

EXPLORE

the world in a whole new way



Ultra

High Resolution Isotope Ratio Mass Spectrometer

Do you want to discover a new

The Thermo Scientific™ Ultra™ High Resolution IRMS sets a new standard in advanced gas isotope ratio measurements and paves the way forward to the exploration of novel isotopic tracers and exciting discoveries in earth and atmospheric sciences, climate research, petroleum geochemistry, noble gas applications and beyond.

Ultra-high resolution is the key to uncovering the isotopic anatomies of molecules and revolutionizes the field of clumped isotopes, molecule fragment measurements and site-specific isotope analysis.



... world of mass spectrometry?



Overcome the limitations of conventional gas IRMS

The Ultra HR-IRMS is the ideal tool to realize previously inaccessible IRMS measurements. Ultra-high resolution enables interference-free measurements of species that are afflicted with isobaric interferences from contaminants, adducts, and isotopologues. This enhances the stable isotope geochemist's toolbox by increasing the number of resolvable isotopologues and results in confidence from knowing your measurement is interference-free.



Ultra-high resolution to separate isobaric interferences



Flexibility to cover multiple applications

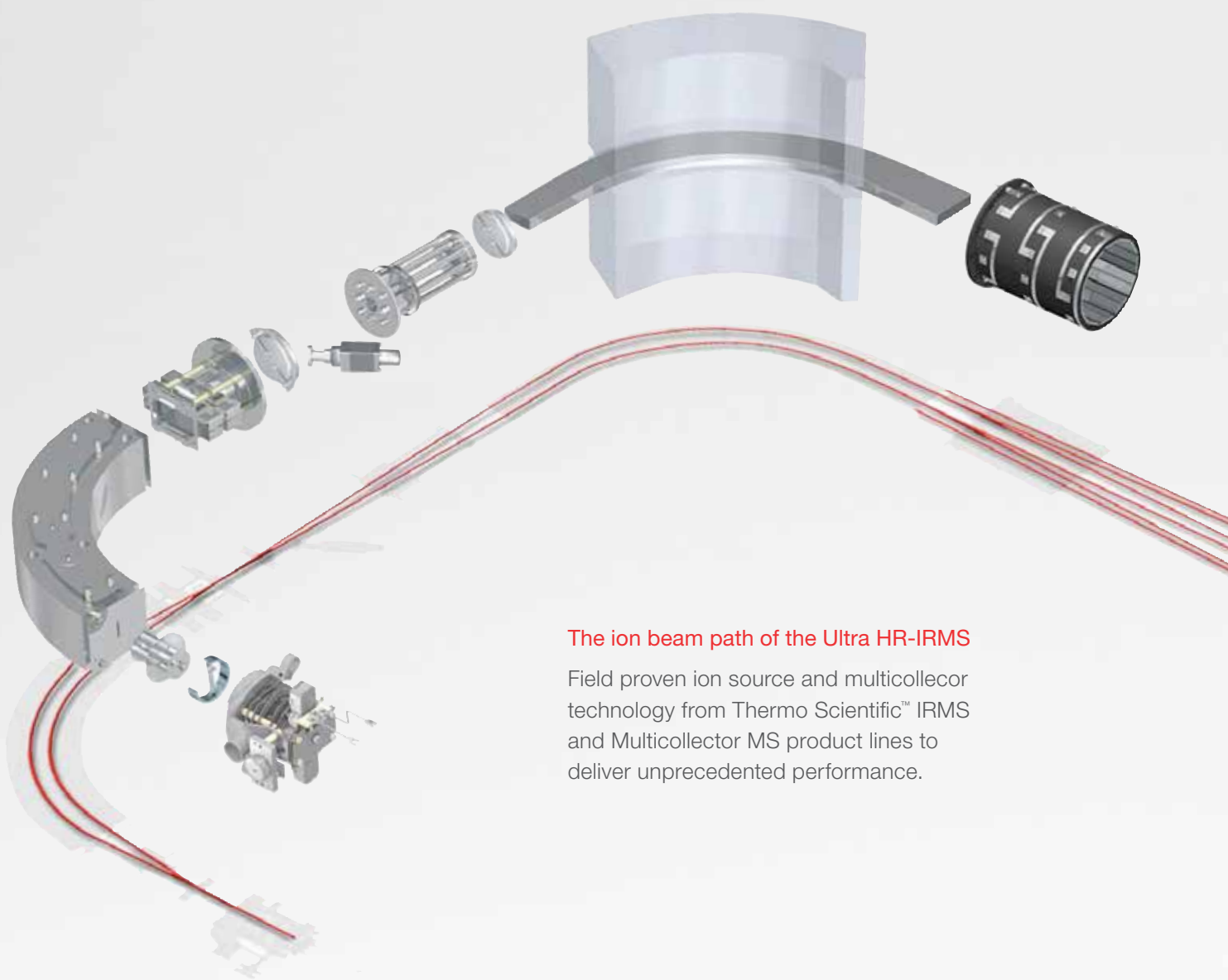


Long-term mass stability and constant resolution



Intuitive graphical software interface

Unlike conventional gas IRMS, the Ultra HR-IRMS employs a variably moveable detector array that allows a flexible setup of multiple collector configurations for a variety of gases. Faraday cups with freely selectable amplification extend the dynamic range of the detector system to 12 orders of magnitude. Thermo Scientific™ $10^{13} \Omega$ Amplifier Technology™ is available for enhanced measurement precision of low intensity ion beams.



The ion beam path of the Ultra HR-IRMS

Field proven ion source and multicollector technology from Thermo Scientific™ IRMS and Multicollector MS product lines to deliver unprecedented performance.

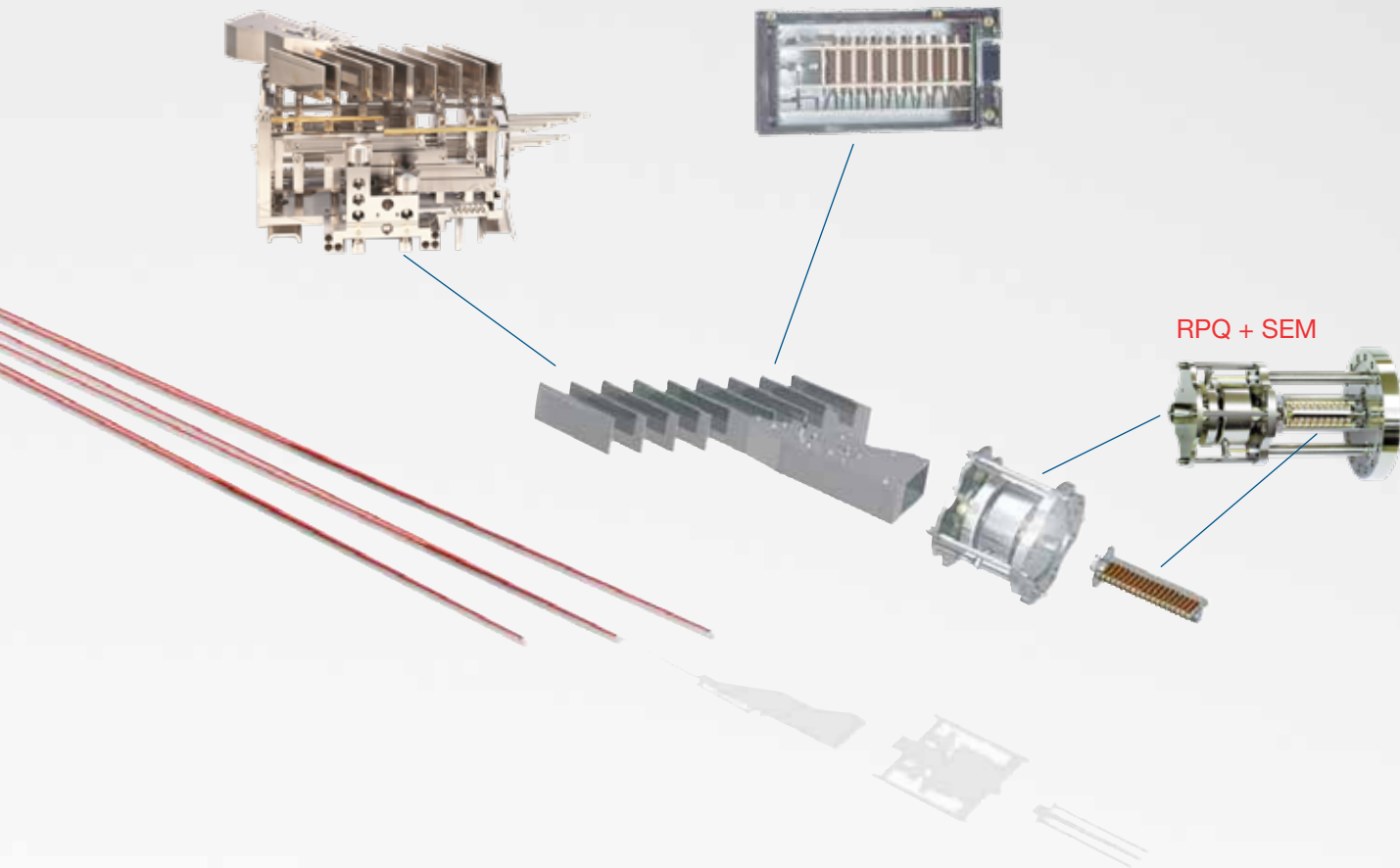
A flexible detection system optimized for the reliable analysis of super rare (clumped) isotope species

For the detection of smallest ion beams, the Ultra HR-IRMS is equipped with moveable compact discrete dynodes (CDD) and a secondary electron multiplier (SEM) with a selectable retarding potential quadrupole (RPQ) filter. An ultra-tight differential vacuum system ensures reduced backgrounds.

