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Gas chromatography-mass spectrometry analysis of volatile organic compounds associated with acridity, nutritional value and medicinal importance in young leaves of *Xanthosoma mafaffa* (Schott)

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Abstract
Cocoyam (*Xanthosoma mafaffa* (Schott)) is an underutilized tropical crop valued for its edible corms and leaves, its leaves are consumed as vegetables in many communities. Beyond their dietary role, cocoyam leaves contain diverse phytochemicals that contribute to its defense, nutrition and medicinal properties. Knowledge of these phytochemicals is important for clarifying their functional mechanisms and potential applications. Gas Chromatography-Mass Spectrometry is a powerful analytical technique which enables the separation, identification and quantification of complex mixtures of bioactive compounds, making it suitable for phytochemical profiling. This study aimed at characterizing the phytochemical profile of young leaves of *Xanthosoma mafaffa*, categorizing them into those associated with acridity, nutritional importance and medicinal relevance. Ethanolic extracts of the leaves were analyzed using GC-MS with a fused silica Elite-1 column and helium as the carrier gas. Mass spectra were interpreted using the NIST library database to identify compounds based on retention time, molecular weight and spectral patterns. Twenty (20) phytochemicals were identified with 3 being associated with acridity, 5 with nutritional importance and 9 being of medicinal relevance. Visualization through pie chart demonstrated that nutritional phytochemicals were of the highest concentration (59%) followed by phytochemicals of medicinal importance (25%) while those associated with acridity (7%). The stacked bar chart revealed that Picolinyl 16-methyl- heptadec-9-enoate with a concentration of 38.38% contributed most to *X. mafaffa*'s nutritional value, N,N'-Bis(salicylidene)-3,3'-bis(aminopropyl)aminocobalt(II) with a concentration of 6.53% contributed most to its medicinal profile, 2- [2,2,3,3,3-Pentafluoro-1-(3-phenoxy- phenylamino)-propylidene]-malononitrile with a concentration of 2.998% contributed most to acridity while those that didn't fall under any of these categories were stacked under the uncharacterized bar. In conclusion *X. mafaffa* leaves are rich in nutritionally and medicinally relevant phytochemicals while acridity is associated with specific phenolic and nitrile compounds.

Keywords: *Xanthosoma mafaffa*, Phytochemicals, GC-MS, Acridity, Nutritional, Medicinal Importance

Introduction

Xanthosoma mafaffa (Schott), is a member of the family Araceae with great economic and nutritional importance. Commonly called cocoyam, it is characterized by a large central corm, surrounding cormels and widely distributed throughout the tropical regions of the world (Ukom *et al*., 2020) [21].

It plays a great role in ensuring food security particularly in Africa, Asia and the Caribbean where it is consumed in most homes. Aside its corms, the leaves represent an essential source of nutrients making up important ingredient in the traditional medicines and delicacies such as *Ekpang Nkukwo* which is popular among the South-Eastern people of Nigeria (Bammite *et al*., 2021) [5].

Xanthosoma spp. leaves are highly nutritional and can be placed on the same level with leafy vegetables. According to Prospére *et al*. (2025), they contain 38.8% carbohydrate, 17.1% protein, 24.3% fiber and 3.2% lipids. Additionally, Spectrophotometric assessment confirmed the presence of potassium, Calcium, magnesium, phosphorus and iron (Prospére *et al*., 2025). Although these nutritional matrices are important in assessing caloric and bulk dietary contributions, they do not cover the full spectrum of functional and organoleptic quality as consumer acceptance and preferences are not just driven by nutrient density but also by flavor and sensory perception which is dictated by secondary volatile metabolome (Bammite *et al*., 2021) [5].

Despite the robust nutritional profile, the anti-nutritional factors consistent with the araceae family constrain the wider and routine use of cocoyam leaves. While the primary cause of cocoyam acridity is the calcium oxalate raphides in synergy with irritant proteins; profilins, its sensory profile may be further compromised by Volatile Organic Compounds (VOCs) which when present, even in trace amounts may contribute to a secondary but persistent chemically desirable or undesirable flavor profile that lingers even after the mechanical acridity has been neutralized by heat treatment greatly impacting sensory perception (Ji *et al*., 2025; Paul *et al*., 2022).

VOCs are highly diverse set of plant metabolites characterized by low molecular weight and high vapour pressures. They include esters, aldehydes, ketones, terpenes, thiols, alcohols, etc. which are responsible for perceived sensory characteristics often affecting human health and contributing to wide-scale nutritional acceptance (Ji *et al*., 2025) [20]. A key objective of phytochemical analysis is the systematic identification and quantification of phytochemicals which is important in correlating their observed biological effects; be it anti-nutritional, nutritional or medicinal, with their underlying chemical composition (Wang *et al*., 2018) [24].

The chemical complexity and low concentration of many VOCs makes the use of a highly sensitive and reliable analytical procedure necessary. Gas Chromatography-Mass Spectrometry (GC-MS) stands as an established core analytical technique for the separation, identification and accurate quantification of volatile compounds in biological samples (Onuoha *et al*., 2022) [18], as it provides the chemical resolution necessary to differentiate closely related isomers and homologous series, as it is sensitive to genetic variation, organ type, and developmental stages which is crucial in plant volatile profiling where subtle structural differences translates into major functional changes (Vallarino *et al*., 2018) [22]. The specific chemical profile of young leaves of *Xanthosoma mafaffa* remains largely uncharacterized (Ashalata *et al*., 2021; Wang *et al*., 2018) [3, 24], hence this research was aimed at analyzing the chemical profile of young leaves of *Xanthosoma mafaffa*, identifying phytochemicals associated with acridity, nutritional value and medicinal importance by GC-MS.

Materials and Methods

Sample collection and Preparation: Young leaves of *Xanthosoma mafaffa* were collected, cleaned to remove debris, air-dried at room temperature and thereafter pulverized into powder. Two (2) g of the leaf powder was macerated in dichloromethane solvent and allowed to stand for 72 hours after which it was filtered using whatman No. 1 filter paper. The filtrate was concentrated by exposing to the air for further drying after which dried extracts were collected and stored in sample bottles at -4 ^{o}c.

GC-MS instrumentation and operating conditions: Analysis was carried out according to the method of Merlin *et al*., (2009) [14]. A GC-MS system fitted with fused capillary column packed with Elite-1 stationary phase was used with Helium; the career gas being in a constant flow rate of 1mL/min. An injection volume of 2 µL of the ethanolic leaf extracts was injected into the GC-MS system and the oven maintained at 290 ^{o}c during the 23 rd min of the run with a hold time of 2 minutes after which mass spectra were obtained under electron impact ionization of 70eV, using a scan interval of 0.5s across a mass range of 40-400 Da.

