



Increase Productivity by Integrating LIMS and EZChrom Elite - a case study

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Joining forces to create a new global leader

- Lyondell Chemical Company and Basell merged to form LyondellBasell Industries on Dec. 20, 2007
- LyondellBasell is...
 - One of the world's largest polymers, petrochemicals, and fuels companies with combined annual revenues of \$44.7 billion*
 - The global leader in polyolefins technology, production and marketing
 - A pioneer in propylene oxide and derivatives
 - A significant producer of fuels and refined products, including biofuels
 - Operator of one of North America's largest full-conversion refineries

**2007 pro forma combined revenues.*

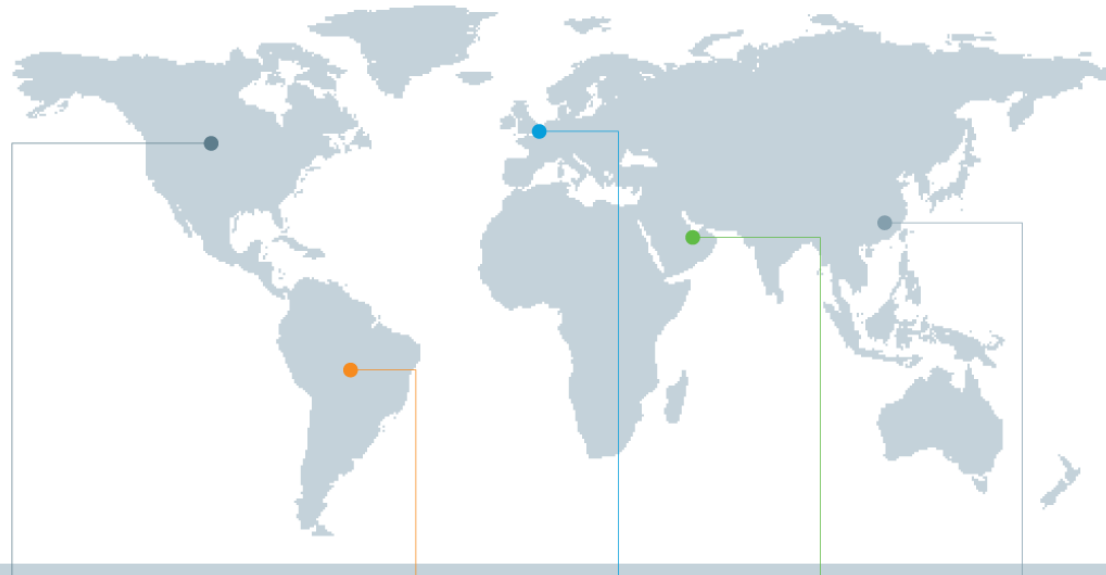
Fast facts

- Four business areas: Polymers, Chemicals, Fuels and Technology
- Delivers exceptional customer value across petrochemical chain
 - Vertically integrated facilities
 - Broad product portfolio
 - Manufacturing flexibility
 - Superior technology base
 - Operational excellence

Chemical industry landscape has changed

- With annual revenues of nearly \$45 billion:
 - Larger than Canon, Disney, Intel, Mitsubishi Electric and Volvo
 - Sales exceed those of DuPont and Bayer
 - Only BASF and Dow are larger

More than 16,000 people worldwide



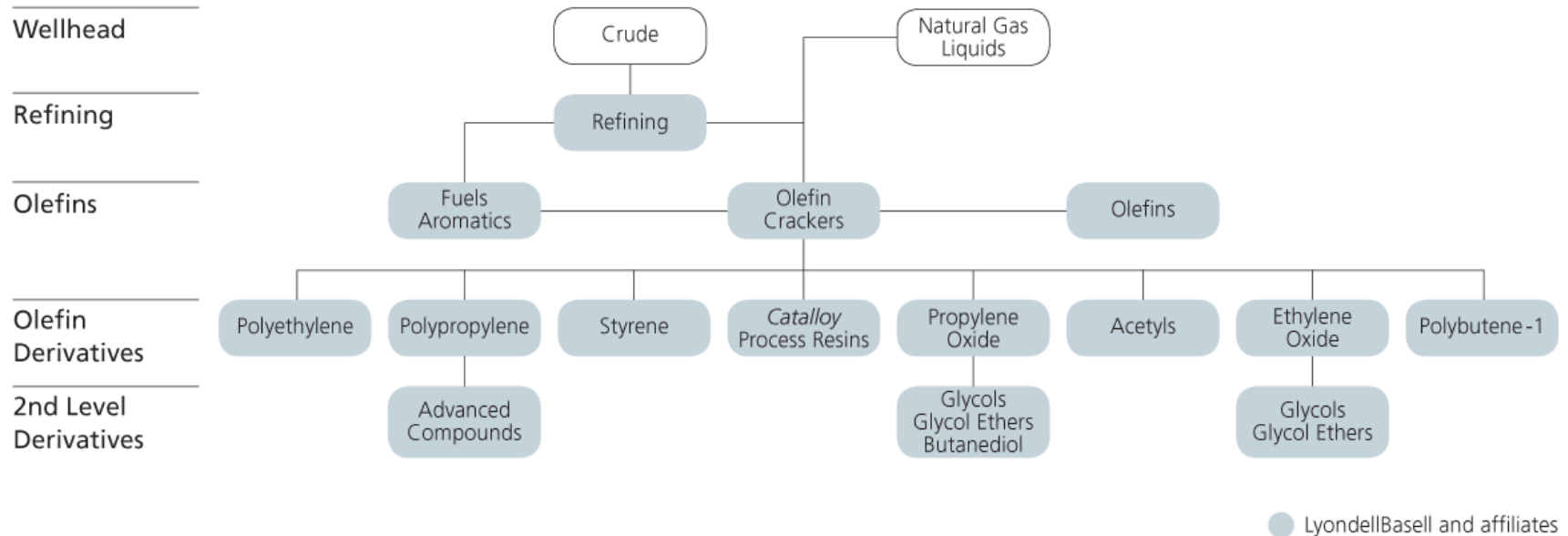
North America		South America		Europe		AFME		Asia Pacific			
Canada	■	Mexico	■	Argentina	■	France	■	Saudi Arabia	■	Australia	■●
Florida	■●	Michigan	●	Brazil	■	Germany	■●			China	■
Georgia	■	New Jersey	■			Italy	■●			Hong Kong	●
Illinois	■	Ohio	■●			Netherlands	○■			Japan	■
Iowa	■	Pennsylvania	●			Poland	■			Korea	■
Louisiana	■	Tennessee	■			Spain	■			Malaysia	■
Maryland	●	Texas	■			UK	■●			Thailand	■

■ Manufacturing ● Technology Centers ○ Worldwide Headquarters

Our leadership

- Volker Trautz – Chief Executive Officer
- Morris Gelb – Executive Vice President, Office of the CEO
- Alan Bigman – Executive Vice President and Chief Financial Officer
- Anton de Vries – President, Polymers Division
- Ed Dineen – President, Chemicals Division
- Norm Phillips – President, Fuels Division
- Bart de Jong – Senior Vice President, Human Resources
- Cees Los – Senior Vice President and General Counsel

