

# LIMS and Instrument Integration: The Perfect Relationship?



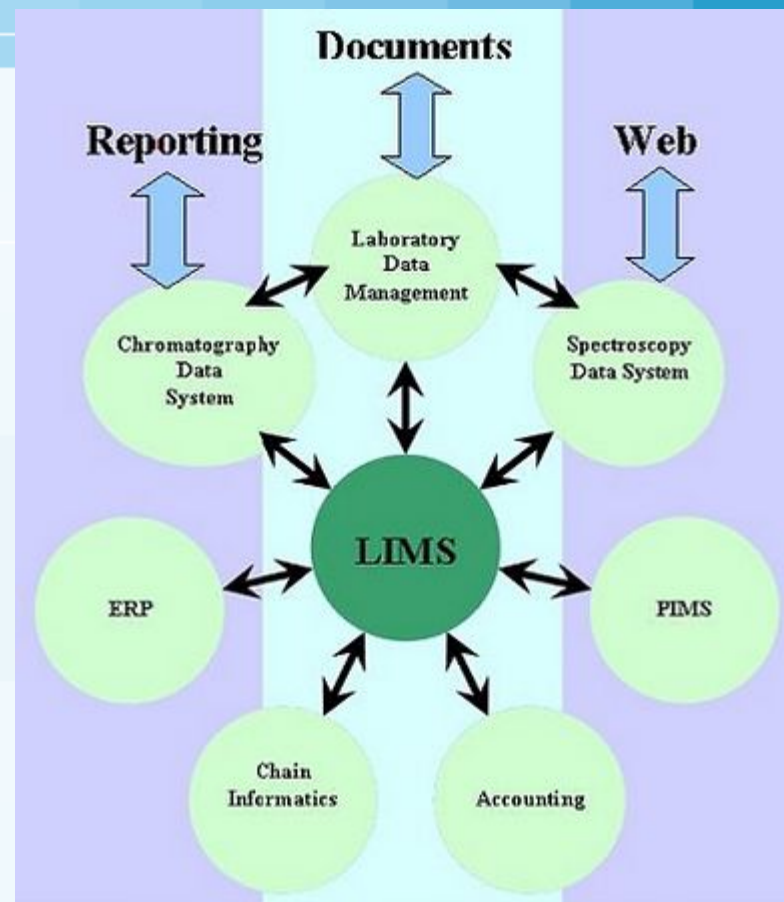
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North Texas Municipal Water District  
2015 National Environmental Monitoring Conference



# What is a LIMS?

It is a system of:

- Software
- Hardware
- People
- Procedures



To manage laboratory data

# Instruments



# Result Entry

- [WS\_Datasheet : Form]

File Edit Insert Records Window Help

Active Samples Archived Samples Maintenance System Configuration Tools Library Files Audit Trail Security Help

Lab#	SampleID:	Collect_Date:	TestID:	TestName:	NumericResult:	Alp	ReportedResult:	Flag:	Units:	Format:	AnalysisDate:	AnalysisTime:	Work
▶ 20080827091	ash-a	7/23/2008	AMMON	Ammonia (as N)	0		0.05	<	mg/L	0.00	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	CL2	Chlorine Residua	0.22		0.22		mg/L	0.00	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	COD	COD, Chemical O	7.5		7.50		mg/L	0.00	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	COND	Conductivity, Fie	0.286		2	<	µS/cm	0	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	Cu	Copper, Cu	0		0.00330	<	mg/L		8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	DO	Dissolved Oxyge	5.96		6.0		mg/L	0.0	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	E. coli	E. coli			"abs: "absent"		MPN / 10		8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	Fe	Iron, Fe	0.211		0.211		mg/L		8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	HARD	Hardness, Total i	120		120		mg/L	0	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	NO3+NO	Nitrogen, Nitrate	0		0.02	<	mg/L	0.00	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	PH-FIEL	pH, Field	8.28		8.28		S. U.	0.00	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	T. Colifo	Total Coliform, C			"pre "present"		cfu / 100		8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	TDS	Residue, Filterab	0.2		1.00	<	g/L	0.00	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	TEMP	Water Temperatu	34.2		34.2		°C	0.0	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	Total P	Total Phosphorus	0.115		0.115		mg/L	0.000	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	TSS-Fie	Total Suspended	30		30		mg/L	0	8/7/2008	11:00:10 A	88
20080827091	ash-a	7/23/2008	TURBIDI	Turbidity	24		24		NTU	0.0	8/7/2008	11:00:10 A	88

