Technical Information

File-based Interfaces of the QIAgility® Setup Manager Software

Introduction

This document describes the file-based interfaces of the QIAgility Setup Manager software.

The software supports XML files in QIAGEN Data Exchange Format (QDEF) that describe plates as well as adapters containing tubes. This file format enables the seamless transfer of plates (or adapters with tubes) together with a corresponding list of samples from one instrument to the next in a workflow. First, the XML output file describing the output labware of the QIAcube® HT Prep Manager software is imported as a sample input file into the QIAgility Setup Manager software to describe the samples on the input labware. Then, the XML output file describing the output labware of the QIAgility Setup Manager software is imported as the sample input file into the Q-Rex® Software for Rotor-Gene® Q instruments.

The software is able to read or directly import sample input files during experiment setup, avoiding errors from manually typing in sample ID and position information. The software supports .xml format, as well as a simple .csv or .txt format. When an experiment is finished, the system optionally generates an XML output file describing the output labware. While a report is generated as a PDF for optimized printing, the additional XML output file is intended for automated computer processing.

Figure 1. The QIAgility system

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Overview of file-based interfaces

Table 1. Files that can be transferred to and from the QIAgility Setup Manager software

File type	Description
Sample input file (.csv)	File in .csv format that can be used to import sample information for the input labware.
Sample input file (.xml)	File in .xml format that can be used to import sample information for the input labware; e.g., created by the QIAcube HT Prep Manager software for a sample prep.
Output file (.xml)	File in .xml format describing the output labware and its contents, optimized for electronic data transfer or computational parsing.
Output file in cycler format	Output labware file in cycler-specific format optimized for electronic data transfer to the used thermal cycler. User can opt to create this file after a run via XSL transformation, based on the output labware file in .xml format. This option is available only if the format .xslt is part of the cycler definition. Details are not described in this document.

Location in the file system

The usual storage place for input and output files can be defined under **User Settings** in the **Configuration** environment of the software. Whenever the user imports a file as a sample list or creates an output file after run, a dialog box opens to navigate through the file system starting at the directory defined in User Settings.

Initially, files are located in the following directories:

- For sample input: C:\Users\Public\QIAGEN\QIAgility\SampleFiles
- For output: the same directory as the experiment itself. If this has not been changed for the experiment, these are located at C:\Users\Public\QIAGEN\QIAgility\Experiments

The system supports the use of network folders. Make sure to check the network connection to make network folders available.

Description of file formats

The following sections describe file types supported by the QIAgility Setup Manger software that are relevant to transferring labware and sample information. Each file type is described by a set of tables and examples.

Note: The labware files in .xml format provided by QIAGEN instrument software are digitally signed with a checksum to ensure data integrity. To prevent unauthorized manipulation, the software checks the file signature during sample list import and displays a warning when the signature is invalid. Import is, however, still possible.

Output file (.xml)

The output file (.xml) uses the QIAGEN Data Exchange Format to describe plates as well as adapters containing tubes. This format supports the convenient transfer of plate (or adapters with tubes) information together with a sample list from one instrument to the next, enabling seamless information flow between the QIAcube HT Prep Manager software, the QIAgility Setup Manager software and the Q-Rex Software for Rotor-Gene Q instruments. The XML output file describing the output labware of the QIAcube HT Prep Manager software is imported as the sample input file into the QIAgility Setup Manager software to describe the input labware. Then, the XML output file describing the output labware of the QIAgility Setup Manager software is imported as the sample input file into the Q-Rex Software.

This file type also supports populating the output labware with information from 2 (or more) runs. Save an output labware file after the first run. Then, during experiment setup of the second run, load this first output labware file. The filled positions described by the file are automatically blocked for the second run. After the second run, save the output file again to create a complete description of the output labware with information from both runs.

A labware file in .xml format contains numerous elements. These elements are described in the following tables, each followed by an example. In the tables:

- Name is the name of the XML element or attribute
- Data type is Node for XML elements or the data type of an attribute
- Content is a description of the content of an element or attribute
- # is the cardinality for contained elements (i.e., how often this element is contained)
- Range/Format describes restriction,s where appropriate

PlateFile — The Root Element

PlateFile is the root element that contains all other elements of a labware file. Table 2 lists the contained elements and attributes.