Variable multicollector

CDD (disassembled)

RPQ + SEM



High resolving power is the key to high mass resolution

In contrast to conventional IRMS, the resolving power of the Ultra HR-IRMS is increased from ~1,000 to >30,000. This is achieved by:

- Optimized beam morphology by double-focusing of both ion energy and angular divergence
- A small source slit (entrance slit), which narrows the beam diameter
- An aperture lens further narrows the beam diameter

Building upon the resolving power ability, a mass resolution sufficient to separate all methane isotopologues and adducts of the same cardinal mass is obtained by:

- A larger ion beam path radius which results in larger “beam separation”
- A small collector slit (exit slit) which results in narrow peak plateaus

Choose the setup that fits your needs

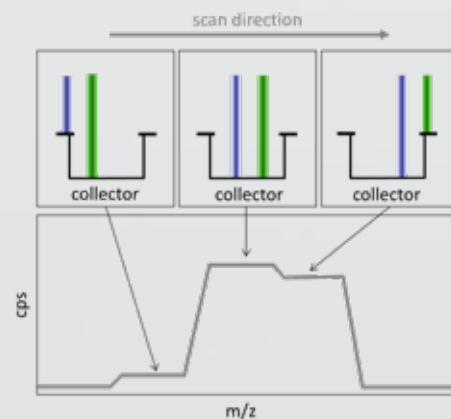
Maximum transmission



The contribution of two species on the peak intensity cannot be deciphered for species that share the same cardinal mass. Highest transmission is achieved.

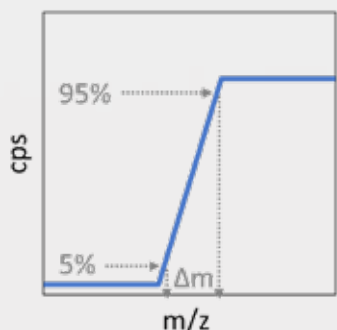
- wide source slit (resolving power >1,800)
- wide ion beams
- wide collector slit

High resolving power



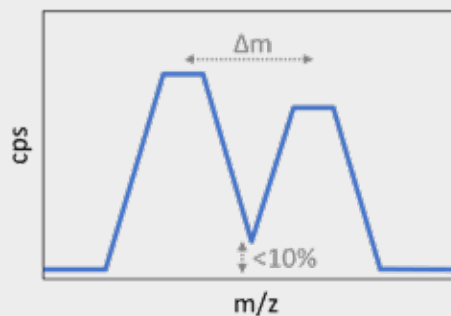
Resolving power is a measure of the steepness of a peak flank.

Resolving power is defined as $M/\Delta M$, where ΔM is calculated on a peak flank between 5% and 95% of its total height. Resolving Power is determined by the ion beam morphology.



Mass resolution is a measure of the ability to separate two peaks from another.

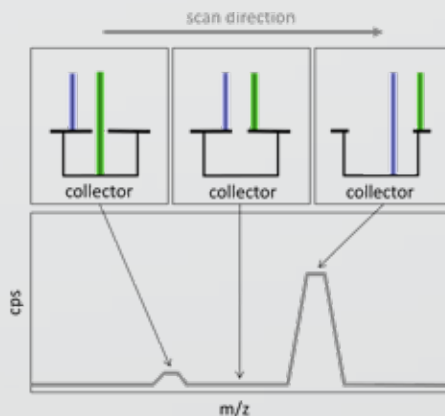
Mass resolution is defined as $M/\Delta M$, where ΔM is the distance between 2 mass peaks that are separated by a valley $<10\%$ of the intensity of the smaller peak.



High mass resolution

The two species of the same cardinal mass are partially resolved at increased resolving power. Interference-free measurement is possible on the peak shoulders.

- medium source slit (resolving power $> 12,000$), or
- narrow source slit (resolving power $> 30,000$)
- narrow ion beams
- wide collector slit



At high resolving power, maximum mass resolution is achieved when a small collector slit is selected. The ion beams of the two species of the same cardinal mass are fully separated.

