

SmartNotes



How does the Thermo Scientific Qtegra™ ISDS Software assist me in routine operation in a GxP compliant laboratory?

I am performing routine, trace elemental analysis of samples in a GxP laboratory. What tools or features does the Thermo Scientific Qtegra Intelligent Scientific Data Solution™ (ISDS) Software provide to assist me in my daily operating procedures?

What is the Qtegra ISDS Software?

The Qtegra ISDS Software is an instrument agnostic software platform employed across the Thermo Scientific™ Qnova™ ICP-MS and the Thermo Scientific ICP-OES portfolio. With the same workflow, functionality and look and feel across multiple instruments, analysts are empowered and can flexibly switch between different techniques eliminating any barrier from learning a completely new software package.

Qtegra ISDS Software has a logical, streamlined interface that intuitively provides the analyst with the appropriate tools at each point in the analytical workflow. Within a modular framework, a series of dedicated 'plug-ins' provide hardware control of the Thermo Scientific analytical tool as well as a wide range of accessory devices (e.g. autosampler or autodilution liquid sample handling systems) from industry standard suppliers. This approach is carried through into data acquisition with dedicated plug-ins available for routine evaluations as well as for more specialized quantification techniques used for example, in time resolved analysis for laser ablation and speciation analyses (using Ion Chromatography, High Performance Liquid Chromatography or Gas Chromatography), as well as for the direct characterisation of nanoparticles using single particle ICP-MS.



Is Qtegra ISDS Software 21 CFR Part 11 compliant?

No software package can be said to be compliant with respect to 21 CFR Part 11. Qtegra ISDS Software does however support the user by providing the required tools to implement the correct (procedural, administrative and technical) controls in order to be compliant with 21 CFR Part 11.

What is the underlying data structure used by Qtegra ISDS Software?

Qtegra ISDS Software is classed as Category 3 (Non-Configured Product) under the GAMP 5 guidelines as no structural modifications or customization of the software concerning user-specific procedures are possible. Data produced by instruments controlled by Qtegra ISDS Software is stored in a file system based on data containers called LabBooks. Just as with a physical, paper lab book in a Laboratory, the Qtegra ISDS LabBook maintains a complete set of electronic records and metadata from each and every stage of the analysis, i.e.:

- The instrument hardware parameters used to acquire data
- The method parameters used during data acquisition
- The raw data from the instrument
- The calculation method(s) performed on the raw data
- Log messages that occurred during measurement
- Information on electronic signatures
- The complete audit trail

The Qtegra ISDS LabBook therefore provides a complete, encapsulated repository that tracks the entire data acquisition workflow, from analysis to result, in both native and human readable formats.

Is it possible to access Qtegra ISDS Software files through other software, e.g. third party programs?

No, Qtegra ISDS Software data files are not accessible using other software packages. Qtegra ISDS LabBooks are encrypted using a secure 256 bit AES key, and can only be opened in the Qtegra ISDS Software environment. All measurement data is stored in a protected folder to restrict access.

How many different user levels are available?

During installation Qtegra ISDS Software creates five different Microsoft® Windows® user account groups that are named according to common laboratory roles and responsibilities: User, Analyst, Supervisor, Manager and Administrator. Local or domain based Windows user accounts are then associated to one (or more) of the Qtegra ISDS user groups to allow access to the software, ensuring that only authorized individuals can use the system. The Qtegra ISDS user groups can be renamed to allow for additional flexibility when working with already defined SOPs.

How does Qtegra ISDS Software control access of users to particular functions?

Only user accounts with membership of one the Qtegra ISDS user groups are able to access Qtegra ISDS Software, protecting it from unauthorized access. A further level of security is available through the use of a dedicated Access Control manager that provides System Administrators with the tools to restrict access to specific actions/tools within Qtegra ISDS Software, allowing for a high degree of flexibility and security in GxP laboratories. All changes are automatically tracked in an audit trail.

