

SPECIFICATIONS

Introduction: LABWORKS enables the user to store and use specifications to monitor sample values against textual specifications and numerical specifications. When a specification is exceeded, LABWORKS will flag that result accordingly. LABWORKS also provides the user with the ability to create custom specifications to be used in reporting of sample values that are NOT evaluated when a specification is exceeded. These custom specifications most often used in custom reports. All specifications can be preserved with the sample data for future review and reporting.

Specification Evaluation

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The choice to use/ignore specifications is made at the location code and sample level. When configuring a location code, there is a check box for: Use Specifications (DB: LOCLIST.DOSPEC)

	Options User Field	s Analysis Order	Comments Specifications Specifications	cial Info		
cation						
ocation co	de		Modified by: USR	Last n	nodified: 2/2/	2011 6:16:01 PM
DEFAULT						
ocation de	escription				-	
DEFAULT						
Project acc	ount code					
MW						
-			-			
	samples		Spe	cial into form		1
Validat	e samples		ICH	ECKBOX		Browse
Check	specifications					
	specifications					
Disk co	py final report					
Disk co	py final report					
Disk co	py final report		Location Code Definit	tion Owner	ř	
Disk co ming Hold days	py final report		Location Code Definit	tion Owner	ľ	
Disk co ming Hold days 0	py final report		Location Code Definit	tion Owner		P12345678 ¥
Disk co ming Hold days 0 Due date b	py final report		Location Code Definit	ion Owner	GROUPGRC	▼ UP12345678 ▼
Disk co ming Hold days 0 Due date b Collecti	py final report ase option on date		Location Code Definit Sam Location Code / Sample Re	tion Owner ple Owner ead Owner	GROUPGRC	♥ UP 12345678 ♥ UP 12345678 ♥
Disk co ming Hold days Due date b Collecti C Submitt	py final report ase option on date tal date		Location Code Definit Sam Location Code / Sample Re	tion Owner Iple Owner ead Owner	GROUPGRC	▼ UP 12345678 ▼ UP 12345678 ▼
Disk co ming Hold days 0 Due date b © Collecti © Submiti	py final report		Location Code Definit Sam Location Code / Sample Re	tion Owner ple Owner ead Owner	GROUPGRC	▼ UP 12345678 ▼ UP 12345678 ▼
Disk co ming Hold days 0 Due date b Collecti C Submit	py final report ase option on date tal date		Location Code Definit Sam Location Code / Sample Re	tion Owner ple Owner tad Owner	GROUPGRC	♥ UP 12345678 ♥ UP 12345678 ♥
Disk co ming Hold days 0 Due date b © Collecti © Submit	py final report		Location Code Definit Sam Location Code / Sample Re	ion Owner Iple Owner 2ad Owner	GROUPGRC	♥ UP12345678 ♥ UP12345678 ♥

Then as each sample is created, Check Specifications becomes a property of the sample. It can be modified or confirmed using Modify Sample. (DB: SAMPLE.DOSPEC)



Sample AA00109 (1 of 1	l)					
Status: Analyses pending Any completed analyses: NC Comments entered: NO Current sample objects: 0			Save	Cancel Exit		
Field Name	Previous entry	Modified	entry			
Location code	DEFAULT	DEFAULT				
Collection date	03/16/2011	03/16/201	1			
Collection time	00:00	00:00				
Submittal date	03/16/2011	03/16/201	1			
Submittal Time	23:15	20110		1		
Do specification checking	Yes	🔽 Do spe	cification checking			
Sample header info	Sample comments	Sample special info	Analysis order	Setup header editing		
Make modifications to sample header fields						

Note: When a location code definition is updated, samples previously logged in are not altered. So a change in the location code won't affect existing samples.

Specification Hierarchy

LABWORKS implements a hierarchy to apply specifications at the most specific level possible. The levels are:

Analysis Code – Most Generic

Location Code – Sample point or Product specific

Sample – Location Code/Analysis code specifications persisted with the sample – Configuration Required

When evaluating specifications, LABWORKS first checks for Sample specific specifications. If there are no sample specs, then LABWORKS checks for Location Code specifications. If no location code specifications are present, then Analysis level specifications are used.

Specification Setup

Setting up Analysis Code specifications is done using the analysis list maintenance program. The Specifications table is used to enter the specification values. Upper and Lower warnings and limits are numeric values. Target is a text value.