- narrow source slit (resolving power $> 30,000$)
- narrow ion beams
- narrow collector slit

How do we maintain peak stability over long time periods?

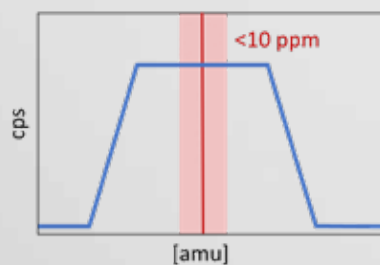
The design of the Ultra is dedicated to uncompromised system stability. Built around a single rigid ion optic bench, with outstanding magnet field regulation, the Ultra HR-IRMS provides long-term peak stability and constant mass resolution. This is the prerequisite for reliable high resolution IRMS measurements of narrowest peak plateaus.

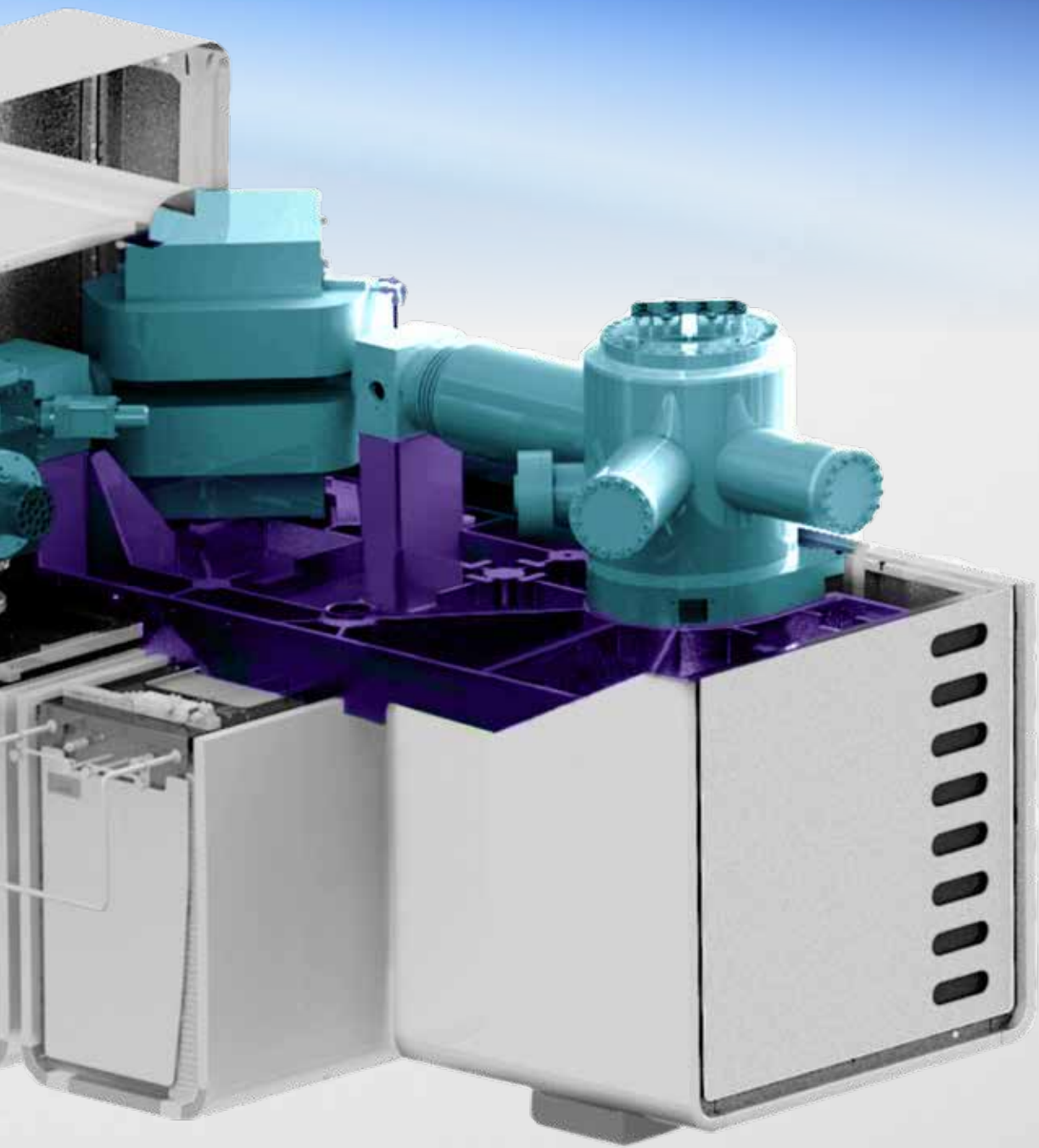
A scientific design for maximum system stability

All hardware components (shaded light turquoise) relevant to the guiding of the ion beam path are covered and mounted on a monolithic platform (shaded dark purple). Ultimate magnet field stability is enabled by active temperature stabilization of electronics. A laminated, water-cooled magnet minimizes hysteresis effects and fast magnet scanning.

