

Application News

No.A461

Spectrophotometric Analysis

Classification and Profiling of Food Containers by Principal Component Analysis with Their UV-Visible-NIR Spectra

There are various types of containers for foods and beverages, but aside from their fundamental purpose of "containing" these items, they also play a role in protecting the food contents from such influences as the external atmosphere, light, etc. With respect to protection from light, for example, it is important to evaluate their effectiveness as a UV barrier. Here, we investigated the transmittance of ultraviolet to near-infrared light in polyethylene terephthalate (PET) bottles used primarily as containers for soft drinks such as juice and tea. The results of measurement using 14 types of PET bottles indicated a difference in transmittance between the ultraviolet and near-infrared regions. Further, by applying multivariate analysis using principal component analysis to the measurement, it was possible to classify the bottles on a two-dimensional graph. Further, a comparison of the results obtained from the same measurement using polystyrene food containers with those of the PET bottles indicated a large difference in transmittance. This paper introduces the results of this analysis.

■ Samples and Results of Measurement

Using the SolidSpec-3700DUV UV-VIS-NIR spectrophotometer, measurements were conducted on 8 juice, 3 tea, and 3 mineral water PET bottle samples, respectively, for a total of fourteen points of measurement (A-N). The samples, cut to several centimeters square using a cutter, were measured using an integrating sphere. Fig. 1 shows an image of a sample mounted in the integrating sphere, and the measurement results are shown in 2 separate groups in Fig. 2 and Fig. 3. The measurement conditions are shown in Table 1. In cases where a separate film had been pasted onto the PET surface, the film was peeled away from the target measurement site.

An overview of the spectra reveals few differences in the visible region, while the differences are more pronounced in the ultraviolet and near-infrared regions. It is believed that this variation might be attributable to factors such as different additives and thickness, with differences in thickness likely having a large effect. The thicknesses of the PET bottles measured with a caliper (0.05 mm units) and their original contents are shown, respectively, in Table 2. The spectra in the ultraviolet region (250 nm - 500 nm) of Fig. 2 and Fig. 3 are shown in expanded views in Fig. 4 and Fig. 5, respectively, and those spectra in the near-infrared region (1600 - 2400 nm) are shown expanded in Fig. 6 and Fig. 7, respectively. Comparing Table 2 and Fig. 4 - Fig. 7, it is clear that the thicker the sample the lower the transmittance, and the thinner the sample the higher the transmittance. Notably, the thickest sample, Sample E with a 0.55 mm thickness, showed the lowest transmittance overall, and the thinnest sample, Sample N with a 0.10 mm thickness, showed the highest transmittance.

Ultraviolet rays accelerate the degradation of food, and near-infrared rays have a heating effect. On the other hand, visible light is associated with the "appearance" or "look" of substances in containers. A difference in transmittance

between the ultraviolet and near-infrared regions was seen in the 14 types of PET bottles subjected to measurement, while there was not much difference in the results associated with the visible region.

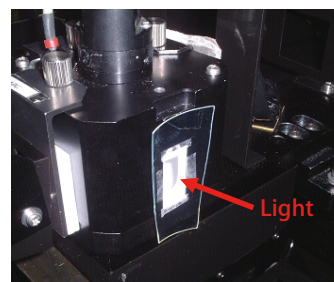


Fig. 1 Photograph of Sample Mounted in Integrating Sphere

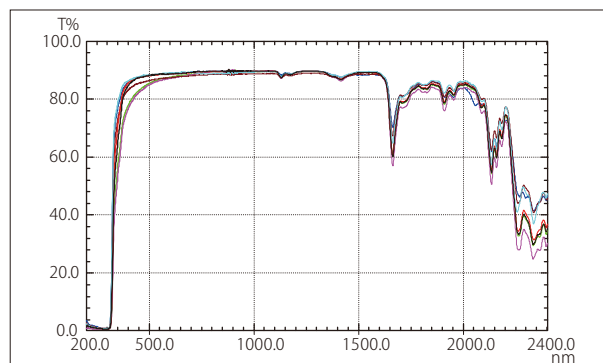


Fig. 2 Transmittance Spectra of Samples A to G
(Red: A, Blue: B, Green: C, Black: D, Red Purple: E, Brown: F, Light Blue: G)

