



Untargeted Metabolomic and Elemental Profiling of Ancient Stepwell Waters

Saloni Sachdeva & Indira P Sarethy*

Department of Biotechnology, Jaypee Institute of Information Technology, Uttar Pradesh, 201309 India

Article info

Article history:

Received: 18 July 2025

Revised: 16 December 2025

Accepted: 16 January 2026

Keywords:

Bioactive compounds, Inductively Coupled Plasma Mass Spectrometry, Ultra Performance Liquid Chromatograph with Electrospray Ionization and Quadrupole-Time of Flight Mass Spectrometer

Abstract

Gandhak-ki-baoli, an ancient stepwell, long revered for its therapeutic properties, represents untapped natural reservoir of bioavailable sulfur and bioactive compounds. In this study a multidisciplinary analytical approach was employed to investigate the physicochemical and biochemical characteristics of stepwell water and its surrounding geological matrix. Inductively Coupled Plasma Mass Spectrometry (ICP-MS) revealed a notable concentration of sulfur (~61 ppm) in the rock samples, while water profiling confirmed a mineral-rich composition indicative of redox-influenced hydrochemical environment. Ultra Performance Liquid Chromatography coupled with Electrospray Ionization and Quadrupole-Time-of-Flight-Mass-Spectrometry (UPLC–ESI–QToF–MS) identified 20 bioactive compounds exhibiting antimicrobial, antioxidant, and anti-inflammatory properties. Therapeutic potential is attributed to (1) membrane-permeabilizing saponins, such as digitonin, which may enhance the permeation of mineral and bioactive compounds through epidermal layers, and (2) bioactive phenolics and flavonoids, such as coumarin, capable of deep dermal absorption. These findings offer a detailed chemical and metabolomic profile of this historic stepwell, underscoring its significance as a unique reservoir with potential biological relevance and applications that warrant further investigation.

Introduction

Freshwater ecosystems represent the physical manifestations of interactions between society and the biosphere. These habitats sustain themselves while also undergoing modifications to meet societal needs. On a localized scale, inland water bodies play a fundamental role in regulating the absorption and transportation of resources, such as nutrients and waste, as well as microclimate regulation and the provision of the domestic

water supply (Vári et al., 2021). On a broader scale, they are vital components of the biogeochemical cycle, global carbon budget, climate variability, and land-use change. Beyond addressing environmental and social needs, these freshwater resources also provide cultural benefits, including their spiritual and aesthetic significance, which fosters a sense of belonging among the communities that rely on them (Tallar & Suen, 2017; Ncube et al., 2021). In addition to their ecological and cultural importance, freshwater inland water bodies,

* Corresponding Author
e-mail: indira.sarethy@mail.jiit.ac.in

especially, ancient stepwells, serve as reservoirs of bioactive compounds with potential biotechnological and pharmaceutical applications (Sachdeva & Sarethy, 2024).

Specifically, mineral-rich freshwater bodies such as soda lakes, volcanic crater lakes, and sulfur springs have long been associated with human health benefits, both through direct therapeutic use in balneotherapy (Protano et al., 2024) and via microbial metabolites with antimicrobial, antioxidant, and cytotoxic properties that hold promise for pharmaceutical industries (Alrumman et al., 2019; Bawane & Yele, 2025). These waters typically contain major anions such as chloride, bicarbonate, sulfate, sulfide, or other sulfurous compounds, and dissolved carbon dioxide, along with soluble cations including magnesium, calcium, and sodium, as well as silicates. Their composition is further enriched by trace elements such as manganese, selenium, zinc, and boron. Collectively, these minerals shape the physicochemical properties of the water and confer broadly recognized health benefits, including improved skin hydration, accelerated wound healing, reinforcement of the skin barrier, and protection against oxidative stress. Among them, sulfur plays a particularly distinctive role: it governs redox balance, drives microbial specialization, and directly mediates therapeutic outcomes such as anti-inflammatory, antibiofilm, antioxidant, and wound-healing effects (Mourelle et al., 2024). Given the recognized dermatological benefits of mineral-rich freshwater environments, waters with well-defined mineral compositions have been incorporated into commercially prominent skincare formulations (Figueiredo et al., 2023), supported by clinical evidence demonstrating benefits in skin hydration, inflammation modulation, and barrier repair (Cacciapuoti et al., 2020). Examples include skincare products developed using thermal waters from Avène, La Roche-Posay, Vichy, Uriage, and Saint-Gervais. In addition, sulfur-based actives remain highly relevant in dermocosmetic formulations, with contemporary products leveraging sulfur's antimicrobial, keratolytic, anti-inflammatory, and sebum-regulating properties to manage acne-prone and irritated skin (Chen et al., 2025). However, when present in excess in natural settings, minerals such as bicarbonate, selenium, boron, chloride, and iron may provoke adverse effects ranging from local skin irritation to systemic toxicity, particularly with prolonged or unregulated exposure. This underscores the need for defined safety thresholds that preserve therapeutic efficacy while minimizing health risks. Yet, internationally

harmonized regulations for medicinal waters remains poorly established. Japan stands as one of the few exceptions, with formal balneotherapy standards that classify springs based on their dominant ions, for example, sulfur (≥ 2 mg/kg), iron (≥ 10 mg/kg), and alum (≥ 1 mg/kg) each linked to specific therapeutic applications, including dermatological care, microbial skin control, anemia management, and tissue repair (Ministry of the Environment, 2019).

Against this backdrop, the sulfur-rich waters of Gandhak-ki-baoli present a unique opportunity to investigate both their traditional therapeutic and cosmetic applications, and their untapped potential as a source of bioactive compounds and minerals. To date, no systematic scientific evaluation of their mineral composition or bioactivity has been reported, highlighting the novelty of the present study. Gandhak-ki-baoli is an ancient rectangular freshwater stepwell established in 1230 AD by Shams ud-Din Iltutmish, the first Muslim king to govern over Delhi. Its purpose was to collect rainfall during a time of extreme water scarcity in Delhi. The baoli is located at 28.5208° N, 77.1817° E and is part of the Mehrauli Archaeological Park, near the Qutab Minar Complex. The name "Gandhak" translates to "sulfur," derived from the stench emitted by the water in the baoli. Despite various anthropogenic activities and climatological changes over the years, the advantageous sulfur characteristic of this pristine ecosystem has persisted, making it an appealing research subject for scientific study.