Keeping narrowest peak plateau positions stable

Peak stability is typically <10 ppm/h (CO_2 at mass 44). This corresponds to an instrumental scattering of the peak position in the range of a few tenth of millimasses.





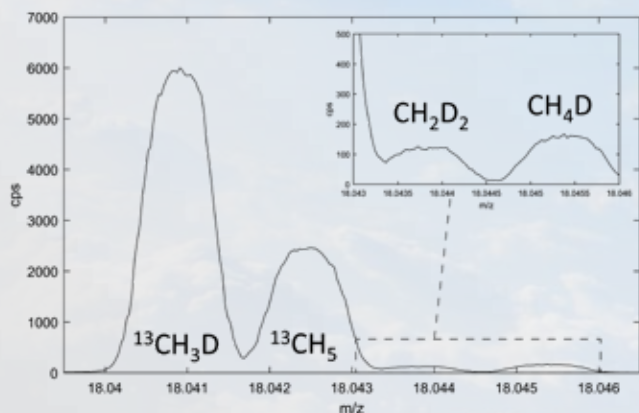
One instrument for multiple applications...

- Fragment measurements (^{13}C , ^{17}O , ^{18}O , CO , ...)
- Clumped isotopes (CH_2D_2 , DD , $^{18}\text{O}^{18}\text{O}$, $^{15}\text{N}^{15}\text{N}$, ...)
- Position specific isotope analyses (C_3H_8 , C_2H_6 , N_2O , ...)
- Separation of adducts ($\text{DD} - \text{H}_2\text{D}$, $^{15}\text{N}^{15}\text{N} - ^{14}\text{N}^{16}\text{O}$, ...), contaminants ($^{13}\text{CO}_2 - ^{14}\text{N}^{15}\text{NO}$, $^{17}\text{O} - \text{OH}$, ...), and isotopologues ($\text{CH}_2\text{D}_2 - ^{13}\text{CH}_3\text{D}$, ...)
- Studying source chemistry

Clumped methane

Recommended reading: Eldridge et al. (2019), Douglas et al. (2017)

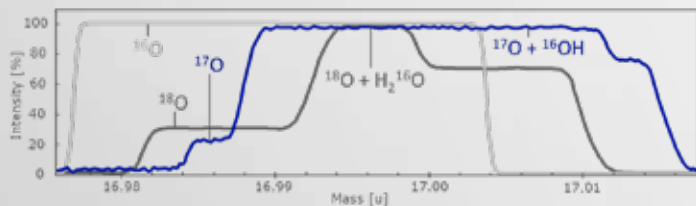
Petroleum science, biochemistry: Doubly-substituted methane (CH_2D_2) is fully separated and directly measurable at high mass resolution.



Oxygen fragments in CO_2

Recommended reading: Adnew et al. (2019)

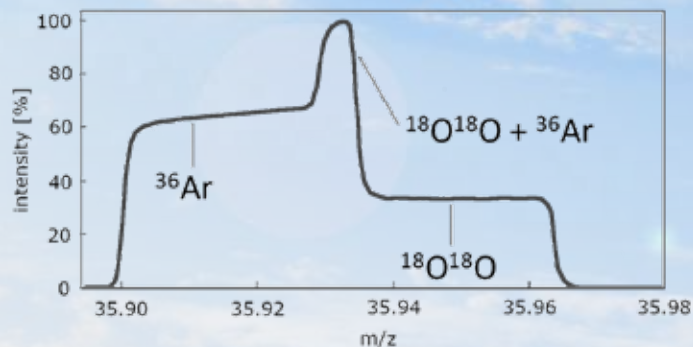
Paleoclimate reconstruction, carbonate formation temperatures: Separation of water molecules from oxygen fragments at high mass resolving power allows the direct determination of triple oxygen isotope compositions from CO_2 .



Clumped oxygen

Recommended reading: Laskar et al. (2019)

Atmospheric chemistry, ozone chemistry: The interference-free analysis of all clumped oxygen species is enabled by separation from various contaminants at high mass resolving power.

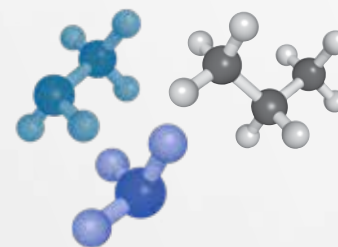


Position-specific ^{13}C in propane

Recommended reading: Piasecki et al. (2018), Clog et al. (2017)

Natural gas systems, biochemistry: Measurement of clumped and/or position-specific signatures in natural gases extends the classical bulk isotopic systematics of hydrocarbons.

