



labSuite 3.1 For Waters Empower

User Guide

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1. Introduction

The labSuite is designed as an extension to the Waters Empower® software. This program delivers data which can be useful and important both for laboratory management as well as for key users, regarding performed analytical measurements.

In network installations the Waters Empower software provides users with all information on the measured samples of a single project. It is easy to keep track of contents and purities of samples, calculate releases or compare spectra. But whenever a question does not refer to a specific project, the data must be located by opening a global project view. The Empower global projects function meets its limits when trying to search for very specific information or when trying to compare CustomFields. Moreover, it works only useably up to a small number of projects selected at the same time.

Now, the labSuite for Waters Empower offers a completely new possibility in gathering, combining, comparing and reorganizing information which is already present in the database. By a much more flexible and enlarged way of evaluating this information fully new dimensions are offered in terms of controlling and managing chromatography data.

1.1 Brief Overview

In the following a short description of the single modules is given. For a detailed guide of how to work with these modules please refer to section „2. User Guide“ of this document.

1.1.1 System Usage Rate

This module performs statistical evaluations on the utilization of chromatography systems. The labSuite differs between productive run times and inoperative stand times of your systems. Regarding stand times the labSuite distinguished between shorter gap times, where a productive use would not be possible due to e.g. system preparation or the short interval between two runs, and larger idle times, where a productive use would be possible, but has not been performed. This way a statistical evaluation of the productive usage of chromatography systems within a defined period is performed and gives helpful information about the efficiency and productivity of a laboratory and might also deliver arguments for the purchase of new systems. All information is shown in numeric values and as bar or pie

chart as well.

1.1.2 Injection Tracking

This tool retrieves and counts all injections which have been performed and displays them together with all related information according to the selected query configuration. This way it can e.g. be displayed on which system the selected injections have been run in a specific project. Or one can get an overview of all injections from various projects in a single table where grouping and sorting is easily performed. The labSuite also reads and displays all Sample CustomFields with their contents. Therefore, it is very simple to keep track of batch numbers, column IDs or any other information which you would like to get. Additionally, the customer gets the total number of injections per query item.

1.1.3 SampleSet Tracking

This module works similar to Injection Tracking, but based on SampleSets. This way it can be displayed, which SampleSets have been run on a specific chromatography system. As SampleSet CustomFields are reported as well it can be shown for example which pipette has been used during sample preparation in case such pipette numbers are entered into Empower.

1.2 Technical Aspects

The labSuite will compile all important information from your existing Waters Empower Database and copy them into its own database. This "Data Warehouse" contains information on existing and removed Waters Empower data (such as deleted or archived data) and is updated after a defined interval.

The labSuite for Waters Empower will use and analyze this Data Warehouse to provide you with information on generated data.

1.3 Definitions

Parameter	Definition/Description
Usage Time	Sum of the duration Sample Set(s) were running on a system. The duration is calculated as End Time - Start Time of a Sample Set.
Stand Time	Max Usage Time - Usage Time. This is the time no Sample Set is running on a system. This time can be defined either as Gap Time or Idle Time depending on the configured Gap Limit.
Gap Limit	A user-defined value which defines the limit between Gap Time and Idle Time. As a default 4 hours are set.
Gap Time	$\text{Stand Time} \leq \text{Gap Limit}$. This is the time no Sample Set was running on a system and which is less or equal than the defined Gap Limit. This time describes e.g. the duration between two Sample Sets, where no additional measurement is possible or the time which is needed to set up a system.
Idle Time	$\text{Stand Time} > \text{Gap Limit}$. This time describes the duration where a system is not used productively.
Reporting Period	Period which is evaluated. Can be unlimited (No Date), a single date, or a defined period specified by dates.
Max Usage Time	Observed period during the defined Reporting Period. This value can be configured by e.g. omitting weekends, night hours(daily availability in %) or public holidays.

Max Usage Time 247	Whole Reporting Period with no omissions. Seven days a week, 24 hours a day. A more detailed description is given in section 3 of this document.
Net Usage	$(\text{Usage Time} / \text{Max Usage Time}) * 100\%$
Gross Usage	$((\text{Usage Time} + \text{Gap Time}) / \text{Max Usage Time}) * 100\%$
Net Usage 247	$(\text{Usage Time} / \text{Max Usage Time}_{247}) * 100\%$

2. User Guide

2.1 General Aspects

2.1.1 Purpose of this User Guide

This user guide describes the basic functionality of the program. It does not give examples or recommendations for the practical operation on use cases.

2.1.2 User Administration and Access Rights

The labSuite does not have an own user administration. The access rights are defined by a specific Empower UserGroup. Therefore, it is necessary to define a UserGroup with all users who should have access to the labSuite. Additionally, a Project needs to be created on which the labSuite UserGroup is given access to. This UserGroup and Project needs to be entered during installation of the labSuite.

For the current version privileges for the single users of the labSuite cannot be restricted, i.e. everybody using the labSuite can operate with the program to the full extent.

2.1.3 Starting the Program

For starting the program, Empower does not need to run, but must at least be installed on the respective client as client version.



The login data to the labSuite corresponds to the Empower login data.



2.2 The labSuite Main Window

After having started the program the following view appears.



From here, a selection of the desired evaluation module (Usage Rate, Injection Tracking or Sample Set Tracking) is possible by choosing the respective item in the menu bar.

2.3 The Single Evaluation Modules

As already mentioned, the program consists of four evaluation modules which work independently from each other. A short description of the functionality of these evaluation types has already been given above. In the following the handling is described more in detail.

