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REVIEW ON FTIR-BASED MOLECULAR FINGERPRINTING OF AYURVEDIC HERBS AND FORMULATIONS

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ABSTRACT
Fourier Transform Infrared (FTIR) spectroscopy has emerged as a rapid, non-destructive, and reliable analytical technique for the evaluation of Ayurvedic drugs. This review focuses on the application of FTIR-based molecular fingerprinting in herbal, polyherbal, herbo-mineral, and Bhasma formulations. Relevant literature from peer-reviewed journals was analyzed to understand the role of FTIR in identifying functional groups, chemical bonding, and organic–inorganic interactions. FTIR spectra of various Ayurvedic drugs consistently show characteristic absorption bands such as O–H, N–H, C–H, C=O, and C–O, which correspond to phytochemicals like phenols, alkaloids, proteins, and glycosides, as well as metal–oxygen bonds in Bhasma. These spectral patterns provide a unique chemical fingerprint that helps in authentication, detection of adulteration, and assessment of batch consistency. The study also highlights that organic functional groups in herbo-mineral formulations arise from herbal processing (Bhāvanā), while inorganic signatures are due to transformations during Māraṇa. Despite its advantages, FTIR has limitations such as overlapping peaks and lack of quantitative accuracy. Overall, FTIR plays a crucial role in the quality control and standardization of Ayurvedic medicines, and its integration with other analytical techniques can further enhance scientific validation and global acceptance.

KEYWORDS: FTIR spectroscopy, Ayurvedic medicines, Molecular fingerprinting, Quality control.

INTRODUCTION
Ayurveda, as described in India's Vedic literature, represents a comprehensive system of preventive as well as curative healthcare and is literally known as the "science of life." It is a traditional, natural healing system recognized as the oldest scientific medical system of the Indian subcontinent, dating back to ancient times.

This holistic system of medicine employs herbs, metals, minerals, and their formulations for therapeutic purposes.[1] Herbs have been used as therapeutic agents since ancient times, but growing demand has led to issues of adulteration and misuse. To address this, modern approaches such as herbal fingerprinting have been developed to authenticate and differentiate herbal medicines. By using analytical techniques to analyze specific components, fingerprinting provides a characteristic profile of the constituents present in a herbal product.[2]

Rasa Śāstra is a specialized branch of medicine that focuses on the pharmacological use of metals and minerals and the preparation of formulations with broad therapeutic potential. These medicines are characterized by rapid action, low dosage, rapid action, tastelessness, improved palatability and long shelf life. Analytical studies form a crucial component of scientific research, as they provide essential information regarding the safety, efficacy, stability, and possible contraindications of such preparations.[3]

Ayurvedic Bhasmas are highly significant in the management of various diseases, but their purity is essential to prevent adverse effects on human health. Therefore, their evaluation involves the use of modern analytical techniques such as TEM, SEM, EDX, XRD, DLS, and FTIR, along with classical Ayurvedic tests.[4]

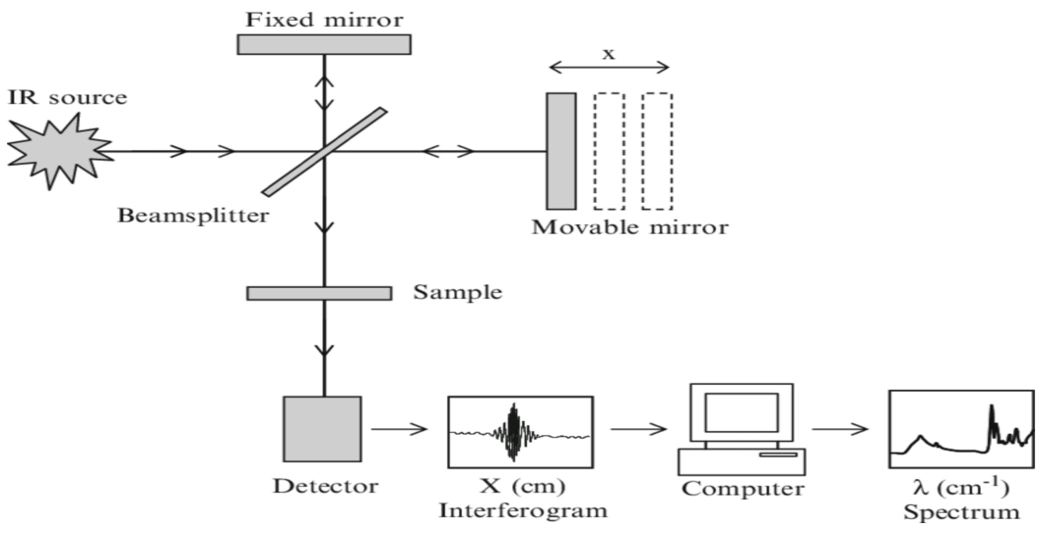
Fourier Transform Infrared (FTIR) spectroscopy is a rapid, non-destructive, and reliable technique for identifying functional groups and chemical bonds in samples. It is especially useful in Ayurvedic formulations as it can analyze complex herbal, herbo-mineral, and Bhasma preparations. FTIR helps in confirming phytochemical groups, organic–inorganic interactions, and chemical transformations during Śodhana and Māraṇa. Hence, it plays an important role in the quality control and standardization of Ayurvedic medicines.[5]

