

Smart Notes



Qtegra ISDS Software: Your lab assistant for Gas IRMS analysis

Laboratories tasked with the analysis of isotopes and elements can rely on the Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution (ISDS) Software to eliminate any barrier from flexibly switching between different techniques for achieving world beating results.

With the same look and feel across multiple instruments, analysts are empowered to effectively use their time in laboratory, even for the most challenging analysis setups. Whether you are investigating individual compounds in complex mixtures using Gas Chromatography or reconstructing global temperatures millions of years ago with clumped isotopes, Thermo Scientific™ Isotope Ratio Mass Spectrometry (IRMS) portfolio covers your application. With Qtegra ISDS Software, your intelligent lab assistant, you are assured:

- Transparency
- Flexibility
- Simplicity
- Innovation



Transparency

We fully understand that in order to trust your software, you first need to understand what it is doing, and that is why transparency is central to the design of Qtegra ISDS Software.

Where is the information available?

Explanations of various method and data evaluation parameters are available within the software to teach you how the software is operating in the background, enabling you to optimize your analysis to achieve high quality results.

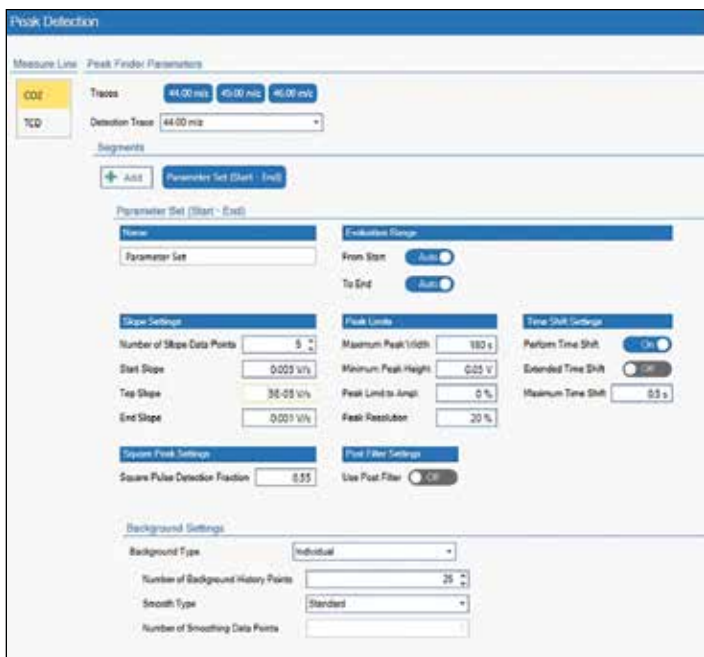


Figure 1. Qtegra ISDS Software: peak detection parameters setup

For every data evaluation module, there is a comprehensive explanation of the mathematics available in the software.

Flexibility

Research often means pushing the boundaries of what is possible. Qtegra ISDS Software provides you with complete flexibility to continue to push the boundaries and make new discoveries within Gas IRMS.

How do I control peripheral devices?

For IRMS systems connected to multiple peripheral devices, Qtegra ISDS Software allows you to switch seamlessly between the different peripheral devices, scheduling back-to-back runs using different peripheral devices. For non-standard IRMS systems, Qtegra ISDS Software provides you with free rein to create and control your unique peripheral device using the Hardware Panel Configurator.

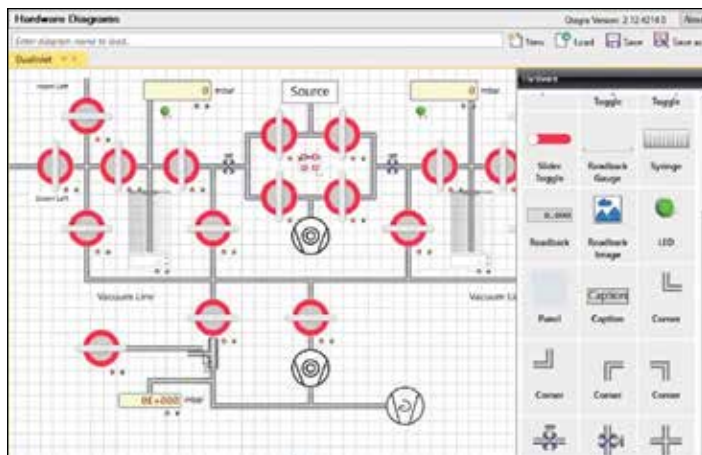


Figure 2. Qtegra ISDS Software: Hardware Panel Configurator

Can I control when my analysis begins?

Have you just performed maintenance and want to wait for the system to stabilize? The Qtegra LabBook scheduler provides you with the flexibility to decide exactly when you want to perform your IRMS analysis. The measurement can be performed immediately, at desired time or added to a queue of Labbooks.

How is my data handled?

Qtegra ISDS Software data evaluation contains many powerful tools that give you total flexibility to evaluate your data. Samples can be grouped into batches and your data can be evaluated against external reference material, allowing you to perform all your data processing within the software so that it is fully traceable and transparent for the future. Your compounds of interest can be easily labeled by Qtegra ISDS Software's Click&Identify approach, allowing you to build up your global Compounds library for quick peak identification and data organization. Also, Qtegra ISDS Software allows you to export all aspects of your data, from chromatograms, to system control metadata through to isotope ratio results, providing you with complete ownership of your data.

How do I troubleshoot my instrument?

