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Original Article

Metabolite Profiling Using Fourier Transform Infrared Spectroscopy (FTIR) Technique of three Traditional Iraqi Medicinal Plants Cordia myxa, Passiflora caerulea, and Chrysanthemum morifolium

Aswan Aziz Ibrahim Badawi Al-Mohammadi[1], Suhair Sabah Mahmoud Ali Al-Rawi[2], Sahar Nasser Muhammad Bakr Al-Ani[3], Ibtihal Mohsen Mansour Hassan Al-Sanafi[4]

[1,3]Anbar University, College of Science, Department of Biology, Iraq

[2]Ibb University, Yemen, College of Science, Microbiology, Department of Biology, Iraq

[4]University of Basra, College of Science, Department of Biology, Iraq

Abstract: The secondary metabolites found in plants have a wide range of biological actions. Investigation of plant chemicals should lead to the development of new pharmaceuticals as well as the identification of novel phytocompounds for use in the synthesis of complex substances and the identification of effective treatments. As part of the preparation for FTIR analysis, Peak (Wave number cm-[l]), (Type of Intensity, Bond and Functional group assignment) were As part of the preparation for FTIR analysis, Peak (Wave number cm-[l]), (Type of Intensity, Bond and Functional group assignment) were 668.21 (Stretch, C-Cl, alkyl halides), 674.76 (Stretch, C-Cl, alkyl halides), 819.15 (Bending, =C–H, Alkenes), 869.19 (Bending, =C–H, Alkenes), 924.32 (Bending, =C–H, Alkenes), 1009. 65 (Stretch, C-F, alkyl halides), 1241.28 (Stretch, C-F, alkyl halides), 1313.52 (Stretch, C-F, alkyl halides), and 1417.68 (Stretch, C-F, alkyl halides). In conclusion the identification of bioactive chemical compounds is based on the peak area, retention time molecular weight and molecular formula. As part of the preparation for FTIR analysis, Peak (Wave number cm-[l]), (Type of Intensity, Bond and Functional group assignment) were more than thirty functional groups.

Keywords: Metabolite Profiling, FTIR, Traditional Iraqi Medicinal Plants.

Corresponding Author: Aswan Aziz Ibrahim Badawi Al-Mohammadi †, Anbar University, College of Science, Department of Biology, Iraq

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Introduction:

Throughout history, people have relied on the medicinal properties of plants for a wide range of ailments. In recent years, there has been a resurgence of interest among scientists in studying these plants for their chemical makeup and biological functions. The borage family counts Cordia myxa among its flowering plant members [1]. Tropical Africa, tropical Asia, the Americas, and the area extending from the eastern Mediterranean to the eastern Indian subcontinent are just a few of the many places you might find Cordia myxa, a broad-leaved deciduous tree, growing [2]. The fruit, which is initially pale and light in colour, starts to ripen in July or August and gradually becomes darker. The translucent pulp, which is rich in mucilage and has a pleasant flavour when ripe, is nearly transparent. In traditional medicine, the fruit has a broad range of applications, particularly in Asia, Africa, and the Middle East. The fruit has a long history of use as a diuretic, cough suppressant, and remedy for respiratory infections and sore throats because of its demulcent qualities. Abscesses, rheumatic discomfort, ringworm, and anthelminthic infections can all be alleviated by using the pulp [3]. Cordia myxa has been found in scientific literature to possess a variety of beneficial effects, including those on the immune system, inflammation, pain, parasites, insects, the cardiovascular system, the respiratory system, the gastrointestinal tract, and overall health .

Although there is a lack of quantitative data, previous research has established that the harmless pyrrolizidine alkaloid macrophylline is present. In addition, there were 6 Polycyclic Aromatic Hydrocarbons (PAHs) detected in Cordia myxa samples from the area, with a total value of 411.6 ng/g [4, 5]. Research suggests that low-income rural populations could benefit from incorporating cordia myxa fruit into their cereal-based diets as an additional source of carbs and protein due to the fruit's high fibre and protein content .

An integral aspect of traditional medicine is the utilisation of medicinal herbs. The Romans utilised Cordia myxa, one of these plants, for its medicinal purposes in the second and third century A.D. The Cordia myxa fruit, often called "Bumber" in the local dialect, is one of the most numerous genera in the Boraginaceae family—with over 300 species—found largely in the Wormer region but also in other parts of the world. Among the most common names are Lasura, Burgund dulu wanan, Pidar, Panugeri, Naruvilli, Geduri, and Assyrian plim. Its native range is tropical places with the ideal geophysical conditions, yet it may be found growing mainly all over the world, primarily in Asia. Myxodium cordia. The antioxidant agents found in dichotoma seeds are readily available and beneficial [6, 7]. Because it has the highest concentrations of sucrose, glucose, and fructose as well as a high total dietary fibre content, which helps lower the risk of many diseases, Cordia myxa is a sweeter fruit .

