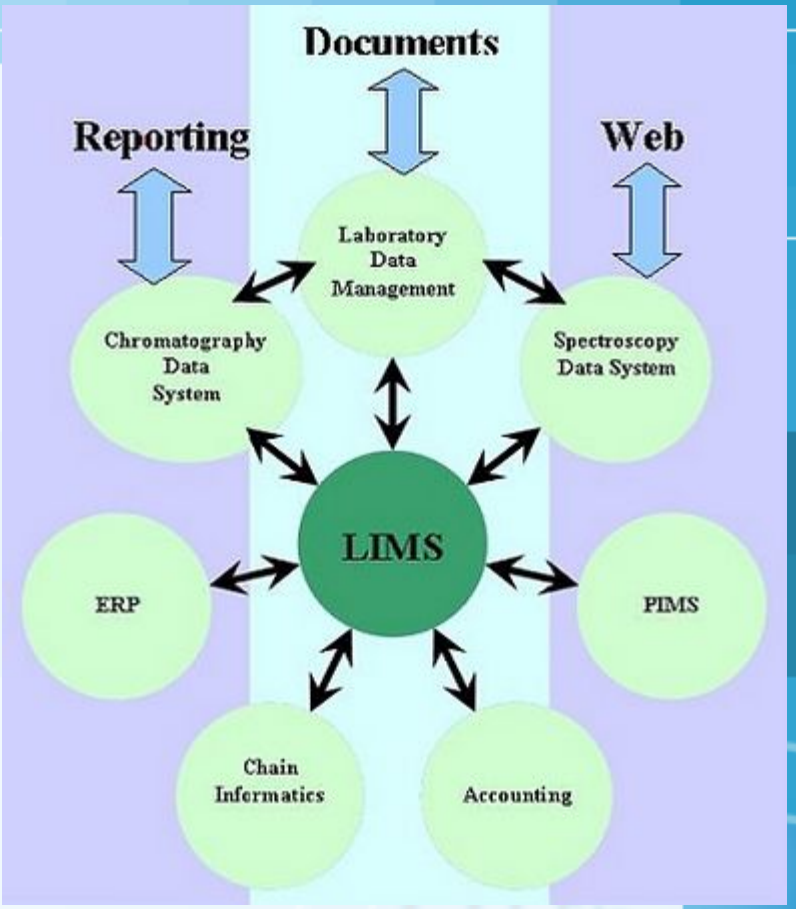
LIMS and Instrument Integration: The Perfect Relationship?

Elizabeth Turner
North Texas Municipal Water District
2015 National Environmental Monitoring Conference

What is a LIMS?

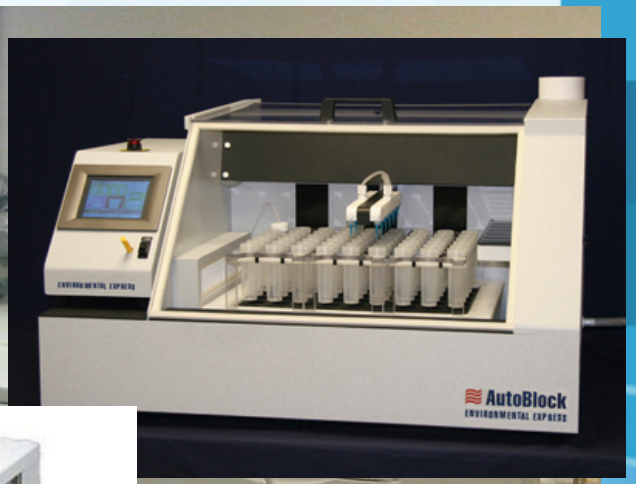
It is a system of:

- Software
- Hardware
- People
- Procedures

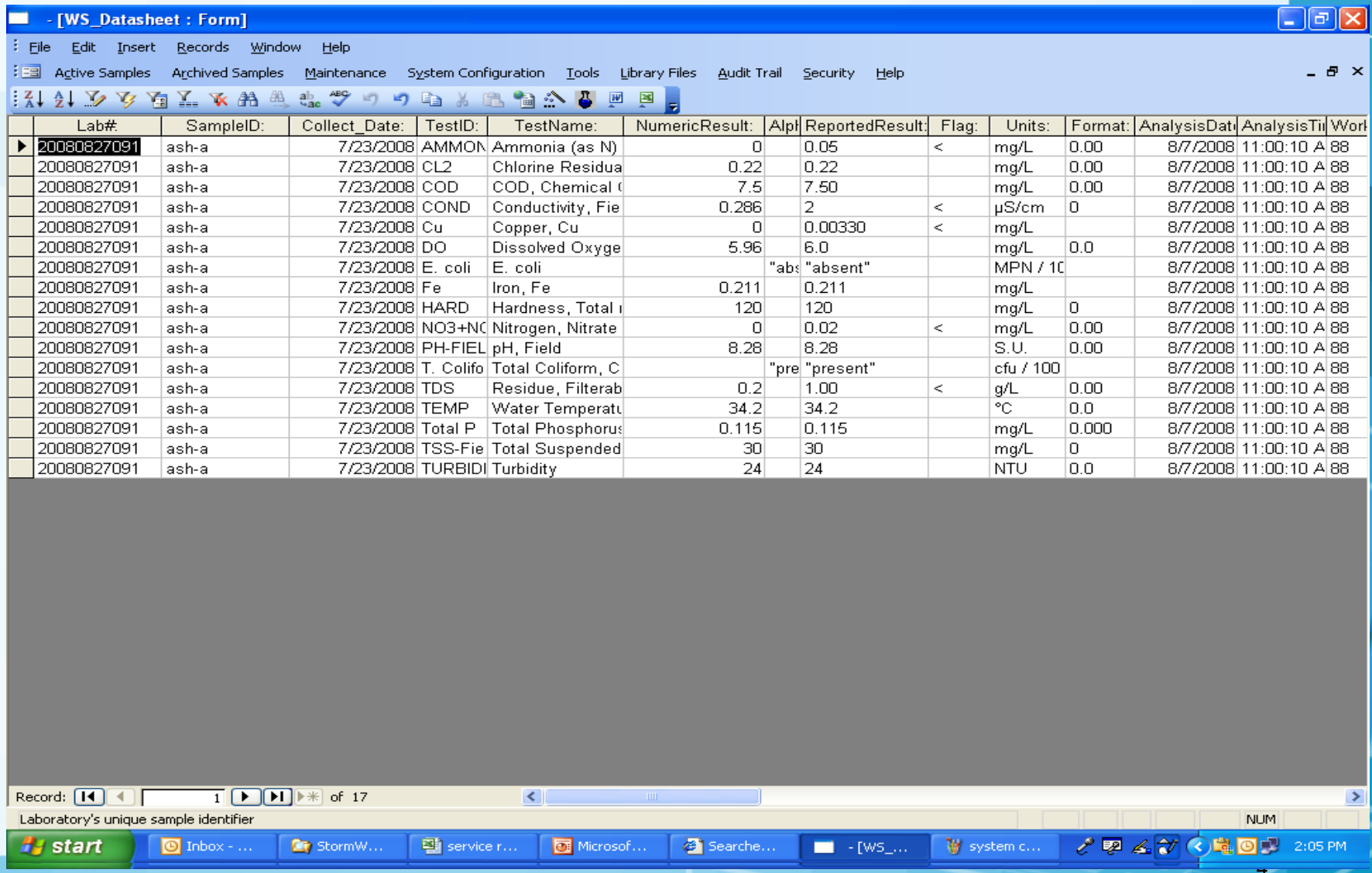


To manage laboratory data

Instruments



Result Entry



Need Identified

Problem:

An efficient way to store, readily retrieve, share and report analytical data

Solution:

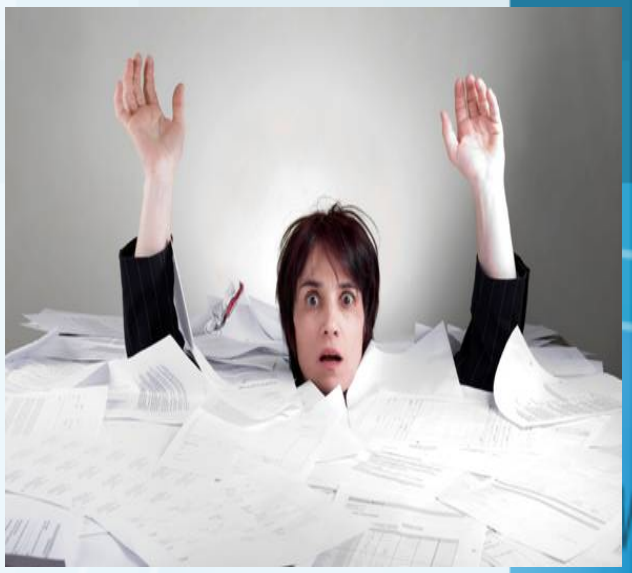
Laboratory Information Management System (LIMS) – Instrument Integration

LIMS Functions

Function	Features
Data and information capture	data entry; file transfers and simple barcode entries; communication with laboratory devices such as data collection instruments or robotic devices
Data analysis and reports	Perform calculations, result verification, data analysis with integrated analytical procedures that link different types of experimental data or integrated external software systems, reports notification system
Laboratory management	Workflow scheduling and monitoring; inventory, sample storage, and tracking systems, decision-making process, revenue and costs tracking, and multi-site project management
System management	Disk backup and recovery, system performance tuning, links to external communications

Instrumentation Integration

- Reduction in transcription errors
- Audit trail
- Increased efficiency
  - Reduced time for data entry
  - Bidirectional transfer



Integration Considerations

- Network Security
  - Instruments allowed on network?
- Unidirectional – sends only data to LIMS
- Bidirectional – sample/ batch data to instrument, results to LIMS
- Use of middleware
- Data to import
  - Raw data, calculated data
  - Quality control data (calibration, spikes, etc.)

Integration Considerations

- Result evaluation
  - Review results before import into LIMS or after?
- Where are calculations performed?
  - Dilutions
  - Dry weight
- Costs
  - Charge per instrument
  - Charge per interface
  - One time cost

Paper to Electronic Example:

Lab Instrument

There is built in logic within most parsing programs that allows the analyst to check some initial validity of their data before importing into the LIMS.

LIMS

This validation includes logic checks against the data range of the results.