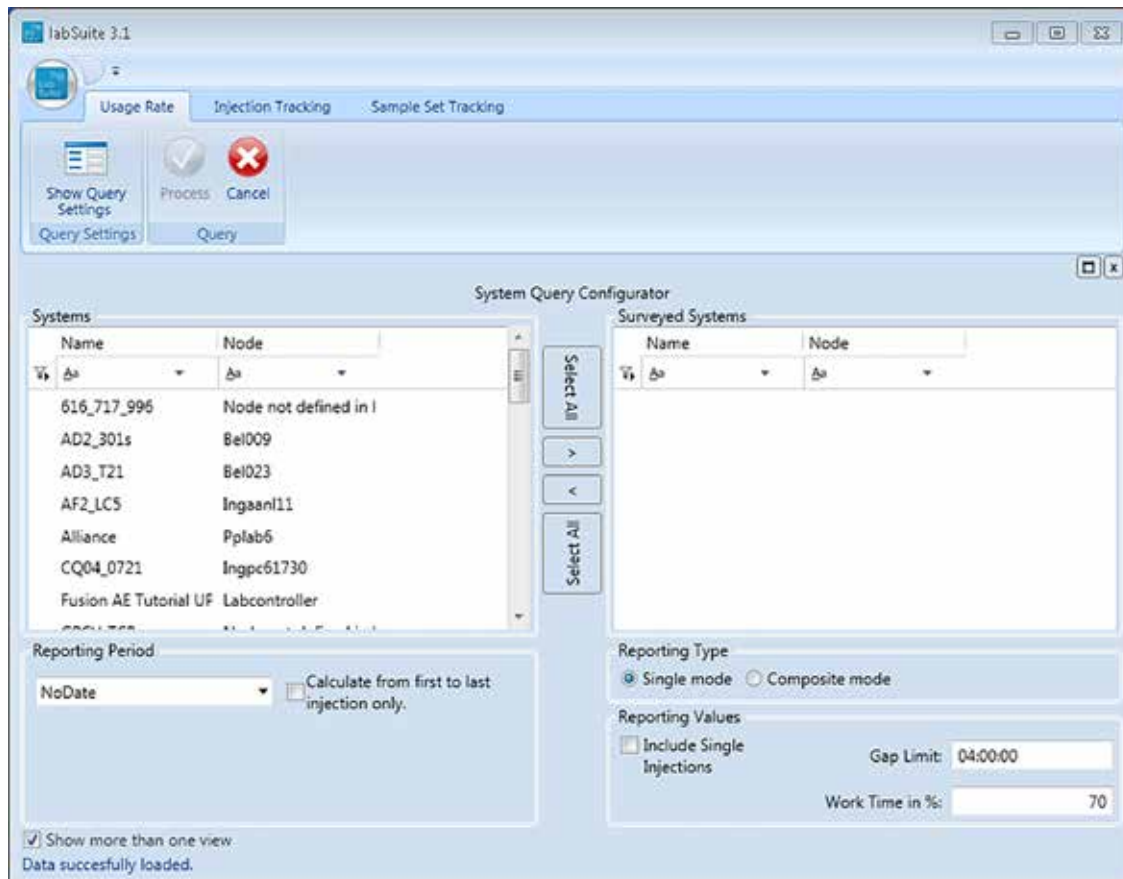
2.3.1 Usage Rate

2.3.1.1 Calculation

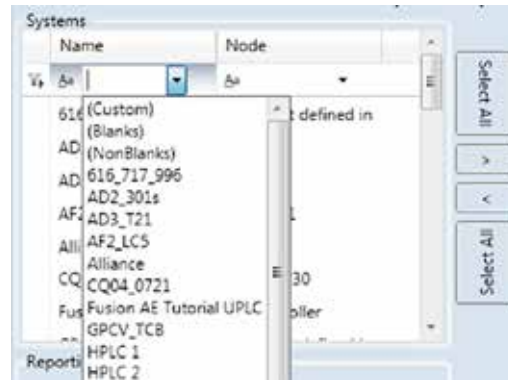
Please compare the definitions of the single parameters in section „1.3 Definitions“. A more detailed description for the single evaluation options is given in section „2.3.1.2 Configuring a Query“ below.

2.3.1.2 Configuring a Query

In order to start a query, the query settings need to be defined first. By selecting the button ‘Show Query Settings’ the current settings are displayed.



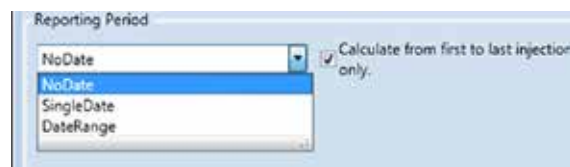
In the left section all available systems are shown. The program includes all systems, which are present in the database no matter whether they are currently configured, have been deactivated or even been deleted in Empower. Once a measurement has been performed on a system, an entry is generated in the Empower database and this entry is considered by the labSuite. In order to get a better overview on the systems of interest a filter can be applied either for 'System Name' or the 'Empower Node'.



A selection of the systems to be evaluated can then be made by the arrows in the middle of the window. For selecting specific systems, the desired systems need to be marked first (a multiple choice is performed by pressing CTRL and the left mouse button) a selection/deselection is then performed by the arrow buttons or the 'Select All' function.

The arrow buttons showing to the right perform a selection for the survey, the arrow buttons showing to the left will perform a deselection. The systems on which the evaluation will be based on are displayed in the right table called 'Surveyed Systems'.

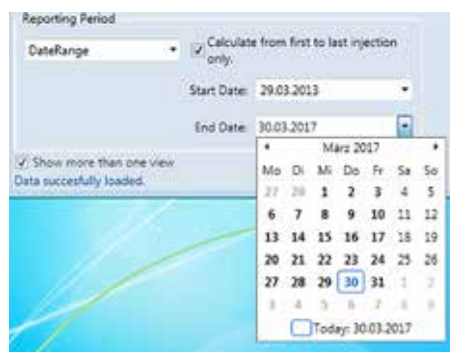
A further restriction to the query can be defined by the Reporting Period. When selecting 'no date' no restriction by time is given and all data present in the database are during calculation.



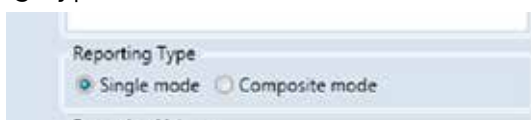
Additionally, a 'SingleDate' can be defined or a 'Date Range'. It is not possible to define a time by hours and minutes when an evaluation should start or end. Except for 'SingleDate' a further restriction can be added defining if the whole time of the selected period should be used as base for the calculation or if the evaluation period should start with the first injection performed during this time and end with the last one. This option can be activated by setting a checkmark for 'Calculate from the first to last injection only'. In some cases the selected period might overlap with SampleSets or Injections, meaning that the start and/or end date of the SampleSet and/or Injection lies outside the given period. In those

cases only usages are considered which are inside the specified period. This means, the MaxUsageTime247 cannot increase, but decrease using this option. Compare also the overview given in section 3.

This option will then define a MaxUsageTime247 for each system individually, starting with the first injection ever performed on the system and ending with the last injection found in the database related to the system with regard to the specified Reporting Period. The dates can be selected from the calendar or can be typed directly into the line.



Further on a Reporting Type can be defined.



The user needs to decide whether each system should be considered individually (Single mode) or if the surveyed systems should be evaluated as a single unit (Composite mode). Using Composite Mode does not mean that the single values are added together, but that first of all the UsageTimes and MaxUsageTime247 of each system is considered and is put on a single time line. All other time values will then depend on the composite Usage Time and composite MaxUsageTime247.

Finally, special Reporting Values need to be defined.



If the option Include Single Injections is not activated only injections which are part of a SampleSet are considered during the calculation.

