IMPLEMENTATION OF A LABORATORY INFORMATION MANAGEMENT SYSTEM (LIMS) TO MANAGE GENOMIC SAMPLES

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Submitted to the faculty of the School of Informatics
in partial fulfillment of the requirements
for the degree of
Master of Science in Laboratory Informatics,
Indiana University

May 2012

Accepted by the Faculty of Indiana University,
in partial fulfillment of the requirements for the degree of Master of Science
in Laboratory Informatics

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Dedicated to Keri, Jack, and Ava

Your love and support made this possible

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ACKNOWLEDGEMENTS

I would like to thank the faculty and staff at the School of Informatics at Indiana University Purdue University at Indianapolis for their support during my time in the Laboratory Informatics Graduate program.

I would like to thank Dr. Mahesh Merchant for being my academic advisor and serving as my thesis committee chair. I would also like to thank Dr. Narayanan Perumal and Joseph Turpin for serving on my thesis committee. Their support and patience was critical in helping complete this project.

I would like to thank LabWare for supplying software and licensing. I would also like to thank the many LabWare consultants who supported my work and answered my many questions for this project.

ABSTRACT

Derick Witty

IMPLEMENTATION OF A LABORATORY INFORMATION MANAGEMENT SYSTEM (LIMS) TO MANAGE GENOMIC SAMPLES

A Laboratory Information Management Systems (LIMS) is designed to manage laboratory processes and data. It has the ability to extend the core functionality of the LIMS through configuration tools and add-on modules to support the implementation of complex laboratory workflows. The purpose of this project is to demonstrate how laboratory data and processes from a complex workflow can be implemented using a LIMS.

Genomic samples have become an important part of the drug development process due to advances in molecular testing technology. This technology evaluates genomic material for disease markers and provides efficient, cost-effective, and accurate results for a growing number of clinical indications. The preparation of the genomic samples for evaluation requires a complex laboratory process called the precision aliquotting workflow. The precision aliquotting workflow processes genomic samples into precisely created aliquots for analysis. The workflow is defined by a set of aliquotting scheme attributes that are executed based on scheme specific rules logic. The aliquotting scheme defines the attributes of each aliquot based on the achieved sample recovery of the genomic sample. The scheme rules logic executes the creation of the aliquots based on the scheme definitions.

LabWare LIMS is a Windows® based open architecture system that manages laboratory data and workflow processes. A LabWare LIMS model was developed to implement the precision aliquotting workflow using a combination of core functionality and configured code.

CHAPTER ONE: INTRODUCTION AND BACKGROUND

Introduction

Laboratory processes are driven by the ability to manage, access, and analyze the data generated in the laboratory. As laboratory evaluation and measurement technologies have evolved, laboratories are creating, analyzing, and storing an increasing amount of laboratory data. Historically, laboratories have created custom in-house systems to manage their laboratory data and workflows. Software developers would evaluate the critical laboratory processes and then formulate customized code to build a system that automated those processes. These in-house systems were typically rigid and made process changes or system upgrades difficult and time-consuming to implement due to the customization and complexity of the code. A staff of developers with a critical skill set had to be retained to maintain and support the system. A customized system can be designed to meet the functional requirements of a laboratory, but typically do not allow for system enhancements as laboratory processes evolve (Bradburn, n.d.).

Due to the limitations of the custom in-house systems, laboratories began adopting commercial of the shelf (COTS) systems like the Laboratory Information Management System (LIMS) for managing their laboratory data and workflows. The core functionality of a LIMS is to support common laboratory workflow processes. Laboratory processes outside of this core functionality are also supported through user interfaces with configuration tools that allow for the enhancement of the LIMS to manage these specialized processes *(Off-the-shelf Integration for Labs*, 2006). A LIMS is built on an open architecture platform where additional functionality supported from the manufacturer can also be added. These enhancements are added as functional modules or software updates that can be imported into the LIMS (*LabWare Technical Manual*, 2009). The configuration tools and functional module imports are designed in a way that a laboratory user without technical development skills can mange the laboratory process changes and system upgrades of a LIMS. A key advantage of using the LIMS model is that the design supports the immediate laboratory functionality, but also allows for flexibility to manage future functional needs of the laboratory (Bradburn, n.d.).

A LIMS is an ideal solution for managing complex laboratory workflows such as the genomic sample precision aliquotting workflow. The precision aliquotting workflow processes samples into precisely created aliquots based on the recovery of the genomic material. Genomic samples have become an important part of the drug development process due to advances in molecular testing technology (Sanders, 2011). This technology is based on the ability to evaluate genomic samples in the form of isolated DNA and RNA for efficient, cost-effective, and accurate results for a growing number of clinical indications. An increasing number of pharmaceutical companies are collecting and storing genomic samples from every patient enrolled in every clinical trial ("Molecular Testing", 2009). These genomic samples are processed into aliquot containers where they are evaluated using an existing molecular testing procedure, or stored indefinitely for future use as more analytical tools become available. The specificity of the molecular testing requires critical care in the preparation of the genomic samples. The potential downstream applications require a large variety of aliquot outputs from the genomic samples. The content of each genomic sample aliquot output is defined by a highly customizable aliquotting scheme and determined by the recovered sample concentration. The aliquotting scheme is pre-defined for each sample and is dependent upon the intended use of the genomic sample. The aliquotting scheme defines the output attributes for each aliquot based on the sample recovery and determines the creation of aliquots into a variety of volumes and sample concentrations. The precision aliquotting workflow is the process of preparing the genomic samples for the creation of specific aliquots as determined by the aliquotting scheme.

The precision aliquotting workflow is a complex laboratory workflow that requires accurate preparation of the genomic samples to support the molecular testing applications. Management of the precision aliquotting workflow by a LIMS would greatly benefit the efficiency and effectiveness of the workflow for a laboratory. The purpose of this project is to demonstrate how the management of genomic samples within a laboratory using the precision aliquotting workflow can be implemented into a LIMS.

Background

The processing of genomic samples for the preparation of aliquots at a clinical laboratory is a multi-step process. Parent genomic samples are logged into the system, processed, and then genomic sample aliquots are output. An example of a genomic sample precision aliquotting workflow is summarized in Figure 1.

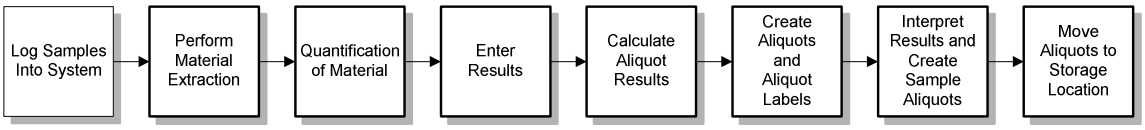


Figure 1: Precision Aliquotting Workflow

For a typical clinical laboratory, the aliquotting scheme is pre-defined for each genomic sample linked to a clinical trial. For a given clinical trial, the intended use of the genomic samples is premeditated. A protocol document outlines the specific objectives of the clinical trial and details how each sample will be used to generate laboratory data. An aliquotting scheme is defined based on the expected use of the genomic sample aliquots. The pre-definition of the aliquotting scheme is important to ensure that the genomic samples are handled consistently during aliquot preparation.

The precision aliquotting workflow starts with the parent samples being received into the laboratory. The parent samples are typically whole blood or blood products that must first be processed to extract and purify the genomic material. The parent samples are logged into the system and linked to a clinical trial. This linkage will associate the genomic sample to the aliquotting scheme. The genomic material is extracted and purified from each parent sample using the defined extraction protocol. The extracted material is reconstituted in a volume of extraction protocol specific reagent and then evaluated on an instrument to measure the concentration and quality of the genomic sample. The measured parent sample concentration is the key result value for calculating the aliquotting scheme. All of the genomic sample results are calculated, reviewed for errors, and approved. Based on the achieved sample concentration and the aliquotting scheme attributes, the appropriate number of aliquots are created, and the expected content of each aliquot is calculated. Aliquot labels with specific aliquot information are created and applied to aliquot containers. Preparation of the aliquots is performed manually by interpreting the aliquot results and physically transferring the genomic material into the aliquot containers. Depending on the complexity of the aliquotting

scheme, the genomic material may require a dilution or adjustment before preparing the aliquots. The aliquots are ready for storage, downstream testing, or for transfer to another system.

The precision aliquotting workflow could be implemented into a laboratory in different ways. The aliquotting schemes are built upon a set of calculations that evaluate the achieved genomic sample concentration against the critical values of the scheme to create the aliquots. A laboratory could automate the aliquotting scheme calculations by using a basic spreadsheet program to execute the calculations that a user manually enters. This solution is limited because it would only automate the aliquotting scheme calculations and not support the other parts of the workflow. Users would have to use other tools to manage those parts of the workflow. From a manual handling perspective, a clinical trial could potentially generate thousands of genomic samples for processing. Managing large data sets within a spreadsheet is very labor intensive and easily prone to errors. Another limitation of this solution is that the spreadsheets that are used within a regulated environment, like a clinical laboratory, are typically required to be validated. The validation of these calculation spreadsheets can be difficult to document and time-consuming to perform depending on the spreadsheet design. The spreadsheet solution is not ideal because it would only support limited process automation and lack efficiency in managing a high throughput of samples.

Another strategy for managing the precision aliquotting workflow within a laboratory is to build a customized in-house laboratory system. These systems are typically built from the ground up using customized code to manage proprietary laboratory processes. The custom in-house solution could automate many parts of the workflow. The aliquotting schemes could be defined in the in-house system and automatically applied to the genomic samples to calculate the aliquot results. One of the major limitations of the in-house system is that it is built on highly-customized code. This requires a large amount of effort to develop and often lacks flexibility when having to adapt to changing laboratory processes (Bradburn, n.d.). The diversity of potential aliquotting schemes will require frequent system enhancements and updates. Modifications to in-house systems have to be performed by developers with a specialized

skill set. The in-house solution to manage the precision aliquotting workflow is limited by a lack of flexibility to handle process changes.

The ideal strategy for managing the precision aliquotting workflow is to implement the workflow into a COTS LIMS. The clinical trial industry can choose from a large number of LIMS products for managing laboratory workflows. Systems such as StarLIMS®, LabVantage Sapphire, Thermo Fisher Scientific Nautilus™, and LabWare LIMS are marketed as being total solutions for handling laboratory data and managing process efficiency within the regulated clinical laboratory environment. Their core functionality manages common laboratory processes such as sample handling, instrument interfaces, inventory, result reporting and many others. The core functionality provides a standardized starting point for configuring workflows. Additional functionality can be implemented by the user through the configuration tools or by adding component modules that are available as add-ons from the manufacturer. This is a distinct advantage over an in-house solution where a developer is required to modify customized code to add functionality. A LIMS is built on an open architecture platform where functionality can be extended through enhancement modules and software updates that can easily be imported.

A commercial LIMS has functionality that is built on time-tested industry best-practices. The combination of built-in core functionality with the availability of tools to configure processes and the availability of functional upgrades gives LIMS a distinct advantage over using spreadsheets or custom in-house systems. A LIMS supports a model of flexibility that can be updated as laboratory processes change. The suite of functionality built into a LIMS gives it the ability to manage complex workflows. The precision aliquotting workflow is a complex workflow that could be automated through the configuration of LIMS functionality. Implementation of a precision aliquotting workflow in LIMS would offer an opportunity to efficiently and effectively manage genomic samples in a laboratory.

CHAPTER TWO: METHODS

Development of the precision aliquotting workflow was performed in the base version of LabWare LIMS V6. LabWare LIMS is a Windows® based open architecture system that allows for complete configuration of clinical laboratory processes. It contains all of the components of a standard LIMS. LabWare's core platform supports most common laboratory-related functions (*LabWare Technical Manual*, 2009). It is designed to support user-defined configurations and customized code to meet the needs of the laboratory.

LabWare LIMS does provide out-of-box functionality to perform aliquotting, but it does not fully support the precision aliquotting process. LabWare has the ability to create aliquots automatically on sample events or manually from a menu option (*LabWare Technical Manual*, 2009). The Sample Login Template can be configured to automatically aliquot by setting the *Aliquot On* field to a sample event such as 'Sample Logged' or 'Sample Received'. An aliquot sample is created for each test logged to the parent sample. This functionality does not work with the precision aliquotting model. When the core functionality executes the sample event that creates the aliquots, the test results are not yet available to determine the number of aliquots that need to be created. For precision aliquotting, the number of aliquots that need to be created for each genomic sample is determined by the achieved concentration result.

LabWare LIMS also has the ability to create aliquots manually using the 'Aliquot' menu option found in Batch Manager, Folder Manager, or from the Main Menu (*LabWare Technical Manual*, 2009). When the 'Aliquot' function is accessed, LabWare displays a dialog prompting the user to select the tests to move to a new aliquot sample. A screenshot of the out-of-box aliquotting window is displayed in Figure 2.

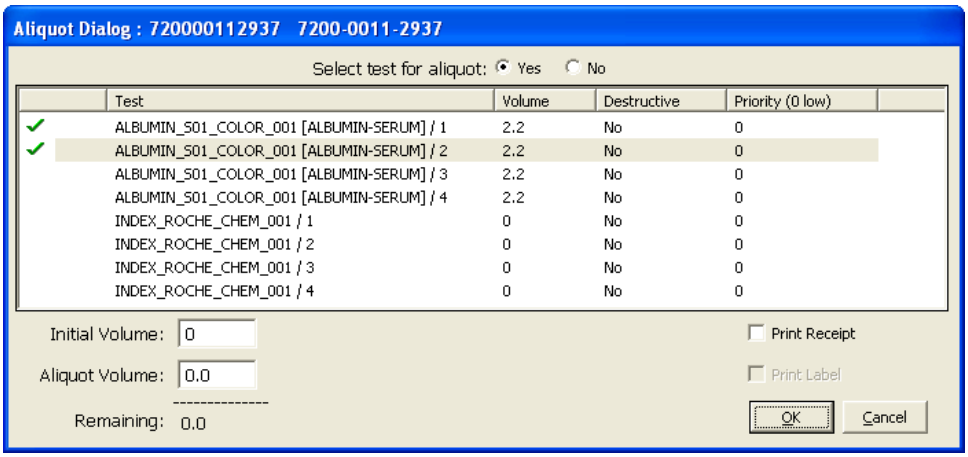


Figure 2: LabWare Core Aliquot Interface

Because the LabWare core functionality does not fully support the precision aliquotting workflow, a custom solution would have to be developed. The precision aliquotting workflow will be implemented in LabWare LIMS using a combination of base functionality and custom code.

The configuration and customization performed in LabWare LIMS to implement the precision aliquotting workflow will support the ability of a user to create and organize genomic samples, define aliquotting scheme attributes, define rules to execute schemes, create aliquot labels, and display aliquotting instructions. Sample Login Templates are configured to manage the creation of samples within LabWare. The templates are configured to allow a user to link specific information such as clinical trial protocol, the aliquotting scheme, and testing methods. Batch Manager will be used to group samples together for processing within a single user interface. It is linked to all of the major workflow functionality in LabWare such as result entry, result review, and label printing. Batch Manager will also be customized to display reports that can display results and processing instructions. The Parent Child Record Editor (PCRE) is a user interface that will be configured to link parent and child tables together. This interface will be used to manage the aliquotting scheme details into a set of parent and child tables. The Rules Manager is an interface that allows a user to configure logic driven rules to process inputs and perform actions (Rules Engine, 2007). This interface will be used to define the rules scheme logic that executes the aliquotting scheme definitions and creates the aliquots.

LabWare Configuration

Installation of LabWare LIMS was performed according to the V6 Installation Manual. LabWare issued a temporary license file and the software has been used in accordance with the user agreement. The data used in LabWare LIMS was managed using a Microsoft Access® database.

LabWare LIMS is built on an open architecture. Periodic updates, enhancements, and maintenance fixes are available for download from LabWare.com for a user with sufficient privileges. The table in Appendix A contains the list of module upgrades that were added to the base LabWare V6 version to enhance the functionality of this model.

Static and dynamic objects were created and configured for the development of the precision aliquotting workflow. A list of the database objects created in the configuration of this model is in Appendix B. LabWare LIMS uses a plugin for Crystal Reports that allows reports generated in Crystal Reports to be called and rendered within LabWare screens. LabWare provided a temporary license for access to Crystal Reports 2008® and it was used for all reports created in this model. A summary of the enhanced functionality for configuring the precision aliquotting model follows in this section.

The term genomic sample refers to large set of sample types commonly processed in a clinical laboratory. One of the most common is double stranded DNA. In the context of this model, the configuration of the precision aliquotting workflow will be based on the genomic sample type of purified DNA.

Analysis

LabWare defines a test as the analysis definition. The analysis definitions are configured for each test on the ANALYSIS table. Two analyses were created for this model: DNA_EXTACT_001 and DNA_ALIQUOT.

The DNA_EXTACT_001 Analysis is the test that is added to each DNA Parent Sample. It is linked to a *Common Name* of 'DNA_PARENT' and an *Analysis Type* of 'NUCLEIC_ACID'. An Analysis is linked to a result through the COMPONENT table. This table defines the result, units, decimal places, and any component calculations for a result. DNA_EXTACT_001 is made up of the results that are important for measuring the quantity and quality of the DNA purified from the parent sample. The *A260* and

A280 components capture the measured absorbance of the sample from a spectrophotometer. The *Concentration* component is a calculated result based on the achieved A260 value multiplied by the Beers-Lambert Constant for double stranded DNA (dsDNA) of 50. The concentration is used as the critical value for determining the aliquotting scheme. The *Purity* component is a calculated component that determines the quality of the recovered sample. The parent sample purity is calculated by A260/A280. A summary of the components are displayed in Table 1.

Component	**Type**	**Unit**	**Decimal**	**Calculation**
A260	Numeric	-	3 dp	-
A280	Numeric	-	3 dp	-
Concentration	Calculation	µg/mL	1 dp	A260 * 50
Purity	Calculation	mL	3 dp	A260/A280

Table 1: Components for DNA_EXTACT_001

The DNA_ALIQUOT Analysis is added to each aliquot created from the aliquotting scheme. It has a *Common Name* of 'DNA' and an *Analysis Type* of 'NUCLEIC_ACID'. It is made up of three components. The result for each component is set based on the achieved parent sample concentration and the aliquotting scheme definitions. The *DNA Concentration* component contains the calculated aliquot sample concentration. The *DNA Volume* component contains the volume of the aliquot sample. The *DNA Yield* component is the weight of DNA in the aliquot sample. A summary of the components is displayed in Table 2.

Component	**Type**	**Unit**	**Decimal**	**Calculation**
DNA Concentration	Numeric	µg/mL	1 dp	-
DNA Volume	Numeric	mL	3 dp	-
DNA Yield	Numeric	µg	1 dp	-

Table 2: Components for DNA_ALIQUOT

Aliquotting Scheme Tool

The aliquotting scheme tool is managed in LabWare LIMS using PCRE. The aliquotting scheme will be defined on a custom table with fields that capture the scheme attributes. An aliquotting scheme is subcategorized into a scheme type. An aliquotting scheme can be a simple scheme type or a complex scheme type. Simple schemes split the genomic sample into equal aliquots. A complex scheme will direct a user to create

specific aliquots at specific concentrations, volumes, and yields. The complex scheme will have calculations to handle every possible outcome. Example workflows of the simple and complex schemes are displayed in Figure 3.

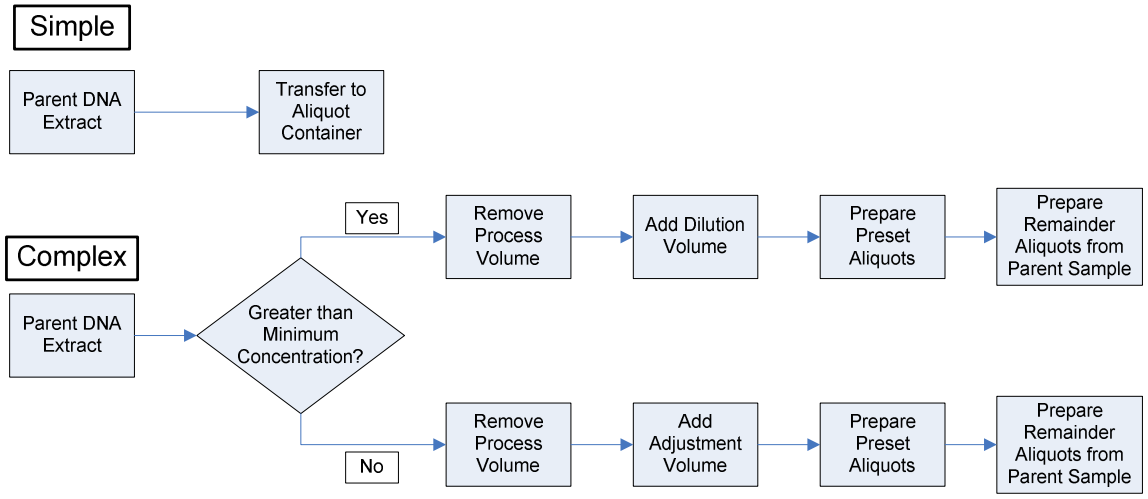


Figure 3: DNA Aliquot Scheme Type

The primary table is the *Aliquot Scheme* table (Database Table: X_ALIQUOT_SCHEME). This table contains the scheme level information. Through PCRE, tables *Scheme Aliquots*, *Aliquot Instruction Steps*, and *Label Design* are linked as child tables. Table *Scheme Aliquots* (Database Table: X_ALQT_INSTRUCTION) contains the individual aliquot level definitions. Table *Aliquot Instruction Steps* (Database Table: X_ALQT_INSTR_STEPS) stores the definitions for the aliquot instructions. Table *Label Design* (Database Table: X_ALIQUOT_LABEL_DISPLAY) contains the information for defining the Aliquot Labels.

Aliquot Scheme Table

The *Aliquot Scheme* parent table allows a user to define the scheme level parameters that drive the precision aliquotting definition. The table design is displayed in Figure 4.

