

# Escape the Trap

Six ways that Agilent Q-TOF technology  
will help you achieve excellent spectral quality





## Find Answers Beyond the Peak Shape

To stay ahead of your analytical challenges, you need an instrument with many strengths. Unlike ion traps that emphasize mass resolution and mass accuracy capabilities, Agilent Q-TOF also combines the power of uncompromised in-spectra detection with high dynamic range and fast analysis.

An Agilent Q-TOF can help your lab increase productivity and data confidence by:

1. Providing wide dynamic range
2. Quantifying more compounds
3. Delivering constant resolution
4. Reducing required samples
5. Delivering isotope ratio fidelity
6. Producing more results

# 1. Providing Wide Dynamic Range



The most important aspect in analytical science is the ability to reliably detect and quantify compounds. Ultrahigh resolution mass spectrometry is useless if compounds with low abundance cannot be reliably detected when in the presence of high abundance compounds. Although ion trap technologies can be extremely sensitive in clean and simple matrices, real-life samples are complex and contain many coeluting major and minor compounds. These conditions often result in analytes interfering with other analytes.

Agilent Q-TOF technology delivers wide in-spectra dynamic range to achieve reliable detection, quantitation, and identification for everyday samples even when other abundant compounds are present.

## Want to enhance the sensitivity of electrospray ionization?

The Agilent Jet Stream Technology ion source uses superheated nitrogen to improve droplet desolvation and ion generation for a stronger signal and reduced noise. That means you get the highest sensitivity for most analytes—and response that is at least five-fold higher than electrospray ionization.

## Ion traps

Spectral dynamic range:  
3.5 orders

## Maximum dynamic range lets you detect and quantify more compounds—the most important aspect in analytical science

In complex samples, low and high abundant compounds are coeluting, requiring maximum dynamic range for quantitation with in-spectra confirmation.

## Agilent Q-TOF

Spectral dynamic range:  
5 orders



## 2. Quantifying More Compounds



All mass spectrometers encounter signal saturation, but the impact of this is different depending on the technology used.

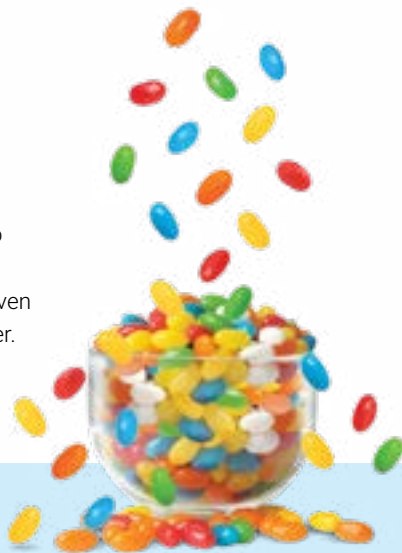
All ion trap designs, including electromagnetic FT instruments, have a common problem: the number of charges accumulated in the trap impacts mass analysis performance. Because trap-based mass analysis is susceptible to interfering charges, technologies implement a mechanism to control the number of charges (gain) during trapping and analysis. When a complex sample is analyzed there are many partially or fully coeluting compounds with various abundances. The ion trap gain control mechanism limits the number of total ions in the trap at the expense of detecting lower abundance ions, compromising limits of detection, delivering poorer precision for the less abundant analytes.

On the other hand, Agilent Q-TOF technology is not dependent on trapping, as ions are separated in space and do not interfere with other ions. With Agilent Q-TOF technology, saturation effects occur at signal detection and only very highly abundant ions are affected. Other ions that are not highly abundant are reliably detected and not impacted by an abundant coeluting compound.

### Are you detecting all your ions—even lower-abundance ions?

#### Ion traps

High-resolution ion traps have a limited capacity to store/trap ions, so lower abundant ions may not even get into the mass analyzer.



#### Agilent Q-TOF

Agilent Q-TOF technology separates ions in space, ensuring maximum accuracy and precision across the entire mass range, even if some ions are highly abundant.



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# 3. Delivering Constant Resolution



Mass spectrometry is routinely used with LC (liquid chromatography), GC (gas chromatography), or CE (capillary electrophoresis) to separate complex samples and improve the detection, quantitation, and identification of the analytes present. To achieve accurate quantitation, a minimum of 12 to 15 data points is required over the chromatographic peak. In addition, different modes of operating the mass spectrometer to provide more compound information, such as data-dependent or Quadrupole Resolves All Ions (Q-RAI) experiments, increase the need for high-speed mass spectral acquisition.

Agilent Q-TOF technology provides constant mass resolution independent from acquisition rate. This is not possible to achieve with high-resolution ion trapping instruments. When faster scan rates are required on an ion trapping instrument, the trap must be filled, scanned, and emptied in smaller and smaller amounts of time. Resolution and mass accuracy are a function of trap scanning time; as scanning time decreases, so does the actual resolution.

