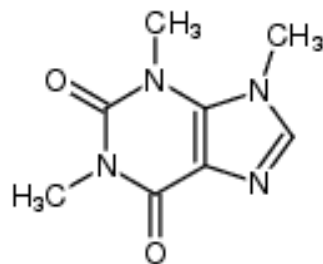


The screenshot displays the ChemAxon UGM (Ultimate Graphical Method) interface. At the top, it shows a chemical reaction scheme for the synthesis of a complex molecule. Below the reaction, there is a table of reagents and their quantities.

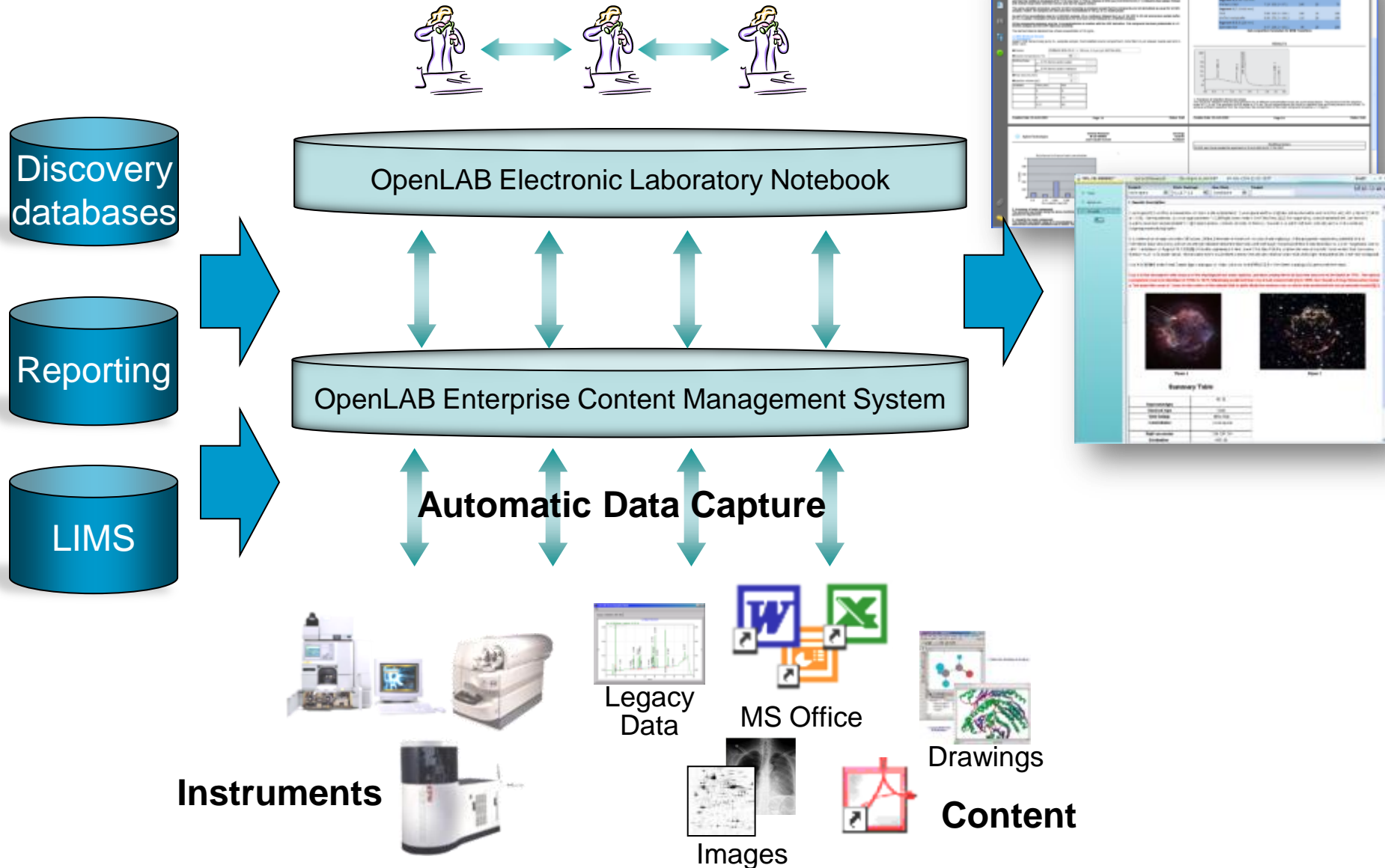
Reagent	Chemical Structure	Address	FW	A	B	Qty.	Purity	Level	Amount	U	Volume
Reagent 1			228.25			1.00 mg	10.00	normal	0.25 g		
Reagent 2			228.25			1.00 mg	10.00	normal	0.25 g		
Reagent 3			94.09			1.00 mg	10.00	normal	0.25 g		0.04 mL
Reagent 4			138.12			1.00 mg	10.00	normal	0.25 g		0.04 mL

