

# Increasing the Chemical Information Obtained in a Polymer Industry Quality Control Environment with the SQ Detector 2

## GOAL

To demonstrate the benefits of coupling the SQ Detector 2 and a Photo Diode Array (PDA) Detector to the ACQUITY UPLC® System, compared with using ACQUITY UPLC-PDA detection alone.

## BACKGROUND

Many Quality Control (QC) laboratories routinely use HPLC or UPLC® chromatographic separation coupled to analog detectors, such as a PDA Detector or a Refractive Index (RI) Detector. While such analysis techniques can provide valuable QC data, some components under investigation may not be detected. Physicochemical characteristics of certain compounds can prevent a sufficient response from being obtained.

Mass detection offers a powerful and flexible tool for the QC analyst, and can be used in conjunction with analog detectors. The ability to easily change the ion source on a mass detector means that a wide range of different classes of compounds, with different structures and properties, can be analyzed on a single instrument. Analytical parameters can be established to ensure the detection of all components of interest by acquiring unambiguous, non-selective data.

Quick and simple QC protocols can be implemented with a single quadrupole mass spectrometer, offering manufacturing companies valuable financial and time savings while maximizing return on investment.

The SQ Detector 2 is a powerful, flexible tool for Quality Control laboratories.

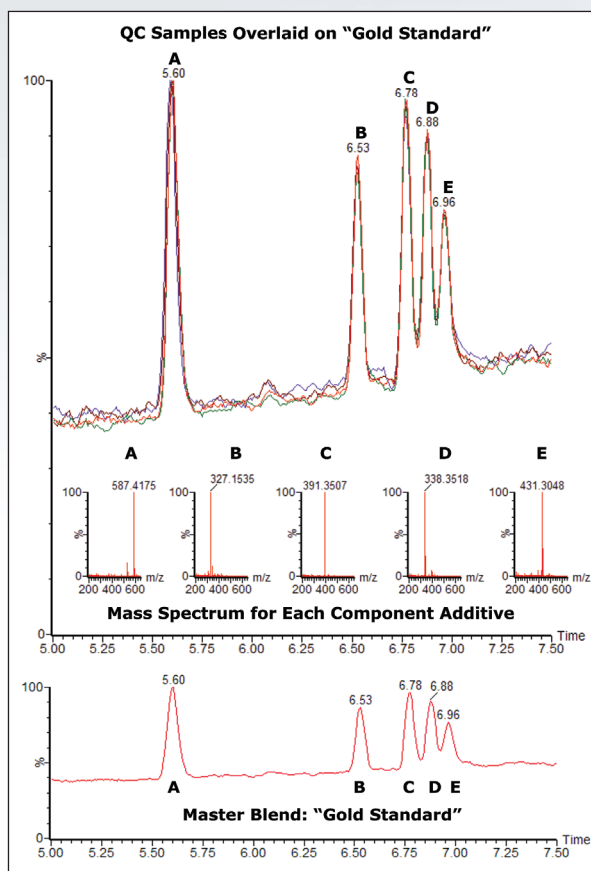
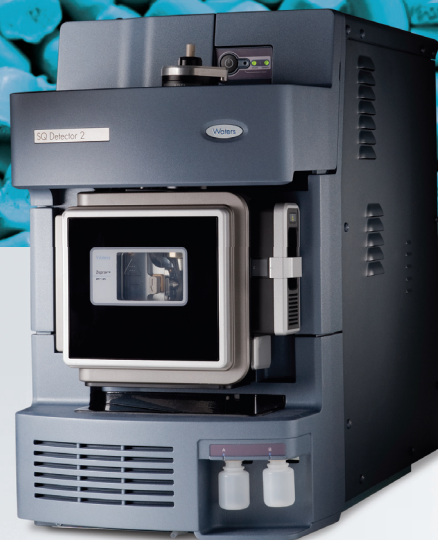


Figure 1. Molecular mass information can be obtained from mass spectra, along with chromatographic retention times and an overall batch fingerprint.

## THE SOLUTION

A Waters® SQ Detector 2 was coupled to an ACQUITY UPLC System. The SQ Detector 2 was fitted with an Atmospheric Pressure Photo Ionization (APPI) source. The APPI source offers an alternative to the more familiar ElectroSpray Ionization (ESI) or Atmospheric Pressure Chemical Ionization (APCI) sources that are also used with mass spectrometers. APPI is the ideal choice for analyzing compounds, such as polymers and polymer additives, because it is equally effective at ionizing low mass and high mass, polar and non-polar species. APPI is a complementary technique to ESI and APCI, offering complete flexibility for the QC analyst.