No aspect of Qtegra ISDS Software is locked for the end-user. This means that you have total flexibility to troubleshoot your instrument and diagnose problems. In-built diagnostics tools allow you to perform tests on your system and determine immediately if the system is performing to specification.

Simplicity

Ultimate flexibility should not equate to complexity. Qtegra ISDS Software is designed to make your analysis simpler without compromising on flexibility or transparency. Automatic features, templates and guided workflows are built into the software to boost your lab's productivity.

How do I get my system prepared for the analysis?

The Get Ready button automatically performs the daily routine instrument start-up procedures that you would normally perform manually such as peak center and autotune. You can also run extended performance checks such as peak flatness test, amplifiers test or linearity checks to make sure that your instrument is set-up and ready to produce high quality data.



Figure 3. Qtegra ISDS Software: Get Ready feature

How can I see my isotope ratios?

Calibrated isotope ratios, blank and interference corrections are all provided by Qtegra ISDS Software via the click of a button, making your data evaluation simple. Raw isotope ratios are calculated in real time with continuous quality control checks to prevent loss of unique samples and ensure the high quality of your data.

Where is my data?

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.

Innovation

Qtegra ISDS Software sets the bar in Gas IRMS software with its unique array of tools designed to improve the accuracy and precision of your isotope measurement.

LIDI 2 Software Workflow for clumped isotope analysis

Clumped isotope analysis allows us to investigate rare isotopologues for paleoclimate reconstruction. Such sophisticated analysis is challenged by factors such as minor fluctuations in lab temperature and uneven crimping of sample and reference capillaries. Thermo Scientific™ LIDI 2 Software Workflow overcomes these challenges for Dual Inlet measurements by matching the reference and sample signal intensities using a mathematical fitting procedure. Qtegra ISDS Software can reference your sample isotope ratios to interpolated reference isotope ratios with the same beam intensity, resulting in improvements in both accuracy and precision of your isotope ratio.

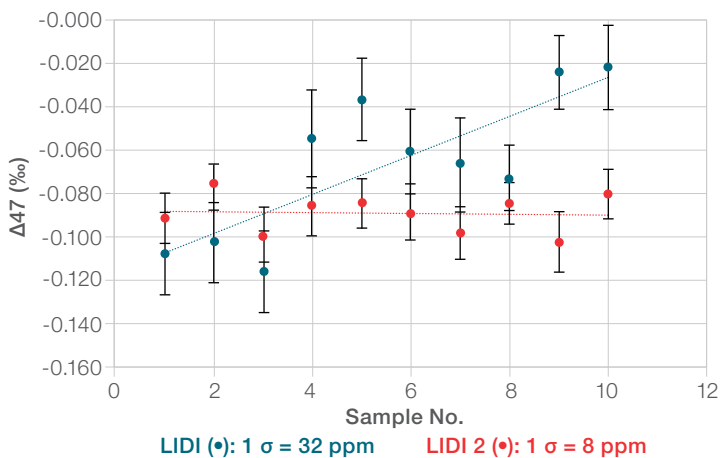


Figure 4. Significant improvement in data precision (red) achieved by LIDI 2 Software Workflow powered by Qtegra ISDS Software

SmartEA Option for elemental analysis of low μg to high mg sample sizes

Elemental Analysis Isotope Ratio Mass Spectrometry (EA-IRMS) analysis of samples with a diverse range of elemental concentrations can create an analytical challenge which is solved by Thermo Scientific™ SmartEA™ Option. SmartEA Option is a feature of Qtegra ISDS Software allowing for dilution of the signal of the most highly concentrated elements, such that the mass spectrometer detectors do not become saturated, yet the very low elemental concentrations are analyzed with sufficient signal-to-noise ratio to produce reliable results. You can set up a method that will bring all sample peaks within a narrow range of intensity, allowing for unattended analysis to deliver high precision results.

Helium Management Module for EA-IRMS analysis

As the demand for helium is high and availability globally has been under pressure, laboratories suffer from higher cost per analysis and in some cases increased system downtime. A solution to alleviate these concerns is provided by Helium Management (HeM) Module for Thermo Scientific™ EA IsoLink™ IRMS System. The HeM Module controlled by Qtegra ISDS Software has been designed to significantly lower helium consumption per sample analysis and therefore increases the number of samples processed per helium gas bottle without affecting data accuracy and precision.

Temperature ramped GC for EA-IRMS

Reduce EA-IRMS analysis times per sample by using temperature ramped GC feature driven by Qtegra ISDS Software. Based on chromatography principles, the EA IsoLink IRMS System provides you with excellent peak shapes and increased sample throughput, without analytical compromise.

Qtegra ISDS Software for Gas IRMS

Join us on our journey with Qtegra ISDS Software. Flexibility and transparency to fully understand your Gas IRMS analysis. Simplicity to boost your lab's productivity. Innovation to guarantee you world-beating isotope ratio results.



Thermo Scientific™ EA IsoLink™ IRMS System, for analysis of bulk sample material



Thermo Scientific™ GC IsoLink II™ IRMS System, for analyzing volatile compounds within a sample



Thermo Scientific™ LC IsoLink™ IRMS System, for analyzing polar compounds within a sample



Thermo Scientific™ GasBench Plus System, On-line gas preparation and introduction system



Thermo Scientific™ Kiel IV™ Carbonate Device, for analysis of carbonate samples

Find out more at thermofisher.com/QtegraIRMS