



Study of the composition of silymarin determined by IR spectroscopy

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Abstract

Silymarin contains several hydroxyl and phenolic groups as well as aromatic rings, so its FTIR spectrum typically shows characteristic bands of: phenolic -OH group stretching and bending, aromatic C=C stretches from the flavonoid structure. C-O stretches from ether and ester bonds.

Each component of silymarin (e.g., silybin, silydianin, silychristin) will contribute to the overall FTIR spectrum, but the peaks mentioned above are generally indicative of the presence of silymarin in an extract or formulation.

Keywords: Composition, silymarin, spectroscopy, FTIR

Introduction

Contact sports such as rugby, American football, and ice hockey are among the most physically demanding athletic activities, combining strength, speed, and frequent player-to-player collisions. While they promote fitness and social engagement, they also pose a high risk of acute and chronic injuries. Understanding silymarin is a complex mixture of flavonoids, primarily derived from the seeds of the *Silybum marianum* plant, commonly known as milk thistle. It is widely studied for its hepatoprotective (liver-protecting) properties and is often used in herbal medicine for treating liver disorders. Silymarin is not a single compound but rather a combination of flavonolignans and flavonoids. The major constituents are:

- Silybin (Silibinin) is the most active and abundant flavonolignan, accounting for about 50-70% of the silymarin mixture.
- Silydianin is another flavonolignan present in smaller amounts.
- Silychristin is a flavonolignan that is also a component of silymarin.
- Flavonoids include these compounds like quercetin, taxifolin, and others, though they are present in smaller amounts.

Silymarin is typically a yellowish-brown powder. Silymarin is relatively insoluble in water but is soluble in organic solvents like ethanol, methanol, and acetone. This characteristic is important when preparing extracts for use in supplements or pharmaceutical applications. Silymarin's components vary in molecular weight, but for silybin (its major component), the molecular weight is approximately 482 g/mol^[1, 5].

Silymarin is most well-known for its liver-protecting effects. It has antioxidant properties, scavenging free radicals and reducing oxidative stress in liver cells. It also supports liver regeneration and inhibits the binding of toxins to liver cell receptors.

It exhibits anti-inflammatory effects, which may help reduce liver inflammation and promote healing in liver diseases such as hepatitis or cirrhosis. Silymarin reduces oxidative stress by increasing the levels of antioxidant enzymes like

superoxide dismutase (SOD) and glutathione. Some studies suggest that silymarin may have potential anticancer properties, particularly in inhibiting the growth of certain types of tumors. It's been studied for its effects on liver cancer, but further research is needed. There's some evidence suggesting that silymarin can have antiviral effects, particularly in reducing the impact of viruses like hepatitis C.

By neutralizing free radicals, it helps prevent oxidative damage to liver cells. Silymarin helps stabilize liver cell membranes, making them less susceptible to damage by toxins. Silymarin prevents toxins, including certain drugs and alcohol, from binding to liver cell receptors, thereby reducing liver damage. Silymarin promotes the regeneration of liver cells by stimulating protein synthesis in hepatocytes (liver cells). Silymarin can regulate the activity of various enzymes involved in detoxification and metabolism. Silymarin is commonly used as a treatment for liver-related diseases such as: chronic hepatitis, cirrhosis, fatty liver disease, liver damage due to alcohol or drug toxicity.

It's also used as a general antioxidant supplement to support health and reduce the risk of oxidative damage^[6, 12].

Due to its antioxidant and anti-inflammatory effects, it is sometimes included in skincare products aimed at protecting the skin from oxidative stress and premature aging. Some studies indicate that silymarin may help protect against liver damage caused by chemotherapy drugs, though clinical evidence is still developing.

Silymarin is generally considered safe when used in recommended doses. However, high doses or prolonged use might cause gastrointestinal disturbances such as nausea or diarrhea.

It may interact with certain medications, such as those metabolized by the liver, including some anticoagulants, statins, and anticancer drugs. Therefore, it is advisable to consult a healthcare provider before use, particularly for individuals on other medications.

It is typically not recommended during pregnancy or breastfeeding unless otherwise advised by a healthcare professional.

Silymarin has low bioavailability due to poor solubility in water. However, its bioavailability can be enhanced by

using it in combination with other substances (e.g., phospholipids) or in liposomal formulations that improve absorption.

Silymarin, with its hepatoprotective, antioxidant, and anti-inflammatory properties, is a valuable natural compound, especially for individuals dealing with liver-related conditions. While research continues to explore its full potential in other therapeutic areas, its primary use remains in liver health. Its properties make it a promising natural supplement, though it's always important to consider potential interactions with other medications and consult a healthcare provider before use^[13, 19].