Table 2. PlateFile elements and attributes

Name	Data type	Content	#	Format/Range
SchemaVersion	Integer	The schema-version of the file format		≥ 1
PlateId	String	The (unique) ID of the labware, taken from the barcode on the labware, or generated by the software		Not empty
Description	String	A description of the plate and/or its purpose, entered into the comment field of the run step.		
Modifications	Node	A list of Modification entries. See page 5 for details.	1	n/a
PhysicalLayout	Node	Information about type and layout of the labware. See page 6 for details.	1	n/a
PlateContent	Node	Information about the content of the labware positions. See page 7 for details.	1	n/a
ProcessHistory	Node	Information about the processes that lead to the content of the labware. This is a list of ProcessLog elements. See page 12 for details.	1	n/a
OtherInfo	Node	Not used by the software. See page 15 for details.	0..1	n/a

```
<!-- This is a technical example of an output file. It has no biological value.
PlateID - ID of the output labware, in this example automatically generated by the
QIAgility Setup Manager Software -->
<PlateFile xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:xsd="
http://www.w3.org/2001/XMLSchema" SchemaVersion="1" PlateId="90945_20150920_234630"
Description="Comment entered on Run step.">
  <Modifications>
  <PhysicalLayout LabwareName="96_200_ABI_4316813" LabwareType="ABI MicroAmp® Optical
  96-Well Reaction Plate, 0.1 ml" QiagenMaterialNumber="1087409">
  <PlateContent>
  <ProcessHistory>
</PlateFile>
<!-- QIAsymphony_CHECKSUM TW5tbxsdeTEz1D25O9avPpGSnsF+pew4xVCr5cDo7qY=-->
```

Figure 2. Example of a PlateFile.

PlateFile.Modifications

Modifications contains the list of modifications made to a labware file, and each modification holds a list of references to other items (e.g., documents, mails, etc.).

Table 3. Modifications elements and attributes

Name	Data type	Content	#	Format/Range
Modifications	Node	The list of modifications to a labware file	1	n/a
Modification	Node	Information about a single modification	*	n/a
TimeStamp	Date Time	Date and time when the modification was made	1	XML-Standard
Operator	String	The name or ID of the system operator who made the modification	1	Not empty
Comment	String	Comment entered in the comment field of the run step	0..1	Not empty
System	String	Name of the (software) system used to make the modification; e.g., QIAgility	1	Not empty
SerialNumber	String	Serial number of the system used to make the modification; e.g., serial number of the QIAgility instrument	1	Not empty
Software	String	Name of the software used to make the modification; e.g., "QIAgility" for the QIAgility Setup Manager software	1	Not empty
SoftwareVersion	String	Version of the software used to make the modification; e.g., version of the QIAgility Setup Manager software	1	Not empty
References	Node	A list of arbitrary references. Not used by the software	0..1	n/a
Reference	Node	Information about a single reference	*	n/a
Name	String	Name of the reference	1	Not empty
Type	String	An arbitrary type	1	
Comment	String	Detailed explanation of the reference	1	Not empty
OtherInfo	Node	See page 15 for details	0..1	n/a
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

```
<PlateFile xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:xsd="
http://www.w3.org/2001/XMLSchema" SchemaVersion="1" PlateId="90945_20150920_234630"
Description="Comment entered on Run step.">
  <Modifications>
    <Modification TimeStamp="2015-09-21T00:13:25.2820992+02:00" Operator="John Smith"
    Comment="Comment entered on Run step." System="QIAgility" SerialNumber="90945"
    Software="QIAgility" SoftwareVersion="1.0.0.107" />
  </Modifications>
  <PhysicalLayout LabwareName="96_200_ABI_4316813" LabwareType="ABI MicroAmp® Optical
  96-Well Reaction Plate, 0.1 ml" QiagenMaterialNumber="1087409">
```

Figure 3. Example of Modifications.

PlateFile.PhysicalLayout

PhysicalLayout describes the physical labware, i.e., the layout of the plate or the adapter holding tubes. This information allows downstream systems to identify the labware type for correct handling (e.g., pipetting) and enables other systems to display the labware with correct position numbering and order.