A blend of five polymer additives was analyzed to illustrate the benefits of using mass spectrometric detection compared with PDA detection. The blend was comprised of **A.** an antioxidant, Irganox 245; **B.** a UV absorber, 2-Hydroxy-4-(octyloxy)-benzophenone; **C.** a plasticizer, Diethylhexyl phthalate (DEHP); **D.** a slip agent, Erucamide; and **E.** an optical brightener, Uvitex OB.

Figure 1 shows a series of QC sample chromatograms overlaid on a master blend “Gold Standard” chromatogram. The Gold Standard represents the correct analytical profile of the polymer additive blend. Not only can analysts obtain retention time information and a characteristic fingerprint for the polymer additive blend, they can also acquire information about the molecular mass. The mass spectrum for each chromatographic peak shows unique information about each component of the blend.

Figure 2 shows a comparison between PDA data and mass spectrometric data for the five-component polymer additive blend. The data were acquired simultaneously, with the PDA Detector in line with the SQ Detector 2. The PDA Detector acquired data over the range 190 to 500 nm – while the SQ Detector 2 acquired data in full scan mode over the range  $m/z$  50 to 800. Figure 2 shows that all five components were easily detected in the mass chromatogram; however, erucamide was not detected by the PDA Detector. No wavelength in the acquired range showed a response for erucamide.

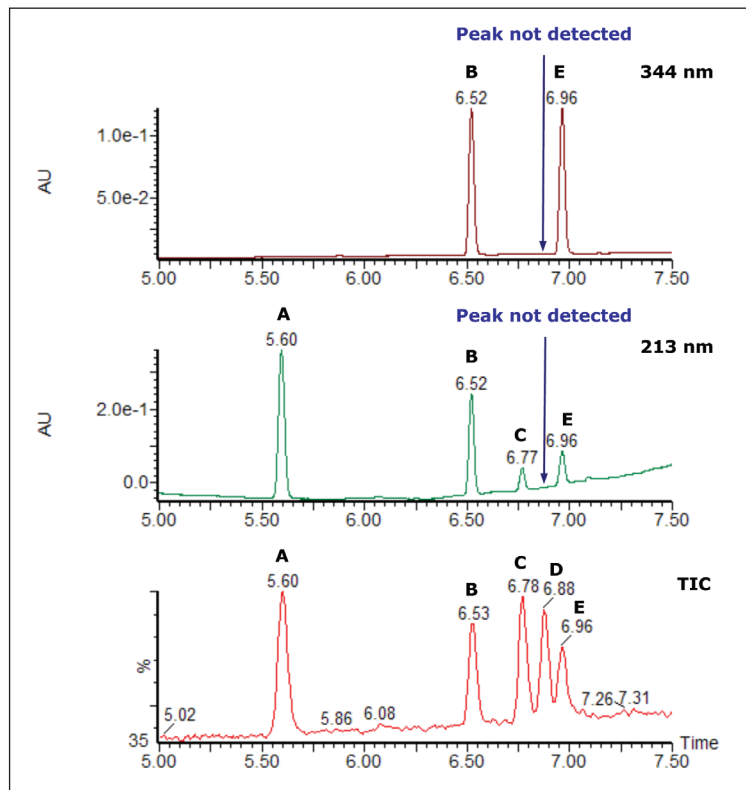


Figure 2. A comparison of PDA data with mass spectrometric data shows that component *D*, erucamide, was not detected by the PDA Detector, but was detected using the SQ Detector 2.

## SUMMARY

The SQ Detector 2 with an APPI source was successfully used to analyze a five-component polymer additive blend. A PDA Detector was included in line with the mass spectrometer.

Using an APPI source with the SQ Detector 2, a QC analysis method was developed that enabled the detection of all components of the polymer additive blend. The PDA Detector did not show a response for the slip agent erucamide. The SQ Detector 2 offers additional selectivity and flexibility to the analyst through the provision of alternative ion sources, proving a powerful tool to meet diverse analytical challenges in any QC environment.

# Waters

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