⇒ Setup delegates for absent reviewers
- ⇒ Link of approval request and related document - No more searching for the data required for an approval.
- ⇒ Full traceability of review progress at any time



Result: Streamlined process completed in days - not weeks

Wrap-up

Agilent OpenLAB ECM

- Build with compliance in mind!



Your benefits

- Easy hands-off storage and archiving
- Scalable from 1 to n instruments and users
- Based on standard Microsoft components, no more discussions with IT!
- Used by 100dreds of customers worldwide, guaranteed development
- Paperless activities fully supported
- PACA on audit trail for pro-active management
- Stream lined processes with BPM!



OpenLAB CDS 2



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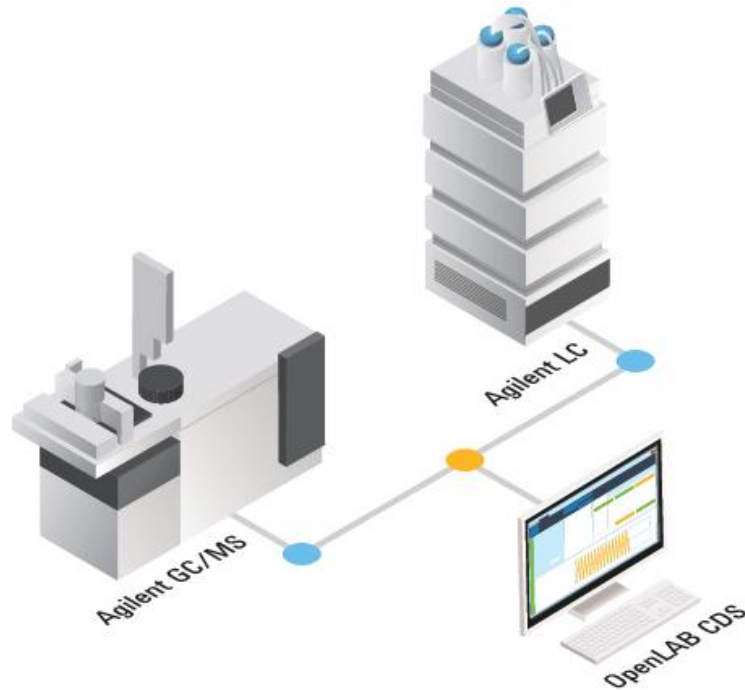


Next Evolution of OpenLAB CDS

“OpenLAB CDS 2.0 - One data system for chromatography and mass spectrometry – Agilent GC, LC, core MS along with third-party instruments.”



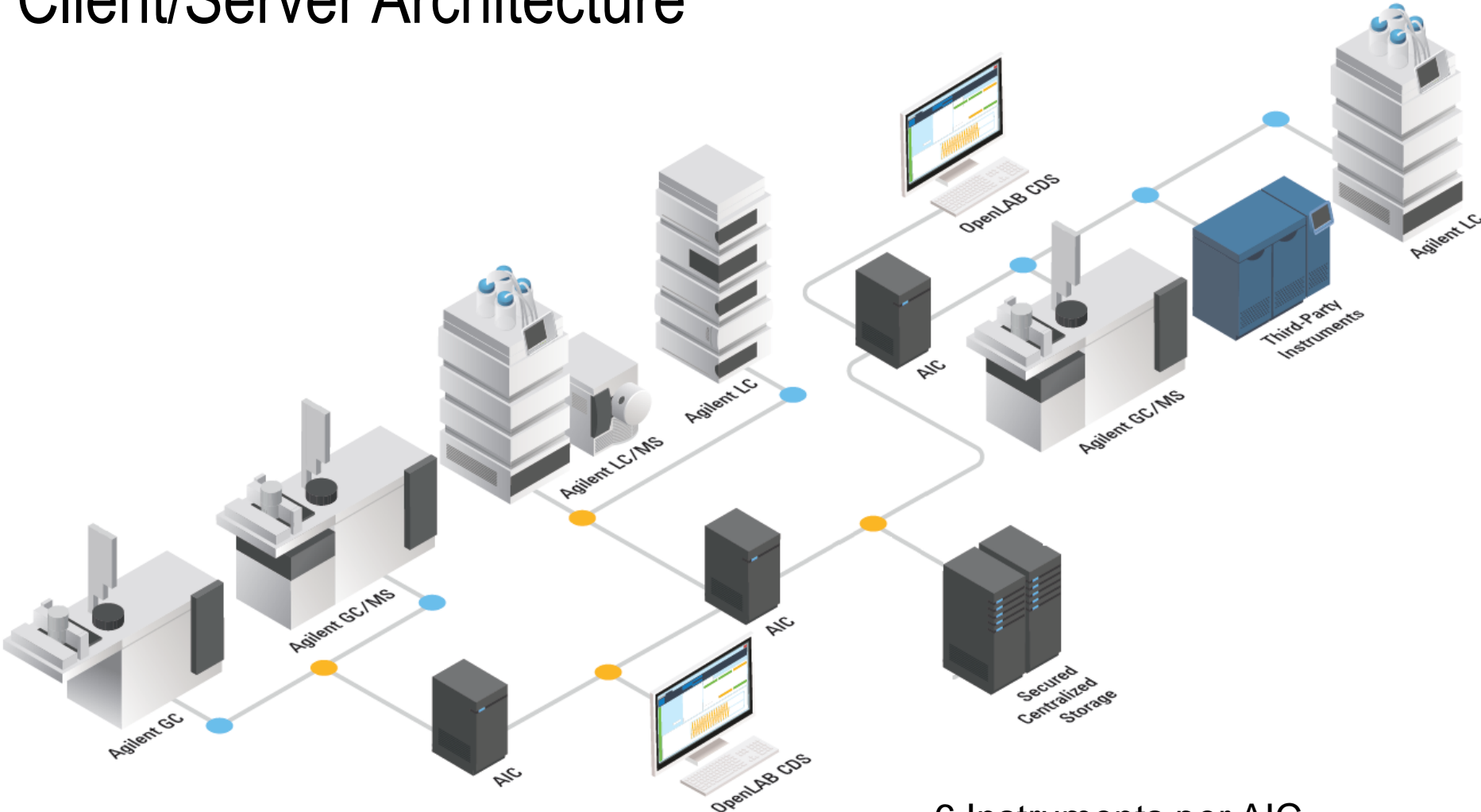
OpenLAB CDS 2.0 Workstation



M8410AA Werkstation en komt met 2 instrument licenties

4 * GC / LC or
2 * MS or
2 * 3D LC

Client/Server Architecture



6 Instruments per AIC
200+ instruments supported

See only what you need when you need it

The image displays the Agilent OpenLAB software interface, which is designed for efficient data acquisition and analysis. The interface is divided into several functional areas:

