

# Application News

## No. A454

### Spectrophotometric Analysis

## Identification Test for D-Galactose and Xylitol Using the Pharma Report Program

- Program for Identification Test, Acceptance Check and Pre-Shipment Check -

The Pharma Report program, a module of the LabsolutionsIR software, makes it easier than ever to conduct all operations using a single click and to view all related information on a single screen. This program is intended for simple identification testing of samples according to procedures specified in the Japanese Pharmacopoeia. As a test method, it provides three critical reporting functions: peak detection, spectral output and report generation. Here, we introduce measurement examples of D-galactose and xylitol as described in the Japanese Pharmacopoeia.

In addition to the samples described in the Japanese Pharmacopoeia, by specifying a characteristic peak of interest, this test can be utilized for pre-shipment inspection and product acceptance of raw materials in the fields of medicine, foods and chemicals, etc.

### Pharma Report Program

The sixteenth edition of the Japanese Pharmacopoeia specifies that regarding identification of a substance, when the spectrum of a specimen and the Reference Spectrum of the substance expected to be found or the spectrum of the Reference Standard exhibit similar intensities of absorption at the same wavenumbers, the specimen can be identified as being the substance expected to be found. Because the test method is programmed to accomplish each specified procedure separately, for example, comparison of a spectrum with that of a standard or identification of a peak at a specified wavelength, the three functional approaches included in the software are selected depending on the final test objective.

- Peak detection
- Spectrum output
- Report generation

The operation flow of the Pharma Report Program is shown in the flowchart of Fig. 1.

First, sample information is entered (or edited) for the identification test to be conducted using the [Edit Comp.] button in the window shown in Fig. 2. Here, up to 20 samples can be entered. The advanced settings for each sample are entered using the window shown in Fig. 3. Information, including the name of each component, the test method, measurement conditions, standard spectrum, in addition to the reference wavenumber and permissible error values are entered prior to starting the analysis.

The program is started by clicking the component name button as shown in Fig. 2. Then, selection is made to either load the measured infrared spectrum or conduct measurement of an infrared spectrum followed by the specified testing procedure. Finally, a data printout is generated according to the three test methods selected in advance.

The conventional method of spectrum confirmation required as much as 10 minutes for analysis, depending on the sample. Using this program, however, the analysis results can be obtained very quickly, often within 1 to 3 minutes when the sample is registered beforehand.

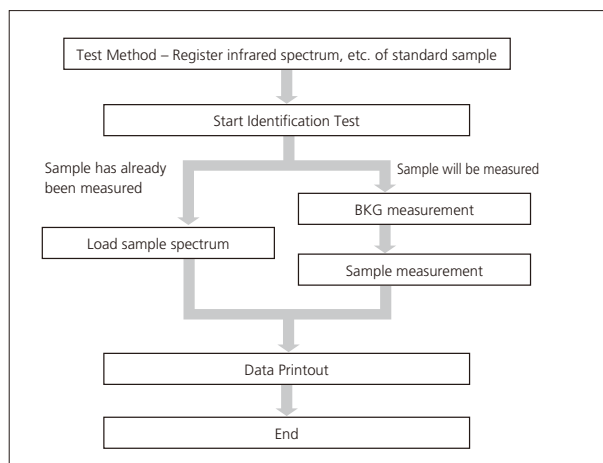


Fig. 1 Flowchart of Program

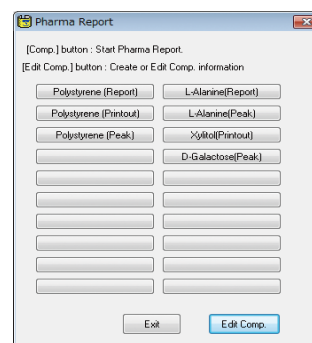


Fig. 2 Execution Window of Pharma Report Program

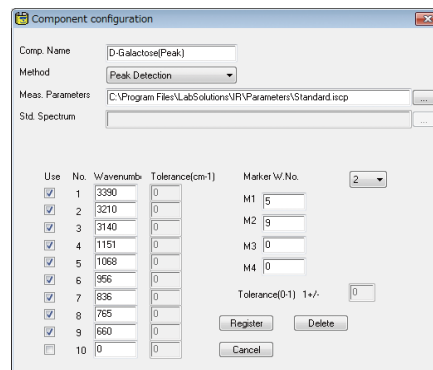


Fig. 3 Parameter Setting Window

### Test Method – Peak Detection

In peak detection, the detection of peaks is conducted in the measured spectrum based upon previously recorded peak values from a stored reference sample. The software routine allows for up to ten peak wavenumbers to be specified. In addition, up to four peaks can be specified to conduct identification by peak intensity ratio matching.

