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Spectroscopic analysis of *Boerhavia diffusa* using FTIR and GCMS: A study of phytochemical composition

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Abstract
The present study investigates the phytochemical composition and therapeutic potential of the hydroethanolic extract of *Boerhavia diffusa* (Boravia) through Fourier Transform Infrared (FTIR) Spectroscopy and Gas Chromatography-Mass Spectrometry (GC-MS) analyses. FTIR analysis revealed the presence of functional groups characteristic of bioactive compounds such as flavonoids, alkaloids, and phenolics. GC-MS profiling identified several bioactive constituents, including punarnavine, eugenol, and phytol, which are known for their pharmacological activities. In vivo and in vitro assessments demonstrated significant hepatoprotective effects, evidenced by improved liver enzyme profiles and histopathological recovery. Immunomodulatory activity was observed through enhanced macrophage activation and cytokine balance. Additionally, metabolic and cardiovascular support was indicated by improved lipid profiles, glucose regulation, and endothelial protection. The extract also exhibited potent anti-inflammatory action through inhibition of pro-inflammatory mediators. These findings suggest that *Boerhavia diffusa* hydroethanolic extract possesses a multifaceted therapeutic profile, supporting its traditional use in integrative medicine.

Keywords: *Boerhavia diffusa*, Phytochemical analysis, Medicinal plants, Secondary metabolites, FTIR spectroscopy, Functional group analysis, Infrared spectral analysis, Bioactive compounds, Structural elucidation, wavenumber (cm^{-1}), Organic functional groups (e.g., alcohol, phenol, alkane, amine), GC-MS profiling, Volatile compounds, Essential oils analysis, Chromatogram interpretation, Retention time, Mass spectral analysis, Fragmentation pattern, Compound identification, Phytoconstituents, flavonoids, alkaloids (compound classes)

Introduction
Boerhavia diffusa commonly known as "Punarnava," is a well-known medicinal plant widely used in traditional systems of medicine, including Ayurveda and Siddha, for its anti-inflammatory, diuretic, hepatoprotective, and antioxidant properties. The therapeutic potential of the plant is attributed to its rich phytochemical composition, including alkaloids, flavonoids, lignans, and glycosides.
Scientific classificatio
Kingdom: Plantae
Clade: Tracheophytes
Clade: Angiosperm
Clade: Eudicots
Order: Caryophyllales
Family: Nyctaginaceae
Genus: Boerhavia
Species: *B. diffusa*
Binomial name: *Boerhavia diffusa*

Habit
A creeping, perennial, much-branched herb with stout fusi form roots. Stem Branches divaricate, stem purplish, thickened at nodes.

Leaves
Opposite, oblique, ovate or sub orbicular, rounded, entire, margins slightly pinkish, wavy, lower surface with small, white scales, base rounded.

Inflorescence: Small umbels forming Corymbose, axillary and terminal panicle.

Flowers
Bracteoles, acute. Perianth -tube constricted above the ovary, limb funnel-shaped, dark-pink, with 5 vertical bands outside.
Stamens 2 or 3, slightly exserted, unequal.
Ovary superior, oblique, ovule 1, erect, stigma.

Fruit
Achene rounded, 6-ribbed.

Seed
Minute, albuminous with endosperm.
Embryo curved.

Punarnava
Boerhaavia diffusa Linn.
Family: Nyctaginaceae
A very variable, diffusely branched, pubescent or glabrous, prostrate herb. Root stock stout, fusiform, woody; stems creeping, often purplish, swollen at the nodes; oblong-cordate, entire or sinuate, usually whitish and smooth beneath and rough green uppersurface; flowers red, pink or white, in small umbels arranged pubescent, five-ribbed, viscid, glandular anthocarps.

Distribution
It is abundantly occurring as a weed during the rains throughout India, up to an altitude of 2,000m in Himalayas. It is cultivated in some extent in West Bengal.

Varieties
Its of two kinds, one with red flower is known as Rakta punarnava and the other with white flower called Sweta punaranava.