Table 4. PhysicalLayout elements and attributes

Name	Data type	Content	#	Format/Range
LabwareName	String	ID of the labware (plate or tube). Allows downstream systems to identify which physical labware this file describes. The name may be unintelligible: "148_25_QIAGEN_981313."	1	Not empty
LabwareType	String	A more readable name of the used labware, such as "QIAGEN Rotor-Disc 100"	1	Not empty
QiagenMaterialNumber	String	Dedicated SAP number for QIAGEN labware or a material number for non-QIAGEN labware	0..1	
LabwareLayout	Node	A brief collection of information about the quantity and alignment of labware positions. This information is useful for software that displays the labware content to the user, but has no access to labware description.	1	n/a
Alignment	String	"Rectangular" if the labware has a strict rectangular arrangement in columns and rows and positions are named in a chessboard scheme. All other alignments (e.g., rings, triangles, Rotor-Gene 4-strip adapter) are "Irregular".	1	(enum) Either Rectangular or Irregular
NumberOfPositions	Integer	Number of physical positions on the labware. Not the number of Position elements in the PlateContent (see page 7), which can be lower.	1	≥ 1
NumberOfRows	Integer	The number of rows of the position alignment. Used only if Alignment is "Rectangular". "0" if Alignment is "Irregular".	0..1	≥ 0
NumberOfColumns	Integer	The number of columns of the position alignment. Used only if Alignment is "Rectangular". "0" if Alignment is "Irregular".	0..1	≥ 0
RowLabeling	String	Determines if position rows are labeled with letters or with numbers (usually letters). Used only if Alignment is "Rectangular".	0..1	(enum) Either Alphabetic or Numeric
ColumnLabeling	String	Determines if position columns are labeled with letters or with numbers (usually numbers). Used only if Alignment is "Rectangular".	0..1	(enum) Either Alphabetic or Numeric
PositionNumberingScheme	String	For rectangular labware, "ByRow" indicates that position counting is performed along rows (i.e., all positions in the first row, then the second row, and so on). "ByColumn" indicates that counting is performed along the columns. "Linear" is assigned to all non-rectangular labware.	1	(enum) Either ByRow, ByColumn or Linear
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

```
<Modifications>
<PhysicalLayout LabwareName="96_200_ABI_4316813" LabwareType="ABI MicroAmp® Optical
96-Well Reaction Plate, 0.1 ml" QiagenMaterialNumber="1087409">
    <!-- Alignment - one of Rectangular, Irregular; PositionNumberingScheme - one of
    ByRow, ByColumn -->
    <Layout Alignment="Rectangular" NumberOfPositions="96" NumberOfRows="8"
    NumberOfColumns="12" RowLabeling="Alphabetic" ColumnLabeling="Numeric"
    PositionNumberingScheme="ByRow" />
</PhysicalLayout>
<PlateContent>
```

Figure 4. Example of PhysicalLayout for a 96-well plate.

```
<Modifications>
<PhysicalLayout LabwareName="148_25_QIAGEN_981313" LabwareType="QIAGEN Rotor-Disc
100" QiagenMaterialNumber="981313">
<!-- Alignment - one of Rectangular, Irregular; Irregular for rotor discs -
NumberOfRows, NumberOfColumns are irrelevant in this case -->
    <Layout Alignment="Irregular" NumberOfPositions="100" NumberOfRows="0"
    NumberOfColumns="0" RowLabeling="Alphabetic" ColumnLabeling="Numeric"
    PositionNumberingScheme="Linear" />
</PhysicalLayout>
<PlateContent>
```

Figure 5. Example of PhysicalLayout for a QIAGEN Rotor-Disc 100.

PlateFile.PlateContent

PlateContent describes the content of the labware positions. Only positions that contain liquid must be listed in this element, however, empty positions may also appear.

Table 5. PlateContent elements and attributes

Name	Data type	Content	#	Format/Range
Description	String	Not used by the software	0..1	
Positions	Node	A list of position descriptions for positions with meaningful or non-empty content, though not necessary all physical labware positions.	1	n/a
Position	Node	Description of one position of the labware	*	n/a
Index	Integer	Index of the position according to the labware PositionNumberingScheme	1	≥ 1
Label	String	Label of the position on the physical labware. For example, "A1" for rectangular labware. The Index in string format (i.e., "1") is used for non-rectangular labware.	1	
Row	Integer	Indicates the row number of the position. Used only if the Alignment is "Rectangular". "0" if the Alignment is "Irregular".	0..1	≥1
Column	Integer	Indicates the column number of the position. Used only if the Alignment is "Rectangular". "0" if the Alignment is" Irregular".	0..1	≥1
Description	String	Not used by the software	0..1	

