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Original Research

Pharmaceutical and Medical Applications of Fourier Transform Infrared Spectroscopy (FTIR), and Nuclear Magnetic Resonance (NMR)

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Abstract:

In the domains of pharmaceuticals and microbiology, there are a number of analytical techniques and among these popular techniques is the infrared spectroscopy. Among the various techniques employed in the optical spectroscopy FTIR or Fourier transform infrared spectroscopy is considered to be one of the most efficient. This is a chemical method that uses infrared radiation at a specific wavelength to study the peak vibrations of a given chemical compound to identify the structure of the compound. This is the most efficient analysis when compared to the other two and does not harm the chip in any way. Overall, it is useful in assessing the values of any biotechnology pharmaceutical in both solid and liquid forms as well as any other detergent form. This paper presents a brief overview of Fourier transform infrared spectroscopy (FTIR) in multiple fields of specializations including biochemistry, geochemistry and the analysis of some herbal medicines and oils.

Since herbs are mixtures of multiple components for which every component possesses unique properties and characteristics, analytical chemists still work with challenging problems while doing pharmacognostic analysis of medicinal herbs. Ensuring quality of the raw materials used and the finished herbal products was mainly achieved through Chemical Analysis that involves the use of instruments such as Gas Chromatography, Mass Spectrometer, and High-Performance Liquid Chromatography. When one considers the vast popularity of using this technique in areas such as microbiology, pharmaceuticals, and the food and bev- erage industries, along with many others, the lack of spe- cific applications of infrared (IR) spectroscopy for analyzing herbs has been somewhat astonishing. This essay lays the following objectives: firstly, to provide future researchers with a basis for further study on plant analysis with herbs as an interest; secondly, to elongate the use of Fourier transform infrared spectroscopy in the field of herbal analysis in particular. Hence, a case study was made employing sound chemometric tools like PCA and SIMCA for obtaining the necessary chemical insights from the infrared spectra. The above stated method can effectively help in the authentication of a wide number of herbal samples and can also serve to provide a measure of assurance to quality control.

There are many instruments that can be used for qualifying and quantifying substances namely nuclear magnetic resonance (NMR). Further, data reduction can be performed using NMR since the technique is quantitative in nature. Quantitative nuclear magnetic

resonance (qNMR) has dual uses in the pharmaceutical industry: The key goals of the analysis were the identification and quantification of medications. When it comes to the primary phase in drug development, a small sample is best suited for trials and testing. Therefore, to maximise value from minimised cost, time, and quantity of samples, this method has to be given priority. This method is quite revolutionary in the characterization of formulations and the identification of IPC samples particularly for contaminants, active medicinal substances, and residual solvents. Meanwhile, the political aspect of the pharmaceutical business reveals that qNMR is regularly employed to qualify virtually any drug product, as pointed out by analysts. Both proportional and referential methods come into handy when one is seeking to attach a specific figure to a given segment in both process control samples as well as final products.

Keywords: FTIR, Geochemical research, Biological, food ingredients.

Introduction:

Analytical chemistry is the branch of chemistry that deal with the micro determination of elements or compound and analytical method involves simple handling of samples, hence sample preparations of solid substance is not time consuming. The procedure of elemental analysis conducted through an X-Ray Fluorescence Spectroscopy (XRF) and the proposed vibrational deformations of chemical limits were explained through Fourier Transform Infrared Spectroscopy (FTIR). Many scientists, especially in the field of organic chemistry and biochemical research, have long realised the potential of applying Fourier transform infrared spectroscopy as an analytical procedure. Also, it can quantitatively and qualitatively analyze as to what the sample appears to contain, and how much of it is present in an unknown sample. Using the specified theory permits samples to be analyzed in various states, including the solid, liquid, pasting, powder, furnished, and gaseous states [1]. This is an approach that provides a rapid analysis time, requires little sample preparation, and requires limited sample volumes. And just how it works might be virtually explained as the abilities organic for every person. It is possible to check how effective FTIR spectroscopy is for the qualitative identification of minerological composition of mixes in natural compounds, such as postglacial deposits containing sand and such, and it may even provide rather valuable minerogical data [2]. He mentioned that attempts to merge IR with biology were initiated in the early 1910s with the intention to utilize IR spectroscopy for analyzing the chemicals contained in living beings. It could be done by the late 1940s, when the technique was successfully applied for the investigation of biological samples; at the present time, infrared spectroscopy constitute one of standard tools used for the description of biomolecules. In the past, the FTIR technique was employed in several different capacities all of which were linked to microbes in the 1950s. During the current year, several research papers have been published describing the application of infrared spectroscopy, particularly using infrared (IR) spectroscopy for bacterial identification. While it is true that various strains of bacteria have distinct IR spectra, a 1959 acclaimed review of the subject concluded to the effect that it was impossible to speak of bacteria identification as a practical process if one was to consider IR techniques, and as such, could not therefore be classified as a scheme.