MATERIALS AND METHODS

The present study is a narrative review based on published research articles describing the application of Fourier Transform Infrared (FTIR) spectroscopy in Ayurvedic drug analysis. Relevant literature was sourced from peer-reviewed journals such as *AYU*, *International Journal of Ayurveda and Pharma Research (IJAPR)*, *International Journal of Research in AYUSH and Pharmaceutical Sciences (IJRAPS)*, and *Journal of Drug Research in Ayurvedic Sciences (JDRAS)* and the Elsevier book *Membrane Characterization*. FTIR studies on single herbal drugs, polyherbal formulations, herbo-mineral preparations, and Bhasma were included, with interpretation based on established FTIR principles and functional-group assignments.

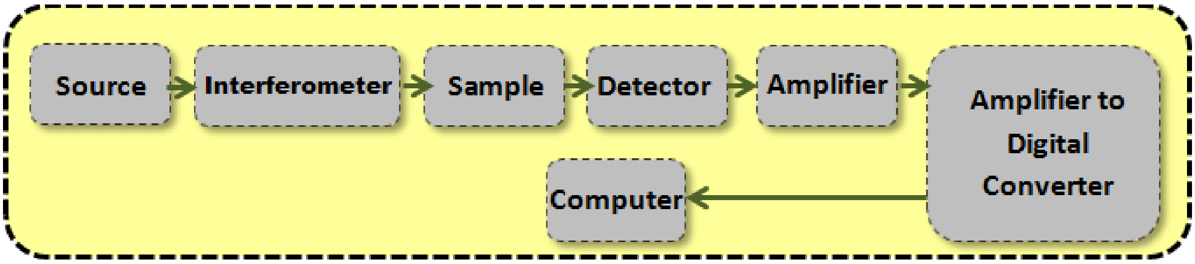
PRINCIPLE AND WORKING OF THE TECHNIQUE

Fourier Transform Infrared (FTIR) spectroscopy is an analytical technique based on the principle that molecules absorb infrared radiation at specific frequencies corresponding to their vibrational energy levels. In an FTIR spectrophotometer, a broad beam of IR radiation from a black-body source passes through an interferometer, where it is split and recombined to produce an interferogram containing information from all frequencies simultaneously. This interferogram then interacts with the sample, which absorbs characteristic frequencies depending on its functional groups and molecular structure. The detector records the resulting signal, and computer software applies Fourier transformation to convert the interferogram into a conventional IR spectrum (4000–400 cm^{-1}). The obtained spectrum provides characteristic absorption bands that enable identification of functional groups and structural features of the compound.[6]



Instrumentation

A Fourier Transform Infrared (FTIR) spectrometer mainly consists of an IR source, a Michelson interferometer, a sample compartment, a detector, and a computer system. The IR source emits broadband infrared radiation, which enters the interferometer where it is split by a beam splitter and reflected by fixed and moving mirrors to generate an interferogram. This modulated beam passes through the sample, where specific frequencies are absorbed according to molecular vibrations. The detector records the interferogram, and a computer applies a Fourier transform to convert it into a conventional IR spectrum representing absorbance or transmittance versus wavenumber.[6]



Sample Preparation for FTIR Analysis

For FTIR analysis, samples were prepared following standard procedures reported in the literature. Herbal and polyherbal samples were dried and finely powdered, while herbo-mineral and Bhasma samples were uniformly triturated to achieve fine particle size. The samples were analyzed either by the KBr pellet method, in which the powdered sample was mixed with spectroscopic-grade potassium bromide and pressed into transparent pellets, or by ATR-FTIR, which allows direct analysis with minimal preparation. Adequate drying was ensured to minimize moisture interference and obtain reproducible spectra in the mid-infrared region (4000–400 cm^{-1})