Product diversity and vertical integration



Product breadth and diverse markets

- LyondellBasell products are basic elements used to make products that people depend on every day

Diverse end markets

- Refining & Fuels
- Building & Construction
- Transportation
- Textiles & Furnishings
- Packaging
- Consumer
- Other



Estimate based on revenue

Global Capacity Positions

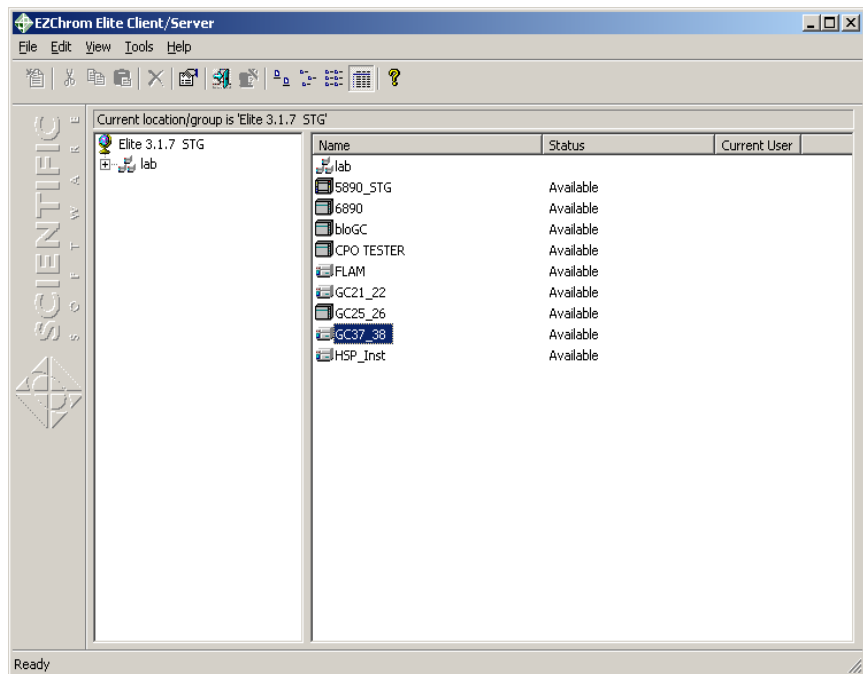
- #1 Global – Polyolefins and Polypropylene Compounding
- #1 Global – Propylene Oxide
- #1 Global – Polyolefin Licensing
- #1 Global – Polypropylene Catalysts
- #1 Global – Polypropylene
- #3 Global – Polyethylene
- #2 Global – Oxygenated Fuels
- #2 Global – Propylene Glycol & Propylene Glycol Ethers
- #5 Global – Light Olefins (Ethylene & Propylene)
- Refining Capacity – 373,000 barrels per day

Laboratory operations

- High level operation
 - Receive sample
 - Acknowledge / Create in LIMS
 - Add / Remove tests
 - Testing
 - Instrument
 - Gravimetric
 - Etc.
 - Report
 - Data Entry
 - Release

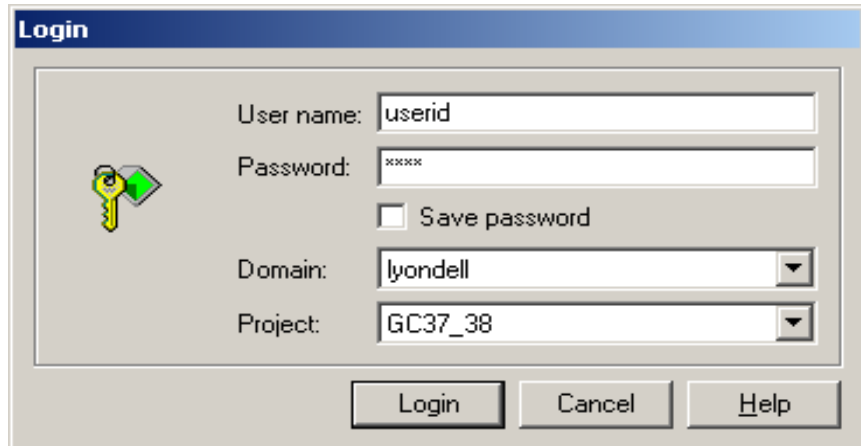
Sample submission – manual process

- Launch Application



Sample submission – manual process

- Open instrument
 - Authentication required
 - Project selection required



Login

User name: userid

Password: xxxx

Save password

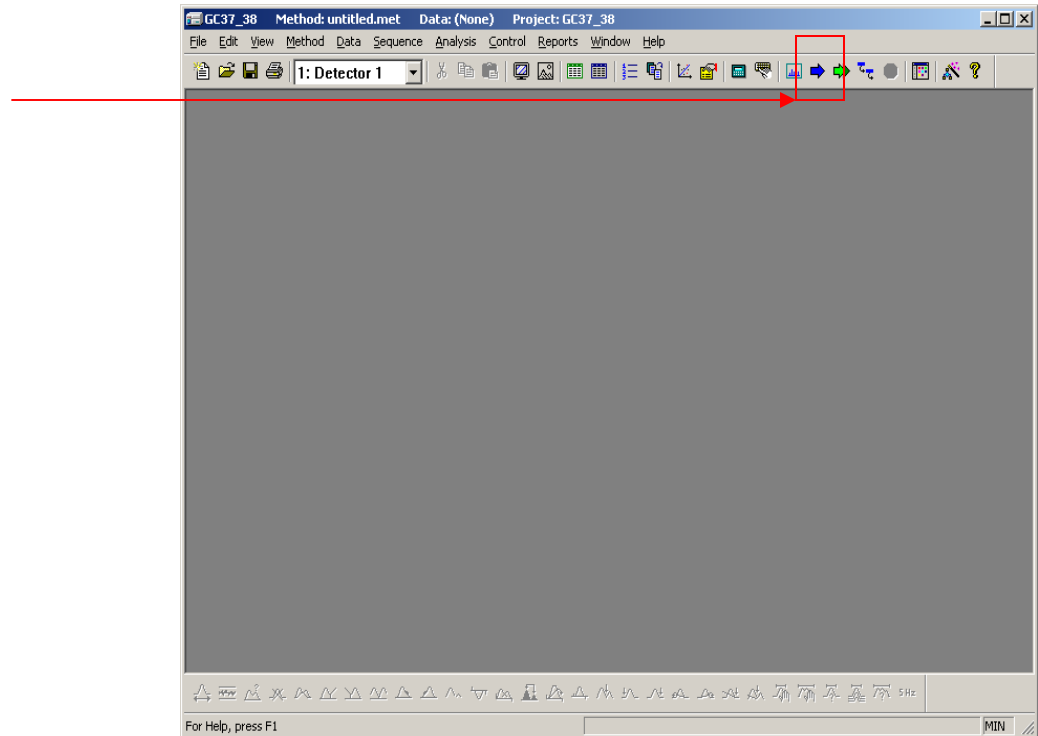
Domain: lyondell

Project: GC37_38

Login Cancel Help

Sample submission – manual process

- Initiate Data Acquisition.



