SHIMADZU
Excellence in Science

Application News

Fourier Transform Infrared Spectrophotometer IRXross™/IRSpirit™ Series

Identification Testing of *Myo*-Inositol Conforming to the European Pharmacopoeia (EP)

H. Iwamae

User Benefits

- Smooth identification testing is possible with the IRXross, which offers both high sensitivity and excellent operability, and the IRSpirit, a compact FTIR, by using the IR Pilot™ dedicated program included as a standard.
- IR Pilot is beneficial in routine analysis work including identification testing because the optimum measurement conditions can be set and accessed easily.
- The "peak designation judgment" function, which was newly added to IR Pilot, enables automatic pass/fail judgments based on wavenumbers specified by the user.

■ Introduction

The instrument control/data analysis software LabSolutions™ IR of the new IRXross and the IRSpirit compact FTIR (Fig. 1) includes the dedicated program IR Pilot as a standard feature, enabling simple measurement/analysis of four types: identification testing, contaminant analysis, quantitative analysis, and film thickness measurement. With this dedicated program, all steps from the actual measurement to analysis and printout can be performed automatically by the correct procedure merely by following the guidance on the screen. IR Pilot offers a total of 23 dedicated application programs as standard. It is also possible to register the entire analysis flow after a measurement and start the analysis from the main menu with one click from the next time.

This article introduces an example of identification testing of *myo*-inositol, which is an additive used in foods and pharmaceutical products, in accordance with the European Pharmacopoeia (EP).

Fig. 1 Appearance of IRXross (Left) and IRSpirit (Right)

■ *Myo*-Inositol

Myo-inositol is one type of cyclitol, which is listed as 1,2,3,5/4,6-inositol or (1R,2R,3S,4S,5R,6S)-cyclohexane-1,2,3,4,5,6-hexanol in the IUPAC nomenclature of chemistry (IUPAC: International Union of Pure and Applied Chemistry), and is a compound that exists universally in many animals and plants. Fig. 2 shows its chemical structural formula. *Myo*-inositol is the most generally distributed of the 9 isomers of inositol and is known as a water-soluble vitamin-like active substance. In addition to using an ingredient in infant formula and dietary supplements, it is also used as a liver hydrolysate preparation. *Myo*-inositol is included in various standards, including the EP and the United States Pharmacopeia (USP), and in Japanese Pharmaceutical Excipients 2018 and Japan's 9th Edition of Specifications and Standards for Food Additives (JSFA-IX), which specify identification tests utilizing the infrared spectrum.

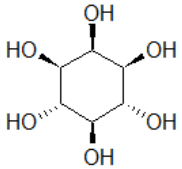


Fig. 2 Chemical Structural Formula of *Myo*-Inositol $C_6H_{12}O_6$

■ Identification Testing of *Myo*-Inositol

Monographs 1805 of the European Pharmacopoeia EP10.6 describes an identification test method for *myo*-inositol using infrared spectroscopy, in which the sample is compared with *myo*-inositol CRS (CAS Registry Number (CAS RN®): 87-89-8). The identification test in this article was conducted on the assumption that the infrared spectrum registered in the search software KnowItAll Spectroscopy Edition (Wiley Science Solutions) is the spectrum of the standard sample. Since EP Monographs 1805 does not mention the peak wavenumber to be confirmed or the allowable range of deviation (allowable error), 12 main peak positions were selected for this experiment. The allowable error between the sample and *myo*-inositol CRS was set at within 1.0 cm^{-1} from the measured resolution of 2 cm^{-1}.

A potassium bromide (KBr) pellet (φ 4 mm) was prepared as the test sample, and its infrared spectrum was measured. Table 1 shows the measurement conditions, and Fig. 3 shows the acquired infrared spectrum.

Table 1 Measurement Conditions

Instrument	: IRXross Fourier transform infrared spectrophotometer (KBr window)
Resolution	: 2 cm^{-1}
Accumulation	: 45 times
Apodization function	: SqrTriangle
Detector	: DLATGS

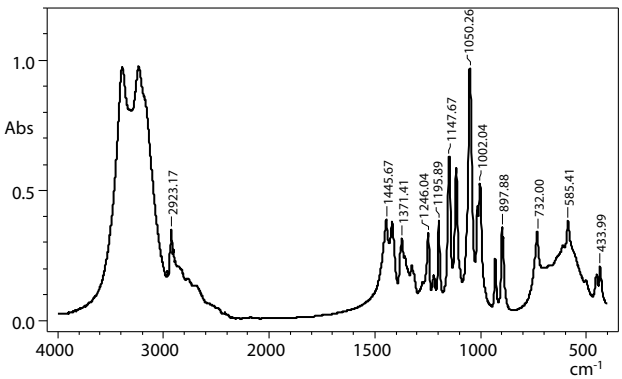
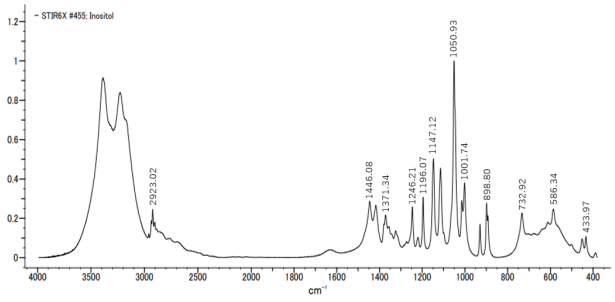


Fig. 3 Infrared Spectrum of Test Sample

Fig. 4 shows the infrared spectrum assumed here as the standard sample. Table 2 summarizes the peak wavenumber positions and the errors of the wavenumbers for the 12 main peak positions used in this experiment.