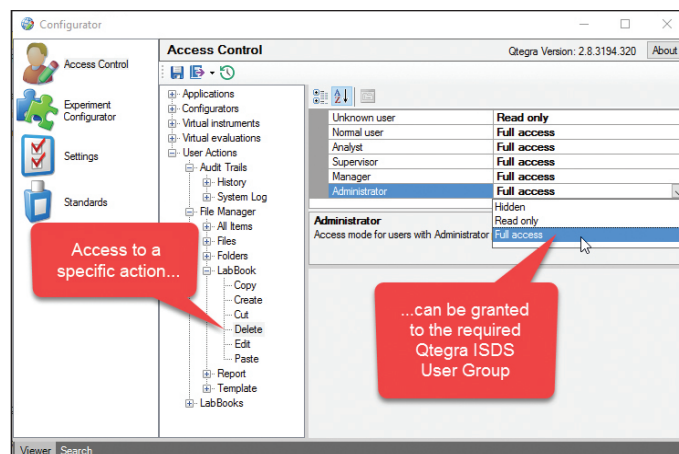


Figure 1. A dedicated Access Control manager allows for a high level of granularity when defining access to functions within Qtegra ISDS Software.

Does Qtegra ISDS Software provide audit trails?

The Qtegra ISDS Software automatically generates permanent audit trails to track all changes within the software environment. Commenting is supported within audit trails to allow for additional flexibility. All audit trails can be reviewed in a single click and can be directly exported as electronic and hardcopy versions. All audit trails are encrypted, read-only files that cannot be accessed outside of the Qtegra ISDS Software. Information in audit trails cannot be edited or deleted. Audit trails cannot be disabled without an automated, permanent record of this change being made.

Time	User	Comment	Key	Old value	New value
11/15/2017 9:47 AM	EMEAjullian.wills	Settings change	Settings.ExperimentEditor/2ICFR11Compliant	False	True
11/15/2017 9:45 AM	EMEAjullian.wills	Turned off 2ICFR11 Compliance	Settings.ExperimentEditor/2ICFR11Compliant	True	False
11/15/2017 9:44 AM	EMEAjullian.wills	Set 2ICFR11 System Log to active	Settings.ExperimentEditor/2ICFR11Compliant/SystemEventLog	False	True

Figure 2. An example Qtegra ISDS Software audit trail that shows complete ‘When?, Who?, Why? and What?’ traceability. Audit trails can be exported in a variety of formats including PDF for archiving.

The System Log in the Qtegra ISDS Software is an electronic audit trail that automatically tracks user account changes in the Qtegra ISDS Software. Events such as successful and unsuccessful log-ins, the creation and deletion of user accounts as well as membership changes in the Qtegra ISDS Software user account groups, etc., are tracked with clear explanatory text and date/time stamps. The audit trail can be filtered for display based on a series of criteria: event type, time period, account. Results can be exported as different file formats (including .pdf) for archiving purposes.

The LabBook – the data repository for analyses made in Qtegra ISDS Software – contains an electronic audit trail that automatically tracks operator entries and actions that create or modify electronic records created during routine analyses providing full ‘When?, Who?, Why? and What?’ traceability. No electronic records for data acquisition and manipulation are ever deleted within Qtegra ISDS Software. Automatic entries in the LabBook audit trail are made for routine tasks such as method creation and data acquisition. Each time the LabBook is manually saved, the user is prompted for a comment that is displayed in the audit trail for easy identification.

Does the Qtegra ISDS Software offer a dedicated tool for Software IQ/OQ?

Qtegra ISDS Software includes an extensive toolset for the performance of software IQ/OQ. Installation Qualification (IQ) is executed when the Qtegra ISDS Software is initially installed. During the IQ process, the tool verifies that all files are installed in the correct locations, and their integrity is verified via comparison of checksums. During the Operational Qualification (OQ) process, the data evaluation algorithms of the software are checked for consistency. The verification of the correct function of the software is accomplished through an example file that is checked for accuracy of results. A printable electronic report is generated for archiving. The IQ/OQ process can be performed whenever it is required (for example after updates to the computer system, such as an operating system change) to meet established company SOPs.

