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Application of Fourier Transform Infrared Spectroscopy (FTIR) for Quantitative Analysis of Pharmaceutical Compounds

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ABSTRACT

Fourier Transform Infrared Spectroscopy (FTIR) is an infrared spectroscopy equipped with a Fourier transform for detection and analysis of spectral results. This method is used to qualitatively and quantitatively analyze organic and inorganic molecules with a wavenumber range of 14000 cm^{-1}–10 cm^{-1}. Based on these wavenumbers, the infrared region is divided into three regions, namely near infrared, mid infrared, and far infrared. The tool used in this method is an FTIR spectrophotometer whose working principle based on the interaction between the energy and the material. This method are fast, non-destructive, simple sample preparation, ease of use, using little solvent so it is environmentally friendly when compared to other HPLC and spectroscopic methods. But the sampling space in this method is relatively small so that it can block infrared rays. The research method that used is systematic literature review (SLR) from 20 research articles in national and international journals with publication years between 2005-2023. Based on the results of quantitative analysis of amoxicillin, pentoxyphylline, ciprofloxacin, diclofenac sodium, sodium ceftriaxone, ibuprofen, valsartan, and cefadroxil compounds in drugs can be analyzed using this method because they include organic compounds and are analyzed in the mid infrared. All concentrations of compounds analyzed meet the content requirements according to the Indonesian Pharmacopoeia IV Edition, which is not less than 90% and not more than 110%.

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ABSTRAK

Spektroskopi Fourier Transform Inframerah (FTIR) adalah spektroskopi inframerah yang dilengkapi dengan transformasi Fourier untuk deteksi dan analisis hasil spektral. Metode ini digunakan untuk menganalisis molekul organik dan anorganik secara kualitatif dan kuantitatif dengan rentang bilangan gelombang 14000 cm^{-1}–10 cm^{-1}. Berdasarkan bilangan gelombang tersebut, daerah infra merah dibedakan menjadi tiga daerah yaitu inframerah dekat, inframerah tengah, dan inframerah jauh. Alat yang digunakan dalam metode ini adalah spektrofotometer FTIR yang prinsip kerjanya berdasarkan interaksi antara energi dan material. Keunggulan metode ini adalah cepat, tidak merusak, preparasi sampel sederhana, mudah digunakan, menggunakan sedikit pelarut sehingga ramah lingkungan jika dibandingkan dengan metode HPLC dan spektroskopi lainnya. Metode penelitian yang digunakan adalah systematic literature review (SLR) dari 20 artikel penelitian di jurnal nasional dan internasional dengan tahun terbit antara 2005-2023. Berdasarkan hasil analisis kuantitatif terhadap senyawa amoksisilin, pentoksifilin, ciprofloxacin, natrium diklofenak, natrium ceftriaxone, ibuprofen, valsartan, dan cefadroxil dalam obat dapat dianalisis menggunakan metode ini karena termasuk senyawa organik dan dianalisis pada inframerah tengah. Seluruh konsentrasi senyawa yang dianalisis memenuhi persyaratan kandungan menurut Farmakope Indonesia Edisi IV, yaitu tidak kurang dari 90% dan tidak lebih dari 110%.

Kata Kunci: Spektroskopi; FTIR; Analisis Kuantitatif; Obat; Senyawa Dalam Obat

1. Introduction

Pharmaceutical preparations consist of drugs, medicinal ingredients, traditional medicines, and cosmetics. Pharmaceutical dosage forms consist of three types, namely solid, semisolid, and liquid preparations. Examples of solid preparations are tablets, capsules, powders, pills, suppositories, and ovules. Examples of semisolid preparations are ointments, pastes, gels, creams, lotions, and linaments. Examples of liquid preparations are syrups, suspensions, elixirs, emulsions, injections, and guttae [1].

Drugs are one of the pharmaceutical preparations that are very important in health services. The drug can be considered as chemical, animal as well as vegetable substances Drugs can be used to treat diseases, relieve symptoms, prevent diseases, or diagnose diseases [2]. According to Law of the Republic of Indonesia Number 36 of 2009 concerning health, drugs are materials or combinations of materials, including biological products used to affect or investigate physiological systems or pathological states in the context of determining diagnosis, prevention, cure, recovery, health improvement and contraception, for humans [3].

