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GC-MS and FTIR analysis of bioactive phytochemicals from ethanolic leaf extracts of *Aloe secundiflora, Tephrosia vogelii* & *Nicotiana tabacum*

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Abstract
In the current study ethanol leave extracts of *Aloe secundiflora, Nicotiana tabacum* and *Tephrosia vogelii* were examined using Fourier Transform Infrared Spectroscopy (FTIR) and Gas Chromatography-Mass Spectrometry (GC-MS) to determine the key functional groups and phytochemical constituents. The FTIR spectra indicated the occurrence of functional characteristic peaks of primary and secondary amines, amides, alkanes, alkenes, aromatic and aliphatic amines in leaf extracts of *Nicotiana tabacum* while for *Aloe secundiflora* it indicated the presence of characteristic peaks associated with alcohols, phenols, alkanes, aldehydes, primary amines, aromatic and aliphatic amines functional groups. The FTIR spectra of *Tephrosia vogelii* indicated the presence of functional characteristic peaks of alcohols, phenols, alkanes, aldehydes, primary amines, nitro compounds, aromatics, aliphatic and aromatic amines. Alkanes, aromatic and aliphatic amines were present in all the three leaf extracts. The analysis using GC-MS for the ethanol leaf extracts of *Aloe secundiflora* indicated the presence of 25 phytochemical constituents, *Nicotiana tabacum* indicated 15 phytochemical constituents and *Tephrosia vogelii* indicated 7 phytochemical constituents.
The two techniques complemented each other especially in detection of alkanes, alcohols and aromatic amines since both methods showed their presence.

Keywords: Phytochemicals, FTIR analysis, GC-MS analysis, *Aloe secundiflora, Nicotiana tabacum, Tephrosia vogelii*

Introduction
Plants produce a wide range of biochemical compounds through both primary and secondary metabolic pathways. These metabolites frequently contribute to plant defense mechanisms, participate in signaling processes, affect enzymatic and hormonal functions, and possess therapeutic properties. Today, it is crucial to evaluate the phytochemical composition of medicinal plants using advanced scientific techniques and analytical methods. FT-IR spectroscopy is a powerful analytical technique widely employed for the investigation of phytochemical groups, enabling the identification and characterization of chemical bonds within biological samples, including various plant parts. Previous studies on Indian medicinal plants have highlighted the significance and effectiveness of this method (Chandra, 2019) [5].
An important aspect of plant research involves the identification of biologically active compounds, which serves as a foundation for subsequent biological and pharmacological investigations (Casuga *et al*., 2016) [3]. Phytochemicals possessing antimicrobial and antioxidant properties hold great potential in controlling diseases in both plants and humans. The detection and characterization of these compounds from various plant species serve as the initial step in harnessing their medicinal and agricultural potential. In agricultural practices, incorporating antimicrobial phytochemicals into Integrated Disease Management strategies can help minimize the harmful residual impacts associated with synthetic chemical use (Mansoori *et al*., 2020) [12].
Medicinal plants contain various bioactive compounds that demonstrate potent pharmacological effects, including antibacterial, antifungal, anticancer, anti-inflammatory, and antioxidant activities. The therapeutic potential of these bioactive compounds should be assessed to determine their efficacy in the treatment of various diseases. Herbal medicines are commonly derived from crude plant extracts that contain a complex mixture of diverse phytochemical constituents (Konappa *et al*., 2020) [10].

Farmers often use synthetic pesticides as a fast pest management solution to control diseases and protect yields. However, the residues of these pesticides are highly toxic and have harmful effects on non-target organisms, thereby negatively affecting biodiversity. Moreover, the reckless and unsystematic use of these pesticides has resulted in the development of resistant pathogen strains and the resurgence of diseases. Consequently, there is a growing need to develop more effective and selective pesticides for managing plant diseases. Plant-derived, environmentally friendly botanical pesticides offer a viable alternative to synthetic chemicals. Notably, these bioactive compounds tend to be less toxic and are biodegradable, making them more sustainable for agricultural use (Mansoori *et al*., 2020) [12].

Throughout human history, medicinal plants have been valuable sources of bioactive compounds traditionally used to treat various human ailments. The global significance of medicinal plants is underscored by the reliance of approximately 70-90% of the population on herbal medicines as a primary component of healthcare systems (Mlozi *et al*., 2022a) [13]. Indeed, many people, especially in developing countries, rely on herbal medicines, likely because they are more affordable for those with limited financial resources. Traditionally, herbal medicines have been administered in various forms, including decoctions, pastes, and infusions, for the treatment of human ailments such as fungal infections of the skin (Mlozi *et al*., 2022a) [13].

The defensive efficacy of medicinal plants against natural antagonists is largely attributed to the secondary metabolites they synthesize. These compounds, characterized by diverse functional groups, confer a range of chemical properties that enable plants to resist herbivores, insect predation, and pathogenic microorganisms, thereby enhancing their survival. Recently, there has been increasing scientific interest in the exploration and characterization of these secondary metabolites, with the aim of developing natural bioactive compounds for the treatment of human diseases (Mlozi *et al*., 2022b) [13].

The initial screening of medicinal plants by spectrometric and chromatographic methods provides basic information on chemical and pharmacological activities, which helps to select the biologically active plants. In recent years, Fourier-transform infrared (FTIR) and gas chromatography-mass spectrometry (GC-MS) have become widely used for detecting functional groups and identifying various bioactive therapeutic compounds found in medicinal plants.

GC-Mass spectrometry (MS) is a highly efficient, rapid, and precise analytical technique used for the detection of a wide range of compounds, including alcohols, alkaloids, nitro compounds, long-chain hydrocarbons, organic acids, steroids, esters, and amino acids, requiring only a minimal volume of plant extract for analysis. (Konappa *et al*., 2020) [10]. Therefore, in this current study, the GC-MS technique was used to detect and identify the phytochemical compounds present in the medicinal plants; *Nicotiana tabacum, Aloe secundiflora* and *Tephrosia vogelii.*

Tephrosia vogelii is an indigenous plant in several tropical regions of Africa and has been introduced to many areas globally. This plant is a member of the Fabaceae family and the Teprosia genus. Owing to its traditional application in fishing practices, *Tephrosia vogelii* is commonly referred to as 'fish bean' or 'fish-poison bean' in English, and as *utupa* in the Swahili-speaking regions. Historically, it has been utilized for generations as a natural pesticide and a fishing biotoxin. However, its use for these purposes has recently been prohibited due to concerns over its ecological toxicity (Mlozi *et al*., 2022a) [13].

