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Comparative Leaf Metabolomics Reveals Distinct Chemical Profiles and Putative New Metabolite Records in *Ailanthus integrifolia* subsp. *integrifolia* and *Ailanthus triphysa*

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ABSTRACT

The genus *Ailanthus* (Simaroubaceae) is recognized for its rich phytochemical diversity, yet information on *A. integrifolia* subsp. *integrifolia* and *A. triphysa* remains limited and is largely confined to studies of bark and resin. Here, we address this knowledge gap by providing the first comparative metabolomic and histochemical characterization of these taxa using ultra-performance liquid chromatography–electrospray ionization–quadrupole time-of-flight mass spectrometry (UPLC-ESI-QTOF-MS) and histochemical staining. A total of 240 and 256 metabolites were putatively annotated in *A. integrifolia* subsp. *integrifolia* and *A. triphysa*, respectively, with only 55 compounds shared between species, revealing substantial interspecific chemical divergence. Both taxa were dominated by terpenoid-derived metabolites, including quassinoids, triterpenoids, and steroidal compounds, but differed markedly in secondary metabolite composition. Quassinoids, including nigakilactone H in both, nigakilactone A in *A. triphysa*, and bruceine A in *A. integrifolia* subsp. *integrifolia*, were tentatively detected and represent putative first reports from these taxa. *A. triphysa* exhibited greater diversity of terpenoid subclasses and a phenolic profile dominated by ellagitannins and hydrolyzable tannins, whereas *A. integrifolia* subsp. *integrifolia* was characterized by extensive lignan, coumarin, and flavonoid diversification. Several additional metabolite classes, including specialized alkaloids, polyacetylenes, peptide derivatives, and uncommon phenolic subclasses, may further expand the known chemical diversity of *Ailanthus* and Simaroubaceae. Histochemical analyses localized terpenoids, phenolics, and alkaloids primarily within epidermal and palisade mesophyll tissues, suggesting roles in foliar defense and photoprotection. These findings constitute the first comprehensive leaf metabolomic resource for these *Ailanthus* species and provide a foundation for future chemotaxonomic, ecological, and pharmacological investigations.

INTRODUCTION

The Simaroubaceae family has attracted significant research interest since the 1930s due to its phytochemical diversity. This family is distinguished by quassinoids, specialized metabolites that serve as taxonomic markers due to their exclusive biosynthesis within Simaroubaceae species (Almeida et al., 2007; Alves et al., 2014). Notably, family members also produce alkaloids, triterpenes, steroids, coumarins, anthraquinones, flavonoids, and other bioactive compounds (Barbosa et al., 2011).

The genus *Ailanthus* exhibits particularly high chemical diversity, with approximately 200 documented compounds. Quassinoids, terpenoids, and alkaloids were the major constituents (Kundu and Laskar, 2010). Phytochemical studies have shown that polar solvents, particularly ethanol and methanol, are most effective for extracting secondary metabolites from *Ailanthus* species (Bhatt & Dhyani, 2012; Albouchi et al., 2013).

Despite extensive documentation across the genus, significant knowledge gaps exist for specific species. Phytochemical studies on *A. integrifolia* and *A. triphysa* remain limited, with existing research focused primarily on bark and resin components rather than leaf chemistry. Available data indicate phenols, flavonoids, aldehydes, and hydrocarbons in *A. integrifolia* bark (Kosuge et al., 1994), while *A. triphysa* leaves contain alkaloids, flavonoids, steroids, and terpenoids (Yadav et al., 2019; Ali et al., 2018). To date, no comparative phytochemical analysis of *A. integrifolia* subsp. *integrifolia* and *A. triphysa* from Philippine populations have been documented. Histochemical studies on the members of the genus are also limited.

Given these gaps, leaf tissues represent a critical yet underexplored target for phytochemical investigation, as they are primary sites of secondary metabolite biosynthesis and accumulation (Yuan et al., 2024). The present study provides the first comparative leaf metabolomic characterization of *A. integrifolia* subsp. *integrifolia* and *A. triphysa* from the Philippines using ultra-performance liquid chromatography–electrospray ionization–quadrupole time-of-flight mass spectrometry (UPLC-ESI-QTOF-MS). In addition, selected classes of secondary metabolites were localized within leaf tissues through histochemical analyses. Specifically, this study aimed to: (1) profile and putatively identify leaf metabolites of both species using untargeted UPLC-ESI-QTOF-MS metabolomics; (2) compare their chemical diversity and species-specific metabolomic signatures; and (3) determine the tissue localization of major phytochemical classes, including terpenoids, phenolics, and alkaloids.

By generating the first comprehensive leaf metabolomic dataset for these *Ailanthus* species, this work expands current knowledge of chemical diversity within the genus and provides new insights into the chemotaxonomy of Simaroubaceae for future ecological, pharmacological, and evolutionary investigations.

MATERIALS AND METHODS

Collection of Plant Materials

Leaf samples of *A. integrifolia* subsp. *integrifolia* were collected from Kanluran Road, Los Baños, Laguna, Philippines (14°09'54" N, 121°14'07" E; 80 m a.s.l.), while those of *A. triphysa* were collected from Brgy. Ilijan, Batangas City, Batangas, Philippines (13°37'57" N, 121°04'08"

E; 20 m a.s.l.). Mature, healthy leaves from the 4th–5th nodes of vegetative branches were sampled, and leaflets were randomly selected along the rachis. Species identities were verified by Assistant Prof. Jiro T. Adorador from the University of the Philippines Los Baños Museum of Natural History. Leaf voucher specimens were deposited in the Plant Biology Division Herbarium in College of Arts and Sciences, UPLB with the following deposition numbers: *A. triphysa* (PBDH 7966) and *A. integrifolia* subsp. *integrifolia* (PBDH 7967).

Leaf Methanolic Extraction

Sample Drying

Leaf samples of *A. integrifolia* subsp. *integrifolia* and *A. triphysa* were thoroughly washed with tap water to remove surface contaminants. The samples were then air-dried and placed in properly labeled brown paper bags. Subsequently, the leaves were then oven-dried using a Cassel convection oven at a temperature below 40 °C to prevent degradation of phytochemicals. Sample weights were recorded every four hours until a constant weight was achieved, indicating complete drying. The drying process required approximately 1-2 weeks.

Methanolic Extraction

Dried leaf samples of *A. integrifolia* subsp. *integrifolia* and *A. triphysa* were milled. The milled samples were then soaked in methanol solvent with a 1:10 w/v ratio for 24 hours. The methanol extracts were then filtered using a standard filter paper (diameter: 90 mm) to obtain the filtrate. The extracts were then dried under reduced pressure on a rotary evaporator to remove the solvent. The resulting extracts were stored in amber bottles prior to the phytochemical profiling. The percent extraction yield was determined for each sample using the formula:

$$\text{Extraction Yield (\%)} = \frac{\text{weight of crude extract (g)}}{\text{weight of original sample (g)}} \times 100$$

Leaf Phytochemical Profiling by UPLC-ESI-QTOF-MS

Sample Preparation

Approximately 10 mg of each dried sample was prepared and diluted to 10 mL with LC-MS grade methanol. The samples were filtered using 0.2 µm polytetrafluoroethylene (PTFE) syringe filter into clear LC-MS vials. Methanol solvent was used as a blank for the analysis, while quercetin was used as the standard for system suitability.

Instruments and Data Acquisition

Untargeted metabolite profiling of methanolic leaf extracts was performed using a Waters ACQUITY I-Class UPLC system coupled to a Waters Xevo G2-S QTOF mass spectrometer (Waters Corporation, Milford, MA, USA). Chromatographic separation was achieved on a Waters ACQUITY HSS C18 column (2.1 × 100 mm, 1.8 µm) maintained at 30 °C. The mobile phases consisted of (A) ultrapure water containing 0.1% formic acid and (B) acetonitrile containing 0.1% formic acid. Gradient elution was performed at a flow rate of 0.25 mL min⁻¹ as follows: 15–40% B (0–1.67 min), 40–55% B (1.67–5.00 min), 55–75% B (5.00–6.67 min), 75–80% B (6.67–10.84 min), 80–95% B (10.84–13.34 min), 95–15% B (13.34–15.01 min), and 15–5% B (15.01–18.00 min). The injection volume was 2 µL, and PDA spectra were recorded from 200–500 nm.

The mass spectrometer was calibrated using 0.5 mM sodium formate, with leucine-enkephalin (m/z 556.2771) used as the lock mass. Data were acquired using MassLynx 4.2 in positive electrospray ionization (ESI⁺) and data-independent acquisition (MSE) mode over an m/z range of 50–1500 Da. Instrument settings included a capillary voltage of 3.0 kV, cone voltage of 40 V, source offset of 80 V, source temperature of 120 °C, desolvation temperature of 450 °C, desolvation gas flow of 600 L h⁻¹, cone gas flow of 100 L h⁻¹, and collision energies of 6 eV (low energy) and 30–50 eV (high energy).

UPLC-MS Data Processing

Raw UPLC–MS data were processed using Waters CONNECT (UNIFI) software for peak detection and putative metabolite annotation. Compounds were annotated by matching accurate mass, isotopic pattern, and MS/MS fragmentation spectra against the Waters Screening Library and Traditional Medicine Library. Chemical structures of annotated metabolites were generated using ChemDraw 25.5.0.6237 and MolDraw.

Leaf Histochemical Detection of Selected Secondary Metabolites

Histochemical analyses were conducted to localize selected classes of secondary metabolites within leaf tissues. For each species, three fresh leaf samples were used in the analysis. Thin transverse sections were obtained from the leaflet blades and midribs using a handheld microtome (Euromex MT.5503).

Sections were processed immediately to minimize metabolite diffusion and were subjected to specific histochemical staining procedures corresponding to the targeted phytochemical classes, as described below:

Terpenoids

Terpenes and essential oils were detected by staining the sections with Neutral Red for 20 minutes. After staining, sections were gently rinsed with distilled water. Positive reactions were characterized by the development of red coloration in the stained tissues. The procedure was based on the method reported by Konarska et al. (2021).

Phenols

Phenolic compounds were localized using a 10% ferric chloride solution. Sections were incubated for 30 minutes and subsequently rinsed with distilled water. The presence of phenolic compounds was indicated by the formation of gray to black coloration in the tissues. This staining method followed the protocol described by Mercado et al. (2024).

Alkaloids

Alkaloid localization was performed using Dragendorff's reagent. Sections were stained and subsequently rinsed with distilled water, followed by washing with a 5% sodium nitrite solution for 20 minutes to enhance color development and remove excess reagent. The presence of alkaloids was indicated by the appearance of yellow to reddish-orange coloration within the tissues. The staining protocol followed the methodology described by Hashimoto et al. (1990).

RESULTS

Leaf Methanolic Extraction

The percent yield of the methanolic extract of the leaf samples of the two Philippine-native *Ailanthus* species is shown in Table 1.

The extraction yield of *A. triphysa* was calculated to be 12.95%, based on a crude extract weight of 6.37 g obtained from 49.20 g of the original sample. In comparison, *A. integrifolia* subsp. *integrifolia* exhibited a lower extraction yield of 8.57%, with 2.10 g of crude extract recovered from 24.50 g of plant material. These results indicate that *A. triphysa* produced a higher extraction yield than *A. integrifolia* subsp. *integrifolia* under the same extraction conditions.

Leaf Phytochemical Profiling by UPLC-ESI-QTOF-MS

This study putatively identified and compared the phytochemical profiles of methanolic leaf extracts from *A. integrifolia* subsp. *integrifolia* and *A. triphysa* using UPLC-ESI-QTOF-MS analysis. Identified compounds were classified into eight major chemical classes namely (1) Terpenoids, (2) Phenolics, (3) Flavonoids, (4) Alkaloids, (5) Lipid Compounds, (6) Amino acids and Polypeptides, (7) Organic Acids, and (8) Other Compounds to facilitate comparison of their chemical diversity.

Table 2 presents the 240 putatively identified phytochemical compounds and their tentative assignments for *A. integrifolia* subsp. *integrifolia*, while Table 3 shows the corresponding 256 compounds for *A. triphysa*. Compounds were organized according to major chemical classes and ranked within each class based on their signal intensities. The MS¹ and MS² base peak, total ions, and PDA-UV chromatograms are presented in Figures 1-2.

As observed, *A. triphysa* exhibited a higher diversity with 256 compounds, in comparison with the 240 compounds identified in *A. integrifolia* subsp. *integrifolia*. The observed differences in phytochemical diversity between the two species are consistent with their respective extraction yields. *A. triphysa*, which exhibited a higher extraction yield (12.95%), also showed greater

phytochemical diversity, compared to *A. integrifolia* subsp. *integrifolia*, which yielded 8.57%. This relationship suggests that the increased crude extract recovery from *A. triphysa* reflects a higher abundance of methanol-extractable compounds, which is supported by its broader chemical class representation.

A summary of the phytochemical class diversity between the two Philippine-native *Ailanthus* species is shown in Table 4.

As summarized, terpenoids constituted the most abundant class in both species, with 144 compounds detected in *A. integrifolia* subsp. *integrifolia* and 147 in *A. triphysa*. Of these, 40 terpenoids were shared, while 104 and 107 were unique to *A. integrifolia* subsp. *integrifolia* and *A. triphysa*, respectively.

Phenolic compounds were more diverse in *A. triphysa* (54) compared to *A. integrifolia* subsp. *integrifolia* (37), with only five shared compounds. Similarly, *A. triphysa* exhibited higher diversity in alkaloids (14) and amino acids and polypeptides (6). In contrast, *A. integrifolia* subsp. *integrifolia* contained a higher number of flavonoids (25) and lipid compounds (18) than *A. triphysa* (13 flavonoids, 8 lipid compounds). Notably, no shared alkaloids, organic acids, or amino acids and polypeptides were observed between the two species.

In total, only 55 compounds were shared between the two species, while 185 compounds were unique to *A. integrifolia* subsp. *integrifolia* and 201 were unique to *A. triphysa*. This disparity indicates substantial interspecific chemical divergence. Such distinct phytochemical profiles reflect species-specific biochemical capacities between the two *Ailanthus* species and further support their chemotaxonomic differentiation.

Leaf Histochemical Detection of Selected Secondary Metabolites

To provide additional information on phytochemical presence in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*, histochemical localization of selected major classes of compound, specifically terpenoids, phenols, and alkaloids, was conducted using established histochemical techniques. Table 5 shows the summary of the localization of different compounds in the leaves upon staining with specific detecting reagents.

Terpenoids

Terpenoids were detected as red colorations in neutral red–stained tissues. Both species exhibited similar tissue localization patterns for terpenoids, indicating comparable distribution within the leaf. Very high detection was consistently observed in dermal tissues, particularly in the epidermal cells of both the midrib and leaf blade. This dominance in epidermal layers suggests that terpenoids are strongly associated with surface tissues.

Terpenoids were also detected in ground tissues, with greater accumulation in the palisade mesophyll compared to the spongy mesophyll. In the midrib, terpenoids were dispersed within parenchymatous ground tissues, while vascular tissues showed only limited staining. These observations indicate that terpenoids in *Ailanthus* leaves are primarily associated with epidermal and photosynthetically active tissues rather than being concentrated within vascular elements. Representative micrographs are shown in Figs. 3g – 3i for *A. integrifolia* subsp. *integrifolia* and Figs. 3j – 3l for *A. triphysa*.

Phenols

Phenolic compounds were detected as gray to black precipitates following staining with 10% ferric chloride. Both species exhibited similar tissue localization patterns, but differed in relative abundance. Phenolic compounds were detected in dermal tissues, specifically in the upper and lower epidermal cells of both the midrib and leaf blade. Notably, epidermal staining was more intense in *A. triphysa* than in *A. integrifolia* subsp. *integrifolia*, indicating a higher accumulation of phenolic compounds in surface tissues of the former.

These compounds were also detected in the ground tissues. In leaves, stronger staining was observed in the palisade mesophyll relative to the spongy mesophyll. In the midrib, phenolics were dispersed throughout the parenchymatous region, although fewer localized deposits were observed in *A. integrifolia* subsp. *integrifolia* compared to *A. triphysa*. Phenolic compounds were additionally detected in vascular tissues of both leaves and midribs. Figs. 4a - 4c and 4d -4f shows the localization of the phenolic compounds in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*, respectively.

Alkaloids

Alkaloids were detected as brown to black colorations in Dragendorff-stained tissues. Both *Ailanthus* species exhibited alkaloid presence across all examined tissue types, although staining intensity varied. In dermal tissues, alkaloids were detected in epidermal cells, with consistently stronger staining in the lower epidermis than in the upper epidermis in both species.

In ground tissues, alkaloids were detected in mesophyll cells, occurring in both palisade and spongy mesophyll. In the midrib, alkaloid localization extended into the parenchymatous region beneath the epidermis. They were also observed in association with vascular tissues, though staining intensity in these regions was comparatively lower. The localization of alkaloid compounds are exhibited in Figs. 4g - 4i for *A. integrifolia* subsp. *integrifolia* and Figs. 4j - 4l for *A. triphysa*.

DISCUSSION

Leaf Methanolic Extraction

The differences of the percent yield of the two *Ailanthus* species could be attributed to the variation of the phytochemical composition and plant tissue characteristics. Previous studies have shown that extraction yield is strongly influenced by the abundance of solvent-soluble secondary metabolites such as phenolics, terpenoids, and flavonoids (Azwanida, 2015; Do et al., 2014). *A. triphysa* may have possessed a higher concentration of methanol-extractable compounds, leading to greater crude extract recovery.

Additionally, environmental factors such as plant age and growing conditions are known to affect biosynthesis and accumulation of secondary metabolites (Gobbo-Neto & Lopes, 2007). These ecological variables may also have contributed to the observed differences of methanolic crude extracts.

Terpenoids and Derivatives

UPLC–MS analysis revealed 144 putatively annotated terpenoid-related features in *A. integrifolia* subsp. *integrifolia* and 147 in *A. triphysa*. Both species were dominated by pentacyclic and tetracyclic triterpenoids and quassinoids; however, *A. integrifolia* subsp. *integrifolia* exhibited relatively greater representation of steroidal terpenoids, norisoprenoids, and related steroid-like metabolites, whereas *A. triphysa* displayed a broader subclass distribution that included triterpenoid saponins, withanolide-like steroids, and cardenolide-like metabolites (Figures 5–6). These patterns indicate subtle species-level differentiation in terpenoid composition despite comparable metabolite richness.

Both species shared a conserved core of terpenoid scaffolds, including oleanane-, ursane-, cycloartane-, and tirucallane-type triterpenoids, together with quassinoids such as nigakilactone H. The recurrent detection of these biosynthetically distinct skeletons is consistent with conserved triterpenoid and quassinoid biosynthetic capacities within *Ailanthus* and Simaroubaceae. Many of these compounds, or closely related analogues, have previously been reported primarily from bark, heartwood, fruits, and roots of *A. altissima* and *A. excelsa* (Joshi et al., 2003; Zhao et al., 2005; Alves et al., 2014), suggesting that core *Ailanthus* terpenoid chemistry may also be expressed in foliar tissues.

Several metabolites detected in this study extend previously reported organ-level distributions within the genus. In *A. integrifolia* subsp. *integrifolia*, putative oleanane-, ursane-, tirucallane-, and cycloartane-type triterpenoids, including 3-epi-ursolic acid-related features, correspond to compounds previously reported from fruits or bark of other *Ailanthus* species. Likewise, *A. triphysa* contained putative betulin, betulinic acid, and multiple oleanane-, lupane-, and tirucallane-type metabolites previously reported from fruits, bark, or heartwood of *A. altissima* and *A. excelsa* (Joshi et al., 2003; Zhao et al., 2005). These assignments remain provisional pending structural confirmation but suggest a broader organ-level distribution of common triterpenoid scaffolds than previously recognized. A summary of the major comparative terpenoid features of both species is presented in Table 6.

At the family level, the foliar terpenoid profiles strongly reflect established Simaroubaceae chemotaxonomic characteristics, particularly the occurrence of quassinoids and structurally diverse triterpenoids. The tentative identification of nigakilactone H in both species and nigakilactone A in *A. triphysa* is consistent with reports from stems of *Picrasma quassioides* (reported as *P. ailanthoides*) (Murae et al., 1969, 1971) and *Quassia amara* (Dou et al., 1996). Likewise, bruceine A, annotated in *A. integrifolia* subsp. *integrifolia*, has been reported from dried fruits of *Brucea javanica* (Nakao et al., 2009). These observations suggest that quassinoid-associated metabolic signatures may also occur in foliar tissues of *Ailanthus* and may represent the first putative reports of these compounds in *A. triphysa* and *A. integrifolia* subsp. *integrifolia*.

The tentative annotation of cucurbitacin B in *A. triphysa*, previously reported from petioles of *Simarouba glauca* (Kandaswamy et al., 2024), further supports the occurrence of shared triterpenoid-based chemistry within Simaroubaceae. Similarly, melianol- and melianodiol-related features correspond to tirucallane-type triterpenoids reported from *Simarouba*, *Toona*, and other

Sapindales taxa (Polonsky et al., 1977; Mao et al., 2026). These observations are consistent with current models that place tirucallane-type intermediates at the center of quassinoid and related terpenoid diversification within Simaroubaceae (Chuang et al., 2022).

Across both species, the consistent detection of oleanane-, ursane-, lupane-, and tirucallane-type metabolites agrees with previous phytochemical reports from *Simarouba*, *Castela*, and *Picrasma* (Alves et al., 2014). In addition, limonoid-like mass spectral features observed in both species are consistent with the shared tirucallane ancestry underlying the biosynthetic divergence of limonoids in Rutaceae and Meliaceae and quassinoids in Simaroubaceae (Pham et al., 2025; Mao et al., 2026).

In contrast, lower terpenoids detected in leaf tissues, including monoterpenes, sesquiterpenes, and carotenoid-derived norisoprenoids such as dihydroactinidiolide and ionone derivatives, are broadly distributed across angiosperms (Yuan et al., 2016; Jin et al., 2025). Their occurrence in both species is therefore more likely to reflect conserved volatile and photosynthesis-associated metabolism than chemotaxonomically informative traits at the genus or family level.