Name	Data type	Content	#	Format/Range
Content	Node		1	n/a
ContentId	String	ID of the content in the position. This is the Sample ID, the control name or the standard name.	1	Not empty
LiquidType	String	Describes the liquid in the position: "Sample " for samples, "Standard " for positions of a standard series, "None Template Control" for a control of type NTC, "Assay Control" for a control of an IC-target, "Control" for any other control	1	String
OriginalLiquidType	String	Describes the liquid type of the origin: "Control" for controls, "Standard" for positions of a standard series, "Sample" for samples	0..1	String
InternalControlName	String	Not used by the software	0..1	String
Volume	Double	Amount of liquid in the position (in microliters)	0..1	
State	String	Describes whether the content is still usable: "Valid" indicates no known problems; a "Unclear" denotes that there might be problems with the content (e.g., there was a liquid level detection warning, but the user ignored it after visual inspection); "invalid" labels a sample that is defect for some reason. "Removed" and "Empty" are not used by the software. Note: lowercase terms are permitted. QIAgility Setup Manager uses lowercase terms.	1	(enum) Either Valid, Unclear, invalid, unknown, Removed or Empty
Concentration	Node	Used only for standards and samples. In the case of samples, used only if the sample concentration was defined in the sample editor or by sample file import. Indicates Name, Value, Unit and Base of the concentration. For samples, the concentration is expressed as Concentration = Value Units per Base; e.g., Concentration = 31415 ng per µl.	0..1	n/a
Name	String	QIAgility Setup Manager uses "StdConcentration" for standards and "Concentration" for samples	0..1	Not empty
Value	Double	The concentration value; e.g., 0.736.	1	
Unit	String	For standards, the concentration unit is defined entirely in Unit (e.g., Unit = "copies/µl"). In contrast, concentration units of samples are defined by the two attributes Unit and Base; that is, Unit = "ng", Base = "µl".	1	Not empty
Base	String	Used only for samples and is always "µl"	0..1	
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a
Origins	Node	Lists the origin(s) of the content, i.e., from which position(s) on the input labware the content was produced (see page 10). Used only for samples.	0..1	n/a
Results	Node	Lists results for the content (see page 11). Not used by the software.	0..1	n/a
KitIds	Node	Lists IDs of kits that affected the content of the position (see page 11)	0..1	n/a
KitId	String	A kit ID	*	Not empty
TargetIds	Node	A list of target IDs, referring to the targets in the position (see page 11)	0..1	n/a
TargetId	String	A target ID	*	Not empty

Name	Data type	Content	#	Format/Range
IssueLinks	Node	A list of IDs for issues that affected the content of this position (see page 11)	0..1	n/a
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

```
<PlateContent>
<!-- Positions - list of all positions on the output labware -->
  <Positions>
<!-- Index - index, Row and Column irrelevant, Label - label on output labware
  -->
    <Position Index="0" Row="0" Column="0" Label="A1">
    <!-- ContentID - sample ID for samples; LiquidType - one of None Template
    Control, Control, Standard, Sample; OriginalLiquidType - one of Control,
    Standard, Sample; Volume - volume after run; State - one of valid, invalid,
    unclear -->
      <Content ContentId="NTC GAPDH + GPCR-like 5" LiquidType="Non Template
      Control" OriginalLiquidType="Control" Volume="20" State="valid">
        <KitIds>
          <KitId Id="204774" />
        </KitIds>
        <TargetIds>
        <!-- Software assigns IDs to defined targets; for target information
        refer to the process history below -->
          <TargetId Id="6756a9de-82df-401e-8fed-ca629f3b406d" />
          <TargetId Id="c4d7aa59-cdc3-43e2-b2d7-69b6a8d25f17" />
        </TargetIds>
      </Content>
    </Position>
```

Figure 6. Example of PlateContent for a control on a QIAGEN Rotor-Disc.

```
    <Position Index="78" Row="0" Column="0" Label="G7">
      <Content ContentId="Standard 1" LiquidType="Standard" OriginalLiquidType=
      "Standard" Volume="20" State="valid">
        <KitIds>
          <KitId Id="204774" />
        </KitIds>
        <TargetIds>
          <TargetId Id="c4d7aa59-cdc3-43e2-b2d7-69b6a8d25f17" />
        </TargetIds>
        <Concentration Name="StdConcentration" Value="100" Unit="copies/µl" />
      </Content>
    </Position>
    <Position Index="79" Row="0" Column="0" Label="G8">
      <Content ContentId="Standard 2" LiquidType="Standard" OriginalLiquidType=
      "Standard" Volume="20" State="valid">
        <KitIds>
          <KitId Id="204774" />
        </KitIds>
        <TargetIds>
          <TargetId Id="c4d7aa59-cdc3-43e2-b2d7-69b6a8d25f17" />
        </TargetIds>
        <Concentration Name="StdConcentration" Value="10" Unit="copies/µl" />
      </Content>
    </Position>
    <Position Index="80" Row="0" Column="0" Label="G9">
```

