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Comparative Phytochemical Profiling of Methanolic Extracts of Different Parts of White Dandelion (*Taraxacum coreanum*) using Hybrid Ion-mobility Q-TOF MS

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Abstract : *Taraxacum coreanum*, known as the native Korean white dandelion, has been historically used in traditional medicine due to its various therapeutic properties. However, the specific benefits and mechanisms of white dandelion in alleviating particular symptoms or diseases remain uncertain due to the complexity of its phytochemical profile. In this study, we aimed to elucidate the phytochemical profiles of methanolic extracts of different parts of the white dandelion (flower, leaf, stem, and root) using hybrid ion-mobility Q-TOF MS. Using the trapped ion mobility-based PASEF technique, 3715 and 2114 molecular features with MS2 fragments were obtained in positive and negative ion modes, respectively, and then a total of 360 and 156 phytochemical compounds were annotated by matching with a reference spectral library in positive and negative ion modes, respectively. Subsequent feature-based molecular networking analysis revealed the phytochemical differences across the four different parts of the white dandelion. Our findings indicated that the methanolic extracts contained various bioactive compounds, including lipids, flavonoids, phenolic acids, and sesquiterpenes. In particular, lipids such as linoleic acids, lysophosphatidylcholines, and sesquiterpenoids were predominantly present in the leaf, while flavonoid glycosides and lysophosphoethanolamines were notably enriched in the flower. An assessment of the total phenolic content (TPC) and total flavonoid content (TFC) of the methanolic extracts revealed that the majority of phytochemicals were concentrated in the flower. Interestingly, despite the root extract displaying the lowest TPC and TFC values, it exhibited the highest radical scavenging rate when normalized to TPC and TFC, suggesting a potent antioxidant effect. These findings and further investigations into the biological activities and medicinal potential of the identified compounds, particularly those exclusive to specific plant parts, may contribute to the development of novel therapeutic agents derived from white dandelion.

Keywords : white dandelion, phytochemical, ion-mobility, Q-TOF, bioactive compound, molecular network, antioxidant activity

Introduction

Dandelion (*Taraxacum* sp.) has been widely used in many forms of traditional medicine for centuries offering health benefits by acting as a diuretic or potentially boosting the immune system to help fight infections.[1] Dandelion is known to be full of potent antioxidants that help neutralize harmful free radicals and may help prevent chronic diseases.[2,3] Besides, it is also reported to have diverse medicinal effects on various diseases or symptoms.[4,5] For instance, extracts from dandelion leaves have shown hypolipidemic effects in high cholesterol-fed rats,[6] while inulin found in its roots influences the development of healthy intestinal microflora.[7] Moreover, compounds like chicoric and chlorogenic acids, present in dandelion, have been reported to regulate blood sugar levels by enhancing insulin secretion.[8,9]

Dandelion is generally considered safe as a food by the Food and Drug Administration.[10] It can be used as a whole plant, but each part of dandelion has also been used for different purposes.[11] The flower, known for its antioxidant components, is commonly used as a tea, while the root is good for liver detoxification,[12] and is valued for its abundant triterpene, taraxasterol, and high contents of fibers, minerals, and vitamins.[3] The leaf is favored for kidney and stomach health and is often used in salads, whereas the entire plant is used for digestive and fever relief.

Recent years have seen extensive studies on the phyto-

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chemical composition of dandelion, revealing a plethora of bioactive compounds such as flavonoids, phenolic acids, and sesquiterpenes. Notably, flavonoid glucosides like luteolin-7-*O*-glucoside and luteolin-7-*O*-rutinoside, along with hydrocinnamic acid, are known to be predominant in dandelion leaves,[11] and chicoric acid and monocaffeoyltartaric acid are known to be found in dandelion flowers, roots, and leaves.[13] However, there remains much to uncover about the phytochemical profiles of different dandelion parts and their potential therapeutic applications.

Various analytical techniques have been employed to explore dandelion's phytochemical profiles. Jung et al. demonstrated different metabolite profiles of three species of *Taraxacum* (*T. coreanum, T. officinale, and T. platycarpum*) using ^{1}H NMR and GC-MS analysis.[14] LC-SPE-NMR was utilized to characterize antimicrobial compounds in dandelion root extracts.[5] Recent advancements include the use of (U)HPLC coupled with high-resolution mass spectrometry to investigate the profiles of a variety of natural products such as herbal extracts, mulberry fruit, and olive oil.[15]

Among a variety of *Taraxacum* species, in particular, *T. coreanum* (also called the white-flowering Korean dandelion) is a local cultivar of dandelion in Korea and some regions of China, and only a few studies have been reported on *T. coreanum,*[16-22] whereas most of the phytochemical profiling and biological studies have focused on *Taraxacum officinale* (common dandelion species).[3,8,23-25] It was reported that *T. coreanum* extracts attenuate LPS-induced inflammatory responses and intestinal barrier dysfunction.[21] Mo et al. also characterized inositol derivatives and phenolic compounds from the roots of *T. coreanum*.[26] However, scientific evidence supporting the medicinal or dietary use of white dandelion, particularly the specific potential benefits of the different plant parts, still remains insufficient.

This study aims to elucidate the phytochemical profiles of methanolic extracts from four different parts of white dandelion using hybrid ion-mobility quadrupole time-of-flight mass spectrometry (Q-TOF MS). Ion-mobility spectrometry (IMS) separates ions based on their size, shape, and charge, in addition to mass, thereby enhancing the resolution of complex mixtures. When combined with Q-TOF MS, this multi-dimensional separation technique allows for a clearer differentiation of compounds that might overlap in conventional LC-tandem MS analysis, providing significantly richer information. A feature-based molecular networking (FBMN) analysis was applied to delineate the plant part-specific phytochemical profiles based on MS/MS data. The insights gained from this investigation can inform the development of pharmaceutical and medicinal applications utilizing bioactive ingredients from white dandelion.

