GC-MS

What is the benefit of high mass resolving power on the Orbitrap Exploris GC Series?

Why do I need high mass resolving power from Orbitrap technology?

- Resolve target analytes from interfering compounds and matrix ions of similar mass.
- Achieve sub-ppm mass accuracy to give data certainty in compound identification.
- Sub-ppm mass accuracy enables narrow mass extraction windows (± 5 ppm) to give high selectivity, which in turn makes peak detection algorithms efficient.
- Easily increase scope of analysis through full scan accurate mass data acquisition (Figure 1).
- Quickly and confidently propose elemental compositions for the identification of unknown features.
- Retrospective data processing of samples long after data acquisition.
- Have high mass resolving power and sensitivity. No compromise.

Figure 1. Analytical approaches to increase scope of analysis through full scan high-resolution, accurate-mass data

With resolving power of up to 240,000 and consistent sub-ppm mass accuracy, the Thermo Scientific™ Orbitrap Exploris™ GC 240 mass spectrometer is a unique laboratory tool for targeted and discovery workflows, where screening, quantitation, compound identification, and structural elucidation applications are required.

High-resolution Orbitrap mass spectrometry has been available with both liquid and gas chromatography for many years and has proven to be a highly valuable analytical technique.[1-4] More recently, the technology in gas chromatography moved to join the Thermo Scientific Orbitrap Exploris Mass Spectrometer series. This new platform of a benchtop hybrid quadrupole-Orbitrap mass spectrometer opens up research opportunities in a system with a significantly reduced footprint, saving both energy and raw materials. The benchtop hybrid quadrupole-Orbitrap mass spectrometer provides new possibilities for increased mass accuracy, sensitivity, and selectivity for GC-amenable compounds. Figure 2 shows how the resolving power is in the ideal range for volatile small molecules, with resolving power increasing with lowering *m/z*.

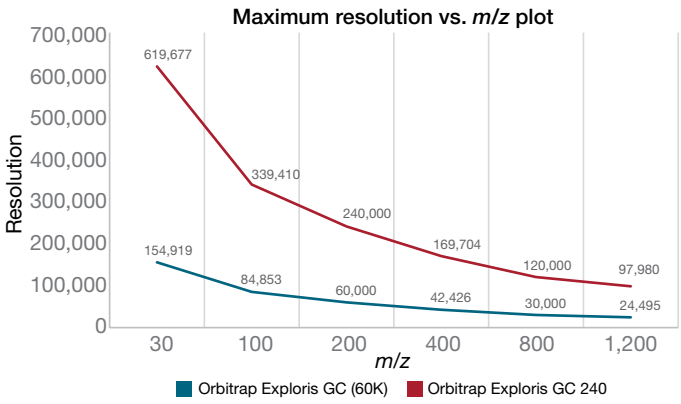

Figure 2. Resolution across the mass range on Orbitrap Exploris GC Series instruments increases with lowering *m/z*, giving higher selectivity in the expected range of volatiles.

The impact of mass resolution on selectivity for targeted analysis

High-resolution, accurate-mass (HR/AM) experiments typically provide a full scan analysis of a sample, and for small molecule analyses, the scan range is typically 50–600 Da. Orbitrap technology provides the required selectivity to resolve the target compound from other compounds or from matrix ions of similar mass. For targeted compound analysis, the accurate mass of the diagnostic ion is extracted with a narrow mass extraction window (typically < 5 ppm). This narrow window is possible only when the instrument provides sufficient mass accuracy, for which high mass resolving power is essential. However, when two mass profiles overlap, the measured mass profile is the sum of the two individual profiles. This overlap results in the incorrect assignment of the mass of the target compound. The problem is demonstrated in Figure 3, where a QuEChERS leek extract in acetonitrile was analyzed four times at resolving powers of 15K, 30K, 60K, and 120K (*m/z* 200).

Being able to separate two compounds that are close in mass is one of the significant advantages of high-resolution accurate mass. This is demonstrated in Figures 4A-C where the compounds flurenol methyl ester $C_{15}H1_2O_3$ *m/z* = 240.0781 and dimetilan $C_{10}H_{16}N_4O_3$ *m/z* = 240.1217 were analyzed at equal intensity at three different resolving power levels of 30,000, 60,000, and 240,000. The zoomed spectra show excellent separation at all resolution levels, with improvements at 60K and 240K showing the clear benefits. When analyzed at 10:1 ratio (Figure 5), there is still good separation and mass accuracy. The latter reflects the real world where compounds will be at varying intensities, and it is essential that mass accuracy is maintained to make confident identifications.

