

The source for news and tips of interest to users of MSC-LIMS, an affordable laboratory information management system for small labs.

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Welcome

Welcome to **MSC-LIMS** *Insights*.

This newsletter will help current MSC-LIMS users get the most out of their software, and will complement the product literature and demo that prospective users can find on our web site at <u>www.msc-lims.com</u>.



Join our mailing list for more information. Sign up at <u>www.msc-lims.com/lims/maillist.html</u>.

This newsletter is for and about MSC-LIMS users. We welcome your comments, and your suggestions for topics you would like to see addressed in upcoming issues. Please send your thoughts to <u>newsletter@msc-lims.com</u>.

MSC-LIMS and SQL Server

As we announced in the <u>previous issue</u> of this newsletter we are currently developing MSC-LIMS version 5.0 for SQL Server. MSC-LIMS 5.0 replaces the earlier Access back end database with a SQL Server database for improved reliability, scalability, and security.

While many MSC-LIMS sites with large databases welcome the move to a SQL Server database, we understand that others may have questions. In this and future newsletters we will address some of these questions.

What are the benefits with SQL Server?

Reliability. SQL Server databases are not subject to corruption that may occur with an Access database in a multi-user installation due to bad network connections or workstation crashes. SQL Server databases can be restored up to the point of failure, whereas an Access database can only be restored to its last backup.

Scalability. The number of LIMS users and the size of the database can increase significantly without the performance degradation encountered with an Access database.

Security. SQL Server databases are inherently more secure than an Access database. MSC-LIMS 5.0 will use SQL Server's Windows authentication so once logged on to Windows you can start MSC-LIMS without any additional login.

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From the Developer

Since we announced the upcoming SQL Server version of MSC-LIMS in the <u>previous issue</u> of *MSC-LIMS Insights*, development has proceeded and we recently delivered an early version to one customer for testing.

If you have a large MSC-LIMS database, many users or could otherwise benefit from a SQL Server version and would like to test the early version, please let us know. We hope to have a couple more sites testing the early SQL Server version later this year. See "MSC-LIMS and SQL Server" in this issue for more information.

As always, please let us know if you have any comments, questions, or concerns about MSC-LIMS or our long term plans. We always welcome your thoughts.

in Cell

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How to Query Completed, Unreported, and Unapproved Batches

If yours is a commercial lab you likely work primarily with sample batches in MSC-LIMS. You log samples by batch, even for single-sample batches. You report results by batch so that one final report has results for all samples in a single batch. And you generate invoices by sample batch.

When you rely on sample batches in MSC-LIMS, you will find it helpful to query samples by batch status. This article shows you how to query completed, completed and unreported, and unapproved batches.

All queries in MSC-LIMS query samples. For example, when you perform a query with a batch number criterion, you are asking the LIMS to find all samples with that batch number or all samples in the batch. The result of your query is still a list of samples. When you need to query batches with specific criteria such as completed batches, remember that the results of the query will still be a list of samples in batches matching your criteria. That may be confusing so let's look at a few examples.

Completed Batches

To query completed samples we only need to enable the Completed option on the Additional tab of the query controls. However, to find completed batches where all samples in the batch are complete requires a subquery or nested query using a Structured Query Language (SQL) expression. A subquery produces a set of data that can be used as part of a query criterion.

Without checking each individual analysis in the sample, we can find a completed sample simply by looking for a non-blank completed date since the LIMS automatically detects when all analyses have a result and adds the completed date. With a subquery we can generate a set of batch numbers for completed batches by finding batches where the number of sample IDs in the batch is equal to the number of nonblank completed dates in the batch. We can then find samples within completed batches by finding samples with a batch number in the set of batch numbers produced by the subquery.

To query completed batches first add the following SQL expression to the SQL Expressions screen on the Setup menu.

Name: Completed Batches

SQL: Batch IN (SELECT Batch FROM Sample GROUP BY Batch HAVING Count(SampleID) = Count(CompletedDate))

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You can now use the Completed Batches expression as a criterion anywhere you query samples by selecting the expression from the pick list on the SQL tab of the query controls. And you can combine the expression with any other criteria. For example, if you want to find all batches completed for customer ABC Company received this month, select the customer, enter the received date range, and select the Completed Batches SQL expression.

Completed Unreported Batches

If you are using the System Configuration screen option that automatically sets sample reported dates, you can extend our previous example and find completed and unreported batches with two subqueries. Just as in our previous example, the first subquery generates a set of batch numbers for completed batches. The second subquery generates a set of batch numbers where the number of samples in the batch is different than the number of non-blank reported dates in the batch to reveal unreported batches. The intersection of the sets resulting from these two subgueries is a list of batches that are both completed and unreported. To query samples in completed unreported batches add the following expression to the SQL Expressions screen then select the expression on the SOL tab of the query controls.