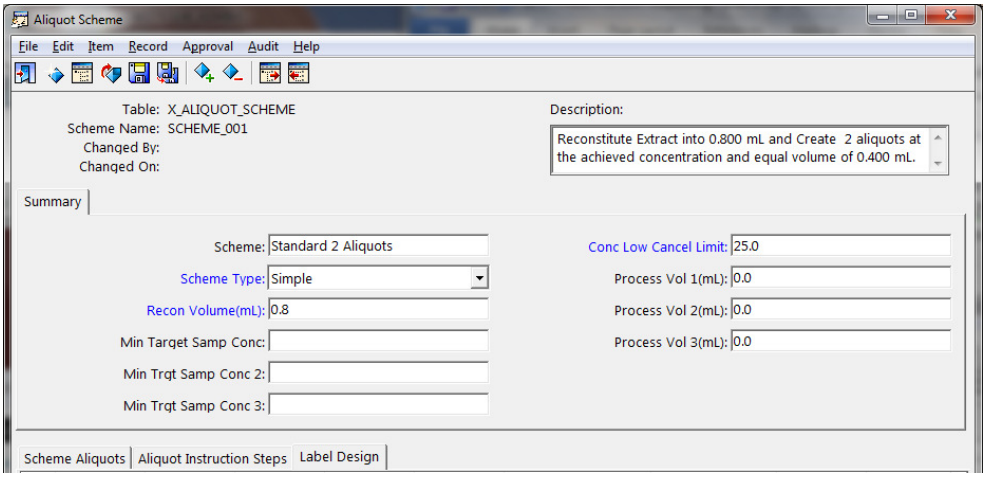


Figure 4: Aliquot Scheme Table

The *Scheme Name* field is the key field for a unique scheme name. LabWare recommends using a consistent nomenclature for identifying each scheme. The simple nomenclature used in this model is 'Scheme_001'.

The *Description* field contains the text that describes the intent of the aliquotting scheme.

The *Scheme* field contains the short descriptive name of the scheme.

The *Scheme Type* field is a mandatory field and is linked to list X_SCHEME_TYPE and identifies the scheme as 'Simple' or 'Complex'. This field is mandatory and drives the execution or the scheme rules.

The *Recon Volume (mL)* field is a mandatory field and contains the reconcentration sample volume. This is the volume of parent DNA sample that is available after extraction for precision aliquotting. This field is mandatory and is used in many of the aliquot calculations.

The *Min Target Samp Conc*, *Min Trgt Samp Conc 2*, and *Min Trgt Samp Conc 3* fields store the critical concentration values that determine the intervals of how the achieved sample concentration will calculate the DNA sample results. For simple schemes, the fields can be set to null. For complex schemes, at a minimum, the *Min Target Samp Conc* field should be defined. A user can define how the scheme rules are executed based on the definitions of the target concentration fields.

The *Conc Low Cancel Limit* field is a mandatory field and stores the minimum acceptable sample concentration for a DNA sample. The user can define rules to cancel or reject tests based on an achieved sample concentration result that exceeds this limit.

The *Process Vol 1(mL), Process Vol 2(mL), Process Vol 3(mL)* fields store processing volumes. The processing volume is a volume of sample that is removed from the parent sample and typically adjusted or diluted to create preset aliquots. Only a complex aliquot scheme will have a process volume defined.

Scheme Aliquots Table

The *Scheme Aliquots* table facilitates the definition of each aliquot. A user can define the concentration, volume, and yield of any aliquot that will be created. The aliquotting scheme is made up of a number of aliquots. A subset of the total aliquots can be defined by an aliquot group. A user can define the number of aliquots to be associated with each aliquot group. The aliquot group is associated through Rules Manager with a concentration target range defined on the *Aliquot Scheme* table. The achieved concentration is evaluated by the scheme rules logic and the creation of aliquots is executed according to the definition of the *Scheme Aliquots* table. The table is displayed in Figure 5.

Scheme Aliquots | Aliquot Instruction Steps | Label Design

	Aliquot Name	Aliquot Group	Group Order	Aliquot Type	Concentration(ug/mL)	Volume(mL)	Yield(ug)
1	Alqt A1	Target Schen	1.00000	Preset 1	200.0	0.100	20.0
2	Alqt A2	Target Schen	2.00000	Preset 1	200.0	0.100	20.0
3	Alqt A3	Target Schen	3.00000	Preset 1	200.0	0.100	20.0
4	Alqt A	Target Schen	4.00000	Remainder	Original Concentration	0.200	Calculate
5	Alqt B	Target Schen	5.00000	Remainder	Original Concentration	0.200	Calculate
6	Alqt C	Target Schen	6.00000	Remainder	Original Concentration	0.200	Calculate
7	Alqt A1	Alt 1 Scheme	1.00000	Preset 1	Original Concentration	Calculate	20.0
8	Alqt A2	Alt 1 Scheme	2.00000	Preset 1	Original Concentration	Calculate	20.0
9	Alqt A3	Alt 1 Scheme	3.00000	Preset 1	Original Concentration	Calculate	20.0
10	Alqt A	Alt 1 Scheme	4.00000	Remainder	Original Concentration	Equal Remaining Volume	Equal Remaining Yield
11	Alqt B	Alt 1 Scheme	5.00000	Remainder	Original Concentration	Equal Remaining Volume	Equal Remaining Yield
12	Alqt C	Alt 1 Scheme	6.00000	Remainder	Original Concentration	Equal Remaining Volume	Equal Remaining Yield
13	Alqt A1	Alt 2 Scheme	1.00000	Remainder	Original Concentration	0.900	Calculate

Figure 5: Scheme Aliquots Table

The *Aliquot Name* field is a free text field that allows a user to define the name of the aliquot. During aliquot creation, the aliquot name is set on the SAMPLE.X_ALQT_NAME field.

The *Aliquot Group* field is a list field linked to List X_ALQT_GROUP. A user defines the aliquot group for a set of aliquots that should get processed together in the same way. The grouping of aliquots is linked to the target concentration fields on the *Aliquot Scheme* table.

The *Group Order* field is an integer field that sets the order that the aliquots will be created. It is configured by the user.

The *Aliquot Type* field is a list field that links to List X_ALIQUOT_TYPE. It links the defined aliquot to a processing volume field on the *Aliquot Scheme* table. For example, the list entry 'Preset_1' links to the *Process Vol 1* field.

The *Concentration(ug/mL)*, *Volume(mL)*, and *Yield(ug)* fields are list fields that are linked to List X_ALQT_ACTION, but allow free-text entry. The fields relate directly to the components on DNA Aliquot Analysis 'DNA_ALIQUOT'. The user has the abilty to enter a concentration, volume, or yield target value for each aliquot. The list entries include settings for 'Calculate', 'Original Concentration', 'Equal Remaining Yield', and 'Equal Remaining Volume'. Execution of the scheme rules evaluates these field defintions to set the results on each aliquot. In order to accurately set the scheme aliquots details, a user will have to have a good working knowledge of the aliquotting scheme before being able to accurately define the fields in this table.

Aliquot Instruction Steps

The *Aliquot Instruction Steps* table allows a user to define the specific instructions for preparing the aliquots. These are displayed through a user interface to provide the step by step instructions on how to prepare the aliquots. This table works in conjunction with the *Aliquotting Steps* table (Database Table: X_ALIQUOTTING_STEPS) and the *Aliquot Step Variable* table (Database Table: X_ALQT_STEP_VARBLS). Both tables contian the static data that drive the creation and display of the aliquotting instructions. These two tables can be configured in the Table Explorer. The table is displayed in Figure 6.

Scheme Aliquots | Aliquot Instruction Steps | Label Design

	Step Num	Alqt Group	Alqt Name	Alqt Step	Alqt Step Desc
1	1.00000	Target Schen		RECON_SAMPL	Reconstitute extract in |RECON_VOLUME| mL of Diluent.
2	2.00000	Target Schen		PROCESS_VOL1	Remove |PROCESS_VOLUME1| mL of Parent Sample and transfer to a Processing Tube.
3	3.00000	Target Schen		ADD_VOLUME	Add |ADD_VOLUME| mL of Diluent to the Processing Tube and mix.
4	4.00000	Target Schen	Alqt A1	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
5	5.00000	Target Schen	Alqt A2	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
6	6.00000	Target Schen	Alqt A3	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
7	7.00000	Target Schen	Alqt A	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
8	8.00000	Target Schen	Alqt B	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
9	9.00000	Target Schen	Alqt C	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
10	1.00000	Alt 1 Scheme		RECON_SAMPL	Reconstitute extract in |RECON_VOLUME| mL of Diluent.
11	2.00000	Alt 1 Scheme		PROCESS_VOL1	Remove |PROCESS_VOLUME1| mL of Parent Sample and transfer to a Processing Tube.
12	3.00000	Alt 1 Scheme		ADJUST_VOLU	Add |ADJUST_VOLUME| mL of Parent Sample to the Processing Tube and mix.
13	4.00000	Alt 1 Scheme	Alqt A1	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
14	5.00000	Alt 1 Scheme	Alqt A2	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
15	6.00000	Alt 1 Scheme	Alqt A3	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
16	7.00000	Alt 1 Scheme	Alqt A	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
17	8.00000	Alt 1 Scheme	Alqt B	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
18	9.00000	Alt 1 Scheme	Alqt C	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
19	1.00000	Alt 2 Scheme		RECON_SAMPL	Reconstitute extract in |RECON_VOLUME| mL of Diluent.
20	2.00000	Alt 2 Scheme	Alqt A1	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.

Figure 6: Aliquotting Instruction Steps table.

The *Step Num* field is a numeric field that detemines the order the instruction step should appear on the user interface. The user can manually configure the order of the steps.

The *Alqt Group* field is a list field that links to List X_ALQT_GROUP. This field links the set of aliquotting steps to an aliquot group and corresponds to the aliquot group on the *Scheme Aliquots* table. Each aliquot group should have a set of aliquot instructions defined..

The *Alqt Name* field is a formula list field that returns a listing of the user created alqt names created on the *Scheme Aliquots* table. The field links the aliquot step to a particular aliquot from the aliquot group. This allows the aliquot specific name to be passed into the instruction step for selection by the user.

The *Alqt Step* field links to the aliquotting steps table (Database Table: X_ALIQUOTTING_STEPS). This table contains the user created aliquotting steps that will get displayed in the user interface. A screenshot of the table is displayed in Figure 7.

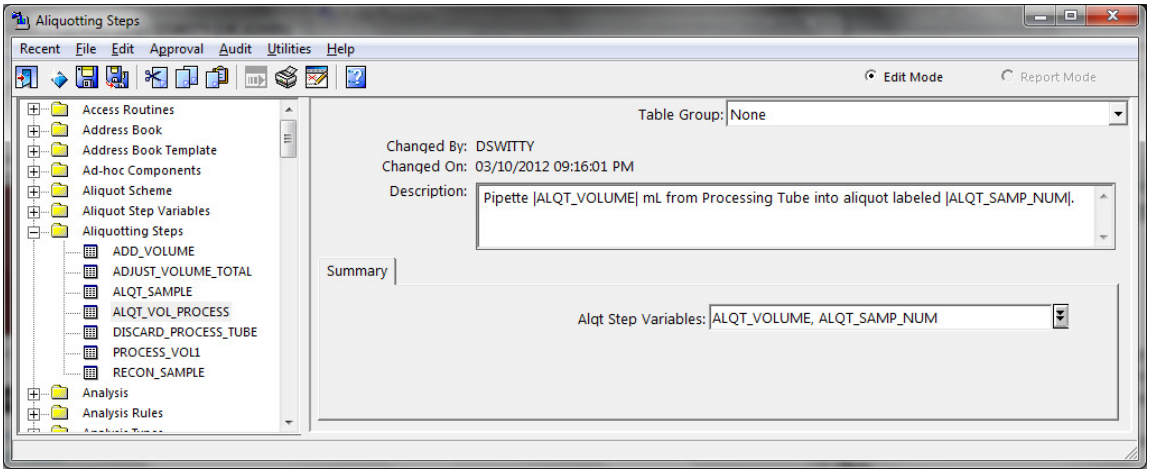


Figure 7: Aliquotting Steps Table

The *Description* Field is a free text field that is designed to work with Subroutine RULE_SET_INSTR_STEPS. This subroutine pulls the important information for the creation of the Aliquots into context. The user can create an aliquot instruction step by configuring an aliquot step statement. The user can insert scheme specific data into the statement by selecting a variable name from the *Aliquot Step Variable* table. The variables are input into the statement and enclosed in "|" (pipes). The user then adds the variables to the *Alqt Step Variables* field. This field is a multi-select list that links to the *Aliquot Step Variable* table. This table is a static data table that links the aliquot step variable to the developer created variable that is in context in processing subroutine RULE_SET_INSTR_STEPS. The code uses a string replace function to replace the variable with the actual value. The table is displayed in Figure 8.

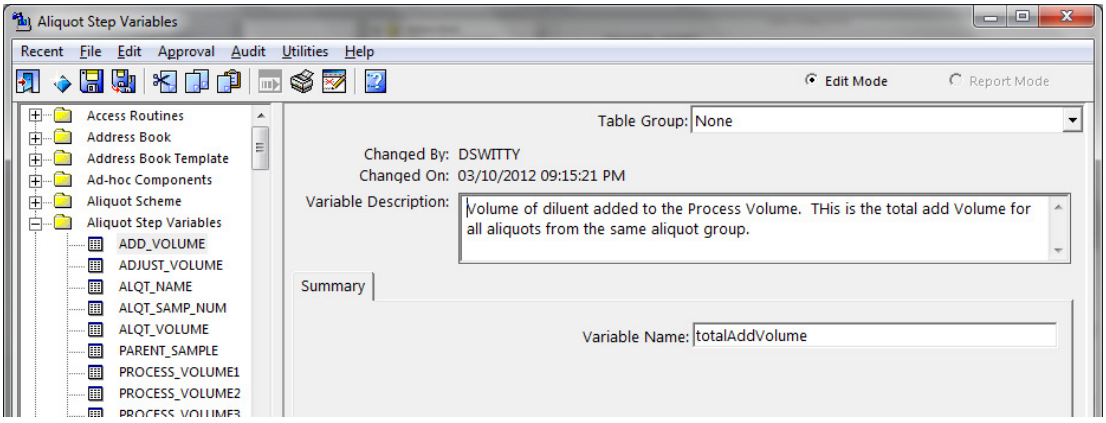
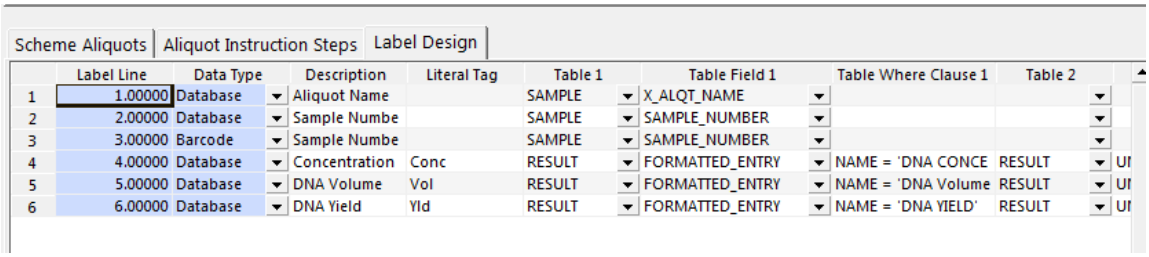


Figure 8: Aliquot Step Variables

The *Alqt Step Desc* field displays the aliquot instruction step description linked to the user selected aliquot step.

Label Design

The *Label Design* table allows the user to configure the aliquot specific information that displays on the aliquot label. Aliquot labels for this model are generated by code and displayed in Crystal Reports for demonstration purposes. LabWare supports label printing using third party software. The table is displayed in Figure 9.



	Label Line	Data Type	Description	Literal Tag	Table 1	Table Field 1	Table Where Clause 1	Table 2	
1	1.00000	Database	Aliquot Name		SAMPLE	X_ALQT_NAME			
2	2.00000	Database	Sample Numbe		SAMPLE	SAMPLE_NUMBER			
3	3.00000	Barcode	Sample Numbe		SAMPLE	SAMPLE_NUMBER			
4	4.00000	Database	Concentration	Conc	RESULT	FORMATTED_ENTRY	NAME = 'DNA CONCE	RESULT	UI
5	5.00000	Database	DNA Volume	Vol	RESULT	FORMATTED_ENTRY	NAME = 'DNA Volume	RESULT	UI
6	6.00000	Database	DNA Yield	Yld	RESULT	FORMATTED_ENTRY	NAME = 'DNA YIELD'	RESULT	UI

Figure 9: Label Design Table

The *Label Line* field is a numeric field that allows the user to determine the order that the line will appear on the label.

The *Data Type* field is a list field linked to list X_LABEL_DATA_TYPE. The available entries are 'Barcode', 'Database', and 'Literal Value'. The data type of 'Barcode' enforces that the returned database value field displays in a barcode format. For this model, the barcode is configured in Crystal Reports and is set to code128. The data type of 'Database' is used when a value stored in the database should be displayed. The database field is determined by the user defined *Table, Field*, and *where Clause* fields. The data type of 'Literal Value' returns the free text value entered in the *Literal Tag* field by the user.

The *Description* field is a free text field that allows a user to identify the record. This field is for documenting the source or intent of the field. It is used for informational purposes only and does not appear on the report or label.

The *Literal Tag* field is a free text field that allows a user to enter static information for display on the label. The literal tag can be a stand alone value if the data type is set to 'Literal Value', or can be used in conjunction with a database field if the data type is set to 'Database'.

The *Table, Table Field, and Table Where Clause* fields are designed to allow a user to fetch specific information from the database. Each set should be configured to return a single value. A user can set the record to return up to three distinct database field records. The *Table* field is a configured list that allows a user to only select the SAMPLE, TEST, and RESULT tables. The *Table Field* field is a configured list field that only returns database fields from the selected Table. The *Table Where Clause* is a free text field that allows a user to enter a where restriction formatted in SQL for the corresponding table field. A user can select up to three different data fields to appear on a single label line, but is limited by the size of the label and the number of characters that can fit onto a single line.

Rules Manager

The LabWare Rules Manager (Rules Engine Module M0467) adds logic defined functionality where a user can define input data and configure the system to perform actions based on database triggers (*Rules Engine*, 2011). The advantage of using the Rules Manager is that after the initial subroutines and inputs are developed by a LabWare developer, an end user without specialized training can configure a rule set. The aliquot scheme calculations will be calculated by the rule set that is defined for each aliquotting scheme.

A rule set is configured by defining a set of triggers, inputs, actions, and rules. The *Trigger* tab is where the database event that executes the rule set is defined. A user can configure the rule to trigger on an event such as record updated or record inserted on a selected table or a table field that is changed or is changed to a specific value. The *Inputs* tab allows a user to pull data into context for the execution of a rule. The data can come from related database fields, subroutines, SQL statements, or even literal static values. The *Actions* tab allows a user to define the evaluations to execute within the rule set. The action types can be set to 'Add Flags', 'Set Variables', call LIMS functions, or call a subroutine. Depending on the action type the user can set the variables to be passed into the action. The *Rules* tab is where the user defines the logic that sets the inputs and actions into a series of If/Then statements to evaluate the data. The Rules Manager

interface allows a user to configure complex rules using the pre-defined objects without having to write new code.

Sample Login Template

DNA parent samples are logged into LabWare using the Sample Login Template DNA_PARENT_SAMP. The user can access the sample interface by selecting the *Get Template* button to open Sample Login Template DNA_PARENT_SAMP. The user can fill out the form to enter the critical information about the samples about to be logged. In the context of a clinical trial, all of the fields have meaning and may drive certain functionality. In the context of this model, the *Genomic Alq Scheme* field is the only mandatory entry. This field links the logged sample to the aliquotting scheme so that the rule set can process the appropriate aliquotting scheme definitions. The *Aliquot Template* field is linked to Sample Login Template 'DNA_ALQT_SAMP'. This template is linked to Sample ID Configuration object DNA_ALQT_CONFIG. This configuration sets the aliquots created from parent samples logged using the DNA_PARENT_SAMP template with a naming convention of DNA-Aliquot-'sample number'. A screenshot of the sample login temple is displayed in Figure 10.

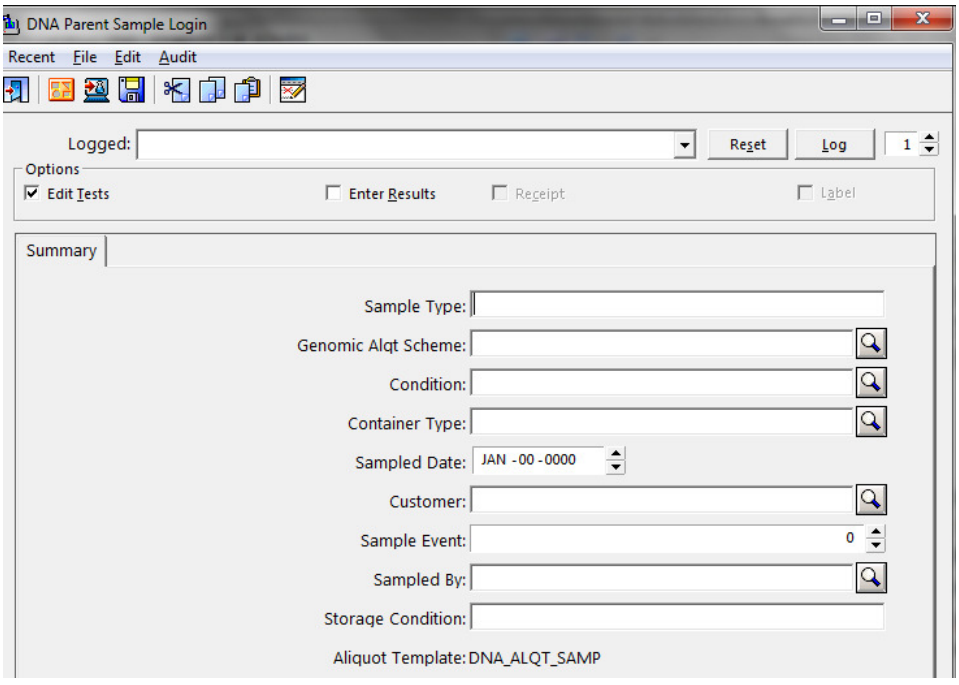


Figure 10: Sample Login Template

Batch Manager

In a typical clinical laboratory, samples are grouped together for processing. LabWare uses Batch Manager to group similar samples into batches (*LabWare Technical Manual*, 2009). The batch template for grouping DNA parent samples is defined by Batch Tests Template 'DNA_BATCH'. The Batch Tests Template controls a large number of out of box functionality, but only the functions critical to the precision aliquotting workflow will be discussed here. The batch naming convention is defined by setting the name prefix to 'DNA' and the Id config to 'Default'. This will result in each new batch being named in the format 'DNA-mmddyy-00'. The *Analysis Link* field is set to 'Name' and the *Analysis Link Key* is set to the DNA Parent Analysis 'DNA_EXTACT_001'. This field controls which tests can be assigned to the batch. The *Batch Report* field is linked to the Crystal Report 'DNA Batch Summary Report'. This report is configured in Crystal Reports 2008 and displays a summary of the parent sample, aliquots, and aliquot instructions for each sample in the batch. The *Object Class* is set to 'Sample'. The Object Class sets the sample related data to the BATCH_OBJECTS table. The *Batch Type* field is set to 'Sample / Test Batch'. This allows only samples with specified tests equal to the Analysis Link Key to be added to the Batch. This is useful in this application as only samples with the specified DNA test can be added to the batch.