Instrument Integration Checklist

Designation: E1578 – 13

Standard Guide for
Laboratory Informatics

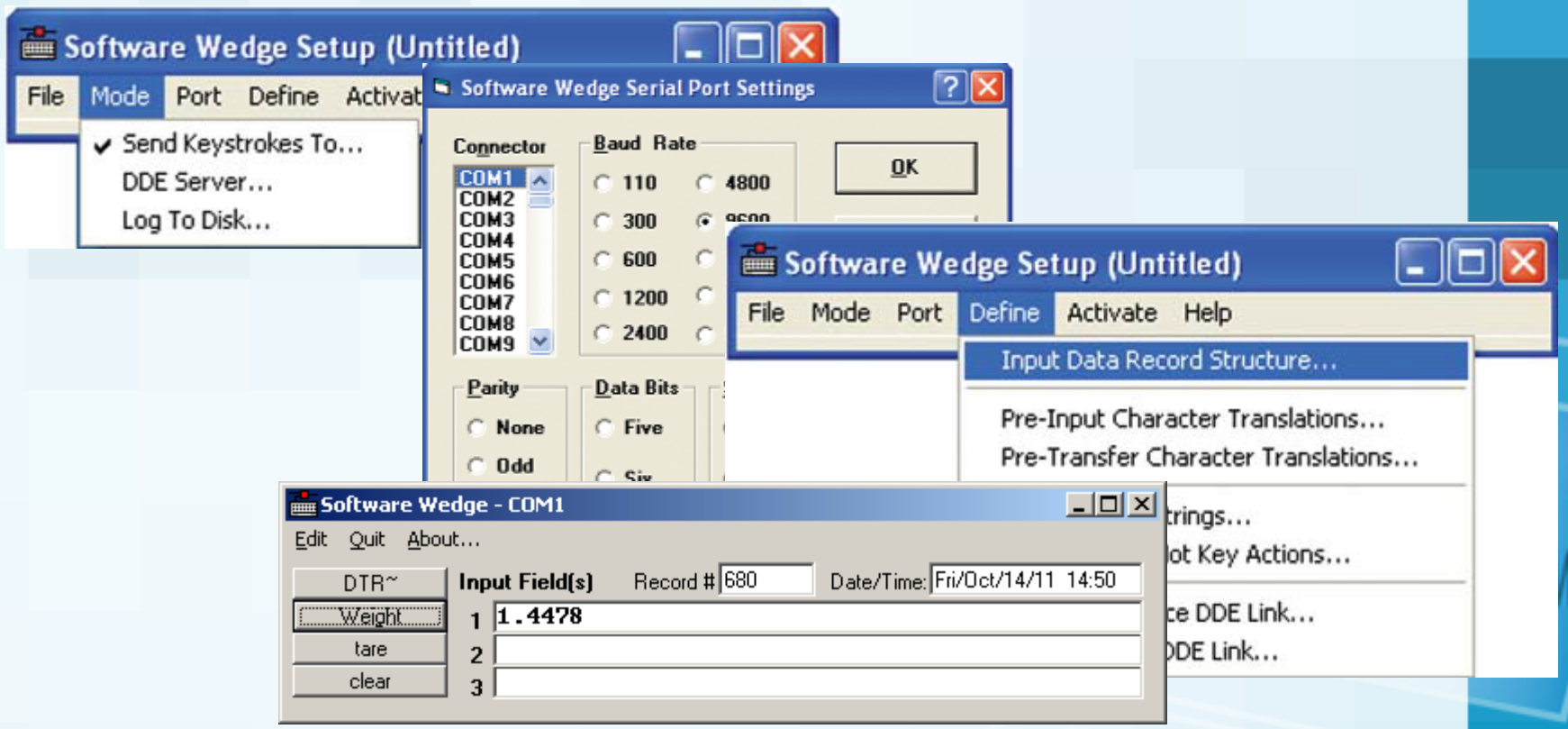
TABLE X1.1 *Continued*

# (Fig. 3)	Laboratory Informatics Functions / Requirements
E-6-4	The system should capture the personnel or instrument information relating to the results/ determinations entered into the system.
E-6-5	In cases where instruments interface with the system, the system should accept the results uploaded from the instrument.
E-6-6	In cases where instruments interface with the system, the system should transfer the sequence of unknown samples and control standards to the instrument.
E-6-7	The system should support integration with simple laboratory instruments via RS 232 connection.
E-6-8	The system should support bi-directional interface with complex laboratory instrumentation software.