# ChemAxon UGM

May 19<sup>th</sup>, 2010



# OpenLAB: Integrated informatics portfolio



# Announcing the Agilent OpenLAB Portfolio

## *Integrating Laboratory Informatics*

### OpenLAB Electronic Lab Notebook (ELN)

- Helps scientists capture and manage experimental details
- Secures intellectual property and improves collaboration
- Multi-discipline; biology, synthetic/medicinal chemistry, analytical Chemistry

### OpenLAB Enterprise Content Manager (ECM)

- The central repository for all laboratory data
- Interfaces to both Agilent and non-Agilent data systems
- Enables searching, management, archiving and reporting

### OpenLAB Chromatography Data System (CDS)\*

- Highly scalable distributed data system
- Supports both ChemStation & EZChrom Elite CDS workflows
- Provides multi-technique, multi-vendor instrument control

\*Coming soon

**OpenLAB**  
CAPTURE • ANALYZE • SHARE

# User workflow and experiment management

## OpenLAB ELN

- Optimize
  - Reduce time between process steps
  - Expedite access to results
- Collaborate
  - Share data across disciplines
  - Re-use experiment procedures
  - Learn from others results
- Secure
  - Safeguard intellectual property
  - Provide data-traceability

The screenshot displays the OpenLAB ELN software interface. At the top, it shows the project ID 'ATL-198-000013', the batch number 'Batch 1', and the date '10-MAR-2009 14:55 EDT'. Below this, there is a table of batch records with columns for Batch #, Structure, Address, Formula, MW, Name, Exp. Name, Mass, Cost, Yield, Purity (%), and Other Yield. The first row shows a batch with a chemical structure and a yield of 88.00%.

Below the table, there is a section for 'Batch Properties' with fields for 'Measured MW', 'Batch Name', 'Batch Remark', and 'Analysis of M'. There is also a section for 'General Properties' with fields for 'Appearance', 'Feeder', 'Mixture', and 'Public Release'.

At the bottom, there is a table of 'Analysis Results' with columns for Sample, Analysis, Result, Req. Status, Analysis #, Analysis Method, and Comments. The table shows several analysis results for different samples, including 'MFC for Stability', 'Content Uniformity', 'Molecular Weight', 'Molecular Weight by MS', 'Molecular Weight by MS', and 'Content Uniformity'.

# OpenLAB ELN: Search and re-use protocols and methods

Kalabie ELN by Agilent Technologies, Inc.

M-DR-000030\* Standard Synthesis Dominique ROUX 20-AUG-2009 18:05 CEST Draft

Project: Chemotherapy Work Package: Line Item: Target:

Design  
Protocol  
Results  
Context

Fast protocol creation with standard sentences and dynamic forms

Molecule links directly to composition table

1. 3,3-dimethyldioxirane, 35.0 °C, 10.0 bar

20-AUG-2009 18:11 add [M-DR-000001.002 \(18 573.96 ml, 5.00 g/l, 0.32 mol, 1.00 eq.\)](#) and [3,3-dimethyldioxirane \(91.01 ml\)](#) into reactor  
heat

[M-DR-000030](#)

The mixture was stirred for  mn at  °C, and filtered.

The mixture was stirred in  for  mn, and filtered.

09-APR-2010 04:23 09-APR-2010 04:23 CEST

30m later purify

The mixture was stirred for  mn at  °C, and filtered.