Data acquisition and component Identification: The injected extract yielded chromatographic peaks which corresponded to the separated components based on retention times after which identification of phytochemicals was done by comparing the acquired mass spectra against the National Institute of Standards and Technology library. Compound identity was assigned as they were found to be in line with the mass spectral fragmentation, retention time behaviour, and molecular weight information relative to the library entries.

Quantification and Reporting: The relative percentage of each component was calculated by comparing its average peak area to the sum of all peak areas in the chromatogram and for each compound identified, compound name, retention time, molecular formula, molecular weight and percentage area was documented as the main analytical output.

Statistical analysis: Data was entered into Microsoft Excel and analyzed. Descriptive statistics was used for the visualization of the result.

Results

The GC-MS profile confirms the complexity of *Xanthosoma mafaffa*'s leaf secondary metabolome, bridging its nutritional capacity and its documented pharmacological potentials. A total of twenty (20) phytochemicals were identified and categorized into three major categories, acridity, nutritional importance and medicinal importance while those which did not fit into these three categories were labelled uncategorized.

In Table 1, three phytochemicals were identified to be associated with acridity in young leaves of *Xanthosoma mafaffa*. 2- [2,2,3,3,3-Pentafluoro-1-(3-phenoxy-phenylamino)-propylidene] malononitrile; a hazardous halogenated organic compound had the highest concentration of2.998% followed by Butaperazine with a concentration of 2.111%.

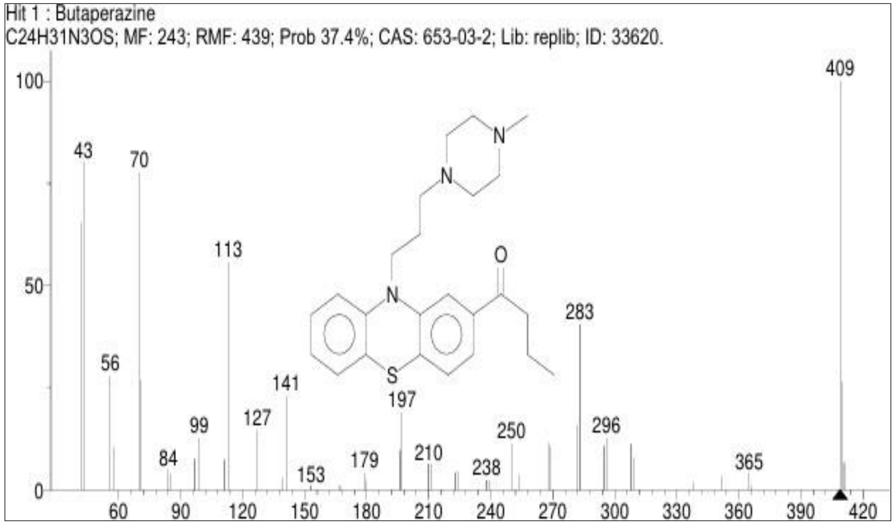
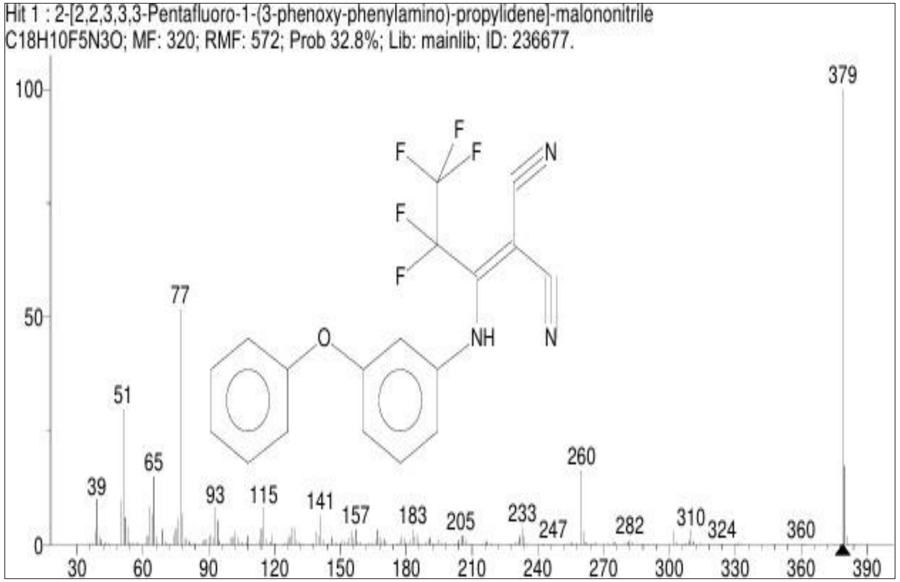
Five phytochemicals were identified as those of nutritional importance in young leaves of *X. mafaffa*. Picolinyl16-methyl-heptadec-9-enoate; an energy and lipid source with a potential for cholesterol metabolism having the highest concentration of 38.379% and Glycine, N-methyl-n-propoxycarbonyl-, dodecyl ester; an N-methyltransferase precursor and methionine metabolism regulator with a concentration of 14.119% was the second most nutritional compound (Table 2).

Table 3 shows phytochemicals of medicinal importance of which N, N'-Bis(salicylidene)-3,3'- bis(aminopropyl) aminocobalt(II) with an antitumor potential had the highest concentration of
6.553% followed by 5,12-Naphthacenedione,6,8,11-tris(acetyloxy)-8- [(acetyloxy)acetyl]- 7,8,9,10-tetrahydro-1-methoxy-,(R) with an antitumor and antimicrobial potential having a concentration of 3.303% being second.

Figure 1 shows the Percentage Contribution of Phytochemicals to acridity, nutritional, medicinal importance and uncharacterized in the chemical profile of young leaves of *X. mafaffa*. From the chart, phytochemicals of nutritional importance with a concentration of 59% had the highest contribution to the chemical profile followed by phytochemicals of medicinal importance with a concentration of 25% and the least being phytochemicals associated with acridity with a concentration of 7%.