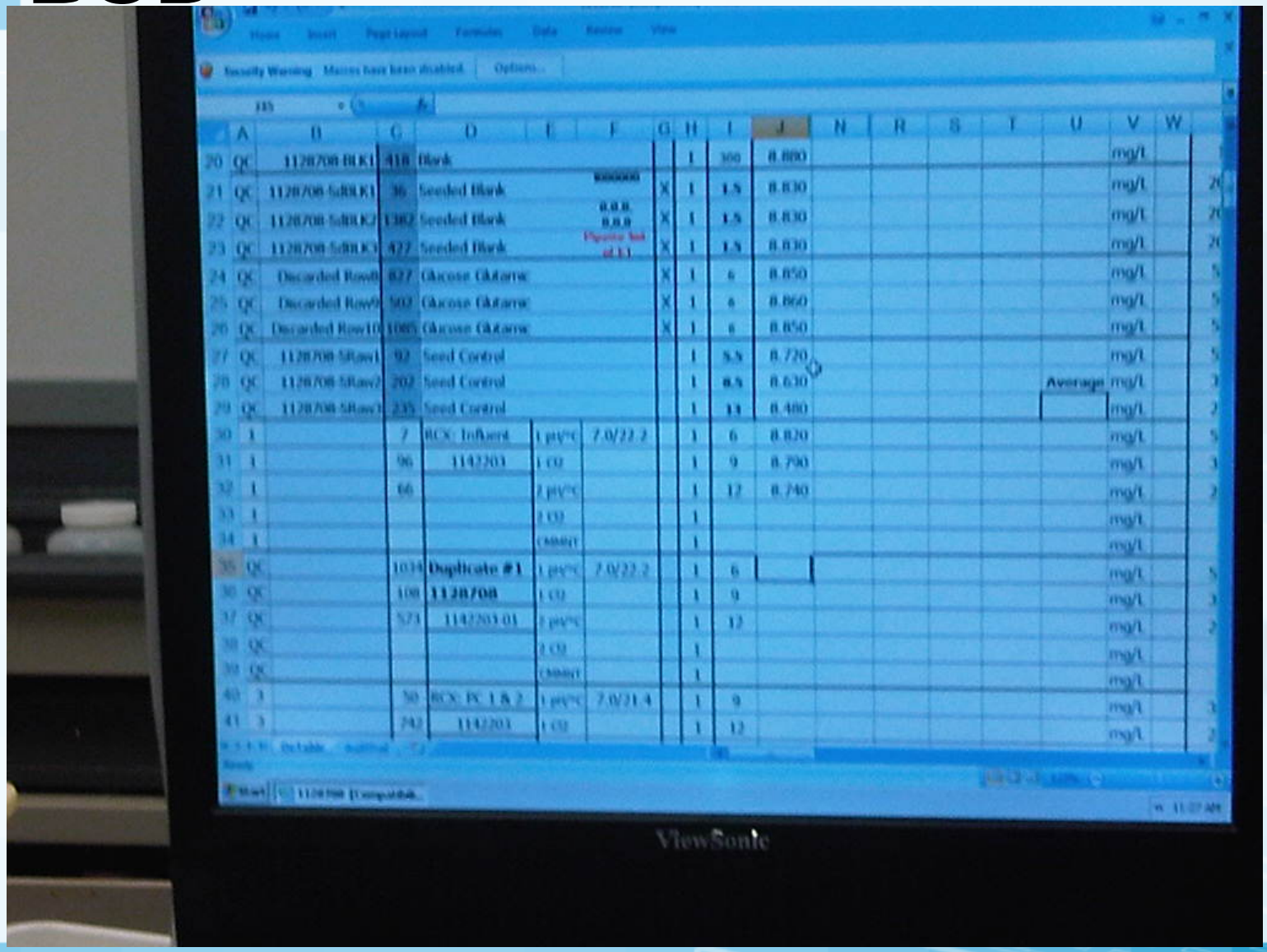
Interfacing Assumption

Only sophisticated instruments can be integrated

If it has an RS232 or USB Port....



BOD

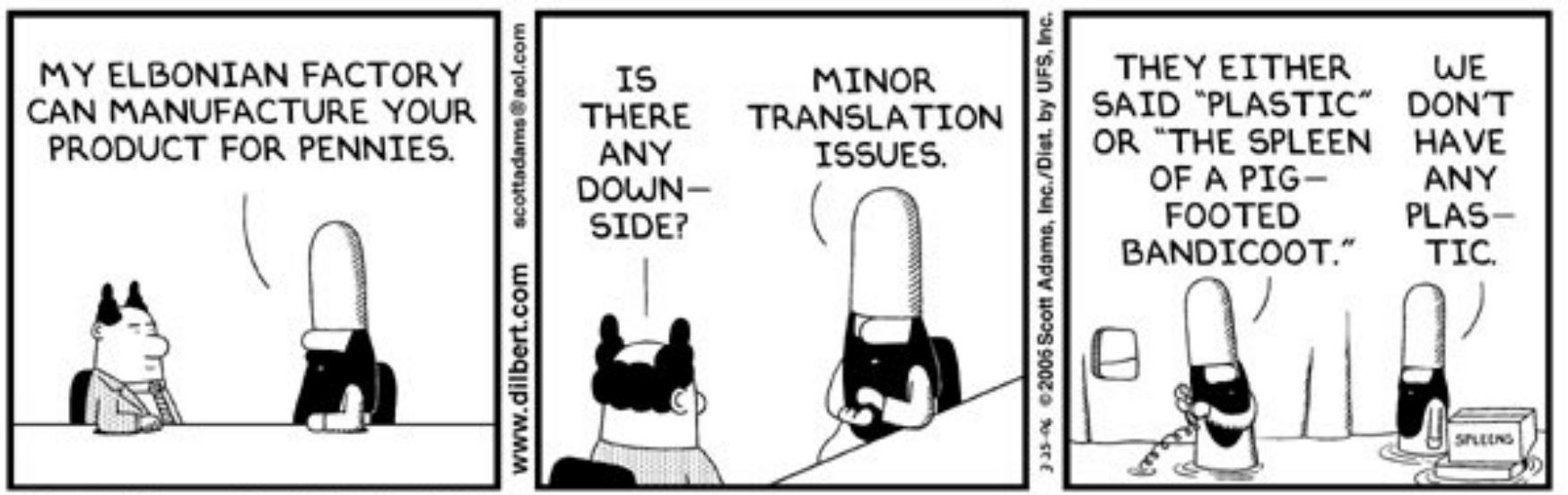


Interfacing Assumption

All instruments “speak the same language”

Integration

Instrument – LIMS Translator



© Scott Adams, Inc./Dist. by UFS, Inc.

