Agilent Laboratory Informatics

Maximising Laboratory Throughput with OpenLAB

2 Oktober 2012

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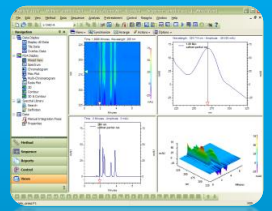
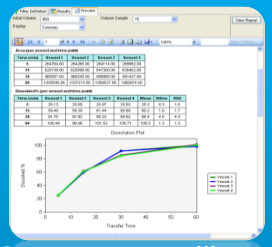
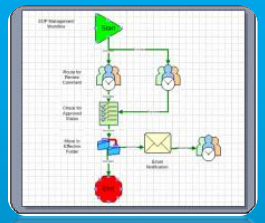
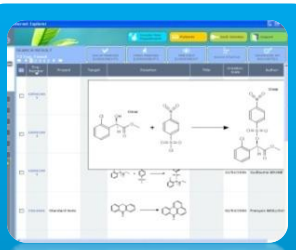
Produkt Spezialist Laborinformationssysteme
Life Science & Chemical Analyses

Agilent OpenLAB - *The Operating System for the Laboratory*

Scientific Data Management	Chromatography Data System	Reporting	Business Process Management	Electronic Lab Notebook
				
OpenLAB Enterprise Content Management (ECM)	OpenLAB Chromatography Data System with Multi-Vendor Control (CDS)	OpenLAB Intelligent Reporter	OpenLAB Business Process Management (BPM)	OpenLAB Electronic Lab Notebook (ELN)

Agilent OpenLAB Manage Instruments, People, Process & Content !

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

- Web-based, n-tier architecture scalable from small lab to global implementation
- Integrating framework for 3rd party applications and techniques.

The unfortunate Problem 1
Paper and Data handling

From chaos…

To a single search in seconds…

AGILENT OPENLAB ECM

SCIENTIFIC DATA MANAGEMENT

Agilent OpenLAB ECM *(Enterprise Content Manager)*

ECM

Processes

SOP Management

Instrument Management

Content Uniformity

Instruments


GC/MS


GC


UV-vis


LC/MS


LC

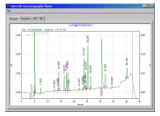

ICP-MS

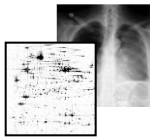

Lab-on-a Chip


CE

Content


MS Office


Legacy Data

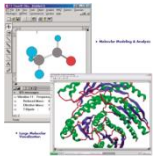

Images


PDF


ELN

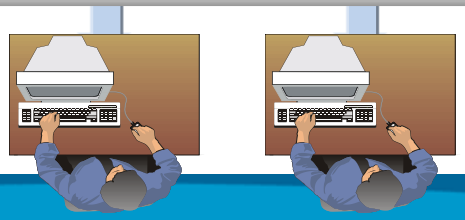

LIMS


Research


Drawings

Intranet

Internet

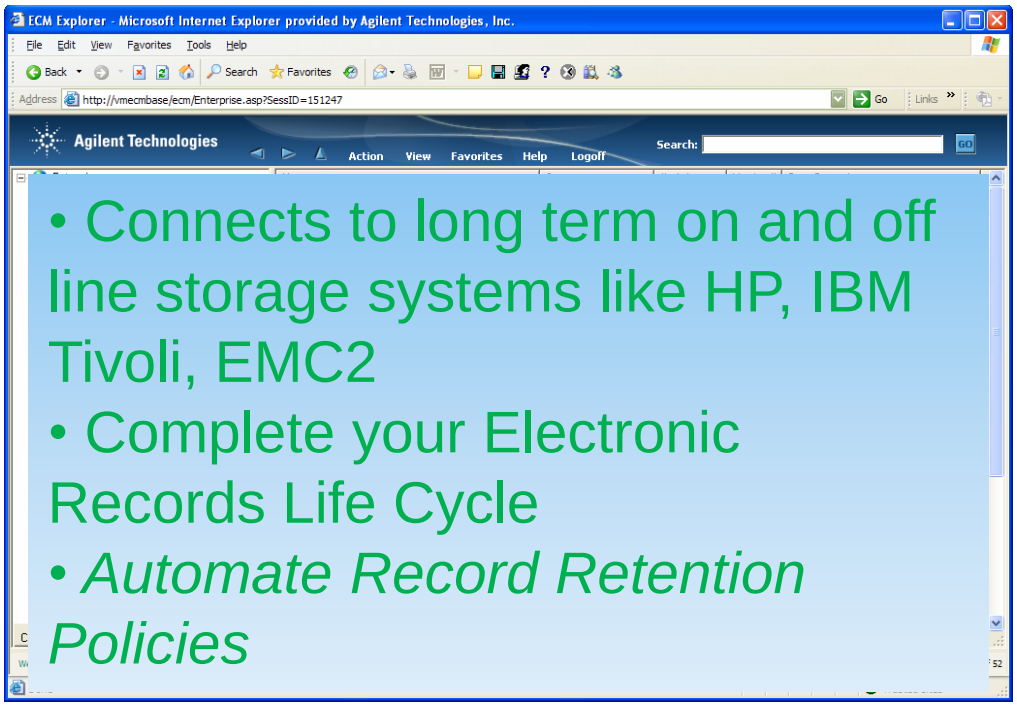


Centrally Store and Protect All Data Using OpenLAB ECM

More than just a Scientific Data Management System SDMS

Manage and organize ALL electronic content regardless of source in a 21 CFR Part 11 way.

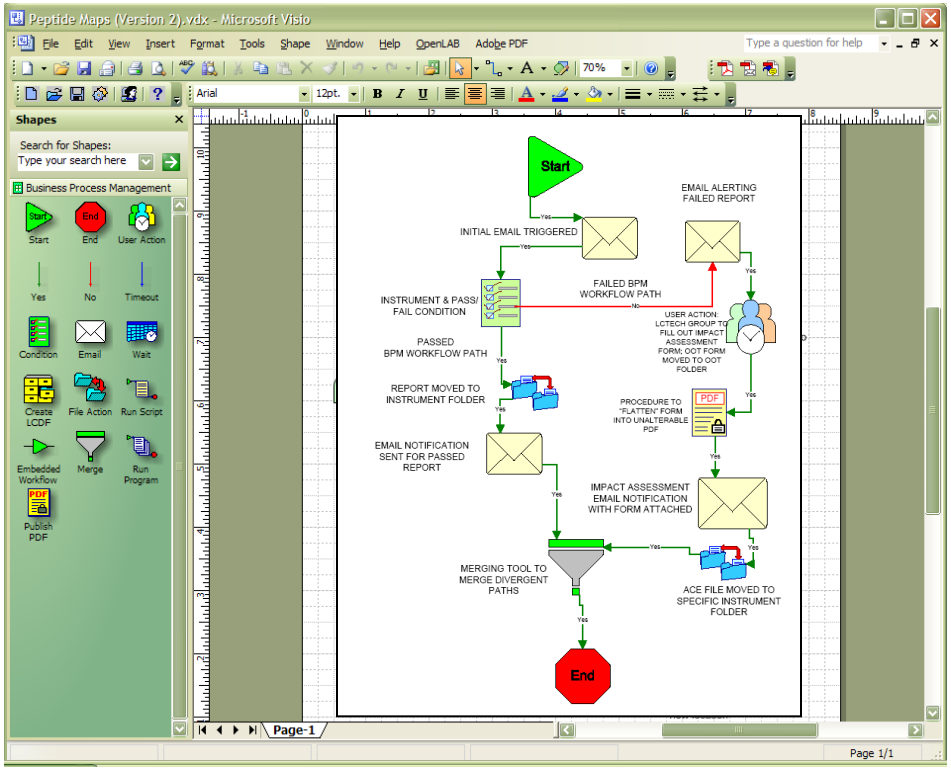
- Analytical Data
- Chromatography results
- Photographs and images
- PDF files and forms
- Scanned paper files
- Email
- Microsoft Office files
- Electronic reports
- ANY electronic content



Agilent OpenLAB BPM *(Business Process Management)*

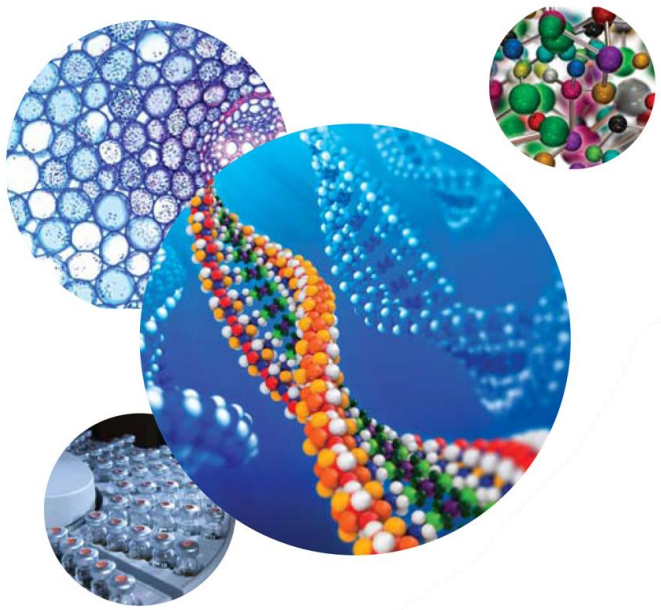
ECM

Automate the Information Flow in your Lab



BPM example of a Pharma Case Study!!!!!