A DNA batch is created by opening Batch Manger from the LabWare main menu option File > Batch Manager and by selecting File > New. The user is prompted to select a template and can choose Batch Tests Template 'DNA_BATCH'. The new batch is assigned a name and is immediately opened. After the Batch is saved, DNA parent samples can be added to the batch by selecting menu option Edit > Add Samples. The Sample Browse window opens and a user can select a sample to add to the batch.

The user enters results from Batch Manager by selecting menu Run > Enter Results. Batch Manager also allows the user to enter results from multiple samples using the result entry Grid. From menu Options > Result Entry by Test or Options > Result Entry Sample, the user can view all of the samples in the batch in a spreadsheet style grid. Samples with analysis DNA_EXTACT_001 can enter results for the A260 and A280 components. The results for purity and concentration will be automatically

calculated. When all the results for a test are entered and the sample is saved, the test status updates to 'Complete'.

The user reviews results from Batch Manager by selecting menu Run > Review. Like Result Entry, the user can review multiple samples from the same dialog window. From Menu Options > Review by Test or Options > Review by Sample, the user can view all samples in the batch in a spreadsheet grid. For this model, review only occurs at the test level. When the test is reviewed, the status of the test is updated to 'Authorized'.

The Report tab on each batch will display Crystal Report 'DNA Batch Summary Report'. This report was configured in Crystal Reports 2008 and linked to the Batch Tests Template. The report displays all the DNA parent samples assigned to the batch. Depending on the sample test status, the Batch Summary Report displays a page for each sample with a section for the parent sample data, a section with the associated DNA aliquot information, and a section with the DNA aliquotting instructions. A sample report is displayed in Figure 11.

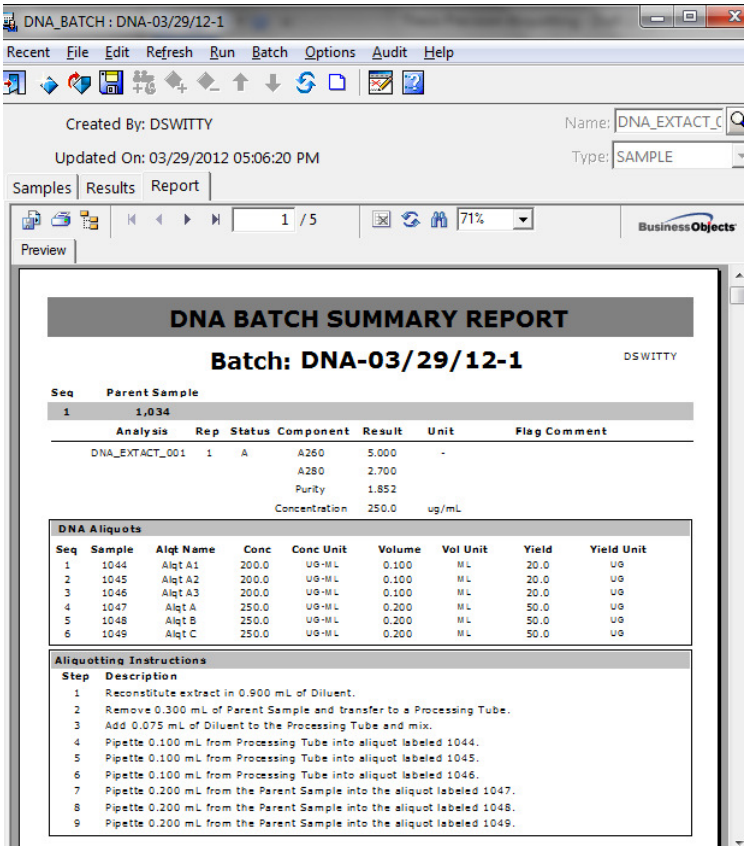


Figure 11: DNA Batch Summary Report

A custom Menu Routine is configured on the Batch Tests Template to allow the user to generate aliquot labels. From Batch Manager the user selects Options > Print Aliquot Labels to call Menu Routine BM_PRINT_ALQ_LABELS. The function prompts the user to select a sample from the current batch that has aliquots (SAMPLE.ALIQUOT = 'T'). The routine then checks the aliquot label definitions based on the Aliquot Scheme Label Design table. The aliquot information for each sample aliquot is formatted and rendered in the Crystal Report 'Aliquot Label Display'. A sample report is displayed in Figure 12.

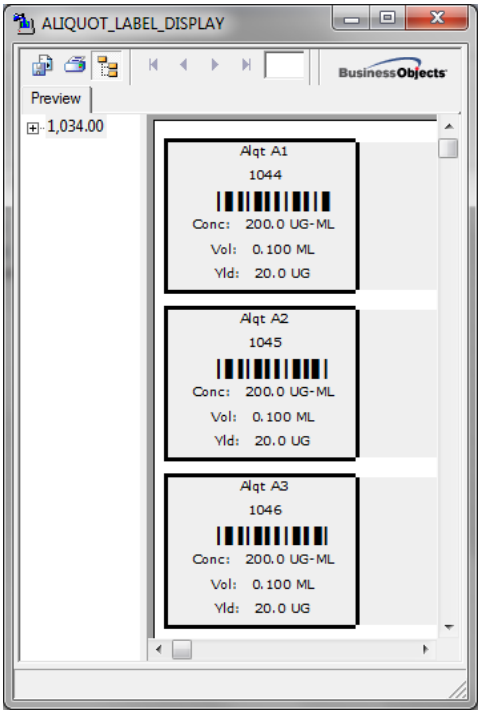


Figure 12: Aliquot Label Display

CHAPTER THREE: RESULTS

For this model, two aliquotting schemes are configured for demonstrating and testing the design: SCHEME_001 and SCHEME_002.

Simple Aliquot Scheme: SCHEME_001

SCHEME_001 is a simple aliquotting scheme. The objective of the scheme is to reconstitute the parent extract into 0.800 mL and create 2 aliquots at the achieved concentration in an equal volume of 0.400 mL. If the achieved DNA concentration is greater than the concentration low cancel limit of 25 µg/mL, then the test is authorized and the aliquots are created. If the DNA concentration is less than the concentration low cancel limit, then the test is rejected and a replicate test is added. If the replicate test has a DNA concentration less than the concentration low cancel limit, then the test is canceled and aliquots are not created. The workflow is displayed in Figure 13.

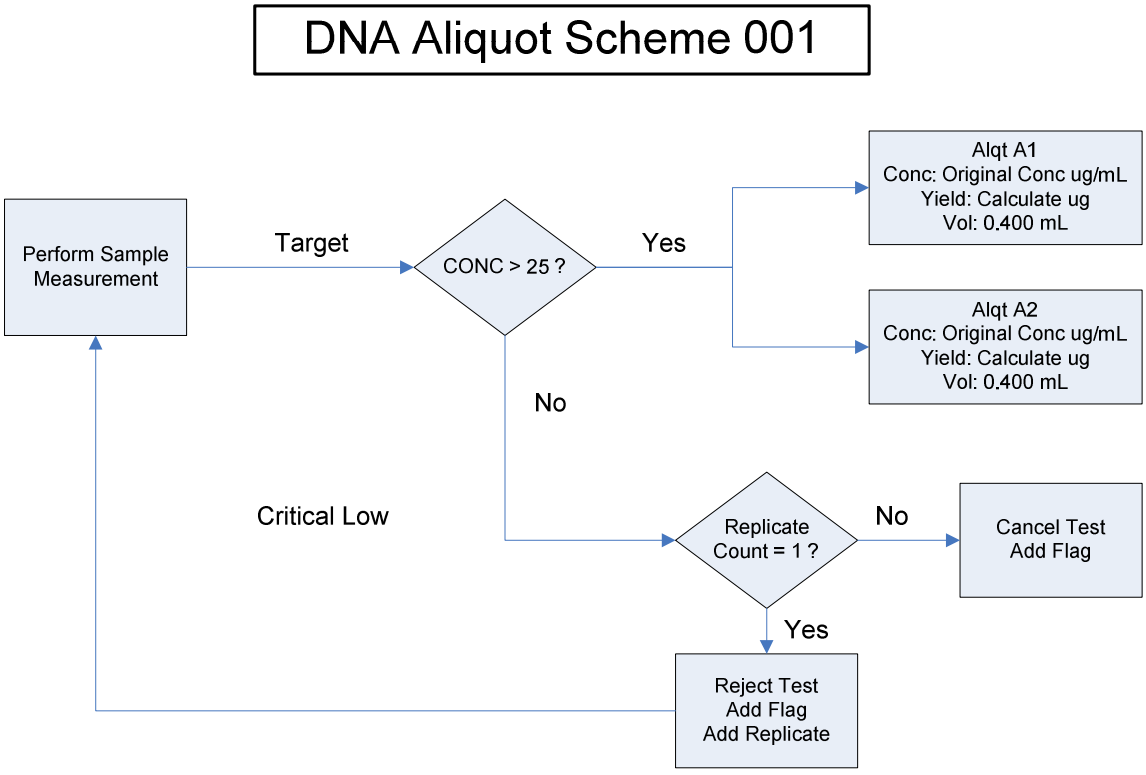


Figure 13: Workflow - DNA Aliquot Scheme 001

The aliquotting scheme for SCHEME_001 can be reviewed by selecting the Parent Child Record Editor button from the main toolbar and selecting table *Aliquot Scheme* and opening record SCHEME_001. The critical aliquotting scheme values for SCHEME_001 are the *Scheme Type* which is set to 'Simple', the *Recon Volume* which is set to 0.800 mL, and the *Conc Low Cancel Limit* which is set to 25 µg/mL. Because the scheme has a scheme type of 'Simple', the *Minimum Target Fields* and the *Process Volume* fields are set to null or zero. The aliquotting scheme configurations are displayed in Figure 14.

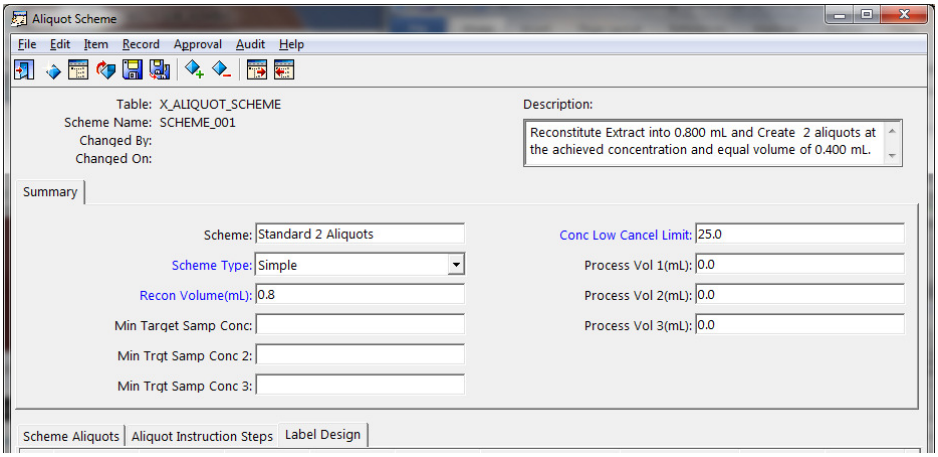


Figure 14: Aliquot Scheme Configurations – SCHEME_001

The *Scheme Aliquots* table is configured to create two aliquots in a single group called the Target group. The Target Group will create each aliquot at the original concentration in a volume of 0.400 mL. The *Yield* is set to calculate from the concentration and volume. The *Scheme Aliquots* table configurations are displayed in Figure 15.

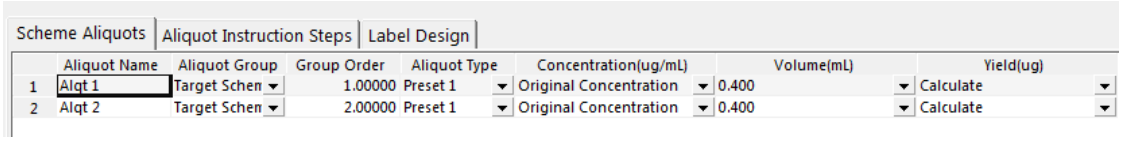


Figure 15: Scheme Aliquots Configurations – SCHEME_001

The *Aliquot Instructions Steps* table is configured to work with the target aliquot group. Aliquots in the target group are created by adding the reconstitution volume to the

parent sample, then transferring 0.400 mL of parent sample into each of the two aliquots. The *Aliquot Instruction Steps* table configuration is displayed in Figure 16.

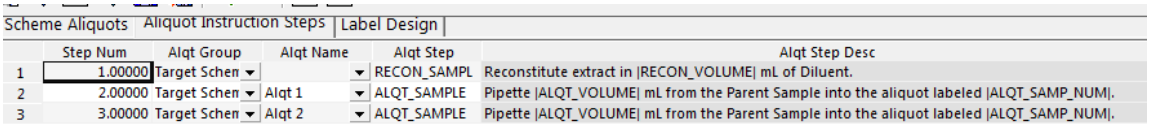


Figure 16: Aliquot Instruction Steps Configuration – SCHEME_001

The *Label Design* table is configured to display 5 lines of data on the label. The first line will display the aliquot scheme name from SAMPLE.X_SCHEME_NAME. The second line displays the aliquot name from SAMPLE.X_ALQT_NAME. The next line will display a literal value of 'dsDNA'. The next line will display the SAMPLE.SAMPLE_NUMBER in barcode format. The last line of the label will display the sample number from the SAMPLE.SAMPLE_NUMBER. The *Label Design* table configuration is displayed in Figure 17.

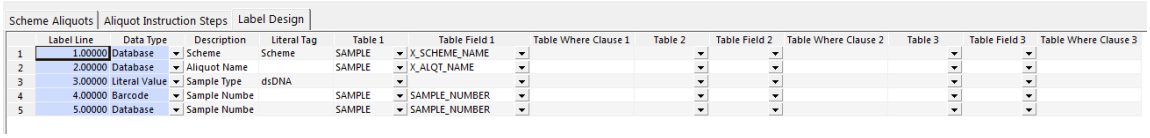


Figure 17: Label Design Configuration – SCHEME_001

Rules Manager Configuration – SCHEME_001

To execute the aliquotting scheme, rule set 'DNA_SIMPLE_SCHEME' was configured. The *Summary* tab was configured with a description of 'DNA Aliquotting Simple Scheme' with the *Enabled* boolean set to 'T'. The *Summary* tab is displayed in Figure 18.

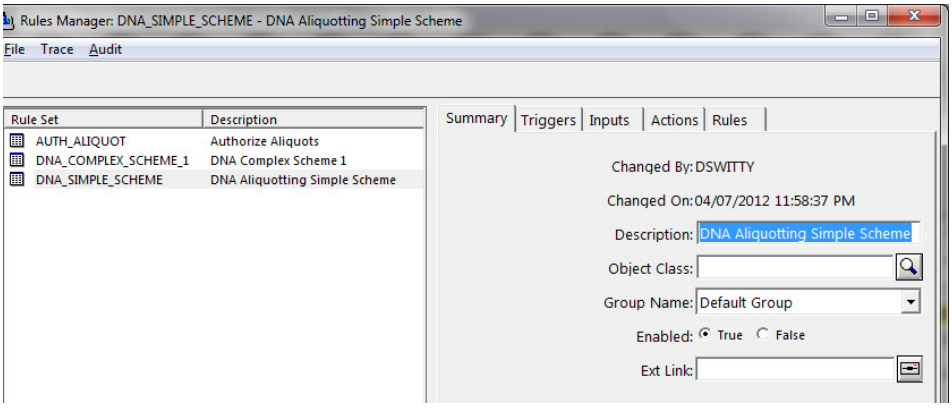


Figure 18: Rules Manager – DNA_SIMPLE_SCHEME Summary Tab

The *Triggers* tab is configured to execute the rule set when a test with analysis DNA_EXTACT_001 has the status field updated to 'Authorized'. The configured *Triggers* tab is displayed in Figure 19.

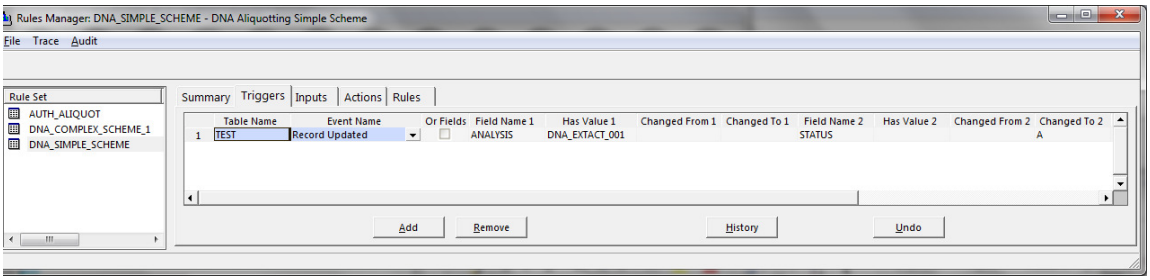


Figure 19: Rules Manager – DNA_SIMPLE_SCHEME Triggers Tab

The *Inputs* tab is configured to feed the appropriate values into the rule actions. A summary of the inputs and their function is displayed in Table 3.

Input	**Source**	**Description**
CUR_BATCH_NAME	Object Field	TEST.BATCH
CUR_ANALYSIS	Literal	Returns value "DNA_EXTACT_001"
REJECT_REASON	Literal	Returns value "Test Result out of Range, Reject Test"
CONC_CRITICAL_LOW	SQL Query	select CONC_LOW_CAN_LIMIT from X_ALIQUOT_SCHEME where SCHEME_NAME = {ALQ_SCHEME}
CANCEL_REASON	Literal	Returns value "DNA Concentration out of Range. Test Cancelled."
REP_COUNT	Object Field	TEST.REPLICATE_COUNT
CUR_TEST_NUM	Object Field	TEST.TEST_NUMBER
NUM_RESULT	Object Field	RESULT.NUMERIC_ENTRY
ALT_ANALYSIS	Literal	Returns value "DNA_ALIQUOT"
CUR_SMP_NUM	Object Field	TEST.SAMPLE_NUMBER
CONC_RESULT	SQL Query	SELECT ENTRY FROM RESULT WHERE TEST_NUMBER = {CUR_TEST_NUM} and NAME = 'CONCENTRATION'
ALQ_SCHEME	Object Field	SAMPLE.X_SCHEME_NAME
ALQT_SCHEME_TYPE	SQL Query	SELECT SCHEME_TYPE FROM X_ALIQUOT_SCHEME WHERE SCHEME_NAME = {ALQ_SCHEME}

Table 3: Rules Manager – DNA_SIMPLE_SCHEME Input Summary

The *Actions* tab is configured to execute the critical functions of Adding Test Replicates, Rejecting Tests, Cancelling Tests, Setting the Aliquot Group, Adding Aliquots, and Updating Aliquot Results. A summary is displayed in Table 4.

Action	**Action Type**	**Subroutine**	**Inputs**
ADD_TEST_REP	Subroutine	ADD_TEST_SUB	Sample Number for Current Test: CUR_SMP_NUM Current Analysis: CUR_ANALYSIS Current Batch Name: CUR_BATCH_NAME Number of Test to Add: 1 Maximum Replicates to add: 2
REJECT_TEST_SUB	Subroutine	REJECT_TEST	Test Number to Reject: CUR_TEST_NUM Sample Number of Tests: CUR_SMP_NUM Analysis: CUR_ANALYSIS Type of Flag: REJECT Reject Reason: REJECT_REASON
CANCEL_TEST_SUB	Subroutine	CANCEL_TEST	Test Number to Cancel: CUR_TEST_NUM Sample Number of Tests: CUR_SMP_NUM Analysis: CUR_ANALYSIS Type of Flag: CANCEL CANCEL REASON: CANCEL_REASON
SET_ALQT_GRP_TARGET	Function	SET_ALQT_GRP_TARGET	Aliquot Group: alqtGroup Target Aliquot Group: alqtGroup

			Aliquot Group Value: TARGET
ADD_DNA_ALIQUOT	Subroutine	ADD_DNA_ALIQUOT	Current Sample Number: CUR_SMP_NUM Current Test Number: CUR_TST_NUM Aliquot Analysis: ALT_ANALYSIS Aliquot Scheme: ALQ_SCHEME Concentration Result: CONC_RESULT
UPDATE_ALQT_RSLTS	Subroutine	UPDATE_ALIQUO_RSLTS	Current Sample Number: CUR_SMP_NUM Current Test Number: CUR_TST_NUM Aliquot Analysis: ALT_ANALYSIS Aliquot Scheme: ALQ_SCHEME Concentration Result: CONC_RESULT

Table 4: Rules Manager DNA_SIMPLE_SCHEME Actions Tab Summary

The *Rules* Tab is configured to evaluate the aliquot scheme type. If the scheme type does not equal 'SIMPLE', the rule set stops and exits the evaluation. If the scheme type is 'SIMPLE', the parent sample concentration result is evaluated against the concentration low cancel limit. If the parent concentration is greater than the concentration low cancel limit, then action 'SET_ALQT_GRP_TARGET executes a function to set the aliquot group to 'TARGET'. Action ADD_DNA_ALIQUOT executes subroutine RULE_SUB_ADD_ALIQUOTS which checks the aliquotting scheme to determine the number of aliquots to create. The subroutine adds the aliquots and then adds the analysis 'DNA_ALIQUOT' to each aliquot. The system then sets the aliquot name and aliquotting scheme on the aliquot sample. Action 'UPDATE_ALQT_RSLTS' executes subroutine 'RULE_SET_ALQT_RESULTS' which fetches the aliquot specific

attributes for each aliquot and sets the aliquot results on the 'DNA_ALIQUOT' analysis. LabWare then updates the test status to 'Complete'. The subroutine then writes the aliquot information to the X_ALQT_INSTRUCTION table for use in a Crystal Report. When all of the aliquots are created, the subroutine runs subroutine 'RULE_SET_INSTR_STEPS' which fetches the scheme aliquotting instructions and writes the final translated aliquotting steps to the X_ALQT_REPORT_STEPS for display in a Crystal Report.