The concept which underlies infrared spectroscopy is the variation of absorptance (or emittance) of a sample with wavelength of infra-red radiation. [9] One of the possibilities of the application of IRA concerns the molecular structure elucidation. These motions are comprised of vibrations within an infrared spectrum of a polyatomic molecular compound

and depend on atomic mass, bond strength, and intra or inter molecular interactions. Thus, one may be able to 'decode' the specific presence of an organic molecule in question in its Infra-Red spectrum in a way that is different from that of other compounds, even other isomers having similar infra-red absorption spectra. The most effective type of identification by the use of IR spectra involves absorption spectra; spectra of most of the substances are henceforth identifiable when reference spectra are available. Far infrared is the frequency region on the electromagnetic spectrum as a whole which is extended from 12800 cm−1 to 10 cm−1. There are three categories of the infrared spectrum, which is divided by the way light behaves while traversing natural molecules [3, 4]. It provide some advantages compared with other types of spectroscopy, for example internal wavelength calibration excess Connes, high optical throughput excess Jacquinot, and wave number(s) simultaneity excess Fellgett. In general, fluorine is used to enhance the SNR which in turn increases the sensitivity and makes spectroscopic analysis to have high reliability and generate accurate procedures [5, 6]. Figures 1 and 2 exhibit two graphics of chosen closely planted species analyzed by HATR and FTIR spectra, respectively. The stretching of OH, NH which are more frequently found in proteins and carbohydrates are comparable with a localise absorption band at around 3400 cm 1. There are strong signals specific to lipids and carbohydrates that can be observed at 3000 cm−1, which belonged to the CH stretching vibrational band. The out of plane bending CH bond temperature sensitive absorption band was completely shielded by other bands which were around 1200-1500 cm−1. The nature of these vibrations is revealed by three protein absorption bands, Amide I, Amide II, and Amide III at about 1680 cm−1 (C = O), 1550 cm−1 (NH), and 1250 cm−1 (CN) respectively. Also, the isolated carbonyl groups are identified by the absorption of light at about 1745 cm-1 which indicates that lipid membrane and cell wall pectin may involve chemicals with ester groups. This band on flowers is due to the subtype of acids such as lauric acid, myristic acid, palmitic acid, dodecenoic acid which are present between 1600 and 1420 cm−1 but they are somehow overlapping with other bands at this range. In the fingerprint region, bands are noted in the region of approximately 1,100 cm−1 which might be owed to C-H bending, C-O stretching or C-C stretching prototype. In these absorption bands, the elements that were found responsible are the carbohydrates in the flower [7–10]. The absorption band indicating that substances containing ester are present in the lipid membrane and cell wall pect in is mainly composed of carbohydrates, which are interesting.

