

# How is Qtegra ISDS Software enhancing Gas IRMS analysis?



The Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution (ISDS) Software is carefully optimized to deliver simplicity, efficiency and quality in your Gas Isotope Ratio Mass Spectrometry (IRMS) laboratory. The software platform is built on four pillars: **Workflow, Data Management, Scalability and Compliance**. Each pillar delivers user experience that is based around simplicity. Qtegra ISDS Software has a logical, streamlined interface that intuitively provides the analyst with the appropriate tools at each point in the analytical workflow. Extensive automation of tasks reduces the requirements for manual intervention. With the same look and feel across multiple instruments, analysts are empowered and can flexibly switch between different techniques, saving you time training operators and working with your results.



## Workflow: How do I get from sample to results?

Qtegra ISDS Software has an intelligent workflow (Figure 1) that drives you from sample to result, without compromising on flexibility. This intelligent yet flexible approach minimizes operator tasks between sample receipt and generation of the final result, dramatically boosting laboratory productivity.

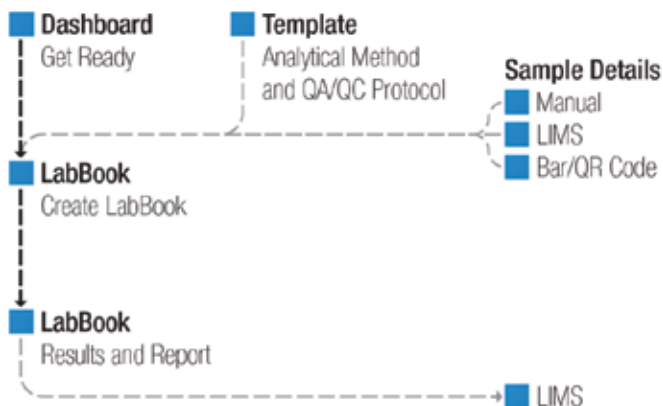


Figure 1. Qtegra ISDS Software Workflow

The **Get Ready** function on your **Dashboard** sets up your system automatically, saving you time and ensuring consistent system performance (Figure 2). For Gas IRMS systems, Get Ready will perform the daily tasks such as peak center and autotune, and also allow for extended performance checks, all in one place.

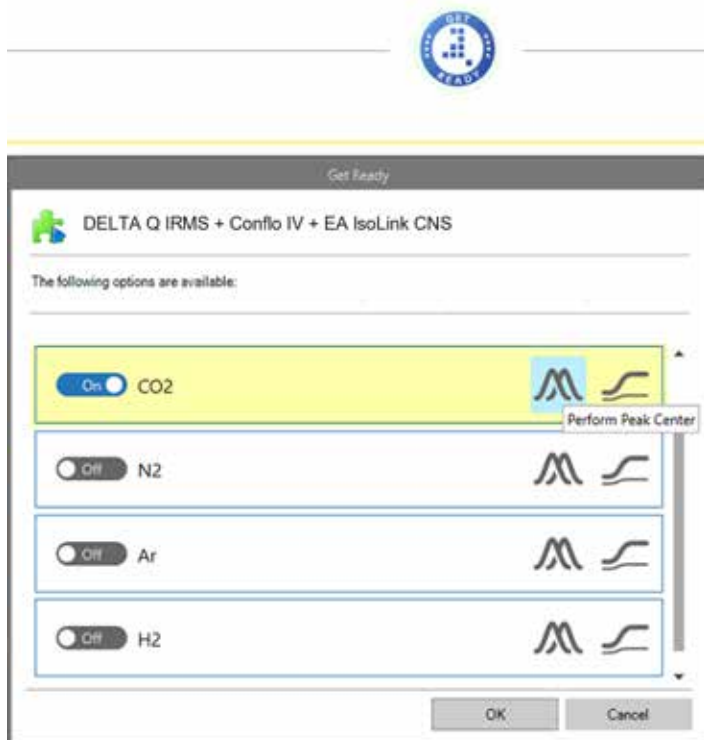


Figure 2. Qtegra ISDS Software: GetReady feature

Knowing that your system is ready for analysis, you can start to prepare your analysis by setting up the **LabBook**. The Labbook is home to everything surrounding your sample analysis: the method, the data evaluation, the results and the QA/QC.

