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IDENTIFICATION OF FUNCTIONAL GROUPS AND CHEMICAL PROFILING OF IPOMOEA PARASITICA USING FTIR SPECTROSCOPY

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Research Paper

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ABSTRACT

The chemical profile of *Ipomoea parasitica* was investigated using Fourier-transform infrared (FTIR) spectroscopy to identify the functional groups present in its methanol and AgNps extracts. Leaves and stems of *Ipomoea parasitica* were collected from natural habitats in Andhra Pradesh, India, and subjected to Soxhlet extraction with methanol and water. The resulting extracts were analyzed using FTIR spectroscopy with potassium bromide (KBr) pellets to determine their functional group composition. The FTIR spectra revealed prominent O-H stretching peaks at 3318.90 cm^{-11}, 3292.16 cm^{-1}, and 3270.18 cm^{-1}, indicative of alcohols and phenols. C-H stretching peaks at 2943.07 cm^{-1} and 2839.56 cm^{-1} confirmed the presence of alkanes. The analysis also identified C=C stretching at 1634.04 cm^{-1} and multiple peaks in the 1760-1400 cm^{-1} range, suggesting a diverse mixture of alkenes. Additionally, C-O stretching peaks at 1207.96 cm^{-1}, 1153.96 cm^{-1}, and 1356.32 cm^{-1} highlighted the presence of alcohols, carboxylic acids, esters, and ethers. C-N stretching at 1054.20 cm^{-1} indicated aromatic and aliphatic amines. Peaks for C-I and carbonyl groups further elucidated the presence of Iodo compounds and carbonyl-containing compounds. The FTIR analysis underscores the diverse chemical composition of *Ipomoea parasitica*, with functional groups that may have significant biological and practical implications. The presence of phenolic compounds suggests potential antioxidant or antimicrobial properties, while the broad array of functional groups indicates varied biological activities. Understanding the chemical profile of *Ipomoea parasitica* can inform its potential applications in pharmaceuticals, agriculture, and other fields. This is the first report of identification of functional groups from *Ipomoea parasitica* (leaves and stem).

No. of Pages: 10 **References: 29**

Keywords: Fourier-transform infrared (FTIR) spectroscopy, *Ipomoea parasitica*, AgNps, Functional groups, Alkanes, Phenolic compounds.

1. Introduction

About 59 genera and 1900 species make up the family Convolvulaceae, which occurs in mostly tropical and warm temperate parts of the world (Staples & Brummitt, 2007). Twining or climbing woody or herbaceous plants with heart-shaped leaves and funnel-shaped flowers make up this family. *Ipomoea,* with 500–600 species, has the most Convolvulaceae species diversity (Austin & Huáman, 1996). *Ipomoea* has around 650 species, nearly half of which are in the Americas and Asia (Mabberley, 2017). Around 65 *Ipomoea* species have been found in southern and western India (Undirwade & Bhadane, 2017).

Ipomoea parasitica was found in Indian states in the 20th century, Biju (2002) from Kerala and Tamil Nadu,

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Shimpale (2012) from Maharashtra, Pal (2012) from Andhra Pradesh and Chhattisgarh, Ravi kiran Arigela, L. Paramesh and Rajesh (2020) from Telangana contributed to *Ipomoea parasitica* history in India. Undirwade et al. (2015) and Undirwade & Bhadane (2017) found more records in Maharashtra. The species inhabits Kerala, Tamil Nadu, Karnataka, Maharashtra, Andhra Pradesh, Chhattisgarh and Telangana.

Traditionally, *Ipomoea* plants were used to cure renal difficulties, constipation, colic, digestive diseases, inflammatory, allergic reactions and more. Recently, scientific interest in the *Ipomoea* genus has increased. Significant chemical and pharmacological advances in this genus have shown it. Some species had antibacterial, analgesic, spasmolytic, spasmogenic, hypotensive, psychotomimetic, and anticancer activities. Pharmacological research supports various traditional medicine uses.

Despite extensive research on certain *Ipomoea* species, species like *I. parasitica* still remain unstudied. Due to their bioactive potency, the glycolipids, phenolic chemicals, and alkaloids likely account for most of this genus's actions. The extraction of novel active chemicals from this *I. parasitica* species may offer many future research opportunities with great scientific significance.