If the parent sample concentration is less than the concentration low cancel limit, the rule checks the number of replicates on the current test. If the TEST.REPLICATE_COUNT = '1', then action REJECT_TEST_SUB executes subroutine RULE_SUB_CANCEL_REJECT_TEST which rejects the current test and sets a flag using the 'Default' flag template and sets the reject reason on the flag. Action ADD_TEST_REP then runs subroutine RULE_SUB_ADD_TEST which adds a replicate test to the currently selected sample.

If the parent sample concentration is less than the concentration low cancel limit a second time, the rule checks that the TEST.REPLICATE_COUNT is not equal to '1' and runs action CANCEL_TEST_SUB. Subroutine RULE_SUB_CANCEL_REJECT_TEST reactivates the authorized test so that LabWare can cancel the test. A cancel flag is added using the 'Default' flag template and a user created cancel reason gets added to the flag. The rule logic is displayed in Figure 20.

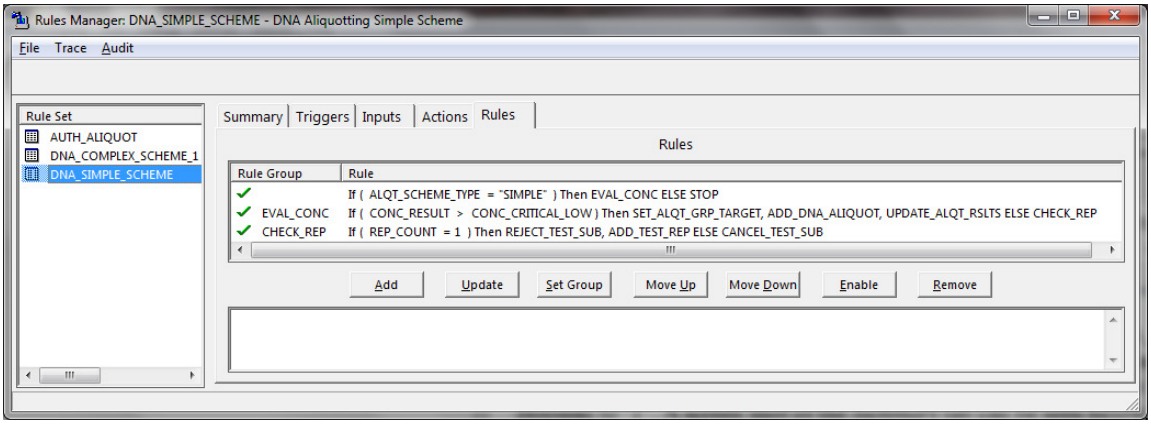


Figure 20: Rules Manager – DNA_SIMPLE_SCHEME – Rules Tab Configuration

Rule Set AUTH_ALIQUOT was defined to auto-authorize the DNA_ALIQUOT analysis once the test is updated to a status of 'Complete'. The *Summary* tab is configured to set the description to 'Authorize Aliquots', set the Object Class to 'TEST', and set the Enabled Boolean to 'T'. The *Summary* tab is displayed in Figure 21.

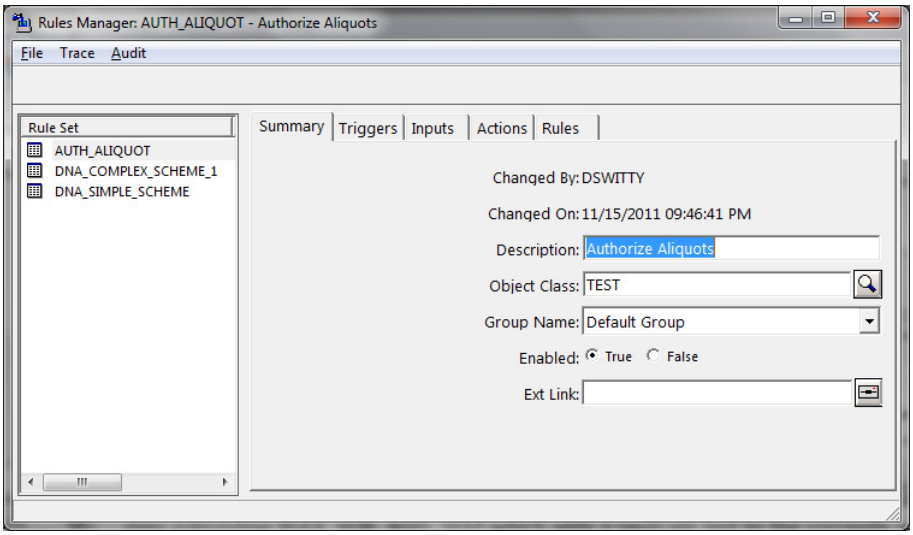


Figure 21: Rules Manager – AUTH_ALIQUOT Summary Tab Configuration

The *Triggers* tab is configured by the user to execute the rule set when the TEST.ANALYSIS field is equal to 'DNA_ALIQUOT' and the TEST.STATUS field is updated to 'C'. The *Triggers* tab is displayed in Figure 22.

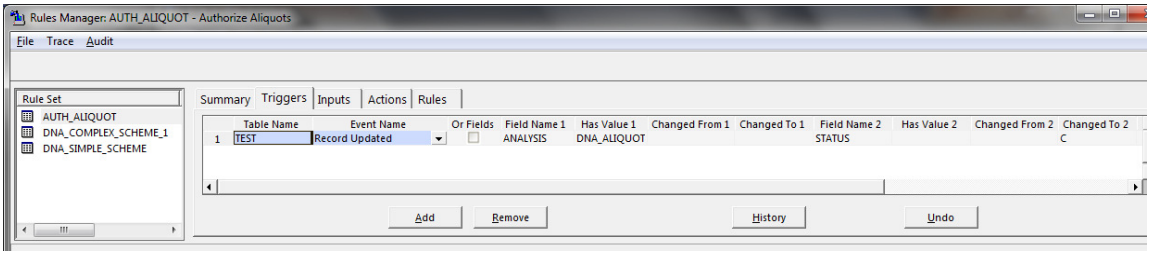


Figure 22: Rules Manager – AUTH_ALIQUOT Triggers Tab Configuration

The *Inputs* tab is configured to feed the appropriate values into the rule actions. A summary of the inputs are displayed in Table 5.

Input	**Source**	**Description**
CUR_TEST_STATUS	Object Field	TEST.STATUS
CUR_TEST_NUM	Object Field	TEST.TEST_NUMBER
CUR_SMP_NUM	Object Field	TEST.SAMPLE_NUMBER

Table 5: Rules Manager – AUTH_ALIQUOT Inputs Tab

The *Actions* tab is configured to execute the authorization of the DNA aliquot analysis. A screenshot of the *Actions* tab configuration is displayed in Figure 23.

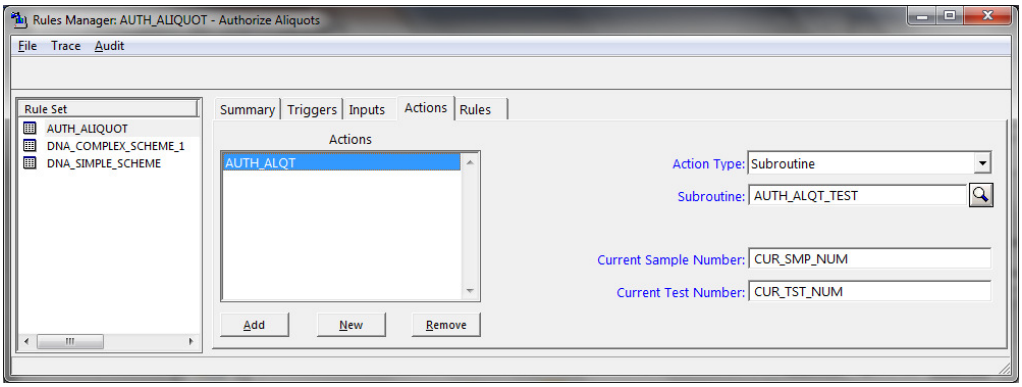


Figure 23: Rules Manager – AUTH_ALIQUOT Actions Tab Configuration

The *Rules* tab is configured to check the current status of the test. If the status is complete, then the Action AUTH_ALQT calls subroutine RULE_AUTH_ALQT which authorizes the current test. The configured *Rules* tab is displayed in Figure 24.

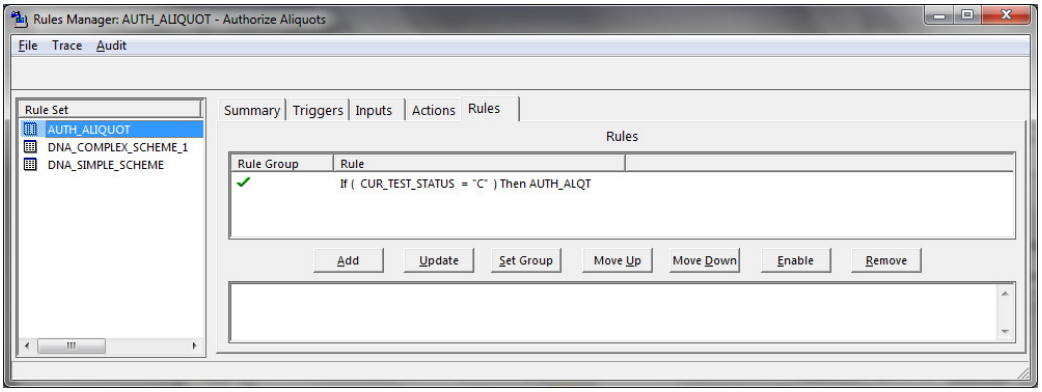


Figure 24: Rules Manager – AUTH_ALIQUOT Rules Tab Configuration

SCHEME_001 Design Evaluation

To demonstrate the design of Aliquot SCHEME_001, three samples have been logged into the system by selecting the Sample Interface button from the main menu and using Sample Login Template 'DNA_PARENT_SAMP'. Samples 1101, 1102, and 1103 are logged and added to batch 'DNA-04/08/12-01' by opening Batch Manager from the main menu icon and selecting the template DNA_BATCH. A screenshot of the batch is displayed in Figure 25.

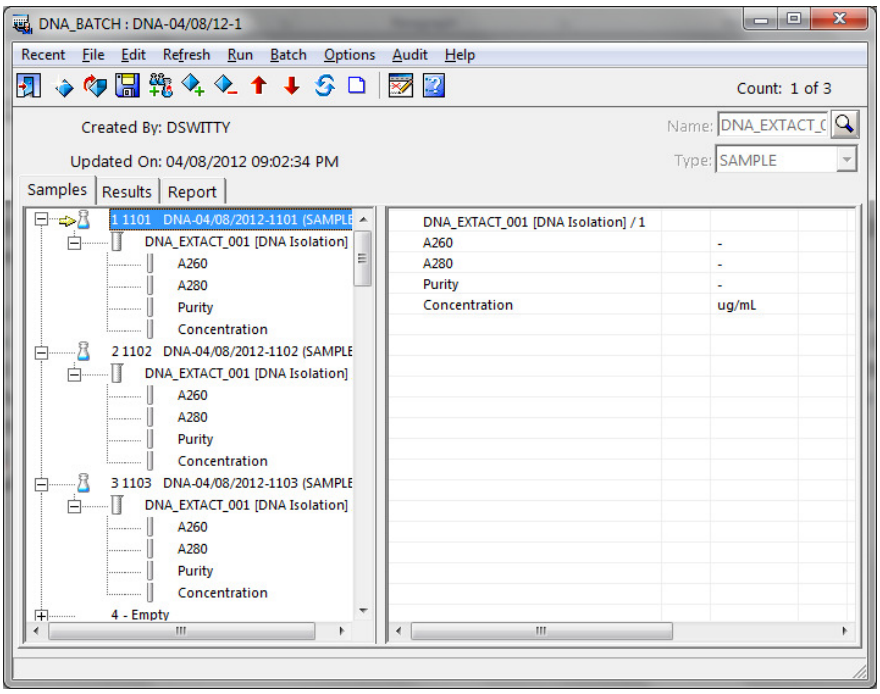


Figure 25: DNA Batch DNA-04/08/12-01 for Testing SCHEME_001

The samples in the batch are resulted by selecting the Options > Result Entry by Test to open the resulting grid. The entered values are displayed in the screenshot in Figure 26.

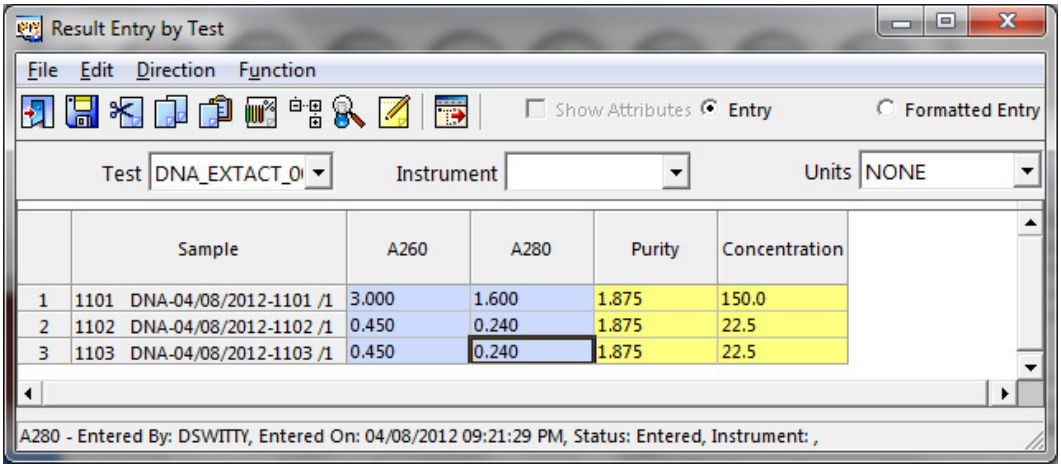


Figure 26: DNA Batch DNA-04/08/12-01 Entered Results

The entered results are saved and the tests are authorized by selecting Options > Grid Review by Test. The user will set the review level to test, highlight each record, and click on the authorize button.

Sample 1101 produced an achieved concentration greater than the concentration low cancel limit of 25 µg/mL. On test authorization, Rule Set DNA_SIMPLE_SCHEME determines that the concentration of 150 µg/mL is greater than the concentration low cancel limit and sets the Aliquot Group to 'TARGET'. The rule then adds two aliquots which is the scheme defined number of aliquots for the target group. The results of each aliquot are set based on the *Scheme Aliquots* table for the scheme. For both aliquots, the concentration is equal to the original concentration of 150 µg/mL, the volume is equal to 0.400 mL, and the DNA yield calculated from the concentration and volume is equal to 60 µg. When the DNA_ALIQUOT analysis test was updated to complete, rule set 'AUTH_ALIQUOT' fired which auto-authorized the test on each aliquot of sample 1101. The aliquot instructions are generated and all of the information is displayed in the Batch Summary Report which can be seen by saving the batch and clicking on the *Report* tab. A screenshot of the Batch Summary Report is displayed in Figure 27.

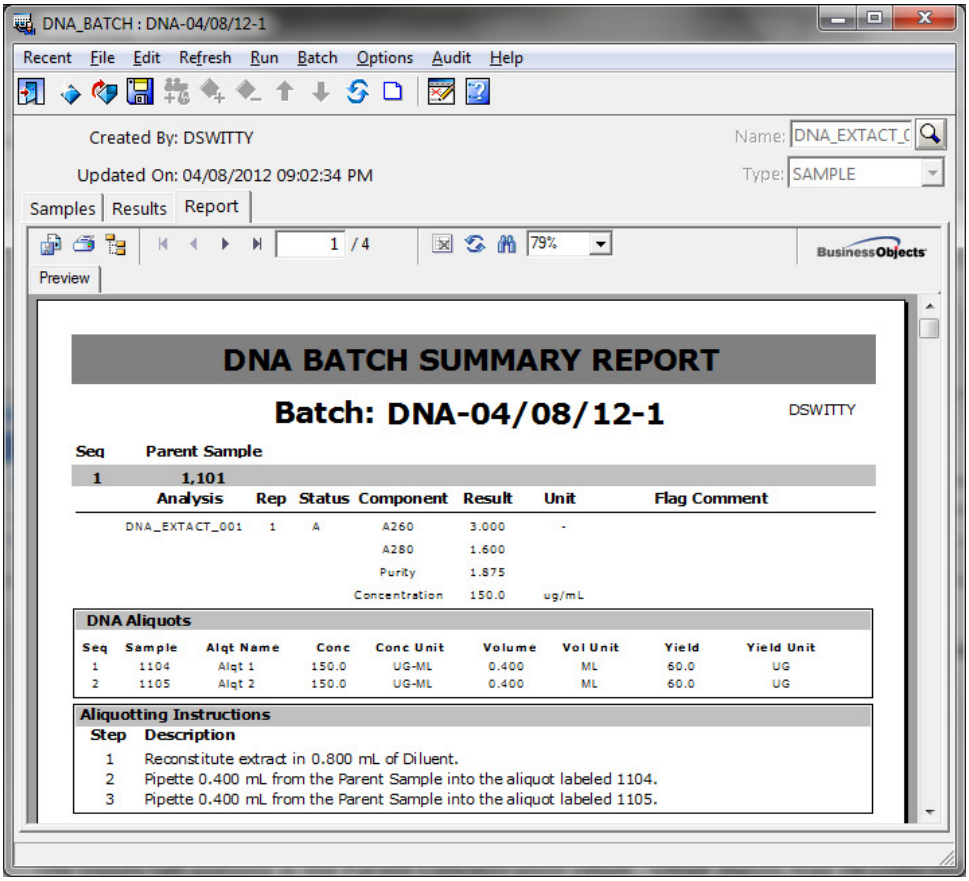


Figure 27: Batch Summary Report for Parent Sample 1101

Sample 1101 produced aliquots and a user can select the Options > Print Aliquot Labels to generate the aliquot labels. The labels are produced with the five fields defined on the *Label Design* table on the aliquotting scheme. A screenshot of the labels is displayed in Figure 28.

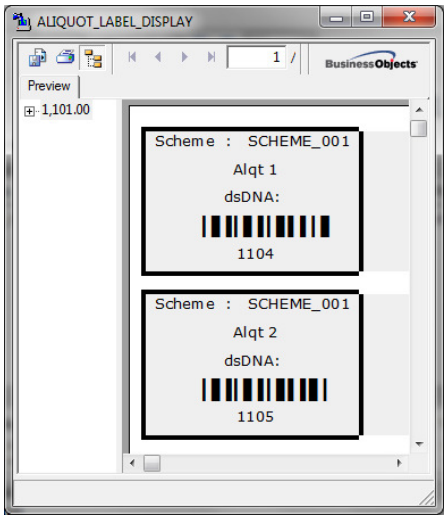


Figure 28: Aliquot Labels for Parent Sample 1101

The concentration for sample 1102 is 22.5 µg/mL which is less than the concentration low cancel limit. On test authorization, rule set DNA_SIMPLE_SCHEME determines that the parent concentration is below the concentration low cancel limit of 25 µg/mL. The rule then checks the TEST.REPLICATE_COUNT and determines that the replicate count is equal to 1. The rule rejects the test and adds a flag with the defined rejection comment. The rule then adds a replicate DNA_ALIQUOT test for confirmation testing. A screenshot of the batch for sample 1102 with a flag attached and a replicate test added is displayed in Figure 29.