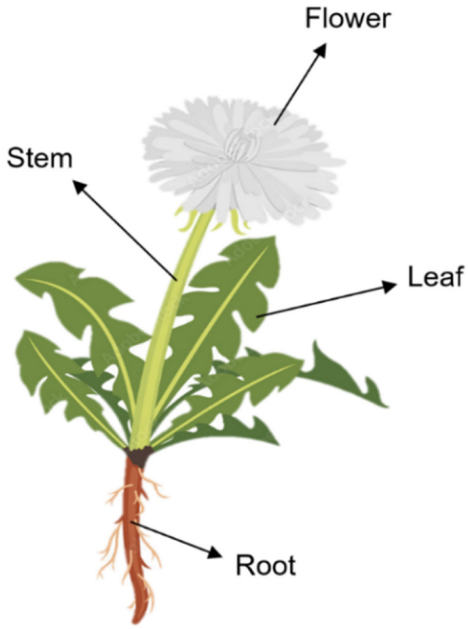

Figure 1. Illustration of four parts of white dandelion (flower, leaf, stem, and root) used in this study.

Experimental

Preparation of methanolic extracts of white dandelion

White dandelion was obtained from the Seongeosan Farm (Cheonan, Korea). The whole white dandelion was washed with water and then cut into parts (flower, leaf, stem, and root) with clean scissors (Figure 1). Four portions of white dandelion samples were lyophilized and ground using an analytical mill (A11 Basic, IKA, Korea). The powder of each portion was subjected to extraction with methanol (1 g/40 mL) using ultrasonication at 40°C for 30 min. The resulting solutions were left at room temperature for 30 min for phase-separation, and then supernatants were collected. The supernatants were filtered with a 0.45 μm Teflon syringe filter to remove insoluble materials. The filtrates were dried under a gentle nitrogen stream, and then reconstituted with methanol for LC-MS analysis.

Assessment of total phenolic and flavonoid contents

Total phenolic (TPC) and flavonoid (TFC) contents of the methanolic extracts of white dandelion were measured using a Folin-Ciocalteu assay[27,28] and a $NaNO_2$-$Al(NO_3)_3$-NaOH colorimetric assay,[29,30] respectively, with minor modifications. For the TPC assay, 100 μL of the extracts were added to a tube containing 50 μL of Folin-Ciocalteu reagent and 650 μL of deionized water, followed by the addition of 200 μL of 7.5% Na_2CO_3 solution. The mixtures were incubated at room temperature in the dark for 30 min. After the incubation, the absorption of samples was measured at a wavelength of 765 nm using a spectrophotometer. The

results were expressed in mg equivalent of gallic acid (GAE) per g dry weight of the sample.[31] For TFC, the extracts (each 100 μL) were mixed with 5% sodium nitrate (30 μL) and water (640 μL), and then placed for 5 min to ensure the oxidation of hydroxyl residues of flavonoids. After the addition of 10% aluminum chloride (30 μL), the mixtures were incubated for 6 min, and 200 μL of 1M sodium hydroxide solution was added to the mixtures to quench the reaction, followed by incubation at 25C for 30 min. The absorption of the resulting solution was measured at 510 nm. The total flavonoid content of the extract was expressed as mg catechin equivalents (CE) per gram of sample.[29] The absorbance of samples subtracted from the absorbance of the blank was used to calculate the TPC and TFC.

Antioxidant scavanging assay

The antioxidant potential of the extract was determined using a DPPH radical scavenging assay, as demonstrated previously.[27,28] 100 μL of the sample was added to a mixture of freshly prepared DPPH solution (0.1 mM in methanol) and deionized water. The mixture was incubated for 15 min at 37°C in the dark and the reduction in absorbance at 517 nm, corresponding to the radical scavenging activity, was measured by a spectrophotometer. A standard curve was obtained with different concentrations of Trolox (0.005 and 1.0 mM), and the results were expressed in mM Trolox equivalents (TE) per g dry weight of sample corresponding to the inhibition ratio of Trolox (%).

UPLC equipped with hybrid ion-mobility Q-TOF tandem MS analysis for phytochemicals

Phytochemical profiling of the methanolic extracts of white dandelion was performed on a timsTOF flex system, a hybrid ion-mobility quadrupole time-of-flight mass spectrometer (Bruker Daltonics, Bremen, Germany) coupled with an ACQUITY UPLC™ system (Waters, Milford, MA), as previously described.[32] Two microliters of the extracts were injected and separated on an ACQUITY HSS T3 column (1.8 μm, 2.1 100 mm) at a flow rate of 300 μL/min, at 40°C. The gradient was established using mobile phase A (0.1% formic acid in water) and mobile phase B (acetonitrile): 2% B for 2 min, 2–10% for 1 min, 10–25% for 7 min, 25–65% for 4.5 min, ramped up to 98% and held for 3 min, and back to 2% B maintained for 1.5 min for column conditioning. The eluate was introduced into the timsTOF flex MS through an ion source with an electrospray potential of 4.5 kV for positive ion mode and -3.6 kV for negative ion mode, respectively. The optimal values for MS parameters were as follows: 20 eV for collision energy, 2.2 bar for the nebulizer, 10 L min^{-1} and 220C for dry gas and dry temperature, respectively, and a mass range of 20 to 1300 *m/z*, with a mobility range of 0.45 to 1.45 Vs cm^{-1}. Full-scan MS data were acquired in the mass range of 20–1300 Da with collision energy set between 20–50 eV in both positive and negative modes. The parallel accumulation–serial fragmentation (PASEF) method was utilized to maximize isolation efficiency and MS/MS speed of precursors while maintaining full sensitivity,[33] as previously demonstrated.[32] For the TIMS analyzer, accumulation and ramp times were configured at 100 ms each, and ion mobility was scanned from 0.45 to 1.45 Vs/cm^2. Within a cycle of 0.53 s, one full TIMS-MS scan and two PASEF MS/MS scans were acquired. Data acquisition was performed using timsControl ver. 4.5 software (Bruker Daltonics).

