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Application News

High Performance Liquid Chromatograph Mass Spectrometer LCMS-2050

Simple Screening Analysis of Detergent Using a Single Quadrupole Mass Spectrometer

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User Benefits

- Simple screening analysis of the components included in detergents such as surfactants can be performed with a single quadrupole LC-MS.
- Because of the direct injection by flow injection, high throughput analysis (1 min/1 sample) can be achieved.
- By performing multivariate analysis of the mass spectra obtained using eMSTAT Solution™, the characteristic components can be easily found.

■ Introduction

Detergents like dishwashing detergents contain various components such as surfactants. In order to develop detergents that have greater detergency and are skin-friendly, it is necessary to select the appropriate type and quantity of surfactants. Therefore, for the development and manufacture of detergents, it is extremely important to understand the information on the components included in the detergents. Also, dishwashing detergents are often mixed into beverages and foods. So detailed analysis and rapid screening of dishwashing detergents are important for foreign matter inspection.

This Application News describes a method using flow injection and a single quadrupole LC-MS for simple screening of the components in dishwashing detergents. Because samples are injected by flow injection, high throughput analysis is possible and useful for multi-sample analysis. When the sample volume is small, a probe electrospray ionization mass spectrometer, as introduced in Application News No. B118, is useful. Even several µL of a sample can be analyzed.

■ Samples and Pretreatment

Seven types of commercial dishwashing detergent were analyzed. In the sample pretreatment, each sample was diluted 1,000-fold with an aqueous solution of 70 % methanol. At dilution, 30 ppm of reserpine and chloramphenicol were added as internal standards.

■ Instruments and Analytical Conditions

The analysis was performed using a system combining the Nexera™ series and the LCMS-2050, as shown in Fig. 1. The LCMS-2050 single quadrupole mass spectrometer is compact, but it affords excellent ease of use and performance.

Fig. 1 Nexera™ and LCMS-2050 System

Normally, direct injection of samples by flow injection without a column can contaminate the mass spectrometer easily. However, the LCMS-2050 is highly robust, and even if it is contaminated, it is easily maintained, so it is suitable for flow injection analysis. The analytical conditions are shown in Table 1.

Table 1 Analytical Conditions

[Flow Injection Conditions] (Nexera XR)	
Flowrate:	0.1 mL/min (0 min)→0.05 mL/min (0.1 min) →0.1 mL/min (0.65 min) →1 mL/min (1 min)
Mobile Phase:	Water / Methanol = 30:70
Injection Volume:	1 µL
[MS Conditions] (LCMS-2050)	
Ionization:	ESI/APCI (DUIS™), Positive and Negative mode
Mode:	Scan (*m/z* 50-2000)
Interface Voltage:	+3.0 kV / -2.0 kV
Nebulizing Gas Flow:	2.0 L/min
Drying Gas Flow:	5.0 L/min
Heating Gas Flow:	7.0 L/min
Desolvation Temp.:	450 °C
DL Temp.:	200 °C

■ Data Analysis

The mass spectrum data obtained were converted into JCAMP format in LabSolutions™ LCMS, and multivariate analysis was performed using eMSTAT Solution. eMSTAT Solution includes statistical analysis mode and discriminant analysis mode, and even those who are not familiar with statistical analysis can easily perform data analysis in accordance with the purpose (Fig. 2). Each sample was analyzed five times to prepare datasets for multivariate analysis. The mass spectrum data obtained by positive mode and negative mode were corrected using reserpine and chloramphenicol, respectively.

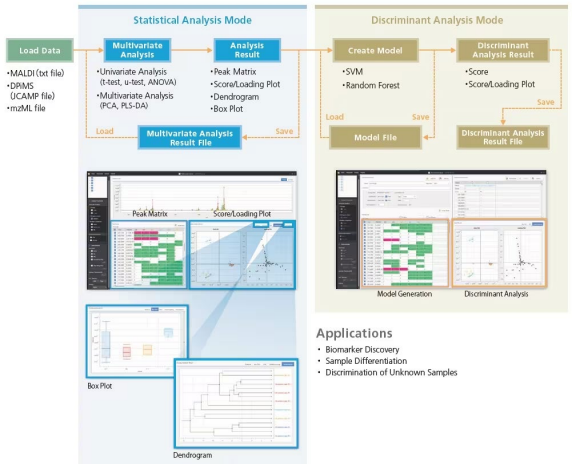

Fig. 2 eMSTAT Solution™ Work Flow

■ Simple Screening Analysis

As a result of analyzing seven types of dishwashing detergent, 263 peaks (maximum *m/z* 1390.49) were detected in positive mode, and 171 peaks (maximum *m/z* 802.36) were detected in negative mode. The results of principal component analysis (PCA) on the data obtained in positive mode are shown in Fig. 3. From the viewpoint of the first principal component in the score plot, dishwashing detergents A-D were classified on the left and dishwashing detergents E-G on the right. From the viewpoint of the second principal component, dishwashing detergents A-D were classified into different classes. On the other hand, dishwashing detergents E-G were plotted in close positions and showed similar trends.