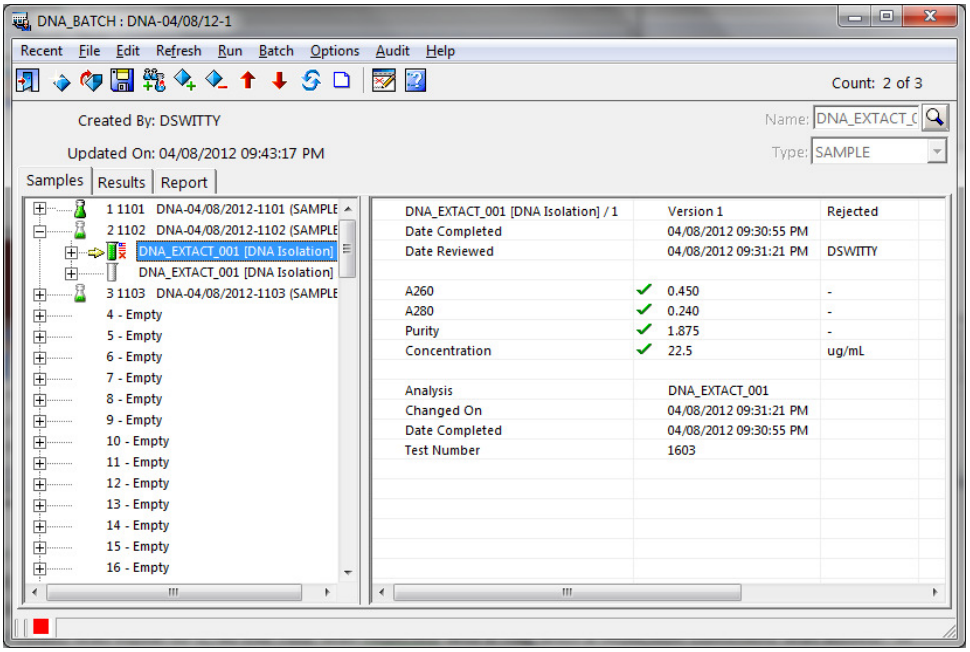


Figure 29: Batch DNA-04/08/12-01 Sample 1102 Replicates and Flag

The replicate test added to 1102 produces a concentration greater than the concentration low cancel limit. The rule set DNA_SIMPLE_SCHEME will determine that the concentration of 150 µg/mL is greater than the concentration low cancel limit. The rule will set the aliquot group to 'TARGET' and add two aliquots. For both aliquots, the concentration is equal to the original concentration of 150 µg/mL, the volume is equal to 0.400 mL, and the DNA yield is calculated and set to 60 µg. When the DNA_ALIQUOT analysis test is updated to 'Complete', rule set 'AUTH_ALIQUOT' fires to auto-authorized the test on each aliquot of sample 1102. The aliquot instructions are generated and all of the information is displayed in the Batch Summary Report which can be viewed by saving the batch and clicking on the *Report* tab. A screenshot of the Batch Summary Report is displayed in Figure 30.

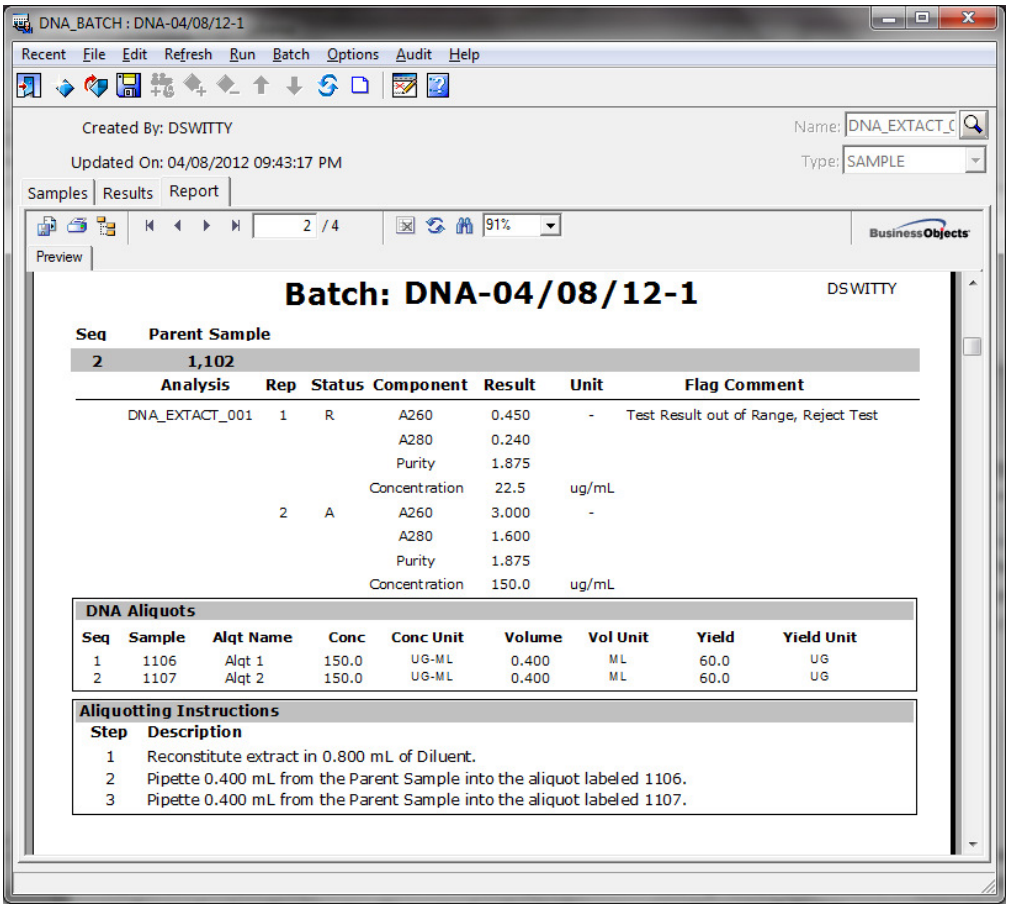


Figure 30: Batch Summary Report for Parent Sample 1102 with two Replicates

Sample 1102 produced aliquots, and a user can generate the labels by selecting the Options > Print Aliquot Labels menu option. A screenshot of the labels is displayed in Figure 31.

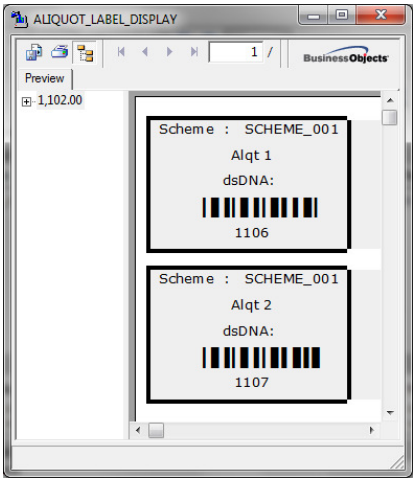


Figure 31: Aliquot Labels for Parent Sample 1102

The concentration for sample 1103 is 22.5 µg/mL, which is less than the concentration low cancel limit. On test authorization, rule set DNA_SIMPLE_SCHEME determines that the parent concentration is below the concentration low cancel limit of 25 µg/mL. The rule then checks the TEST.REPLICATE_COUNT and determines that the replicate count is equal to 1. The rule rejects the test and adds a flag with the defined rejection comment. The rule then adds test replicate DNA_ALIQUOT to sample 1103.

The replicate test for 1103 produces another value less than the concentration low cancel limit. On test authorization, the rule set DNA_SIMPLE_SCHEME determines that the concentration of 22.5 µg/mL is less than the concentration low cancel limit. The rule logic then determines that the replicate count is not equal to one. The current test is canceled and a flag is added with the defined cancel reason. A screenshot of sample 1103 in the batch with both test replicates canceled is displayed in Figure 32.

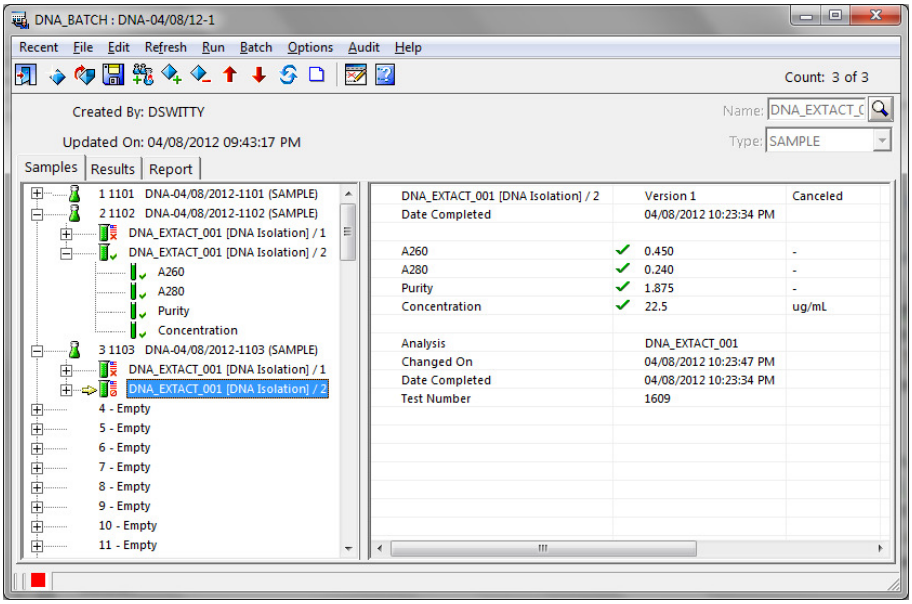


Figure 32: Batch DNA-04/08/12 Sample 1103 with Rejected and Cancelled Replicates

Because sample 1103 did not produce a concentration that produces viable aliquots, the rule set did not create any aliquots or aliquot instructions. A screenshot of the Batch Summary Report is displayed in Figure 33.

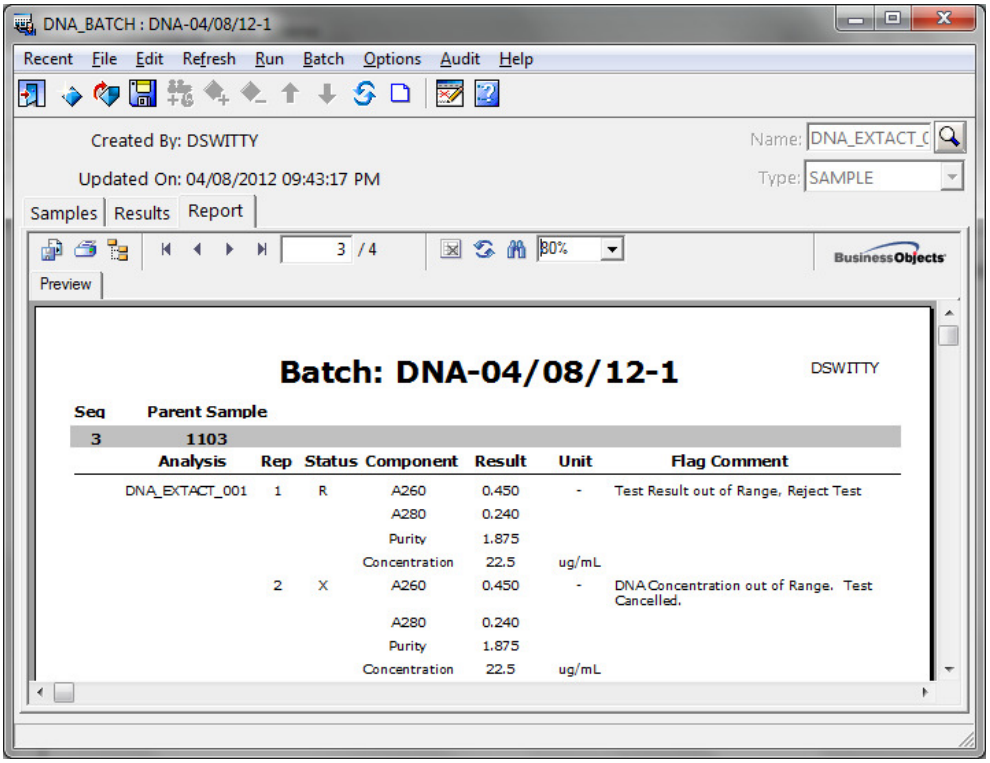


Figure 33: Batch Summary Report for Sample 1103

Complex Aliquot Scheme: SCHEME_002

SCHEME_002 is a complex aliquotting scheme. The objective of the scheme is to reconstitute the extract into 0.900 mL. If the parent sample concentration is greater than or equal to 200 µg/mL, then the target scheme is used. The target scheme creates 3 aliquots at a volume of 0.100 mL at a concentration of 200 µg/mL. The remaining sample is split into 3 equal remainder aliquots of 0.200 mL at the original concentration.

If the parent concentration is less than 200 µg/mL and greater than or equal to 50 µg/mL, then the ALT_1 scheme is used. The ALT_1 scheme creates 3 aliquots at a yield of 20 µg in an adjusted volume and a concentration equal to the original concentration. The remaining sample is split into 3 aliquots at the original concentration in equal remaining volume.

If the parent concentration is less than 50 µg/mL and greater than the concentration low cancel limit value of 10 µg/mL, then the ALT_2 scheme is used. The ALT_2 scheme creates one aliquot of 0.900 mL at the original concentration.

If the DNA concentration is less than the concentration low cancel limit, then the test is rejected and a replicate test is added. If the replicate test has a DNA concentration less than the concentration low cancel limit, then the test is canceled and aliquots are not created. A summary of SCHEME_002 is displayed in Figure 34.

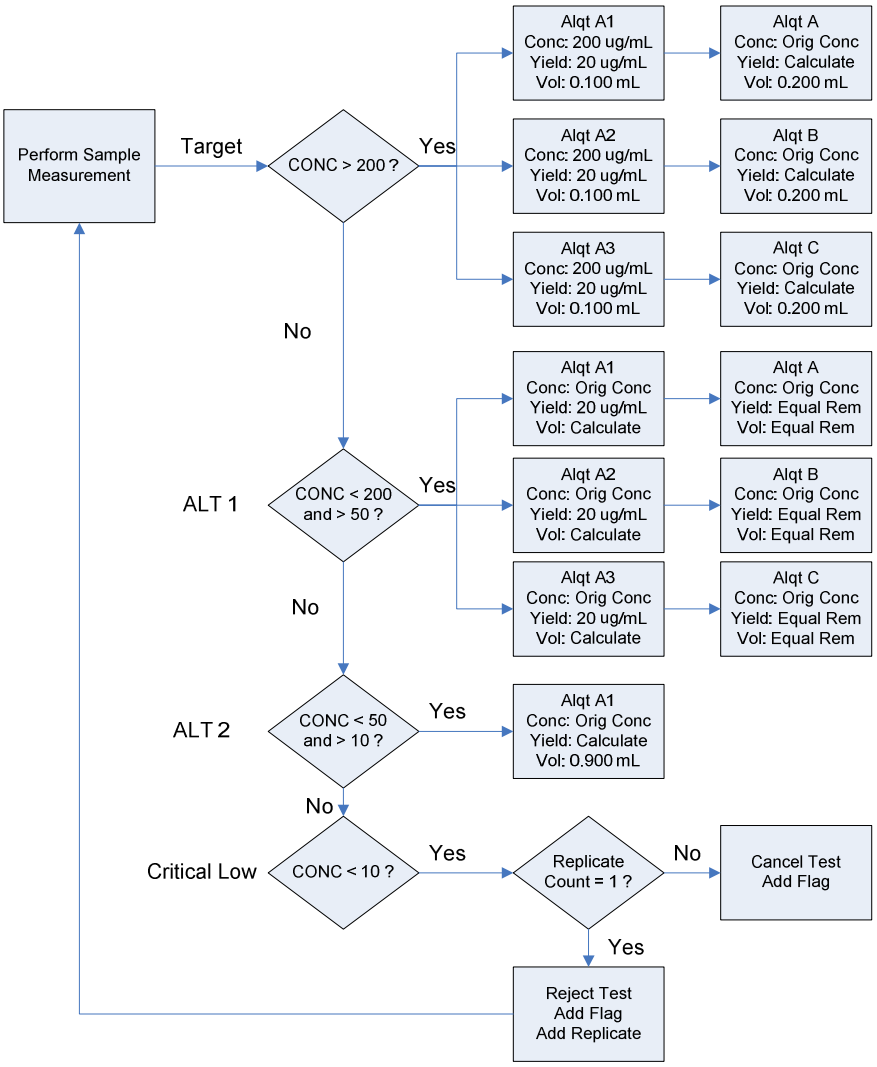


Figure 34: Workflow – DNA Aliquot Scheme: SCHEME_002

The aliquotting scheme values for SCHEME_002 are defined by opening the Parent Child Record Editor from the Main Menu Toolbar, selecting the *Aliquot Scheme* table, and opening the SCHEME_002 record. For SCHEME_002, the *Scheme Type* is set to 'Complex 01', the *Recon Volume* is set to 0.900 mL, and the *Conc Low Cancel Limit* is set to 10 µg/mL. The *Min Target Samp Conc* is set to 200 µg/mL and the *Min Trgt Samp*

Conc 2 is set to 50 µg/mL. In the context of this scheme, the concentration hierarchy is defined that the 'Target' group of aliquots is created when the parent concentration is greater than or equal to 200 µg/mL. The 'Alt 1' group of aliquots is created when the parent concentration is less than 200 µg/mL and greater than or equal to 50 µg/mL. The 'Alt 2' group of aliquots is created when the parent concentration is less than 50 µg/mL, but greater than the concentration low cancel limit. The *Process Volume 1* field is set to 0.300 mL. This links to the preset 1 subset of aliquots within each aliquot group defined on the *Scheme Aliquots* table. The preset 1 group of aliquots is created by removing 0.300 mL from the parent sample for preparing sample volume dilutions or adjustments. A screenshot of the aliquotting scheme configuration is displayed in Figure 35.

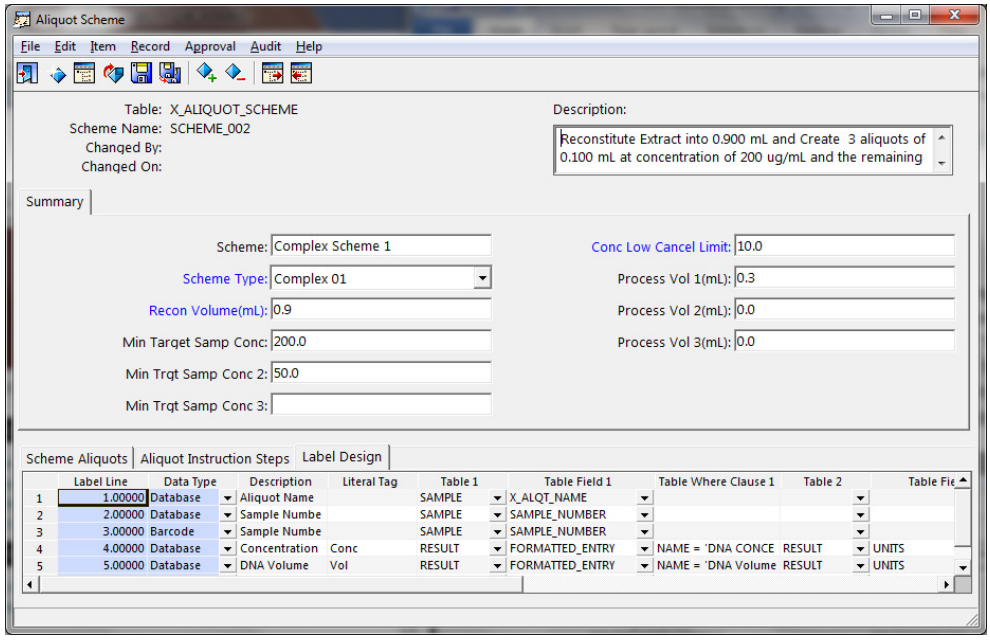


Figure 35: Aliquot Scheme Configurations – SCHEME_002

The *Scheme Aliquots* table is configured with a Target Group, Alt 1 Group, and Alt 2 group. The aliquot group that gets created is dependent upon the parent sample achieved concentration.

The Target Group will create six aliquots. The first three aliquots will have an aliquot type of 'Preset 1' and work with the *Process Vol 1* field on the *Aliquot Scheme* table. Aliquots Alqt A1, Alqt A2, and Alqt A3 are configured to produce an aliquot with a concentration of 200 µg/mL, a volume of 0.100 mL, and a yield of 20 µg. The last three aliquots have an aliquot type of 'Remainder'. Aliquots Alqt A, Alqt B, and Alqt C

will each have an aliquot produced that has a concentration equal to the original concentration, a volume equal to 0.200 mL, and a yield that is calculated based on the concentration and volume.

The Alt 1 Aliquot Group will also create six aliquots. The first three aliquots have an aliquot type of 'Preset 1' and work with the *Process Vol 1* field on the *Aliquot Scheme* table. Aliquots Alqt A1, Alqt A2, and Alqt A3 are configured to produce an aliquot with a concentration equal to the original concentration, a volume that is calculated off of the yield and the concentration, and a yield of 20 µg. The last three aliquots have an aliquot type of 'Remainder'. Aliquots Alqt A, Alqt B, and Alqt C will each have an aliquot produced that has a concentration equal to the original concentration, a volume equal to the remaining volume divided by three, and a yield that is equal to the remaining yield divided by three.

The Alt 2 aliquot group will create a single aliquot. Alqt A1 is configured to have a concentration equal to the original concentration, a volume of 0.900 mL, and a yield calculated from the concentration and volume. A screenshot of the *Scheme Aliquots* table configuration is displayed in Figure 36.

Scheme Aliquots | Aliquot Instruction Steps | Label Design

	Aliquot Name	Aliquot Group	Group Order	Aliquot Type	Concentration(ug/mL)	Volume(mL)	Yield(ug)
1	Alqt A1	Target Schen	1.00000	Preset 1	200.0	0.100	20.0
2	Alqt A2	Target Schen	2.00000	Preset 1	200.0	0.100	20.0
3	Alqt A3	Target Schen	3.00000	Preset 1	200.0	0.100	20.0
4	Alqt A	Target Schen	4.00000	Remainder	Original Concentration	0.200	Calculate
5	Alqt B	Target Schen	5.00000	Remainder	Original Concentration	0.200	Calculate
6	Alqt C	Target Schen	6.00000	Remainder	Original Concentration	0.200	Calculate
7	Alqt A1	Alt 1 Scheme	1.00000	Preset 1	Original Concentration	Calculate	20.0
8	Alqt A2	Alt 1 Scheme	2.00000	Preset 1	Original Concentration	Calculate	20.0
9	Alqt A3	Alt 1 Scheme	3.00000	Preset 1	Original Concentration	Calculate	20.0
10	Alqt A	Alt 1 Scheme	4.00000	Remainder	Original Concentration	Equal Remaining Volume	Equal Remaining Yield
11	Alqt B	Alt 1 Scheme	5.00000	Remainder	Original Concentration	Equal Remaining Volume	Equal Remaining Yield
12	Alqt C	Alt 1 Scheme	6.00000	Remainder	Original Concentration	Equal Remaining Volume	Equal Remaining Yield
13	Alqt A1	Alt 2 Scheme	1.00000	Remainder	Original Concentration	0.900	Calculate

Figure 36: Scheme Aliquots Configurations – SCHEME_002

The *Aliquot Instructions* table is configured to work with all three aliquot groups. The target aliquot group has nine steps. First, the sample is reconstituted. Then the 'Process Volume 1' is removed. The calculated 'Add Volume' of diluent is added to the process sample and mixed. Aliquots Alqt A1, Alqt A2, and Alqt A3 are created. Then aliquots Alqt A, Alqt B, and Alqt C are created from the remaining parent sample.