Data processing and compound identification

The acquired LC-MS/MS spectra were subjected to data processing.[32] Feature extraction and compound identification were processed using MetaboScape ver. 6.0.2 (Bruker Daltonics). The intensity threshold and minimum 4D peak size were set to 350 counts and 80 points, respectively. For ion deconvolution, in positive ion mode, the primary ions ($[M+H]^+$, $[M+Na]^+$, and $[M+K]^+$) as well as the common ion ($[M+H-H_2O]^+$) were utilized. In negative ion mode, ion deconvolution was carried out using the primary ions ($[M-H]^-$ and $[M+Cl]^-$) and the common ion ($[M-H-H_2O]^-$). The tolerances for feature annotation in MetaboScape were as follows: *m/z* 5 ppm for narrow and 10 ppm for wide, mSigma 20 for narrow and 50 for wide, MS/MS 850 for narrow and 400 for wide, ΔCCS 1.5% for narrow and 3.5% for wide. Based on these parameters the similarity between the spectral library and measured spectrum for annotated compounds of interest was evaluated. Spectral libraries including Bruker MetaboBASE® Personal Library 3.0, Bruker HMDB Metabolite Library 2.0, Bruker NIST 2020 Mass Spectral Library, and Bruker Summer MetaboBASE Plant Library were employed for the identification of phytochemicals.

Feature-based molecular networking analysis

Mass spectral similarity-based molecular networking with untargeted tandem mass spectrometry data was performed using the feature-based molecular network (FBMN) method on the Global Natural Products Social Molecular Networking (GNPS) web platform.[34,35] The data were collected on a tims-TOF flex in Parallel-Accumulation Serial Fragmentation (PASEF) mode, and processed with MetaboScape. Results obtained by using MetaboScape were then exported as a feature quantification table (.TXT format) and an MS2 spectral summary (.MGF format) and uploaded to the GNPS web platform for molecular networking analysis with the FBMN workflow. The parameters for the generation of molecular networks using FBMN were as follows: precursor ion mass tolerance of 0.02 Da; fragment ion mass tolerance of 0.02 Da; minimum pairs cosine score of 0.7; Network TopK of 10; maximum connected component size of 100; minimum matched fragment ions of 6; minimum cluster size of 2, and no MSCluster.

The molecular networks generated were visualized via Cytoscape v.3.10.0.[36] The data including collision cross-section (CCS) values and additional spectral annotations, which were obtained from spectral library searches in MetaboScape, were integrated to display the molecular networks. The molecular networking job in GNPS can be accessed at https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=62ec357a217746f198a7839833e1dd99 for positive ion mode data and https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=b8c4ea7d6b964d11a76ea891de61469a for negative ion mode data.

Results and Discussion

Assessment of TPC, TFC, and antioxidant activity of methanolic extracts of four parts of white dandelion

The total flavonoid and phenolic contents (TFC and TPC) and corresponding antioxidant activities using DPPH assay were determined for four different parts–flower, stem, leaf, and root–of the white dandelion, as previously demonstrated.[32] Among these plant parts, the flower exhibited the highest concentration of total phenols at 5.87 mg GAE/g sample, closely followed by the leaf at 5.83 mg GAE/g sample, the stem at 1.88 mg GAE/g sample, and finally, the root at 1.51 mg GAE/g sample (Table 1). In terms of total flavonoids, the leaf stood out with the highest concentration at 34.41 mg CE/g sample, followed by the flower at 18.96 mg CE/g sample, the stem at 2.44 mg CE/g sample, and the root at 1.32 mg CE/g sample (Table 2), indicating that the phytochemical components (i.e., phenolic and flavonoid compounds) of white dandelion were mostly enriched in the flower and the leaf.

Looking at the scavenging efficiency normalized by TPC, interestingly, the root displayed a higher value of 37.4 compared to the flower at 14.9, with the stem and leaf showing slightly lower values of 9.4 and 8.9, respectively (Table 1). Additionally, the scavenging efficiency normalized by TFC was particularly notable for the root at 42.8, contrasting with values of 7.2, 4.6, and 1.5 for the stem, flower, and leaf, respectively (Table 2). This highlights the existence of a stronger anti-oxidant potential of certain phenolic and flavonoid components in the root.

In summary, the total contents of phenolic and flavonid compounds were predominantly observed in the leaf and flower parts of the while dandelion. However, the antioxidant efficiency of the root was notably higher compared to the other parts, suggesting the presence of significant antioxidant compounds within the root of white dandelion.

Table 1. Total phenolic content (TPC) and corresponding antioxidant scavenging activity of four parts of white dandelion.

Sample	mg GAE / g sample	Scavenging activity (%)	Scavenging rate normalized by TPC
flower	5.87	87.2	14.9
leaf	5.83	51.7	8.9
stem	1.88	17.6	9.4
root	1.51	56.4	37.4

Table 2. Total flavonoid content (TFC) and corresponding antioxidant scavenging activity of four parts of white dandelion

Sample	mg CE / g sample	Scavenging activity (%)	Scavenging rate normalized by TFC
flower	18.96	87.2	4.6
leaf	34.41	51.7	1.5
stem	2.44	17.6	7.2
root	1.32	56.4	42.8

Comparison of phytochemical profiles between four parts of white dandelion

To comparatively investigate the phytochemical profiles of four different parts of white dandelions (i.e., flower, stem, leaf, and root), each methanlic extract was subjected to UPLC/hybrid ion-mobility Q-TOF MS analysis in both positive and negative ion modes. The separation was initially performed *via* a UPLC system based on the constituents' polarity through reversed-phase chromatography, resulting in the distinct total ion chromatograms of the samples (Figure 2). The subsequent separation was done based on the conformational differences in ion mobility spectroscopy, yielding a total of 3715 and 2114 molecular features with MS2 fragmentations obtained from the positive and negative ion modes, respectively. The enhanced annotation of these complicated molecular features was illustrated by the TIMS MS heat maps in Supplementary Figure S1. Subsequently, 360 and 156 compounds were identified by matching with reference spectral libraries in the positive and negative ion modes, respectively.

