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Nota applicativa

The Use of TrendPlot Software for Routine Monitoring of Polymer QC Tandem Quadrupole Data

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This is an Application Brief and does not contain a detailed Experimental section.

Abstract

In this application brief we use TrendPlot Software within TargetLynx Application Manager for tracking routine polymer QC data, and to rapidly identify out-of-specification materials.

Benefits

TrendPlot Software within TargetLynx Application Manager provides rapid and simple QC data tracking.

Introduction

Product Quality Control (QC) is vitally important in manufacturing industries. The impact of sub-standard raw materials or a poor quality final product can be huge in terms of factory productivity, workers' time and financial costs.

Strategies to mitigate the occurrences of process shutdown or product recall include implementing stringent QC testing procedures. Materials used during manufacture may be sampled and analyzed multiple times and in replicate throughout the production cycle, which generates large quantities of valuable QC data. Processing and mapping these data can be complex and time-consuming.

Collating and viewing information about different materials simultaneously may prove challenging where important gradual trends, measurement shifts, or systematic biases might be overlooked. It is vital to detect an out of control trend long before the material becomes out of specification by utilizing an automated and standardized approach. Identifying such a trend offers manufacturers the opportunity to take reparative action before significant production costs are incurred.

Results and Discussion

Waters Xevo TQD, with an Atmospheric Pressure Photo Ionization (APPI) source, coupled to an ACQUITY UPLC System, were used to acquire quantitative QC data for various widely-used polymer additives. The Xevo TQD was operated in MRM mode to ensure maximum sensitivity and selectivity for the compounds of

interest.

Multiple injections were acquired over an extended period of time. The MRM data were processed using TargetLynx Application Manager. TargetLynx automatically detects and quantifies mass spectral data using a simple, customizable processing method. TrendPlot can then display these data in a variety of analyst-defined ways.

Figure 1 shows QC data for the optical brightener Uvitex OB. In this example, each daily batch was sampled twice (sample A and sample B), and TrendPlot was used to automatically plot the integrated area for each chromatographic peak. TrendPlot also offers the ability to add statistical limits to the graphs. In Figure 1, the central green band represents two standard deviations (SD) and the outer orange bands represent three SD for the acquired data.