Verification step	State
Verification of the prerequisites for IQ/OQ	OK
Gathering system information	OK
Verification of installed files	OK
Verification of all required references	OK
Verification of LabBook evaluations	OK

System Information	
Current time	9/23/2017 7:18:37 PM
Computer name	DEBRE-BLPLJC2
User name	EMEAjullian.wills
Operating system	Windows 10
Windows folder	C:\WINDOWS
Net runtimes	.NET 2.0.50727.4927 (Service Pack 2) .NET 3.0.30729.4926 (Service Pack 2) .NET 3.5.30729.4926 (Service Pack 1) .NET 4.0.0.0 .NET 4.6.01586
System locale	English (United States)
User locale	English (United States)
Thousands separator	.
Decimal separator	.
List separator	.
Processor count	4
Processor detail	Intel® Family 6 Model 78 Stepping 3 Intel(R) Core(TM) i5-6300U CPU @ 2.40GHz

Figure 3. IQ/OQ report generated by the Qtegra ISDS Software Qualification tool.

In order to further ensure integrity of the software installation, each time the Qtegra ISDS Software is initialized a repeat IQ to check file integrity is automatically performed with any issue flagged in a permanent log file.

How can Qtegra ISDS Software assist with Performance Qualification of my instrument?

Performance Qualification (PQ) assures that the daily performance of the instrument meets defined expectations, ultimately demonstrating that the instrument is suitable for a given analytical task.

In contrast to Installation Qualification and Operational Qualification (IQ/OQ), the analyst is responsible for defining the criteria used for PQ and for establishing applicable protocols, e.g. through the use of Standard Operating Procedures (SOPs).



In order to assist with system validation and to ensure accurate and consistent performance, Qtegra ISDS Software provides a “Get Ready” capability. With a single click, an exhaustive verification of instrument performance can be triggered (Figure 4). This assessment can be automatically performed on initial startup but can also be scheduled at any time, for example when switching between analysts or work periods.

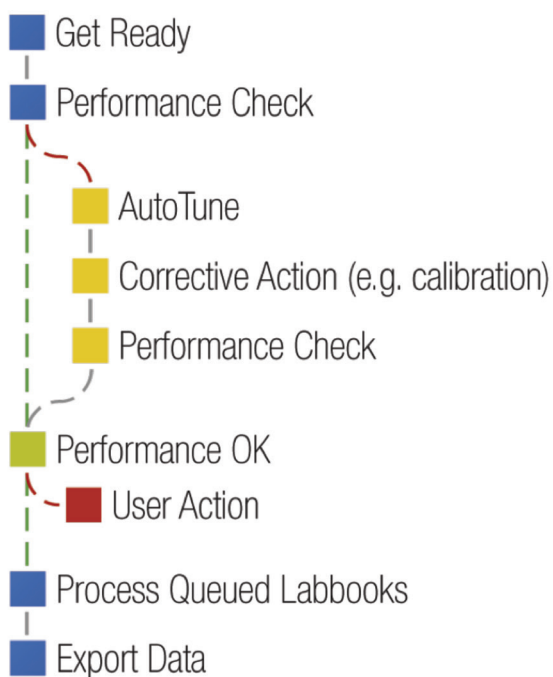


Figure 4. Get Ready instrument performance verification workflow and automated system set-up.

If all of the performance goals are met, the instrument can start to process queued LabBooks of analyses. If any corrective actions are required however, for example an autotune to improve sensitivity, they are automatically triggered and a repeat performance check is performed. Reports for each step in the process allow for complete traceability.

Which parameters are checked as part of the Get Ready routine?

As part of the Get Ready procedure, all the required instrument modes are automatically checked for consistent operation. With ICP-MS for example, the relevant parameters include sensitivity across the mass range, plasma conditions (e.g. oxide and doubly charged formation) as well as interference suppression through the use of kinetic energy discrimination (KED). Mass resolution and calibration accuracy are also assessed.

How can I monitor instrument performance over time?

Reports from autotunes and performance checks are automatically stored within the Qtegra ISDS Software file structure as encrypted files that cannot be user modified or accessed outside of the Qtegra ISDS Software. Autotune and performance reports can be exported in electronic – PDF – or hardcopy versions for archiving. Changes in instrument parameters are permanently recorded to allow for a complete instrument history to be maintained. Additionally, during a LabBook based sequence of analyses, the applied instrument settings and their corresponding readback values are saved into the LabBook to allow for complete traceability at any time.

