Characterization And Quantization Of Medicinal Drugs Using Biomedical Optical Spectroscopy Methods

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Abstract—**In India, there are two types of Medical Treatment Systems (MTS) using various drugs namely, English Medical Treatment Systems (EMTS) and Ayurveda, Unani and Siddha Treatment System (AUSTS).The experiments for medicinal drugs were carried out with the help of biomedical optical spectroscopy techniques such as Ultra violet/Visible, Fourier Transform Infrared and Fourier Transform-Raman. The spectral analysis indicated that the specific functional groups of the drug materials have almost the same chemical characteristics. The following functional groups are present N=C=O, -N=C=S,-N=C=N-, -N3, O=C-C , O=C-N,C=C-N, C=C-C and CH_3, CH_2 & CH.**

Keywords- **Fourier transform infra red spectroscopy, medical treatment system, ayurveda, unani and siddha treatment system, potassium bromide.**

I INTRODUCTION

All over the world, plants have been used in traditional medicine for several thousand years. In India, medicinal plants as a group comprise approximately 8000 species, and of that fifty percent account for all the higher flowering plant [1] species in India. The knowledge of medicinal plants has been accumulated in the course of many centuries, based on different medicinal systems [1] such as Ayurveda, Unani and Siddha. In a large number of countries, the human population depends on medicinal plants for treating various illnesses as well as for livelihood. The World Health Organization (WHO) estimated that 80% of population of the developing countries relies on traditional medicines, mostly plant drugs, for their primary health care needs. The objective of this research is to identify the various chemical groups present in the five important medicinal drugs given for gastric problems by both types of physicians. The number of reported cases of gastric problem [2] is steadily increasing in both industrialized and developing countries, in spite of the fact that significant progress has been achieved in the

identification of gastric problems at the molecular level, using FTIR spectroscopy and other advanced technologies of bio-optics. Spectroscopic investigations on pharmaceutical samples are of great importance now. Vibrational spectral studies of many pharmaceutical drugs are extensively carried out by many scientists. So far nobody has made an attempt to study the chemical characteristics [2] of the Brown and green samples.

II EXPERIMENTAL SET UP

A. FTIR

In the FTIR, the design of the optical pathway produces a pattern called an interferogram. The interferogram is a complex signal, but its wave like pattern contains all the frequencies that make up the infrared spectrum. A mathematical operation known as the Fourier Transform (FT) can separate the individual absorption frequencies with the interferogram producing a spectrum virtually identical to that obtained with a dispersive spectrometer. The advantage of an FTIR instrument is that, it acquires the interferogram [8] in less than a second. It is thus possible to collect dozens of interferograms of the same sample and accumulate them in the memory of a computer. When a Fourier transform is performed on the sum of the accumulated interferogram, a spectrum with a better SNR can be plotted. An FT-IR instrument is capable of greater speed and sensitivity than the dispersion instrument. There are three basic spectrometer components in an FTIR system: the radiation source, the interferometer, and the detector. The same types of radiation sources are used for both dispersive [8] and Fourier Transform spectrometers. The source is more often water-cooled in FTIR instruments to provide better power and stability. In contrast, a completely different approach is taken in an FTIR spectrometer to differentiate and measure the absorption at the component frequencies. The monochromator is replaced by an

interferometer, which divides the radiant beams, generates an optical path difference between the beams [9], then recombines them in order to produce repetitive interference signals measured as a function of the optical path difference by a detector.

B. Detector

When the mirror is moved at a constant velocity, the intensity of the radiation reaching the detector varies in a sinusoidal manner to produce the interferogram output. The interferogram is the record of the interference signal. It is actually a time domain spectrum, and records the detector response changes versus time [12] within the mirror scan. If the sample happens to absorb at this frequency, the amplitude of the sinusoidal wave is reduced by an amount proportional to the amount of the sample in the beam. The extension of the same process to three component frequencies results in a more complex interferogram, which is the summation of three individual modulated waves. In contrast to this simple, symmetric interferogram, the interferogram produced with a broadband IR source displays extensive interference patterns. It is a complex summation of superimposed sinusoidal waves, each wave corresponding to a single frequency. When this IR beam is directed through the sample, the amplitudes of a set of waves are reduced by absorption, if the frequency of this set of waves is the same as one of the characteristic frequencies of the sample. The interferogram contains information of the entire IR region to which the detector is responsive. A mathematical operation known as the Fourier transformation converts the interferogram (a time domain spectrum displaying intensity versus time within the mirror scan) into the final IR spectrum, which is the familiar frequency domain spectrum showing intensity versus frequency.