Figure 1. *Ipomoea parasitica* (Kunth) G. Don Plant.

2.0 Materials and Methods

2.1 Plant Materials

Fresh plant leaves and stems of *Ipomoea parasitica* were collected from natural habitats in Araku, Visakhapatnam, Andhra Pradesh, India in December of 2021. Identified by detailed study and relevant literature were authenticated by Prof. Dr. S.B. Padal, Dept. of. Botany, Andhra University, Visakhapatnam Andhra Pradesh, India. The collected leaves and stems were transferred to the laboratory under controlled conditions to maintain their freshness and prevent degradation. The leaves were cleaned with distilled water to remove any contaminants before proceeding with further experiments.

2.2 Preparation of Plant Extract

The leaves and stems were air-dried for 10 days in a shaded, well-ventilated area to prevent direct sunlight and moisture. After drying, the leaves and stems were pulverized into a fine powder using a mechanical grinder. The Soxhlet was equipped with 50 g of leaf powder and 50 g of stem powder separately and 500 ml of methanol solvent and device running constantly for 72 h. At the end of the extraction period, the extract was concentrated using vacuum evaporator to remove the solvent and obtain a dried extract.

2.3 Preparation of 1mM Silver nitrate stock solution ($AgNO_3$):

The Silver Nitrate ($AgNO_3$) was purchased from Sigma Aldrich Chemicals. An accurately weighed 16.9 mg of silver nitrate was dissolved with 100 ml of MilliQ water and stored in amber color bottle until further use.

2.4 Preparation of Silver nanoparticles:

Five millilitres of methanol extracts from the leaf and stem of *I. parasitica* were combined with 100 millilitres of 1 mM aqueous silver nitrate solution and

incubated at room temperature in the dark for the reduction to Ag+ ions. After 15 minutes, the solution's colour changed from colourless to yellowish-brown, suggesting the creation of silver nanoparticles (AgNps). The yellowish-brown solution of silver nanoparticles was isolated by centrifugation at 10,000 rpm for 20 minutes. The supernatant was discarded, and the pellets were collected. This dried extract was then sent for Fourier-transform infrared (FTIR) analysis to identify the functional groups present.

2.5. FTIR Analysis

For Fourier-transform infrared (FTIR) analysis, 1 mg of each dried extract powder was mixed with 10 mg of potassium bromide (KBr) and compressed in to translucent sample discs using a hydraulic press. The FTIR spectra were recorded using a spectrometer (Shimadzu, Japan) within the region of 4000 to 400 cm ^{1}, employing the standard KBr pellet technique. This allowed for the identification of the functional groups present in the extracts of *Ipomoea parasitica (*Pramila *et al.*, 2012).

3.0 Results

The FTIR spectrum was used to identify the functional groups of the active components based on the peak values in the infrared radiation region. The FTIR spectrum of the *Ipomea parasitica* plant extracts, methanolic extracts, leaves, stems, and AgNps in the form of a KBr pellet is shown in Figures 1,2, 3, and 4. The height absorption at 3318.90 cm^{-1} is due to the O-H stretching in the extract, indicating the presence of the alcohol/phenol functional group, as represented in Tables 1, 2, 3, and 4 (with the range between 3200-3600 cm^{-1}. The band at 2108.24 cm^{-1} corresponds to the C C stretching vibration, suggesting the presence of silicon compounds (within the range of 2050-2235 cm^{-1}. The absorption peak at 1634.04 cm^{-1} is due to the C=C stretching, characteristic of alkenes, which falls within the range of 1610-1680 cm^{-1}.

Additionally, the peak at 552.07–456.60 cm^{-1} is attributed to C-I and S-S bonds, associated with aliphatic iodo compounds (in the range of 600-450 $cm^{-1.}$ The absorption at 3292.16 cm^{-1} is due to O-H stretching, denoting alcohol/phenol groups (range of 3200-3600 cm^{-1}. The peak at 2107.96 cm^{-1} indicates C≡C stretching related to silicon compounds (within 2250-2050 cm^{-1}. The C=C stretching observed at 1637.80 cm^{-1} suggests the presence of alkenes. Peaks at 1207.96 cm^{-1} and 1153.96 cm^{-1} correspond to C-O stretching in alcohols, carboxylic acids, esters, and ethers (range of 1360-1180 cm^{-1}) and aliphatic amines (1300-1050 cm^{-1}, respectively. Additionally, C-N stretching at 1054.20 cm^{-1} is indicative of aromatic amines (range of 1250-1020 cm^{-1}).