Can I integrate Qtegra ISDS Software with my existing LIMS?

Qtegra ISDS Software provides a series of features to integrate with Laboratory Information Management Systems (LIMS). Sample details from a LIMS export can be merged with template defined rules to generate a complete Sample List for routine acquisition with just a couple of mouse clicks. In this process, the sample label, autosampler rack position as well as information on sample dilution performed during the preparation stage can be automatically transferred into the Qtegra ISDS Software. Flexible mapping controls allow for simple cross reference between potentially differing sample metadata, or for translation between different languages. After acquisition, data export (as .csv or .xml files) back into the LIMS system can be automatically performed per analysis and/or after completion of the entire LabBook.

Can I change users during data acquisition, for example when there is a shift change during a running sequence?

Yes, it is possible to log off and on using different user accounts during data acquisition. Access to Qtegra ISDS Software is securely managed through the use of Windows user groups and specific permissions given to users by System Administrators as previously described. LabBook scheduling and data acquisition however is controlled by a system wide Windows service process that is completely independent from the active Windows user account. The active user submitting the LabBook for data acquisition is captured in the LabBook audit trail until a new user makes a change. An additional advantage of keeping data acquisition separate from user accounts is that it's not necessary to have the Qtegra ISDS Software user interface (UI) open during data acquisition.

Can I store my data on a remote location, e.g. a server?

Complete electronic records consisting of raw data and metadata from an analysis are stored in the Qtegra ISDS LabBook data container. By default these are saved to a secure folder on the local hard drive of the instrument control PC. From this initial location, links to external folders can be created inside the Qtegra ISDS File Manager, for example, to allow access to external hard drives for local backup or to network servers for backup or data distribution. It is not recommended to initially save running LabBooks to external locations in case of network instability. A backup facility is provided within Qtegra ISDS Software to allow for automated backups of LabBooks directly after analysis.

Can I manipulate my data on a separate PC?

In order to free up the instrument control PC in busy laboratories, it can be useful to perform further data evaluation, generate reports etc. on a different PC. The default Qtegra ISDS Software license allows for up to three additional software installations on PCs that are used for data evaluation only. In this way, LabBooks can either be stored on a central data storage device (e.g. a server) and manipulated as required or accessed directly from the original data storage location on the instrument control PC. All changes to the data set are tracked in the audit trail that's integral to the Qtegra ISDS LabBook data container.

Can I generate electronic or hardcopy reports of the results from my analyses?

In addition to a series of supplied report templates, Qtegra ISDS Software includes a powerful report template editor to allow the creation of custom reports. Reports can be configured to include detailed information on any aspect from the original data source, the LabBook (Figure 5). In this way, complete traceability of the entire acquisition process is possible, including LabBook creation and acquisition date and times, instrument identification and information about users acquiring and modifying the data set. Company logos can be added to reports for personalization.

The resulting reports can be archived as PDF files or hardcopy versions. The Qtegra ISDS Software allows the automatic generation of a report print out (and/or PDF export) directly after measurement. All report parameters can be renamed to take into account local language or meet company specific nomenclature to allow for ease of data handling, for example in LIMS systems.

Can I define my own calculations in the Qtegra ISDS Software?

The basic calculation algorithms that take raw intensities from the instrument and convert them into final, reportable concentration data within Qtegra ISDS Software are not user-definable. All steps in the calculation process are documented, validated and can be easily demonstrated and checked for accuracy using standard spreadsheet applications such as Microsoft Excel®.

Once the final concentration data has been obtained however, a range of additional calculations can be made directly within the Qtegra ISDS Software. This is particularly useful for users in regulated laboratory environments who may face issues with traceability when using external software packages such as Microsoft Excel.

You can perform simple mathematical functions within a single LabBook. For example, you can sum the concentrations of different elements, useful if you are performing screen analyses to check if the total elemental concentration is above the limit specified by a supplier.

