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Chemical Diversity, Bioactivity Potential, and Toxicity Risks of *Dioscorea bulbifera* and *Xanthosoma robustum* Leaves: A Comparative GC–MS Study

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Abstract

Leaves of Dioscorea bulbifera and Xanthosoma robustum are widely used in traditional medicine for the management of various health conditions. Despite their ethnomedicinal relevance, there is limited comparative information on their phytochemical composition and associated safety profiles. Comprehensive chemical profiling is necessary to validate their therapeutic claims, identify bioactive constituents, and assess potential toxicological risks linked to indiscriminate or excessive consumption. Gas chromatography–mass spectrometry (GC-MS) was used to identify and compare phytochemical constituents present in the leaf extracts of D. bulbifera and X. robustum. The detected compounds were classified based on chemical structure and reported biological activities, with emphasis on shared constituents and compounds with known or suspected toxic effects. A total of 34 compounds were identified in D. bulbifera leaves, predominantly comprising low-molecular-weight aromatic hydrocarbons, aldehydes, alcohols, cycloalkanes, and furan derivatives, which are associated with antimicrobial and antioxidant activities. In contrast, X. robustum contained 62 compounds, including long-chain alcohols, esters, nitrogen-containing heterocyclic compounds, and aromatic metabolites, suggesting possible roles in enzyme modulation, lipophilicity, and anticancer-related activities. The presence of shared phytochemicals indicates overlapping pharmacological potential. However, potentially harmful compounds such as benzene, toluene, and trichloroacetic acid derivatives were also detected. The study supports the traditional medicinal use of both plants while highlighting significant phytochemical diversity and potential safety concerns. The detection of toxic constituents underscores the need for proper processing, dosage regulation, and detoxification strategies to ensure safe therapeutic application.

Keywords: Bioactivity; *Dioscorea bulbifera;* GC-MS; Phytochemicals; *Xanthosoma robustum*

1. Introduction

Plants constitute a rich reservoir of bioactive secondary metabolites that are largely responsible for their diverse therapeutic effects. *Dioscorea bulbifera* L., widely referred to as aerial potato or aerial yam, and *Xanthosoma robustum*, commonly known as the elephant ear plant, are tropical species of notable ethnomedicinal importance. Both plants have been traditionally employed for their antimicrobial, anti-inflammatory, and antioxidant activities. *Dioscorea bulbifera* L. (Figure 1) is a twining, herbaceous climbing vine that develops both large and small basal tubers. The plant exhibits a vigorous and invasive growth pattern, often exceeding 20 meters in length, enabling it to dominate and suppress surrounding vegetation (Dray and Rayamajhi, n.d.). In addition to its subterranean tubers, the species produces aerial tubers along its climbing stems. These structures are edible and have long been utilized in traditional medicine, underscoring the plant's recognized ethnopharmacological relevance (National Tropical Botanical Garden, 2007).

Figure 1: Aerial tubers (bulbils) and leaves of *Dioscorea bulbifera* L.

Xanthosoma robustum (Figure 2) is characterized by its expansive, broad leaves with conspicuous venation, features that make it easily recognizable. These leaves are commonly used both as a food source and in traditional healing practices (Kew Science). Its distinctive morphology, together with a diverse profile of phytochemicals, underpins the plant's importance in ethnomedicine.

Figure 2: Corms and leaves of *Xanthosoma robustum*

Although *Dioscorea bulbifera* (family Dioscoreaceae) and *Xanthosoma robustum* (family Araceae) are taxonomically distinct, both species contain a range of secondary metabolites with significant pharmacological relevance. Nonetheless, differences in their phytochemical composition are likely to influence their therapeutic performance, safety profiles, and possible toxic effects.

According to Mohanty et al. (2021), the primary and secondary metabolites present in the bulbils of *D. bulbifera* contribute substantially to its nutraceutical importance, indicating potential applications in addressing antimicrobial resistance. The plant is extensively utilized in traditional Indian and Chinese medical systems for diverse therapeutic purposes (Ghosh et al., 2015). Studies have shown that its bulbils possess notable anti-diabetic properties, as demonstrated through both in vitro and in silico approaches (Rapotatoajhi et al., 2024). In addition, extracts from the stem tubers exhibit strong antioxidant capacity, largely attributed to their bioactive secondary constituents (Odeghe et al., 2020).

Further investigations reveal that *D. bulbifera* leaves contain compounds with potential use as biopesticides (Oksari et al., 2025). Mainasara et al. (2021) identified a total of 39 secondary metabolites in the methanolic leaf extract of the plant. Dihydrodioscorin isolated from *D. bulbifera* has been reported to inhibit fungal growth at a

concentration of 0.1% (Wang et al., 2009). Moreover, bioactive compounds such as epicatechin, myricetin, isovanillic acid, and vanillic acid found in the bulbils have demonstrated the ability to enhance immune defense against cardiovascular diseases in experimental animal models (Vasanthi et al., 2019). The bulbils are also nutritionally valuable, containing appreciable amounts of proteins, carbohydrates, minerals, and vitamins (Bolaniran et al., 2019; Bennett et al., 2024). However, high intake levels have been associated with suppression of mononuclear macrophage phagocytic activity (Cui et al., 2016). Additionally, the steroidal compound diosgenin—an important precursor in the synthesis of contraceptives and cortisone—has been successfully isolated from *D. bulbifera* (Jayachandran et al., 2016).