Protein, fat, carbs, ash, and minerals like potassium, sodium, calcium, iron, and zinc are all abundant in Cordia myxa fruit. Saponins, glycosides, trepenoids, alkaloids, phynolic acids, gum, and mucilage are abundant in Cordia myxa.In addition to its anti-inflammatory, anti-arthritic, diuretic, astringent, demulcent, and expectorant properties, Cordia myxa fruit is commonly used to treat chest and urinary infections, wound healing, and a host of other common health issues [8, 9.]

Secondary Metabolites

The metabolic process yields metabolites as its byproducts and intermediates. Small molecules are typically the only ones referred to as metabolites. Among metabolites' many roles are those of fuel, structure, signalling, enzyme stimulation and inhibition, catalytic activity (often in the form of a cofactor), defence, and relationships with other creatures. There is a wide variety of organic compounds produced by plants, and most of them don't seem to have any role in the development or growth process.

The distribution of these chemicals, which are often known as secondary metabolites, might vary among certain taxonomic groupings in plants. The potential to modify the synthesis of bioactive plant metabolites through tissue culture technology has attracted significant interest in recent years, driven by the growing commercial significance of secondary metabolites [11]

It is possible to regularly develop sterile conditions for the establishment of cell and tissue culture technologies from explants (leaves, stems, roots, and meristems) of plants in order to multiply and harvest secondary metabolites. It has been observed that commercial medicinal plants can produce secondary metabolites in vitro using plant cell suspension cultures. The utilisation of plant cell cultures has circumvented numerous obstacles in the synthesis of

plant secondary metabolites, which are distinctive sources for medicines, food additives, flavours, and other commercial materials1. The generation of secondary metabolites can be greatly enhanced by organised cultures, particularly root cultures [12]. To put it simply, secondary metabolites are chemical substances that did not play a primary role in an organism's regular development, growth, or reproduction2. Such metabolites are those that are typically formed as mixtures of closely related members of a chemicalfamily, are typically produced in a phase subsequent to growth, do not function in growth (though they may have a survival function), are produced by specific taxonomic groups of microorganisms, and have unusual chemical structures .

In contrast to primary metabolites, which cause death instantly, secondary metabolites might have a more subtle effect on an organism's attractiveness, fertility, or survivability over time, or even have no discernible effect at all [13]. In many cases, they only apply to a small subset of species within a given phylogenetic group. Along with other interspecies defences, they are crucial in plants' defences against herbivory4. Not long ago, secondary metabolites were used by humans as a kind of medication, flavouring, and even recreational drug.

CLASSIFICATION

Some ways to categorise secondary metabolites include their chemical structure (e.g., sugar-containing rings), composition (e.g., nitrogen-containing or non-containing), solubility in different solvents, or the route of synthesis (e.g., phenylpropanoid, which generates tannins). As well as often grouped based on the pathways they take throughout biosynthesis [14]. Phenolics, Terpenes and Steroids, and Alkaloids, Flavanoids10 are the three main classes of big molecules.There may be serious repercussions for some of them .

The term "alkaloids" was initially used to describe plant-based basic chemicals that contained nitrogen and had pharmacological activity. Additionally, they have the ability to obstruct ion channels, inhibit enzymes, or disrupt neurotransmission, leading to hallucinations, clumsiness, convulsions, nausea, and even death.

Terpenes

Terpenes are among the most widespread chemically diverse groups of natural products. Terpenes are a unique group of hydrocarbon-

based natural products whose structures may be derived from isoprene. Terpenes are classified by the number of 5-carbon units [15]. The function of terpenes in plants is generally considered to be both ecological and physiological: Allelophathy, Insecticidal, Insect pollinators, Plant hormone (Abscisic acid, gibberlellin).

Flavonoids

With more than 4500 different representatives known thus far, the flavanoids constitute an enormous class of phenolic natural products. Present in most plant tissues, often in vacuoles, flavonoids can occur as monomers, dimmers and higher oligomers [16]. Flavonoids comprise a diverse set of compounds and perform a wide range of functions. Specific flavonoids can also function to protect plants against UV-B irradiation. The flavonoids consist of various groups of plant metabolites which include chalcones, aurones, flavanones, isoflavonoids, flavones, flavonols, leucoanthocyanidins, catechins, and anthocyanins.