Quickly insert images and searchable annotate

Opened Exp.  
Characters

Start Kalabie ELN by Agilent T... Kalabie ELN by Agilent... EN 9:23 PM

# Experiment results in OpenLAB ELN...

The screenshot displays the OpenLAB ELN interface for project ATL-MB-000013. The top navigation bar includes Project ID, Cost Center (Reaction Development), Lab ID (Project Alpha), and Hazard Level (Process A). A table lists batches, with one entry for ATL-MB-000013.002 showing a chemical structure, formula C<sub>22</sub>H<sub>27</sub>N<sub>9</sub>O<sub>4</sub>S, MW 474.58, and a name 1-[4-ethoxy-3-(6,7-...]. Below this, a 'General Properties' section shows 'Measured MW' as 474.60 and 'Batch Type' as 'Final Product'. A 'Samples' section lists various analysis requests. A table at the bottom shows the status of these requests, including 'HPLC for Stability', 'Content Uniformity', and 'Matabolite ID'.

Batch #	Structure	Additive	Formula	MW	Name	Exp. Mass	Mass	Load	Yield	Purity (%)	Chem. Yield
ATL-MB-000013.002	<chem>C22H27N9O4S</chem>		C <sub>22</sub> H <sub>27</sub> N <sub>9</sub> O <sub>4</sub> S	474.58	1-[4-ethoxy-3-(6,7-...	1.070.34 g	g		77.00	99.00	67.76

Sample	Analysis	Request	Req. Status	Analysis #	Analysis Status	Comments
ATL-MB-000013.002-S1	HPLC for Stability	ATL-MB-000022	Draft			
ATL-MB-000013.002-S5	Content Uniformity	ATL-MB-000017	Assigned			
ATL-MB-000013.002-S2	Matabolite ID	ATL-MB-000025	Accepted	ATL-MB-000026	Draft	
ATL-MB-000013.002-S3	Matabolite ID	ATL-MB-000018	Assigned			
ATL-MB-000013.002-S2	Structure Confirmation by MS	ATL-MB-000018	Assigned			
	Structure Confirmation by MS	ATL-MB-000018	Assigned			
	Content Uniformity	ATL-MB-000025	Accepted	ATL-MM-000001	Draft	

Quickly manage measured or calculated sample properties

Manage multiple batches and split samples for analysis

Direct link to resulting analysis experiment and results

Monitor status of analysis requests

# Experiment report contains all data and results

## Data traceability and IP protection

**REACTION**

Type : Bromidation

M-DR-000001.002 → M-DR-000030.001

**PLANNING**

Compound	MW	Eq	Mole	Purity	Mass	C	Volume
M-DR-000001.002	282.12	1.00 eq	0.32 mol	98.00	1.00 µg	5.00 g/l	18573.96 ml
3,3-dimethyloxirane	74.06	1.00 V	0.20 mol	99.00		2.00 µg/ml	91.01 ml

**PROTOCOL**

Time	Description
20-AUG-2009 18:11	add M-DR-000001.002 (18 573.96 ml; 5.00 g/l; 0.32 mol; 1.00 eq.) and 3,3-dimethyloxirane (91.01 ml) into reactor heat
	M-DR-000030
	The mixture was stirred for <input type="text" value="20"/> mn at <input type="text" value="32"/> °C, and filtered.
	The mixture was stirred in ice <input type="text" value="30"/> for <input type="text" value="30"/> mn, and filtered.
09-APR-2010 04:23	09-APR-2010 04:23 CEST
30m later	purify
	The mixture was stirred for <input type="text" value="54"/> mn at <input type="text" value="54"/> °C, and filtered.

extract M-DR-000030.001 (299.00 µg; 98.00 %)  
M-DR-000030.003 (200.00 µg; 0.00 %)

**RESULTS**

Agilent Technologies Standard Synthesis  
M-DR-000030  
Dominique ROUX Chemotherapy

Batch	Structure	Formula	MW	Name	Exp. Mass	Mass	Yield	Purity [%]	Chem. Yield
M-DR-000030.001		C22H29NO5	387.48		250000.00.00 µg	299.00 µg	0.00		98.00
M-DR-000030.003		C22H29NO5	387.48		250000.00.00 µg	200.00 µg	0.00		0.00

Batch compounds

Batch	Structure	Formula	MW	Ratio
M-DR-000030.001		C22H29NO5	387.48	100
M-DR-000030.003		C9H15IO2	282.12	10
M-DR-000030.003		C22H29NO5	387.48	90