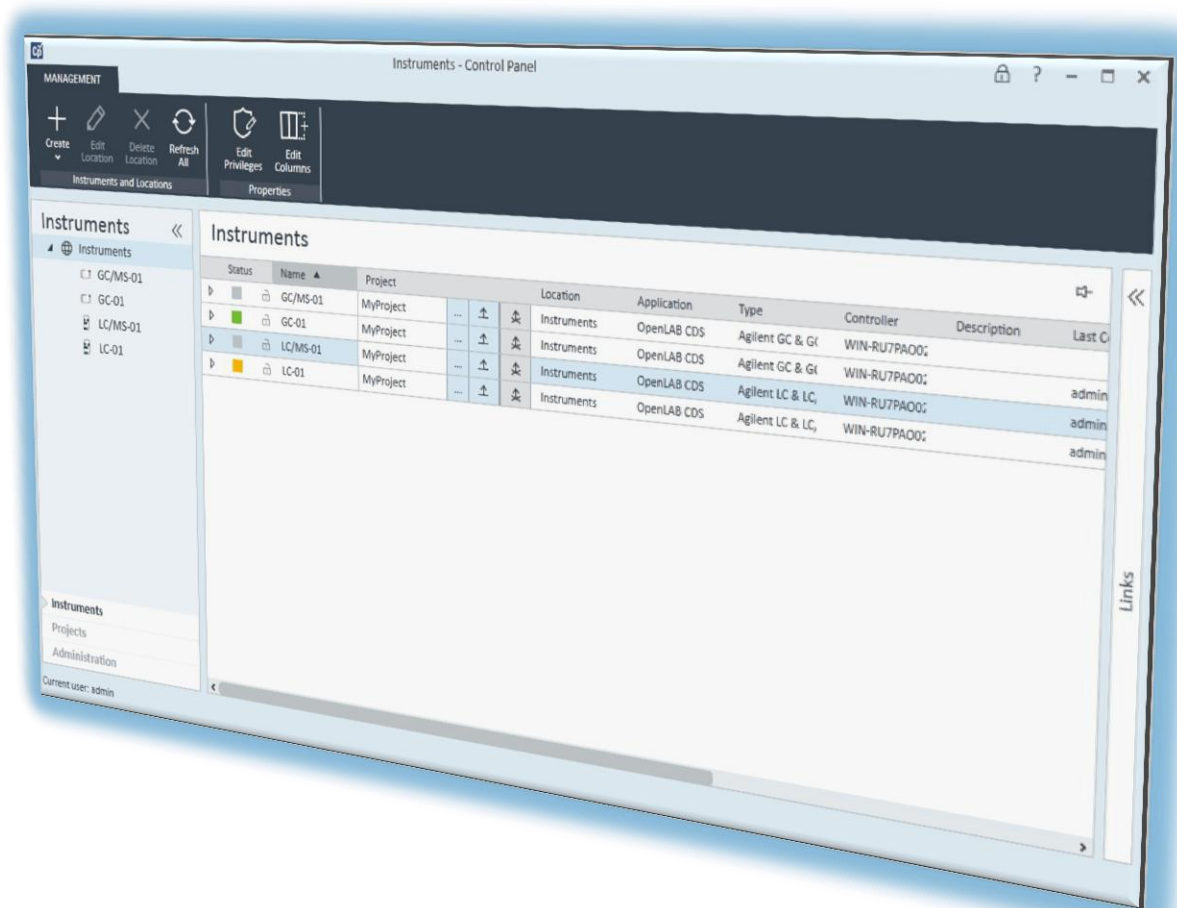
- Run Queue:** A table listing the status of various samples, including columns for Status, Type, Name, User, Acquisition Method, and Details.
- Instrument Status:** A dashboard providing real-time monitoring of key components: Sampler (5.00 µL), Grad. Pump (100.0, 0.0, 0.00 mL/min, 1.00 bar), Column Oven (24.64 °C), and VWD (250 nm).
- Online Signals:** A section for monitoring instrument parameters such as Grad. Pump Pressure, Flow, and Column Oven Temperature, with a corresponding time-series plot.
- Chromatograms:** A main window showing the chromatogram with a zoomed-in view of a specific peak region, highlighting the signal intensity and retention time.
- Peak Table:** A table summarizing the detected peaks, including their retention times, areas, heights, and concentrations.

Peak	Area	Height	Height%	Amount	Concentration	Start time (min)
2.448	0.620	2.349	1.40			
43.455	11.002	21.690	12.90			
30.123	7.627	8.817	5.25			
37.358	9.459	14.899	8.97			
59.278	15.009	26.812	15.96			
55.426	14.033	24.339	14.48			
5h.774	17.966	39.205	23.46	3.746 mg		3.746

View your entire lab at a glance

Central point for

- Instrument management
- Administration
- Launching instruments
- License management
- Access to log files



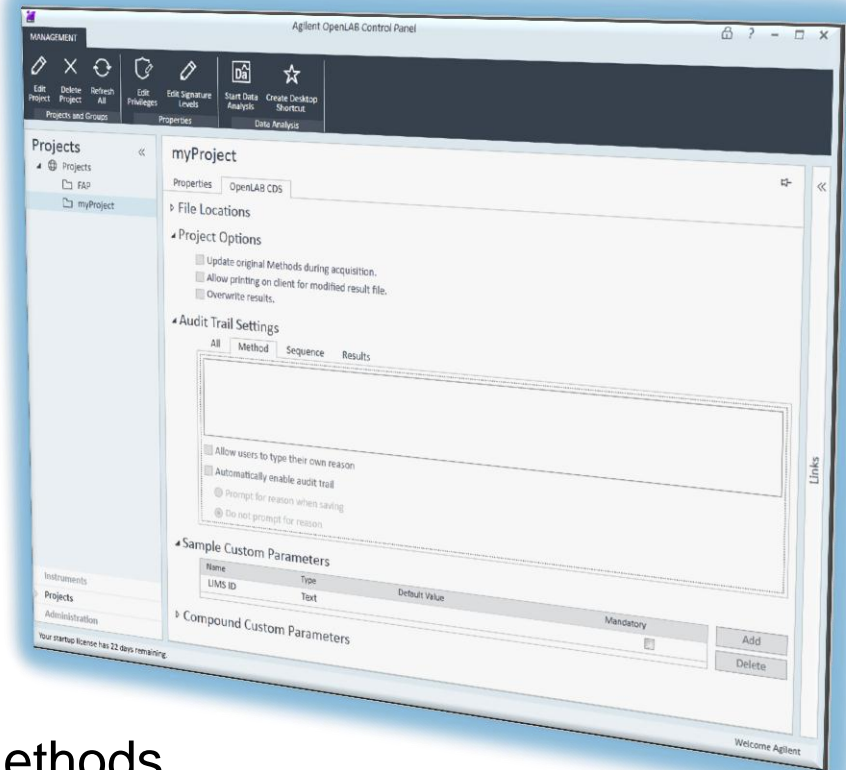
Data and Methods – Some Aspects

Projects

- Organize data context
- Reflect organizational structure
- Specific access rights and settings
- Custom fields on sample and compound level

Methods

- Dedicated acquisition and processing methods
- Copy of the methods is stored with the result set
 - Allows adaption of the method in the context of the result container
 - Master method can be updated from local method (requires privilege)



MS Support in OpenLAB CDS 2.0

Support of Agilent LC/MSD and GC/MSD instruments

MS Tuning and Calibration

MS based Quantitation with reference spectra confirmation

GC/MS NIST library searches

Compound Confirmation and Estimation of Sample Purity
(LC/MS)