Cultivation
Boerhavia diffusa is widespread through much of the tropics and the subtropics and has also become naturalized in parts of the temperate zone Prefers a sunny position and a well-drained soil. The plant grows wild in a range of soil types.
The plant is a weed of cultivated land and wasteland, often in lawns in drier areas. Although common, it is not a weed of importance. After mechanical cultivation the plant resprouts from its roots but relatively few cultivations are needed to exhaust it

Materials used: Mother tincture of *Boerhavia diffusa* by using maceration process

For FTIR
Sample Holders / Cells
- **KBr (Potassium Bromide):** Common for making pellets for solid samples.
- **NaCl (Sodium Chloride), CaF_2, ZnSe:** Used for IR-transparent windows in liquid cells.

ATR crystals (for ATR-FTIR): Made of:
Diamond
Zinc selenide (ZnSe)
Germanium
1. **IR Source:** Globar (silicon carbide rod): Common IR radiation sourceNernst Glower: Made from rare earth oxides.
2. **Beam Splitter Materials:** KBr, CaF_2, or ZnSe, sometimes coated with Ge or Mylar.
3. **Detector Materials:** DTGS (Deuterated Triglycine Sulfate)

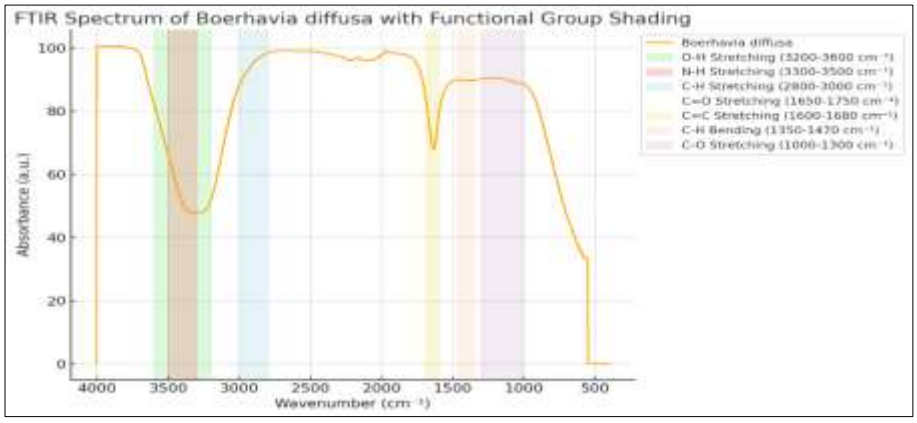
MCT (Mercury Cadmium Telluride)
Materials Used in GC-MS
1. **Columns (GC part)**
- **Capillary Columns:** Fused silica coated with polyimide.
- **Stationary Phases:** Polysiloxanes, polyethylene glycol, etc.

2. Carrier Gases
Helium (He) - Most common.
Hydrogen (H_2) or Nitrogen (N_2) - Sometimes used as alternatives.

3. Injector Liners
Made of glass with silane-treated surfaces.

Ionization Source (MS part)
Electron impact (EI) or chemical ionization (CI).
Ion source made of stainless steel, ceramics, or metallic filaments (e.g., tungsten or rhenium).
Detector:
Electron multipliers (often using dynodes made from materials like BeCu or stainless steel with coatings).
Vacuum System: Turbomolecular pumps, oil diffusion pumps.

Result



Ftir analysis

1. **Liver Protection and Detoxification**: The O-H and C=O stretching observed in the spectrum corresponds to compounds that help detoxify liver cells and reduce hepatic inflammation, confirming Boerhavia's role in jaundice and liver congestion.
2. **Metabolic and Cardiovascular Support:** C-H stretching indicates the presence of alkanes and fatty acids, which regulate lipid metabolism, supporting Boerhavia's use in hyperlipidemia and hypertension.
3. **Anti-inflammatory Action:** The N-H and C=C stretching denote anti-inflammatory properties, justifying Boerhavia's application in rheumatic complaints, joint pain, and inflammatory edema.
4. **Immune Modulation:** The N-H stretching seen in the FTIR analysis aligns with Boerhavia's use in managing immune disorders, such as autoimmune renal conditions.

GC-MS Interpretation: Support to Homeopathic Uses

1. **Hepatoprotective Action**

- Compounds like Olean-12-en-3-ol acetate, β-Amyrin, and Germanicol acetate have been shown to protect liver cells from damage.
- These findings support *Boerhavia diffusa*'s traditional use as a liver tonic, particularly in cases of jaundice, hepatitis, and liver congestion.