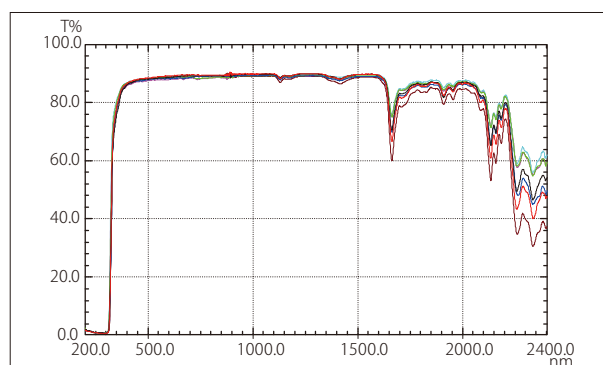


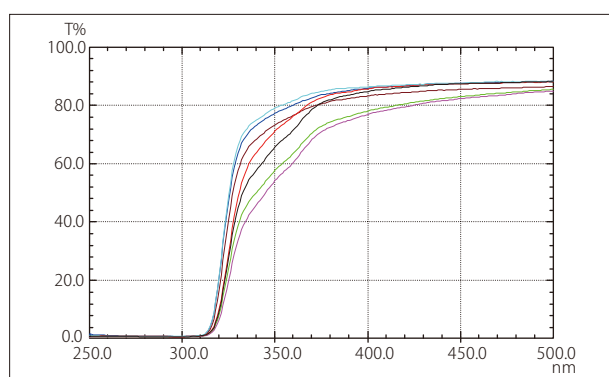
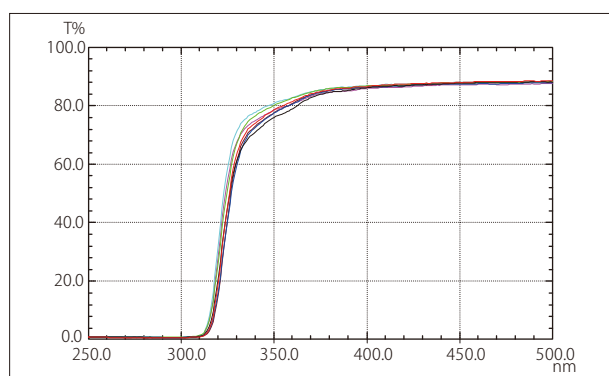
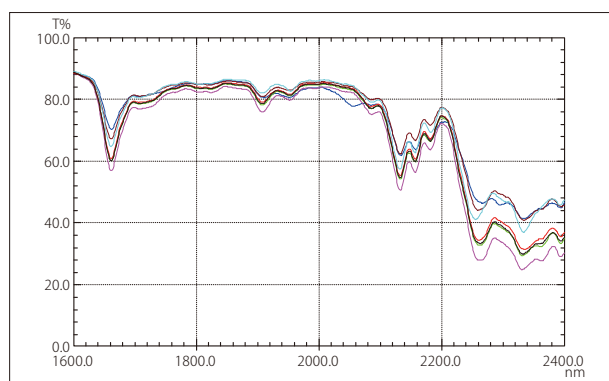
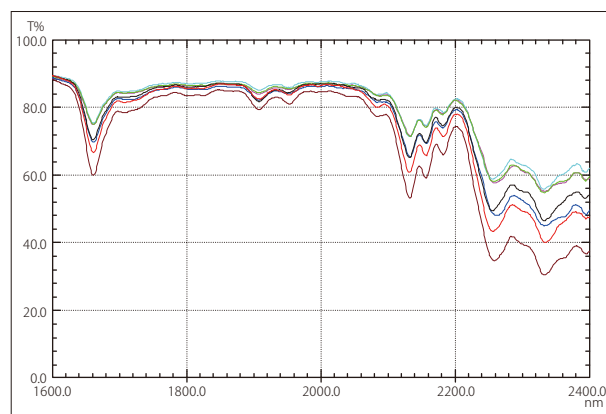
Fig. 3 Transmittance Spectra of Samples H to N
(Red: H, Blue: I, Green: J, Black: K, Red Purple: L, Brown: M, Light Blue: N)

Table 1 Analytical Conditions

Instrument	: Shimadzu SolidSpec-3700DUV UV-VIS-NIR spectrophotometer
Measurement wavelength range	: 200 nm to 2400 nm
Scan speed	: Medium
Sampling pitch	: 1.0 nm
Photometric value	: Transmittance
Slit width	: (12) nm
Detector switching wavelengths	: 870 nm, 1650 nm

