Nota de aplicación

The Advantages of Using GC-MS/MS for the Analysis of Trace Components in Complex Matrices

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This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief investigates the advantages of Waters Micromass Quattro micro GC for the analysis of trace components from carp extract.

Benefits

Highest degree of sensitivity and selectivity

Introduction

The application of GC-MS for trace analysis is common place in the modern laboratory. Over time, required limits of detection decrease, whilst the sample matrices to be analysed become more complex.

Extraction and cleanup methods can aid the analyst by reducing the complexity of the final sample extract, but can also be time consuming, inefficient, and costly.

The high selectivity of GC-MS/MS allows the simplification of cleanup procedures while maintaining high selectivity and sensitivity when targeting trace components in complex sample extracts

Results and Discussion

Waters Micromass Quattro micro GC offers three possible acquisition modes for quantitative analysis: full scan, selected ion recording (SIR) and multiple reaction monitoring (MRM).

To investigate the difference between these modes, a calibration standard and an extracted Carp sample were injected in each mode.

First, the calibration standard and the matrix extract were acquired in full scan mode, scanning from 50 to 600 Da. From these chromatograms, selected compound specific mass chromatograms viewing peaks from the molecular ion cluster of an internal standard (*m/z* 317.9) and analyte (*m/z* 305.9) were generated.

Figures 1 and 2 present the extracted mass chromatograms for the calibration standard (Figure 1) and the Carp extract (Figure 2) in full scan mode. As can be seen from the chromatograms, the peaks for the calibration standard are clearly visible, but no information can be obtained from the matrix extract.