Phenolics and Derivatives

A. integrifolia subsp. *integrifolia* yielded 37 putatively annotated phenolic compounds distributed across several subclasses, with lignans and coumarins being the most prominent, accompanied by alkyl phenols, stilbenoids, phenylpropanoids, anthraquinones, and other minor phenolic groups. In contrast, *A. triphysa* exhibited greater phenolic richness, with 54 putative compounds, and a strongly uneven subclass distribution dominated by tannins, particularly ellagitannins and related hydrolyzable tannin derivatives. Additional subclasses included phenylpropanoids, lignans, anthraquinones, xanthones, diarylheptanoids, phthalides, and secoiridoid-related metabolites. These patterns suggest a tannin-enriched phenolic profile in *A. triphysa* and relative enrichment of lignans and coumarins in *A. integrifolia* subsp. *integrifolia* (Figures 7–8).

Despite these differences, both species shared several putative phenolic metabolites, including ginkgolic acid and bakuchiol (alkyl phenols), (–)-lariciresinol and glehlinoside A (lignans), and blestrianol D (stilbenoid). The recurrence of these structurally distinct compounds is consistent with conserved phenylpropanoid- and polyketide-derived metabolic frameworks within the genus, although confirmation of individual identities will require isolation and spectroscopic analysis. A summary of the comparative phenolic features is presented in Table 7.

The phenolic profiles observed here are broadly consistent with previous reports from *Ailanthus*. Earlier studies documented simple phenolic acids, hydroxycinnamate derivatives, and coumarins from bark, twigs, leaves, fruits, and reproductive structures of *A. integrifolia*, *A. altissima*, *A. excelsa*, and *A. triphysa* (Kosuge et al., 1994; Shu-Hua et al., 2003; Jin et al., 2009; Albouchi et al., 2013; Andonova et al., 2024; Cocîrlea et al., 2024; Ray et al., 2025). Accordingly, the detection of phenylpropanoid-related acids, simple phenols, and multiple coumarin derivatives in both species agrees with established genus-level phenolic chemistry.

More recent studies have expanded the known phenolic diversity of *Ailanthus* through the isolation of lignans and neolignans from root bark and samaras of *A. altissima* (Zhang et al., 2020; Shi et al., 2020; Yuan et al., 2025). Within this context, the prominence of lignan-related metabolites in leaves of *A. integrifolia* subsp. *integrifolia*, including kadsurenin E and B, (–)-lariciresinol, secoisolariciresinol, lappaol B, glehlinoside A, erythro-dihydroxydehydrodiconiferyl alcohol, (–)-olivil, japenol, and neoarctin B, represents a notable extension of lignan occurrence to

foliar tissues. While lignans are not unprecedented in *Ailanthus*, their apparent abundance in leaves suggests organ-specific variation in lignan accumulation within the genus.

In contrast, *A. triphysa* was characterized by a strong representation of ellagic acid, ellagic acid derivatives, and hydrolyzable tannin-related features. Although earlier studies emphasized low-molecular-weight phenolic acids and coumarins (Shu-Hua et al., 2003), investigations of *A. altissima* and *A. excelsa* have demonstrated that ellagic acid and HHDP-galloylglucose derivatives are recurrent components of *Ailanthus* phenolic chemistry (Albouchi et al., 2013; Caramello et al., 2021; Andonova et al., 2023; Ray et al., 2025). The putative detection of castalagin, laevigatin A, geraniin, euphormisin M1, pedunculagin, tellimagrandin I, isochebolic acid, neochebolic acid, and HHDP-glucose therefore likely reflects an existing tannin-related metabolic capacity within the genus, although the apparent dominance of ellagitannins has not previously been reported for *A. triphysa*.

At the family level, the observed phenolic profiles align closely with established Simaroubaceae chemistry. Simple phenolic acids, gallates, hydroxycinnamates, and coumarins are widely reported from *Quassia*, *Castela*, *Picrasma*, *Picrolemma*, *Simarouba*, and *Brucea* (Alves et al., 2014). Likewise, hydrolyzable tannin constituents, including gallic acid, methyl gallate, apiosyl gallate, ellagic acid, and HHDP derivatives, are well documented in *Quassia*, supporting the interpretation that the ellagitannin-rich profile of *A. triphysa* falls within the metabolic potential of Simaroubaceae.

The putative detection of lignans, together with xanthone-, diarylheptanoid-, phthalide-, and secoiridoid-related metabolites, suggests interspecific modulation of secondary metabolism within *Ailanthus*. Pending structural confirmation, the latter subclasses may represent potential first reports for the genus or family and may further expand the known phenolic diversity of Simaroubaceae.

The phenolic patterns observed here are also consistent with the close phylogenetic relationship of Simaroubaceae to Rutaceae and Meliaceae (Pirani et al., 2022). Rutaceae are typically characterized by simple phenolic acids, coumarins, and hydrolyzable tannins (Kanes et al., 1993; Abeysinghe et al., 2007; Moshood et al., 2023), whereas Meliaceae frequently exhibit diversification of lignans, galloyl-derived phenolics, coumarins, and stilbenes across multiple organs (Ainazzahra et al., 2025). Consequently, the lignan-enriched profile of *A. integrifolia* subsp. *integrifolia* and the ellagitannin-dominated chemistry of *A. triphysa* can be interpreted as lineage- and organ-specific expressions of phenylpropanoid- and tannin-derived metabolic capacities shared across the Simaroubaceae–Meliaceae–Rutaceae clade rather than departures from established Sapindales phenolic patterns.

Flavonoids and Derivatives

A total of 25 flavonoids and flavonoid-related metabolites were putatively annotated in the leaves of *A. integrifolia* subsp. *integrifolia*, compared with 13 in *A. triphysa*. The flavonoid profile of *A. integrifolia* subsp. *integrifolia* spanned multiple subclasses, including flavones (six compounds), flavone glycosides (five), isoflavonoids (three), flavanones (three), coumestans (two), and isoflavanquinones (two), together with single representatives of flavonols, flavonol glycosides, flavanol glycosides, isoflavone glycosides, and chalcones. This distribution reflects a chemically diverse flavonoid profile comprising both aglycones and conjugated forms, as well as prenylated, methoxylated, and quinone-containing derivatives.

In contrast, the flavonoid profile of *A. triphysa* was comparatively restricted. Of the 13 annotated flavonoids, nine were flavonol glycosides, while the remainder comprised one isoflavone glycoside, one isoflavone, and two flavanones. The predominance of glycosylated flavonols and limited representation of other subclasses indicate a narrower flavonoid profile relative to *A. integrifolia* subsp. *integrifolia*. Comparative flavonoid profiles are summarized in Table 8 and Figures 9–10.

Comparison with previous studies indicates that the flavonoid chemistry of *A. triphysa* largely conforms to established *Ailanthus* chemotypes. Across the genus, leaf flavonoid profiles are typically dominated by flavones, flavonols, and their glycosides, including apigenin, luteolin, kaempferol, quercetin, and astragalin (Loizzo et al., 2007; Jin et al., 2009). Consistent with these reports, most flavonoids detected in *A. triphysa*, including trifolin, kaempferol glucuronides, and rhamnosylated flavonol derivatives, overlap with compounds previously reported from *A. triphysa* and other *Ailanthus* species (Shu-hua et al., 2003; Lee et al., 2013; Liu et al., 2025). Minor differences, such as additional glucuronidated derivatives, may represent putative new records pending structural confirmation.

In contrast, the flavonoid profile of *A. integrifolia* subsp. *integrifolia* showed limited correspondence with previous reports. Existing phytochemical studies of this species have focused primarily on bark tissues and documented flavanone glycosides such as naringin and neoeriocitrin (Kosuge et al., 1994). The present analysis revealed a substantially broader array of putative flavonoids, including flavones and flavone glycosides, coumestans (coumestrol and corylidin), isoflavonoids (ophiopogonone derivatives), isoflavanquinones (abruquinones A and D), chalcones (psorachalcone A), and prenylated flavanones (kushenol B and X). To the best of current knowledge, these metabolites have not previously been reported from *A. integrifolia* and therefore represent putative new species records. Moreover, because earlier studies were restricted to bark tissues, this study constitutes the first characterization of leaf flavonoid chemistry in the species.

At the family level, the flavonoid profiles observed here reveal both conserved and divergent features within Simaroubaceae. Flavonol glycosides appear to be widespread, as demonstrated by vitexin in *Q. amara* leaves (Fabre et al., 2012) and kaempferol derivatives in *Simarouba versicolor* (Arriaga et al., 2002), supporting the view that flavonol glycosylation is a conserved metabolic trait. In contrast, the broader subclass diversity observed in *A. integrifolia* subsp. *integrifolia*, particularly the occurrence of isoflavonoids, isoflavanquinones, coumestans, and chalcones, appears atypical based on currently available Simaroubaceae data. Reports from other genera, including *Eurycoma longifolia* and *B. javanica*, generally describe more restricted flavonoid profiles dominated by flavone glycosides and related phenolics (Ruan et al., 2019; Norazhar et al., 2025).

Comparison with other Sapindales families provides additional context. Rutaceae are characterized primarily by flavanones and their glycosides (Alam et al., 2022), although overlap occurs through shared flavone and flavonol subclasses (Alves et al., 2014). The occurrence of chalcones and prenylated flavonoids in Rutaceae (Kiplimo et al., 2011; Eom et al., 2016) parallels the detection of psorachalcone A and prenylated flavanones in *A. integrifolia* subsp. *integrifolia*. Meliaceae show even closer correspondence, with reports of flavonols, flavone glycosides, catechins, and diverse prenylated and methoxylated flavonoids across several genera (Pereira et al., 2012; Jaafar et al., 2016; Ainazzahra et al., 2025). The detection of prenylated flavanones, isoflavonoids, and quinone-containing flavonoids in *A. integrifolia* subsp. *integrifolia* is therefore consistent with broader patterns of flavonoid diversification within Sapindales.

Overall, *A. triphysa* conforms to a conserved flavonol glycoside-dominated flavonoid chemotype characteristic of *Ailanthus* and broadly reflected across Simaroubaceae. In contrast, *A. integrifolia* subsp. *integrifolia* exhibits a more diverse flavonoid profile characterized by expanded subclass representation and the occurrence of isoflavonoids, isoflavanquinones, coumestans, chalcones, and prenylated flavanones, highlighting substantial species-level variation in flavonoid metabolism within the genus.

Alkaloids and Derivatives

Methanolic leaf extracts of *A. integrifolia* subsp. *integrifolia* yielded nine tentatively annotated alkaloids representing diverse structural classes, including indole alkaloids (1-carboethoxy- β -carboline, corynoxine, penniclavine), steroidal alkaloids (hupehenine, pingbeinine), a steroidal alkaloid glycoside (hupehemonoside), a quinolizidine alkaloid (dictysine), a triterpene alkaloid (cimicifugadine), and a phenethylamine alkaloid (ephedradine A).

In contrast, *A. triphysa* exhibited a broader alkaloid profile comprising 14 putatively annotated compounds, including indole/ β -carboline derivatives (β -carboline-1-propionic acid, 1-vinyl-4-methoxy- β -carboline, 4,9-dimethoxy-1-vinyl- β -carboline, and 1-formyl-4-methoxy- β -carboline), a tropane alkaloid (2 α ,3 β -dihydroxy nortropane), pyridine alkaloids (arecoline, gentiatibetine, guvacoline), a steroidal alkaloid glycoside (zhebeinoside), a benzyloquinoline alkaloid (narceine), a steroidal alkaloid (pingbeidinose), a phenethylamine alkaloid (ephedradine B), a glycosylated alkaloid (aristolactam Ia N- β -D-glucopyranoside), and a quinoline alkaloid (6-hydroxykynurenic acid). Representative alkaloid structures are shown in Figures 11–12, while comparative profiles are summarized in Table 9.

Both species contained indole/ β -carboline-type alkaloids, consistent with the established prominence of this class in *Ailanthus*. However, *A. triphysa* exhibited greater apparent subclass diversity, including pyridine-, tropane-, quinoline-, benzyloquinoline-, and phenethylamine-type alkaloids, whereas *A. integrifolia* subsp. *integrifolia* contained fewer annotated alkaloids but retained considerable structural diversity.

Several alkaloids detected in *A. triphysa* correspond to compounds previously reported from other *Ailanthus* species. β -Carboline-1-propionic acid has been isolated from the root bark of *A. altissima* and the wood of *A. triphysa* (reported as *A. malabarica*) (Ohmoto & Koike, 1984; Aono et al., 1994), whereas 1-vinyl-4-methoxy- β -carboline (dehydrocrenatine) has been reported from leaves of *A. altissima* and extracts of *Q. amara* (Joshi et al., 1977; Souleles & Waigh, 1984; Tada et al., 2009). Although structurally related β -carboline derivatives have previously been reported from bark and roots of *A. triphysa* (Joshi et al., 1977), the detection of these compounds in leaves extends their known organ-level distribution and may represent new plant-part records within the genus.

For *A. integrifolia* subsp. *integrifolia*, the tentative identification of 1-carboethoxy- β -carboline is noteworthy because structurally related β -carboline derivatives, such as 1-methoxycarbonyl- β -carboline, have previously been isolated from *A. altissima* leaves (Souleles & Kokkalou, 1989). To date, no alkaloids have been reported from *A. integrifolia* subsp. *integrifolia*; consequently, all alkaloids detected here may represent putative first records for the taxon pending structural confirmation.

These observations are consistent with extensive phytochemical studies demonstrating that β -carboline and canthin-6-one alkaloids are the principal nitrogenous secondary metabolites of

Ailanthus. Such compounds have been reported from *A. altissima*, *A. excelsa*, and *A. triphysa*, particularly in root bark, stem bark, and wood tissues (Joshi et al., 1977; Ohmoto et al., 1976–1981; Cordell et al., 1978; Varga et al., 1980; Souleles & Waigh, 1984; Aono et al., 1994; Kim et al., 2016; Zhao et al., 2017; Caramello et al., 2021; Shao et al., 2023). Notably, canthin-6-one alkaloids were not detected in either Philippine-native species. This absence may reflect tissue-specific biosynthesis, developmental stage, ecological influences, or extraction-related factors because previous studies have largely focused on bark and wood tissues.

At the family level, β -carboline and canthin-6-one alkaloids are widely distributed across Simaroubaceae, including *Brucea*, *Picrasma*, *Picrolemma*, *Simaba*, *Simarouba*, and *Eurycoma* (Alves et al., 2014; Vikas et al., 2017). β -Carboline-1-propionic acid and related β -carbolines have been reported from *B. antidysenterica*, *Q. amara*, *E. harmandiana*, *E. longifolia*, and *P. quassioides* (Kanchanapoom et al., 2001; Kuo et al., 2003; Tada et al., 2009; Lee et al., 2009; Taniguchi et al., 2012; Makong et al., 2019; Kwon et al., 2018), reinforcing their chemotaxonomic significance within the family.

Against this background, several alkaloids tentatively annotated in the present study appear atypical for both *Ailanthus* and Simaroubaceae. These include phenethylamine alkaloids (ephedradine A/B), the quinolizidine alkaloid dictysine, steroidal alkaloids and glycosides (hupehenine, pingbeinine, hupehemonoside, zhebeininoside), the benzylisoquinoline alkaloid narceine, the tropane alkaloid $2\alpha,3\beta$ -dihydroxy nortropane, and pyridine alkaloids such as arecoline, guvacoline, and gentiatibetine. Likewise, the tentative detection of the quinoline alkaloid 6-hydroxykynurenic acid in *A. triphysa* is noteworthy because quinoline alkaloids are characteristic markers of Rutaceae (Soares, 2007), a family closely related to Simaroubaceae within Sapindales (APG IV, 2016). While these annotations may reflect previously unrecognized biosynthetic capacity, they do not conform to the established phytochemical profile of Simaroubaceae and therefore require validation through targeted isolation and structural elucidation.

Lipid Compounds

Untargeted UPLC–MS analysis revealed a chemically richer lipid profile in *A. integrifolia* subsp. *integrifolia* than in *A. triphysa*. The former was characterized by diverse polyacetylenes, sterol esters, phospholipids, fatty acids, and fatty acid esters, whereas *A. triphysa* contained fewer lipid classes, consisting mainly of sterol esters, fatty acids, limited polyacetylenes, and the long-chain alkane octacosane (Figure 13). Despite these differences, both species shared panaxynol, faltarindiol, cholesteryl palmitate, and vernolic acid, suggesting conserved lipid metabolic pathways alongside species-specific variation (Table 10).

Polyacetylenes are associated with antimicrobial, antifeedant, and allelopathic activities (Minto, 2008), whereas long-chain alkanes are major constituents of cuticular waxes involved in protection against water loss and environmental stresses (Shepherd & Wynne Griffiths, 2006; Xue et al., 2017). The prominence of octacosane in *A. triphysa* may also be associated with species-specific epidermal characteristics, although this relationship requires further anatomical investigation.

Previous studies of *A. triphysa* have reported fatty acids, aldehydes, and fatty acid esters from vegetative tissues (Shu-Hua et al., 2003; Thongnest et al., 2017; Yadav et al., 2019), many of which were not detected here. These differences likely reflect methodological biases, as GC–MS with ethyl acetate preferentially detects volatile and semi-polar metabolites, whereas LC–MS

with methanol is better suited for polar lipids such as phospholipids and sterol esters (Dai & Mumper, 2010; Niessen, 2006; Saini et al., 2021). Environmental factors, including salinity, drought, temperature, and irradiance, may have also contributed to the observed lipid variation between the coastal habitat of *A. triphysa* and the inland habitat of *A. integrifolia* subsp. *integrifolia*, although this requires experimental validation (Shepherd & Wynne Griffiths, 2006; Xue et al., 2017; Yao et al., 2021).

Within *Ailanthus*, lipid studies have focused primarily on seed oils, with *A. altissima* reported to contain fatty acids, phytosterols, tocopherols, and phospholipids, including phosphatidylethanolamine (Andonova et al., 2024). The present findings extend the occurrence of sterol esters and phosphatidylethanolamines to leaf tissues and suggest that polyacetylenes and fatty acid esters may represent previously undocumented foliar metabolites pending targeted confirmation. Similar lipid classes have been reported from seeds of *S. glauca*, *Q. amara*, and *B. javanica* (Amerine, 1974; Patil & Murthy, 2020; Zhang et al., 2018), but the present study highlights the comparatively limited knowledge of foliar lipid chemistry in *Ailanthus*, Simaroubaceae, and Sapindales more broadly (Adeyeye & Adesina, 2015; Nadeem et al., 2016; Romsdahl et al., 2022).

Organic Acids

The present UPLC–MS analysis tentatively annotated pantothenic acid (vitamin B5) as the only detectable organic acid in *A. integrifolia* subsp. *integrifolia*, whereas anthranilic acid (2-aminobenzoic acid) and nicotinic acid were detected in *A. triphysa* (Figure 14; Table 11).

Pantothenic acid is a ubiquitous primary metabolite synthesized by plants and serves as the precursor of coenzyme A, which is essential for central metabolic processes including fatty acid metabolism and the tricarboxylic acid cycle (Coxon et al., 2005; Leonardi & Jackowski, 2007; Czumaj et al., 2020). Consequently, its apparent detection only in *A. integrifolia* subsp. *integrifolia* should not be interpreted as evidence of biological absence in *A. triphysa*. Small organic acids often exhibit poor retention on reversed-phase chromatographic systems and variable ionization efficiencies, making their detection highly dependent on extraction procedures and chromatographic conditions (Haselberg et al., 2019). Improved recovery of low-molecular-weight organic acids has been demonstrated using targeted extraction and specialized chromatographic approaches (Huang et al., 2014), suggesting that additional organic acids may have been present but remained below detection limits in the present workflow.

The detection of anthranilic acid in *A. triphysa* is biochemically plausible because it functions as a precursor in quinoline alkaloid biosynthesis (Grundon, 1988). Although this observation does not confirm pathway activity, the co-occurrence of anthranilic acid and a putatively annotated quinoline alkaloid in the same species is consistent with its endogenous occurrence. Likewise, the tentative annotation of nicotinic acid is supported by reports from the related simaroubaceous species *Odyndea klaineana* (reported as *Hannoa undulata*), from which nicotinic acid was recovered using methanolic extraction (Uraku et al., 2022).

Reports from other Sapindales taxa, particularly Rutaceae, have documented a wide range of organic acids, including citric, malic, oxalic, and succinic acids, when appropriate analytical methods are employed (Violeta et al., 2010). These observations further suggest that the limited organic acid profiles detected here likely reflect methodological constraints associated with untargeted UPLC–MS analysis rather than true biochemical absence. Nevertheless, all annotations remain tentative and require confirmation through targeted analyses and structural validation.

Amino Acids and Polypeptides

The UPLC–MS analysis revealed differences in amino acid- and peptide-related metabolites between the two *Ailanthus* species (Figure 15; Table 12). *A. integrifolia* subsp. *integrifolia* yielded a single putatively annotated amino acid derivative, morusimic acid E, whereas *A. triphysa* contained four amino acids (valine, proline, glutamine, and tyrosine) and two peptide-like metabolites, heterophyllin A and an *N*-benzoyl-phenylalanine derivative, indicating greater diversity of these metabolites in *A. triphysa*.

The occurrence of valine, proline, and tyrosine in *A. triphysa* is consistent with previous reports from *A. altissima* and *A. excelsa*, suggesting that these amino acids are common constituents of the genus (Kim et al., 1977; Nag & Matai, 1994; Lee, 2008; Khokhani et al., 2012). By contrast, glutamine has not previously been reported in *Ailanthus* and may represent a putative new genus record. Likewise, the tentative annotation of morusimic acid E in *A. integrifolia* subsp. *integrifolia*, previously reported only from *Morus alba* fruits (Kusano et al., 2002), represents a putative new record for both *Ailanthus* and Simaroubaceae.

Information on amino acid and peptide chemistry remains limited within Simaroubaceae. The detection of valine and tyrosine agrees with reports from *S. glauca* (Govindaraju et al., 2009), whereas the peptide-like metabolites heterophyllin A and the *N*-benzoyl-phenylalanine derivative have not previously been documented in the family. Although these compounds have been reported from unrelated angiosperms (Jakupovic et al., 1987; Talapatra et al., 1983; Yang et al., 2003; Wu et al., 2004; Nwodo et al., 2014; Hua, 2016), their occurrence in *Ailanthus* requires confirmation through targeted isolation and structural elucidation.

Other Compounds

Several metabolites outside the major phytochemical classes were tentatively annotated. *A. integrifolia* subsp. *integrifolia* exhibited a relatively simple profile comprising pyrophaeophorbide A, phenanthrene, adenosine, senkyunone, and anemonin (Figure 16), whereas *A. triphysa* displayed greater diversity with the additional detection of L-noradrenaline, heterodendrin, indolylmethyl glucosinolate, methyl- β -D-fructopyranoside, 2-(*p*-anisyl)-5-methyl-1-hexene, and senkyunolide (Figure 17; Table 13).