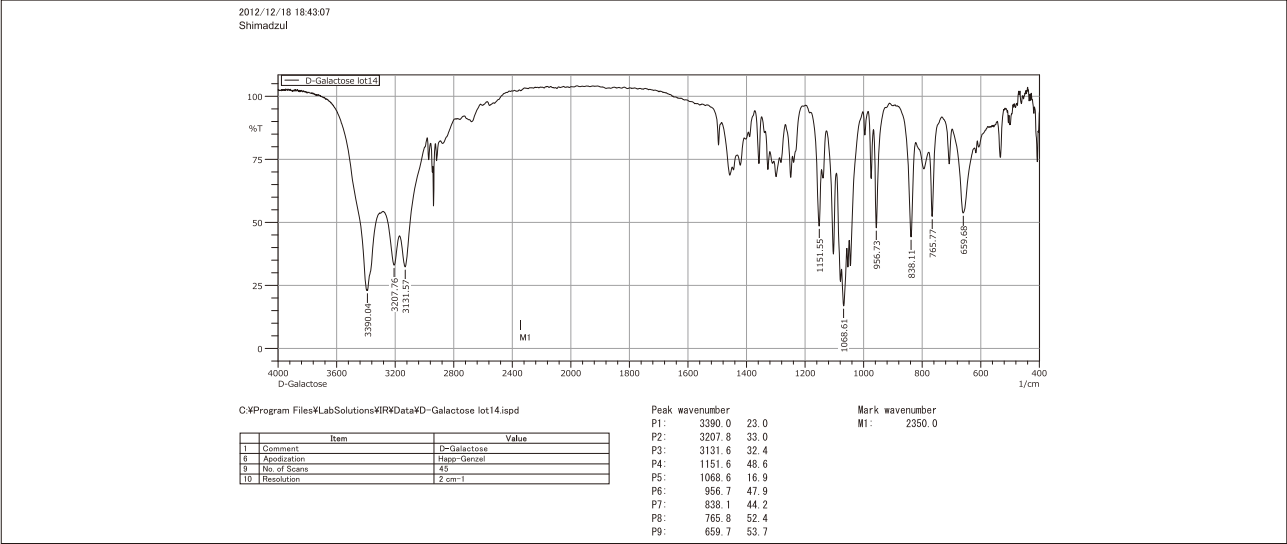


Fig. 4 Output Example of Peak Detection – D-Galactose

For example, the Japanese Pharmacopoeia specifies as follows regarding identification of D-galactose: "Determine the infrared absorption spectrum as directed in the potassium bromide disk method under Infrared Spectrophotometry: it exhibits absorption at the wavenumbers of about 3390 cm<sup>-1</sup>, 3210 cm<sup>-1</sup>, 3140 cm<sup>-1</sup>, 1151 cm<sup>-1</sup>, 1068 cm<sup>-1</sup>, 956 cm<sup>-1</sup>, 836 cm<sup>-1</sup>, 765 cm<sup>-1</sup> and 660 cm<sup>-1</sup>." Here, following measurement of D-galactose by the potassium bromide disk method, identification testing was conducted using peak detection. Fig 4 shows the printed output of a d-galactose test example.

■ Test Method – Spectrum Comparison

In the spectrum output mode, the standard spectrum and measured sample spectrum are printed side by side. For example, the Japanese Pharmacopoeia specifies as follows regarding identification of Xylitol: "Determine the infrared absorption spectrum of Xylitol, previously dried, as directed in the potassium bromide disk method under Infrared Spectrophotometry, and compare the spectrum with the Reference Spectrum: both spectra exhibit similar intensities of absorption at the same wavenumber." The effectiveness of this method is that verification can be conducted by visually comparing the sample spectrum with the reference spectrum.

■ Test Method – Report Generation

Report generation offers a more objective assessment of the spectral output indicating the same absorption values at the same wavenumbers in the compared spectra. The peak wavenumbers and peak intensity ratios of a previously recorded standard spectrum are compared with those of the sample spectrum, and judgment of acceptance is conducted based on a permissible error value. Evaluation can be conducted using wavenumber values for up to 10 peaks and absorption intensity ratios for up to 4 peaks. The permissible error ranges of peak wavenumbers and intensity ratios can be arbitrarily set. Here, after measuring xylitol by the potassium bromide disk method (KBr), confirmation testing was conducted using the report generation feature. The acceptance judgment results shown in Fig. 5 were obtained by merely calling up the sample spectrum and the standard spectrum.

■ Conclusion

Here, we introduced the Pharma Report Program. Included with this software is the Food Additives Identification Program, which features the same operation procedures as those used in the Pharma Report Program. Because the standard spectra (listed in the Food Additives Compendium) are included in the software, measurement can be conducted very quickly and conveniently.

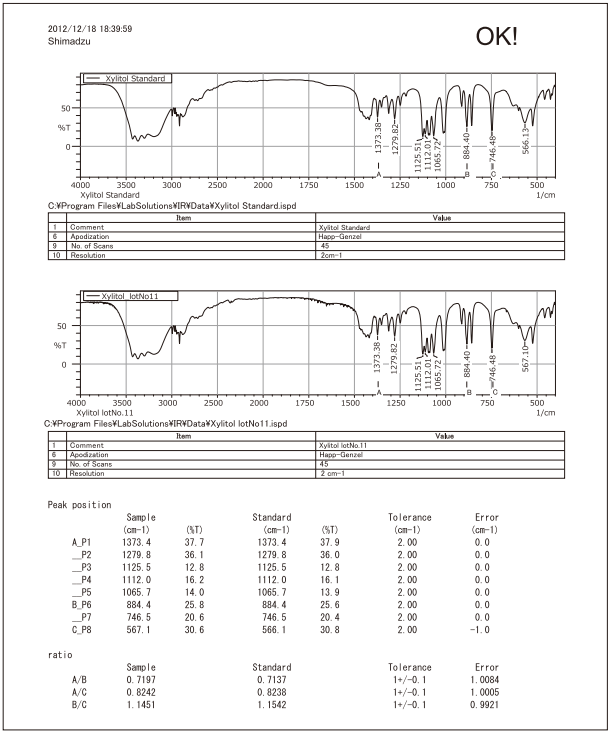


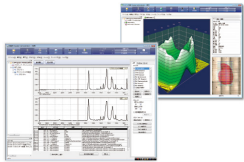
Fig. 5. Report Generation Output Example – Xylitol

[References]  
The Japanese Pharmacopoeia, Sixteenth Edition, edited by Pharmaceutical and Medical Device Regulatory Science Society of Japan



# Related Products

Some products may be updated to newer models.



> LabSolutions IR  
Analytical Data System for FTIR

# Related Solutions

> Price Inquiry

> Product Inquiry

> Technical Service /  
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