

## 29. THE IR SPECTROPHOTOMETRY APPLICATIONS IN THE STUDY OF PHYSICAL AND CHEMICAL COMPATIBILITY OF SOME ACTIVE SUBSTANCES

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**Introduction:** The qualitative aspects of infrared spectroscopy are one of the most powerful attributes of this diverse analytical technique. IR spectrophotometric method is a modern method, which is used to identify the molecular structure of the drug substances based on the spectrum, resulting from the interaction of light with certain functional groups, bonds and structural units. IR spectrophotometric method was used in this study to determine the physical and chemical compatibility of izohydrofural, methyluracil and benzocaine by interpretation of the spectrum of pure and mixed substances.

**Purpose and objective:** To apply the IR spectrophotometric method in the research of physical and chemical compatibility of izohydrofural, methyluracil and benzocaine. This study will prove the possibility of a combination of izohydrofural, methyluracil and benzocaine in the same dosage form.

**Materials and methods:** In this research it was used the active substances: izohydrofural, methyluracil and benzocaine, and FT-IR Bruker Equinox 55 spectrometer.

**Results:** The infrared spectrum of a molecule is considered to be a unique physical property and it is a characteristic of the molecule. It is based on the fact that the structural features of the molecule, whether they are the backbone of the molecule or the functional groups attached to the molecule, produce characteristic and reproducible absorptions in the spectrum. This information can indicate whether there is backbone to the structure and, if so, whether the backbone consists of linear or branched chains. Next it is possible to determine if there is unsaturation and/or aromatic rings in the structure. Finally, it is possible to deduce whether specific functional groups are present. If detected, one is also able to determine local orientation in the group and its location in the structure. IR spectrophotometry is rich in information and it can be used in the chemical and physical compatibility studies of the drugs. An infrared absorption spectrum often contains a bewildering array of sharp peaks and minima. Peaks useful for the identification of functional groups are located in the shorter-wavelength region of the infrared, from about 2.5 to 8.5 mm, where the positions of the maxima are only slightly affected by the carbon skeleton of the molecule. Identifying functional groups in a molecule is seldom sufficient to positively identify the compound. For the study of physical and chemical compatibility of the drugs, there were interpreted the spectrum of each drug substances. Then it was analyzed the spectrum of the mixture of the chemical substances. After that, it was overlapped the infrared spectrum of each chemical substance with the infrared spectrum of the mixture. If the substances are physically and chemically compatible, then it must be present the same characteristic absorption bands of chemical functional groups both in the spectrum of each substance and in the spectrum of the mixture. The infrared spectrum of the mixture of izohydrofural, methyluracil and benzocaine has the most characteristic absorption bands of each substance, which indicates the physical and chemical compatibility of the molecules of the substances.

**Conclusions:** It was used the IR spectrophotometry to research the physical and chemical compatibility of some active, chemical substances.

**Keywords:** Physical and chemical compatibility, infrared spectroscopy

## 30. ISOFLAVONES-STRUCTURE, PROPERTIES, APPLICATIONS

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**Introduction:** Isoflavones are a class of organic compounds and biomolecules related to the flavonoids. Isoflavones are produced almost exclusively by the members of the *Fabaceae* (i.e., *Leguminosae*, or bean) family. Some are termed antioxidants because of their ability to trap singlet

oxygen. Some isoflavones, in particular soy isoflavones, when studied in populations eating the soy protein, have indicated that there is a lower incidence of breast cancer and other common cancers because of its role in influencing sex hormone metabolism and biological activity through intracellular enzymes, protein synthesis, growth factor actions, malignant cell proliferations, differentiation and angiogenesis. However some critics claim that isoflavones can increase the incidence of epithelial hyperplasia and cause goitre and hyperthyroidism. Isoflavones remain the subject of many scientific studies, as illustrated by the more than 1700 scientific publications mentioning isoflavones in their title or abstract. Most of these studies show that isoflavones may have some health benefit.

**Materials and methods:** bibliographic study of plants producing isoflavones - soybean (*Glycine max* L.), green bean (*Phaseolus vulgaris* L.), alfalfa sprout (*Medicago sativa* L.), mung bean sprout (*Vigna radiata* L.), cowpea (*Vigna unguiculata* L.), kudzu root (*Pueraria lobata* L.). The analysis of methods used for the separation and standartization of isoflavones: Nuclear Magnetic Resonance (NMR), UV-VIS, MS, high-performance liquid chromatography (HPLC).

**Results:** Most protocols of the sample preparation for isoflavone determination in soymilk and other liquid soybean products involves tedious freeze-drying and time-consuming extraction procedures. We report a facile and rapid magnetic solid-phase extraction (MSPE) of isoflavones from soymilk for subsequent high-performance liquid chromatography electrospray ionization tandem mass spectrometry (HPLC-ESI-MS/MS) analysis. The extraction was based on the selective binding of the isoflavones to baicalin-functionalized core-shell magnetic nanoparticles (BMNPs). The HPLC method is the most suitable choice for the identification of flavonoids as separation methods are well established and coupling with the MS is easy. For the isolation of flavonoids from liquid samples (drinks) or of physiological fluids typically are addressed in two ways: the first one is based on liquid-liquid extraction, and the second SPE. An interlaboratory study was conducted to evaluate a method for determining total soy isoflavones in dietary supplements, dietary supplement ingredients, and soy foods. Isoflavones were extracted using aqueous acetonitrile containing a small amount of dimethylsulfoxide (DMSO) and all 12 of the naturally occurring isoflavones in soy were determined by HPLC with UV detection using apigenin as an internal standard.

**Conclusions:** Isoflavones are found in high concentrations in the vegetable, fruit and vegetable flavonols in most of the human diet.

**Keywords:** isoflavones, soybean, antioxidants

### 31. PHARMACEUTICAL QUALITY OF *TILIAE FLOS* COMMERCIAL SAMPLES: CHEMICAL COMPOSITION - BIOLOGICAL ACTIVITY CORRELATION

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**Introduction.** *Tiliae flos* represents flowers and bracts harvested from *Tilia sp.*, well-known medicinal species widely used in traditional medicine. Sedative, immunomodulatory, antispasmodic and carminative properties represent the premises of usage also in modern therapy. Currently, most of the scientific data for linden chemical composition comes from Mexico, whereas Romanian endemic species have scarce studies. **The main objective** of the present study was to assess the pharmaceutical quality of five linden tea commercial samples according with Pharmacopoeial provisions. Also, we intended to prove a direct correlation between the chemical composition of the plant material and the biological properties.

**Material and methods.** The samples were bought from different pharmacies from Iasi and they were given numbers from 1 to 5; samples 1 and 2 were packed as 50 g bags and 3-5 were sachets (1.5g) packages. In order to identify the plant species we started with macroscopic and microscopic analysis. To assess the chemical composition we extracted 5g of each sample with