Table 2 Thickness of PET Samples

Sample Name	Thickness (mm)
A (juice type)	0.40
B (juice type)	0.30
C (juice type)	0.50
D (juice type)	0.35
E (juice type)	0.55
F (juice type)	0.25
G (juice type)	0.40
H (juice type)	0.35
I (green tea)	0.25
J (green tea)	0.15
K (green tea)	0.35
L (mineral water)	0.15
M (mineral water)	0.35
N (mineral water)	0.10


Fig. 4 Expanded Spectra of Fig. 2 (Ultraviolet Region)
(Red: A, Blue: B, Green: C, Black: D, Red Purple: E, Brown: F, Light Blue: G)

Fig. 5 Expanded Spectra of Fig. 3 (Ultraviolet Region)
(Red: H, Blue: I, Green: J, Black: K, Red Purple: L, Brown: M, Light Blue: N)

Fig. 6 Expanded Spectra of Fig. 2 (Near-Infrared Region)
(Red: A, Blue: B, Green: C, Black: D, Red Purple: E, Brown: F, Light Blue: G)

Fig. 7 Expanded Spectra of Fig. 3 (Near-Infrared Region)
(Red: H, Blue: I, Green: J, Black: K, Red Purple: L, Brown: M, Light Blue: N)

■ Classification and Profiling of PET Bottles by Principal Component Analysis

We attempted to classify and conduct variance analysis of the above 14 PET points using Principal Component Analysis (PCA)¹⁾. Fig. 8 shows a scores plot²⁾ of the first principal component (PC-1) plotted along the horizontal axis, and the second principal component (PC-2) plotted along the vertical axis. In the scores plot, the closer the points are to one another, the more similar are the samples. For example, samples C and E, and samples J, L and N can be considered similar to one another, respectively. The spectra of samples C and E are shown in Fig. 9, and those of samples J, L and N are shown in Fig. 10. The spectra in the respective groups are clearly similar.

Fig. 11 shows a loadings plot³⁾. Viewing the loadings plot makes it easy to grasp the characteristics of the sample points on the scores plot. It is clear that the loading vector³⁾ components corresponding to nearly all the wavelength data plotted along the horizontal axis (1st principal component axis) from the center to the right are plotted as positive values. That indicates that the further to the right the samples are positioned in the scores plot of Fig. 8, the higher the transmittance will be overall, and that can be confirmed by looking at Fig. 12, which shows the spectra of samples J, L and N plotted to the right in Fig. 8 and samples C and E which are plotted to the left.

On the other hand, looking at the vertical axis (2nd principal component axis) of Fig. 11, the loading vector components corresponding primarily to the wavelengths of the ultraviolet region data are plotted with large positive values. That indicates that the further upward the samples are positioned in the scores plot of Fig. 8, the higher will be the transmittance in the ultraviolet region, and that can be confirmed by looking at Fig. 13, which shows the spectra of samples M and G plotted in the upper region and samples C and E which are plotted in the lower region. Thus, by using Principal Component Analysis, a large number of samples can be represented on a 2-axis graph consisting of characteristic axes (principal component axes).

Furthermore, we will also describe the use of a vertical axis for a third principal component that captured another characteristic. Fig. 14 is a scores plot with a horizontal axis for the first principal component, and a vertical axis for a third principal component. Only B is plotted in an upward isolated manner. This suggests that B has some characteristic that sets it apart from the other samples. Looking at Fig. 15 and its expanded version Fig. 16, which compare B with A, K and N, it is apparent that the shape of the spectrum of B in the near-infrared region is different from those of the other samples. The shape of B in the wavelength vicinities indicated with the red arrows is noticeably different from the others. The fact that this difference was detected in the scores plot suggested that some type of additive, etc. had been added to the PET of sample B. Using principal component analysis, it is possible to find a sample having features and characteristics that are quite different from those among a large number of samples.