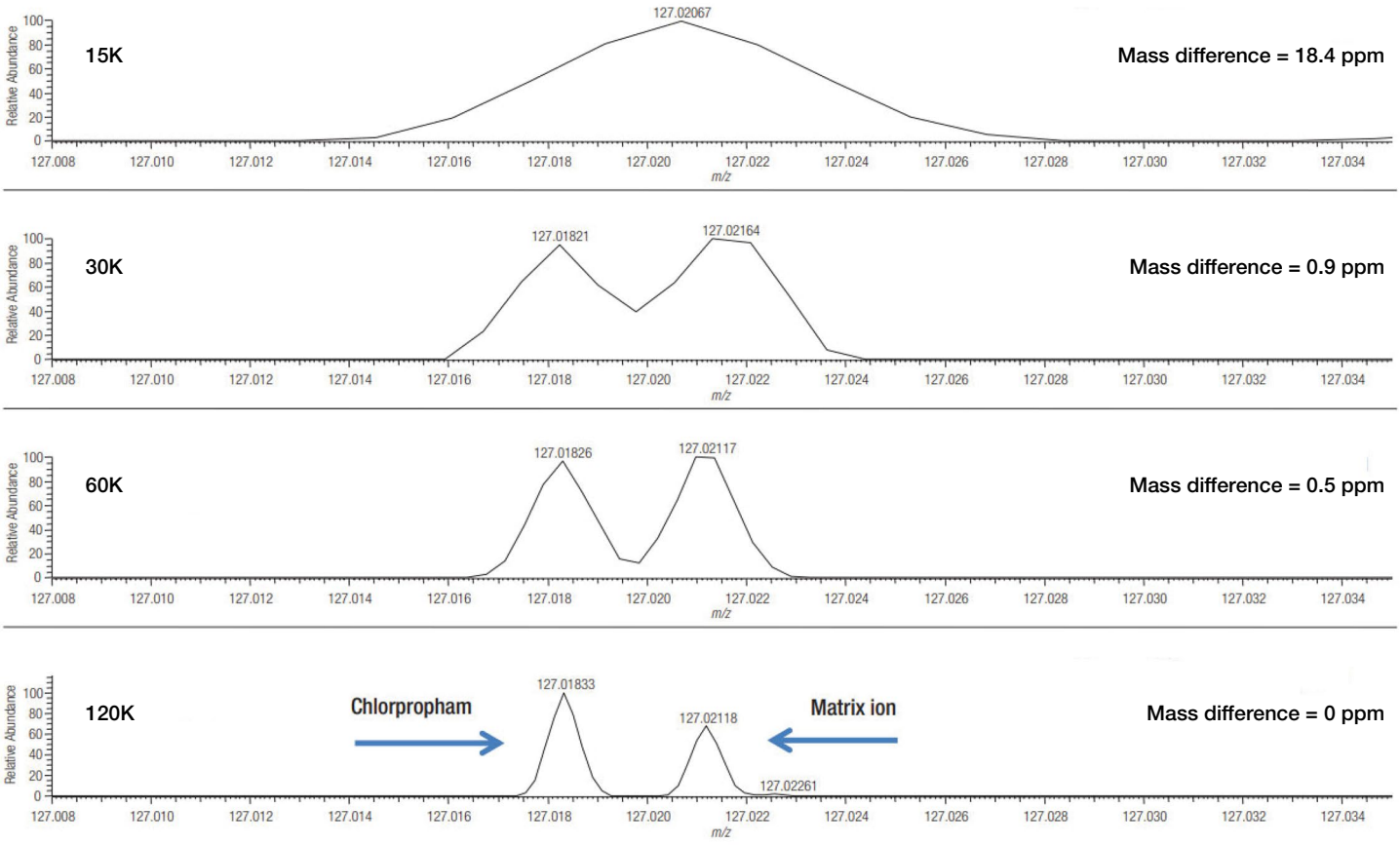

Figure 3. Effect of resolving power on mass accuracy of an analyte in matrix. Mass profiles of chlorpropham 10 ng/g in leek acquired at resolutions of 15K, 30K, 60K, and 120K. Matrix interference at 15K and 30K prevents separation of the pesticide from the interference and higher-than-expected mass difference. Chlorpropham is resolved at 60K and 120K with improvements in mass accuracy.