Sample submission – manual process

- Required information/knowledge

- Sample ID
- Method
- Data path
- Data filename
- Sample Amount
- ISTD Amount
- Multipliers
- Divisors
- Vial number
- Volume
- Description
- Print Option

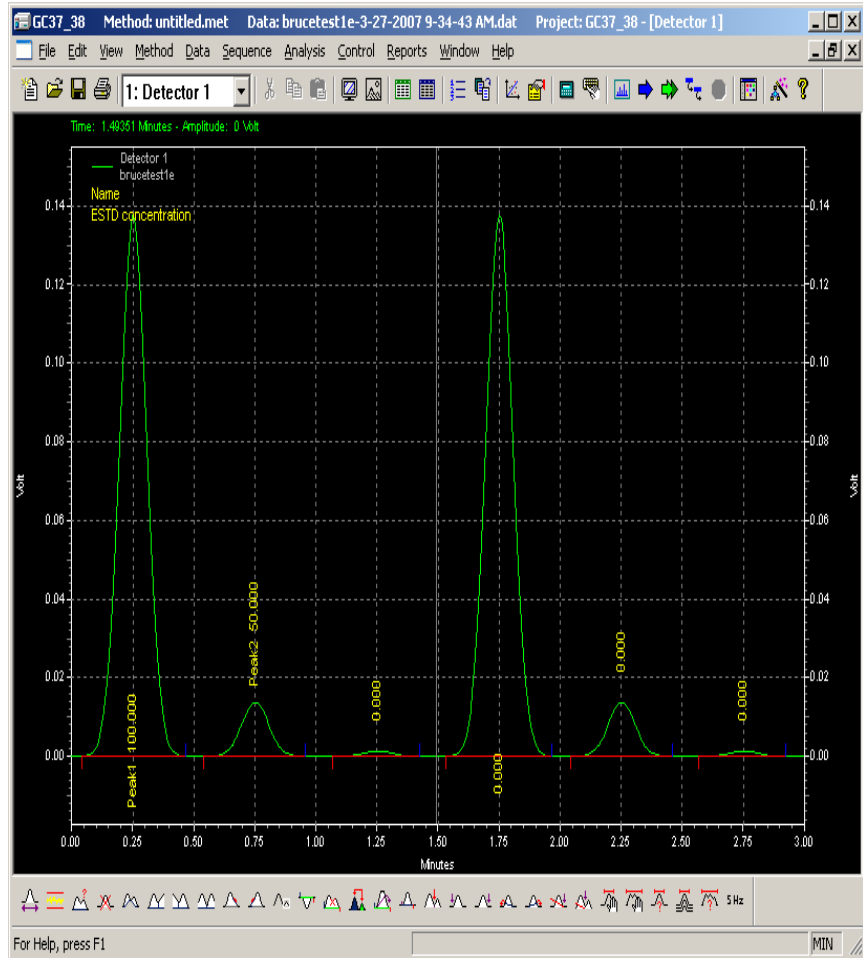
- Defaults may / may not be correct
- Can always edit values
- Prone to ‘typos’

The screenshot shows the 'Single Run Acquisition' dialog box. It contains the following fields and options:

- Run information:** Sample ID, Method, Data path (\\ddcaps01\stg_elite\$\projects\GC37_38\Data), Data file, Number of reps (1), and Print method report checkbox.
- Amount values:** Sample amount (1), Internal standard amount (1), Multiplication factors (1, 1, 1), and Dilution factors (1, 1, 1).
- Autosampler:** Vial (1), Injection volume (0.5 uL), and Tower (N/A).
- Calibrate:** Calibrate checkbox, Calibration level (1), and checkboxes for Clear all calibration, Clear calibration for level, Print calibration report, Clear replicates, and Average replicates.
- Buttons:** Start, Cancel, Help, and Description... (bottom right).
- Begin run:** Immediately dropdown and a circular icon.

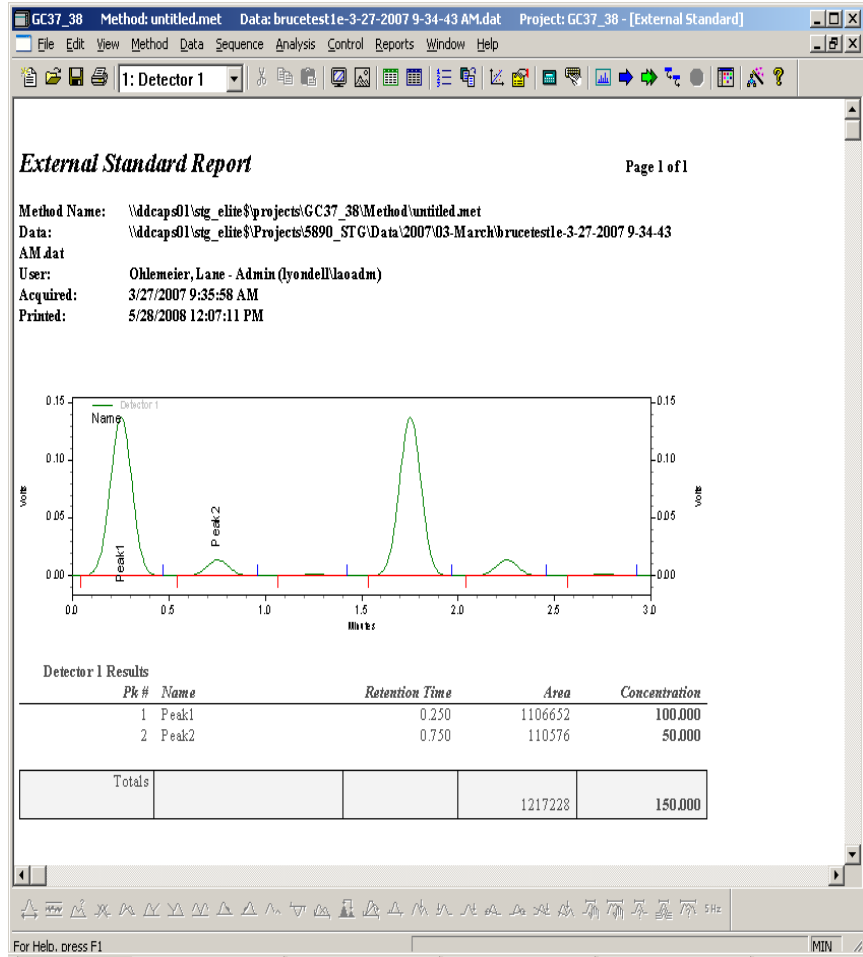
Sample submission – manual process

- Post Acquisition



Data entry – manual process

- Report
 - View on screen
 - Print
 - Printing may require additional steps if ‘automatic’ printing not selected when sample was submitted



