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SPECTRAL AND CHROMATOGRAPHIC ANALYSIS METHODS OF THE SAFINOL SUBSTANCE

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Abstract

Safinol is a biologically active compound with anticoagulant activity that has potential pharmaceutical applications. Studying its physicochemical characteristics is necessary for determining the molecular structure and composition of the substance. In this work, spectral and chromatographic analytical methods were used to investigate Safinol. Ultraviolet (UV) spectrophotometry, infrared (IR) spectroscopy, and high-performance liquid chromatography (HPLC) were applied to identify structural features and determine the presence of active components.

UV spectrophotometric analysis revealed absorption bands characteristic of aromatic chromophoric systems. The obtained spectrum showed similarities with the spectrum of salicylic acid, suggesting that aromatic fragments are present in the Safinol structure.

IR spectroscopy confirmed the presence of several functional groups in the compound. The analysis detected absorption bands corresponding to carboxylate ions, methylene groups, and N–C bonds. These spectral features indicate that the Safinol molecule contains organic structural fragments associated with these functional groups.

Chromatographic analysis was performed using HPLC to determine the composition of the substance. The chromatographic results confirmed the presence of salicylic acid derivatives in the Safinol sample. The retention time of the standard salicylic acid peak was observed in the range of 6–8 minutes. Quantitative analysis showed that the content of salicylic acid derivatives in Safinol ranges from 2.85 to 2.95 μg/g.

The obtained results demonstrate that spectral and chromatographic methods provide reliable information about the structure and composition of Safinol. These analytical techniques are effective for the identification and quality control of biologically active pharmaceutical substances.

Keywords: Safinol, spectral analysis, UV spectrophotometry, IR spectroscopy, HPLC, salicylic acid.

Introduction

The study of biologically active substances is an important direction in pharmaceutical chemistry. Identification of the structure and composition of such compounds is necessary for evaluating their biological activity, safety, and stability. Modern analytical methods allow researchers to determine the chemical structure of pharmaceutical substances and to control their quality.

Spectral methods such as UV and IR spectroscopy are widely used for identifying functional groups and studying electronic transitions in organic molecules. Chromatographic techniques, particularly high-performance liquid chromatography are effective tools for separating, identifying and quantifying chemical compounds in complex mixtures.

Safinol is considered a promising anticoagulant substance. Therefore, investigation of its structural characteristics and composition using reliable analytical methods is essential.

The purpose of this study was to analyze the Safinol substance using spectral and chromatographic techniques and to determine the presence of salicylic acid derivatives within the compound.

Materials and Methods

The analysis of the Safinol substance was performed using several instrumental methods.

For UV spectrophotometric analysis, 10 mg of Safinol and 10 mg of salicylic acid were dissolved in distilled water. The solutions were treated in an ultrasonic bath for 5 minutes to ensure complete dissolution. Spectral measurements were carried out using a UV-1280 UV-VIS spectrophotometer.

Infrared spectroscopic analysis was performed using an IRTracer-100 Fourier transform infrared spectrometer equipped with a diamond/ZnSe prism. Spectra were recorded in the range of 4000–400 cm^{-1} with a resolution of 4 cm^{-1}.

For chromatographic analysis, a high-performance liquid chromatography (HPLC) system Agilent-1200 with a C18 column (5 µm, 4.6 × 150 mm) was used. The mobile phase consisted of 0.1% trifluoroacetic acid and acetonitrile (70:30). The flow rate was 1.0 mL/min, and the injection volume was 20 µL. Detection was performed at 254 nm.

Results and Discussion

The UV spectral analysis of Safinol showed absorption maxima typical for aromatic compounds. The spectrum demonstrated similarities to the spectrum of salicylic acid, indicating the presence of aromatic chromophoric groups in the compound. Slight shifts in the absorption maxima suggest structural differences between Safinol and pure salicylic acid as shown in Fig.1

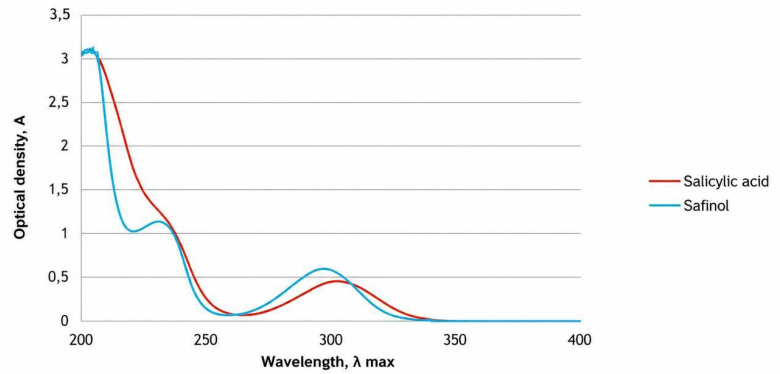


Figure 1. Proportionality of the UV spectrophotometric analysis of Safinol and salicylic acid.