- There is no data standard for laboratory instruments
  - AnIML (Analytical Information Markup Language) an emerging data standard for laboratory instruments covering multiple analytical techniques
  - XML is popular
  - CSV and TXT files are also used

Data Translation

- The interface will need to present the data in a format that the LIMS is able to understand.
- Every LIMS has a unique format that is required for interface/LIMS communications.
- ASCII files, ODBC and proprietary transactions are among the most common methods of transferring data.
- To transfer data via ODBC or API requires a full understanding of LIMS tables and table structure.

Interfacing Assumption

Every LIMS can interface with every instrument

Yes but……

- May take time to develop interface
- May only be unidirectional
- May require a 3rd party vendor

Example Outputs

BOD Analyzer

1436308A.txt - Notepad

File Edit Format View Help

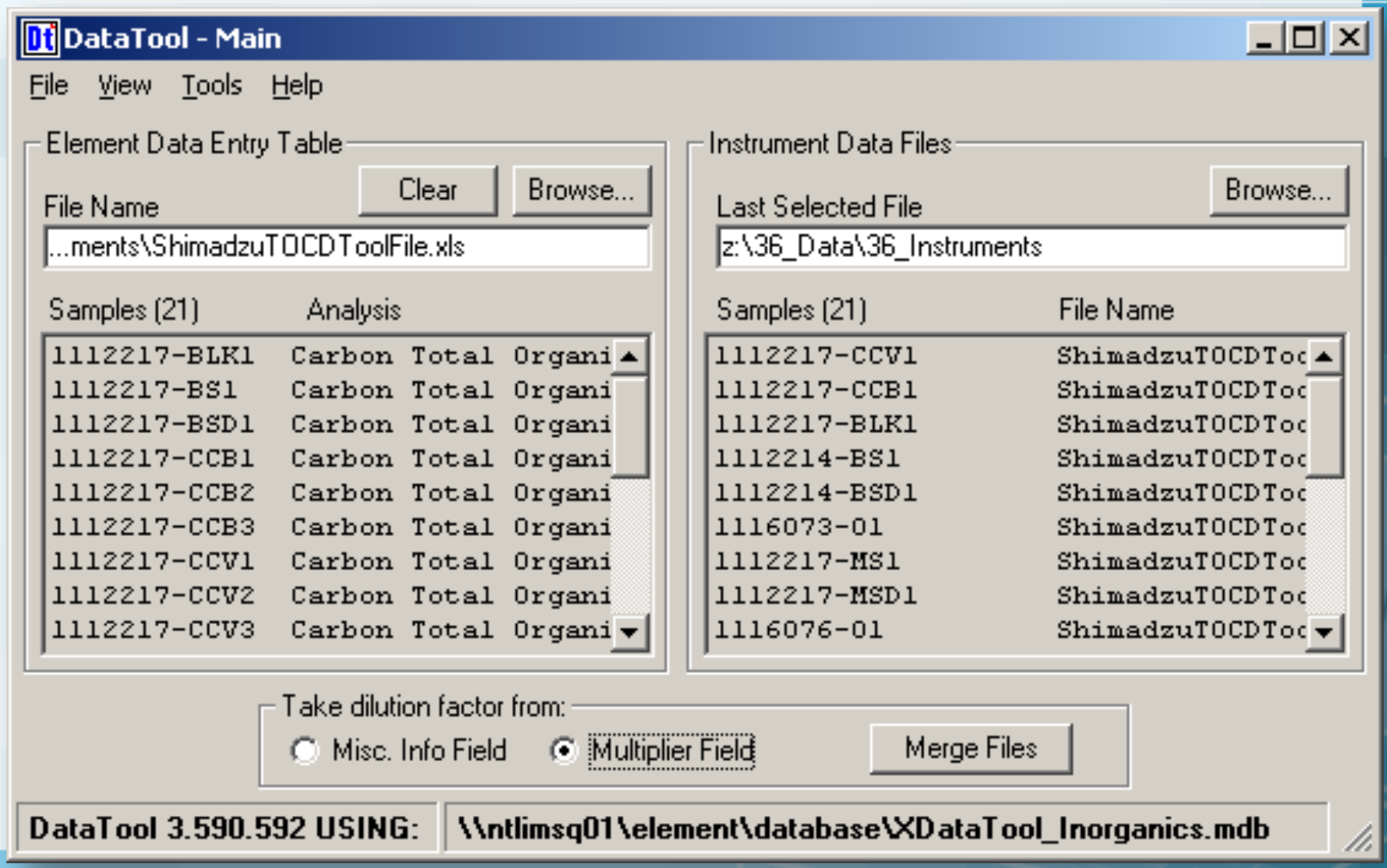
```
"Header Info","Skalar_BOD","1436308A","12/29/2014 11:54:00 AM","hfs","1/3/2015 7:15:54 AM","rcb","Calculated","-0.28","0.3172241","168.7776","","0",""
"1","Tray03","1","Blank","1436308-BLK1","0","1","0","8.43","19.2","12/29/2014 11:56:00 AM","8.88","20","1/3/2015 7:16:52 AM","-0.4499998","","","","","","-5%D","","","",""
"2","Tray03","2","Blank","1436308-BLK1","0","1","0","8.41","19.3","12/29/2014 11:57:46 AM","8.84","20","1/3/2015 7:17:33 AM","-0.4300003","","","","","","-5%D","","","",""
"3","Tray03","3","Blank","1436308-BLK1","0","1","0","8.42","19.3","12/29/2014 11:59:33 AM","8.76","20","1/3/2015 7:18:11 AM","-0.3400002","","","","","","-4%D","","","",""
"4","Tray03","4","SeedBlank","1436308-SdBlk","0","1","2","8.4","19.3","12/29/2014 12:01:29 PM","7.86","20","1/3/2015 7:19:11 AM","0.5399995","","","","","","6%D","","","",""
"5","Tray03","5","SeedBlank","1436308-SdBlk","0","1","2","8.42","19.4","12/29/2014 12:03:25 PM","8.19","20","1/3/2015 7:19:56 AM","0.2300005","","","","","","3%D","","","",""
"6","Tray03","6","SeedBlank","1436308-SdBlk","0","1","2","8.42","19.3","12/29/2014 12:05:20 PM","8.2","20","1/3/2015 7:20:40 AM","0.2200003","","","","","","3%D","","","",""
"7","Tray03","7","Standard","1436308-BS1","6","1","2","8.41","19.4","12/29/2014 12:07:21 PM","4.48","20","1/3/2015 7:22:07 AM","3.93","164.7776","168.7776","","","","47%D","","","",""
"8","Tray03","8","Standard","1436308-BS1","6","1","2","8.41","19.4","12/29/2014 12:09:19 PM","4.41","20","1/3/2015 7:23:02 AM","4","168.2776","","","","","","48%D","","","",""
"9","Tray03","9","Standard","1436308-BS1","6","1","2","8.41","19.4","12/29/2014 12:11:14 PM","4.31","20","1/3/2015 7:24:03 AM","4.1","173.2776","","","","","","49%D","","","",""
"10","Tray03","10","Seed","1436308-SettRaw","0","1","6","8.35","19.4","12/29/2014 12:13:09 PM","6.59","20","1/3/2015 7:25:17 AM","1.76","","","","","","21%D","","","",""
"11","Tray03","11","Seed","1436308-SettRaw","0","1","10","8.25","19.4","12/29/2014 12:15:08 PM","5.14","20","1/3/2015 7:26:23 AM","3.11","0.311","","","","","38%D","","","",""
"12","Tray03","12","Seed","1436308-SettRaw","0","1","14.5","8.16","19.4","12/29/2014 12:17:15 PM","3.47","20","1/3/2015 7:27:36 AM","4.69","0.3234482","","","","","57%D","","","",""
"13","Tray03","13","Sample","1453010-01","4","1","0","8.42","19.4","12/29/2014 12:18:58 PM","6.26","20","1/3/2015 7:28:49 AM","2.16","162","162.8","","","","26%D CV3=1.2%","","","",""
"14","Tray03","14","Sample","1453010-01","7","1","0","8.36","19.4","12/29/2014 12:20:41 PM","4.51","19.9","1/3/2015 7:30:02 AM","3.849999","165","","","","","46%D","","","",""
"15","Tray03","15","Sample","1453010-01","10","1","0","8.34","19.5","12/29/2014 12:22:26 PM","2.96","20","1/3/2015 7:31:16 AM","5.38","161.4","","","","","65%D","","","",""
"16","Tray03","16","Sample","1436308-DUP1","4","1","0","8.41","19.5","12/29/2014 12:24:15 PM","7.02","20","1/3/2015 7:32:45 AM","1.39","","","","","","17%D Delta<2.00","","","",""
"17","Tray04","1","Sample","1436308-DUP1","7","1","0","8.39","19.5","12/29/2014 12:26:00 PM","4.69","20","1/3/2015 7:34:02 AM","3.7","158.5714","157.5857","","","","44%D CV2=0.9%","","","",""
"18","Tray04","2","Sample","1436308-DUP1","10","1","0","8.35","19.5","12/29/2014 12:27:45 PM","3.13","20","1/3/2015 7:35:18 AM","5.22","156.6","","","","","63%D","","","",""
"19","Tray04","3","Sample","1453010-03","6","1","0","8.4","19.5","12/29/2014 12:29:27 PM","5.62","20","1/3/2015 7:36:27 AM","2.78","139","138.2222","","","","33%D CV3=5.2%","","","",""
"20","Tray04","4","Sample","1453010-03","9","1","0","8.41","19.5","12/29/2014 12:31:09 PM","4.49","20","1/3/2015 7:37:31 AM","3.92","130.6667","","","","","47%D","","","",""
"21","Tray04","5","Sample","1453010-03","12","1","0","8.37","19.5","12/29/2014 12:32:40 PM","2.57","20","1/3/2015 7:38:51 AM","5.8","145","","","","","60%D","","","",""
```

