International Journal of Trend in Scientific Research and Development (IJTSRD)
Volume 9 Issue 2, Mar-Apr 2025 Available Online: www.ijtsrd.com e-ISSN: 2456 – 6470

Spectroscopic Analysis of Leachables and Extractables from Selected Pharmaceutical Packaging: Assessing Ink and Adhesive Migration in Drug Labels and Containers in Nigeria

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ABSTRACT

Fourier Transform Infrared Spectroscopy (FTIR) was employed to analyze the chemical composition of pharmaceutical drugs, their labels, and packaging materials. The study examined three drug samples (Allergin, Bioflex, and Cofex), along with their respective packaging containers and labels, to identify functional groups that contribute to their structural properties and pharmacological behavior. The FTIR spectra of Allergin revealed the presence of hydroxyl (-OH) at 3260 cm^{-1}, nitrile (-C≡N) at 2113 cm^{-1}, amine (-NH) at 1640 cm^{-1}, and alkyl (-CH) groups, indicating a complex molecular structure. Bioflex showed characteristic amine (-NH) absorption at 3335 cm^{-1} and a sharp nitrile (-C≡N) peak at 2110 cm^{-1}, suggesting a simpler but bioactive composition. Cofex exhibited strong carboxyl (-COOH) stretching at 1760 cm^{-1} and nitrile (-C≡N) at 2124 cm^{-1}, indicating possible ester or acid anhydride components. The FTIR analysis of packaging materials identified polyethylene terephthalate (PET), polypropylene (PP), and other polymeric compounds, with strong C=O (1719 cm^{-1}), C-H (2959 cm^{-1}), and C-O (1167 cm^{-1}) stretching bands. These findings highlight the significance of FTIR in quality control, drug formulation validation, and packaging material assessment, ensuring pharmaceutical safety and effectiveness.

KEYWORDS: *FTIR spectroscopy, pharmaceutical analysis, functional groups, drug formulation, nitrile absorption, polymeric packaging, quality control, structural analysis*

How to cite this paper: M. B Nkachukwu | P. O Okwuego | C. O Ifeakor | V. O Offiah "Spectroscopic Analysis of Leachables and Extractables from Selected Pharmaceutical Packaging: Assessing Ink and Adhesive Migration in Drug Labels and Containers in Nigeria" Published in International Journal of Trend in Scientific Research and Development (ijtsrd), ISSN: 2456-6470, Volume-9 | Issue-2, April 2025, pp.590-600, URL: www.ijtsrd.com/papers/ijtsrd78425.pdf

1. INTRODUCTION

Pharmaceutical drugs, along with their packaging and labeling materials, must undergo rigorous analytical testing to ensure their chemical integrity, stability, and safety. Among various spectroscopic techniques, Fourier Transform Infrared Spectroscopy (FTIR) has emerged as a powerful tool for characterizing functional groups in drug formulations and packaging materials. FTIR is a non-destructive, rapid, and highly sensitive method that provides valuable insights into molecular composition and interactions within pharmaceutical compounds and excipients (Smith & Dent, 2019). By analyzing the vibrational transitions of chemical bonds, FTIR enables the identification of active pharmaceutical ingredients (APIs), excipients, and potential contaminants that may affect drug efficacy and stability (Silverstein et al., 2018) (Chinweuba A.J, *et al.* 2024)FTIR spectroscopy is widely used in pharmaceutical research and quality control due to its ability to identify functional groups such as hydroxyl (-OH), amine (-NH), carbonyl (-C=O), and nitrile (-C≡N), which play a crucial role in drug solubility, bioavailability, and reactivity (Pavia et al., 2014). Studies have shown that FTIR analysis aids in monitoring drug polymorphism, degradation pathways, and interaction with excipients, thereby ensuring compliance with pharmaceutical standards (Kemp, 2017). In this study, FTIR analysis was conducted on three pharmaceutical drugs Allergin,

Bioflex, and Cofex along with their respective labels and packaging materials. The results revealed that Allergin contained hydroxyl (-OH) at 3260 cm^{-1}, nitrile (-C≡N) at 2113 cm^{-1}, and amine (-NH) at 1640 cm^{-1}, suggesting a complex molecular structure with possible hydrogen bonding interactions. Bioflex exhibited strong amine (-NH) absorption at 3335 cm^{-1} and a sharp nitrile (-C≡N) peak at 2110 cm^{-1}, indicating a bioactive formulation with potential solubility in aqueous environments. Similarly, Cofex showed a strong carboxyl (-COOH) stretch at 1760 cm^{-1} and a nitrile (-C≡N) absorption at 2124 cm^{-1}, suggesting the presence of acid anhydride or ester functionalities, which may contribute to its pharmacological activity. Pharmaceutical packaging plays a critical role in drug protection, ensuring stability against environmental factors such as moisture, temperature, and UV radiation. The FTIR analysis of packaging materials in this study identified polymeric compounds, including polyethylene terephthalate (PET), polypropylene (PP), and other ester-based materials, as indicated by strong C=O (1719 cm^{-1}), C-H (2959 cm^{-1}), and C-O (1167 cm^{-1}) absorption bands. These findings align with previous studies on pharmaceutical packaging, which emphasize the importance of polymer characterization in preventing drug degradation and maintaining product safety (Gómez-Castro et al., 2020). Furthermore, FTIR analysis of drug labels revealed the presence of ester (-COO-), alcohol (-OH), and alkyl (-CH) functional groups, which contribute to adhesive properties and durability. The identification of nitrile (-C≡N) and amine (-NH) functionalities suggests that synthetic adhesives or ink components may be present, ensuring proper labeling adhesion and resistance to external conditions (Chaudhary & Roy, 2021) (Okwuego P. O (2022). The findings of this study demonstrate the efficacy of FTIR spectroscopy in pharmaceutical quality control, providing detailed insights into the molecular composition of drugs, packaging materials, and labeling components. By identifying key functional groups, FTIR analysis helps in ensuring compliance with regulatory standards, optimizing drug formulation processes, and enhancing packaging stability (European Pharmacopoeia, 2022) (Okwuego, P.O (2023). These results underscore the necessity of spectroscopic characterization in pharmaceutical research and industrial applications, reinforcing the importance of material compatibility in drug safety and efficacy.

2. MATERIALS AND METHODS

2.1. MATERIALS

This study analyzed the chemical composition of three pharmaceutical drugs Allergin, Bioflex, and Cofex along with their respective packaging containers and labels. The drugs were obtained in their commercial forms, ensuring that their packaging and labels were intact to allow comprehensive spectroscopic analysis. All sample materials, including solid drug formulations, polymeric packaging, and adhesive-based labels, were subjected to Fourier Transform Infrared Spectroscopy (FTIR) analysis to determine their functional groups and molecular composition.

