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Application News

No. A535

Spectrophotometric Analysis

Taking Advantage of the Contaminant Library

Accuracy and speed are necessary when determining the cause of contaminants. There are many causes of contamination that lead to complaints, such as contamination originating from a company's own production line to consumers inadvertently introducing contaminants themselves, and therefore contaminant analysis requires considerable knowledge and experience.

This article introduces an example of contaminant analysis using a contaminant library that consolidates Shimadzu's experience and analysis know-how.

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Contaminant Library Overview

The contaminant library can be used in the same way as the standard library by adding it as an option to the LabSolutions IR software, which performs instrument control and data analysis on Shimadzu's FTIR instruments. Unlike commercially-available libraries that only contain data on single components, this contaminant library contains as many as 485 entries including mixtures such as actually collected contaminants (provided by water supply and food companies) and gaskets, and therefore achieves a remarkably improved search accuracy. Furthermore, while conventional contaminant libraries have only provided notation of component names, which made identifying the source of contaminants difficult, this library employs notation that allows inference of contamination sources.

In addition to infrared spectra obtained through measurement using a single reflection ATR attachment, the contaminant library contains detailed information including sample images, major elements, color, shape, hardness, and metallic luster. Since all included samples have also undergone EDX analysis, the corresponding EDX profile database can be viewed as a PDF file for samples that appear in the contaminant library search results. This contains the qualitative profile and quantitative analysis results.

Example of Contaminant Analysis

FTIR analysis was performed on contaminant 1 detected on a production line. Table 1 lists the instruments and analysis conditions. Fig. 1 shows the measurement result and search result from the contaminant library. With the top search result being bone particle, the contaminant was considered a mixture of calcium phosphate and protein. The peak around 1750 cm^{-1} (C=O group derivative) present in contaminant 1 can be considered to be due to the influence of cooking oil.

Fig. 2 shows the EDX profile database of bone particle, which was indicated in the library search result. Performing EDX analysis enabled verification of the presence of Ca and P, which are the main components of bone. Since this corroborates the FTIR analysis results, this example demonstrates the benefits of analysis using both FTIR and EDX instruments.

Table 1 Instruments and Analysis Conditions

Instruments	:	IRAffinity-1S, MIRacle10 (Diamond prism)
Resolution	:	4 cm^{-1}
Accumulation	:	40
Apodization	:	Happ-Genzel
Detector	:	DLATGS