Your **sample details** can be manually input or imported. For the analysis setup you can use a **template** containing the complete predefined measurement protocol including gas configuration, system timings, internal standards, or sequence rules. Intelligent templates are provided within the software but are also completely customizable using previously measured samples as a starting point (Figure 3).

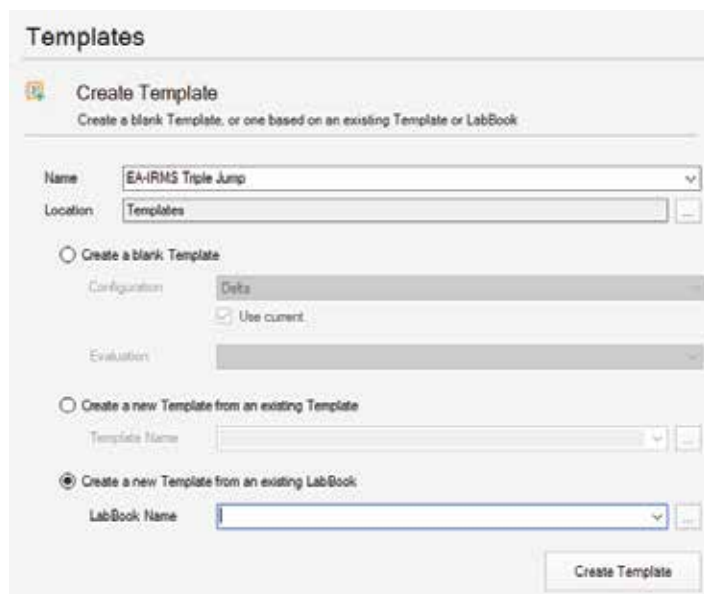


Figure 3. Qtegra ISDS Software: templates

The templates contain comprehensive quality control tests that can be fully integrated into your workflow. The intelligent template enables continuous data quality monitoring and rule-based automatic interaction on failures, such as repeat analysis and automatic dilution of samples outside the calibration range.

The LabBook allows you to display the key method parameters in a simple Drag&Drop layout, enabling you to easily tune your method.

The analysis begins as soon as you schedule a LabBook. Data is processed on the fly so your results are ready immediately. Your LabBook contains sample lists and fully interactive display of results, allowing you to dive into relevant areas of your data (Figure 4).



Figure 4. Qtegra ISDS Software: results display

### Data Management: Is there a direct route to relevant data?

Once an analysis has been made, the Qtegra ISDS Software LabBook provides a layered approach to results through a series of views, where data can be displayed, queried and instantly recalculated. This layered approach quickly directs the user to relevant areas of data, aiding your manual data review, maximizing your productivity.



Figure 5. Qtegra ISDS Software: chromatograms overlay

Qtegra ISDS Software LabBook allows you to focus in on specific chromatograms, easily re-define peak backgrounds, or overlay chromatograms to monitor interferences and much more (Figure 5).

Whether you are interested in  $\delta^{13}\text{C}$ ,  $\delta\text{D}$  or  $\Delta_{47}$ , Qtegra ISDS Software LabBook data evaluation modules are available so that you can immediately see your isotope ratio result.

Fast searches across multiple LabBooks can be performed directly within **Qtegra LabBook Query**. Can't remember when you analyzed a sample? Then search for results based on metadata or data contexts. The data can be queried over multiple LabBooks simultaneously. Want to export data from multiple analytical runs? Data can be combined from several LabBooks; for example, to assess long term reproducibility of quality control results.

Once reviewed, you have several options where to send your data. A "What you see, is what you get" (WYSIWYG) **data report tool** enables simple reporting of all relevant results. All information – whether it is graphical or data – can be instantly exported as an image or as text.

Additionally, **full integration with LIMS** is supported. Sample lists can be imported from LIMS into pre-defined protocol templates, incorporating the full range of quality control checks. Comprehensive, user-definable reports allow for flexible export to external LIMS software packages.

## Scalability: How to expand without adding complexity?

Whether you are challenged with globalization or consolidation, Qtegra ISDS Software allows organizations to deploy in a familiar environment. Qtegra ISDS Software scalability provides a balance between mainstream capabilities and specialized functions: focusing on the immediate task and creating awareness of greater possibilities.