Example Outputs

```
'DLZ - Summary Report"
'Sample ID:","1506128-02"
'Sample Date/Time:","Wednesday, February 11, 2015 20:10:19"
'Sample Description:"
'Batch ID:","1504015"
'Initial Sample Quantity (mg):"
'Sample Prep Volume (mL):"
'Aliquot Volume (mL):"
'Diluted To Volume (mL):"
'Method File:","C:\NexIONData\Method\200.8 (samples)101613.mth"
'Analyst  :","lmacias"
'Intensities"
'I/S","Analyte","Mass","Conc. Mean","Unit","Conc. RSD","Meas. Intens. Mean"
'|-","Li",6,,"ppb",,536933.313
'|  ","Be",9,0.005672,"ppb",16.076,25.000
'|  ","Na",23,S,"ppm",S,S
'|  ","Mg",24,15.585557,"ppm",1.304,235113096.440
'|  ","Mg",25,15.848597,"ppm",1.923,31696453.630
'|  ","Mg",26,16.282950,"ppm",2.824,36347239.079
'|  ","Al",27,16.512011,"ppb",3.091,320537.641
'|  ","K",39,20.445506,"ppm",0.101,432341572.132
'|  ","Ca",44,111.051123,"ppm",0.956,89795421.050
'|  ","Sc",45,,"ppb",,739951.120
'|  ","V",51,6.552038,"ppb",3.645,271807.856
'|  ","Cr",52,0.733155,"ppb",5.500,27656.753
'|  ","Fe",54,0.035377,"ppm",1.512,84880.436
'|  ","Mn",55,1.952747,"ppb",1.171,52326.663
'|  ","Fe",56,0.091809,"ppm",0.526,7117155.729
'|  ","Fe",57,0.320618,"ppm",1.365,205566.544
'|  ","Ni",58,3.839623,"ppb",1.198,47077.637
'|  ","Co",59,0.310297,"ppb",2.251,8038.928
'|  ","Ni",60,5.811787,"ppb",1.818,33745.149
'|  ","Cu",63,26.569484,"ppb",2.157,322171.454
'|  ","Zn",64,48.464628,"ppb",3.175,264298.748
'|  ","Cu",65,22.913944,"ppb",2.527,117646.248
'|  ","Zn",66,42.986799,"ppb",2.651,116094.313
'|  ","Zn",68,42.250997,"ppb",2.282,70906.910
'|>","Ge",74,,"ppb",,94431.381
'|  ","As",75,7.042137,"ppb",1.482,27755.604
'|  ","Se",78,-0.159974,"ppb",77.765,7623.919
'|  ","Se",82,1.066629,"ppb",3.528,360.693
'|  ","Y",89,,"ppb",,771779.699
'|  ","Ag",107,0.006552,"ppb",12.402,161.668
'|  ","Cd",111,0.030106,"ppb",12.276,153.668
'|  ","In",115,,"ppb",,1055104.580
'|  ","Sb",121,0.386290,"ppb",0.233,7135.115
'|-","Sb",123,0.388037,"ppb",1.912,5195.258
'|-","Ba",137,45.750489,"ppb",0.857,259931.175
'|  ","Ba",138,47.869800,"ppb",0.290,1689812.579
'|  ","Tb",159,,"ppb",,1382581.021
```