The annotated phytochemical compounds were further categorized into nine classes according to the classification results obtained from ClassyFire.[37] According to the classification results, phytochemical compounds annotated from both positive and negative data were categorized into distinct classes such as 'lipid and lipid-like molecules', 'organoheterocyclic compounds', 'organic acid and derivatives', 'benzenoids', 'organic oxygen compounds', 'phehylpropanoids and polyketides', 'nucleosides, nuleotides, and analogues'. Additionally, exclusive to the positive ion mode dataset were compounds categorized as 'organic nitrogen compounds', 'organometallic compounds', and 'hydrocarbons'. Conversely, the 'lignans, neolignans and related compounds' class was solely identified within the negative ion mode dataset (see Figures 3A and 3C, and Supplementary Tables S1 and S2). Further details regarding the chemical attributes of these compounds including RT, CCS, mass errors and compound classes, can be found in the Supplementary Datasets. Note that if the components identified with the same 'Compound Name' have different

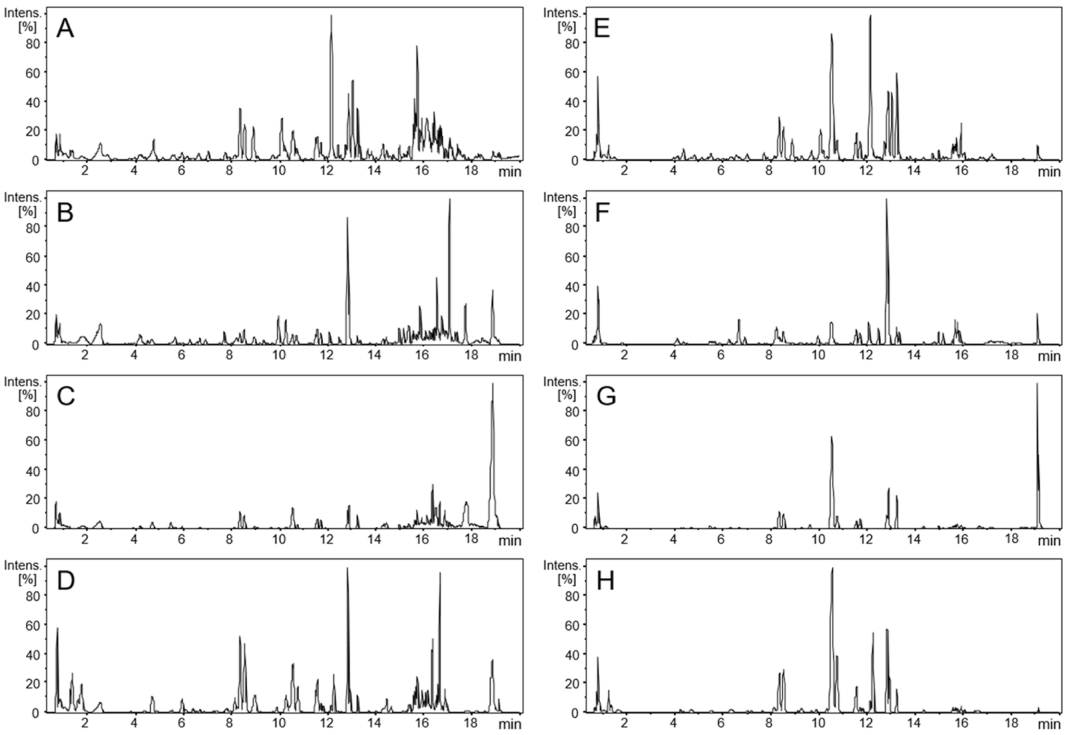

Figure 2. Total ion chromatograms obtained from four different parts of white dandelion via positive (A, B, C, and D) and negative (E, F, G, and H) ion modes. A and E, flower; B and F, leaf; C and G, stem; D and H, root.

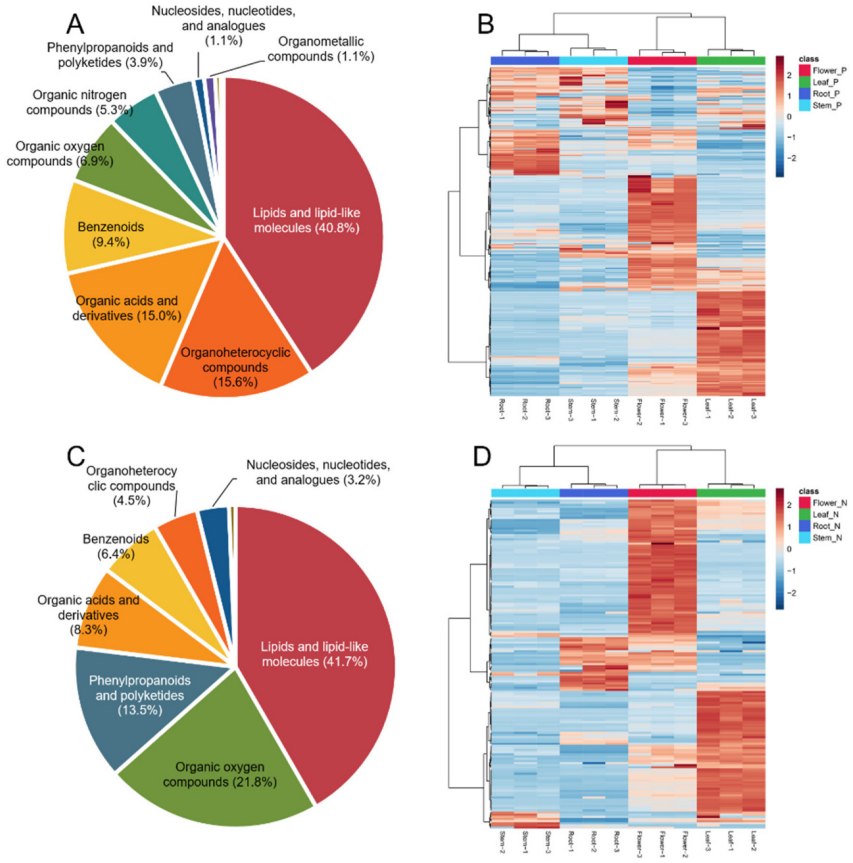

Figure 3. Pie charts showing the distribution of molecular classes of phytochemical compounds identified by positive (A, C) and negative (B, D) ion modes from methanolic extracts of white dandelion. The contribution of each of these groups was estimated based on the LC-MS peak-frequency of the total. Heatmaps showed the phytochemicals from white dandelion in positive (C) and negative (D) ion modes. The heatmaps were displayed with the compounds fitted in the criterion of p-value < 0.05, variable importance in projection (VIP) score > 1 and |fold change| > 2.

RT or CCS values, there is a possibility that they could be isomers not present in the library used for the search; therefore, they were not excluded from the list.

As shown in the Venn diagrams of the phytochemical compounds identified from different parts of white dandelions (Supplementary Figure S2), most of the compounds (~70% of the total) were found in all parts, but certain compositions were observed in specific parts. To identify the key phytochemical constituents dominant in each part, the annotated compounds were presented in heatmaps. As depicted in Figures 3B and 3D, the flower and leaf are the most enriched sources of the phytochemical compounds. Further investigation into their molecular networking analysis was conducted.

