[TECHNOLOGY BRIEF]

Rapid Analysis of Complex Heterogeneous Mixtures for Active Components in Cosmetic Products

GOAL

To employ Waters® Atmospheric Solids Analysis Probe (ASAP) as a sample inlet for mass spectrometry to directly analyze heterogeneous samples and eliminate sample preparation.

BACKGROUND

Active components, such as UV absorbers are widely used in formulated personal care products, including sun block and over-the-counter facial creams. These components are constantly under examination for quality control, thermal stability or shelf life, and photochemical stability. The sample matrix is a heterogeneous complex mixture that includes components as diverse as pigments, oils, emulsions, and functional or active organic chemicals. Typical analyses of these types of materials include the use of conventional analytical tools, such as NMR, LC, or LC/MS. These techniques require time-consuming workup procedures that include precipitation, extraction, filtration, separation, and evaporation. ASAP can provide mass spectra of mixtures within seconds without sample workup, which streamlines the workflow when monitoring mixtures in targeted analysis.

Streamline your workflow when monitoring mixtures in targeted analyses with ASAP, which provides mass spectra of mixtures within seconds – no sample workup required.

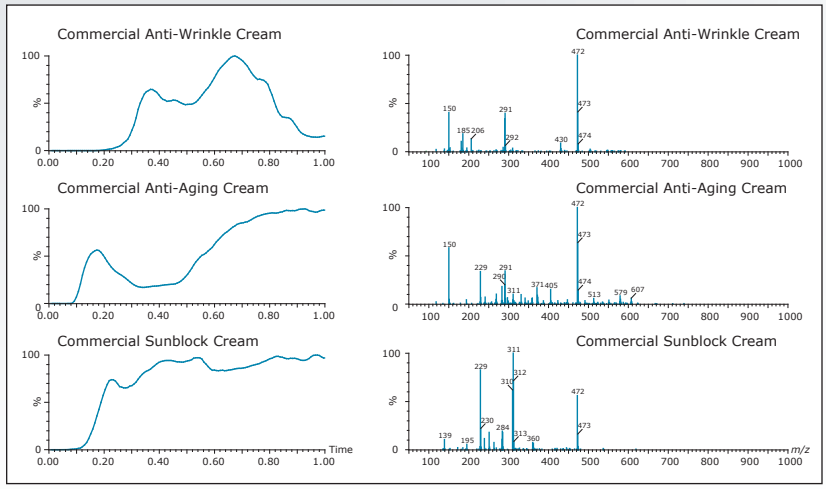

Figure 1. The complex sample spectra were recorded for the bulk sample without dilution, extraction, or any sample pre-treatment. Note that both negative and positive ionization were collected – positive ionization data are displayed.

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THE SOLUTION

A tandem quadrupole mass spectrometer with an ASAP probe was used to analyze critical components in formulated products, without the need for extensive sample preparation or isolation of the analyte from a heterogeneous matrix. The sample was loaded onto a glass tube on the probe by dipping its tip directly into the product mixture. The probe was inserted into the MS source at atmospheric pressure. Desolvation gas heated to 350 °C was used to volatilize the analytes. Mass spectra were acquired in two minutes using both APCi positive and negative mass scan modes. The targeted analytes were isolated from matrix interference based on confirmatory fragmentation.

A complex data set is displayed in the collected spectra, shown in Figure 1, which provide a summation of information from a wide array of product components. Utilizing a targeted workflow approach, an evaluation of the data set focused on expected and other typical components in the various products.

Employing a wide array of collision conditions for the target analyte list, the sample components were analyzed to determine appropriate fragmentation conditions.

Based on the collision cell conditions for each component in the target analyte list, a schedule of MRM scans was established. The samples were then reanalyzed using the ASAP sampling method, and the resulting thermal desorption chromatograms were collected, as shown in Figure 2.

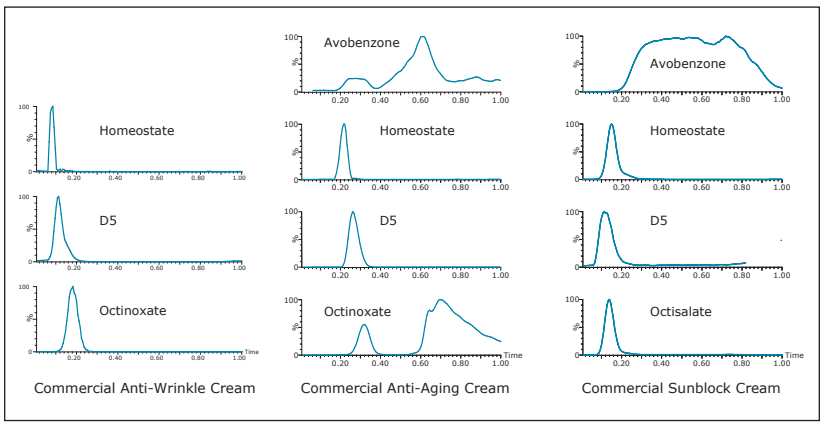

Figure 2. Thermal desorption chromatograms for the target analyte list using MS/MS data. Each thermal chromatogram was processed using a simple smoothing function to provide consistent data over the acquisition range.

Analysis of active ingredients in personal care products was routinely conducted using ASAP as a mass spectrometer inlet with a total analysis time of two minutes. This technique allowed for direct sample introduction, without the need for sample preparation. Complex sample matrix interferences were easily addressed with a targeted analysis using established fragmentation patterns produced in the collision cell, which resulted in unique analyte detection.

SUMMARY

- Using ASAP as a sample inlet for analysis of heterogeneous sample matrices allows for collection of characteristic mass spectra and analysis of relative concentration of components in a product mixture.
- This analytical approach can be used to monitor key ingredients, as well as to profile product integrity.
- ASAP can provide critical data and increased analysis capacity with minimal specialized operator training required to support researchers, as well as production operations.

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