Traditionally, the study of ancient structures like this have focused on examining broken stone or rock surfaces for biodeterioration and conducting biogeological research. However, the primary objective of the current research is to explore the bioactive metabolites and sources of sulfur, which may offer medicinal benefits to the water. Fig. 1 depicts the state-of-the-art approach of this present study for comprehensive analysis of the objectives. Furthermore, the Gandhak-ki-baoli stepwell represents an ideal natural system for studying extreme conditions, owing to its consistently high sulfur content and stable redox environment throughout the year.

Materials and methods

1. Sample collection and processing

Samples of surface water and rock were obtained from Gandhak-ki-baoli (28.5207° N, 77.1853° E) (Fig. 2), an ancient stepwell situated near the water extraction

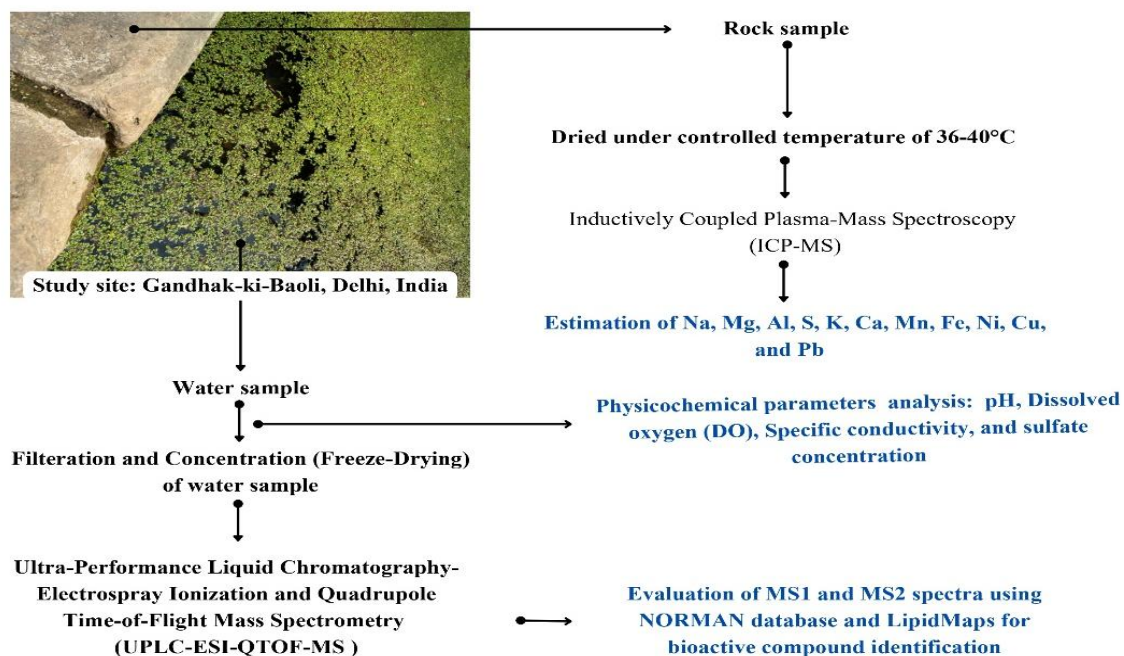


Fig. 1 Schematic representation of methodology

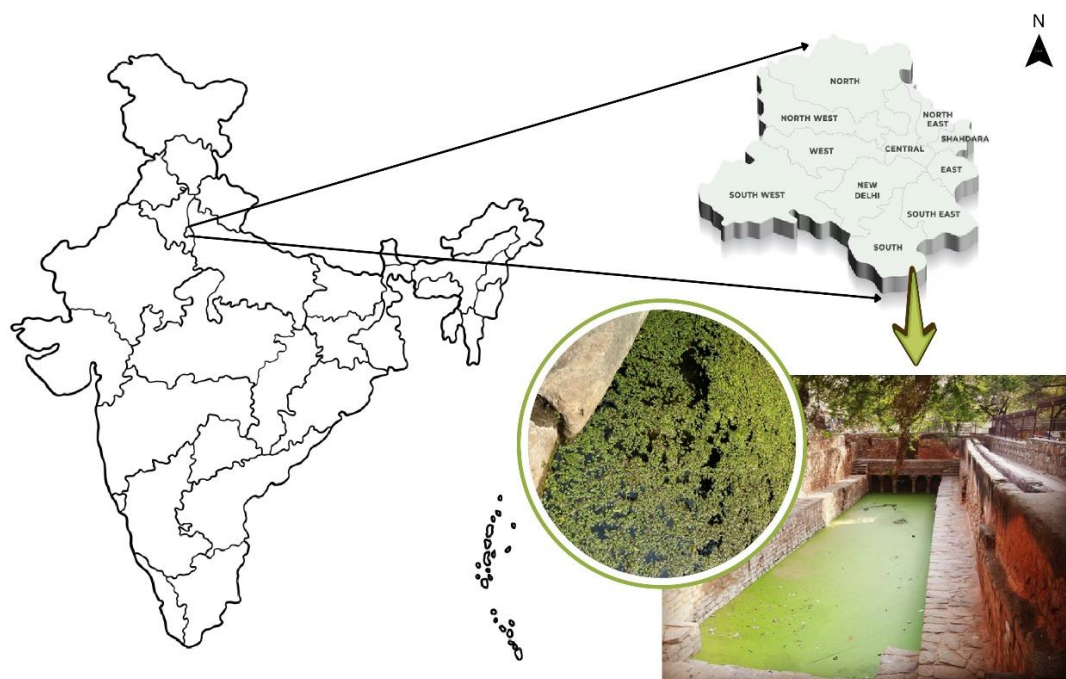


Fig. 2 Study site, Gandhak-ki-baoli, which is located within the Mehrauli Archeological Park in Delhi

location utilized by the local communities. Samples were collected in February 2024 (winter season) when water levels were stable, minimizing seasonal variation. The pooled water sample was collected at a depth of 10–15 cm using sterile plastic bottles, employing the methodology outlined in ISO 5667-1:2020. The collected samples were appropriately labeled and immediately stored in a container and kept in an insulated icebox at $4 \pm 1^\circ\text{C}$ to preserve their integrity and prevent any degradation until subsequent analysis.