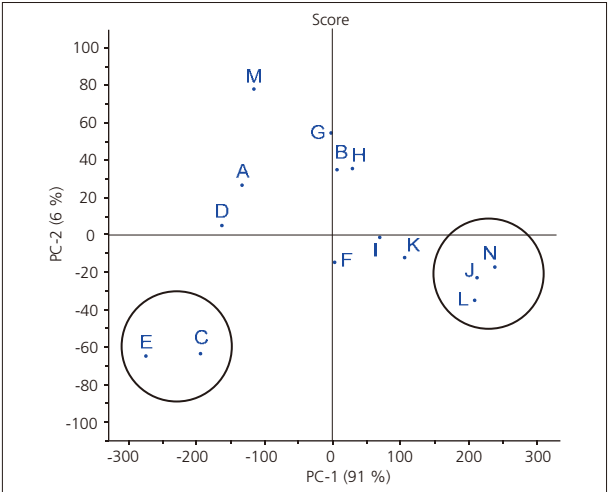


Fig. 8 Scores Plot

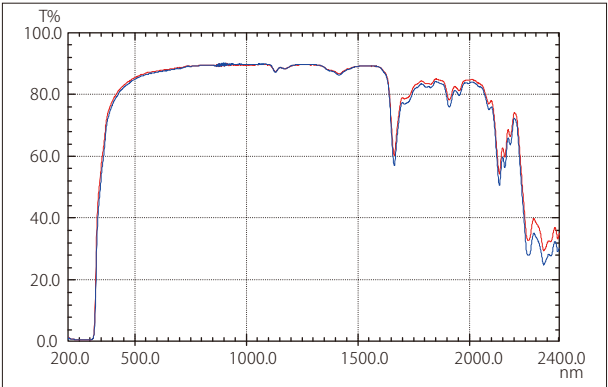


Fig. 9 Spectra of C and E (Red: C, Blue: E)

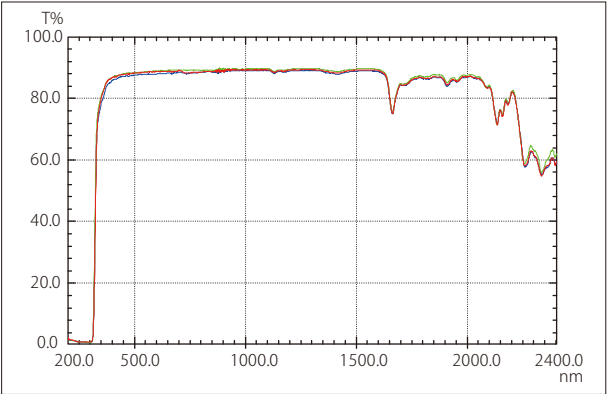


Fig. 10 Spectra of J, L and N (Red: J, Blue: L, Green: N)

