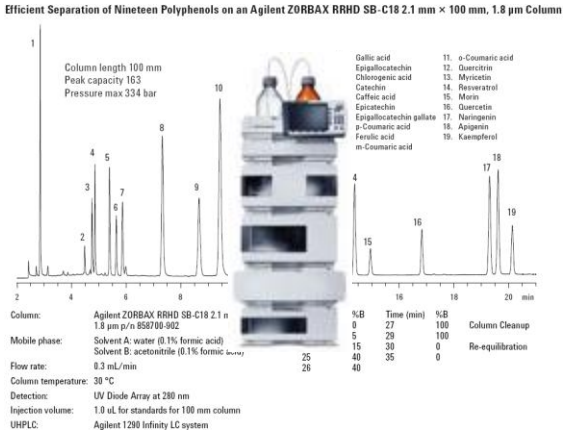
An informed way to manage information

penLAB

Steve Brown
Rich Mutkoski
Agilent Technologies



Laboratory Data Collection, Analysis, Interpretation and Management

Agenda

Overview of OpenLAB (CDS, ELN, ECM)

OpenLAB CDS Remote Control (AIC)

OpenLAB Collaboration (remote access)

OpenLAB Demo

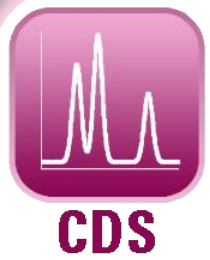
Wrap up and Questions

Challenges for Laboratories

- *Record Keeping - Paper*
- *Data Overload*
- *Access to Data and Instruments (remotely)*
- *Collaboration*

- *Regulatory Compliance (CLIA, 21CFRpart11, CBER…)*
- *IP Protection*
- *Data Integrity*
- *Turn Over in labs (training)*
- *Multiple Sources of Data and Instrumentation*

Agilent OpenLAB Laboratory Software Suite



OpenLAB CDS

Chromatography Data System

Workstation, Networked, Distributed

- ChemStation, EZChrom workflows
- Agilent and Non Agilent Instrument Control (Multi-vendor)
- OpenLAB ECM Intelligent Reporter
- Regulated and non-regulated modes
- Web-based options

OpenLAB ECM

Enterprise Content Manager

Scientific Data Management System

- Data archiving
- Instrument vendor neutral
- Viewers, filters, converters
- Agilent workstation aware!
- Time stamp/audit trail
- Report capture
- E-signatures
- Regulatory compliance
- TNF conversion (LTDA)

OpenLAB ELN

Electronic Lab Notebook

Capture, Organize, Collaborate, Protect

- Smart, high productivity alternative to paper notebooks
- IP protection and compliance features
- Simplifies and accelerates lab work
- Smart data import and dynamic forms
- Simple web-based client
- Analytical request module

OpenLAB

Professional Services

Integration of OpenLAB Solutions

- Speeds full utilization of OpenLAB software & instruments
- Maximizes the return on investment in OpenLAB
- Accelerates OpenLAB adaptation to existing workflows

OpenLAB ELN

ELN

OpenLAB ELN

Electronic Lab Notebook

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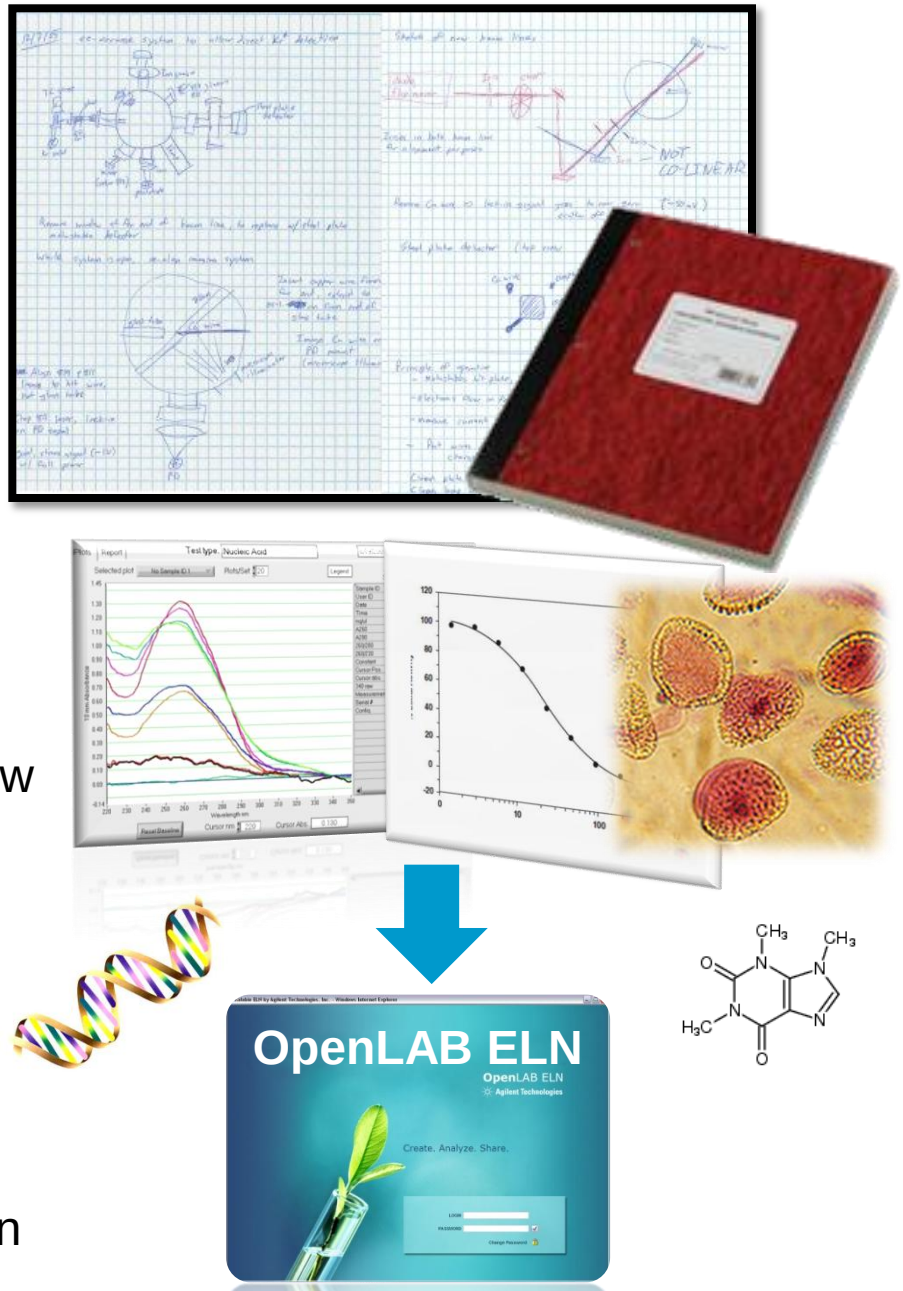
Agilent OpenLAB ELN

Electronic Lab Notebook

A Web-based ELN which enables you to…

- Document, manage and share across multiple disciplines with a single solution
- Search and collate disparate data sources into single experiment
- Reduce cycle times with integrated workflow processing and improve lab efficiency
- Integrate with existing information systems

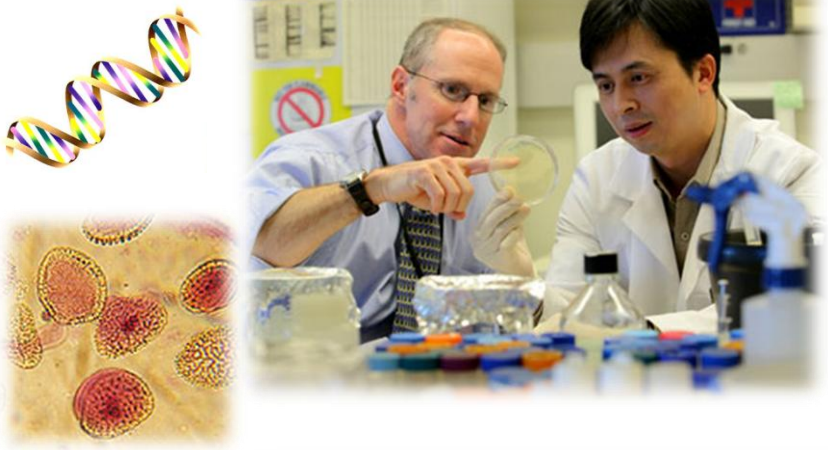


Resulting in…

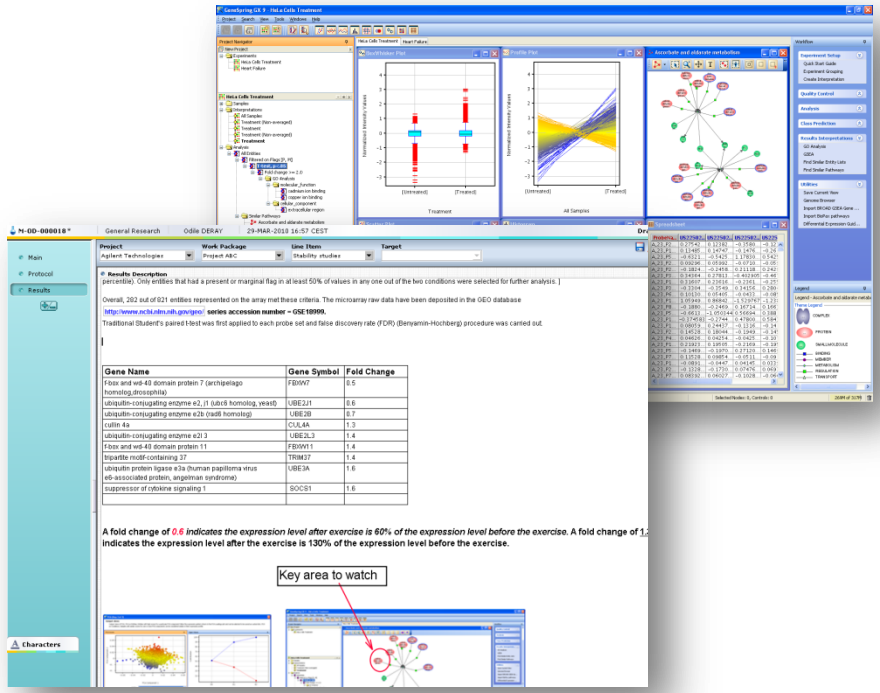
- Improved efficiency and data quality
- More secure Intellectual Property protection