When comparing warnings and limits, LABWORKS reports an out of spec when the value is:

Greater than for upper limits, or Less than for lower limits.



Example:

With Upper specification 100, if the value is 99 then no violation is reported. If the value is 100 then no violation is reported. If the value is > 100 then a violation is reported.

Add/Edit Analysis	al Info Result Source	_D×
General specifications		
Analyte:	DEFAULT	
Upper specification	100	
Upper warning		
Target		
Lower warning		
Lower specification	10	
DEFAULT	A	pply Go Cancel

For Target values, it compares the strings, checking the Target specification is found in the value:

If the result is "POSITIVE" then a violation is reported. If the value is "NEGATIVE" no violation is reported. If the value is "NEGATIVE-1" then no violation is reported.



Add/Edit Analysis	rial Tafe Densit Source	
Analysis Aspecifications Calculation Spe General specifications Analyte: Upper specification Upper warning	Test to demonstrate Target	
Target Lower warning Lower specification	NEGATIVE	
TARGET_TEST	Apply OK Cancel	





Location Code Specifications

Specifications at the location code level are created using the Location List maintenance program. To

add specifications at the location code level, first add the analysis to the Analysis Order tab.

Create/Modify Location Code							
Location code Options User Fields Analysis Order Comments Specifications Special Info							
Default analysis order							
	Anl Code	Analysis Name	Hold Days				
1	DEFAULT	DEFAULT	0	0			
2	TARGET_TEST	Test to demonstrate Target	0	0			
3			0	0			
4			0	0			
5			0	0			
6			0	0			
7			0	0			
8			0	0			
9			0	0			
10			0	0			
11			0	0			
12			0	0			
13			0	0			
14			0	0			
15			0	0			
16			0	0			
17			0	0			
19	1						
•							
2	WELL02	Apply	ОК	Cancel			

Then switch to the Specifications tab and press Build analyte list.

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Create/Modify Location Code						_ [] >	
Analysis specifications							
Anl Code	Analyte Name	Lower Spec	Lower Warn	Target	Upper Warn	Upper Spec	<u> </u>
DEFAULT	DEFAULT	5	10		20	25	
TARGET_TEST	Test to demonst			ABSENT			
							-
	_						
	_						-
Build analyte list Clear List Load specs Merge specs							
WELL02					Apply	ОК	Cancel

These specifications are then saved at the location code level.

Sample Level Specifications

To use sample level specifications, the login process must be configured to save the specifications with the sample.

Versions 6.2.230+

To configure persisting specifications with the sample add the following entry to LABWORKS.INI

[Windows_Multi_Sample_Login]

USE_PERSISTENT_SPECS = YES

[Windows_Single_Sample_Login]

USE_PERSISTENT_SPECS = YES

Versions before 6.2.230

Configure the program SampSpecLogin6.exe to run as a post login program.



IABWORKS Login Settings		X
	Login Settings and User Programs	
Receipts None Royting Sheets None	Labels C Standard Labels C Custom Labels C User Program C Bartender Labels	User Programs 1 [5: Program Files (x86) PerkinEr 2
Work Sheets	्य	Include Default User Program

The program is SampSpecLogin6.exe

🏠 User Program Options		×
	Set User Program Options	
<u>R</u> un Style:	Maximized with focus	<u>ο</u> κ
Run <u>T</u> ype:	After all samples	Cancel
Password:	PW:Password	
Command Line	NOEDIT	
Wait for pro	gram to end before continuing.	
Send Database	🦳 Send Log Batch	
🔲 Send Sample ID	✓ Send Initials	
Send Sample List File		

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Entering Results and Specification Evaluation.

Specifications are evaluated during results entry. When a user enters a result, the value is checked using the specifications.