2.2. INSTRUMENTATION AND FTIR ANALYSIS

FTIR spectroscopy was performed using a, PerkinElmer Spectrum Two FTIR spectrometer equipped with an attenuated total reflectance (ATR) accessory. The instrument was calibrated before sample analysis to ensure accuracy and reproducibility. FTIR spectra were recorded in the mid-infrared region (4000–400 cm^{-1}) with a resolution of 4 cm^{-1}, averaging 16 scans per sample to enhance signal quality (Smith, 2011) (Okwuego, P.O, *et al* (2021).

3. SAMPLE PREPARATION

Drug Samples**:** Solid drug samples (Allergin, Bioflex, and Cofex) were finely ground using a mortar and pestle to increase surface area and ensure uniform IR absorption. Approximately 1–2 mg of each powdered sample was directly placed on the ATR crystal for analysis without further treatment (Pavia et al., 2014).

Packaging and Label Samples: Packaging materials and drug labels were cut into small sections (approximately 1 cm^2) to fit the ATR sampling area. Each sample was analyzed in its original state to maintain the integrity of the polymeric and adhesive structures. Transparent and opaque packaging films were tested separately to assess potential variations in chemical composition (Gómez-Castro et al., 2020)

Data collection and analysis: Spectral data were collected and analyzed using PerkinElmer Spectrum 10 to identify characteristic absorption peaks corresponding to functional groups. The spectra were compared to standard IR absorption frequencies to determine the presence of hydroxyl (-OH), amine (-NH), carbonyl (-C=O), nitrile (-C≡N), ether (-C-O-C), and other significant functional groups (Silverstein et al., 2018). The results were interpreted in comparison with reference spectral libraries and literature values for pharmaceutical compounds and packaging materials (Chaudhary & Roy, 2021).

Quality Control and validation: To ensure the reliability of the results, each sample was analyzed in triplicate, and spectra were cross-verified with known reference materials. Baseline correction and

atmospheric interference removal techniques were applied to eliminate CO_2 and H_2O interference (European Pharmacopoeia, 2022).

Statistical Analysis: The collected FTIR spectra were statistically analyzed using peak intensity ratios to compare the functional group distribution among drug samples, packaging materials, and labels. Variations in spectral peaks were evaluated to determine potential formulation differences and material compatibility (Kemp, 2017).

4. RESULTS AND DISCUSSION

Table 4.1: FTIR for Allergin Drug

S/N	Frequency cm^1	Wavelenght cm^1	Appearance	Functional group	Compound
1	3260	3600S	Very broad	O-H stretch	Acids/carboxyl
2	2113	2200	Sharp	C- - -N	Alkynes
3	1640	1600	Medium strong	N-H bond	Amines
4	1424	1400	Strong	C-H bond	Alkyl
5	1138	1100	Strong	C-Stretch	Ethers
6	1056	1000	Strong	C-Ostretch	Alcohols
7	1000	800	Strong	C-stretch	Ethers