The absorption peak at 3270.18 cm^{-1} is due to O-H stretching in alcohols/phenols (range of 3200-3600 cm^{-1}). The N-H stretching observed at 3105.15 cm^{-1} is associated with aliphatic amines (3000-3300 cm^{-1}). Peaks at 3007.97 cm^{-1} and 2943.07 cm^{-1} are related to O-H and C-H stretching, indicating alcohols/phenols (3200-3600 cm^{-1}) and alkanes (2970-2850 cm^{-1}), respectively. C=C stretching observed at 1689.96 cm^{-1}, 1642.96 cm^{-1}, 1581.57 cm^{-1}, 1546.97 cm^{-1}, 1516.64 cm^{-1}, 1452.22 cm^{-1}, and 1430.38 cm^{-1} suggests alkenes (within the range of 1760-1400 cm^{-1}). Various C-O stretching peaks observed at 1356.32 cm^{-1}, 1282.44 cm^{-1}, 1269.37 cm^{-1}, 1188.82 cm^{-1}, 1176.97 cm^{-1}, 1152.82 cm^{-1}, and 1108.58 cm^{-1} are associated with alcohols, carboxylic acids, esters, ethers (1360-1180 cm^{-1}), aliphatic amines (1300-1050 cm^{-1}), and aromatic amines (1250-1020 cm^{-1}).

Finally, the peak at 3257.80 cm^{-1} corresponds to O-H stretching in alcohols/phenols (range of 3200-3600 cm^{-1}). The peak at 3008.83 cm^{-1} denotes N-H stretching, related to aliphatic amines (3000-3300 cm^{-1}). C-H stretching observed at 2942.96 cm^{-1} indicates alkanes (2970-2850 cm^{-1}). The peaks at 1669.76 cm^{-1} and 1643.56 cm^{-1} are related to C-H stretching in carbonyl groups (1760-1690 cm^{-1}). The C=C stretching at 1582.01 cm^{-1}, 1453.56 cm^{-1}, and 1550.48 cm^{-1} suggests alkenes (1760-1600 cm^{-1}). The C-O stretching peaks at 1176.64 cm^{-1}, 1106.49 cm^{-1}, 1297.87 cm^{-1}, 1358.80 cm^{-1}, 1154.27 cm^{-1}, and 1227.83 cm^{-1} are associated with alcohols, carboxylic acids, esters, ethers (1360-1180 cm^{-1}), and aliphatic amines (1300-1050 cm^{-1}).

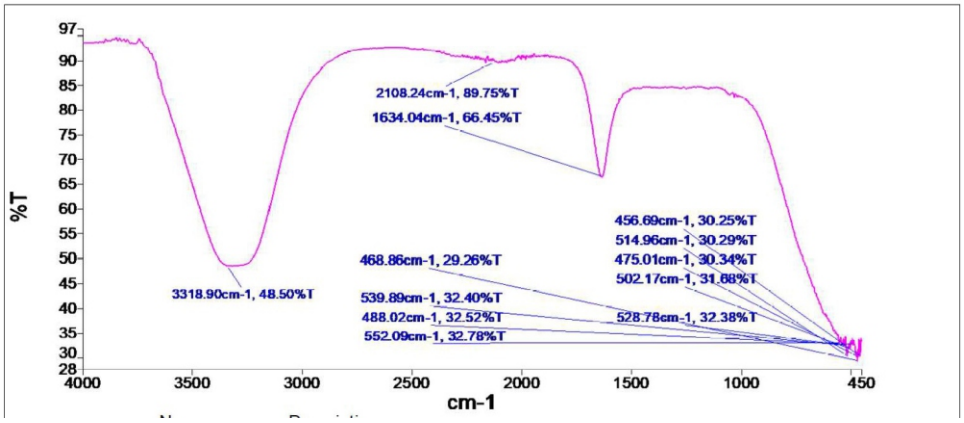

Figure 2: FTIR analysis of *Ipomoea parasitica* plant leaf methanol extract.