The detection of phenanthrene is consistent with previous reports from *A. altissima* var. *altissima* (reported as *A. glandulosa*) (Ernst, 1974). Although phenanthrenes are widespread among angiosperms (Toth et al., 2017), they remain poorly documented in Simaroubaceae and may represent an underreported component of *Ailanthus* chemistry. Similarly, the occurrence of phthalides (senkyunone and senkyunolide) extends observations beyond their better-known distribution in *Apium graveolens*, *Angelica sinensis*, *Ligusticum chuanxiong*, and *Cajanus cajan* (Li et al., 2025; Yao et al., 2025; Gao et al., 2025). The tentative detection of anemonin is likewise chemically plausible, as butenolides have been reported from related Sapindales families, including Rutaceae and Meliaceae, as well as Simaroubaceae-associated lineages (Fo et al., 1996; Duran-Pena et al., 2023).

Several metabolites detected exclusively in *A. triphysa* should be interpreted cautiously because they are not characteristic of *Ailanthus* or Simaroubaceae. L-noradrenaline has been reported from diverse plant families, including Rutaceae (Odjakova & Hadjiivanova, 1997; Tang

et al., 2023), heterodendrin from Fabaceae and Sapindaceae (Yulvianti & Zidorn, 2021), and indolylmethyl glucosinolate primarily from Brassicaceae (Umoh, 2020; Bischoff, 2021). Likewise, methyl- β -D-fructopyranoside and 2-(*p*-anisyl)-5-methyl-1-hexene have been reported from unrelated angiosperms (Li et al., 2004; Qing-bo et al., 2011; Alrasheid et al., 2018; Wang et al., 2017) but not from *Ailanthus*. These results suggest greater miscellaneous metabolite diversity in *A. triphysa*; however, because several annotations fall outside the established phytochemical profile of *Ailanthus* and Simaroubaceae, targeted isolation, MS/MS comparison with authentic standards, and structural elucidation are required to confirm their occurrence and assess their chemotaxonomic significance.

Metabolic Patterns in A. integrifolia subsp. integrifolia and A. triphysa

The occurrence of shared metabolites between the two *Ailanthus* species supports the presence of conserved metabolic traits within the genus, whereas the broader metabolite spectrum of *A. triphysa* suggests species-specific chemical diversification. Several detected compounds also exhibit affinities with metabolites reported from other Sapindales families, indicating potential chemotaxonomic significance at the order level.

Differences between the UPLC–MS-derived phytochemical profiles obtained here and those reported previously may reflect phytogeographic, biological, and methodological factors. Secondary metabolite composition is strongly influenced by geographic origin and local environmental conditions, resulting in substantial chemical variability (Omwango et al., 2024; Imran et al., 2024). Likewise, differences in solvent polarity and extraction protocols can bias the classes of compounds recovered (Chatepa et al., 2024), whereas the greater sensitivity of UPLC–MS enables detection of low-abundance and highly polar metabolites that may have been overlooked using earlier analytical approaches (Custodio-Mendoza et al., 2024).

The higher chemical diversity observed in *A. triphysa*, despite the apparent absence of foliar oil glands found in *A. integrifolia* subsp. *integrifolia*, suggests that adaptation and defense may be achieved through alternative metabolic strategies independent of specialized secretory structures. Secondary metabolites play critical roles in plant responses to biotic and abiotic stresses by functioning as antioxidants, antimicrobial agents, herbivore deterrents, osmoprotectants, and signaling molecules (Akula & Ravishankar, 2011; Isah, 2019; Divekar et al., 2022; Kumar et al., 2023). Their biosynthesis is frequently induced by environmental stressors, including salinity, drought, high irradiance, pathogen attack, and herbivory (Akula & Ravishankar, 2011; Yeshi et al., 2022).

The *A. triphysa* individuals examined in this study were collected from a coastal environment characterized by exposure to salt spray, strong solar radiation, wind exposure, periodic water limitation, and pathogen pressure. Such conditions are known to promote the production and diversification of phenolics, flavonoids, terpenoids, alkaloids, and other specialized metabolites that contribute to stress tolerance and defense (Yeshe et al., 2022; Kumar et al., 2023). Numerous studies have demonstrated that environmental stress can increase both the concentration and diversity of secondary metabolites as part of an adaptive response (Akula & Ravishankar, 2011; Isah, 2019). The elevated metabolite diversity detected in *A. triphysa* is therefore consistent with the hypothesis that specialized metabolism contributes to adaptation under environmentally challenging conditions (Divekar et al., 2022; Isah, 2019; Akula & Ravishankar, 2011; Yeshe et al., 2022).

The simultaneous occurrence of elevated metabolite diversity and domatia in *A. triphysa* further suggests the integration of direct and indirect defense mechanisms. Secondary metabolites provide direct protection against herbivores, pathogens, and abiotic stressors, whereas domatia may facilitate associations with beneficial mites that suppress herbivores and fungal pathogens (Romero & Benson, 2005; Pireda et al., 2017). The coexistence of these traits suggests a coordinated defense strategy in which chemical defenses and mutualistic interactions operate complementarily to enhance plant fitness. In contrast, the foliar oil glands of *A. integrifolia* subsp. *integrifolia* may represent an alternative defense strategy involving localized production, storage, or secretion of specialized metabolites.

Overall, the compounds detected in the present study but absent from previous reports may reflect genuine chemical variation arising from species-specific biology, environmental conditions, and improved analytical coverage. Although the present annotations remain putative, several metabolites may represent previously unreported records for these species and warrant confirmation through targeted isolation and structural characterization.

Leaf Histochemical Detection of Selected Secondary Metabolites

Histochemical investigations in *Ailanthus* remain scarce and have largely focused on resin localization in the bark of *A. excelsa* (Shah et al., 1986). In the present study, histochemical analyses revealed a broadly conserved tissue-level distribution of terpenoids, phenolics, and alkaloids in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. In both species, these metabolites were concentrated primarily in dermal and ground tissues, particularly epidermal cells and palisade mesophyll, with comparatively limited localization in vascular tissues.

The predominance of terpenoids in epidermal and mesophyll tissues is consistent with reports from other Simaroubaceae, where lipid-reactive stains have revealed terpenoid-rich deposits in parenchymatous tissues, oleoresin-containing idioblasts, cortical regions, and mesophyll cells (Shah et al., 1986; Saraiva et al., 2003; Macedo et al., 2005; Campagna et al., 2012; Tolke et al., 2022). Likewise, phenolic compounds were widely distributed across dermal, ground, and vascular tissues but exhibited stronger localization in epidermal and palisade mesophyll cells. Similar distributions of tannins and flavonoids have been documented in *Simarouba glauca*, *Picramnia sprucei*, and *Castela tweedii* (Saraiva et al., 2003; Campagna et al., 2012; Sundharamoorthy et al., 2025). Alkaloids were also broadly distributed throughout epidermal, mesophyll, and vascular-associated tissues, corresponding to patterns reported in *S. glauca* (Sundharamoorthy et al., 2025).

Comparable localization patterns occur in related Sapindales families. In *Zanthoxylum* species (Rutaceae), terpenoids and essential oils occur in secretory cavities, epidermal cells, and parenchymatous tissues, whereas phenolic compounds are concentrated in epidermal and vascular-associated regions (Andrade et al., 2020; Fladzinski et al., 2024). Similarly, in *Azadirachta indica* (Meliaceae), terpenoids are localized in mesophyll tissues and tannins in epidermal and midrib regions (Rodrigues et al., 2020). These observations suggest that tissue-level localization of secondary metabolites is broadly conserved among chemically related Sapindales taxa.

The concentration of terpenoids, phenolics, and alkaloids in epidermal tissues is consistent with Optimal Defense Theory, which predicts preferential allocation of defensive compounds to tissues exposed to the greatest risk of herbivory or pathogen attack (McKey, 1974; Rhoades & Cates, 1976; Zangerl & Bazzaz, 1992). Epidermal cells constitute the first physical and biochemical barrier encountered by herbivores and pathogens, while phenolic compounds

accumulated in these tissues additionally contribute to UV protection, oxidative stress mitigation, and antimicrobial defense (Agati et al., 2012). The localization of metabolites within palisade mesophyll is also consistent with known biosynthetic pathways, particularly the plastid-localized MEP pathway responsible for terpenoid biosynthesis (Cheng et al., 2025). Because palisade cells are rich in chloroplasts, they provide an important cellular environment for metabolite production as well as defense.

Alkaloid accumulation in epidermal and ground tissues further reflects established compartmentalization mechanisms in which potentially toxic metabolites are stored away from sensitive metabolic processes while remaining available for defense (Wink & Roberts, 1998; Facchini, 2001). Conversely, the comparatively limited concentration of secondary metabolites in vascular tissues may reflect functional constraints associated with transport and structural support, a pattern similarly observed in other woody taxa (Franceschi et al., 2005).

Overall, the histochemical profiles of *A. integrifolia* subsp. *integrifolia* and *A. triphysa* reveal a shared anatomical framework for secondary metabolite accumulation that closely parallels patterns reported throughout Simaroubaceae. These observations are strongly supported by the UPLC–ESI–QTOF–MS results, which identified terpenoids, phenolics, and alkaloids as the dominant metabolite classes in both species. Notably, the stronger phenolic staining observed in *A. triphysa* corresponds with its higher phenolic diversity relative to *A. integrifolia* subsp. *integrifolia*.

CONCLUSION

This study provides the first integrated metabolomic and histochemical characterization of leaf secondary metabolites in the two *Ailanthus* species *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. Untargeted UPLC–ESI–QTOF–MS analysis revealed substantial chemical diversity in both taxa, with terpenoids representing the dominant metabolite class, followed by phenolics, flavonoids, alkaloids, and lipid-related compounds. Although both species shared a conserved chemical framework consistent with established Simaroubaceae phytochemistry, they exhibited pronounced interspecific differences in metabolite composition, with *A. triphysa* showing greater overall metabolite richness and broader subclass diversity, while *A. integrifolia* subsp. *integrifolia* was relatively enriched in lignans, coumarins, steroidal terpenoids, and structurally diverse flavonoids. Histochemical analyses demonstrated that terpenoids, phenolics, and alkaloids are predominantly localized in epidermal and palisade mesophyll tissues, with stronger phenolic staining in *A. triphysa*, corresponding to its higher phenolic diversity. Collectively, the metabolomic and histochemical evidence indicate that, despite retaining core chemical traits characteristic of Simaroubaceae, the two species exhibit distinct patterns of secondary metabolites and tissue-level allocation. These findings establish the first chemical and anatomical framework for leaf secondary metabolism in the two *Ailanthus* species and provide a foundation for future chemotaxonomic, ecological, and pharmacological studies, pending targeted compound isolation, structural confirmation, and expanded population-level sampling.

DECLARATIONS

Abbreviations

UPLC-ESI-QTOF-MS - Ultra-Performance Liquid Chromatography–Electrospray Ionization–Quadrupole Time-of-Flight Mass Spectrometry

MEP Pathway – Methylerythritol Phosphate Pathway

APG – Angiosperm Phylogeny Group

Ethics approval and consent to participate

Collection of *A. triphysa* in Brgy. Ilijan, Batangas City, Batangas, was conducted with permission from the landowner, Mr. Porfirio T. Silang. *A. integrifolia* subsp. *integrifolia* was collected along Kanluran Road, within UPLB campus but outside the Mt. Makiling Forest Reserve (as verified by the Makiling Center for Mountain Ecosystems), with research collection permitted.

Consent for publication

Not applicable

Availability of data and materials

All data generated or analysed during this study are included in this published article and its supplementary information files.

Competing interests

The authors declare that they have no competing interests.

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Authors' contributions

J.D.L.V. conceived the study, conducted the experiments with assistance from E.C.V., performed the data analysis and interpretation, and wrote the original manuscript draft. R.C.N. supervised the chemical analyses, contributed to the interpretation of metabolomic data, as well as critically reviewed the manuscript. E.C.V. and N.S.B. contributed to the study design and provided substantial revisions. All authors reviewed and approved the manuscript.

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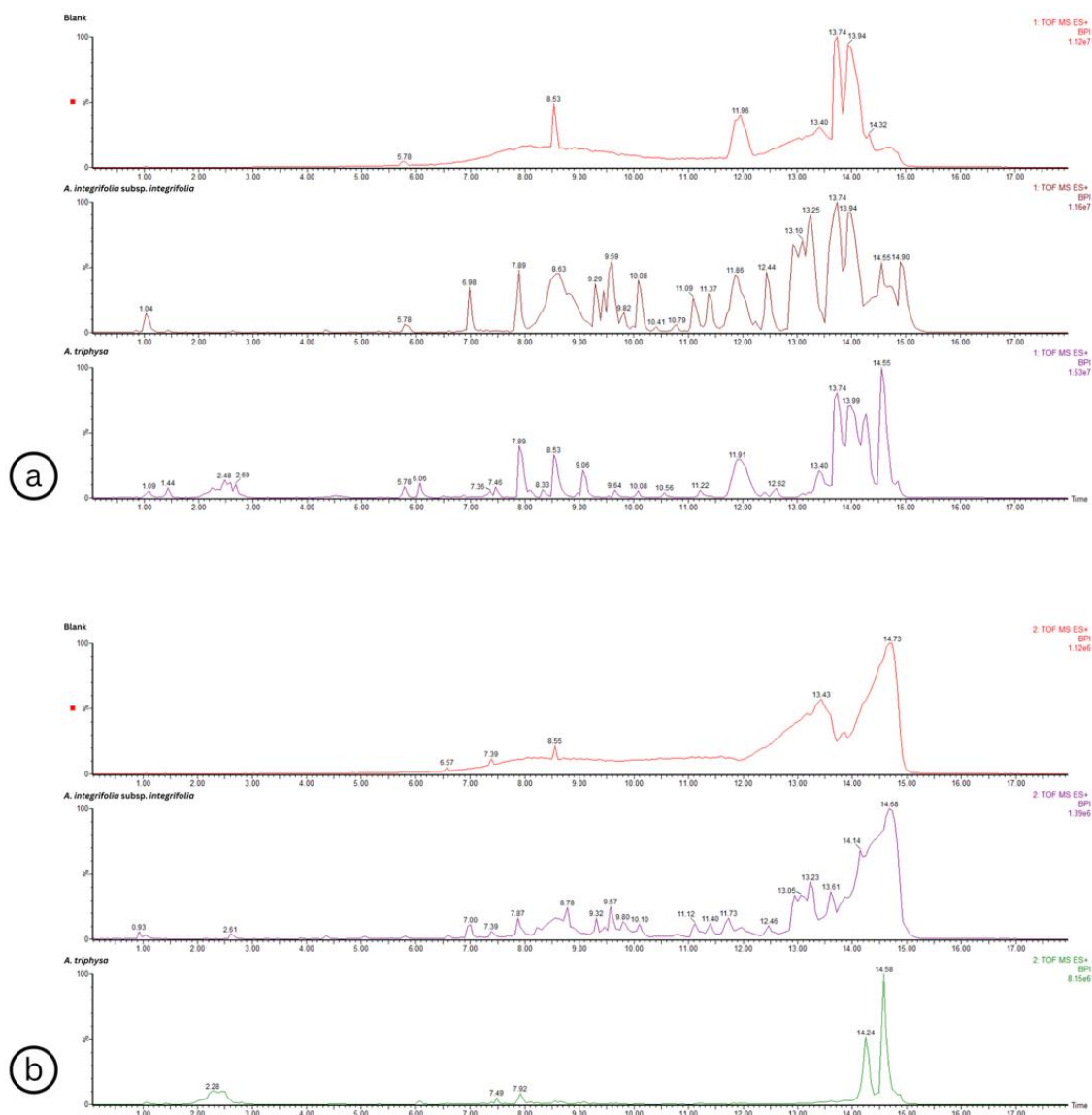


Figure 1. MS1 (A) and MS2 (B) base peak chromatograms of the two *Ailanthus* species and the blank used in the UPLC–ESI–QTOF–MS analyses.

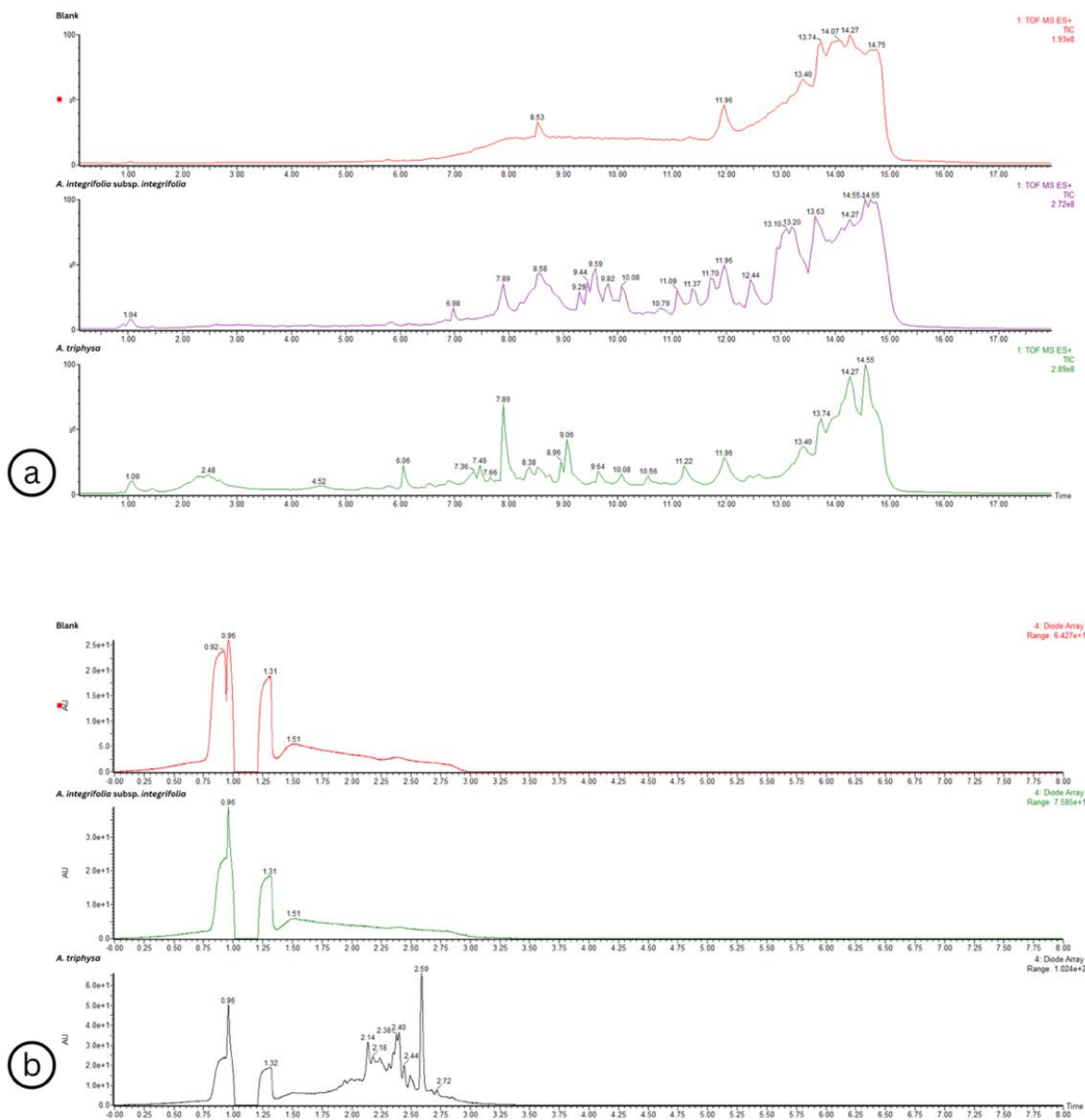


Figure 2. Total ion (A) and photodiode array/ultraviolet (PDA/UV) (B) chromatograms of the two *Ailanthus* species and the blank used in the UPLC–ESI–QTOF–MS analyses

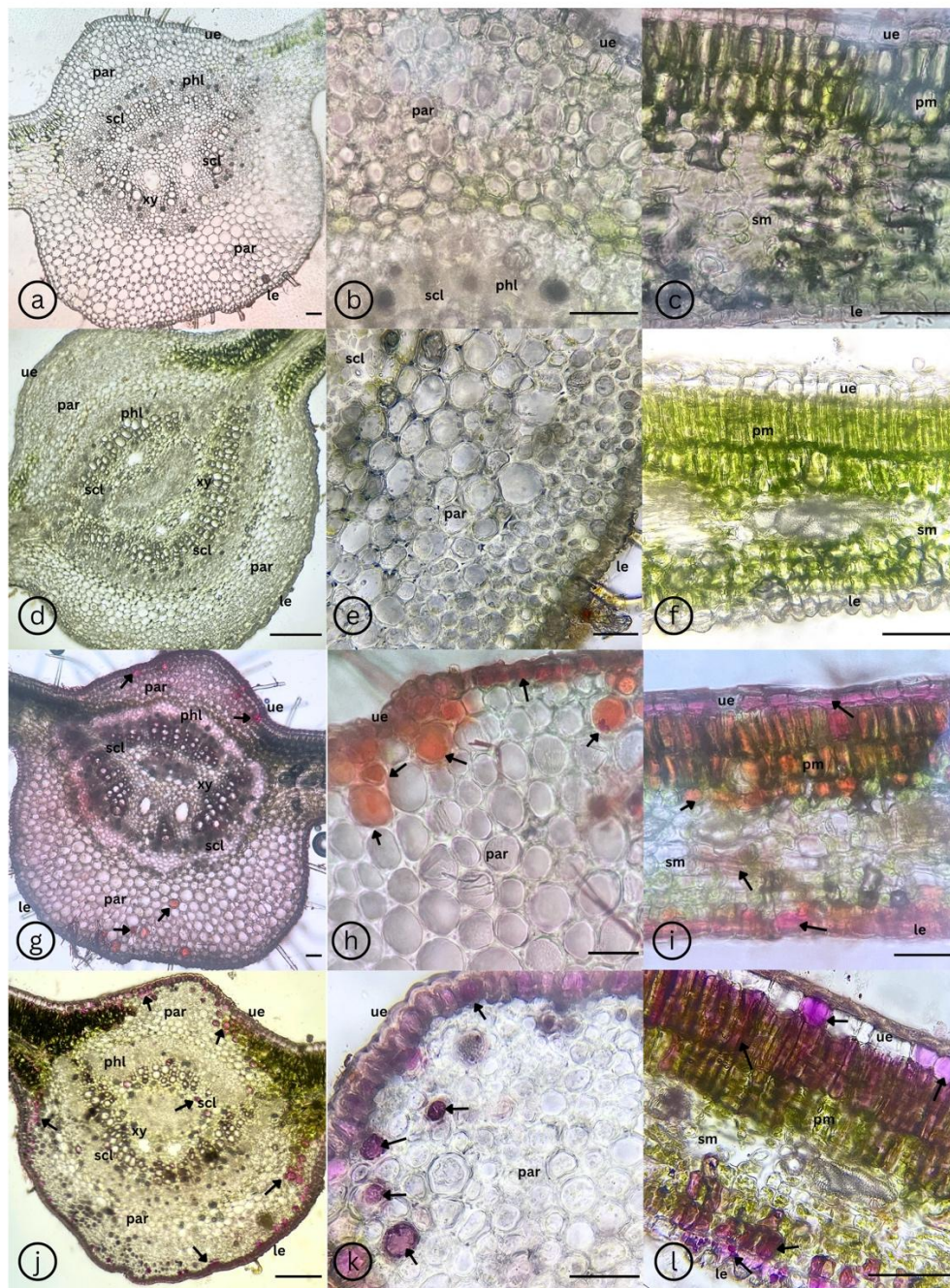


Figure 3. Histochemical localization of terpenoids in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. (A)–(F) Unstained control sections (A)–(C), *A. integrifolia* subsp. *integrifolia*; (D)–(F), *A. triphysa*. (G)–(L) Neutral red-stained sections showing terpenoids as red-stained cells (arrows) (G)–(I), *A. integrifolia* subsp. *integrifolia*; (J)–(L), *A. triphysa*. Midrib (A), (D), (G), (J); midrib detail (B), (E), (H), (K); and leaf blade (C), (F), (I), (L) sections. Abbreviations: ue, upper epidermis; pm, palisade mesophyll; sm, spongy mesophyll; scl, sclereid; le, lower epidermis; par, parenchyma; phl, phloem; xy, xylem. Scale bar = 0.05 mm