Figure 7. Example of PlateContent for a standard on a QIAGEN Rotor-Disc.

```
<Position Index="13" Row="2" Column="1" Label="B1">
  <Content ContentId="sample 13" LiquidType="Sample" OriginalLiquidType=
  "Sample" Volume="25" State="valid">
    <Origins>
      <Origin ProcessId="5f37ac24-945b-4e9d-9c80-96d84ad88aa1" PlateId=
      "90945_20150921_001325" PositionName="B1" ContentId="sample 13" />
    </Origins>
    <KitIds>
      <KitId Id="204254" />
    </KitIds>
    <TargetIds>
      <TargetId Id="8505b707-9fbf-4590-851d-6ad37aa8ff90" />
    </TargetIds>
  </Content>
</Position>
```

Figure 8. Example of PlateContent for a sample with ID "sample 13" in position B1 on a 96-well plate.

Origins

Table 6. Origins elements and attributes

Name	Data type	Content	#	Format/Range
Origin	Node		*	
ProcessId	String	ID of the process that generated input for the Origin. The process to which this ID belongs is listed in the ProcessHistory element (see page 12). In most cases, this ID refers to a QIAgility run.	1	Not empty
PlateId	String	ID of the input labware from which the position content originated	1	Not empty
PositionName	String	Name of the position (e.g., "A1") on the input labware from which the position content originated	1	Not empty
ContentId	String	The ContentId of the Position in the Origin. This is usually the sample ID, as entered in the sample editor or imported as an input file.	0..1	Not empty
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

```
<Position Index="4" Row="0" Column="0" Label="A5">
  <Content ContentId="1" LiquidType="Sample" OriginalLiquidType="Sample"
  Volume="20" State="valid">
    <Origins>
      <Origin ProcessId="e65bc92c-3478-4ef0-a1f0-af743839521b" PlateId=
      "90945_20150920_230114" PositionName="A1" ContentId="1" />
    </Origins>
```

Figure 9. Example of Origin for a sample „1" in position "A5" that originated from sample „1" in position "A1" of the input labware.

KitIds

Content of a position can be affected by one or more kits —a box with reagents sold by a vendor —during processing. Kit boxes are usually equipped with a barcode that identifies the product and may contain additional information, like kit expiration date or production lot number.

Kit IDs described in this section reference to more extensive kit information in the **MetaData** element of **ProcessHistory** (see page 13).

TargetIds

Target IDs described in this section reference more extensive target information in the **MetaData** element of **ProcessHistory** (see page 13).

Results

The **Result** element has the same structure as the **Concentration** element and is not used by the software.

Table 7. Results elements and attributes

Name	Data type	Content	#	Format/Range
Result	Node	Not used by the software	*	
Name	String	Name, Value, Unit and Base of the Result. The Result is expressed as Name = Value Units per Base (e.g., some Name = 31415 copies per µl)	1	Not empty
Value	Double	See description under Name	1	Not empty
Unit	String	See description under Name	1	Not empty
Base	String	See description under Name	0..1	Not empty
OtherInfo	Node	See page 15	0..1	n/a

IssueLinks

Content of a position can be affected by one or more “issues” during its processing lifetime, such as a pipetting problem. Content links to relevant issues listed in the ProcessHistory by including the respective issue ID.

Table 8. IssueLink elements and attributes

Name	Data type	Content	#	Format/Range
IssueLink	Node		*	
IssueId	String	Unique ID of an issue found in the Issues element of a ProcessLog (see Table 9)	1	Not empty
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