Aloe species have been recognized for their medicinal value since the fourth century, with leaf constituents identified as the bioactive agents responsible for a range of therapeutic effects, including antibacterial, antifungal, and antiviral activities. *Aloe secundiflora* occurs in semi-arid areas and open grasslands of both Kenya and Tanzania. The leaf exudate of this species has been utilized in ethnoveterinary medicine for treating bacterial infections, controlling ectoparasites, and managing certain viral diseases. In poultry, for instance, the exudate has been widely used as a preventive measure against Newcastle disease virus and as a treatment for fowl typhoid, coccidiosis, and other gastrointestinal conditions. The phytochemistry of the leaf exudate of this variant of *A. secundiflora* from this locality has not, however, been studied (Rebecca *et al*., 2003) [15].

Nicotiana tabacum L. is an annual plant widely cultivated in various countries for its economically valuable leaves, which are processed into tobacco products. The plant typically grows to a height of 1-2 meters, and nicotine is present in nearly all parts, though its concentration varies depending on factors such as species, soil type, and climatic conditions. In addition to nicotine, *N. tabacum* contains other phytoconstituents, including polyphenols, pyridine alkaloids, and amino acids, with nicotine comprising approximately 90-95% of the total pyridine content. According to reports from the World Health Organization (WHO), approximately 1.3 billion individuals globally consume nicotine through tobacco products, and its usage is expected to rise due to the substance's highly addictive nature (Faoziyat Adenike *et al*., 2019) [7].

Experimental methods and materials

Study Area: The research study was conducted in Elgeyo Marakwet County, specifically within the Keiyo North Sub-county. Leaf samples of *Nicotiana tabacum* and *Aloe secundiflora* were collected from Tambach Ward, while *Tephrosia vogelii* leaf samples were obtained from Kamariny Ward, both located within Keiyo North Sub-county.

Collection, identification and extraction of plant material

Fresh leaves from each plant species were harvested from the designated sampling sites and taxonomically identified by a specialist in the Department of Biological Sciences, School of Pure and Applied Sciences, Mount Kenya University. The collected leaves were rinsed with distilled water, oven-dried at 40 °C for 72 hours, and subsequently ground into a fine powder using a mechanical mill. Precisely 300 grams of powdered plant material from each species was subjected to extraction using 70% ethanol (FF ethanol water, 7:3 v/v) through maceration with continuous agitation for 24 hours. The resulting mixture was then filtered, and the filtrate concentrated under reduced pressure at 50 °C using a rotary evaporator. The concentrated extract was stored in glass bottles for subsequent bioassay analysis (dos Santos *et al*., 2016) [6].

Fourier transform infrared spectrometry (FTIR) Analysis: Thirty milliliters of the ethanol extract (from 2g of the plant) were combined with dry potassium bromide (KBr) (300 mg) of spectroscopic grade purity (AR) using a mortar pestle grinded to fine powder and the mixture was compressed into thin tablets under a pressure of approximately $5x10^6$ Pa in an evacuated die, resulting in a clear, transparent disc with a diameter of 13 mm and a thickness of 1 mm. The IR spectra and peaks were recorded at room temperature using a BRUKER alpha model FTIR machine between 4000- 400 cm^{-1} equipped an air cooled DTGs were recorded. Each analysis was done twice for confirmation.

Fourier Transform Infrared (FTIR) spectroscopy was utilized to determine the functional groups present in the phytochemical constituents of the plant samples by analyzing the characteristic absorption peaks within the infrared region. The ethanolic extracts of the plant samples were analyzed using FTIR spectroscopy, and the functional groups of the constituent compounds were identified by interpreting the characteristic peak intensities and ratios. The FTIR peak values and corresponding functional groups are presented in Figures 1-3 and Tables 1-3. Various functional groups of different compounds present in the plant sample were identified.

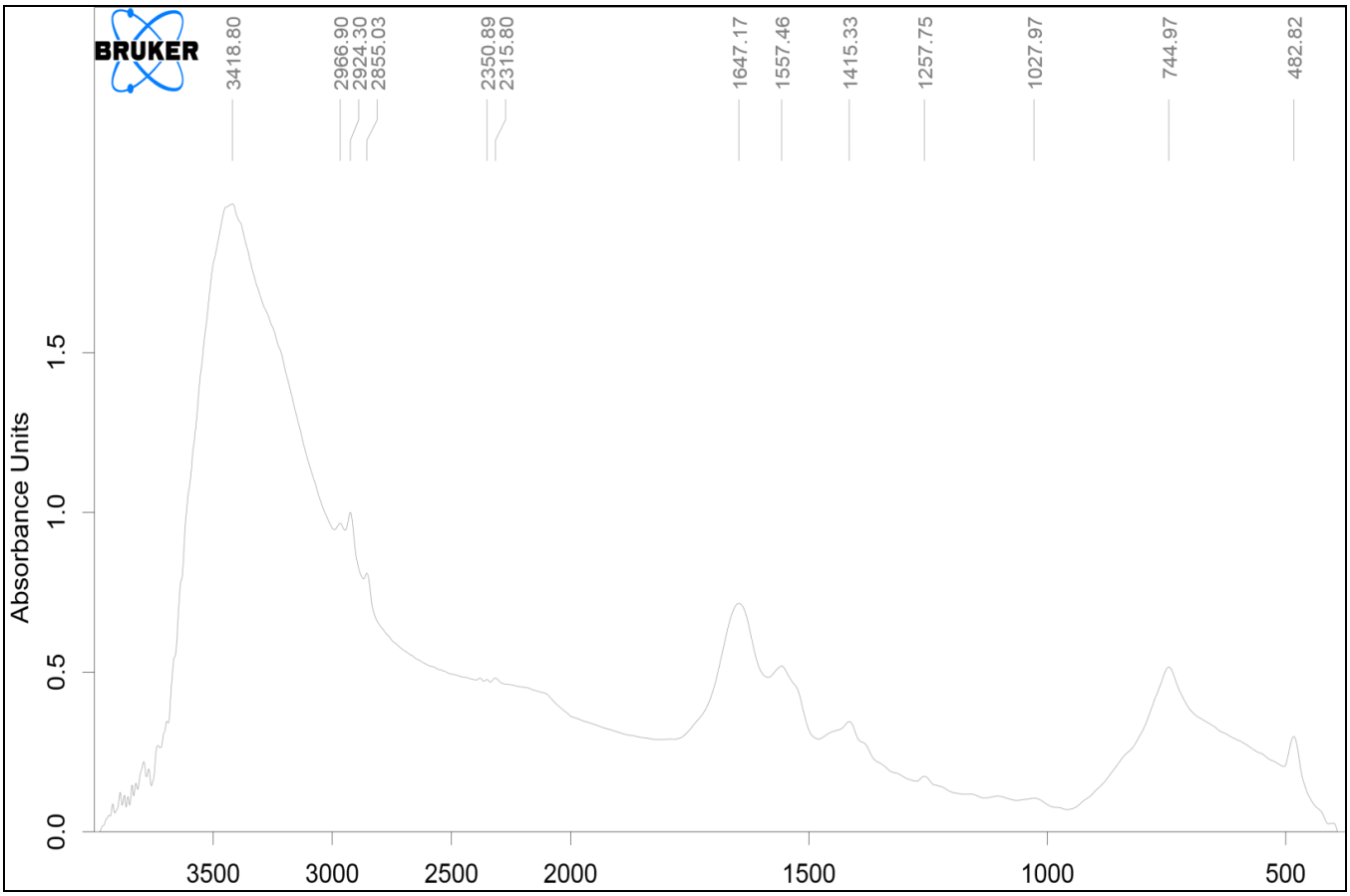


Fig 1: FTIR Spectrum of *Nicotiana tabacum*

Wavenumber cm^{-1}

Table 1: FTIR absorption peaks and corresponding functional groups identified in the leaf extracts of *Nicotiana tabacum*.