ADVANCES IN PRODUCTION AND THE CREATION OF SECONDARY METABOLITES

Pharmacists, food scientists, and chemical engineers have a one-of-a-kind resource in plant secondary metabolites. Furthermore, they supply unique resources that are utilised in several domains. For metabolites that are challenging to get by chemical synthesis or plant extraction, plant cell culture has emerged as a potential option [17]. This is in addition to directly extracting these chemicals or derivatives from plants and using chemical synthesis. There have been several attempts over the years to use plant cell culture technologies to produce secondary metabolites, but there are still numerous biological and technical obstacles.

The poor production of secondary metabolites in plant cell cultures is a big hurdle [18]. Treatment with different elicitors, signal compounds, and abiotic stresses are some of the strategies for culture production of these metabolites that have been developed based on this principle. Plant secondary metabolites primarily serve to protect

plants from herbivores, insects, and pathogens, but they can also help plants survive other biotic and abiotic stresses. It is true that several of these therapies do a good job of increasing the production of secondary metabolites in plants, both in vivo and in vitro [19, 20]. Still, it's not often productive enough for use in industry.

These FTIR spectra for each GLV were obtained by experimentally running and laboratory processing a large amount of data already collected from an FTIR instrument, primarily using PC-based software. Experimental preparation for Fourier transform infrared spectroscopy (FTIR) analysis involved turning a small quantity of crushed leaf samples into pellets using KBr and simultaneously pressing the examined mixture into a thin layer. Concurrently, data was gathered in the wave number range of 4000 cm1 to 500 cm1 in order to gather reliable and researched information regarding the transmission of infrared light. All experimental samples were run through three independent tests in this case; untreated KBr pellets served as a control.

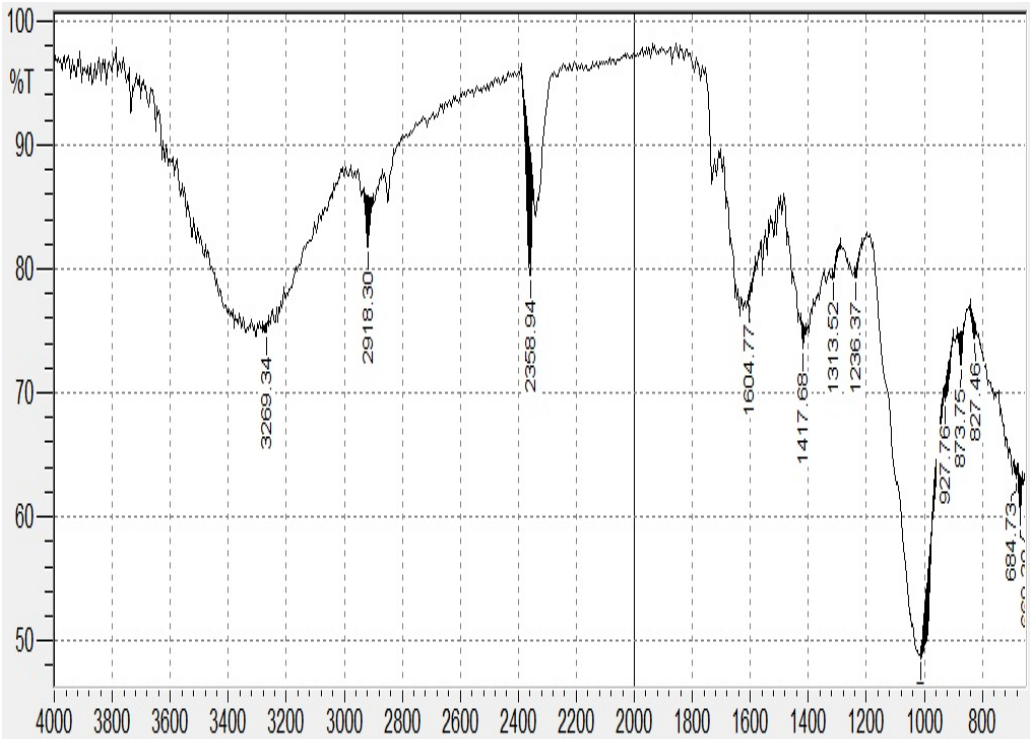
The nutritional and therapeutic properties of the Cordia myxa fruit have led to its global cultivation. Some chemicals in the fruit extract were identified and their relative concentrations were reported, and initial phytochemical screening was carried out. A hot maceration process was used to extract the ethanol. We looked for sugars, proteins, glycosides, alkaloids, flavonoids, phenolic chemicals, saponins, and tannins in the extract. To determine the identities and relative amounts of the volatile chemicals, Gas Chromatography-Mass Spectroscopy was employed [11, 12]. Except for saponins, all of the substances that were investigated were detected in the fruit. GC-MS revealed that the fruit contains phytol, linoleic acid, olealdehyde, stigmastanol, γ-sitosterol, a number of esters and phosphate ester-derivatives, and a fat-soluble version of ascorbic acid [13]. While quantitative analysis is still pending, the study's findings indicate that the fruit contains numerous bioactive chemicals that have cytotoxic, anti-inflammatory, hyperlipidemic, hyperglycemic, and thyroid-inhibiting effects. Is the fruit's chemical makeup anything that needs further research?not merely the ephemeral elixir.