- **Agilent OL BPM option:**
  - **Automate a process in the laboratory without any programming knowledge**
  - **Control the flow of information for data review, electronic signoff, electronic notifications**
  - **Manage and schedule instrument maintenance through BPM**



CDS ECM ELN SERVICES

AGILENT OPENLAB ELN

ELECTRONIC LAB NOTEBOOK

The unfortunate Problem 1
Paper and Data handling

ELN

From chaos…

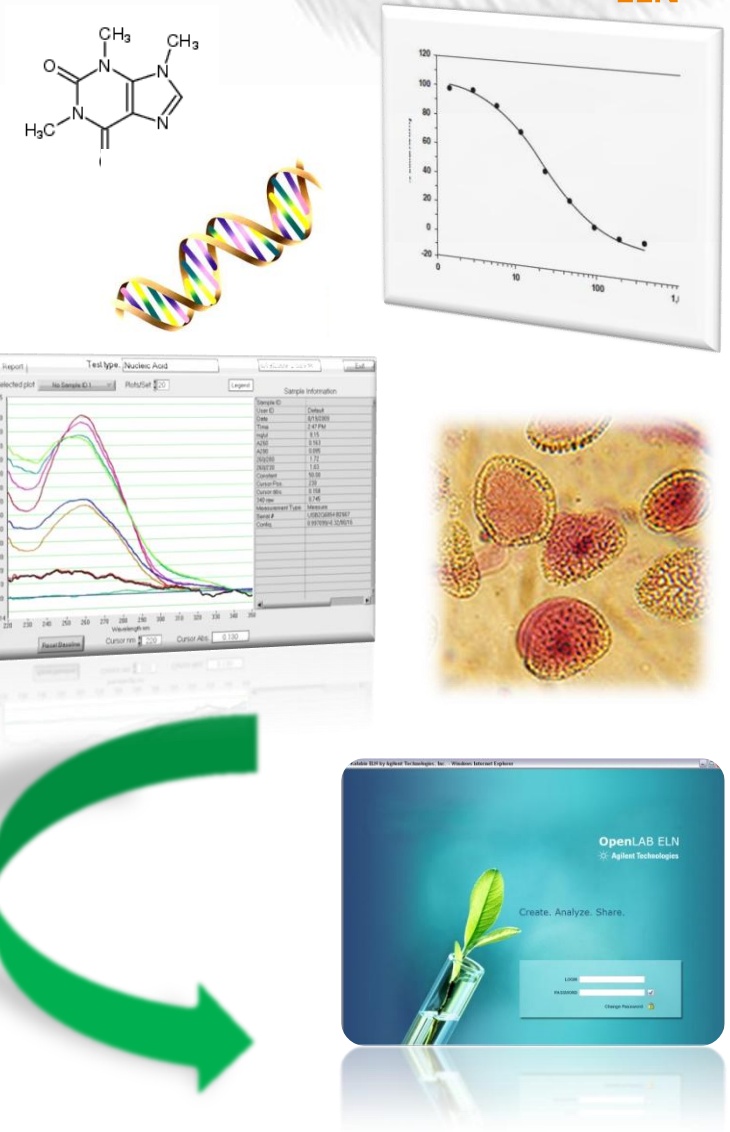
To a single search in seconds…

Agilent OpenLAB ELN *(Electronic Laboratory Notebook)*

ELN

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



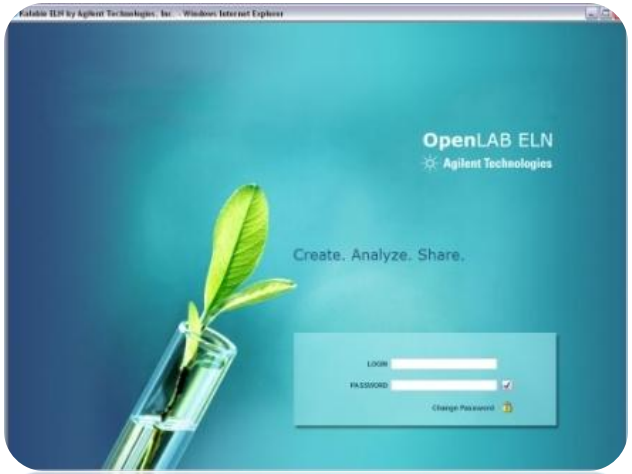
Resulting in…

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

Agilent OpenLAB ELN *(Electronic Laboratory Notebook)*

OpenLAB ELN is an open architecture, highly flexible electronic lab notebook that simplifies and accelerates the documentation process and facilitates cross-team collaboration

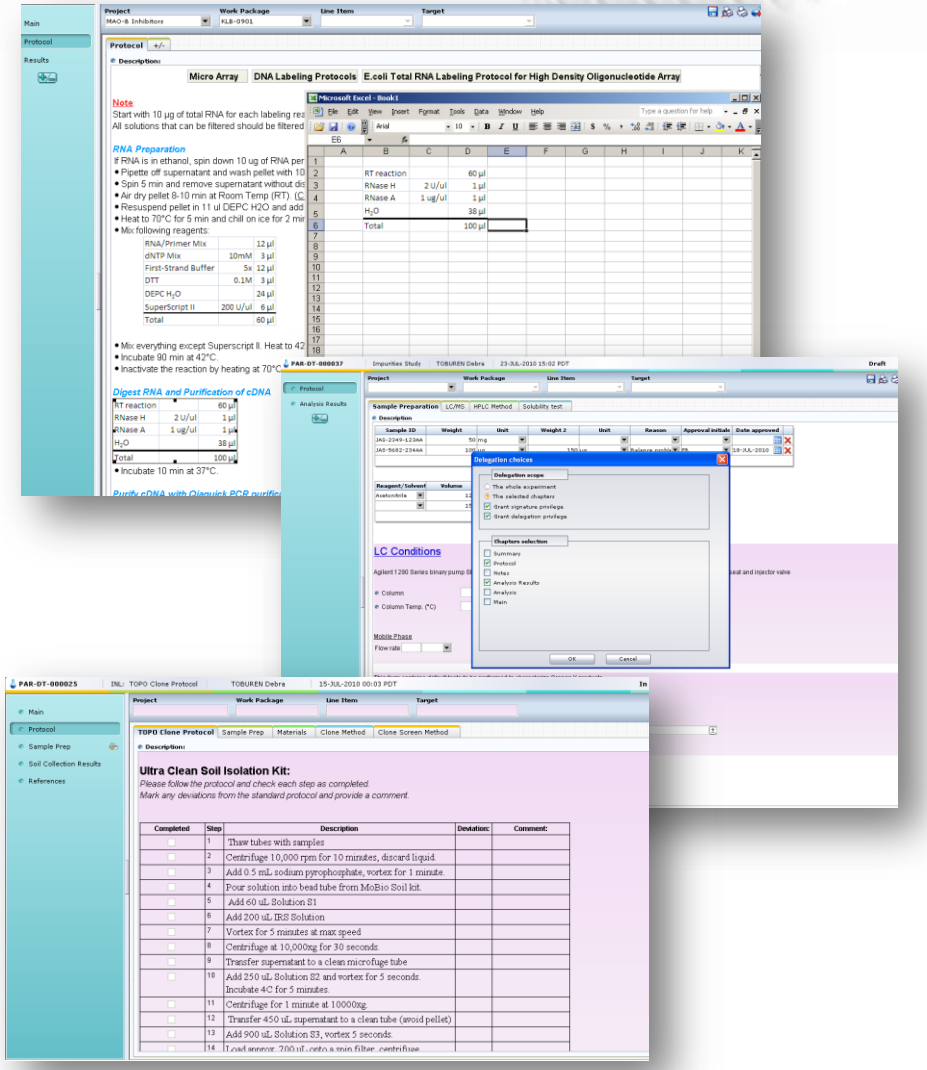
- Integrated into the OpenLAB framework
  - Consistency with OpenLAB architectural values
  - Connectivity with OpenLAB ECM and CDS
- Multidisciplinary
  - Synthetic Chemistry
  - Biology/Genomics
  - Analytical Chemistry
  - Formulations
- Superior IP Protection
  - SAFE (user authentication) and Surety AbsoluteProof (data integrity)



An ELN Tailored to Your Working Environment

ELN

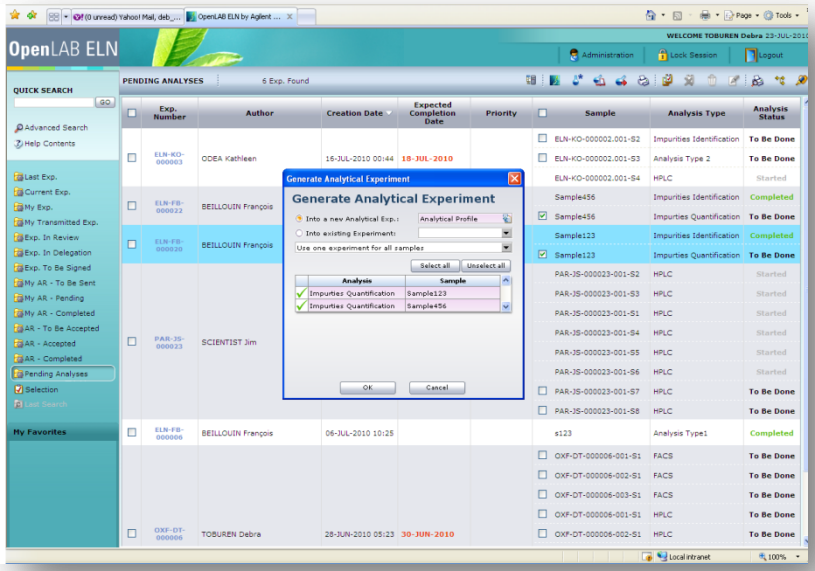
- Quickly setup an experiment and capture data.
- Mirror your workflow with experiment templates, forms and form fields
- Ability to search - review experimental data across multiple researchers
- Complete and transparent auditing activities