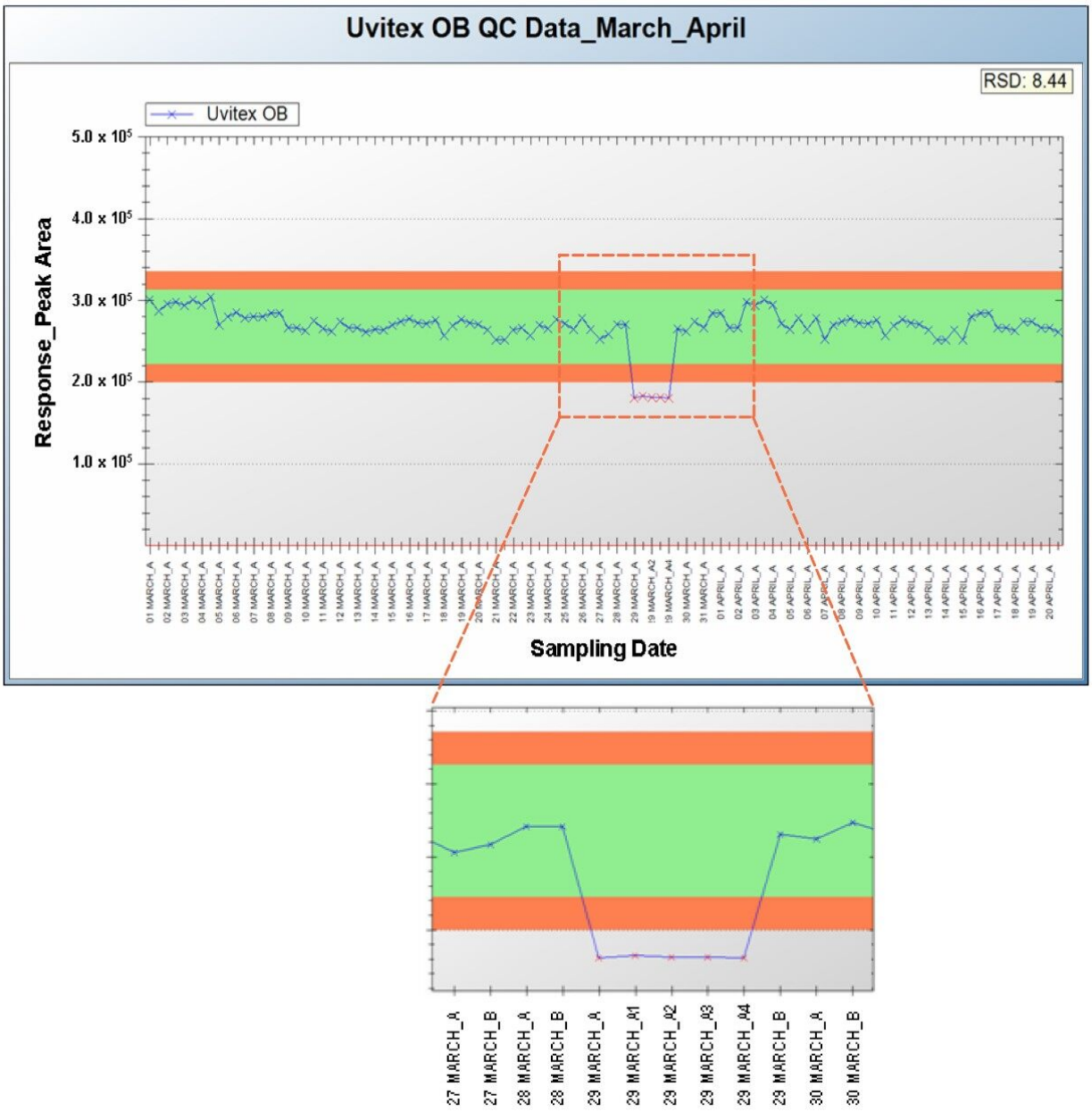

Figure 1. TrendPlot showing QC data for the optical brightener Uvitex OB. The magnified section shows that Sample A on March 29 fell outside acceptable manufacturing specifications.

On March 29, Sample A fell below the three SD limit. This was recognized immediately and the same sample was reanalyzed four times. Each subsequent result was added to the TrendPlot graph, and it was simple to identify the batch as unacceptable.

Figure 2 shows QC data for dibutyl phthalate (DBP), a polyvinyl chloride (PVC) softener, and 2-hydroxy-4-

(octyloxy)-benzophenone, a UV absorber. Information for different materials can either be plotted as shown in Figure 2, or overlaid on a single axis. In the polymer, the two additives were each expected to be present at 10% ±1%. The 10% level is marked on each graph, and the acceptable manufacturing limits of ±1% are shown by the green band.