PlateFile.ProcessHistory

Table 9. PlateFile.ProcessHistory elements and attributes

Name	Data type	Content	#	Format/Range
ProcessLog	Node		*	
LogId	String	A generated unique ID	1	Not empty
Name	String	Brief description of the process; e.g., "Assay setup" for the actual QIAgility run, "Input Plate Created" as a reference if the sample IDs were entered into the QIAgility software (referred from the Origin element).	1	Not empty
MetaData	Node	Process properties, like start and end time (see page 13)	1	
ProcessSteps	Node	A list of qualitative steps performed during the process (see page 14)	1	
Issues	Node	A list of issues that occurred during the process (see page 15)	0..1	
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

```
</PlateContent>
<ProcessHistory>
<!-- Details about the run -->
<ProcessLog LogId="e65bc92c-3478-4ef0-a1f0-af743839521b" Name="Input Plate
Created">
<MetaData StartTime="2015-09-20T22:04:32.6395729+02:00" EndTime=
"2015-09-20T22:59:30.9961241+02:00" GeneratingSystem="QIAgility" SerialNumber=
"90945" Software="QIAgility" SoftwareVersion="1.0.0.107" Description="QIAgility"
>
<ProcessSteps>
</ProcessLog>
<ProcessLog LogId="d4947d7c-5e79-4b61-aba2-d770c2e4c336" Name="Assay Setup">
<MetaData StartTime="2015-09-20T22:04:32.6395729+02:00" EndTime=
"2015-09-20T22:59:30.9961241+02:00" GeneratingSystem="QIAgility" SerialNumber=
"90945" Software="QIAgility" SoftwareVersion="1.0.0.107" Description="QIAgility"
>
<ProcessSteps>
</ProcessLog>
</ProcessHistory>
</PlateFile>
<!-- QIAsymphony_CHECKSUM p9Bgw+KVa59MBn15+33zZ69K8ScijFWIpw8GsXm8dbY=-->
```

Figure 10. Example of ProcessHistory with generated input labware and actual run

MetaData

MetaData contains general information about a process.

Table 10. MetaData elements and attributes

Name	Data type	Content	#	Format/Range
StartTime	DateTime	Start time of the process	1	XML-Standard
EndTime	DateTime	End time of the process	1	XML-Standard
GeneratingSystem	String	Name of the system on which the process ran. “QIAgility” for this software.	1	Not empty
SerialNumber	String	Serial number of the instrument on which the process ran.	1	Not empty
Software	String	Name of the software from the system that ran the process. “QIAgility” for this software.	1	Not empty
SoftwareVersion	String	Version of the software that ran the process.	1	Not empty
Description	String	Description of the process. “QIAgility” for this software.	0..1	
WorklistNames	Node	Names of the worklists used in the process. Not used by the software.	0..1	
WorklistName	Node		*	
Name	String	Filename of a worklist used to perform a process	1	Not empty
Kits	Node	Kits used for a process	0..1	
Kit	Node	Details about a kit	*	
KitId	String	Barcode on the kit box (or other identifier, like a GUID).	1	Not empty
Name	String	Name of the kit, e.g., “Rotor-Gene Multiplex PCR Kit (400)”	1	Not empty
Lot	String	Kit lot number, usually derived from the kit barcode. "Kit Lot not provided" if not available.	1	
ExpiryDate	DateTime	Kit expiration date, usually derived from the kit barcode. If no expiration date is provided, “Dec 31, 2999” (effectively meaning that the kit never expires)	1	XML-Standard
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a
Targets	Node	Targets used for the run	0..1	
Target	Node	Details about a target	*	
TargetId	String	A target ID used in the positions Content to refer to this description	1	Not empty
Name	String	Name of the target, e.g., “GAPDH”	1	Not empty
Type	String	Type of target: “Test”, “Reference” or “IC”	1	Not empty
Reporter	String	Reporter of the target, e.g., “HEX”	0..1	Not empty
Content	String	Content of the target	0..1	Not empty
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

Figure 11. Example of MetaData with kit and target description.

ProcessStep

Each process consists of several process steps, which are described in the **ProcessHistory** element.

Table 11. ProcessSteps elements and attributes

Name	Data type	Content	#	Format/Range
Index	Integer		1	≥ 1
Name	String	Name of the step, as listed in the task list of the run step	1	Not empty
Description	String	Description of the step	0..1	Not empty
StartTime	DateTime	Start time of the step	1	XML-Standard
EndTime	DateTime	End time of the step	1	XML-Standard
Status	String	"Ok" if successfully completed, "Failed" if the step or one of its sub-steps failed	1	(enum) Either OK or Failed
SubSteps	Node	A list of child process steps, the same as ProcessHistory.ProcessSteps	0..1	
OtherInfo	Node	Not used by the software (see page 15)	0..1	n/a

```
    </MetaData>
    <ProcessSteps>
      <ProcessStep Index="1" Name="Prepare Reaction Mix Base" Description=
      "Prepare Reaction Mix Base" StartTime="2015-09-20T22:07:16.3979393+02:00"
      EndTime="2015-09-20T22:07:16.7209578+02:00" Status="Ok" />
      <ProcessStep Index="2" Name="Prepare Standard Series" Description=
      "Prepare Standard Series" StartTime="2015-09-20T22:09:11.1405022+02:00"
      EndTime="2015-09-20T22:09:11.469521+02:00" Status="Ok" />
      <ProcessStep Index="3" Name="Prepare Target Reaction Mix" Description=
      "Prepare Target Reaction Mix" StartTime="2015-09-20T22:15:12.3091599+02:00"
      EndTime="2015-09-20T22:15:12.6091771+02:00" Status="Ok" />
      <ProcessStep Index="4" Name="Distribute Liquids to Output Plate" Description
      ="Distribute Liquids to Output Plate" StartTime=
      "2015-09-20T22:59:10.187934+02:00" EndTime=
      "2015-09-20T22:59:11.6590181+02:00" Status="Ok" />
    </ProcessSteps>
```

Figure 12. Example of ProcessStep for an assay setup run.