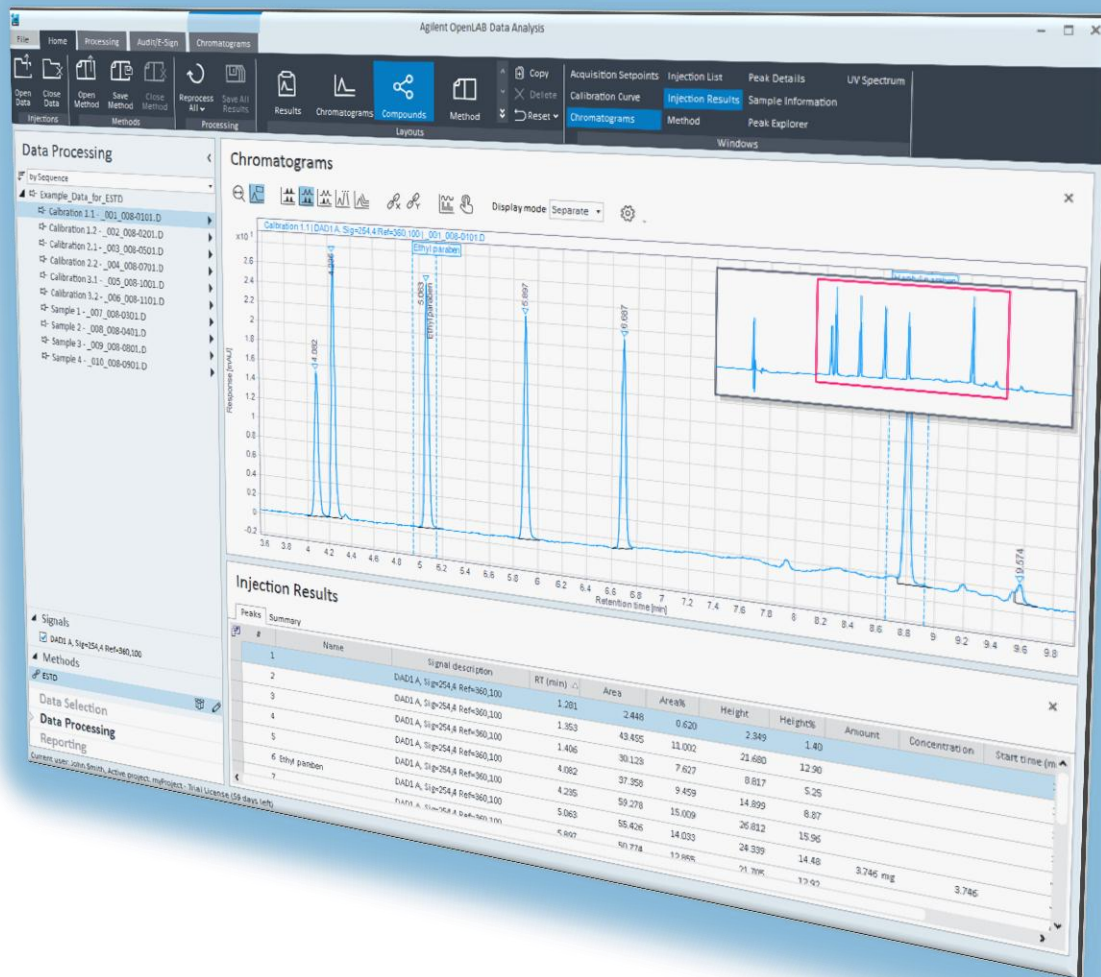
Extracting spectra at specific time or peak based

Reporting of MS data



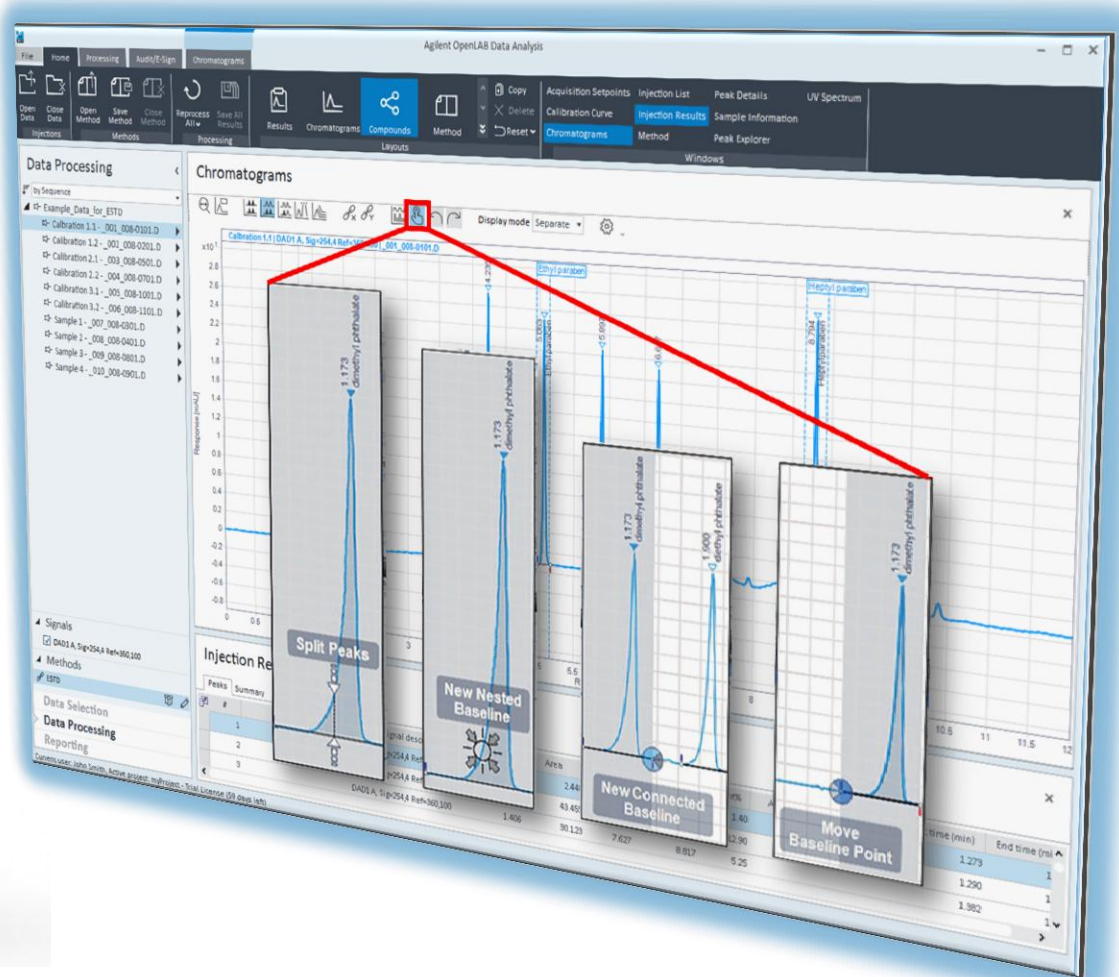
OpenLAB CDS 2.0 – Data Analysis

- One tool for LC/GC/3D UV/MS data analysis
- UI adapts to selected data type
- High processing performance
- One-click manual integration
- Fast data review with Peak Explorer
- Advanced Audit Trail Review
- Custom Calculation Designer
- eSignature