In *Xanthosoma* species, various plant parts including leaves, fruits, and seeds have been reported to contain oxalic acid ($C_2H_2O_4$), a compound considered potentially harmful when consumed in high amounts. Oxalic acid forms both soluble and insoluble salts, including oxalate ions and calcium oxalate crystals, which are implicated in the formation of kidney stones when present at elevated dietary levels (Nina et al., 2020). Furthermore, Kato et al. (1996) isolated four hydroperoxysterols from the aerial parts of *X. robustum*, which exhibited antibacterial activity against *Micrococcus luteus*, *Bacillus subtilis*, and *Escherichia coli*.

Despite these findings, there remains limited comparative information on the detailed chemical composition of the leaves of *D. bulbifera* and *X. robustum*, as well as the implications for their therapeutic efficacy and safe use in ethnomedicine. This study aims to address this gap by conducting a comparative gas chromatography–mass spectrometry (GC–MS) analysis of hexane leaf extracts from both species. The objectives are to identify, categorize, and compare their phytochemical constituents, highlight bioactive compounds associated with pharmacological activities, and assess potential safety concerns related to their medicinal application.

2. Materials and Methods

All reagents employed in this study were of analytical grade, sourced from BDH, Labtech Chemicals, and Ken Light Laboratories, and were used as received without any additional purification steps.

2.1 Plant Collection and Identification

Leaves of *Xanthosoma robustum* were harvested from a farm in Toru-Orua Community, Bayelsa State, Nigeria, while leaves of *Dioscorea bulbifera* were obtained from a farm in Agbura Community, Bayelsa State, Nigeria. Botanical identification of both plant materials was carried out at the Department of Biological Sciences, University of Africa, Toru-Orua.

2.2 Preparation of Samples

Leaves of *Dioscorea bulbifera* and *Xanthosoma robustum* were air-dried for 21 days, ground into a fine powder using an electric blender, and preserved in a desiccator prior to subsequent analyses.

2.3 Bioactive Chemicals

The extracts were analyzed using an Agilent 6890 gas chromatograph coupled with an Agilent 5973 mass selective detector (MSD), equipped with an Agilent 7683 Series automatic liquid sampler and a META X5-coated fused-silica capillary column (30 m × 0.25 mm internal diameter, 0.25 µm film thickness) with a maximum temperature limit of 325 °C. High-purity helium was employed as the carrier gas at a constant flow rate of 1.0 mL/min.

A 1 µL portion of each sample was introduced in split mode at a ratio of 20:1. The temperatures of the MS source and quadrupole were maintained at 230 °C and 150 °C, respectively, while the injector, transfer line, and ion source were set at 280 °C. Mass spectral data were collected over a scan range of 50–550 amu under an ionization energy of 70 eV, with the electron multiplier voltage automatically adjusted.

Identification of bioactive compounds was achieved by matching retention times and mass spectra with entries in the 2014 National Institute of Standards and Technology (NIST) library, which contains more than 590,000 reference spectra. This approach enabled the assignment of compound identities, including their molecular weights, formulas, structural features, and fragmentation patterns.

3. Results and Discussion

The phytochemical constituents detected in the hexane leaf extracts of *Dioscorea bulbifera* and *Xanthosoma robustum* are presented in Tables 1 and 2, respectively. A comparative classification of the compounds identified in both extracts is provided in Table 3, while the corresponding GC-MS chromatograms are illustrated in Figures 3 and 4.

Table 1: Phytochemicals detected in hexane leaf extract of *Dioscorea bulbifera* using Gas Chromatography-Mass Spectrometry (GC-MS)

S/N	Retention Time (min)	Compound Name	Peak Area (%)	Match Probability (%)	Molecular formula	Molecular weight
1.	1.293	1-Butanol, 2-methyl	0.82	89.2	$C_5H_{12}O$	88
2.	1.338	1,3-Butadiene, 2-fluoro	0.50	97.0	C_4H_5F	72
3.	1.449	Hexane, 3-ethyl	0.95	73.1	C_5H_{18}	114