Big Four Concentration Screen						
Report Date - 11/29/2017 12:44:28 PM						
Instrument Summary:						
Instrument Name: ICAP Q						
Serial Number: 03281R						
LabBook Summary:						
LabBook Name: Paracetamol Tablets 05OCT16_1.imexp						
LabBook Path: _Application Data\Workspace\LabBooks\QC						
Number of Samples: 61						
Number of Results: 61						
LabBook Started: 10/5/2016 4:37:45 PM by: ICP-MS						
LabBook Changed: 11/29/2017 12:06:19 PM by: EMEA\julian.wills						
Sum of Concentrations:						
ID:	Start Time:	Arsenic	Cadmium	Mercury	Lead	Sum of Big 4
PRC-0266	10/5/2016 5:42:26 PM	0.4 ppb	0.1 ppb	0.6 ppb	0.2 ppb	1.29 ppb
PRC-0274	10/5/2016 6:06:49 PM	0.1 ppb	0.0 ppb	0.6 ppb	2.8 ppb	3.50 ppb
PRC-0276	10/5/2016 6:10:59 PM	0.1 ppb	0.0 ppb	0.2 ppb	1.4 ppb	1.88 ppb
PRC-0277	10/5/2016 6:13:05 PM	0.4 ppb	0.0 ppb	0.2 ppb	0.8 ppb	1.40 ppb
PRC-0278	10/5/2016 6:15:10 PM	0.1 ppb	0.0 ppb	0.2 ppb	0.5 ppb	0.78 ppb
PRC-0279	10/5/2016 6:17:16 PM	0.1 ppb	0.0 ppb	0.1 ppb	0.6 ppb	0.79 ppb
1 / 1						

Figure 5. Use of sum function in Qtegra ISDS Software reports to display the sum of recorded concentrations in a single analysis. As can be seen, flexible, per column definition of reported decimal places is possible.

How can Qtegra help me to demonstrate successful validation of my methods?

A range of powerful Quality Control (QC) tools are provided as part of the default Qtegra ISDS Software installation and these can be configured to demonstrate successful method validation against national and international measurement protocols. For example, the U.S. Pharmacopeial Convention (USP) Chapter '<233> - Elemental Impurities – Procedures', requires that six independent samples spiked at a defined concentration level are repeatedly analyzed to test the complete preparation and quantification method.

The calculation of recoveries is accomplished using the Quality Control features implemented in the Qtegra ISDS Software. Through an automated procedure, the concentration amount recovered for a given analyte is calculated based on the comparison of results from the (unspiked) sample and the sample spiked at a known concentration of the target elements.

The flexible reporting tool supplied in Qtegra ISDS Software allows a printable record to be generated that shows the recovery results for each replicate as well as the average recovery and repeatability results from all six analyses (Figure 6) to meet the USP <233> requirements. The results can then be archived as hardcopy or in a variety of formats including PDF.

Repeatability Results														
Report Date - 11/29/2017 4:16:04 PM														
Instrument Summary:														
Instrument Name: ICAP Q														
Serial Number: 03281R														
LabBook Summary:														
LabBook Name: Paracetamol Tablets 05OCT16_1.imexp														
LabBook Path: _Application Data\Workspace\LabBooks\QC\Used for SmartNote														
Number of Samples: 61														
Number of Results: 61														
LabBook Started: 10/5/2016 4:37:45 PM by: ICP-MS														
Last change time: 11/29/2017 4:15:07 PM by: EMEA\julian.wills														
Repeatability Results:														
ID:	51V (KED)	63Ni (KED)	59Co (KED)	65Cu (KED)	75As (KED)	95Mo (KED)	101Ru (KED)	103Rh (KED)	105Pd (KED)	111Cd (KED)	189Ir (KED)	195Pt (KED)	202Hg (KED)	208Pb (KED)
Repeatability- 1	102 %	100 %	101 %	100 %	106 %	100 %	100 %	100 %	100 %	101 %	102 %	102 %	103 %	104 %
Repeatability- 2	101 %	100 %	101 %	99 %	106 %	99 %	99 %	99 %	99 %	102 %	102 %	100 %	102 %	103 %
Repeatability- 3	98 %	97 %	98 %	98 %	104 %	98 %	98 %	98 %	98 %	99 %	100 %	99 %	101 %	103 %
Repeatability- 4	101 %	99 %	99 %	99 %	105 %	99 %	98 %	98 %	98 %	100 %	101 %	100 %	103 %	122 %
Repeatability- 5	99 %	96 %	97 %	97 %	102 %	98 %	97 %	97 %	97 %	99 %	100 %	99 %	101 %	102 %
Repeatability- 6	98 %	97 %	97 %	97 %	101 %	99 %	98 %	98 %	97 %	98 %	100 %	98 %	101 %	102 %
Av. Recovery	100 %	98 %	99 %	98 %	104 %	99 %	98 %	98 %	98 %	100 %	101 %	100 %	102 %	106 %
Repeatability	2 %	2 %	2 %	1 %	2 %	1 %	1 %	1 %	1 %	2 %	1 %	1 %	1 %	8 %
1 / 1														