Fourier Transform Infrared spectroscopy (FTIR) is an infrared spectroscopy equipped with a Fourier transform for detection and analysis of spectrum results [4]. FTIR is an analytical technique for analyzing organic and inorganic molecules with wavenumber ranges, as: 14000 cm^{-1}–10 cm^{-1}. Based on these wavenumbers, the infrared areas are divided into three areas, such as near infrared (14000 cm^{-1}–4000 cm^{-1}) vibration-sensitive overtone, mid infrared (4000 cm^{-1}–400 cm^{-1}) relating to the vibrational energy transition of a molecule that provides information about functional groups in the molecule, and far infrared (400 cm^{-1}–10 cm^{-1}) to analyze molecules containing heavy atoms such as inorganic compounds. For compound analysis is usually done in the medium infrared area [5].

In the FTIR method, the tool used for analysis is the FTIR spectrophotometer. The working principle of this method is the interaction between energy and material. Some

infrared that passes through the gap to the sample is absorbed by the sample and others are transmitted through the sample surface so that the infrared light passes through the detector and the measured signal is then sent to a computer and recorded in the form of peaks [5]. The advantages of this method over other spectroscopic methods are fast, non-destructive, ease of use, and almost all compounds show absorption of infrared radiation. Compared to high performance liquid chromatography (HPLC), this method is simpler in sample preparation and uses only a small or no solvent so that it is friendly to the environment [6]. The disadvantage of this method is that the sampling space is relatively small, which can block infrared rays [5]. The validation parameters in this method are precision, accuracy, linearity, limit of detection (LOD), and limit of quantification (LOQ) [7].

FTIR can be used for both qualitative and quantitative analysis. In qualitative analysis, it is used to determine the structure and functional groups of a compound being analyzed. Functional group analysis of a compound is carried out by comparing the absorbance bands formed in the infrared spectrum using a comparison compound spectrum [4]. Quantitative analysis is used to determine the concentration of a compound from the analyzed sample. The principle in quantitative analysis is that the energy absorbed at a given wavenumber is proportional to the number of energy-related bonds, so with a greater concentration of compounds [8]. Therefore, this method can help in the identification phase of potential drug compounds in new drug development.

According to Law Number 36 of 2009 concerning Health in paragraph 1 of article 105, pharmaceutical preparations in the form of drugs and medicinal raw materials must meet the requirements in the Indonesian Pharmacopoeia or other standard books. One of the parameter requirements of the drug is said to be of good quality if the drug has met the specified concentration requirements. Quality control is an important part of how to make good drugs to ensure that each drug made always meets [6]. Therefore, each drug must be analyzed for its concentration quantitatively using various existing analytical methods. This study provides an explanation of the use of FTIR for quantitative analysis of compounds in drugs so that it can be used for the development of analysis methods that are simple, cheap, fast, and environment-friendly.

2. Methods

This study uses the systematic literature review (SLR) method with a qualitative approach to determine the use of Fourier Transform Infrared spectroscopy (FTIR) for quantitative analysis of compounds in drugs. The scientific articles used were obtained from Google Scholar, Science Direct, and NCBI pages. Journal searches were based on inclusion criteria using the keywords "quantitative analysis of compounds in drugs using Fourier Transform Infrared spectroscopy (FTIR)" or "use of Fourier Transform Infrared spectroscopy (FTIR)". Inclusion criteria in this study include research articles from national and international journals with publication years between 2005-2023 and using English or Indonesian. The research subject is Fourier Transform Infrared spectroscopy (FTIR) and the research topic is quantitative analysis of compounds in drugs using Fourier Transform Infrared spectroscopy (FTIR). Journals that meet the criteria and are in accordance with the research variables are then analyzed descriptively and then presented in tabular form. This literature review uses 20 articles from national and international journals that have been published and in accordance with the criteria.