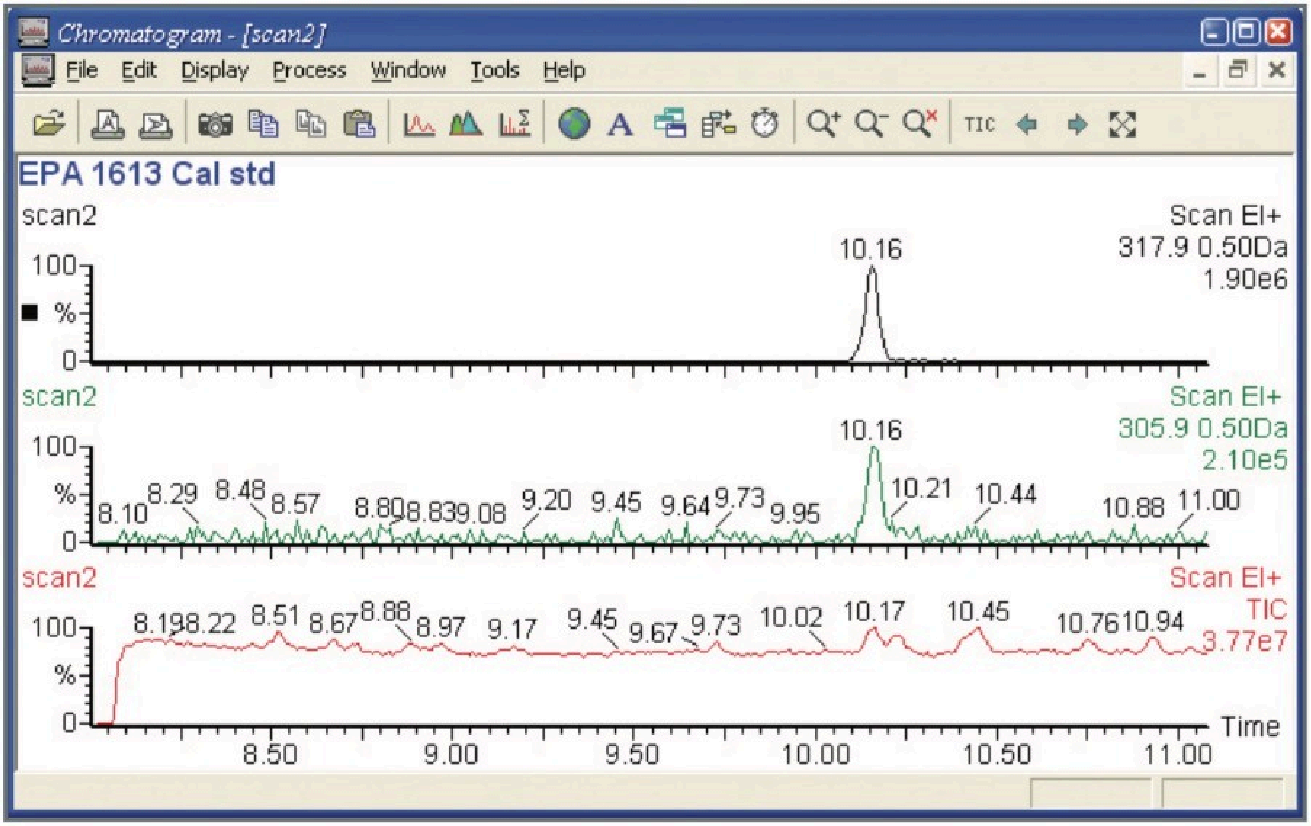

Figure 1. Full scan calibration standard injection.

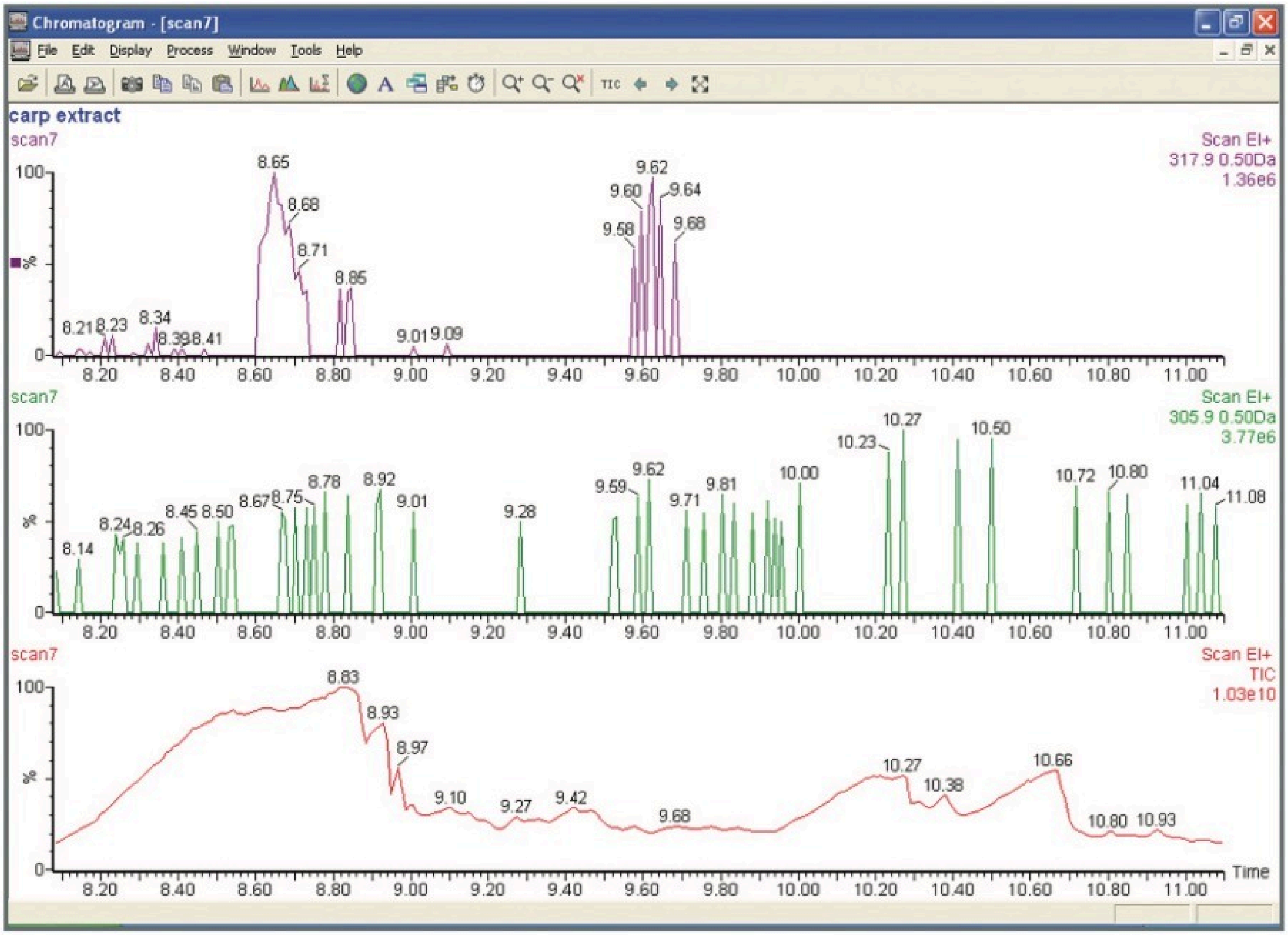

Figure 2. Full scan Carp extract injection.