Figure 2 shows the individual contribution of phytochemicals in the categories which they belong. For phytochemicals associated with acridity, 2- [2,2,3,3,3-Pentafluoro-1-(3-phenoxy-phenylamino)-propylidene]-malononitrile with a concentration of 2.998% represented by the red segment had the highest contribution, for phytochemicals of nutritional importance, Picolinyl 16-methyl-heptadec-9-enoate with a concentration of 38.379% represented by the yellow segment, had the highest contribution and for phytochemicals of medicinal importance, N,N'- Bis(salicylidene)-3,3'-bis(aminopropyl)aminocobalt(II) with a concentration of 6.530% represented by the green segment had the highest contribution. The phytochemicals which did not fit into the 3 categories, was represented by the uncharacterized bar.

Table 1: Volatile Organic Compounds Associated with Acridity in Young Leaves of *X. mafaffa* (Schott)

S/N	Compound Name	Molecular formular	Retention Time (Min.)	Relative Aboundance (%)	Acrid Effect	Chromatogram
1	Butaperazine	$C_{24}H_{31}N_3OS$	18.387	2.111	▪ Blured Vission ▪ Central Nervous System depression ▪ Dry mouth	
2	2- [2,2,3,3,3-Pentafluoro-1-(3-phenoxy-phenylamino)-propylidene]-malononitrile	$C_{18}H_{10}F_5N_3O$	22.200	2.998	▪ Hazardous halogenated organic compound	

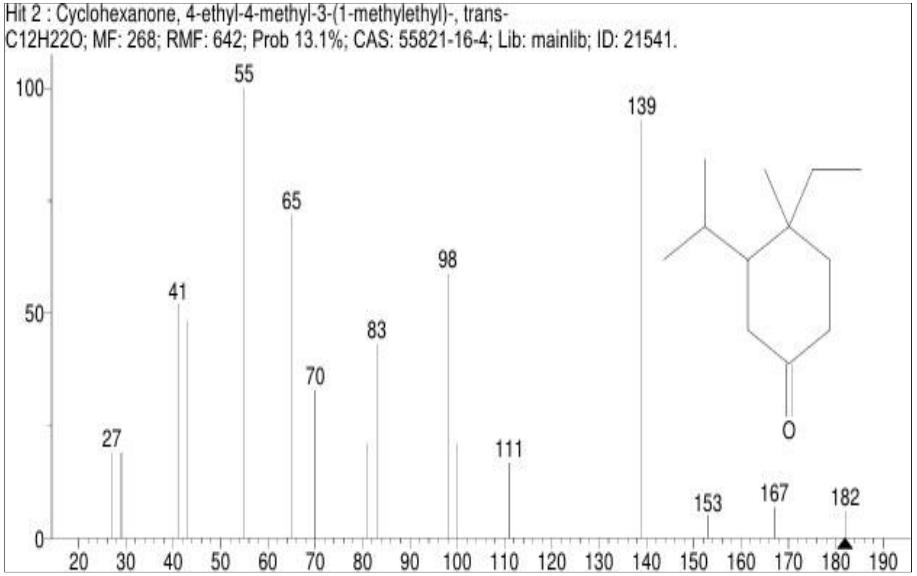
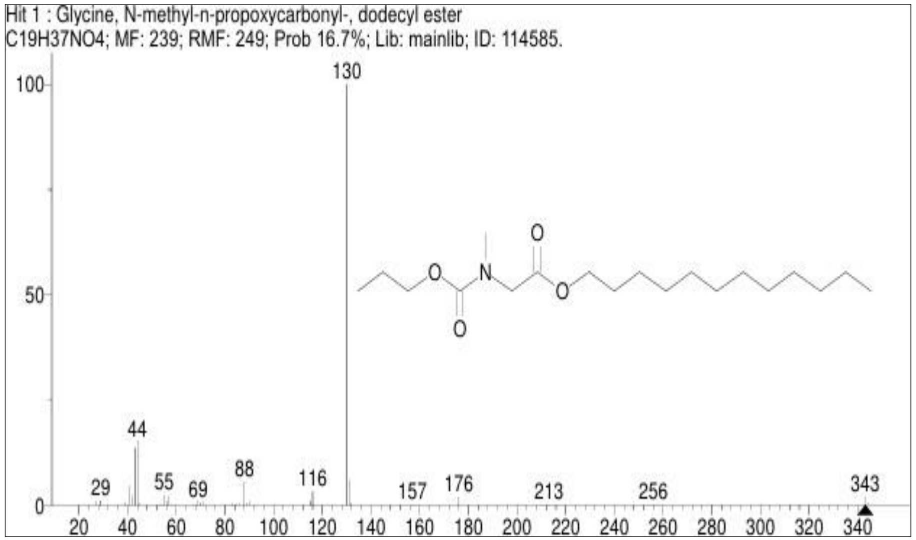
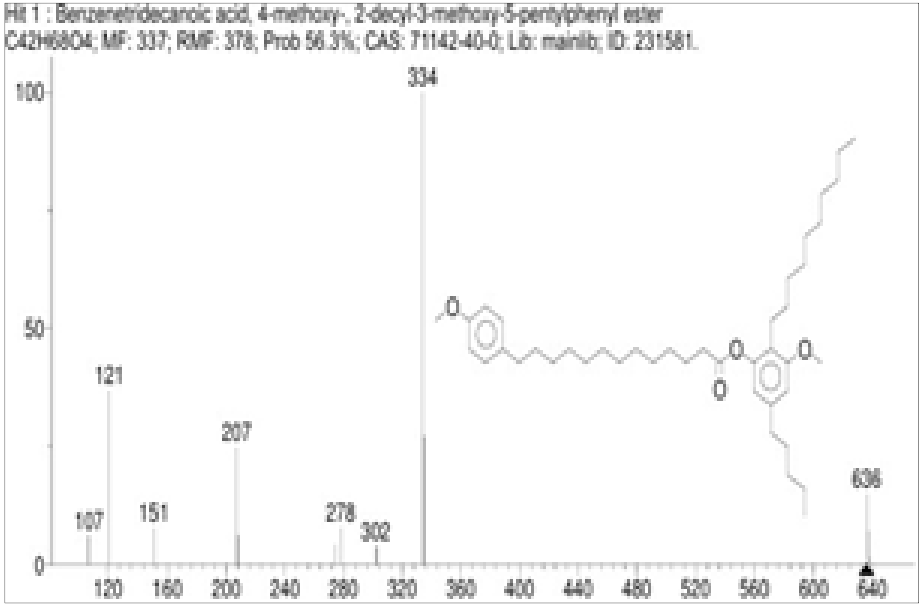
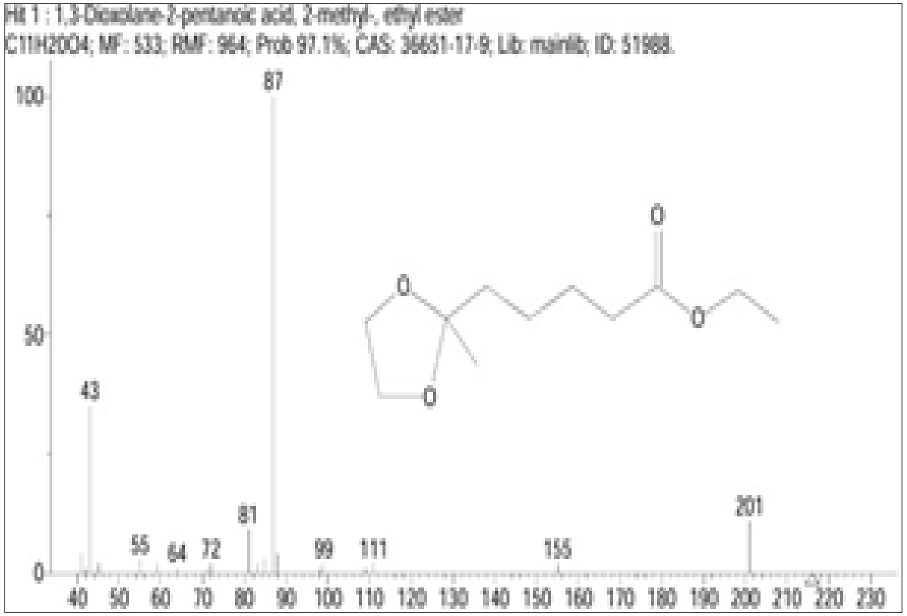
3		$C_{12}H_{22}O$	17.770		▪ Skin and Eye Irritation ▪ Mucous memrane irritation ▪ Gastrointestinal irritation	
	Phenol,2,4,6-triiodo			1.995		

