



Using Triple Quadrupole MS, a precursor ion is chosen from the mass spectrum of the compound. The first quadrupole filters this and allows it to pass the 'second quad', which in today's instruments is a hexapole or octapole. This serves as a collision cell where the single ion is further fragmented using a collision gas, usually Argon. The resulting product ions are then separated further in the 'third quad'. When using this technique, Multiple Reaction Monitoring (MRM) is applied whenever possible. In these cases, one or two ions are monitored - one is used for quantitation calculations and the other for compound confirmation.

When multiple target compounds are co-eluting, the quadrupoles and collision cell are rapidly switching electrical potentials, thereby removing the previously created ions to prevent 'cross talk'. This is crucial when it comes to the accurate identification and analysis of components to the critical levels required for pesticide residue applications. Modern equipment, such as the Shimadzu High Efficiency UF sweeper collision cell, can perform 600 MRM transitions per second with no cross talk. This allows collection of the maximum number of data points during the passage of a component 'peak' through the detector, giving the optimum quantitation precision.

It is now also possible to use 'Fast GC' columns to reduce conventional analysis times by a factor of three or four. These columns produce much smaller peak widths and require data sampling rates three to four times faster than conventional columns. An example of using such a column to analyse trace level PBDE is shown in Figure 1. This analysis was carried out using the Shimadzu Ultra Fast (UF) MS detector incorporating Advanced Scanning Protocol (ASSP).

Whilst the MRM technique for trace level determination of target compounds produces excellent results, it has the drawback of not providing any additional information about the presence of non-target compounds. For that, 'FullScan' data is required. In the past, this required a second analysis of the sample. Now, however, the ultra fast capabilities of modern instruments allow both MRM and FullScan data acquisition in a single run.

Both sets of data are available in a single data file, making possible trace level quantitation of target compounds and automatic qualitative analysis of every compound present in the sample. This halves the number of analyses required, minimises the analytical variables and dramatically reduces the time for a complete analysis.

Figure 2 shows an example of a combined MRM/FullScan analysis of metabolites in rat urine.

### QuEChERS Procedure

The QuEChERS method is a streamlined approach that has been readily accepted by many pesticide residue analysts. This method makes it easier and less expensive for analytical chemists to examine pesticide residues in foodstuffs.

During the procedure, the analyst homogenises the sample in a blender. Sample is then placed in a centrifuge tube with reagent and agitated for one minute. The reagents used depend on the type of sample, with variables depending on the structure and type of matrix. Following this the sample is put through a cleanup column prior to chromatography analysis. With QuEChERS, eight samples can be prepared in 45 minutes.

### Simultaneous Scan / MRM Data in a single run 600 transition/sec MRM and 20,000 amu/sec Scan Speed

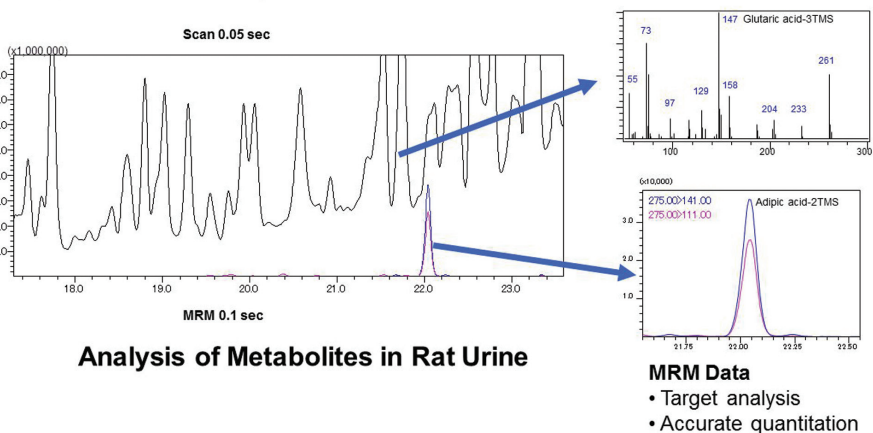


Figure 2: MRM/FullScan analysis of metabolites in rat urine using the Shimadzu Triple Quad GCMS

### Conclusion

Triple Quadrupole MS is a powerful tool for fast and accurate analysis of a wide range of compounds in complex matrices. Modern high-performance instruments provide the correct data in one quick instrument run, rather than the several steps previously required. The added capability to run a full scan and MRM simultaneously, instead of these being two separate procedures, opens up multiple opportunities for an extensive range of analytical procedures within short timeframes.

The need for speed when running complex analyses will continue to become more crucial in the future, especially in dynamic application areas such as pesticide residue testing. The techniques described above are used not only in food testing but also in determining pesticide degradation by-products in water, sediment, and soils. These new technologies and practices are going a long way to meet the analytical speed and sensitivity demands across multiple testing applications and will continue to support analysts in

meeting the increasingly stringent regulatory requirements in pesticide residues and other controlled areas.

For more information on how Triple Quadrupole MS can improve your analysis, visit [www.shimadzu.com](http://www.shimadzu.com)

### References

1. Regulation (EC) No 396/2005 of the European Parliament and of the Council of 23 February 2005 on maximum residue levels of pesticides in or on food and feed of plant and animal origin and amending Council Directive 91/414/EEC