Peak frequency (cm^{-1})	Chemical bond	Functional group
3418.80	N-H stretch	Primary, secondary amines, amides
2924.30	C-H stretch	Alkanes
1647.17	-C=C- stretch	Alkenes
1415.33	C-C stretch	Aromatics
1257.75	C-N stretch	Aromatic amines
1027.97	C-N stretch	Aliphatic amines

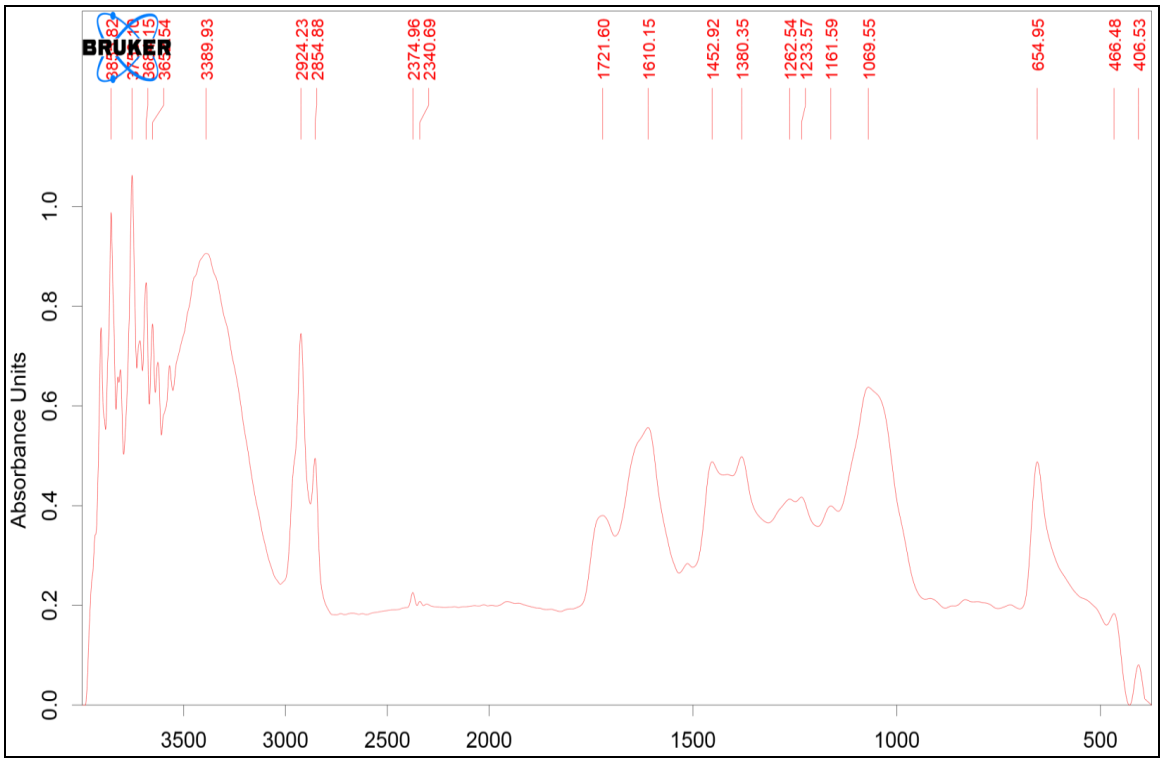


Fig 2: FTIR Spectrum of *Aloe secundiflora*

Wavenumber cm^{-1}

Table 2: FTIR absorption peaks and corresponding functional groups identified in the leaf extracts of *Aloe secundiflora*.

Peak frequency (cm^{-1})	Chemical bond	Functional group
3399.96	O-H stretch	Alcohols, phenols
2924.60	C-H stretch	Alkanes
2854.92	C-H stretch	Alkanes
1721.60	C=O stretch	Aldehydes, saturated aliphatic
1610.15	N-H bend	Primary amines
1452.92	C-H bend	Alkanes
1262.54	C-N stretch	Aromatic amines
1233.57	C-N stretch	Aliphatic amines
1069.55	C-N stretch	Aliphatic amines

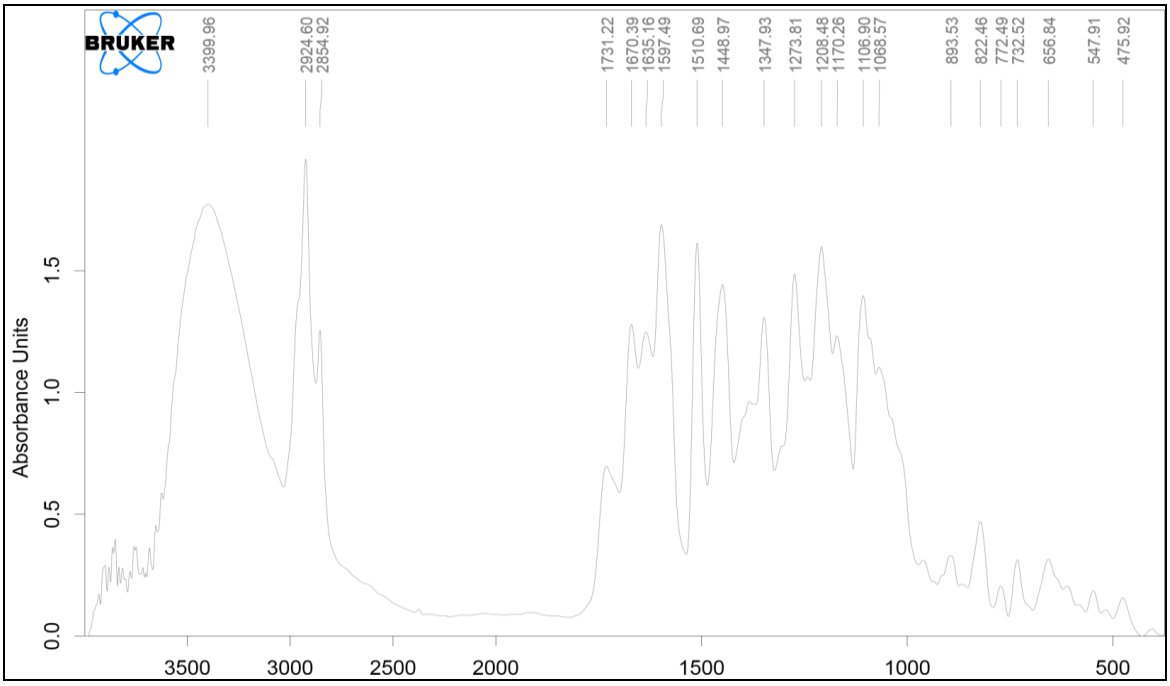


Fig 3: FTIR Spectrum of *Tephrosia vogelii*

Wavenumber cm^{-1}

Table 3: FTIR absorption peaks and corresponding functional groups identified in the leaf extracts of *Tephrosia vogelii.*

