SHIMADZU

Application News

Spectrophotometric Analysis — No.A399

Introduction of Japanese Pharmacopoeia Program

The upgraded version of IRsolution Ver. 1.40 that will be provided with the new Fourier Transform Infrared Spectrophotometer IRAffinity-1 is equipped as standard with the formerly optional "Pharma Report Program".

The program, which enables simple identification testing according to the Japanese Pharmacopoeia, is introduced here in this Application News.

■ Pharma Report Program

The Pharma Report program features the following 3 functions to support identification testing.

• Peak detection
• Spectrum output
• Report creation

Appropriate use of the above functions can be used to compare a measured spectrum with a reference spectrum to conduct evaluation.

■ Peak Detection Feature

In peak detection, peaks corresponding to substances in the measured sample spectrum are detected. Up to 10 peaks can be specified. In addition, wavenumbers of particular interest can be displayed as marked wavenumbers (4 points maximum). Simply loading the sample spectrum and peak table of the constituent peaks allows display of the output results, like those shown in Fig. 1. The identification test evaluation method is effective when conducting confirmation (whether or not a specified peak is present) based on absorption wavenumber. In addition, it can also be used for conducting comparisons with the reference infrared absorption spectra contained in the Japanese Pharmacopoeia.
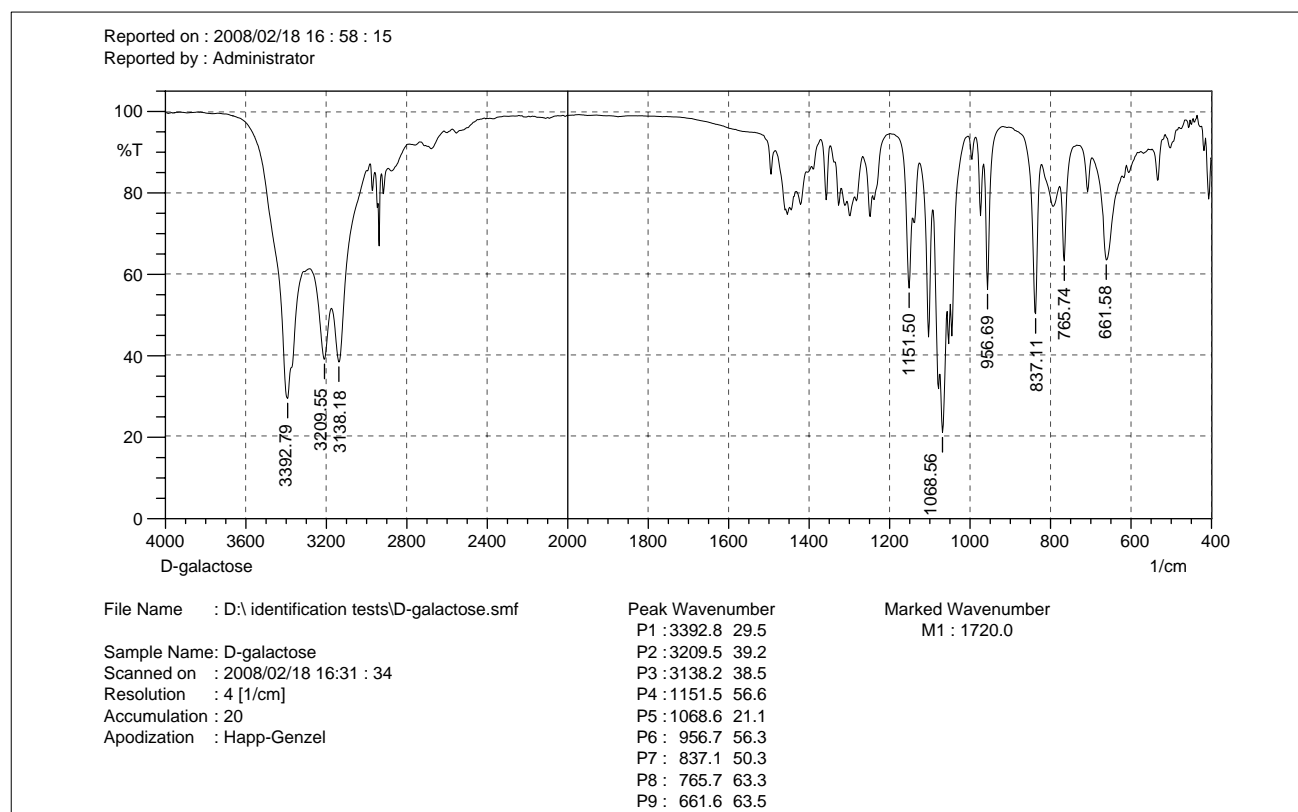
Reported on : 2008/02/18 16 : 58 : 15
Reported by : Administrator

