

# Agilent SureMass

## Technical Overview

### Abstract

Full spectrum GC/MS data have historically relied on conventional manual analysis or algorithmic deconvolution to extract and identify chemical components found in complex mixtures where chromatographic coelution may occur. Available deconvolution algorithms are capable of determining even trace level components under challenging chromatographic conditions. However, these algorithms are often optimized for nominal resolution scanning mass spectrometer techniques (for example, quadrupole MS), and may not produce optimal results for high resolution full spectrum mass analyzers, such as time-of-flight (TOF). This technical overview discusses a novel signal processing algorithm (SureMass) for chemical component detection, designed specifically for high-resolution profile MS data from the Agilent TOF-based MS systems, available for use with the 7200 Series GC/Q-TOF platforms.



**Agilent Technologies**

## Introduction

Prominent deconvolution techniques based on retention time and elution profile matching of extracted ion chromatograms (EICs) continue to be an extremely powerful tool for GC/MS users (Figure 1). These signal processing techniques are well suited to deal with spectral data generated from scanning GC quadrupole mass spectrometer (GC/MSD) instruments. Such deconvolution tools are commonplace in the many laboratories with GC/MSD systems.

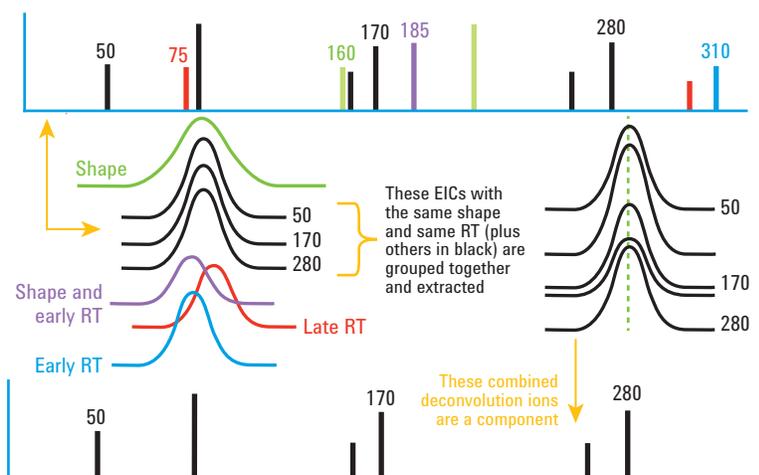


Figure 1. Time and profile-based deconvolution.

Despite the analytical power of this established deconvolution technique, it has been designed and optimized predominantly for data from nominal mass scanning instruments such as the GC/MSD. Data from high-resolution accurate mass instruments, such as the Agilent 7200 Series GC/Q-TOF systems, do not necessarily derive maximum utility from this conventional approach. Processing speed, component detectability, and replicate repeatability are all affected when applying approximating treatments to complex data types. The richness of chromatographic detail and broad spectral information from high-resolution accurate mass data tests the limits of performance for EIC-based component detection. To make better use of the high-resolution accurate mass data generated by the GC/Q-TOF, an innovative signal processing algorithm for feature detection and deconvolution has been developed by Agilent.

Agilent SureMass is a novel chemical feature detection algorithm designed specifically for high-resolution MS profile data, such as that which is generated by 7200 Series GC/Q-TOF systems. This advanced technique processes the full spectrum, high-resolution TOF MS profile data as a continuous 3-dimensional array (retention time,  $m/z$ , and abundance) rather than as a set of EICs. Based on the concept of persistent 3-dimensional spectral ridges and associated chemical features, SureMass is designed to accommodate MS detection characteristics that may vary on the chromatographic timescale. This is an important aspect of the algorithm – just as conventional (nominal mass) deconvolution incorporates abundance corrections for spectral skewing associated with scanning mass spectrometers, SureMass includes the ability to adapt to changes in MS measurement characteristics ( $m/z$  value, intensity) based on changing experimental conditions. By considering practical instrument performance characteristics in designing the signal processing algorithm, improved results can be generated compared to previously available techniques.

Performance characteristics of TOF MS have a defined impact on acquired data. This becomes apparent when viewing the entirety of a TOF data file in three dimensions. Chemical features are visible as apexes along persistent ridge signals. These ridges are present along the time domain, and extend upwards to form a feature during the elution of a component. Ridges emanate from low-level chemical signals. Notably, these ridges are not necessarily static in the  $m/z$  domain. Due to changes in experimental conditions throughout the duration of data acquisition, there may be a trackable change in measured  $m/z$  values. SureMass is able to extract ridges following these trackable patterns.