The pooled surface water sample was filtered through $0.22\ \mu\text{m}$ PES syringe filters that removed the suspended solids and retained the dissolved analytes, followed by physicochemical analysis. Subsequently, the water sample was subjected to a freeze drier using Alpha 1–2 LSCbasic (Martin Christ, Germany) under vacuum ($0.37\ \text{mbar}$) at -55°C for approximately 30 h to concentrate the water sample for better detection of compounds using LC-MS. The rock sample was weighed, followed by oven-drying at a controlled temperature of $36\text{--}40^\circ\text{C}$ for 72 h until a constant weight was attained. The analysis of metals in the rock sample was conducted using ICP-MS with a multi-standard calibration approach.

2. Analysis of physicochemical parameters and metals

The water samples collected from the stepwell underwent analysis to determine the sulfate content (mg/L), dissolved oxygen (DO), specific conductivity ($\mu\text{S/cm}$), and pH, following the established protocols outlined by APHA (APHA, 2012). The pH and specific conductivity were measured using a multimeter, while DO and sulfate were estimated using the Winkler and methylene blue method, respectively. DO was determined by titration method, in which oxygen was fixed with manganese sulfate and alkaline iodide-azide, producing a manganese hydroxide precipitate. Upon acidification with sulfuric acid, iodine equivalent to the DO content was liberated and titrated with standardized $0.025\ \text{N}$ sodium thiosulfate using starch as an endpoint indicator. The concentration of DO was calculated using the Eq. 1.

$$\text{DO} \left(\frac{\text{mg}}{\text{L}} \right) = \frac{V \times N \times 8 \times 1000}{V_s} \quad \text{Eq. 1}$$

where, V = volume of $\text{Na}_2\text{S}_2\text{O}_3$ used (mL), N = normality of $\text{Na}_2\text{S}_2\text{O}_3$, and V_s = volume of the water sample (mL)

Sulfate concentration was determined by the methylene blue spectrophotometric method. In this procedure, sulfate ions were precipitated as BaSO_4 using BaCl_2 -gelatin, followed by reaction with methylene blue to form a

stable blue complex. Absorbance was measured at $665\ \text{nm}$ with a UV-Vis spectrophotometer (UV-1800, Shimadzu Corporation, Japan), and concentrations were obtained from a calibration curve prepared with sulfate standards ($1\text{--}20\ \text{mg/L}$). The sulfate concentration was expressed using Eq. 2.

$$\text{SO}_4^{2-} \left(\frac{\text{mg}}{\text{L}} \right) = \frac{(C \times V)}{V_s} \quad \text{Eq. 2}$$

where, C = concentration obtained from the calibration curve (mg), V = final extract volume (mL), and V_s = sample volume (mL)

For the rock sample obtained from the stepwell, an Inductively Coupled Plasma-mass Spectroscopy (ICP-MS 7900 with UHMI, Agilent Technologies, Inc., Santa Clara, CA, USA) analysis was conducted to estimate Na, Mg, Al, S, K, Ca, Mn, Fe, Ni, Cu, and Pb as per protocols described by Silva et al. (2013). Upon arrival at the laboratory, the oven-dried rock sample was weighed, finely powdered, and subjected to acid digestion using concentrated HNO_3 and HF in Teflon vessels. The digested extracts were diluted to volume with ultrapure water before analysis. The calibration process involved the use of multi-element standard solutions using TraceCERT Multi-Element Standard Solution (Sigma-Aldrich Co., Ltd., Germany) with varying concentrations ($10, 20, 50, 100$, and $200\ \mu\text{g/L}$), and accuracy was validated with procedural blanks. The results obtained from the analysis were reported in parts per billion (ppb).

3. UPLC-(ESI)-QToF-MS metabolite profiling

A Chromatographic analysis was carried out utilizing an Acquity Ultra Performance Liquid Chromatograph (UPLC) system (2D nanoACQUITY, Waters, USA) coupled with a QTOF mass spectrometer (SYNAPT G2, Waters, USA), which was coupled with a Quadrupole-Time of Flight mass spectrometer (QToF-MS). The QToF-MS instrument featured electrospray ionization (ESI) and was operated at a nominal mass resolution of $20,000$, under the control of MassLynx 4.1 software.

The chromatographic separation was accomplished using an ACQUITY UPLC BEH C 18 column ($2.1 \times 100\ \text{mm}$, $1.8\ \mu\text{m}$, Waters India Pvt. Ltd., Bangalore) maintained at 35°C . The mobile phase consisted of two phases: phase A composed of methanol:water ($5:95$), and phase B composed of methanol:water ($95:5$), both containing 0.1% formic acid. A gradient program was employed with a flow rate of $0.3\ \text{mL/min}$, starting with 90% A from 0 to $0.5\ \text{min}$, transitioning to 50% A at $4.5\ \text{min}$, followed by a shift from 50% to 2% A between

4.5 and 8 min, maintaining 2% A from 8 to 11 min, returning to 90% A from 11 to 11.5 min, and concluding with 90% A from 12 to 14 min. The injection volume was 5 μ L, and the samples were kept at 15°C throughout the analysis. Furthermore, for mass spectroscopy, the heated ESI source and the transfer capillary were both operated at 120°C and 500°C, respectively, with a capillary voltage of 3 kV, and a cone gas flow of 50 L/h. While the reference mass of leucine enkephalin (m/z 556.2771 in positive and m/z 554.2670 in negative polarity) was used for mass correction with a flow rate of 10 μ L/min at a concentration of 2 μ g/mL at every 10-sec interval. Data acquisition was performed using the MSE function in continuum mode, acquiring the MS1 and MS2 spectra and covering the mass-to-charge ratio (m/z) range of 50–1200. For further processing, in the untargeted evaluation, the m/z of the resulting features was compared against the NORMAN database along with Lipid Maps as per Horai et al. (2010) and Fahy et al. (2007), respectively.