**ANALYTICAL FORMS**

General properties

Batch	Dialicator	Deliv. mass
M-DR-000030.001	No	
M-DR-000030.003	No	200.0000 µg
M-DR-000030.004	No	

Samples

Batch	Sample	Container Type	Mass	Destination
M-DR-000030.001	M-DR-000030.001-S1			
M-DR-000030.003	M-DR-000030.003-S1	Vial 100mL	100.00 µg	Deep Freeze (-50°C)
	M-DR-000030.003-S2	Vial 10ml	100.00 µg	Fridge 5°C

**ANALYSIS**

Batch	Sample	Analysis	Request	Req. Status	Analysis #	Analysis Status
M-DR-000030.001	M-DR-000030.001-S1	HPLC	M-DR-000032	Accepted	M-JD-000004	Draft
	M-DR-000030.001-S1	HPLC	M-DR-000032	Accepted	M-JD-000004	Draft
	M-DR-000030.001-S1	HPLC	M-DR-000032	Accepted	M-JD-000004	Draft
Batch		Solvent				

# Improved research efficiency for three sites, in three countries...

- "Compound registrations increased 15 % versus the year before."
  - Hans Troost, Business Analyst, Solvay Pharmaceuticals
- Increase personal productivity
  - Easily check pending experiments, experiments to sign or pending requests
  - Browse 'my experiments', create favorites based on search criteria
  - QuickSearch across experiments and documents
  - Register and search molecule and reactions

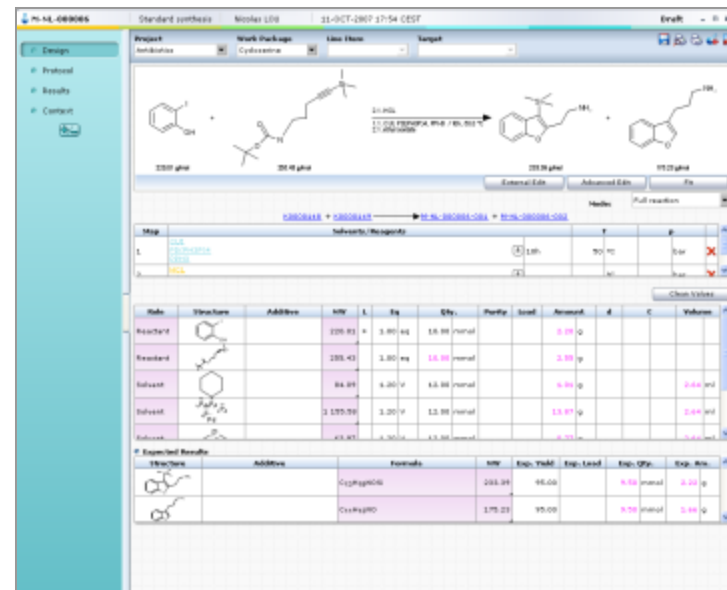
The screenshot shows the 'SEARCH RESULT' page in the Kalabie application. It features a table with the following data:

Exp. Number	Reaction	Result Batch	Result Yield (%)	Site
8-19-008815	<chem>CC(=O)O.CC(=O)O&gt;&gt;CC(=O)OC(=O)C</chem>	8-19-008815-001 8-19-008815-002	43.05 63.09	Baslin
8-19-008813	<chem>CC(=O)O.CC(=O)O&gt;&gt;CC(=O)OC(=O)C</chem>	8-19-008813-002 8-19-008813-001	97.79 89.36	Baslin
8-19-008812	<chem>CC(=O)O.CC(=O)O&gt;&gt;CC(=O)OC(=O)C</chem>			Baslin
8-19-008803	<chem>CC(=O)O.CC(=O)O&gt;&gt;CC(=O)OC(=O)C</chem>			Baslin

The screenshot shows the 'ADVANCED EXPERIMENT SEARCH' page in the Kalabie application. It includes search filters for 'Generic Criteria' and 'Structure Search', and a 'Result List Columns' section with options for 'Available Columns' and 'Selected Columns'.