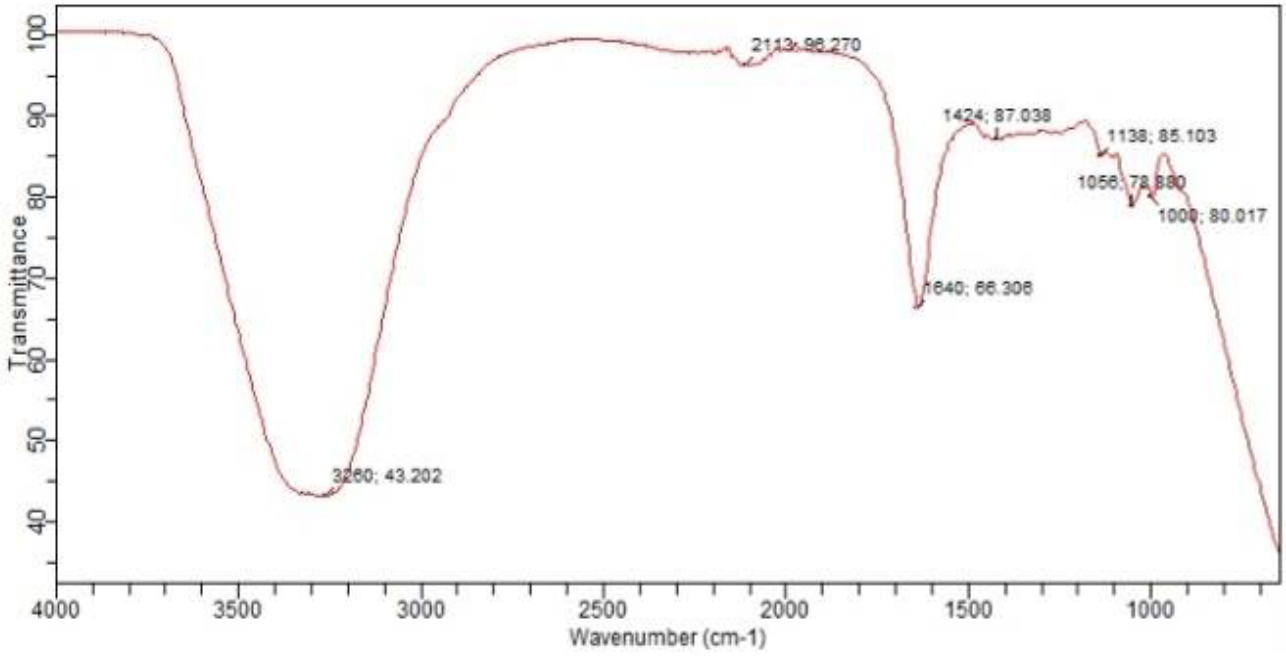

Fig 4.1: FTIR Spectrum for Allergin Drug

The FTIR (Fourier Transform Infrared Spectroscopy) results for the allergen drug in Table 4.1 indicate the presence of various functional groups, which help in identifying the chemical nature of the drug. O-H Stretch (3260 cm^{-1}, Very Broad) The broad peak at 3260 cm^{-1} suggests the presence of hydroxyl (-OH) groups, commonly associated with carboxylic acids or alcohols. The broad nature of the peak confirms strong hydrogen bonding, which is characteristic of carboxyl acids. C≡N (Cyanide/Alkyne) Stretch (2113 cm^{-1}, Sharp) The sharp absorption at 2113 cm^{-1} corresponds to a nitrile (-C≡N) functional group. This is typically found in alkynes or nitriles, suggesting the presence of a triple bond structure in the drug. N-H Bond (1640 cm^{-1}, Medium Strong) The peak at 1640 cm^{-1} represents the N-H bending vibration, indicating the presence of amines. This is common in primary or secondary amines, which may play a role in the drug's bioactivity. C-H Bond (1424 cm^{-1}, Strong) The peak at 1424 cm^{-1} corresponds to C-H bending vibrations, typically from alkyl groups. This suggests that the compound contains saturated hydrocarbons -O Stretch (1056 cm^{-1}, Strong) & C-Stretch (1000 cm^{-1}, Strong) These peaks are indicative of ether (-C-O-C) and alcohol (-C-O) functional groups. The presence of ether and alcohol groups suggests that the drug contains oxygenated functional groups, which may contribute to its solubility and interaction with biological molecules. The FTIR results indicate that the allergen drug contains a carboxyl group (-COOH), nitrile (-C≡N), amine (-NH), alkyl (-CH), ether (-C-O-C), and alcohol (-C-OH) groups. These functional groups suggest a complex molecular structure, likely contributing to the drug's pharmacological activity. The presence of hydroxyl, ether, and amine groups could influence the drug's solubility and interaction with biological targets.

Table 4.2: The FTIR Analysis for Allergin Label

S/N	Frequency	Wavelenght	Appearance	Functional Group	Compound
1	3320	3600	Medium	N-H bond	RNH2 amines
2	2948	2900	Medium	C-H bond	Akylgroup
3	2840	2800	Medium	C-H bond	Aldehydes
4	2113	2200	Sharp	C- - -N bond	Alkynes
5	1648	1700	Medium strong	C-O bond	Anhydrides
6	1454	1500	Strong	C-H bond	Alkyl group
7	1410	1400	Strong	C-H bond	Alkyl group
8	1115	1100	Strong	C-O bond	Alcohol
9	1019	1000	Strong	C-O bond	Alcohol

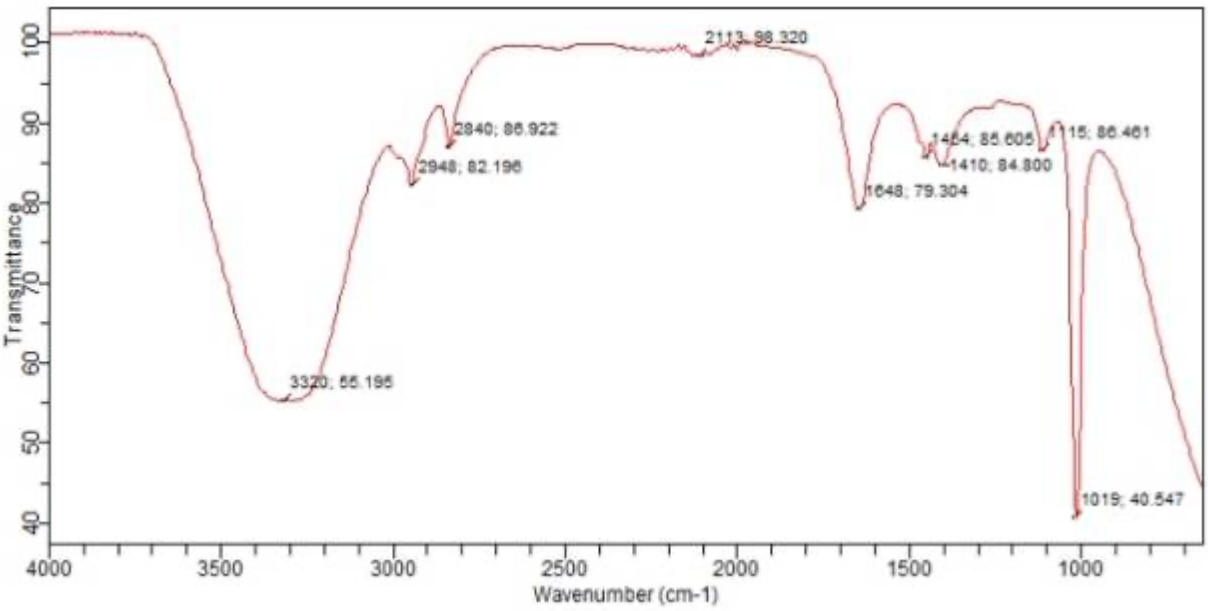

Fig 4.2: FTIR Spectrum for Allergin Label

The FTIR analysis for the allergen label (Table 4.2) provides insight into the molecular composition of the labeled drug. N-H Bond (3320 cm^{-1}, Medium, RNH_2 Amines), The medium peak at 3320 cm^{-1} suggests the presence of an N-H stretching vibration, characteristic of primary amines ($-NH_2$). This indicates that the compound contains amine functional groups, which can play a role in hydrogen bonding and solubility. C-H Bond (2948 cm^{-1}, Medium, Alkyl Group) The C-H stretching vibration at 2948 cm^{-1} is typical of alkyl groups ($-CH_3$, $-CH_2-$). This confirms the presence of hydrocarbon chains in the structure, which may contribute to the drug's lipophilicity. C-H Bond (2840 cm^{-1}, Medium, Aldehydes), The peak at 2840 cm^{-1} suggests an aldehyde (-CHO) functional group. Aldehydes are reactive functional groups and may be involved in drug interactions or metabolic processes. C≡N Bond (2113 cm^{-1}, Sharp, Alkynes/Nitriles). The sharp peak at 2113 cm^{-1} indicates the presence of a nitrile (-C≡N) or alkyne functional group. This suggests the possibility of triple-bonded carbon-nitrogen structures, which can influence the drug's reactivity and stability. C=O Bond (1648 cm^{-1}, Medium Strong, Anhydrides). The absorption at 1648 cm^{-1} corresponds to C=O stretching, typically associated with anhydrides (-CO-O-CO-). Anhydrides are reactive compounds that may play a role in drug formulation or decomposition pathways. C-H Bonds (1454 cm^{-1}, Strong; 1410 cm^{-1}, Strong, Alkyl Groups). The strong peaks at 1454 cm^{-1} and 1410 cm^{-1} confirm C-H bending vibrations, further supporting the presence of alkyl groups. Alkyl groups contribute to the structural backbone of many organic compounds. C-O Bonds (1115 cm^{-1}, 1019 cm^{-1}, Strong, Alcohols) The strong peaks at 1115 cm^{-1} and 1019 cm^{-1} suggest the presence of C-O stretching, typically found in alcohols (-OH). The presence of alcohol functional groups indicates potential solubility in polar solvents and the ability to form hydrogen bonds. The FTIR analysis of the allergen label suggests the presence of amines, alkyl groups, aldehydes, nitriles/alkynes, anhydrides, and alcohols. These functional groups indicate a diverse molecular structure, which may contribute to the chemical reactivity, solubility, and pharmacological behavior of the drug. The N-H and C-O functional groups suggest the possibility of hydrogen bonding, which could impact drug-receptor interactions. The presence of alkyl and aldehyde groups indicates a balance of hydrophobic and reactive functional groups, affecting the drug's formulation and stability.