Data entry – manual process

- Data Entry
 - Must locate / navigate to entry screen in LIMS
 - Hard copy generally needed to facilitate data entry
 - After data is entered, changes must be saved

LabVantage
SAPPHIRE

Data Entry

Collapse All Save Changes Release Dataset Un-Release Dataset Show Key

CXOPSM2-0068001-0011 (T-850 EB PROD(E-853))

SamplePoint(SamplePointId Description)	SampleId	SchedDate
CXOPSM2-0068001-0011(T-850 EB PROD(E-853))	S-022008-487866	29-Nov-2007 5:00 AM
Batch	Lot	Notes

ACX0753/1 Desc: ACX#753 EB PRODUCT GC

Release / Un-Release

Previous two results

ETHYLBENZENE	99.71 wt%	S-082007-480496
	99.71 wt%	S-082007-480121
PO	10 ppm	S-082007-480496
	10 ppm	S-082007-480121
BENZENE	41 ppm	S-082007-480496
	41 ppm	S-082007-480121
NONAROMATICS	32 ppm	S-082007-480496
	27 ppm	S-082007-480121
TOLUENE	799 ppm	S-082007-480496
	717 ppm	S-082007-480121
CUMENE	130 ppm	S-082007-480496
	131 ppm	S-082007-480121
STYRENE	322 ppm	S-082007-480496
	336 ppm	S-082007-480121
n-XYL FNF	271 ppm	S-082007-480496

Done Local intranet

Sample statistics

- Amongst all LBI laboratories running chromatographic analysis via EZChrom Elite and LabVantage Sapphire LIMS
- ~27,000 samples/mo
- ~450,000 data points
- Average 16 points / sample



Sample submission – manual process

- ~ 1.5 minute to:
 - Launch EZChrom Elite
 - Log into instrument
 - Open Single run dialog
 - Enter required information
 - Start



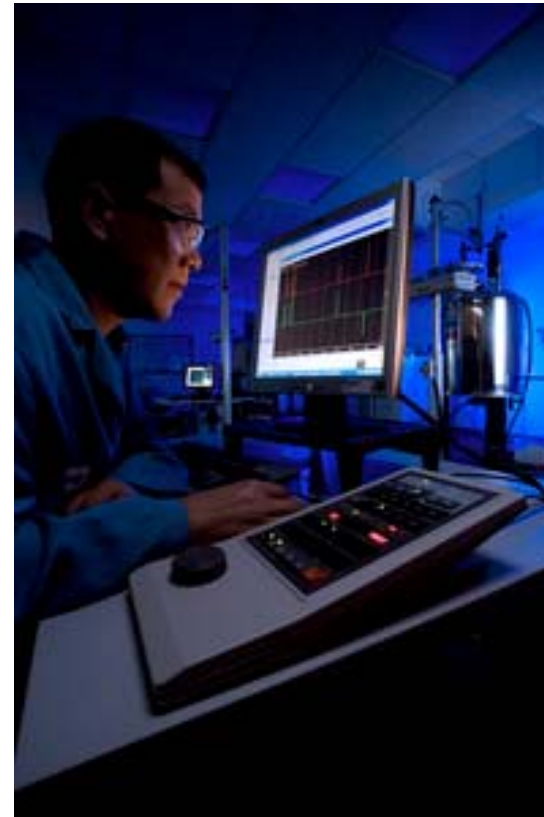
- Translates to

$$\frac{1.5 \text{ Minutes}}{\text{sample}} * \frac{27,000 \text{ Sample}}{\text{Month}} = 8100 \text{ hours / year}$$

- Equals 3.9 years of labor for sample submission

Data entry – manual process statistics

- ~ 1 minute for 16 data points
- Translates to 27,000 min/yr.
 - 450 hours / month
 - 5400 hours / year
 - ~ 2.5 years of labor



Sample submission + data entry

- Total time expenditure of sample submission and data entry
 - Approximately 6.4 years of labor
- Over a normal shift
 - Repetitive
 - Prone to errors (typos)
- What can be done?

Automation

Let the computers do the heavy lifting



Automation capabilities

- What can it do for me?
- Sample Submission
 - Store predetermined configurations.
 - Instrument/Project/Method/Factors/volumes/etc
 - Build filenames in a uniform manner
 - SxID + Desc + date stamp + nnnn.dat
 - Pre-populate fields
 - SxID
 - Description
 - Etc
 - Reduces input errors
 - Decreases setup time

Automation capabilities

- What can it do for me?
- Data Entry
 - Upon completion of data acquisition, automatically transfer and populate data fields in LIMS
 - Reduces data entry labor to ZERO
 - Reduces data entry errors
 - Transposed numbers
 - Decimal place errors

Automation – how do you do it?

- Requirements – High Level
 - Means of holding preconfigured settings
 - Leverage the database in LIMS
 - Means of presenting configuration options to end users for selection
 - Web pages inherent to the LIMS
 - Zero footprint
 - Handoff of user settings from LIMS to CDS
 - Mechanism for data transfer from CDS back to LIMS