Table 1: FTIR Peak Values and Corresponding Functional Groups in *Ipomoea parasitica* leaf methanol Extracts.

S. No	Peak values(cm^{-1})	Bond	Functional groups assigned
1.	3318.90	O-H stretching	Alcohol/ phenol
2.	2108.24	CC stretching vibration	Silicon Compounds.
3.	1634.04	C=C stretching	Alkenes
4.	552.07	C-I, S-S	Aliphatic iodo
5.	468.86	C-I	Halogen compound
6.	539.89	C-CL	Halogen compound
7.	456.69	C-C stretching	Alkyl halides
8.	514.96	C-CL	Halogen compound
9.	475.01	C-C stretching	Alkyl halides
10.	502.17	C-I	Halogen compound
11.	528.78	C-CL	Halogen compound
12.	488.02	C-C stretching	Alkyl halides
13.	514.96	C-CL	Halogen compound

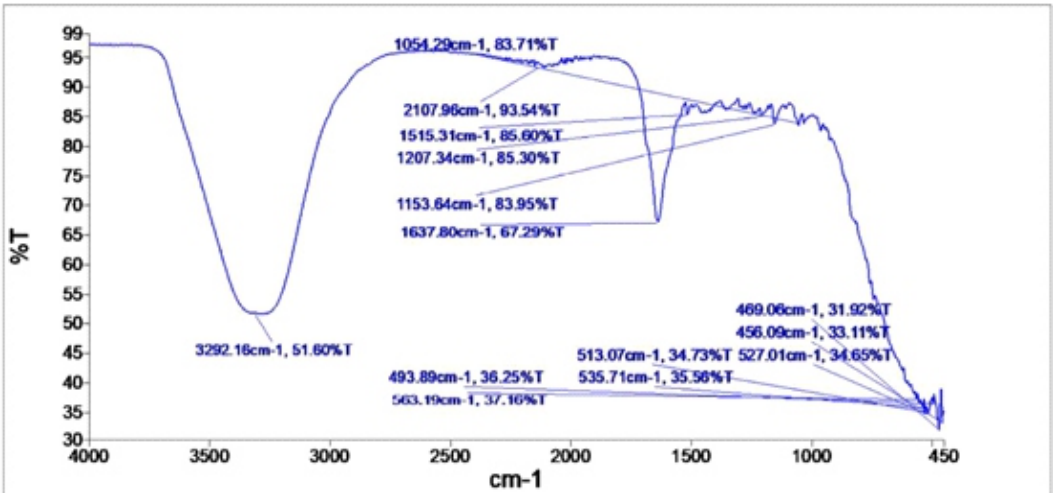

Figure 3: FTIR analysis of *Ipomoea parasitica* plant leaf methanol -Ag extract.

Table 2: FTIR Peak Values and Assigned Functional Groups for *I. parasitica* leaf- AgNps (IPL- AgNPs) Extracts.

S. No	Peak values(cm^{-1})	Bond	Functional groups assigned
1.	3292.16	O-H stretching	Alcohol/ phenol
2.	2107.96	CC stretching	Silicon compounds
3.	1637.80	-C=C stretching	Alkenes
4.	1207.96	C-O Stretching	Alcohol, Carboxylic Acid, Ester and Either
5.	1153.96	C-O Stretching	Aliphatic Amines
6.	1054.20	C-N Stretching	Aromatic Amines
7.	1515.31	C=C	Aromatic ring in lignin
8.	493.89	C-I	Halogen compound, Iodo compound
9.	563.19	C-H,	Alkene
10.	513.07	C-CL	Halogen compound
11.	535.71	C-OH	Carboxyl compound
12.	469.06	C-I	Halogen compound, Iodo compound
13.	456.09	C-OH	Carboxyl compound