Analytical Chemistry Workflow

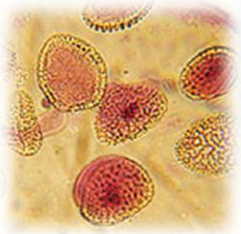
ELN

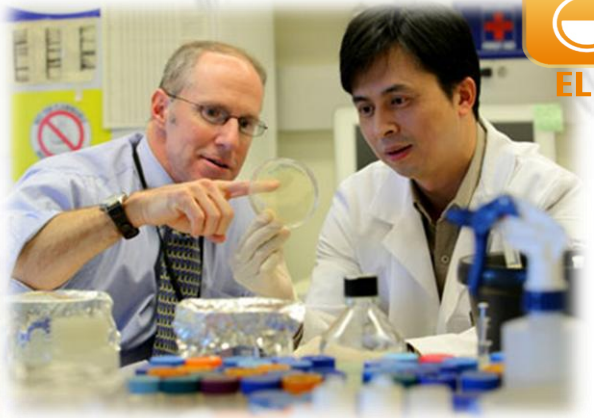
- Generate quickly reports across multiple samples and techniques
- Reduce cycle time from request to result
  - Check status, queue requests
  - Easy tracking of procedures and details
  - Reduce time for routing document approval
- Import directly from instruments
  - ChemStation, Empower, MassHunter*
  - Small devices (balances, pH meters, etc)
- Capture images, chromatograms, spectra; fully searchable annotations
- Setup experiments quickly with standard sentences and templates



Focus on Biology

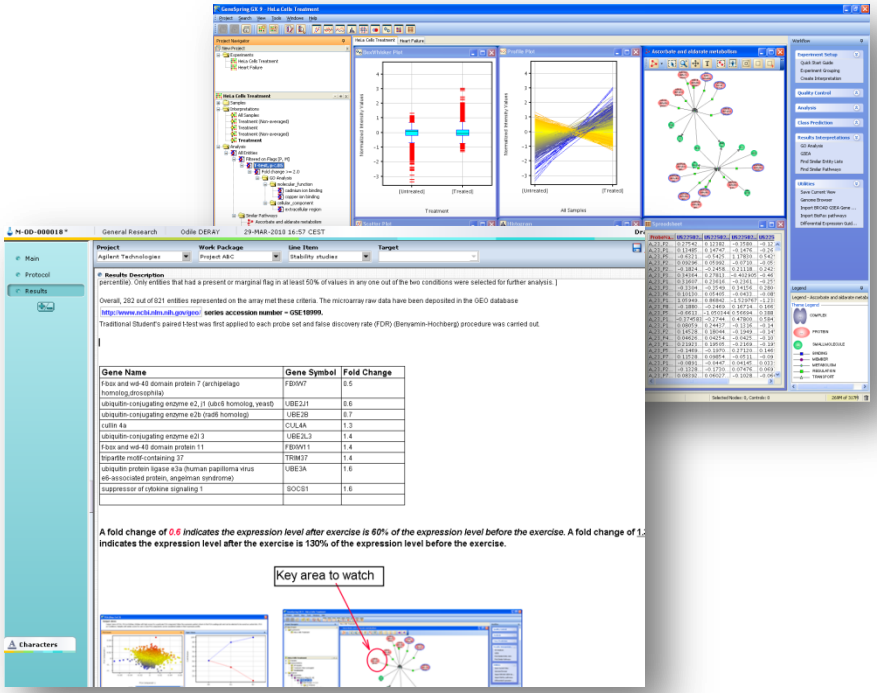
- Cell biology
- Proteomics
- Molecular biology
- Genomics
- Toxicology





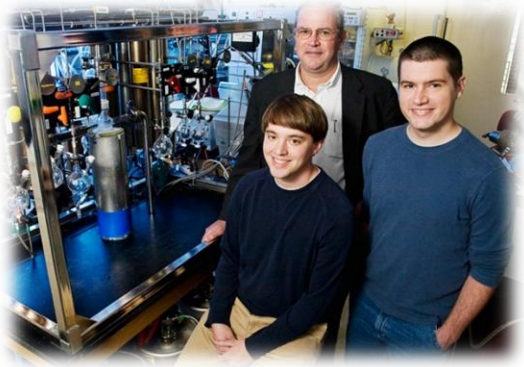
ELN

- 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
  - GeneSpring, MassHunter, VectorNTI…

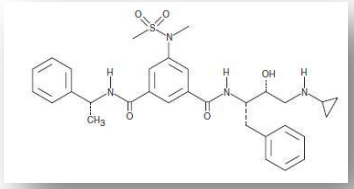


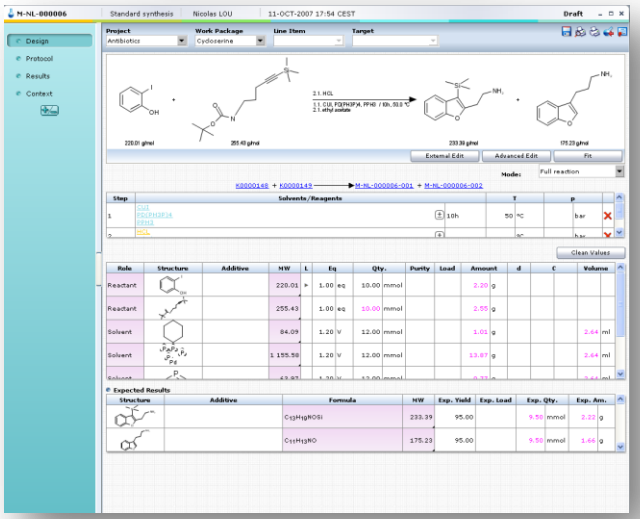
Focus on Synthetic Chemistry

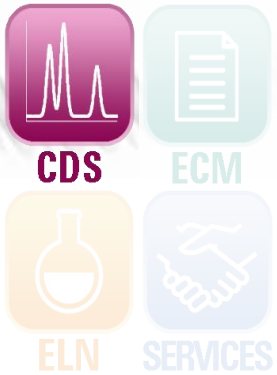
ELN



- Search and re-use synthesis knowledge from across the lab or organization
- Plan, search and design reactions
- Access commercial sourcing and registration systems
- Create favorites for commonly used reagents and solvents
- Manage batches, split samples and submit for analysis directly from the experiment







AGILENT OPENLAB CDS

CHROMATOGRAPHY DATA SYSTEM

Agilent OpenLAB CDS *(Chromatographic Data System)*

What is OpenLAB CDS?

OpenLAB CDS is:

- The consolidation of ChemStation and EZChrom under the new OpenLAB architecture
- The next major revision of Agilent ChemStation, EZChrom and OpenLAB ICM with significantly enhanced functionality
- …initially available in two flavors as EZChrom Edition and as ChemStation Edition of OpenLAB CDS

OpenLAB CDS: Enhanced Functionality

1. **Unmatched Scalability**
   - From workstation to enterprise distributed data systems; adapting to the needs of YOUR laboratory via a consolidated architecture
2. **A Central Control Panel**
   - With lab-at-a-glance functionality for better laboratory management via a new Shared Services application
3. **New Custom and Advanced Reporting**
   - Easy setup of advanced reports for improved productivity, via OpenLAB Intelligent Reporting
4. **More intuitive and more flexible result review and reprocessing options**
   - Create virtual “reprocessing-only” sequence for flexible result recalculation or keep acquisition sequence setup for full data integrity

All this via a “non-disruptive upgrade”

- The next major revision of ChemStation and EZChrom/OpenLAB ICM offers backwards compatibility of data, methods and workflows; protecting your investment
- Designed with usability in mind