Issue

Table 12. Issue elements and attributes

Name	Data type	Content	#	Format/Range
IssueId	String	A unique identifier for an issue. This identifier is linked to the positions affected by the issue.	1	Not empty
Description	String	Description of the issue, i.e., why the issue is noteworthy	1	Not empty
TimeStamp	DateTime	Time when the issue occurred	1	XML-Standard
OtherInfo	Node	Not used by the software (see next section)	0..1	n/a

OtherInfo

OtherInfo is not used by the software. Most entities described in the previous sections are extendable because they include the optional element OtherInfo, which in turn contains a list of name/value pairs. These pairs are of two types:

- Simple; merely a name and a value. The value may be of type string, int, uint, long, float, double, or DateTime.
- Complex; includes a name and value, but the value again holds a list of name/value pairs. This recursive data structure allows for more complex data to be stored in OtherInfo.

The names must be unique at each respective level and may not be empty or consist of blank spaces.

Table 13. OtherInfo elements and attributes

Name	Data type	Content	#	Format/Range
OtherInfo	Node		0..1	n/a
Simple	Node		*	n/a
Name	String	Name of the simple value	1	Not empty
Value		Simple value	1	See description above
Complex	Node		*	n/a
Name	String	Name of the complex value	1	Not empty
Value	Node	List of enclosed simple pairs of complex values	1	n/a
Simple	Node		*	n/a
Name	String	Name of the simple value	1	Not empty
Value		Simple value	1	as above
Complex	Node		*	n/a
Name	String	Name of the complex value	1	Not empty
Value	Node	Node for ad infinitum additions, if required	1	n/a

An example of the use of **OtherInfo** is shown in Figure 13, with a possible corresponding screen display on the right. Note that:

- **OtherInfo** contains five elements, four simple ones and one complex, which in turn contains one simple and two complex structures.
- There are two elements with name “e” (the Euler constant without decimal comma and the elementary charge). They do not interfere with each other because they reside within different parent pairs.

```
<OtherInfo>
  <Simple Name="I. Newton" Value="If I have seen further, it is by standing on the shoulders
of giants."/>
  <Simple Name="e" Value="2718"/>
  <Simple Name="Pi" Value="3.14159"/>
  <Complex Name="Physical Constants">
    <Value>
      <Complex Name="Universal">
        <Value>
          <Simple Name="G" Value="6.6738480E-11"/>
          <Simple Name="c" Value="299792458"/>
          <Simple Name="h" Value="6.6260695729E-34"/>
        </Value>
      </Complex>
      <Complex Name="Electromagnetic">
        <Value>
          <Simple Name="Z0" Value="376.730313461"/>
          <Simple Name="e" Value="1.60217656535E-19"/>
        </Value>
      </Complex>
      <Simple Name="g" Value="9.81"/>
    </Value>
  </Complex>
  <Simple Name="Landing of Apollo 11" Value="1969-07-21T03:56:00"/>
</OtherInfo>
```

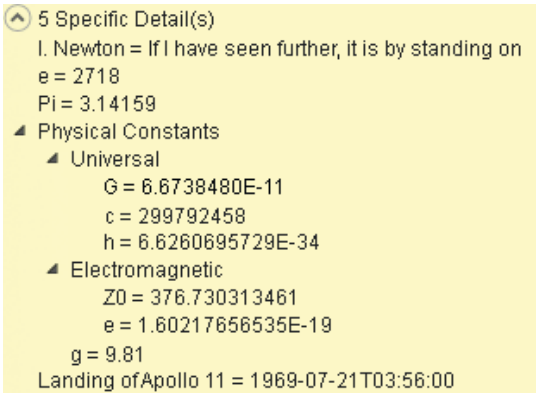

Figure 13. Example of the use of OtherInfo, including a possible display on the screen.