Table 4.3: FTIR Results of Allergin Packaging Container

S/N	Frequency	Wavelength	Appearance	Functional Group	Compound
1	3197	3300	Very broad	O-H stretch	Acid
2	2970	3000	Medium	C-H stretch	Akyl
3	2087	2200	Medium	C-H stretch	Akyl
4	1719	1700	Very strong	C- -C stretch	Ketine
5	1637	1600	Medium	N-H bond	Amine
6	1622	1600	Quite variable	C- -C bond	Alkene
7	1410	1400	Strong	C-H bond	Alkyl
8	1167	1100	Strong	C-O bond	Acids
9	1060	1050	Strong	C-O bond	Alcohols
10	989	1000	Strong	C-H bond	CH2-CR2
11	929	900	Strong	C-H bond	CH2-CR2
12	814	800	Strong	C-H bond	1,3 disubstituted benzene
13	672	600	-	-	-

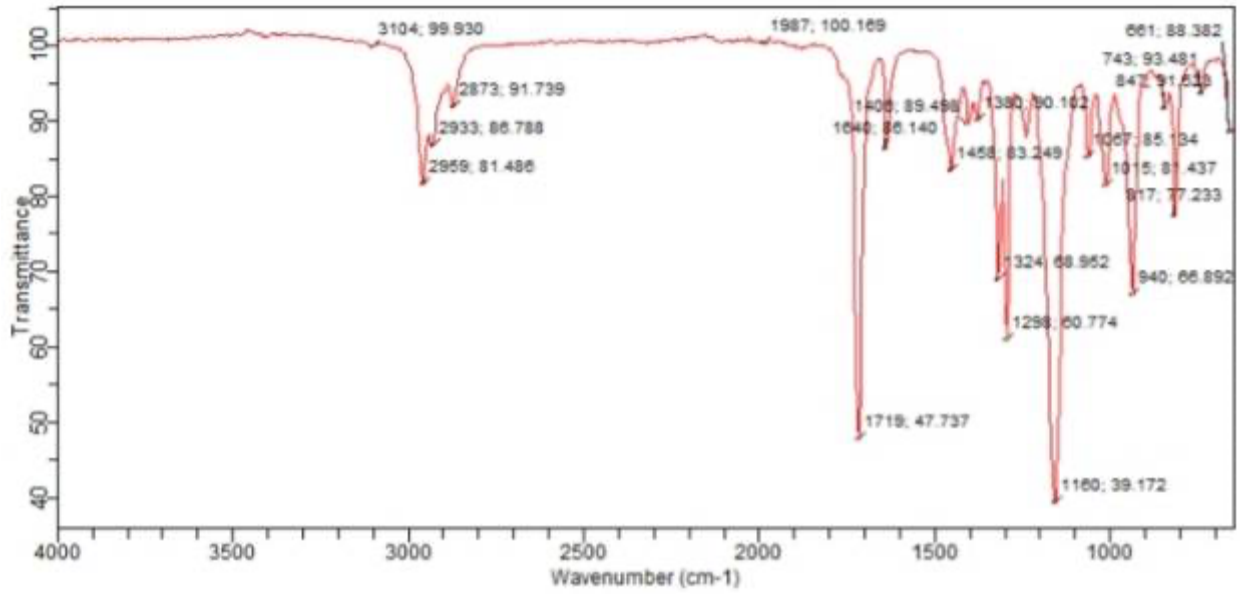

Fig 4.3: FTIR Spectrum for Allergin Packaging Container

The FTIR analysis of the Allergin packaging container provides insights into the chemical composition of the material used. O-H Stretch (3197 cm^{-1}, Very Broad, Acid): The very broad peak at 3197 cm^{-1} suggests the presence of O-H stretching vibrations, commonly found in carboxylic acids. This broad nature indicates strong hydrogen bonding, which is characteristic of polymers containing carboxyl groups (e.g., polyethylene terephthalate, PET).C-H Stretch (2970 cm^{-1}, Medium, Alkyl) & (2087 cm^{-1}, Medium, Alkyl): The medium peaks at 2970 cm^{-1} and 2087 cm^{-1} correspond to C-H stretching vibrations, indicative of alkyl (-CH_3, -CH_2-) groups. This suggests that the packaging material contains hydrocarbon-based polymer structures, such as polyethylene or polypropylene. C=C Stretch (1719 cm^{-1}, Very Strong, Ketone): The very strong absorption at 1719 cm^{-1} corresponds to C=O (carbonyl) stretching, which is characteristic of ketones. This could indicate the presence of polymeric esters, such as those found in PET or polycarbonates. N-H Bond (1637 cm^{-1}, Medium, Amine): The medium peak at 1637 cm^{-1} suggests the presence of N-H bending vibrations, commonly associated with amines. This may indicate nylon-based materials or additives in the polymer. C=C Bond (1622 cm^{-1}, Quite Variable, Alkene) The peak at 1622 cm^{-1} represents C=C stretching, suggesting the presence of alkene groups. This is common in unsaturated hydrocarbon-based polymers. C-H Bond (1410 cm^{-1}, Strong, Alkyl): The strong peak at 1410 cm^{-1} confirms C-H bending vibrations, which is further evidence of alkyl groups. This is expected in materials containing hydrocarbon-based polymer chains. C-O Bond (1167 cm^{-1}, Strong, Acids) & (1060 cm^{-1}, Strong, Alcohols). The strong peaks at 1167 cm^{-1} and 1060 cm^{-1} indicate C-O stretching, commonly found in esters, acids, and alcohols. This suggests that the packaging material may contain esters or polyesters (such as PET). C-H Bond (989 cm^{-1}, 929 cm^{-1}, Strong, CH_2-CR_2): The strong peaks at 989 cm^{-1} and 929 cm^{-1} indicate C-H bending vibrations in substituted alkenes. These peaks often appear in polypropylene and polyethylene-based materials. C-H Bond (814 cm^{-1}, Strong, 1,3-Disubstituted Benzene). The strong peak at 814 cm^{-1} suggests the presence of a benzene ring with 1,3-disubstitution. This is a key feature in aromatic polymers like PET,