D-galactose

File Name	: D:\ identification tests\D-galactose.smf	Peak Wavenumber	Marked Wavenumber
		P1 : 3392.8 29.5	M1 : 1720.0
Sample Name: D-galactose		P2 : 3209.5 39.2	
Scanned on	: 2008/02/18 16:31 : 34	P3 : 3138.2 38.5	
Resolution	: 4 [1/cm]	P4 : 1151.5 56.6	
Accumulation : 20		P5 : 1068.6 21.1	
Apodization	: Happ-Genzel	P6 : 956.7 56.3	
		P7 : 837.1 50.3	
		P8 : 765.7 63.3	
		P9 : 661.6 63.5	

Fig.1 Output Example of Peak Detection (D-Galactose)

■ Spectrum Output Feature

The spectrum comparison feature operates so that the sample spectrum and the standard spectrum are printed along with one another. In the identification method published in the Japanese pharmacopeia general test methods for infrared absorption spectral measurement, it states that "a sample and standard substance are confirmed to be the same substance if the absorption intensities at the same wavenumbers are equivalent in the absorption spectra of the sample and reference sample when comparing the two spectra. (omitting the last part[∗])" Visual confirmation of the sample and standard spectrum can be conducted when using the spectrum comparison feature. Fig. 2 shows an example of the spectrum output. The upper spectrum is that of the standard substance, and the lower is that of the sample.
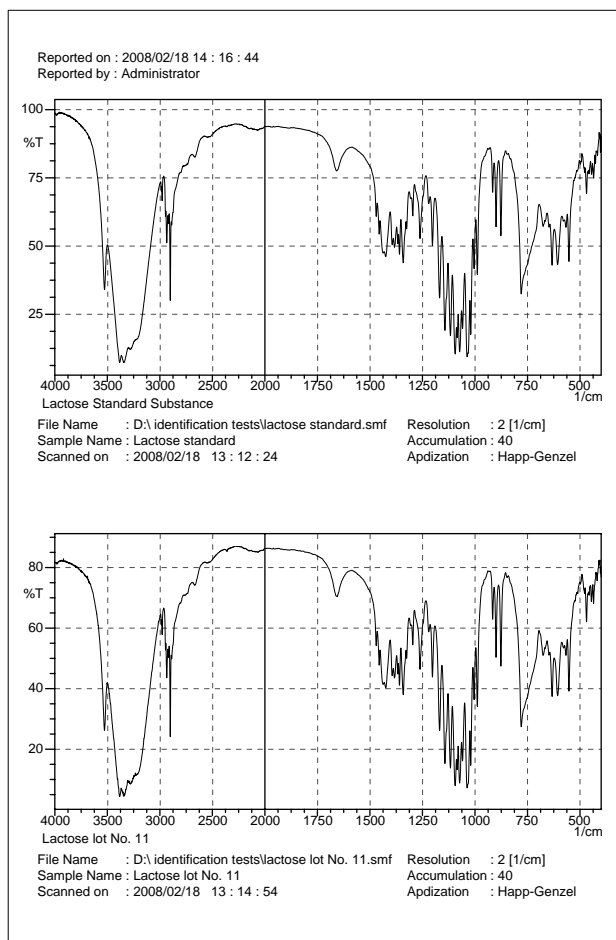
■ Report Creation Feature