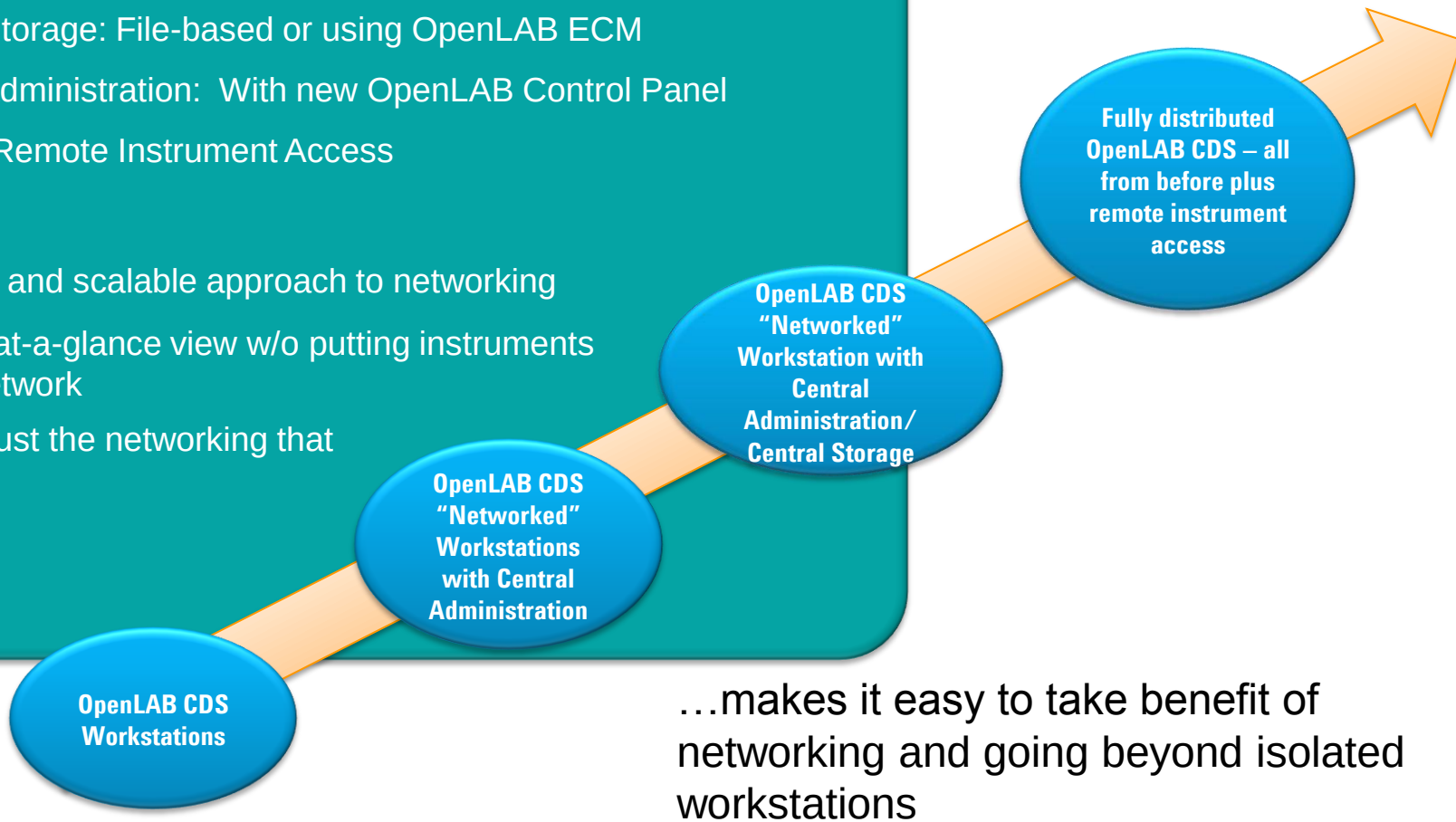
OpenLAB CDS: Scalable in Storage, Lab Management and Administration

Flexible stepwise adaption of networking:

- Central Storage: File-based or using OpenLAB ECM
- Central Administration: With new OpenLAB Control Panel
- Local or Remote Instrument Access

Benefits:

- Stepwise and scalable approach to networking
- Get Lab-at-a-glance view w/o putting instruments on the network
- Choose just the networking that you need



…makes it easy to take benefit of networking and going beyond isolated workstations

OpenLAB CDS – Workstation Configuration

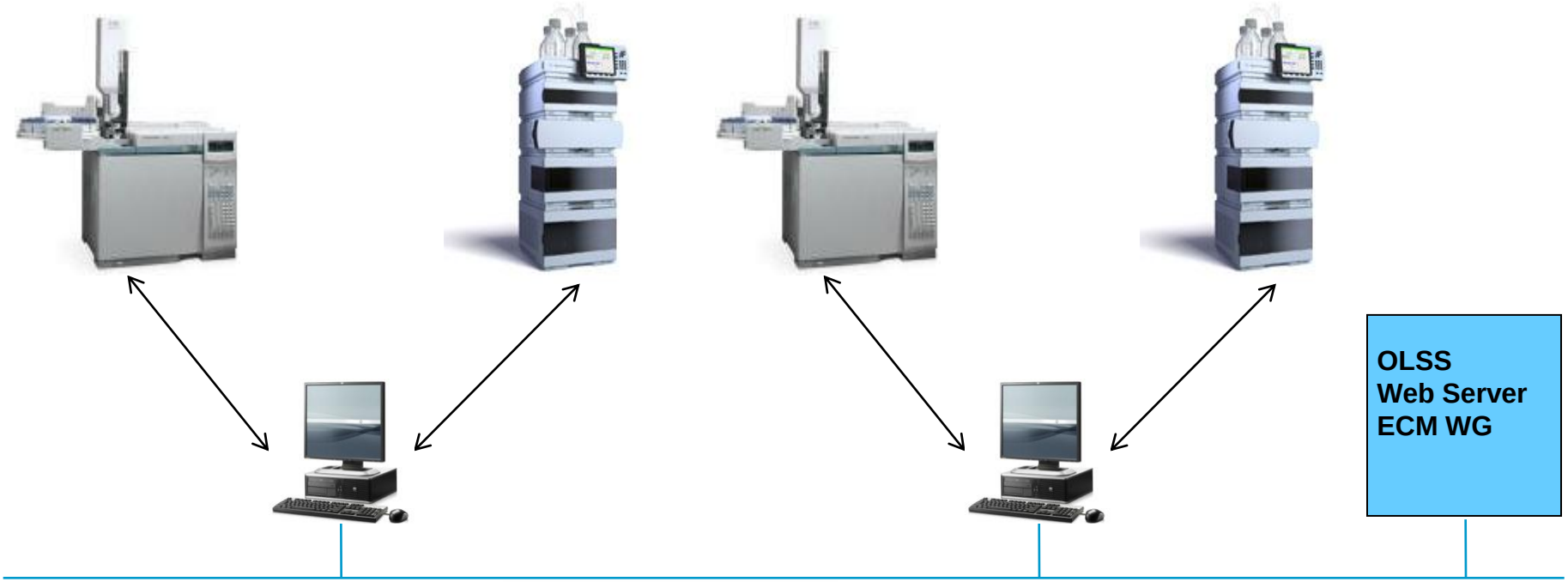
OpenLAB CDS Configurations: Workstation-only

- **Instrument Control:** Local on each workstation
- **Administration:** Local OpenLAB Control Panel on each workstation
- **Storage:** Local on each workstation
- **Benefits:**
  - Simple to install/upgrade
  - Complete network-independence

Fits well with:

- Laboratories who just bought a new instrument and need software to run it
- Current ChemStation/EZChrom laboratories with limited budget wanting to benefit from new features

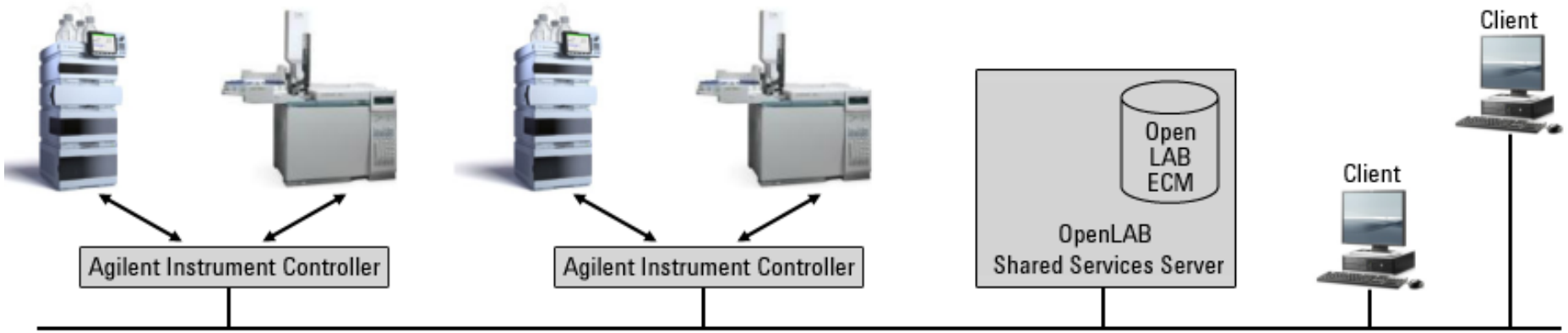
OpenLAB CDS: Networked Workstations compliant



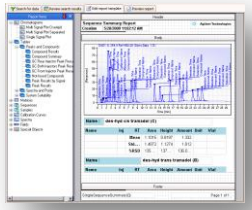
Lab at a Glance

OpenLAB CDS – Fully Distributed Configuration

OpenLAB CDS Configurations: Distributed Chromatography Data Systems



- **Instrument Control:** Remote access via Agilent Instrument Controllers (AICs) from anywhere
- **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
  - Remote instrument access from anywhere
  - Buffered data acquisition
  - Remove PCs from the laboratory – save precious benchspace



Optional Database reporting

Fits well with:

- Laboratories in need for a fully distributed CDS, who look for a database storage of their data for searching and reporting

OpenLAB CDS: The Control Panel

Central point for:

- Lab-at-a-glance view
- Administration of users, storage and instruments
- Launching ChemStation or EZChrom instruments

New look and feel:

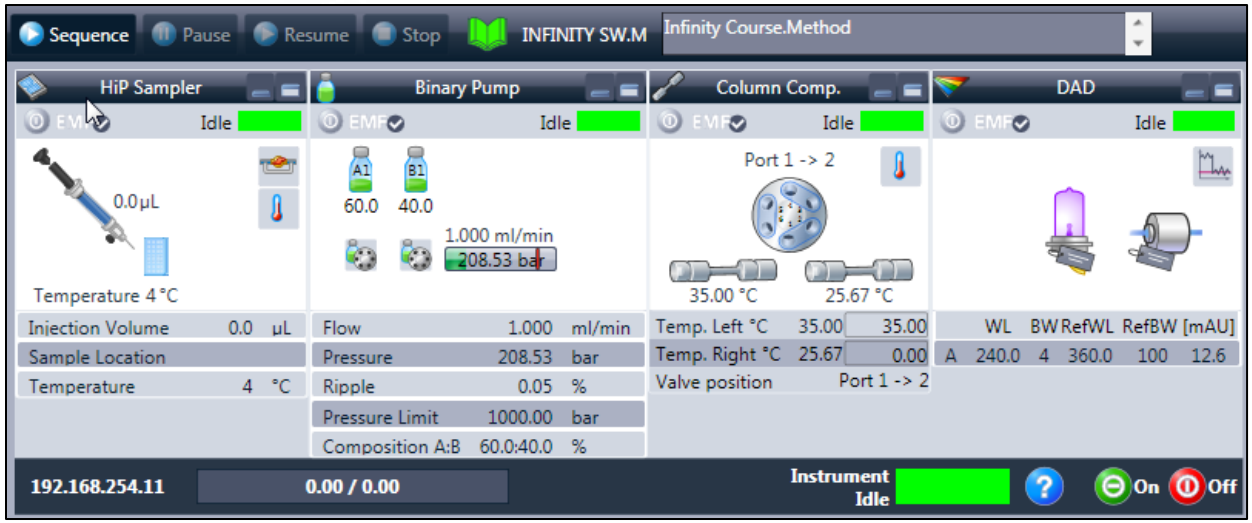
- Intuitive
- Easy-to-use

– **Support and troubleshooting:**

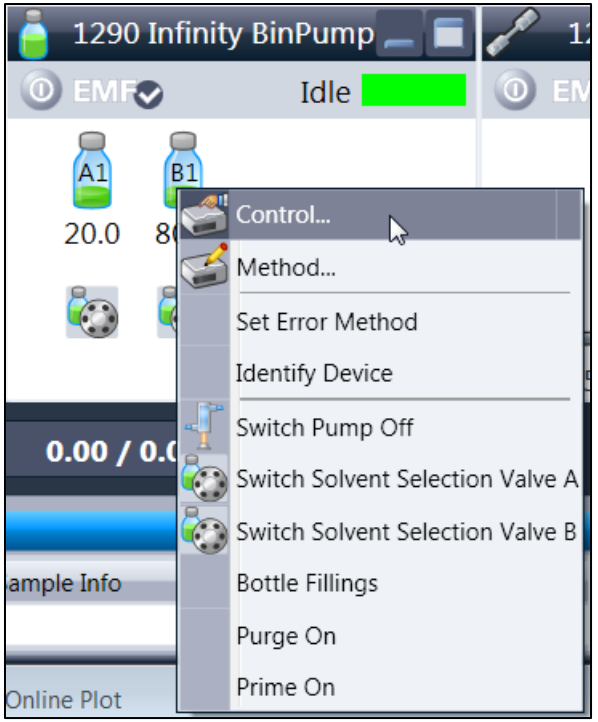
– Central access to all config and log files

SUPERRIOR INSTRUMENT CONTROL

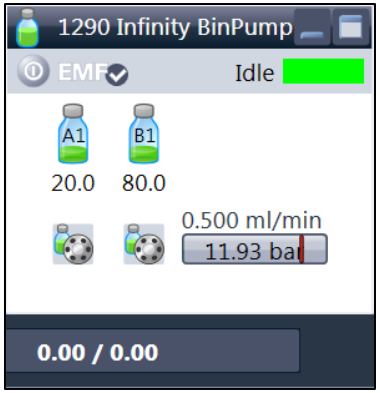
CDS



Right -click for Menu



Module with Status



Multi Vender Instrument Control in the OpenLAB CDS

✓Agilent 7820, 7890, 6890, 6850, 5890II, Micro GC & Headspace Systems
✓Agilent 1100 / 1120 / 1200 LC and 1290LC

Plus

Shimadzu*
✓Hitachi partly*
✓Perkin Elmer
Thermo*
✓Varian
✓Waters
✓Jasco
✓Vici
✓CTC

New drivers being continually added…
Clarus series x00 just released
Available over „DriverCentral soon
X80 will follow

*Driver currently not available from vendor due to missing Win 7 Support

OpenLAB CDS: Intelligent Reporting

Intuitive report template generation with drag & drop and interactive report preview functionality

Pre-configured report items (tables, graphics, matrices) make it easy to generate custom reports

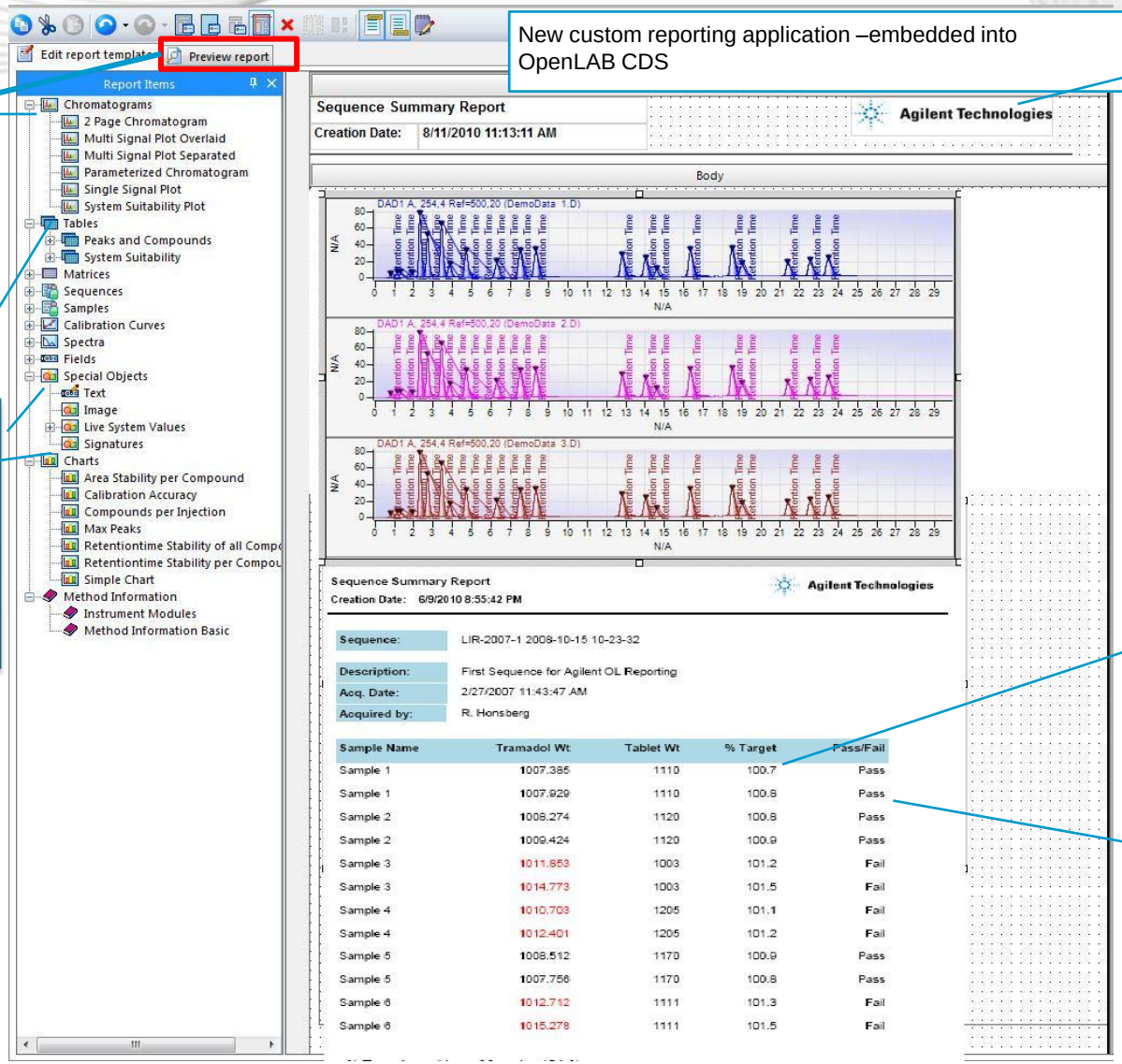
All current reporting options in ChemStation and EZChrom remain available

New custom reporting application –embedded into OpenLAB CDS

Easily include graphics such as your company logo

Embedded custom calculation functionality to calculate final results
– here %label claim

Intelligent Reporting:
Including limit checks into report
Decision-based result representation (pass/fail)



Minor component analysis

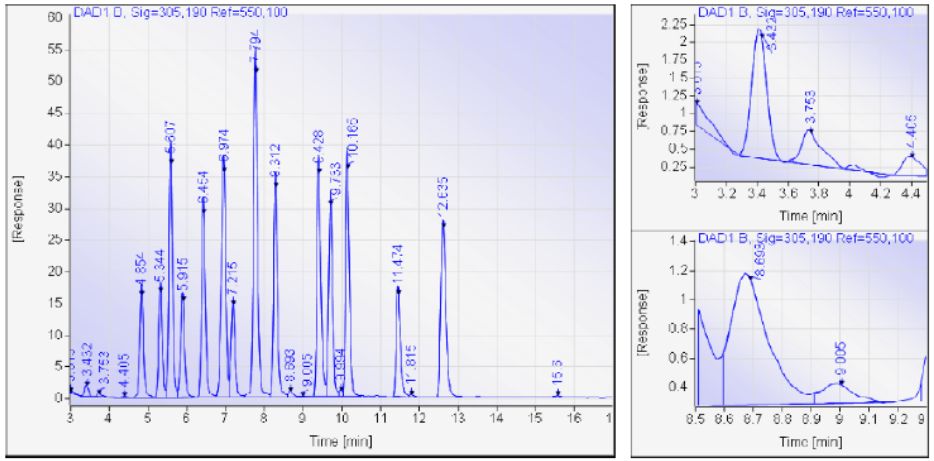
Multiple chromatograms or spectra per page