# For the synthetic chemists...

- Plan and design reactions using standard chemistry tools
  - ChemAxon bundled
  - Integrate with Symyx, Accelrys and ChemDraw
- Seamless integration with existing registration systems and sourcing databases
- Create favorites for commonly used reagents and solvents
- Quick experiment setup with standard sentences and templates
- Create batches, split samples and submit for analysis directly from the experiment
- Reduce redundant experiments; search across reactions and molecules



**Green Chemistry, also called sustainable chemistry, is a practical philosophy encouraging the design of products and processes that reduce or eliminate the use and generation of hazardous substances. Whereas environmental chemistry is the territory of the natural environment, and of related chemical reactions, green chemistry needs to reduce and prevent pollution at its source. In 1990 the Pollution Prevention Act was passed in the United States. This act played a crucial role in the development of green chemistry.**

**A Reaction, an environmentally required.**

As a chemical philosophy, green chemistry derives from organic chemistry, inorganic chemistry, biochemistry, analytical chemistry, and green physical chemistry. However, the philosophy of green chemistry tends to focus on industrial applications. Combined this with toxic chemistry what tends to favor academic applications, although industrial applications are possible. The focus is on minimizing the hazard and maximizing the efficiency of any chemical process. It is applied to environmental chemistry which focuses on chemical processes to be understood.

In 2002 Royal Society identified three key developments in green chemistry: use of separate catalytic systems as green solvent, application of hydrogen peroxide for clean oxidations and the use of hydrogen in experiments. Methods of transport of reagents in applying green chemistry are supercritical water oxidation, or water reactions and microwave reactions.

# Chemaxon Inside....

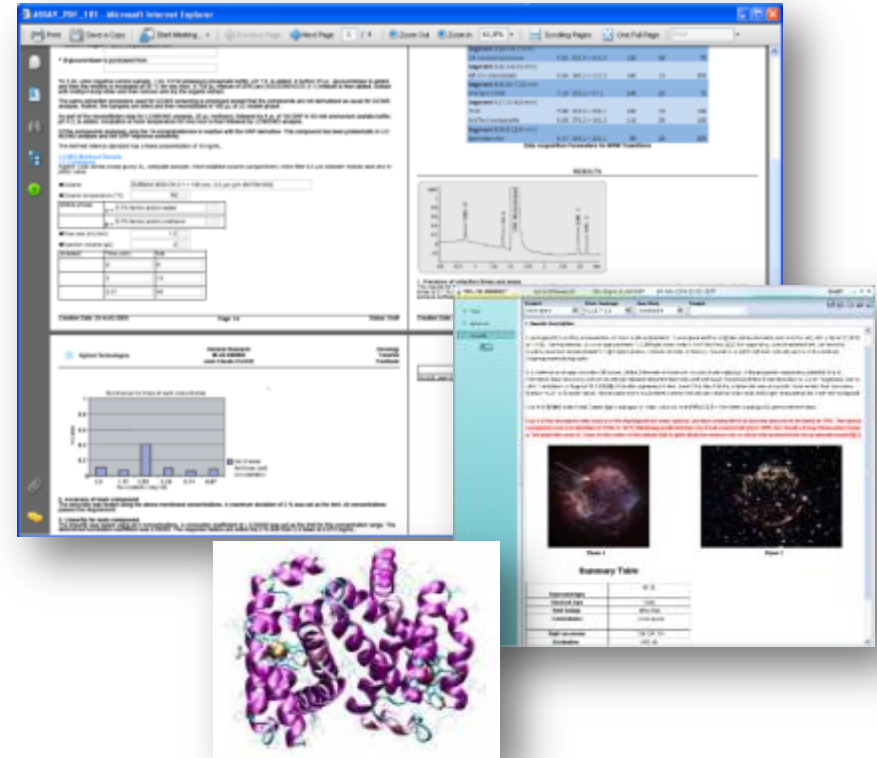
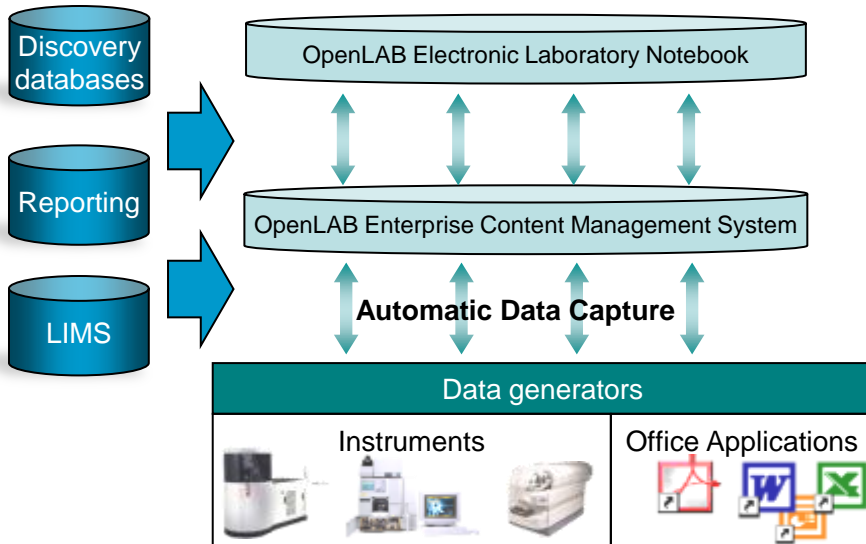
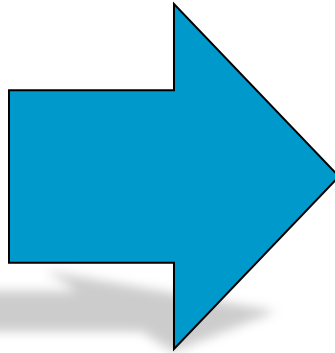
The screenshot displays the Chemaxon software interface. At the top, the window title is "M-FB-000009" and the status bar shows "Standard synthesis", "François BEILLOUIN", and "28-MAY-2009 16:13 CEST". The main workspace shows a chemical reaction scheme. The reactant is a benzimidazole derivative with a chlorine atom and a carboxylic acid group, labeled "(S)" and "307.8 g/mol". The reaction conditions are "1. Benzene, THF 2.3M, 78.0 °C". The product is the corresponding methyl ester. Below the reaction, there are buttons for "External Edit", "Advanced Edit", and "Fit". A table below the reaction shows the mapping from "M-FB-000008.001" to "M-FB-000009.002".

