

## Rapid Fingerprinting Tools for a Food Production and QC Environment

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Waters Corporation

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### Abstract

This application brief develops a robust and rapid screening tool that can be used to automatically determine the identity and quality of food ingredients within a couple of minutes.

### Benefits

The SQ Detector 2 provides a rapid and robust approach to determine ingredient identity or quality.

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### Introduction

Food and beverage manufacturers frequently need to test the purity and identity of their incoming raw materials. Tools that allow rapid testing on incoming raw materials entering the factory floor are beneficial for quick turnarounds.

While other analytical techniques already exist within this area it is often useful to obtain a mass spectral fingerprint of the products being tested, as it can provide additional information for troubleshooting if issues arise.

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The Engineered Simplicity of the SQ Detector 2 allows the technology to be accessible to all levels of expertise, including operators who may be new to MS technology.

The Waters SQ Detector 2 has experimental flexibility: inlets to the MS can be changed, and there are many different ways to interpret the data depending on the results needed. Data interpretation needs to be easy and rapid for the user. MarkerLynx XS Software has the capability of displaying analyzed results pictorially, so that non-conforming products can be seen.



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## Results and Discussion

The SQ Detector 2, along with the ASAP Probe and MarkerLynx XS Software data processing, were used to rapidly analyze edible oils. Four different types of oils were assessed and analyzed; three of which were omega-6 oils: evening primrose oil, starflower (borage) oil, and CoQ10 in sunflower oil; the fourth was omega-3 fish oil.

The oil was placed onto the tip of a glass capillary (no dilution or sample prep was performed in this

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case), and directly analyzed using the ASAP Probe and the SQ Detector 2.

Within two minutes the probe temperature was ramped up so the sample could be desorbed from the glass tip and into the source of the SQ Detector 2. Full scan data were collected for each sample in order to provide a mass spectral fingerprint of each sample.

Figure 1 shows the full scan data at different time points in the desorption process (spectra shown in red). It is possible to see the mass spectral change as the temperature was increased. The mass spectral fingerprint summed over the entire acquisition time is shown in purple. Data were collected for these samples in the  $m/z$  range 50 to 1200.

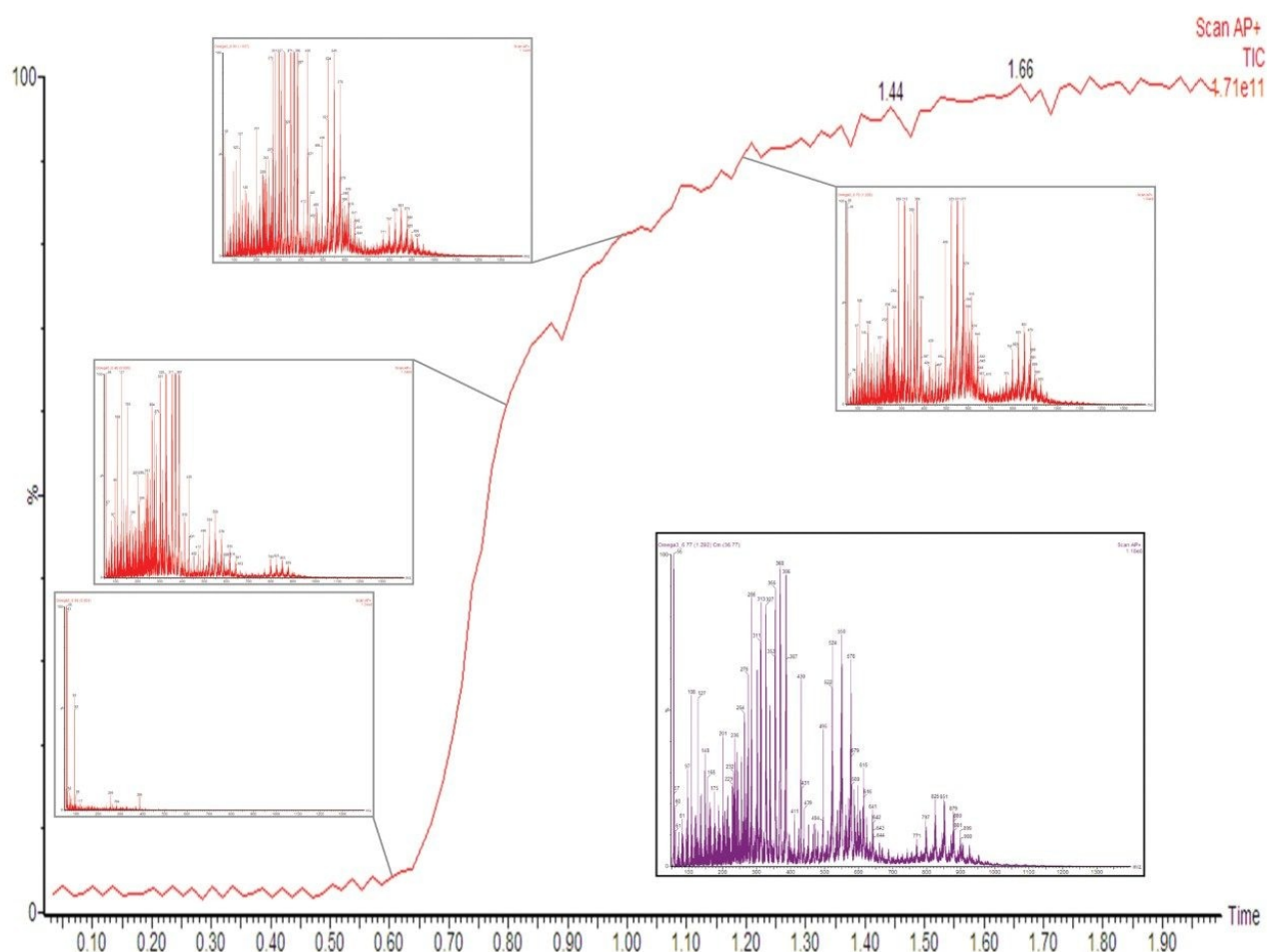


Figure 1. Spectra from ASAP-SQ Detector 2 analysis of fish oil: the red spectra show specific times during the temperature ramp; the purple spectrum was combined over the entire acquisition time.