Results and discussion

1. Physicochemical parameters

The higher sulfate concentration of 256.19 mg/L (Table 1) in the analyzed habitat suggests that SO_4^{2-} acts as a significant electron acceptor in anoxic environments, potentially influenced by the dissolution of the brick aggregates used in its construction (Margalef-Martí et al., 2023). The restricted nature of the environment, coupled with limited external inputs, emerges as a significant determinant of the observed ion levels. Corroborating this observation, the presence of the biological sulfate cycle, in conjunction with other nutrient cycles, near the interface of water and sediment, as substantiated by sulfur data derived from ICP-MS analysis, further bolsters the evidence.

Table 1 Selected physical and chemical characteristics of the ancient stepwell, Gandhak-ki-baoli. The water sampled as surface grabs at a depth of 10–15 cm

Parameters	Calculated value
Sulfate (SO_4^{2-}) (mg/L)	256.19
Dissolved oxygen (mg/L)	2
Specific conductivity ($\mu\text{S}/\text{cm}$)	783
pH	7.21

The pH of water serves as a significant indicator of its alkaline or acidic properties and plays a pivotal role in determining water quality. In the case of Gandhak-ki-baoli, the water pH is reported to be neutral, with a

value of 7.21. Previous studies by Brahmacharimayum et al. (2019) have established that sulfur-reducing bacteria (SRB) generally thrive within a neutral to alkaline pH range, specifically between pH 7 and 9.5. However, it is crucial to note that extreme pH values can have distinct impacts on microbial processes, exhibiting an inverse relationship with the solubility of metal sulfides, which can ultimately hinder the reduction process. Electrical conductivity refers to the measure of dissolved substances or ions present in water. In the case of the stepwell, the higher electrical conductivity (EC) can be ascribed to a multitude of factors. One plausible explanation is the occurrence of active biological interactions, such as microbial metabolism and the decomposition of organic matter, which release ions into the water (Borch et al., 2010). Furthermore, the disintegration of salts from the brick aggregates utilized in the construction of the baoli can also contribute to the increased EC. Molecular oxygen, despite its significance in biogeochemical cycles, exhibits limited solubility in water. Consequently, oxic-anoxic interfaces are established in diverse environments where distinct aerobic and anaerobic processes take place within separate zones. Likewise, the water sample under consideration demonstrates relatively low levels of dissolved oxygen (DO), measuring 2 mg/L, and indicating oxic conditions. In such conditions, heterotrophic SRB employ sulfate or other anions as their terminal electron acceptor (Ito et al., 2002). Preliminary microbiological assessment indicated the presence of SRBs (as illustrated in Fig. 3), as anaerobic enrichment on Postgate B medium produced characteristic black iron sulfide (FeS) precipitates. This finding aligns with the neutral pH and low dissolved oxygen conditions of the stepwell.

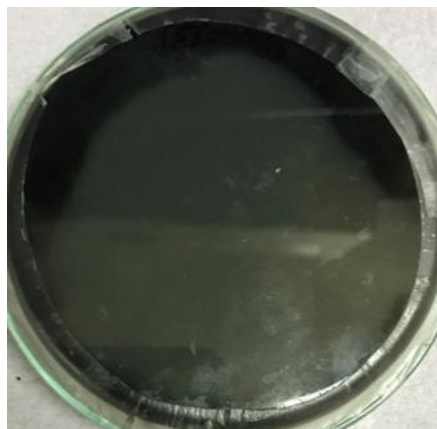


Fig. 3 Black FeS precipitates formed during anaerobic enrichment on Postgate B medium, indicating sulfate-reducing bacterial activity

Inductively coupled plasma mass spectrometry (ICP-MS) is a precise and sensitive method used to analyze and quantify elements in the parts-per-billion range. It involves ionizing the elements in a sample and measuring their masses using a mass spectrometer. Table 2 presents the data obtained from the ICP-MS analysis. The sediment of Gandhak-ki-baoli, dating back to the 13th century, contains a total sulfur concentration of 60898.12 ppb, far exceeding the Japanese balneotherapy threshold for sulfur springs (≥ 2 mg/kg) (Ministry of the Environment, 2019). The elevated levels of sulfur (S), sodium (Na), potassium (K), magnesium (Mg), and calcium (Ca) in the sediment are commonly associated with the chemical weathering of building materials during interactions between the sediment and water, as explained by Jingfu et al. (2016). This phenomenon, as noted by Gaur et al. (2022), also plays a role in increasing the sediment's salinity and electrical conductivity. The collective results indicate that the major ionic composition in the ancient stepwell Gandhak-ki-baoli is primarily governed by processes such as base ion exchange, salt dissolution, and silicate weathering. Although iron and alum concentrations were not the primary focus, any detectable levels could be contextualized against the Japanese standards for ferruginous ($\text{Fe} \geq 10$ mg/kg) and alum rich-water ($\text{Al} \geq 1$ mg/kg), which are linked to therapeutic indications including dermatological care, microbial skin control, and tissue repair (Ministry of the Environment, 2019).