**Q-TOF resolution is independent from acquisition speed, so you can capture your lowest abundant compounds.**



### Ion traps

At low speeds, ion traps achieve their highest resolution.



### Ion traps

At high speeds, the resolution in ion traps drops substantially, leading to unresolved compounds and interferences.



### Agilent Q-TOF

At all speeds, Agilent Q-TOF technology offers uncompromised resolution to resolve compounds, every time.

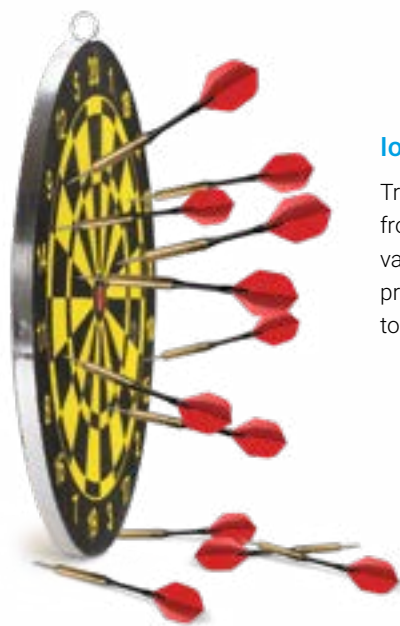
## 4. Reducing Required Samples



No one wants to analyze more samples than necessary to get the right answer. Running extra samples is costly in time and money. Furthermore, it may not be possible to get additional samples from material that is difficult to collect. How many samples to run should be dependent on your experiment and not the instrument being used to measure the sample. Reducing instrument-required sample runs starts with the instrument design. Trapping instruments by design generate a spectrum from a single ion sample leading to more variation in the measured signal.

Agilent Q-TOF technology measures thousands of ion transients to create a high quality, low variance mass spectrum. This results in mass data with low relative standard deviations. Data with lower RSDs (higher precision) require fewer samples to be run to achieve the required statistical power for your experiment.

**Will the number of samples you run depend on your experiment—or your instrument?**



### Ion traps

Trapping instruments generate a spectrum from a single ion sample, which leads to more variation in the measured signal. To get a precise value, multiple measurements need to be made.



### Agilent Q-TOF

Agilent Q-TOF technology measures thousands of ion transients to create a high-quality, low-variance mass spectrum. With far less variation in the experiment compared to ion traps, less samples need to be measured to give the same results.

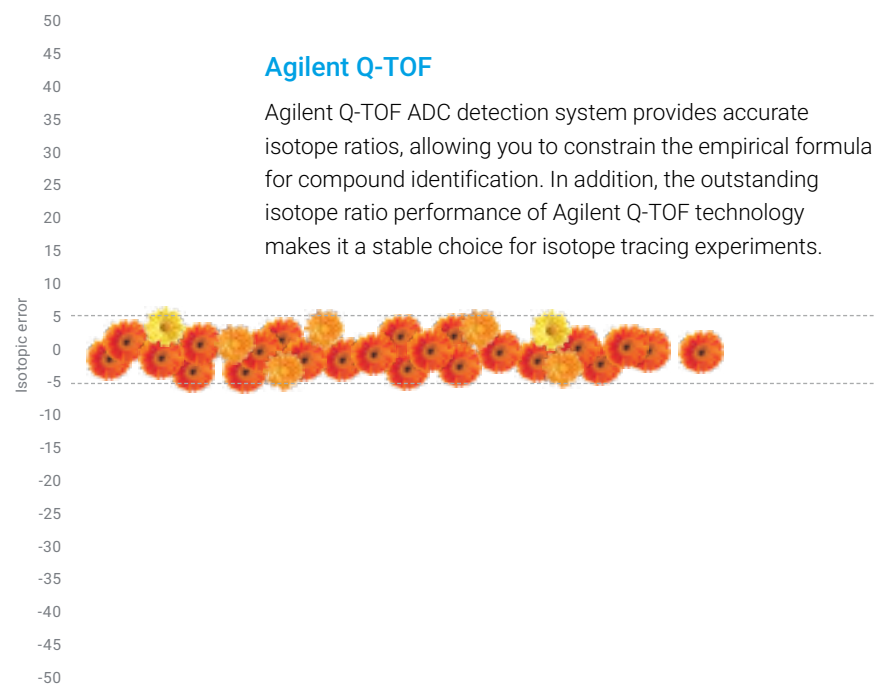
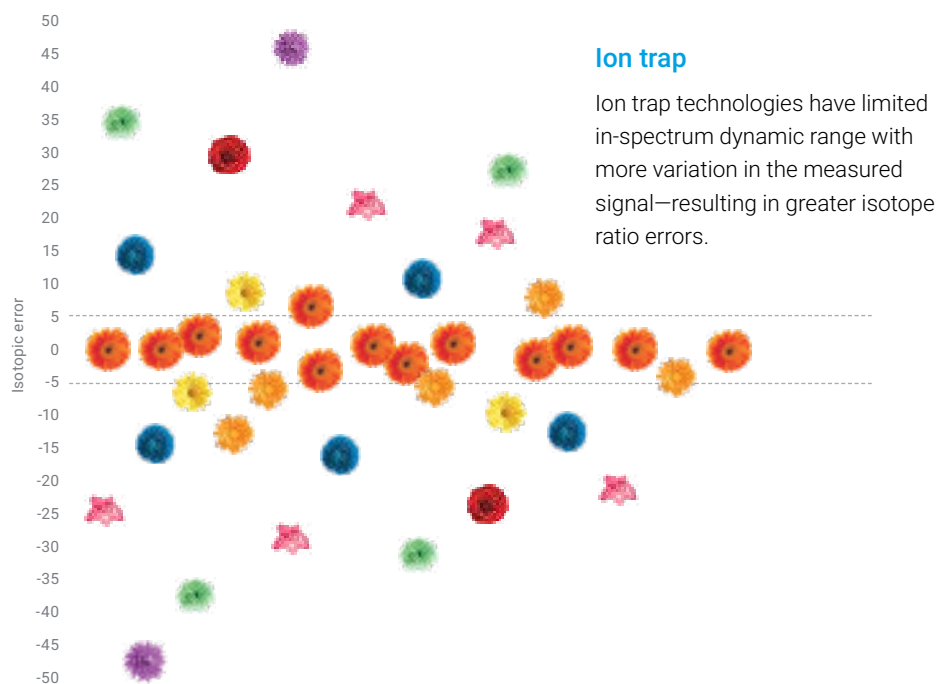
# 5. Delivering Isotope Ratio Fidelity