Data collected from the SQ Detector 2 can be automatically interpreted and viewed using MarkerLynx XS Software, shown in Figure 2, which uses Principal Component Analysis (PCA) to find and group samples that have similar characteristics.

In Figure 2, each color represents a different incoming raw material. It can be seen that multiple injections of each product grouped well together were well separated from the other samples analyzed using this rapid approach. Data can be easily visualized with MarkerLynx XS Software, which allows the user to clearly see variations between products.

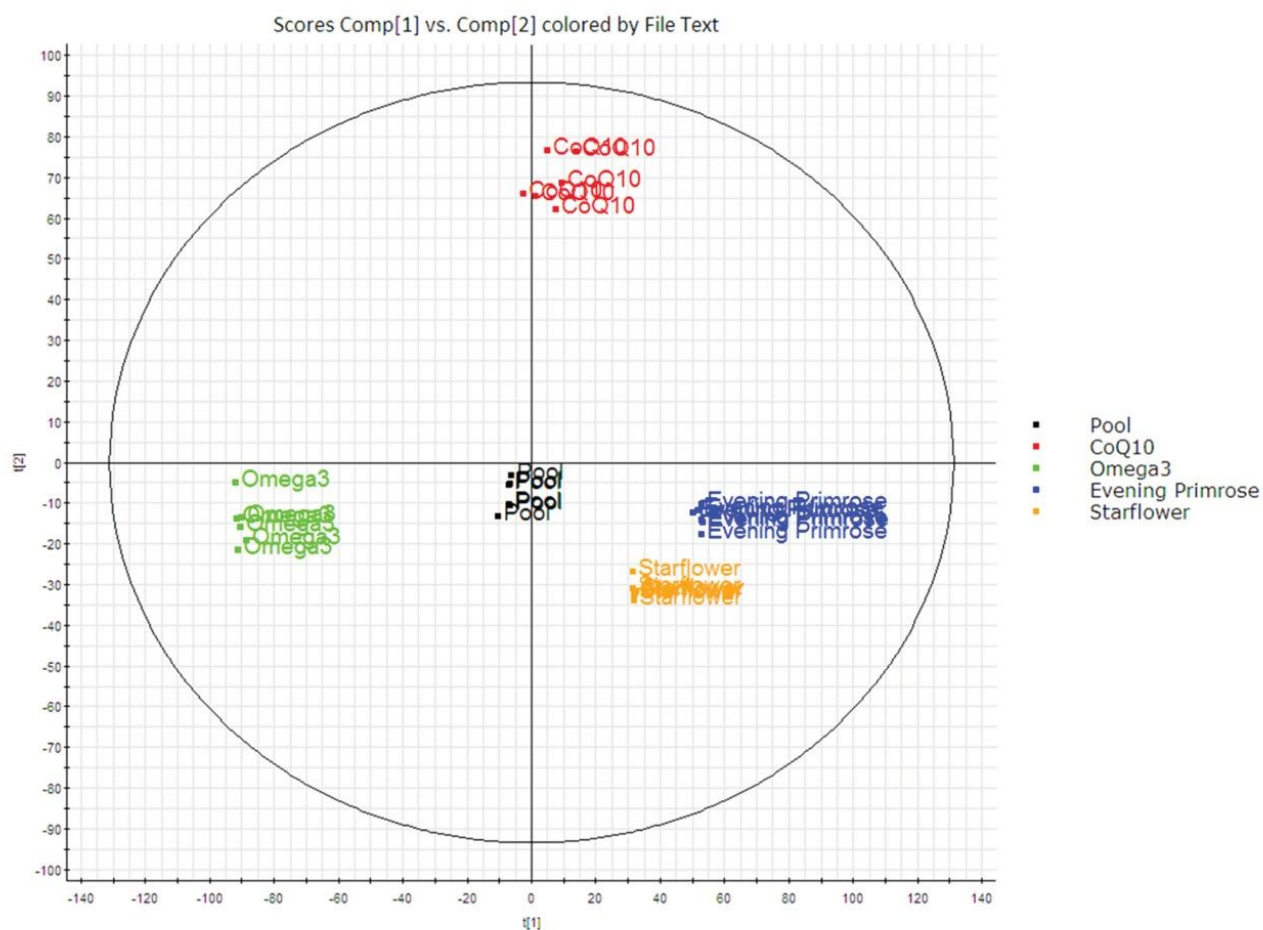


Figure 2. Sample view within MarkerLynx XS: the software provides the user with an easy way of viewing product variation / change.

The total system solution described in this application brief provides a rapid and robust approach that allows analysts to determine either the ingredient identity or quality of a sample.

## Conclusion

The ASAP Probe and SQ Detector 2, combined with MarkerLynx XS data processing, was used to

successfully screen ingredients that are used within the food and dietary supplements industry.

This approach is easy to adapt in any food production or QC environment to help rapidly analyze incoming samples.

The SQ Detector 2 has been designed to provide users with maximum versatility and minimum setup effort. Combining the SQ Detector 2 with MarkerLynx XS Software allows easy data interpretation to support the detection of potentially non-conforming products in a factory or QC environment.

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[Progenesis QI Software <https://www.waters.com/134790655>](https://www.waters.com/134790655)

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