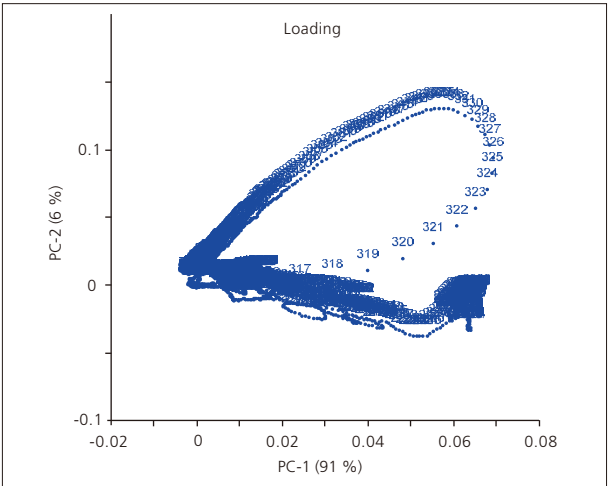


Fig. 11 Loadings Plot (Upper) Loading

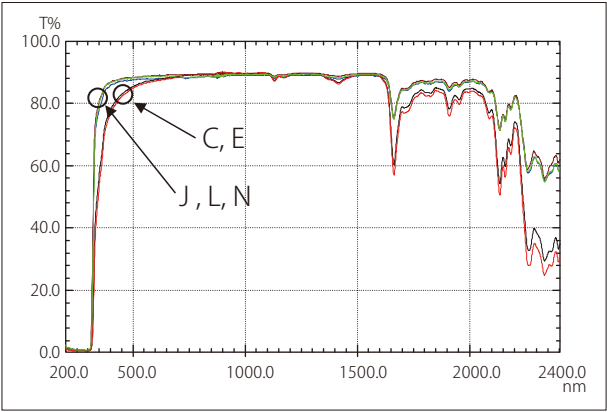


Fig. 12 Spectra for J, L and N Group and C and E Group

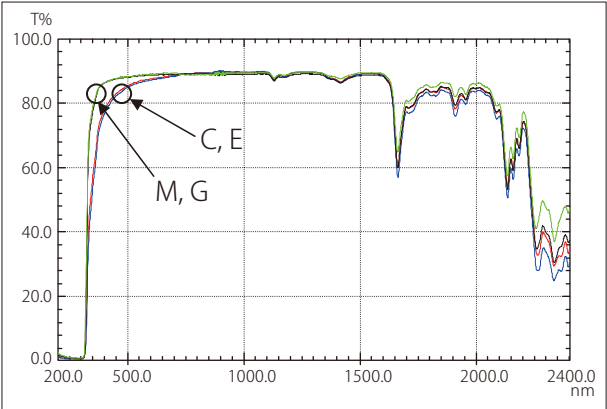


Fig. 13 Spectra for M and G Group and C and E Group

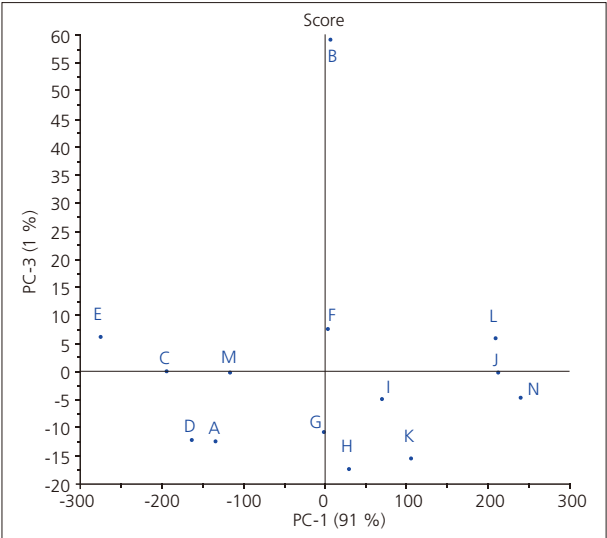


Fig. 14 Scores Plot (Upper) Score

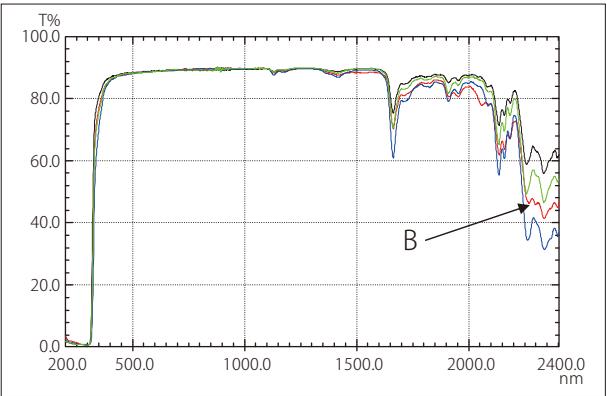


Fig. 15 Spectra for B and Group of A, K and N (Red: B, Blue: A, Green: K, Black: N)

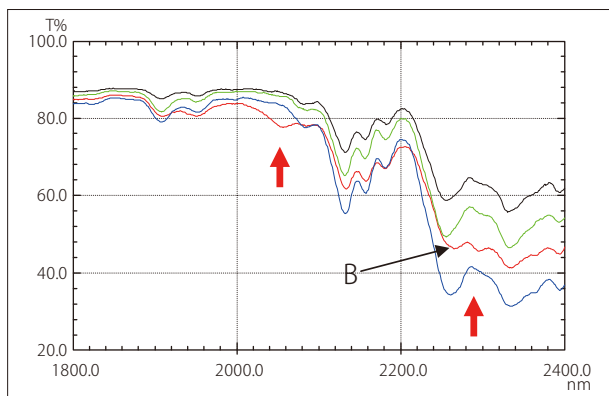


Fig. 16 Spectra for B and Group of A, K and N
(Red: B, Blue: A, Green: K, Black: N)

■ Comparison of Polystyrene Containers and PET Bottles

We conducted a comparison of polystyrene (abbreviated below as PS) containers and PET bottles. The transparent PS measurement samples consisted of a lid used for a "cup soup" container (sample (1)), and the cover (sample (2)) of a food pack. The sample thicknesses, measured with a caliper, are shown in Table 3, and the measurement results are shown in Fig. 17. Fig. 17 presents a comparison of the PS samples with the PET samples A, K and N, and clearly indicates a great difference in the spectra of these two materials. Fig. 18 and Fig. 19 show expanded sections of ultraviolet region from 250 to 500 nm and the near-infrared region from 1600 to 2400 nm, respectively. PS clearly exhibits greater transmittance in the ultraviolet region than PET, and even greater transmittance in the near-infrared region above 1600 nm.