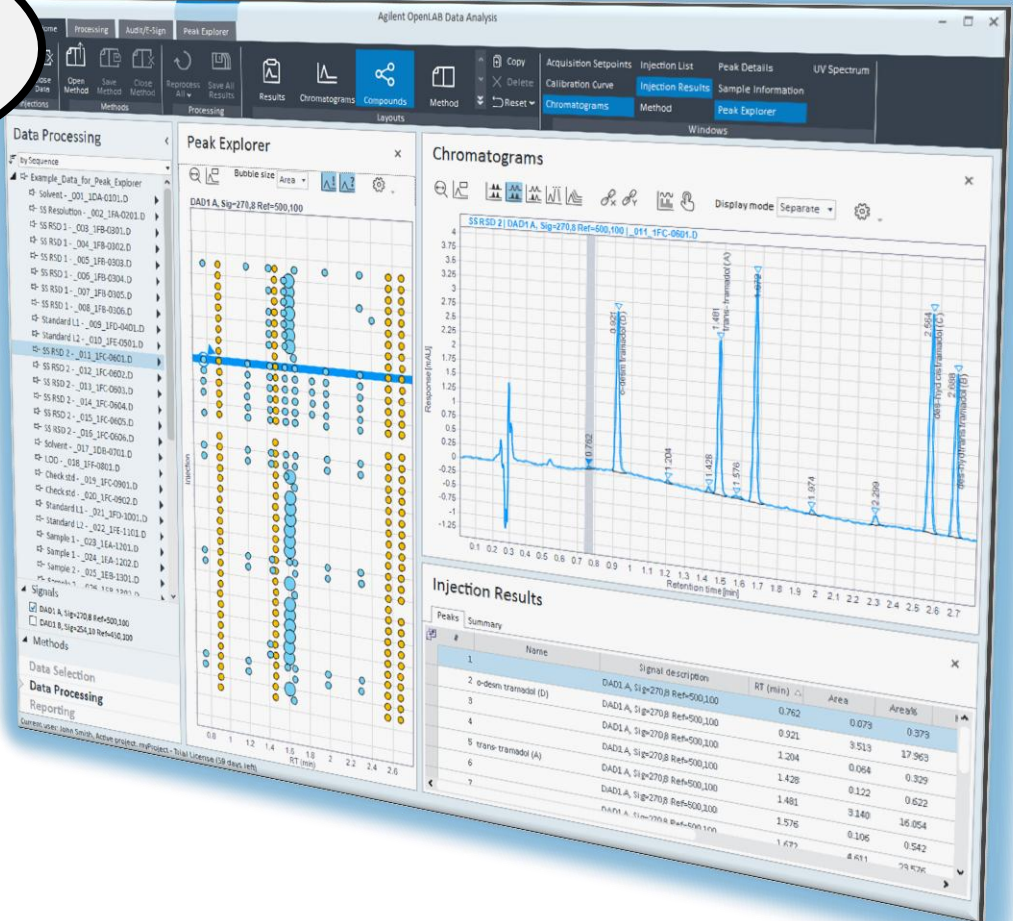
One-Click Manual Integration

Great, I always get
the tool that I need
when I need it -
automatically!



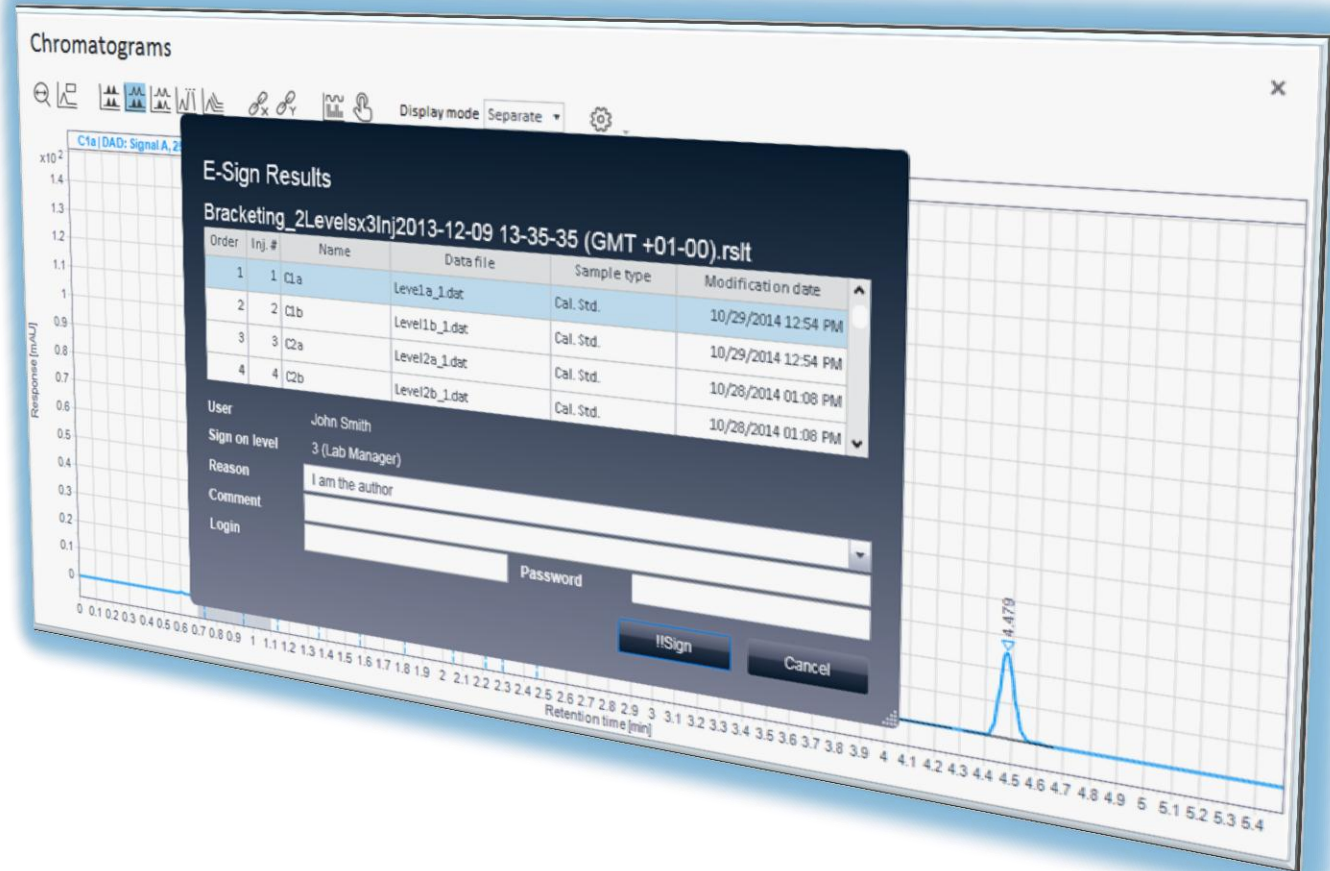
Get new insights into your data

Wow, now I can find anomalies at first glance – even within hundreds of chromatograms and peaks!