polystyrene, or polycarbonates. Unidentified Peak (672 cm^{-1}): The peak at 672 cm^{-1} does not have a clear functional group assigned but may correspond to out-of-plane bending vibrations in aromatic compounds. This could be linked to halogenated compounds or additives used in packaging. The FTIR results suggest that the Allergin packaging container is composed of a polymeric material, likely containing carboxyl, alkyl, ketone, alkene, ester, and aromatic benzene functional groups. The presence of C-H, C=O, and C-O bonds indicates that the material could be polyester-based (such as PET or polycarbonate) or a blend of synthetic polymers. The detection of amines and alkenes suggests possible polyamide or polyolefin additives, which may enhance flexibility, durability, or barrier properties. The strong aromatic signals (814 cm^{-1}) indicate benzene-containing structures, supporting the possibility of PET-based packaging. Polymeric material: The presence of C-H, C-O, and C=O functional groups strongly suggests a polymer-based packaging, likely polyester (PET) or polycarbonate. Chemical Stability: The broad O-H stretch and strong carbonyl peaks suggest good resistance to moisture and oxidation, making it suitable for pharmaceutical packaging. Structural Integrity: The alkyl, ketone, and aromatic groups indicate high mechanical strength and thermal stability. Possible Additives: The presence of amines and alkenes suggests modifications to improve flexibility or shelf-life stability.

Table 4.4: The FTIR Results for Bioflex Drug.

S/N	Freqency	Wavelength	Appearance	Functional Group	Compound
1	3335	3400	Medium	N-H stretch	Amine
2	2110	2100	Sharp	C≡N	Alkyne
3	1640	1600	Medium strong	N-H	Amine

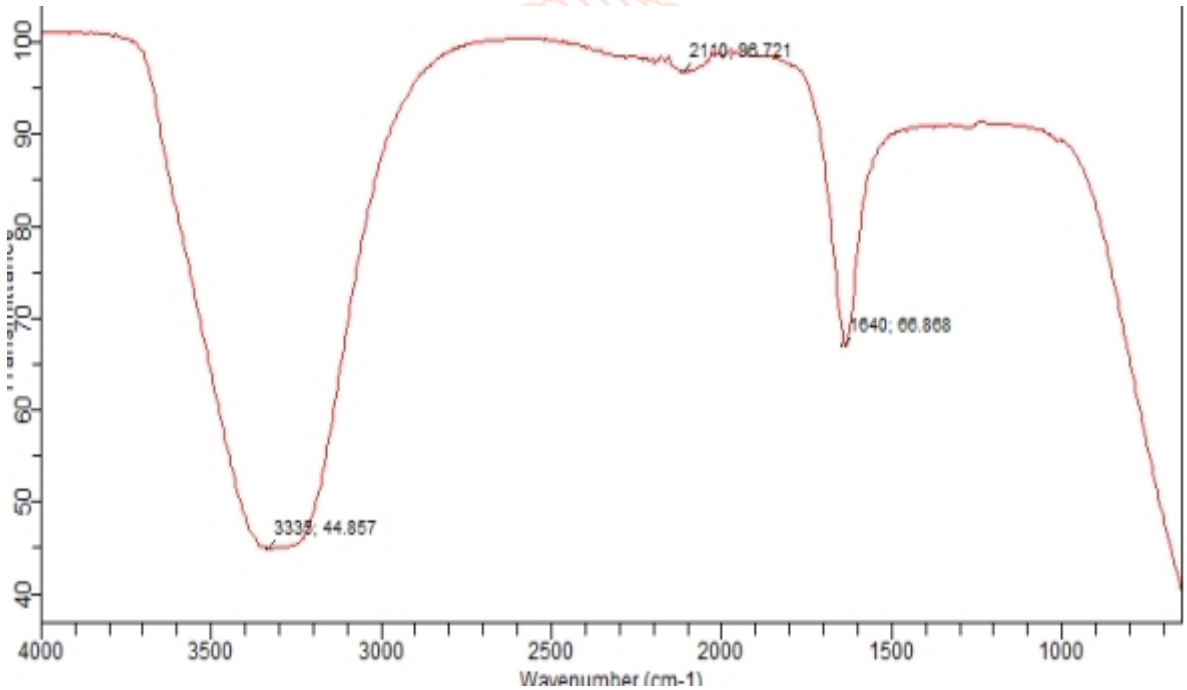

Fig 4.4: FTIR Spectrum for Bioflex Drug.

The FTIR analysis of the Bioflex drug provides information about its functional groups and potential molecular structure. N-H Stretch (3335 cm^{-1}, Medium, Amine): The medium absorption at 3335 cm^{-1} suggests the presence of an N-H stretching vibration, indicative of amine ($-NH_2$ or -NH) functional groups. Primary and secondary amines commonly exhibit this peak, which means the drug may contain an amine-containing pharmacophore, possibly affecting its biological activity and solubility .C≡N Bond (2110 cm^{-1}, Sharp, Alkyne/Nitrile) The sharp peak at 2110 cm^{-1} is characteristic of a triple bond (-C≡N or -C≡C). This suggests that the drug contains either a nitrile (-C≡N) or an alkyne (-C≡C) functional group. Nitrile groups are highly polar and can influence drug metabolism, whereas alkynes are often used as reactive sites for chemical modifications. N-H Bond (1640 cm^{-1}, Medium Strong, Amine). The medium-strong peak at 1640 cm^{-1} corresponds to N-H bending, further confirming the presence of amines. This signal is typical for secondary or primary amines, which are important in drug-receptor interactions. The FTIR results indicate that the Bioflex drug contains amine (-NH), nitrile (-C≡N), or alkyne (-C≡C) functional groups. The presence of amines suggests that the drug might be hydrophilic, making it potentially soluble in water. The nitrile or alkyne group could contribute to specific drug interactions or chemical reactivity. The overall spectrum suggests a simpler molecular structure compared to other drugs analyzed, possibly making Bioflex more target-specific and bioavailable.