From the product information of dishwashing detergents, the peak at *m/z* 163.28 which was characteristic of dishwashing detergent A is considered to be butyl carbitol (stabilizing agent). The peak at *m/z* 230.32 which was characteristic of dishwashing detergents B-D is considered to be alkylamine oxide (C12, amphoteric surfactant). On the right side of the loading plot, many peaks with 44 Da intervals such as *m/z* 649.53, 693.48, 737.51, and 781.52 were observed.

Fig. 4 shows the mass spectrum of dishwashing detergent G. A characteristic mass spectrum with peaks at 44 Da intervals was observed. From the product information of dishwashing detergent G, it is considered that these peaks were from a polyoxyethylene alkyl ether (nonionic surfactant).

■ Conclusion

This Application News describes an example of a simple screening analysis of dishwashing detergent using a single quadrupole LC-MS. By statistically analyzing the mass spectrum data obtained, it was possible to classify each dishwashing detergent and identify its characteristic components. Since the sample is injected by flow injection, the throughput of this method is high (1 min/1 sample), allowing rapid analysis of a large number of samples. Therefore, this method is useful for the screening analysis of detergents in product development and foreign matter inspection.

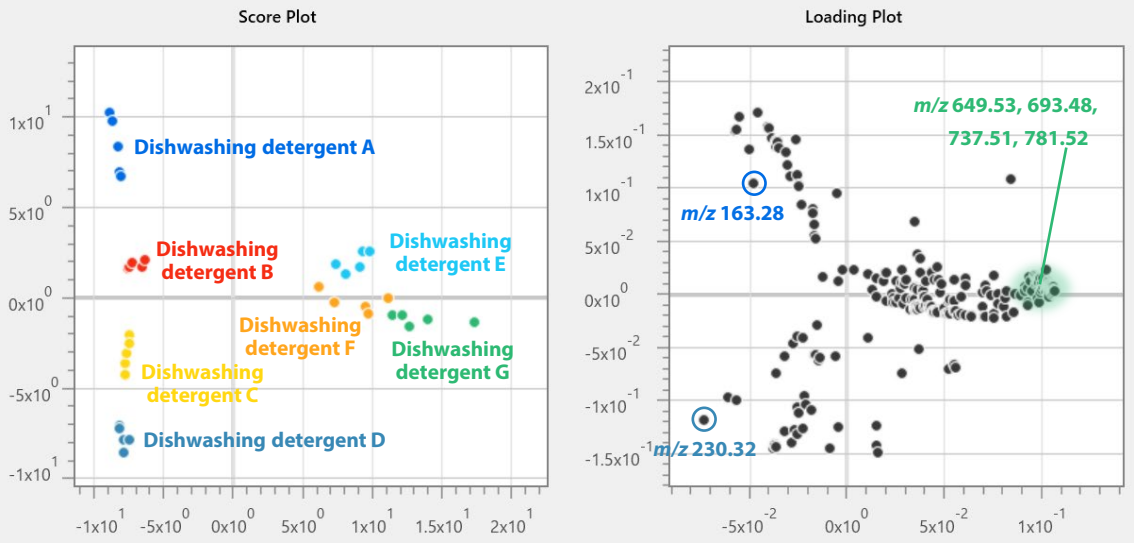

Fig. 3 PCA Results (Positive Mode)

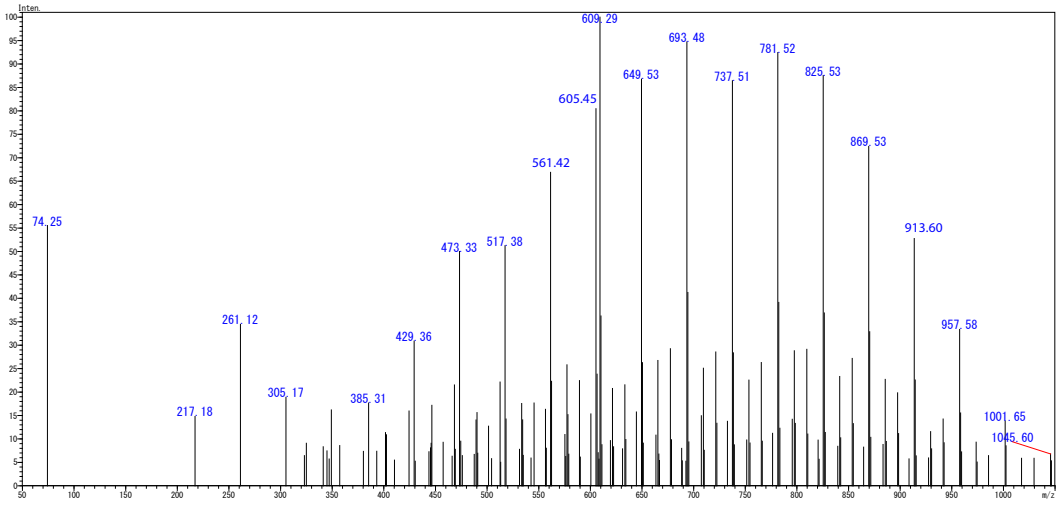

Fig. 4 Mass Spectrum of Dishwashing Detergent G (Positive Mode)

<Related Application News>

1. Analysis of Contaminated Samples by DPiMS-2020 (1): Detection of Surfactants in Beverages Application News No.B118

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