Peak frequency (cm^{-1})	Chemical bond	Functional group
3399.96	O-H stretch	Alcohols, phenols
2924.60	C-H stretch	Alkanes
1731.22	C=O stretch	Aldehydes, saturated aliphatic
1597.49	N-H bend	Primary amines
1510.69	N-O asymmetric stretch	Nitro compounds
1448.97	C-C stretch (in-ring)	Aromatics
1347.93	N-O symmetric stretch	Nitro compounds
1273.81	C-N stretch	Aromatic amines
1106.90	C-N stretch	Aliphatic amines

Discussion

FT-IR is a widely utilized technique for identifying chemical constituents and elucidating compound structures, and it is an essential method for identifying medicines in the pharmacopoeias of many countries. FTIR can be used to determine the structure of unknown compositions and analyze the intensity of absorption spectra, which is linked to the molecular composition or the content of chemical groups. The FTIR method detects the vibrations of bonds within chemical functional groups and produces a spectrum that can be considered a biochemical or metabolic 'fingerprint' of the sample (Article Nazneen Bobby, 2012) [1].

The FTIR technique serves as an effective tool for detecting various organic and inorganic compounds in plant materials. In the current study, FTIR analysis was performed on dried leaf samples of *Nicotiana tabacum*, *Aloe secundiflora*, and *Tephrosia vogelii*. From the FT-IR spectra, it is evident that each band corresponds to distinct absorption peaks of the functional groups present in the sample. Screening of functional groups indicate the presence of amides, alkanes, alkenes, aliphatic and aromatic amines, primary amines, secondary amines in *Nicotiana tabacum* leaf extracts (Fig 1 and Table 1). Leaf extracts of *Aloe secundiflora* revealed the presence of alcohols, phenols, alkanes, aldehydes, primary amines, as well as aromatic and aliphatic amines (Fig 2 and Table 2).

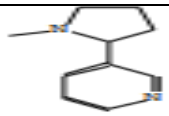
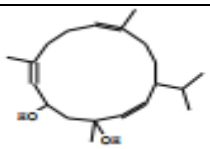
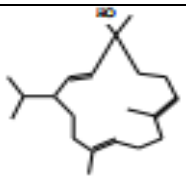
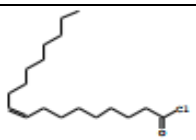
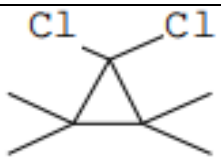
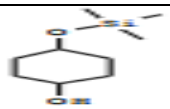
Analysis of functional groups in the leaf extracts of *Tephrosia vogelii* indicated the presences of alcohols, phenols, alkanes, aldehydes, primary amines, nitro compounds, aromatics, aromatic amines and aliphatic amines (Fig 3 and Table 3). The presence of various phytochemical groups in the plant samples suggests their potential medicinal value. Among these, phenolic compounds are particularly important, as they play a key role in the biosynthesis and structural development of lignin in plants. Phenolics are aromatic benzene ring compounds with one or more hydroxyl groups, produced by plants primarily for protection against stress and pathogen attacks. Additionally, plants rich in phenolics are excellent sources of antimicrobial agents. In addition, phenolic compounds contribute to various physiological and ecological functions, including the incorporation of phytochemicals that facilitate pollination, pigmentation for camouflage, and defense mechanisms against herbivores (Chandra, 2019b) [5].

Alkanes (identified in all the three leaf extracts) which are abundantly present in almost all biological organisms, providing ecological and metabolic functions by serving as a source of carbon and energy. Amines constitute a fundamental component of amino acids, which are the building blocks of proteins in all living organisms. Therefore, amino groups play a vital role in both plant and animal biological processes. FTIR has been used to analyze the functional groups of phytoactive compounds present in the leaf and stem extracts of the *Wedelia biflora* (Gowry *et al*., 2015) [8], leaf extracts of *Albizia lebbeck* (Article Nazeen Bobby, 2012) [1] and leaf extracts of *Nicotiana plumbaginifolia* (Chandra, 2019a) [5]. The results indicated that different extracts contain different phytochemical compounds, for example, *Nicotiana plumbaginifolia* leave extracts contain phenols, protein, acid, alcohol and ether (Chandra, 2019b)[5] while leaf extracts of *Albizia lebbeck* contain amide, alkynes, alkanes, carboxylic acids, alkenes, aromatics, aliphatic amines and alkyl halides compounds (Article Nazneen Bobby, 2012) [1].

Gas chromatography-mass spectrometry (GC-MS) analysis

Phytochemical analysis of the leaf ethanolic extracts was conducted using the GC-MS facility at Jomo Kenyatta University of Agriculture and Technology (JKUAT). The analysis was conducted using an Agilent 7010B Triple Quadrupole GC-MS system (manufactured in Germany). A 2 µL aliquot of each sample was injected in splitless mode. Phytochemical compounds were separated using an HP-5 capillary column (30 m length, 0.250 mm internal diameter, and 0.25 µm film thickness; Agilent Technologies), with helium as the carrier gas. The flow rate of the mobile phase was maintained at a constant 0.2 mL/min. Samples were dissolved in a methanol-dichloromethane mixture (2:3 ratio), and mass spectrometric analysis was performed in electron ionization (EI) mode at 70 eV. A Flame Ionization Detector (FID) was used, with a scan range of *m/z* 40 to *m/z* 500. The oven temperature was initially set at 40 °C for 5 minutes, then ramped to 250 °C and held for 9 minutes, followed by a final increase to 280 °C, which was maintained for an additional 14 minutes. The total running time was 35 min. The identification of phytochemical structures and names was based on their molecular weights (*m/z*) obtained from GC-MS chromatograms. This was achieved by comparing the spectral peaks with reference data available in the National Institute of Standards and Technology (NIST) libraries