Table 2 Concentration of major and minor ions using ICP-MS

Parameters	Calculated value (ppb)
34 S	60898.12
23 Na	21381.49
24 Mg	21350.05
39 K	10119.15
43 Ca	6250.88
56 Fe	138.12
55 Mn	51.36
207 Pb	31.61
27 Al	14.72
208 Pb	13.24
60 Ni	11.23
63 Cu	1.77
206 Pb	0.004

2. UPLC-(ESI)-QToF-MS metabolite profiling

After analyzing the peaks and annotating them using both MS1 and MS2 scans, the researchers found 75 specific peaks with m/z values matching the target metabolite within a tolerance range of 0.001–2 ppm. The compounds identified through MassBank belong to various natural compound classes, namely, Monosaccharides, Saponins, Alkaloids, Lignane, Esters, Terpenoids, Catechins, Flavones, Indolizidines, and Catechins (Supplementary Table 1), while using LIPID MAPS the identified compounds were found to belong to Fatty esters, Fatty Acids and Conjugates, Octadecanoids, Steroids, Eicosanoids, Oxidized glycerophospholipids, Glycerophosphoinositols, Glycerophosphoglycerols, Phosphosphingolipids, and Triradylglycerols (Supplementary Table 2). Table 3 presents an exhaustive overview of

Table 3 Identification of natural products via UPLC-(ESI)-QToF-MS and their medicinal potential, found in water from ancient stepwell, Gandhak-ki-baoli

Category of natural metabolite	m/z ratio	Adduct	Predicted compound	Potential application	Reference
Triterpenoid saponin	127.0266	+ve	Asiaticoside	Wound healing property	Hillman et al. (2022)
	779.0623, 779.1534, 779.2447, 779.3361, 779.4273, 779.5179, 779.6082, 780.2749	+ve	Bacoside A3	Anti-bacterial property (more known for neuroprotective effect)	Parai et al. (2017)
Terpenoids	133.0837	+ve	2,6-Cyclolycopene-1,5-diol	Anti-oxidant property (a metabolite of lycopene) *	Yang and Ling (2025)
Saponins	856.959, 857.0596	+ve	Paclitaxel	Anti-cancer property	Yang and Ling (2025)
	218.1794, 274.2209, 714.3149, 714.3985, 714.4822, 714.5657, 714.649, 857.1595, 857.2599, 857.3598	+ve	Ginsenoside	Anti-inflammatory Property	Mao et al. (2022)
	781.2772, 783.2927	+ve	Digitonin	Cell membrane permeabilization property	Verleur and Wanders (1993)
Alkaloids	189.0811	+ve	Chelidinin	Anti-inflammatory property	Yang et al. (2011)
	190.0836	+ve	Tetrandrine	Anti-inflammatory property	Chen et al. (2022)
	219.0813	+ve	19S-Methoxytubotaiwine	Anti-microbial and anti-cancer properties*	Yang & Ling (2025)
	175.0215	-ve	Isomajidine	Anti-oxidant and anti-cancer properties	Gülçin et al. (2011)
	219.9169	-ve	Mitragynine	Anti-inflammatory property*	Yang & Ling (2025)

Table 3 (Continue)

Category of natural metabolite	m/z ratio	Adduct	Predicted compound	Potential application	Reference
Glycosides	194.0946	+ve	5(S)-5-carboxystrictosidine	Anti-cancer property (Precursor in indole <i>alkaloid biosynthesis</i>) *	Yang & Ling (2025)
	275.2234	+ve	Madecassoside	Anti-inflammatory property	Shen et al. (2019)
	615.2955	+ve	Soyasapogenol B base + O-HexA-Hex-Pen	Anti-inflammatory property*	Yang & Ling (2025)
	740.2629	+ve	Kaempferol-3-O-robinoside- 7-O-rhamnoside	Anti-oxidant and anti-inflammatory properties*	Yang & Ling (2025)
	757.29, 760.3234	+ve	Cyanidin 3- (2G-glucosylrutinoside)	Anti-oxidant property	Čižmarová et al. (2023)
Flavanoid	203.0554	+ve	Procyanidin	Anti-inflammatory property	Hughes-Formella et al. (2006)
	301.0765	+ve	Eriodictyol-7-O- neohesperidoside	Anti-oxidant and anti-inflammatory properties*	Yang & Ling (2025)
	319.1227	+ve	Perrottetin	Anti-inflammatory property*	Yang & Ling (2025)
	952.0541, 952.277	+ve	Hyperoside	Wound healing property	Elloumi et al. (2022)
	952.1652, 952.3884	+ve	Myricitrin		
	116.9841	−ve	Epicatechin	Anti-inflammatory and anti-oxidant properties	Čižmarová et al. (2023)
	131.0248	−ve	Chrysanthellin A	Anti-inflammatory property	Park et al. (2012)
	136.9853	−ve	6-Methoxyluteolin	Anti-inflammatory property	Zhou et al. (2020)
	160.9056	−ve	Hesperetin	Anti-inflammatory property	Lietal.(2016);Čižmarová et al. (2023)
	164.9006	−ve	Rhamnetin	Anti-inflammatory property	Antunes-Ricardo et al. (2015)
	170.9487	−ve	Baicalein	Anti-inflammatory property	Wang et al. (2022); Čižmarová et al. (2023)
	195.8796	−ve	Cyanidin-3-O-galactoside	Anti-inflammatory and anti-oxidant properties	Heetal.(2017);Čižmarová et al. (2023)
Phenolic compound	250.1366	+ve	4-Coumaroyl Choline	Anti-oxidant and antimelanogenic properties	Boo (2019)
	782.2904	+ve	Coumarin	Anti-oxidant and anti-bacterial properties	Sharifi-Rad et al. (2021); Ecevit et al. (2022)
Carotenoid	522.1959	+ve	Lycopene	Anti-oxidant property	Franco et al. (2021)
Cyclohexa-depsipeptide	784.2958	+ve	Beauvericin	Anti-inflammatory property	Wu et al. (2013)
Mycotoxin					

Remark: * The reported biological activities are based on the known bioactivities of the broader phytochemical classes (e.g., flavonoids, terpenoids, and alkaloids) reported in the literature. Exact activities of the predicted compounds may vary.