4.	1.557	Furan, 2,5-dihydro-3-methyl	1.26	94.1	C_5H_8O	84
5.	1.592	3-Buten-2-ol, 2-methyl	0.69	93.9	$C_5H_{10}O$	86
6.	1.733	Benzene	5.14	81.9	C_6H_6	78
7.	1.884	2,4-Hexadiyne	7.34	86.5	C_6H_6	78
8.	2.328	1,3-Butadiene-1-carboxylic acid	11.11	97.8	$C_5H_6O_2$	98
9.	2.671	1,5-Hexadien-3-yne, 2-methyl	4.49	91.5	C_7H_8	92
10.	2.723	Toluene	1.92	80.5	C_7H_8	92
11.	3.237	Acetic acid, dichloro	6.95	99.0	$C_2H_2Cl_2O_2$	128
12.	3.531	2,4-Octadiyne	12.15	78.3	C_8H_{10}	106
13.	3.780	Bicyclo[2.1.1]hex-2-ene, 2-ethenyl	2.35	83.1	C_8H_{10}	106
14.	3.845	Benzene, 1,3-dimethyl	4.49	62.4	C_8H_{10}	106
15.	3.906	Bicyclo[3.1.0]hexan-2-ol	2.04	91.2	$C_6H_{10}O$	98
16.	3.985	3-Methyl-2-thiophenecarboxaldehyde	2.82	86.0	C_6H_6OS	126
17.	4.063	Ethanone, 1-(4-methyl-1H-imidazol-2-yl)	2.77	97.0	$C_6H_8N_2O$	124
18.	4.106	Cyclopropane, 1-methyl-2-pentyl	1.24	52.0	C_9H_{18}	126
19.	4.123	2-Dodecenal, (E)	1.87	83.0	$C_{12}H_{22}O$	182
20.	4.174	4-Methyl-1,4-heptadiene	1.10	67.4	C_8H_{14}	110
21.	4.240	1,2-Dipropylcyclopropene	1.30	84.2	C_9H_{16}	124
22.	4.394	Benzeneacetaldehyde	4.67	88.9	C_8H_8O	120
23.	4.534	1-Hexen-4-yne, 3-ethylidene-2-methyl	2.44	90.8	C_9H_{12}	120
24.	4.630	Benzene, 1-ethyl-2-methyl	0.40	63.3	C_9H_{12}	120
25.	4.657	2-Hexene, 3,5-dimethyl	0.36	69.0	C_8H_{16}	112
26.	4.716	Benzene, 1-ethyl-4-methyl	0.68	63.1	C_9H_{12}	120
27.	4.754	Cyclohexane, (2-methylpropyl)	0.24	93.6	$C_{10}H_{20}$	140
28.	4.807	Benzene, cyclopropyl	0.04	48.6	C_9H_{10}	118
29.	4.895	Benzene, 1,2-diethyl	0.42	87.9	$C_{10}H_{14}$	134
30.	4.933	Naphthalene, decahydro-, trans	0.18	66.9	$C_{10}H_{18}$	138
31.	5.024	Benzene, 2-ethyl-1,4-dimethyl	0.08	57.1	$C_{10}H_{14}$	134
32.	5.087	Undecane	0.42	55.0	$C_{11}H_{24}$	156
33.	5.234	Naphthalene, decahydro-2-methyl	0.07	74.9	$C_{11}H_{20}$	152
34.	5.571	Dodecane	0.04	62.2	$C_{12}H_{26}$	170

Table 2: Phytochemicals identified from the hexane leaf extract of *Xanthosoma robustum* leaves using Gas Chromatography-Mass Spectrometry (GC-MS)

S/N	Retention Time (min)	Compound Name	Peak Area (%)	Match Probability (%)	Molecular formula	Molecular weight
1.	1.677	2-Furanmethanol	2762	91.4	$C_5H_6O_2$	98
2.	1.976	1,3-Butadiene-1-carboxylic acid	5540	97.8	$C_5H_6O_2$	98
3.	2.150	Methylenecyclopropanecarboxylic acid	1713	0.90	$C_5H_6O_2$	98
4.	2.333	1,6-Heptadiyne	6139	92.2	C_7H_8	92
5.	2.349	Benzene, [(methylsulfinyl)methyl]-	4870	4.01	$C_8H_{10}OS$	154
6.	2.368	1,5-Heptadien-3-yne	1683	88.2	C_7H_8	92
7.	2.431	1,5-Hexadien-3-yne, 2-methyl-	1245	5.64	C_7H_8	92
8.	2.722	Benzene, [(methylsulfinyl)methyl]-	1453	4.01	$C_8H_{10}OS$	154
9.	2.805	2-Pentyn-1-ol	2965	87.5	C_5H_8O	84