Materials and methods

Fourier transform infrared (FTIR) spectra of the silymarin were obtained in the range of 400 to 4000 cm^{-1} using a FTIR Spectrophotometer (Shimadzu Corp.) (Fig.1) by the diffuse reflectance method.

Results and discussions

The FTIR spectrum of silymarin is shown in Fig. 2.



Fig 1: Spectrophotometer Shimadzu

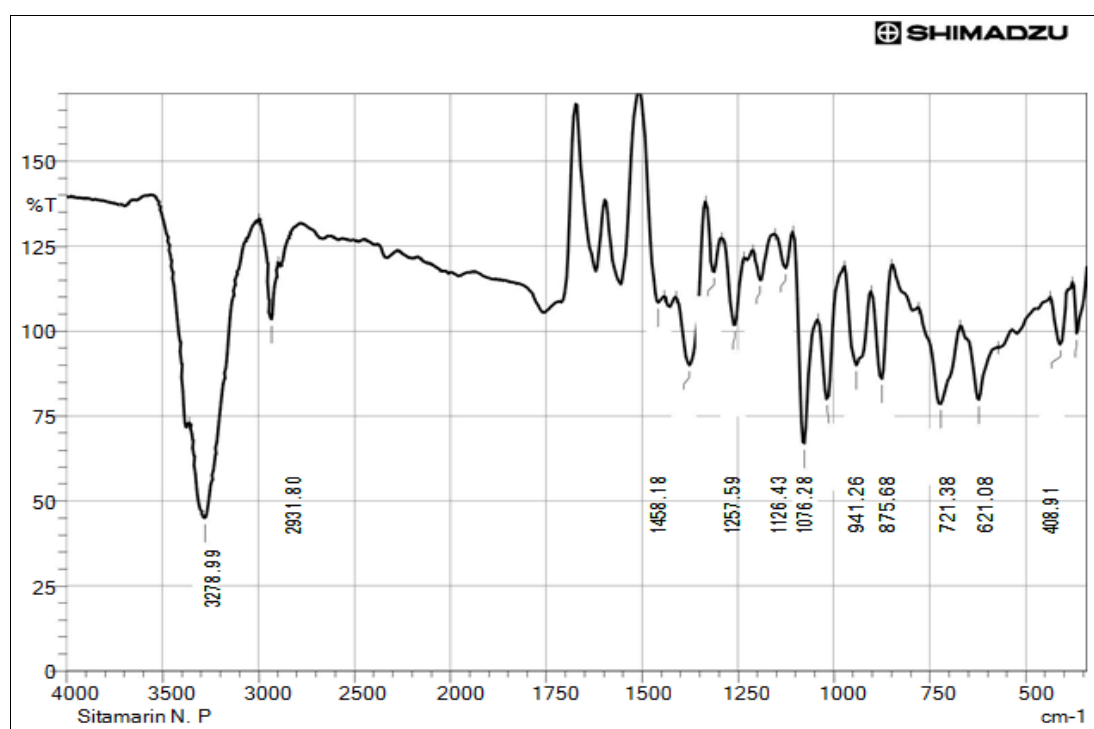


Fig 2: Spectrum of silymarin

The FTIR spectrum of silymarin would show several important peaks that can be attributed to its flavonoid and flavonolignan components. Here are some of the key regions to look for:

Hydroxyl group (-OH) stretching is around 3200-3550 cm^{-1} . This broad absorption band is due to the stretching vibration of hydroxyl groups (-OH), which are present in the flavonoid structures of silymarin.

Aromatic C-H stretching is around 2900-3000 cm^{-1} are the C-H stretching vibrations from the aromatic rings of the flavonoid and flavonolignan structures typically show absorption in this region.

Aromatic C=C stretching is around 1500-1600 cm^{-1} are this corresponds to the stretching vibrations of the conjugated carbon-carbon double bonds in the aromatic rings (C=C)

typical of flavonoid structures.

C-O stretching is around 1200-1300 cm^{-1} are the C-O stretching vibrations from the ether or ester bonds in the flavonoid and flavonolignan portions of silymarin are often observed in this region.

Aromatic C-H bending is around 800-900 cm^{-1} are this region typically shows the out-of-plane bending of C-H bonds from the aromatic rings.

C-O-C stretching is around 1050-1150 cm^{-1} are this is associated with the stretching vibrations of the C-O-C ether linkages found in the silymarin structure, especially in the flavonolignans.

Phenolic -OH bending is around 1360-1380 cm^{-1} are this corresponds to bending vibrations of the phenolic -OH group.

Conclusions

The given IR spectra of silymarin shows the principle peaks such as $>C=C<$ Aromatic 1508 cm^{-1} and $-O-H$ stretch $1083,1157,1269\text{ cm}^{-1}$, $-COOH$ carboxylic acid 1732 cm^{-1} indicate that above IR spectra is of silymarin which is identified and proved.

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