The calibration standard and Carp extract were then injected in SIR mode, monitoring the ions of interest for the internal standard (*m/z* 317.93) and analyte (*m/z* 305.89). Figures 3 and 4 present the acquired chromatograms for the calibration standard (Figure 3) and the matrix extract (Figure 4).

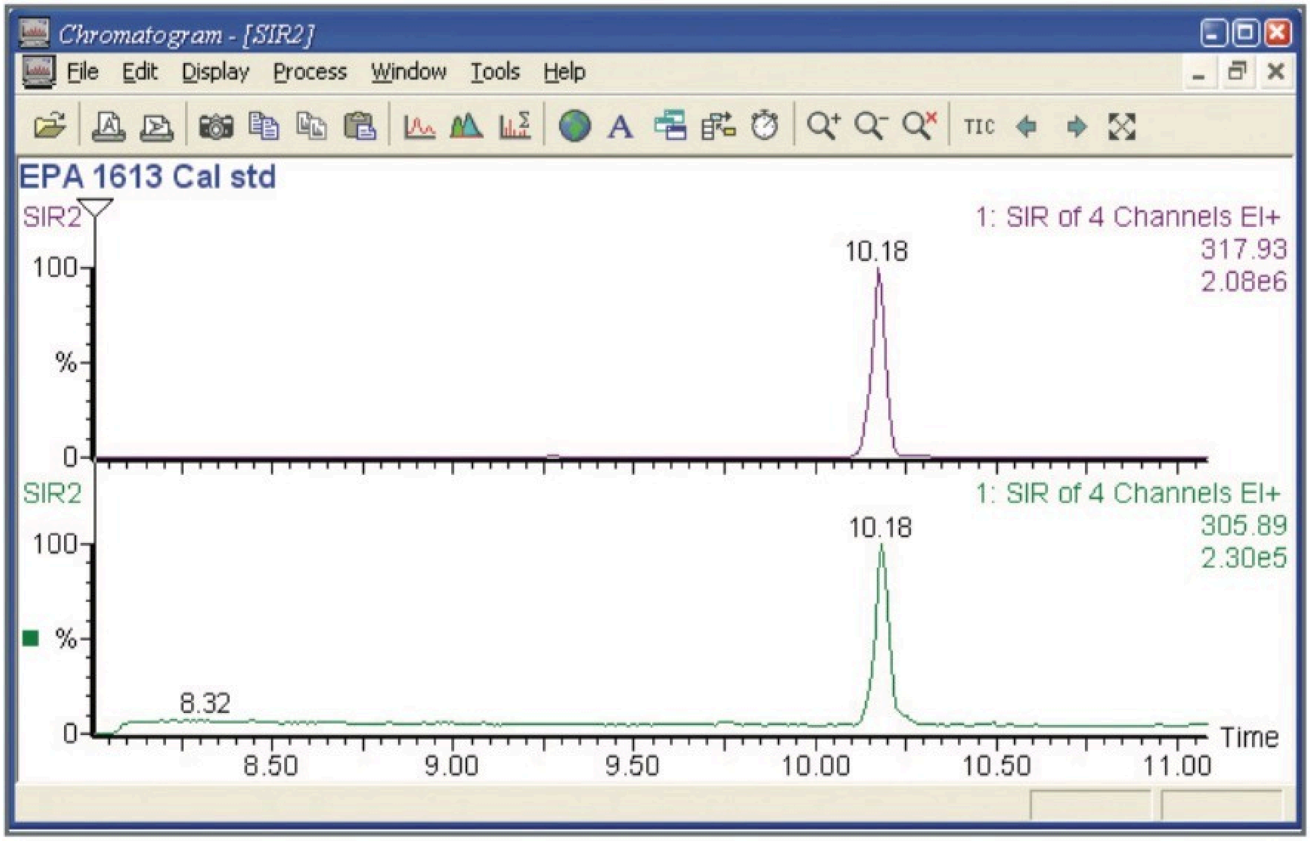

Figure 3. SIR calibration standard injection.