OpenLAB ELN

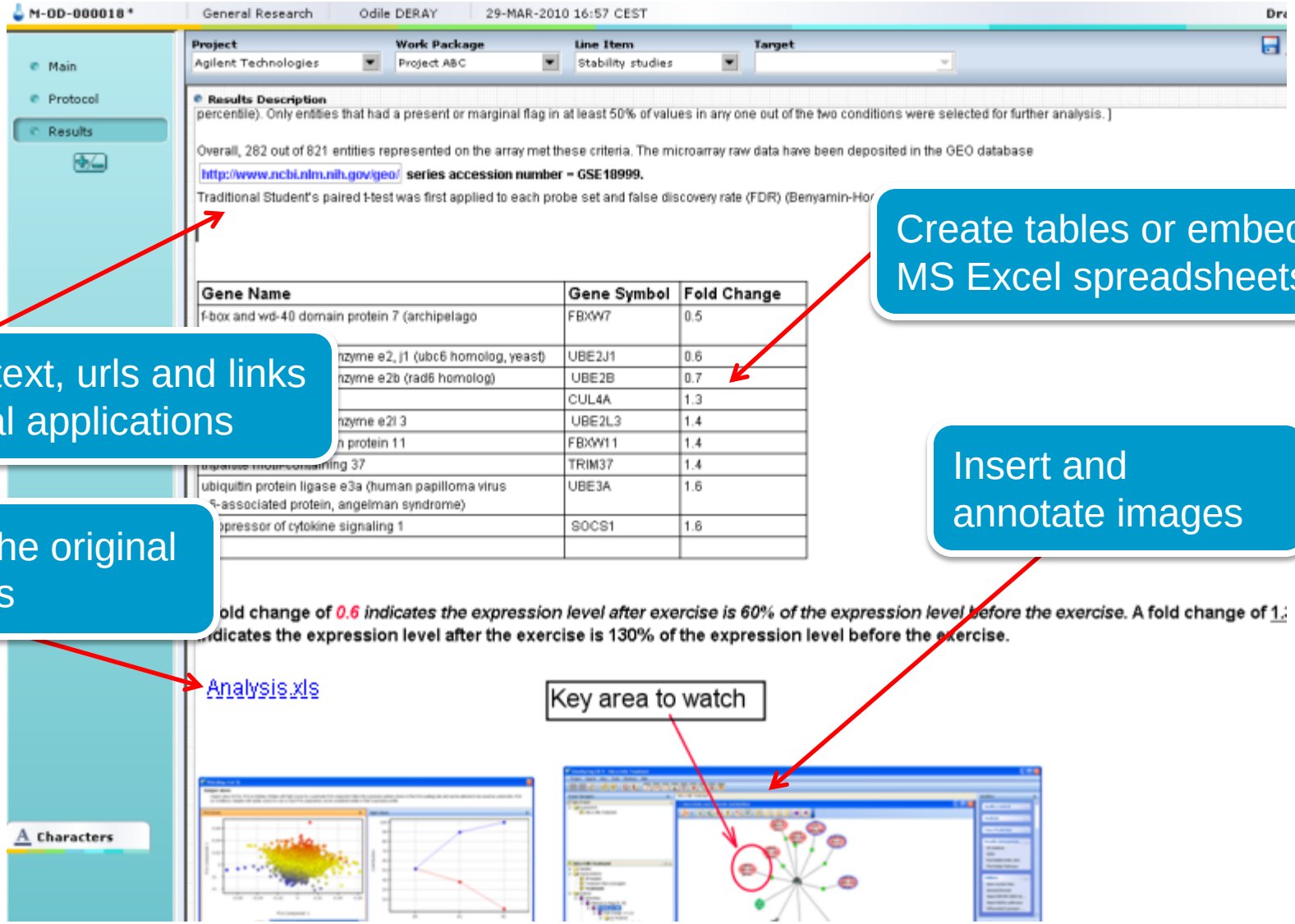
- Cell biology and Molecular biology
- Genomics and Proteomics
- Chemistry (synthetic and analytical)
- Toxicology and Forensics
- General R&D



- Rich text environment for free-form data entry
- Insert images, searchable annotations
- Re-use protocols and methods
- Clone previous experiments
- Link to external sources (e.g. websites, documents)
- Import files, data and results from other applications