The Alt 1 aliquot group also has nine steps. First the sample is reconstituted, and then the 'Process Volume 1' is removed. The calculated 'Adjust Volume' is removed from the parent sample and added to the process sample and mixed. Aliquots Alqt A1, Alqt A2, and Alqt A3 are created. Then Aliquots Alqt A, Alqt B, and Alqt C are created from the remaining parent sample.

The Alt 2 aliquot group only has two steps. The sample is reconstituted, and then the entire parent sample volume is added to aliquot Alqt 1. A screenshot of the *Aliquot Instruction Steps* table configuration is displayed in Figure 37.

Scheme Aliquots | Aliquot Instruction Steps | Label Design

	Step Num	Alqt Group	Alqt Name	Alqt Step	Alqt Step Desc
1	1.00000	Target Schen		RECON_SAMPL	Reconstitute extract in |RECON_VOLUME| mL of Diluent.
2	2.00000	Target Schen		PROCESS_VOL1	Remove |PROCESS_VOLUME1| mL of Parent Sample and transfer to a Processing Tube.
3	3.00000	Target Schen		ADD_VOLUME	Add |ADD_VOLUME| mL of Diluent to the Processing Tube and mix.
4	4.00000	Target Schen	Alqt A1	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
5	5.00000	Target Schen	Alqt A2	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
6	6.00000	Target Schen	Alqt A3	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
7	7.00000	Target Schen	Alqt A	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
8	8.00000	Target Schen	Alqt B	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
9	9.00000	Target Schen	Alqt C	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
10	1.00000	Alt 1 Scheme		RECON_SAMPL	Reconstitute extract in |RECON_VOLUME| mL of Diluent.
11	2.00000	Alt 1 Scheme		PROCESS_VOL1	Remove |PROCESS_VOLUME1| mL of Parent Sample and transfer to a Processing Tube.
12	3.00000	Alt 1 Scheme		ADJUST_VOLU	Add |ADJUST_VOLUME| mL of Parent Sample to the Processing Tube and mix.
13	4.00000	Alt 1 Scheme	Alqt A1	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
14	5.00000	Alt 1 Scheme	Alqt A2	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
15	6.00000	Alt 1 Scheme	Alqt A3	ALQT_VOL_PRO	Pipette |ALQT_VOLUME| mL from Processing Tube into aliquot labeled |ALQT_SAMP_NUM|.
16	7.00000	Alt 1 Scheme	Alqt A	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
17	8.00000	Alt 1 Scheme	Alqt B	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
18	9.00000	Alt 1 Scheme	Alqt C	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.
19	1.00000	Alt 2 Scheme		RECON_SAMPL	Reconstitute extract in |RECON_VOLUME| mL of Diluent.
20	2.00000	Alt 2 Scheme	Alqt A1	ALQT_SAMPLE	Pipette |ALQT_VOLUME| mL from the Parent Sample into the aliquot labeled |ALQT_SAMP_NUM|.

Figure 37: Aliquot Instruction Steps Configuration – SCHEME_002

The *Label Design* table is configured to display 6 lines of data on the label. The first line displays the aliquot name from SAMPLE.X_ALQT_NAME. The next line will display the SAMPLE.SAMPLE_NUMBER of the aliquot followed by the SAMPLE.SAMPLE_NUMBER in barcode format. The next three lines are configured to display the aliquot results. A tag of 'Conc', 'Vol', or 'Yld' is followed by the RESULT.FORMATTED_RESULT and the RESULT.UNITS where the component name equals 'DNA Concentration', 'DNA Volume', or 'DNA Yield'. A screenshot of the *Label Design* table configuration is displayed in Figure 38.

Scheme Aliquots | Aliquot Instruction Steps | Label Design

	Label Line	Data Type	Description	Literal Tag	Table 1	Table Field 1	Table Where Clause 1	Table 2	Table Field 2	Table Where Clause 2	Table 3	Table Fi
1	1.00000	Database	Aliquot Name		SAMPLE	X_ALQT_NAME						
2	2.00000	Database	Sample Numbe		SAMPLE	SAMPLE_NUMBER						
3	3.00000	Barcode	Sample Numbe		SAMPLE	SAMPLE_NUMBER						
4	4.00000	Database	Concentration	Conc	RESULT	FORMATTED_ENTRY	NAME = 'DNA CONCE	RESULT	UNITS	NAME = 'DNA CONCE		
5	5.00000	Database	DNA Volume	Vol	RESULT	FORMATTED_ENTRY	NAME = 'DNA Volume	RESULT	UNITS	NAME = 'DNA Volume		
6	6.00000	Database	DNA Yield	Yld	RESULT	FORMATTED_ENTRY	NAME = 'DNA YIELD'	RESULT	UNITS	NAME = 'DNA YIELD'		

Figure 38: Label Design Configuration – SCHEME_002

Rules Manager Configuration – SCHEME_002

To execute the aliquotting scheme, rule set 'DNA_COMPLEX_SCHEME_1' was configured. The *Summary* tab was configured with a *Description* of 'DNA Complex Scheme 1' and the *Enabled* Boolean set to 'T'. The *Summary* tab is displayed in Figure 39.

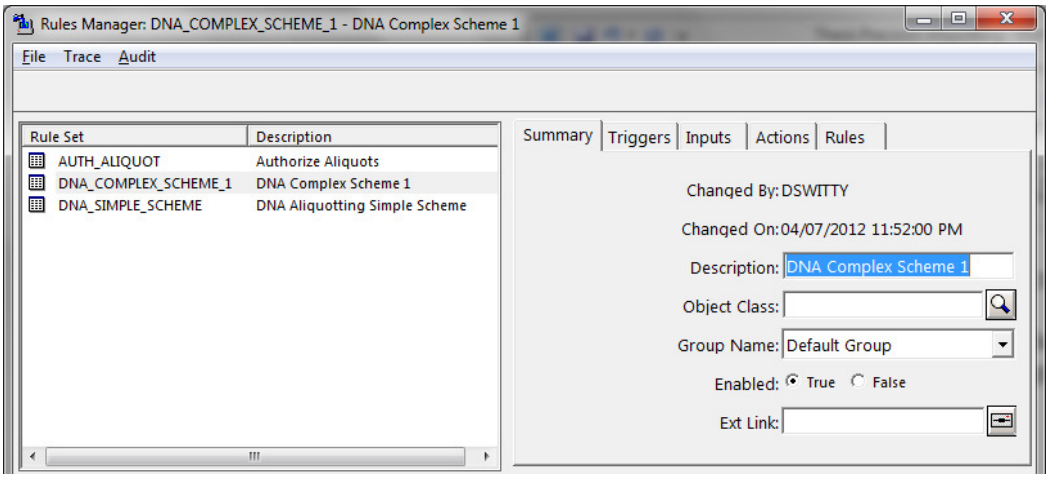


Figure 39: Rules Manager – DNA_COMPLEX_SCHEME_1 Summary Tab

The Triggers tab is configured to execute the rule set when a test with Analysis DNA_EXTACT_001 gets the *Status* field updated to 'Authorized'. The configured *Triggers* tab is displayed in Figure 40.

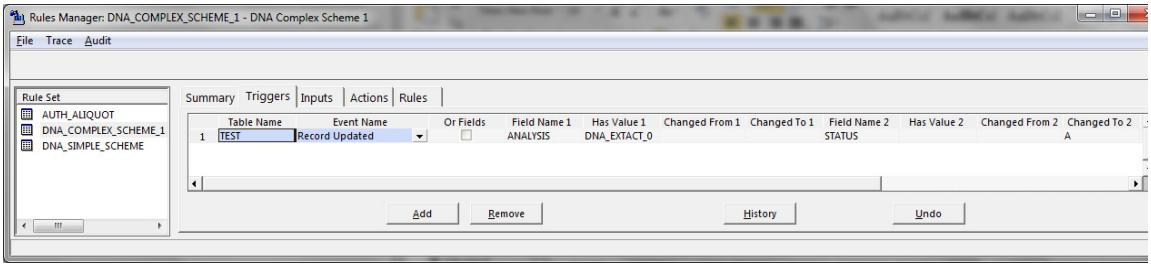


Figure 40: Rules Manager – DNA_COMPLEX_SCHEME_1 Triggers Tab

The *Inputs* tab is configured to feed the appropriate values into the rule actions. A summary of the inputs is displayed in Table 6.

Input	**Source**	**Description**
REP_COUNT	Object Field	TEST.REPLICATE_COUNT
ALQT_SCHEME_TYPE	SQL Query	SELECT SCHEME_TYPE FROM X_ALIQUOT_SCHEME WHERE SCHEME_NAME = {ALQ_SCHEME}
ALQ_SCHEME	Object Field	SAMPLE.X_SCHEME_NAME

CONC_RESULT	SQL Query	SELECT ENTRY FROM RESULT WHERE TEST_NUMBER = {CUR_TEST_NUM} and NAME = 'CONCENTRATION'
CUR_TEST_NUM	Object Field	TEST.TEST_NUMBER
CUR_SMP_NUM	Object Field	TEST.SAMPLE_NUMBER
ALT_ANALYSIS	Literal	Returns value “DNA_ALIQUOT”
CUR_ANALYSIS	Literal	Returns value “DNA_EXTACT_001”
CUR_BATCH_NAME	Object Field	TEST.BATCH
TARGET_CONC_1	SQL Query	select MIN_TARGET_SAMP_CONC from X_ALIQUOT_SCHEME where SCHEME_NAME = {ALQ_SCHEME}
TARGET_CONC_2	SQL Query	select MIN_TRGT_SAMP_CONC_2 from X_ALIQUOT_SCHEME where SCHEME_NAME = {ALQ_SCHEME}
TARGET_CONC_3	SQL Query	select MIN_TRGT_SAMP_CONC_3 from X_ALIQUOT_SCHEME where SCHEME_NAME = {ALQ_SCHEME}
REJECT_REASON	Literal	Returns value “Test Result out of Range, Reject Test”
CONC_CRITICAL_LOW	SQL Query	select CONC_LOW_CAN_LIMIT from X_ALIQUOT_SCHEME where SCHEME_NAME = {ALQ_SCHEME}
CANCEL_REASON	Literal	Returns value “DNA Concentration out of Range. Test Cancelled.”

Table 6: Rules Manager – DNA_COMPLEX_SCHEME_1 Input Summary

The *Actions* tab is configured to execute the critical functions of Adding Test Replicates, Rejecting Tests, Cancelling Tests, Setting the Aliquot Group, Adding Aliquots, and Updating Aliquot Results. A summary is displayed in Table 7.

Action	**Action Type**	**Subroutine**	**Inputs**
CANCEL_TEST_SUB	Subroutine	CANCEL_TEST	Test Number to Cancel: CUR_TEST_NUM Sample Number of Tests: CUR_SMP_NUM Analysis: CUR_ANALYSIS Type of Flag: CANCEL CANCEL REASON: CANCEL_REASON
REJECT_TEST_SUB	Subroutine	REJECT_TEST	Test Number to Reject: CUR_TEST_NUM Sample Number of Tests: CUR_SMP_NUM Analysis: CUR_ANALYSIS Type of Flag: REJECT Reject Reason: REJECT_REASON
ADD_TEST_REP	Subroutine	ADD_TEST_SUB	Sample Number for Current Test:

			CUR_SMP_NUM Current Analysis: CUR_ANALYSIS Current Batch Name: CUR_BATCH_NAME Number of Test to Add: 1 Maximum Replicates to add: 2
SET_ALQT_GRP_ALT1	Function	SET_ALQT_GRP_ALT1	Aliquot Group: alqtGroup Target Aliquot Group: alqtGroup Aliquot Group Value: ALT_1
SET_ALQT_GRP_TARGET	Function	SET_ALQT_GRP_TARGET	Aliquot Group: alqtGroup Target Aliquot Group: alqtGroup Aliquot Group Value: TARGET
UPDATE_ALQT_RSLTS	Subroutine	UPDATE_ALIQUO_RSLTS	Current Sample Number: CUR_SMP_NUM Current Test Number: CUR_TST_NUM Aliquot Analysis: ALT_ANALYSIS Aliquot Scheme: ALQ_SCHEME Concentration Result: CONC_RESULT
ADD_DNA_ALIQUOT	Subroutine	ADD_DNA_ALIQUOT	Current Sample Number: CUR_SMP_NUM Current Test Number: CUR_TST_NUM Aliquot Analysis: ALT_ANALYSIS Aliquot Scheme: ALQ_SCHEME Concentration Result: CONC_RESULT
SET_ALQT_GRP_ALT2	Function	SET_ALQT_GRP_ALT2	Aliquot Group: alqtGroup Target Aliquot Group: alqtGroup Aliquot Group Value: ALT_2

Table 7: Rules Manager – DNA_COMPLEX_SCHEME_1 Actions Tab Summary

The *Rules* tab is configured to evaluate the aliquot scheme type. If the scheme type does not equal 'COMPLEX_01', the rule stops and the evaluation ends. If the scheme type is 'COMPLEX_01', the parent sample concentration result is evaluated against the target rule. If the concentration is greater than the target concentration 1, then action 'SET_ALQT_GRP_TARGET executes and sets the aliquot group to 'TARGET'.

Action ADD_DNA_ALIQUOT executes subroutine RULE_SUB_ADD_ALIQUOTS which checks the aliquotting scheme to determine the number of aliquots to create. The subroutine adds the aliquots, adds the 'DNA_ALIQUOT' analysis to each aliquot, and then sets the aliquot name and aliquot scheme on each aliquot sample. The rule executes action 'UPDATE_ALQT_RSLTS' which runs subroutine 'RULE_SET_ALQT_RESULTS' which fetches the aliquot specific settings for the target aliquot group from the aliquotting scheme and sets the aliquot results on the 'DNA_ALIQUOT' analysis. The subroutine then writes the aliquot information to the X_ALQT_INSTRUCTION table for use in a Crystal Report. When all of the aliquots are created, the subroutine 'RULE_SET_INSTR_STEPS' fetches the scheme aliquotting instructions and writes the final formatted aliquotting steps to the X_ALQT_REPORT_STEPS for display in a Crystal Report.

If the parent sample concentration is less than the target concentration 1 and greater than the minimum target concentration 2, then action 'SET_ALQT_GRP_TARGET executes and sets the aliquot group to 'ALT_1'. Action ADD_DNA_ALIQUOT executes subroutine RULE_SUB_ADD_ALIQUOTS which checks the aliquotting scheme to determine the number of aliquots to create. The subroutine adds the aliquots, then adds the 'DNA_ALIQUOT' analysis to each aliquot and sets the aliquot name and aliquot scheme on each aliquot sample. The rule executes action 'UPDATE_ALQT_RSLTS' which runs subroutine 'RULE_SET_ALQT_RESULTS' to fetch the aliquot specific settings for the Alt 1 aliquot group from the aliquotting scheme and set the aliquot results on the 'DNA_ALIQUOT' analysis. The subroutine then writes the aliquot information to the X_ALQT_INSTRUCTION table for use in a Crystal Report. When all of the aliquots are created, subroutine 'RULE_SET_INSTR_STEPS' fetches the scheme aliquotting instructions and writes the final formatted aliquotting steps to the X_ALQT_REPORT_STEPS for display in a Crystal Report.

If the parent sample concentration is less than the minimum target concentration 2, but greater than the concentration low cancel limit, then action 'SET_ALQT_GRP_TARGET executes and sets the aliquot group to 'ALT_1'. Action ADD_DNA_ALIQUOT executes subroutine RULE_SUB_ADD_ALIQUOTS which

checks the aliquotting scheme to determine the number of aliquots to create. The subroutine adds the aliquots, then adds the 'DNA_ALIQUOT' analysis to the aliquot and sets the aliquot name and aliquot scheme on the aliquot sample. The rule executes action 'UPDATE_ALQT_RSLTS' which runs subroutine 'RULE_SET_ALQT_RESULTS' to fetch the aliquot specific settings for the Alt 2 aliquot group and sets the aliquot results on the 'DNA_ALIQUOT' analysis. The subroutine then writes the aliquot information to the X_ALQT_INSTRUCTION table for use in a Crystal Report. When all of the aliquots are created, subroutine 'RULE_SET_INSTR_STEPS' executes and fetches the scheme aliquotting instructions and writes the final formatted aliquotting steps to the X_ALQT_REPORT_STEPS table for display in a Crystal Report.

If the parent sample concentration is less than the concentration low cancel limit, the rule checks the number of replicates on the current test. If the TEST.REPLICATE_COUNT = '1', then action REJECT_TEST_SUB executes subroutine RULE_SUB_CANCEL_REJECT_TEST which rejects the current test, sets a flag using the 'Default' flag template, and sets the defined reject reason. Action ADD_TEST_REP then runs subroutine RULE_SUB_ADD_TEST which adds a replicate test to the currently selected sample.

If the TEST.REPLICATE_COUNT is not equal to '1', then Action CANCEL_TEST_SUB runs subroutine RULE_SUB_CANCEL_REJECT_TEST which reactivates the authorized test to allow LabWare to then cancel the test. A cancel flag is added using the 'Default' flag template and the rule defined cancel reason is added to the flag. A screenshot of the rule logic is displayed in Figure 41.

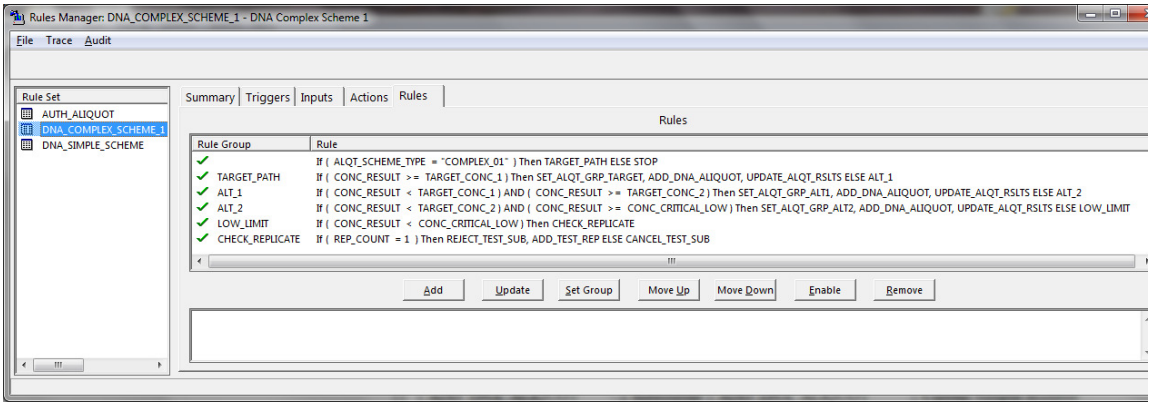


Figure 41: Rules Manager – DNA_COMPLEX_SCHEME_1 Rules Tab Configuration

Rule Set AUTH_ALIQUOT was defined to auto-authorize the DNA_ALIQUOT analysis added to DNA aliquots once the test is updated to a status of complete. This rule is described in the previous section and works will all aliquot samples with the 'DNA_ALIQUOT' analysis assigned.

SCHEME_002 Design Evaluation

To demonstrate the design of Aliquot SCHEME_002, four samples have been logged into the system by selecting the Sample Interface button from the main menu and using the Sample Login Template DNA_PARENT_SAMP. During the login process, the samples are linked to SCHEME_002. Samples 1108, 1109, 1110, and 1111 have been logged and added to batch 'DNA-04/10/12-01' by opening Batch Manager from the Main Menu icon and selecting the template DNA_BATCH. A screenshot of the batch and samples is displayed in Figure 42.

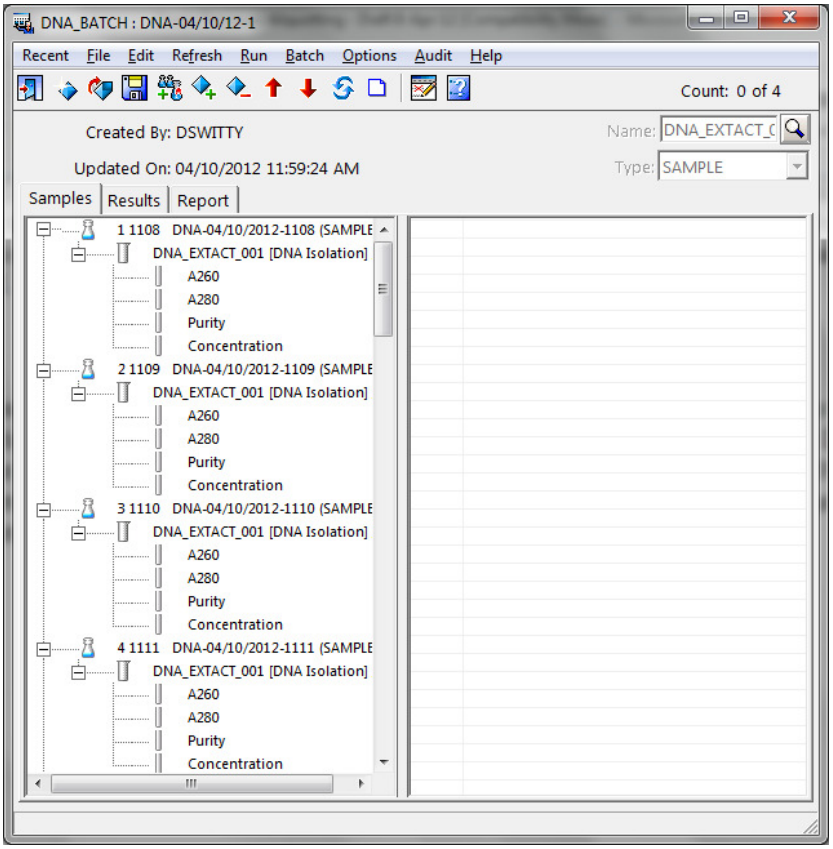


Figure 42: DNA Batch DNA-04/10/12-01 for Testing SCHEME_002

The samples in the batch are resulted by selecting the Options > Result Entry by Test to open the resulting grid. The entered values are displayed in the screenshot in Figure 43.