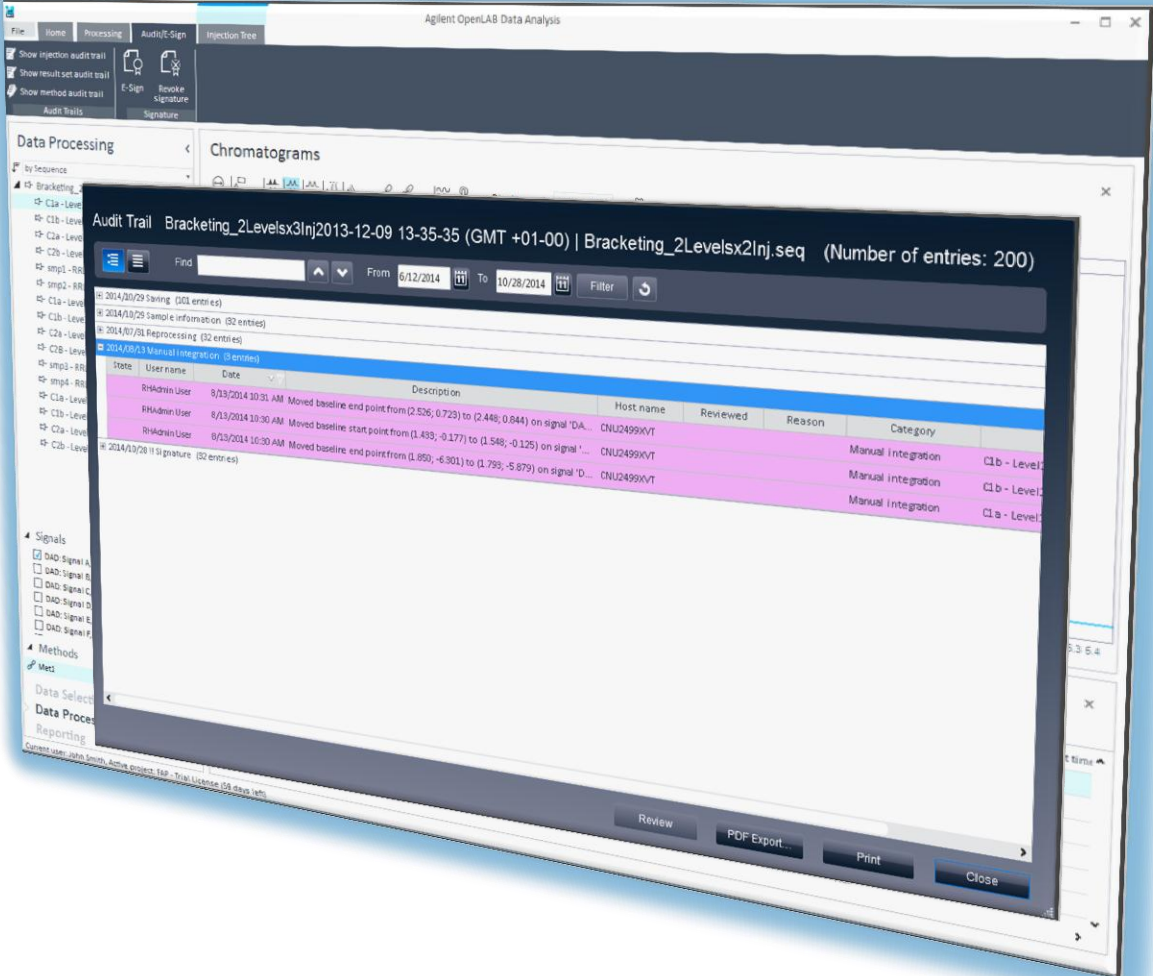
E-Signatures

In Data Analysis
Up to 5 levels
Reportable



Advanced Audit Trail Review

- Documented review
- Audit categories
- Full text searchable



Sample Scheduler for OpenLAB

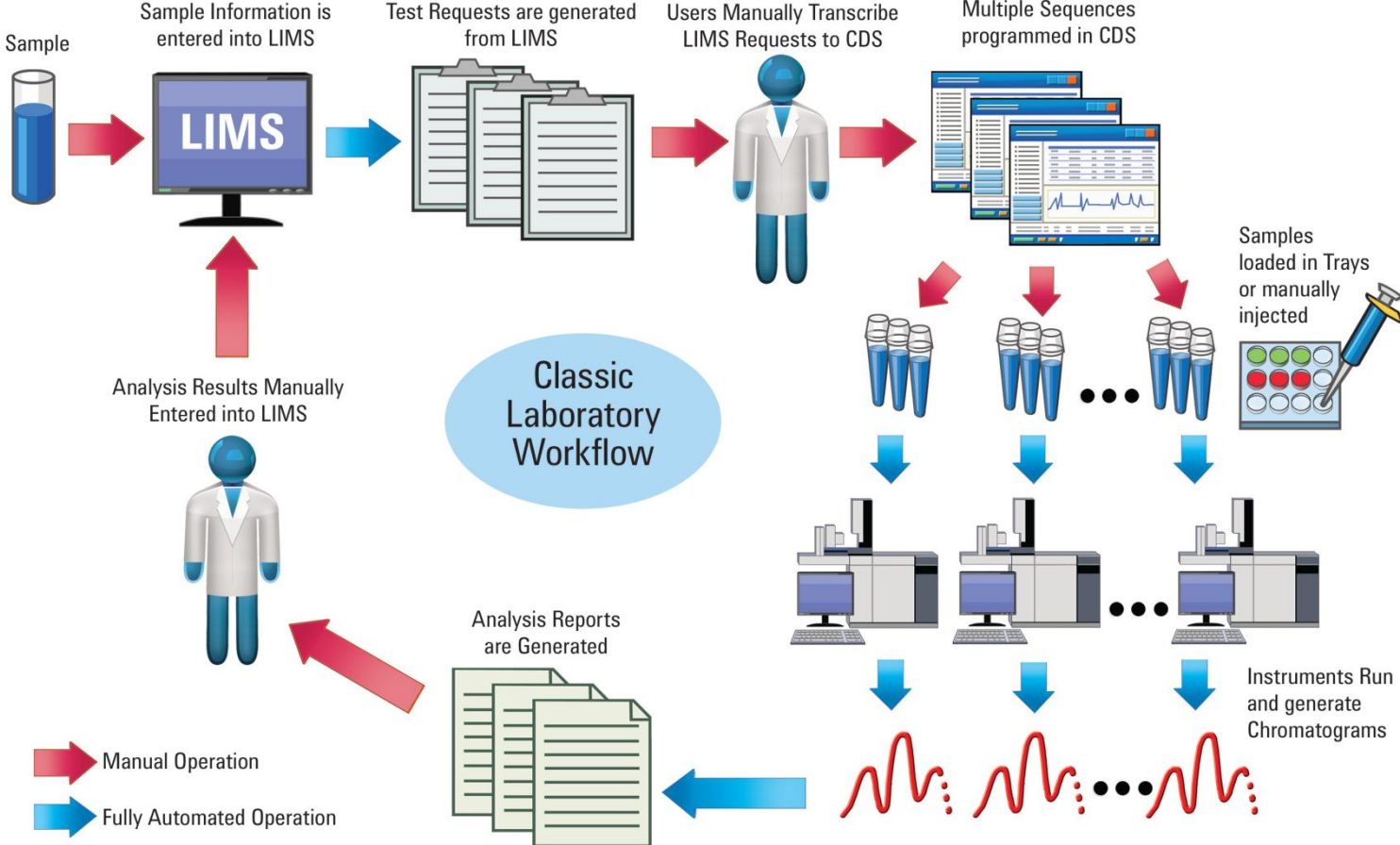
Configurable out-of-the-box LIMS interface