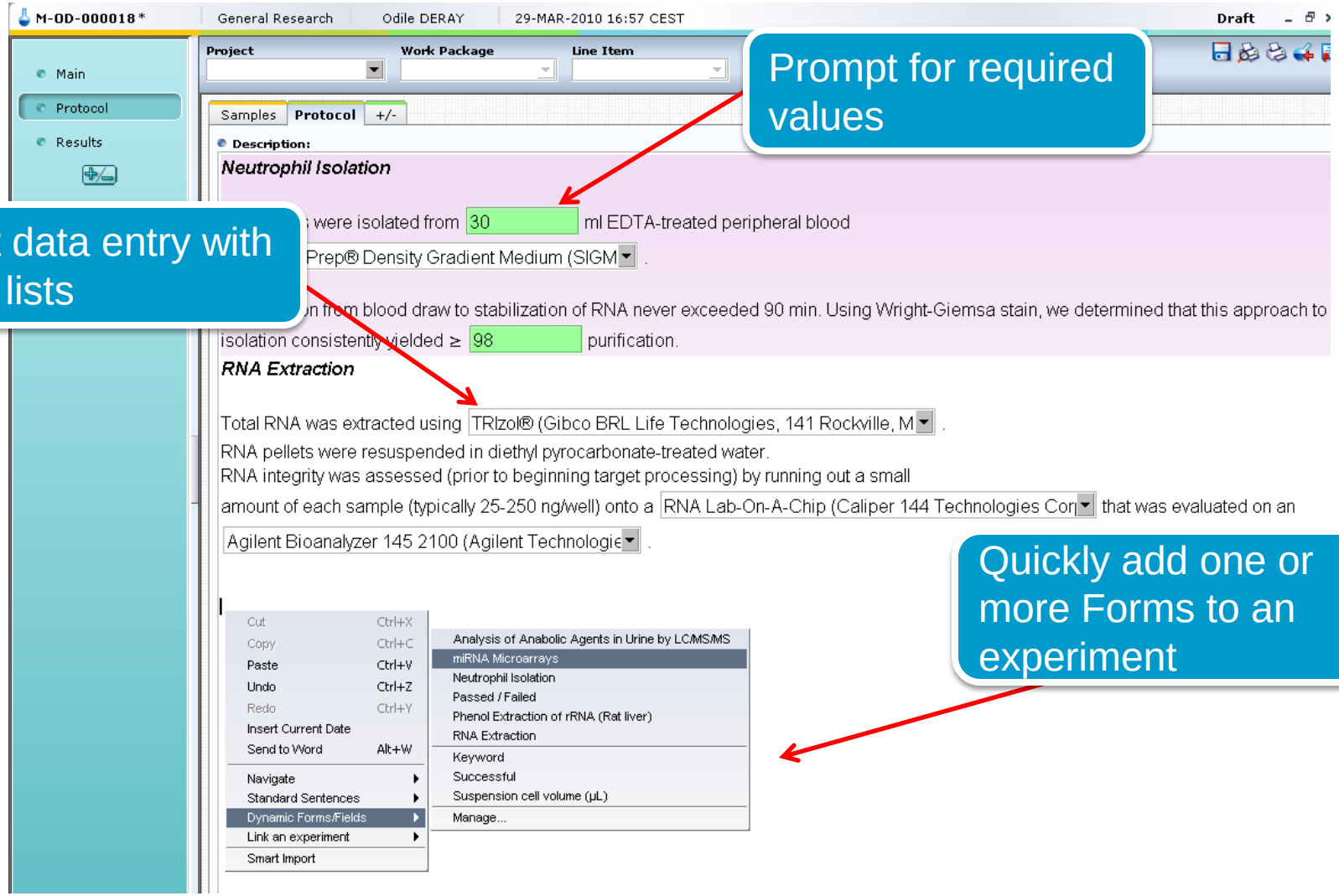


Experiment results in OpenLAB ELN…

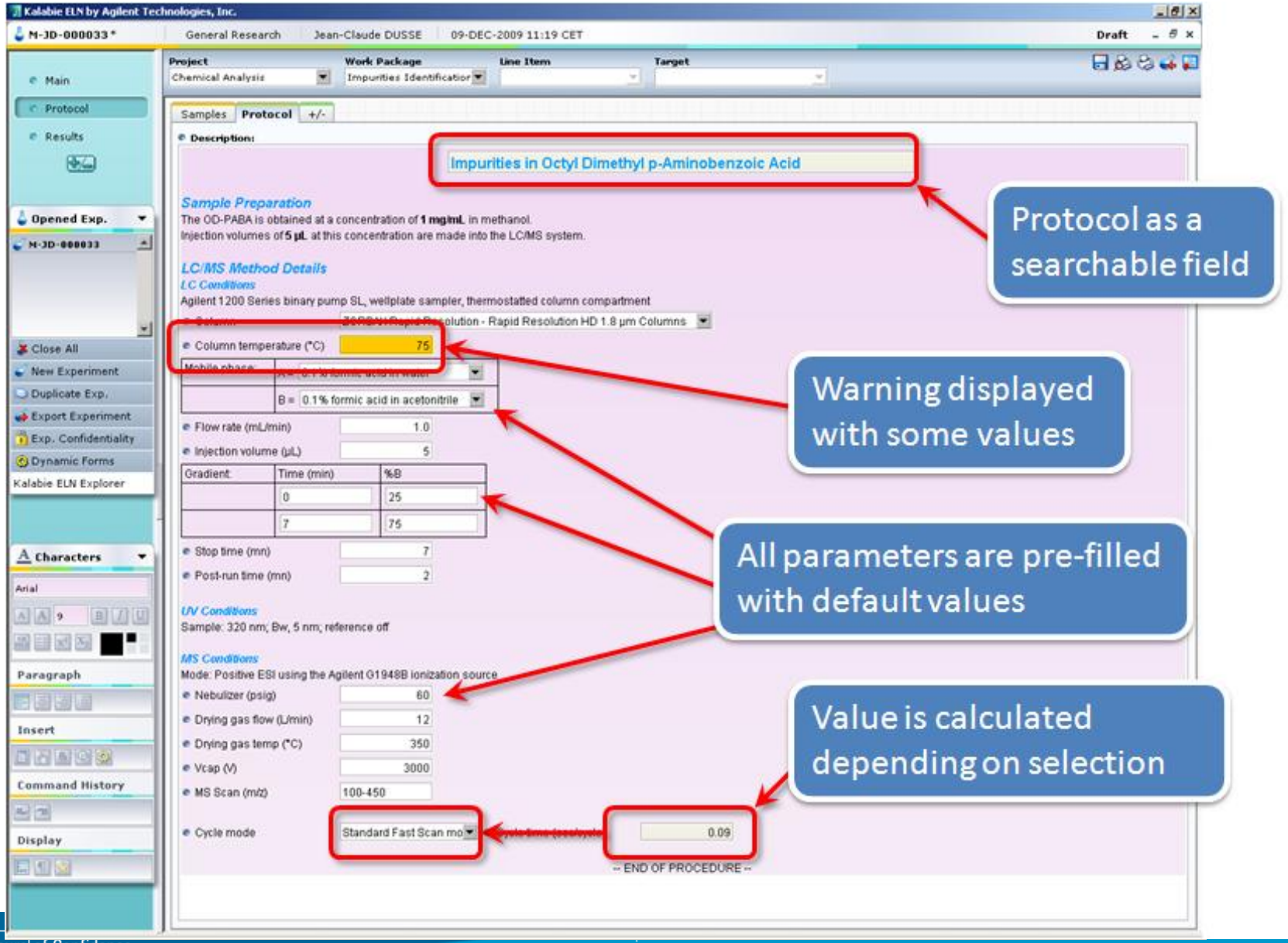


Case Study:

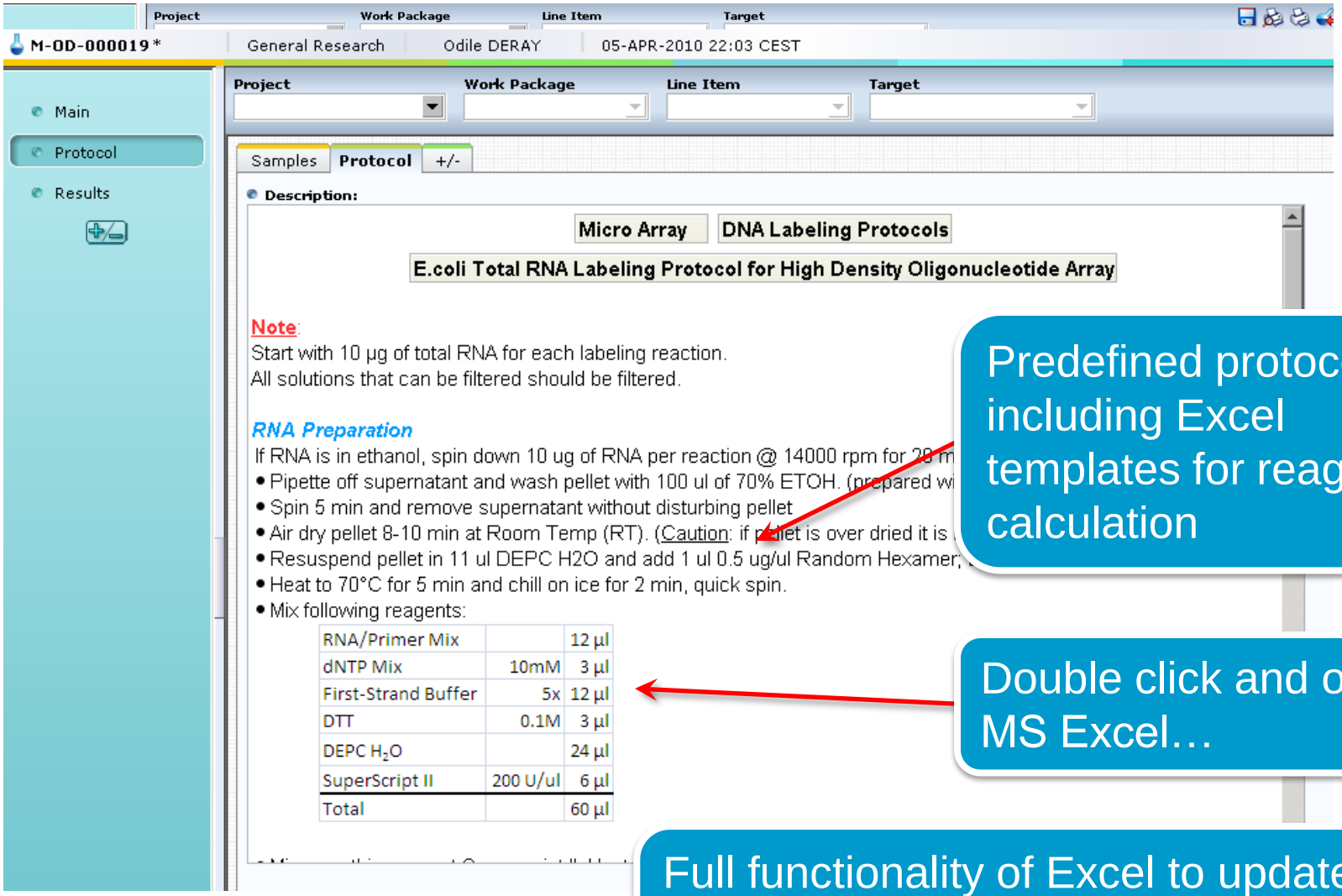
Quickly enter protocol details with Experiment Templates