Name: Completed Unreported Batches

SQL: Batch IN (SELECT Batch FROM Sample GROUP BY Batch HAVING Count(SampleID) = Count(CompletedDate)) AND Batch IN (SELECT Batch FROM Sample GROUP BY Batch HAVING Count(SampleID) <> Count(ReportedDate))

Unapproved Batches

If you are using sample approval in MSC-LIMS, you can find unapproved samples by simply selecting the Unapproved option on the Additional tab of the query controls. In an unapproved sample, the only incomplete analysis is the defined "Approval" analyte. Therefore, an unapproved batch is a batch where all samples in the batch are unapproved. Multiple subqueries are also required to find unapproved batches. The first subquery finds samples having only one incomplete analysis. The second subquery finds samples with an incomplete "Approval" analyte. The intersection of the sets produced by these two queries yields a list of unapproved samples. If the count of unapproved samples in a batch is equal to the total number of samples in the batch then the batch is unapproved. To query samples in unapproved batches add the following expression to the SQL Expressions screen then select the expression on the SQL tab of the query controls.

Name: Unapproved Batches

SQL: Batch IN (SELECT Batch FROM Sample WHERE Batch IS NOT NULL AND ((Sample.SampleID IN (SELECT SampleID FROM SampleAnalysis WHERE AnalysisResult IS NULL AND ResultTypeID IS NULL GROUP BY SampleID HAVING Count(AnalysisID) = 1)) AND (Sample.SampleID IN (SELECT SampleID FROM SampleAnalysis WHERE AnalysisID=999 AND AnalysisResult IS NULL AND ResultTypeID IS NULL))) GROUP BY Batch HAVING Count(SampleID) = (SELECT Count(SampleID) FROM Sample AS S2 WHERE S2.Batch = Sample.Batch))

Replace 999 in the expression above with the internal AnalysisID for your "Approval" analyte. To find the AnalysisID open any sample query dialog and select the Unapproved check box on the Additional tab, click Query, then select the SQL tab and find 'WHERE AnalysisID=n' in the 'SQL for last query' field. Replace 999 with n.

Like any sample query, a query using one of the above SQL expressions produces a list of samples. You can get a list of just the batch numbers by exporting to Excel. Export a Sample Summary report of the queried samples to the generic MSC-LIMS Export Template, delete all but the Batch column then use the Remove Duplicates option on the Data tab.

Using Excel's Formula Evaluator

The example Excel export templates installed with MSC-LIMS use formulas to display LIMS data on a report worksheet. Some of the formulas may be lengthy and difficult to comprehend. If you need to modify one of these formulas, wonder why your formula results in an error, or just want to understand how the formula works, Excel's formula evaluator is a handy tool.

Understanding how a lengthy formula calculates the final result can be difficult because of nested functions and logical tests. In Excel 2010 or newer, the formula evaluator solves a formula one step at a time allowing you to see how the formula is calculated.

Let's take a look at an example. If you export a Sample Summary report to the Final Report Example template, you will find this formula to display the result for the first analyte in the first sample in cell N25:

```
=IF(ISBLANK(INDEX(AnalysisResultFormatted,
ROW() - ROW(OneAnalysisResults) + 1)),
"",INDEX(AnalysisResultFormatted, ROW() -
ROW(OneAnalysisResults) + 1))
```

With cell N25 selected, select Evaluate Formula in the Formula Auditing group on the Formulas tab.



Use the Evaluate button to view the value of the underlined portion of the formula. The result will appear in italics.

Evaluate Formula	
Report!\$N\$25	Evaluation: = IF(ISBLANK(INDEX(<i>AnalysisData!\$W\$2:\$W\$14</i> , <u>ROW()</u> - ROW (OneAnalysisResults) + 1)), ",INDEX(AnalysisResultFormatted, ROW() - ROW(OneAnalysisResults) + 1))
To show the result of the appears italicized.	underlined expression, dick Evaluate. The most recent result Evaluate Step In Step Out Gose

Continue clicking the Evaluate button to view each underlined step in the formula's calculation and its italicized result. If there is a result for the first analyte in the first sample (i.e. cell N25 is not blank) the final evaluation step in the formula will appear as shown below.

Evaluate Formula		? ×
Reference: Report!\$N\$25	E <u>va</u> luation: = IF(FALSE, #N/A, <i>AnalysisData1\$W\$2</i>)	*
To show the result of the appears italicized.	ne underlined expression, dick Evaluate. The most recent result	<u>C</u> lose

After fully evaluating the original lengthy formula, we can see the formula has been reduced to a simple IF function in the form IF(condition, result_if_true, result_if_false). Since cell W2 on the AnalysisData sheet does have a value (i.e. there is a result for the first sample's first analyte), the result of the nested ISBLANK function as the condition portion of the IF function is FALSE. Therefore, the result of the IF function is the value in cell W2 on the AnalysisData sheet.

Whether you are developing a complex formula or just trying to understand an existing formula, use Excel's formula evaluator to visually break the formula down to a series of simple calculation steps. Add this tool to your Excel arsenal and you will quickly understand and troubleshoot daunting formulas.

MSC-LIMS and SQL Server

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Integration. While integrating LIMS data with external applications has always been possible, some will find it easier to integrate with SQL Server databases.

What are the tradeoffs with SQL Server?