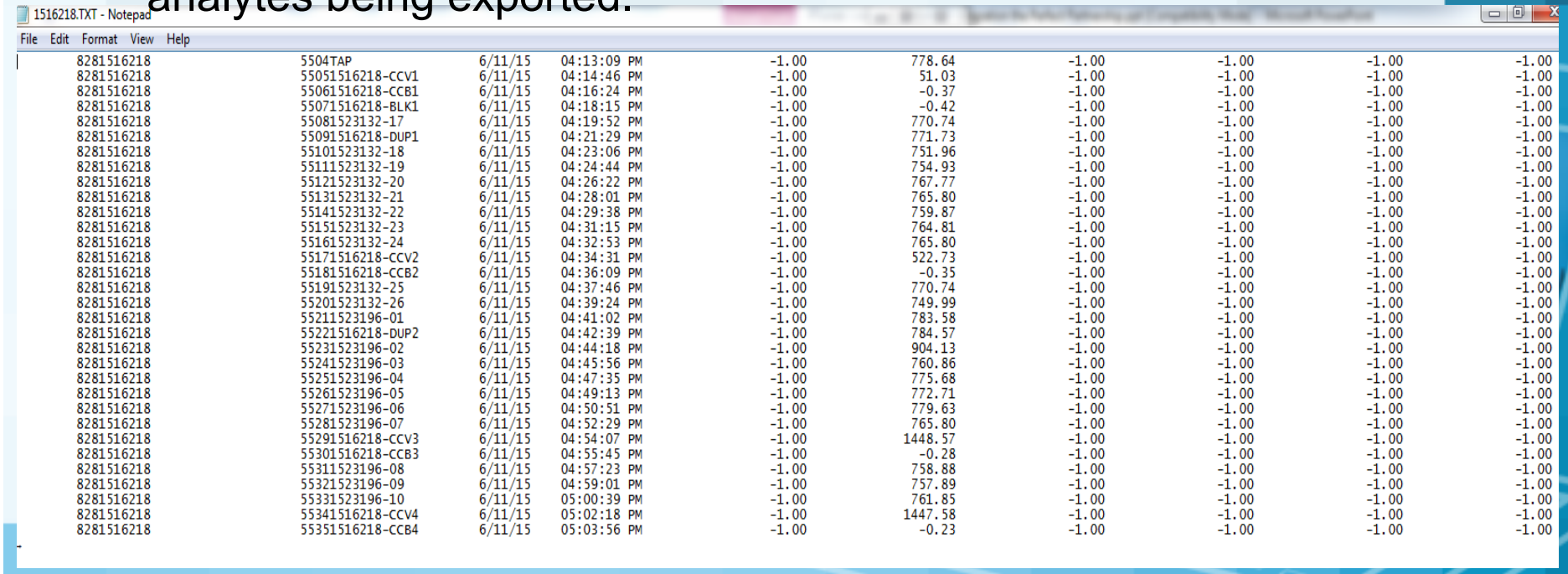
ICP-MS

Instrument Integration data tool



Example Issue - Titrator

- Instrument exports a pivot table report that has no analyte specification.
- The analyte columns are determined by the way the user develops the report that is exported.
- Once the columns were specified by the user then the analytes in those columns were mapped within parser to the specific analytes being exported.