Advantages of FTIR

- Requires only a very small amount of sample, which is ideal for limited or valuable materials.
- Rapid technique – spectra can be obtained within a short time.
- Non-destructive analysis, allowing the same sample to be analyzed repeatedly.
- Enables high reproducibility, helping to verify and confirm results.
- High sensitivity for detecting different functional groups present in a sample.
- Requires minimal or no sample preparation, saving time and reducing errors.
- Suitable for complex samples such as herbal drugs, biological tissues, and herbo-mineral formulations.[7]

Limitation of FTIR

- FTIR is primarily a qualitative technique; accurate quantification of metallic, mineral, or bioactive constituents in complex formulations and Bhasma is difficult without rigorous calibration.
- Overlapping absorption bands are common in polyherbal and herbo-mineral formulations, making spectral interpretation challenging.
- Strong water absorption in herbal extracts can mask important functional group bands, especially in transmission FTIR.
- In ATR-FTIR, spectra of Bhasma and mineral-based preparations may show band shifts and intensity variations due to refractive index differences and limited penetration depth.
- FTIR has low sensitivity for trace elements, limiting detection of minor metallic constituents.
- It cannot provide complete structural, crystalline, or elemental information for metals and minerals.[8]

Literature Review of FTIR Studies on Ayurvedic Drugs

Withania somnifera

S. No.	Wavenumber (cm^{-1})	Functional Group / Bond	Type of Compound	Phytochemical Correlation
1.	3440 cm^{-1}	O–H stretching	Phenolic compounds	Phenolics, flavonoids
2.	2924 cm^{-1}	C–H / Carboxylic acid stretching	Carboxylic acids	Withanolides, organic acids
3.	1540 cm^{-1}	N–O stretching	Nitro compounds	Alkaloids, nitrogen-containing compounds
4.	1004 cm^{-1}	C–O stretching	Ethers / glycosidic linkages	Alkaloids, nitrogen-containing compounds

TINISPORA CORDIFOLIA[9]

Sample	Wavenumber (cm^{-1})	Functional Group Identified	Chemical / Phytochemical Indication
Aqueous Extract	2956, 2825	C–H and O–H stretching	Alcohols, aliphatic chains
	1566, 1401, 1277	C–C and N–O stretching	Aromatic cyclic compounds
	827, 664, 559	C–C, aldehyde vibrations	Long-chain aliphatic compounds, aldehydes
Guduchi Satva	3307, 2931	O–H and C–H stretching	Alcohols, polysaccharides

	1664	C=O stretching	Ketone group
	1337, 1149, 1076	C–O, C–C, C–H bending, N–O stretching	Aromatic and nitrogen-containing compounds
	996, 926, 860, 763, 706	C–C and C=C stretching	Long-chain aliphatic compounds

Amrtadi Churna[10]

Batch 1 (cm-1)	Batch 2(cm-1)	Batch 3(cm-1)	Bond type	Functional group
3851.15	3853.08	3854.04	Unknown	Unknown
3735.44	3734.48	3736.41	Unknown	Unknown
3390.25	3414.35	3401.82	N-H stretching	Amide
2931.27	2350.8	2933.2	Alkyl C-H stretch	Alkane
2355.62	Absent	2356.59	Unknown	Unknown
1708.62	1712.48	1708.62	C=O stretching	Aldehyde/ketone
1621.84	1622.81	1621.84	C=C bending	Aromatic
1539.88	1536.99	1540.85	N-O asymmetric stretch	Nitro compound
1449.24	1445.39	1450.21	C-H Bending	Alkanes
1348	1351.86	1381.75	C–H rock	Alkanes
1220.72	1220.72	1221.68	C–N stretch	aliphatic amines
1044.27	1047.16	1043.3	C–O stretch	Alcohols/carboxylic acids/esters/ethers
872.63	875.52	873.6	=C–H bend	Alkenes
764.64	760.78	762.71	C-H bending	Aromatics
672.07	670.14	670.14	Alkene C-H bending	Alkynes