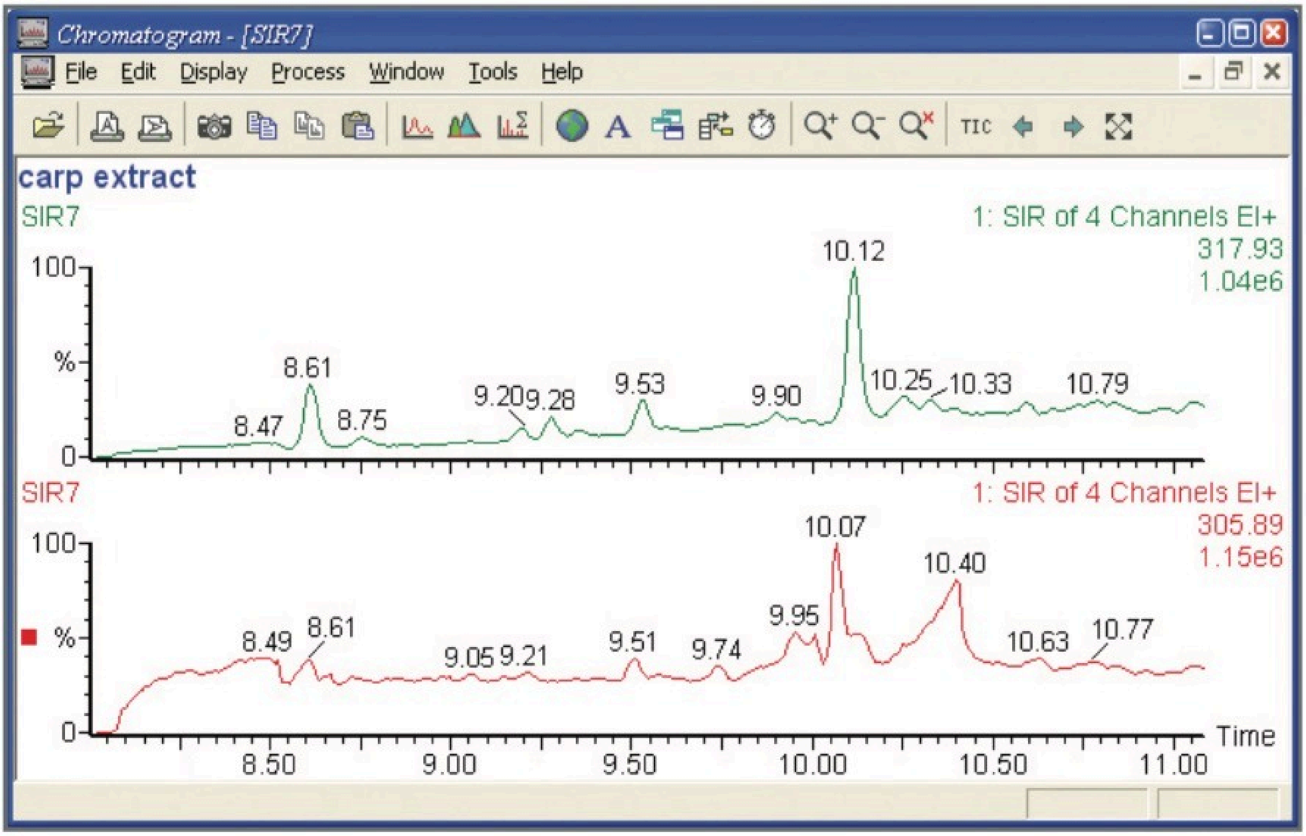

Figure 4. SIR Carp extract injection.

The calibration standard shows much improved signal to noise (S/N) ratios for both the internal standard and analyte peaks; however, the matrix injection shows a vast improvement when compared with full scan analysis, but does not show good selectivity for the internal standard. The analyte trace does not really offer any true quantitative information.

The instrument was then tuned in daughter ion mode, tuning on daughters of heptacosa. The calibration standard and matrix extract were then acquired in muliple reaction monitoring (MRM) mode, monitoring compound specific transitions. In this mode of operation, the first quadrupole monitors the precursor mass, which then undergoes collisionally induced fragmentation in a collision cell, aided by the prescence of a collision gas and collision energy (eV). The second quadrupole then monitors the product mass, which is normally selected to be a compound specific fragment. Figures 5 and 6 present the calibration standard injection (Figure 5) and the matrix extract injection (Figure 6).