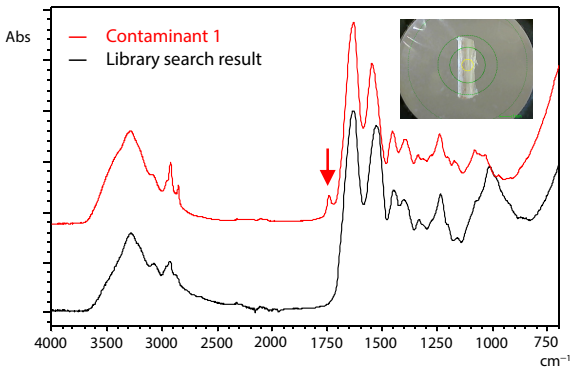


Fig. 1 Measurement Result and Search Result of Contaminant 1

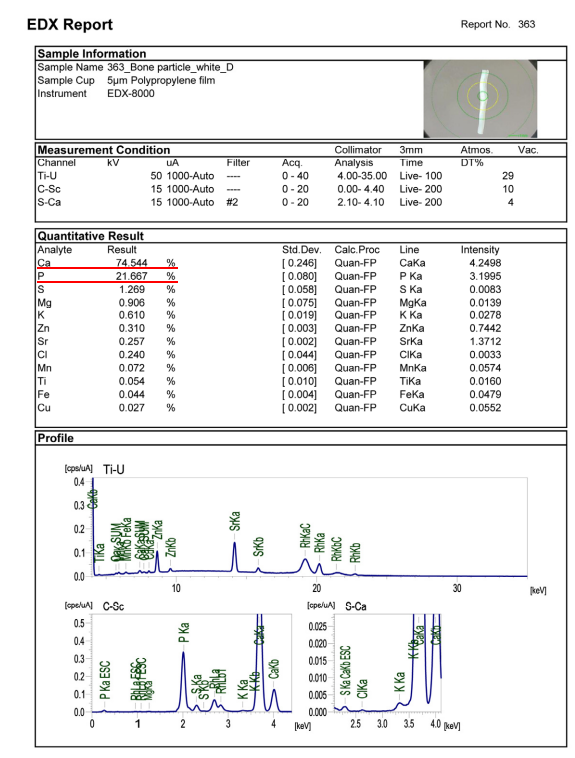
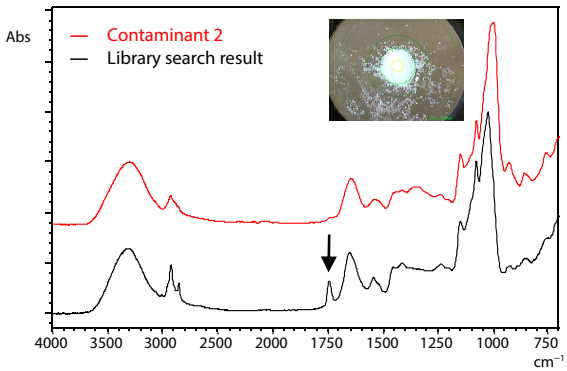


Fig. 2 EDX Profile Database of "Bone Particle"

Next, FTIR analysis was performed on contaminant 2 that was detected on a food production line. Fig. 3 shows the measurement result and the search result from the contaminant library. The top search result was a cluster of starch. While this contains starch, cooking oil, and protein, since the peak around 1750 cm^{-1} (C=O group derivative) is hardly visible in contaminant 2 we can deduce that even if cooking oil was present in the contaminant, it would be minute.
Fig. 4 shows the EDX profile database of the cluster of starch that was indicated in the library search result. While salt (NaCl) was detected in the database, presumably from Na and Cl contained in food, almost no metallic elements were detected in contaminant 2.
This leads to the possibility that contaminant 2 is an ingredient whose main components are starch and protein.
Lastly, Table 2 lists an example of data in the contaminant library.



Library information: Cluster of starch Materials; Starch, Cooking oil (Triacylglycerol), Protein Major elements; Cl, Na Color; Brown Shape; Cluster Hardness; Hard Metallic luster; No Technique; ATR (Ge)

Fig. 3 Measurement Result and Search Result of Contaminant 2

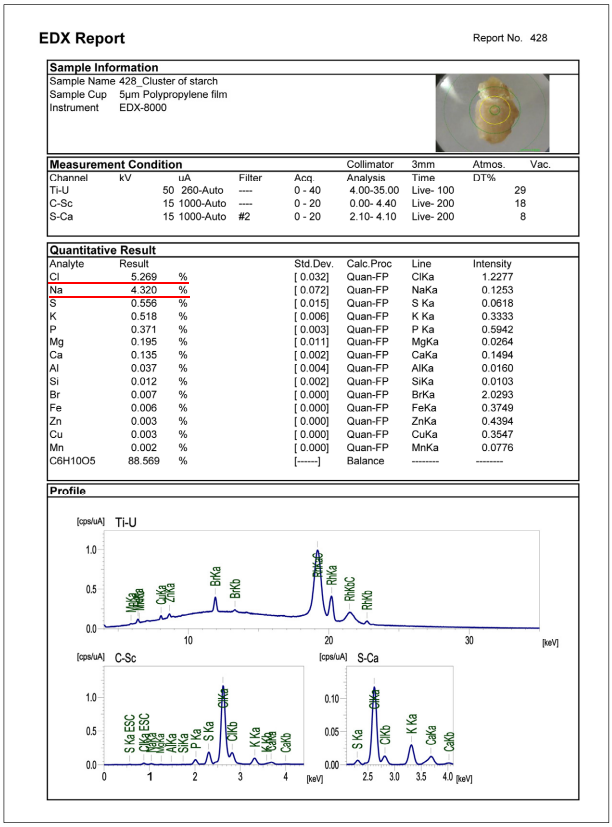


Fig. 4 EDX Profile Database of "Cluster of starch"