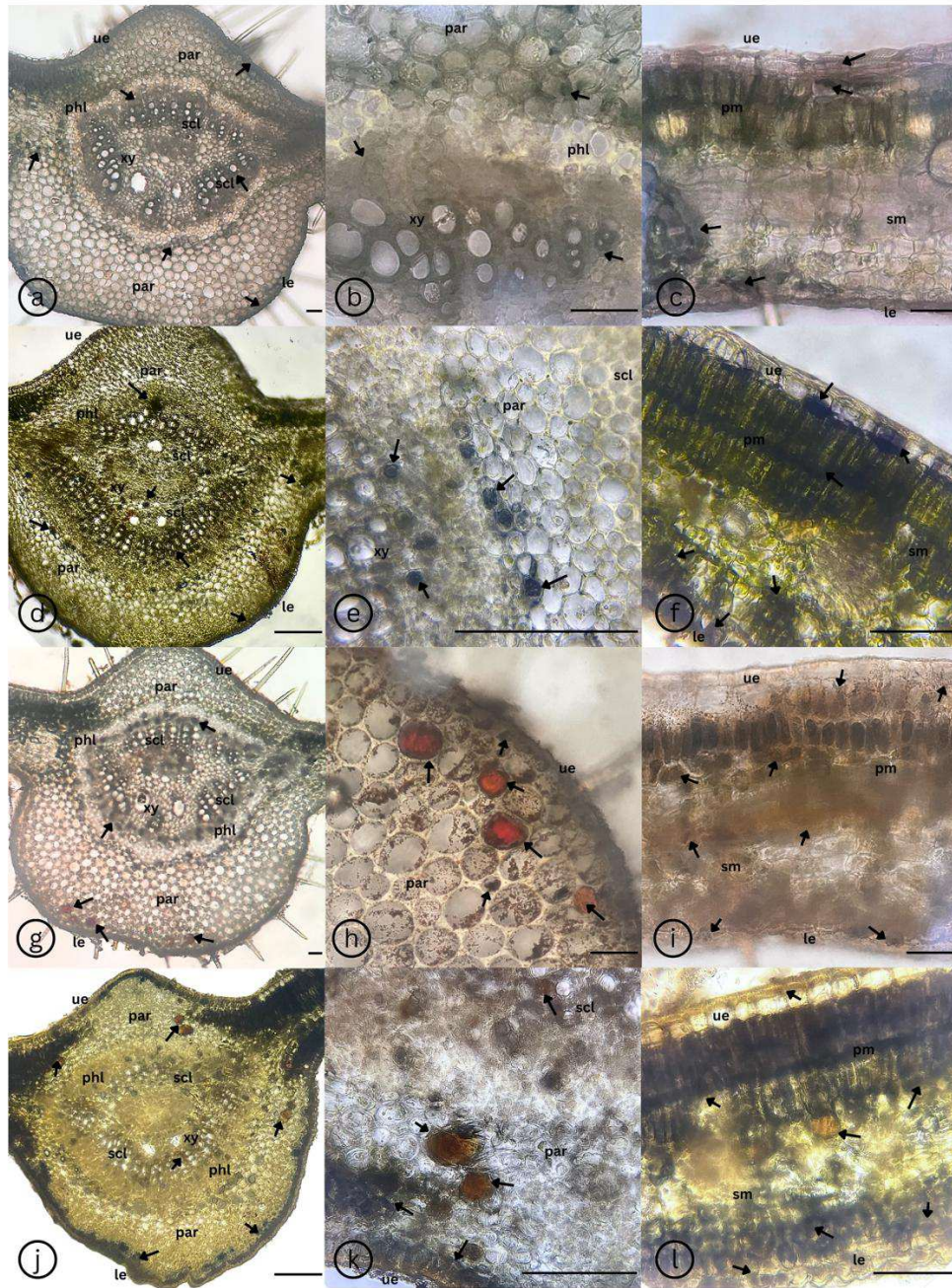


Figure 4. Histochemical localization of phenols and alkaloids in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. (A)–(F) Sections stained with 10% ferric chloride showing phenols as black-gray tissues (arrows) (A)–(C), *A. integrifolia* subsp. *integrifolia*; (D)–(F), *A. triphysa*. (G)–(L) Sections stained with Dragendorff reagent showing alkaloids as brown-black cells (arrows) (G)–(I), *A. integrifolia* subsp. *integrifolia*; (J)–(L), *A. triphysa*. Midrib (A), (D), (G), (J); midrib detail (B), (E), (H), (K); and leaf blade (C), (F), (I), (L) sections. Abbreviations: ue, upper epidermis; pm, palisade mesophyll; sm, spongy mesophyll; scl, sclereid; le, lower epidermis; par, parenchyma; phl, phloem; xy, xylem. Scale bar = 0.05 mm.

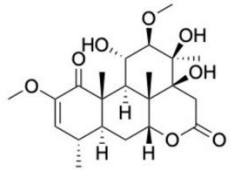
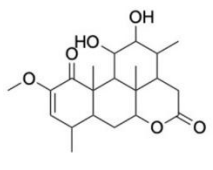
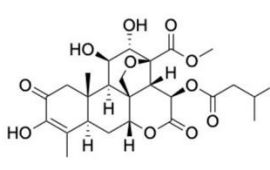
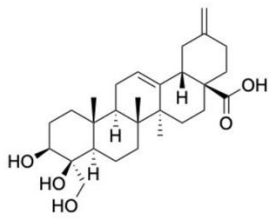
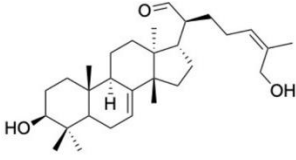
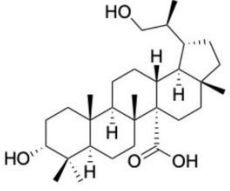
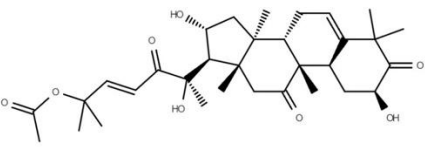
Quassinoids		
		
Nigakilactone H	Nigakilactone A**	Bruceine A*
Oleanane triterpenoid	Tirucallane triterpenoid	
		
3β,4β,23-Trihydroxy-24,30-dinorolean-12,20(29)-dien-28-oic acid	(24Z)-3β,27-Dihydroxy-7,24-tirucalladien-21-al*	
Lupane triterpenoid	Cucurbitane triterpenoid	
		
(20S)-3α,29-Dihydroxylupan-27-oic acid*	Cucurbitacin B	

Figure 5. Structural diversity of representative triterpenoids of the Philippine-native *Ailanthus* species as annotated by the UPLC-ESI-QTOF-MS analysis. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

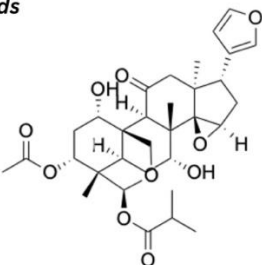
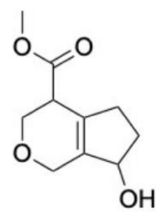
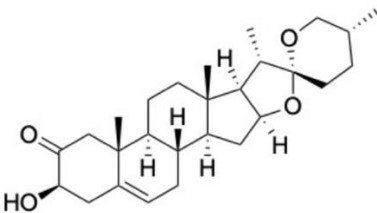
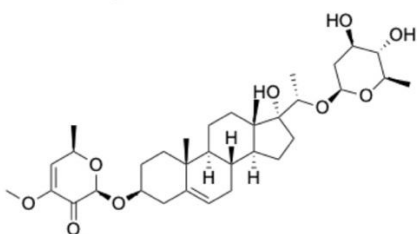
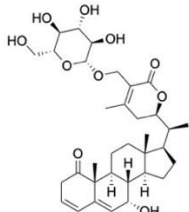
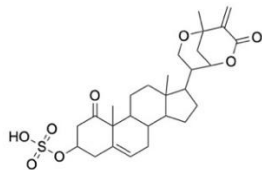
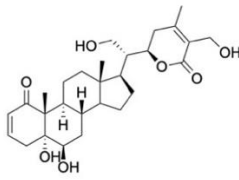
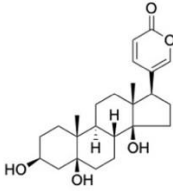
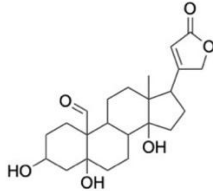
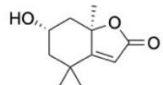
Limonoids  Azedarachin C	Iridoid  1,4α,5,7α-Tetrahydro-7-hydroxy-cyclopenta[c]pyran-4-carboxylic methyl ester*
Steroid  Diosgenone	Steroidal Glycoside  Periplocoside M**
Withanolides  Daturametelin I**  Daturametelin F*  Withafastousin E**	
Cardenolides  Telocinobufagin**  Strophanthidine  Digiprolactone	

Figure 6. Representative terpenoid subclasses identified in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species.

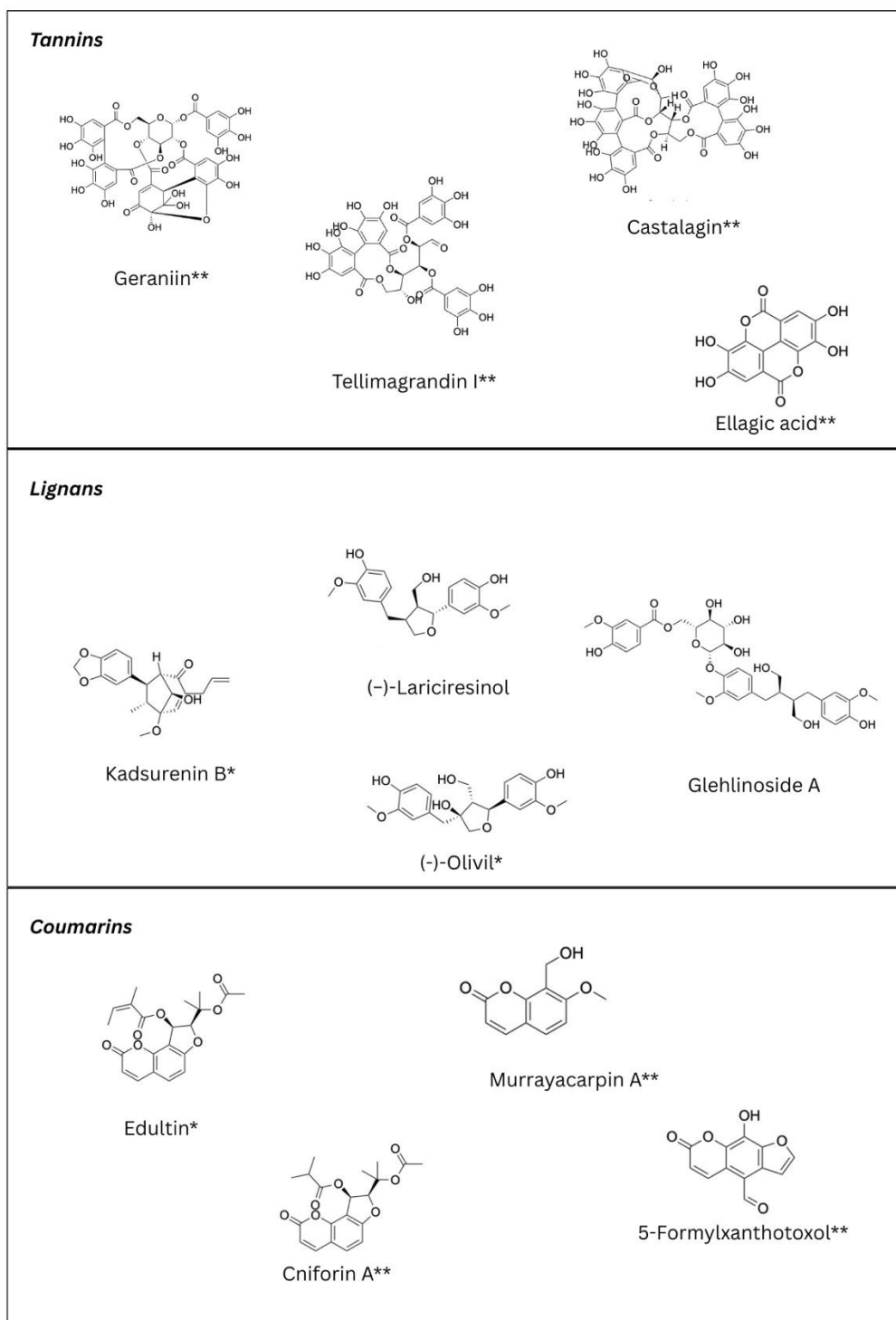


Figure 7. Structural diversity of representative lignans, tannins, and coumarins compounds identified from two Philippine-native *Ailanthus* species. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

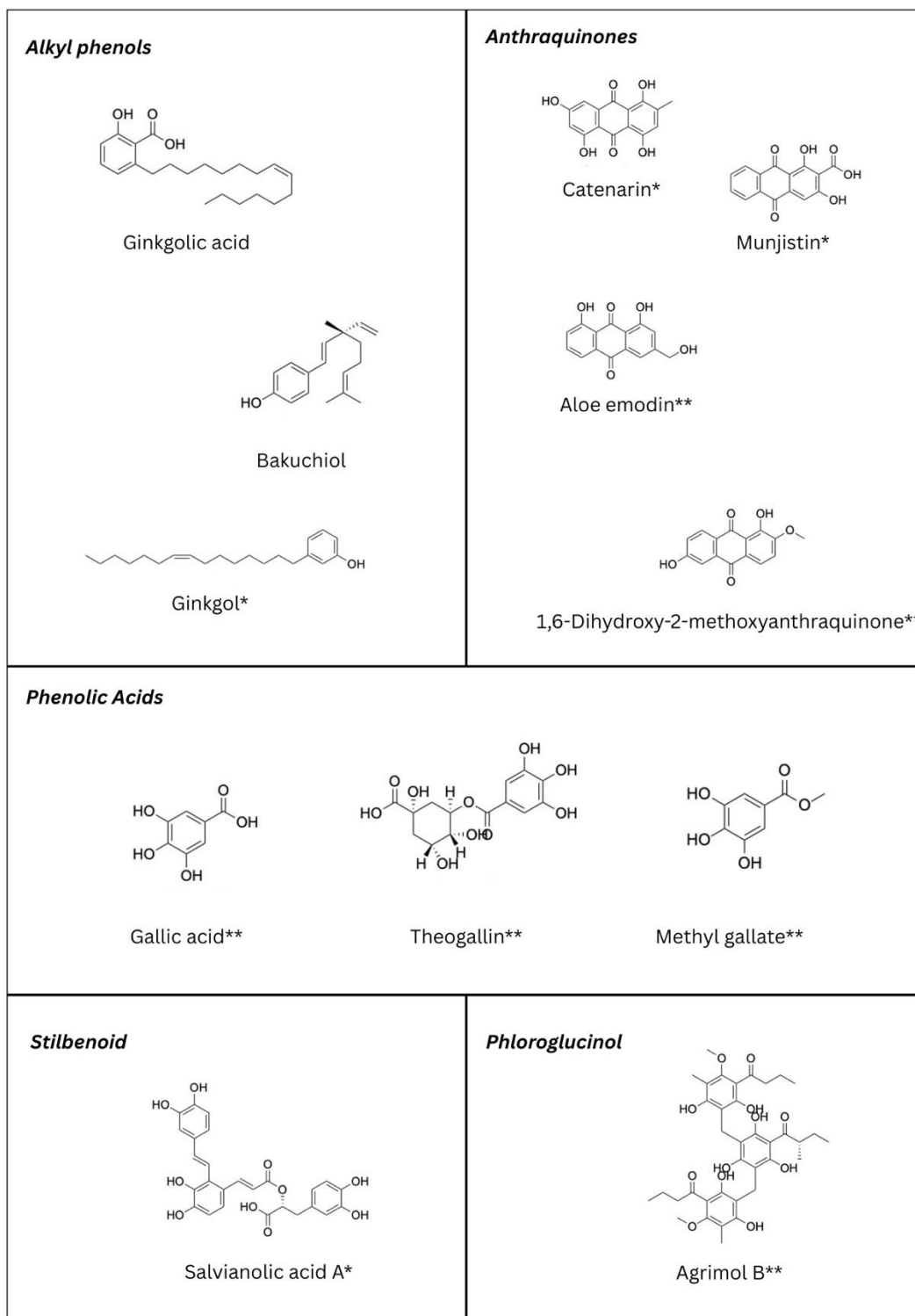


Figure 8. Representative phenolic subclasses identified in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

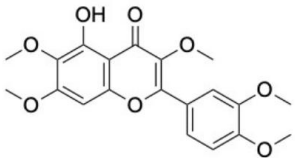
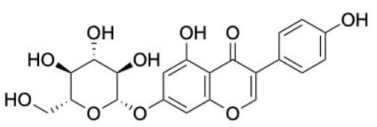
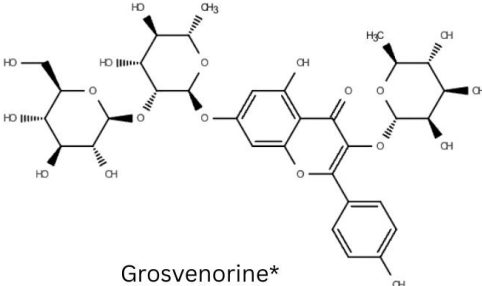
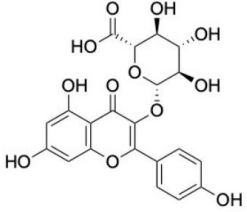
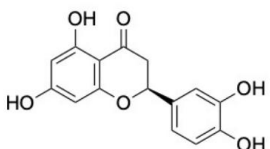
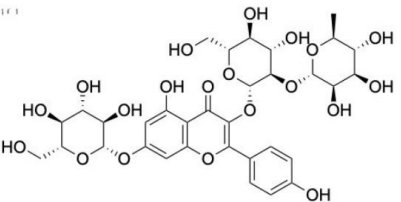
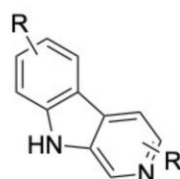
Flavone  Artemitin*	Isoflavone  Genistin
Flavanols  Grosvenorine*  Kaempferol 3-O-glucuronide**	
Flavanone  Eriodictyol**	Flavanol  Kaempferol 3-O-neohesperidoside-7-O-rhamnoside

Figure 9. Representative flavonoid subclasses identified in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

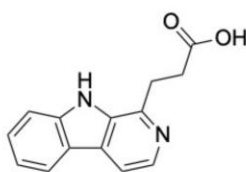
Isoflavanone 6-Aldehydo-isoophiopogonone B*	Isoflavanquinone (3R)-Abruquinone A*
Coumestan Coumestrol*	Chalcone Psorachalcone A*

Figure 10. Representative structures of flavonoid subclasses exclusively identified in *A. integrifolia* subsp. *integrifolia*

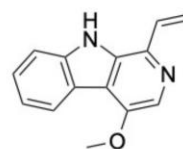
**β -Carboline Alkaloids
(Indole)**



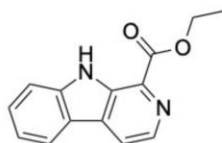
β -Carboline scaffold



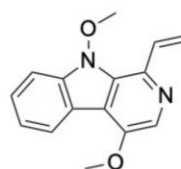
β -Carboline-1-propionic acid**



1-vinyl-4-methoxy- β -carboline
(Dehydrocrenatine)**



1-carboethoxy- β -carboline
(Kumujian A)*



4,9-dimethoxy-1-vinyl- β -carboline
(Picrasidine D)**

Figure 11. Structural diversity of β -carboline alkaloid compounds annotated from the two *Ailanthus* species. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