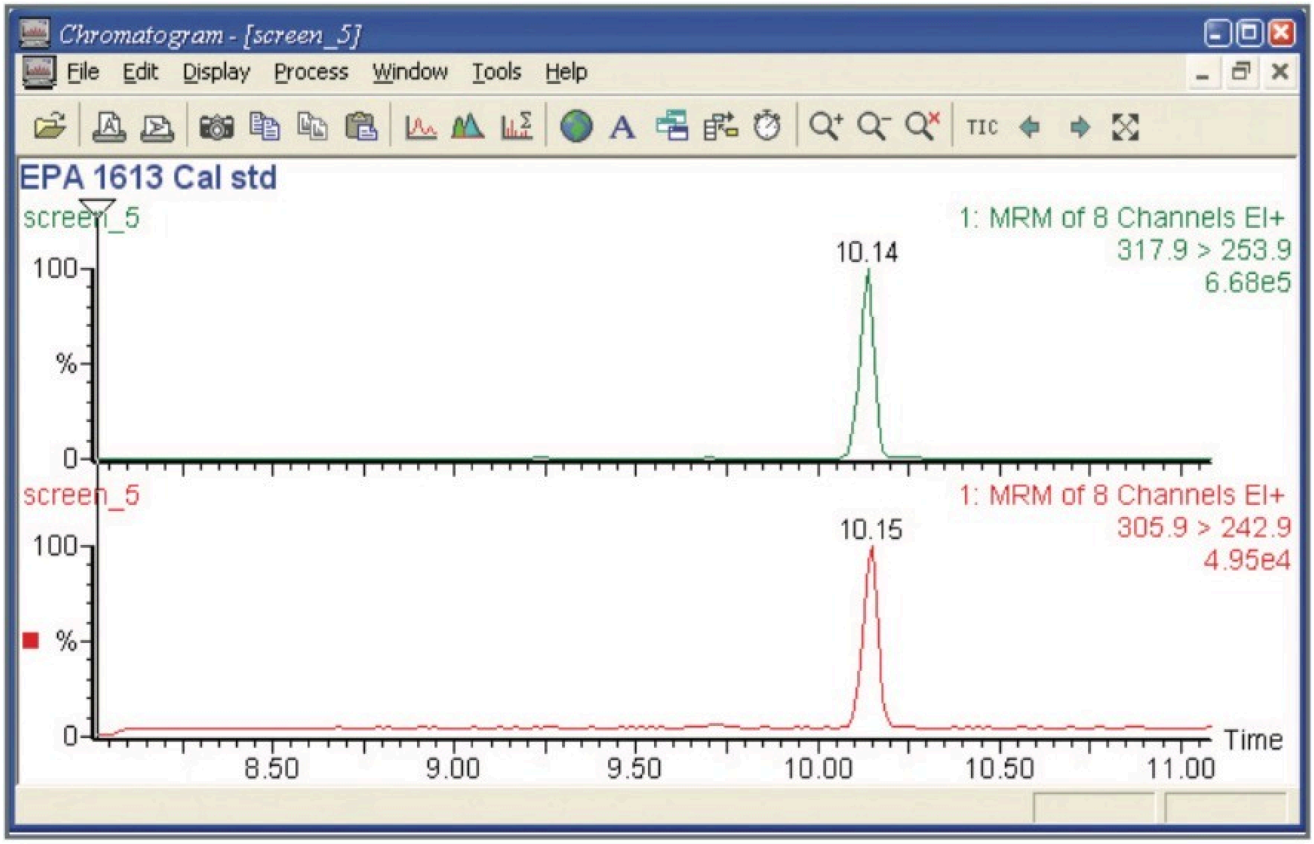

Figure 5. MRM calibration standard injection.