OpenLAB ELN – Predefined Forms



Using Dynamic Forms and Excel in OpenLAB ELN

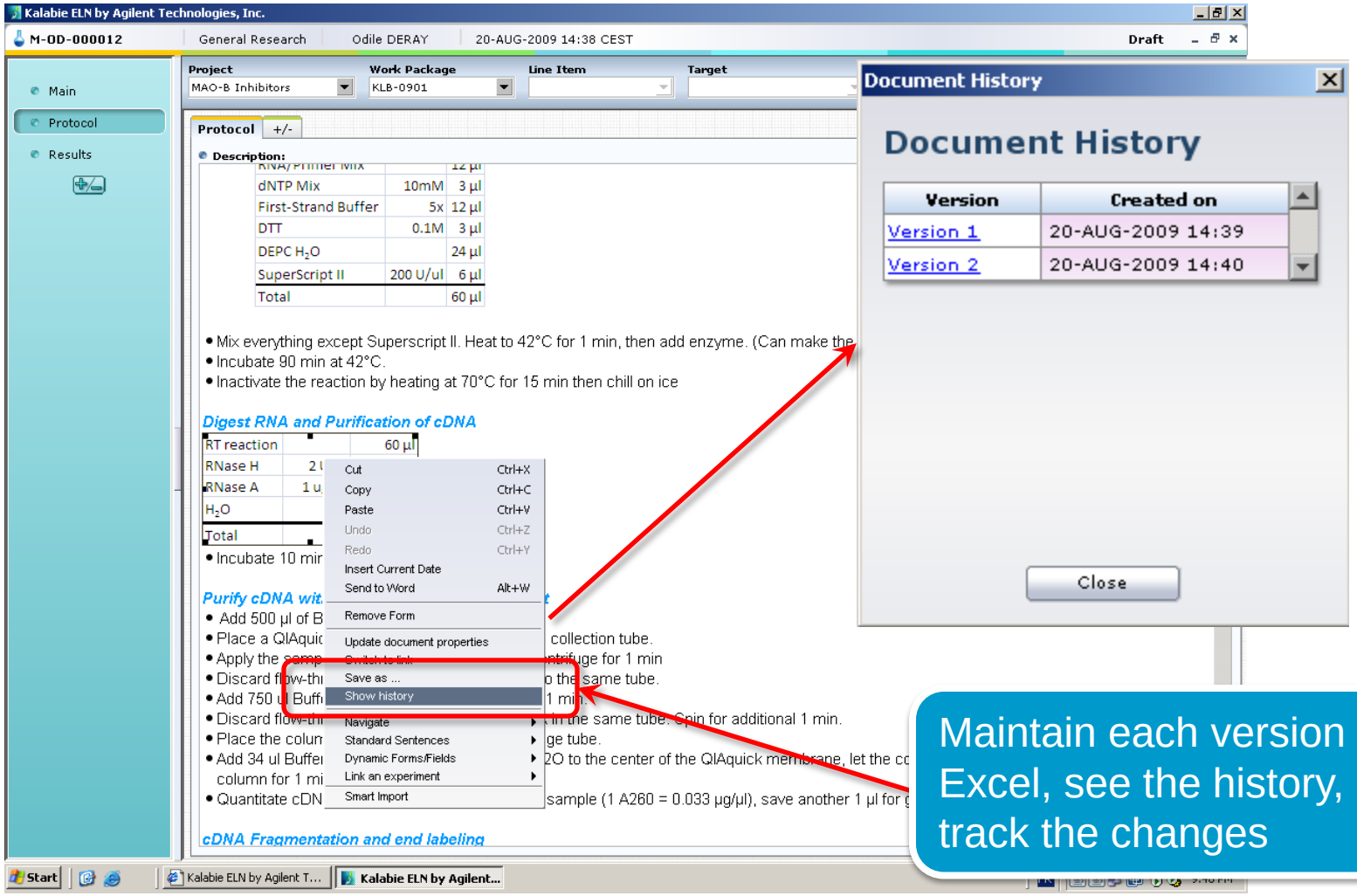


Predefined protocol including Excel templates for reagent calculation

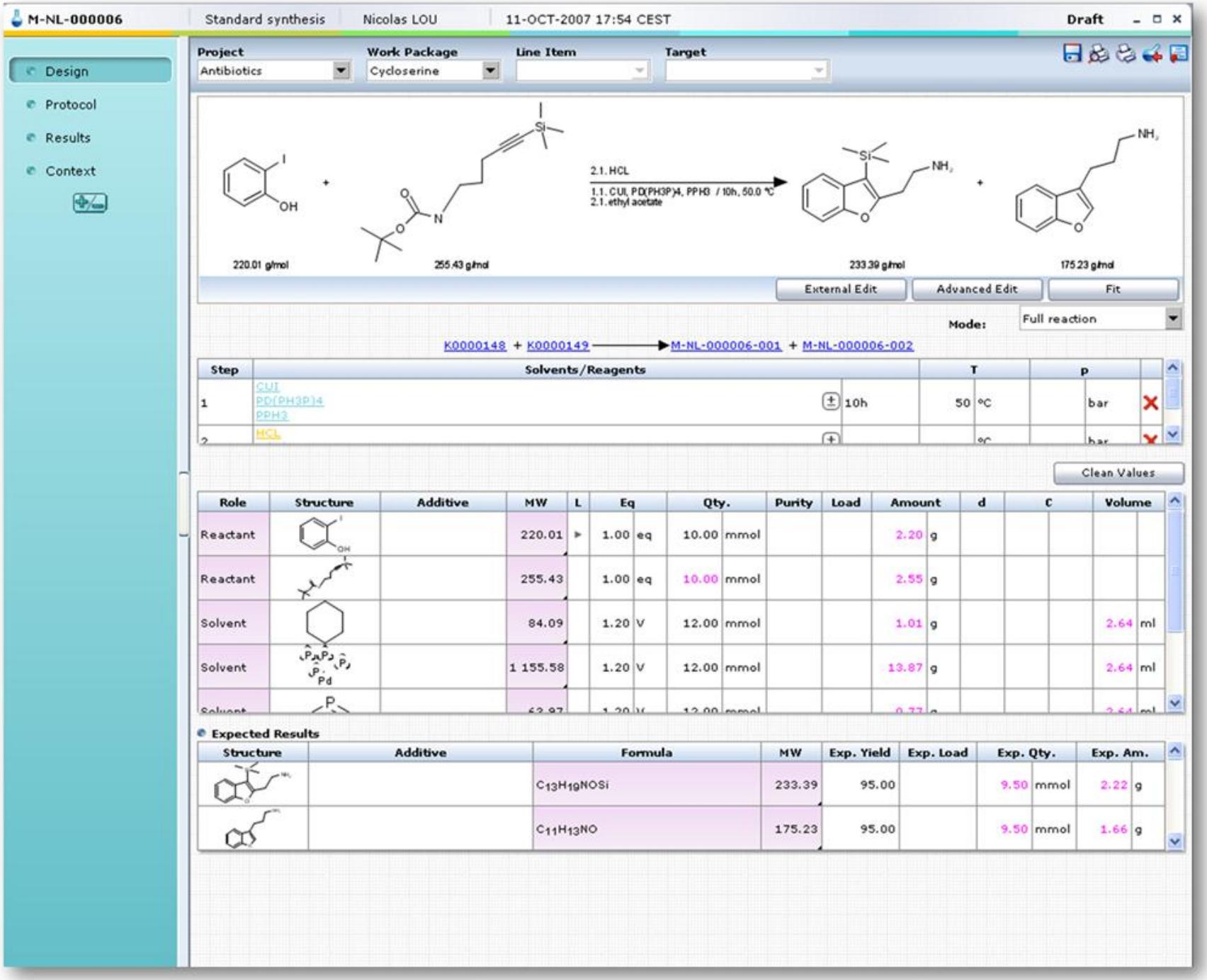
Double click and open MS Excel…

Full functionality of Excel to update values, add calculations, graphics and macros

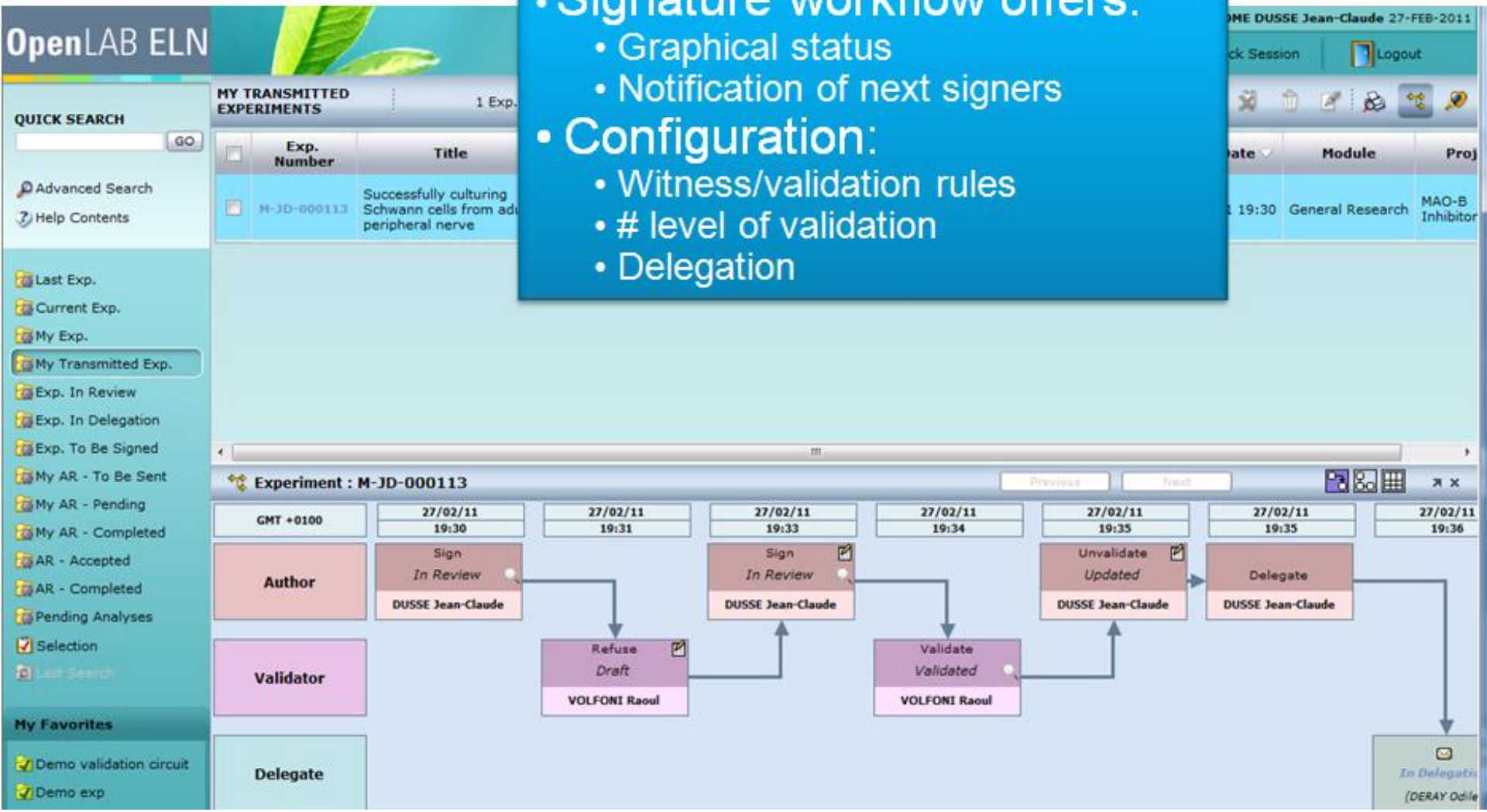
Managing changes within MS Excel



Maintain each version of Excel, see the history, track the changes


M-NL-000006
Standard synthesis
Nicolas LOU
11-OCT-2007 17:54 CEST
Draft
Design
Protocol
Results
Context
Project
Antibiotics
Work Package
Cycloserine
Line Item
Target
2.1. HCL
1.1. CUI, PD(PH3P)4, PPH3 / 10h, 50.0 °C
2.1. ethyl acetate
220.01 g/mol
255.43 g/mol
233.39 g/mol
175.23 g/mol
External Edit
Advanced Edit
Fit
Mode:
Full reaction
K0000148 + K0000149 → M-NL-000006-001 + M-NL-000006-002
Step
Solvents/Reagents
T
p
1
CUI
PD(PH3P)4
PPH3
10h
50 °C
bar
2
HCL
°C
bar
Clean Values
Role
Structure
Additive
MW
L
Eq
Qty.
Purity
Load
Amount
d
C
Volume
Reactant
220.01
1.00 eq
10.00 mmol
2.20 g
Reactant
255.43
1.00 eq
10.00 mmol
2.55 g
Solvent
84.09
1.20 V
12.00 mmol
1.01 g
2.64 ml
Solvent
1 155.58
1.20 V
12.00 mmol
13.87 g
2.64 ml
Expected Results
Structure
Additive
Formula
MW
Exp. Yield
Exp. Load
Exp. Qty.
Exp. Am.
C13H19NOSi
233.39
95.00
9.50 mmol
2.22 g
C11H13NO
175.23
95.00
9.50 mmol
1.66 g

- Signature workflow offers:
  - Graphical status
  - Notification of next signers
- Configuration:
  - Witness/validation rules
  - # level of validation
  - Delegation



