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Tips and techniques from the laboratory experts.

If you've had your laboratory run low-level polyaromatic hydrocarbons (PAHs) or other low level analyses, chances are you have heard of Gas Chromatography/Mass Spectroscopy-Selective Ion Monitoring (GC/MS-SIM). Over the years clients have asked us "What's the difference between GC/MS-Full Scan and GC/MS-SIM?" To address this question we must start with the basics. (For our example we will be talking about a standard quadrupole mass spectrometer using electron ionization.)

GC/MS is an instrumental analytical technique comprised of a gas chromatograph and a mass spectrometer. In general, the GC is used to separate complex chemical mixtures into individual components. Once separated, the chemicals can be identified and quantified by the mass spectrometer.

Before analysis can occur a sample must be prepared, usually by extracting the analytes of interest into a liquid solvent phase. This extract is then injected into the GC where it is swept onto a separation column by an inert carrier gas such as hydrogen or helium. The analytes in the mixture are carried through the column by the carrier gas where they are separated from one another by their interaction between the coating (stationary phase) on the inside wall of the column and the carrier gas. Each analyte interacts with the stationary phase at different rates. Those that react very little move through the column quickly and will exit into the mass spectrometer before those analytes having longer interaction and retention times.

When the individual analytes exit the GC column they enter the ionization area (ion source) of the MS. Here they are bombarded with electrons which form ionized fragments of the analyte. These ionized fragments are then accelerated into the quadrapole via a series of lenses and separated based on their mass to charge ratio. This separation is accomplished by applying alternating RF frequency and DC voltage to diagonally opposite ends of the quadrapole, which in turn allows a specific mass fragment to pass through the quadrapole filter. From here the fragments enter the mass detector (electron multiplier) and are recorded. The MS computer graphs a mass spectrum scan showing the abundance of each ionized mass fragment.

A GC/MS system in Full Scan mode will monitor a range of masses know as mass to charge ratio (abbreviated m/z). A typical mass scan range will cover from 35-500 m/z four times per second and will detect compound fragments within that range over a set time period. Laboratories have extensive computer libraries containing mass-spectra of many different compounds to compare to the unknown analyte spectrum. The Full Scan mode is quite useful when identifying unknown compounds in a sample and providing confirmation of results from GC using other types of detectors.

Operation of a GC/MS in SIM mode allows for detection of specific analytes with increased sensitivity relative to full scan mode. In SIM mode the MS gathers data for masses of interest rather than looking for all masses over a wide range. Because the instrument is set to look for only masses of interest it can be specific for a particular analyte of interest. Typically two to four ions are monitored per compound and the ratios of those ions will be unique to the analyte of interest. In order to increase sensitivity, the mass scan rate and dwell times (the time spent looking at each mass) are adjusted.

When properly setup and calibrated, GC/MS-SIM can increase sensitivity by a factor of 10 to 100 times that of GC/MS-Full Scan. Because unwanted ions are being filtered, the selectivity is greatly enhanced providing an additional tool to eliminate difficult matrix interferences.

The ability of the mass spectrometer to identify unknowns in the full scan mode and quantitiate know target analytes in the SIM mode, makes it one of the most powerful tools available for trace level quantitative analysis in the lab today.

For more information on GC/MS-Full Scan and GC/MS-SIM contact Columbia Analytical Services, Inc. at 360.577.7222 or visit www.caslab.com.

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