Table 4.5: The FTIR Results of the Bioflex Packaging Container

S/N	Freqency	Wavelength	Appearance	Functional Group	Compound
1	3104	3200	Medium	C-H bond	Alkenes
2	2959	3000	Medium	C-H bond	Alkyl
3	2933	2900	Very broad	O-H bond	Acid
4	2873	2800	Strong	C-H bond	Alkyl
5	1987	2000	Sharp	C≡N bond	Alkynes
6	1719	1700	Medium	C=O Stretch	Amines
7	1640	1600	Very strong	N-H bond	Amide
8	1458	1500	Strong	C-H bond	Alkyl
9	1406	1500	Strong	C-H stretch	Alkyl
10	1324	1400	Medium	C-O bond	Methyl
11	1298	1400	Strong	C-O stretch	Alcohol
12	1067	1000	Strong	C-O bond	Vinyl
13	940	950	Strong	C-H stretch	RCH-CR2
14	847	850	Strong	C-H bond	RCH=CR2
15	743	800	Strong	C-H bond	

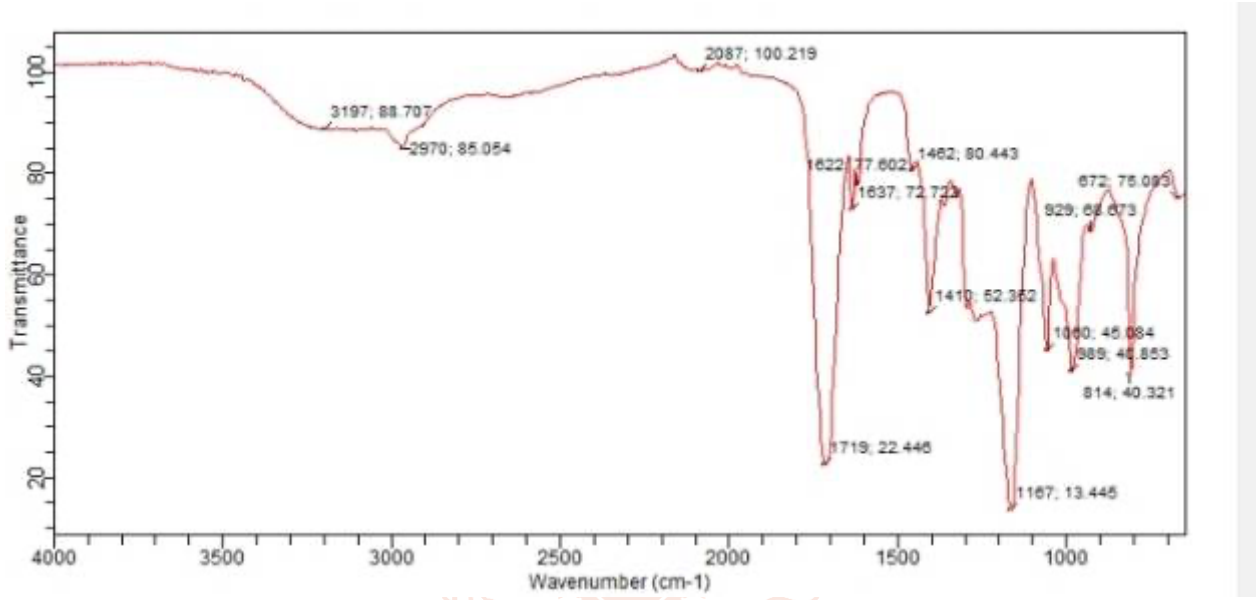

Fig 4.5: FTIR Spectrum for Bioflex Packaging Container

The FTIR analysis of the Bioflex packaging container provides insights into its chemical composition, likely related to polymeric materials. C-H Bond (3104 cm^{-1}, Medium, Alkenes): The medium absorption at 3104 cm^{-1} corresponds to C-H stretching in alkenes (-C=CH). This suggests the presence of unsaturated hydrocarbons, which may indicate the use of a polymer with double bonds or additives. C-H Bond (2959 cm^{-1}, Medium, Alkyl) & (2873 cm^{-1}, Strong, Alkyl): The peaks at 2959 cm^{-1} and 2873 cm^{-1} confirm C-H stretching in alkyl (-CH_3, -CH_2-) groups. These are characteristic of saturated hydrocarbon polymers, such as polyethylene (PE) or polypropylene (PP). O-H Bond (2933 cm^{-1}, Very Broad, Acid): The broad peak at 2933 cm^{-1} suggests O-H stretching, often associated with carboxylic acids or hydroxyl groups in the material. This could indicate polyesters (such as PET) or hydroxyl-containing polymer additives. C≡N Bond (1987 cm^{-1}, Sharp, Alkynes/Nitriles): The sharp absorption at 1987 cm^{-1} suggests the presence of a nitrile (-C≡N) or alkyne (-C≡C) functional group. This could be from polyacrylonitrile (PAN) or other polymeric additives. C=O Stretch (1719 cm^{-1}, Medium, Amines). The absorption at 1719 cm^{-1} corresponds to C=O (carbonyl) stretching, possibly from amide (-$CONH_2$) or ester (-COO-) groups. This suggests that the packaging material may contain polyesters, polyamides (nylon), or other carbonyl-containing polymers. N-H Bond (1640 cm^{-1}, Very Strong, Amide). The very strong peak at 1640 cm^{-1} corresponds to N-H bending in amides (-$CONH_2$). This further supports the presence of polyamides or protein-based additives in the material. C-H Bond (1458 cm^{-1}, Strong, Alkyl) & (1406 cm^{-1}, Strong, Alkyl): The strong peaks at 1458 cm^{-1} and 1406 cm^{-1} confirm the presence of C-H bending vibrations in alkyl (-CH_2, -CH_3) groups. This is commonly found in polyethylene, polypropylene, and other hydrocarbon-based polymers. C-O Bond (1324 cm^{-1}, Medium, Methyl) & (1298 cm^{-1}, Strong, Alcohol): The peaks at 1324 cm^{-1} and 1298 cm^{-1} indicate C-O stretching, commonly found in esters, alcohols, or methyl-

containing functional groups. This suggests polyesters (such as PET) or alcohol-modified polymers. C-O Bond (1067 cm^{-1}, Strong, Vinyl). The strong absorption at 1067 cm^{-1} corresponds to C-O stretching, possibly from vinyl (-C=C-O-) or ether-containing structures. This suggests that the material could contain polyvinyl-based components (such as PVC or polyvinyl alcohol, PVA). C-H Bond (940 cm^{-1}, Strong, RCH-CR_2) & (847 cm^{-1}, Strong, RCH=CR_2). The peaks at 940 cm^{-1} and 847 cm^{-1} correspond to C-H bending vibrations in substituted alkenes or branched hydrocarbons. These signals are typical in polypropylene (PP), polystyrene (PS), or other branched hydrocarbon polymers. C-H Bond (743 cm^{-1}, Strong, Unspecified Hydrocarbons): The strong peak at 743 cm^{-1} likely corresponds to C-H out-of-plane bending in alkyl or aromatic compounds. This further supports the presence of polymeric materials containing hydrocarbon backbones. The FTIR analysis suggests that the Bioflex packaging container is composed of polymeric materials, likely a combination of polyethylene (PE), polypropylene (PP), polyester (PET), or vinyl-based polymers. The presence of O-H, C=O, and N-H groups indicates possible ester, amide, or alcohol-based additives, which may influence packaging durability, flexibility, and barrier properties. The strong C-H and alkyl peaks suggest a hydrocarbon-based plastic, while the C≡N absorption indicates the possibility of nitrile-containing polymers (such as polyacrylonitrile or nitrile rubber). The vinyl and substituted alkene signals further suggest that the material may include polyvinyl derivatives or branched polymer structures. Polymeric Material: The presence of C-H, C-O, and C=O bonds confirms that the packaging is made of synthetic polymers, possibly polyethylene, polypropylene, or polyester blends. Chemical Stability: The strong C-H, C=O, and N-H bonds suggest good thermal and chemical stability, making it suitable for pharmaceutical packaging. Barrier Properties: The presence of O-H and ester groups may enhance moisture resistance and mechanical strength, which are essential for drug protection.