Minor Component Analysis

Creation Date: 6/9/2010 3:57:45 PM

Agilent Technologies

Sample_Name PAH



Region 1 Peaks

RT	Area	Area Percent
3.432	12.4342	0.40
3.435	19.6959	0.23
3.753	4.5677	0.15

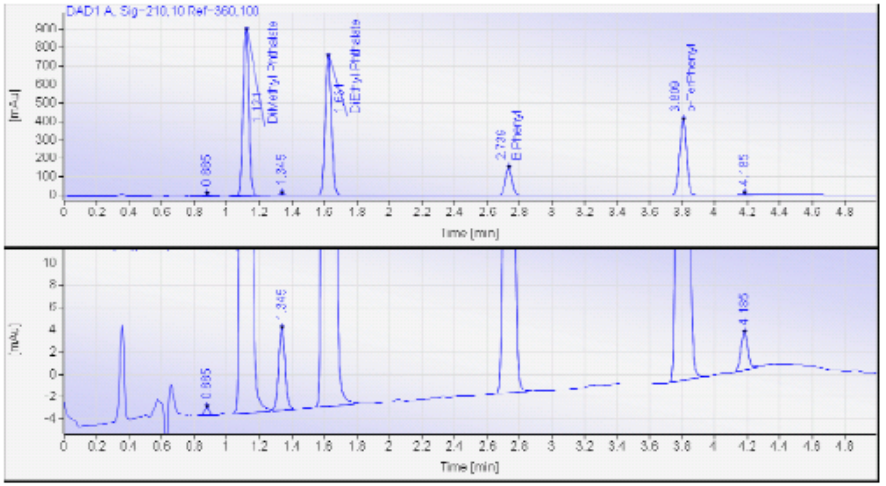
Region 2 Peaks

RT	Area	Area Percent
8.688	19.2821	0.22
8.693	8.2108	0.27
9.005	0.9892	0.03

Enhanced Result Review

Enhanced Result Review: Chromatograms in multiple scale on one page

Instrument:	AglTrnLab1412		
Inj. Date/Time:	4/11/2007 9:58:20 PM	**Operator:**	Roy McCune
Acq. Method:	CSEXAMPLE.M	**Injection:**	1 of 1
Proc Method:	CSEXAMPLE.M	**Data file:**	SIG1000019.D
Inj. Volume:	5		



Sample Name: AglTrnLab1412

Name	Signal	RT	Area	Height	Amount	Unit
DiMethyl Phthalate	DAD1A	1.121	2168.8835	908.1318	10.284	ng/ul
DiEthyl Phthalate	DAD1A	1.631	2015.7975	757.8688	11.601	ng/ul
BiPhenyl	DAD1A	2.739	425.5811	140.9147	9.870	ng/ul
o-TerPhenyl	DAD1A	3.809	1187.6146	405.9807	10.420	ng/ul

Intelligent: Flagging of Out-of-Spec values

- Flag outliers by pass/fail criteria using conditional formatting
- Automatically sort results, etc.

System Suitability Test Failed tests are marked red

	Amount	RSD(RT)	RSD(Area)	HW-Resolution	PW	K'	S/N
des-hyd cis tramadol (C)	0.804	0.019	1.456	15.247	-0.041	21.547	10.076
des-hyd trans tramadol (B)	0.748	0.025	1.846	3.854	-0.135	22.639	7.584
o-desm tramadol (D)	0.816	0.059	2.648		0.281	7.088	7.813
TRAMADOL	1004.590	0.057	0.099		42.381	5.150	2094.055
trans- tramadol (A)	0.812	0.065	2.346	6.892	0.100	11.992	7.931

List of NOT found compounds is empty

Applied rules for system suitability test
1.1 Precision of areas must be < 2 % rsd
1.2 Precision of retention times must be < 0.5 % rsd
1.3 Resolution must be > 2 for all peaks
1.4 Maximum peak width must be < 0.08 min at half height.
1.5 k´ must be 5 < k' < 25
1.6 Signal-to-noise ratio must be > 50 for all peaks

Calibration Test Failed tests are marked red

Compound and Calibration lvl		Amount	% Level	RSD(RT)	RSD(Area)
des-hyd cis tramadol (C)	1	0.821	0.082	0.285	1.127
	2	0.104	0.103	0.265	25.604
des-hyd trans tramadol (B)	1	0.765	0.076	0.268	1.992
	2	0.079	0.078	0.313	17.515
o-desm tramadol (D)	1	0.815	0.081	0.773	1.359
	2	0.093	0.092	0.933	14.671
TRAMADOL	1	1000.474	100.000	0.639	0.300
	2	100.654	100.000	0.532	0.082
trans- tramadol (A)	1	0.831	0.083	0.573	4.311
	2	0.089	0.089	0.526	13.703

All calibrated compounds found

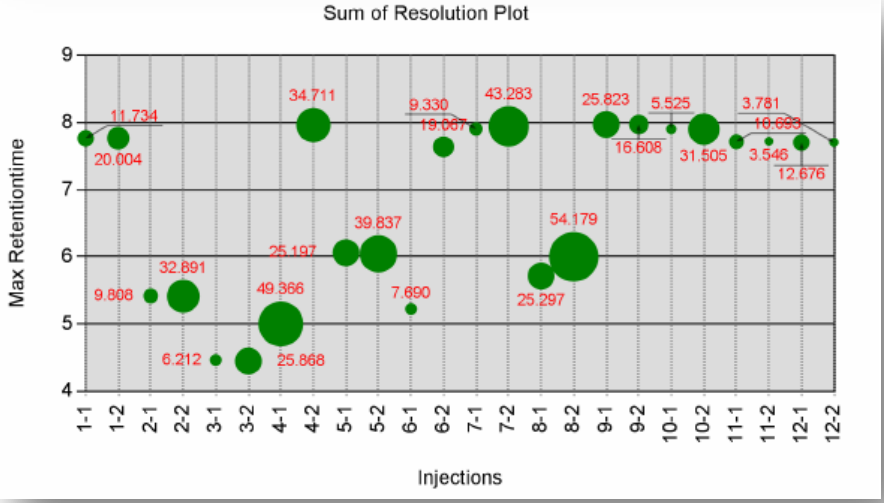
Powerful: Method Development Report

- Summary table with overview of found peaks and sum of peak resolution
- Summary bubble plot shows a graphical representation of the results

Method Development Results Summary

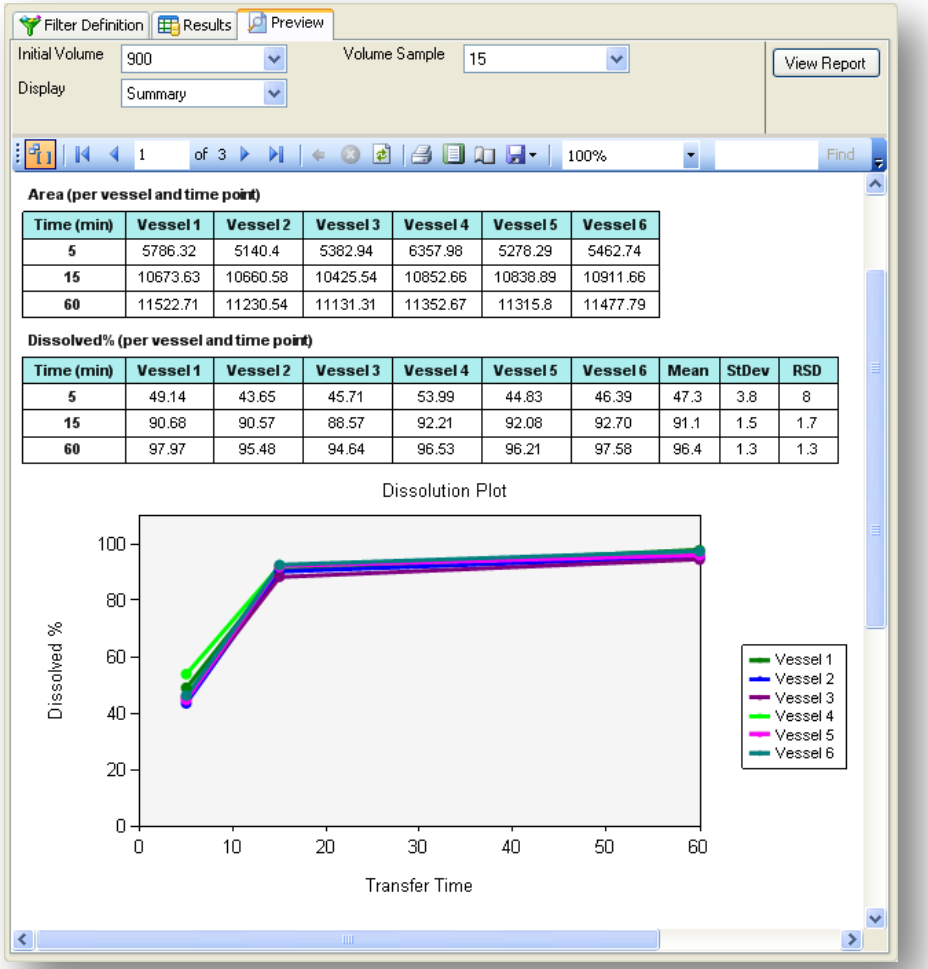
Sequence :	METOPROLOL100N2008-07-30
Signal:	DAD1 B, Sig=230,10 Ref=360,100
Min. Area%:	0.5