The principle of position-specific analysis is based on the measurement of molecule fragments and their isotopologues.



Biochemistry

Paleoclimate

Mineralogy and Petrology

Climatology

Paleoenvironments

Petroleum industry

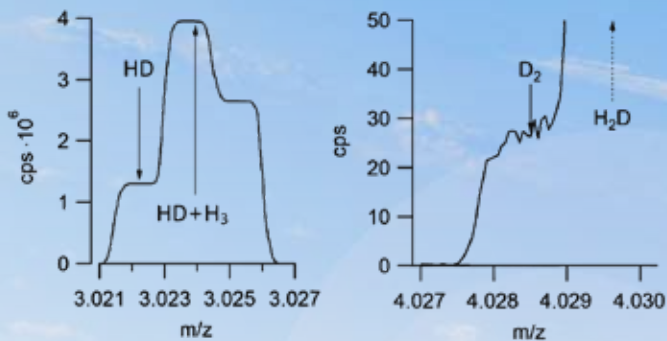
Environmental sciences

Atmospheric sciences

Clumped hydrogen

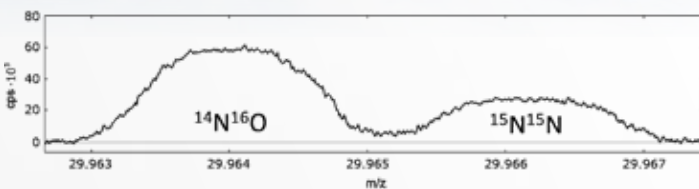
Recommended reading: *Popa et al. (2019)*,

Atmospheric chemistry, H₂ cycling: All isotopologues of hydrogen, even the rare DD, can be analyzed free of interferences at natural abundance levels at high mass resolving power.



Clumped nitrogen

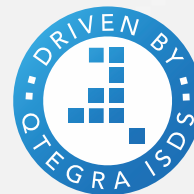
Denitrification, atmospheric chemistry: The clumped nitrogen molecules (¹⁵N¹⁵N) can be fully separated from ¹⁴N¹⁶O adduct ions at high mass resolution.



...Explore the world in a whole new way

Bringing advanced isotope ratio data into the reach of every user

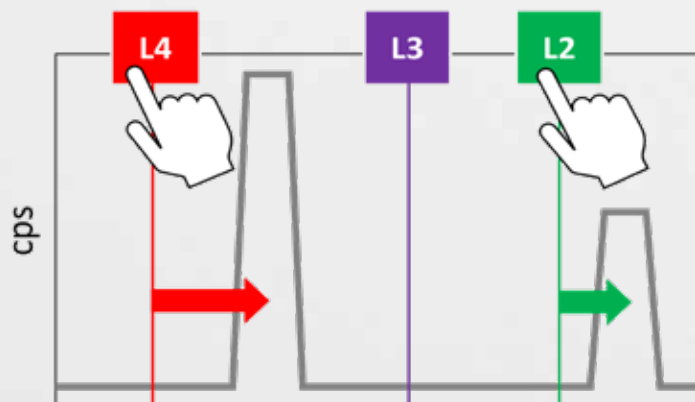
The Ultra HR-IRMS is operated by Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution (ISDS™). It provides extensive control for optimized analytical conditions and offers all the flexibility required for the most demanding applications.



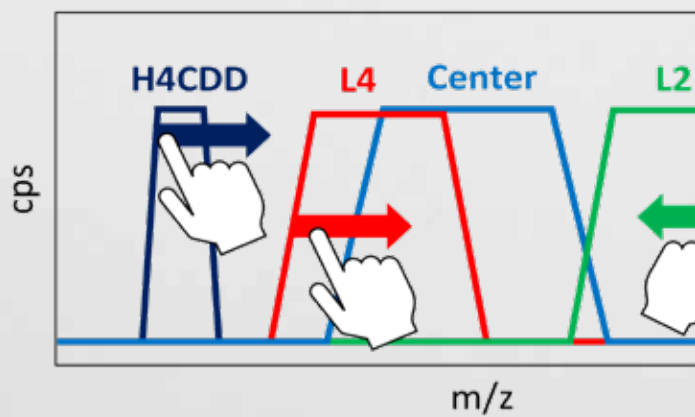
Graphical collector positioning and instrument setup

Collector configurations are easily set up using both ion counters and Faraday cups with software-selectable amplification. The “drag & drop” function allows for graphical peak alignment and the collectors are automatically driven to the exact position.