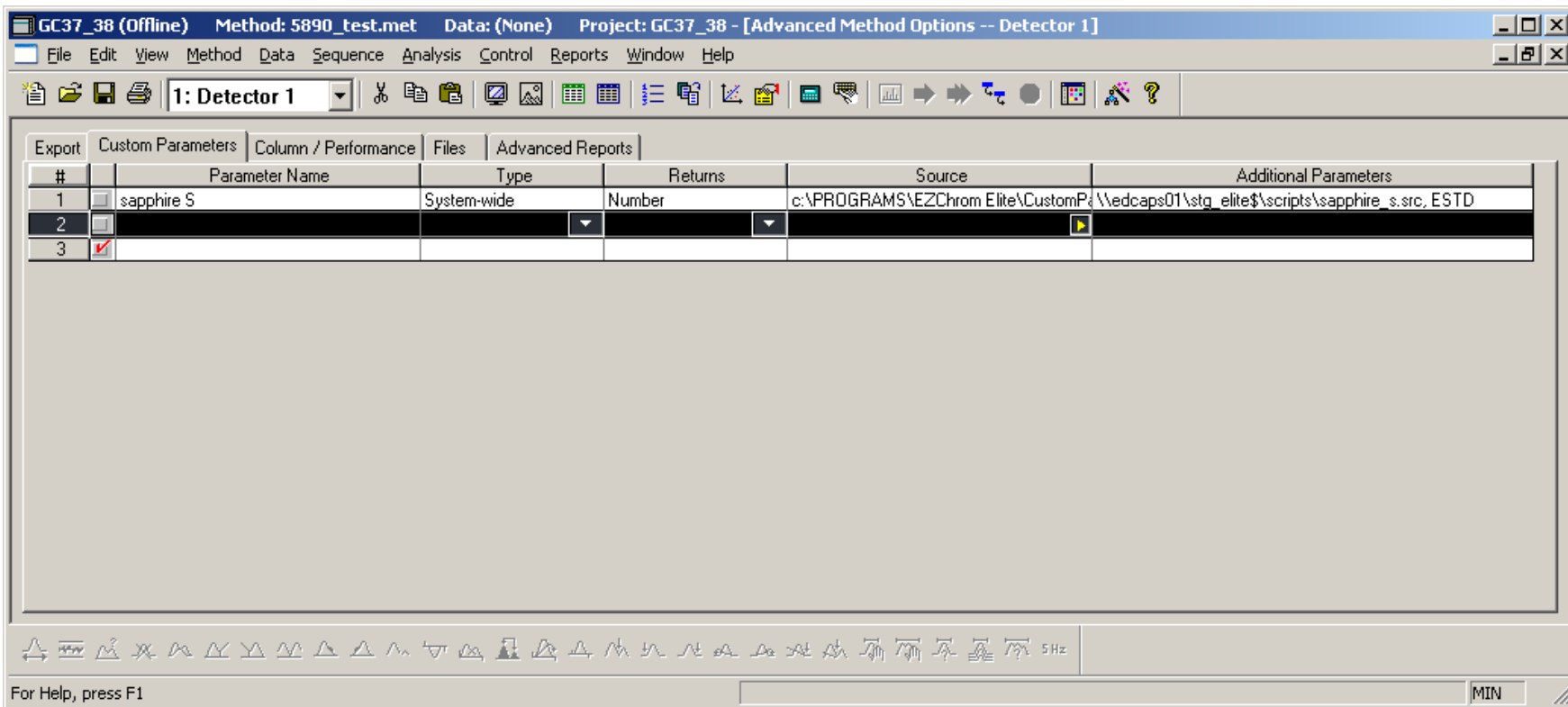
LIMS configuration

- In the LIMS - Super Users correlate Instruments with:
 - Method
 - Detector
 - Factors
 - Edit flag
 - Test (LIMS)
 - Project
 - Misc.
- Information stored in DB

The screenshot shows a window titled "Edit Instru_Method" with a tabbed interface. The "Categories" tab is active, and there is a "Notes" checkbox. The "Instru_Method Id" is 000000000000027. The "Instru Methoddesc" is ACQ0742.MBAC.PIC.WT0742. The "Instrument Id" is GC21_22. The "Method Id" is GC22.ACQ742.net and the "Detector" is 2. There are links for "Labels Id" (GC2) and "Site Id" (D0). A "Cannot be Modified?" label is present. The "Internal Standard" is 1, with "High Throughput?" checked and "Manual Vial?" unchecked. The "Dilution Factor" is 1, with "Paramet Id" (ACQ742) and "Variant Id" (D0). The "Sample Amount" is 1, with "Version Id". The "Vial Number" is 1. The "Injection Volume" is 0.5, with "Project Id" (GC21_22). The "Injection Type" is Autosampler. The "Seq File Dir:" is %project%\GC21_22\sequence. The "Data File Dir:" is %project%\GC21_22\data. The "Method File Dir:" is %project%\GC21_22\method. "OK" and "Cancel" buttons are at the bottom right.

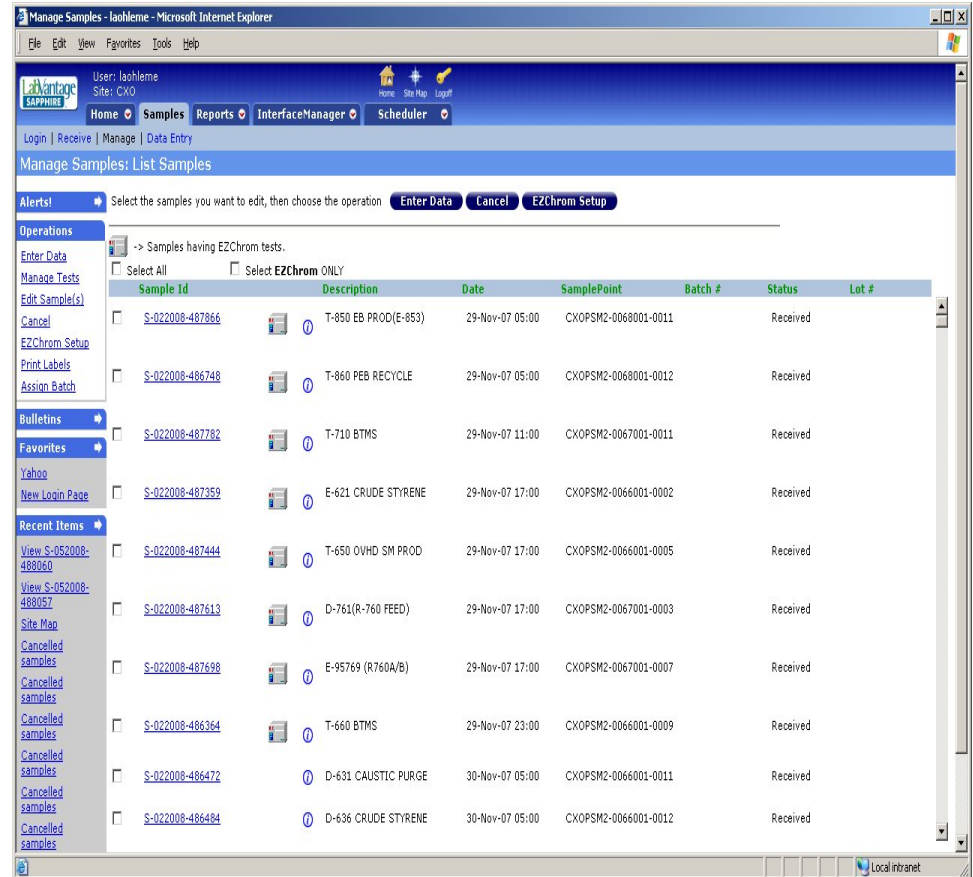
EZChrom configuration

- To facilitate the automatic transfer back to the LIMS. A custom parameter running a VBScript file is employed in each method.