OpenLAB ECM

OpenLAB ECM

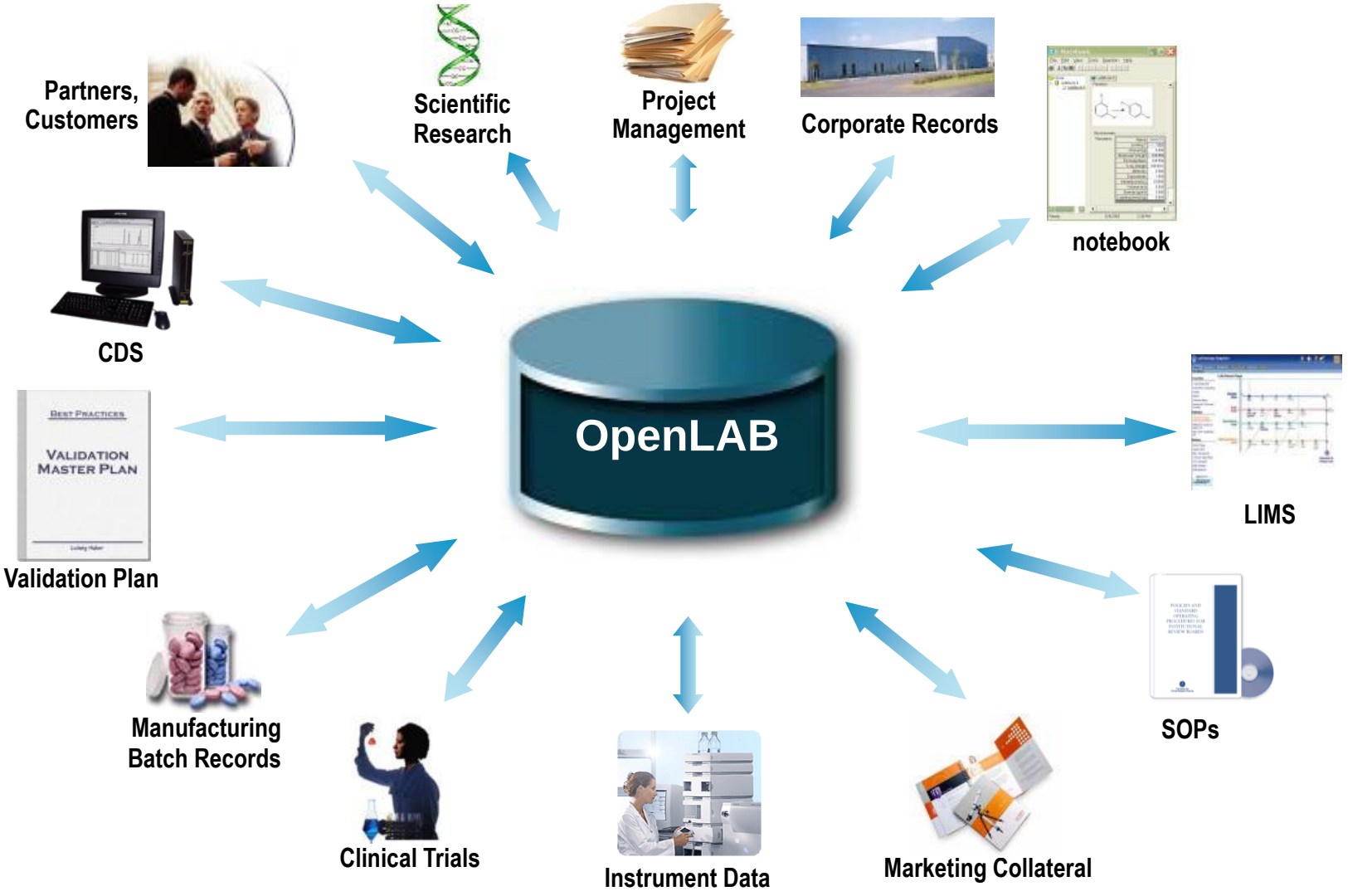
Enterprise Content Manager

Scientific Data Management System

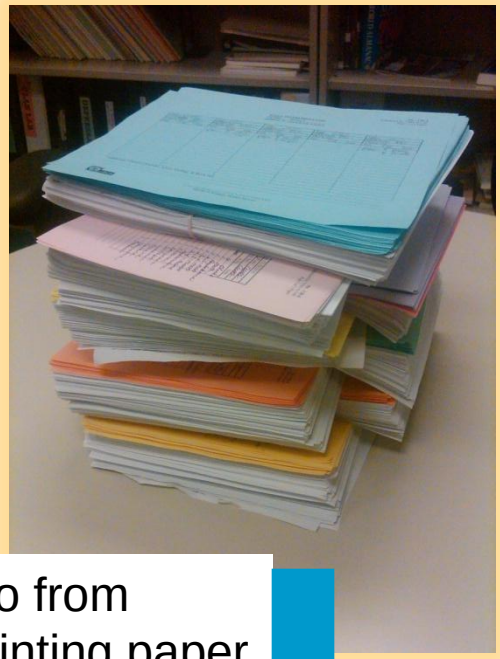
- Data archiving
- Instrument vendor neutral
- Viewers, filters, converters
- Agilent workstation aware!
- Time stamp/audit trail
- Report capture
- E-signatures
- Regulatory compliance
- TNF conversion (LTDA)

OpenLAB can store any electronic data

- *Central data storage in a compliance environment*

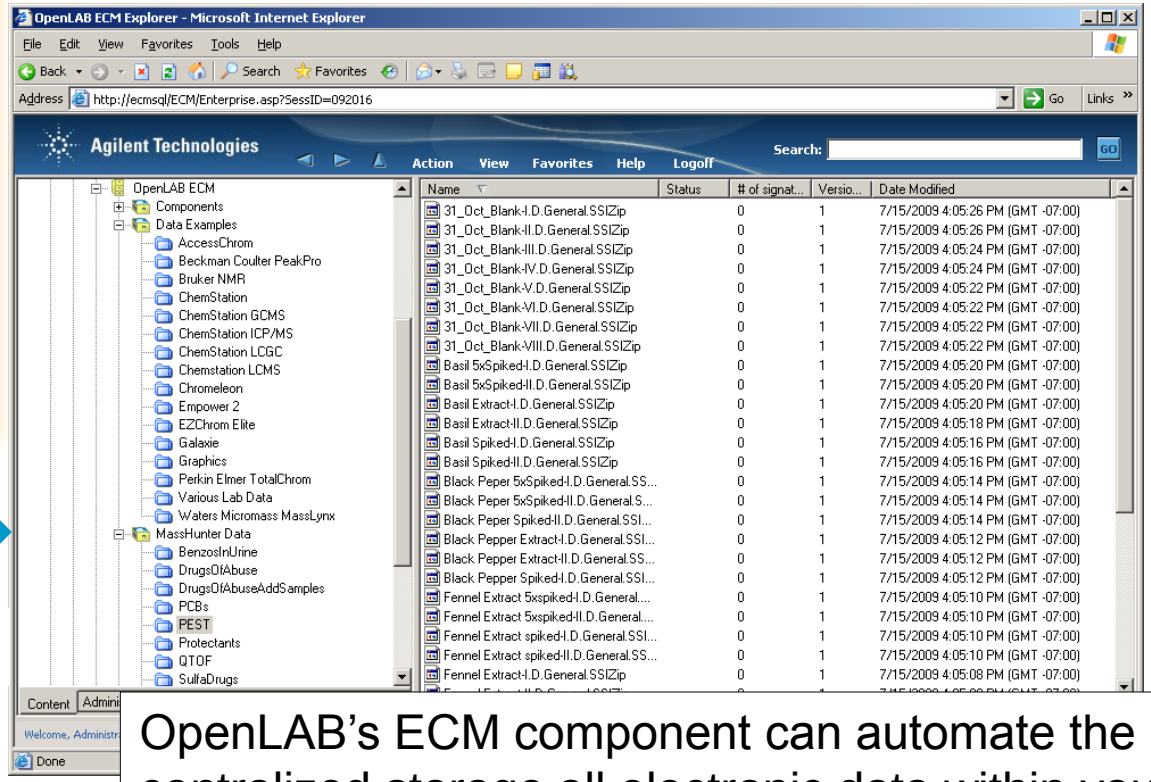


Generating and Storing Electronic Data in OpenLAB



Go from printing paper

To OpenLAB



OpenLAB's ECM component can automate the centralized storage all electronic data within your laboratory – both raw analytical and report data.