Conclusion

While the data included in this library is useful for contaminant analysis since it contains the analysis results of actual contaminants, even higher accuracy in analysis can be achieved through the accumulation of samples detected as contaminants in a custom user library.
The EDX-FTIR contaminant finder/material inspector software, EDXIR-Analysis, which was released in 2016, contains data files of both FTIR and EDX analyses enabling integrated analysis using both data types. As demonstrated in the example of contaminant 1, in some cases performing EDX analysis may provide useful information for contaminant samples that prove difficult to identify with FTIR analysis alone. In contaminant analysis, a multifaceted approach which covers both organic and inorganic contaminants is very effective. For details, refer to Application News No. A522A.

Table 2 Example of Data in the Contaminant Library

	Name	Comment
Water Supply-Related Contaminants	Pipe slip packing	Pipe slip packing Materials; Polyethylene (PE) Major elements; below 1% Color; Black Shape; Resin/Ring Hardness; Hard Metallic luster; No Technique; ATR (Ge)
	Sealing tape	Sealing tape Materials; Polytetrafluoroethylene (PTFE) Major elements; F Color; White Shape; Film Hardness; Soft Metallic luster; No Technique; ATR (Ge)
	Coating of inner wall_1	Coating of inner wall_1 Materials; Polystyrene (PS), Acrylic resin Major elements; Cl Color; Brown Shape; Fragment Hardness; Soft Metallic luster; No Technique; ATR (Ge)
	Mold	Mold Materials; Protein, Silicate Major elements; below 1% Color; Brown Shape; Mold Hardness; Soft Metallic luster; No Technique; ATR (Ge)
	Coating in pump_white	Coating in pump_white Materials; Polyamide (Nylon 11), Titanium dioxide (TiO_2) Major elements; Ti, Na Color; White Shape; Scraping Hardness; Brittle Metallic luster; No Technique; ATR (Ge)
Food-Related Contaminants	Piece of plant material	Piece of plant material Materials; Plant epidermis (Cellulose), Vegetable fat (Triacylglycerol) Major elements; Cl, Na Color; Brown Shape; Cluster Hardness; Soft Metallic luster; No Technique; ATR (Ge)
	White hair	White hair Materials; Human hair (Protein) Major elements; S Color; White Shape; Fiber Hardness; Soft Metallic luster; No Technique; ATR (Ge)
	Nail	Nail Materials; Nail (Keratin) Major elements; S Color; White Shape; Fragment Hardness; Hard Metallic luster; No Technique; ATR (Ge)
	Bone particle_brown	Bone particle_brown Materials; Bone particle (Calcium phosphate, Protein) Major elements; Ca, P, Mg Color; Brown Shape; Stick Hardness; Hard Metallic luster; No Technique; ATR (Ge)
	Stapler1	Stapler1 Materials; Zinc stearate (Adsorbate on metal surface) Major elements; Fe, P Color; Black Shape; Stick Hardness; Hard Metallic luster; Yes Technique; ATR (Ge)
	Glass fragment	Glass fragment Materials; Glass (SiO_2) Major elements; Pb, Si, K, Na, Zn Color; Transparency Shape; Cluster Hardness; Hard Metallic luster; No Technique; ATR (Ge)
	Stainless steel_1	Stainless steel_1 Materials; Unidentified (Adsorbate on metal surface) Major elements; Fe, Cr, Ni, Mn Color; Silver Shape; Metal Hardness; Hard Metallic luster; Yes Technique; ATR (Ge)

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