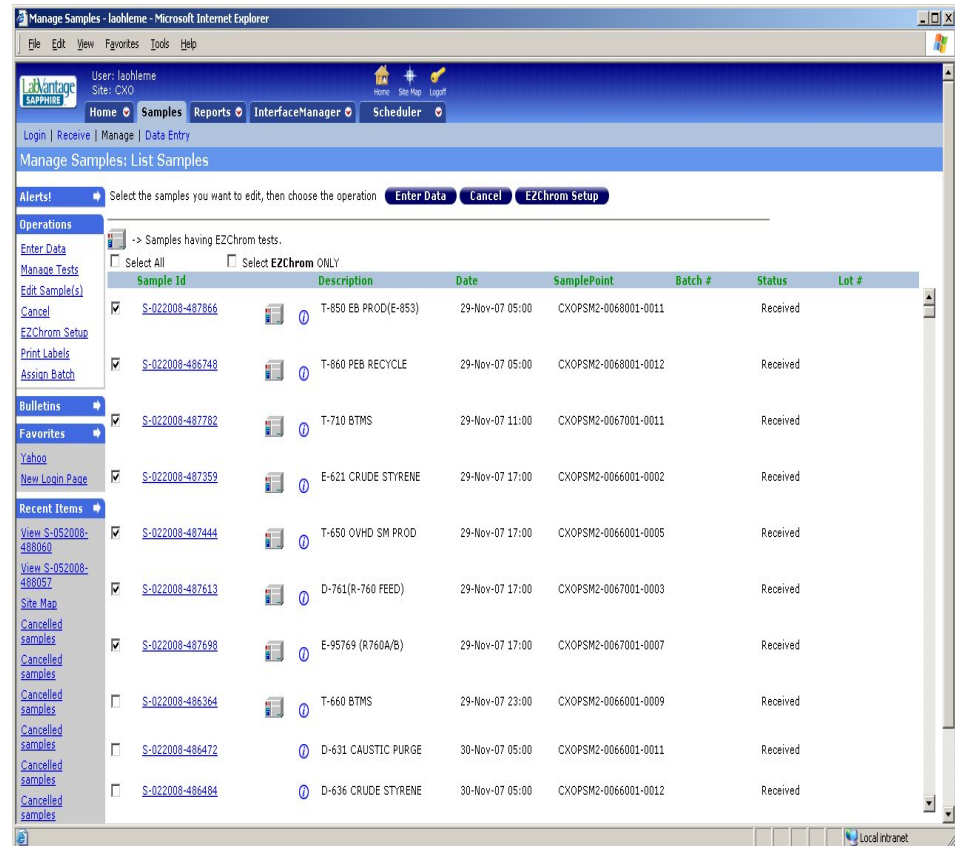
Automation interface – user experience

- User navigates to “Backlog” page
- Samples designated as “EZChrom” samples show with an instrument icon



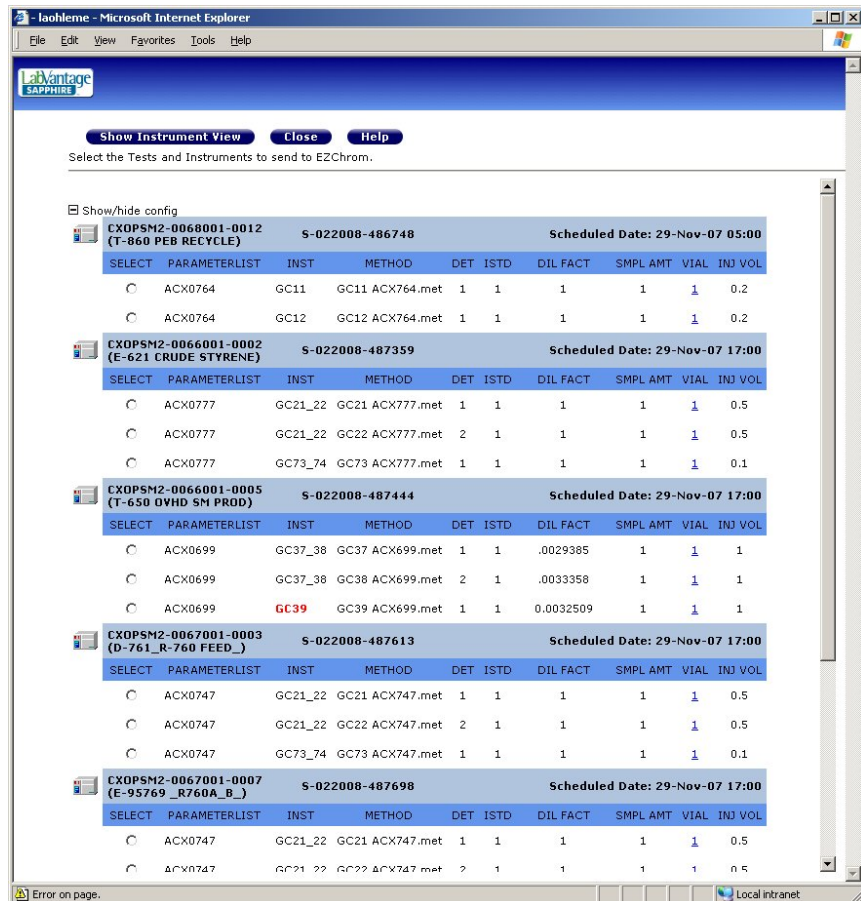
Automation interface – user experience

- Select samples for analysis
- Click “EZChrom Setup”



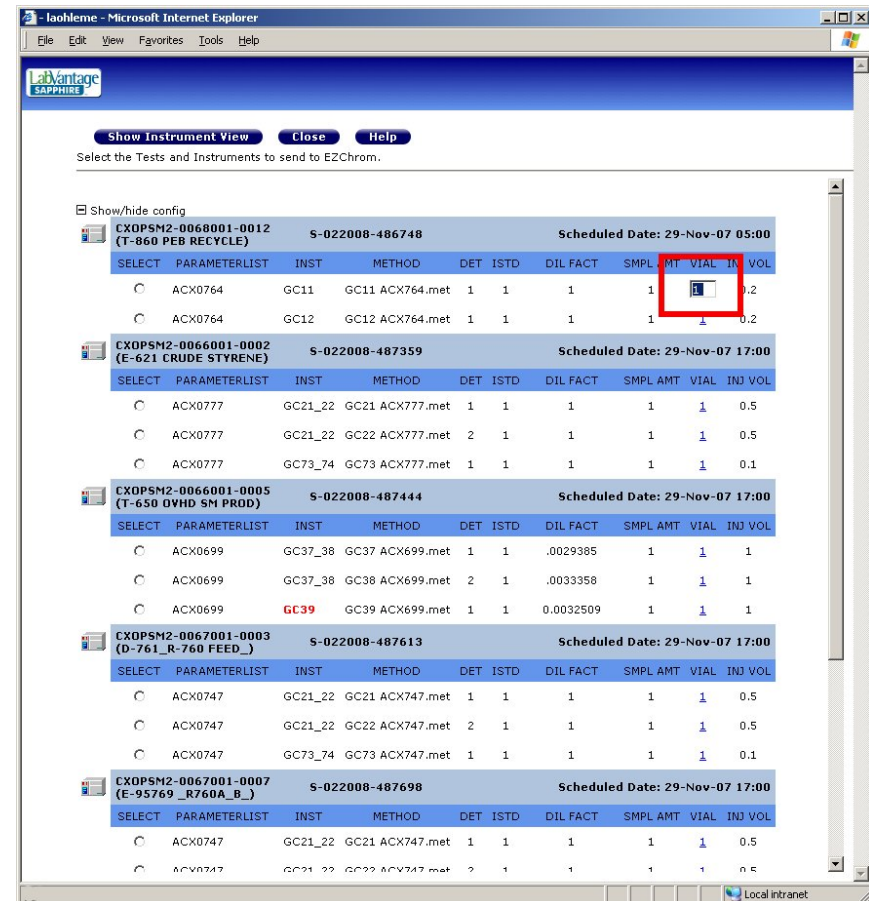
Automation interface – user experience

- User is presented with:
 - Sample point and description
 - Sample ID
 - Scheduled Date
 - Preconfigured combinations
 - Test
 - Instrument
 - Method
 - Factors
 - Amounts
 - May / May not be editable



Automation interface – user experience

- Editable values
 - Shown as a typical hyperlink



Automation interface – user experience

- Out of service instruments
 - Shown in red
 - May be due to:
 - Out of calibration
 - Hardware issues
 - Etc.