Table 2: Volatile Organic Compounds of Nutritional Importance in Young Leaves of *X. mafaffa* (Schott)

S/N	Compound Name	Molecular formula	Retention Time (Min.)	Relative Abundance (%)	Nutritional Relevance	Chromatogram
1	Glycine,N-methyl-n-propoxycarbonyl-,dodecyl ester	$C_{19}H_{37}NO_4$	4.442	14.119	▪ N-methyltransferase precursor ▪ Regulation of methionine metabolism	

2	Benzenetridecanoic acid,4-methoxy-,2-decyl-3-methoxy-5-pentylphenyl ester	$C_{42}H_{68}O_4$	6.188	2.007	▪ Energy source	
3	1,3-Dioxolane-2-pentanoic acid,2-methyl-,ethyl ester	$C_{11}H_{20}O_4$	19.086	2.15	▪ Flavouring agent ▪ Enhances sensory quality and palatability	

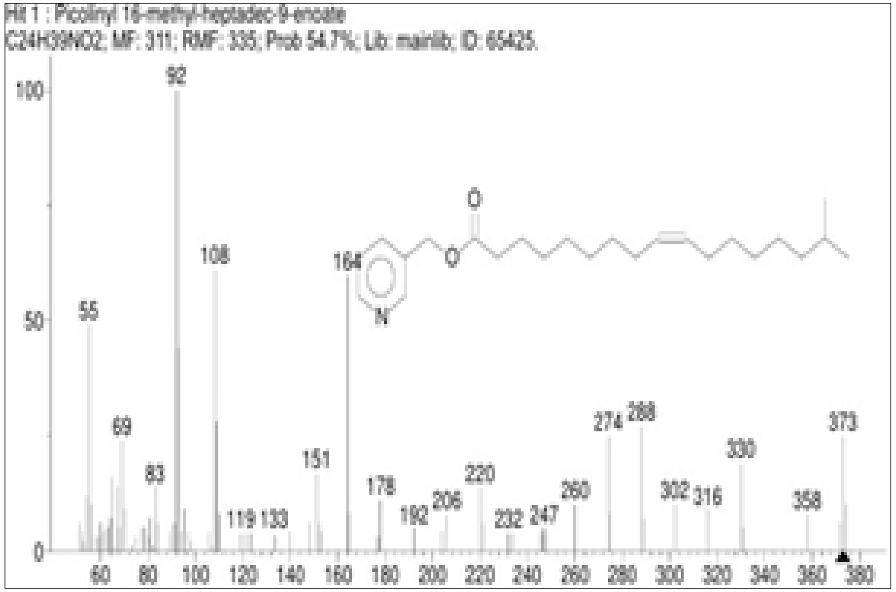
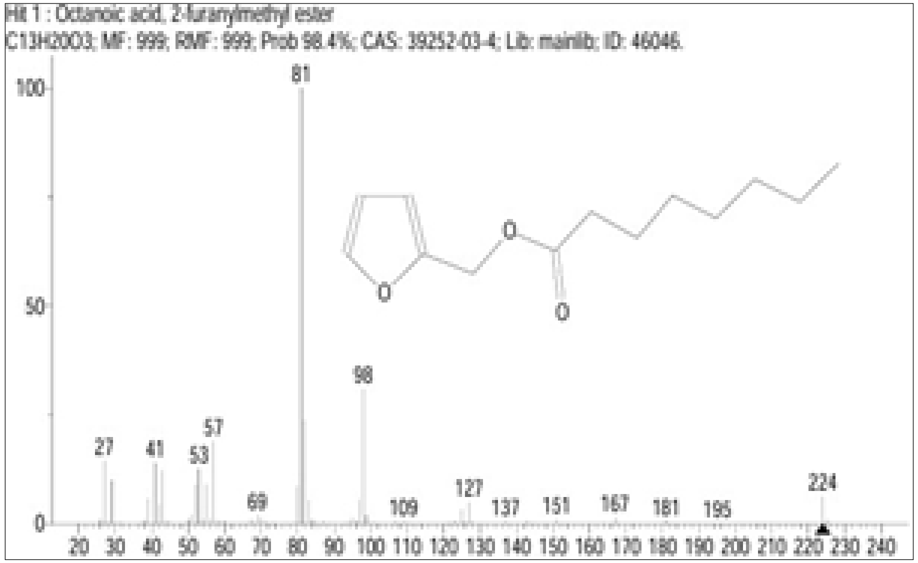
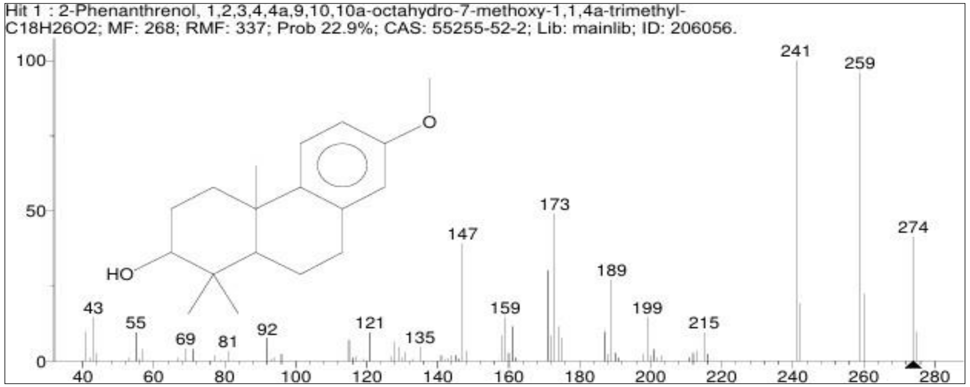
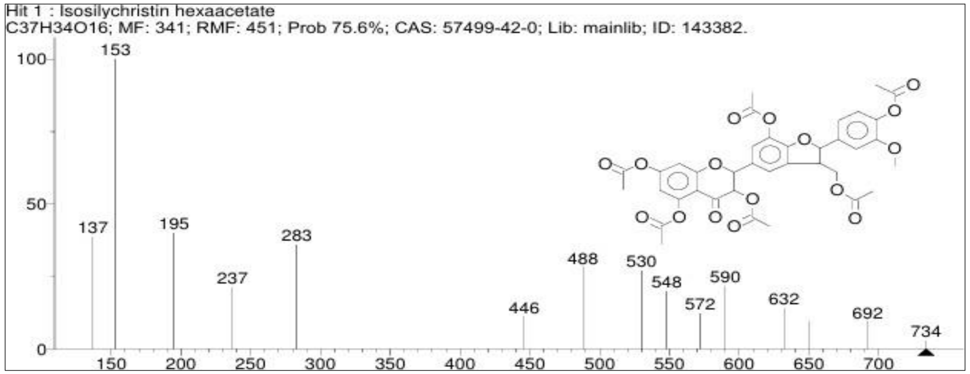
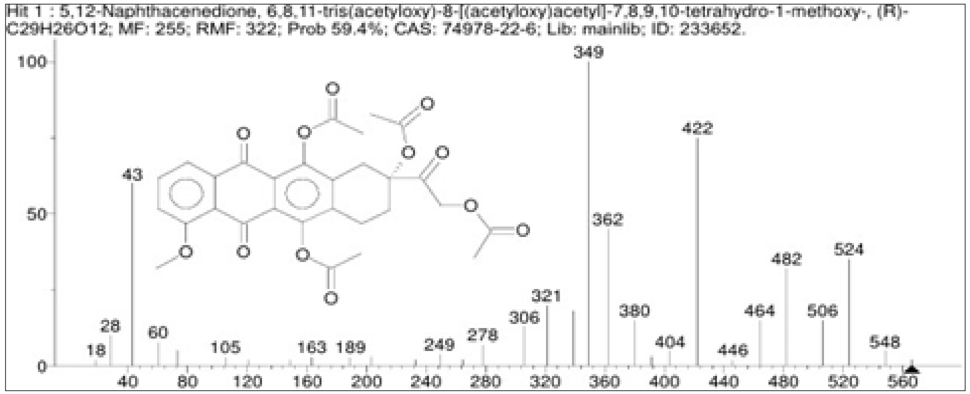
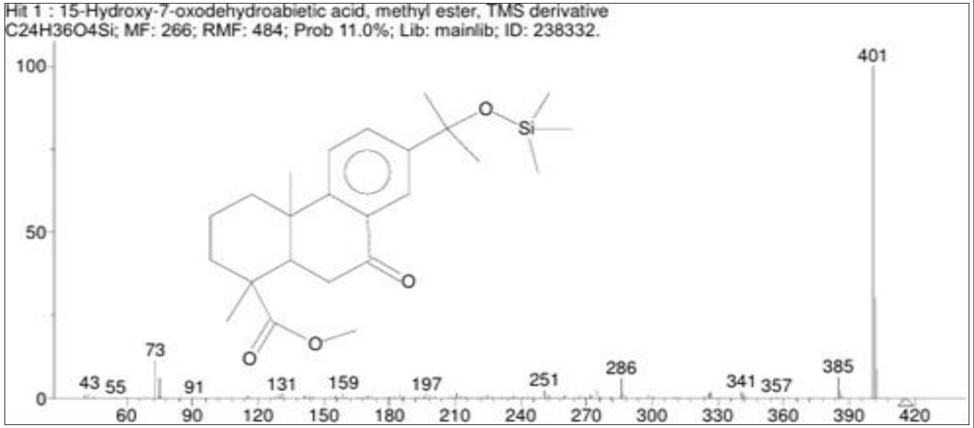