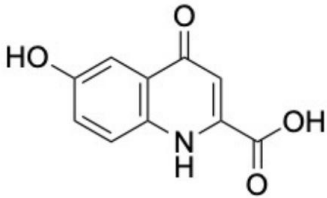
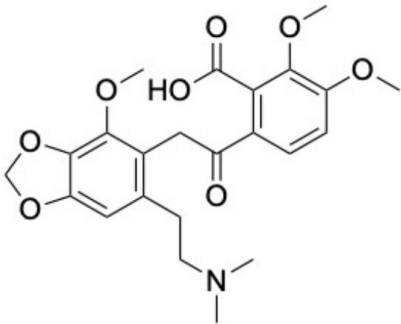
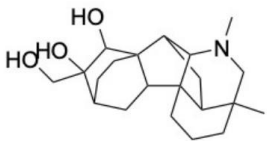
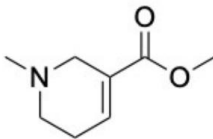
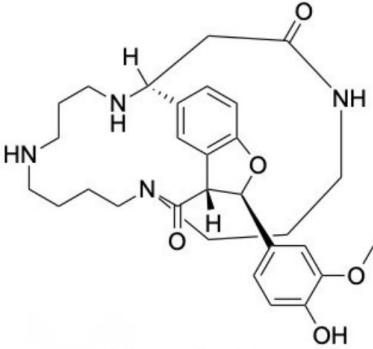
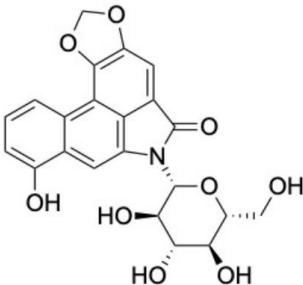
Quinoline Alkaloid  6-hydroxykynurenic acid**	Benzyloquinoline Alkaloid  Narceine**
Quinolizidine Alkaloid  Dictysine**	Pyridine Alkaloid  Arecoline**
Phenethylamine Alkaloid  Ephedradine B**	Glycosylated Alkaloid  Aristolactam Ia N-β-D-glucopyranoside**

Figure 12. Representative alkaloid subclasses identified in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

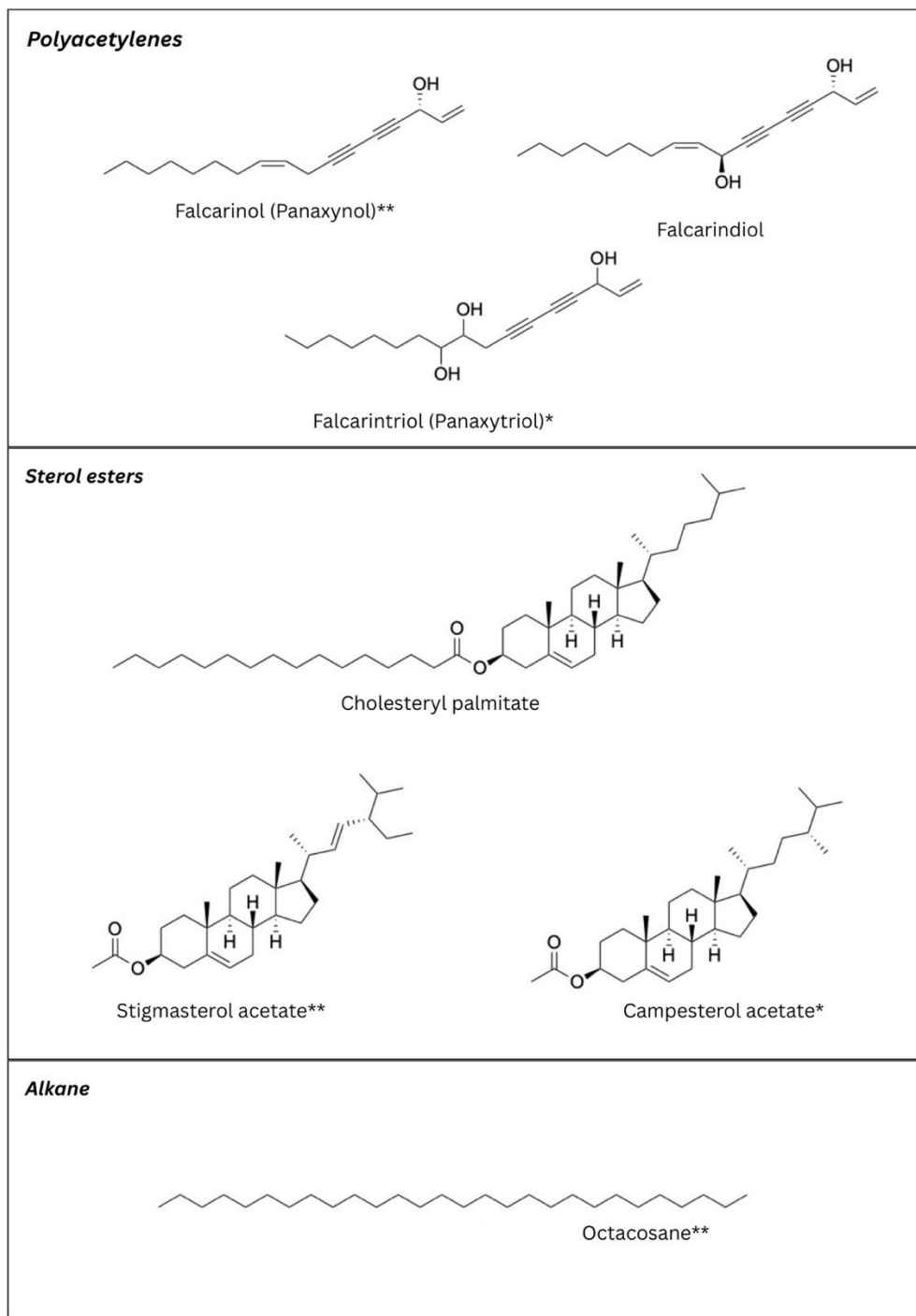


Figure 13. Representative lipid subclasses identified in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

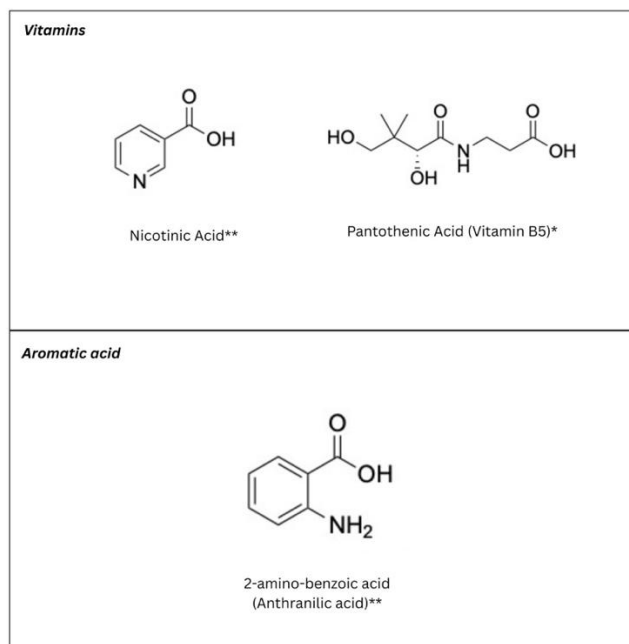


Figure 14. Representative organic acid metabolites identified in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

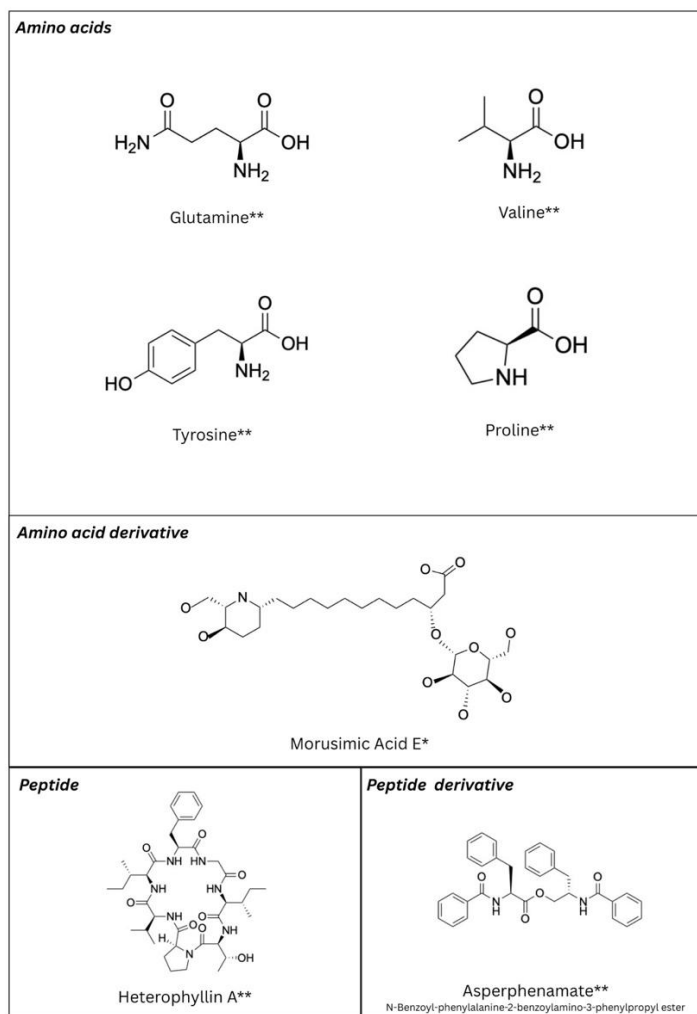


Figure 15. Representative free amino acids and polypeptides identified in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*. * = detected in *A. integrifolia* subsp. *integrifolia*; ** = detected in *A. triphysa*; no symbol = detected in both species

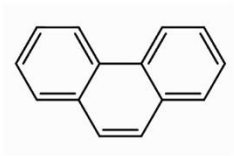
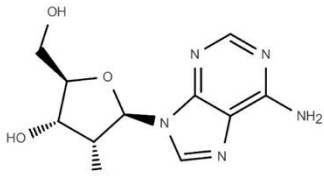
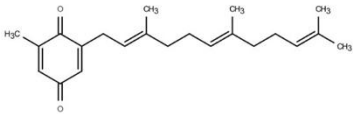
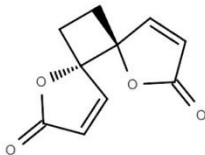
Polycyclic Aromatic Hydrocarbon  Phenanthrene	Nucleoside  Adenosine
Phthalide  Senkyunone	Butenolide  Anemonin

Figure 16. Unique miscellaneous metabolites identified exclusively in the leaves of *A. integrifolia* subsp. *integrifolia*

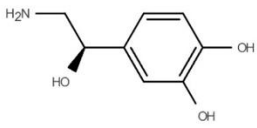
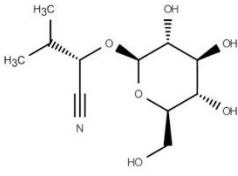
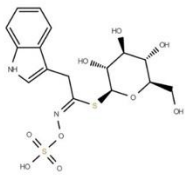
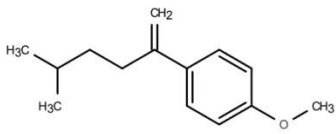
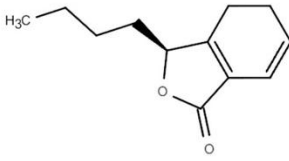
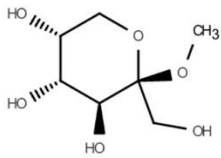
Catecholamine  Phenanthrene	Cyanogenic glycoside  Heterodendrin
Glucosinolate  Indoylmethyl glucosinolate	Aromatic hydrocarbon  2-(p-anisyl)-5-methyl-1-hexene
Phthalide  Senkyunolide	Sugar glycoside  methyl-β-D-fructopyranoside

Figure 17. Unique miscellaneous metabolites identified exclusively in the leaves of *A. triphysa*.

Table 1. Percent extraction yield of methanolic leaf extracts of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

SAMPLE	WEIGHT OF ORIGINAL SAMPLE (g)	WEIGHT OF CRUDE EXTRACT (g)	EXTRACTION YIELD (%)
<i>A. integrifolia</i> subsp. <i>integrifolia</i>	24.50	2.10	8.57
<i>A. triphysa</i>	49.20	6.37	12.95

Table 2. Putative metabolites identified in the methanolic extract of *A. integrifolia* subsp. *integrifolia* obtained by UPLC-ESI-QTOF-MS ranked from the highest intensities and categorized according to compound class

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
1.	(24Z)-3 β ,27-Dihydroxy-7,24-titucalladien-21-al	456.3603	457.3694	3.8261	9.3448	370395.3750	Triterpenoid	Kim et al. (2025)
2.	(24Z)-3 β ,27-Dihydroxy-7,24-titucalladien-21-al	456.3603	457.3693	3.5718	9.8275	169827.2500	Triterpenoid	
3.	Paeonolide F	510.3345	511.3415	-0.5199	9.6453	61457.2656	Triterpene lactone	He et al. (2010)
4.	Lucialdehyde A	438.3498	439.3592	4.9441	13.7719	58033.1563	Triterpenoid	
5.	11-Deoxy-23-acetate alisol B	498.3709	499.3786	0.9260	14.3728	52389.9961	Triterpenoid	Kim et al. (2025)
6.	Xanthophyll	568.4280	569.4342	-1.9159	14.3071	49130.8945	Carotenoid	Kanehisa et al. (2025)
7.	5-Dehydrokarounidiol	438.3498	439.3579	2.0224	10.4284	47799.0820	Triterpenoid	Kim et al. (2025)
8.	Iridobelamal A	474.3709	475.3792	2.1930	7.8980	40804.5234	Triterpenoid	
9.	(20S)-3 α ,29-Dihydroxylupan-27-oic acid	474.3709	475.3799	3.5083	9.4290	38063.3828	Triterpenoid	Yang et al. (2008)
10.	Nigakilactone H	424.2097	425.2161	-2.1251	11.3624	30001.3047	Quassinoid	Kim et al. (2025)
11.	Rubiprasin B	500.3866	501.3938	-0.1479	11.1333	25169.9414	Triterpenoid	
12.	25-Dehydroxy-11-acetate alisol A	514.3658	515.3719	-2.3300	7.9179	25047.7285	Triterpenoid	
13.	Abrisapogenol A	458.3760	459.3848	3.3079	14.8059	23744.9590	Triterpenoid	
14.	Lucialdehyde A	438.3498	439.3576	1.1915	11.4240	22269.9570	Triterpenoid	
15.	Iridobelamal A	474.3709	475.3795	2.7406	9.8341	22227.3770	Triterpenoid	
16.	Siraitic acid A	472.3189	473.3254	-1.5850	9.7373	18615.0195	Triterpenoid	
17.	16-O-Acetylisoiridogermanal	516.3815	517.3891	0.6368	10.0776	18100.8496	Triterpenoid	
18.	Rubiatrionol	458.3760	459.3826	-1.4762	14.3758	17382.4004	Triterpenoid	
19.	Rubiatrionol	458.3760	459.3835	0.5697	8.3756	16659.1445	Triterpenoid	
20.	Isonarthogenin	430.3083	431.3164	1.9094	8.7848	14863.0361	Steroid	Kim et al. (2025)
21.	Trametenolic acid	456.3603	457.3685	1.9930	8.9290	14215.2959	Triterpenoid	
22.	Ruscogenin	430.3083	431.3161	1.2096	7.7905	13748.7217	Steroidal sapogenin	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
23.	23-Acetate alisol B	514.3658	515.3718	-2.4357	8.2082	11237.1416	Triterpenoid	
24.	3-Acetylaleuritolic acid	498.3709	499.3773	-1.8072	13.9181	10637.0000	Triterpenoid	
25.	Diosgenone	412.2977	413.3055	1.1553	8.7764	10302.8086	Steroid	
26.	Methyl 2 α -methoxyursolate	500.3866	501.3950	2.3161	13.3231	10029.1904	Triterpenoid	Li et al. (2021)
27.	Diosgenin	414.3134	415.3217	2.4994	11.4155	9789.2559	Steroidal sapogenin	Kim et al. (2025)
28.	16-O-Acetylisoiridogermanal	516.3815	517.3879	-1.6861	9.8139	9683.8408	Triterpenoid	Ito et a. (1998)
29.	Δ 3,5-Deoxytigogenin	396.3028	397.3107	1.5536	11.1128	7987.3403	Steroidal sapogenin	Minghe and Yanyong (1983)
30.	3 β ,4 β ,23-Trihydroxy-24,30-dinorolean-12,20(29)-dien-28-oic acid	458.3032	459.3114	1.9376	7.7185	6389.8413	Triterpenoid	Kim et al. (2008)
31.	Olibanumols J	460.3916	461.3999	2.1423	11.1373	5449.5415	Triterpenoid	Kim et al. (2025)
32.	Poricoic acid DM	528.3451	529.3512	-2.2734	7.7993	5151.3272	Triterpenoid	
33.	Farnesyl acetate	264.2089	265.2166	1.4709	11.3194	5128.1460	Sesquiterpenoid	
34.	3 β -Hydroxy-12,17-diene-28-nordeane-23-al	424.3341	425.3409	-1.0830	14.3727	4386.3477	Triterpenoid	Begum et al. (2010)
35.	Dehydroabietic acid	300.2089	301.2172	3.2168	13.2615	4295.9331	Diterpenoid	
36.	Curculigenin B	476.3866	477.3945	1.4062	10.0762	3371.9841	Steroidal sapogenin	
37.	Poricoic acid AM	512.3502	513.3561	-2.5426	8.3035	3217.3743	Triterpenoid	
38.	Siraitic acid C	440.2927	441.3007	1.7680	7.7115	3208.7883	Triterpenoid	Kim et al. (2025)
39.	Androsta-4-ene-3,17-dione	286.1933	287.2015	3.2139	13.2615	3150.3140	Steroid	
40.	20(R)-Protopanaxatriol (Protopanaxatriol)	476.3866	477.3947	1.7784	10.5018	3095.4871	Triterpenoid	
41.	Hyodeoxycholic acid	392.2927	393.2980	-4.8421	12.3170	2845.9299	Bile acid	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
42.	(22E,24R)-5 α ,8 α - Epidioxysterosta-6,9,22- trien-3 β -ol	426.3134	427.3217	2.4940	12.7944	2539.0437	Sterol	Lee et al. (2020)
43.	Tsugaric acid B	528.3815	529.3890	0.3985	13.5949	2317.8921	Triterpenoid	Kim et al. (2025)
44.	Cimicidanol	484.3189	485.3255	-1.3108	4.1516	2222.2422	Triterpenoid	
45.	3-O-(2'E,4'Z-Decadienoyl) ingenol	498.2981	499.3039	-3.0266	7.9521	2142.6387	Diterpenoid	
46.	Strophanthidine	404.2199	405.2262	-2.3589	7.5827	2125.9739	Cardenolide	
47.	24-Acetate alisol A	532.3764	533.3810	-4.9685	14.7032	2060.5669	Triterpenoid	
48.	Poricoic acid E	500.3138	501.3227	3.3488	7.8856	2042.6161	Triterpenoid	Frolova and Ovodov (1971) Kim et al. (2025)
49.	Eleutheroside K	734.4605	735.4657	-2.8230	14.0566	1998.8585	Triterpenoid saponin	
50.	Xantholide B	232.1463	233.1533	-1.2733	9.5893	1982.3648	Sesquiterpene lactone	
51.	Δ 7-Stigmasterol	410.3549	411.3624	0.5777	9.4549	1975.7474	Sterol	de Blas and del Valle Gonzalez (1996)
52.	Meldenin	454.2719	455.2807	3.3549	13.2723	1856.0050	Limonoid	Kim et al. (2025)
53.	23-Acetate alismaketone A	530.3607	531.3659	-4.0257	6.8311	1820.0783	Triterpenoid	de Blas and del Valle Gonzalez (1996)
54.	Δ 7-Stigmasterol	410.3549	411.3629	1.7819	9.7833	1690.7384	Sterol	Kim et al. (2025)
55.	Furanodiene	216.1514	217.1585	-0.9922	9.5742	1649.2932	Sesquiterpenoid	Morin et al. (2002)
56.	α -Estradiol	272.1776	273.1854	1.7686	9.5129	1580.3491	Steroid	Kim et al. (2025)
57.	Songoroside A	588.4026	589.4094	-0.7404	12.4100	1516.6458	Triterpenoid saponin	Kim et al. (2025)
58.	Bufalin	386.2457	387.2521	-2.4169	12.8294	1493.2202	Cardenolide	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
59.	23-Acetate alisol K	526.3294	527.3348	-3.5994	7.8509	1489.1462	Triterpenoid	Kim et al. (2025)
60.	Dihydroactinidiolide	180.1150	181.1218	-2.6073	5.9448	1464.7427	Norisoprenoid	
61.	Hexanorcucurbitacin F	404.2563	405.2616	-4.6906	10.4720	1436.5331	Triterpenoid	
62.	Digiprolactone	196.1099	197.1163	-4.4540	3.3007	1403.0077	Cardenolide	
63.	Poricoic acid C	482.3396	483.3464	-0.9826	12.2909	1346.6317	Triterpenoid	
64.	23-Acetate alisol K	526.3294	527.3389	4.1142	8.2399	1297.1588	Triterpenoid	Tian et al. (2007)
65.	1,1,6-Trimethyl-1,2-dihydronaphthalene	172.1252	173.1322	-1.4731	9.5551	1265.1328	Norisoprenoid	
66.	25-Anhydrocimigenol-3-O- β -D-xylopyranoside	602.3819	603.3891	-0.0183	7.7717	1261.1549	Triterpenoid saponin	
67.	Phytolaccagenic acid	516.3451	517.3526	0.4441	11.9942	1212.0128	Triterpenoid	
68.	Bornyl transcinamate	284.1776	285.1847	-0.6764	9.5929	1209.2899	Monoterpenoid	
69.	Ar-turmerone	216.1514	217.1585	-0.8363	13.2221	1195.1151	Sesquiterpenoid	Kim et al. (2025)
70.	Cordilin	413.3294	414.3369	0.5424	6.4807	1171.8118	Sesquiterpene lactone	
71.	Arteannuin A	206.1307	207.1371	-4.2383	3.4651	1121.1605	Sesquiterpene lactone	
72.	13,17-Epoxy alisol A	506.3607	507.3676	-0.9023	6.2718	1106.4187	Triterpenoid	
73.	23,27-Dihydroxypennogenin	462.2981	463.3051	-0.7405	14.7818	1104.5198	Steroidal sapogenin	
74.	12 β -Hydroxycimigenol	504.3451	505.3533	1.9346	7.5196	1067.8403	Triterpenoid	Di-Fan et al. (2014)
75.	Vellardiol	236.1776	237.1846	-1.4339	7.8830	1055.1726	Sesquiterpenoid	
76.	Picfeltarraegenin I	484.3189	485.3260	-0.4074	4.9197	1015.8164	Triterpenoid	
77.	Ganoderenic acid C	516.3087	517.3173	2.5186	8.6456	991.4171	Triterpenoid	Kim et al. (2025)
78.	8 β ,9 α -Dihydroganoderic acid J	516.3087	517.3157	-0.5499	7.4836	968.5094	Triterpenoid	
79.	Poricoic acid F	498.3345	499.3407	-2.2202	11.9956	967.9709	Triterpenoid	
80.	Astramembranin II	622.4081	623.4175	3.3911	14.7571	941.7677	Triterpenoid saponin	Bohlmann et al. (1984)
81.	Florilenalin angelate	346.1780	347.1848	-1.3907	4.1961	934.0776	Sesquiterpene lactone	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
82.	Terrestrosin I	1096.5302	1097.5400	2.4130	12.4757	918.4000	Steroidal saponin	Kim et al. (2025)
83.	Terrestroside F	562.3870	563.3930	-2.2455	12.6163	904.2220	Steroidal saponin	
84.	ArteamisinineI	206.1307	207.1371	-3.9141	2.8391	899.9670	Sesquiterpene lactone	
85.	Methyl pachymate	542.3971	543.4062	3.3375	13.7168	897.4012	Triterpenoid	Kim et al. (2025)
86.	Elculentic acid	502.3294	503.3361	-1.1545	4.5393	857.6414	Triterpenoid	Zhang et al. (2023)
87.	3,7,11-Trimethyl-2,6,10-dodecatrienoic methyl ester	250.1933	251.2007	0.4990	7.8965	836.3911	Sesquiterpenoid	Kim et al. (2025)
88.	Oxyphyllenodiol B	238.1569	239.1645	1.2526	13.6531	831.0637	Sesquiterpenoid	
89.	Lindestrene	214.1358	215.1430	-0.2546	13.1323	816.7642	Sesquiterpene lactone	
90.	Ganolucidic acid B	502.3294	503.3389	4.3665	6.3726	788.5637	Triterpenoid	Zhao et al. (2017)
91.	Eremanthin	230.1307	231.1384	1.7099	13.6552	766.7073	Sesquiterpene lactone	
92.	Tracheloionoside	516.2571	517.2639	-0.8240	3.0101	759.4714	Norisoprenoid	
93.	Quinatoside A	588.3662	589.3706	-4.9361	4.6259	757.8966	Triterpenoid saponin	Kim et al. (2025)
94.	Stigmast-4-ene-3,6-dione	426.3498	427.3586	3.5533	9.4830	752.5208	Steroid	
95.	Palbinone	358.2144	359.2212	-1.3646	6.0815	731.9964	Steroid	
96.	Columbin	358.1416	359.1492	0.7791	7.4802	720.6404	Diterpenoid	Wang et al. (2004)
97.	5 α ,8 α -Epidioxysterosta-6,22-dien-3 β -ol	428.3290	429.3351	-2.7828	8.3551	713.1148	Steroid	
98.	1,1,6-Trimethyl-1,2-dihydronaphthalene	172.1252	173.1319	-3.1766	7.9045	660.5829	Norisoprenoid	
99.	Daturametelin F	534.2287	535.2351	-1.7560	14.2217	647.6747	Withanolide	Kim et al. (2025)
100.	2 α ,3 α ,23-Trihydroxy-olean-12-en-28-oic acid methyl ester	502.3658	503.3738	1.4667	9.2143	613.5010	Triterpenoid	Li et al. (2012)