The screenshot shows a web browser window displaying a configuration management interface. The interface lists several instrument configurations, each with a table of parameters. The third configuration, for instrument 'CXOPSM2-0066001-0005 (T-650 OVHD SM PROD)', has a red box around the 'GC39' entry in the 'INST' column. The table columns are: SELECT, PARAMETERLIST, INST, METHOD, DET, ISTD, DIL FACT, SMPL AMT, VIAL, and INJ VOL.

SELECT	PARAMETERLIST	INST	METHOD	DET	ISTD	DIL FACT	SMPL AMT	VIAL	INJ VOL
<input type="radio"/>	ACX0764	GC11	GC11 ACX764.met	1	1	1	1	1	0.2
<input type="radio"/>	ACX0764	GC12	GC12 ACX764.met	1	1	1	1	1	0.2
<input type="radio"/>	ACX0777	GC21_22	GC21 ACX777.met	1	1	1	1	1	0.5
<input type="radio"/>	ACX0777	GC21_22	GC22 ACX777.met	2	1	1	1	1	0.5
<input type="radio"/>	ACX0777	GC73_74	GC73 ACX777.met	1	1	1	1	1	0.1
<input type="radio"/>	ACX0699	GC37_38	GC37 ACX699.met	1	1	.0029385	1	1	1
<input type="radio"/>	ACX0699	GC38	GC38 ACX699.met	2	1	.0033358	1	1	1
<input type="radio"/>	ACX0699	GC39	GC39 ACX699.met	1	1	0.0032509	1	1	1

Automation interface – user experience

- When selection is complete, user selects “Show Instrument View”
- All selections will be displayed in a table view grouped by instrument
- All information required for the run is in the page; however, only enough information is shown to identify the sample

LabVantage
SAPPHIRE

Submit to EZChrom Cancel Preview Close

Select the Tests and Instruments to send to EZChrom.

Credentials:
UserID:
Enter your WINDOWS password:

Print All

GC11		Sequence:GC11_28-MAY-2008_1011264.seq			Print: <input type="checkbox"/>
DET	SAMPLEID	SAMPLEPOINT	VIAL	FILENAME	
1	S-022008-486748	CXOPSM2-0068001-0012-T-860 PEB RECYCLE	2	S-022008-486748_T-860_PEB_ACX0764_29-Nov-07_0500_1_6912.dat	

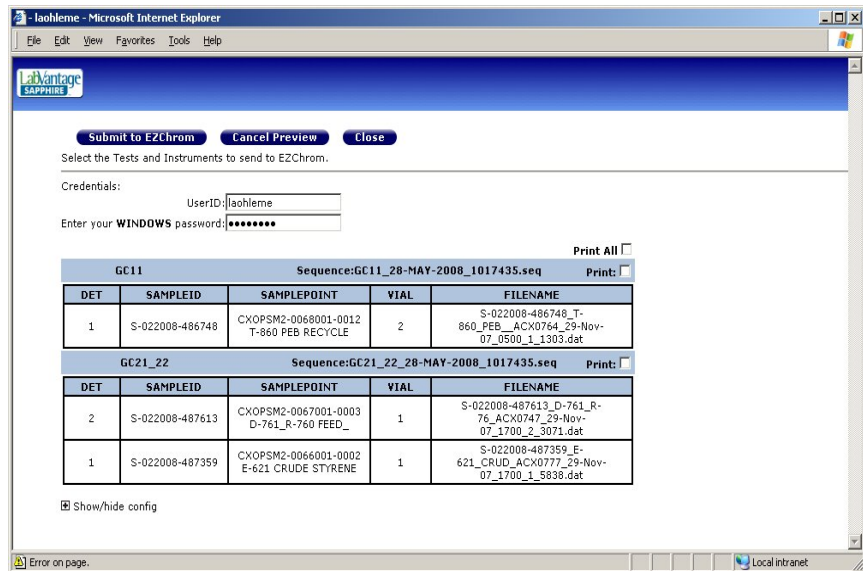
GC21_22		Sequence:GC21_22_28-MAY-2008_1011279.seq			Print: <input type="checkbox"/>
DET	SAMPLEID	SAMPLEPOINT	VIAL	FILENAME	
1	S-022008-487359	CXOPSM2-0066001-0002-E-621 CRUDE STYRENE	1	S-022008-487359_E-621_CRUD_ACX0777_29-Nov-07_1700_1_9064.dat	
2	S-022008-487613	CXOPSM2-0067001-0003-D-761_R-760 FEED_	1	S-022008-487613_D-761_R-76_ACX0747_29-Nov-07_1700_2_2955.dat	