The Gap Limit is necessary to distinguish between Gap Times and Idle Times. All

time values which are below this limit will be regarded as 'Gap Time'. If no limit is defined all times where no data acquisition has taken place is considered as 'Idle Time'. The 'Gap Limit' can be a value between 00:00:00 and 23:59:59.

The value for Work Time in % is necessary to distinguish between 'Reporting Period' and 'MaxUsageTime' (compare section „1.3 Definitions“). Whereas the 'MaxUsageTime247' is identical to the 'Reporting Period' The MaxUsageTime is used to consider e.g. night hours. A value of e.g. 70% means that only 16.8 hours a day are counted for the defined evaluation period. A value between 0 and 100 can be set.

2.3.1.3 Starting and Canceling a Query

The query is started by the green 'Process' button.



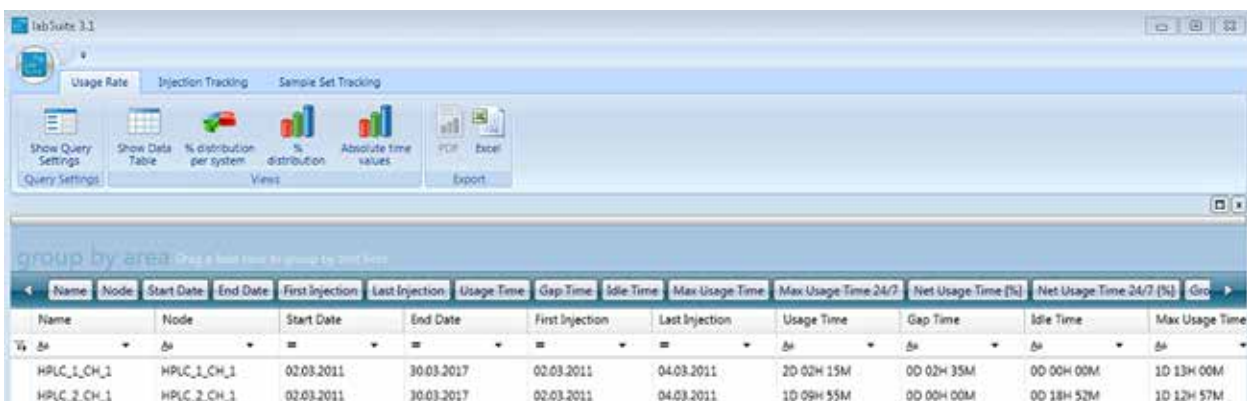
When the processing job is completed the view will switch over to the table view of the results.

For canceling a query, i.e. discarding the current query settings, the red 'Cancel' button needs to be selected. The view will then switch back to the result view of the last query.

2.3.1.4 Displaying Results

Table View

When the processing job is finished a result view will be displayed. The first view shows a data table.



Name	Node	Start Date	End Date	First Injection	Last Injection	Usage Time	Gap Time	Idle Time	Max Usage Time	Max Usage Time 24/7	Net Usage Time (%)	Net Usage Time 24/7 (%)	Group
HPLC_1_CH_1	HPLC_1_CH_1	02.03.2011	30.03.2017	02.03.2011	04.03.2011	2D 02H 15M	0D 02H 35M	0D 00H 00M	1D 13H 00M				
HPLC_2_CH_1	HPLC_2_CH_1	02.03.2011	30.03.2017	02.03.2011	04.03.2011	1D 09H 55M	0D 00H 00M	0D 18H 52M	1D 12H 57M				

A description of the single fields is given in section 1.4. The fields 'Start Date' and 'End Date' describe the selected Reporting Period, the Fields 'FirstInjection' and 'LastInjection' describe the date of the first and last injection for the respective system during the selected Reporting Period.

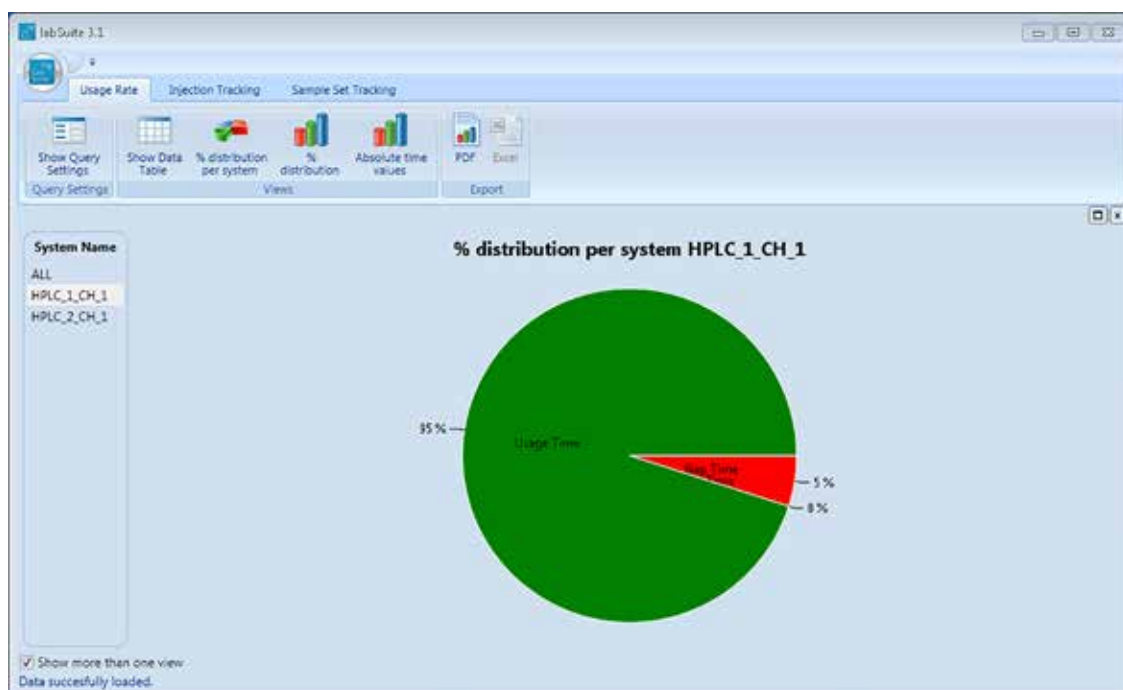
From the table view it is easy to get to a chart view by simply clicking on the button of the desired chart.