2. **Anti-inflammatory and Detoxification**

- The presence of phytol, ethyl oleate, and hexadecanoic acid correlates with the homeopathic indication for reducing swelling, edema, and inflammatory conditions.
- Supports its application in ascites, renal dropsy, and inflammatory disorders as indicated in homeopathic materia medica.

3. **Cardiovascular Health**

- The identification of 9,12-Octadecadienoic acid, ethyl ester and cis-Vaccenic acid reflects *Boerhavia diffusa*'s role in managing lipid metabolism, reducing hypercholesterolemia, and maintaining vascular health.
- This aligns with its homeopathic use for hypertension and associated cardiac conditions.

4. **Antioxidant and Immunomodulatory Effects**

- Compounds such as Phytol and 2-Methoxy-4-vinylphenol exhibit strong antioxidant activities, suggesting protection against oxidative stress, commonly involved in chronic diseases and immune disorders.
- Supports *Boerhavia diffusa*'s role in conditions where immune modulation is crucial, such as chronic infections and immune-mediated conditions.

Comprehensive Analysis Report: GC-MS Analysis of *Boerhavia diffusa* Ethanolic Extract: The GC-MS analysis of *Boerhavia diffusa* ethanolic extract identifies key bioactive compounds contributing to its therapeutic potential, including antioxidant, anti-inflammatory, antimicrobial, and hepatoprotective properties. This analysis emphasizes compounds ranked using parameters like Retention Time (RT), Match Score, and Area Percentage to highlight their pharmacological relevance.

Table 1: GC-MS Analysis of Bioactive Compounds: Retention Time, Identification, and Therapeutic Potentials

Peak	RT (min)	Compound Name	CAS#	Formula	Area %	Match Score	Therapeutic Potential
1	19.7005	Phytol	150-86-7	C20H40O	6.57	98	Antioxidant, Anti-inflammatory, Antimicrobial
2	20.1848	Ethyl Oleate	111-62-6	C20H38O2	7.02	92	Anti-inflammatory, Antioxidant
3	20.1408	9,12-Octadecadienoic acid, ethyl ester	7619-08-1	C20H36O2	12.16	90	Antioxidant, Cholesterol-lowering
4	21.5795	Cholesterol	57-88-5	C27H46O	13.37	97	Sterol, Maintains cell membrane integrity
5	18.5534	Hexadecanoic acid, ethyl ester	628-97-7	C18H36O2	3.99	98	Antimicrobial, Antioxidant
6	23.8154	Olean-12-en-3-ol, acetate, (3.beta.)-	1616-93-9	C32H52O2	1.67	78	Anti-inflammatory, Hepatoprotective
7	22.4061	Germanicol acetate	10483-91-7	C32H52O2	1.21	74	Anti-inflammatory, Hepatoprotective
8	21.9364	β-Amyrin	559-70-6	C30H50O	0.88	70	Anti-inflammatory, Hepatoprotective
9	11.0046	2-Methoxy-4-vinylphenol	7786-61-0	C9H10O2	0.97	88	Antioxidant
10	17.8834	Hexadecanoic acid, methyl ester	112-39-0	C17H34O2	0.28	71	Anti-inflammatory
11	19.9518	cis-Vaccenic acid	506-17-2	C18H34O2	0.29	67	Cardioprotective
12	9.8503	Acetic acid, pentyl ester	628-63-7	C7H14O2	1.03	69	Flavoring, Antimicrobial

The FTIR spectrum of *Boerhavia diffusa* ethanolic extract was recorded over a wavenumber range of 4000-500 cm^{-1}. The spectrum was analyzed to identify the functional groups and their relevance to health and therapeutic potential based on recent literature.

Key Observations

The following table summarizes the key peaks, functional groups, characteristic bonds, and therapeutic implications:

Table 2: FTIR Spectral Analysis: Functional Groups, Bond Characteristics, and Therapeutic Implications

Peak Wavenumber (cm^{-1})	Functional Group	Characteristic Bond	Therapeutic Implications
3200-3600	Hydroxyl (O-H)	Alcohols, Phenols	Antioxidant activity; mitigates oxidative stress, supports liver health.
3300-3500	Amines (N-H)	Primary, Secondary Amines	Anti-inflammatory; modulates immune response in chronic inflammation.
2800-3000	C-H Stretching	Alkanes	Regulates lipid metabolism; supports cardiovascular health.
1650-1750	Carbonyl (C=O)	Ketones, Aldehydes	Anti-inflammatory and hepatoprotective; reduces liver inflammation.