1516218.TXT - Notepad

File Edit Format View Help

8281516218	5504TAP	6/11/15	04:13:09 PM	-1.00	778.64	-1.00	-1.00	-1.00	-1.00
8281516218	55051516218-CCV1	6/11/15	04:14:46 PM	-1.00	51.03	-1.00	-1.00	-1.00	-1.00
8281516218	55061516218-CCB1	6/11/15	04:16:24 PM	-1.00	-0.37	-1.00	-1.00	-1.00	-1.00
8281516218	55071516218-BLK1	6/11/15	04:18:15 PM	-1.00	-0.42	-1.00	-1.00	-1.00	-1.00
8281516218	55081523132-17	6/11/15	04:19:52 PM	-1.00	770.74	-1.00	-1.00	-1.00	-1.00
8281516218	55091516218-DUP1	6/11/15	04:21:29 PM	-1.00	771.73	-1.00	-1.00	-1.00	-1.00
8281516218	55101523132-18	6/11/15	04:23:06 PM	-1.00	751.96	-1.00	-1.00	-1.00	-1.00
8281516218	55111523132-19	6/11/15	04:24:44 PM	-1.00	754.93	-1.00	-1.00	-1.00	-1.00
8281516218	55121523132-20	6/11/15	04:26:22 PM	-1.00	767.77	-1.00	-1.00	-1.00	-1.00
8281516218	55131523132-21	6/11/15	04:28:01 PM	-1.00	765.80	-1.00	-1.00	-1.00	-1.00
8281516218	55141523132-22	6/11/15	04:29:38 PM	-1.00	759.87	-1.00	-1.00	-1.00	-1.00
8281516218	55151523132-23	6/11/15	04:31:15 PM	-1.00	764.81	-1.00	-1.00	-1.00	-1.00
8281516218	55161523132-24	6/11/15	04:32:53 PM	-1.00	765.80	-1.00	-1.00	-1.00	-1.00
8281516218	55171516218-CCV2	6/11/15	04:34:31 PM	-1.00	522.73	-1.00	-1.00	-1.00	-1.00
8281516218	55181516218-CCB2	6/11/15	04:36:09 PM	-1.00	-0.35	-1.00	-1.00	-1.00	-1.00
8281516218	55191523132-25	6/11/15	04:37:46 PM	-1.00	770.74	-1.00	-1.00	-1.00	-1.00
8281516218	55201523132-26	6/11/15	04:39:24 PM	-1.00	749.99	-1.00	-1.00	-1.00	-1.00
8281516218	55211523196-01	6/11/15	04:41:02 PM	-1.00	783.58	-1.00	-1.00	-1.00	-1.00
8281516218	55221516218-DUP2	6/11/15	04:42:39 PM	-1.00	784.57	-1.00	-1.00	-1.00	-1.00
8281516218	55231523196-02	6/11/15	04:44:18 PM	-1.00	904.13	-1.00	-1.00	-1.00	-1.00
8281516218	55241523196-03	6/11/15	04:45:56 PM	-1.00	760.86	-1.00	-1.00	-1.00	-1.00
8281516218	55251523196-04	6/11/15	04:47:35 PM	-1.00	775.68	-1.00	-1.00	-1.00	-1.00
8281516218	55261523196-05	6/11/15	04:49:13 PM	-1.00	772.71	-1.00	-1.00	-1.00	-1.00
8281516218	55271523196-06	6/11/15	04:50:51 PM	-1.00	779.63	-1.00	-1.00	-1.00	-1.00
8281516218	55281523196-07	6/11/15	04:52:29 PM	-1.00	765.80	-1.00	-1.00	-1.00	-1.00
8281516218	55291516218-CCV3	6/11/15	04:54:07 PM	-1.00	1448.57	-1.00	-1.00	-1.00	-1.00
8281516218	55301516218-CCB3	6/11/15	04:55:45 PM	-1.00	-0.28	-1.00	-1.00	-1.00	-1.00
8281516218	55311523196-08	6/11/15	04:57:23 PM	-1.00	758.88	-1.00	-1.00	-1.00	-1.00
8281516218	55321523196-09	6/11/15	04:59:01 PM	-1.00	757.89	-1.00	-1.00	-1.00	-1.00
8281516218	55331523196-10	6/11/15	05:00:39 PM	-1.00	761.85	-1.00	-1.00	-1.00	-1.00
8281516218	55341516218-CCV4	6/11/15	05:02:18 PM	-1.00	1447.58	-1.00	-1.00	-1.00	-1.00
8281516218	55351516218-CCB4	6/11/15	05:03:56 PM	-1.00	-0.23	-1.00	-1.00	-1.00	-1.00

Example Issue – Discrete Analyzer

- Instrument software requested dilution factor
- Only exported calculated data
- Dilution factor entered in LIMS
- Dilution factor applied by BOTH instrument and LIMS
- Solution: only enter dilution factor in LIMS
- Configured to acquire the dilution factor from an appendage to the lab id number (1525100-01@5)

Example Issue – ICP-MS

- Instrument has collision cell (KED) option
- KED mode ok for Clean Water Act analysis but not Safe Drinking Water Act analysis
- Different detection limits for standard mode and KED mode
- Solution: Two instrument names
- Analyst enters appropriate instrument name during import

Summary

- Instrument integration is beneficial
- Libraries exist for most common instruments
- Interfaces may need to be customized based on instrument, laboratory process
- Important to understand instrument data files and LIMS table structure

Acknowledgements

- Bobby Sims, NTMWD Assistant LIMS Administrator
- Ed Howland, NTMWD LIMS Administrator