Record: 1 of 17

Laboratory's unique sample identifier

NUM

start | Inbox - ... | StormW... | service r... | Microsof... | Searche... | - [WS\_... | system c... | 2:05 PM

# **Need Identified**

## **Problem:**

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

## **Solution:**

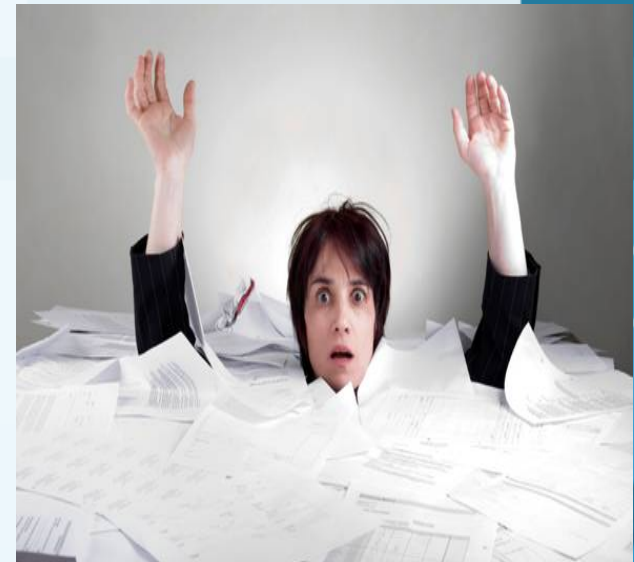
Laboratory Information Management System (LIMS) – Instrument Integration

# LIMS Functions

<b>Function</b>	<b>Features</b>
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	<del>Perform calculations, result verification,</del> 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