Thermo Fisher Scientific provides a full range of instrumentation for the analysis of elements and isotopes. Qtegra ISDS Software is the unifying platform that links our innovative and market leading hardware to your application. **Qtegra ISDS Software is standardized from instrument to instrument.** This minimizes the requirement for specialist operators and dramatically reduces the requirement for extensive cross training. Qtegra ISDS Software promotes collaboration and provides capabilities that allow organizations to standardize:

- Harmonized workflow
- Streamlined method development and validation
- Multi-vendor accessory control for LC, GC, lasers and other sampling devices

- Standardized data format
- Secure user access and tracking

**Qtegra ISDS Software is simple to install and configure.** An intuitive drag-and-drop instrument configurator provides a bespoke system configuration for your particular application. Each Thermo Scientific Gas IRMS system comes pre-deployed with Qtegra ISDS Software to ensure rapid system set-up and security of system settings.

**Qtegra ISDS Software is modular,** so it provides a flexible framework in which instrument and accessory plug-ins are combined into a single workflow. In addition to the instrument plug-in, Qtegra ISDS Software provides integrated plug-ins for autosamplers, autodilutors as well as major chromatography systems. Qtegra ISDS Software for Gas IRMS comes with a plug-in for Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) Software, providing seamless communication to gas chromatography devices (Figure 6). We also provide a software plug-in development kit to allow third-party manufacturers to interface their technology seamlessly to the powerful Qtegra ISDS Software.

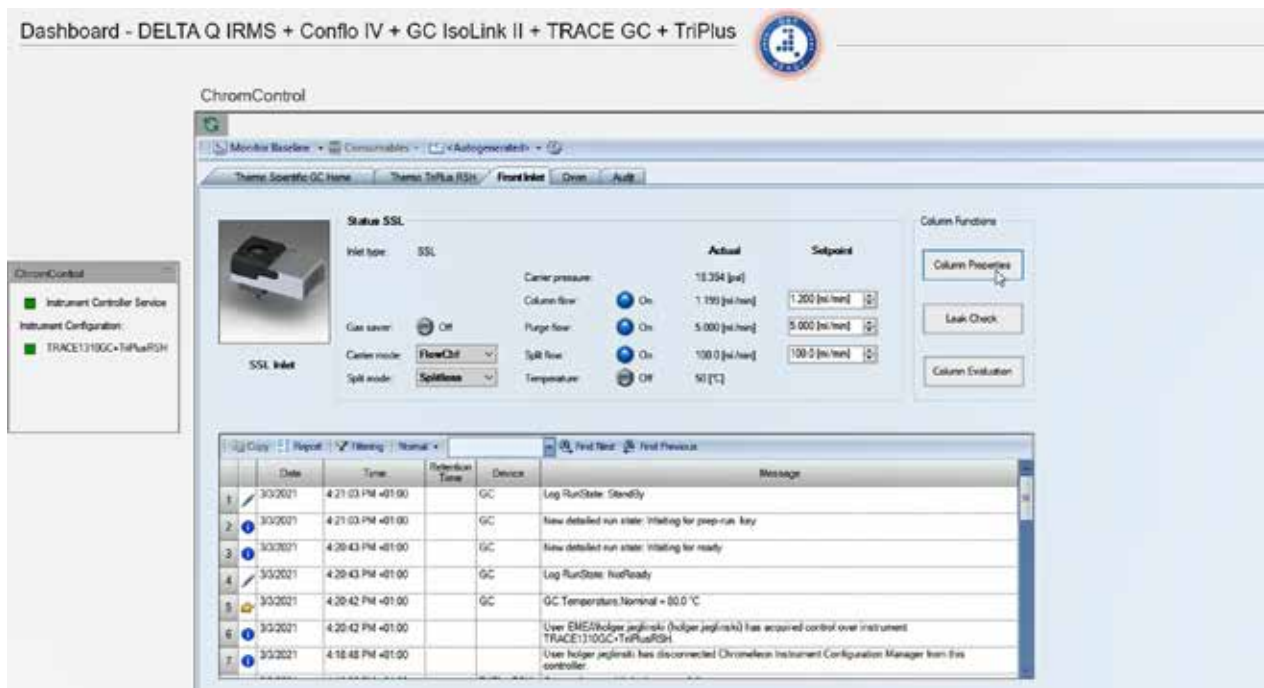


Figure 6. Qtegra ISDS Software: ChromControl

## Compliance: Will new technology create a compliance challenge?

Qtegra ISDS Software recognizes the challenge to meet rising standards of quality and to comply with rigorous regulatory requirements by including the necessary tools for you to rapidly meet your compliance goals. Qtegra ISDS Software security supports the administrator by creating a controlled environment to ensure that the system is configured to comply with GxP and 21 CFR Part 11 regulations. This is achieved with a full range of features, including:

- Audit trails
- Open/closed system control
- Electronic signatures
- Identification codes and passwords
- Tools for integrated data management
- Full record change traceability

Qtegra ISDS Software ensures the utmost integrity and traceability for all of your raw data, metadata, and reported results. Access control in Qtegra ISDS Software is provided by the Microsoft Windows® User Management system that is flexible, secure and customizable. Users are defined with privileges, roles, and access groups (Figure 7). Qtegra ISDS Software enables you to establish audit trails, assign access privileges, set password expiry, and automated log-outs due to inactivity. Multi-level security is provided for every task. Qtegra ISDS Software also helps you manage your compliance on a day-to-day basis with such capabilities as secure time-stamped audit trails. Records can be easily reviewed so you can apply the appropriate electronic signatures. All data is relationally stored, so full documentation is automatic and complete, saving you time during compliance audits.

Configurator

**Access Control**

The Access Control applet of the Configurator tool allows the Administrator to control the User Actions.

Save History Export

User Action	USER GROUPS						
	System Administrator	Administrator	Data Administrator	Manager	Supervisor	Analyst	User
▲ Audit Trails							
> ▲ History							
Export	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
View	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
▸ System Log							
▲ File Manager							
▸ All Items							
▲ Files							
Delete	Prohibited	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed
Export	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Import	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
▸ Folders			Prohibited				
▲ LabBook							
Copy	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Create	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Cut	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Delete	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Edit	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Paste	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
▲ Report							
Copy	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Create	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Cut	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Delete	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Edit	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
Paste	Prohibited	Allowed	Allowed	Allowed	Allowed	Allowed	Allowed
▸ Template							
▸ LabBooks							
▸ Dashboard							

Figure 7. Qtegra ISDS Software: privileges, roles, and access groups

## Qtegra ISDS Software driven – the journey has begun

Qtegra ISDS Software is developed using a platform-based approach; it is a core control software across different analytical devices. Cross-device training and adoption of new instrumentation is faster and easier, allowing for increased flexibility in modern multi-technique laboratories.

The range of instruments running Qtegra ISDS Software is ever expanding.

Supported Instruments	
Technology	Instrument
Gas Isotope Ratio MS	Thermo Scientific™ Ultra™ High Resolution IRMS
	Thermo Scientific™ 253 Plus™ 10 kV IRMS
	Thermo Scientific™ DELTA Q™ IRMS
	Thermo Scientific™ EA IsoLink™ IRMS System
	Thermo Scientific™ GC IsoLink II™ IRMS System
	Thermo Scientific™ LC IsoLink™ IRMS System
	Thermo Scientific™ GasBench Plus IRMS System
	Thermo Scientific™ Kiel IV Carbonate Device
ICP-OES	Thermo Scientific™ iCAP™ 7000 Series ICP-OES
	Thermo Scientific™ iCAP™ 7000 Plus Series ICP-OES
	Thermo Scientific™ iCAP™ PRO Series ICP-OES
ICP-MS	Thermo Scientific™ iCAP™ Q ICP-MS
	Thermo Scientific™ iCAP™ RQ ICP-MS
	Thermo Scientific™ iCAP™ TQ ICP-MS
	Thermo Scientific™ iCAP™ TQs ICP-MS
	Thermo Scientific™ iCAP™ TQe ICP-MS
Multicollector ICP-MS	Thermo Scientific™ Neoma™ MC-ICP-MS
Noble Gas MS	Thermo Scientific™ Argus VI™ Noble Gas MS
	Thermo Scientific™ Helix SFT™ Noble Gas MS
	Thermo Scientific™ Helix MC Plus™ Noble Gas MS

Find out more at [thermofisher.com/QtegraIRMS](https://thermofisher.com/QtegraIRMS)

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