Single UI for routing samples to any instrument

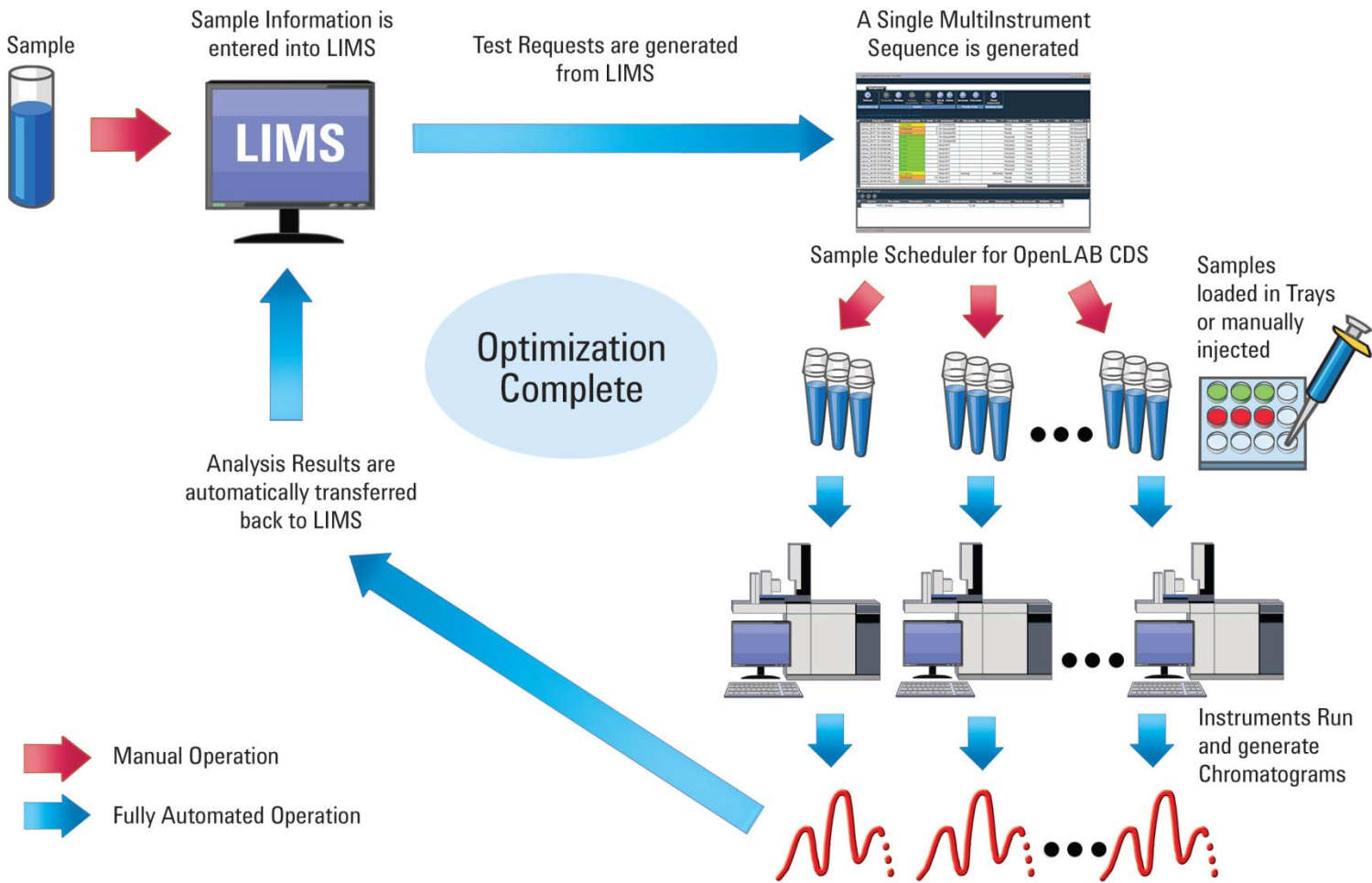
Walk-up interface for ad-hoc samples



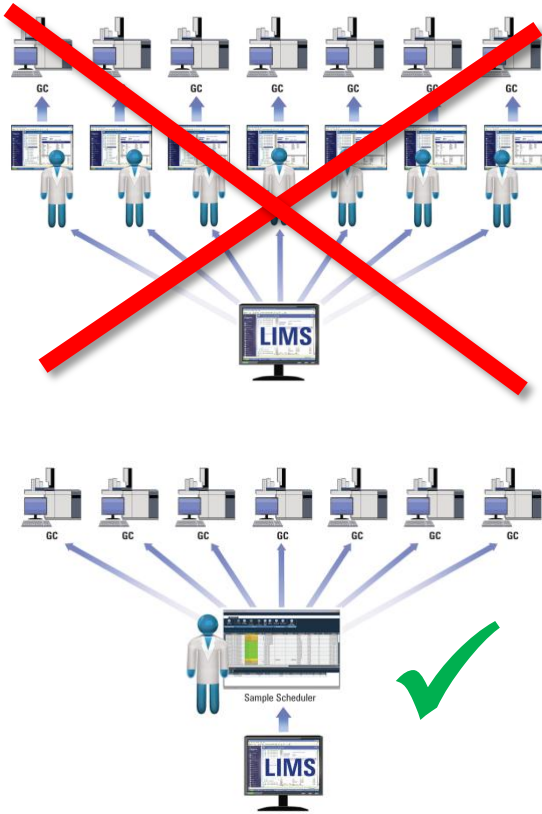
Want a short cut to more reliable results?



Close the gap between the LIMS and instruments



Lab wide sequencing across instruments



SampleScheduler for OpenLAB CDS Client

File Home Actions Edit View Manage

Refresh Schedule Wait Restart Stop Stop Instrument Sooner Later Show notifications

Analysis Table

Drag a column header here to group by that column.

Identifier	Sample name	State	Priority	Analysis time	Project	I.L. Laboratory	Instrument	Acq. method	Proc. method
USE Template with alter...	<U>-<A>	Scheduled	3		Quality	B27	GC1	GC1.amx	
Alternative2-<D>-<U>-<A>	<U>-template	Waiting			Quality	B27	GC3	GC3-ter.amx	GC1-calibrat
ffron-SCHAdmin_2015-06...	aaaaa	Incomplete			Quality	B27	GC2	GC2.amx	GC1-calibrat
alternative Instr-LIMS_10...	ffron-SCHOperator-TOTAL	Ended			Quality			GC2.pmx	GC2.pmx
ffron-SCHAdmin_2015-06...	Sample-<D>	Waiting On Error			Quality	B27	GC2	GC2.amx	
commandA1	Sample-<D>-<D>	Holding			Quality		GC1	GC1.amx	GC1-calibrat
commandA10	Sample-<D>-<D>	Holding			Quality	3800		3800.amx	
ffron-SCHAdmin_2015-06...	Sample-20150612 140618	Error			Quality				
ffron-SCHAdmin_2015-06...	Sample-20150612 140709	Stopped			Quality				
ffron-SCHAdmin_2015-06...	Sample-20150612 140900	In Progress			Quality				
ffron-SCHAdmin_2015-06...	Sample-20150612 140924	Stopped		0.8/1 (min)	Quality	3800			
ffron-SCHAdmin_2015-06...	Sample-20150615 144600	Ended			Quality	3800		3800.amx	
GC1-command-1_2	Sample-7890_Labo-ffron...	Scheduled			Quality	3800		3800.amx	
GC1-1_1	Sample-GC1-20150615 14...	Ended			Quality	3800		3800.amx	
GC1-1_2	Sample-GC1-20150615 14...	Submitted			Quality	3800		3800.amx	
testGC1-4min_1	Sample-GC1-20150615 14...	Submitted			Quality	3800		3800.amx	
	test	Incomplete			Quality	7890_Labo		3800.amx	
					R&D	GC1		3800.amx	GC2.pmx
						GC1		GC1.amx	GC2.pmx
						GC1		GC1.amx	GC2.pmx
						GC1		GC1.amx	GC2.pmx