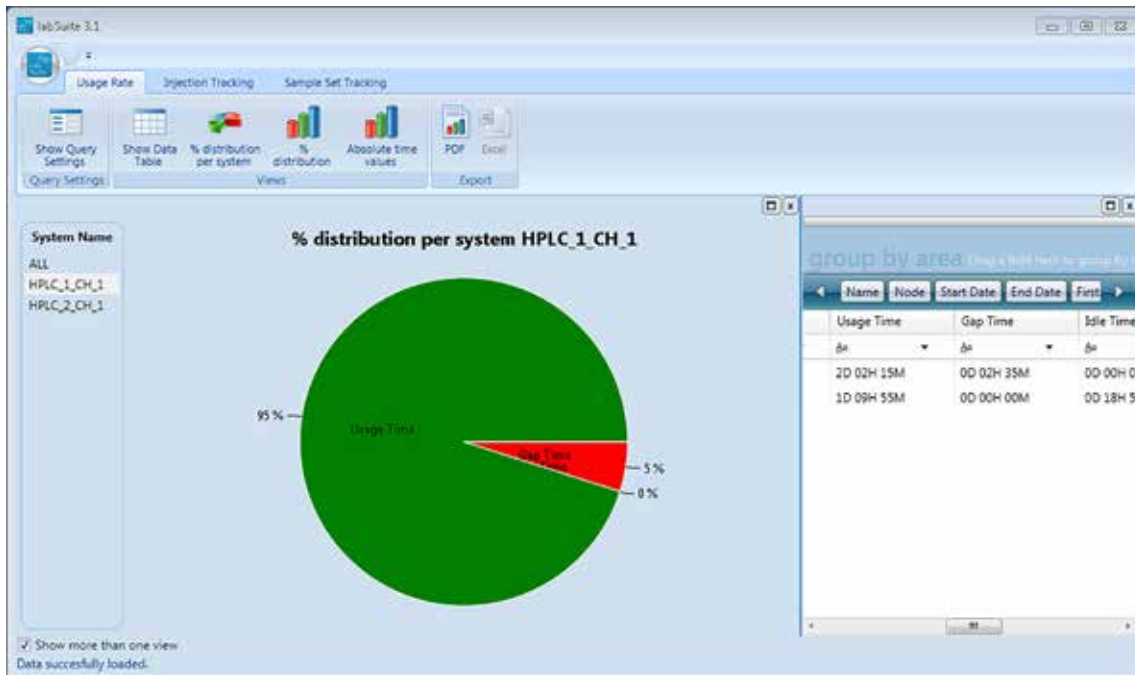
When switching to a chart view the selection made in table view does not influence the presentation in the chart views.

Pie Chart View

The Pie Chart View can be reached from the button '% distribution per system'. Here a pie chart is given showing the distribution of 'Usage Time', 'Gap Time' and 'Idle Time' for the current selection. On the left side a list of all systems which are part of the selection is displayed. Just select the system of interest in this table and the related pie chart is shown.

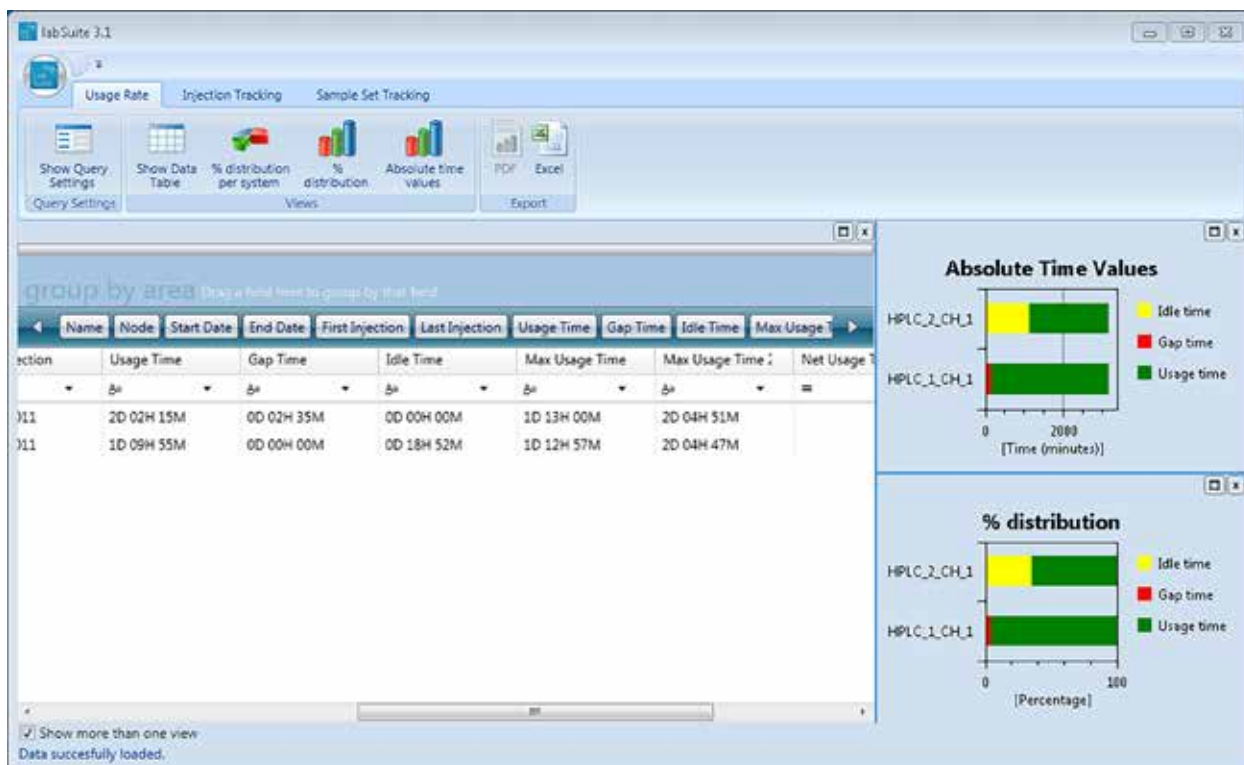


By selecting the 'show more than one view'-function in the lower left corner of the window, previously loaded views are displayed in the same window. Up to three views can be displayed together.



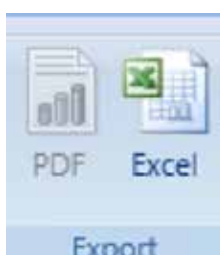
Bar Chart View

Two bar chart views are offered. One presenting the distribution in percent and one showing the absolute values in minutes.