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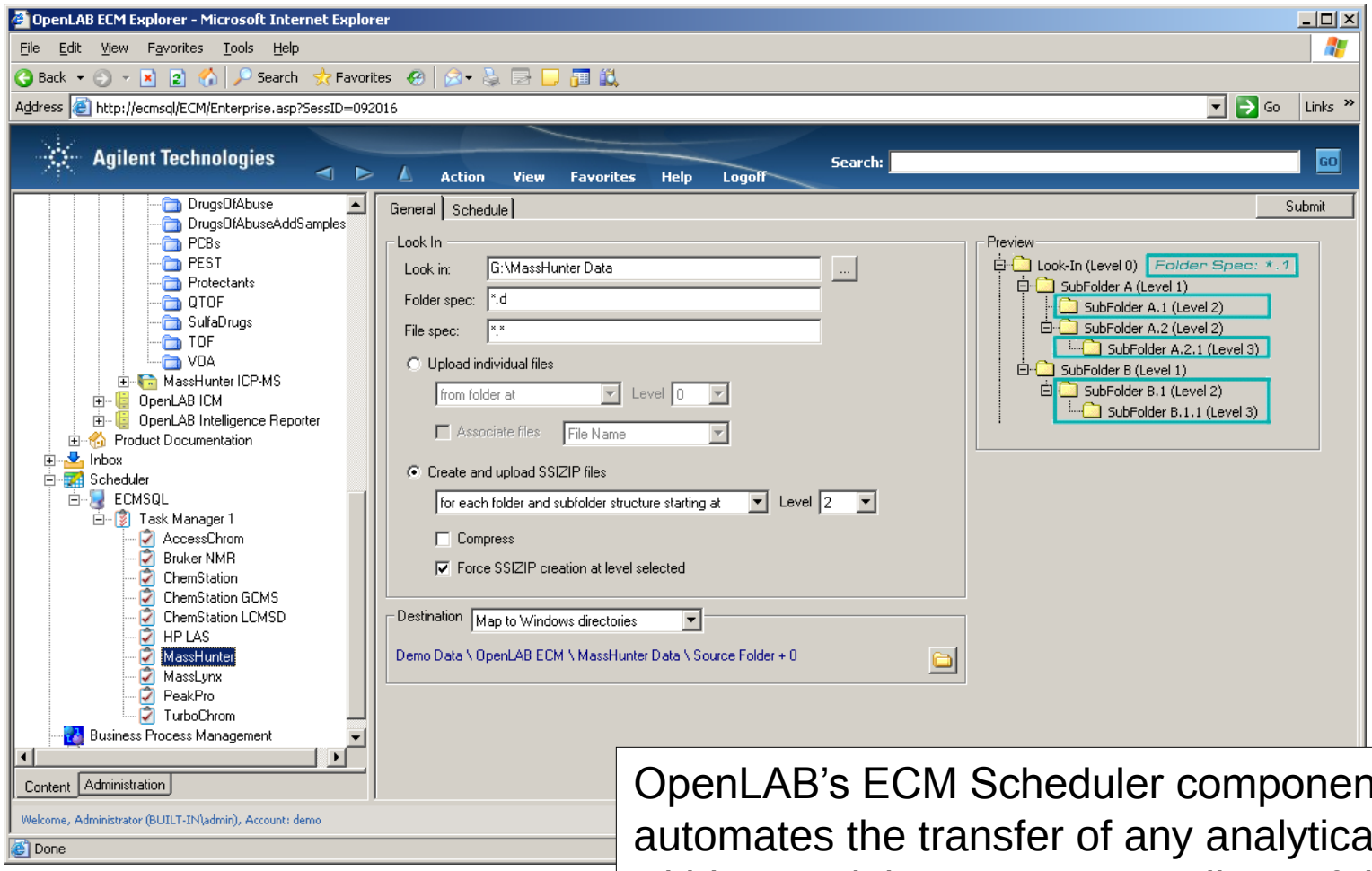
Automated Data Collection with OpenLAB



OpenLAB's ECM Scheduler component automates the transfer of any analytical data within your laboratory – regardless of the instrument vendor.

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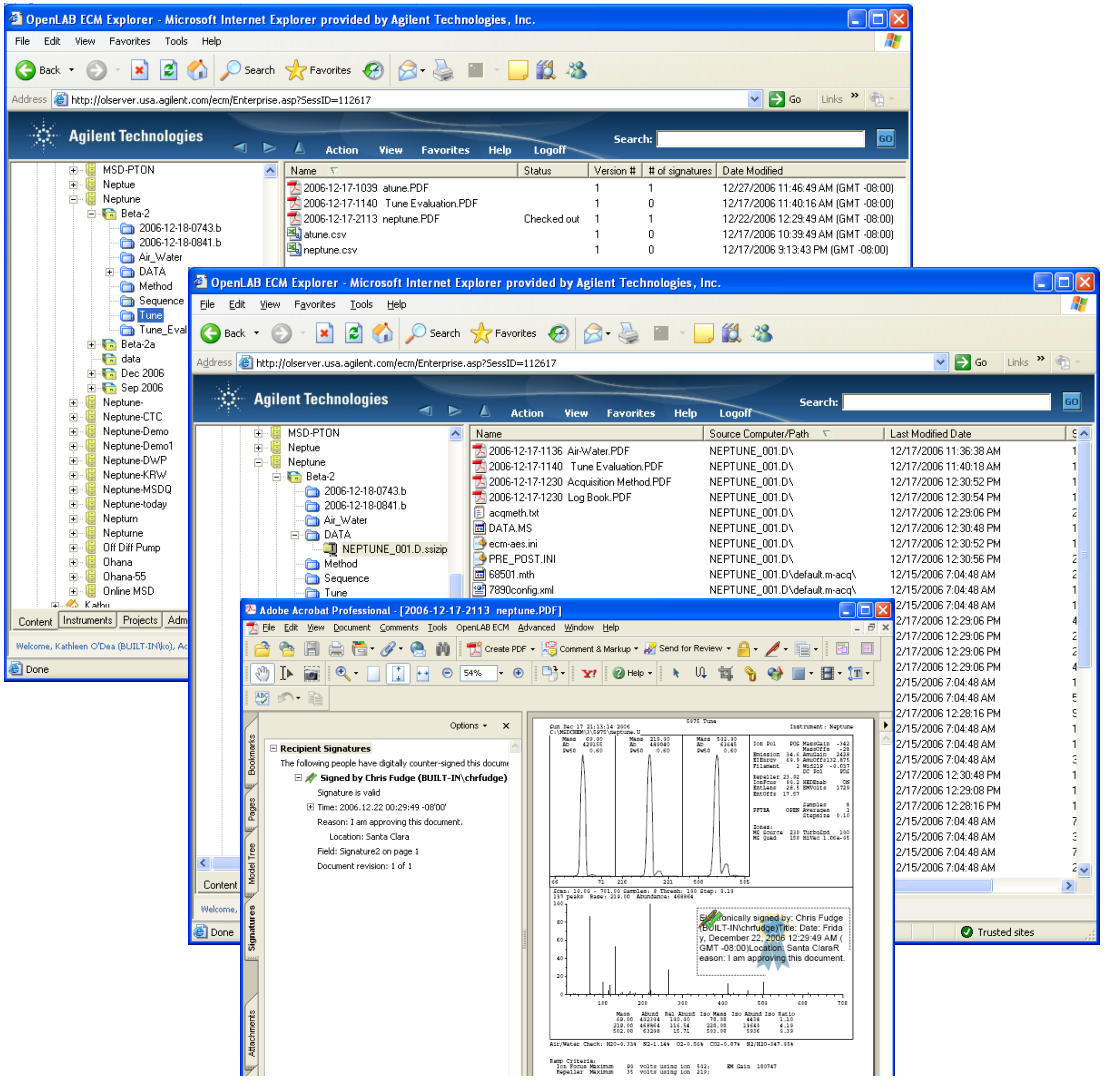
Electronic Signature of PDF Files in OpenLAB



- The PDF files that are stored in the Air_Water, Tune, and Tune_Eval folders can be signed with the Adobe PDF signature tool.
- This tool encrypts a visible signature within the PDF file.
- The signature is present when the file is viewed, printed, or removed from the ECM.
- Signing the PDF files with the Adobe PDF Signature tool requires Adobe Acrobat (not Reader)
- PDF files that are stored inside the SSIZIP file can not be signed individually.

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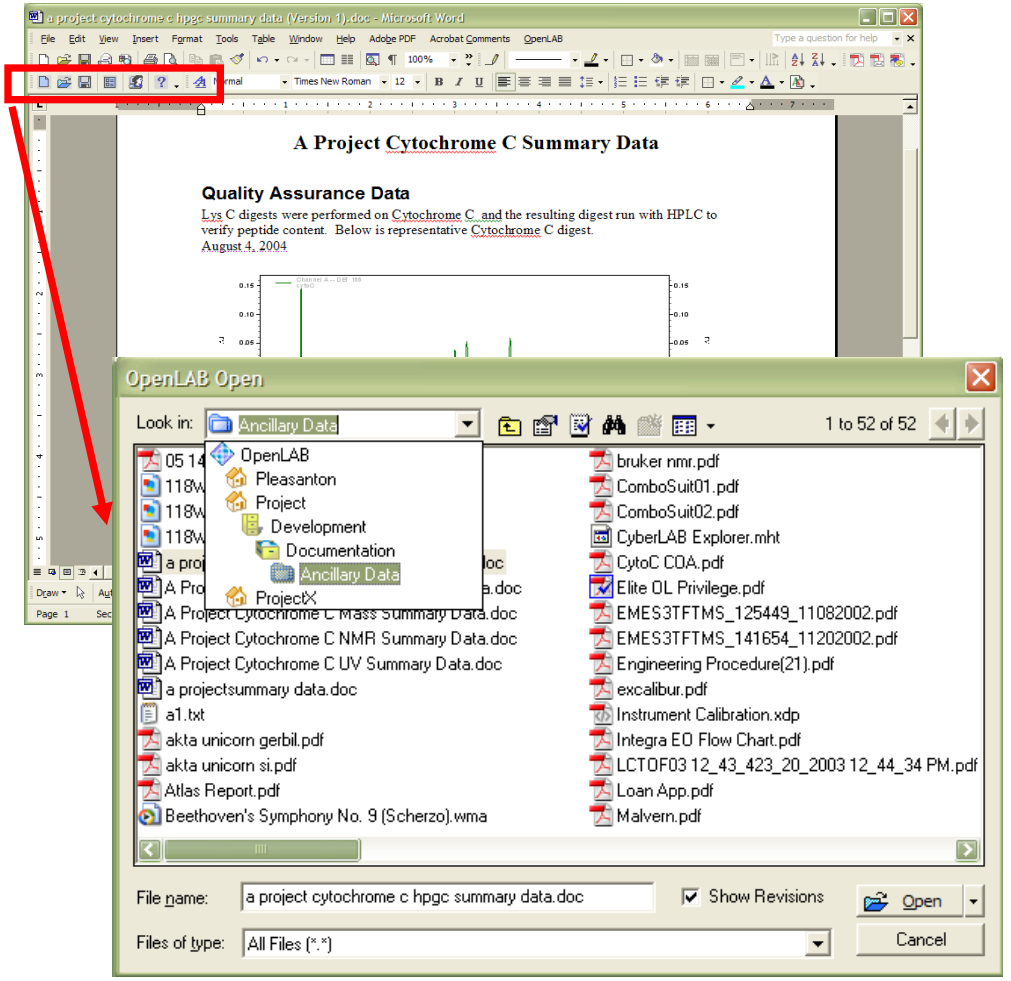
Interacting with Content from Desktop Applications