Table 3 Thickness of PS Samples

Sample Name	Thickness (mm)
(1)	0.30
(2)	0.10

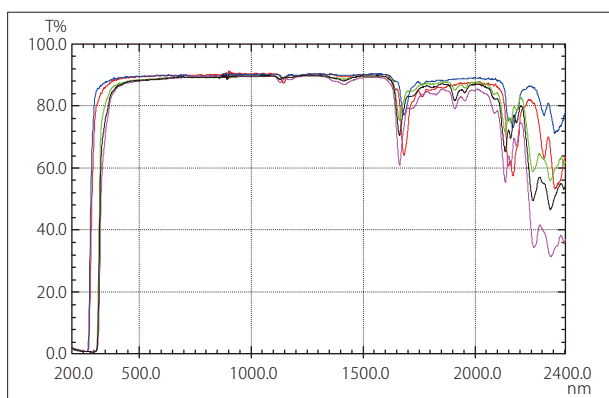


Fig. 17 Comparison Between Spectra of PS Samples and PET Samples
(Red: PS (1), Blue: PS (2), Reddish Purple: A (PET), Black: K (PET), Green: N (PET))

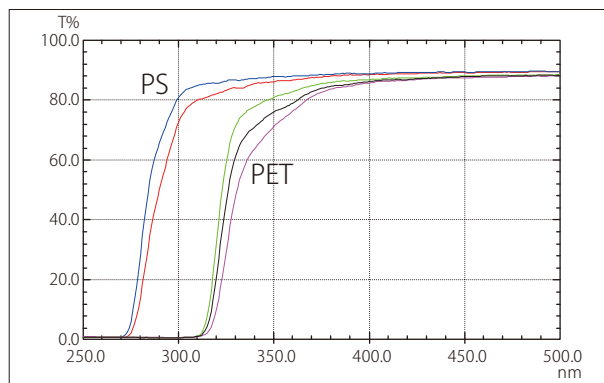


Fig. 18 Expanded Spectra of Fig. 17 (Ultraviolet Region) (Red: PS (1), Blue: PS (2), Reddish Purple: A (PET), Black: K (PET), Green: N (PET))

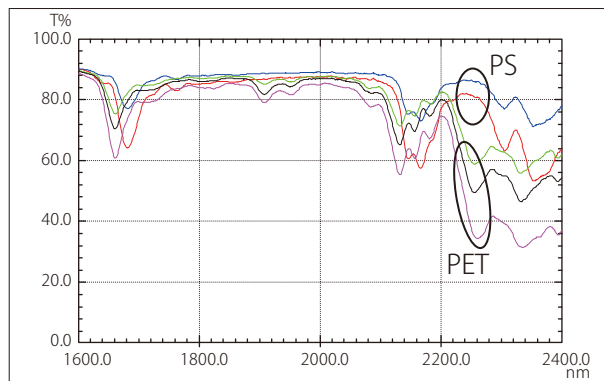


Fig. 19 Expanded Spectra of Fig. 17 (Near-Infrared Region) (Red: PS (1), Blue: PS (2), Reddish Purple: A (PET), Black: K (PET), Green: N (PET))

■ Conclusion

Results obtained from measurement of a large number of PET bottles indicated that there are differences in the transmittance of ultraviolet and near-infrared radiation. Since infrared radiation accelerates the degradation of food products, and near-infrared radiation has a heating effect, it is important from the standpoint of protecting food contents that transmittance of these types of radiation be understood. The transmittance of visible light can be associated with the "appearance" or "look" of substances in containers, but this did not appear to present a significant difference in any of the samples. By applying multivariate analysis using principal component analysis to the measurement results, we were able to classify the PET bottles from the standpoint of transmittance, and further, we were able to find one sample which displayed a unique spectral pattern. In addition, as a result of comparing the polystyrene containers with the PET bottles, polystyrene was found to permit greater transmittance of both ultraviolet and near-infrared light. By combining spectroscopy with multivariate analysis, it is possible to evaluate food containers from various perspectives.

- 1) The calculations were conducted using the Unscrambler® multivariate analysis software. The Unscrambler® is a trademark or registered trademark of CAMO Software. Regarding the analysis shown here, principle component analysis was conducted using mean-centering.
- 2) A scores plot is a 2-dimensional graphic representation of each sample point projected on two loading vectors expressed in multidimensional space. For more on "loading vector" refer to Note 3 below.
- 3) A loadings plot is obtained by plotting the components corresponding to each loadings vector of the first principal component and second principal component (or a combination of other principal components) using two-dimensional coordinates. Here, the loadings vector is obtained by calculating the eigenvalues of the data matrix

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