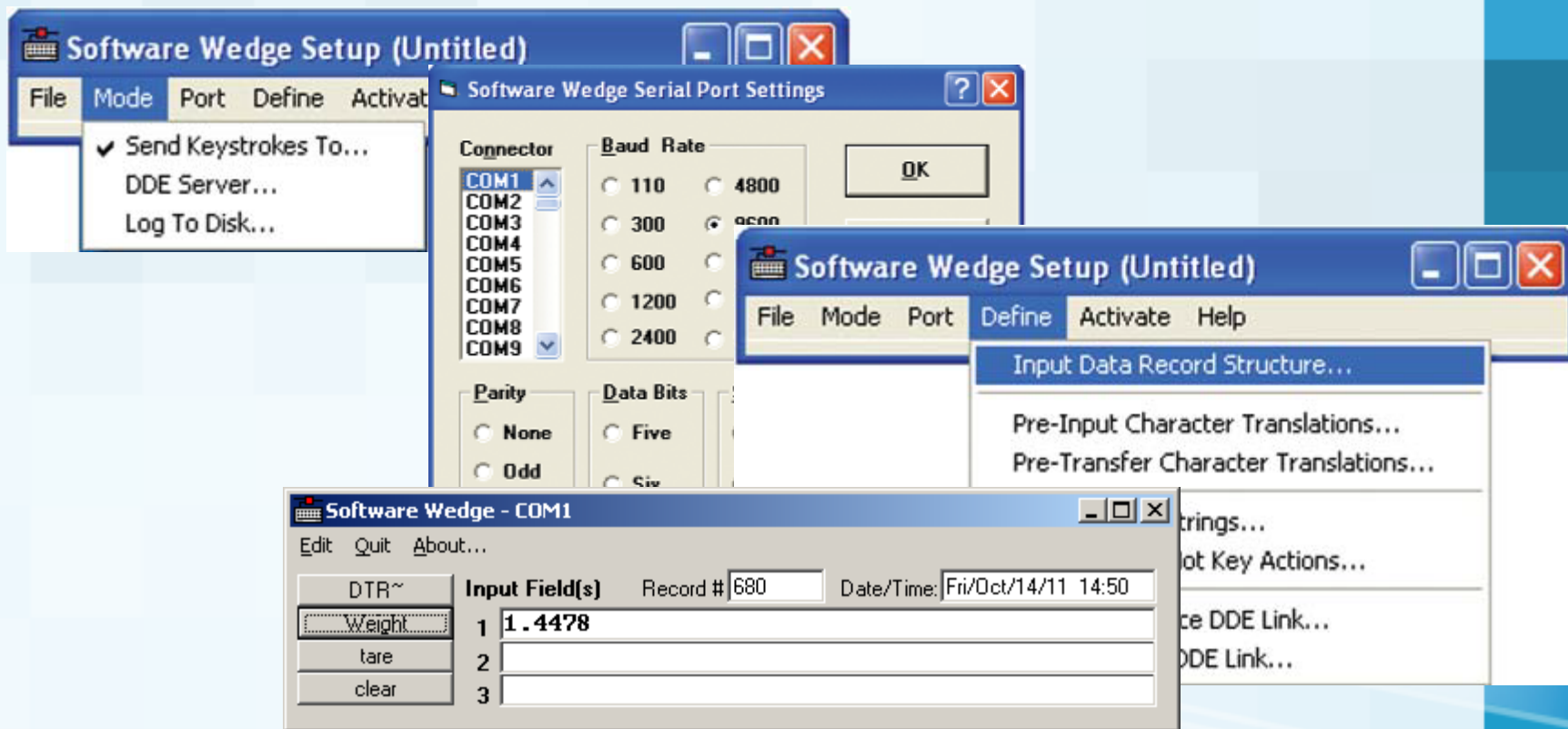
TABLE X1.1 *Continued*

# (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

Microsoft Excel spreadsheet showing BOD data. The spreadsheet includes a security warning and a data table with columns A through W and rows 20 through 41.

	A	B	C	D	E	F	G	H	I	J	N	R	S	T	U	V	W
20	QC	1120700-BLK1	418	Blank					1	300	0.880					mg/l	
21	QC	1120700-5-BLK1	36	Seeded Blank		0.000	X	1	1.5	0.830						mg/l	20
22	QC	1120700-5-BLK2	1382	Seeded Blank		0.000	X	1	1.5	0.830						mg/l	20
23	QC	1120700-5-BLK3	422	Seeded Blank		0.000 <i>(Duplicate test of 1)</i>	X	1	1.5	0.830						mg/l	20
24	QC	Discarded Row8	827	Glucose Glucose			X	1	6	0.850						mg/l	5
25	QC	Discarded Row9	502	Glucose Glucose			X	1	6	0.860						mg/l	5
26	QC	Discarded Row10	1085	Glucose Glucose			X	1	6	0.850						mg/l	5
27	QC	1120700-5Row1	92	Seed Control				1	8.5	0.720						mg/l	5
28	QC	1120700-5Row2	202	Seed Control				1	8.5	0.630				Average		mg/l	3
29	QC	1120700-5Row3	235	Seed Control				1	14	0.480						mg/l	2
30	I		7	BCX: Influent	1 pt/c	7/0/22.2		1	6	0.820						mg/l	5
31	I		96	1142703	1 CO			1	9	0.790						mg/l	3
32	I		66		2 pt/c			1	12	0.740						mg/l	2
33	I				1 CO			1								mg/l	
34	I				(blank)			1								mg/l	
35	QC		1034	Duplicate #1	1 pt/c	7/0/22.2		1	6							mg/l	5
36	QC		108	1120700	1 CO			1	9							mg/l	3
37	QC		571	1142703.01	1 pt/c			1	12							mg/l	2
38	QC				1 CO			1								mg/l	
39	QC				(blank)			1								mg/l	
40	I		50	BCX: DC 1 & 2	1 pt/c	7/0/21.4		1	9							mg/l	3
41	I		742	1142703	1 CO			1	12							mg/l	2