The detector signal is sampled at small, precise intervals during the mirror scan. The sampling rate is controlled by an internal, independent reference, a modulated monochromatic

beam from a Helium Neon (HeNe) laser [12] focused on a separate detector. Using commercially available software and highly flexible graphical tools, results are obtained that cause confusion, rather than providing solutions to the urgent clinical problems. Thus, it is unreseasonable to claim that astral contraction wave activity plays a dominant role in intra gastric fluid motions, on the bases of the results of the computer stimulation of a flow caused by the prescribed indentations of the surface boundaries (20,21). Also, in view of the fundamental mechanical property of the tissues and their softness, it is unwise to argue for the dependence of the stress-strain states on the radii or curvature of the visceral organs. More than 20% of our population is expected to exceed 85 years of age by the year 2030 (20); hence, the gastroenterologist in the twenty first century will be increasingly confronted with digestive diseases in the elderly population. Gastrointestinal disease is the second most common reason for the hospital admission of elderly patients, a patients group that accounts for four times as many hospitalizations as younger patients do (21).

III MATERIALS AND METHODS

Molecular composition

The Brown sample consists of the following traditional plants such as Piper nigrum: 10 mg, Glycyrrhiza glabra: 200 mg, Aloe vera: 5 mg, Embelia ribes: 20 mg, Elettaria cardamom: 20 mg, Myrstica fragrants: 20 mg, Caryophyllus aromatious: 20 mg, Perula foetida: 20 mg, phyllanthus emblica: 20 mg, Coriandrum sativum: 20 mg, Musa paralisica: 10 mg, Cinnamomum zevlanica: 10 mg, Zingiber efficinate: 10 mg. The orange sample consists of the following composition: Ispaghula Husk (Mentago ovata): 85.57%, Methylparaban: 0.2%, Propylparaban: 0.02%. The composition of green sample each 1 ml (20 drops approx.) contains: Pudina Satva:

0.0337 ml (Mentha piperata), Purified Water Q.S, Alcohol IP : 10% , V/V Colours: Tartrazine Yellow Spra, C.I.No.19140: 0.0585 mg , Alizarine Cyanine Green: F.C.No. 61570:0.0553 mg. The molecular formula of one of the compositions of the Blue sample is 1-[5-(1,3-Benzodioxol-5-yl)-1-oxo-2,4-petadienyl] $C_{17}H_{19}NO_3$ and it can be isolated from black pepper (Piper nigrum) and other Piper species. Black pepper contains 6% to 9% piperine by weight. Piperine is tasteless, but its stereoisomer, chavicine, is the active ingredient in black pepper, that provides its characteristic taste. The Loss of pungency during the storage of black pepper is attributed to the slow isomerization of chavicine into piperine, when all these chemical compounds react with the macromolecules such as proteins, fatty acids and glucose. The entire structure is changed and sometimes it gives excellent results for gastric problems.

IV Results and Discussions

The C=C asymmetric stretching vibrations occur in the region of 2037cm^{-1} in the FTIR spectra. As solids or liquids, primary aliphatic amines absorb in the region 3434cm^{-1} – 3450cm^{-1}, and exhibit a broad band of medium intensity. In a dilute solution in non-polar solvents, two bands are observed for primary amines due to N-H asymmetric and symmetric vibrations in the range 3550cm^{-1} – 3250cm^{-1}. The relative intensity of the bands due to the hydroxyl stretching decreases with an increase in the concentration with additional broader bands appearing at lower frequencies 3580cm^{-1} – 3200cm^{-1}.In aminobenzoesaesure the hydroxyl stretching occurs at 3434cm^{-1} in the FTIR spectra[16]. From the above band assignments, the sample under experiment shows a very strong band at 3434cm^{-1} in the FTIR spectrum due to N-H and O-H stretching.The carbonyl groups exhibit a strong absorption band due to C=O (saturated aldehyde) vibration at 1728cm^{-1}. In fluorouracil, the bands observed at 1642cm^{-1} in the FTIR were assigned to C = O asymmetry stretching vibration[17]. A strong band at 1728cm^{-1} is assigned to

C = O carbonyl stretching of nalidixic acid[18]. The band at 1642cm-1, which is close to the literature range is assigned for C = O stretching[19] in benzocaine. Keeping this in mind, the sharp band present in the expected region at 1728cm^{-1} in the FTIR spectrum is ascribed to be due to C = O stretching vibration. The C-N stretching absorption of primary aliphatic amines is weak, and occurs in the region 1119cm^{-1}-973cm^{-1}. Secondary aliphatic amines have bands of medium intensity at 1178cm^{-1} – 1140cm^{-1}. The band in the region 1217cm^{-1} in the FTIR are assigned to the C – N symmetrical stretching of the compound fluorouracil[17]. On this analogy, the bands at 1217cm-1 in the FTIR spectra of the drug sample are assigned to C – N vibrations. The bands due to C – O stretching vibrations are strong and occur in the region 1217cm^{-1} - 1119cm^{-1}. In aminobenzoesaeure, a strong band occurs near 1119cm^{-1} in the FTIR spectra and is assigned to C-O stretching vibration[16]. In benzocaine, the very strong and sharp peak at 1217cm^{-1} has been assigned to the C-O stretching. Taking the above band assignments, 1119cm^{-1} and 973cm^{-1} in the FTIR spectrum of the sample under experiment, are assigned to C-O vibration. A number of C-H in plane deformation bands occur in the region 973cm^{-1} – 901cm^{-1}, the bands being sharp, but of weak to medium intensity. However these bands are not normally of important for interpretation purposes although they can be used. The aromatic C-H out-of-plane deformation bands occur below 700cm^{-1}. The bending vibration are generally found at lower wave numbers. The frequencies observed at 775cm^{-1}, 705cm^{-1}, 676cm^{-1}, 592-491cm^{-1} are assigned to O=C-C , O=C-N , C=C-N and C=C-C bending of the pyrimidine ring in the FTIR spectra of Xanthine, and the C-N-C bending vibrations are assigned at 498cm^{-1} and 428cm^{-1} [19,20]. Using the above analogy, the bands at 901cm^{-1} -775cm^{-1} is due to C-H in-plane deformation[21]. The bands at 676cm^{-1} are due to C-H out-of-plane deformation / C-C=O deformation(Figure 1)