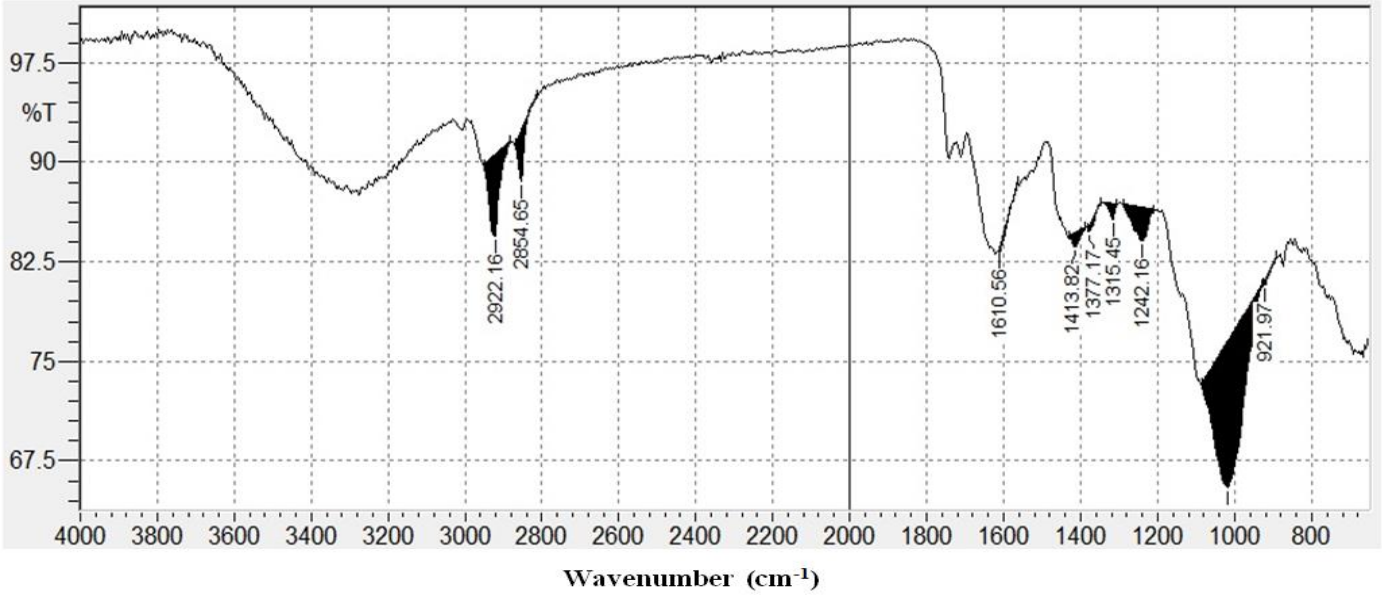

Figure 1. Fourier-transform infrared spectroscopic profile solid analysis of *Chrysanthemum* morifolium

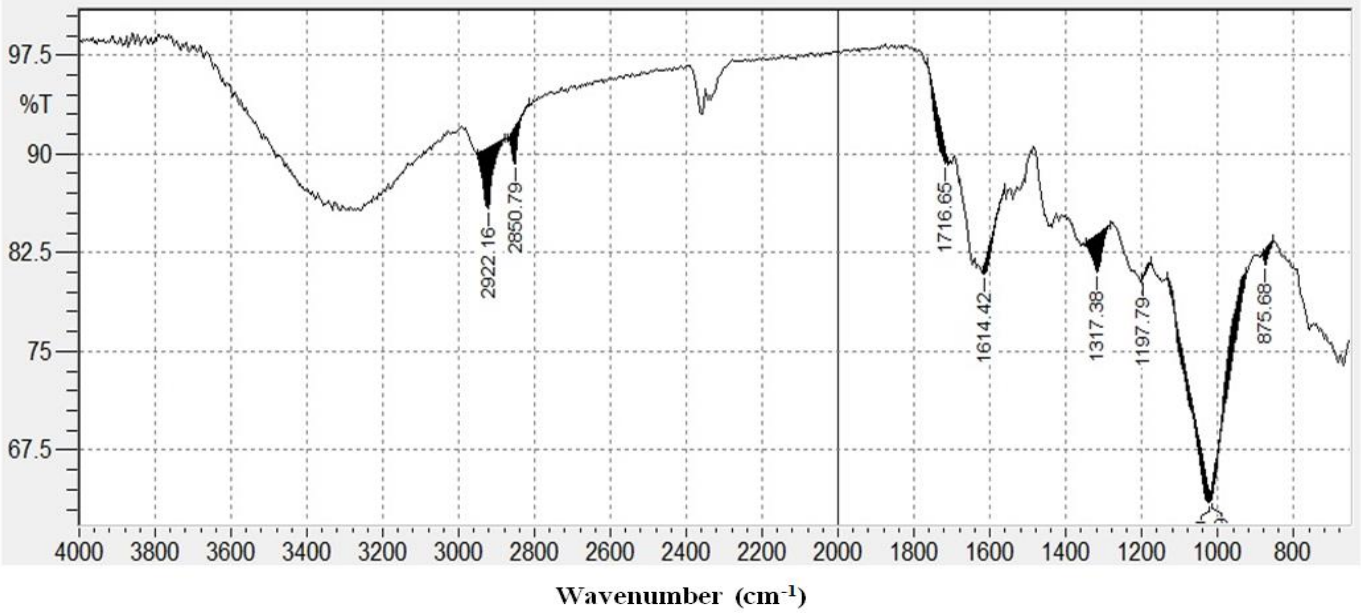

Figure 1. Fourier-transform infrared spectroscopic profile solid analysis of *Passiflora caerulea* .