Checksum

Like other labware files in .xml format generated by QIAGEN instrument software, the file is digitally signed with a checksum to ensure data integrity. The checksum is a trailing line in the XML file, like: <!– QIAsymphony_CHECKSUM characterswhichresembletherackfileschecksum=–>

Input file (.xml)

Sample information for the input labware can be imported as an XML file during experiment setup. To import a file of this type, select the file type .xml in the **File** dialog (preselected). After import, the sample list is displayed for selecting.

If the labware type cannot be found in the list of supported labware, the import is not possible.

The file is expected to be digitally signed with a checksum (as described for the output file). To prevent unauthorized manipulation, the software checks the file signature during import and presents a warning when the signature is missing or invalid. However, an import is always possible.

The format of the XML file for sample input is the same as for the output file. For sample import, the software takes information from the elements listed in Table 14 (for details about the elements, refer to the description of the output file).

Table 14. Elements used for sample import (.xml)

Information	XML element	Description
Labware type	PhysicalLayout	The software uses the attributes LabwareName, LabwareType and QiagenMaterialNumber to find labware in the list of supported labware. The corresponding labware is selected as input labware type if the labware is supported and marked as available in the Labware Manager of the software. If the software cannot find the described labware in the list of supported labware, the file cannot be imported. The software creates positions in the sample list according to the layout information, using the attributes Alignment, NumberOfPositions, NumberOfRows, NumberOfColumns, RowLabeling, ColumnLabeling and PositionNumberingScheme.
Sample ID	ContentId	Taken from the PlateContent in the Positions list of the PlateContent element. The software fills the ContentId into the correct Sample ID field according to the Position element.
Concentration	Value	From Concentration of the Content element at the position
Description	–	Not imported

Sample input file (.csv)

Sample information for the input labware can be imported from a .csv file during experiment setup.

A sample input file (.csv) is a simple comma-separated .csv or .txt file that contains a header line and several lines describing single sample positions. The input labware type is not described in the file.

To import a file of this type, select the file type .csv or .txt in the File dialog. After import, select the input labware type in the software. The sample list can be viewed or corrected after import by clicking Define samples.

The expected components of the file are described in Table 15. Comma (,) is expected as the field delimiter.

Table 15. Description of sample input files (.csv or .txt)

Parameter	Dimension	Range	Description
WellPosition	String	A1–P24 | 1–n	Sample position on a plate or adapter. Input must fit the position naming of the plate or adapter (e.g., A1, B1, …; or 1, 2, ...) and may not exceed the geometric capacity of the input labware type. Positions can be listed in any order. Empty sample positions are supported, i.e., they can be just not listed.
SampleID	String	(not empty)	The sample ID, which does not necessarily have to be unique
Concentration	Double	(empty) | 0–10,000	Concentration of sample in ng/µl. For documentation purpose only. The value does not influence the experiment settings or pipetting. For decimals, use the (English) number format #.# with up to 18 decimal places. Period (.) is expected as the decimal delimiter. Do not use a digit grouping symbol (i.e., comma (,) as thousand delimiter) because it disrupts the file format.
Description	String	(empty) | String	Additional comments or description. Use quotation marks (" ") if the description includes a comma (,). See the provided example.

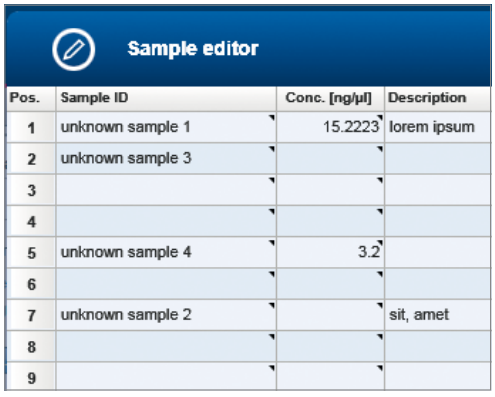

Figure 14. Sample input after import from the example .csv files described below.

The above sample input for the QIAgility results from either of the following .csv files.

A .csv file for a rectangular plate or adapter

```
WellPosition,SampleId,Concentration,Description
A1,unknown sample 1,15.2223,lorem ipsum
B1,unknown sample 2,,"sit, amet"
B3,unknown sample 3,,
A2,unknown sample 4,3.2,
```

A .csv file for an irregular plate or adapter

```
WellPosition,SampleId,Concentration,Description
1,unknown sample 1,15.2223,lorem ipsum
7,unknown sample 2,,"sit, amet"
2,unknown sample 3,,
5,unknown sample 4,3.2,
```

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