Name	Inositol
CAS Registry Number	87-89-8
Catalog Number	109102
Formula	C6H12O6
InChI	InChI=1S/C6H12O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-12H/t1-,2-,3-,4+,5-,6-
InChI Key	CDAISMWEOUEBRE-GPIVLXJGSA-N
Instrument Name	Bruker Tensor 27 FT-IR
Melting Point	222 - 227 °C
Mol.Weight	180.156 g/mol
Purity	>98%
Source of Sample	Spectrochem Pvt. Ltd.
Source of Spectrum	Bio-Rad Laboratories, Inc.
Technique	KBr1

Fig. 4 Infrared Spectrum of *Myo*-Inositol (CAS Registry No.: 87-89-8)
(Source: Search Software KnowItAll Spectroscopy Edition)

Table 2 Main Peak Wavenumbers and Errors

Peak wavenumber in Fig. 3 (cm^{-1})	Peak wavenumber in Fig. 4 (cm^{-1})	Error of wavenumber (cm^{-1})
2923.17	2923.02	0.15
1445.67	1446.08	0.41
1371.41	1371.34	0.07
1246.04	1246.21	0.17
1195.89	1196.07	0.18
1147.67	1147.12	0.55
1050.26	1050.93	0.67
1002.04	1001.74	0.30
897.88	898.80	0.92
732.00	732.92	0.92
585.41	586.34	0.93
433.99	433.97	0.02

According to Table 2, peaks could be confirmed at the same wavenumbers and the largest error of the wavenumbers was 0.93 cm^{-1}. Therefore, it can be surmised that the measured sample is *myo*-inositol.

■ Higher Efficiency in Identification Testing by Using IR Pilot

As described above, an identification test was carried out by comparing the peak positions in the infrared spectra of a standard sample and the test sample. The following introduces an example of labor-saving in this operation.

Sample measurement and peak detection can be automated by using the IR Pilot dedicated program, which is provided with the IRXross and the IRSpirit as a standard feature.

IR Pilot is a convenient program that can simplify the entire workflow in identification test, from measurement and analysis of the target sample to printout, merely by selecting the four items ① Analysis purpose, ② Measurement technique, ③ Accessory to be used, and ④ Necessary data process in accordance with the guidance shown on the screen.

The measurement under the optimum conditions, as shown in Table 1, is possible merely by selecting "Identification test corresponding to pharmacopoeia," "Transmission spectroscopy," and "KBr pellet." By using "Peak pick" and "Peak designation judgment" for the analysis after the measurement, it is possible to prepare a report that includes detection of the main peaks and the detection results, compare the infrared spectra of the standard sample and test sample at the specified peak wavenumbers, and make a pass/fail judgment by a simple procedure.

The following explains this procedure using the condition setting screen of "Peak designation judgment" as an example (see Fig. 5). Here, the major peak positions were registered referring to the infrared spectrum of *myo*-inositol (CAS Registry No.: 87-89-8) registered in the search software KnowItAll Spectroscopy Edition. When performing an identification test, the user should purchase a standard sample and acquire the infrared spectrum. A maximum of 10 peak wavenumbers can be used in the comparison, and a maximum of 4 peak intensity ratios can be set. The test sample is judged as Pass if the error of the wavenumbers is within the allowable range set by the user. If the user registers the program after executing the analysis, only the background (BKG) measurement and the sample measurement operations are necessary when conducting identification tests in the future. In addition to the national pharmacopoeias, this system can also be used in identification tests by other official analysis methods.

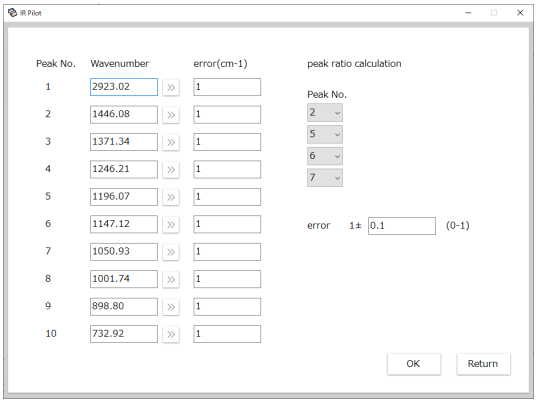


Fig. 5 Condition Setting Screen for Peak Designation Judgment

■ Conclusion

An identification test was conducted for *myo*-inositol, which is a type of additive used in food and pharmaceutical products. Measurement and peak detection conforming to the European Pharmacopoeia (EP) were carried out, and agreement of the absorbed wavenumbers of the test sample with the spectrum of an assumed standard sample was confirmed. If a standard sample is prepared, the entire process, including the pass/fail judgment, can be carried out automatically, allowing further labor-saving in identification tests. In identification tests based on official analysis methods, IR Pilot saves the user the time and trouble required to set analysis conditions and prepare reports, resulting in more efficient testing.

<Reference>
European Pharmacopoeia (EP 10.6), Monographs, *myo*-inositol

01-00308-EN First Edition: Apr. 2022

Shimadzu Corporation
www.shimadzu.com/an/