In order to get ready for FTIR analysis, the following parameters were used: Peak (wave number cm^{-1}), Type of Intensity, Bond, and Functional group assignment. As part of the preparation for FTIR analysis, Peak (Wave number cm^{-1}), (Type of Intensity, Bond and Functional group assignment) were 668.21 (Stretch, C-Cl, alkyl halides), 674.76 (Stretch, C-Cl, alkyl halides), 819.15 (Bending, =C–H, Alkenes), 869.19 (Bending, =C–H, Alkenes), 924.32 (Bending, =C–H, Alkenes), 1009. 65 (Stretch, C-F, alkyl halides), 1241.28 (Stretch, C-F, alkyl halides), 1313.52 (Stretch, C-F, alkyl halides), and 1417.68 (Stretch, C-F, alkyl halides).

Plants produce helpful natural compounds called secondary metabolites through a process called secondary metabolism. It seems that as cells mature and undergo morphological differentiation during plant growth, they produce certain secondary metabolites, which are associated with the induction of morphological [14–18] differentiation. It has been noted that differented tissues produce significantly more secondary metabolites in vitro than non-differentiated or less-differentiated tissues.

These metabolites have many benefits, such as fast product recovery, plant cultures being a lifesaver when dealing with difficult or expensive plants, and easy cell line selection for high secondary metabolite yields [19, 20]. Since the field of plant metabolic engineering is rapidly expanding, there are many more examples that might be given.

Although metabolic engineering represents a significant advance, focusing solely on genes will not address the several challenges that have impeded the commercialization of plant secondary metabolites [21–25]. In addition, recent developments in plant cell cultures have the potential to open up new avenues for the commercial, cost-effective production of plants, cells, and compounds, regardless of how uncommon or exotic they may be. Biosynthetic pathways of target chemicals in plants and microbes are generally still poorly understood [26, 27], necessitating approaches to build molecular and cellular level data. Problems in the generation of secondary metabolites from cultured plant cells have been explained through case-by-case studies [28, 29] due to the complicated and incompletely known nature of plant cells in-vitro cultures. Up to this point, many useful secondary phytochemicals have been successfully produced by advanced research using unstructured callus or suspension cultures; nonetheless, there are instances where production calls for highly differentiated micro plant or organ cultures.



Wavenumber (cm-1)

Figure 1. Fourier-transform infrared spectroscopic profile solid analysis of Cordia myxa

Table 1. Fourier Transform Infrared Spectroscopy (FTIR) peak values of solid analysis of *Cordia myxa*.