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
101.	Evobioside	682.3564	683.3609	-4.1595	12.9570	600.5976	Cardenolide	Kim et al. (2025)
102.	Methyl 2 α ,3 β -diacetyloxy-lup-20(29)-en-28-oate	570.3920	571.4013	3.5208	11.2627	585.3763	Triterpenoid	
103.	Methyl lucidenate Q	474.2981	475.3045	-1.9283	6.4289	571.4534	Triterpenoid	
104.	Isolinderoxide	244.1463	245.1529	-2.7467	9.5872	552.6382	Sesquiterpenoid	
105.	3-epi-Dehydropachymic acid	526.3658	527.3733	0.3814	10.1898	529.1206	Triterpenoid	Kim et al. (2025)
106.	24-Acetate alisol F	530.3607	531.3671	-1.7472	9.2192	525.8785	Triterpenoid	
107.	Neotigogenin	416.3290	417.3350	-3.0679	9.9977	518.9655	Steroidal sapogenin	
108.	Ergosta-4,6,8(14),22-tetraen-3-one	392.3079	393.3159	1.7419	11.9854	516.6885	Steroid	
109.	Columbin	358.1416	359.1487	-0.4999	5.8893	508.0333	Diterpenoid	
110.	Dehydroisoandrosterone	288.2089	289.2170	2.7362	12.5391	501.5777	Steroid	
111.	16-Oxy-acetoxypachymic acid	570.3920	571.3998	0.8163	11.7443	483.2833	Triterpenoid	
112.	Eremanthin	230.1307	231.1382	1.1213	10.0305	481.9249	Sesquiterpene lactone	
113.	Manogenin	446.3032	447.3095	-2.2139	7.7145	474.4408	Steroidal sapogenin	Kim et al. (2025)
114.	Apocynoside I	386.1941	387.2007	-1.7180	2.9797	474.2283	Norisoprenoid glycoside	
115.	Siraitic acid E	456.2876	457.2932	-3.6769	8.2365	473.9745	Triterpenoid	
116.	1,4 α ,5,7 α -Tetrahydro-7-hydroxy-cyclopenta[c]pyran-4-carboxylic methyl ester	196.0736	197.0800	-4.4039	2.8060	472.9397	Iridoid	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
117.	Cimidahuside G	620.3924	621.4006	1.4635	7.5036	468.8549	Triterpenoid saponin	
118.	Dehydrobaimuxinol	236.1776	237.1851	0.6247	12.9377	429.3370	Sesquiterpenoid	
119.	Lindestrene	214.1358	215.1427	-1.7898	9.5801	428.5193	Sesquiterpenoid	
120.	2 β -Acetoxypterodontic acid	292.1675	293.1733	-4.9478	12.8343	428.0921	Sesquiterpenoid	Zhao et al. (1997)
121.	Salviolone	268.1463	269.1533	-1.1794	9.5949	411.6866	Diterpenoid	Kim et al. (2025)
122.	Mogroside III	962.5450	963.5528	0.4747	8.9501	391.2280	Triterpenoid saponin	
123.	β -Santonin	246.1256	247.1322	-2.5375	3.7961	387.3353	Sesquiterpene lactone	Coggon and Sim (1969)
124.	Xantholide A	230.1307	231.1379	-0.3692	13.2606	372.5962	Sesquiterpene lactone	Kim et al. (2025)
125.	12-Hydroxymethyl abietate	332.2351	333.2427	0.7784	7.8977	348.7627	Diterpenoid	Fujita (1966)
126.	Methyl protoneograccillin	1078.5560	1079.5620	-0.9826	12.4723	343.9324	Steroidal saponin	Kim et al. (2025)
127.	1 α ,2 α ,3 β ,19 α ,23-Pentahydroxyurs-12-en-28-oic acid-28-O- β -D-xylopyranoside	652.3823	653.3927	4.8296	14.4363	342.9377	Triterpenoid saponin	Gupta and Singh (1989)
128.	Prosapogenin 1	706.3928	707.4001	-0.0510	8.0506	337.0853	Triterpenoid	Kim et al. (2025)
129.	14-Acetoxy-7 β -(3-ethyl-cis-crotonoyloxy)-1 α -(2-methylbutyryloxy)-notonipetranone	490.2931	491.2999	-0.9199	6.9218	332.6719	Sesquiterpenoid	Kikuchi and Suzuki (1992)
130.	Trachelosperoside F	682.3564	683.3651	2.0881	3.4957	315.9858	Triterpenoid saponin	Abe and Yamauchi (1987)
131.	Oriediterpenol	304.2402	305.2466	-3.1184	2.9634	313.8095	Diterpenoid	
132.	Platycodigenin	520.3400	521.3468	-0.9930	5.6912	299.2898	Triterpenoid	Kim et al. (2025)
133.	Darutigenol	322.2508	323.2569	-3.5828	2.9632	298.9439	Diterpenoid	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
134.	Ganoderenic acid H	512.2774	513.2833	-2.6363	11.1953	287.5980	Triterpenoid	Kim et al. (2025)
135.	Aduncin	294.1103	295.1167	-3.1215	3.0329	286.5992	Sesquiterpene lactone	
136.	Cynanoside M	720.3721	721.3784	-1.3166	10.5223	278.5585	Steroidal glycoside	
137.	(S)-Shihulimonin A	502.1839	503.1889	-4.4656	2.6000	274.5948	Limonoid	
138.	Phytolaccagenin	532.3400	533.3464	-1.5713	9.0873	268.0999	Triterpenoid	
139.	Bruceine A	522.2101	523.2175	0.2672	4.6550	260.8688	Quassinoid	
140.	Oxyphyllenone A	210.1256	211.1326	-1.4213	3.5246	245.0144	Sesquiterpenoid	
141.	Schizonol	168.1150	169.1218	-2.8712	6.4311	238.0913	Monoterpenoid	
142.	Ecdysterone-3-O- β -D-glucopyranoside	642.3615	643.3710	3.3942	6.8468	219.0581	Steroidal glycoside	Meng et al. (2001)
143.	Xysmalogenin	372.2301	373.2367	-1.5771	8.7920	199.7052	Cardenolide	Kim et al. (2025)
144.	Nimbolidin E	738.3615	739.3661	-3.6846	5.2855	183.0546	Limonoid	Fan et al. (2022)
<i>Phenolics</i>								
145.	Schininallyl ol	344.1624	345.1692	-1.2099	4.8925	3830.9180	Coumarin	Kim et al. (2025)
146.	Kadsurenin E	344.1624	345.1693	-0.9186	4.4237	2575.8064	Lignan	Xiao et al. (2021)
147.	6-Methoxyl-7-hydroxycoumarin	192.0423	193.0488	-3.9005	3.0626	2231.1306	Coumarin	Kim et al. (2025)
148.	trans-Octadecyl-ferulate	460.3553	461.3630	0.9432	13.2653	2124.2014	Phenyl-propanoid	
149.	2-(p-Anisyl)-5-methyl-1-hexene	204.1514	205.1587	0.0690	13.1253	1908.5414	Phenyl-propanoid	N/A
150.	6,7-Dimethoxy-8-hydrocoumarin	222.0528	223.0606	2.1917	9.8432	1603.0907	Coumarin	Kim et al. (2025)
151.	Ginkgol	302.2610	303.2687	1.3671	13.0056	1340.7157	Alkyl phenol	
152.	(-)-Lariciresinol	360.1573	361.1641	-1.2427	5.9297	1109.3851	Lignan	
153.	Secoisolariciresinol	362.1729	363.1799	-0.9319	6.8353	837.4276	Lignan	
154.	Munjistin	284.0321	285.0395	0.3522	10.8997	783.0469	Anthraquinone	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Phenolics</i>								
155.	Kadsurenin B	342.1467	343.1542	0.4380	5.8737	772.6404	Lignan	
156.	Scroside A	830.2845	831.2889	-3.3665	14.7783	770.4665	Phenolic glycoside	
157.	Ginkgolic acid	346.2508	347.2588	2.0101	13.1123	770.0274	Alkyl phenol	
158.	(3'R)-3'- Hydroxycolumbianadin	344.1260	345.1325	-2.1486	2.6452	606.8580	Coumarin	
159.	Cniforin A	374.1366	375.1433	-1.3024	4.5288	595.7785	Coumarin	
160.	Terminalic acid	316.2038	317.2097	-4.4198	9.0873	584.3855	Tannin	
161.	Bakuchiol	256.1827	257.1911	4.2879	7.1558	544.7750	Alkyl phenol	
162.	5,7,2'-Trihydroxy-6- methyl-8-methoxy-3(S)- (4'- methoxybenzyl)chroman- 4-one	360.1209	361.1268	-3.8432	2.5977	504.8470	Homoiso-flavanone	Kim et al. (2025)
163.	Lappaol B	550.2203	551.2254	-3.9365	5.6021	503.1157	Lignan	
164.	2,4,6- Trimethoxyacetophenone	210.0892	211.0956	-4.1914	3.3192	482.6811	Phenolic ketone	
165.	Torachryson-8-O- β -D- glucopyranoside	408.1420	409.1484	-2.2270	2.3059	476.2373	Phenolic glycoside	
166.	Isoscopoletin	192.0423	193.0488	-3.9188	6.4331	472.2955	Coumarin	Liu et al. (2003)
167.	2,3,5,4'- Tetrahydroxystilbene-2- O- β -D-glucopyranoside	406.1264	407.1331	-1.4178	2.3623	412.2290	Stilbenoid	Li et al. (2022)
168.	Glehlinside A	674.2575	675.2667	2.8673	3.5177	410.8204	Lignan	
169.	1-Hydroxy-4,7- dimethoxy-1-(2- oxopropyl)-1H- phenanthren-2-one	326.1154	327.1213	-4.2247	2.6597	403.1143	Phenanthrene derivative	Kim et al. (2025)

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Phenolics</i>								
170.	Blestrianol D	452.1624	453.1678	-4.1931	7.4254	387.6117	Stilbenoid	He et al. (2017)
171.	Cnidimol B	292.0947	293.1018	-0.6717	3.9157	376.9676	Chromone	Kim et al. (2025)
172.	Catenarin	286.0477	287.0546	-1.5685	3.7578	356.8241	Anthraquinone	
173.	(-)-trans-Khellactone	262.0841	263.0906	-2.8875	4.0285	344.0387	Coumarin	
174.	Erythro- dihydroxydehydrodicon iferyl alcohol	392.1471	393.1532	-3.0214	2.5452	339.3587	Lignan	Kim et al. (2025)
175.	(-)-Olivil	376.1522	377.1583	-3.0576	2.5167	335.7830	Lignan	
176.	Edultin	386.1366	387.1432	-1.6251	3.9821	289.0012	Coumarin	
177.	Salvianolic acid A	494.1213	495.1282	-0.8272	5.2174	216.3659	Stilbenoid	
178.	Ginnol (Celidoniol)	424.4644	425.4731	3.3158	8.7792	212.2388	Phenyl-propanoid	
179.	Japenol	376.1522	377.1587	-2.0965	5.3891	202.1938	Lignan	
180.	Neoarctin B	742.2989	743.3053	-1.2033	6.4252	196.4743	Lignan	
181.	Neociwujiaiphenol	402.1679	403.1761	2.4140	6.7257	190.9762	Alkyl phenol	
<i>Flavonoids</i>								
182.	3,8-Di-C- glucosylapigenin	594.1585	595.1649	-1.4977	2.2071	3599.5073	Flavone	Chopin and Dellamonica (1980)
183.	Baicalein	270.0528	271.0597	-1.4101	4.4266	1322.6620	Flavone	Kim et al. (2025)
184.	Coumestrol	268.0372	269.0446	0.4211	10.0633	1134.6733	Coumestan	
185.	Kushenol X	440.1835	441.1893	-3.3135	11.3647	1078.0580	Flavanone	
186.	5,6,4'-Trihydroxy-7- methoxyflavone	300.0634	301.0703	-1.0981	4.5583	1005.2659	Flavone	
187.	2"-O-Glucosyl- isoswertisin	608.1741	609.1801	-2.1502	2.7612	837.9870	Flavone	Zhu et al. (1989)
188.	6-Aldehyde-7-methoxy- isoophiopogonone B	354.1103	355.1182	1.6807	11.2184	833.2169	Isoflavonoid	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED D M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Phenolics</i>								
189.	Corylidin	368.0896	369.0966	-0.7298	5.1206	770.9944	Coumestan	Kim et al. (2025)
190.	(3R)-Abruquinone D	378.1315	379.1379	-2.0970	2.3351	738.6246	Isoflavanquinone	Chun-qing and Zhi-bi (1998)
191.	6-Aldehydo- isoophiopogonone B	340.0947	341.1022	0.7506	10.9003	679.1965	Isoflavonoid	Kim et al. (2025)
192.	Sagittatoside B	646.2262	647.2308	-4.0589	14.1686	670.2140	Flavonoid glycoside	
193.	Methyl ophiopogonone B	326.1154	327.1227	-0.1433	9.6065	610.2789	Isoflavonoid	
194.	Artemitin	388.1158	389.1220	-2.8226	2.6749	567.5644	Flavone	Stochmal et al. (2001) Chun-qing and Zhi-bi (1998)
195.	Apigenin-7-O- β -D- glucuronopyranoside	444.1056	445.1122	-1.7260	2.3090	560.9239	Flavonoid glycoside	
196.	(3R)-Abruquinone A	360.1209	361.1276	-1.6188	2.8122	560.3216	Isoflavanquinone	
197.	Kaempferol 3-O- neohesperidoside-7-O- rhamnoside	740.2164	741.2242	0.7270	2.3015	549.1459	Flavonoid glycoside	Kim et al. (2025)
198.	Leachianone G	356.1260	357.1330	-0.8244	4.0756	534.4315	Flavanone	
199.	Genistin	432.1056	433.1118	-2.6539	2.6187	514.5518	Flavonoid glycoside	
200.	Grosvenorine	740.2164	741.2231	-0.8026	2.6426	456.1973	Flavonol	
201.	Sophorabioside	578.1636	579.1697	-1.9376	2.7327	400.2047	Flavonoid glycoside	
202.	Kushenol B	492.2512	493.2597	2.5803	11.5425	312.2854	Flavanone	
203.	5-O-Desmethylnobiletin	388.1158	389.1221	-2.4710	3.1997	291.9493	Flavone	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
Phenolics								
204.	5-Hydroxy-6,7-dimethoxyflavone-4'-O-β-D-glucoside	476.1319	477.1370	-4.5727	3.0412	238.7299	Flavonoid glycoside	Kim et al. (2025)
205.	5,7,3',4'-Tetramethoxyflavone	342.1103	343.1173	-0.9515	10.3667	228.4044	Flavone	
206.	Psorachalcone A	340.1311	341.1383	-0.2651	3.3988	224.8951	Chalcone	
Alkaloids								
207.	1-Carboethoxy-β-carboline	240.0899	241.0965	-2.7995	2.5560	2151.4131	Indole Alkaloid	Han et al. (1985)
208.	Dictysine	347.2460	348.2518	-4.4551	11.9926	674.7780	Quinolizidine alkaloid	
209.	Cimicifugadine	613.3615	614.3700	2.0159	9.1859	490.7060	Triterpene alkaloid	Kim et al. (2025)
210.	Corynoxeine	382.1893	383.1952	-3.4268	6.1953	478.0096	Indole Alkaloid	
211.	Hupehemonoside	591.3771	592.3832	-2.0447	9.0675	404.4321	Steroidal alkaloid glycoside	
212.	Huphenine	415.3450	416.3520	-0.7334	6.6283	344.7093	Steroidal alkaloid	
213.	Ephedradine A	492.2737	493.2821	2.3943	7.6328	337.0627	Phenethyl-amine alkaloid	
214.	Pingbeinine	445.3556	446.3650	4.7076	8.5618	250.5259	Steroidal alkaloid	
215.	Penniclavine	270.1368	271.1435	-2.2261	6.9413	233.6509	Indole Alkaloid	
Lipid Compounds								
216.	Panaxynol	244.1827	245.1910	4.1093	13.1046	26101.8203	Polyacetylene	Kim et al. (2025)
217.	Falcarindiol	260.1776	261.1850	0.4557	9.4727	6800.0068	Polyacetylene	
218.	Palmitic acid-3β-sitosterol ester	800.6530	801.6640	4.5876	14.7598	5179.2822	Sterol ester	Walter (1963)
219.	Lobetyolinin	558.2312	559.2362	-4.1364	14.7426	4484.7183	Polyacetylene	Kim et al. (2025)
220.	Campesterol acetate	442.3811	443.3893	2.2226	12.4425	3085.3879	Sterol ester	
221.	Lobetyolinin	558.2312	559.2364	-3.7919	14.1750	2950.5100	Polyacetylene	
222.	Vernolic acid	296.2351	297.2411	-4.3514	13.8497	2295.6082	Fatty acid	
223.	Cholesteryl palmitate	624.5845	625.5932	2.2592	13.7720	2220.2390	Sterol ester	

Table 2. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
Lipid Compounds								
224.	Ethyl palmitoleate	282.2559	283.2637	1.8623	10.7056	1528.8878	Fatty acid ester	Yoon et al. (2011)
225.	Panaxydol	260.1776	261.1856	2.7557	13.2598	1368.0096	Polyacetylene	
226.	Panaxytriol	278.1882	279.1959	1.6497	10.5129	1029.4171	Polyacetylene	
227.	Ciryneol C	282.1387	283.1473	4.9910	14.0031	849.9122	Polyacetylene	
228.	Ethyl pentadecanoate	270.2559	271.2638	2.5453	10.9758	663.8510	Fatty acid ester	
229.	Ciryneol A	320.1988	321.2055	-1.5585	11.1455	452.4031	Polyacetylene	Kim et al. (2025)
230.	2-Eicosenal	294.2923	295.3002	2.1917	11.6866	408.1368	Fatty aldehyde	
231.	Arachidonic acid	304.2402	305.2477	0.7202	9.2609	373.4691	Fatty acid	
232.	Ethyl linoleate	308.2715	309.2801	4.0197	11.0281	250.9288	Fatty acid ester	
233.	Phosphatidyl ethanolamines	745.5622	746.5714	2.5991	8.2300	236.2152	Phospholipid	
Amino Acids and Polypeptides								
234.	Morusimic acid E	507.3043	508.3112	-0.7965	11.6726	219.0474	Amino acid derivative	Kim et al. (2025)
Organic Acids								
235.	Vitamin B5	219.1107	220.1173	-3.1454	1.7973	1757.1880	Vitamin	Kim et al. (2025)
Other Compounds								
236.	Pyropheacophorbide A	534.2631	535.2714	1.9982	10.1522	4201.6167	Chlorophyll derivative	Kim et al. (2025)
237.	Phenanthrene	178.0783	179.0853	-1.0107	14.2904	924.6709	Polycyclic aromatic hydrocarbon	
238.	Adenosine	267.0968	268.1034	-2.4188	1.0684	654.8619	Nucleoside	
239.	Senkyunone	326.2246	327.2316	-0.6828	9.0944	601.8473	Phthalide	
240.	Anemonin	192.0423	193.0488	-3.7360	9.4232	563.5779	Butenolide	

Table 3. Putative metabolites identified in the methanolic extract of *A. triphysa* obtained by UPLC-ESI-QTOF-MS ranked from the highest intensities and categorized according to compound class