IR spectroscopic analysis revealed several characteristic absorption bands corresponding to different functional groups. A weak band at 3383 cm^{-1} indicated the presence of a small amount of moisture. Absorption bands at 1629 cm^{-1} and 1573 cm^{-1} corresponded to vibrations of the –COONa group. Additional bands observed near 1487 cm^{-1} and 1444 cm^{-1} were associated with methylene and carboxylate groups.

Stretching vibrations of methylene groups were detected near 2902 cm^{-1}, while vibrations attributed to N–C bonds appeared in the region of 1249–1143 cm^{-1}. In the fingerprint region, several absorption bands corresponding to substituted benzene rings were also observed as shown in Fig.2, the reluts indicate.

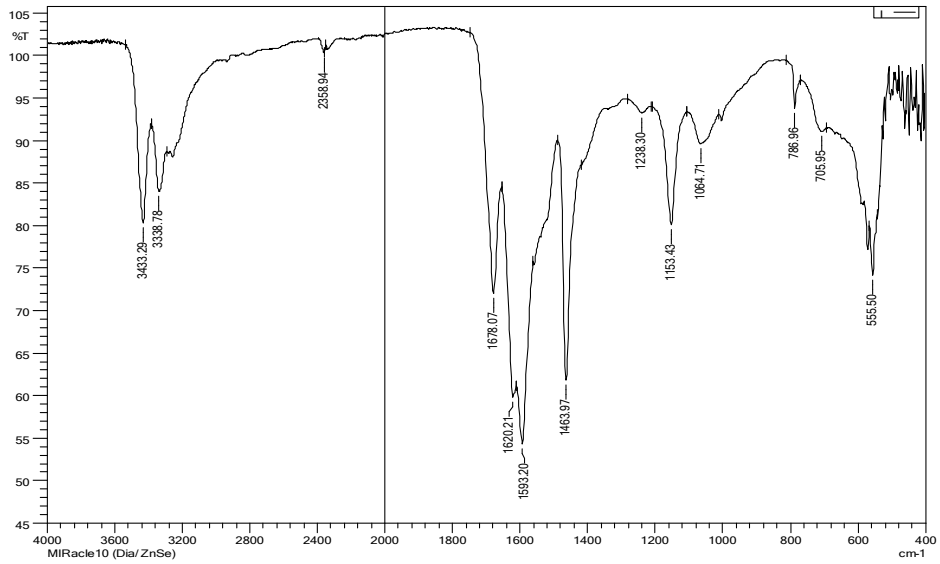


Figure 2. IR spectrum results of the Safinol substance.

Chromatographic analysis confirmed the presence of salicylic acid derivatives in the Safinol substance. The chromatogram showed a retention time similar to the standard salicylic acid peak. Quantitative analysis demonstrated that the concentration of salicylic acid derivatives ranged from 2.85 to 2.95 µg/g as shown in Fig.3

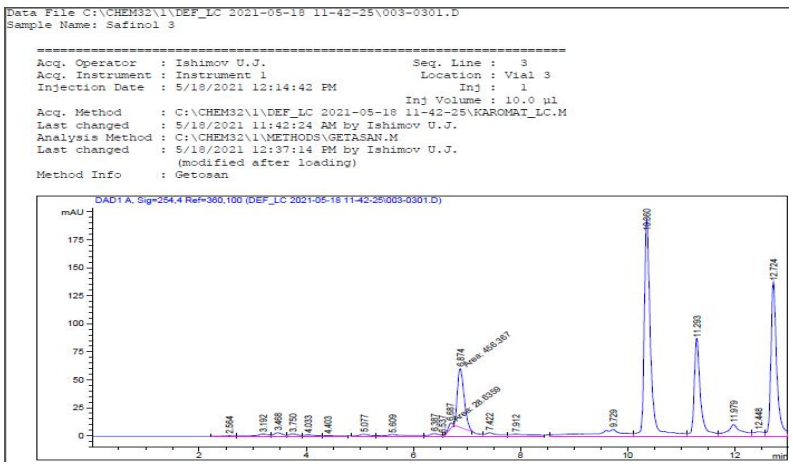


Figure 3. Demonstration of the salicylic acid in the Safinol substance.

Conclusion

The results of this study show that spectral and chromatographic analytical methods are effective tools for the investigation of the Safinol substance. UV spectrophotometry revealed the presence of aromatic chromophoric systems, while IR spectroscopy allowed the identification of functional groups such as carboxylate ions, methylene fragments, and N–C bonds.

Chromatographic analysis using HPLC confirmed the presence of salicylic acid derivatives and allowed their quantitative determination. The concentration of these derivatives in the Safinol sample was found to be between 2.85 and 2.95 µg/g.

The combination of UV, IR, and HPLC techniques provides reliable information about the structure and composition of Safinol and can be used for its analytical characterization and pharmaceutical quality control.

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