No.	Peak (Wave number cm-1)	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Type of Intensity	Bond	Type of Vibration	Functional group assignment	Group frequency
1.	668.21	59.416	3.865	677.01	663.51	2.859	0.176	Strong	C-Cl	Stretch	alkyl halides	600–800
2.	674.76	63.115	0.860	690.52	678.94	2.285	0.038	Strong	C-Cl	Stretch	alkyl halides	600–800
3.	819.15	74.505	1.152	840.96	821.68	2.387	0.081	Strong	=C–H	Bending	Alkenes	650-1000
4.	869.19	72.300	2.593	885.33	866.04	2.555	0.131	Strong	=C–H	Bending	Alkenes	650-1000
5.	924.32	69.360	0.661	931.62	900.76	4.511	0.180	Strong	=C–H	Bending	Alkenes	650-1000
6.	1009. 65	48.730	0.709	1012.63	933.55	18.575	0.677	Strong	C-F	Stretch	alkyl halides	1000-1400
7.	1241.28	79.328	0.352	1240.23	1217.08	2.182	0.052	Strong	C-F	Stretch	alkyl halides	1000-1400
8.	1313.52	79.285	1.798	1315.45	1290.38	2.296	0.008	Strong	C-F	Stretch	alkyl halides	1000-1400
9.	1417.68	73.681	0.430	1425.40	1408.04	2.204	0.073	Medium	C=C	Stretch	Aromatic	1400-1600
10.	1604.77	77.448	9.752	1608.63	1581.63	2.817	0.060	Bending	N-H	Stretch	Amide	1550-1640
11.	2358.94	79. 466	3.998	2389.80	2349.30	2.488	0.880	Unknown	-	-	-	-
12.	2918.30	81.850	1.636	2931.80	2899.01	2.468	0.286	Strong	C-H	Stretch	Alkane	2850-3000
13.	3269.34	74.844	0.747	3280.92	3261.63	2.381	0.034	Bending	N-H	Stretch	Amide	3100-3500

Table 2. FT-IR peak values of solid analysis of *Passiflora caerulea.*

No.	Peak (Wave number cm-1)	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Type of Intensity	Bond	Type of Vibration	Functional group assignment	Group frequency
1.	875.68	81.563	1.123	881.47	854.47	2.266	0.084	Strong	=C–H	Bending	Alkenes	650-1000
2.	1016.49	63.828	0.776	1020.34	925.83	12.733	0.091	Strong	C-F	Stretch	alkyl halides	1000-1400
3.	1024.20	63.550	0.936	1132.21	1020.34	16.466	0.352	Strong	C-F	Stretch	alkyl halides	1000-1400
4.	1197.79	80.489	0.124	1199.72	1176.58	2.079	0.004	Strong	C-F	Stretch	alkyl halides	1000-1400
5.	1317.38	81.051	2.838	1346.31	1284.59	5.107	0.417	Strong	C-F	Stretch	alkyl halides	1000-1400
6.	1614.42	80.833	0.751	1618.28	1562.34	4.241	0.112	Bending	N-H	Stretch	Amide	1550-1640
7.	1716.65	89.259	0.978	1764.87	1710.86	1.969	0.261	Strong	C=O	Stretch	Acid	1700-1725
8.	2850.79	89.239	2.861	2870.08	2814.14	2.088	0.208	Strong	C-H	Stretch	Alkane	2850-3000
9.	2922.16	85.898	4.577	2951.09	2879.72	3.716	0.655	Strong	C-H	Stretch	Alkane	2850-3000

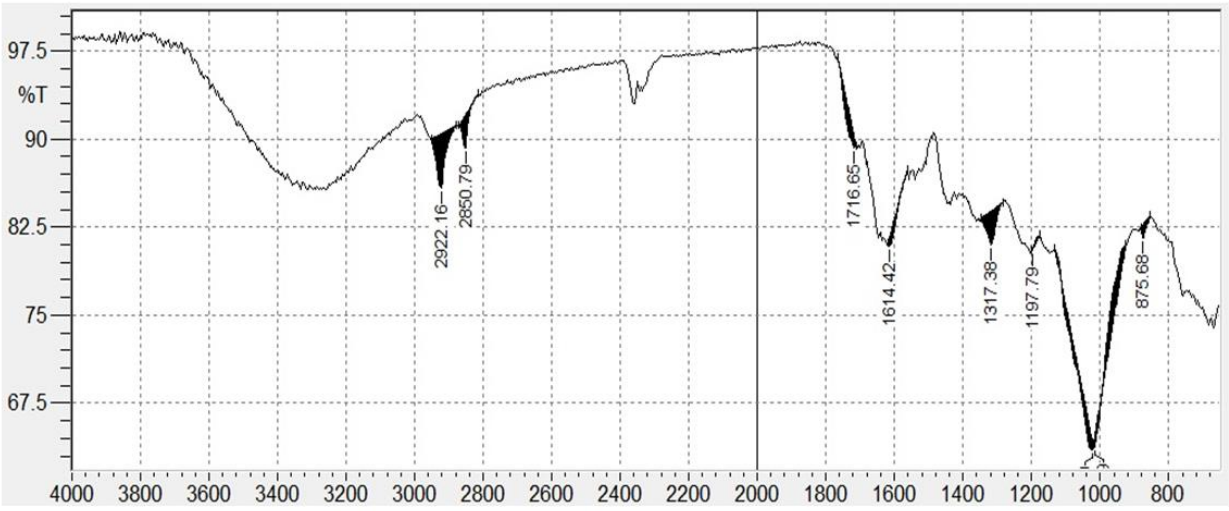


Figure 2. Fourier-transform infrared spectroscopic profile solid analysis of *Passiflora caerulea* .