Show/hide config

Error on page. Local intranet

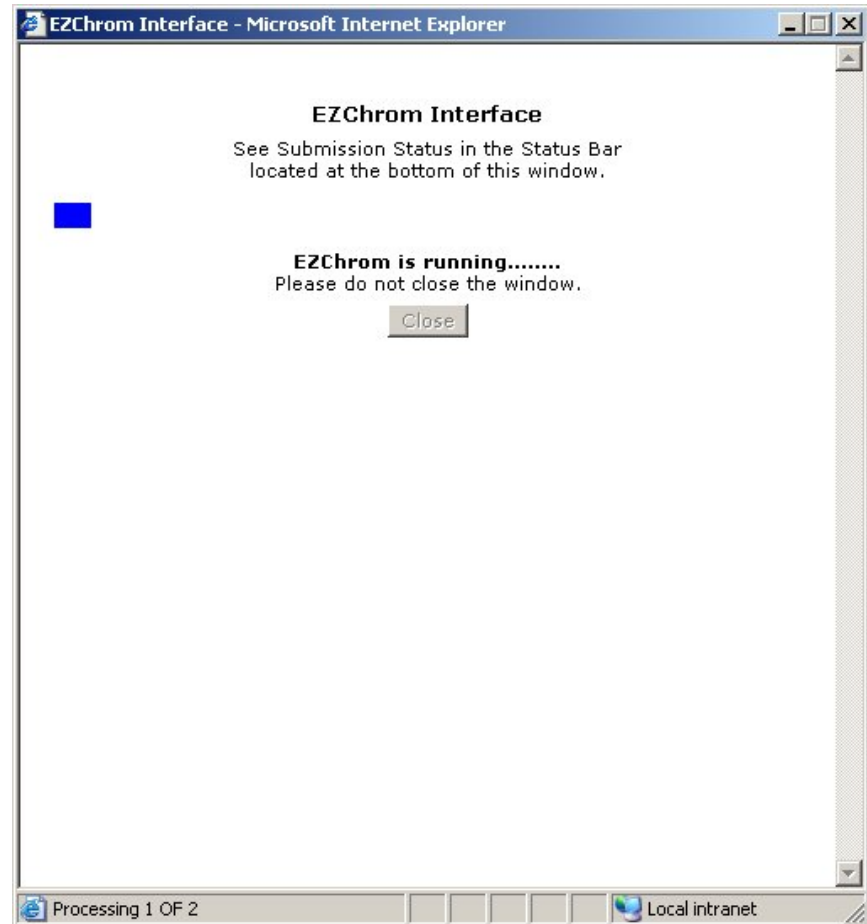
Automation interface – user experience

- Some configuration available at this point
- User can click and drag samples to change order of injection
- Print allows for the “custom report” to automatically print at the completion of data acquisition (optional)
- Credentials entered only once for all instruments
- This can be ‘canceled’ and user will be returned to prior screen if modifications are needed. Prior selections will be retained



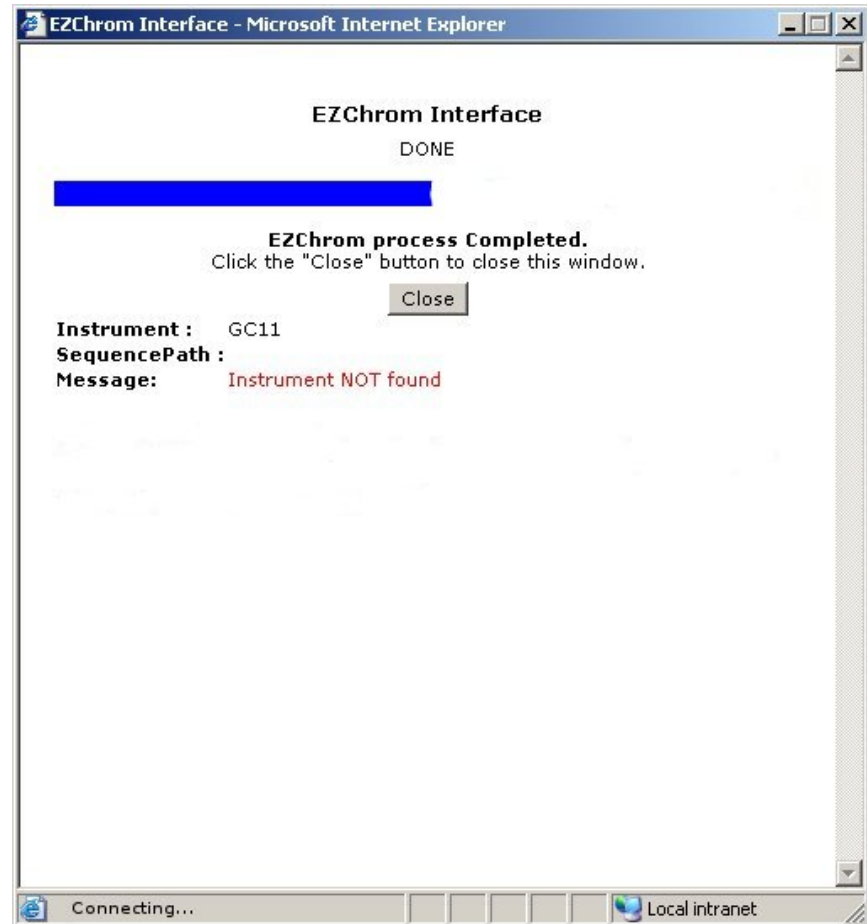
Automation interface – user experience

- When user is satisfied with selections, samples are submitted
- New window opens showing status of submissions



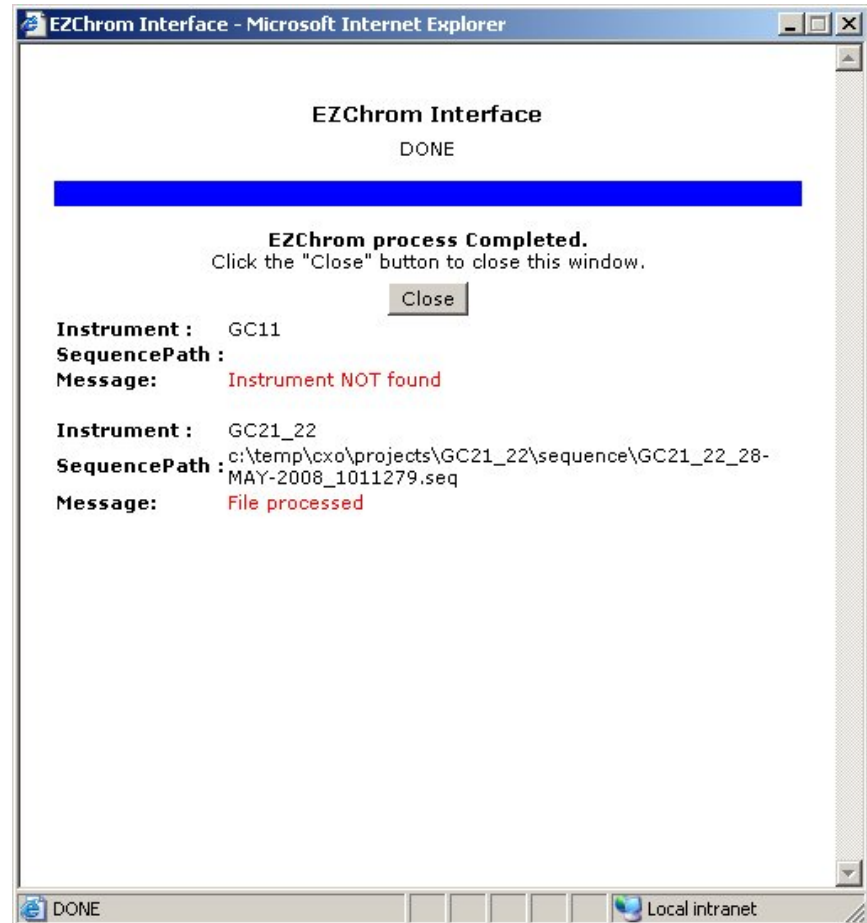
Automation interface – user experience

- A status bar displays the % of completion
- A message specific to each instrument is displayed



Automation interface – user experience

- After all processing is complete, user will see status of all submissions.



Automation – what did we accomplish?

- Labor Savings
 - Starting Instruments
 - ~50% reduction in time
 - Data Entry
 - 100% reduction
 - Total Savings
 - ~ 4.45 years labor!
- Data integrity
 - LIMS value matches instrument output
 - Does not guarantee ‘good’ data
 - Setup misconfiguration
 - Greatly reduced
 - Sample tested on wrong instrument

Acknowledgements

- Agilent
- LyondellBasell Laboratory Staff
- LyondellBasell Information Technology Organization

Thank you for your attention

Q&A

