The Analysis of Sunscreen UV Filters Agents and Preservatives

INTRODUCTION

UV filter agents and preservatives are widely used in a broad range of applications, including cosmetic and personal care products, household products, plastics, paints, and adhesives. Regulatory bodies, such as governments, have set guidelines and regulatory requirements to protect the health and safety of consumers, and to ensure product quality. The analysis of these agents is crucial to ensure compliance with FDA regulations.

METHODS

Data Acquisition and Processing:
All data were acquired and processed using Empower® 3 software for chromatography data. The Waters ACQUITY UPLC System with PDA detector was used for this analysis.

Standards:

1. 2-Phenoxyethanol [122-99-6]
2. Homosalate [118-56-9]
4. Propylparaben [94-13-3]
5. Oxybenzone [117-50-1]
6. Avobenzone [70356-09-1]
7. Octinoxate [5466-77-3]
8. Octylacate [118-80-5]
9. Homosalate [118-56-9]

UPLC conditions:

Column: BEH C18, 2.1 x 100 mm, 1.7 μm
Flow rate: 0.8 mL/min
Column temp.: 50 °C
Injection: 3 μL
Detection: PDA 251 to 500 nm
Sampling rate: 20 pts/s
Filter response: 0.1 s
Injection: 3 μL
Mobile phase A: 0.05 v% of TFA in H2O
Mobile phase B: 0.05 v% of TFA in CH3CN

Linear gradient: 5% B to 100% B in 7 min

Figure 1 shows the chemical structures of four UV filter agents (1-4) and five UV filter agents (5-9) discussed in this paper. These compounds are among the most commonly used ingredients in commercial sunscreen products in personal care and cosmetic products. A mixture of 1-9 was separated using a Waters ACQUITY UPLC System with a 2.1 x 100 mm BEH C18 Column using a seven-minute linear gradient method (5% B to 100%).

The solvents employed for the separation are common, easy to prepare and suitable for use with mass spectrometry detectors, if needed. 0.05 v% TFA in H2O (mobile phase A) and 0.05 v% TFA in CH3CN (mobile phase B).

RESULTS AND DISCUSSION

PDF-timed wavelength chromatograms were plotted using theAreas of each analyte. This can increase the detection limit when the analysis have very different limits and add quantification. Figure 2 shows an overlay of 12 replicate injections of PDF-timed wavelength chromatograms. Visual examination shows the overall reproducibility is excellent. Despite the similar structures of each chromatogram, the components are well resolved by the 7-minute linear gradient method. Two impurities in the mixture that previously co-eluted are now separated.

Peak 10 is an unknown impurity in the acetate (6 standard) whereas peak 11 is aomer of homosalate (9). The Empower 3 report table in Figure 2 shows the % RSD ranges from 0.02% to 0.04%. Retention time reproducibility is a good indicator of the robustness and suitability of UPLC with BDD column chemistry for preservatives and sunscreens.

To confirm peak identities and provide assurance regarding spectral peak purity or “non-convolution” a user can build a PDF library and perform library matching and peak purity analysis through Empower 3 Software.

Figure 3 shows (a) spectra extracted from PDF chromatograms of standards (1-9) that were used to create a library with names, concentrations, and retention times.

Empower 3 uses Spectral Contrast theory to quantitatively compare the shapes of UV spectra during library matching and peak purity analysis. The match angle or purity angle indicates how closely the spectra overlap. A spectral contrast angle of 0° means that the spectra perfectly match and the compounds these spectra represent are identical; a 90° angle means that the two spectra do not overlap and that the compounds are different.

The Threshold Angles are an indicator of “uncertainty” or non-identities. If the Match or Purity (Spectral Contrast) Angle is less than the Match or Purity Threshold Angle, this indicates that the differences between the spectra are non-identities and the match is “good” or the peak is spectrally pure.

CONCLUSION

The Waters ACQUITY UPLC System with PDA Detection and Empower 3 Software provide sensitive, baseline resolved, rapid separations with automated library matching.

This has been demonstrated with a rapid, reproducible separation of a mixture of nine of the most commonly used organic sunscreen and biocides in cosmetics and personal care products.

The easy-to-use experimental conditions are suitable for raw material suppliers, cosmetics, and personal care product formulators.

Applications include quality control, new product development, and troubleshooting.

References