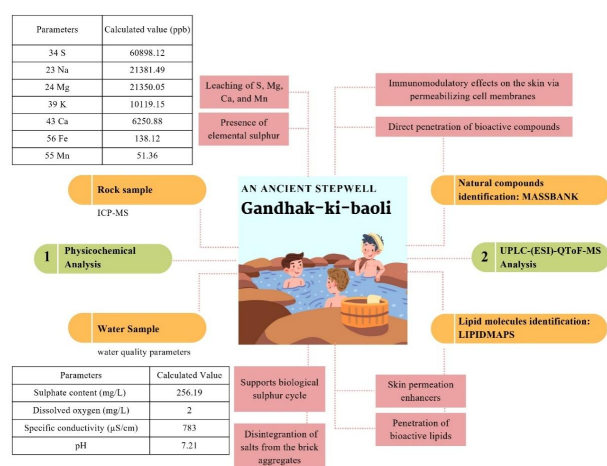


Fig. 4 Graphical representation of the bioactive compounds identified through LC-MS analysis and their potential therapeutic relevance in the treatment of skin diseases

compounds obtained from the two databases, including their reported bioactivity concerning the treatment of skin diseases (as illustrated in Fig. 4).

Among these substances, terpenes, terpenoids, fatty acid esters, and glycols have shown considerable potential as skin permeation enhancers, effectively increasing the therapeutic efficacy of compounds in treating superficial dermal infections (Patil & Saraogi, 2014). On the other hand, saponins, especially digitonin have the capacity to render cell membranes more permeable and dissolve membrane constituents (Sudji et al., 2015), which increases the availability of bioactive compounds (phenolic and non-phenolic compounds) along with minerals (as per ICPMS results) such as sulfur, magnesium, calcium bicarbonate, and manganese that have immune system-modulating effects on skin conditions like dermatitis (Cacciapuoti et al., 2020). In conjunction with the aforementioned findings, the results of metagenomic

analysis (Accession: PRJNA905208) (National Center for Biotechnology Information, 2022) also highlight the presence of abundant microbes associated with sulfur metabolism, notably *Sulfuricurvum kujiense*, a bacterium constituting 5.4% of the overall biodiversity. This bacterium demonstrates the capability to engage in S (0) organo-mineralization through the utilization of dissolved organic compounds, thereby enabling it to effectively stabilize and store bioavailable sulfur (in the form of S (0)) externally to its cellular structures (Cron et al., 2019). Additionally, significant bioactive potential was observed in two rare actinomycetes, *Microbacterium proteolyticum* GKB-017 and *Kocuria flava* GKB-021, through GC-MS metabolite fingerprinting and bioactivity screening; notably, both strains were isolated from the same baoli environment (Sachdeva & Sarethy, 2025). In addition to healthcare and pharmacological benefits, the water holds the potential to benefit the food and cosmetic industries with Lycopene as bioactive pigments; and Hyperoside, Myricitrin, Procyanidin, Madecassoside and Rhamnetin as protectants from UV-mediated inflammation. However, it was determined that 27.3% of the compounds under scrutiny were not sourced from natural origins (Fig. 5).

Instead, they were classified as synthetic antibiotics, fragrance compounds, herbicides, fungicides, and substances associated with industrial and personal care products, possibly originating from domestic waste that has been dumped into the stepwell.

For thousands of years, natural products have been critical in replenishing the pharmaceutical pipeline by exhibiting anti-inflammatory, antioxidant, analgesic, and antitumoral activities. In this study, utilizing the detection method employed, coumarin, characterized by its fused benzene and α -pyrone rings, was identified at elevated intensity, indicating the potential to exert substantial antioxidant activity, leading to reduced edema and inflammation (Sharifi-Rad et al., 2021) in addition to antibacterial efficacy against a variety of clinically relevant ailments (Ecevit et al., 2022). Furthermore, Yourick and Bronaugh (1997) reported that coumarin exhibits rapid penetration into human skin, with an absorption rate exceeding 97% within a 6-h period, a phenomenon that could be bolstered by the presence of saponins, polysaccharides, and lipids in the water sample. Flavanoids, the most abundant class of natural products