There are so many famous spectroscopic techniques that are currently used commonly in the many labs for many types of spectroscopic studies; they are normally used for material analysis. Until recently, we have seen that the infrared (IR) spectroscopy prominently used to obtain qualitative data in analytical chemistry. Which consisted in defining the extensive regular specific and characteristic properties of many compounds. IR spectroscopy still remains a good quantitative analytical method, despite the lack of accuracy and presence of interference with some probe types, due to the chemometric developments and software advances with proper artificial intelligence abilities on top of increased and engineering of complex instrumental technologies. Of all the different types of IR spectroscopy, Fourier transform infrared spectroscopy, often abbreviated as FTIR, is a relatively new but highly effective technique that has effectively revived interest in the application of IR spectroscopy. Infrared spectroscopy is a process in which electromagnetic radiations exhibit energy absorptions in the infrared spectrum while passing through molecules. Molecules are depicted at different kinds of over excited vibrational as well as rotational energy levels due to energy absorption. A compact and characteristic spectrum was defined [11, 12]. Due to the innovations in fourier transform infrared spectroscopy technology, a multipurpose tool for the both quantitative and qualitative study has been established. [6] Though it is a destructive and real time technique, FTIR is unable to identify the unknown compound type in the liquid, gas, and solid samples as well as not capable of measuring the amount of it. As for the mentioned dipoles, it is important to note that they are affected by vibrations. Turning to the case of the molecule, radiation denotes the change in the dipole moment or in this case, the molecule can be described as IR active. Whether polar bonds exist or the structure is an asymmetric one—duration of the link has no bearing—the dipole moment for IR-inactive species is zero. (Infrared) inert: Unlike the London dispersion forces, the other type of force that occurs between molecules is known as dipole dipole forces or also known as polar bonding and are found on symmetrical molecules. Controlling the frequency is also directly related to energy levels which makes it useful in applications such as Infrared spectroscopy where the energy levels of the chemical bonds are measured in terms of frequency.

In comparison with the infrared absorption spectra of other chemicals, such as isomers, the spectra of an organic compound can definitely be detected, since they leave a ‘fingerprint.’ Infra-red (IR) radiation can be described as an electromagnetic wave having a frequency that is slightly lower

than that of the visible light hence the nomenclature. The use of chromato chromatography in combination with IR spectroscopy is increased due to the fingerprinting capabilities of the instrument, supplementing chromatographic complex mixtures. Combinatorial chemistry, a new filed used today involves the use of a high throughput automated analysis technique refer to as HPLC-FTIR. Neglecting the water vapor line around 3700 cm-1, the whole spectrum of around 4000-400 cm-1 is suitable for scanning most substances in the forms of solid, liquid, or gaseous states [13]. The energy range of the laser pulses in this case was thus lower than the commonplace values for the electron excitation in molecules, but it sufficed to lift the molecules to their first vibrational states. By applying better equiments, the infrared spectra of the samples at low picogram level can also be identified. This method is referred to as the ‘‘workhorse’’ of analytical research because it possesses an outstanding ability to detect samples in different contexts.

FT-IR spectra used in the field of biology:

Intact microbial cell FT-IR spectra serve as unique, fingerprint-like signatures for applications such as : First, the investigator should determine the specific species and strains of microbes that exist; Sec, it is important to determine the intracellular components and structures including endospores, storage compounds, and inclusion bodies; Third, the investigator must ascertain substrates that cause the metabolic production of carbon dioxide. This is because as talked by (iv), growth-dependent phenomena and cell-drug interactions are characterised by. Spectral contours [14–17] and artificial neural networks were employed to extract specific information through the utilization of methods that involves resolution enhancement, differential spectroscopies and techniques on pattern recognition techniques including factor, cluster and linear discriminant analysis. Light microscope is interesting when used a spectrometer because you get to see some interesting uses from it. In medicine, the application of pharma- ceuticals, water quality analysis, and microbial strain collections, the use of FTIR with whole cells is considered the industry standard.

This sector you are in, whether processing, retailing or production of foods, microbial identification is the most crucial analysis that has to be carried out for effective food safety and quality assurance. Blood chemistry tests including enzymes, proteins and lipids; hormones and endocrines are some of the key components that are analyzed by biochemical tests while serotyping involves the identification of bacteria by their antigen and antibodies. The conventional method of performing these tests includes the culture of bacteria in a given medium type like selective agar or broth for a few days before subjecting the microbial sample to specific tests that reveal the existence of the given species[18, 19]. The delay in decision making on the counter arguments may result in slow actions to take the right precautions to remedy the food contaminations. Thus, at least in the food sector, rapid and direct microbiological examination may prove to be an essential and constructive tool. Traditional biochemical analyses of individual bacteria species have proved very difficult due to the fact that microbial cells are resistant to analysis when they are intact; however, with the application of Fourier transform infrared spectroscopy or FTIR, microbial cells are analyzable yielding complex, unique, and reproducible biochemical fingerprints.

Herbal medication evaluations:

Some of the chemicals found in sources such as herbals can only have his or her structures elucidated by infrared (IR) spectroscopy. In phytochemical research, it has the potential of being a “fingerprinting” mechanism where it is utilized in the comparison of synthetic products and natural ones [20, 21]. Actually IR spectrum is not very straightforward as it is composed of many lines that can be difficult to interpret or use in certain operations, and because of that the skills required are high. Initial scans of plant using the same species can differ in certain ways, and these differences may not be easily discernible with the naked eye. Consequently, there are many more

possibilities to apply the infrared spectroscopy in other fields apart from the herbal analysis, for example in food and beverages, microbiology, pharmaceuticals and etc. Chemometric methods have become a Webster tool in the frame of the scientific community due to development in computer technology which makes the process of the analysis faster and shorter amount of time for the development of the products [22–24]. The commonly used method of analyzing data that have more than one variable when there is no prior knowledge about the samples under consideration is through a technique that can be best described as pattern recognition and one of them is Principal Components Analysis (PCA). It is also important to note that infrared spectrum analysis has also used the supervised classification techniques which utilizes SIMCA, which involves the establishment of the PCA model for grouping of the unknown sample in line with the defined class model.