The FTIR spectrum of Amrtadi churna correlates well with its herbal ingredients—Gokshur, Amalaki, and Guduchi—by showing characteristic functional group peaks. The band around 3390–3414 cm^{-1} (N–H stretching) indicates alkaloids from Guduchi, while peaks at 1708–1712 cm^{-1} (C=O) and 1621–1622 cm^{-1} (aromatic C=C) confirm phenolic compounds and tannins from Amalaki. Additionally, peaks near 2931 cm^{-1} and 1445 cm^{-1} (C–H stretching/bending) suggest aliphatic chains and support the presence of steroidal or triterpenoid (Steroidal and triterpenoid compounds mainly contain hydroxyl (–OH), carbonyl (C=O), double bonds (C=C), and in triterpenoids, carboxylic (–COOH) groups) compounds from Gokshur. Thus, the FTIR profile confirms the contribution of each ingredient to the formulation's phytochemical composition.

Hridayarnava Rasa[11]

S. No	Wavenumber (cm^{-1})	Functional Group / Bond	Type of Vibration	Interpretation
1	3876–3421	O–H, N–H	Stretching	Hydroxyl groups & amines (from herbal components)
2	2922, 2853	C–H	Stretching	Aliphatic chains (organic compounds)
3	1612	C=O	Stretching	Carboxylic acids / amide groups
4	1383	C–H / N–O	Bending	Methyl groups / nitro compounds
5	1115	C–O	stretching	Alcohols, ethers, esters
6	883–791	C–H	Bending	Aromatic ring structures
7	651–614	C–Cl	Stretching	Halogen compounds
8	504	C–Br	Stretching	Brominated compounds
9	456	C–I	Stretching	Iodinated compounds

The functional groups observed in the FTIR spectrum of Hridayarnava Rasa are present mainly due to the herbal processing (Bhavana), purification (Shodhana), and incineration (Marana) steps involved in its preparation. During Bhavana, herbal liquids such as Triphala Kwatha and Kakamachi Swarasa are added, which contain various organic compounds like alcohols, phenols, amines, and carboxylic acids. Triphala contains minor alkaloids with functional groups like –NH, –OH, C=O, and aromatic C=C, whereas Kakmachi is rich in steroidal alkaloids (solanine, solasonine, etc.) having –NH, –OH, C–H, C=C, and glycosidic (–O–) groups. Halogen FTIR bands (C–Cl/C–Br) usually come from mineral salts or impurities, not from the herbal ingredients.

MAKRDHWAJ[12]

Wavenumber (cm^{-1})	Functional Group / Bond	Chemical / Structural Indication
3658, 3431	O–H, N–H	Alcohols, phenols, amines
2923, 2850	C–H (alkyl)	Presence of alkyl chains
1632	C=C	Aromatic or conjugated systems
1513	N–O	Nitro compounds
1385	C–H (methyl)	Methyl groups
1112	C–N	Amines / nitrogen-containing compounds
742	C–H (aromatic)	Aromatic ring structures

The organic functional groups observed in the FTIR spectrum of Makaradhwaja, such as O–H, C–H, C=C, and C=O, mainly originate from the herbal materials used during its preparation, particularly Aloe vera juice and Hibiscus flower juice in the Bhavana (levigation) process. (Aloe vera shows –OH, C=O, C–O (polysaccharides, anthraquinones), while Hibiscus shows –OH, C=O, aromatic C=C, and C–O–C (flavonoids, anthocyanins) .These plant materials contain phytochemicals like phenols, alcohols, proteins, and organic acids, which contribute to O–H, N–H, and C=O functional groups. During the high-temperature Kupipakwa process, these organic constituents undergo chemical transformations, leading to the formation of new compounds and stabilization of functional groups such as C=C and C–H.

Yashad bhasam[13]

Wavenumber (cm^{-1})	Functional Group / Bond	Stage / Chemical Indication
517–576 (<800)	Zn–O	Formation of zinc oxide (incineration stage)
~1371	C–H	Presence of organic groups in final stages
1657–1739	C=C, C=O	Aromatic and carbonyl compounds
~1227	C–N	Nitrogen-containing compounds
3000–3740	O–H	Hydroxyl groups (alcohols/phenols)

The major peaks observed in the FTIR spectra of Yashad Bhasma after purification and in final product shows the presence of C=C, C=O and C-H bonds. The source of organic group in final product is due to the plant material used during preparation, which contains several organic compounds eg. Azardica indica (neem) contains azadirachtin and derivatives basically terpin and lomonoids.