Table 4: GC-MS Identified Chemical Constituents in Leaf Extracts of *Nicotiana tabacum*

No	RT (min)	Compound name	Chemical structure	Molecular formula	CAS#	Molecular weight	Area%
1	6.408	Undecane		$C_{11}H_{24}$	1120-21-4	156	0.80
2	10.517	(S)-3-(1-methyl-2-pyrrolidinyl) Pyridine		$C_{10}H_{14}N_2$	54-11-5	162	33.40
3	16.500	7,11,15-Trimethyl-3-methylenehexadec-1-ene		$C_{20}H_{38}$	504-96-1	278	3.28
4	20.475	methyl (E)-octadec-7-enoate		$C_{19}H_{36}O_2$	2345-29-1	296	0.32
5	23.017	(4E,8E,13Z)-12-Isopropyl-1,5,9-trimethyl-4,8,13 - cyclotetradecatriene-1,3-diol		$C_{20}H_{34}O_2$	7220-78-2	306	3.07
6	23.613	Hexadec-12-en-1-yl oxiranecarboxylate.		$C_{19}H_{36}O_3$	7501-44-2	312	3.02
7	25.358	(1R,2E,4S,7E,11E)-4-Isopropyl-1,7,11-trimethylcyclotetradeca-2,7,11-trienol		$C_{20}H_{34}O$	25269-17-4	290	0.59
8	25.639	(9Z)-octadec-9-enoyl chloride		$C_{18}H_{33}ClO$	112-77-6	300	0.95
9	26.209	3, 7, 11, 15-Tetramethyl-hexadecyl acetate.		$C_{17}H_{40}O_5Si_2$	0-00-0	380	0.30
10	26.414	Oxiran-2-ylmethyl (9Z)-octadec-9-enoate		$C_{21}H_{38}O_3$	0-00-0	338	37.60
11	26.766	Hexadec-12-en-1-yl oxirane carboxylate.		$C_{19}H_{36}O_3$	0-00-0	312	5.94
12	28.881	1,1-Dichloro-2,2,3,3-tetramethylcyclopropane		$C_7H_{12}Cl_2$	3141-45-5	166	3.81
13	29.218	Cyclohexane-1,4-diol		$C_9H_{20}O_2Si$	54725-70-1	188	2.04
14	29.846	2-hydroxypropyl octadec-9-enoate		$C_{21}H_{40}O_3$	0-00-0	340	4.11
15	34.018	(Z)-3-(Z)-13-octadecadien-1-ol.		$C_{18}H_{34}O$	0-00-0	266	0.77

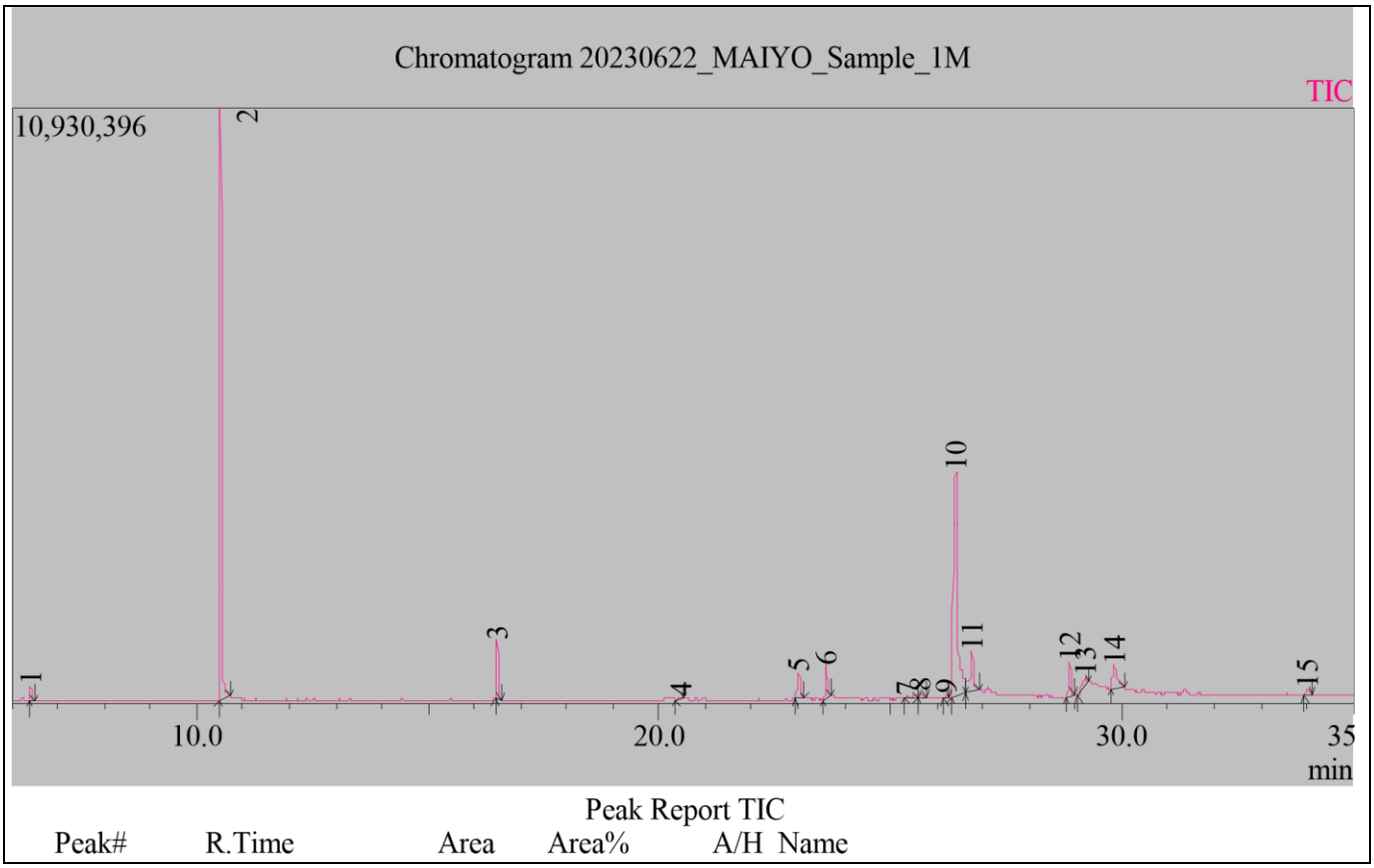
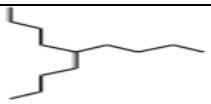
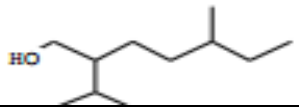


Fig 4: GC MS chromatogram for *Nicotiana tabacum* leave extract

Table 5: GC-MS Identified Chemical Constituents in Leaf Extracts of *Tephrosia vogelii*

