

One of the greatest challenges in sample analysis lies in the detection of a large number of target compounds in complex matrices, many of which are present at low levels.

## For this type of application, the following features are essential:

- · Accurate mass-high resolution full spectral acquisition
- · Low level detection
- · Simplified acquisition method development
- · Easily automated qualitative analysis
- Batch processing for target compounds



The matrix has a great impact on the analysis



Removable Ion Source

## A powerful way to screen for hundreds of compounds in complex matrices

MassHunter Data Analysis Software:

- Use "Find by Formula" algorithm to search for compounds with or without Retention Time
- Both unit or accurate mass El spectral libraries can be utilized to screen the accurate mass El GC/Q-TOF data
- Full spectum data provides complete information that allows for retrospective analysis - without rerunning your samples - so that you can search with a different library or for specific compounds of interest
- Full spectrum accurate masshigh resolution data enables the identification of unexpected peaks or unknown compounds
- Intuitive quantitation using MassHunter Quantitative Analysis

For more information, visit: agilent.com/chem/gcms\_qtof



# **Agilent Technologies**

## **Screening Workflow**

In complex samples, it is challenging to search for low level components. With the accurate mass-high resolution capabilities of the GC/Q-TOF, screening for hundreds of low level compounds can be readily achieved.

Vegative lons	Scoring	Results	Result Filters	Fragment Confirmation
A Formula Source		A Formula Matching		Positive lons
Source of form	ulas to confi	m		
These form	mulas: 🛕			
C14H12C	03			A
C14H12C (type a co	D3 omma-separ	ated list of f	ormulas, e.g., "Cl	6H6, CH4")
C14H12C (type a co	D3  omma-separ d exchange	ated list of f	ormulas, e.g., "C	6H6, CH4")
C14H12C (type a co	D3 omma-separ d exchange	ated list of f file (.CEF):	iormulas, e.g., "Ci	6H6, CH4")
C14H12C (type a co	D3  omma-separ d exchange	ated list of f file (.CEF):	iormulas, e.g., "C	6H6, CH4")
C14H12C (type a co Compound Database	03  omma-separ d exchange / Library	ated list of f	iormulas, e.g., "C	6H6, CH4")

Use a mass or elemental formula to search a chromatogram for a single compound - or use a library to search for multiple compounds. Retention time can be used for increased confidence. *Retention Time Locking is a standard feature of the Agilent 7890 GC.* 



Fragment extraction window

With the high resolution GC/Q-TOF, you can readily generate Extracted Ion Chromatograms (EIC) to isolate the compound of interest. High resolution data facilitates identification of trace level targets in a complex matrix.



Isotope pattern matching

The MassHunter Qualitative Analysis software includes Molecular Formula Generation tools that will assign empirical formulas to mass peaks with an overlay of the theoretical isotope pattern (abundance and spacing).

Screening for hundreds of compounds can be achieved using the Agilent 7200 GC/Q-TOF coupled with the Agilent 7890B GC and MassHunter software.

## **Further readings:**

Agilent 7200 Series GC/Q-TOF: Resolve your most challenging applications (5991-4806EN)

For more information, please visit: www.agilent.com/chem/gcms\_qtof

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