This "sample and standard substance are confirmed to be the same substance if the absorption intensities at the same wavenumbers are equivalent in the absorption spectra of the sample and reference sample" mentioned above is applied straightforwardly in report creation, with a pass/fail judgment assigned on the basis of comparison of the peak positions and peak intensity ratios of the sample and standard spectra. Evaluation is based on up to 10 peak positions and up to 4 of those peak intensity ratios. The tolerance values of the peak positions and peak intensity ratios can freely set. The pass/fail judgment result like that shown in Fig. 3 can be obtained by merely loading the sample and standard spectra and the peak table of those substances

(∗) Reference : 15th Revision Japanese Pharmacopoeia Society of Japanese Pharmacopoeia Edition
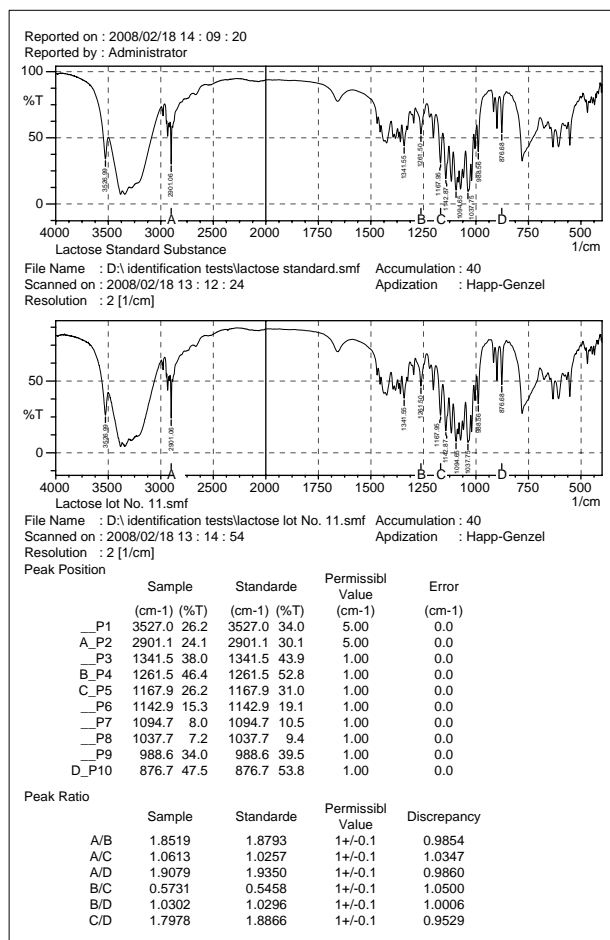

Fig.2 Output Example of Spectrum Comparison (Lactose)

Peak Position

	Sample		Standarde		Permissibl Value	Error
	(cm-1)	(%T)	(cm-1)	(%T)	(cm-1)	(cm-1)
__P1	3527.0	26.2	3527.0	34.0	5.00	0.0
A_P2	2901.1	24.1	2901.1	30.1	5.00	0.0
__P3	1341.5	38.0	1341.5	43.9	1.00	0.0
B_P4	1261.5	46.4	1261.5	52.8	1.00	0.0
C_P5	1167.9	26.2	1167.9	31.0	1.00	0.0
__P6	1142.9	15.3	1142.9	19.1	1.00	0.0
__P7	1094.7	8.0	1094.7	10.5	1.00	0.0
__P8	1037.7	7.2	1037.7	9.4	1.00	0.0
__P9	988.6	34.0	988.6	39.5	1.00	0.0
D_P10	876.7	47.5	876.7	53.8	1.00	0.0

Peak Ratio

	Sample	Standarde	Permissibl Value	Discrepancy
A/B	1.8519	1.8793	1+/-0.1	0.9854
A/C	1.0613	1.0257	1+/-0.1	1.0347
A/D	1.9079	1.9350	1+/-0.1	0.9860
B/C	0.5731	0.5458	1+/-0.1	1.0500
B/D	1.0302	1.0296	1+/-0.1	1.0006
C/D	1.7978	1.8866	1+/-0.1	0.9529

Fig.3 Output Example of Report Creation (Lactose)

Related Solutions

> Price Inquiry

> Product Inquiry

> Technical Service / Support Inquiry

> Other Inquiry