It is an essential tool important in deducing the structures of organic molecules, and one of the most trusted is the infrared spectra. And since FTIR spectroscopy costs less than traditional method, more user-friendly, comes with shorter time of turn around and is quite reproducible, this method is registering a steady growth today. More FTIR systems are being applied to determine qualities of herbs due to advancement in FTIR methods and its correlation with computational or mathematically enabled approaches like two dimensional correlation analysis [25]. Herbal raw materials here undergo quality and quantity analysis with an FTIR among other equipment. Thus, infrared spectroscopy is a reliable, quick, and cost-effective approach to identify the flavonoid levels in extracts of medicinal plants. Compared relative to rather archaic, energetically demanding, expensive, and time-consuming spectroscopic and [26-28] chromatographic techniques, IR spectroscopy can offer analytical information if in synergy with sophisticated chemo metres. Several native South African medicinal plant leaf extracts were analyzed for flavonoid content using partial least square and linear discriminant methods and compared after being extracted with ultrasonication and maceration.

It is practically impossible to find any plants that are free from variation because basically, variation is natural in everything that grows. It is possible that samples harvested within the same region and samples harvested in other areas of the globe may have substantial differences in quality. Therefore, in order to ensure the quality of crude herbs, the identification of their geographic origin is crucial before they go through the processes of extraction and formulation of a finished product [29, 30]. Since it is not convenient to devote much time and effort to the conventional wet chemical analysis, the manufacturers of herbal products are always on the lookout for more effective as well as less-costly modes of verifying their products. The authors purposively aimed at developing a system which would be capable of rapidly identifying quality using Infrared spectroscopic data coupled with statistical and mathematically derived techniques for data reduction so as to obtain relevant specifics.

Existing quality control is rather weak and there is an urgent need for improvement, as pharmacovigilance regulation of herbal medicine is not adequately established or sufficient, and there are necessary adjustments necessary because of increased consumption and usage of herbal medicine. I took the time to sum up external factors that may influence the quality of herbal medications; some of the factors include geographical location, growing period, and the production method among others. Some of the challenges that are faced in assessing pharmacognosy of herbal medicine include; the following; The level of difficulty that comes when dealing with a compound mix of herbs. The quality control of herbs has mainly relied on the conventional techniques such as the separation techniques in the HPLC and the gas chromatography in addition to the mass spectroscopy. A ‘basic’ sample preparation does not require such investment in time and money to develop a technique [31, 32]. The benefits of the IR spectroscopy are as follows: the method is rapid; usually the samples do not require

preparation before analysis; cost of analysis is low; it is a non destructive technique; and it is an environmetally friendly technique, and the physical and chemical properties of a sample can be predicted from its IR spectrum. This device has developed over time and is helpful to assess raw materials and food quality, and for assessing processes. These collections of bonds are the basis of an older technique for studying the structure of organic molecules, the infrared spectra contain a great deal of structural information [33]. The current appeal of Fourier transform infrared (FTIR) spectroscopy is increasing for several reasons, namely due to its low cost of operation, simplicity of use, fast workmanship, high reliability of the method, and virtually noiseless sound production. In recent years, evaluation methods with mathematics or calculating tool, such as 2D synchronous correlation analysis and FTIR, are gradually applied for the quality assessment of herbs.

The process of identifying oils and fats:

Some fats and oils key quantities such as iodine value (IV) and saponification number (SN) which are fundamental in the processing of fats and oils can be measured using conventional procedures that may take a considerable amount of time. Although appealing in the abstract when used in dispersive equipment, and when coupled with transmission sampling techniques in early studies, the idea has not received much attention at all. There are several suggestions, which have been discussed previously, to suggest that using infrared spectroscopy can be a good method to deduce IV. For the comparability of the results, both Fourier Transform Infrared Spectroscopy (FTIR) method and Fourier Transform Infrared Spectroscopy/Attenuated Total Reflectance (FTIR/ATR) based on the peak height were used We received samples of IV and SN from vegetable oil processor or else purchased locally. The samples were taken in triplicate, meaning that for every analysis three separate samples were run. The times taken to analyze and predict for both IV and SN remained below 2 mm/sample time, and all the samples were investigated thoroughly with a heated (65°C) ATR crystal. Analyzing the results of the FTIR readings of the IV and SN It could be deduced, that they were within k3, albeit this was with much lesser time and effort analytically. 0 and 2. One unit was derived from the chemical values obtained from the results of each test 5 units in total. This is enough for ordinary controlling of quality and exclude extra setting in the quality control program. It is clear that fats and oils will use Fourier transform infrared spectroscopy in the future in some applications. Consequently, it is evident that the peroxide value study of the oil degradation could be the most valid study. An increased peroxide peak is observed in the FTIR spectrum when oil is heated over an ATR crystal[34] , showing that the initial peroxide load and further prospective oxidation of oils may be determined. Therefore, in a closed system, oxidation of oil on an ATR crystal is actually feasible, similar to the active oxygen method. Therefore, with FTIR, one can analyze typical fat and oil samples in a single run.

Evaluation of Polymers:

Contrary to the traditional view, which treated the polymer products as a single kind of species, the polymer molecules formed complicated groups with different chemical compositions and structures. The observed multiple polymer population was further separated into the individual population type of polymers by using a method of coupled chromatography with infrared spectroscopy which James L. Dwyer and his fellow used to analyse the polymers. As for the polymer characterization, there is no question that combined with proper sample preparation FTIR could provide more information in no time. The composition and structure of dispersed phase makes it necessary to look at the physical properties of the polymers since it defines the phase morphology [35, 36]. The work ing method in LC-FTIR, which has analyzed LC instrumentation including FTIR in conjunction with the interpretive of the infrared software that may be valuable for the polymer scientist and synthesis chemist.

Use of Fourier Transform Infrared Spectrophotometry for the Analysis of Pharmaceutical Medications:

For the quantitative and accurate measurement of acetylsalicylic acid (ASA) in different pharmaceutical products, a novel, efficient and fast FTCIR spectrometry method was developed. Thus he discovered that it is possible to determine which component of drug combinations is the active uses an element by comparing the KBr spectra obtained by traditional methods. Data analysis involved Beer Law lambert's, major components regression (PCR+) and partial least square (PLS) chemo metrics. The authors carried out an experiment to determine the possibility of using Beer-Lambert law to determine ASA in pharmaceutical products at the wavelength 1605. 49 cm1. The authors suggest considering the PCR+ method [36] since it yielded very comparable results to the PCR-RS method, and the RSD (3. Pharmaceutical items' biotin (vitamin H) and ascorbic acid (vitamin C) contents of several pharmaceutical items were quantified by employing Fourier, transform infrared spectroscopy in the Short time frame. By means of ordinary KBr spectra, active substance profiles in the formulations of medications were determined. In analyzing the data, chemometrics and the Beer-Lambert law are used while the method of calibration consists of linear regression. In fact the vitamin C is one of the necessary nutrients whose presence is felt many of the higher primates. Thus, the majority of animals, mammals in particular, as well as birds and some fish do not need it, while a minor portion that does is represented by guinea pigs and approximately 20% of all mammals. The microbial synthesis of the hydrophilic vitamin, H or B7, is a ring of tetrahydrothiophene, bridged to another ring of tetrahydroimidizalone.

The Use of Fourier Transform Infrared Spectroscopy in Combination with Chemometrics for the Purification and Verification of Food Oils and Fats

Economic motives conspire to substitute high-quality, expensive edible fats and oils and other foods containing these commodities with inferior, comparatively inexpensive materials. Authentication examination of food products has employed some specific analytical techniques, most of which require particularly involved sample preparation steps and the need to employ costly instrumental equipment. Hence, for these authentication goals, inline and reliable solutions are recommended and implemented. This work has highlighted the use of infrared spectroscopy entailing chemometrics for the authentication which has been laden by numerous extensive reports. The review uncovered three new things: This is based on the following observations: (1) chemometrics as an analytical data treatment is crucial for turning the FTIR spectra into consumable data; (2) FTIR among the analytical techniques has been used as the most reported techniques in fats and oil authentication analysis; and (3) FTIR spectroscopy anchored on chemometric has been used for fats and oils authentication. The subsequent evolution in certificating and warranting the qualities of oils for fats is to propose, create and harmonise Fourier transform infrared spectroscopy chemometrics.