ViewSonic

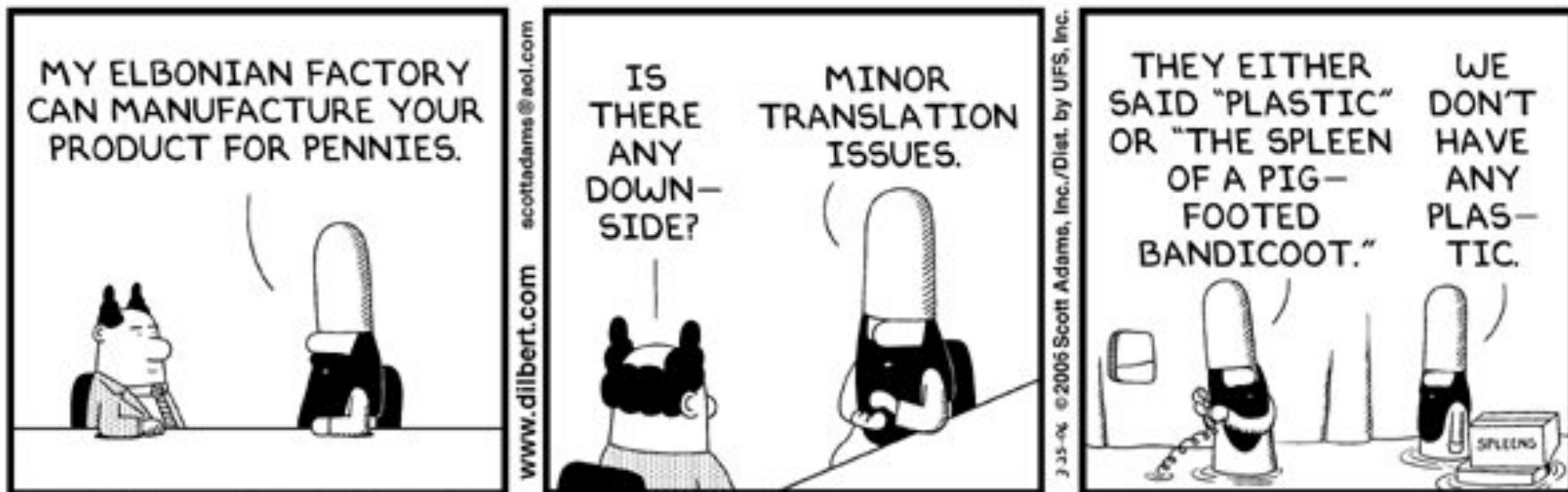
# Interfacing Assumption

All instruments “speak the same language”