Materials

Amoxicillin tablets, pentoxyfillin tablets, ciprofloxacin tablets, sanmol tablets, diclofenac sodium tablets, sodium seftriaxone tablets, ibupirac tablets, valsartan tablets, kalmicetine capsules, and reconstituted cefadroxil dry syrup.

3. Results and Discussion

Drugs are one of the pharmaceutical preparations used to treat disease, relieve symptoms, prevent disease, or diagnose disease [2]. Pharmaceutical preparations in the form of drugs and medicinal raw materials must meet the concentration requirements specified in the Indonesian Pharmacopoeia or other standard books to ensure that each drug made always meets quality requirements in accordance with its intended use [6]. Therefore, each drug must be analyzed for its concentration quantitatively using various existing analytical methods. FTIR spectrophotometers can be an alternative choice for quantitative analysis of compounds in drugs because most of the compounds in drugs are organic compounds [5].

A sample analyzed must be prepared before being analyzed using a FTIR spectrophotometer. Solid drug samples such as tablets and capsules must be smoothed to reduce the particle size so that they can be easily dissolved in the appropriate solvent. Liquid medicine samples such as dry syrup that have been reconstituted must be reconstituted with the appropriate solvent so that the powder can dissolve completely. To assist the sample dissolution process, it can be assisted by heating to the appropriate temperature so that the analyzed compound is not damaged by high temperatures [9]. Things that need to be considered in the selection of solvents are that they must be able to dissolve the sample perfectly, do not contain conjugated double bonds, are colorless, must be inert, and have high purity [10].

Table 1. Data from quantitative analysis of compounds in drugs using FTIR

Sample	Compound	Solvent	Wavenumber	Concentration	Description	Resource
Amoxicillin Tablets	Amoxicillin	Aquadest	1815 – 1736 cm^{-1}	100,4%	Mid infrared	[11]
Pentoxyfillin Tablets	Pentoxyfillin	Methanol	3000 – 2750 cm^{-1}	101,7%	Mid infrared	[10]
Ciprofloxacin Tablets	Ciprofloxacin	Methanol	1707 cm^{-1}	98,65%	Mid infrared	[12]
Sanmol Tablets	Paracetamol	Methanol	1668 cm^{-1}	102,69%	Mid infrared	[13]
Diclofenac Sodium Tablets	Diclofenac sodium	KBr (potassium bromide)	1550 – 1605 cm^{-1}	100,25%	Mid infrared	[14]
Sodium Seftriaxone Tablets	Sodium Seftriaxone	Aquadest	4000-400 cm^{-1}	101%	Mid infrared	[15]
Ibupirac Tablets	Ibuprofen	Chloroform	1648-1783 cm^{-1}	100,5%	Mid infrared	[16]
Valsartan Tablets	Valsartan	KBr (potassium bromide)	1732 cm^{-1}	101%	Mid infrared	[17]

Kalmicetine capsules	Chloramphenicol	Methanol	1694,1 cm^{-1}	100,8%	Mid infrared	[6]
Reconstituted cefadroxil dry syrup	Cefadroxil	Aquadest	1636,55 cm^{-1}	100,3%	Mid infrared	[18]

Amoxicillin is an organic compound that is very soluble in water that has a functional group C=O [11]. Pentoxyfillin is an organic compound soluble in methanol and chloroform that has O-H functional groups [10]. Ciprofloxacin is an organic compound soluble in methanol and alcohol that has a functional group C=O [12]. Paracetamol is an organic compound soluble in water and methanol that has C=C and C-H functional groups [13]. Diclofenac sodium is an organic compound soluble in methanol and potassium bromide which has a C=O functional group [14]. Sodium ceftriaxone is a water-soluble organic compound that has a C=O functional group [15]. Ibuprofen is an organic compound soluble in chloroform and acetone that has a functional group C=O [16]. Valsartan is an organic compound soluble in potassium bromide that has a C-H functional group [17]. Chloramphenicol is a water-soluble organic compound and methanol that has a C-H functional group [6]. Cefadroxil is a water-soluble organic compound that has a C-H functional group [18]. Compounds that can be analyzed using an FTIR spectrophotometer are organic and inorganic compounds so that all of these compounds can be analyzed quantitatively using an FTIR spectrophotometer. FTIR is an analytical technique for analyzing organic and inorganic molecules with a wavenumber range of 14000 cm^{-1}–10 cm^{-1} [5]. The solvent used needs to be adjusted to the solubility of the compounds contained in the sample and meet the requirements of the existing solvent. In Table 1, it shows that all solvents used are in accordance with the solubility of each compound present.