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
1.	Prosapogenin 2	560.3349185	561.3435	2.400194	6.096200466	114769.77	Triterpenoid	Kim et al. (2025)
2.	12-Deoxywithastramonolide	470.2668389	471.2755	2.981012	7.945663452	102711.6	Withanolide	
3.	Withametelin G	470.2668389	471.2755	2.856361	7.496209145	87900.508	Withanolide	Baig et al. (2020)
4.	Withametelin G	470.2668389	471.2749	1.750612	6.094381332	52708.375	Withanolide	
5.	Paeonolide F	510.3345246	511.3415	-0.65222	11.24584198	38803.684	Triterpene lactone	He et al. (2010)
6.	Nigakilactone H	424.209718	425.2161	-2.08053	11.36730862	31937.59	Quassinoid	
7.	Roburic acid	440.3654308	441.3734	1.463468	13.11184025	30052.039	Triterpenoid	Kim et al. (2025)
8.	1 α ,7 β -Di(4-methylseneciocyloxy)oplopa-3(14)Z,8(10)-dien-2-one	442.2719243	443.2795	0.717607	6.092999458	17469.104	Sesquiterpenoid	Yaoita et al. (1999)
9.	Poricoic acid E	500.3137891	501.3218	1.478628	6.093520164	14208.956	Triterpenoid	Kim et al. (2025)
10.	Poricoic acid F	498.3345246	499.3428	1.948002	12.43893623	13392.942	Triterpenoid	
11.	Daturametelin D	436.2613596	437.2675	-2.48912	10.58079815	12128.167	Withanolide	
12.	Ganolucidic acid B	502.3294392	503.3373	1.069824	6.573443413	11280.352	Triterpenoid	
13.	3-Epiursolic acid	456.3603454	457.3692	3.369635	9.829660416	10651.523	Triterpenoid	
14.	23-Acetate alisol K	526.3294392	527.3379	2.213607	8.241868973	10466.8	Triterpenoid	
15.	Daturametelin A	600.3298331	601.3347	-4.08728	4.622598648	10041.649	Withanolide	
16.	Belamcandal	528.3450893	529.3522	-0.33448	7.206793308	9607.9629	Triterpenoid	
17.	2-Hydroxyesculentic acid	518.3243538	519.3315	-0.33467	3.89519453	9605.4043	Triterpenoid-derivative	
18.	Paeonolide G	512.3137891	513.3231	3.930963	9.032273293	9483.6807	Triterpene lactone	Yang et al. (2020)
19.	Phytolaccagenic acid	516.3450893	517.3533	1.897148	8.020344734	9196.7432	Triterpenoid	Kim et al. (2025)
20.	23-Acetate alisol K	526.3294392	527.3369	0.328075	7.322202682	9150.3496	Triterpenoid	
21.	(25R)-Spirostan-4-ene-3,12-dione	426.2770097	427.2846	0.810721	7.321075916	8894.6426	Steroid	
22.	Iridobelamal A	474.3709101	475.3802	4.179892	9.766801834	8068.1655	Triterpenoid	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
23.	3-Epiursolic acid	456.3603454	457.3689	2.812886	9.341803551	7375.7505	Triterpenoid	Kim et al. (2025)
24.	Poricoic acid B	484.3188745	485.3249	-2.52973	4.867298126	7164.6201	Triterpenoid	
25.	Elculentic acid	502.3294392	503.3356	-2.14652	4.805521011	6807.0962	Triterpenoid	Zhang et al. (2023)
26.	Ambrolal	438.3497807	439.3574	0.731207	11.43327332	6781.499	Triterpenoid	Yang et al. (2011)
27.	Withafastuosin E	488.2774036	489.2855	1.600497	7.947486877	6474.3779	Withanolide	Kim et al. (2025)
28.	Diosgenin-3,6-dione	426.2770097	427.2852	2.185599	12.43983746	6168.189	Steroid	
29.	Ganoderic acid α	574.3141831	575.3201	-2.38434	10.60497475	6052.2559	Triterpenoid	Kim et al. (2025)
30.	Cucurbitacin B	558.3192684	559.3273	1.400945	7.284403324	5876.251	Triterpenoid	
31.	Curculigenin C	458.3759955	459.3829	-0.90528	14.7950716	5233.8438	Steroidal sapogenin	Kim et al. (2025)
32.	5-Dehydrokarounidiol	438.3497807	439.3574	0.707524	10.45073032	5078.0205	Triterpenoid	
33.	Prosapogenin 3	896.4769509	897.4806	-3.99466	7.036279202	5058.3696	Triterpenoid	Kim et al. (2025)
34.	Neocimisine	576.3298331	577.3361	-1.67825	11.26698208	4559.4438	Triterpenoid saponin	
35.	2 α ,3 α ,23-Trihydroxy-olean- 12-en-28-oic acid methyl ester	502.3658247	503.3747	3.094282	8.890688896	4261.3472	Triterpenoid	Li et al. (2012)
36.	Daturametelin C	468.2875744	469.2967	3.925052	9.68820858	4001.7881	Withanolide	Kim et al. (2025)
37.	Bufotalin	444.2511889	445.2576	-2.00411	7.201224804	3948.9236	Cardenolide	
38.	Poricoic acid D	514.3294392	515.3372	0.883891	7.492887974	3743.4849	Triterpenoid	Yaoita et al. (1999)
39.	1 α -Angeloyloxy-7 β -(4- methylseneciolyloxy)oplopa -3(14)Z,8(10)-dien-2-one	428.2562743	429.265	3.358138	7.938891411	3668.3618	Sesquiterpenoid	
40.	8 β ,9 α -Dihydroganoderic acid J methyl ester	530.3243538	531.3328	2.142839	12.44570827	3428.1306	Triterpenoid	Yi et al. (2009)
41.	Poricoic acid E	500.3137891	501.3224	2.570424	7.918638706	3415.6528	Triterpenoid	Kim et al. (2025)

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
42.	2 α ,3 α ,24-Trihydroxyolean-11,13(18)-dien-28-oic acid methyl ester	500.3501746	501.3593	3.738372	9.59475708	3295.6626	Triterpenoid	Tchunte Tchuenmogne et al. (2017)
43.	Methyl kulonate	484.35526	485.3636	2.193073	12.23330116	3226.9634	Triterpenoid	Kim et al. (2025)
44.	Esculentagenin	546.3192684	547.3278	2.344953	12.43890095	3123.5225	Triterpenoid	
45.	Esculentoside F	812.419436	813.4243	-2.90542	9.570521355	3004.281	Triterpenoid saponin	
46.	3-Hydroxy-12,14-diene-27-nordeane-28-nic acid	454.3083098	455.3151	-1.13258	7.809821129	2935.6418	Nortriterpenoid	N/A
47.	Digiprolactone	196.1099444	197.1167	-2.73593	3.29647851	2807.0835	Cardenolide	Kim et al. (2025)
48.	(25R)-Spirostan-3,6,12-trione	442.2719243	443.2787	-1.11934	4.684856892	2692.6377	Steroidal sapogenin	Xu et al. (1998)
49.	Telocinobufagin	402.2406242	403.2491	2.931977	7.942273617	2643.1206	Cardenolide	Kim et al. (2025)
50.	Melianol	612.3298331	613.3371	-0.05652	9.696967125	2474.7275	Triterpenoid	
51.	Paeonenolide F	510.3345246	511.3424	1.226464	9.530531883	2448.7314	Triterpene lactone	He et al. (2010)
52.	Ganoderic acid G	532.3036184	533.311	0.201447	9.56033802	2360.488	Triterpenoid	
53.	Ganoderenic acid B	514.2930537	515.3	-0.63759	9.148253441	2343.873	Triterpenoid	
54.	Poricoic acid AM	512.3501746	513.3558	-3.25042	8.392131805	2262.936	Triterpenoid	Kim et al. (2025)
55.	Tsugaric acid B	528.3814748	529.3879	-1.5713	13.61667728	2229.6338	Triterpenoid	
56.	5-Dehydrokarounidiol	438.3497807	439.3581	2.478795	13.69818878	2179.7644	Triterpenoid	
57.	25(S)-Ruscogenin	430.3083098	431.3156	-0.0011	8.77067852	2154.7568	Steroidal sapogenin	
58.	Bufalin	386.2457096	387.2512	-4.68952	12.82840252	2098.999	Cardenolide	
59.	Methyl lucidenate P	532.3036184	533.3105	-0.70416	8.422442436	2051.6929	Triterpenoid	
60.	Withafastuosin E	488.2774036	489.2849	0.534583	7.508662701	1940.2562	Withanolide	
61.	Siraitic acid B	470.3032245	471.3105	-0.06333	8.416387558	1724.8662	Triterpenoid	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
62.	3-epi-Dehydropachymic acid	526.3658247	527.3706	-4.69203	10.02452374	1687.359	Triterpenoid	Mahato et al. (1981)
63.	Neohecogenin-3-O- β -D-glucopyranoside	592.3611333	593.3676	-1.30794	5.766927719	1684.4785	Steroidal saponin	
64.	Diosgenone	412.2977451	413.3065	3.518002	8.777817726	1683.304	Steroid	
65.	Marsdenoside H	956.4980802	957.5044	-0.97905	14.15917778	1649.1671	Steroidal glycoside	
66.	3-O-(2'E,4'Z-Decadienoyl) ingenol	498.2981391	499.3033	-4.32706	11.26442528	1643.1284	Diterpenoid	Kim et al. (2025)
67.	Betulinic acid	456.3603454	457.3687	2.435552	8.795861244	1628.6411	Triterpenoid	
68.	Daturametelin J	632.3196624	633.3246	-3.66018	8.262569427	1572.9784	Withanolide	
69.	Daturametelin H	598.3141831	599.3196	-3.13928	7.961038589	1536.6744	Withanolide	
70.	Isolinderoxide	244.1463299	245.1542	2.221654	9.095147133	1444.474	Sesquiterpene	
71.	Soyasaponins I methyl ester	940.5395511	941.544	-3.02847	7.927937031	1434.1018	Triterpenoid saponin	Rios et al. (2012)
72.	Abrisapogenol E	474.3709101	475.3788	1.289025	9.343858719	1383.4501	Triterpenoid	
73.	Rubiatriol	458.3759955	459.3823	-2.1373	8.353288651	1377.9417	Triterpenoid	
74.	Biatractylolide	462.2770097	463.2825	-3.94162	7.775570869	1290.7384	Sesqui-terpenoid	
75.	Majoroside F3	800.492207	801.4976	-2.38784	9.095776558	1266.3451	Steroidal saponin	
76.	25-Hydroxy-3-epi-dehydrotumulosic acid	500.3501746	501.3566	-1.61484	9.000000954	1265.2223	Triterpenoid	Kim et al. (2025)
77.	Phytolaccagenin	532.3400039	533.3494	3.904088	9.087179184	1219.6876	Triterpenoid	
78.	Methyl ganoderate B	530.3243538	531.3304	-2.33294	12.82720852	1201.0221	Triterpenoid	
79.	Periplocoside M	604.3611333	605.3705	3.415167	9.245533943	1141.3752	Steroidal glycoside	
80.	Nigakilactone A	378.2042387	379.2126	2.881914	7.216326714	1095.3832	Quassinoid	
81.	Cynatratoside C	778.4139567	779.4198	-1.89615	7.223145962	1090.1707	Steroidal saponin	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
82.	11 α ,12 α -Epoxy-3 β ,23-dihydroxy-30-norolean-20(29)-en-28,13 β -olide	470.3032245	471.3102	-0.55103	6.585600853	1073.9523	Triterpenoid	N/A
83.	Polyphyllin G	1048.545424	1049.549	-3.97618	6.639892101	1034.8569	Steroidal saponin	Kim et al. (2025)
84.	5,6,7,7 α -Tetrahydro-4,4,7 α -trimethyl-2(4H)-benzofuranone	180.1150298	181.1218	-2.59547	5.936564922	1017.8639	Mono-terpenoid	Kerk et al. (2018)
85.	Hecogenin-3-O- β -D-glucopyranosyl(1 $\rightarrow$ 4)- β -D-galactopyranoside	754.4139567	755.4194	-2.39851	7.285889626	974.88947	Steroidal saponin	Wu et al. (1996)
86.	20-Hydroxylganoderic acid G	548.298533	549.3073	2.746103	8.013954163	941.17834	Triterpenoid	
87.	Poricoic acid B	484.3188745	485.3251	-2.21873	3.946381807	929.2251	Triterpenoid	
88.	Olibanumols J	460.3916455	461.3976	-2.91411	11.12848854	876.95953	Triterpenoid	Kim et al. (2025)
89.	23-Acetate alismaketone A	530.3607393	531.3681	0.151769	9.203015327	872.14105	Triterpenoid	
90.	Eburicoic acid	470.3759955	471.3818	-3.21309	10.4340353	826.06781	Triterpenoid	
91.	Siraitic acid C	440.2926598	441.2992	-1.69909	7.676539421	825.00244	Triterpenoid	
92.	Withametelin E	486.2617536	487.2688	-0.52297	7.94411087	807.78601	Withanolide	
93.	Rhapontisterone C	508.3400039	509.348	1.31624	12.83343887	807.02435	Phyto-ecdysteroid	Guo et al. (1991)
94.	Neohecogenin acetate	472.3188745	473.3256	-1.19467	3.843609571	747.87921	Steroidal sapogenin	Marker and Lopez (1947)
95.	Hederagenin 3 β ,23-acetonide	512.3865601	513.3913	-4.89671	11.64729023	747.65881	Triterpenoid	Chakroborty et al. (2023)
96.	22-Hydroxy-25(R,S)-furostan-5-en-12-one-3 β ,22,26-triol-26-O- β -D-glucopyranoside	608.3560479	609.3644	1.822353	7.519083977	723.33948	Steroidal glycoside	N/A
97.	Dehydroabietic acid	300.2089301	301.216	-0.81215	13.31380844	718.27185	Diterpenoid	Kim et al. (2025)

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
98.	Cimiaceroside A	618.3767833	619.3821	-3.12277	6.566445351	714.24377	Triterpenoid saponin	Kim et al. (2025)
99.	Arteannuin A	206.1306798	207.1372	-3.72667	2.925526857	689.30127	Sesquiterpene lactone	
100.	Hexanorcucurbitacin F	404.2562743	405.262	-3.81671	10.46108341	680.19055	Triterpenoid	
101.	Picfeltarraenin IA	762.4190421	763.4239	-3.15515	10.41745377	647.23126	Triterpenoid saponin	
102.	Polyporusterone B	476.3137891	477.3204	-1.42311	3.90629077	634.22144	Steroid	
103.	Esculentoside D	694.3928273	695.3996	-0.7641	4.605885029	633.86896	Triterpenoid saponin	Ito et a. (1998)
104.	16-O-Acetylisoiridogermanal	516.3814748	517.3878	-1.83042	10.06758213	631.94696	Triterpenoid	
105.	Abrusoside A	646.3716979	647.3759	-4.68856	6.872922421	619.4715	Triterpenoid saponin	
106.	23,27-Dihydroxypennogenin	462.2981391	463.3046	-1.66393	14.78032875	595.48053	Steroidal sapogenin	
107.	3 β ,4 β ,23-Trihydroxy-24,30-dinorolean-12,20(29)-dien-28-oic acid	458.3032245	459.3105	-0.09281	3.901440382	590.25269	Triterpenoid	
108.	Quinatoside C	720.4084774	721.4165	1.020552	5.621268749	587.91815	Triterpenoid saponin	Kim et al. (2025)
109.	Betulin	442.3810808	443.3885	0.424818	12.21482182	582.34515	Triterpenoid	
110.	(3 β ,12 β ,16 β)-12-Acetoxy-16,23-epoxy-9,19-cyclolanost-22-ene-24-one-3-O- β -D-xylopyranoside	644.3924334	645.399	-1.08507	9.883335114	576.95465	Triterpenoid saponin	N/A
111.	Ganoderenic acid G	512.2774036	513.2835	-2.3519	8.020517349	567.50555	Triterpenoid	Kim et al. (2025)
112.	Actein	676.3822626	677.3894	-0.22825	4.69209671	561.24292	Triterpenoid saponin	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
113.	Ganoderic acid H	572.298533	573.3051	-1.186	4.051460266	553.966	Triterpenoid	
114.	Bornyl transcinnamate	284.17763	285.1857	2.696418	9.685900688	517.35669	Mono-terpenoid	
115.	Tumulosic acid	486.3709101	487.3779	-0.663	13.37252045	514.54382	Triterpenoid	
116.	Strophanthidine	404.2198888	405.2288	4.07976	7.706426144	514.40265	Cardenolide	
117.	Tetrahydroxyurs-12-en-28-oic acid	504.3450893	505.3519	-0.99078	9.693921089	512.0191	Triterpenoid saponin	Yuan et al. (2008)
118.	Mudanpioside D	510.1737264	511.182	1.894966	2.753979445	511.17282	Monoterpene glycoside	
119.	1,1,6-Trimethyl-1,2-dihydronaphthalene	172.1252005	173.1323	-0.79173	7.937543392	508.70157	Norisoprenoid	
120.	Cimicifugoside H2	634.3716979	635.3774	-2.45006	5.358248711	493.86758	Triterpenoid saponin	Kim et al. (2025)
121.	Linderazulene	210.1044651	211.1121	1.691378	9.092419624	479.4733	Sesqui-terpenoid	
122.	Nimbolidin D	726.3615272	727.3672	-2.22167	7.687717915	453.61911	Limonoid	
123.	Lablab saponin I	1082.529774	1083.532	-4.9629	6.782077789	452.18967	Triterpenoid saponin	
124.	7 β -(3-Ethyl-cis-crotonoyloxy)-14-hydroxy-1 α -(2-methylbutyryloxy) notonipetranone	448.282489	449.2877	-4.69326	2.487339973	449.58548	Sesquiterpenoid	Kikuchi and Suzuki (1992)
125.	Xantholide B	232.1463299	233.154	1.811582	9.688477516	444.10999	Sesquiterpene lactone	Kim et al. (2025)
126.	Curculigo saponin G	782.4816423	783.49	1.33712	10.572649	443.45053	Triterpenoid saponin	Xu et al. (1992)
127.	Lucidenic acid N (LM1)	460.282489	461.2908	2.234739	6.093472481	440.26627	Triterpenoid	
128.	Daturametelin I	616.3247478	617.3295	-4.01264	3.710426569	439.02063	Withanolide	Kim et al. (2025)
129.	Cimidahuside I	678.3979127	679.4045	-1.0498	5.593960762	433.1557	Triterpenoid saponin	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Terpenoids</i>								
130.	Neohecogenin-3-O- β -D-xylopyranosyl(...)-glycoside	1194.566948	1195.573	-0.70166	8.349611282	406.29727	Steroidal saponin	Li et al. (1990)
131.	Methyl 2 α -hydroxyursolate	486.3709101	487.38	3.626746	9.847201347	389.80164	Triterpenoid	Kim et al. (2025)
132.	3-O-Formyl-20R,21-epoxyresibufogenin	428.2198888	429.2254	-4.06169	8.35577774	364.46484	Cardenolide	Kino et al. (2007)
133.	Azedarachin C	586.2777976	587.2859	1.336443	2.979445696	352.82428	Limonoid	Kim et al. (2025)
134.	Clerodendrin	622.1169994	623.123	-2.11745	1.074236274	346.97791	Diterpenoid	Sakinah et al. (2025)
135.	6,17-Epoxyathyrol-5,15-diacetate-3-phenylacetate	552.2723183	553.2816	3.570925	8.362355232	346.3259	Diterpenoid	Sakinah et al. (2025)
136.	25-O-Acetyl-7,8-didehydrocimigenol-3-O- β -D-xylopyranoside	660.387348	661.3943	-0.51411	5.808300495	336.38699	Triterpenoid saponin	Sun et al. (2016)
137.	Androsta-4-ene-3,17-dione	286.1932801	287.1995	-3.73085	13.31116676	335.66013	Steroid	Kim et al. (2025)
138.	Cholestenone	384.339216	385.3483	4.691395	12.86777401	332.04358	Steroid	Hu and Chen (1997)
139.	Chrysanthediol A	236.17763	237.1854	2.002016	12.60749722	331.16843	Sesquiterpenoid	
140.	1,1,6-Trimethyl-1,2-dihydronaphthalene	172.1252005	173.1325	0.113202	9.684750557	305.13519	Norisoprenoid	Kim et al. (2025)
141.	Mubenoside A	884.4769509	885.4798	-4.94578	11.51193523	281.3143	Triterpenoid saponin	
142.	Apocynoside I	386.1940679	387.2007	-1.6187	2.38448	278.49014	Norisoprenoid glycoside	Liu et al. (2003)
143.	Dehydroisoandrosterone	288.2089301	289.2164	0.827323	12.60964012	273.27399	Steroid	
144.	Cimidahuside D	692.3771773	693.3845	0.098667	5.343167305	238.15292	Triterpenoid saponin	Kim et al. (2025)
145.	Neotigogenin-3-O-multiglycoside	1004.51921	1005.53	3.848576	6.084420681	229.98277	Steroidal saponin	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
Terpenoids								
146.	Zederone	246.1255944	247.133	0.609953	3.787692308	218.55418	Sesquiterpenoid	Kim et al. (2025)
147.	Lindestrene	214.1357652	215.144	4.574203	9.68194294	186.18074	Sesquiterpene lactone	
Phenolics								
148.	Ellagic acid	302.0062672	303.0138	0.913358	2.714730024	65939.758	Tannin	Kim et al. (2025)
149.	Laevigatin A	802.0864871	803.0942	0.510471	2.124437809	22511.584	Tannin	
150.	7-Hydroxy-1-methoxy-2-methoxyxanthone	286.0477381	287.0551	0.295445	2.827385426	20073.691	Xanthone	Mochamad et al. (2024)
151.	1,3-Dihydroxy-2-hydroxymethylanthraquinon e-3-O-β-D-xylopyranoside(1→6)-β-D-glucopyranoside	564.1479056	565.1553	0.148657	2.312623501	11373.795	Anthraquinone	Kim et al. (2025)
152.	2-Acetylemodin_1	312.0633881	313.0704	-0.905	2.605144024	8456.0293	Anthraquinone	Kim et al. (2025)
153.	Castalagin 2,3-(S)-	934.071231	935.0802	1.846773	2.413781881	4735.8735	Tannin	
154.	Hexahydroxydiphenoyl-D-glucose	482.0696553	483.0753	-3.41324	1.970894456	3121.8982	Tannin	Kim et al. (2025)
155.	1,7-Diphenyl-6(E)-hepten-3-one	264.1514153	265.1588	0.451856	7.931313515	2612.9976	Phenyl-propanoid	
156.	4-O-Acetyl-caffeic acid	222.0528234	223.0611	4.331116	9.838912964	2532.9399	Phenyl-propanoid	Kim et al. (2025)
157.	Norbergenin	314.063782	315.0706	-1.39956	2.00387907	2523.7722	Phenolic glycoside	
158.	6-Hydroxyaloeemodin	286.0477381	287.0547	-1.09692	4.590468884	2473.3062	Anthraquinone	Zhang et al. (2004)
159.	Deoxyschizandrin	416.2198888	417.2261	-2.55631	5.503927708	1746.0841	Tannin	
160.	Tellimagrandin I	786.0915725	787.0956	-4.12001	2.729388952	1694.9208	Tannin	Haslam and Uddin (1967)
161.	Isochebulic acid	356.0379612	357.0447	-1.43027	1.070447922	1501.9928	Tannin	
162.	Neochebulic acid	356.0379612	357.0447	-1.51441	1.457219005	1392.8191	Tannin	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Phenolics</i>								
163.	3-O-Methyl ellagic acid	316.0219172	317.0285	-2.19495	2.805012703	1291.6312	Ellagic acid derivative	
164.	Geraniin	952.0817957	953.091	2.02179	2.293144464	1164.8839	Dehydroellagitann in	
165.	Pedunculagin	784.0759225	785.0808	-3.00429	3.553444386	1056.6775	Tannin	Kim et al. (2025)
166.	Asaricin	192.0786442	193.0854	-2.83125	2.083775282	997.58118	Phenylpropanoid	
167.	5-Hydroxy-1,7- diphenylheptan-3-one	282.1619799	283.1693	0.164877	7.932971001	841.17438	Phenylpropanoid	
168.	Gallic acid	170.0215233	171.0283	-3.05638	1.999985814	759.32581	Phenolic acid	
169.	Mulberrofuran O	646.2202827	647.2276	0.081787	14.17082691	703.80298	Stilbenoid	
170.	Nortrachelogenin 8'-O- β - glucoside	536.1893765	537.1961	-1.1002	2.85577178	686.17487	Lignan	Chen et al. (2018)
171.	Evodionol	248.104859	249.1112	-3.85223	2.508055449	680.61609	Phenylpropanoid	
172.	Dehydrodiisoeugenol	326.1518092	327.1589	-0.46123	6.210541725	651.87708	Lignan	
173.	Ginkgolic acid	346.250795	347.2579	-0.52309	13.10512924	630.26392	Alkyl phenol	
174.	1,4-Dihydroxy-2- methoxybenzene	140.0473441	141.0543	-2.29182	1.049572468	628.27863	Phenol	Kim et al. (2025)
175.	Bakuchiol	256.1827154	257.1909	3.39475	7.168935776	598.62897	Alkyl phenol	
176.	Aloe-emodin	270.0528234	271.0597	-1.6296	2.909784079	575.77057	Anthraquinone	
177.	3-O-trans-Feruloylquinic acid	368.1107322	369.1178	-0.54083	3.158830881	574.07196	Phenylpropanoid	
178.	Citrusin A	538.2050266	539.2116	-1.32341	2.603666544	555.69019	Lignan	
179.	Amurenlactone A	368.1107322	369.1179	-0.35603	2.76908803	532.84344	Phenylpropanoid	Zhou et al. (2008)
180.	Murrayacarpin A	206.0579088	207.0646	-2.83703	3.143621206	521.88916	Coumarin	Kim et al. (2025)
181.	Agrimol B	682.2989269	683.3069	1.019916	13.12056923	520.41724	Phloroglucinol derivative	
182.	Blestrianol D	452.1623739	453.1674	-4.87843	7.411738396	511.94473	Stilbenoid	He et al. (2017)