10.	2.973	Carbonic acid, but-3-en-1-yl dodecyl ester	1542	4.00	$C_{17}H_{32}O_3$	284
11.	3.087	Cyclopropane, nonyl-	8700	35.6	$C_{12}H_{24}$	168
12.	3.241	2-Dodecene, (Z)-	1146	4.85	$C_{12}H_{24}$	168
13.	3.448	1-Dodecene	4688	4.85	$C_{12}H_{24}$	168
14.	3.748	Carbonic acid, but-3-yn-1-yl undecyl ester	2218	4.29	$C_{16}H_{28}O_3$	268
15.	3.778	1-Undecene, 5-methyl-	9728	63.5	$C_{12}H_{24}$	168
16.	3.806	1-Undecene, 7-methyl-	2496	4.16	$C_{12}H_{24}$	168
17.	3.855	1-Undecene, 10-methyl-	1626	1.20	$C_{12}H_{24}$	168
18.	4.017	3-Octadecene, (E)-	6535	6.70	$C_{18}H_{36}$	252
19.	4.053	9-Octadecene, (E)-	5350	6.44	$C_{18}H_{36}$	252
20.	4.153	Cyclopropane, nonyl	5948	35.6	$C_{12}H_{24}$	168
21.	4.191	2-Dodecene, (Z)-	5647	4.85	$C_{12}H_{24}$	168
22.	4.465	1-Decanol	6176	50.2	$C_{10}H_{22}O$	158
23.	4.513	1-Hexen-4-yne, 3-ethylidene-2-methyl-	2118	90.8	C_9H_{12}	120
24.	4.571	2,3-Heptadien-5-yne, 2,4-dimethyl-	2076	3.30	C_9H_{12}	120
25.	4.598	Cyclohexane, 1,2,4-tris(methylene)-	1109	0.80	C_9H_{12}	120
26.	4.652	1-Aminobenzotriazole	6792	96.9	$C_6H_6N_4$	134
27.	4.798	Benzaldehyde	5119	0.96	C_7H_6O	106
28.	4.959	4-Ethynyl-1-methylpyrazole	8882	96.7	$C_6H_6N_2$	106
29.	5.055	2,4,6-Cycloheptatrien-1-one	1386	0.96	C_7H_6O	106
30.	5.177	[1,2,3,4]Tetrazolo[1,5-a]pyridine, 6-methyl-	2992	0.74	$C_6H_6N_4$	134
31.	5.332	4-Ethynyl-1-methylpyrazole	9880	96.7	$C_6H_6N_2$	106
32.	5.463	1-Cyclohexene, 1-ethynyl	8946	80.4	C_8H_{10}	106
33.	5.557	1,6-Heptadien-3-yne, 5-methyl-	1473	2.00	C_8H_{10}	106
34.	5.765	p-Xylene	3874	2.00	C_8H_{10}	106
35.	5.806	Dichloroacetic acid, nonyl ester	1818	79.3	$C_{11}H_{20}Cl_2O_2$	254
36.	6.207	Dichloroacetic acid, decyl ester	2485	2.34	$C_{12}H_{22}Cl_2O_2$	268
37.	6.223	Pentadecafluorooctanoic acid, nonyl ester	3037	1.89	$C_{17}H_{19}F_{15}O_2$	540
38.	6.524	Acetic acid, trichloro-, nonyl ester	2688	76.1	$C_{11}H_{19}Cl_3O_2$	288
39.	6.680	Trichloroacetic acid, undecyl ester	1866	2.40	$C_{13}H_{23}Cl_3O_2$	316
40.	6.792	Nonyl heptafluorobutyrate	5852	1.64	$C_{13}H_{19}F_7O_2$	340
41.	6.909	2-Tridecanol	3413	80.0	$C_{13}H_{28}O$	200
42.	7.027	2-Tetradecanol	4131	4.32	$C_{14}H_{30}O$	214
43.	7.068	Acetic acid, trichloro-, nonyl ester	5836	76.1	$C_{11}H_{19}Cl_3O_2$	288
44.	7.297	Trichloroacetic acid, undecyl ester	3732	2.40	$C_{13}H_{23}Cl_3O_2$	316
45.	7.319	Nonyl heptafluorobutyrate	7122	1.64	$C_{13}H_{19}F_7O_2$	340
46.	7.501	Carbonic acid, but-3-yn-1-yl undecyl ester	8923	4.02	$C_{16}H_{28}O_3$	268
47.	7.532	Carbonic acid, but-3-yn-1-yl octyl ester	7903	3.24	$C_{13}H_{22}O_3$	226
48.	7.572	1,5-Heptadien-3-yne	8224	88.2	C_7H_8	92
49.	7.735	1,5-Hexadien-3-yne, 2-methyl-	1272	5.64	C_7H_8	92
50.	7.803	Benzaldehyde, 2-methyl-	1375	70.5	C_8H_8O	120
51.	8.032	Benzaldehyde, 4-methyl-	1502	15.3	C_8H_8O	120
52.	8.265	n-Tetracosanol-1	8811	28.5	$C_{24}H_{50}O$	354
53.	8.327	Behenic alcohol	9969	4.41	$C_{22}H_{46}O$	326
54.	8.511	Octacosanol	1244	4.07	$C_{28}H_{58}O$	410
55.	8.638	Decane, 2-methyl-	1165	53.8	$C_{11}H_{24}$	156
56.	9.061	Benzaldehyde, 3-methyl-	3820	68.0	C_8H_8O	120