2.3.1.5 Reporting

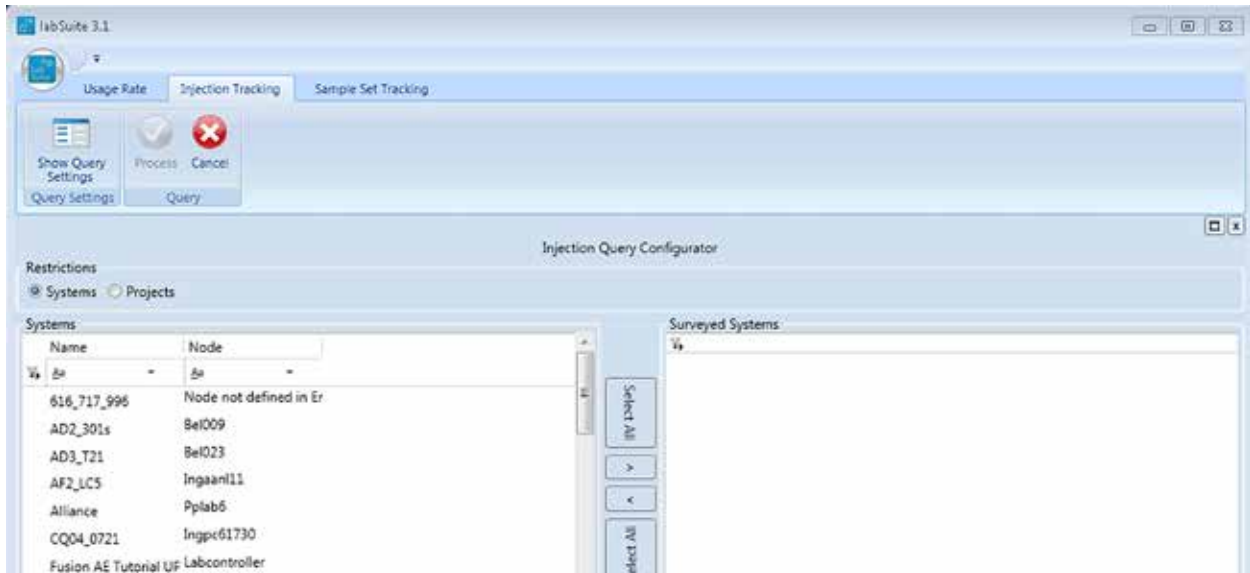
For reporting purposes the table views of the displayed data can be exported as an Excel file.



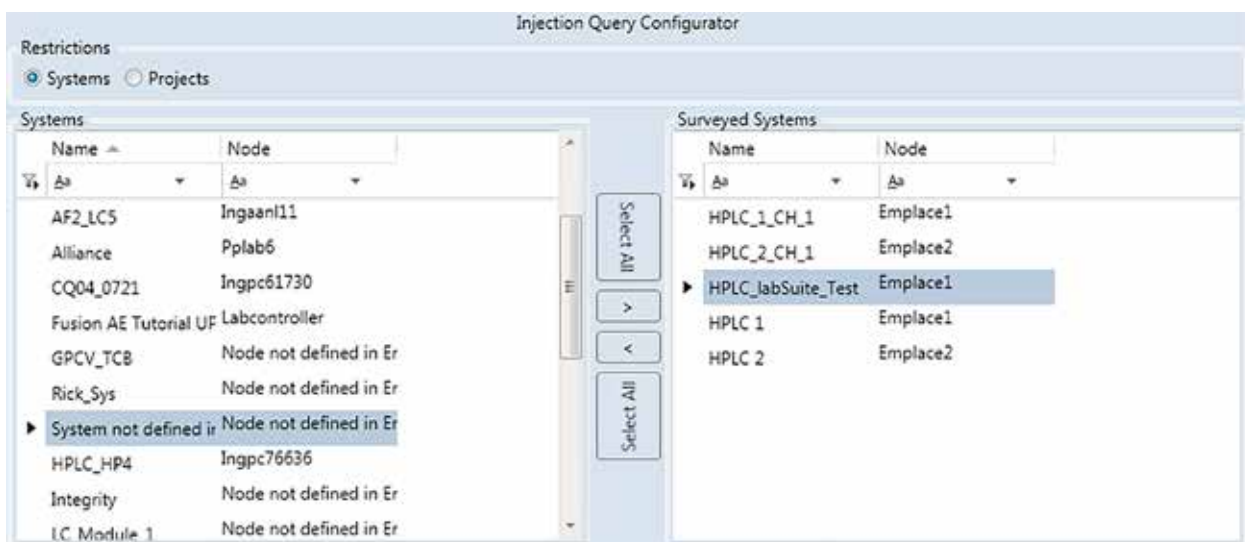
2.3.2 Injection Tracking

2.3.2.1 Configuring a Query

A query can either be based on Empower Projects or on Systems.

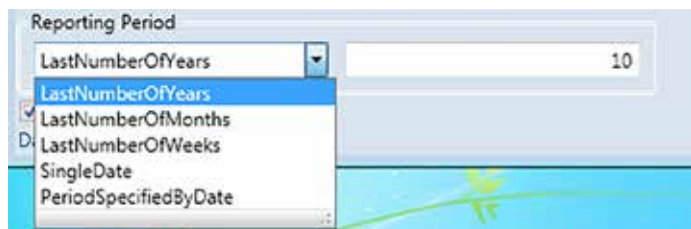


Depending on what is decided to base the query on a list of all items found in the database is given in the table on the left side. Search and selection of either Projects or Systems is performed in the same way as described in section 2.3.1.2.



A reporting period can be defined as well. Here a specific period can be defined

by date or a single date can be selected. Additionally, a query can be based on a period of years, months or weeks. Selecting e.g. Yearly (LastNumberOfYears) and entering a value of 10 means for example that the query is based on the last ten years.



2.3.2.2 Starting and Canceling a Query

The query is started by the green 'Process' button.