Installing SQL Server, backing up and maintaining a SQL Server database, and managing Windows login accounts are tasks that require more thought and planning than equivalent procedures with an Access database.

When will MSC-LIMS 5.0 be available?

An early version of MSC-LIMS for SQL Server is currently installed for testing at one site. We expect additional sites to begin testing the early version later this year. The official release of MSC-LIMS 5.0 will likely occur during the second half of 2018.

Notes from Technical Support

Result High and Low Warning Flags

A user recently asked:

Could you please tell me why when a spec is listed as 11-11.4 and a result is 11.4, LIMS gives an 'H' warning for the result?

The 'H' for high is appearing because the result value is at or above the warning maximum value specified for the analyte in the sample's project. Review the specifications in the Projects setup screen and set the Warning Max field to a value slightly above 11.4 (e.g. 11.40001). Note that the Report Specs field is simply text that allows you to specify an acceptable result for a final report. 'H'igh and 'L'ow flags are appended by comparing the result value to the warning maximum and minimum values.

You can view a sample analysis' specifications by double-clicking the Result Value field (or right-click and choose Result Specifications) in either results entry screen. Specifications are copied to the sample at login from the sample's project. Correcting a project's specifications will affect all future samples. If the analysis does not yet have a result you can correct a sample's analysis specifications using the Update Min/Max button on the Analyses setup screen. See "Understanding Analysis Specifications" in <u>MSC-LIMS</u> Insights No. 22 for more information.

Will there be additional costs for MSC-LIMS 5.0?

Although we have not finalized the price list for version 5.0, we do expect an increase in the cost for Annual Subscriptions. The cost for Annual Maintenance for Full System licensees is also expected to increase. Migrating an existing MSC-LIMS database to SQL Server requires a full copy of Microsoft Access and other utilities from Microsoft. For those who do not have Microsoft Access or prefer assistance, we will offer one-time database migration for an additional fee. Full System licensees with customized systems will also incur a nominal one-time fee to reapply their customizations.

Do I have to upgrade to MSC-LIMS 5.0?

No. While there will be no additional development to MSC-LIMS 4.x, we will continue to support it and you can continue to run version 4.x.

Add an Analysis to Many Projects

A user updating projects asked:

If I wanted to add an analysis to all existing projects, how would I do that? Or do I have to go in to each individual one and make changes?

You do have to add the analysis to each individual project but there are some editing techniques that can help. Open the Projects setup screen, switch to edit mode then click the View All button. Add the analysis to the first project, click or tab off the new analysis record then click the record selector (the box at the far left of the record) and use Ctrl+C to copy. Move to the next project using the project record selectors at the bottom left of the screen or click in the project name field and use Page Down. Click the asterisk new record selector at the bottom of the list of analyses and use Ctrl+V to paste the copied analysis.

Graph a Single Analyte

A user recently asked:

How can I graph a single analyte in the LIMS or in Excel?

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Use the Analyte Comparison report on the Samples menu to create a quick trend graph for a single analyte. In the Analyte Comparison Setup screen, select the single analyte, enter your sample query criteria, enable the "Include Graph(s)" option, click the Query button, then click the Preview button to view the report. The graph will appear below the tabular data on the report's last page.

If you prefer to create your own graph in Excel, export the Analyte Comparison report (with or without the graph) to the generic MSC-LIMS Export Template and the selected analyte's results will be found in worksheet column C labeled "1" for the report's first analyte.

Accessing Excel's Name Manager

A user modifying an Excel export template recently asked:

We need to go to cell B6 and navigate to Insert | Name | Define then select OneSampleResults and extend the column reference range. In Excel 2016 I can't find Insert | Name | Define. Can you direct me?

Although Insert | Name | Define no longer exists on the ribbon in newer versions of Excel, you can still use its keystroke shortcut Alt+I, N, D to open the Name

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Manager. Alternatively, you will find the Name Manager on the Formulas tab of the ribbon. Note that if you insert a column anywhere within the existing OneSampleResults named range, Excel will automatically expand the named range. You can also change the OneSampleResults range to include more columns (e.g. \$A\$4:\$Z\$4) than currently used so you don't have to remember to change it each time you add a new column.

Significant Figure Rounding in Excel

A user developing an Excel final report template with calculations asked:

Is there a way to round columns to 2 significant figures?

Yes, you can round to any number of significant digits in Excel with this generic formula:

=ROUND(number,digits-(1+INT(LOG10(ABS(number)))))

Where 'number' is the value to round and 'digits' is the number of significant digits. To round the value in cell B5 to two significant figures, for example, use this formula in another cell:

=ROUND(B5,2-(1+INT(LOG10(ABS(B5)))))

This section of *MSC-LIMS Insights* is devoted to current users of MSC-LIMS. Here we briefly introduce only the most recent additions to MSC-LIMS.com Customers Only pages. Use your login name and password to log on to the Customers Only section of our website.

File Library

Final Report - N Samples per Page.xlt

This new example Excel final report template includes a sample header preceding each sample's results with a Settings sheet option to specify the number of samples on each page. See the template's Read Me sheet for details.

Contact Us

Questions, comments, suggestions? Reach us at:



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