High-resolution, accurate mass measurement requires many factors beyond just the value of the monoisotopic mass of the compound to obtain reliable compound identification. While fragment information can deliver high quality compound identification, it is not always experimentally feasible or sufficient (e.g. for isobars and enantiomers) and chromatographic retention times may also not be known when profiling complex samples. Isotope ion ratios can be used to improve compound annotation by constraining the compound molecular formula beyond what perfect mass measurement can do.

Ion trapping instruments have limited in-spectrum dynamic range with more variation in the measured signal resulting in greater errors in isotope ratios. The Agilent Q-TOF ADC detection system is designed to provide accurate isotope ratios. This allows the use of isotope ratios acquired on the Agilent Q-TOF to constrain the empirical formula in compound identification. The impressive isotope ratio performance of the Agilent Q-TOF technology makes the instrument a good solution for stable label isotope tracing experiments.

## Agilent Q-TOF instruments deliver the high resolution—and accurate mass-to-isotope measurements—you need for compound identification



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## 6. Producing More Results



Labs are facing the challenge of analyzing more samples. With modern UHPLC technology, you can shorten your LC/MS method times to just minutes, but only if your mass spectrometer can keep up.

Agilent Q-TOF technology can collect data as fast as is needed for modern high-speed HPLC separations. This allows you to analyze more samples in less time by reducing the analytical instrument bottleneck to productivity. Importantly, Agilent's high-resolution, accurate mass Q-TOF acquires data fast without compromising mass spectral performance. Furthermore, the wide dynamic range of Agilent Q-TOF technology permits the detection of low abundance compounds while significantly reducing the need to dilute and re-run samples in order to quantify both high and low-abundance compounds. Taken all together, Agilent Q-TOF technology produces more, high quality results in less time.

### Accelerate your lab's capabilities to run more samples with a fast Q-TOF technology

#### Ion trap

These instruments are limited by the amount of ions the trap can store. To overcome this, typically long gradient times are used to reduce the number of ions at a given time, leading to low sample throughput in the lab.



#### Agilent Q-TOF

Agilent Q-TOF technology eliminates the requirement for trapping ions allowing much faster data acquisition workflows. Your lab can now take full advantage of rapid UHPLC separations to deliver more sample results in less time.





## Look deeper into samples than ever before

Confidently analyze target and nontarget analytes in complex matrices with Agilent Q-TOF instruments. Their simultaneous accuracy, speed, and isotopic fidelity let you minimize false positives, improve database search scores, and generate molecular formulas for unknowns.

What's more, you can move beyond targeted screening restrictions with accurate mass spectral libraries for pesticides, veterinary drugs, mycotoxins, extractables and leachables, forensics, and water contaminants.

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