#	Column / Solvent	# of peaks	Sum Resolution	Max RT
1-1	Chromatographic column: Zorbax SB C18, 2.1x50mm, 1.8µm Solvents: 95% A1: H2O (water+0.2%tfa), 5% B1: ACN (*0,16% TFA)	13	3.488	7.769
1-2	Chromatographic column: Zorbax SB C18, 2.1x50mm, 1.8µm Solvents: 95% A1: H2O (water+0.2%tfa), 5% B1: ACN (*0,16% TFA)	9	5.090	7.771
2-1	Chromatographic column: Zorbax Eclipse Plus, 2.1x50mm, 1.8µm Solvents: 95% A1: H2O (water+0.2%tfa), 5% B1: ACN (*0,16% TFA)	11	6.275	2.866

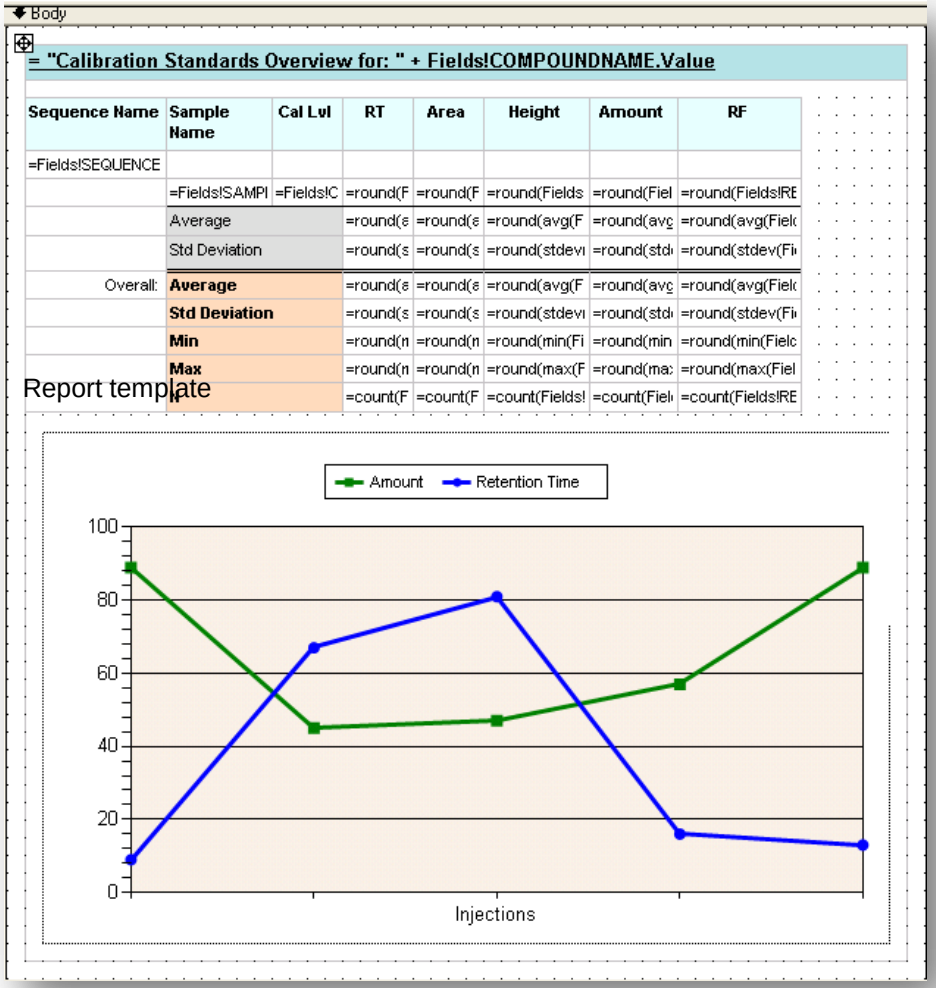


Powerful: Dissolution Testing Report

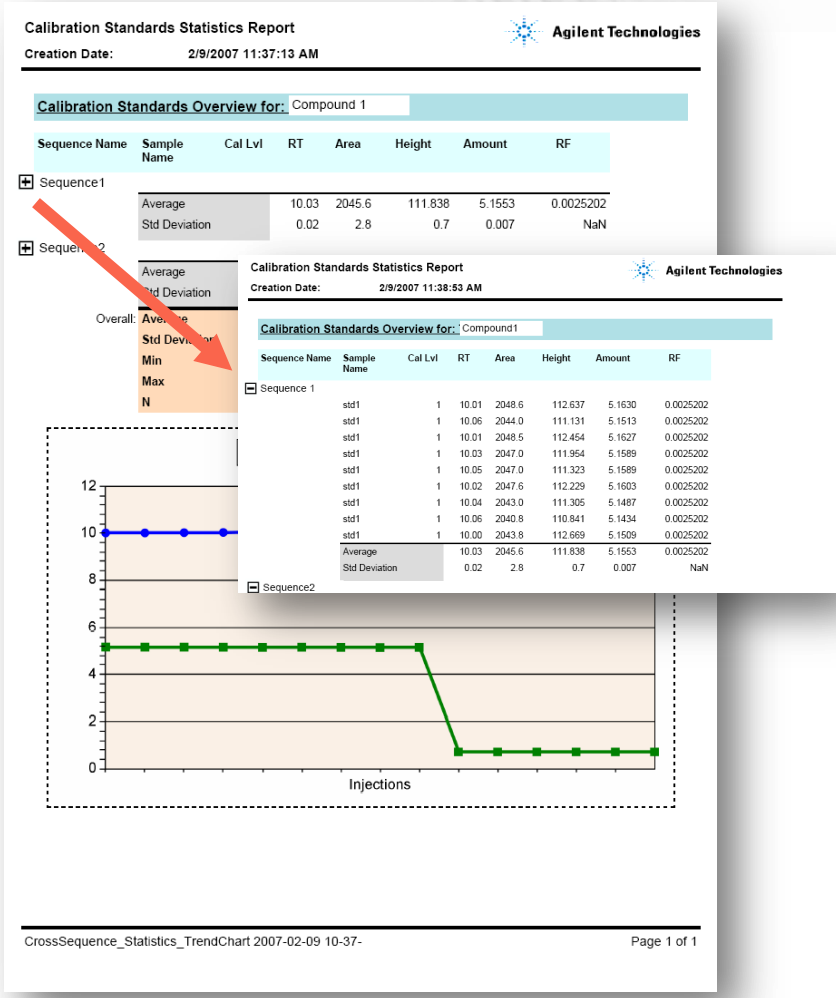
- Reports dissolution profile in table and trend chart format
- Calculates volume correction of samples based on initial volume and volume withdrawn
- Overlay of plots from different vessels



Powerful: Cross Sequence Statistics with Trend Chart *



Report template



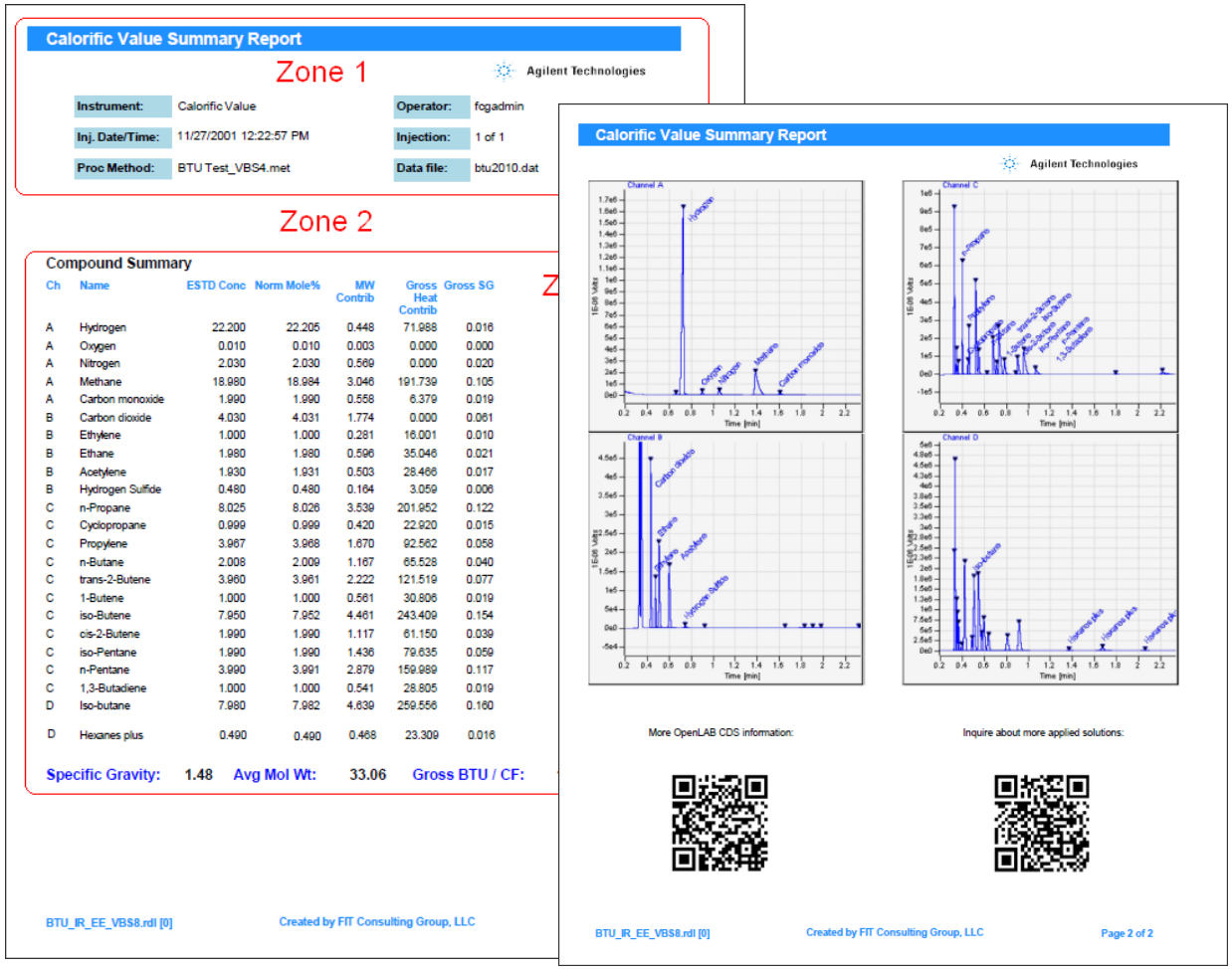
*Requires OpenLAB ECM Intelligent Reporter