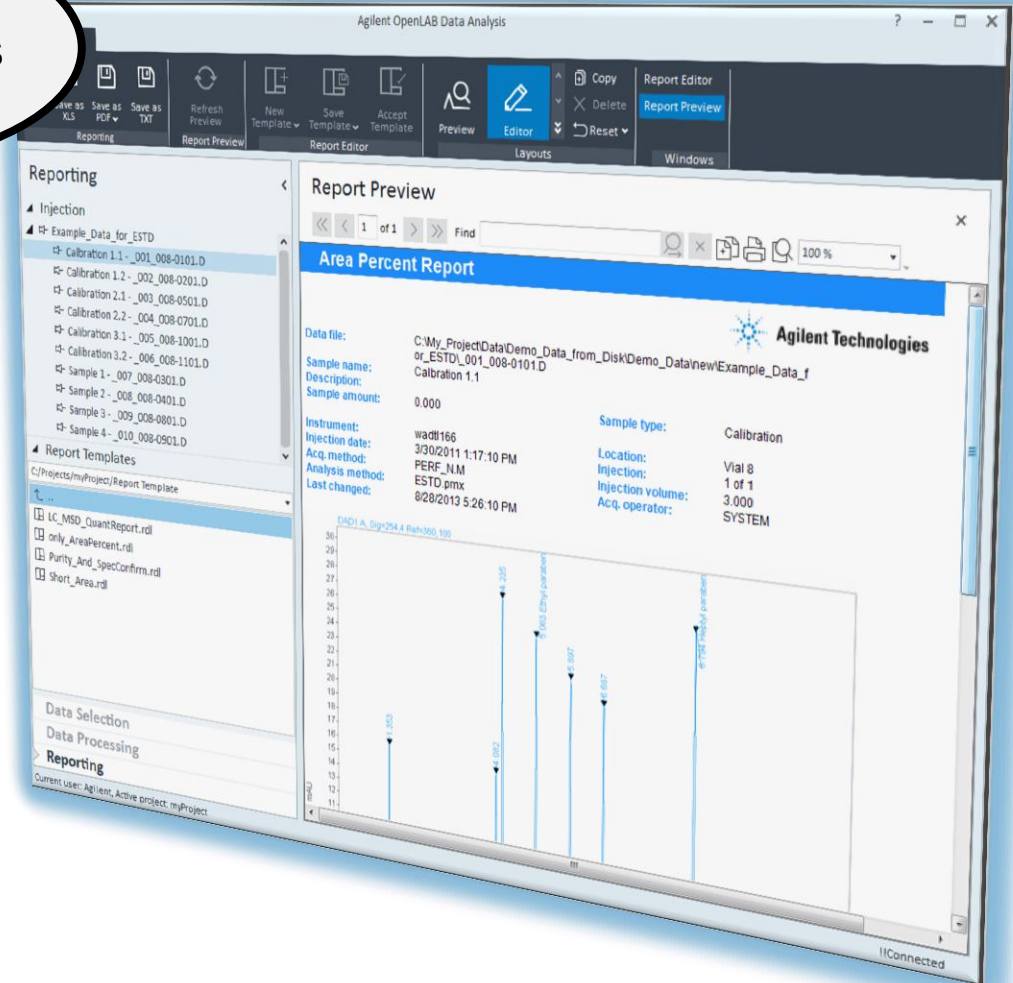
User: ffron-schadmin | No filter applied | Connected

Intelligent Reporting - Complex Reporting Made Easy

Create your report templates via Drag&Drop.

Use interactive reports for your data review.

Apply your business logic in your reports.





OpenLAB ELN

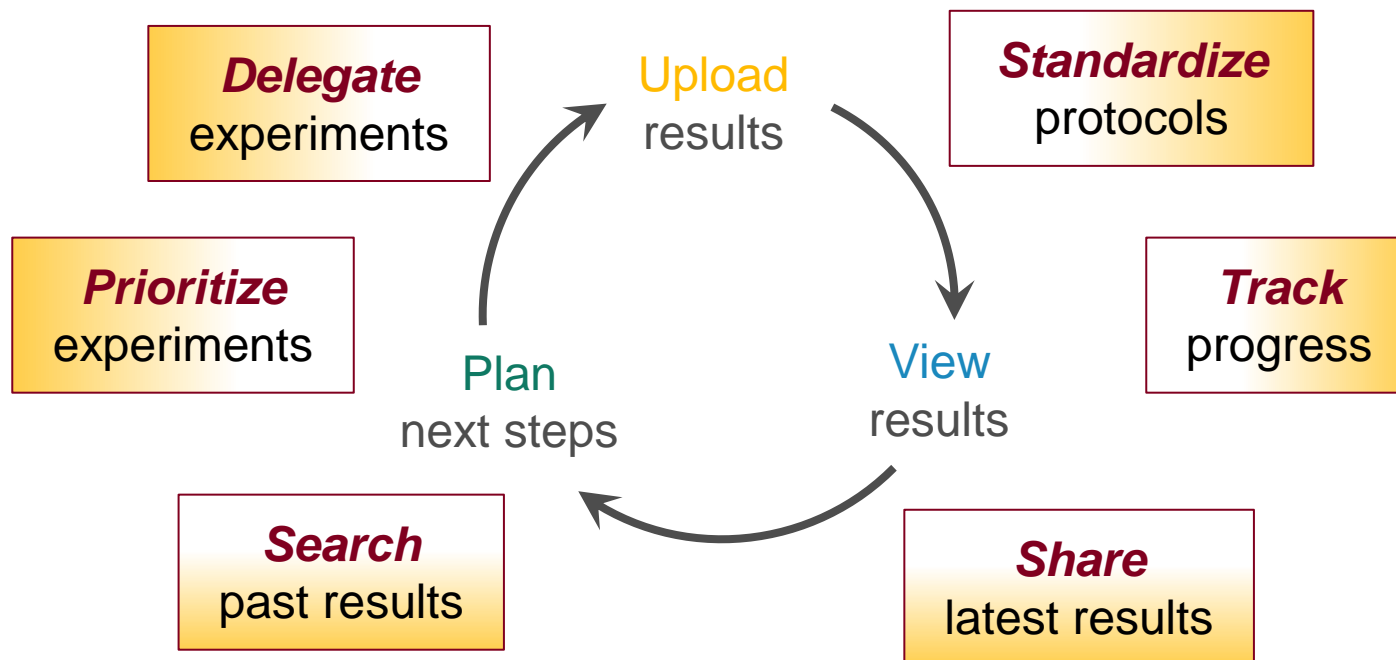


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What is OpenLAB ELN?

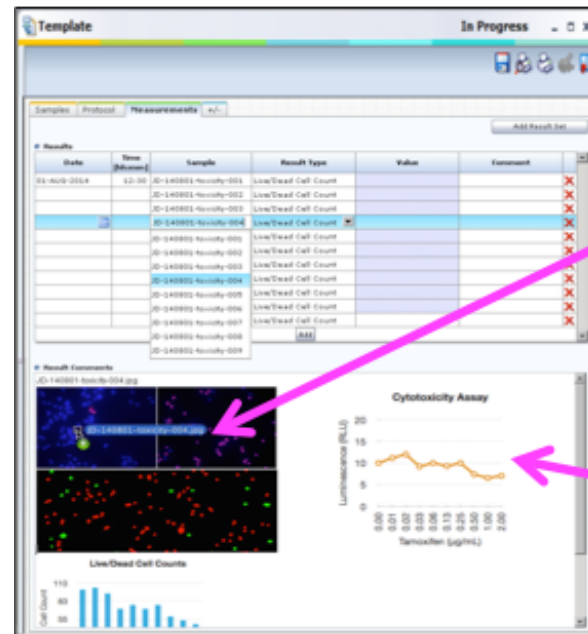
Central Hub between Lab Manager + Lab Employees