A feed fat or oil refers fat and oils for human consumption, are commonly used food products. Thus, the use of feeds and MY is becoming more attractive as an economic feedstock, not only for the food industry but also for oleochemical and pharmaceutical companies. Nutritionists have indicated that in order to ingst fat soluble vitamins such as vitamins A, D, E, and vitamin K, which are essential in the human metabolism, and other essential fatty acids such as oleic, linoleic and alfa-linoleic acids the recommended form is the vegetable oils [9]. Fat and oil are present in majority of foods prepared within many meals, margarine, shortening, vegetable oil, salad dressings and other many products. From this discussion, it becomes obvious that, the factors that define the quality of fats and oils include authenticity, purity, and some of the measures of intrinsic quality which in turn dictate the quality of the food products that contain the fats and oils. S, it becomes apparent that edible oils and fats occupy a prominent position regarding frequently

adulterated food ingredients, using data obtained from Scopus addressing www. scopus. and recognizing online news com, with food adulteration as key terms. Valdes et al. have also recognised that out of all the products, 11 percent of the reported frauds belonged to the fats and oils category, which ranked third in this regard. Food items commonly consumed by Ugandans implicated by this study as being contaminated are as follows: 13% of the contaminated food items have been derived from fishes while the remaining 27% have been derived from meat and animal products. This consolidated concern regarding food product adulteration particularly involving fats and oils has been of bother to practically everybody involved in food industry since the earliest times and civillization. This led to quality deterioration of food products through adulteration while posing health complications in humans [39]. Often, the adulterants that contaminate oil are actually food products and thus health risks arising from fat and oil adulteration may not pose a great threat. However, in areas where people are inclined to suffer severe allergic reactions, results from vegetable oil adulteration have precipitated such adverse health complications as Spanish olive oil syndrome. Multiple methods exist for the adulteration of fats and oils: possible schemes highlighted are; (1) substituting high-quality fats and oils with inferior quality; (2) adulteration through dilution of quality oils with low-quality oils; (3) relabelling palm oils or other premium oils as EVOO; (4) location of origin of the oils; and (5) substituting one grade of olive oil with an even higher grade such as pomace olive oil with EVOO. In ensuring that the specified fats and oils are not counterfeited or spiked, it is prudent to conduct authentication tests on the said commodities [60, 61]. The analysis of the actual sample of oil and fats is performed in order to confirm that the tested oils and fats are corresponding to the information on the label. Conventional techniques summed up for the authentication analysis include the calculation of constants such as saponification and iodine numbers; advanced techniques require complex equipment such as liquid chromatography coupled to mass spectrometer detectors; or the organoleptic examination also forms another approach.

To ensure there is quality fats and oils and food items with these products, several assay techniques that have revolutionized the center and have been examined and implemented in practice. These methods mostly involve spectroscopy, chromatography, plus molecular techniques; they encompass chromatography chemometrics and metabolomics, near infrared spectroscopy chemometrics, Fourier-transform mid infrared Fourier MIR spectroscopy Other methods These methods embraced chemometric techniques plus DNA-based approaches like polymerase chain reaction Because of the uniqueness in FTIR spectra Finger printing property therefore FTIR chemometrics was much documented in the certification of oils plus fats. FTIR, due to its nature and multiplicity, is one of the hardest spectra to interpret out there. However, using the chemometrics and multivariate data analysis, the FTIR spectral data can be transformed and thereafter, chemical information retrieved for use in interpretation and differentiation, for instance, quantification. Using chemometrics for classification, for example, in cases where the samples were real and fake edible fats and oils, the differences were clear [42, 43] While using chemometrics to quantify the samples using multivariate calibration technique made it possible to predict the level of adulteration.

Among the more well-known vibrational spectroscopy techniques is the Fourier transform infrared (FTIR) spectroscopy where coherent electromagnetic radiation identifies the vibrational energy levels on the basis of its interaction with the functional groups in the materials being investigated. ATR-FTIR spectroscopy has recently gained increasing trend in the food sector for authentication examination since the technique is non-destructive and reliable if complemented by chemometric software. This method can thus, both quantitatively and in a subjective manner, differentiate between original and imitation food using the FTIR spectrum features [44]. Infrared (IR) region of the electromagnetic spectrum

includes a range of frequency extending from 14, 000 cm−1 to 50,000 cm−1. This spectrum can be further subdivided into three areas: Near IR region is from 14 000 to 4000 cm-1, Middle IR-from 4000 to 400cm-1 and Far IR-from 400 to 50 cm-1. To further focus our review, we concentrated on the data acquired from the MIR region only because it is the most used in fat and oils authentication tests out of the three regions. For example, in the last few years we witnessed reviews addressing the applicability of FTIR spectroscopy combined with chemometrics in the fields like: biopharmaceuticals, halal food authentication, overall meat and any product derived from it, herbal product discrimination and authentication, and biomedical fluid biomolecule authentication. It must be noted, however, that authentication analysis FTIR spectra are difficult to interpret but with usual software applications in chemometrics together with increased computational capacity, this has not posed a challenge. Chemical information like for example FTIR spectra, chromatograms, etc. can be presented at chemical data and this kind of data could be processed by using chemometric methods practically based on statistics and digital mathematics. Actually, according to the International Chemometrics Society, chemometrics can be defined as the science of using mathematical and statistical techniques for making relationships between chemical data and property pattern including the concentration [46]. The development of chemometric software supported the techniques of Fourier transform infrared spectroscopy (FTIR) on the genuine of culinary oils and fats. Some of the PLS modeling software includes Minitab ®(State College, Pennsylvania, USA), Unscrambler® (Camo Analytics, Molndal, Sweden), SIMCA® (Sartorius,Gottingen, , Germany) and MATLAB's PLS_Toolbox (Mathworks, MA, USA) and there are many more readily available in the market but these are easy to use. Brereton et al discussed the aims and features of the software under consideration Besides, there are other shoulders chemometrics programmes such as R factoextra and FactoMineR The later was effectively used in the process of fats and oils authentication.