Tamra bhasam[14]

Spectral Region (cm^{-1})	Observed Peaks / Range	Functional Group / Assignment	Interpretation
Hydrogen stretching region	Multiple peaks (10–11)	O–H, N–H, C–H	Variation depends on *Shodhana* medium
Triple bond region (2700–1950)	No peaks	C≡C, C≡N absent	Indicates absence of complex triple-bond structures
Double bond region (1950–1550)	~1700 cm^{-1}	C=O stretching (ketones, acids, amides, carbonates)	Presence of carbonyl-containing compounds
	1690–1600 cm^{-1}	C=C, C=N stretching	Indicates alkenes, aromatics, and imines
Aromatic region (1650–1450)	Peaks present	Aromatic ring vibrations	Confirms aromatic compounds
Fingerprint region (1500–700)	~1200 cm^{-1}	C–O–C stretching	Ether or ester linkages
	700–800 cm^{-1}	C–Cl vibrations	Possible halogen-containing compounds
C–H stretching/bending	~2870 cm^{-1}, ~1380 cm^{-1}	Alkyl (aliphatic) & aromatic C–H	Indicates presence of hydrocarbon chains
O–H stretching	3610–3670 cm^{-1}	Free O–H (phenols, low concentration)	Weak hydrogen bonding
	3200–3400 cm^{-1}	Alcohols/phenols	Strong hydrogen bonding
N–H stretching	3400–3500 cm^{-1}	Amines	Presence of nitrogen-containing groups
	2400–3200 cm^{-1}	Ammonium ions	Indicates protonated amines
Carboxylic acid region (1580–1690)	Absent in Bhasma	–COOH group absent	Confirms proper Bhasma formation (*Niramlatva*)

Vajra abharak Bhasma[15]

Spectral Region (cm^{-1})	Observed Peaks / Range	Functional Group / Assignment	Interpretation
3700–3600	Sharp peaks	Free O–H stretching (alcohols)	Presence of non–hydrogen bonded hydroxyl groups
3150–3000	Broad bands	Hydrogen-bonded O–H	Indicates intramolecular H-bonding in hydroxyl groups
2350–2340	Sharp peak	O=C=O stretching	Presence of CO_2 or carbonate groups
1550–1500	Strong absorption	N–O stretching	Indicates nitro compounds
1045–980	Broad, intense bands	Acid anhydride, monosubstituted alkenes	Suggests complex organic functional groups
713–694	Peaks present	Aromatic C–H bending (benzene derivatives)	Confirms aromatic compounds
466–456	Peaks present	Si–O–Si linkage	Confirms siloxane/silicate network
685–500	Bands present	C–Br stretching	Indicates halogen-containing compounds
900–400 (overall)	Multiple bands	Fingerprint region	Confirms complex organic–inorganic structure

The FTIR spectrum of the final product shows both organic and inorganic functional groups, which arise due to the combined effect of ingredients and processing. The presence of O–H groups (3700–3000 cm^{-1}) is due to herbal materials used during Bhavana, such as plant decoctions and cow milk, which contain phenols, alcohols, and tannins.

The broad nature of the peak indicates hydrogen bonding in these compounds. The carbon dioxide peak (2350 cm^{-1}) appears due to atmospheric CO_2 or formation of carbonate during repeated heating cycles (Marana). The N–O peaks (1550–1500 cm^{-1}) arise from nitrogen-containing compounds like alkaloids and other phytochemicals introduced from herbs. The C–O and anhydride peaks (1045–980 cm^{-1}) are due to organic acids, esters, and glycosides present in plant materials.

The aromatic benzene peaks (713–694 cm^{-1}) confirm the presence of flavonoids and phenolic compounds from herbs. Silicate (Si–O–Si) peaks (750–450 cm^{-1}) originate from the main mineral ingredient, Abhraka (biotite mica), which is rich in silicate structures. The halogen peaks (C–Br) are not from plants but are likely due to mineral salts, ash of plant materials (e.g., castor leaves), or trace impurities introduced during processing. Thus, the FTIR spectrum clearly indicates that the final product is a bio-inorganic system, containing both herbal organic compounds and mineral components, which is responsible for its therapeutic activity.