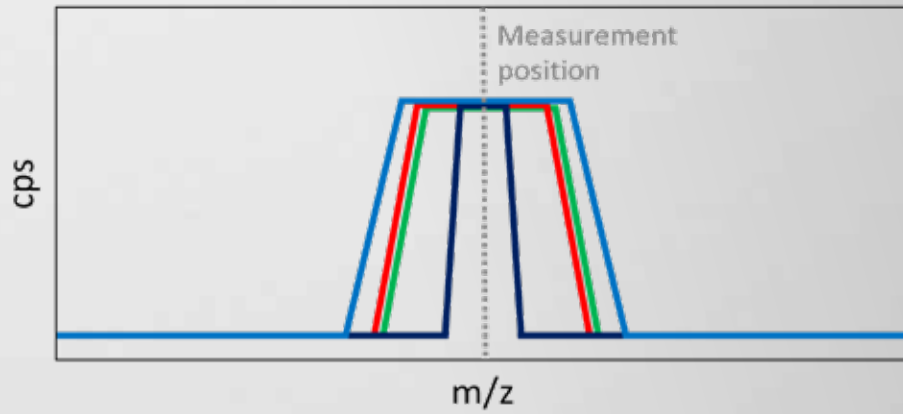
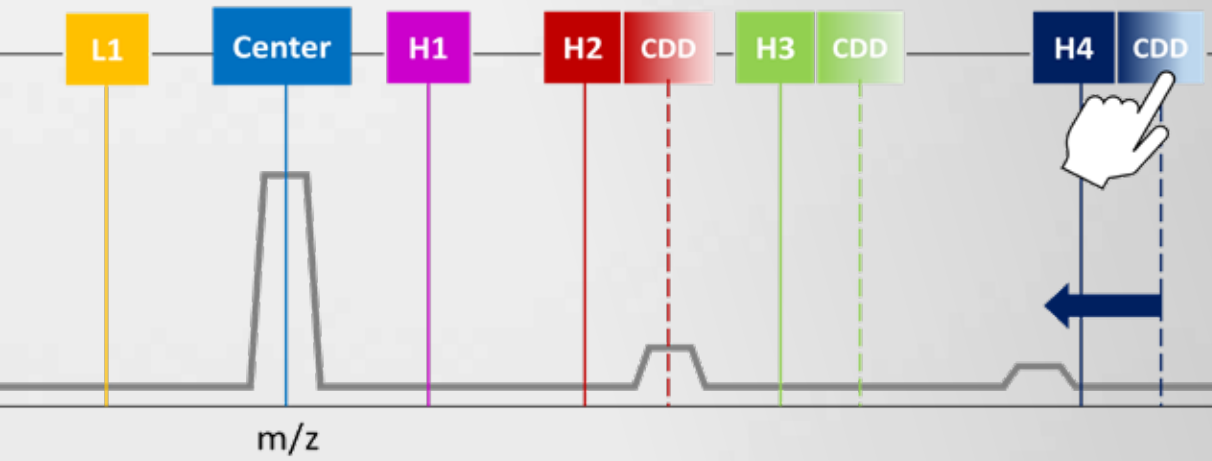
Enhanced measurement precision of low intensity ion beams at high mass resolution is enabled by reproducible software-controlled switching of mass resolution modes and automated peak center routines for maximum peak stability.