57.	9.771	Benzaldehyde, 2-methyl-	1337	70.5	C_8H_8O	120
58.	10.420	2,4-Nonadiyne	2894	80.1	C_9H_{12}	120
59.	10.675	2,3-Heptadien-5-yne, 2,4-dimethyl	4478	3.60	C_9H_{12}	120
60.	10.764	Benzene, 1,2,3-trimethyl-	7816	3.46	C_9H_{12}	120
61.	11.139	Benzene, 1-ethyl-3-methyl-	3101	61.7	C_9H_{12}	120
62	12.145	Benzene, 1-ethyl-2-methyl-	3080	12.8	C_9H_{12}	120

Table 3: Combined Phytochemical Classification of Hexane leaf extracts of *Dioscorea bulbifera* & *Xanthosoma robustum*

S/N	Compound Name	Plant Source	Chemical Class	Sub-Class/ Notes
1	1-Butanol, 2-methyl	*D. bulbifera*	Alcohol	Branched aliphatic alcohol
2	1,3-Butadiene, 2-fluoro	*D. bulbifera*	Halogenated hydrocarbon	Fluorinated alkene
3	Hexane, 3-ethyl	*D. bulbifera*	Alkane	Branched hydrocarbon
4	Furan, 2,5-dihydro-3-methyl	*D. bulbifera*	Furan derivative	Oxygen heterocycle
5	3-Buten-2-ol, 2-methyl	*D. bulbifera*	Alcohol	Unsaturated alcohol
6	Benzene	*D. bulbifera*	Aromatic hydrocarbon	Simple benzene ring
7	2,4-Hexadiyne	*D. bulbifera*	Alkyne	Conjugated diyne
8	1,3-Butadiene-1-carboxylic acid	Both	Unsaturated carboxylic acid	α,β-unsaturated acid
9	1,5-Hexadien-3-yne, 2-methyl	Both	Alkyne/ Alkene	Conjugated dienyne
10	Toluene	*D. bulbifera*	Aromatic hydrocarbon	Methylbenzene
11	Acetic acid, dichloro	*D. bulbifera*	Halogenated acid	Dichloroacetic derivative
12	2,4-Octadiyne	*D. bulbifera*	Alkyne	Conjugated diyne
13	Bicyclo[2.1.1]hex-2-ene	*D. bulbifera*	Bicyclic hydrocarbon	Strained bicyclic ring
14	Benzene, 1,3-dimethyl	*D. bulbifera*	Aromatic hydrocarbon	Xylene isomer
15	Bicyclo[3.1.0]hexan-2-ol	*D. bulbifera*	Alcohol	Bicyclic alcohol
16	3-Methyl-2-thiophenecarboxaldehyde	*D. bulbifera*	Aromatic heterocycle	Thiophene aldehyde
17	Ethanone, 1-(4-methyl-1H-imidazol-2-yl)	*D. bulbifera*	Imidazole derivative	Alkaloid-like heterocycle
18	Cyclopropane, 1-methyl-2-pentyl	*D. bulbifera*	Cycloalkane	Branched cyclopropane
19	2-Dodecenal (E)	*D. bulbifera*	Aldehyde	Long-chain unsaturated
20	4-Methyl-1,4-heptadiene	*D. bulbifera*	Alkene	Unsaturated hydrocarbon
21	1,2-Dipropylcyclopropene	*D. bulbifera*	Cycloalkene	Small cyclopropane
22	Benzeneacetaldehyde	*D. bulbifera*	Aromatic aldehyde	Benzaldehyde derivative
23	1-Hexen-4-yne, 3-ethylidene-2-methyl	Both	Alkene/Alkyne	Conjugated unsaturated hydrocarbon
24	Benzene, 1-ethyl-2-methyl	Both	Aromatic hydrocarbon	Xylene derivative
25	2-Hexene, 3,5-dimethyl	*D. bulbifera*	Alkene	Branched alkene
26	Benzene, 1-ethyl-4-methyl	Both	Aromatic hydrocarbon	Xylene derivative
27	Cyclohexane, (2-methylpropyl)	Both	Cycloalkane	Branched cyclohexane