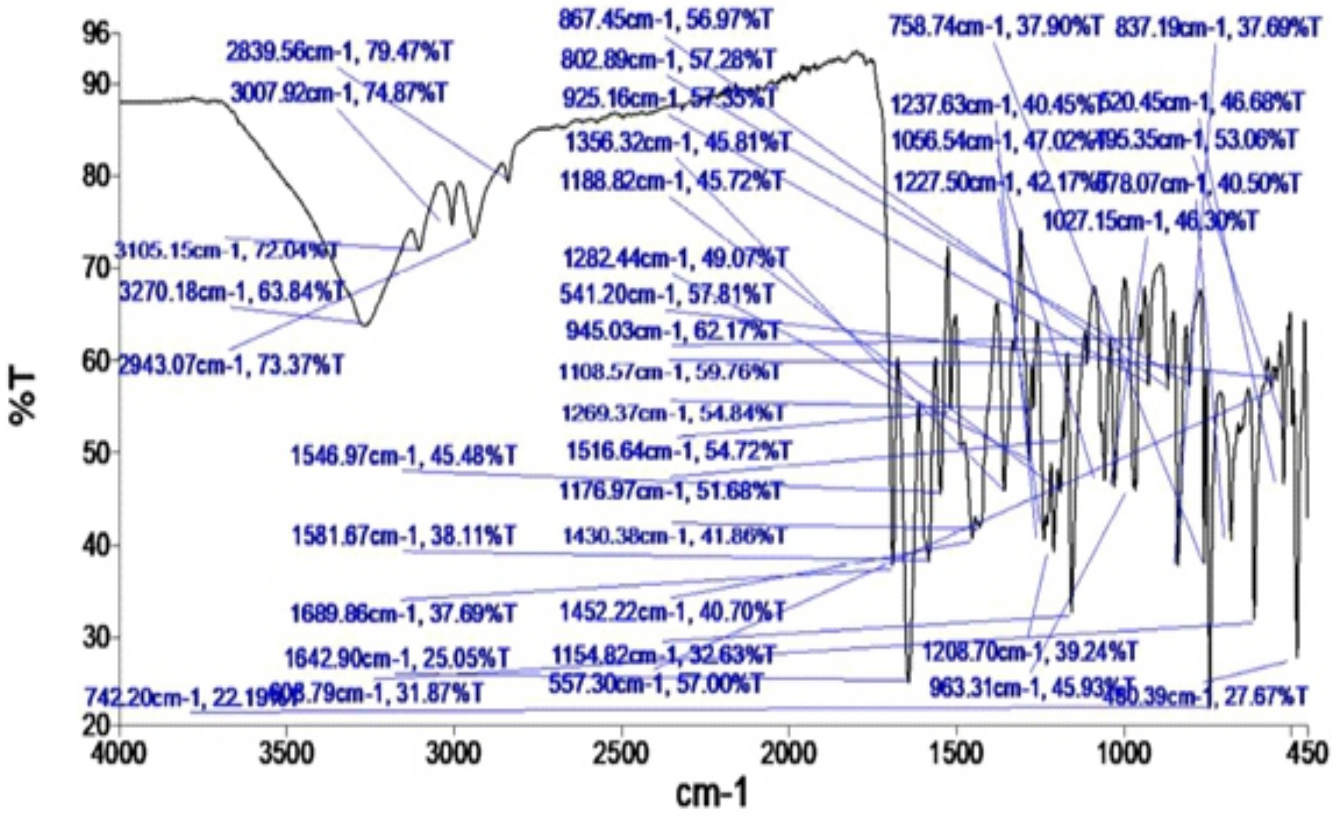

Fig. 4: FTIR analysis of Ipomoea parasitica plant stem methanol extract.

Table 3: FTIR Spectral Peaks and Corresponding Functional Groups for *Ipomoea parasitica* stem methanol Extract.