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Phenolics</i>								
183.	Euphormisin M1	910.1076165	911.117	2.344395	2.226288795	503.66412	Tannin	Yoshida et al. (1994)
184.	Yakuchinone B	310.1568946	311.1638	-1.19333	9.105443001	498.37109	Phenyl-propanoid	
185.	Butylphthalide	190.0993797	191.1069	1.436454	9.100990295	481.19843	Phthalide	
186.	(-)-Lariciresinol	360.1572885	361.1632	-3.68196	5.322453499	463.20996	Lignan	
187.	(-)-Acuminatin	340.1674593	341.174	-2.13835	7.932186127	434.72113	Lignan	
188.	Isobutyl cinnamate	204.1150298	205.1215	-4.12917	2.274156094	420.18558	Phenyl-propanoid	Kim et al. (2025)
189.	5-Formylxanthoxol	230.0215233	231.028	-3.56251	2.252244234	407.74789	Coumarin	
190.	Senkyunolide	192.1150298	193.1218	-2.5854	2.226055861	395.49841	Phthalide	
191.	1,7-Diphenyl-4,6-heptadien-3-one	262.1357652	263.1423	-2.96658	7.937577248	357.25125	Phenyl-propanoid	
192.	Glehlinside A	674.2574561	675.2652	0.762486	3.15752387	340.59442	Lignan	
193.	Ligustrosidic acid	552.1842911	553.1914	-0.21777	2.550342321	335.76855	Secoiridoid	N/A
194.	Polygoacetophenoside	346.0899968	347.0964	-2.56766	1.067258954	335.74121	Phenolic glycoside	
195.	(+)-Acetoxypinoresinol	416.1471177	417.1544	0.119284	3.160834312	331.96588	Lignan	
196.	1,6-Dihydroxy-2-methoxyanthraquinone	270.0528234	271.0601	-0.0655	4.424588203	328.83603	Anthraquinone	
197.	(-)-Secoisolariciresinol-4-O- β -D-glucopyranoside	524.225762	525.2331	0.106269	9.108434677	318.79428	Lignan	
198.	3-O-trans-Coumaroylquinic acid	338.1001676	339.107	-1.16385	3.237043381	313.50333	Phenyl-propanoid	Kim et al. (2025)
199.	Theogallin	344.0743467	345.0811	-1.62134	1.497487783	294.69659	Phenolic acid	
200.	Isopropyl-p-benzyl alcohol	136.088815	137.0957	-3.02571	2.659976721	289.05151	Phenyl-propanoid	N/A
201.	3,8-Dihydroxy-4,10-dimethoxy-7-oxo-benzopyrano-benzopyran	342.0739528	343.0806	-1.75758	2.637146473	278.64081	Xanthone	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
Phenolics								
202.	Gomisin K2	402.2042387	403.21	-3.77063	6.935842991	269.29855	Lignan Phenolic acid ester	Kim et al. (2025)
203.	Methyl gallate	184.0371734	185.044	-2.30113	2.454370737	201.05293		
Flavonoids								
204.	Genistin	432.1056469	433.1132	0.577055	2.617186069	102269.7	Flavonoid glycoside	Kim et al. (2025)
205.	Trifolin	448.1005615	449.1077	-0.28693	2.827460527	15574.616	Flavonoid glycoside	
206.	Pinnatifinoside A	414.0950822	415.1019	-1.17491	2.613270998	6901.4067	Flavonoid glycoside	
207.	Kaempferol-3-glucuronide	464.0954761	465.1022	-1.12169	2.677722692	5965.3623	Flavonoid glycoside	
208.	7-O- α -L-Rhamnosyl-3-O- β - D-glucopyranosyl kaempferol	594.1584703	595.1654	-0.53921	2.171422243	2363.9324	Flavonoid glycoside	Zhang et al. (2025)
209.	Corylinal	282.0528234	283.0594	-2.52108	2.614259243	1890.5391	Isoflavone	Kim et al. (2025)
210.	Kaempferol 3-O- β -D- glucuronopyranoside	462.079826	463.0865	-1.31942	2.838155031	1650.3298	Flavonoid glycoside	Bidel et al. (2015)
211.	Sanggenon J	488.2198888	489.2275	0.689979	14.17398548	766.02936	Flavonoid	Kim et al. (2025)
212.	Patuletin-7-O-(6"- isobutyryl)-glucoside	578.1635557	579.1701	-1.27458	2.463741064	635.6748	Flavonoid glycoside	Heilmann et al. (1999)
213.	Hibiscetin-3-O-glucoside	496.0853054	497.0913	-2.63111	1.091557741	608.54395	Flavonoid glycoside	Kim et al. (2025)
214.	Quercetin-3-O- α -D- glucuronide	478.0747407	479.0809	-2.37596	1.099346042	421.51041	Flavonoid glycoside	Zhang et al. (2010)
215.	Kaempferol 3-O- α -L- rhamnopyranosyl-(1 $\rightarrow$ 2)- β - D-glucuronopyranoside	608.1377349	609.1437	-2.20786	2.734092236	331.33347	Flavonoid glycoside	Tram et al. (2017)

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Phenolics</i>								
216.	Eriodictyol	288.0633881	289.0696	-3.82319	3.400553226	277.95697	Flavanone	Kim et al. (2025)
<i>Alkaloids</i>								
217.	β -Carboline-1-propionic acid	240.0898776	241.0969	-1.23649	2.556115389	3834.5952	Indole alkaloid	Gabriel et al. (2019)
218.	2 α ,3 β -Dihydroxy nortropane	143.0946287	144.1014	-3.21874	1.051625371	3116.5181	Tropane alkaloid	Wang et al. (2020)
219.	Zhebeinoside	593.3927677	594.4003	0.365983	7.68605423	2661.1089	Steroidal alkaloid glycoside	Kim et al. (2025)
220.	Arecoline	155.0946287	156.1014	-3.06318	1.461551905	2445.7542	Pyridine alkaloid	
221.	Narceine	445.1736668	446.1805	-1.07797	2.25590682	1360.8461	Benzylisoquinolin e alkaloid	
222.	Gentiatibetine	165.0789786	166.0858	-2.83109	1.798271775	1183.4198	Pyridine alkaloid	
223.	Pingbeidoside	623.4033324	624.4102	-0.71265	4.590352058	1164.1482	Steroidal alkaloid	
224.	Ephedradine B	522.2842204	523.2929	2.753612	8.088645935	1122.9257	Phenethylamine alkaloid	Taniguchi et al. (2012)
225.	Aristoloctam Ia N- β -D- glucopyranoside	457.1008958	458.1074	-1.66803	3.639207602	987.30432	Glycosylated alkaloid	
226.	6-Hydroxykynurenic acid	205.0375077	206.0441	-3.46268	1.849369526	776.93945	Quinoline alkaloid	
227.	1-Vinyl-4-methoxy- β - carboline	224.094963	225.1018	-1.86978	3.079866171	643.71289	Indole alkaloid	
228.	Guvacoline	141.0789786	142.0856	-4.62407	1.060431242	398.25177	Pyridine alkaloid	Li et al. (1990)
229.	4,9-Dimethoxy-1-vinyl- β - carboline	254.1055277	255.1122	-2.36715	2.782542467	378.94733	Indole alkaloid	Lee et al. (2009)

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
Alkaloids								
230.	1-Formyl-4-methoxy-β-carboline	226.0742276	227.0812	-1.38022	4.545462608	261.73953	Indole alkaloid	Kwon et al. (2018)
Lipid Compounds								
231.	Octacosane	394.4538519	395.4619	1.858607	9.09998703	19331.947	Alkane	Kim et al. (2025)
232.	Cholesteryl palmitate	624.5845317	625.5911	-1.16612	13.77257729	4671.3325	Sterol ester	
233.	Vernolic acid	296.2351449	297.2412	-4.08624	13.84346771	2280.3362	Fatty acid	
234.	5-(3-Hydroxy-4-acetoxybut-1-ynyl)-2,2'-bithiophene	292.0227857	293.029	-3.69562	2.22902298	2141.5603	Polyacetylene	
235.	9,12-Dihydroxy-15-nonadecenoic acid	328.2613596	329.268	-1.94686	11.07800198	1947.1636	Fatty acid	
236.	Panaxynol	244.1827154	245.1902	0.755335	13.11917782	1733.2864	Polyacetylene	
237.	Falcarindiol	260.17763	261.185	0.447241	13.3112154	353.95474	Polyacetylene	
238.	Stigmasterol acetate	454.3810808	455.3899	3.334877	14.36297798	328.50473	Sterol ester	
Amino Acids and Polypeptides								
239.	Heterophyllin A	727.4268618	728.4369	3.851957	5.270575523	4770.958	Peptide	Kim et al. (2025)
240.	Valine	117.0789786	118.0859	-2.77725	1.059782386	1982.4655	Amino acid	
241.	Proline	115.0633285	116.0702	-3.12587	1.054103494	651.58923	Amino acid	
242.	Glutamine	146.0691422	147.0771	4.572498	0.991101801	468.48285	Amino acid	
243.	Tyrosine	181.0738932	182.0805	-3.93137	1.060870647	346.20868	Amino acid	
244.	N-Benzoyl-phenylalanine-2-benzoylamino-3-phenylpropyl ester	506.2205575	507.2284	1.146129	8.130856514	321.49973	Peptide derivative	
Other Compounds								
245.	Senkyunone	326.2245802	327.2333	4.544189	9.090709686	42889.5	Phthalide	Kim et al. (2025)
246.	Pyrophaeophorbide A	534.263091	535.2684	-3.71729	10.12847519	4703.0283	Chlorophyll derivative	
247.	Adenosine	267.0967539	268.1036	-1.70291	1.0558604	2278.9985	Nucleoside	

Table 3. Continued...

NO.	COMPOUND NAME	EXPECTED MASS (DA)	OBSERVED M/Z	MASS ERROR (PPM)	OBSERVED RT (MIN)	RESPONSE	SUBCLASS	SUBCLASS REF.
<i>Other Compounds</i>								
248.	L-Noradrenaline	169.0738932	170.0807	-2.83751	1.063725471	1391.1941	Catecholamine	
249.	Phenanthrene	178.0782503	179.0851	-2.45789	14.2933054	845.1947	PAH	
250.	Heterodendrin	261.1212373	262.1282	-1.38772	1.059580326	753.87439	Cyanogenic glycoside	
251.	Indolylmethyl glucosinolate	448.0610217	449.0681	-0.51191	2.105507851	608.43781	Glucosinolate	
252.	Anemonin	192.0422587	193.0491	-2.03717	3.054290295	529.77344	Butenolide	
253.	Methyl- β -D-frucopyranoside	194.0790382	195.0856	-3.48019	1.049432755	504.64954	Sugar glycoside	Kim et al. (2025)
254.	2-Amino-benzoic acid	137.0476785	138.0543	-4.93931	1.055743217	410.38254	Aminobenzoic acid	
255.	2-(p-Anisyl)-5-methyl-1-hexen	204.1514153	205.1583	-2.08038	13.2108326	383.0993	Aromatic hydrocarbon	
256.	Nicotinic acid	123.0320284	124.039	-2.80092	1.062405348	227.58852	Vitamin	

Table 4. Comparison of phytochemical class diversity between the two *Ailanthus* species as revealed by UPLC-ESI-QTOF-MS

MAJOR CHEMICAL CLASS	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>	SHARED	UNIQUE TO <i>A. integrifolia</i> subsp. <i>integrifolia</i>	UNIQUE TO <i>A. triphysa</i>
Terpenoids	144	147	40	104	107
Phenolics	37	54	5	32	50
Flavonoids	25	13	1	24	12
Alkaloids	9	14	0	9	14
Lipid Compounds	18	8	4	14	4
Organic Acids	1	2	0	1	2
Amino Acids and Polypeptides	1	6	0	1	6
Other Compounds	5	12	5	0	6
TOTAL	240	256	55	185	201

Table 5. Qualitative histochemical detection of selected phytochemical classes leaf tissues of *Ailanthus integrifolia* subsp. *integrifolia* and *Ailanthus triphysa*

COMPOUND CLASS	DETECTING REAGENT	<i>A. integrifolia</i> subsp. <i>integrifolia</i>			<i>A. triphysa</i>		
		Dermal	Ground	Vascular	Dermal	Ground	Vascular
Terpenoids	Neutral Red	++	+	+	++	+	+
Phenolic Compounds	10% Ferric chloride	+	+	++	++	++	++
Alkaloids	Dragendorff's	+	++	+	+	++	+

+ high detection, ++ very high detection

Table 6. Comparative profile of terpenoid metabolites detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	144	147
Dominant metabolite type	Pentacyclic and tetracyclic triterpenoids, quassinoids, steroidal terpenoids	Pentacyclic triterpenoids, quassinoids, triterpenoid saponins, withanolide- and cardenolide-like metabolites
Quassinoids detected	Nigakilactone H, Bruceine A	Nigakilactone H, Nigakilactone A
Shared terpenoid compounds	Oleanane-, ursane-, cycloartane-, tirucallane-type metabolites; betulinic acid-related compounds; nigakilactone H	
Specialized terpenoid classes	Phytoecdysteroid-like metabolites	Withanolide-like steroids and cardenolide-like metabolites
Some putatively novel compounds/features	Nigakilactone H, Bruceine A, phytoecdysteroid-like metabolites in leaves	Nigakilactone H, Nigakilactone A, Cucurbitacin B, withanolide-like steroids, cardenolide-like metabolites, triterpenoid saponins
Chemotaxonomic implication	Enrichment in steroidal and other related chemistry	Expanded terpenoid subclass diversification and triterpenoid chemistry

Table 7. Comparative profile of phenolic metabolites detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	37	54
Dominant metabolite type	Lignans and coumarins	Hydrolyzable tannins (ellagitannins)
Shared phenolic compounds	Ginkgolic acid, bakuchiol, (–)-lariciresinol, glehlinoside A, blestrianol D	
Putatively novel compounds/features	Dominance of lignans in leaf tissue; extensive lignan diversity	Ellagitannin-dominated leaf chemistry; polymeric hydrolyzable tannins
Chemotaxonomic implication	Lignan–coumarin-enriched chemotype	Ellagitannin-dominated chemotype reflecting strong tannin biosynthesis

Table 8. Comparative profile of phenolic metabolites detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	25	13
Dominant metabolite type	Flavones, flavone glycosides, specialized flavonoids	Flavonol glycosides
Major flavonoid subclasses detected	Flavones, flavone glycosides, flavanones, isoflavonoids, coumestans, isoflavanquinones, chalcones	Flavonol glycosides, flavanones, isoflavones
Shared compound		Genistin
Putatively novel compounds/features	First flavonoid reports for the taxon	Additional glucuronidated and acylated flavonol glycosides
Chemotaxonomic implication	Indicates expanded and atypical flavonoid diversification within <i>Ailanthus</i>	Supports conserved flavonol glycoside-dominated <i>Ailanthus</i> chemotype

Table 9. Comparative profile of alkaloid metabolites detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	9	14
Dominant metabolite type	β -Carboline/indole alkaloids and steroidal alkaloids	β -Carboline alkaloids with multiple additional alkaloid subclasses
Major alkaloid subclasses detected	Indole, steroidal, quinolizidine, triterpene, phenethylamine	Indole/ β -carboline, tropane, pyridine, steroidal, benzyloquinoline, quinoline, phenethylamine
β -Carboline alkaloids detected	1-carboethoxy- β -carboline	β -carboline-1-propionic acid, dehydrocrenatine derivatives
Atypical alkaloid classes detected	Quinolizidine and triterpene alkaloids	Tropane, pyridine, quinoline, benzyloquinoline alkaloids
Putatively novel compounds/features	First alkaloid records for the taxon	Multiple atypical alkaloid subclasses not previously reported in <i>Ailanthus</i>
Chemotaxonomic implication	Supports conserved β -carboline chemistry within <i>Ailanthus</i>	Suggests expanded alkaloid biosynthetic diversity and possible ancestral pathway retention

Table 10. Comparative profile of lipid metabolites detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	18	8
Dominant metabolite type	Polyacetylenes, sterol esters, phospholipids	Sterol esters, fatty acids, long-chain alkane
Shared lipid compounds	Panaxynol, faltarindiol, cholesteryl palmitate, vernolic acid	Panaxynol, faltarindiol, cholesteryl palmitate, vernolic acid
Putatively novel compounds/features	Multiple polyacetylenes and fatty acid ethyl esters in leaves	Foliar occurrence of specialized lipids and cuticular alkane enrichment
Chemotaxonomic implication	Suggests chemically defense-oriented foliar lipid profile	Suggests cuticular and stress-associated lipid specialization

Table 11. Comparative profile of organic acids detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	1	2
Detected organic acids	Pantothenic acid (Vitamin B5)	Nicotinic acid, 2-amino-benzoic acid (anthranilic acid)
Major biochemical relevance	Coenzyme A precursor; fatty acid synthesis and metabolism	Pyridine-derived metabolite involved in cellular metabolism
Previously reported in <i>Ailanthus</i>	No prior report mentioned	Nicotinic acid previously reported in <i>Ailanthus altissima</i>
Chemotaxonomic implication	Putative occurrence in <i>Ailanthus</i> leaves	Supports occurrence of pyridine-derived metabolites within the genus

Table 12. Comparative profile of free amino acids and polypeptides detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	1	6
Dominant metabolite type	Amino acid derivative	Free amino acids and peptide derivatives
Putatively novel compounds	Morusimic acid E	Heterophyllin A; N-benzoyl-phenylalanine derivative; glutamine occurrence in <i>Ailanthus</i>
Chemotaxonomic implication	Species-level unusual metabolite occurrence	Expanded peptide chemistry within Simaroubaceae

Table 13. Comparative profile of miscellaneous metabolites detected in the leaves of *A. integrifolia* subsp. *integrifolia* and *A. triphysa*

COMPARATIVE FEATURE	<i>A. integrifolia</i> subsp. <i>integrifolia</i>	<i>A. triphysa</i>
Number of detected metabolites	5	12
Dominant metabolite type	Chlorophyll derivatives, nucleosides, phthalides, butenolides, and aromatic hydrocarbons	Catecholamines, cyanogenic glycosides, glucosinolates, sugar glycosides, phthalides, and aromatic hydrocarbons
Shared compounds	Pyrophaeophorbide A, phenanthrene, adenosine, senkyunone, anemonin	Pyrophaeophorbide A, phenanthrene, adenosine, senkyunone, anemonin
Putatively novel compounds/features	Occurrence of phenanthrene, phthalide, and butenolide metabolites in <i>Ailanthus</i> leaves	Detection of glucosinolate, cyanogenic glycoside, catecholamine, and aromatic hydrocarbon metabolites not previously reported from <i>Ailanthus</i> or Simaroubaceae
Chemotaxonomic implication	Supports conserved miscellaneous metabolic traits within the genus	Indicates broader metabolic diversification and affinities with metabolites reported from allied Sapindales families