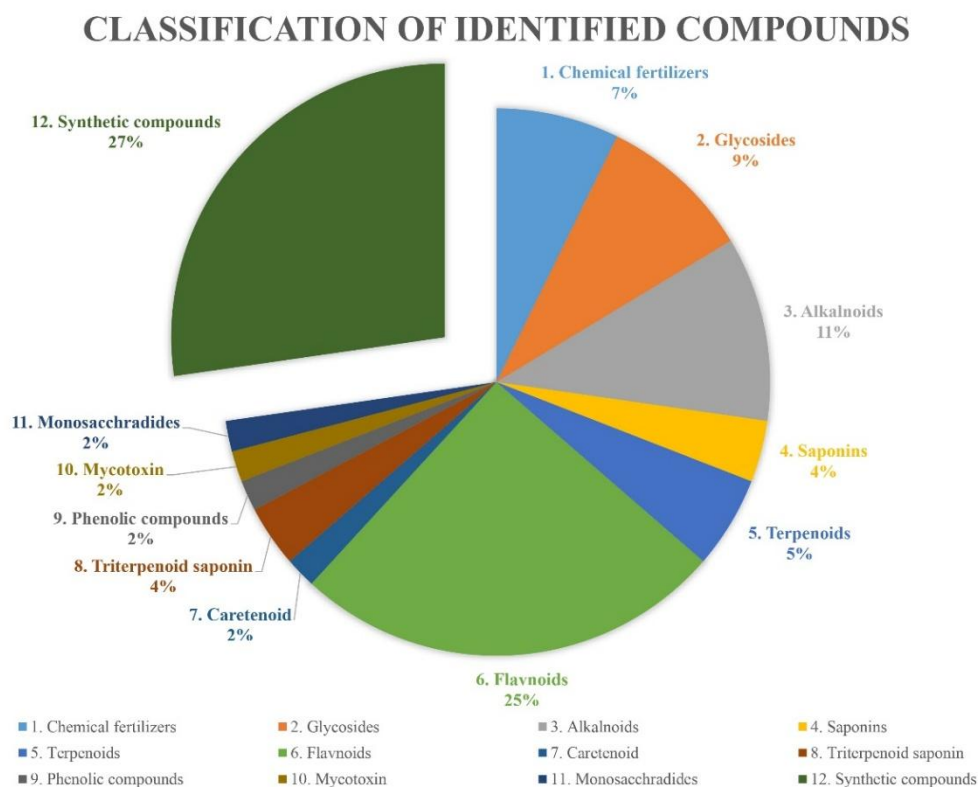


Fig. 5 Taxonomic classification of MassBank-derived compounds

detected, include Hyperoside, Procyanidin, Myricitrin, Perrottetin, Eriodictyol-7-O-neohesperidoside, Cyanidin 3-(2G-glucosylrutinoside), Epicatechin, Chrysanthellin A, 6-Methoxyluteolin, Hesperetin, Rhamnetin, Baicalein, and Cyanidin-3-O-galactoside. These all have a wide range of bioactivity including antioxidant properties that aid in the protection of the skin against oxidative damage produced by free radicals, anti-inflammatory effects, which can help reduce skin inflammation and redness, and potential UV protection (Čižmarová et al., 2023). Furthermore, their capacity to permeate into the deeper layers of the skin highlights their significance in topical applications as anti-inflammatory agents (Merfort et al., 1994).

Additionally, nonphenolic compounds including saponins (digitonin, ginsenoside, asiaticoside, and bacoside A3), followed by Glycosides, Alkaloids, Terpenes and Carotenoid exhibit potent anti-inflammatory, antioxidant and, antimicrobial properties that may contribute to the medicinal properties of water (Hillman et al., 2022). Beauvericin is a significant mycotoxin, characterized by a cyclic lactone trimer comprising N-methylphenylalanyl and D- α -hydroxyisovaleryl residues that possesses beneficial properties, including antifungal, antiviral, anticancer, and antibiotic effects (Wang & Xu, 2012). Moreover, it can penetrate through biological membranes, and shows promise as a potential drug candidate for inflammatory conditions by inhibiting activated T cells (Wu et al., 2013; Taevernier et al., 2015).

Naturally, lipids offer inherent benefits for the skin (Fernandes et al., 2023); some of them may act as pro-inflammatory mediators (oxidized glycerophospholipids), while others may have anti-inflammatory properties. Glycerophosphoinositols and Glycerophosphoglycerols are part of the cell membrane and can influence signaling pathways involved in inflammation (Vessichelli et al., 2017), while Fatty Esters and Fatty Acids, Octadecanoids, Eicosanoids, and Triacylglycerols can modulate inflammation and immune responses in the skin along with potential antimicrobial and antifungal properties, particularly against bacteria (Zhang et al., 2018). Specifically, fatty acids have a selective mechanism against Gram-positive organisms by targeting the structure and function of bacterial cell walls and membranes (Karimi et al., 2015). On the other hand, oxidized Glycerophospholipids (8.7% of the total number of compounds) are compounds that are involved in oxidative stress and inflammation processes in the skin but contribute to the antibacterial effect (Bochkov et al., 2010).

Conclusion

This study presents the first comprehensive physicochemical, elemental, and metabolomic profiling of Gandhak-ki-baoli, an ancient freshwater stepwell in Delhi. ICP-MS revealed exceptionally high sulfur concentrations in the rock matrix along with major cations, while water chemistry indicated stable redox-active conditions. UPLC-ESI-QToF-MS analysis further identified a wide array of bioactive metabolites, including saponins, flavonoids, and phenolics, many of which are associated with antimicrobial, antioxidant, and anti-inflammatory activities. Collectively, these results highlight the elemental and metabolomic richness of the stepwell, supporting its long-standing recognition as a medicinal water source. Although direct biological assays were not undertaken in this preliminary work, the findings establish a reliable chemical baseline for future studies exploring therapeutic, cosmetic, and environmental significance. Importantly, the metabolomic and elemental insights generated here may inform future product development in balneotherapy, cosmeceuticals, and wellness formulations, provided they are pursued in alignment with international regulatory frameworks (e.g., Japanese balneotherapy standards). In doing so, this work bridges traditional heritage knowledge with modern scientific innovation, laying the groundwork for safe and evidence-based applications of stepwell-derived resources.

Acknowledgment

The authors gratefully acknowledge the Jaypee Institute of Information Technology, Noida, for providing the necessary infrastructure and facilities to carry out this research.

Conflicts of interest

The authors declare no conflict of interest.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used ChatGPT (open AI) and Grammarly for language editing and improving the clarity of the manuscript. All scientific content, interpretation, and conclusions were developed by the authors.