Rajat bhasam[3]

Actual peak	Bond	Type of bond	Specific type of bond
2918.94	C - H	Alkyl	Methylene
2850.88	C - H	Alkyl	Methyl
1022.64	C – N	Aliphatic Amine	Any

Pital bhasam[16]

Wavenumber (cm^{-1})	Functional Group	Interpretation
519	Cu–O, Zn–O	Metal oxide bonds
1101	C–O	Organic compounds (alcohols/ethers)
2334	O–H	Hydroxyl group / moisture

The functional groups observed in the FTIR spectrum of Pittal Bhasma are present due to both the processing method and the materials used during its preparation. During the incineration (Marana) process, metals like copper and zinc react with oxygen at high temperatures, leading to the formation of metal oxides (Cu–O and Zn–O bonds), which appear in the lower wavenumber region. At the same time, during the Bhavana (levigation) process, various herbal juices and organic media are used, which introduce organic compounds containing C–O groups that remain adsorbed on the surface of the bhasma particles. Additionally, the presence of O–H groups is due to residual moisture and hydroxyl-containing compounds from herbal ingredients and atmospheric absorption. Thus, the FTIR functional groups arise from a combination of inorganic metal oxide formation and organic constituents from plant-based processing, confirming the herbo-metallic nature of the formulation.

Naga bhasam[17]

Functional groups	A(ν cm-1)	B(ν cm-1)	D(ν cm-1)	G(ν cm-1)	U(ν cm-1)
2- substituted pyridines	417.68	415.82	412.70	417.60, 411.39, 405.63	418.99, 405.87
Halogens	-	612.42	748.11	616.06, 685.34	712.93, 685.74
Aldehydes	866.54	-	867.13	844.48	874.43
Carboxylic acid	930.52, 1456.38	-	-	987.04, 910.18	-
Alkyl amine	-	-	-		1128.26
Tertiary alcohol	1412.78	1384.45	1457.11	1446.84	1421.04
Secondary amides	1636.62, 3448.37	1637.94, 3415.70	1638.08, 3448.54	1632.06, 3445.65	1637.73, 3448.92
Di alkyl ketone	2843.59, 2917.14	2847.31, 2924.96	2925.31	2921.23	2917.14

Hirak bhasam[18]

Peaks	Actual	Functional groups	
	669,712	Aliphatic arganhalogen compounds	From Saidhav
1250+890-800	874	Epoxy & oxirane ring	From Kulittha Kvatha
1150-1100	1016	Aliphatic fluro compounds	From Saidhav
1420-1300	1419	Carboxylate	From Kulittha Kvatha
1815-1770,1820-1775	1792	Acid (acyl) halide, aryl carbonate	From Saidhav
2100=1800	2090	Transition metal carbonyls	From Saindhav and From KulitthaKvatha
	3648,3687,3816,3834,3850,3900	CH bend	From Kulittha Kvatha

Commonly Studied FTIR Markers

FTIR Wavelength Library / Reference Spectra for Ayurvedic Drugs[19]

Wavenumber (cm^{-1})	Functional Group / Bond	Observed in Literature Review (Ayurveda)	Comparative Interpretation
3600–3200	O–H stretching (broad)	Withania, Tinospora, Hridayarnava Rasa, Makardhwaj, Tamra, Vajra Abhraka, Praval	Broad bands confirm phenolics, alcohols, glycosides, and herbal media used during Bhāvanā and Śodhana.
3645–3600	Free O–H (sharp)	Vajra Abhraka, Praval Bhasma	Sharp peaks indicate free hydroxyl groups after mineral processing or carbonate formation.
3500–3300	N–H stretching	Withania, Hridayarnava Rasa, Makardhwaj, Tamra Bhasma	Indicates amines, alkaloids, ammonium ions from herbal processing.
3100–3000	=C–H stretching	Withania, Tinospora, aromatic herbs	Reflects aromatic and unsaturated phytoconstituents
2960–2850	Aliphatic C–H stretching	Almost all herbal, polyherbal, herbo-mineral drugs	Alkyl chains, lipids, organic coatings.
2260–2100	C≡C / C≡N	Generally absent; occasional carbonate/CO_2 in Vajra Abhraka	Absence supports complex natural origin; CO_2 bands explained by carbonates.
1750–1700	C=O stretching	Guduchi Satva, Amṛtādi Cūrṇa, Hridayarnava Rasa, Praval	Esters, acids, ketones from herbs and Sneha.
1680–1630	Amide I / C=C	Proteins (herbs), Makardhwaj, Tamra	Aromatic C=C and protein amide linkages overlap
1650–1550	N–H bending (Amide II)	Withania, Tamra, Nāga Bhasma	Nitrogen-containing compounds.
1600–1450	Aromatic C=C	Most herbal & polyherbal drugs	Aromatic rings dominate herbal fingerprints.
1350–1260	O–H bend / C–N stretch	Withania, Guduchi, Amṛtādi Cūrṇa	Phenols, amines, glycosides
1250–1000	C–O stretching	Sugars, ethers, Satva, polyherbals	Carbohydrates and glycosides.
1150–1050	C–O–C stretching	Guduchi Satva, Amṛtādi Chūrṇa	polysaccharide structures