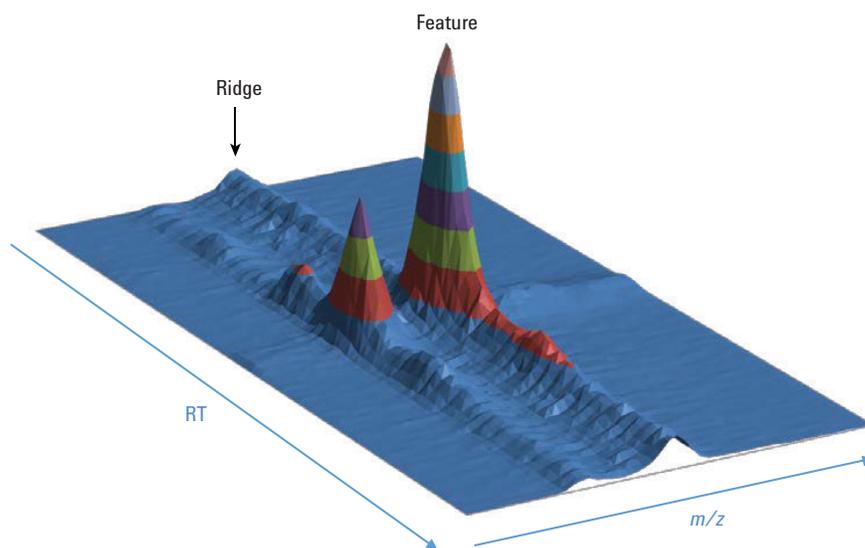


Figure 2. Agilent SureMass three-dimensional signal processing.

## Extracted SureMass Chromatogram (ESM)

The dynamic nature of spectral ridges also applies to their associated chemical features. To make use of this characteristic, SureMass performs variable signal extractions of a chemical feature by incorporating changes in mass assignment during its elution profile. In this way, an Extracted SureMass Chromatogram, or ESM, can be generated. The ESM corresponds to a defined, variable ridge and its associated chemical feature. It is not necessarily a static mass range extraction as is performed with conventional deconvolution using EICs. The ESM is a two-dimensional chromatographic representation of a detected chemical feature extracted from the three-dimensional signal.

The assigned  $m/z$  for an ESM is calculated as the abundance weighted average of  $m/z$  values from contributing spectra that are characterized by signal processing as being below an empirically determined abundance threshold. Discrepancies in  $m/z$  assignment due to changing experimental conditions are minimized, and increased  $m/z$  accuracy is possible regardless of chromatographic complexity and signal intensity.

## Linear Dynamic Range

In addition to the ability to accurately extract chemical component signals, SureMass can interpolate signal intensity for instances when experimental conditions obscure true peak abundance. Typical GC/MS analyses are performed at 5 to 20 Hz spectral acquisition rate. The actual rate chosen will depend on chromatographic peakwidth, and will normally be selected to achieve ~10 to 20 data points across a chromatographic peak for proper characterization. This acquisition rate generates data points on the rising and falling edges of the peak with sufficient frequency to model peak curvatures during these portions of the peak elution profile, even if the true peak abundance between these segments is obscured. These rising and falling sections can then be fit to empirically derived coeluting peak models, providing a complete chromatographic peak profile and intensity characterization even during periods of extreme chromatographic abundance. This technique is used by SureMass when experimental conditions cause the ESM signal to exceed a predetermined abundance level. The linear dynamic range of an analysis can thereby be extended compared to conventional signal extraction techniques. It is often possible to achieve an order of magnitude or more extension of linear dynamic range using SureMass. This enhancement enables extended quantitative accuracy and increased identification confidence through improved spectral library matching.

## **Sensitivity and Precision**

Conventional deconvolution techniques are designed to detect and extract low-level signals in the presence of significant, complex background. SureMass furthers this ability for high-resolution data by following ridge elution profiles to low abundance levels that would typically be obscured by standard EIC extraction. These low-level ridge and associated feature extractions yield greater sensitivity for trace-level components. Additionally, ESM signals include less noise from interferences than conventional EICs with this approach, resulting in a cleaner extracted chromatogram. At low signal levels, this signal quality aspect improves repeatability (peak area/height %RSDs) across replicate injections.

## **Processing Time**

An additional advancement of SureMass over conventional signal processing techniques is the greatly reduced computational time required. By distilling rich spectral and chromatographic data to the relevant information contained in detected ridges and features, the processing of data files using SureMass is made much more efficient than nominal mass deconvolution algorithms. For equivalent analyses, processing speed enhancements of ~100 times compared to earlier techniques are possible. Because SureMass can be applied as a post acquisition technique, it is possible to use this algorithm on previously acquired GC/Q-TOF data sets.

## **Conclusions**

With its novel signal processing technique, Agilent SureMass is able to detect and extract component features with greater sensitivity and accuracy, more reproducibly, across a broader dynamic range, and in less time than any technique previously available for the Agilent 7200 Series GC/Q-TOF. Analytical value from the information-rich, high-resolution MS profile data generated by the GC/Q-TOF can be brought to previously unattainable levels in quantitative, qualitative, and discovery workflows with this new capability. For 7200 Series GC/Q-TOF users, SureMass is available with Agilent MassHunter Quantitative Analysis B.08.00 and Unknowns Analysis B.08.00 as a simple data analysis method parameter within each application.

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