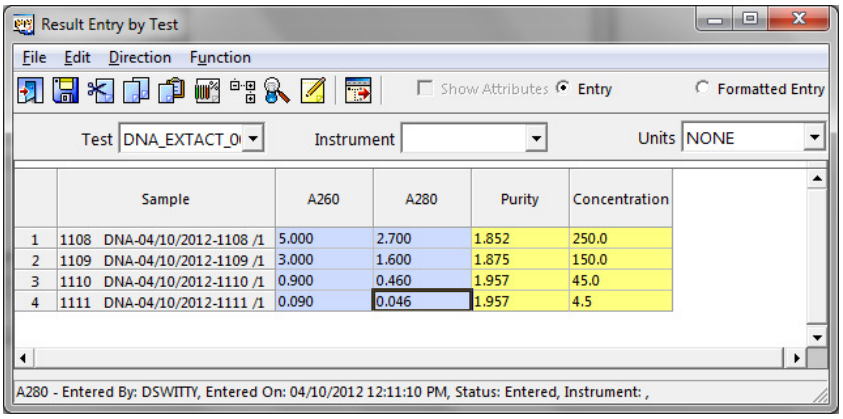


Figure 43: DNA Batch DNA-04/10/12-01 Entered Results

The entered results are saved and the tests are authorized by selecting Options > Grid Review by Test. The user sets the review level to test, highlights each record, and clicks on the 'Authorize' button. The rule set executes on the test authorized event.

Sample 1108 produced an achieved concentration greater than the minimum target concentration 1 of 200 µg/mL. On test authorization, rule set DNA_COMPLEX_SCHEME_1 determined that the concentration of 250 µg/mL is greater than the minimum target concentration 1 and set the aliquot group variable to 'TARGET'. The rule executes the target rule group and adds six aliquots which is the scheme defined number of aliquots for the target group. The results of each aliquot are set based on the *Scheme Aliquots* table definitions for the target scheme. Aliquots Alqt A1, Alqt A2, and Alqt A3 are resulted with a concentration of 200 µg/mL, a volume of 0.100 mL, and a yield of 20 µg. Aliquots Alqt A, Alqt B, and Alqt C are resulted with a concentration of 250 µg/mL, a volume of 0.200 mL, and yield of 50 µg. When the DNA_ALIQUOT analysis test was updated to complete, Rule Set 'AUTH_ALIQUOT' auto-authorized the test on each aliquot of sample 1108. The aliquot instructions are generated and all of the information is displayed in the Batch Summary Report which can be seen by saving the batch and clicking on the *Report* tab. A screenshot of the Batch Summary Report is displayed in Figure 44.

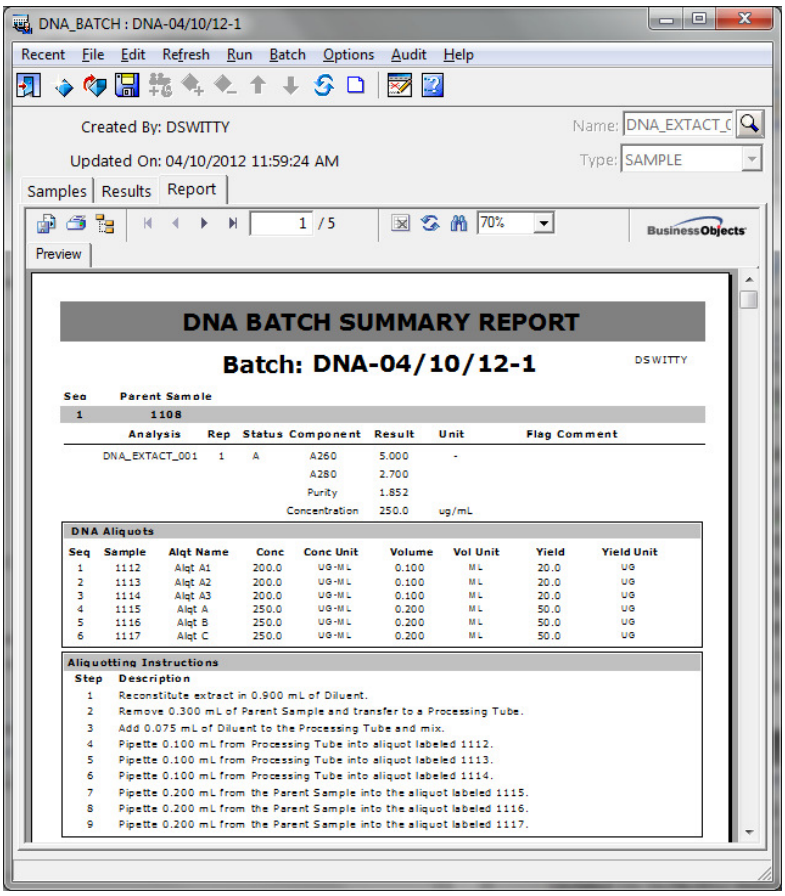


Figure 44: Batch Summary Report for Parent Sample 1108

Sample 1108 produced aliquots and a user can select the Options > Print Aliquot Labels to generate the aliquot labels. The labels are produced with the six fields defined on the *Label Design* table on the aliquotting scheme. A screenshot of the labels is displayed in Figure 45.

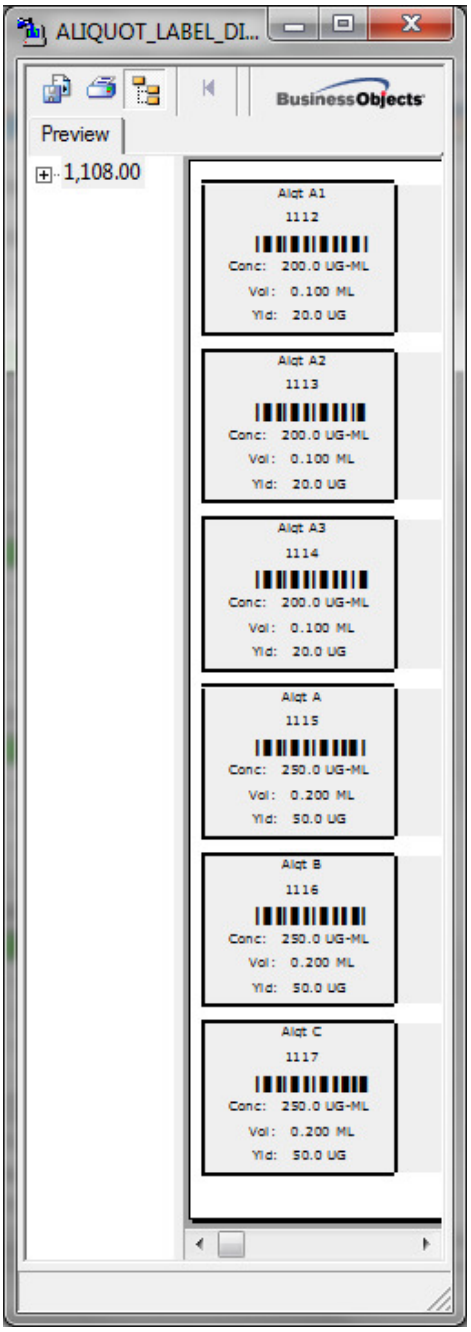


Figure 45: Aliquot Labels for Parent Sample 1108

Sample 1109 produced an achieved concentration less than the minimum target concentration 1 of 200 µg/mL and greater than the minimum target concentration 2 of 50 µg/mL. On test authorization, rule set DNA_COMPLEX_SCHEME_1 determines that the concentration of 150 µg/mL is less than the minimum target concentration 1 and greater than the minimum target concentration 2 and sets the aliquot group to 'ALT_1'.

The rule fires the Alt 1 rule group and adds six aliquots which is the scheme defined number of aliquots for the Alt 1 aliquot group. The results of each aliquot are set based on the *Scheme Aliquots* table definitions for the Alt 1 scheme. Aliquots Alqt A1, Alqt A2, and Alqt A3 are resulted with a concentration of 150 µg/mL, a volume of 0.133 mL, and a yield of 20 µg. Aliquots Alqt A, Alqt B, and Alqt C are resulted with a concentration of 150 µg/mL, a volume of 0.167 mL, and yield of 25 µg. When the DNA_ALIQUOT analysis test is updated to complete, rule set 'AUTH_ALIQUOT' auto-authorizes the test on each aliquot of sample 1109. The aliquot instructions are generated and all of the information is displayed in the Batch Summary Report which can be viewed by saving the batch and clicking on the *Report* tab. A screenshot of the Batch Summary Report is displayed in Figure 46.

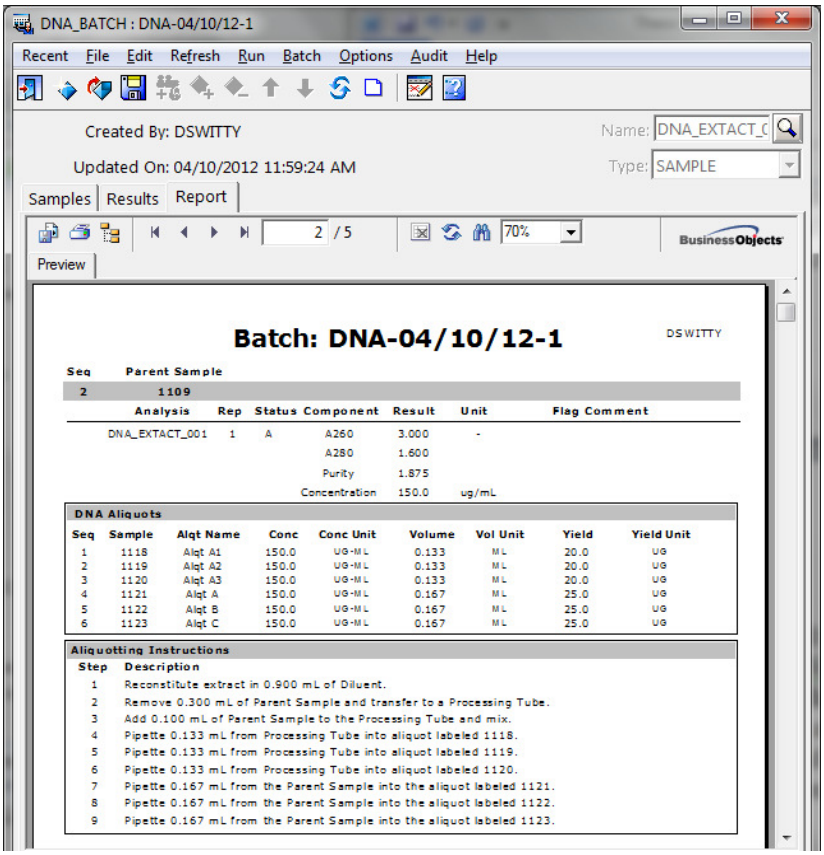


Figure 46: Batch Summary Report for Parent Sample 1109

Sample 1109 produced aliquots and a user can select the Options > Print Aliquot Labels to generate the aliquot labels. The labels are produced with the six fields defined

on the *Label Design* table on the aliquotting scheme. A screenshot of the label is displayed in Figure 47.

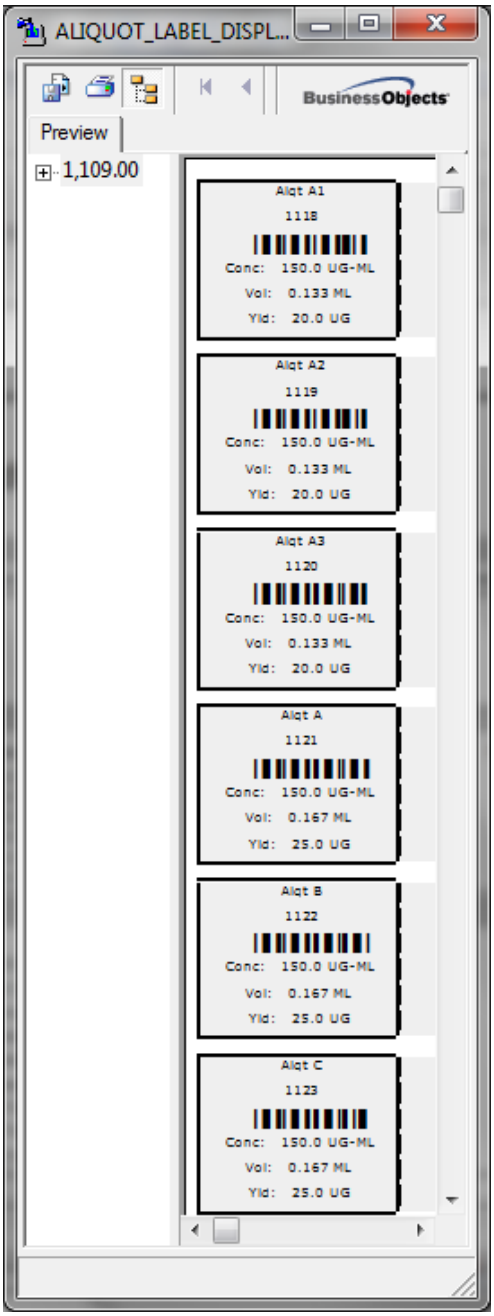


Figure 47: Aliquot Labels for Parent Sample 1109

Sample 1110 produced an achieved concentration less than the minimum target concentration 2 of 50 µg/mL and greater than the concentration low cancel limit of 10 µg/mL. On test authorization, rule set DNA_COMPLEX_SCHEME_1 determines that

the concentration of 45 µg/mL is less than the minimum target concentration 2 and greater than the concentration low cancel limit which set the aliquot group to 'ALT_2'. The rule executes the Alt 2 rule group and it creates one aliquot which is the scheme defined number of aliquots for the Alt 2 aliquot group. The results of each aliquot are set based on the *Scheme Aliquots* table definitions for the Alt 2 scheme. Aliquot Alqt A1 is resulted with a concentration of 45 µg/mL, a volume of 0.900 mL, and a yield of 40.5 µg. When the DNA_ALIQUOT analysis test is updated to complete, rule set 'AUTH_ALIQUOT' auto-authorizes the test on each aliquot of sample 1110. The aliquot instructions are generated and all of the information is displayed in the Batch Summary Report which can be viewed by saving the batch and clicking on the *Report* tab. A screenshot of the Batch Summary Report is displayed in Figure 48.

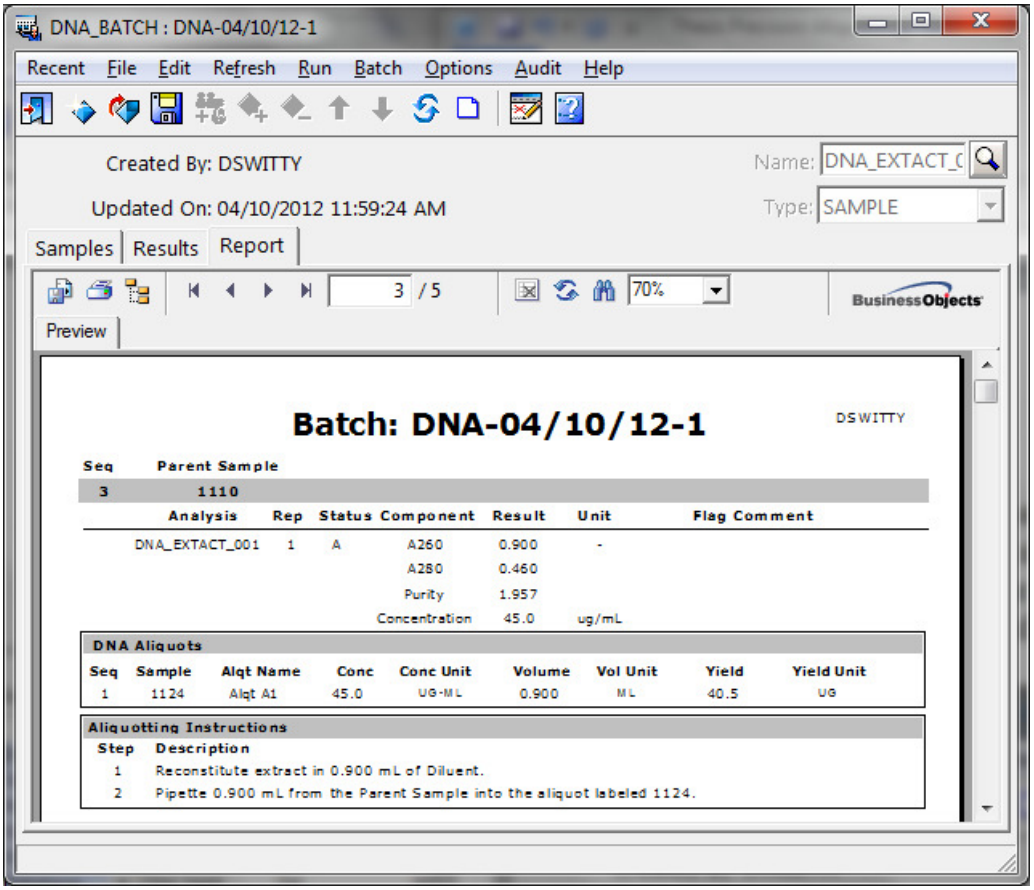


Figure 48: Batch Summary Report for Parent Sample 1110

Sample 1110 produced aliquots, and a user can select the Options > Print Aliquot Labels to generate the aliquot labels. The labels are produced with the six fields defined on the *Label Design* table on the aliquotting scheme. A screenshot of the label is displayed in Figure 49.

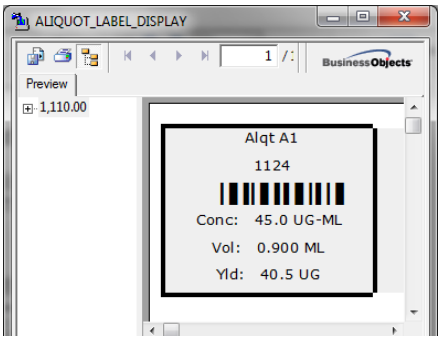


Figure 49: Aliquot Labels for Parent Sample 1110

Sample 1111 produced an achieved concentration of 4.5 µg/mL which is less than the concentration low cancel limit. On test authorization, rule set DNA_COMPLEX_SCHEME_1 determines that the parent concentration was below the concentration low cancel limit of 10 µg/mL and then checks the TEST.REPLICATE_COUNT. The replicate count is equal to 1, the test is rejected, and a flag with the defined rejection comment is added. A replicate DNA_ALIQUOT test is added to sample 1111. A screenshot of the batch for sample 1102 with a flag attached and a replicate test added is displayed in Figure 50.

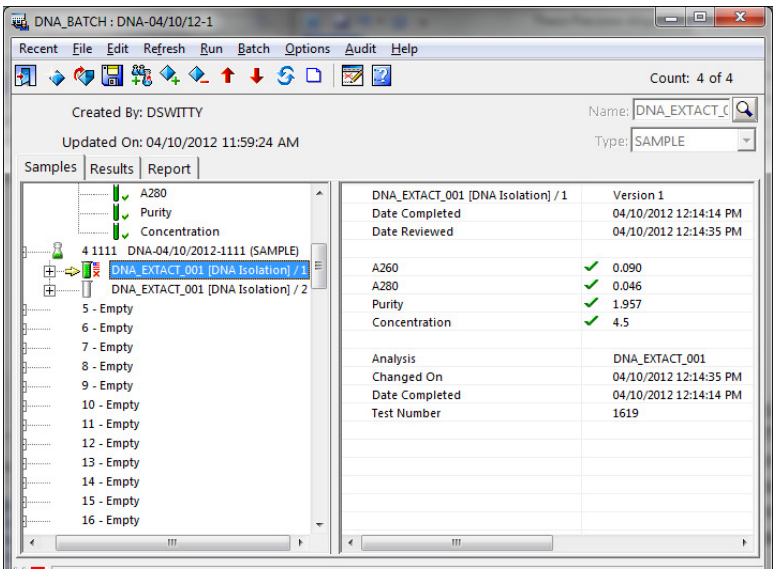


Figure 50: Batch DNA-04/08/12-01 Sample 1111 Replicates and Flag

The replicate test for 1111 produced an achieved concentration value less than the concentration low cancel limit. On test authorization, rule set DNA_COMPLEX_SCHEME_1 determines that the concentration of 4.5 µg/mL is less than the concentration low cancel limit. The rule set then checks the replicate count and determines that it is not equal to 1. The current test is canceled and a flag is added with the defined cancel reason. A screenshot of sample 1111 in the batch is displayed in Figure 51.