FBMN analysis of phytochemicals of four parts of white dandelion

PASEF data from the methanolic extracts of white dandelion were subjected to FBMN analysis using the GNPS web platform (https://gnps.ucsd.edu/).[34] The resulting FBMN categorized the chemical classes of each cluster and were visualized using Cytoscape, where nodes were organized into multiple superclasses including “Phenylpropanoids and polyketides”, “Organic oxygen compounds”, “Organoheterocyclic compounds”, “Organic acids and derivatives”, “Benzenoids”, and so forth (refer to Figure 4).

In the positive ion mode data analysis, a total of 138 clusters, each containing at least two nodes, were identified (see Figure 4A). Noteworthy among these were MN-2, MN-6, MN-15, and MN-17, which revealed crucial aspects of white dandelion's chemical profile. MN-2 exhibited a prevalent presence of purine nucleosides subclass, including guanosine, adenosine, and 5’-methylthioadenosine, distributed uniformly across all four plant parts (Figure 5A). Conversely, compounds such as astragalin and isoquercitrin, known for their therapeutic effects on various diseases,[38,39] were categorized under flavonoid glycosides subclass and were relatively more abundant in the flower or leaf. Additionally, an abundance of carbohydrates, particularly kestose and neighboring nodes, was notably found in the root and leaf. Fructooligosaccharides like kestose are known for their potentially beneficial effects on stimulating the growth of bifidobacterial in the human colon.[40]

The chemical profile of MN-6 was characterized by the prevalence of lipids and lipid-like molecules superclass, particularly linoleic acids and their derivatives, as well as mono/sesquiterpenoids like alpha-curcumene, primarily localized in the leaf. Conversely, terpene lactones such as isoalanotolactone and atractylenolide III, recognized for their apoptotic, antimicrobial, and/or anticancer properties,[41-43] were predominantly detected in the root (refer to Figure 5B). Within MN-14, di and tripeptides were most prominent in the flower (refer to Figure 5C). In MN-17, glycerophosphocholine was found distributed across all four plant parts, with phosphatidylcholines (PCs) being pervasive and lysophosphatidylcholines (LPCs) exhibiting notably higher abundance in the leaf (Figure 5D). LPC, originating from the breakdown of PC by phospholipase

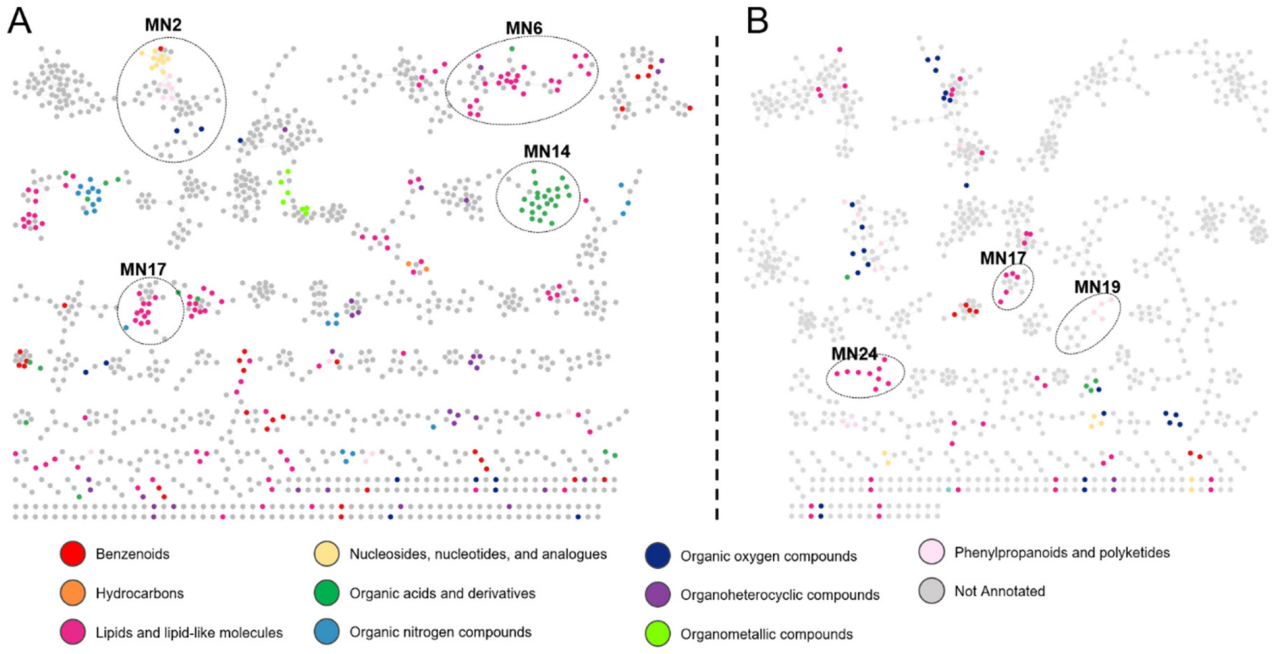

Figure 4. Molecular networks of all the detected features from the methanolic extracts of white dandelion in (A) positive and (B) negative datasets, respectively. Note that the nodes in the molecular networks are highlighted based on their chemical superclass that were annotated based on reference spectral library or GNPS library matches.