28	Benzene, cyclopropyl	*D. bulbifera*	Aromatic hydrocarbon	Cyclopropylbenzene
29	Benzene, 1,2-diethyl	*D. bulbifera*	Aromatic hydrocarbon	Diethylbenzene
30	Naphthalene, decahydro	*D. bulbifera*	Polycyclic hydrocarbon	Hydrogenated naphthalene
31	Benzene, 2-ethyl-1,4-dimethyl	*D. bulbifera*	Aromatic hydrocarbon	Alkyl-substituted benzene
32	Undecane	*D. bulbifera*	Alkane	Long-chain saturated hydrocarbon
33	Naphthalene, decahydro-2-methyl	*D. bulbifera*	Polycyclic hydrocarbon	Hydrogenated naphthalene
34	Dodecane	*D. bulbifera*	Alkane	Long-chain saturated hydrocarbon
35	2-Furanmethanol	*X. robustum*	Furan derivative	Oxygen heterocycle alcohol
36	Methylenecyclopropanecarboxylic acid	*X. robustum*	Cycloalkane carboxylic acid	Small cyclopropane acid
37	1,6-Heptadiyne	*X. robustum*	Alkyne	Linear diyne
38	Benzene, [(methylsulfinyl)methyl]-	*X. robustum*	Aromatic thioether	Sulfur-containing aromatic
39	1,5-Heptadien-3-yne	*X. robustum*	Alkene/Alkyne	Conjugated dienyne
40	2-Pentyn-1-ol	*X. robustum*	Alcohol	Unsaturated alkyne alcohol
41	Carbonic acid esters	*X. robustum*	Ester	Long-chain carbonic esters
42	Cyclopropane, nonyl-	*X. robustum*	Cycloalkane	Branched cyclopropane
43	1-Dodecene	*X. robustum*	Alkene	Long-chain
44	1-Undecene variants	*X. robustum*	Alkene	Branched long-chain
45	3- & 9-Octadecene	*X. robustum*	Alkene	Long-chain monoenes
46	1-Decanol	*X. robustum*	Alcohol	Long-chain primary alcohol
47	1-Aminobenzotriazole	*X. robustum*	Nitrogen heterocycle	Triazole derivative
48	Benzaldehyde & derivatives	*X. robustum*	Aromatic aldehyde	Ortho/meta/para derivatives
49	4-Ethynyl-1-methylpyrazole	*X. robustum*	Pyrazole derivative	Nitrogen heterocycle
50	Cyclohexene, 1-ethynyl	*X. robustum*	Cycloalkene	Unsaturated cycloalkene
51	p-Xylene	*X. robustum*	Aromatic hydrocarbon	Dimethylbenzene
52	Fluorinated esters	*X. robustum*	Fluorinated esters	Perfluoroalkyl esters
53	Long-chain alcohols (C_{24}–C_{28})	*X. robustum*	Fatty alcohols	n-Tetracosanol, behenic, octacosanol
54	Decane, 2-methyl	*X. robustum*	Alkane	Branched hydrocarbon
55	2,4-Nonadiyne	*X. robustum*	Alkyne	Conjugated diyne
56	Benzene alkyl derivatives	*X. robustum*	Aromatic hydrocarbon	Xylenes/ethyl/methylbenzenes