The functional group assignment for the Blue sample is given below(Figure 2). In the wavelength region 2.92 to 2.93µm, a very strong vibrational functional group was assigned to N-H free stretching (2°amine). A very strong CH_3, CH_2 & CH two or three vibrational functional group bands are assigned in the wavelength region 3.41µm to 3.5µm. A medium vibrational band was assigned to the wavelength region 4.67µm to -N=C=O, -N=C=S,-N=C=N-, -N3. In the wave number 1724cm^{-1} a very strong C=O (saturated aldeghyde) was assigned. The wave number 1669cm^{-1} was assigned to the C=O (amide I band) functional group. The frequency region between 6.48to 6.65µm was assigned to the functional group N-H (2°-amide) II band. The vibrational intensity in this frequency region was medium. A medium intensity CH2 & CH3 deformation was assigned to the wave number 1451cm^{-1}. A medium intensity O-H bending (in-plane) was assigned in the wave number 1339cm^{-1}.From the wavelength region 8.25 to 9.67µm, the functional group C-N stretching was obtained with medium intensity. A strong vibrational band =C-H & CH2 was assigned to the wave number 926cm^{-1}.From the wavelength region 12.12 to 12.56µm was assigned to the functional group out-of plane bending. The functional group NH2 & N-H wagging (shifts on H-bending) was assigned to the wavelength region 13.12 to 14.4µm. The C-H deformation was assigned to the wave number 932cm^{-1} and S-S disulfide was found in the wavelength region 20.28 to 21.78µm.

The functional group assignment for the yellow is given as follows(Figure 3). For the 3472cm^{-1} wave number, the N-H (1°-amines) intensity is weak, two bands were assigned and from 3.32 to 3.5µm CH_3, CH_2 & CH 2 or 3 bands were assigned, the intensity was strong. O-H (very broad) was assigned at the wave number 2681cm^{-1}, for this band also, intensity was strong. Phosphine band i.e. P-H was assigned at the wave number 2347cm^{-1}, the intensity was very sharp

and medium. The C=O band was assigned to the wave number 1746cm^{-1} and the intensity was strong. C=O (amide I band) was assigned to the wave number 1655cm^{-1} and the intensity was strong. From 6.83 to 7.26μm, the CH_2 & CH_3 deformation was obtained, and the intensity was medium. From 8.09 to 8.93μm, the C-N band was assigned and the intensity was medium. =C-H & =CH2 was obtained at 10.33 to 10.92μm. CH_2 rocking was obtained at the wave number 722cm^{-1}.The N-H (1°amide, 2 bands) with weak intensity value(Figure 4) was assigned to the wave number 3416cm^{-1}. The carboxyl group C=O (amide I band) with strong intensity was assigned to the wave number 1681cm^{-1} to 1698cm^{-1}. It is obtained that a medium intensity C-N bond at the wave number 1207cm^{-1} to 1027cm^{-1}. C-H bending and ring puckering with strong to medium intensity was assigned to wave numbers 872cm^{-1} to 712cm^{-1}. The CH, CH_2,& CH_3 three bands with strong intensity was assigned to the wave numbers 2985cm^{-1} to 2850cm^{-1}. The S-S disulfide with weak intensity value was assigned to the wave numbers 590cm^{-1} to 492cm^{-1}. The wave number 1609cm^{-1} to 1616cm^{-1} was assigned to amide group namely N-H(1° amide) II band with medium intensity value. The wave number 895cm^{-1} was assigned to the =C-H & =CH_2 with strong intensity value. The wave number 676cm^{-1} to 685cm^{-1} was assigned to NH_2 and N-H wagging (shifts on H-bonding) with very strong intensity. From wave number 600cm^{-1} to 616cm^{-1} very strong intensity C-H deformation was observed. The wave number 1356cm^{-1} to 1451cm^{-1} was assigned to the CH_2 & CH_3 deformation with medium intensity.

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