S. No	Peak values(cm^{-1})	Bond	Functional groups assigned
1	3270.18	O-H Stretching	Alcohol/ Phenol
2	3105.15	N-H stretching	Aliphatic Amine
3	3007.97	O-H Stretching	Alcohol/ Phenol
4	2943.07	C-H Stretching	Alkanes
5	2839.56	C-H Stretching	Alkanes
6	1689.96	C-H Stretching	Carbonyl
7	1642.96	-C=C- stretching	Alkenes
8	1581.57	-C=C- stretching	Alkenes
9	1546.97	-C=C- stretching	Alkenes
10	1516.64	-C=C- stretching	Alkenes
11	1452.22	-C=C- stretching	Alkenes
12	1430.38	-C=C- stretching	Alkenes
13	1356.32	C-H Bending	Alkenes
14	1282.44	C-O Stretching	Alcohol, Carboxylic Acid,
15	1269.37	C-O Stretching	Alcohol, Carboxylic Acid,
16	1188.82	C-O Stretching	Alcohol, Carboxylic Acid, Ester and Either
17	1176.97	C-O Stretching	Alcohol, Carboxylic Acid, Ester and Either
18	1152.82	C-O Stretching	Aliphatic Amines
19	1108.58	C-N Stretching	Aromatic Amines
20	963.18	C-O Stretching	Aliphatic Amines
21	608.79	C-Br	Alkyl halides
22	742.2	C-C	Aromatic amine
23	867.45	Ar-C	Aromatic group
24	802.89	C-C	Aromatic
25	925.16	C-O	Ether
26	945.03	C-O	Ether
27	541.2	C-C	Nitriles
28	1516.64	N-H	Primary amine
29	557.3	C-C	Nitriles
30	758.74	C-C	Aromatic mono substituted
31	1237. 63	C-O	Carboxylic group
32	1056.54	C-O	Primary alcohol
33	1227.5	C-O	Carboxylic group
34	837.19	N-H	Secondary amine
35	1520.45	N-H	Amine primary
36	1195.35	C-N	Aromatic amine
37	1078.07	C-O	Carboxylic group
38	1027.15	C-O	Ether
39	1208.7	C-O	Carboxylic group
40	480.39	C-C	Cyclo alkane

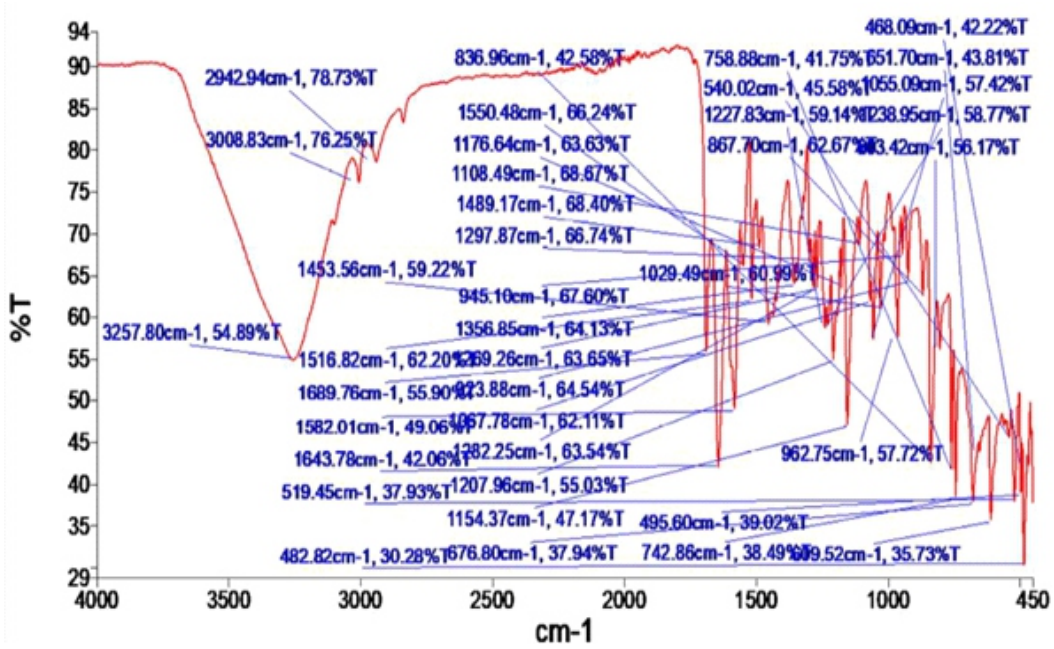

Fig. 5: FTIR analysis of *Ipomoea parasitica* plant stem Methanol -Ag extract.