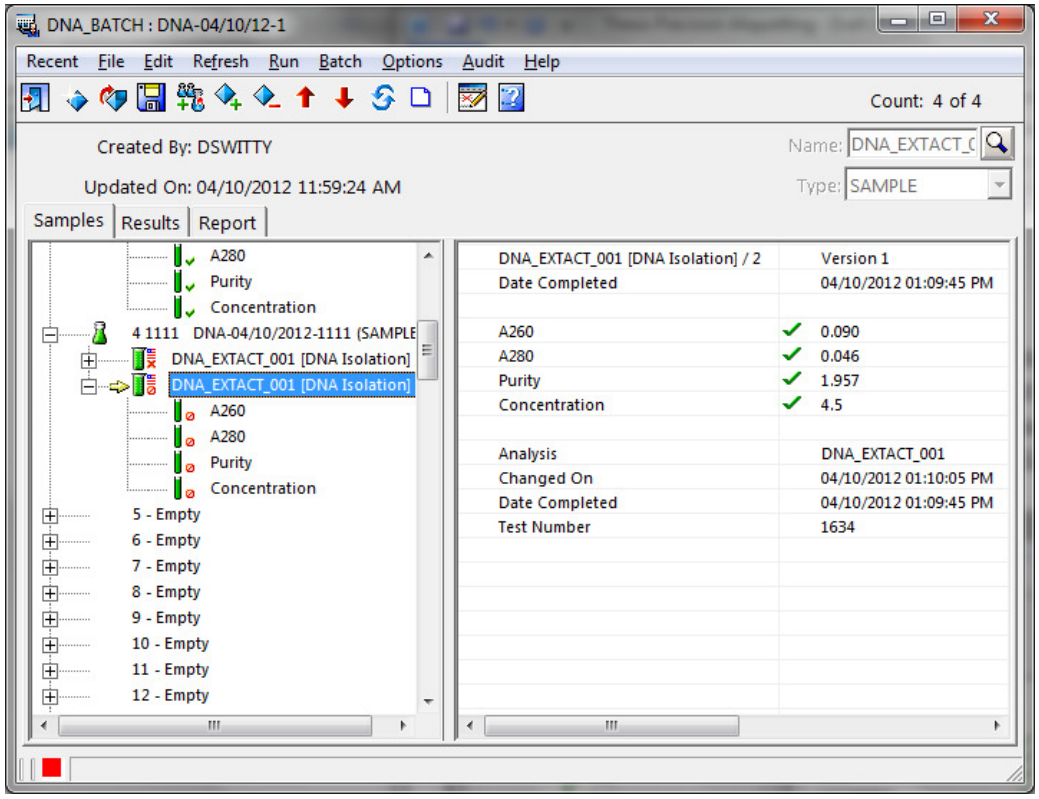


Figure 51: Batch DNA-04/10/12-01 Sample 1111 with Rejected and Cancelled Replicates

Because sample 1111 did not produce a concentration that would produce viable aliquots, the rule set did not create any aliquots or aliquot instructions. A screenshot of the Batch Summary report is displayed in Figure 52.

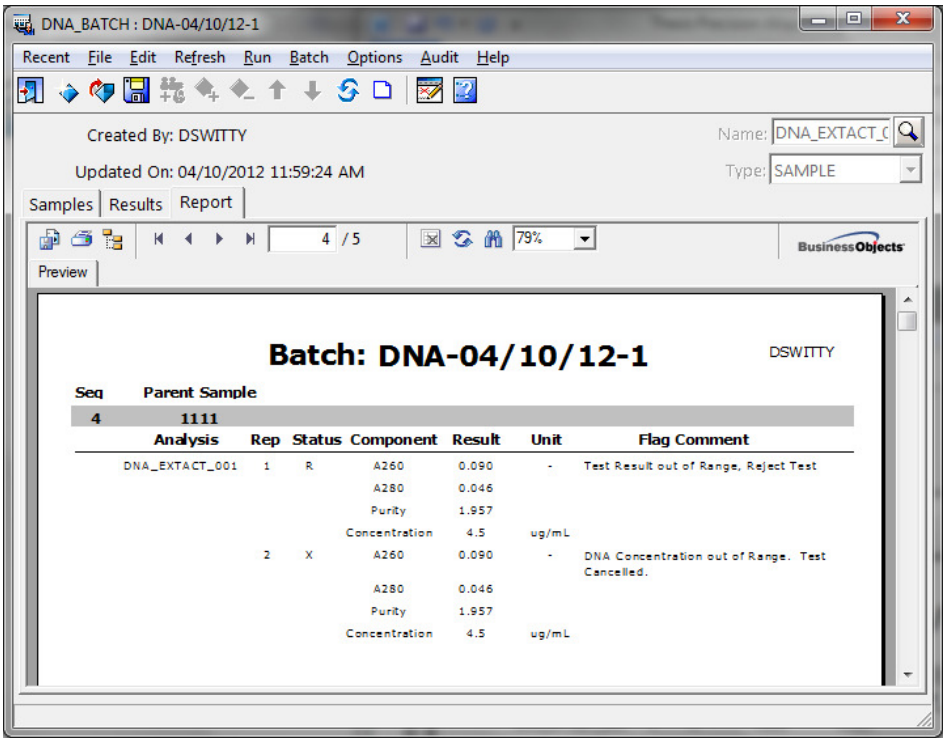


Figure 52: Batch Summary Report for Sample 1111

CHAPTER FOUR: DISCUSSION

The precision aliquotting workflow configured using the LabWare LIMS model successfully created sample aliquots, aliquot instructions, and aliquot labels as defined in the Aliquot Scheme Tool. The development work in building the Aliquot Scheme Tool template supported the ability to define the aliquot schemes for SCHEME_001 and SCHEME_002. The development of the inputs and actions in Rules Manager allowed the creation of the rules logic to execute and implement the aliquotting schemes. The LabWare model also demonstrated the ability to manage the typical functionality required in a laboratory to execute an end-to-end precision aliquotting workflow. A comparison of the typical laboratory functional workflow versus the demonstrated LabWare model is displayed in the summary in Figure 53.

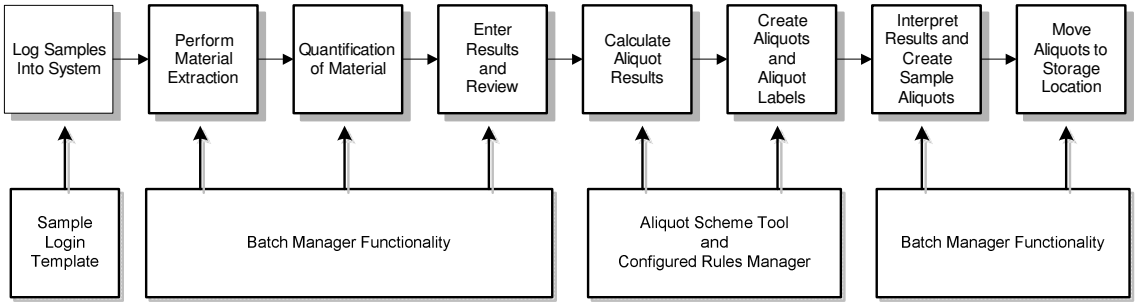


Figure 53: Comparison of Clinical Trial Process with LabWare Model

The ability of LabWare LIMS to be customized and configured to manage laboratory processes and data led to the successful implementation of this precision aliquotting model. Samples that need to be created and logged into the workflow are managed in LabWare using the Sample Login Template. The template can easily be configured to capture the important data that needs to be linked to the sample in the login user interface. In this model the user links the aliquotting scheme to the sample. Batches are LabWare's object for grouping samples and information together. In this model, the batch template was configured to group and organize the genomic samples for DNA testing. The Batch Manager interface links the user to most of the core laboratory functionality managed by LabWare. The DNA extraction and quantification of the genomic samples is performed in batch sets organized using Batch Manager. Batch Manager also links to the result entry and review interfaces. As results become available for entry, the samples can easily be opened in the resulting and review dialogs. Batch

Manager also links to the Batch Summary Report interface. This Crystal Report was developed to display all of the critical aliquotting scheme results and instructions to the user in a single interface.

The creation and resulting of DNA aliquots is defined by the Aliquot Scheme Tool and executed by the scheme rules logic. The combination of the two adds a significant level of efficiency by automating the aliquot creation process. The aliquot scheme also defines the aliquot labels and aliquot instructions. Because the samples are all grouped in a batch, Batch Manager provides the ideal organized user interface for managing aliquot creation, label creation functionality, and displaying the aliquot instructions. The base LabWare functionality combined with the custom design elements in this model provide an efficient and intuitive interface for managing the precision aliquotting workflow.

CHAPTER FIVE: CONCLUSION

The open architecture of a LIMS supported the implementation of a complex laboratory workflow. The ability to extend the core functionality of a LIMS through customization of add-on modules and configuration tools allows for the implementation of most laboratory workflows. The highly configurable LIMS may not require the overhead and specialized support of a system built with customized code (Bradburn, n.d). The adaptability of a LIMS supports the extension of the system life-cycle and the long-term sustainability of the system. As the technology and standard procedures of the laboratory continue to evolve, the configuration of the system can be modified to meet the changing needs of the laboratory. The ability of a LIMS to automate laboratory processes will become increasingly important as workflows become more complex and require the management of the increasing amount of data. The addition of automation into the workflow will support the reduction of laboratory errors and loss of sample. The implementation of a LIMS in the laboratory model demonstrated the ability to manage laboratory workflow processes and data.

The implementation of the precision aliquotting workflow using LIMS demonstrated the ability to significantly improve the management of a process through automation. The creation of a template driven Aliquot Scheme Tool in LabWare provides the user with an intuitive user interface for defining the scheme. The template solution allows a user to define an almost endless variation of aliquotting schemes. The configured Aliquot Scheme Tool promotes a self-sustaining user method of managing the aliquotting scheme. Some aliquotting schemes are very complex and may require experienced laboratory users to define. A user with a basic understanding of LabWare and a working knowledge of aliquotting schemes would be able to create most of the potential schemes within the template tool. The ability of the user to define the schemes allows the laboratory to take ownership of the process without having to rely on a technical support group to load the scheme data. The laboratory users who possess the first-hand experience and knowledge of the aliquotting schemes would have the tools to define them. This increases the efficiency of creating the schemes because it eliminates the need to manage and maintain the knowledge transfer between the laboratory experts and technical groups.

The precision aliquotting workflow scheme rules logic is executed using the LabWare LIMS Rules Manager module. The Rules Manager is an add-on module that adds a large amount of functionality to LabWare LIMS. It is defined by a set of inputs and actions that may be core functionality or a highly customized set of code. The customized code may require a developer to create, but can be configured as universal objects that can be used across rule sets. Once the inputs and actions are prepared, a user can configure the scheme rules logic based on the expected outcome of the aliquotting scheme. The functionality allows the laboratory to own the process of creating the scheme rules logic.

Limitations

The aliquotting scheme definition tools are configured to allow the user to define and implement an aliquotting scheme. Sophisticated users with a strong knowledge base of what attributes make up an aliquotting scheme will be able to successfully and completely configure a scheme. The aliquotting scheme should be configured to account for all possible result outcomes.

Future Enhancements

The precision aliquotting workflow model designed for this project was created to demonstrate the basic functionality in LabWare LIMS. Further development would be required to implement the model in the regulated environment of a clinical laboratory. The Aliquot Scheme Tool requires some knowledge of the basics of defining an aliquot scheme. A great enhancement to the tool would be a validation function that would evaluate the validity and reasonability of the defined scheme attributes. The validation tool should consider both the scheme definitions and the rule set definitions. Within the scheme it is important that every possible scheme scenario is configured. A validation tool would support the user in correctly and accurately defining the scheme.

An extension of the validation tool would be a function to simulate the scheme based on the defined attributes. The simulation tool would allow a user to confirm that the defined scheme produces the expected outputs.

Another enhancement would be the addition of a visual workflow to help the user track samples through the workflow. The basic LabWare user interface opens the different managers using the buttons on the main menu which is not always user-friendly. LabWare does have the ability to incorporate HTML pages into the main interface with links to open specific functionality. A visual workflow could be configured with links to open Login Templates, Batches, and Sample Folders. This would add a user interface with improved functionality and usability.

LabWare LIMS contains core functionality for supporting interfaces with other laboratory systems. Manual result entry is a common bottleneck in a laboratory. In a regulated environment, clinical laboratories are required to implement processes such as double data entry and double review in order to ensure that test results are accurately reported. LabWare has driver configurations available for common laboratory instrumentation where an interface can be implemented to automate the transfer of results into LIMS without the need for manual result entry. If a driver is not available for a specific instrument, LabWare can be configured to accept instrument data. Configuring LabWare to interface with instrumentation and automate result entry would an efficient way to enhance this model.

Another bottleneck in the precision aliquotting workflow is the manual aliquotting. The LabWare workflow model is built on the strategy of a user following the aliquotting instructions to manually transfer the genomic material into the aliquot containers. Several manufactures such as Hamilton, Tecan, and Beckman Coulter offer robotic systems that could be interfaced with LIMS to automate the creation of the aliquots. The aliquot specific data and the aliquotting instructions generated for a sample could be formatted and exported out of LIMS to a robotic system where the aliquots could be created. Interfacing LIMS with a robotic system would enhance the precision aliquotting workflow by decreasing the amount of hands-on tech time while decreasing the potential for transcription errors.

Summary

Through this model, LabWare LIMS functionality demonstrated the ability to manage the precision aliquotting workflow. The Aliquot Scheme Tool and Rules

Manager proved to be capable of defining and executing an aliquotting scheme while maintaining the ability for a user to configure the scheme. The implementation of this model demonstrated the ability of a LIMS to manage a complex laboratory workflow.

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Appendix A – User added LabWare Modules

Module	Description
V601e	Maintenance Release e. Incorporates all maintenance updates up to e.
!M0052-v01_(DatabaseMigrationTool)	Adds Utility Function for managing database updates for Module Additions
!M0298-v01_dev_224_(WorkflowManagement)	Adds Workflow Manager. Allows for the creation of LIMS workflow.
!M0382-v01_dev_007_(Debugger)	Adds Debug Utility function for debugging subroutines.
!M0391-v01_dev_040_(LIMSBasicPart6)	Adds additional LIMS Basic functions.
!M0433-v01_dev_054_(LIMSBasicFunctionsPart7)	Adds additional LIMS Basic functions.
!M0467-v01_dev_032_(RulesEngine)	Adds Rules Manager. This module update adds the Database Tables, LIMS basic functions, and Access Function ID's to run Rules Manager.
!M0493-v01_dev_006_(LIMSBasicFunctionsPart8)	Adds additional LIMS Basic functions.

Appendix B – LabWare Configured Objects

Crystal Report – AliquotLabelDisplay.rpt
Crystal Report – DNA Batch Summary Report.rpt
Crystal Report – DNA Aliquotting Instructions.rpt
Crystal Report – Aliquot Steps SubReport.rpt
Crystal Report – Aliquot Details SubReport.rpt
Aliquot Scheme – SCHEME_001
Aliquot Scheme – SCHEME_002
Aliquot Step Variables – ADD_VOLUME
Aliquot Step Variables – ADJUST_VOLUME
Aliquot Step Variables – ALQT_NAME
Aliquot Step Variables – ALQT_SAMP_NUM
Aliquot Step Variables – ALQT_VOLUME
Aliquot Step Variables – PARENT_SAMPLE
Aliquot Step Variables – PROCESS_VOLUME1
Aliquot Step Variables – PROCESS_VOLUME2
Aliquot Step Variables – PROCESS_VOLUME3
Aliquot Step Variables – RECON_VOLUME
Aliquotting Steps – ADD_VOLUME
Aliquotting Steps – ADJUST_VOLUME_TOTAL
Aliquotting Steps – ALQT_SAMPLE
Aliquotting Steps – ALQT_VOL_PROCESS
Aliquotting Steps – DISCARD_PROCESS_TUBE
Aliquotting Steps – PROCESS_VOL1
Aliquotting Steps – RECON_VOL1
ANALYSIS – DNA_ALIQUOT
ANALYSIS – DNA_EXTACT_001
BATCH_TESTS_TEMPLATE – DNA_BATCH
COMMON_NAME – DNA
COMMON_NAME – DNA_PARENT
CONDITIONS – AMBIENT
CONDITIONS – FROZEN-70
CONDITIONS – REFRIGERATED
CUSTOMERS – WITTY_LABS
FLAG_TEMPLATES – DEFAULT
FOLDER_GROUP
FOLDER_TEMPLATE – DNA_ALQT_INSTR
FOLDER_TEMPLATE – DNA_FLDR_PEND_SAMPS
FOLDER_TEMPLATE – DNA_FLDR_READY_TEST
LISTS – X_ALIQUOT_TYPE
LISTS – X_ALQT_ACTION
LISTS – X_LABEL_DATE_TYPE
LISTS – X_NONE
LISTS – X_SCHEME_TYPE
MENU_ROUTINE – BM_PRINT_ALQ_LABELS
QUERY_TAGS – ALIQUOT_LABEL_DISPLAY
QUERY_TAGS – DNA_FLDE_READY_TESTING

QUERY_TAGS – DNA_FLDR_PEND_SAMP
QUERY_TAGS – FLDR_DNA_INSTRUCTIONS
QUERY_TAGS – FLDR_DNA_PENDING
QUERY_TAGS – FLDR_DNA_SAMPLES
RULE_ACTION_FUNCTIONS – ADD_CUR_REP
RULE_ACTION_FUNCTIONS – SET_ALQT_GRP_ALT1
RULE_ACTION_FUNCTIONS – SET_ALQT_GRP_ALT2
RULE_ACTION_FUNCTIONS – SET_ALQT_GRP_TARGET
RULE_ACTION_SUBROUTINE – ADD_DNA_ALIQUOT
RULE_ACTION_SUBROUTINE – ADD_TEST_SUB
RULE_ACTION_SUBROUTINE – AUTH_ALQT_TEST
RULE_ACTION_SUBROUTINE – CANCEL_TEST
RULE_ACTION_SUBROUTINE – DNA_ALQT_CMPX1_ALT1
RULE_ACTION_SUBROUTINE – DNA_ALQT_CMPX1_ALT2
RULE_ACTION_SUBROUTINE – REJECT_TEST
RULE_ACTION_SUBROUTINE – UPDATE_ALIQUOT_RSLTS
RULE_MASTER_ACTION – ADD_DNA_ALIQUOT
RULE_MASTER_ACTION – REJECT_TEST_FLAG
RULE_MASTER_ACTION – SET_ALQT_GRP_ALT1
RULE_MASTER_ACTION - SET_ALQT_GRP_ALT2
RULE_MASTER_ACTION – SET_ALQT_GRP_TARGET
RULE_MASTER_ACTION – UPDATE_ALQT_RSLTS
RULE_MASTER_INPUT – ALQ_SCHEME
RULE_MASTER_INPUT – ALQT_SCHEME_TYPE
RULE_MASTER_INPUT – ALT_ANALYSIS
RULE_MASTER_INPUT – CANCEL_REASON
RULE_MASTER_INPUT – CONC_CRITICAL_LOW
RULE_MASTER_INPUT – CONC_RESULT
RULE_MASTER_INPUT – CUR_ANALYSIS
RULE_MASTER_INPUT – CUR_COMPONENT
RULE_MASTER_INPUT – CUR_RES_NUM
RULE_MASTER_INPUT – CUR_SMP_NUM
RULE_MASTER_INPUT – CUR_TEST_NUM
RULE_MASTER_INPUT – CUR_TEST_STATUS
RULE_MASTER_INPUT – PARENT_SMP_NUM
RULE_MASTER_INPUT – REP_COUNT
RULE_MASTER_INPUT – TARGET_CONC_1
RULE_MASTER_INPUT – TARGET_CONC_2
RULE_MASTER_INPUT – TARGET_CONC_3
RULE_MASTER_INPUT – TEST_STATUS
SAMPLE_ID_CONFIGURATION – DEFAULT
SAMPLE_ID_CONFIGURATION – DNA_SAMP_LABELS
SAMPLE_LOGIN_TEMPLATES – DNA_ALQT_SAMP
SAMPLE_LOGIN_TEMPLATES – DNA_PARENT_SAMP
SUBROUTINES – ALQT_MODULATOR
SUBROUTINES – DNA_LOG_SAMPLES
SUBROUTINES – DNA_OPEN_SCHEME
SUBROUTINES – FLDR_DNA_ALIQUOTS

SUBROUTINES – FLDR_DNA_PENDING
SUBROUTINES – RULE_AUTH_ALQT
SUBROUTINES – RULE_SET_ALQT_RESULTS
SUBROUTINES – RULE_SET_INSTR_STEPS
SUBROUTINES – RULE_SUB_ADD_ALIQUOTS
SUBROUTINES – RULE_SUB_ADD_TEST
SUBROUTINES – RULE_SUB_ALT_ADD_ALQTS
SUBROUTINES – RULE_SUB_CANCEL_REJECT_TEST
SUBROUTINES – UTIL_ALQT_LABEL_CRYSTAL
TABLE_MASTER - SAMPLE
TABLE_MASTER – X_ALIQUOT_SCHEME
TABLE_MASTER – X_ALIQUOTTING_STEPS
TABLE_MASTER – X_ALQT_INSTR_STEPS
TABLE_MASTER – X_ALQT_INSTRUCTION
TABLE_MASTER – X_ALQT_LABEL_DISPLAY
TABLE_MASTER – X_ALQT_REPORT_STEPS
TABLE_MASTER – X_ALQT_STEP_VARBLS
TABLE_MASTER – X_LABEL_DESIGN
TABLE_MASTER – X_SCHEME_ALQT_INFO
TABLE_TEMPLATE – X_ALIQUOT_SCHEME
TABLE_TEMPLATE – X_ALQT_INSTR_STEPS
TABLE_TEMPLATE – X_LABEL_DESIGN
TABLE_TEMPLATE – X_SCHEME_ALQT_INFO
VISUAL_WORKFLOWS – DNA_HOME_PAGE
UNITS – ML
UNITS – NONE
UNITS – UG
UNITS – UG-ML
UNITS – UL
USERS – DSWITTY
USERS – LW_ADMIN

Appendix C - Vita

Derick Witty

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Education

Master of Science in Chemical Informatics with a Specialization in Laboratory Informatics, Expected June 2012
School of Informatics, Indiana University Purdue University at Indianapolis (IUPUI)
Thesis: Implementation of A Laboratory Information Management System (LIMS) to manage Genomic Samples

Advisor: Mahesh Merchant

Bachelor of Arts in Biology / Minor in Chemistry, May 24, 1997
Franklin College, Franklin IN

Experience

LIMS Database Administrator, Covance Central Laboratory, Indianapolis, IN
September 2008 - Current

- Responsible for design and configuration of laboratory workflows in LIMS.
- Support system testing and validation teams.

Supervisor, Genomics Laboratory, Covance Central Laboratory, Indianapolis, IN
March 2007 – September 2008

- Responsible for supervision, training, and development of lab personnel.
- Responsible for maintaining inspection ready laboratory and participating in customer audits.
- Requirement gathering, development, and user acceptance testing for instrument interfaces.
- Development and validation of clinical testing platforms.

Senior Technologist, Genomics Laboratory, Covance Central Laboratory, Indianapolis, IN
July 1999 – March 2007.

- Responsible for organization of personnel and daily Workflow.
- Clinical laboratory testing including Genomic Sample preparation, PCR, and Genotyping.
- Validation and development of new testing procedures.
- Verification and reporting of patient data.
- Writing of Standard Operating Procedures and Validation Reports.