Table 1. The application of FTIR spectroscopy combined with chemometrics for authentication analysis of oils.

Adulterated Fats and Oils	Adulterants	Wavenumbers (1/λ) Region	Spectral Treatment	Chemometrics Techniques
Extra virgin olive oil (EVOO)	Corn oil (CO) and sunflower oil (SFO)	3027–3000, 1076–860, and 790–698 cm^{-1} for CO and 3012–3000 cm^{-1} for SFO	Derivatization	DA for classification and PLS for quantification
	Soybean oil (SB) and sunflower (SF) oil	3035–670 cm^{-1}	Mean centering	PLS for quantification and PLS-DA for classification
	Canola oil (CaO)	3028–2985 and 1200–987 cm^{-1}	No spectral treatment	PLS for quantification and DA for classification
	Grapeseed oil (GSO) and walnut oil (WO)	3018–3002 and 1200–1000 cm^{-1} for GSO and 3029–2954 and 1125–667 cm^{-1} for WO	No spectral treatment	DA for classification and PLS for quantification
Virgin coconut oil (VCO)	Corn oil (CO) and sunflower oil (SFO)	3028–2983, 2947–1887, and 1685–868 cm^{-1}, (VCO mixed with CO) and combined wavenumbers of 3030–2980 and 1300–1000 cm^{-1} (VCO mixed with SFO)	Derivatization	PLSR for quantification and DA for classification

Pharmacological Applications of Nuclear Magnetic Resonance Spectroscopy

As one might expect, NMR spectroscopy lacks sensitivity which is generally regarded as one of the technique's primary weaknesses. While the signals being compared are kept distinct from each other the sensitivity is more than adequate to aid in API quality assessment. Increase of sensitivity in the recent years is well known due to the microcoil technology, gradient shimming techniques, inverse or cryo probes as well as due to utilization of routinely used high-field spectrometers with the frequencies more than 400 MHz. The following reports gives reasons why it is possible to use nuclear magnetic resonance (NMR) spectroscopy in an identification of the molecular structure of an impurity, which cannot be revealed in a medicine. Despite the high potential of using NMR spectroscopy as an analytical instrument in enforcing quality control on various products, very few international pharmacopoeias have adopted it. However, nuclear magnetic resonance spectra also soon entered as a regular part of quality examinations within the realms of the pharmaceutical industries, especially with regards to ''Big Pharma". With this idea, it will take some time to get the q NMR spectroscopy into the monographs of the international pharmacopoeias. In particular, with PDE-5 inhibitors being as dangerous as similar substances, people interested in natural medicines have developed a vast market for HMs. This has led to it being considered widely as a safe and effective product compared to other traditional medicines since it is all natural. People who inadvertently ingest a synthetic medicine are risking their lives because synthetic medicines are on the increase being mixed with the regular ones in the market [47]. Most of the HMs targeted are those that are advertised to boost the sexual feats in the body of a man. The current-resolution of EM maps versus atomic-level structures of biomacromolecules: Nuclear magnetic resonance spectroscopy is one of the two dominant technologies.

Conclusion

NMR spectroscopy is based on the quantum mechanical phenomenon that nucleus has a characteristic magnetic property. Coulometry with gas evolution, gravimetry, and titrimetry as the three forms all entail using simple reference substances to determines the absolute quantities of reagents. In addition, NMR is often used in modern diagnostic methods in medicine such as magnetic resonance imaging or MRI. The ability of the resonance frequency of a material to increase with the strength of the magnetic field applied to it is one of the major aspects that defines Nuclear Magnetic Resonance (NMR). Thus, nuclear magnetic resonance, NMR, which initially was considered as a powerful phenomenon in physics, has become a stern and multifaceted analytical tool to several fields of science, medicine, and industry. Moreover, the nuclear magnetic resonance (NMR) technique provides unique and universally significant patterns of molecular interaction/motion that contains valuable information about protein function.

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