Figure 6. Use of calculation and reporting features in Qtegra ISDS Software to display results for the USP <233> Repeatability test.

How can Qtegra ISDS Software assist me in documenting changes in my data?

The Qtegra ISDS LabBook contains the acquisition method, raw data, the calculation method and final calculated data. It also contains the complete audit trail to track every stage of the process. A series of automatic entries are made in the audit trail during LabBook based data acquisition. Each time a manual change is made in the LabBook a comment has to be entered that requires a two stage identity check. All comments are tracked in the audit trail.

Qtegra ISDS Software supports the use of non-biometric electronic signatures to ensure that only verified data sets are released for production samples. Multiple levels of signatures are provided and a flexible editor is provided to assign functions to specific Qtegra ISDS User Groups. Changes to electronic signatures are tracked in the LabBook audit trail and signatures (with full 'When?, Who?, Why? and What?') traceability) can be recorded in hard copy or electronic reports.

Does Qtegra ISDS Software provide QC tests?

The default installation of Qtegra ISDS Software contains a wide selection of predefined quality control (QC) tests that are based on the following base types:

- Blank tests to verify the achievable detection limits.
- Calibration tests to monitor accuracy against the concentration calibration.
- Paired sample tests to assess duplicate or serial dilutions.
- Spike tests to verify recovery from various stages in the method.
- Continuous tests to monitor internal standard recovery and signal stability (as raw intensities and/or concentrations) in each analysis.

All tests can be matched to Standard Operating Procedures (SOPs) to meet specific conditions (e.g. acceptable recovery ranges, target elements etc.) and potential corrective actions (e.g. triggering of repeat analysis etc.). Results from QC tests are directly displayed in the software user interface and can be distributed further via data export or generation of printable or electronic records. Additional QC tests can be created as required in order, for example, to comply with existing SOPs.

I can generate a lot of data very quickly. How can Qtegra help me to focus on what's important during my analyses?

Qtegra ISDS Software contains dedicated functions to automatically format results outside of defined ranges to allow for quicker identification of potential issues that may require user action. This includes basic abilities to, for example, identify results from all analyses (not just quality control samples) that lie outside of SOP defined warning or failure boundaries. Additional flexibility allows for concentrations to be compared against detection limits and/or calibration ranges, especially important in laboratories without autodilution capabilities where over calibration range samples are highlighted so that they can be taken from the sample rack, further manually diluted and added to the acquisition.

In the data evaluation (Figure 7) and reporting (Figure 8) steps in the Qtegra ISDS Software workflow, these samples can be automatically 'flagged' to focus attention, e.g. through the use of user definable replacement text or formatting (color coding, font changes etc.).