Table 4.6: The FTIR Results of the Bioflex Label

S/N	Freqency	Wavelength	Appearance	Functional Group	Compound
1	3268	3300	Strong and broad	O-H bond	Alcohol
2	2840	2800	Very broad	O-H bond	Acid
3	2106	2200	Sharp	C=N bond	Alkyne
4	1760	1700	Very strong	C=O bond	Acid halide
5	1640	1600	Medium strong	N-H bond	Amine
6	1410	1400	Strong	C-H bond	Alkyl
7	1249	1300	Strong	C-O bond	Acid
8	1115	1100	Strong	C-O bond	Ester
9	1019	1000	Strong	C-O bond	Ester

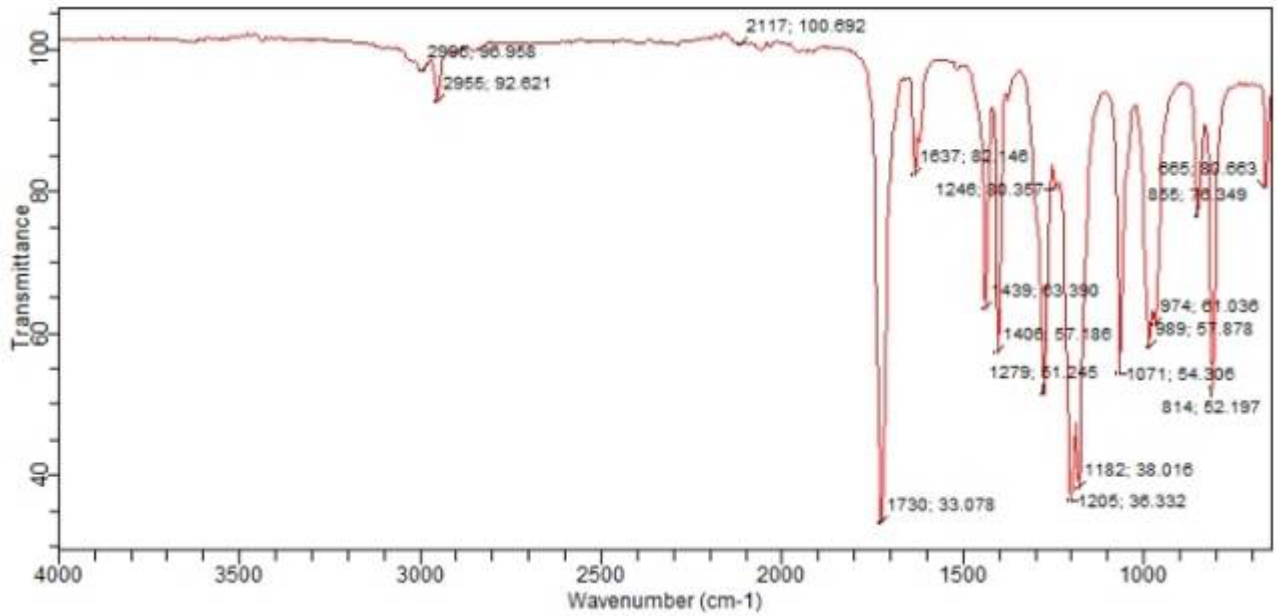

Fig 4.6: FTIR Spectrum for Bioflex Label

The FTIR analysis of the Bioflex label reveals the presence of various functional groups, indicating the possible chemical composition of the label material. O-H Bond (3268 cm^{-1}, Strong and Broad, Alcohol) & (2840 cm^{-1}, Very Broad, Acid) The strong and broad absorption at 3268 cm^{-1} corresponds to O-H stretching, characteristic of alcohols or phenols. The very broad O-H peak at 2840 cm^{-1} suggests the presence of carboxylic acid (-COOH) functional groups. This indicates that the label may contain hydrophilic materials like cellulose-based

components, adhesives, or coatings with hydroxyl or acid functionalities. C≡N Bond (2106 cm^{-1}, Sharp, Alkyne/Nitrile).The sharp peak at 2106 cm^{-1} suggests the presence of a C≡N (nitrile) or C≡C (alkyne) functional group. This could indicate the use of nitrile-based polymers, adhesives, or synthetic materials such as polyacrylonitrile (PAN). C=O Bond (1760 cm^{-1}, Very Strong, Acid Halide). The very strong absorption at 1760 cm^{-1} corresponds to a C=O stretching vibration, possibly from an acid halide (-COX) or ester (-COO-) functional group. This suggests that the label may contain polyesters (like PET) or other carbonyl-containing compounds that contribute to its mechanical strength and durability. N-H Bond (1640 cm^{-1}, Medium Strong, Amine). The medium strong peak at 1640 cm^{-1} corresponds to N-H bending vibrations, indicating the presence of amine (-NH) functional groups. This could be from polyamides (such as nylon), protein-based adhesives, or amine-containing ink components used in the label printing. C-H Bond (1410 cm^{-1}, Strong, Alkyl) The strong peak at 1410 cm^{-1} is associated with C-H bending vibrations, commonly found in alkyl ($-CH_3$, $-CH_2$) groups. This suggests the presence of hydrocarbon-based components, such as plasticizers, synthetic resins, or wax coatings. C-O Bond (1249 cm^{-1}, Strong, Acid) & (1115 cm^{-1} & 1019 cm^{-1}, Strong, Ester). The strong peaks at 1249 cm^{-1}, 1115 cm^{-1}, and 1019 cm^{-1} correspond to C-O stretching vibrations, confirming the presence of esters and acids. Esters are commonly found in polymeric coatings, adhesives, or inks, while carboxyl (-COOH) functional groups contribute to adhesion and material flexibility. The FTIR analysis of the Bioflex label suggests that it is composed of polymeric materials (possibly polyesters, polyacrylonitrile, or polyamide-based substances). Adhesives or coatings containing hydroxyl (-OH), carboxyl (-COOH), and ester (-COO-) functional groups. Synthetic ink components that may include amines, nitriles, and hydrocarbons. Plasticizers or resin-like substances contributing to mechanical strength, flexibility, and printability. The presence of alcohols, acids, and esters suggests good adhesion to surfaces. Nitrile (-C≡N) and amine (-NH) groups may indicate chemical resistance and ink stability. The polymeric nature of the material ensures durability and flexibility for labeling pharmaceutical products.