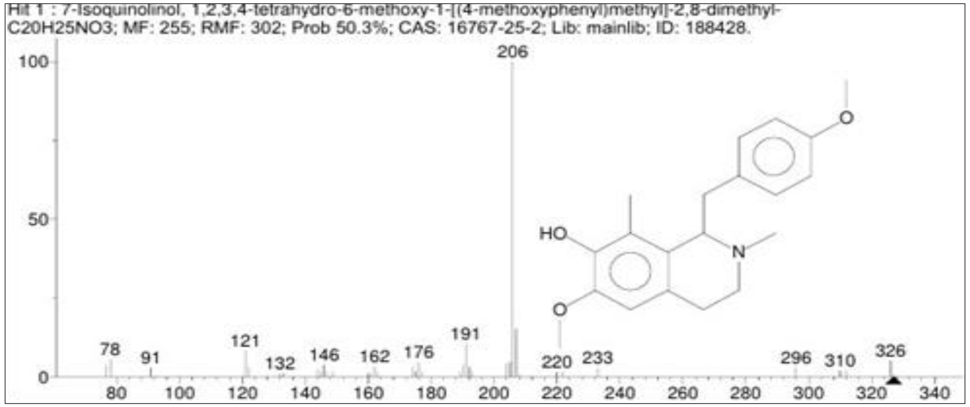
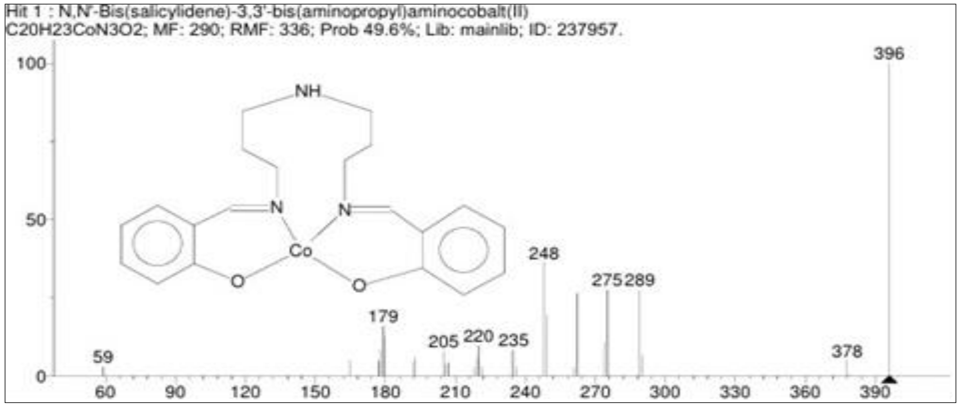
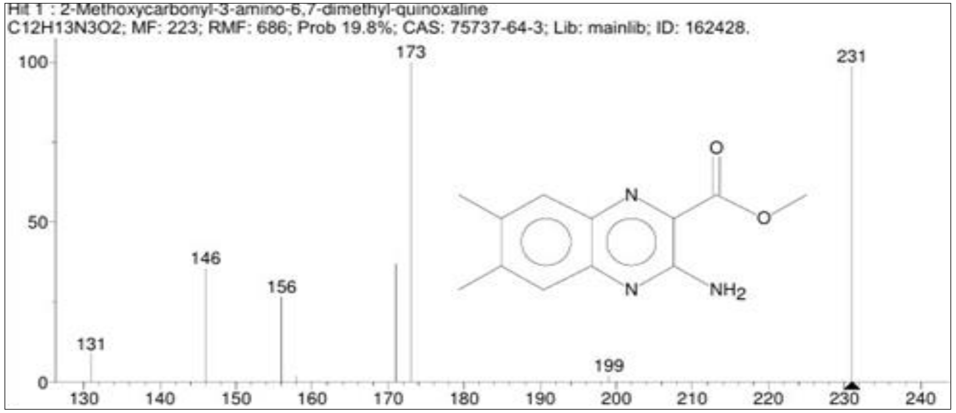
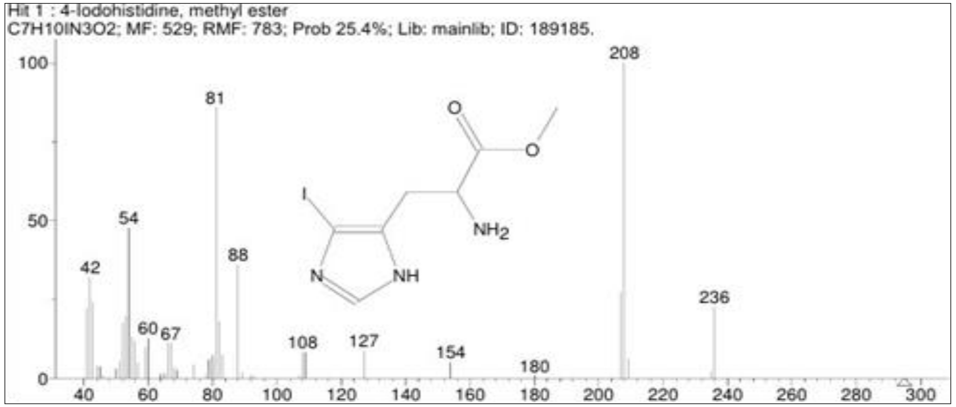
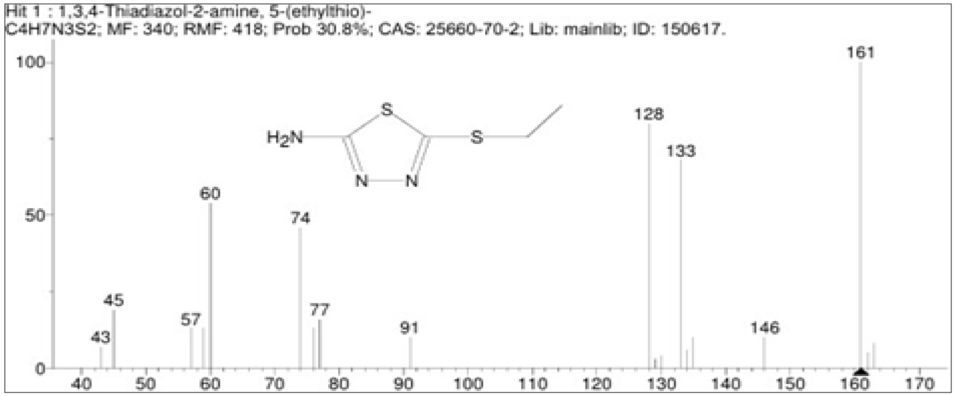
4	Picolinyl 16-methyl-heptadec-9-enoate	$C_{24}H_{39}NO_2$	4.559	38.379	▪ Cholesterol metabolism ▪ Energy soorce ▪ Lipid source	
5	Octanoic acid,2-furanylmethyl ester	$C_{13}H_{20}O_3$	24.301	2.242	▪ Flavouring agent ▪ Enhance sensory profile	