No	Time	Sample Type	Label	75As (KED) (ppb)	103Rh (KED) (%)	
1	3/23/2016 5:51:06 AM	UNKNOWN	Prime	0.001	98.2%	
2	3/23/2016 5:52:44 AM	UNKNOWN	Prime	-0.001	99.7%	
3	3/23/2016 5:54:18 AM	BLK	Calibration Blank	0.000	100.0%	
4	3/23/2016 5:55:53 AM	STD	0.025 ppb ICS2	0.025	99.97%	
5	3/23/2016 5:57:26 AM	STD	0.050 ppb ICS2	0.051	99.37%	
6	3/23/2016 5:58:59 AM	STD	0.100 ppb ICS2	0.100	99.09%	
7	3/23/2016 6:00:33 AM	STD	1.000 ppb ICS2	1.000	100.25%	
11	3/23/2016 6:06:55 AM	UNKNOWN	UN	0.002	100.12%	
12	3/23/2016 6:08:30 AM	QC	QC	OR 5.056	101.1%	
13	3/23/2016 6:10:04 AM	QC	QC	0.002	99.4%	
15	3/23/2016 6:13:14 AM	QC - KCB	Blank (undigested)	0.001	99.1%	
42	3/23/2016 6:55:57 AM	UNKNOWN	28370900	QC FAIL	99.4%	
43	3/23/2016 6:57:33 AM	UNKNOWN	28370904	7.731	99.4%	
44	3/23/2016 6:59:08 AM	UNKNOWN	28370908	QC FAIL	99.4%	
45	3/23/2016 7:00:43 AM	UNKNOWN	28370912	QC FAIL	93.1%	
46	3/23/2016 7:02:17 AM	UNKNOWN	28370918	96.293	96.1%	
47	3/23/2016 7:03:54 AM	UNKNOWN	28370923	100.667	96.0%	
47				1	103.565	95.1%
47				102.122	94.7%	
47				97.768	97.0%	
				100.667	96.0%	
				4.1	1.4	
				1.3	1.3%	
48	3/23/2016 7:05:29 AM	UNKNOWN	28370933	97.436	96.7%	
49	3/23/2016 7:07:03 AM	UNKNOWN	28370936	OR 265.522	W 76.8%	
50	3/23/2016 7:08:39 AM	UNKNOWN	28370940	OR 268.360	W 76.8%	
51	3/23/2016 7:10:14 AM	UNKNOWN	28370955	OR 267.958	W 77.7%	
52	3/23/2016 7:11:48 AM	QC	Blank (undigested)	-0.001	106.1%	
53	3/23/2016 7:13:25 AM	QC - CCV	5.00 ppb CVS	OR 5.134	102.7%	
54	3/23/2016 7:15:00 AM	QC - CCV	0.500 ppb Hg CVS	0.001	105.6%	
55	3/23/2016 7:16:35 AM	UNKNOWN	28371046	14.612	98.2%	
56	3/23/2016 7:18:11 AM	UNKNOWN	28371071	16.840	98.5%	
57	3/23/2016 7:19:45 AM	UNKNOWN	28371087	17.709	98.4%	
58	3/23/2016 7:21:20 AM	UNKNOWN	28378057	52.212	90.3%	
59	3/23/2016 7:22:54 AM	UNKNOWN	28378060	OR 191.639	86.7%	

Figure 7. The Qtegra ISDS Software flags and limits are used in the data evaluation views to automatically highlight values after comparison against defined criteria.