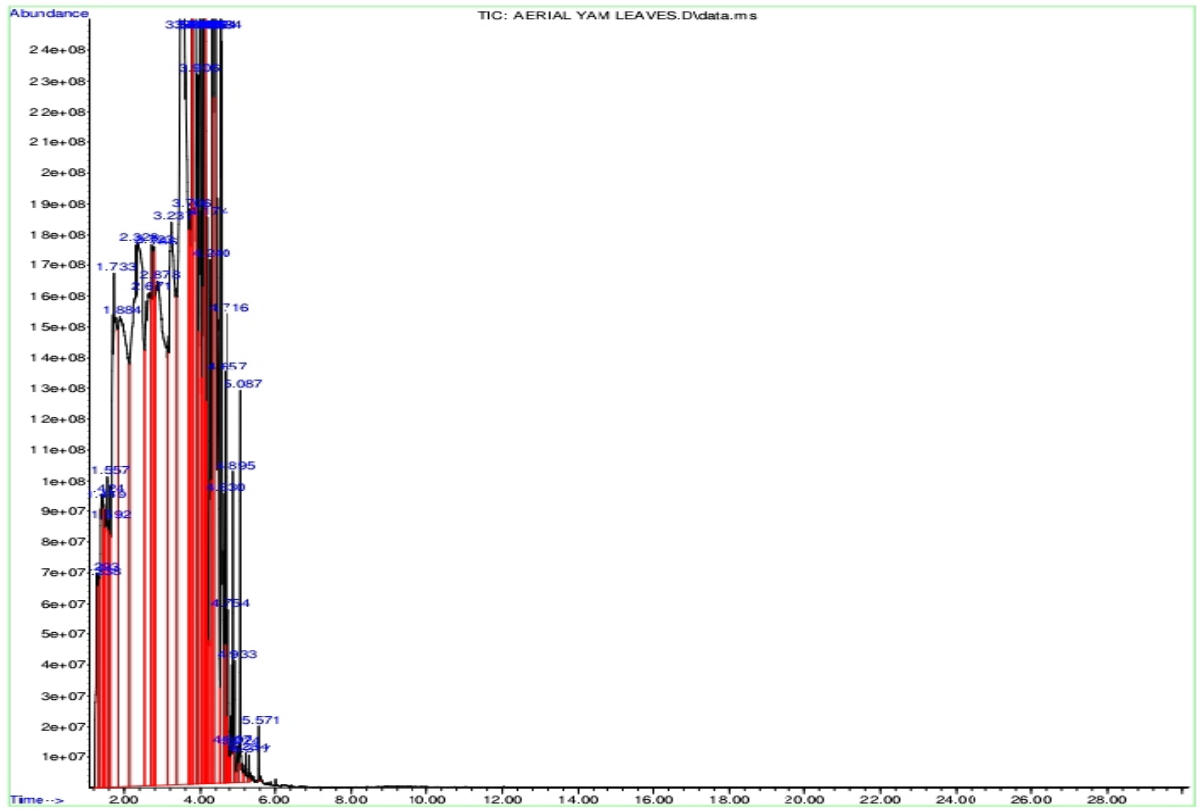

Figure 3: GC-MS chromatogram of hexane leaf extracts of *D. bulbifera*

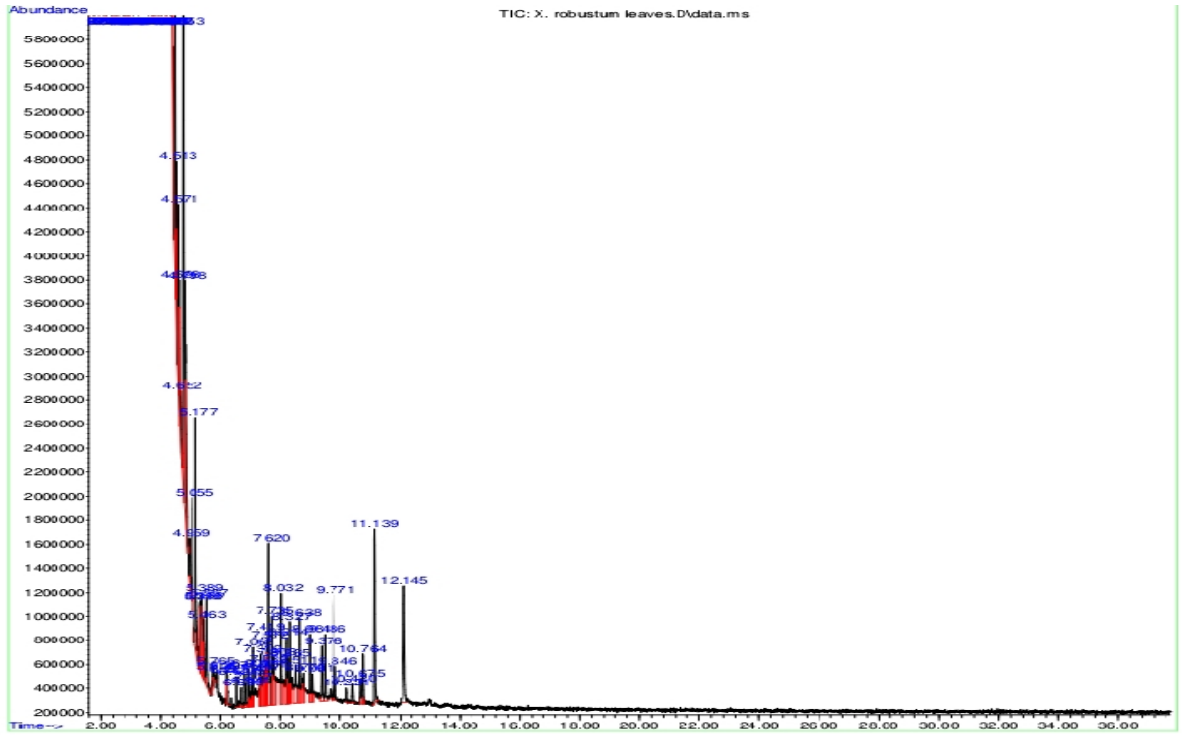

Figure 4: GC-MS chromatogram of hexane leaf extract of *X. robustum*

Dioscorea bulbifera yielded thirty-four (34) phytochemical constituents, as presented in Table 1, while sixty-two (62) compounds were identified in Xanthosoma robustum (Table 2). Comparative profiling demonstrated clear qualitative and quantitative disparities between both leaf samples. The constituents of *D. bulbifera* were largely composed of aromatic hydrocarbons, aromatic aldehydes, low-molecular-weight alcohols, cycloalkanes, and

furan derivatives. In contrast, *X. robustum* displayed a more chemically diverse profile, characterized by long-chain alcohols, esters, nitrogen-containing heterocycles, as well as aromatic compounds. Overall, all identified metabolites were grouped into major chemical classes, including aromatic hydrocarbons, aromatic aldehydes, alcohols, esters, alkanes, alkenes, alkynes, cycloalkanes, furans, and nitrogen-containing heterocycles (Table 3).