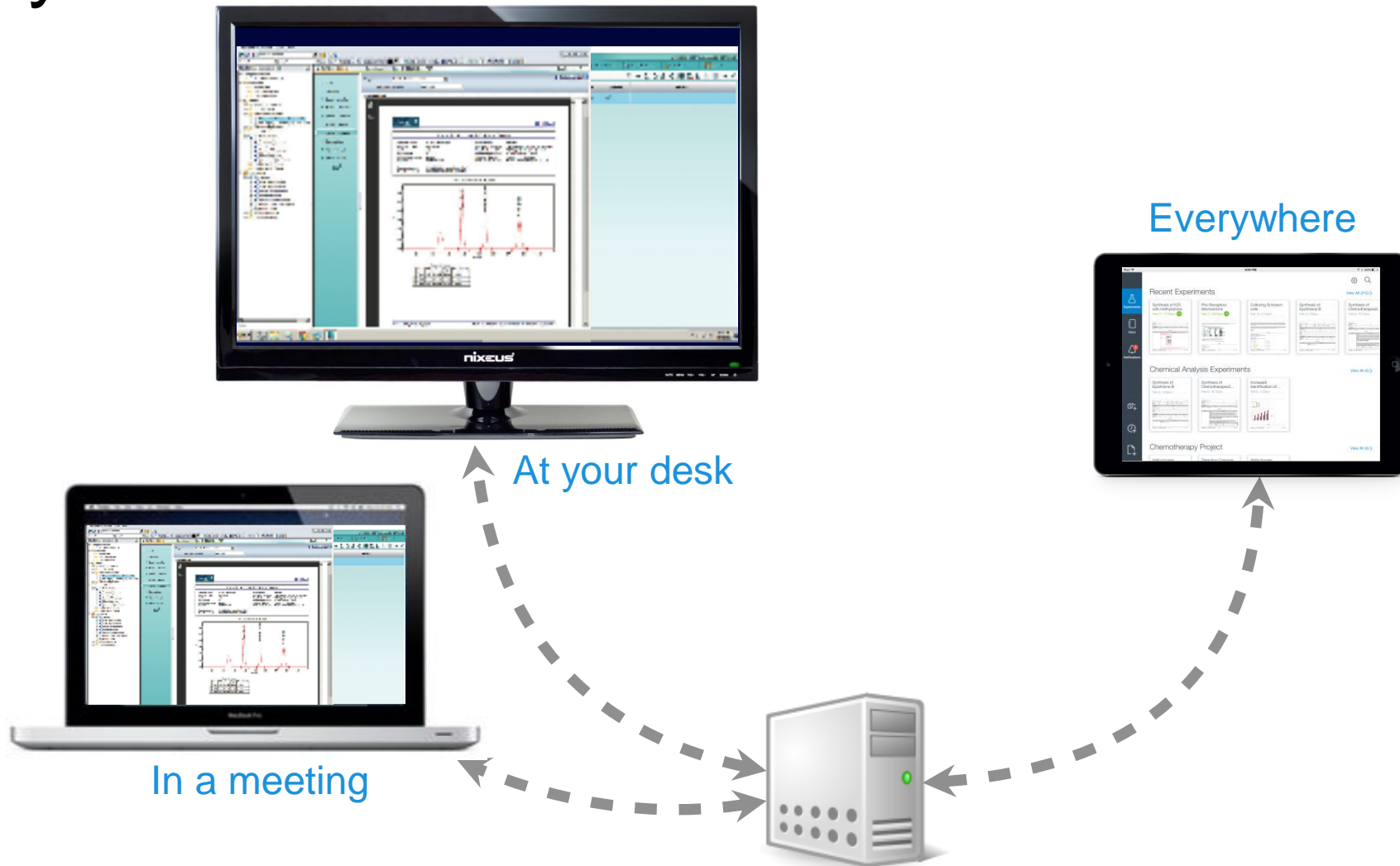
What is OpenLAB ELN?

Capture your **complete experiment** (protocol, analysis, results) – all in one place.

- OpenLAB ELN helps you build connections between disparate data files – by bringing all your files together onto one single notebook page
- Simply drag-drop your files directly onto the page



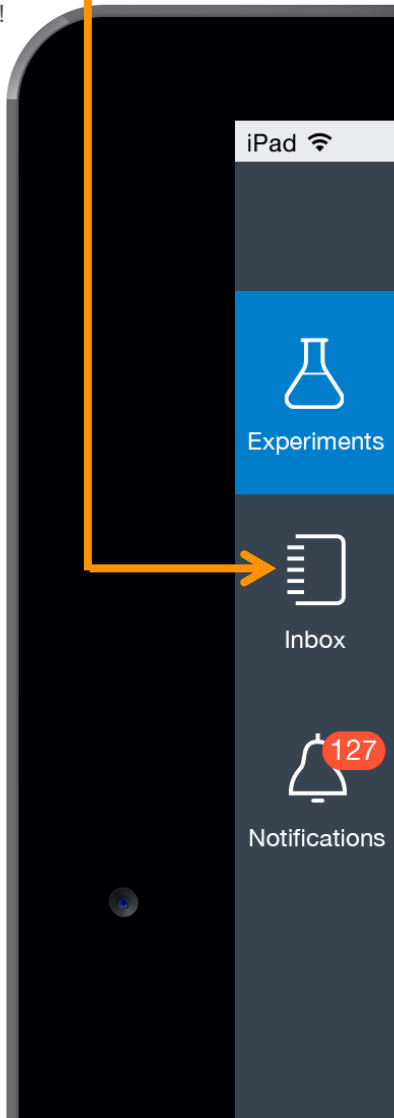
Access OpenLAB ELN – anytime, anywhere



Meet OpenLAB ELN Mobile.

ELN Inbox

Send & receive photos, videos, PDFs, Microsoft Office files, and more!



Author ID

Badges

Quickly see *who* last made changes

Color

Indicators

Quickly see *if* there are new changes

Recent Experiments

Impact of Temperature on...
Sept 14, 2:12 PM SD

Injection volume (µL)
Flow rate (mL/min)
Mobile Phase
Reagent A Reagent B

Time (min)	MS	UV
0.0	0.0	0.0
20.0	0.0	0.0

Gradient:
Time (min) 0.0 10.0 20.0
Flow rate (mL/min) 1.0 1.0 1.0

MS Conditions:
MS Scan (m/z)
Cycle mode
Inlet flow (mL/min)
Carrier gas flow (L/min)
Oven gas temp (°C)

Impurities in Oxytetracycline p. Antibioticos: Acid

Sample Information
The GC/MS data presented is a combination of signals in helium.
Injection volume of 5 µL, all the concentrations are made into the LC/MS system.

LC/MS Method Details
LC Conditions
MS Conditions

Sample: J01-10001-001-001
Injection ID: J01-10001-001-001
Injection Type: New List
Injection: 01-10001-001-001
Injection: 01-10001-001-001

Effect of Trypan Blue on Cells
Sept 14, 2:12 PM

Time (min)	MS	UV
0.0	0.0	0.0
20.0	0.0	0.0

Sample: J01-10001-001-001
Injection ID: J01-10001-001-001
Injection Type: New List
Injection: 01-10001-001-001
Injection: 01-10001-001-001

Impact of Temperature on...
Sept 14, 2:12 PM

Time (min)	MS	UV
0.0	0.0	0.0
20.0	0.0	0.0

Sample: J01-10001-001-001
Injection ID: J01-10001-001-001
Injection Type: New List
Injection: 01-10001-001-001
Injection: 01-10001-001-001

Biology Experiments

Parallel Synthesis Experiment
Sept 14, 3:45 PM SJ

Effect of Benzene on Cells
Sept 14, 2:12 PM SJ

Effects of Insulin on the Potency...
Sept 14, 2:12 PM



Agilent Technologies

Why Agilent OpenLAB ELN?

- | | |
|--|--|
| 1 USER ADOPTION
No programming required. | OpenLAB ELN doesn't require any programming skills to capture data. Simply drag-drop Microsoft Excel files onto a page, or build forms that can include checkboxes, drop-down lists, tables, calendars, and more. |
| 2 SMART IMPORT
Making data capture simpler, faster, and more accurate. | Automatically import data from OpenLAB CDS, other vendors' data systems, or any XML data source. Users can be confident that their data are free of transcription errors and instantly accessible within their experiments. |
| 3 REQUEST MANAGER
Speed up your lab's turn-around time. | OpenLAB ELN streamlines communication by facilitating task delegation and instant, transparent access to completed results. What's more, it increases your lab's productivity by eliminating bottlenecks and track status/results in real time. |
| 4 DYNAMIC FORMS
Flexible, on-demand design. | Dynamic Forms automate repetitive tasks, improve data quality, and simplify scientists' work. You can also minimize human error and structure your workflows (using fields such as text, numbers, tables, DNA sequences, molecules, and more). |
| 5 OPEN ARCHITECTURE
Scalability made simple. | N-tier architecture makes scaling straightforward and easy—whether you're running on-premise or in the cloud. Plus, you can lower your total cost of ownership through minimal upgrade costs, and easy integration with the tools and apps you already use—including LIMS, SDMS, and ERPs. |