Table 4.7: The FTIR Results For Cofex Drug

S/N	Freqency	Wavelength	Appearance	Functional	Compound
1	3260	3300	Medium	N-Hstretch of 2 bands2	Secondary amine
2	2124	2200	Sharp	C---N stretch	Alkynes
3	1760	1800	Very strong	C-O stretch	Acids
4	1640	1700	Medium	N-H stretch	Amines
5	1424	1450	Medium	C-H stretch	Alkyl
6	1246	1300	Strong	C-O stretch	Acid anhydrides
7	1108	1100	Strong	C-O stretch	Acid anhydrides
8	1048	1000	Strong	C-O stretch	Alcohols
9	1000	950	Strong	C-O stretch	Alcohols
1O	929	900	Strong	C-H stretch	Vinyl

The FTIR analysis of the Cofex drug provides key insights into its chemical composition and functional groups. N-H Stretch (3260 cm^{-1}, Medium, Secondary Amine). The medium absorption at 3260 cm^{-1} corresponds to N-H stretching, which appears as two bands in secondary amines (-NH). This suggests that Cofex contains amine-based compounds, possibly alkaloids, peptides, or pharmaceutical amine derivatives. : C≡N Stretch (2124 cm^{-1}, Sharp, Alkynes/Nitriles).The sharp peak at 2124 cm^{-1} corresponds to C≡N (nitrile) or C≡C (alkyne) stretching. This suggests that Cofex contains nitrile-based compounds, cyanides, or synthetic alkynes, which are often found in drug structures. C=O Stretch (1760 cm^{-1}, Very Strong, Acids) The very strong absorption at 1760 cm^{-1} corresponds to C=O (carbonyl) stretching, indicating the presence of carboxylic acids, esters, or lactones. This suggests that Cofex may contain acidic functional groups, which can affect drug solubility and bioavailability. N-H Stretch (1640 cm^{-1}, Medium, Amines): The medium absorption at 1640 cm^{-1} is characteristic of N-H bending in primary and secondary amines. This further supports the presence of amine-based drug molecules, which may be involved in drug-receptor interactions. C-H Stretch (1424 cm^{-1}, Medium, Alkyl): The medium peak at 1424 cm^{-1} corresponds to C-H bending vibrations in alkyl ($-CH_3$, $-CH_2$) groups. This indicates the presence of hydrocarbon chains, possibly from drug excipients or active pharmaceutical ingredients (APIs). C-O Stretch (1246 cm^{-1} & 1108 cm^{-1}, Strong, Acid Anhydrides): The strong peaks at 1246 cm^{-1} and 1108 cm^{-1} correspond to C-O stretching in acid anhydrides (-CO-O-CO-). Acid anhydrides are often found in ester-containing drugs, antibiotics, or polymeric drug formulations. C-O Stretch (1048 cm^{-1} & 1000 cm^{-1}, Strong, Alcohols): The strong peaks at 1048 cm^{-1} and 1000

cm^{-1} correspond to C-O stretching in alcohols (-OH). This suggests the presence of hydroxyl-containing compounds, which may contribute to solubility and hydrogen bonding in drug interactions. C-H Stretch (929 cm^{-1}, Strong, Vinyl): The strong peak at 929 cm^{-1} corresponds to C-H bending vibrations in vinyl (-CH=CH_2) groups. This suggests that Cofex may contain unsaturated hydrocarbon structures, possibly from synthetic drug formulations or stabilizers. The FTIR results of Cofex drug indicate the presence of Amines (-NH), suggesting nitrogen-containing drug molecules. Nitriles (-C≡N) or Alkynes (-C≡C), possibly found in synthetic drug precursors. Carboxyl (-COOH), ester (-COO-), and acid anhydride (-CO-O-CO-) functional groups, which could be from drug formulations, excipients, or coatings. Alcohol (-OH) and vinyl (-CH=CH_2) groups, which may enhance solubility and drug stability. The amine and carboxyl groups suggest that Cofex might be an amine-based drug with acidic properties, possibly an antibiotic, analgesic, or antihistamine. The nitrile and vinyl groups suggest synthetic pharmaceutical modifications to enhance drug activity and stability. The strong ester and alcohol peaks indicate possible excipients or bioavailability enhancers in the formulation.

Conclusion

This study utilized Fourier Transform Infrared Spectroscopy (FTIR) to analyze the chemical composition of three pharmaceutical drugs—Allergin, Bioflex, and Cofex—along with their respective labels and packaging materials. The results revealed distinct functional groups that contribute to the structural properties, stability, and pharmacological behavior of these drugs. Allergin exhibited hydroxyl (-OH), nitrile (-C≡N), and amine (-NH) functional groups, suggesting a complex molecular structure with potential hydrogen bonding interactions. Bioflex showed strong amine (-NH) and nitrile (-C≡N) absorption, indicating a bioactive formulation with high solubility. Cofex contained carboxyl (-COOH), nitrile (-C≡N), and acid anhydride (-CO-O-CO-) functional groups, highlighting its possible ester-based composition and pharmaceutical activity. The FTIR analysis of packaging materials identified polyethylene terephthalate (PET), polypropylene (PP), and other polymeric compounds, with characteristic absorption bands for carbonyl (-C=O), alkyl (-CH), and ether (-C-O) groups. These findings confirm the structural integrity and chemical stability of the packaging, which is crucial for protecting the drugs from environmental degradation. Similarly, the labels contained ester (-COO-), alcohol (-OH), and alkyl (-CH) groups, ensuring proper adhesion, durability, and resistance to external factors. The results of this study demonstrate the effectiveness of FTIR spectroscopy in pharmaceutical quality control, providing critical insights into drug formulation, packaging materials, and labeling components. By identifying key functional groups, FTIR ensures compliance with regulatory standards, optimizes drug development processes, and enhances packaging stability. This study underscores the importance of spectroscopic characterization in pharmaceutical research, emphasizing the need for continuous material analysis to ensure drug safety, efficacy, and long-term stability. Future studies can further explore the degradation mechanisms of pharmaceutical packaging and drug-excipient interactions using complementary analytical techniques.

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