An "Embedded Marvin Sketch" window is overlaid on the main interface. It has a menu bar (File, Edit, View, Insert, Atom, Bond, Structure, Tools, Help) and a toolbar. The main area shows the same chemical reaction scheme as the main workspace, with the reactant labeled "KAL\_ID=0" and the product labeled "KAL\_ID=1". The window also includes a "Role" table, an "Expected Results" section, and a 2D structure editor at the bottom.

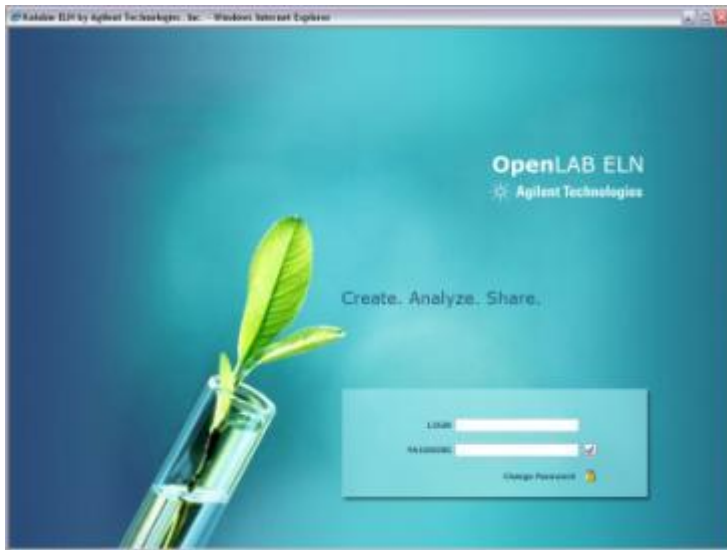
Role	Structure
Reactant	

Expected Results	Structure
Ad	

# Providing a Collaboration Platform



- Enable knowledge management
- Improve IP protection
- Improve regulatory compliance
- Increase productivity



# Questions?