1000–900	=C–H bending	Tinospora, Amṛtādi Chūrṇa	Unsaturation and aromatic substitutions.
900–700	Aromatic C–H (oop)	Hridayarnava, Vajra Abhraka, Praval	Ring substitution patterns retained.
700–500	Metal–O stretching	Yashad (Zn–O), Tamra (Cu–O), Pittal	Oxide formation during Māraṇa.
500–400	Lattice vibrations	Vajra Abhraka, Tamra, Hirak	Indicates silicates and mineral frameworks.

Across all categories, FTIR studies consistently focus on identifying functional group markers rather than individual chemical constituents.

Common FTIR markers

FTIR studies of herbal, herbo-mineral, and Bhasma formulations mainly reveal characteristic functional-group markers rather than specific compounds. Broad O–H and N–H bands (3200–3600 cm^{-1}) are commonly observed, indicating hydroxyl and amine groups derived from herbal processing during Śodhana and Bhāvanā. Aliphatic C–H stretching (3000–2850 cm^{-1}) reflects organic chains and coatings present in herbal and herbo-mineral preparations. Bands between 1820–1600 cm^{-1} correspond to C=O and C=C vibrations, associated with carbonyl and aromatic structures. Nitrogen-containing groups appear as N–O and C–N bands in the 1550–1300 cm^{-1} range. The fingerprint region (1200–600 cm^{-1}) is most diagnostic, confirming sugars and aromatic compounds in herbal drugs, and metal–oxygen bonds, carbonates, and silicates in Bhasma, indicating formation of a stable inorganic core.

Comparison of FTIR with Other Analytical Techniques Used in Ayurvedic Drug Evaluation[3,6,14,20]

Analytical Technique	Information Provided	Role in Ayurvedic Drug Analysis	How it Compares with FTIR
FTIR Spectroscopy	Functional groups, chemical bonding, organic–inorganic interactions	Authentication, chemical fingerprinting, confirmation of Māraṇa and Bhāvanā effects	Primary qualitative screening tool; does not give crystal structure or elemental quantity
X-Ray Diffraction (XRD)	Crystalline phase, lattice structure	Confirms phase transformation of metals/minerals (e.g., Zn → ZnO)	FTIR confirms bond formation; XRD confirms crystal structure
SEM–EDS	Particle size, morphology, elemental composition	Confirms fineness, homogeneity, and elemental purity of Bhasma	FTIR shows bonding; SEM–EDS shows structure and elements
HPTLC / HPLC	Separation and quantification of phytochemicals	Marker-based standardization of herbal/polyherbal drugs	FTIR gives holistic fingerprint; chromatography gives compound-level data
ICP-MS / AAS	Trace and toxic metal quantification	Safety evaluation and pharmacopeial compliance	FTIR indicates chemical form; ICP/AAS gives precise metal concentration

DISCUSSION

FTIR spectroscopy is widely recognized as a rapid, non-destructive analytical tool for quality evaluation of herbal medicines by identifying functional groups and chemical interactions. Its ability to generate a chemical fingerprint enables consistent assessment of raw materials and finished products. FTIR has been used to discriminate different herbal species and monitor batch consistency, making it suitable for quality control protocols in traditional medicine analysis.

Detection of adulteration and substandard quality is one of the most important applications of FTIR spectroscopy in the quality evaluation of Ayurvedic drugs.

Adulteration may occur intentionally, such as the addition of synthetic drugs to herbal formulations for rapid therapeutic effects, or unintentionally due to substitution, improper processing, or poor-quality raw materials.

In genuine herbal and Ayurvedic formulations, FTIR spectra exhibit characteristic absorption bands corresponding to naturally occurring functional groups such as O–H, N–H, C–H, C=O, and C–O. Adulteration alters these spectral patterns by introducing new absorption bands, changing peak intensities, or causing shifts in existing peaks, which can be detected by comparison with authentic reference spectra. A clear example of FTIR-based adulteration detection is reported by Azminah et al., where synthetic pharmaceutical adulterants such as sildenafil citrate, phenylbutazone, and sibutramine HCl were added to herbal products.