The predominance of aromatic aldehydes in *D. bulbifera* is particularly significant, as these compounds are widely reported to exhibit antimicrobial and antioxidant activities. The aldehyde functional group is capable of forming Schiff bases with microbial enzymes, resulting in enzyme deactivation, while the aromatic ring system enhances free radical stabilization and scavenging activity (Odeghe et al., 2021; Aljaafari et al., 2022; Sanguansermsri et al., 2024).

In *X. robustum*, the relatively high abundance of nitrogen-containing heterocycles suggests potential enzyme-modulating and antiproliferative properties, consistent with the established pharmacological importance of heterocyclic bioactive compounds (Mermer et al., 2021; Kumar et al., 2023). Additionally, the prevalence of long-chain alcohols and esters is commonly linked to enhanced lipophilicity, improved membrane permeability, and possible membrane-disruptive bioactivity due to their strong affinity for lipid bilayers (Di et al., 2007).

The moderate occurrence of furan derivatives in both plant species further supports their shared antioxidant and antimicrobial potential, as furan-based compounds are well known for redox activity and membrane-associated antimicrobial mechanisms. Likewise, the detection of alkanes, alkenes, alkynes, and cycloalkanes indicates additional structural diversity and possible involvement in enzyme–substrate interactions consistent with reported bioactivities of hydrocarbon derivatives (De et al., 2015).

Overall, *D. bulbifera* presents a comparatively simpler phytochemical profile dominated by low-molecular-weight aromatic aldehydes, which may underpin its traditional antimicrobial applications. In contrast, *X. robustum* exhibits a more complex chemical architecture enriched with nitrogen heterocycles and long-chain lipophilic constituents, suggesting broader pharmacological potential. The shared presence of several compound classes in both species further indicates overlapping and potentially complementary bioactivities, thereby supporting their ethnomedicinal relevance.

Despite the presence of bioactive metabolites with therapeutic promise, both plants also contain compounds of toxicological concern that warrant careful evaluation. *D. bulbifera* contains benzene and toluene, which are recognized for their neurotoxic and carcinogenic effects at elevated exposure levels (IARC, 2018; ATSDR, 2000; Bennett & Ebisintei, 2024; Bennett & Ebisintei, 2025). Similarly, *X. robustum* contains trichloroacetic-acid–related derivatives such as acetic acid, trichloro-, nonyl ester, and (Z)-4-decen-1-ol, trifluoroacetate, which have been associated with mucosal irritation and potential systemic toxicity (New Jersey Department of Health and Senior Services; Trichloroacetic acid – an overview).

These observations underscore the necessity for appropriate processing techniques, purification strategies, and strict dosage regulation in order to minimize toxicity while maximizing therapeutic efficacy.

4. Conclusions

The combined GC-MS analysis demonstrates substantial phytochemical diversity in *Dioscorea bulbifera* and *Xanthosoma robustum*, underscoring both species as significant reservoirs of bioactive constituents. *D. bulbifera* is predominantly characterized by low-molecular-weight aromatic hydrocarbons and aldehydes, a chemical profile consistent with its reported antimicrobial and antioxidant properties. In contrast, *X. robustum* displays a more complex phytochemical architecture enriched with long-chain alcohols, esters, and nitrogen-containing heterocyclic compounds, suggesting broader pharmacological potential, including enzyme-modulatory, anticancer, and lipophilic bioactivities. The occurrence of shared metabolites, such as 1,3-butadiene-1-carboxylic acid, indicates overlapping therapeutic relevance and provides a biochemical rationale for their concurrent use in ethnomedicinal practices. Collectively, this comparative phytochemical profiling offers robust chemical justification for the traditional applications of these plants while identifying promising molecular leads for future pharmacological exploration.

Notwithstanding their therapeutic potential, the detection of toxic constituents such as benzene, toluene, and trichloroacetic-acid derivatives raises significant safety concerns. These compounds are associated with carcinogenic, neurotoxic, and systemic toxic effects, thereby necessitating caution in their medicinal application. Accordingly, the development of effective processing and detoxification strategies, alongside standardized dosage guidelines, is essential to mitigate health risks while retaining therapeutic efficacy.

In the context of increasing global interest in plant-derived therapeutics, these findings advance current understanding of *D. bulbifera* and *X. robustum* as dual sources of both valuable and potentially hazardous phytochemicals. This provides a scientific foundation for safer utilization, more informed clinical investigations, and the development of evidence-based herbal formulations.

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Conceptualization, V.B.; Methodology, V.B.; Software, V.B and S.U.; Validation, V.B and S.U.; Formal Analysis, V.B; Investigation, V.B and S.U.; Resources, V.B and S.U.; Data Curation, V.B.; Writing—Original Draft, V.B.; Writing—Review & Editing, V.B.; Supervision, V.B and S.U.

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Nomenclature

Term/Abbreviation	Definition
ANOVA	Analysis of Variance
GC-MS	Gas Chromatography-Mass Spectrometry
D. bulbifera	*Dioscorea bulbifera*
X. robustum	*Xanthosoma robustum*

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