Index	Start Time	Sample Type	Label	75As (KED)	103Rh (KED)
1	3/23/2016 5:51:06 AM	UNKNOWN	Prime	0.001 ppb	98.207 %
2	3/23/2016 5:52:44 AM	UNKNOWN	Prime	-0.001 ppb	99.684 %
3	3/23/2016 5:54:18 AM	BLK	Calibration Blank	0.000 ppb	100.000 %
4	3/23/2016 5:55:53 AM	STD	0.025 ppb ICS2	N/A	99.970 %
5	3/23/2016 5:57:26 AM	STD	0.050 ppb ICS2	0.051 ppb	99.372 %
6	3/23/2016 5:58:59 AM	STD	0.100 ppb ICS2	0.100 ppb	99.099 %
7	3/23/2016 6:00:33 AM	STD	1.000 ppb ICS2	1.000 ppb	100.252 %
11	3/23/2016 6:06:55 AM	UNKNOWN	UN	0.002 ppb	100.123 %
12	3/23/2016 6:08:30 AM	QC	QC	OR 5.056	101.440 %
13	3/23/2016 6:10:04 AM	QC	QC	0.002 ppb	99.400 %
15	3/23/2016 6:13:14 AM	QC	QC	0.001 ppb	99.100 %
42	3/23/2016 6:55:57 AM	UNKNOWN	28370900	QC FAIL	99.400 %
43	3/23/2016 6:57:33 AM	UNKNOWN	28370904	7.731 ppb	99.400 %
44	3/23/2016 6:59:08 AM	UNKNOWN	28370908	QC FAIL	99.400 %
45	3/23/2016 7:00:43 AM	UNKNOWN	28370912	QC FAIL	93.118 %
46	3/23/2016 7:02:17 AM	UNKNOWN	28370918	96.293 ppb	96.075 %
47	3/23/2016 7:03:54 AM	UNKNOWN	28370923	100.667 ppb	96.036 %
48	3/23/2016 7:05:29 AM	UNKNOWN	28370933	97.436 ppb	96.676 %
49	3/23/2016 7:07:03 AM	UNKNOWN	28370936	OR 265.522	W 76.757
50	3/23/2016 7:08:39 AM	UNKNOWN	28370940	OR 268.360	W 76.757
51	3/23/2016 7:10:14 AM	UNKNOWN	28370955	OR 267.958	W 77.731
52	3/23/2016 7:11:48 AM	QC	Blank (undigested)	-0.001 ppb	106.127 %
53	3/23/2016 7:13:25 AM	QC	5.00 ppb CVS	OR 5.134	107.621 %
54	3/23/2016 7:15:00 AM	QC	0.500 ppb Hg CVS	0.001 ppb	105.610 %
55	3/23/2016 7:16:35 AM	UNKNOWN	28371046	14.612 ppb	98.182 %
56	3/23/2016 7:18:11 AM	UNKNOWN	28371071	16.840 ppb	98.545 %

Figure 8. The same data conditional formatting displayed in the evaluation views is carried through into reports that can be automatically sent to a printer (and/or as a CSV export) to trigger manual corrective actions.

How can I monitor my analytical results over time?

In order to review, for example, the results obtained for a routine quality control standard, a LabBook Query function is provided in the Qtegra ISDS Software that can search and filter results across multiple LabBooks. Figure 9 shows the LabBook Query interface that allows analysts to search for results obtained for a given analysis based on location, analysis date, method parameters, naming and comments. Data components from the resulting analyses can then be compiled into a single data export or electronic or printed report.

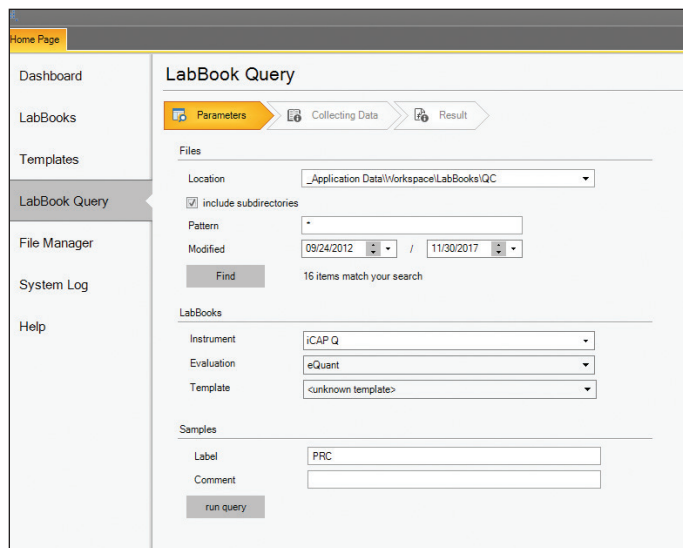


Figure 9. The Qtegra ISDS Software LabBook Query interface is used to search and subsequently extract information for analyses in multiple LabBooks.

How can Qtegra ISDS Software assist me when I want to expand my analytical capabilities?



With the flexible framework provided by the use of plug-ins in Qtegra ISDS Software, it's simple to expand analytical abilities to add, for example, autodilution capabilities in combination with the appropriate hardware and software plug-ins. A completely new technique, for example speciation or nanoparticle analyses, can be quickly implemented through the addition of the appropriate plug-in within Qtegra ISDS Software. With all plug-ins interfacing into the same basic Qtegra ISDS Software structure there's no difference in workflow with the same look and feel throughout, independent of the analytical task.

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