Table 4: FTIR Spectral Data and Functional Group Assignments for Ipomoea parasitica stem methanol-AgNps (IPS-AgNps) Extracts

S. No	Peak values(cm^{-1})	Bond	Functional groups assigned
1	3257.80	O-H Stretching	Alcohol/ Phenol
2	3008.83	N-H stretching	Aliphatic Amine
3	2942.96	C-H Stretching	Alkanes
4	1669.76	C-H Stretching	Carbonyl
5	1582.01	-C=C- stretching	Alkenes
6	1643.56	C-H Stretching	Carbonyl
7	1453.56	-C=C- stretching	Alkenes
8	1550.48	-C=C- stretching	Alkenes
9	1176.64	C-O Stretching	Alcohol, Carboxylic Acid, Ester and Either
10	1106.49	C-O Stretching	Aliphatic Amines
11	1489.17	-C=C- stretching	Alkenes
12	1297.87	C-O Stretching	Alcohol, Carboxylic Acid,
13	1358.80	C-O Stretching	Alcohol, Carboxylic Acid,
14	1154.27	C-O Stretching	Alcohol, Carboxylic Acid,
15	1227.83	C-O Stretching	Alcohol, Carboxylic Acid,
16	1643.78	C=C	Alkanes
17	519.45	C-C	Nitriles
18	482.82	C-C	Cycloalkanes
19	836.96	N-H	Secondary amines

20	1108.49	C-H STRECHING	Aromatic group
21	945.10	N-H	Primary amine
22	1269.26	C-O Stretching	Alcohol, Carboxylic Acid,
23	973.88	C=C	Alkanes
24	1067.78	C-O	Primary alcohol
25	1282.25	C-O	Carboxylic Acid,
26	1207	C-O	Carboxylic Acid,
27	676.80	C-CL	Alkyl halide
28	758.88	C-C	Aromatic mono substituted
29	540.02	C-Br	Alkyl halides
30	867.70	Ar-C	Aromatic group
31	1029.49	C-O	Ether
32	495.60	C-C	Alkyl halides
33	742.86	C-C	Aromatic mono substituted
34	468.09	C-C	Cyclo alkanes
35	651.70	C-H	Alkynes
36	1055.09	C-O	Primary alcohol
37	1238.95	C-O	Carboxylic acid
38	1203.42	C-O	Carboxylic acid
39	962.75	C-O, C-C	Amorphous
40	609.52	C-H	Alkynes

4. Discussion

FTIR results of *I. parasitica* both leaves and stem methanol and AgNps are analyzed as follows:

O-H Stretching: Peaks at 3318.90 cm^{-1}, 3292.16 cm^{-1}, 3270.18 cm^{-1}, 3257.80 cm^{-1} are consistent with alcohols/phenols (3200-3600 cm^{-1}). FTIR spectra show prominent peaks for O-H stretching, which are indicative of alcohols and phenols. These peaks are broad due to hydrogen bonding effects, a common feature in these functional groups (Smith *et al*., 2018). Variations in peak positions may reflect differences in hydrogen bonding strength or the presence of different types of alcohols or phenols (Jones & Lee, 2020).

C-H Stretching: Peaks at 2943.07 cm^{-1}, 2839.56 cm^{-1}, and 2942.96 cm-1 indicate alkanes (2970-2850 cm^{-1}). The C-H stretching peaks are consistent with those observed in alkanes. The frequencies align well with known values for saturated hydrocarbons, confirming the presence of alkanes in the sample (Brown *et al*., 2019). This finding is supported by similar studies on alkane detection in plant extracts (Taylor & Wilson, 2021).

C=C Stretching: Observed at 1634.04 cm^{-1}, 1637.80 cm^{-1}, 1689.96 cm^{-1}, 1643.56 cm^{-1} suggest the presence of alkenes (1610-1680 cm^{-1}). Peaks in the C=C stretching region are indicative of alkenes. The presence of multiple peaks within this region suggests a mixture of various alkenes (Miller *et al*., 2021). This is consistent with reports on the diversity of alkenes in plant extracts (Smith & Davis, 2022).