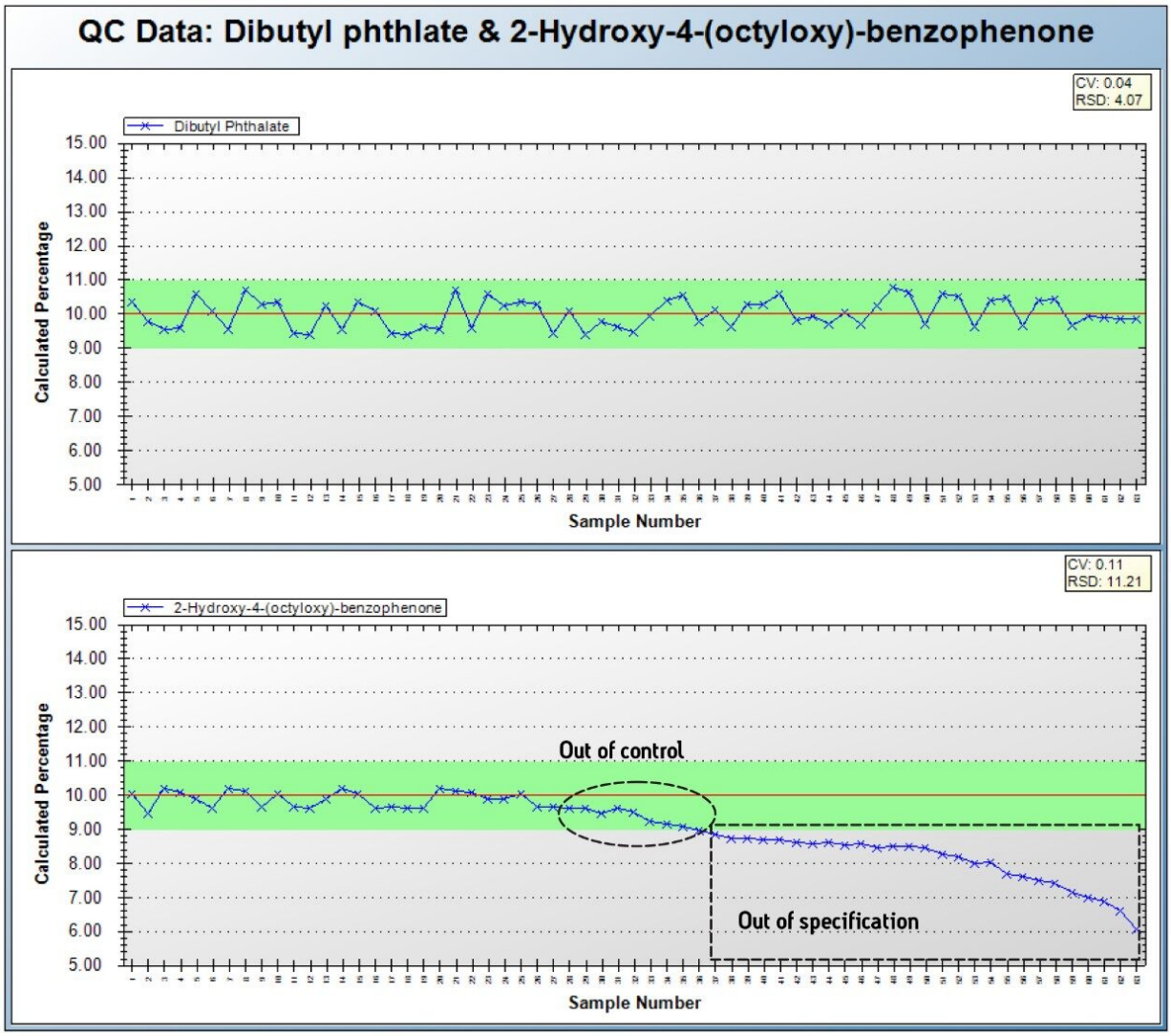

Figure 2. TrendPlot graphs showing QC data for dibutyl phthalate (DBP) and 2-hydroxy-4-(octyloxy)-benzophenone. DBP remained within specification, whereas 2-hydroxy-4-(octyloxy)-benzophenone gradually drifted out of control, leading to out of specification behavior.

We saw that DBP consistently fell within specifications. However, 2-hydroxy-4-(octyloxy)-benzophenone was initially acceptable and then gradually drifted outside specifications. This gradual change in material quality

is often difficult to detect as isolated data points.

Conclusion

TrendPlot Software within Waters' TargetLynx Application Manager was successfully used to monitor polymer additive QC data. TrendPlot Software quickly and easily plots various types of analytical data, and many different aspects of the data can be mapped. New data points can easily be added to an active graph, enabling the tracking of QC data over many months, or even years. TrendPlot offers manufacturers vital, on-going statistics about the quality of valuable raw materials and final products.

Within TrendPlot, QC data for Uvitex OB were monitored statistically using the automatically calculated SD. A single batch was rapidly identified as falling outside prescribed manufacturing specifications. Multiple additive compounds were also monitored simultaneously, and a gradual drift in material quality was observed. This flexible TrendPlot functionality for monitoring QC data offers companies invaluable time and money savings.

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