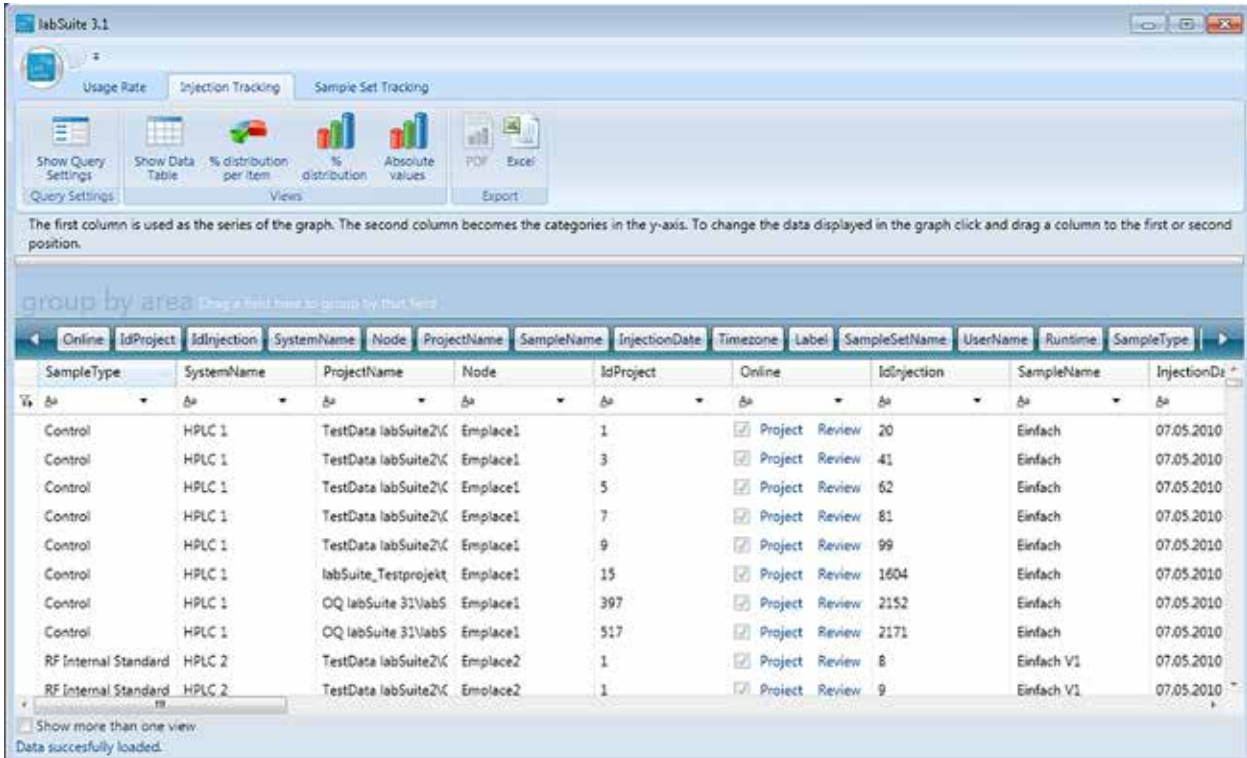


When the processing job is finished the view will switch over to the table view of the results.

For canceling a query, i.e. discarding the current query settings, the red 'Cancel' button needs to be selected. The view will then switch back to the result view of the last query.

2.3.2.3 Displaying Results

After having processed the query the table view of the evaluated data appears.



The screenshot shows the labSuite 3.1 interface. At the top, there are tabs for 'Usage Rate', 'Injection Tracking', and 'Sample Set Tracking'. Below these are icons for 'Show Query Settings', 'Show Data Table', '% distribution per item', '% distribution', 'Absolute values', 'PDF', and 'Excel'. A text box explains: 'The first column is used as the series of the graph. The second column becomes the categories in the y-axis. To change the data displayed in the graph click and drag a column to the first or second position.'

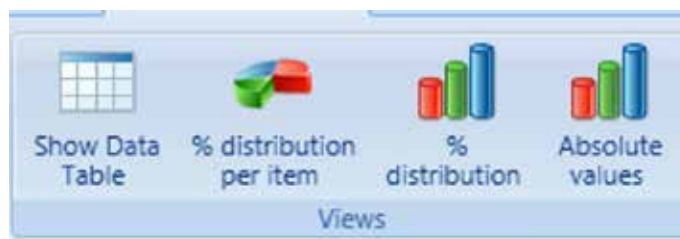
Below this is a 'group by area' section with a dropdown menu. The main part of the interface is a data table with the following columns: Online, IdProject, IdInjection, SystemName, Node, ProjectName, SampleName, InjectionDate, Timezone, Label, SampleSetName, Username, Runtime, and SampleType. The table contains 11 rows of data, including 'Control' and 'RF Internal Standard' entries.

SampleType	SystemName	ProjectName	Node	IdProject	Online	IdInjection	SampleName	InjectionDate
Control	HPLC 1	TestData labSuite2\K	Emplace1	1	<input checked="" type="checkbox"/>	Project Review 20	Einfach	07.05.2010
Control	HPLC 1	TestData labSuite2\K	Emplace1	3	<input checked="" type="checkbox"/>	Project Review 41	Einfach	07.05.2010
Control	HPLC 1	TestData labSuite2\K	Emplace1	5	<input checked="" type="checkbox"/>	Project Review 62	Einfach	07.05.2010
Control	HPLC 1	TestData labSuite2\K	Emplace1	7	<input checked="" type="checkbox"/>	Project Review 81	Einfach	07.05.2010
Control	HPLC 1	TestData labSuite2\K	Emplace1	9	<input checked="" type="checkbox"/>	Project Review 99	Einfach	07.05.2010
Control	HPLC 1	labSuite_Testprojekt	Emplace1	15	<input checked="" type="checkbox"/>	Project Review 1604	Einfach	07.05.2010
Control	HPLC 1	OQ labSuite 31\labS	Emplace1	397	<input checked="" type="checkbox"/>	Project Review 2152	Einfach	07.05.2010
Control	HPLC 1	OQ labSuite 31\labS	Emplace1	517	<input checked="" type="checkbox"/>	Project Review 2171	Einfach	07.05.2010
RF Internal Standard	HPLC 2	TestData labSuite2\K	Emplace2	1	<input checked="" type="checkbox"/>	Project Review 8	Einfach V1	07.05.2010
RF Internal Standard	HPLC 2	TestData labSuite2\K	Emplace2	1	<input checked="" type="checkbox"/>	Project Review 9	Einfach V1	07.05.2010

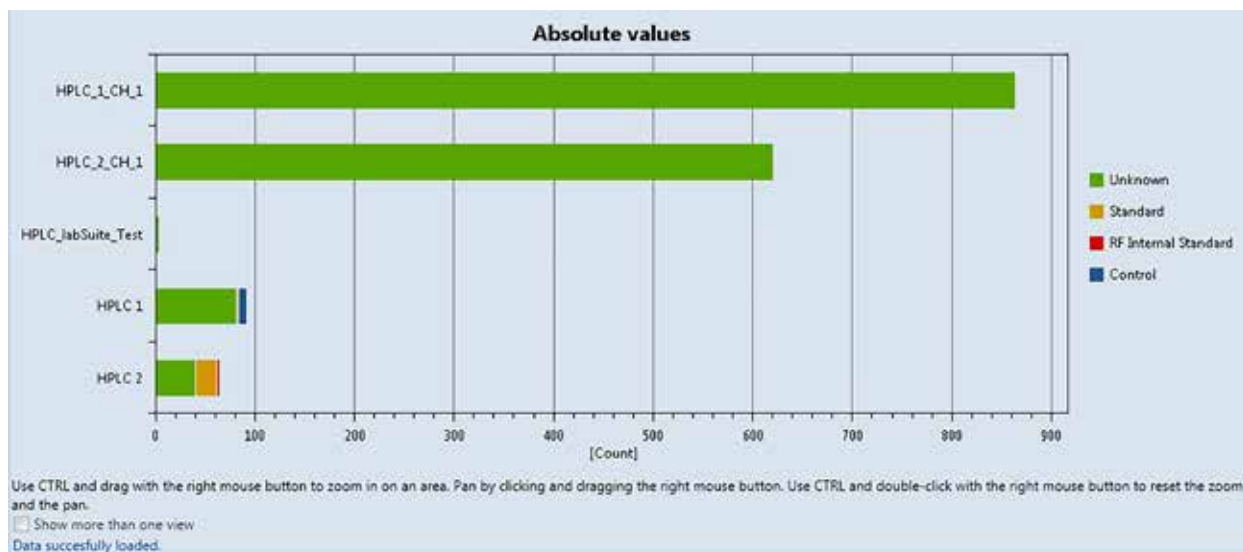
At the bottom of the table, there is a checkbox 'Show more than one view' and a message 'Data successfully loaded.'