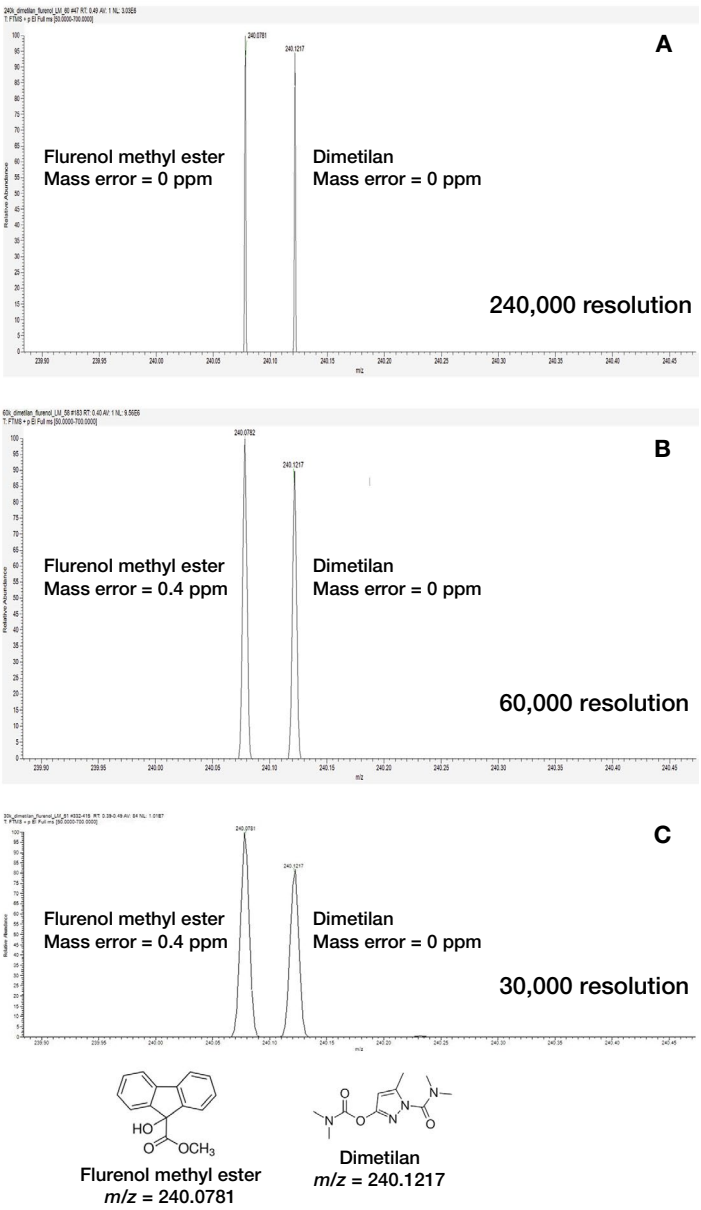

Figure 4. Zoomed spectrum of two similar accurate mass compounds flurenol methyl ester $C_{15}H_{12}O_3$ *m/z* = 240.0781 and dimetilan $C_{10}H_{16}N_4O_3$ *m/z* = 240.1217 acquired at (A) 240,000 resolving power (RP), (B) 60,000 RP, and (C) 30,000 RP

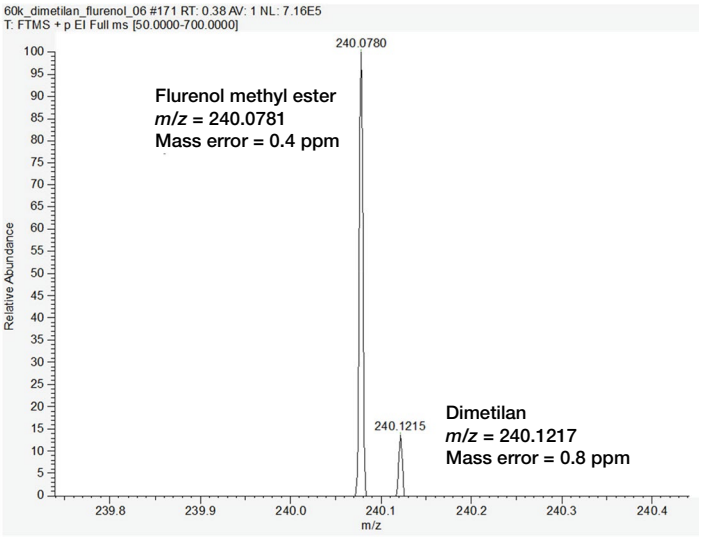

Figure 5. Zoomed spectrum at 10:1 intensity ratio of flurenol methyl ester $C_{15}H_{12}O_3$ *m/z* = 240.0781 and dimetilan $C_{10}H_{16}N_4O_3$ *m/z* = 240.1217 acquired at 60,000 resolving power

References

1. Orbitrap Exploris GC 240 mass spectrometer brochure
2. Orbitrap Exploris GC 240 mass spectrometer product specifications
3. Technical note 10730: Mass resolving power of 240,000: for confident compound identification
4. White paper 003116: Grant application resource: Using the Orbitrap Exploris GC 240 mass spectrometer to accelerate research

Learn more at **thermofisher.com/orbitrapexplorisgc240**

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