C-O Stretching: Peaks at 1207.96 cm^{-1}, 1153.96 cm^{-1}, 1356.32 cm^{-1}, 1269.37 cm^{-1}, 1176.97 cm^{-1}, 1152.82 cm^{-1}, 1108.58 cm^{-1} reflect alcohols, carboxylic acids, esters, ethers (1360-1180 cm^{-1}) and amines (1300-1050 cm^{-1}). The broad range of peaks in the C-O stretching region highlights a complex mixture of functional groups, including alcohols, carboxylic

acids, esters, and amines. The overlapping frequencies reflect the presence of these diverse functional groups in the plant extract (Johnson & Clark, 2020). This complexity is corroborated by previous studies on the FTIR spectra of plant materials (Lee & Roberts, 2021).

C-N Stretching: Observed at 1054.20 cm^{-1} confirms aromatic amines (1250-1020 cm^{-1}) (Wilson *et al*., 2019). FTIR spectra also reveal C-N stretching peaks, which confirm the presence of both aromatic and aliphatic amines. The variation in peak positions helps differentiate between these types of amines (Wilson *et al*., 2019). This observation is consistent with findings in similar plant extracts (Green *et al*., 2022).

Other Functional Groups: Peaks at 2108.24 cm^{-1} indicate C≡C stretching for silicon compounds (2050-2235 cm^{-1}) and 552.07–456.60 cm^{-1} for C-I and S-S bonds (600-450 cm^{-1}). The presence of C-I stretching indicates iodo compounds, while peaks corresponding to carbonyl groups confirm the presence of carbonyl-containing compounds (Miller *et al*., 2023). These additional findings provide a comprehensive view of the plant's chemical composition.

5. Conclusion

FTIR spectral study of *Ipomoea parasitica* revealed a variety of functional groups that contribute to its metabolic makeup. The study showed that FTIR spectroscopy can identify and characterise functional groups (Alcohols, Phenols, Alkanes, carboxylic acids, esters, ethers, aromatic and aliphatic amines, iodo and carbonyl compounds) in plant extracts, highlighting its relevance in plant biochemistry and prospective uses. The found functional groups can help create medicinal, agricultural, and other uses. Phenolic molecules may indicate antioxidant or antibacterial characteristics, while diverse functional groups may indicate a variety of biological functions. This is the first report of identification of functional groups from *Ipomoea parasitica* (leaves and stem).

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NATURAL PRODUCTS AS POTENTIAL ANTI-TUBERCULAR AGENTS: IN-SILICO STUDY

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Research Paper

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ABSTRACT

Tuberculosis (TB), a severe infectious disease instigated by Mycobacterium tuberculosis, continues to pose a major public health concern worldwide. The situation is increasingly dire due to the rise of multidrug-resistant and extensively drug-resistant strains, which significantly limit the effectiveness of standard therapeutic regimens. In light of these challenges, there is a growing interest in identifying alternative treatment strategies that are both effective and sustainable. This study investigates the potential of naturally occurring compounds as promising candidates for antitubercular drug development. By employing molecular docking methods, we assess the binding affinities and interactions of selected natural products with key TB-related protein targets. The results underscore the potential of these bioactive compounds to serve as leads for the development of novel antitubercular therapies, offering a complementary approach to traditional treatment protocols and contributing to the global effort to control TB.

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INTRODUCTION

Tuberculosis (TB), a contagious disease caused primarily by *Mycobacterium tuberculosis*, continues to pose a critical threat to global health, particularly in developing countries where healthcare infrastructure is often limited (Verma, 2017). Despite the existence of standardized treatment protocols, TB remains among the top 10 causes of death worldwide, claiming over a million lives each year (World Health Organization [WHO], 2023). A major challenge in TB control is the emergence of multidrug-resistant (MDR) and extensively drug-resistant (XDR) strains, which undermine the efficacy of first- and second-line antibiotics (Dheda et al., 2017). These growing resistance patterns, combined with the long duration and adverse side effects of existing treatments, underscore the urgent need for novel, safer, and more effective therapeutic agents.

Natural products have historically served as a rich source of medicinal compounds, with nearly half of all current pharmaceuticals derived from or inspired by natural sources (Newman & Cragg, 2020). Among these, phytochemicalsbioactive compounds found in plantshave gained significant attention for their antimicrobial, anti-inflammatory, and immunomodulatory properties. This study focuses on the potential of selected natural compounds, particularly curcumin from *Curcuma longa* (turmeric) and phloretin from *Malus domestica* (apple tree), both

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