In Table 1, it can be seen that amoxicillin tablets containing amoxicillin compounds are analyzed by wavenumber 1815-1736 cm^{-1}. Analysis of pentoxyfilin tablets containing pentoxyfillin compounds was analyzed by wavenumber 3000-2750 cm^{-1}. Analysis of ciprofloxacin tablets containing ciprofloxacin compounds was analyzed by wavenumber 1707 cm^{-1}. Analysis of diclofenac sodium tablets containing diclofenac sodium compounds was analyzed by wavenumber 1550-1605 cm^{-1}. Analysis of sanmol tablets containing paracetamol compounds was analyzed by wavenumber 1668 cm^{-1}. Analysis of sodium ceftriaxone tablets containing sodium ceftriaxone compounds is analyzed by wavenumber 4000-400 cm^{-1}. Analysis of ibupirac tablets containing ibuprofen compounds was analyzed by wavenumber 1648-1783 cm^{-1}. Analysis of valsartan tablets containing valsartan compounds is analyzed by wavenumber 1732 cm^{-1}. Analysis of kalmicetine capsules containing chloramphenicol compounds is analyzed by wavenumber 1694,1 cm^{-1}. Analysis of reconstituted cefadroxil dry syrup containing cefadroxil compounds was analyzed by wavenumber 1636,55 cm^{-1}. All compounds in the drug were analyzed in the mid infrared region because they were in the wavenumber range 4000-400 cm^{-1}.

In FTIR spectrophotometry, certain frequencies absorbed by samples of organic compounds will cause higher vibrations. The determination of drug concentration is in the mid infrared region because this area is used to identify and predict chemical components in organic samples, including drugs [4]. In the infrared spectrum, each type of bond and functional group in the molecular structure has absorption at different infrared wavenumbers according to the vibrational properties of the molecule. The FTIR method makes it possible to determine functional groups in organic compounds, such

as stretching and bending of covalent bonds in molecules. Thus, the analysis of the mid infrared spectrum makes it possible to determine functional groups in organic compounds, including in drugs [19]. Table 1 shows the percentage of compounds in drugs analyzed by FTIR. The concentration of amoxicillin in the sample is 100,4%. The concentration of pentoxyfillin in the sample is 101,72%. The concentration of ciprofloxacin in the sample is 98,65%. The concentration of paracetamol in the sample is 102,69%. The concentration of diclofenac sodium in the sample is 100,25%. The concentration of sodium ceftriaxone in the sample is 101%. The concentration of ibuprofen in the sample is 100,5%. The concentration of valsartan in the sample is 101%. The concentration of chloramphenicol in the sample is 100,8%. The concentration of cefadroxil in the sample is 100,31%. All concentrations of these compounds meet the content requirements according to the Indonesian Pharmacopoeia VI Edition, that the amount of active substance compounds in a drug is not less than 90% and not more than 110% [20].

4. Conclusion

Fourier Transform Infrared spectroscopy (FTIR) is an infrared spectroscopy equipped with a Fourier transform for detection and analysis of spectrum results. This method is used to qualitatively and quantitatively analyze organic and inorganic molecules with a wavenumber range of 14000 cm-1–10 cm-1. Based on these wavenumbers, the infrared region is divided into three regions, such as near infrared, mid infrared, and far infrared. Quantitative analysis of amoxicillin, pentoxyphylline, ciprofloxacin, diclofenac sodium, ceftriaxone sodium, ibuprofen, valsartan, and cefadroxil compounds in the drug was carried out in the mid-infrared region. All compound concentrations meet the content requirements according to the Indonesian Pharmacopoeia VI Edition. Therefore, this method can help in the identification phase of potential drug compounds in new drug development. However, the sampling space of this method is relatively small which may block the infrared rays so it requires improvement to overcome it.

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