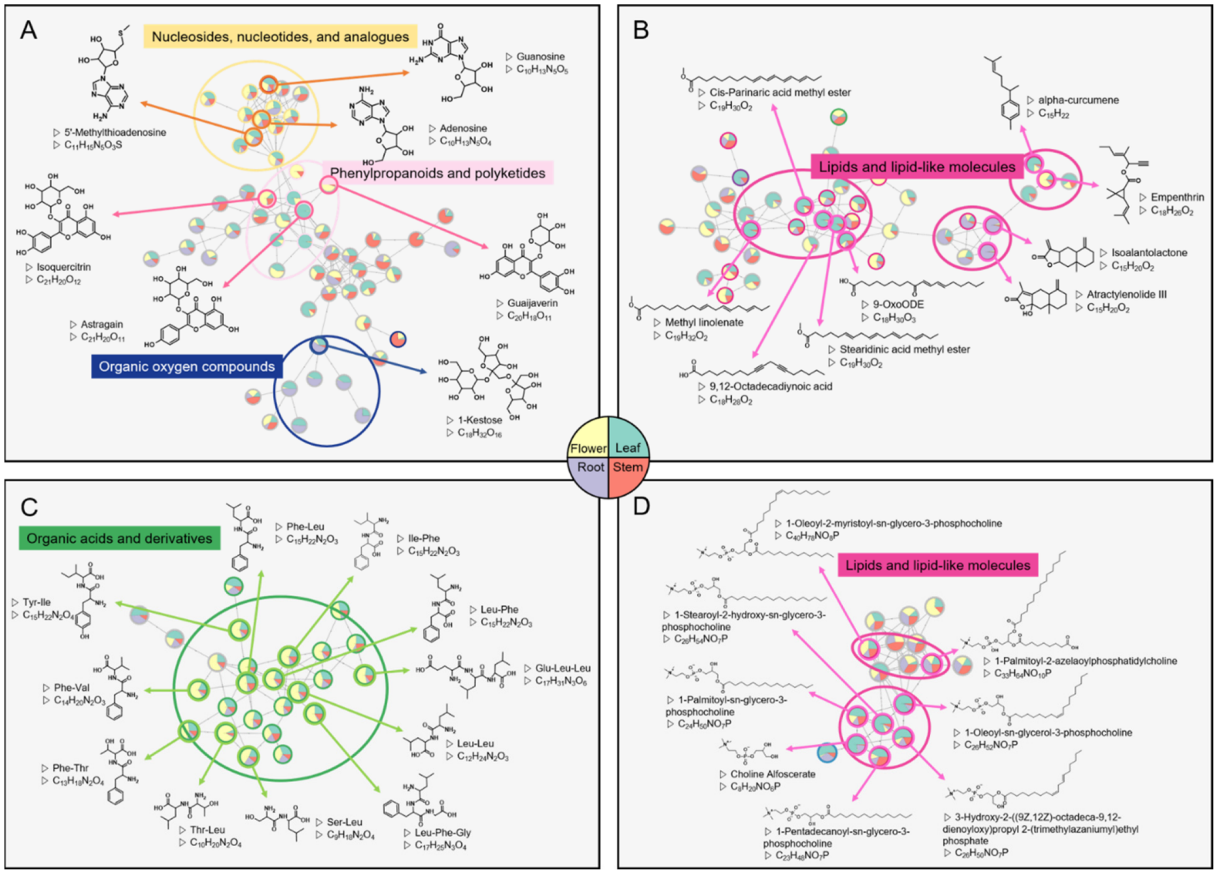

Figure 5. FBMN results of the (A) MN-2, (B) MN-6, (C) MN-14, and (D) MN-17 clusters from positive ion mode datasets. Each node is colored according to the averaged peak intensity of the total of the different plant parts of white dandelion (Color code: flower: yellow, leaf: green, stem: red, root: purple).

enzyme, plays a pivotal role in inflammatory and infectious diseases, insulin resistance, and decreasing blood glucose level.[44,45] Due to the presence of the choline head group, PC or LPC tends to ionize readily in positive ion mode, and the varying distribution patterns of these compounds in white dandelion may be linked to distinct biosynthetic mechanisms driven by differential gene expression.

Analysis of the negative ion mode data revealed 136 clusters, each consisting of at least two nodes (see Figure 4B). Three prominent molecular networks, namely MN-17, MN-19, and MN24, were identified. MN-17 exhibited a superclass of lipids and lipid-like molecules, primarily comprising the glycerophosphoethanolamine subclass, with a higher abundance observed in the flower (as depicted in Figure 6A). It is worth noting the presence of lysophosphoethanol-amines (LPEs) in plants, which are linked to plant resistance against necrotrophs or hemibiotrophic pathogen.[46,47] Meylaers and colleagues reported the antifungal and antibacterial activity of 1-LPE in the housefly.[47] Identified as phenylpropanoids and polyketides in the superclass, MN-19 predominantly featured flavonoid glycosides subclasses exclusive to the flower and leaf, with notable annotations such as luteolin-4'-*O*-glucoside, luteolin-7,3'-di-*O*-glucoside, and kaempferol-7-*O*-glucoside (Figure 6B). Those flavones are a class of representative antioxidants.[48] Comprising a superclass of lipids and lipid-like molecules, MN-24 was annotated with linoleic acids and derivatives subclasses. These compounds were relatively more abundant in the leaf and flower (Figure 6C).

The intricate synthesis of phytochemical compounds often occurs within specific cellular compartments, tissues, or organs of plants.[49,50] These compounds, which encompass a broad range of molecules like flavonoids, alkaloids, and terpenoids, are synthesized through complex biochemical pathways.[51] The exact location of synthesis varies depending on the type of phytochemical and the plant species involved.

For instance, in many plants, specialized organelles such as chloroplasts, mitochondria, and peroxisomes play crucial roles in synthesizing various phytochemicals. Chloroplasts are well-known sites for the synthesis of pigments like chlorophyll and carotenoids,[52] while mitochondria are involved in the synthesis of certain terpenoids and alkaloids.[53] Additionally, the endoplasmic reticulum (ER) and