# Integration

## Instrument – LIMS Translator



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- 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 3<sup>rd</sup> 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%,"",,""
"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%,"",,""
"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%,"",,""
"4","Tray03","4","SeedBlank","1436308-SdB1k","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%,"",,""
"5","Tray03","5","SeedBlank","1436308-SdB1k","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%,"",,""
"6","Tray03","6","SeedBlank","1436308-SdB1k","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%,"",,""
"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%,"",,""
"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%,"",,""
"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%,"",,""
"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%,"",,""
"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%,"",,""
"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%,"",,""
"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% 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","3.8499999","165","",46%,"",,""
"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%,"",,""
"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% 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% 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%,"",,""
"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% 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%,"",,""
"21","Tray04","5","Sample","1453010-03","12","1","0","8.37","19.5","12/29/2014 12:32:40 PM","3.57","20","1/3/2015 7:38:51 AM","5.8","145","",60%,"",,""
```

# 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 :','Imacias'  
'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

**DataTool - Main**

File View Tools Help

Element Data Entry Table

File Name

...ments\ShimadzuTOCDToolFile.xls

Samples (21)	Analysis
1112217-BLK1	Carbon Total Organi ▲
1112217-BS1	Carbon Total Organi
1112217-BSD1	Carbon Total Organi
1112217-CCB1	Carbon Total Organi
1112217-CCB2	Carbon Total Organi
1112217-CCB3	Carbon Total Organi
1112217-CCV1	Carbon Total Organi
1112217-CCV2	Carbon Total Organi
1112217-CCV3	Carbon Total Organi ▼

Instrument Data Files

Last Selected File

z:\36\_Data\36\_Instruments

Samples (21)	File Name
1112217-CCV1	ShimadzuTOCDToC ▲
1112217-CCB1	ShimadzuTOCDToC
1112217-BLK1	ShimadzuTOCDToC
1112214-BS1	ShimadzuTOCDToC
1112214-BSD1	ShimadzuTOCDToC
1116073-01	ShimadzuTOCDToC
1112217-MS1	ShimadzuTOCDToC
1112217-MSD1	ShimadzuTOCDToC
1116076-01	ShimadzuTOCDToC ▼

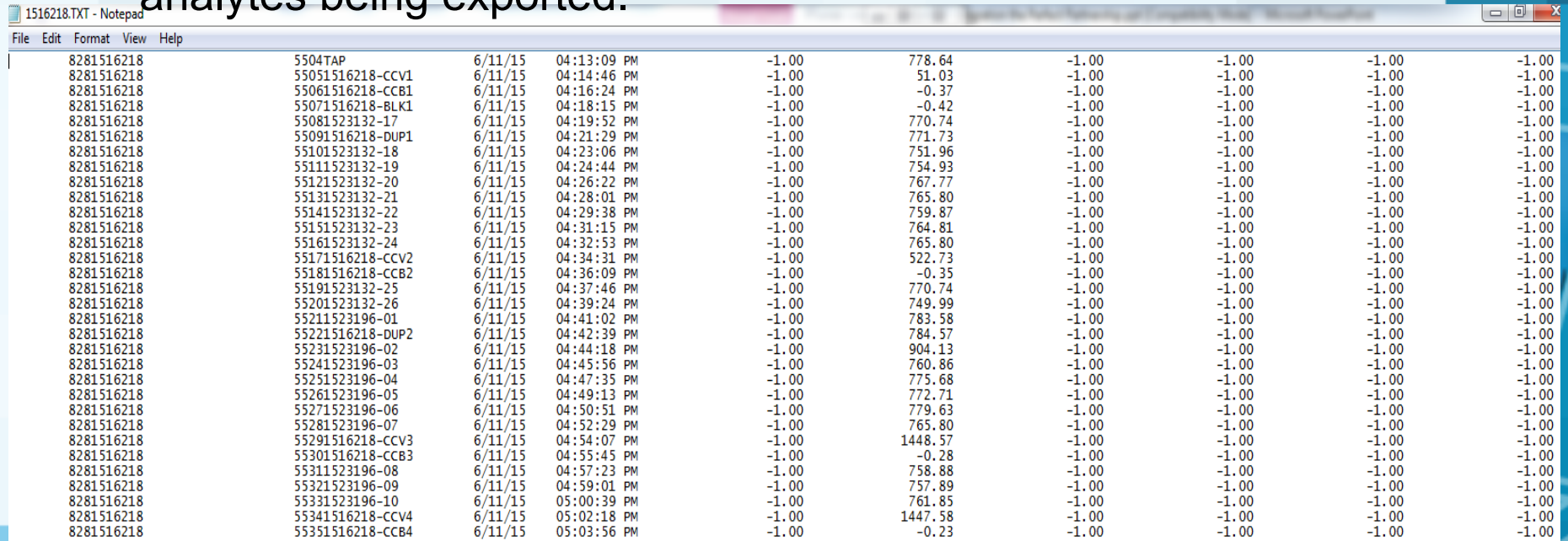
Take dilution factor from:

Misc. Info Field  Multiplier Field

DataTool 3.590.592 USING: \\ntlmsq01\element\database\XDataTool\_Inorganics.mdb

# 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

ID	Sample ID	Date	Time	Value 1	Value 2	Value 3	Value 4	Value 5	Value 6	Value 7
8281516218	5504TAP	6/11/15	04:13:09 PM	-1.00	778.64	-1.00	-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	-1.00
8281516218	55061516218-CCB1	6/11/15	04:16:24 PM	-1.00	-0.37	-1.00	-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	-1.00
8281516218	55081523132-17	6/11/15	04:19:52 PM	-1.00	770.74	-1.00	-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	-1.00
8281516218	55101523132-18	6/11/15	04:23:06 PM	-1.00	751.96	-1.00	-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	-1.00
8281516218	55121523132-20	6/11/15	04:26:22 PM	-1.00	767.77	-1.00	-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	-1.00
8281516218	55141523132-22	6/11/15	04:29:38 PM	-1.00	759.87	-1.00	-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	-1.00
8281516218	55161523132-24	6/11/15	04:32:53 PM	-1.00	765.80	-1.00	-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	-1.00
8281516218	55181516218-CCB2	6/11/15	04:36:09 PM	-1.00	-0.35	-1.00	-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	-1.00
8281516218	55201523132-26	6/11/15	04:39:24 PM	-1.00	749.99	-1.00	-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	-1.00
8281516218	55221516218-DUP2	6/11/15	04:42:39 PM	-1.00	784.57	-1.00	-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	-1.00
8281516218	55241523196-03	6/11/15	04:45:56 PM	-1.00	760.86	-1.00	-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	-1.00
8281516218	55261523196-05	6/11/15	04:49:13 PM	-1.00	772.71	-1.00	-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	-1.00
8281516218	55281523196-07	6/11/15	04:52:29 PM	-1.00	765.80	-1.00	-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	-1.00
8281516218	55301516218-CCB3	6/11/15	04:55:45 PM	-1.00	-0.28	-1.00	-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	-1.00
8281516218	55321523196-09	6/11/15	04:59:01 PM	-1.00	757.89	-1.00	-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	-1.00
8281516218	55341516218-CCV4	6/11/15	05:02:18 PM	-1.00	1447.58	-1.00	-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	-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

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