(1) “Drag & drop” collectors for initial collector alignment



(2) “Drag & drop” peaks for fine adjustment of collector positions



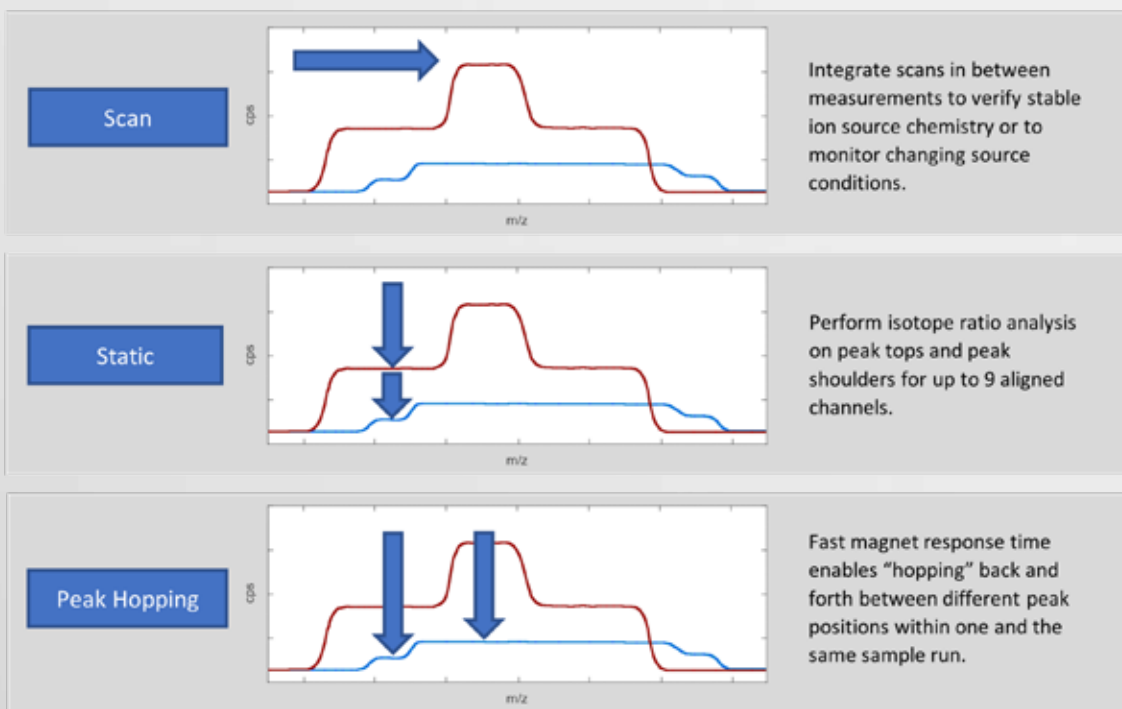
From sample to result

Qtegra ISDS has an intelligent workflow that drives you from sample to result. Once an analysis has been made, the Qtegra ISDS LabBook provides a layered approach to results through a series of views, where data can be displayed and instantly processed with user-defined algorithms.



Automated flexible measurement strategies

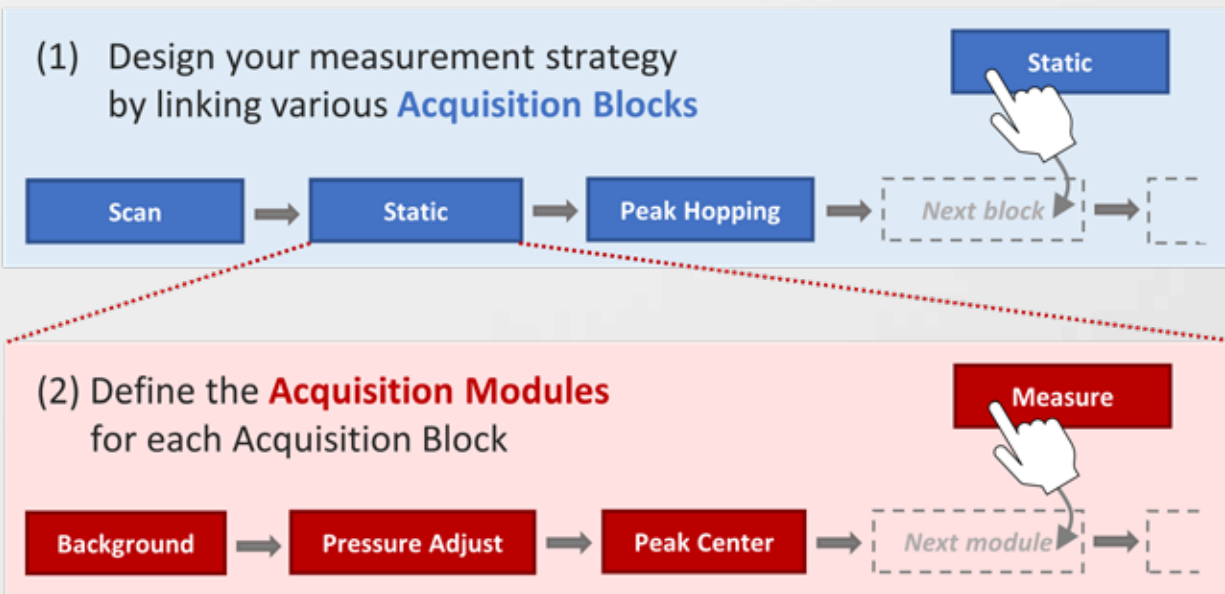
An easy to use graphical interface allows the user to design flexible and complex measurement strategies in an intuitive way. Integrating mass scans, performing static measurements and peak hopping can be combined into a single method.



Intuitive method development

Method development is facilitated by organizing functional modules per “Drag & Drop”:

In a 1st step various acquisition blocks are easily combined to enable comprehensive and coherent measurement strategies. In a 2nd step each data acquisition block is defined by adding different acquisition modules.



References

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