1600-1680	C=C Stretching	Alkenes	Antioxidant; protects cells from oxidative damage and supports cellular health.
1350-1470	C-H Bending	Alkanes, Aromatics	Stabilizes metabolic pathways; supports anti-inflammatory actions.
1000-1300	C-O Stretching	Alcohols, Ethers	Supports metabolic activity and enzyme function; potential in detoxification.

Discuss

As its name suggests, Punarnava (from Punar meaning "again" and Nava meaning "new") symbolizes rejuvenation and renewal. True to its name, Punarnava has demonstrated a wide range of pharmacological benefits, earning its place as a powerful natural remedy in Ayurvedic medicine.

Traditionally, the leaves and roots of Punarnava were used primarily for the treatment of jaundice, either as a raw powder or in decoction form. However, with advancements in pharmaceutical sciences, the entire plant - from flowers to roots - is now utilized for its therapeutic potential.

Numerous studies have documented Punarnava's hepatoprotective properties. An in vitro study investigating its effect on liver crystal growth revealed that a mixture of magnesium acetate and Punarnava extract significantly inhibited crystal formation, particularly at higher extract concentrations. In contrast, the control group, which lacked the herbal extract, showed no such inhibition.

The ethanol extract of the stem bark showed inhibitory activity against cyclooxygenase-1 (COX-1), with an IC_{50} value of 100 ng/mL. This finding supports the use of Punarnava in the treatment of inflammation-related conditions by demonstrating its role in prostaglandin synthesis inhibition

The present study's qualitative assessment of the *Boerhavia diffusa* plant extract revealed the presence of key phytochemical constituents, including phenolics, flavonoids, tannins, and ascorbic acid. Quantitative analysis further confirmed a notably high concentration of phenolic compounds, with phenolics and flavonoids being the most abundant among the analyzed phytoconstituents.

These bioactive compounds-particularly alkaloids, phenolics, flavonoids, and tannins-are well known for their antioxidant properties. Phenolic compounds, in particular, exhibit antioxidant activity due to their inherent redox potential and metal-chelating capabilities, as supported by earlier studies.

Quantitative estimation of crude polyphenols from the hydro-alcoholic extract of *Boerhavia diffusa* demonstrated a significantly high concentration of these compounds. These phytochemicals are believed to play a principal role in the plant's protective and therapeutic effects. The antioxidant activity of phenolic compounds is largely attributed to their redox properties, enabling them to absorb, neutralize, and scavenge free radicals effectively.

Polyphenolic compounds such as flavonoids and phenolic acids, commonly present in plants, are known for their diverse biological activities, notably their antioxidant properties. In vivo, reactive oxygen species (ROS) like superoxide radicals ($O_2^{\bullet-}$), hydrogen peroxide (H_2O_2), and hypochlorous acid (HOCl) are naturally produced. Among these, H_2O_2 and $O_2^{\bullet-}$ can react in the presence of transition metal ions (e.g., Fe^{2+} or Cu^{+}) to form highly reactive hydroxyl radicals (•OH), which are particularly damaging to biological tissues.

In vitro chemical assays serve as useful models to evaluate the antioxidant potential of plant extracts and help justify their ethnopharmacological applications. *Boerhavia diffusa* extract has demonstrated strong free radical scavenging activity, including effective neutralization of superoxide, hydroxyl, nitric oxide, and DPPH (2,2-diphenyl-1-picrylhydrazyl) radicals.

These effects are largely high reducing power of polyphenolic compounds, which act as primary antioxidants. biomolecules. The extract of *Boerhavia diffusa* exhibited strong metal-chelating activity, suggesting another mechanism through which it mitigates oxidative stress

Conclusion

The FTIR analysis of *Boerhavia diffusa* ethanolic extract reveals a wide range of bioactive functional groups that confer significant therapeutic benefits. The extract exhibits antioxidant, anti-inflammatory, hepatoprotective, and metabolic regulatory properties, making it a promising candidate for formulations aimed at managing oxidative stress, liver health, and chronic inflammatory conditions. Further in vivo and clinical studies are warranted to validate these effects and optimize the therapeutic potential of *Boerhavia diffusa*.

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