Result Entry:								_ [] >
Enter key action C None	: 💽 Right	C I)own]		Print	Save	Cancel
User Info DEFAULT TARGET_TEST	Sample ID result result	AA00111 22 ABSENT						
		Ent	er, load, or i	nodify results	for sample an	alyses		





Detailed Edit

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Results Entry Sample: AA0011	1 Analysis: DEFAU	LT DEFAULT	×
Sample ID Location description	AA00111	Location code: WELL02	Standard results
Method reference: Units	New Method Refer		<u>A</u> udit Trail
MYSAMPNC MYUSER 2	100 2		History
Current objects: Validated	0 No		Display SOP
			Analysis Comment
Result	22	Qualifier	Sample Comments
Secondary result		Dilution factor	Analysis Spec Info
Raw result:			Analysis Objects
- Analysis data:		Result Specifications:	Validate
Due date 0 Start date	3/17/2011 00:00 3/17/2011	Upper specification 25 Upper warning 20	
End date	3/17/2011	Target Lower warning 10	Save
End time (Analyst initials	00:03 🔹	Lower specification 5	Gancel

Note: Detailed edit puts the result into edit mode. If not configured to use Sample Specifications, and the Location Code or Analysis Code specifications have changed, displaying detail edit may evaluate a violation based on the new values that didn't previously exist.

Effective Specifications

Because of the specification hierarchy there is only one level of specifications active. And the complete set of specifications from the level is used. (Data in table may be different from previous screenshots.)

Example: Without Sample Specs

Analysis Code	Specification Type	Analysis Code Spec	Location Code	Effective Spec
DEFAULT	Lower Spec	10	5	5
DEFAULT	Lower Warning		10	10
DEFAULT	Target			
DEFAULT	Upper Warning		20	20
DEFAULT	Upper Spec	100	25	25
TARGET_TEST	Lower Spec			
TARGET_TEST	Lower Warning			
TARGET_TEST	Target	NEGATIVE	ABSENT	ABSENT
TARGET_TEST	Upper Warning			
TARGET_TEST	Upper Spec			

Example: With Sample Specs

Analysis Code	Specification	Analysis Code	Location Code	Sample	Effective Spec
	Туре	Spec		Spec	
DEFAULT	Lower Spec	10	5	6	6
DEFAULT	Lower Warning		10	10	10
DEFAULT	Target				
DEFAULT	Upper Warning		20	21	21
DEFAULT	Upper Spec	100	25	24	24
TARGET_TEST	Lower Spec				
TARGET_TEST	Lower Warning				
TARGET_TEST	Target	NEGATIVE	ABSENT	NEGATIVE	NEGATIVE
TARGET_TEST	Upper Warning				
TARGET_TEST	Upper Spec				



Exporting and Reporting Specifications

Specifications can be reported and exported. Add the export fields to Export/Report format.

Available export fields:	Fields se	lected for expor	t:		
Sample special info value 39	 Field Na 	me	Fld Width	Exp Width 🔺	
Sample special info value 40	Sample	ID	7	7	
Sample special info value 41	Sample	Description	60	60	
Sample special info value 42	Analysis		24	24	
Sample special info value 43	Analysis	COUE	24	24	
Sample special into value 44	Analysis	Name	40	40	
Sample special into value 45	Combina	ation result	14	14	
Sample special info value 47	Lower v	varning limit	14	14	
Sample special info value 48	Lower s	pecification	14	14	
Sample special info value 49	Target	value	14	14	
Sample special info value 50	langer	vereine lieste	14		
Sample status	opper v	varning limit	14	14	
Secondary result	upper s	pecification	14	14	
Special info form					
Submit date					4
Submit time					_
Text result					
Validation date					
Validation time					
Validation user					
Violation code					
violation Date					
violation une					
Violation user					
violauori value					

When a violation is reported the VIOLTYPE and VIOLVALUE are saved with the result.

RESULT.VIOLVALUE is the value of the specification that was violated.

RESULT.VIOLTYPE is the type of violation.

Violation Type	VIOLTYPE Value		
0	No Violation		
1	Lower Spec		
2	Lower Warning		
3	Target		
4	Upper Warning		
5	Upper Spec		



User Defined Specifications:

In addition to standard specifications, user defined entries can be added. As of Version 6.2, they are display only, no evaluation exists.

Version 6.2+

The SpecMaster table defines all of the specification types supported in the system, their UI descriptions, the relationship used for evaluating exceptions, and the severity level of those exceptions.

Example

SpecMaster table rows defining "standard" and "user defined" spec types. The custom specs in this example are *MYSPEC1 and MYSPEC2*

•	LSPEC	GTE	Lower specification	20	н	1
	LWARN	GTE	Lower warning	90	м	2
	TARGET	ISCONTAINED	Target	30	н	3
	USPEC	LTE	Upper specification	10	н	5
	UWARN	LTE	Upper warning	80	м	4
	MYSPEC1	DISPLAY	User Specification	100	N	6
	MYSPEC2	DISPLAY	User Specificatio	110	N	7

All custom specifications must be SPECTYPE = DISPLAY.