Reports with interactive elements when viewed online

Intelligent reporting HPI Example

BTU Report Kit

- Technical note
- Report Template
- Data



Calorific Value Summary Report

Zone 1

Agilent Technologies

Instrument:	Calorific Value	Operator:	fcgadmin
Inj. Date/Time:	11/27/2001 12:22:57 PM	Injection:	1 of 1
Proc Method:	BTU Test_VBS4.met	Data file:	btu2010.dat

Zone 2

Compound Summary

Ch	Name	ESTD Conc	Norm Mole%	MW Contrib	Gross Heat Contrib	Gross SG
A	Hydrogen	22.200	22.205	0.448	71.988	0.016
A	Oxygen	0.010	0.010	0.003	0.000	0.000
A	Nitrogen	2.030	2.030	0.569	0.000	0.020
A	Methane	18.980	18.984	3.046	191.739	0.105
A	Carbon monoxide	1.990	1.990	0.558	6.379	0.019
B	Carbon dioxide	4.030	4.031	1.774	0.000	0.061
B	Ethylene	1.000	1.000	0.281	16.001	0.010
B	Ethane	1.980	1.980	0.596	35.046	0.021
B	Acetylene	1.930	1.931	0.503	28.466	0.017
B	Hydrogen Sulfide	0.480	0.480	0.164	3.059	0.006
C	n-Propane	8.025	8.026	3.539	201.952	0.122
C	Cyclopropane	0.999	0.999	0.420	22.920	0.015
C	Propylene	3.967	3.968	1.670	92.562	0.058
C	n-Butane	2.008	2.009	1.167	65.528	0.040
C	trans-2-Butene	3.960	3.961	2.222	121.519	0.077
C	1-Butene	1.000	1.000	0.561	30.806	0.019
C	iso-Butene	7.950	7.952	4.461	243.409	0.154
C	cis-2-Butene	1.990	1.990	1.117	61.150	0.039
C	iso-Pentane	1.990	1.990	1.436	79.635	0.059
C	n-Pentane	3.990	3.991	2.879	159.989	0.117
C	1,3-Butadiene	1.000	1.000	0.541	28.805	0.019
D	Iso-butane	7.980	7.982	4.639	259.556	0.160
D	Hexanes plus	0.490	0.490	0.468	23.309	0.016

Specific Gravity: 1.48 Avg Mol Wt: 33.06 Gross BTU / CF:

BTU_IR_EE_VBS8.rdl [0] Created by FIT Consulting Group, LLC

Calorific Value Summary Report

Agilent Technologies

More OpenLAB CDS information:

Inquire about more applied solutions:

BTU_IR_EE_VBS8.rdl [0] Created by FIT Consulting Group, LLC Page 2 of 2

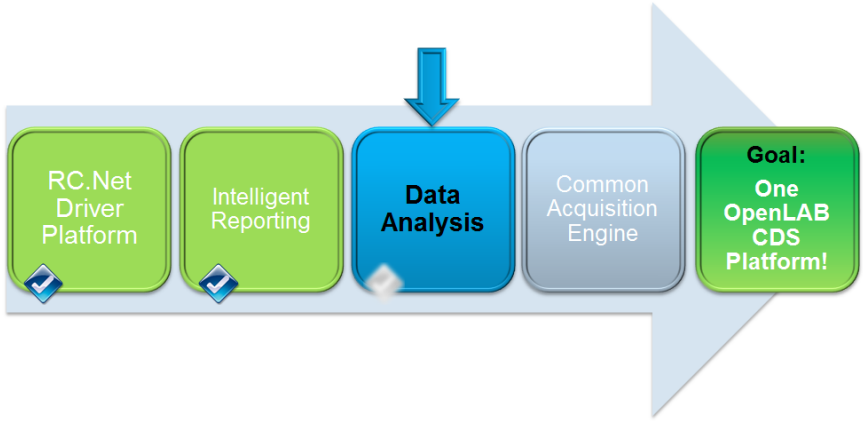
OpenLAB CDS

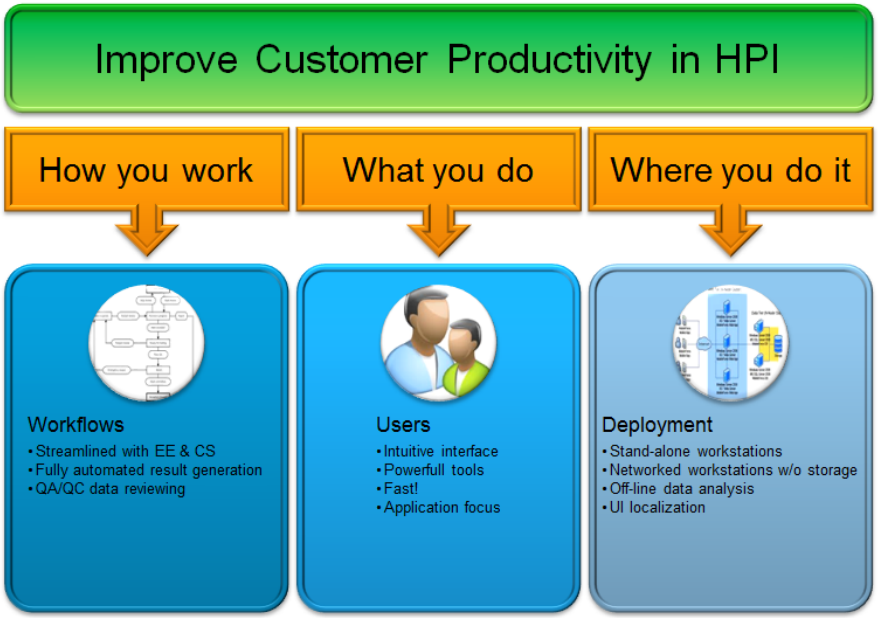
New Data Analysis platform

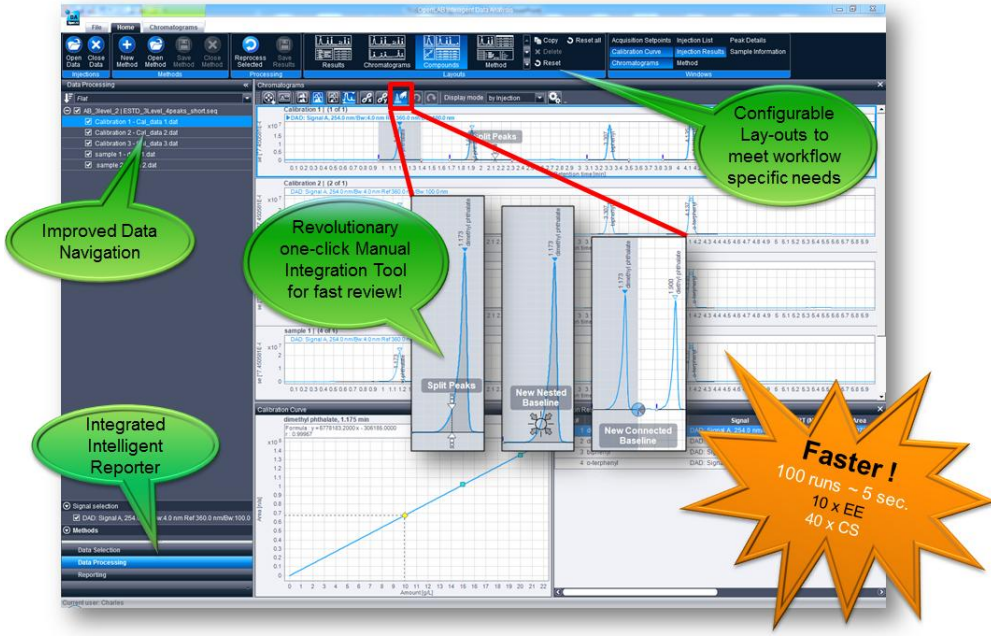
Bringing you an Unique Data Analysis Experience!

OpenLAB Data Analysis: What is it?

- ✓ Next step in OpenLAB **Consolidation** Strategy
- ✓ October Release focuses on **HPI** ASTM D6584 Biodiesel
- ✓ Value Proposition:
  - **Faster** from sample to result
  - **Easier** results with less effort
  - **Smarter** tools to improve your performance







OpenLAB CDS

New OpenLAB Data Store with Lab Applications

Starting
1 Nov 2012 !!!
For smal Customer
up to 15
instruments very
Limited compared
to ECM


Questions
Thank you