No	RT (min)	Compound name	Chemical structure	Molecular formula	CAS#	Molecular weight	Area%
1	5.666	Dodecane		$C_{12}H_{26}$	112-40-3	170	6.70
2	6.221	5-n butylnonane		$C_{13}H_{28}$	17312-63-9	184	3.88
3	7.193	Tetradecane		$C_{14}H_{30}$	629-59-4	198	20.27
4	7.782	4-methyl Tetradecane		$C_{15}H_{32}$	25117-24-2	212	35.20
5	8.132	5-methyl-2-(propan-2-yl) heptan-1-ol.		$C_{11}H_{24}O$	91337-07-4	172	1.88
6	8.704	Hexadecane		$C_{16}H_{34}$	544-76-3	226	25.06
7	9.493	Icosane		$C_{20}H_{42}$	112-95-8	282	7.01

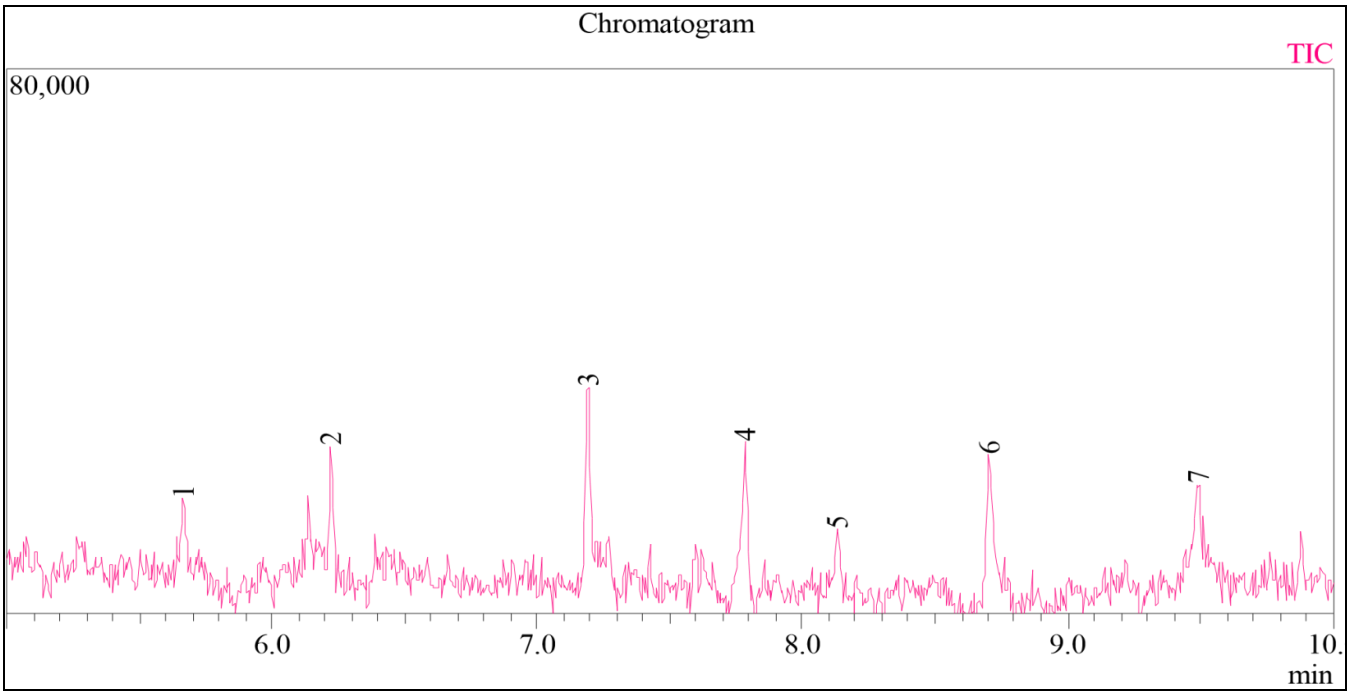
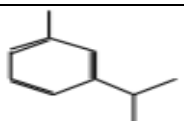
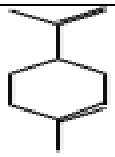
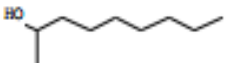
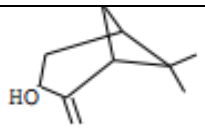
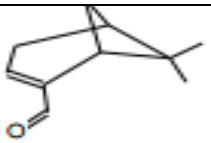
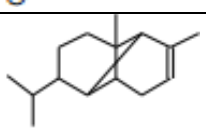
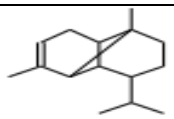
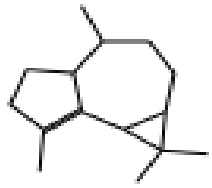
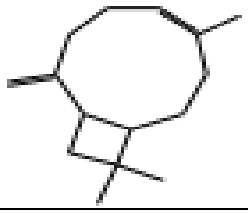
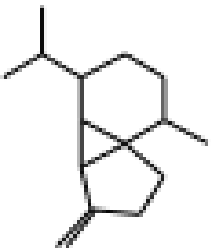
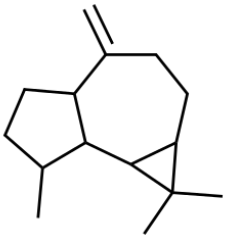
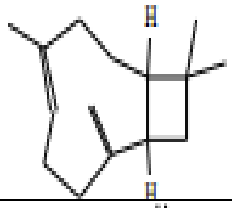
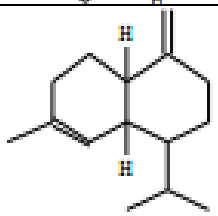
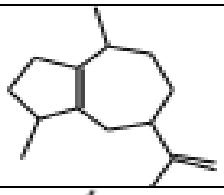
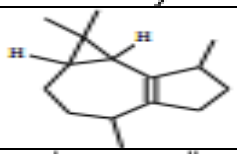
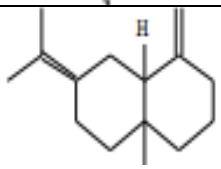
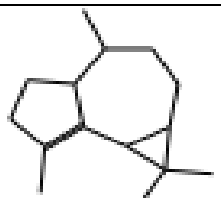
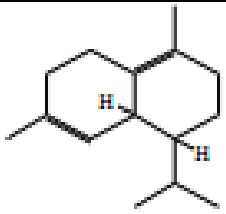
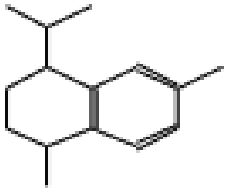
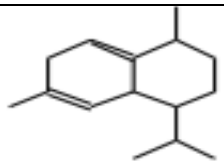
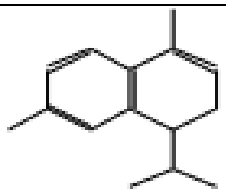
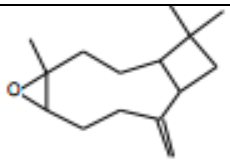
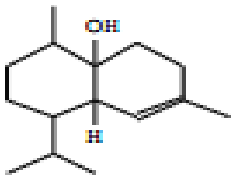
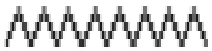