The definition for the chart views is defined by the first two columns of the table view. The first column defines the distribution item applied on a single bar and the second column the Y-axis value of the chart views. The X-axis is given by the number of injections. By drag and drop every column can be moved to the desired position.

By selecting a chart view from the buttons below the view switches over to the respective chart.



Below a bar chart view, 'Absolute values' is given for the table view displayed above.



Here one can for example evaluate how many injections have been run on an Empower system during the selected period and what the ratio is between standard injections and sample injections.

2.3.2.4 Reporting



The reporting functions work in the same way as described in section 2.3.1.5. For reporting purposes the chart can be exported as PDF file.

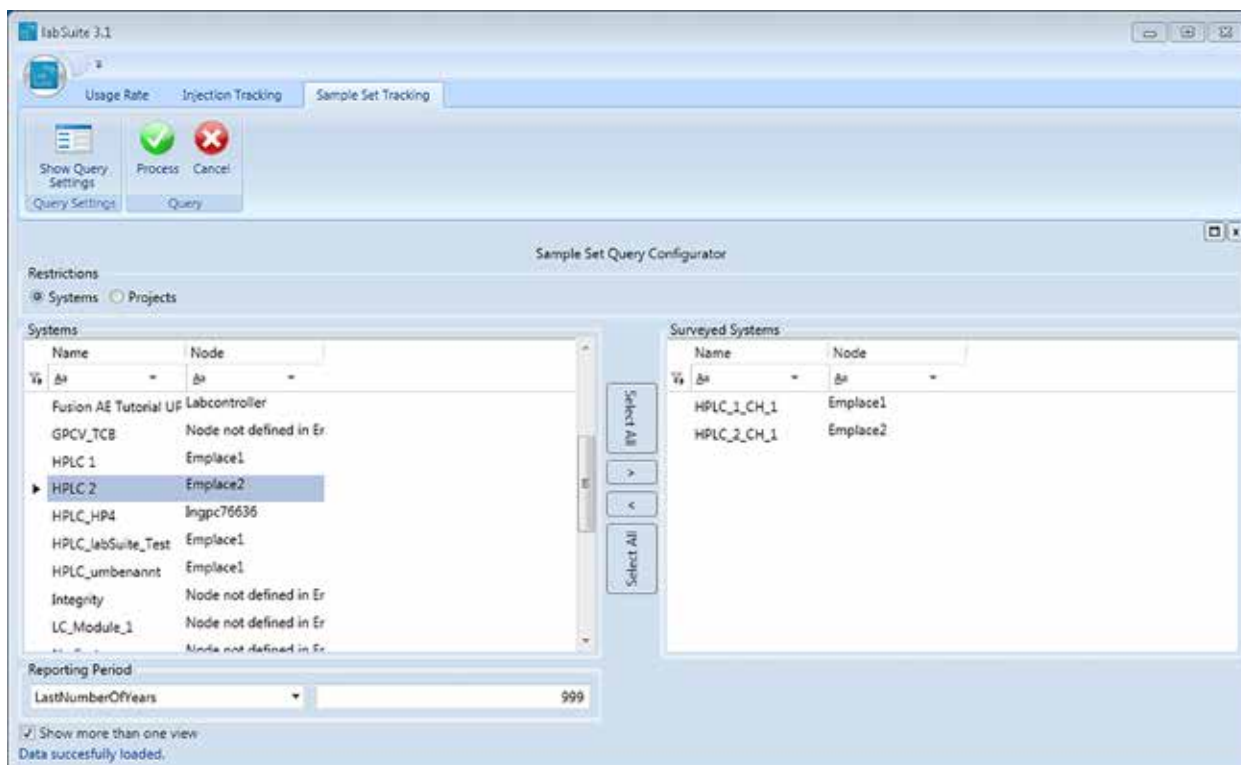
Empower fields displayed in table view for Injection Tracking:

Field Name in Empower	Field Name in labSuite
Acquired by	USERNAME
Database	DATABASE
Date Acquired	INJECTIONDATED
Empower Node	NODE
Instrument Method Name	INSMETHOD_NAME
Label	LABEL
Project Name	PROJECTNAME
Run Time	RUNTIME
Sample Name	SAMPLENAME
Sample Set Name	SAMPLESETNAME
Sample Type	SAMPLETYPE
System Comment	COMMENTS
System Name	SYSTEMNAME

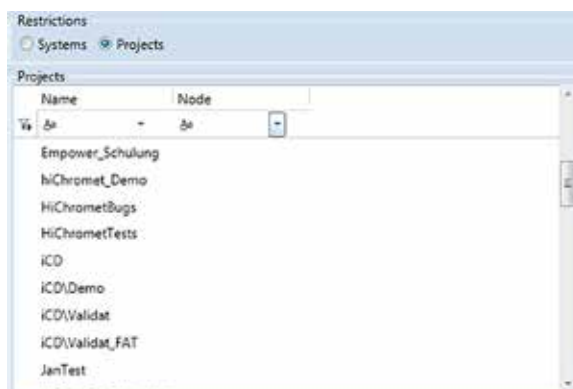
2.3.3 SampleSet Tracking

2.3.3.1 Configuring a Query

Below the main window for 'SampleSet Tracking' is displayed.



An evaluation can be based on either Systems or Projects. For Systems also the Empower Node where the System is connected to is shown. If a System has been connected to different Empower Nodes it appears together with respective Node multiple times in the table. Projects are displayed by the whole Empower Project Path in order to distinguish Projects with the same name but at a different location in the Empower Project hierarchy.