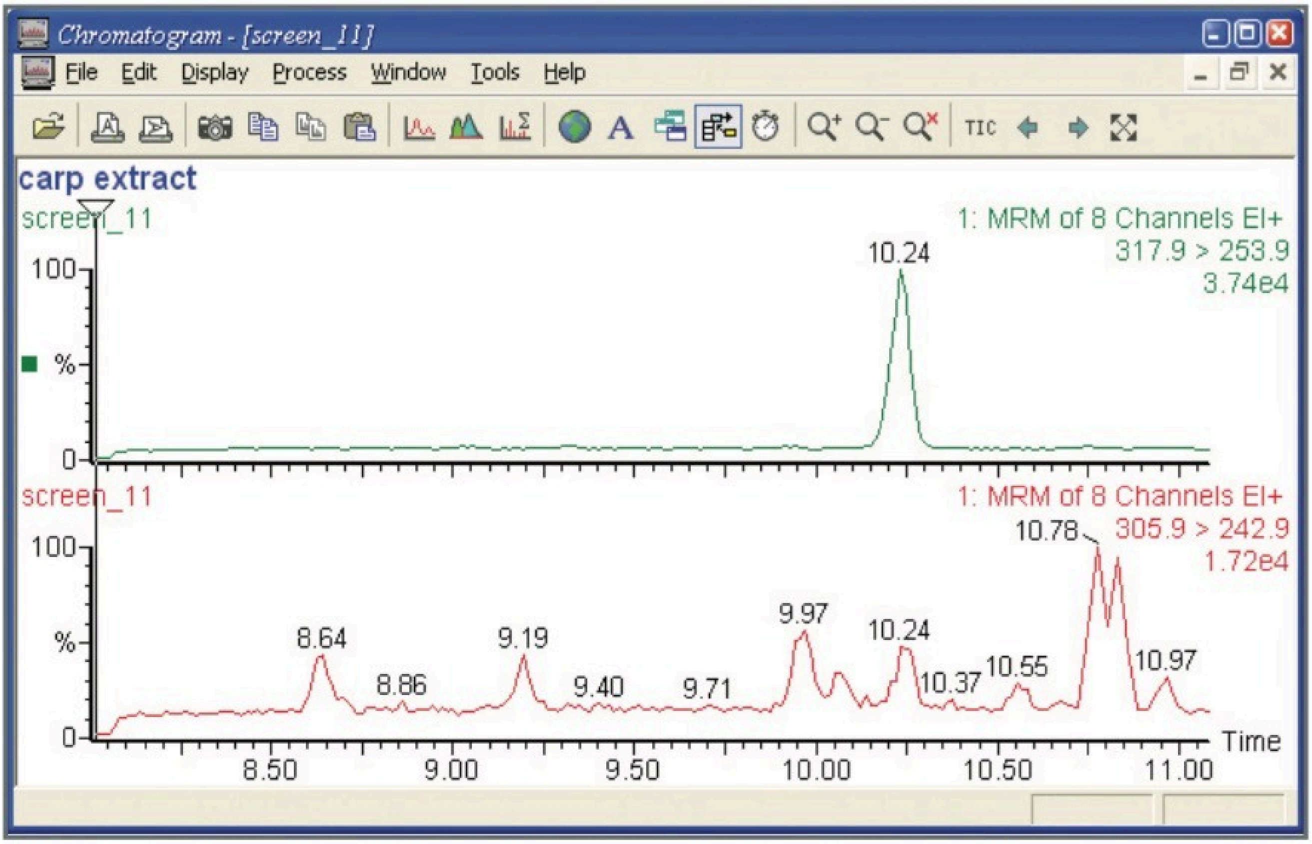

Figure 6. MRM Carp extract injection.

The calibration standard shows similar signal to noise when compared with the SIR standard injection. Upon inspection of the matrix extract chromatogram, it can now be clearly seen that a much higher degree of selectivity is offered by using MRM, with the internal standard (317.9 > 253.9) having good S/N at 10.24 minutes, and an analyte peak (305.9 > 242.9) is now distinguishable at 10.24 minutes. All other peaks seen in the analyte chromatogram are now from other isomers of the target compound.

Conclusion

Full scan analysis has a low degree of selectivity, given that a comparatively wide mass range is acquired, with all masses stored by the data system. Full scan analysis is invaluable for the identification of unknown peaks, and is essential during method development.

SIR analysis gives a much higher degree of selectivity and greater sensitivity when compared with full scan analysis, but when performed on a quadrupole instrument, complex extracts will require a high degree of specific cleanup to enable the analyst to obtain reliable results.

Analysis of complex sample extracts using MRM acquisition offers the analyst the highest degree of sensitivity and selectivity, and can be possibly the only way to obtain reliable results without the need for time consuming clean-up processes, or expensive high resolution instrumentation.

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