Fig 5: GC MS chromatogram for *Tephrosia vogelii* leave extract

Table 6: GC-MS Identified Chemical Constituents in Leaf Extracts of *Aloe secundiflora*

No	RT (min)	Compound name	Chemical structure	Molecular formula	CAS#	Molecular weight	Area%
1	4.350	1-Methyl-3-(1-methylethyl)benzene		$C_{10}H_{14}$	535-77-3	134	2.26
2	4.383	1-methyl-4-prop-1-en-2-yl-cyclohexene		$C_{10}H_{16}$	5989-27-5	136	11.87
3	4.450	3, 7-dimethylocta-1, 3, 6-triene.		$C_{10}H_{16}$	13877-91-3	136	0.80
4	4.841	Undecane		$C_{11}H_{24}$	1120-21-4	156	9.06
5	4.924	Heptyl methyl carbinol		$C_9H_{20}O$	628-99-9	144	0.89
6	5.444	6,6-dimethyl-2-methylenebicyclo [3.1.1]heptan-3-ol		$C_{10}H_{16}O$	547-61-5	152	0.72
7	5.914	6,6-Dimethylbicyclo[3.1.1]hept-2-ene-2-carboxaldehyde,		$C_{10}H_{14}O$	564-94-3	150	0.54
8	7.180	8-isopropyl-1,3-dimethyltricyclo [4.4.0.0(2,7)]dec-3-ene		$C_{15}H_{24}$	14912-44-8	204	0.73
9	7.230	1, 3-dimethyl-8-(1-methylethyl) tricycle [4.4.0.0², ⁷] Dec-3-ene.		$C_{15}H_{24}$	0-00-0	204	9.26

10	7.482	1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4α,4aβ,7bα)]-		$C_{15}H_{24}$	489-40-7	204	1.39
11	7.609	(1R,9S,Z)-4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene		$C_{15}H_{24}$	87-44-5	204	14.43
12	7.664	1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, octahydro-7-methyl-3-methylene-4-(1-methylethyl)		$C_{15}H_{24}$	13744-15-5	204	0.64
13	7.749	1,1,7-trimethyl-4-methylenedecahydro-1H-cyclopropa[e]azulene		$C_{15}H_{24}$	25246-27-9	204	4.18
14	7.925	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (1R,4E,9R)		$C_{15}H_{24}$	68832-35-9	204	1.03
15	7.973	(1S,4aR,8aS)-Decahydro-1-naphthalenyl 4-methylbenzenesulfonate		$C_{15}H_{24}$	6980-46-7	204	8.38
16	8.015	(1S,4S,7R)-1,4-dimethyl-7-prop-1-en-2-yl-1,2,3,4,5,6,7,8-octahydroazulene		$C_{15}H_{24}$	3691-12-1	204	0.60
17	8.065	1,1,4,7-tetramethyl-1a,2,3,4,5,6,7,7b-octahydro-1H-cyclopropa[e]azulene.		$C_{15}H_{24}$	95910-36-4	204	0.76
18	8.136	(8R,8aS)-8,8a-Dimethyl-2-(propan-2-ylidene)-1,2,3,7,8,8a-hexahydronaphthalene		$C_{15}H_{24}$	58893-88-2	204	5.43

19	8.200	(1aR,4R,4aR,7bS)-1,1,4,7-tetramethyl-1a,2,3,4,4a,5,6,7b-octahydrocyclopropa[e]azulene		$C_{15}H_{24}$	489-40-7	204	0.60
20	8.298	1, 2, 3, 5, 6, 8a-hexahydro-4, 7-dimethyl-1-(1-methylethyl) naphthalene.		$C_{15}H_{24}$	483-76-1	204	10.05
21	8.372	(1S,4S)-4-isopropyl-1,6-dimethyl-1,2,3,4-tetrahydronaphthalene		$C_{15}H_{22}$	72937-55-4	202	3.20
22	8.455	(+)-cubenene.		$C_{15}H_{24}$	29837-12-5	204	1.95
23	8.574	(1S)-4,7-dimethyl-1-propan-2-yl-1,2-dihydronaphthalene		$C_{15}H_{20}$	21391-99-1	200	1.06
24	9.012	(1R,4R,6R,10S)-4, 12, 12-trimethyl-9-methylene-5-oxatricyclo [8.2.0.0(4, 6)] dodecane.		$C_{15}H_{24}O$	1139-30-6	220	4.84
25	9.327	(1S,4R,4aS,8aR)-1-Isopropyl-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-4a-ol		$C_{15}H_{26}O$	19912-67-5	222	0.94
26	9.548	Heptadecane		$C_{17}H_{36}$	629-78-7	240	0.57
27	11.360	Nonadecane		$C_{19}H_{40}$	629-92-5	268	3.00
28	13.218	Icosane		$C_{20}H_{42}$	112-95-8	282	0.82