Integration with Desktop Applications like Microsoft Office, Adobe Acrobat

- Open and Save files directly to the content repository from familiar desktop application
- Small OpenLAB toolbar mimics Desktop functions with Content security
- Search the content repository from within the Desktop application for files of interest
- Compare documents or versions stored in the repository



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Remediation Services for Excel Spreadsheets

Cell by Cell auditing capabilities for Excel spreadsheets

Audits cell content changes

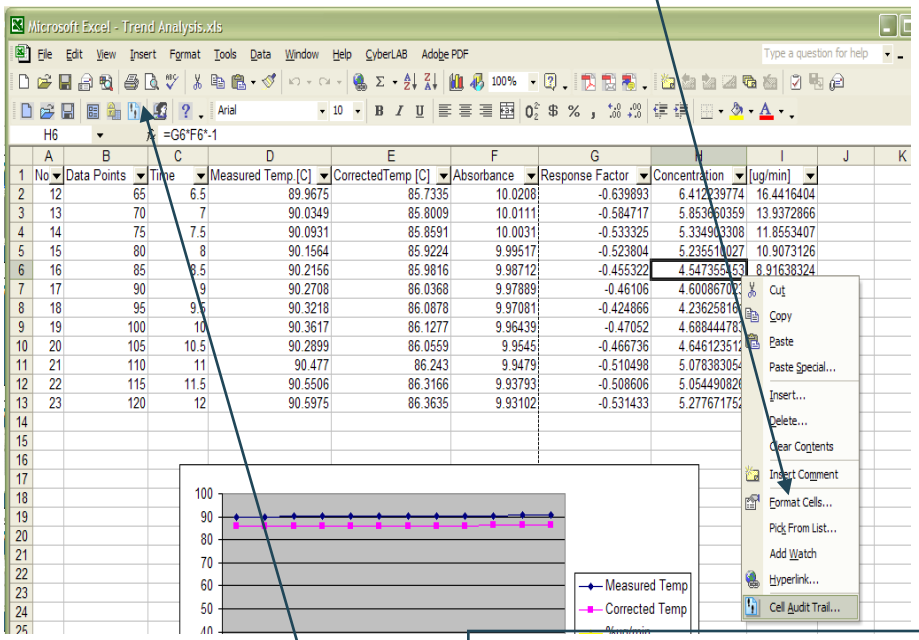
Audits cell formula changes

Audits macro changes

Each audit trail entry captures:

- Date / time of edit
- User ID
- Worksheet name and cell
- Old / New value
- Description & Reason for change

View the entries for a single cell



Or the entire spreadsheet

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OpenLAB CDS

OpenLAB CDS

Chromatography Data System

Workstation, Networked, Distributed

- ChemStation, EZChrom workflows
- Agilent and Non Agilent Instrument Control (Multi-vendor)
- OpenLAB ECM Intelligent Reporter
- Regulated and non-regulated modes
- Web-based options

OpenLAB Control Panel

Central point for:

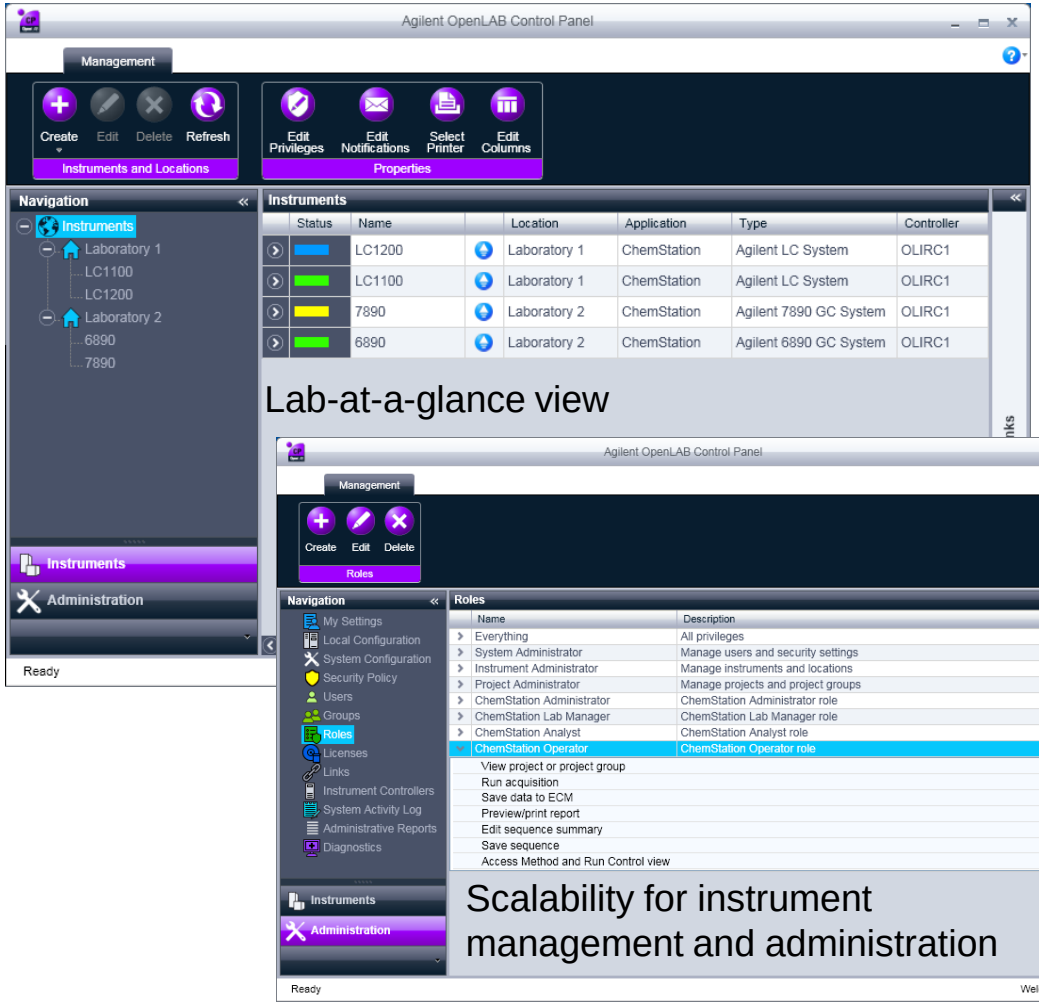
- Launching ChemStation & EZChrom instruments
- “Lab-at-a-Glance” view
- Administration of users, storage and instruments
- User privileges/user security
- Administrative reports

New look and feel:

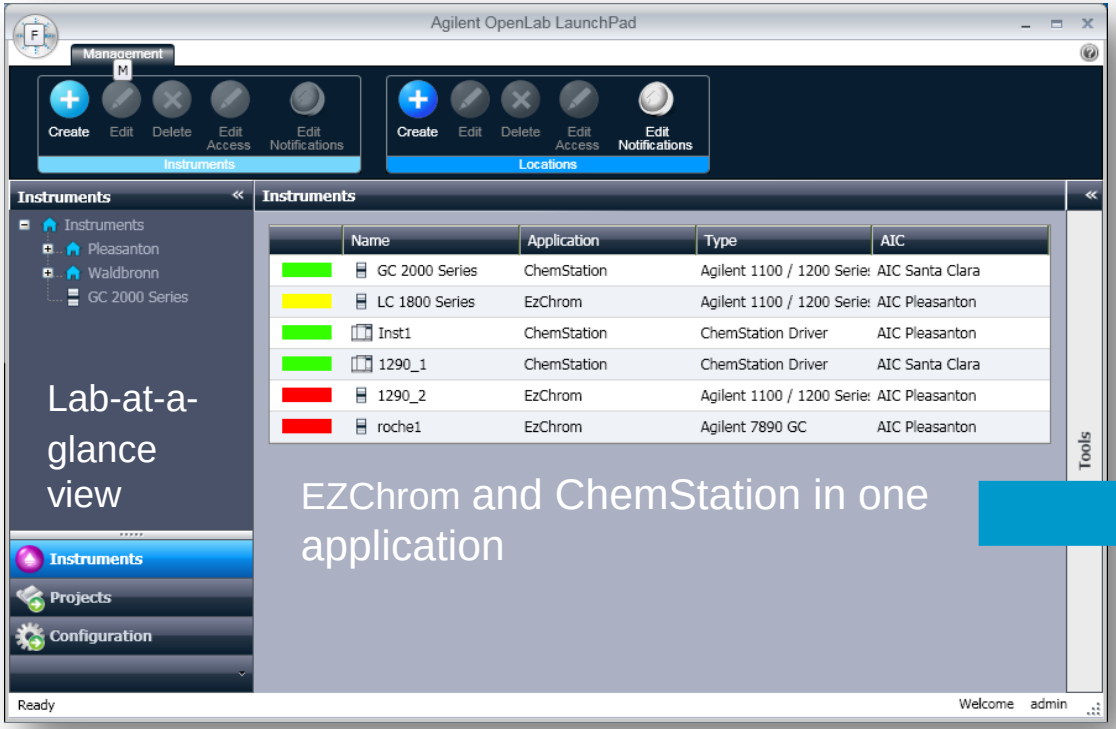
- Intuitive
- Easy-to-use

Support and troubleshooting:

- Central access to all config and log files



OpenLAB Control Panel



Remote lab monitoring

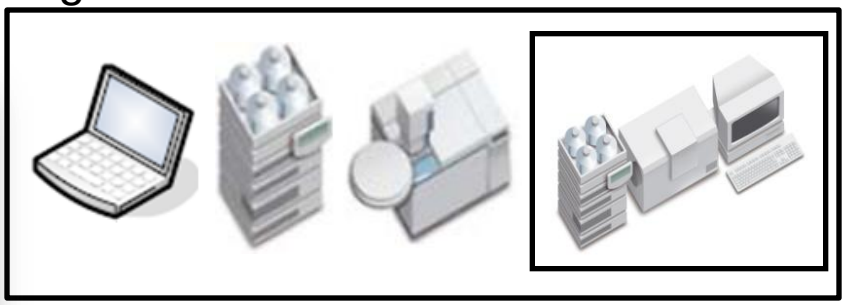
- **Lab at a Glance**
- **Instrument status**
- **System logbook**
- **Any errors**

OpenLAB CDS

Chromatography Data System

Workstation

ChemStation Edition –
Agilent LC/GC/LCMS/CE/AD



Or

EZChrom Edition

Control of Agilent LC/GC Waters, Shimadzu, Varian, PE…

OpenLAB CDS

Server Room

OpenLAB CDS Server(s)
Web, App, File Transfer, IR, SS
SQL or Oracle DB
(DB will be on a separate Server)

Example topology 1: OpenLAB CDS – Example: Local ChemStation

CDS Clients

LC Lab 1

ChemStation Client

GC Lab 1

ChemStation Client

LC Lab 2

ChemStation Client

Mass Spec Lab 1

GC/MS LC/MS ICP-MS

Note: 1200 LC data buffering in instrument

Steve Brown

OpenLAB CDS

Example topology 2: OpenLAB CDS - AIC

Remote Access / Control / Processing / Monitoring

Server Room

OpenLAB CDS Server
Web, App, File Transfer, IR, SS
SQL or Oracle DB
(DB will be on a separate Server)

Shared Services
(remote Monitoring)

CDS Clients

LC Lab 1

AIC

GC Lab 1

AIC

LC Lab 2

AIC

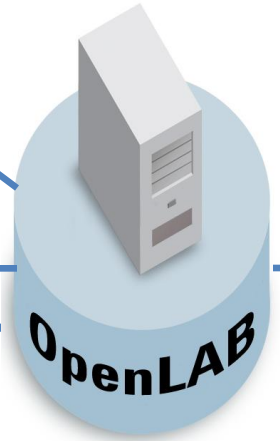
Mass Spec Lab 1

GC/MS LC/MS ICP-MS

Note: 1200 LC data buffering in instrument (flash)

AIC = Agilent Instrument Controller

OpenLAB Intelligence Reporter

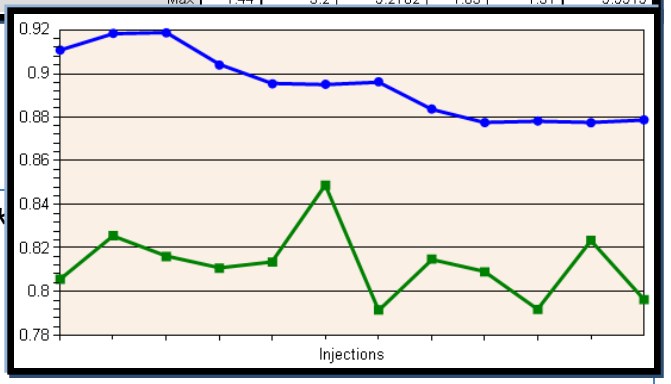


System Suitability Test — Failed tests are marked red

	Amount	RSD(RT)	RSD(Area)	Resolution EP	PW 50%	K'	S/N
des-hyd cis tramadol (C)	0.805	0.789	1.728	15.686	-0.040	21.307	11.308
des-hyd trans tramadol (B)	0.746	0.735	1.908	3.771	-0.127	22.403	8.547
o-desm tramadol (D)	0.823	2.130	2.789		0.291	6.860	9.001
TRAMADOL							
trans- tramadol (A)							

Results QC Samples

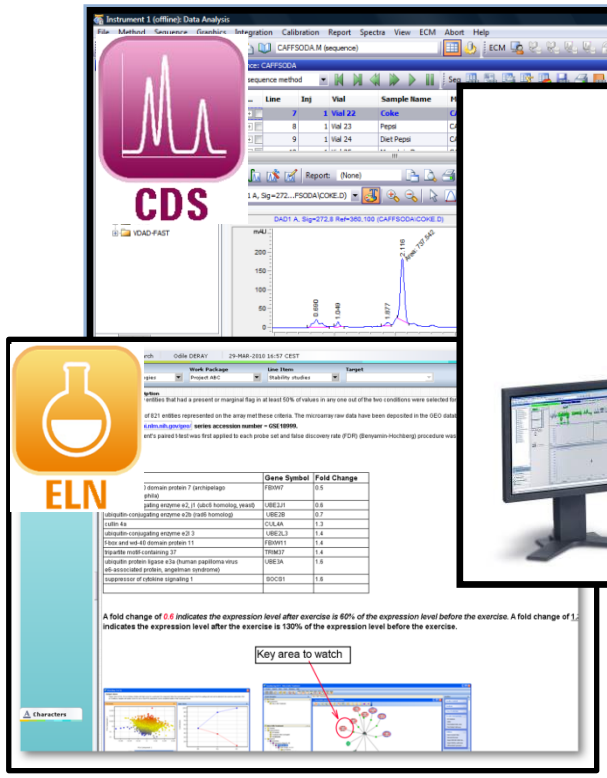
				trans- tramadol (A)			TRAMADOL		
				RT	Area	Amount ()	RT	Area	Amount ()
6	SS RSD 2	3	1FC-0603.D	1.43	3.15	5.1944	1.62	1.28	5.4352
	SS RSD 2	1	1FC-0601.D	1.44	3.16	5.2022	1.63	1.31	5.5515
	SS RSD 2	4	1FC-0604.D	1.43	3.17	5.2243	1.62	1.28	5.4390
	SS RSD 2	5	1FC-0605.D	1.44	3.2	5.2702	1.62	1.3	5.5245
	SS RSD 2	2	1FC-0602.D	1.44	3.17	5.2186	1.62	1.29	5.4773
	SS RSD 2	6	1FC-0606.D	1.44	3.14	5.1764	1.62	1.27	5.3594
			Average	1.44	3.16	5.2143	1.62	1.29	5.4645
			Stand. Dev.	0	0.02	0.0323	0	0.01	0.0691
			Min	1.43	3.14	5.1764	1.62	1.27	5.3594
			Max	1.44	3.2	5.2702	1.63	1.31	5.5515



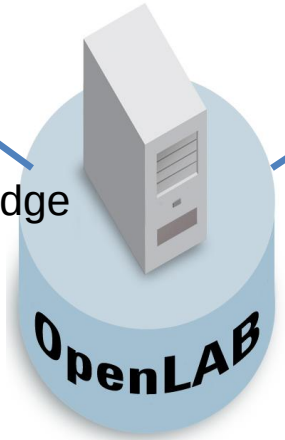
- Reports from CDS Instruments*
- Dynamic report templates
- Database reporting
- Automatic report generation
- Simple to advanced calculations with control charts
- Easily export results to Excel, PDF, or other formats
- Reports and templates managed securely in ECM
- Report templates work across different analysis/sites

Summary: From the Lab Bench to the Desktop - OpenLAB

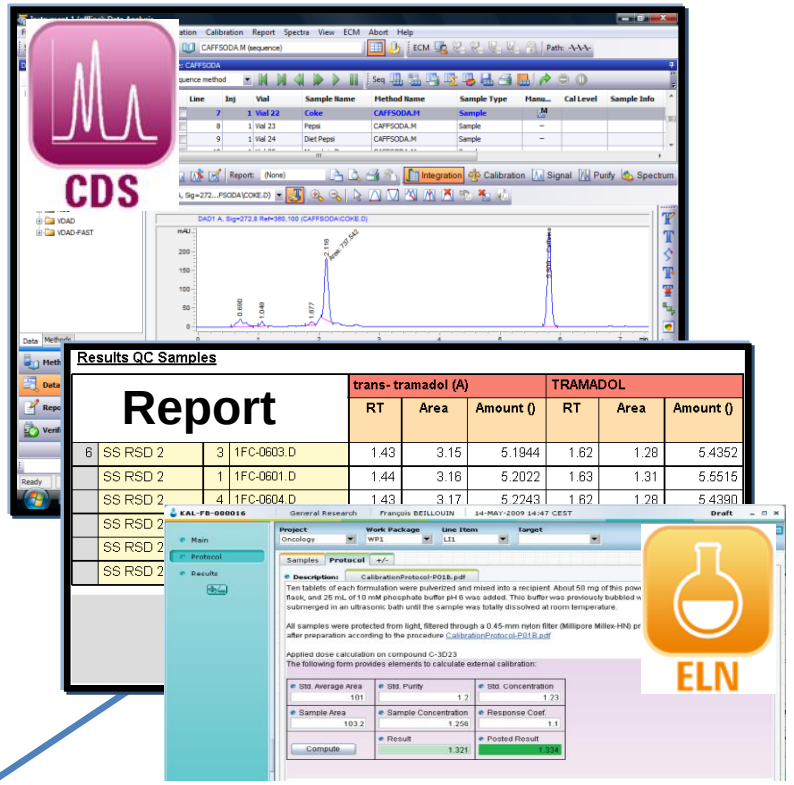
Laboratory



- Centrally store all data, reports, knowledge
- Security, versions, audit trail, e-sig
- OpenLAB unifies data, information and regulatory compliance



Office/Home



- Run & Reprocess from anywhere
- Easily find data and results
- Create custom reports
- Collaborate: ELN (Word, Excel, PDF)

21CFRPart11 Compliance

Steve Brown

Questions

Where to get more information

- http://www.agilent.com/chem/openlabcds

- Agilent Account Managers
  or
- Agilent Informatics Product Specialists
  Linda Johnson 302-636-3805
  linda_johnson@agilent.com

  Steve Brown – West - Midwest
  Marc Mandelbaum – East Coast
  Jonathon McSayles – Midwest to North East
  Steve Miller – Southern States
  Spencer Tse – West Coast