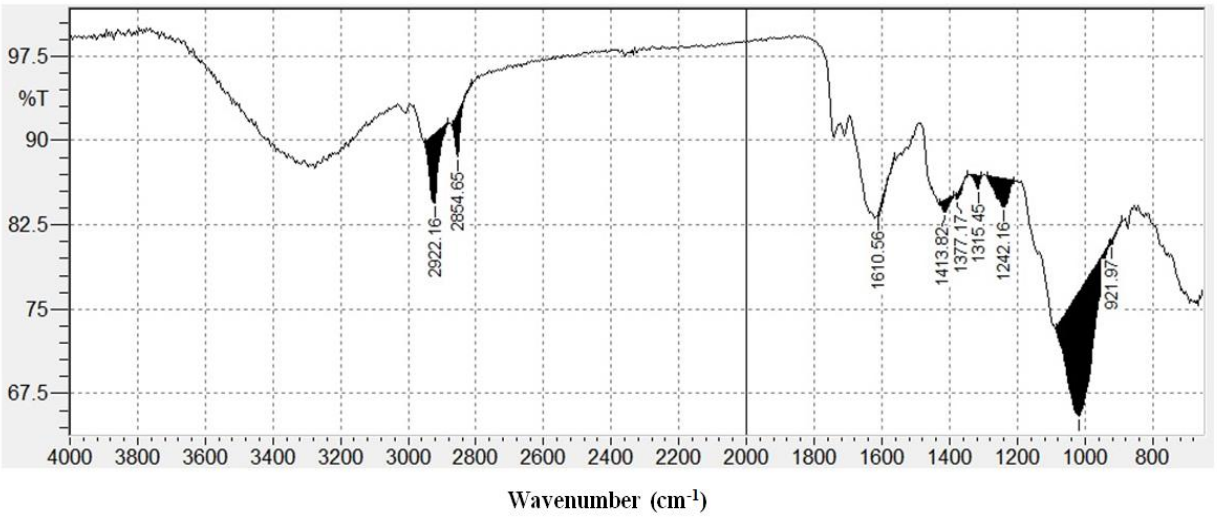


Figure 3. Fourier-transform infrared spectroscopic profile solid analysis of *Chrysanthemum morifolium*

Table 3. FT-IR peak values of solid analysis of *Chrysanthemum morifolium*.

No.	Peak (Wave number cm-1)	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Type of Intensity	Bond	Type of Vibration	Functional group assignment	Group frequency
1.	921.97	80.755	0.353	925.83	891.11	3.028	0.029	Strong	=C–H	Bending	Alkenes	650-1000
2.	1018.41	65.504	11.041	1085.92	927.76	23.417	5.506	Strong	C-F	Stretch	alkyl halides	1000-1400
3.	1242.16	84.097	2.514	1290.38	1209.37	5.590	0.546	Strong	C-F	Stretch	alkyl halides	1000-1400
4.	1315.45	85.759	1.119	1346.31	1305.81	2.555	0.089	Strong	C-F	Stretch	alkyl halides	1000-1400
5.	1377.17	84.830	0.459	1381.03	1348.24	2.185	0.050	Strong	C-F	Stretch	alkyl halides	1000-1400
6.	1413.82	83.609	1.112	1429.25	1390.68	2.888	0.126	Medium	C=C	Stretch	Aromatic	1400-1600
7.	1610.56	83.285	0.261	1612.49	1562.34	3.321	0.044	Bending	N-H	Stretch	Amide	1550-1640
8.	2854.65	88.593	3.783	2870.08	2812.21	2.026	0.291	Strong	C-H	Stretch	Alkane	2850-3000
9.	2922.16	84.451	6.126	2951.09	2881.65	3.790	0.862	Strong	C-H	Stretch	Alkane	2850-3000

CONCLUSION:

The ethanolic extract of *Cordia myxa* , *Passiflora caerulea*, and *Chrysanthemum morifolium* was analyzed, and it was found to contain bioactive phytochemical components. The identification of bioactive chemical compounds is based on the peak area, retention time molecular weight and molecular formula. As part of the preparation for FTIR analysis, Peak (Wave number cm-1), (Type of Intensity, Bond and Functional group assignment) were thirteen functional groups.

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