Table 3: Volatile Organic Compounds of Medicinal Importance in Young Leaves of *X. mafaffa* (Schott)

S/N	Compound Name	Molecular formula	Retention Time (Min.)	Relative Abundance (%)	Medicinal importance	Chromatogram
1	2-Phenanthrenol, 1,2,3, 4,4a,9,10,10a-octahydro-7-methoxy-1,1,4a-trimethyl	$C_{18}H_{26}O_2$	11.374	1.899	-Antioxidant potential	
2	Isosilychristin hexaacetate	$C_{37}H_{34}O_{16}$	4.728	2.437	-Hepatoprotective potential -Antioxidant -Antitumor	
3	5,12-Naphthacenedione,6,8,11-tris(acetyloxy)-8-[(acetyloxy)acetyl]-7,8,9,10-tetrahydro-1-methoxy-,(R)	$C_{29}H_{26}O_{12}$	19.831	3.303	-Antitumour potential -Antimicrobial potential	

4	15-Hydroxy-7-oxodehydroabietic acid,methyl ester,TMS derivative	$C_{24}H_{36}O_4Si$	11.176	1.92	-Antioxidant -Anti-inflammatory	
5	7-Isoquinolinol,1,2,3,4-tetrahydro-6-methoxy-1- [(4-methoxyphenyl) methyl]-2,8-dimethyl	$C_{20}H_{25}NO_3$	22.537	1.929	- Antimalarial -Antimicrobial	
6	N,N'-Bis(salicylidene)-3,3'-bis(aminopropyl) aminocobalt(II)	$C_{20}H_{23}CoN_3O_2$	12.823	6.53	- Has Antitumor potential	

7	2-Methoxycarbonyl-3-amino-6,7-dimethyl-quinoxaline	$C_{12}H_{13}N_3O_2$	13.551	2.54	- Antimicrobial - Antitumor	
8	4-Iodohistidine,methyl ester	$C_7H_{10}IN_3O_2$	19.511	2.122	- Antifungal potential - Antimicrobial potential	
9	1,3,4-Thiadiazol-2-amine, 5-(ethylthio)	$C_4H_7N_3S_2$	14.657	2.006	- Antimicrobial scaffold - Anti-inflammatory agent	

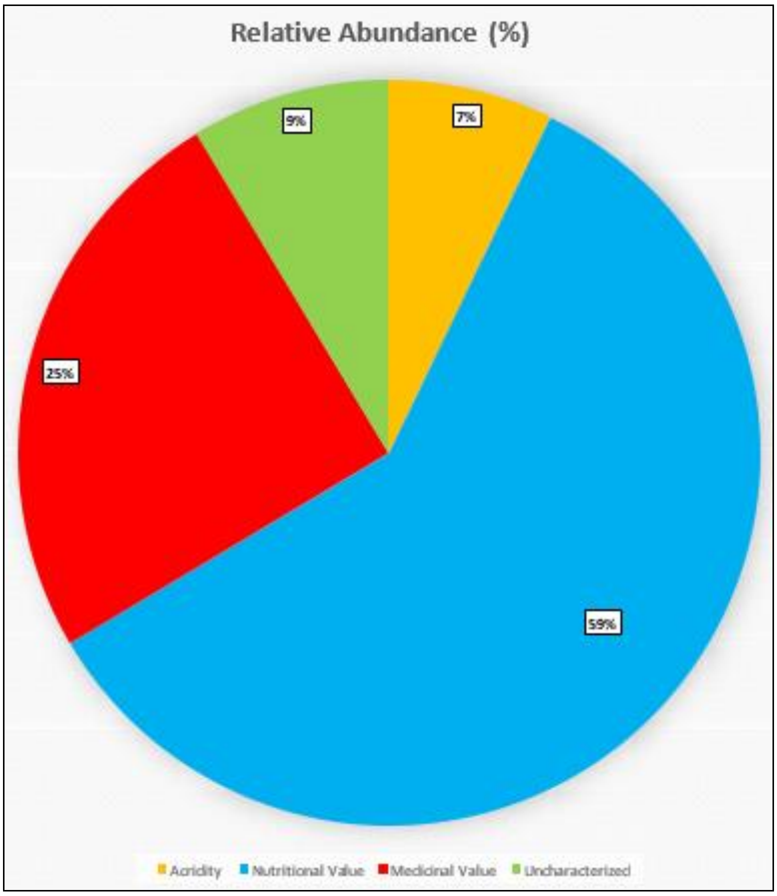


Fig 1: Percentage Contribution of Phytochemicals associated with Acridity, Nutritional value, Medicinal importance and uncharacterized ones in the chemical profile of young leaves of X. mafaffa

Discussion

The traditional use of foliage, particularly young leaves, suggests an understanding in the indigenous food system that these parts possess minimal anti-nutritional factors compared to mature tissues. This long history of consumption makes it important for conducting a comprehensive biochemical analysis to valorize the plant's resources (Prospére *et al*., 2025) [20].

GC-MS analysis is a reliable tool which has been used over the years for the identification of phytochemicals in plants (Eleazu, 2016) [7]. The identified compounds revealed *Xanthosoma mafaffa* as a plant that actively produces and accumulates a wide range of chemical classes; with a high concentration of long-chain fatty acid precursors which has been confirmed as a metabolic energy source.

The phytochemical profile was grouped into acridity, nutritional and medicinal importance which is significant because most phytochemical studies on cocoyam have focused on tubers rather than foliage, leaving a gap in comparative data. Similar GC-MS work on *Colocasia esculenta* tubers reported antioxidant phytochemicals (Eleazu, 2016) [7], but leaf chemistry remains largely unexplored.

In terms of acridity, secondary organic compounds possessing known toxic properties suspected to contribute to overall plant acridity were grouped. Compounds such as phenol,2,4,6-triiodo, butaperazine, and a fluorinated malononitrile derivative were detected. Phenolic compounds are well known contributors to bitterness and acrid taste in plants, and halogenated phenols exhibit strong antimicrobial and irritant properties. Acridity in cocoyam has traditionally been attributed to calcium oxalate raphides (Fang *et al*., 2024) [8], but the presence of reactive phenolics and nitrile derivatives suggests a broader chemical basis. Piperazine derivatives, have been reported in GC- MS screens of alkaloid-rich extracts to act as deterrents to herbivores and cause dermal or mucous membrane irritation in humans thus explaining the traditional need to process cocoyam leaves before consumption (Paul *et al*., 2022). The identification of nitrile derivatives aligns with cyanogenic glycosides reported in cassava and other tropical crops, which are categorized as plant defense compounds (Vetter, 2000) [23].

Nutritionally, the dominant compound picolinyl 16-methyl-heptadec-9-enoate highlights the abundance of fatty acid esters. Fatty acid esters are consistently reported in GC-MS studies of leafy vegetables and oils, contributing to caloric value and membrane structure (Kumar *et al*., 2023; Lisec *et al*., 2006). Babayemi and Adepoju, (2020) [4, 12, 13] similarly reported high levels of fatty acids in leafy vegetables consumed in Nigeria, emphasizing their nutritional importance. The detection of glycine esters, supports amino acid availability, aligning with reports of amino acid derivative in plant GC-MS metabolomics (Lisec *et al*., 2006) [13]. Medium-chain fatty acids such as octanoic acid esters are valued for rapid metabolism and antimicrobial properties, as documented in coconut oil and diary fats (Charlot *et al*., 2022) [6]. Aromatic esters and dioxolane

Derivatives contribute to flavour and antioxidant potential, consistent with the reports of Alam *et al*. (2025) [1] who carried out a GC-MS analysis of plant volatiles. Collectively, these compounds suggest that cocoyam leaves are not only fibrous green leaves but are also nutritionally rich, with potential nutraceutical applications.