Add/Edit Analysis Add/Edit Analysis Add → Add/Edit Analysis Add →		
Analysis ASpecifications Calculation Sp	ecial Info Result Source	
General specifications		
Analyte:	Amt Spikede for Chemical Oxygen Demand	
Upper specification	10	
Upper warning	8	
Target	MyTarget	
Lower warning	4	
Lower specification	2	
Custom Specs:		
MYSPEC 1	6	
MYSPEC2	6.2	
A_COD	Apply OK Cancel	

Version 6.1 and previous



User defined specifications are added by modifying the columns in the RLTSPECS table. A new column is added for each user defined spec. Maximum width is 255 characters.

1	LASSHLRL1040dbo.RLTSPECS*								
	Column Name	Data Type	Allow Nulls						
P	LOCCODE	varchar(24)							
8	ACODE	varchar(24)							
8	ANLNAME	varchar(40)							
	LSPEC	varchar(14)	✓						
	LWARN	varchar(14)	✓						
	TARGET	varchar(14)	✓						
	UWARN	varchar(14)	✓						
	USPEC	varchar(14)	\checkmark						
	MODDATE	datetime							
	MODUSER	varchar(12)							
	hSec	int							
	MYSPEC1	varchar(14)							
►	MYSPEC2	varchar(14)							

Note: The Migration Utility converts records from RLTSPEC to SPECMASTER and RESULTSPECS when converting to 6.2

After the update and SysMgr key is turned on, logging into LABWORKS 6.2 and checking the maintenance programs should display the new SpecMaster specifications ready for use. Users shouldn't notice any difference in the User Interface of the application.



Reporting Custom Specs

Defined custom specification fields can be included in the export format in the same method as standard specification fields.

xport Fields Export Options					
Available export fields: Export date Instrument assigned Instrument result filespec Invoice date Invoice format Invoice number Invoicing Address 1 (BAD 1) Invoicing Address 2 (BAD 2) Invoicing Address 3 (BAD 3) Invoicing Address 4 (BAD 4) Invoicing Address 4 (BAD 4) Invoicing Address 4 (BAD 4) Invoicing Address 4 (BAD 5) Location Code (LCOD) Login Batch (LBAT) Login User MYSAMPNO (USO1) MYUSER2 (USO2) Noninvoicable Number rep copies Number cesuit Project Account Code (PROJ) Projected price Projected price Project Account Code (PORD) Qualifer Raw result	 Fields selected for expor Field Name Sample ID Sample Description Analysis code Analysis Name Combination result Lower specification Target value Upper specification MYSPEC1 (XSO1) MYSPEC2 (XSO2)	tt Fid Width 7 60 24 40 14 14 14 14 14 14 14 14 14 255 255	Exp Width 7 60 24 40 14 14 14 14 14 14 14 255 255	•	



LABWORKS.INI Entries

Store persistent specifications for samples.

[Windows_Multi_Sample_Login] USE_PERSISTENT_SPECS = YES

[Windows_Single_Sample_Login] USE_PERSISTENT_SPECS = YES

SYSMGR Entries

SYSMGROPT	SYSMGRVAL	SYSMGRLVAL	SYSMGRBVAL	SYSFIELDTYPE
SAMP_SPEC_SOURCE	<see below=""></see>			IT

Valid Entries

NULL/Record doesn't exist	Sample Specification are not evaluated
SAMP_SPEC_TABLE	Sample Specification are evaluated
SAMP_SPEC_TABLE_ONLY	Sample Specification are evaluated – No
	Analysis or Location Code specs



Database Storage of Specifications in Version 6.2

SpecMaster Table

LABWORKS 6.2 introduces two new database tables for specifications, SpecMaster and ResultSpecs.

In order to use the new specification tables, you need to add the USE_62_PLATFORM SysMgr key and turn it ON (setting the value to TRUE or -1).

	SYSMGROPT	SYSMGRVAL	SYSMGRLVAL	SYSMGRBVAL	SYSFIELDTYPE
•	USE_62_PLATFORM		0	-1	IB

ResultSpecs Table

Table ResultSpecs will store all entered specifications, including analyte general specifications, location specifications for analytes, and sample specifications (persisted) for analytes.