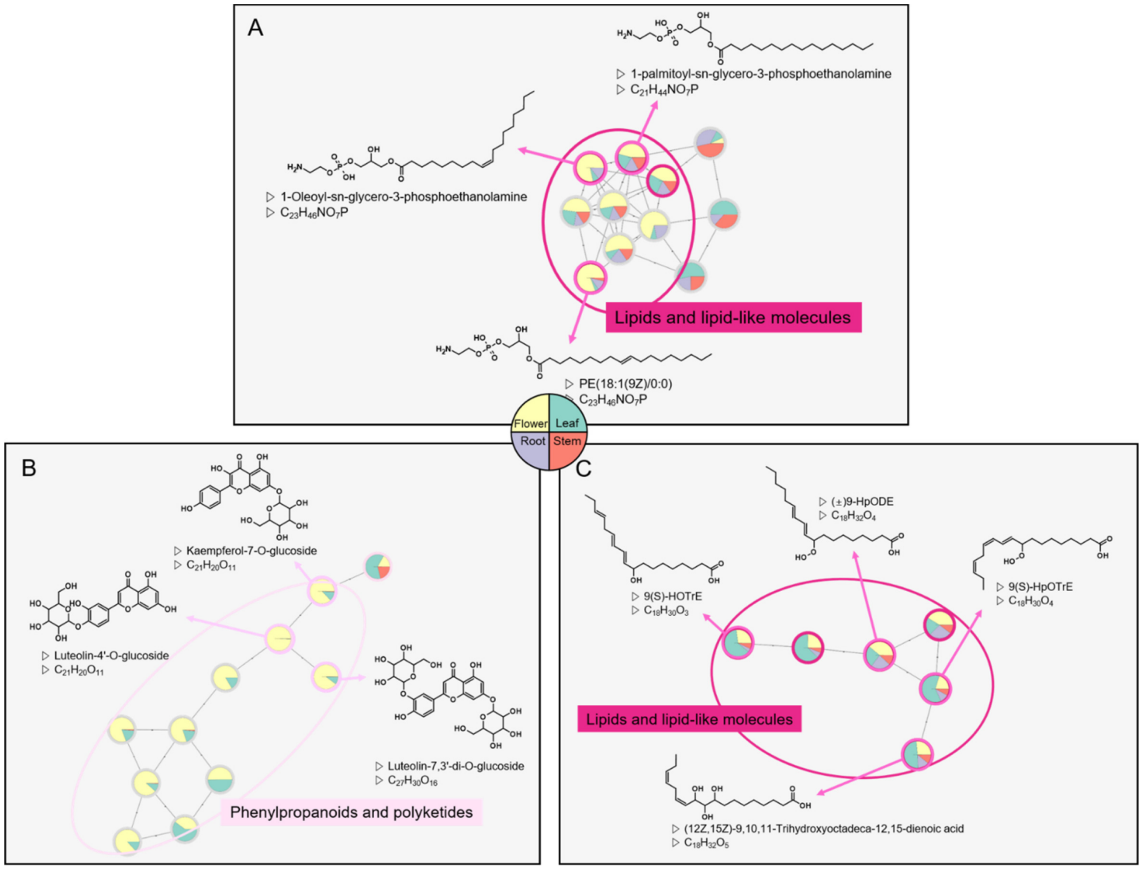

Figure 6. FBMN results of the (A) MN-17, (B) MN-19, and (C) MN-24 clusters from negative ion mode datasets. Each node is colored according to the averaged peak intensity of the total of the different plant parts of white dandelion (Color code: flower: yellow, leaf: green, stem: red, root: purple).

Golgi apparatus are essential for the biosynthesis and packaging of phytochemicals destined for secretion or storage.[54]

Moreover, specific tissues or organs within plants may specialize in the production of particular phytochemicals. For instance, alkaloids are often synthesized in specialized cells within leaves, stems, or roots,[55] while essential oils rich in terpenoids are commonly produced in glandular trichomes located on the surface of leaves or other aerial parts.[56]

Despite significant advancements in plant biochemistry and molecular biology, uncovering the precise cellular, tissue, or organ locations where certain phytochemicals are synthesized remains an ongoing area of research.[57,58] Understanding these processes not only sheds light on plant biology but also holds implications for various fields including medicine, agriculture, and nutrition.

Conclusions

Despite the common use of dandelion in alternative medicine, the benefits and mechanisms of dandelion in alleviating specific symptoms or diseases remain uncertain due to the complexity of its phytochemical profile. In this aspect, the comprehensive phytochemical profiling conducted in this study, utilizing high-resolution ion-mobility Q-TOF MS in conjunction with feature-based molecular networking analysis, offers a detailed insight into the phytochemical composition of white dandelion across its different plant parts.

To date, only one study has reported on the global metabolite profiling of *T. coreanum* using ^{1}H NMR and GC-MS, which identified amino acids, organic acids, and fatty acids,[14] reflecting the intrinsic properties of the analytical instruments applied. To the best of our knowledge, this is the first comprehensive phytochemical profile of *T. coreanum* utilizing LC-MS-based approaches. Our results identified a wide range of compounds, including lipids, flavonoids, and/or oligosaccharides.

This study confirmed that although the flower and leaves of the white dandelion contain the largest amounts of phytochemical compounds, the roots possess unique components, some of which exhibit very high antioxidant activity. In particular, amino acids and various glycosylated flavones were identified in the flowers, highlighting their potential

benefits for antioxidant uptake.

Our findings highlight a predominance of flavonoids, phenols, and terpenes–compounds renowed for their antioxidant, anti-inflammatory, anti-diabetic properties–in the flowers, followed by the leaves, stems, and roots. Additionally, the distinct distribution patterns of various compound classes, such as purine nucleosides, carbohydrates, flavonoid glycosides, and lipids provide valuable insights into the potential bioactive properties and ecological functions of these constituents within the plant matrix.

The exact cellular, tissue, or organ location where these complicated phytochemical compounds are synthesized remains unveiled yet. Identifying this location is crucial for understanding their physiological functions and roles in plant life, as well as for facilitating the isolation of enzymes involved in their biosynthesis. Furthermore, gaining insights into the genes associated with the biosynthesis and accumulation of these compounds is essential for advancing our understanding of plant metabolism and for potential applications in metabolic engineering and biotechnology.[59] Nevertheless, further investigations into the biological activities and medicinal potential of the identified compounds, especially those exclusive to specific plant parts, may contribute to the development of novel therapeutic agents derived from white dandelion.

It is impoartant to note that the phytochemical compounds annotated from the untargeted LC-MS/MS analysis, followed by reference spectral library matches, have not been fully validated. Therefore, further investigation and validation are necessary to confirm the presence of the bioactive compounds of interest.

Furthermore, the solvent selection for the extraction of phytochemical components in natural products is critical because the extraction yield and the composition may vary by the solvent chosen and the chemical characteristics of the target compounds.[60,61] Hence, utilizing different solvents for extraction may reveal diverse phytochemical profiles. Although we investigated the phytochemical profiles of methanolic extracts from different parts of white dandelion, further exploration using alternative extraction solvents could yield additional information on the phytochemical compositions.