Authentic samples lacked strong carbonyl absorption bands, whereas adulterated samples showed prominent

C=O stretching bands at ~1700–1750 cm^{-1} along with additional peaks around 938, 751, and 1292 cm^{-1}, which served as reliable indicators of adulteration (adulteration reference).[21]

FTIR spectroscopy provides a characteristic chemical fingerprint of Ayurvedic herbal, polyherbal, herbo-mineral, and Bhasma formulations by representing the collective vibrational pattern of functional groups rather than individual compounds. Similar to previously reported ATR-FTIR fingerprinting studies, the mid-infrared region (4000–400 cm^{-1}), particularly the fingerprint region (≈1400–400 cm^{-1}), offers formulation-specific spectral patterns that remain consistent for authentic samples prepared under standardized conditions.[7]

FTIR analysis of Ayurvedic formulations reveals characteristic functional groups that directly reflect their composition and pharmaceutical processing. In single herbal drugs such as *Withania somnifera* and *Tinospora cordifolia*, broad O–H and N–H stretching bands in the 3600–3200 cm^{-1} region arise from naturally occurring phenolics, flavonoids, glycosides, proteins, and alkaloids, serving as markers of herbal identity and therapeutic potential. Polyherbal formulations like Amṛtādi Chūrṇa exhibit overlapping bands corresponding to O–H/N–H, C–H, C=O, C=C, and C–O/C–N vibrations due to the cumulative contribution of multiple plant ingredients, generating a reproducible chemical fingerprint that confirms formulation integrity and batch consistency. In herbo-mineral formulations such as Haridrāṇava Rasa and Makardhwaj, the coexistence of organic functional groups and inorganic signatures results from the use of herbal juices and decoctions during Bhāvanā and Kupipāka Rasāyana, leading to stable organic–inorganic interactions rather than complete degradation of organic matter. In metallic and mineral Bhasma including Tamra Bhasma, along with Yashad, Vajra Abhraka, Rajata, Praval, Pittal, Nāga, and Heeraka, prominent low-frequency bands in the 600–400 cm^{-1} region correspond to metal–oxygen or lattice vibrations (such as Cu–O in Tamra Bhasma) formed during Māraṇa, confirming transformation of raw metals and minerals into oxide, carbonate, or silicate forms. The absence or marked reduction of carboxylic acid bands in Tamra Bhasma further supports proper Bhasma formation in accordance with the Ayurvedic principle of *Niramlatva*. Thus, the observed FTIR functional groups collectively provide chemical evidence of formulation composition, processing authenticity, and therapeutic suitability.

Gaps in Current FTIR-Based Research on Ayurvedic Drugs

FTIR spectroscopy in Ayurvedic drug analysis, significant research gaps persist. Most studies lack validated, formulation-specific FTIR marker bands, reporting only general functional group assignments, which limits regulatory and pharmacopeial applicability.In addition, poor sample standardization—including variations in raw material source, processing methods, and sample preparation techniques—leads to spectral variability and reduced reproducibility. The absence of official FTIR reference libraries for Ayurvedic formulations remains a major challenge, highlighting the need for standardized protocols, validated markers, and multi-technique correlation to strengthen scientific validation of Ayurvedic medicines.[6,8]

CONCLUSION

Fourier Transform Infrared (FTIR) spectroscopy is a powerful, rapid, and non-destructive analytical technique that significantly contributes to the quality control, authentication, and standardization of Ayurvedic herbal, herbo-mineral, and Bhasma formulations. By identifying characteristic functional groups, FTIR provides critical evidence of chemical transformations occurring during classical Ayurvedic pharmaceutical processes such as Śodhana, Bhāvanā, and Māraṇa.

FTIR is most effective for confirming formulation identity, organic–inorganic interactions, and batch-to-batch consistency rather than precise quantification of individual constituents. Its integration with advanced analytical tools enhances scientific validation while preserving the traditional integrity of Ayurveda.

Establishment of standardized FTIR reference libraries for classical Ayurvedic drugs, supported by pharmacopeial guidelines, will further strengthen quality assurance, regulatory acceptance, and global credibility of Ayurvedic medicines.

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