Medicinally, several bioactive chemical classes were identified, including flavonolignans, quinones, alkaloids, thiadiazoles, diterpenoides and alogenated amino acids. Isosilychristin hexaacetate is structurally related to silymarin constituents which are known for their hepatoprotective and antioxidant activities (Jaffar *et al*, 2024) [10]. Quinone derivatives resembling anthracyclines are typically classified as cytotoxic agents in pharmacological literatures (Minotti *et al*., 2004; Mohora *et al*., 1999) [15, 17]. Quinoxaline derivatives are reported as antimicrobial and anti- inflammatory compounds (Hanieh and Alfwuaires, 2025) [9], while isoquinoline alkaloids are categorized as analgesic and antimalarial agents (Yun *et al*., 2021). Thiadiazoles are consistently grouped as synthetic pharmacophores with antifungal and anti-inflammatory activities (Anthwal *et al*., 2022) [2], and diterpenoid resin acids such as abietic acid are categorized as anti inflammatory and antimicrobial metabolites (Mohammad *et al*., 2025) [16]. This categorization aligns with pharmacological classifications, though it differs from plant metabolomics studies which often lists these compounds under "Secondary metabolites" without functional grouping. Functionally, these compounds mechanism of action include reactive oxygen species scavenging, enzyme inhibition, DNA intercalation, and microbial membrane disruption, supporting the ethno- medicinal use of cocoyam leaves.

In conclusion the phytochemical characterization of young leaves of *Xanthosoma mafaffa* demonstrates that the plant contains a rich diversity of compounds with functional relevance beyond its traditional dietary use. Acridity was linked to phenolic and nitrile derivatives aside oxalates, nutritional importance was dominated by fatty acid esters and amino acid derivatives while medicinal potential was marked by the presence of flavonolignans, quinones, alkaloids, thiadiazoles, diterpenoids, and rare complexes. By categorizing these phytochemicals according to their functional mechanisms, this study connects chemical composition to ethnobotanical practice. The findings highlight cocoyam leaves as a promising source of nutraceutical and pharmacological agents.

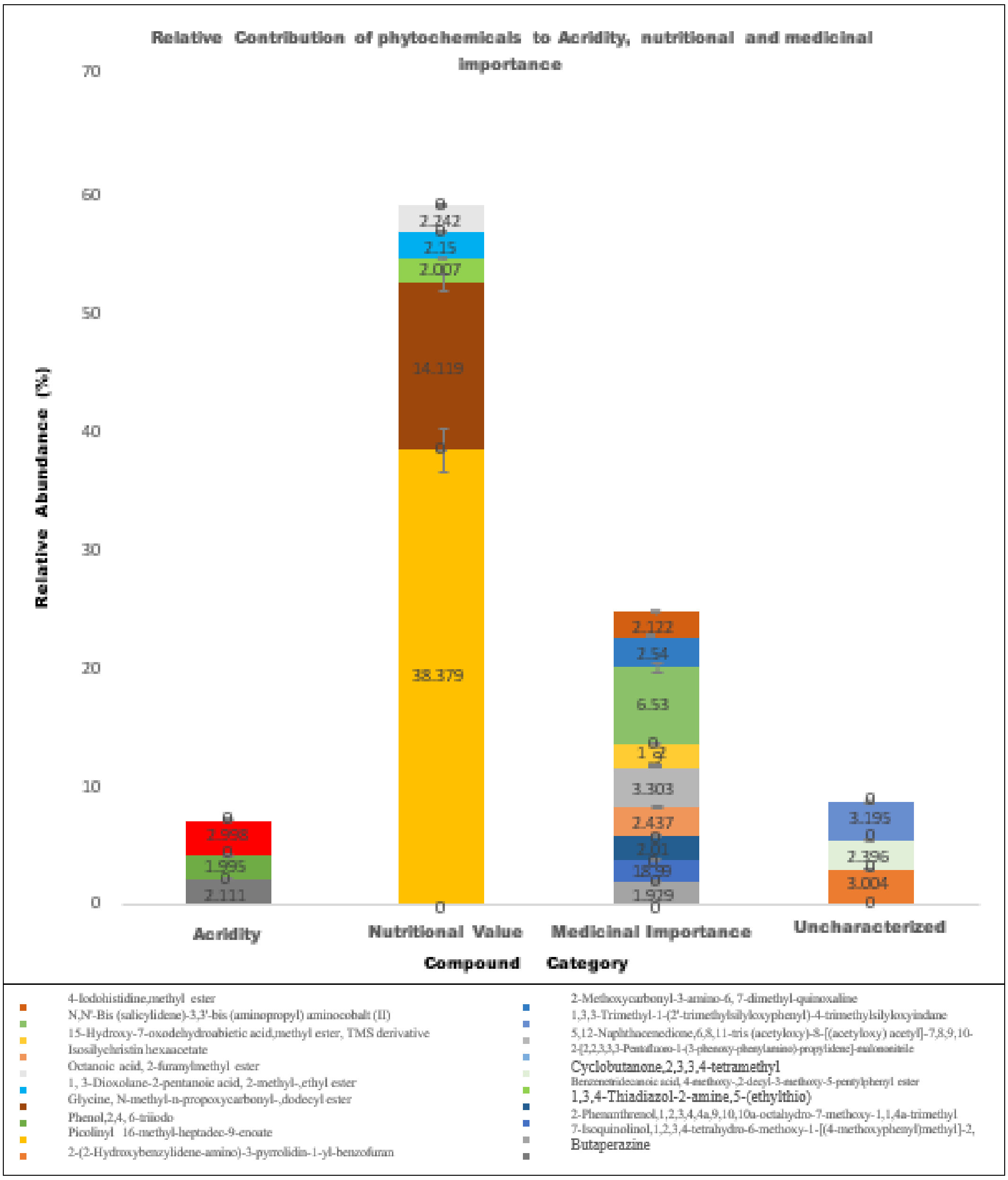


Fig 2: Individual phytochemical contribution to acridity, nutritional, medicinal importance and uncharacterized in young leaves of *X. mafaffa*.

Declarations

Author's contributions: IIN, SMS and OGO designed the study; IIN and IIJ prepared the sample and carried out the extraction procedures; VKA and IIJ carried out the data analysis and interpretation. IIN drafted the manuscript, SMS, VKA and OGO reviewed it while all authors contributed to the development of the final manuscript and approved its submission.

Conflict of Interest: The authors declare no conflict of interest.

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