Acknowledgments

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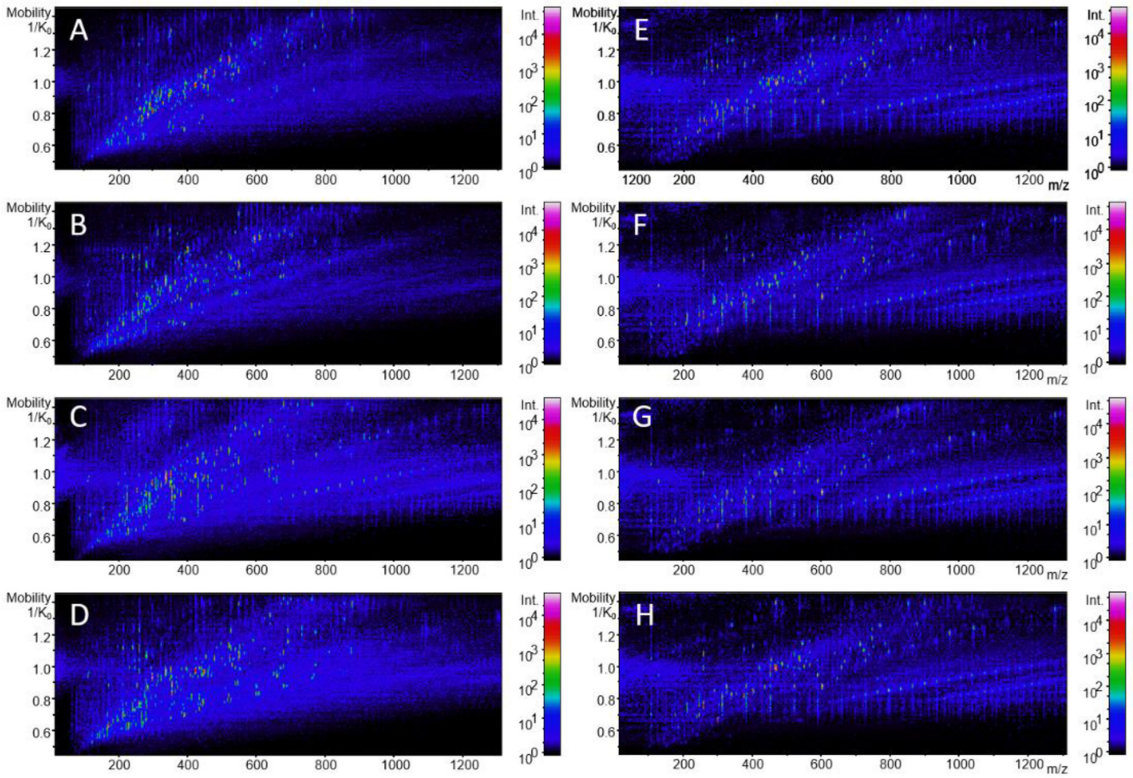
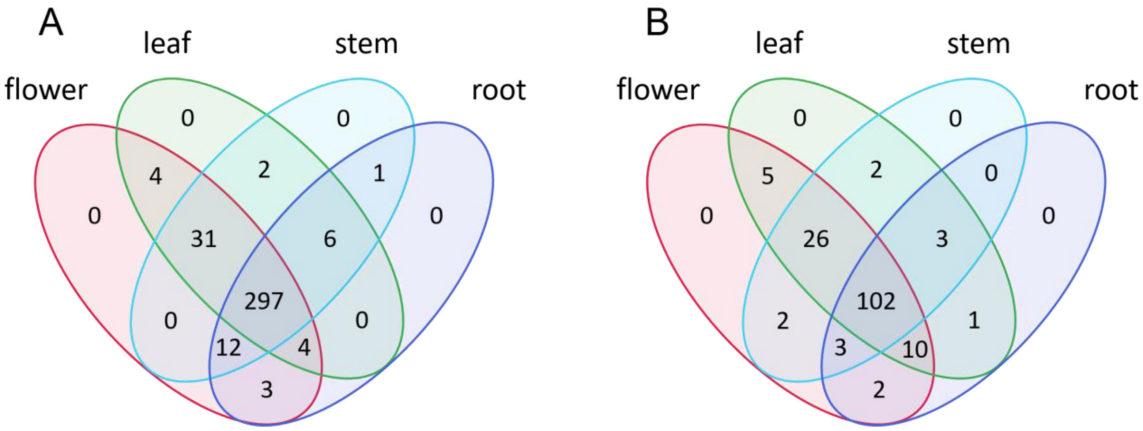
Supplementary



Supplementary Figure S1. TIMS MS Heat maps plotting m/z and $1/k_0$ of molecular features observed via positive (A, B, D, and D) and negative (E, F, G, and H) ion modes. A and E, flower; B and F, leaf; C and G, stem; D and H, root.



Supplementary Figure S2. Venn diagrams displaying the number of phytochemical compounds identified from four parts of white dandelion in (A) positive and (B) negative datasets.

Supplementary Table S1. Superclass level-classification distribution of phytochemical compounds annotated from the methanolic extracts of white dandelion using UPLC/ion-mobility Q-TOF MS in positive ion mode.

No.	Classification (Superclass level)	Total Count	Total Count (%)
1	Lipids and lipid-like molecules	147	40.83
2	Organoheterocyclic compounds	56	15.56
3	Organic acids and derivatives	54	15.00
4	Benzenoids	34	9.44
5	Organic oxygen compounds	25	6.94
6	Organic nitrogen compounds	19	5.28
7	Phenylpropanoids and polyketides	14	3.89
8	Nucleosides, nucleotides, and analogues	4	1.11
9	Organometallic compounds	4	1.11
10	Hydrocarbons	2	0.56
11	NA	1	0.28

Supplementary Table S2. Superclass level-classification distribution of phytochemical compounds annotated from the methanolic extracts of white dandelion using UPLC/ion-mobility Q-TOF MS in negative ion mode.

No.	Classification (Superclass level)	Total Count	Total Count (%)
1	Lipids and lipid-like molecules	65	41.67
2	Organic oxygen compounds	34	21.79
3	Phenylpropanoids and polyketides	21	13.46
4	Organic acids and derivatives	13	8.33
5	Benzenoids	10	6.41
6	Organoheterocyclic compounds	7	4.49
7	Nucleosides, nucleotides, and analogues	5	3.21
8	Lignans, neolignans and related compounds	1	0.64

