Figure 2. Qtegra ISDS Software Dashboard showing the live system status at a glance. All relevant aspects of instrument and acquisition are directly accessible from the list on the left.

One software platform to cover all day-to-day tasks
Qtegra ISDS Software offers full control of all aspects of your measurement from within one software environment, for maximum control and efficiency. All relevant settings are intuitively structured and directly accessible from Qtegra ISDS Software’s landing page – the Dashboard (Figure 3).

From the Dashboard, the user can monitor the live system status, acquire data, view live data in real-time, perform calibration, and directly access Instrument settings such as collector configuration, peak center settings and ion source tuning, and can then create and run the actual acquisition method which is the LabBook.

External referencing
Unknown standards and internal standard materials are analyzed versus an internal laboratory reference gas. Qtegra ISDS Software automatically calculates the delta values of the unknown samples against the external reference material (Figure 5).

Benefits for clumped isotope analysis
Purification Trap control
The automated control of a Purification Trap is fully integrated into Qtegra ISDS Software (Figure 7). Clumped Carbonate analyses are particularly sensitive for contaminants. The Purification Trap can be controlled and monitored directly through the Qtegra ISDS Software. It can be cooled to ~30 °C during CO₂ transfer to the mass spectrometer to hold and retain any non-condensable contaminants in the feed lines running through the system. The Purification Trap can be automatically baked up to 150 °C to release potential contaminants to the waste line.

Qtegra ISDS Software not only drives the Ultra HR-IRMS and the Thermo Scientific™ Kiel IV Carbonate Device, and advanced clumped isotope analyses with Thermo Scientific™ Ultra™ IR-IRMS. We highlight how Qtegra ISDS Software eases advanced clumped isotope analyses with Thermo Scientific™ IRMS and Thermo Scientific™ Kiel IV Carbonate Device and carbonate analyses with Thermo Scientific™ 253 Plus™10 kV instruments, they will immediately feel familiar with others, also available across multiple Thermo Scientific instruments, analysts are empowered to effectively use their time in the laboratory, even for the most challenging analysis setups.

What are the challenges of clumped isotope analysis?
Clumped isotopes refer to isotopic ratios in natural materials which are characterized by having two or more heavy isotopes ([13C] and/or [15N]) and less than the corresponding light isotopes ([12C] and/or [14N]). This isomerism results in systematically elevated carbon and nitrogen mass values, which are difficult to exclude in many data sets. As such, additional processing steps are required to obtain high-quality data.

One software platform to cover all tasks provides maximum control and efficiency.
Qtegra ISDS Software guides the analyst from sample to result with comprehensive flexibility. Guided “top-to-bottom” workflows are ubiquitous throughout the software architecture and assist the analyst during setup of instrument hardware, acquisition procedure step-by-step.

Dashboard
Monitor system live status on the Dashboard, then set up the collector configuration and the ion source tuning under Instrument, finally customize and run your acquisition method under LabBook (red arrows in Figure 3).

TuneBook
The TuneBook is the place to adjust and save your instrument parameters. The workflow guides you (red arrows in Figure 4) through Collector Configuration, previous Tune Sessions, manual and automatic Focus and Peak Shape tuning, and optional Performance Checks.

Figure 4. TuneBook Workflow

LabBook
The LabBook is the place to define the acquisition method. Workflows (red arrows in Figure 5) guide you through all relevant acquisition parameters. This includes Standard material and Delta Calculation definitions as well as parameters of available hardware options, such as Dual Ion, Reference Retr., Carbonate Device, or Purification Trap.

Figure 5. LabBook Workflow

Lidi and Lidi 2 Software Workflow functionality
The introduction of the Long Integration Dual Iret (LIDI) significantly improved the sample utilization by first measuring the whole sample followed by the standard (WIS). Higher sensitivity for smallest carbonate samples is achieved.

In contrast to LIDI, where intensities of sample and reference are compared for a certain time, LIDI 2 Software Workflow goes one step further and matches the reference and sample signal intensities using a mathematical fitting procedure. Qtegra ISDS Software can reference your sample isotope ratio to interpolated reference isotope ratios with the same beam intensity, resulting in even further improvements in both accuracy and precision of your isotope ratio [5]. Figure 6.

Seamless switching between Lidi and Lidi 2 Software Workflow
Qtegra ISDS Software allows for direct switching between LIDI and LIDI 2 Software Workflow method evaluation in a measured LabBook.

Figure 6. Three-day zero environment Z0 data evaluated according to LIDI and LIDI 2 Software Workflow method. 1σ confidence intervals are indicated. Original LIDI data shows correlation with laboratory temperature.

Improved data evaluation
Acquired data can be readily processed and evaluated within the Qtegra ISDS Software by Background Correction. Outlier Test, External Calibration Correction (ECC), and both LIDI and LIDI 2 Software workflows (labeled 1 in Figure 6) processing, and External Referring.

Evaluated data are presented live during the run in the LabBook whereas the statistics and plots for multiple samples can be visualized (Figure 6).

External referencing
Unknown samples and external standard materials are analyzed versus an internal laboratory reference gas. Qtegra ISDS Software automatically calculates the delta values of the unknown samples against the external reference material (Figure 5).

Figure 5. Statistics across multiple samples of a run can be visualized, along with externally referenced delta values of unknown samples. (1) Sample list with individually selectable samples, (2) table of delta values for all individual samples selected, (3) statistics table across all selected samples, (4) visualization of delta values for selected samples, (5) visualization of externally referenced delta values for selected samples.