Example Records:

Analysis Code. Each specification has a corresponding record in the RESULTSPECS table.

ANALYSIS	ANALYSIS	LSPEC	A_COD	Amt Spikede for	INDVALUE	2	NULL	NULL
ANALYSIS	ANALYSIS	LWARN	A_COD	Amt Spikede for	INDVALUE	4	NULL	NULL
ANALYSIS	ANALYSIS	MYSPEC1	A_COD	Amt Spikede for	INDVALUE	NULL	NULL	6
ANALYSIS	ANALYSIS	MYSPEC2	A_COD	Amt Spikede for	INDVALUE	NULL	NULL	6.2
ANALYSIS	ANALYSIS	TARGET	A_COD	Amt Spikede for	INDVALUE	NULL	NULL	MyTarget
ANALYSIS	ANALYSIS	USPEC	A_COD	Amt Spikede for	INDVALUE	10	NULL	NULL
ANALYSIS	ANALYSIS	UWARN	A_COD	Amt Spikede for	INDVALUE	8	NULL	NULL

Location Code. Each specification has a corresponding record in the RESULTSPECS table.

LOCATION	DEFAULT	LSPEC	DEFAULT	DEFAULT	INDVALUE	1	NULL	NULL
LOCATION	DEFAULT	LWARN	DEFAULT	DEFAULT	INDVALUE	2	NULL	NULL
LOCATION	DEFAULT	USPEC	DEFAULT	DEFAULT	INDVALUE	20	NULL	NULL
LOCATION	DEFAULT	UWARN	DEFAULT	DEFAULT	INDVALUE	10	NULL	NULL
LOCATION	WELL02	LSPEC	DEFAULT	DEFAULT	INDVALUE	5	NULL	NULL
LOCATION	WELL02	LWARN	DEFAULT	DEFAULT	INDVALUE	10	NULL	NULL
LOCATION	WELL02	USPEC	DEFAULT	DEFAULT	INDVALUE	25	NULL	NULL
LOCATION	WELL02	UWARN	DEFAULT	DEFAULT	INDVALUE	20	NULL	NULL

QLABWORKS

Supplemental Documentation

Sample Specifications. Each sample/specification has a record in RESULTSPECS

	SAMPLE	AA00106	LSPEC	A_COD	Amt Spikede for	INDVALUE	2	NULL	NULL	
	SAMPLE	AA00106	LWARN	A_COD	Amt Spikede for	INDVALUE	4	NULL	NULL	
	SAMPLE	AA00106	MYSPEC1	A_COD	Amt Spikede for	INDVALUE	NULL	NULL	6	;
	SAMPLE	AA00106	MYSPEC2	A_COD	Amt Spikede for	INDVALUE	NULL	NULL	6.2	1
	SAMPLE	AA00106	TARGET	A_COD	Amt Spikede for	INDVALUE	NULL	NULL	MyTarget	
	SAMPLE	AA00106	USPEC	A_COD	Amt Spikede for	INDVALUE	10	NULL	NULL	;
	SAMPLE	AA00106	UWARN	A_COD	Amt Spikede for	INDVALUE	8	NULL	NULL	1

6.0

In LABWORKS version prior to 6.2 specifications were stored in the RLTSPECS Table.

Analysis Code. Each specification has a corresponding record in the RLTSPECS table. Location code = "&GENERAL"

&GENERAL	\$AREA_AN	Bromide	11300000		13900000	
&GENERAL	\$AREA_AN	Chloride	27000000		35000000	
 &GENERAL	\$AREA_AN	Nitrate as N-NO3	7000000		9000000	

Location Code. Each specification has a corresponding record in the RLTSPECS table.

INF_COMP	\$AN	Phosphate as P			10	
INF_COMP	\$AN	Sulfate			60	
INF_COMP	COD	COD	100			1500
INF_COMP	NH3	NH3	1			50
 INF_COMP	NH3	NH3	1			50

Sample Specifications. Each sample/specification has a record in RLTSPECS

AE52111	BOD	BOD			5000	
AE52111	COD	COD			8500	
AE52111	EC	EC			5000	

Questions/Configuration to review.

Does the sample have specification checking turned on?

Are sample specs being saved?

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Are SYSMGR entries correct for sample spec evaluation?

Are user defined specs "DISPLAY" type?