2.3.3.2 Starting and Canceling a Query

The query is started by the green 'Process' button.

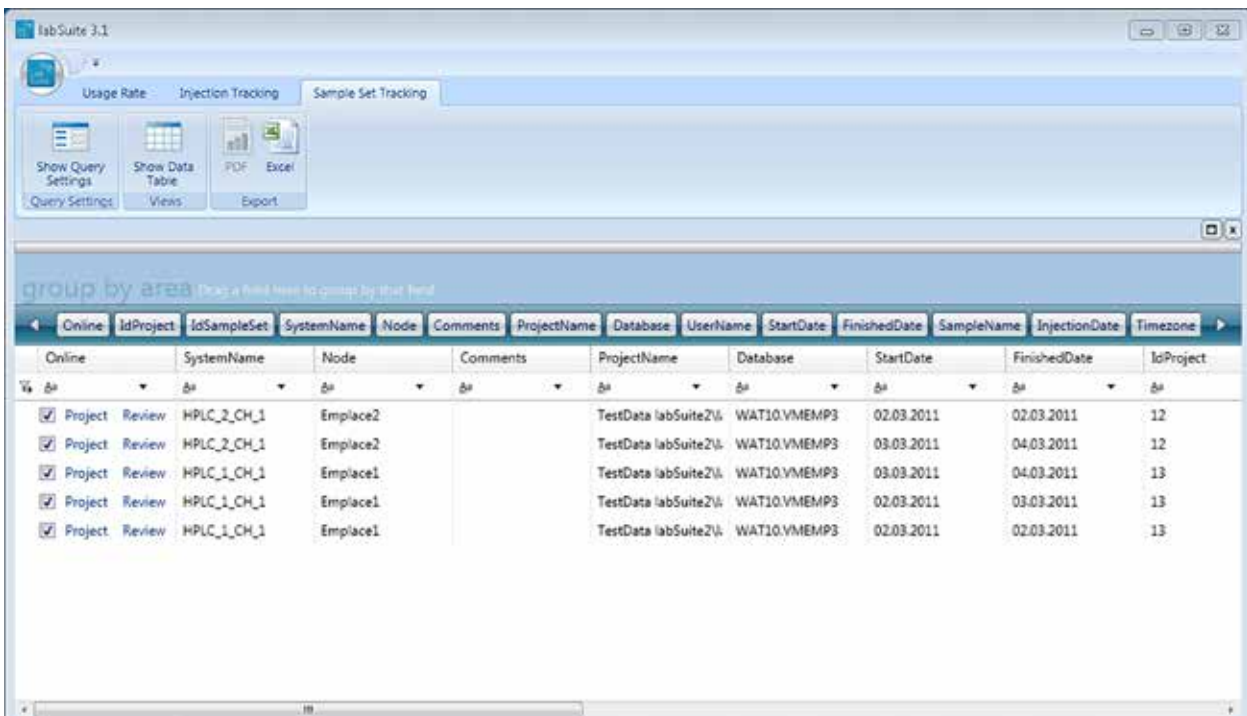


When the processing job is finished the view will switch over to the table view of the results.

For canceling a query, i.e. discarding the current query settings, the red 'Cancel' button needs to be selected. The view will then switch back to the result view of the last query.

2.3.3.3 Displaying Results

After having processed the data the table view appears listing all Sample Sets which are part of the query.



Online	IdProject	IdSampleSet	SystemName	Node	Comments	ProjectName	Database	Username	StartDate	FinishedDate	SampleName	InjectionDate	Timezone
<input checked="" type="checkbox"/>	Project	Review	HPLC_2_CH_1	Emplace2		TestData labSuite2\	WAT10.VMEMP3		02.03.2011	02.03.2011			12
<input checked="" type="checkbox"/>	Project	Review	HPLC_2_CH_1	Emplace2		TestData labSuite2\	WAT10.VMEMP3		03.03.2011	04.03.2011			12
<input checked="" type="checkbox"/>	Project	Review	HPLC_1_CH_1	Emplace1		TestData labSuite2\	WAT10.VMEMP3		03.03.2011	04.03.2011			13
<input checked="" type="checkbox"/>	Project	Review	HPLC_1_CH_1	Emplace1		TestData labSuite2\	WAT10.VMEMP3		02.03.2011	03.03.2011			13
<input checked="" type="checkbox"/>	Project	Review	HPLC_1_CH_1	Emplace1		TestData labSuite2\	WAT10.VMEMP3		02.03.2011	02.03.2011			13

As you can see in the picture above it is not possible to get a chart view in this evaluation mode.

2.3.3.4 Reporting

The reporting functions work in the same way as described in section 2.3.1.5 .

Empower fields displayed in table view for SampleSet Tracking:

Field Name in Empower	Field Name in labSuite
Sample Set Acquired by	USERNAME
Database	DATABASE
Sample Set Finish Date	FINISHEDDATE
Empower Node	NODE
Sample Set Start Date	STARTDATE
Project Name	PROJECTNAME
Sample Set Name	SAMPLESETNAME
Sample Set ID	SAMPLETYPE
System Comment	COMMENTS
System Name	SYSTEMNAME

3. Attachment

Definition of MaxUsageTime247 for the single evaluation modes:

Reporting Period	Calculate from first to last injection only*	Runs have no overlap with Reporting Periods Start and End Time	Runs have an overlap with Reporting Periods Start Time	Runs have an overlap with Reporting Periods End Time	Runs have an overlap with Reporting Periods Start and End Time
No Date	no	MaxUsage247 is from the 1. inj. to the current date	n/a **	n/a **	n/a **
	yes	MaxUsage247 is from the 1. inj. to the last inj.	n/a **	n/a **	n/a **
Single Date	no	MaxUsage247 is 24 hours	MaxUsage247 is 24 hours, only the usage within these 24 hours is considered, overlaps are cut at start and end time of the reporting period		
	(yes)	option not available			
Period by Date	no	MaxUsage247 is from the start date to the end date of the period (equals reporting period)	MaxUsage247 is from the start date to the end date of the period (equals reporting period). Overlaps are cut at start and end time of the reporting period.		
	yes	MaxUsage247 is from the 1. inj. to the last inj. Found within the defined reporting period	MaxUsage247 is from the start date of the reporting period to last injections date	MaxUsage247 is from the first injections date to the end date of the reporting period	MaxUsage247 is from the start date to the end date of the reporting period

It goes without saying that calculated Usage, Gap and Idle Times can only by part of the defined maxusagetime247

* Calculation from the start date of the first injection to either SampleSet Finish Date or in case no Finish

Date exists the last injection start date + Run Time.

** Overlap not possible by definition

4. Contact beyontics

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