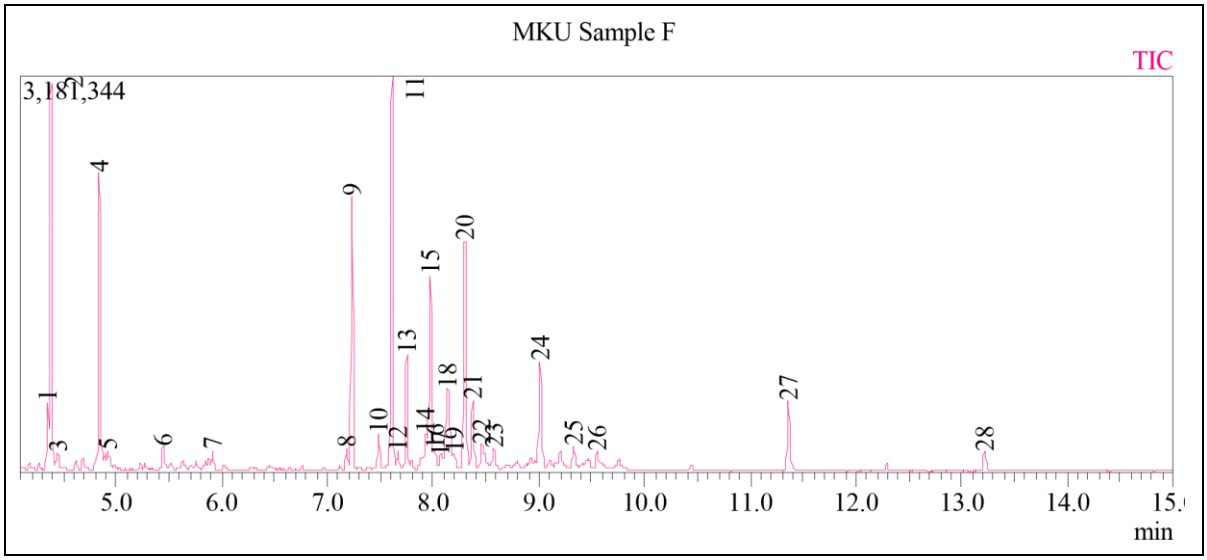


Fig 6: GC MS chromatogram for *Aloe secundiflora* leave extract

Discussions

GC-MS combines two highly effective micro-analytical techniques for analyzing complex mixtures. The gas chromatograph temporally separates mixture components, while the mass spectrometer delivers structural information and quantification of each compound. This integrated approach offers multiple advantages: it enables the qualitative identification of individual compounds through their distinct mass spectral fragmentation patterns—serving as chemical fingerprints—and simultaneously provides quantitative data based on their nominal masses (Nugraha & Nandiyanto, 2021) [14].

In the present study GC-MS analysis identified 28 bioactive compounds in the leaf extracts of *Aloe secundiflora* (Table 6 and Fig 6) and the following three compounds had the highest concentrations (1R,9S,Z)-4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene (14.43%), 1-methyl-4-prop-1-en-2-yl-cyclohexene (11.87%) and 1,2,3,5,6,8a-hexahydro-4, 7-dimethyl-1-(1-methylethyl)naphthalene (10.05%) while the rest (24 compounds) had less than 10% concentrations based on their peak areas. Bioactive compounds present in *Aloe secundiflora* can classified into alcohols (5.56%), phenols (0.94%), alkanes (13.45%), aldehydes (1.43%) and alkenes (78.62%).

GC-MS analysis of the leaf extracts of *Tephrosia vogelii* identified 7 bioactive compounds i.e. dodecane, 5-n butylnonane, Tetradecane, 4-methyl Tetradecane, 5-methyl-2-(propan-2-yl)heptan-1-ol, hexadecane and Icosane while *Nicotiana tabacum* leave extracts revealed the presence of 15 bioactive compounds i.e. undecane, (S)-3-(1-methyl-2-pyrrolidinyl) Pyridine, 7,11,15-Trimethyl-3-methylenehexadec-1-ene, methyl (E)-octadec-7-enoate, (4E,8E,13Z)-12-Isopropyl-1,5,9-trimethyl-4,8,13 -cyclotetradecatriene-1,3-diol, Hexadec-12-en-1-yl oxiranecarboxylate, 1R,2E,4S,7E,11E)-4-Isopropyl-1,7,11-trimethylcyclotetradeca-2,7,11-trienol, (9Z)-octadec-9-enoyl chloride, 3,7,11,15-Tetramethyl-hexadecyl acetate, Oxiran-2-ylmethyl (9Z)-octadec-9-enoate, Hexadec-12-en-1-yl oxiranecarboxylate, 1,1-Dichloro-2,2,3,3-tetramethylcyclopropane, Cyclohexane-1,4-diol, 2-hydroxypropyl octadec-9-enoate and (Z)-3-(Z)-13-octadecadien-1-ol. The leave extracts of *Tephrosia vogelii* indicated the presence of alkanes (98.12%) and alcohols (1.88%) while for *Nicotiana tabacum* indicated presence of amines, alkanes, alkenes, aliphatic amines, primary & secondary amines and amides in different amounts. From the GC-MS results alkanes and alcohols are present in all the three leave extracts in varying quantities. The three leave extracts had been investigated for their pesticidal activity against fall armyworms and the results indicated that *Nicotiana tabacum* had the highest mortality on the second instar larvae followed by leave extracts of *Aloe secundiflora* while *Tephrosia vogelii* had the lowest pesticidal activity against the larvae (Kimutai Maiyo *et al*., 2023) [9]. These findings are evident that the leave extracts can be utilized for management of pests apart from disease control in humans which has been extensively investigated by many researchers (Baeshen *et al*., 2023; Chali & Sime, 2019; Kumar, 2017; Srivastava *et al*., 2020) [2, 4, 11, 16].

Conclusion

Ethnobotanical plants are rich in bioactive phytochemical compounds with significant pharmacological properties and can serve as potential therapeutic alternatives. The biological activities of compounds found in the leaf extracts of *Nicotiana tabacum*, *Aloe secundiflora*, and *Tephrosia vogelii* support their medicinal applications. The study identified major bioactive compounds present in all the extracts. Recognizing these compounds in the plant provides a foundation for assessing its potential health benefits, paving the way for further biological and pharmacological research. Most of the functional groups identified through FTIR analysis corresponded closely with the compounds detected in GC-MS, suggesting that both techniques can complement each other in phytochemical analysis. For example, in the leaf extracts of *Tephrosia vogelii* the FTIR spectra indicated a peak at 2924.60cm^{-1} (Table 3) which is a characteristic peak of C-H stretch associated alkanes and the GC-MS chromatogram showed the presence of alkanes such dodecane, hexadecane & Icosane (Table 5) hence the two techniques complement each other. Similarly, FTIR spectra gave a peak at 3399.96cm^{-1} which is characteristic peak for O-H stretch (Table 3) and the GC-MS chromatogram indicated the presence of an alcohol 5-methyl-2-(propan-2-yl)heptan-1-ol (Table 5) in the leaf extract of *Tephrosia vogelii.* The same observation was seen for the leaf extract

of *Nicotiana tabacum*, characteristic peak at 2924.30cm^{-1} for C-H stretch associated with alkanes in the FTIR spectra (Table 1) while GC-MS chromatogram indicated the presences of undecane an alkane (Table 4). Also the FTIR spectra of *Nicotiana tabacum* showed a characteristic peak at 1257.75cm^{-1} for C-N stretch that associated with aromatic amines (Table 1) and GC-MS chromatogram showed the presence of (S)-3-(1-methyl-2-pyrrolidinyl) Pyridine an amine (Table 4). Similar observations can be seen in the leaf extracts of *Aloe secundiflora*, FTIR spectra showed a characteristic peak at 3399.96cm^{-1} for O-H stretch that is associated with alcohols/phenols (Table 2) while GC-MS chromatogram of the same showed the presence of the following alcohols Heptyl methyl carbinol and 2-Methylene-6,6-dimethylbicyclo[3.1.1]heptan-3-ol.___(Table 6). Also the FTIR spectra showed a characteristic peak at 1721.60cm^{-1} for C=O stretch which is associated with aldehydes (Table 2) while the GC-MS chromatogram indicated presence of 6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-carboxaldehyde an aldehyde (Table 6).

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