References

- Alrumman, S.A., Mostafa, Y.S., Al-Qahtani, S.T.S., Sahlabji, T., & Taha, T.H. (2019). Antimicrobial activity and GC-MS analysis of bioactive constituents of thermophilic bacteria isolated from Saudi hot springs. *Arabian Journal for Science and Engineering*, 44(1), 75–85. <https://doi.org/10.1007/s13369-018-3597-0>
- Antunes-Ricardo, M., Gutiérrez-Urbe, J.A., Martínez-Vitela, C., & Serna-Saldivar, S.O. (2015). Topical anti-inflammatory effects of isorhamnetin glycosides isolated from *Opuntia ficus-indica*. *BioMed Research International*, 2015, 847320. <https://doi.org/10.1155/2015/847320>
- Bawane, P., & Yele, S. (2025). Antibacterial and cytotoxic activity of bioactives from *Paenibacillus dendritiformis* isolated from Lonar Soda Lake, Maharashtra, India. *International Microbiology*. <https://doi.org/10.1007/s10123-025-00682-3>
- Bochkov, V.N., Oskolkova, O.V., Birukov, K.G., Levonen, A.L., Binder, C.J., & Stöckl, J. (2010). Generation and biological activities of oxidized phospholipids. *Antioxidants & Redox Signaling*, 12(8), 1009–1059. <https://doi.org/10.1089/ars.2009.2597>
- Boo, Y.C. (2019). p-Coumaric acid as an active ingredient in cosmetics: A review focusing on its antimelanogenic effects. *Antioxidants*, 8(8), 275. <https://doi.org/10.3390/antiox8080275>
- Borch, T., Kretzschmar, R., Kappler, A., Van Cappellen, P., Ginder-Vogel, M., Voegelin, A., & Campbell, K. (2010). Biogeochemical redox processes and their impact on contaminant dynamics. *Environmental Science & Technology*, 44(1), 15–23. <https://doi.org/10.1021/es9026248>
- Brahmacharimayum, B., Mohanty, M.P., & Ghosh, P.K. (2019). Theoretical and practical aspects of biological sulphate reduction: A review. *Global NEST Journal*, 21(2), 222–224. <https://doi.org/10.30955/gnj.002577>
- Cacciapuoti, S., Luciano, M.A., Megna, M., Annunziata, M.C., Napolitano, M., Patruno, C., ... Fabbrocini, G. (2020). The role of thermal water in chronic skin diseases management: A review of the literature. *Journal of Clinical Medicine*, 9(9), 3047. <https://doi.org/10.3390/jcm9093047>
- Chen, S., Lin, Z., He, T., Islam, M.S., Xi, L., Liao, P., ... Chen, X. (2022). Topical application of tetrandrine nanoemulsion promotes the expansion of CD4⁺Foxp3⁺ regulatory T cells and alleviates imiquimod-induced psoriasis in mice. *Frontiers in Immunology*, 13, 800283. <https://doi.org/10.3389/fimmu.2022.800283>
- Chen, Y.J., Tang, J., Wang, L., & Hua, W. (2025). Sulfur and its derivatives in dermatology: Insights into therapeutic applications—A narrative review. *Journal of Cosmetic Dermatology*, 24(8), e70402. <https://doi.org/10.1111/jocd.70402>
- Čižmarová, B., Hubková, B., Tomečková, V., & Birková, A. (2023). Flavonoids as promising natural compounds in the prevention and treatment of selected skin diseases. *International Journal of Molecular Sciences*, 24(7), 6324. <https://doi.org/10.3390/ijms24076324>
- Cron, B., Henri, P., Chan, C.S., Macalady, J.L., & Cosmidis, J. (2019). Elemental sulfur formation by *Sulfuricurvum kujiense* is mediated by extracellular organic compounds. *Frontiers in Microbiology*, 10, 2710. <https://doi.org/10.3389/fmicb.2019.02710>
- Ecevit, K., Barros, A.A., Silva, J.M., & Reis, R.L. (2022). Preventing microbial infections with natural phenolic compounds. *Future Pharmacology*, 2(4), 460–498. <https://doi.org/10.3390/futurepharmacol2040030>
- Elloumi, W., Mahmoudi, A., Ortiz, S., Boutefnouchet, S., Chamkha, M., & Sayadi, S. (2022). Wound-healing potential of quercetin-3-O-rhamnoside and myricetin-3-O-rhamnoside isolated from *Pistacia lentiscus* distilled leaves in a rat model. *Biomedicine & Pharmacotherapy*, 146, 112574. <https://doi.org/10.1016/j.biopha.2021.112574>
- Fahy, E., Sud, M., Cotter, D., & Subramaniam, S. (2007). LIPID MAPS online tools for lipid research. *Nucleic Acids Research*, 35, W606–W612. <https://doi.org/10.1093/nar/gkm324>
- Fernandes, A., Rodrigues, P.M., Pintado, M., & Tavará, F.K. (2023). A systematic review of natural products for skin applications: Targeting inflammation, wound healing, and photoaging. *Phytomedicine*, 115, 154824. <https://doi.org/10.1016/j.phymed.2023.154824>
- Figueiredo, A.C., Rodrigues, M., Mourelle, M.L., & Araujo, A.R.T.S. (2023). Thermal spring waters as an active ingredient in cosmetic formulations. *Cosmetics*, 10(1), 27. <https://doi.org/10.3390/cosmetics10010027>
- Franco, L., Marchena, A., & Rodríguez, A. (2021). Skin health properties of lycopene and melatonin. *Journal of Dermatology and Skin Science*, 3(1), 26–29. <https://doi.org/10.29245/2767-5092/2021/1.1126>
- Gaur, N., Sarkar, A., Dutta, D., Gogoi, B.J., Dubey, R., & Dwivedi, S.K. (2022). Evaluation of water quality index and geochemical characteristics of surface water from Tawang, India. *Scientific Reports*, 12(1), 1–18. <https://doi.org/10.1038/s41598-022-14760-3>
- Gülçin, İ., Beydemir, Ş., Topal, F., Gagua, N., Bakuridze, A., Bayram, R., & Gepdiremen, A. (2011). Apoptotic, antioxidant, and antiradical effects of majdine and isomajdine from *Vinca herbacea* Waldst. and kit. *Journal of Enzyme Inhibition and Medicinal Chemistry*, 27(4), 587–594. <https://doi.org/10.3109/14756366.2011.604318>
- He, Y., Hu, Y., Jiang, X., Chen, T., Ma, Y., Wu, S., ... Bai, W. (2017). Cyanidin-3-O-glucoside inhibits the UVB-induced ROS/COX-2 pathway in HaCaT cells. *Journal of Photochemistry and Photobiology B: Biology*, 177, 24–31. <https://doi.org/10.1016/j.jphotobiol.2017.10.006>
- Hillman, P.F., Lee, C., & Nam, S.J. (2022). Microbial natural products with wound-healing properties. *Processes*, 11(1), 30. <https://doi.org/10.3390/pr11010030>
- Horai, H., Arita, M., Kanaya, S., Nihei, Y., Ikeda, T., Suwa, K., ... Nishioka, T. (2010). MassBank: A public repository for sharing mass spectral data for life sciences. *Journal of Mass Spectrometry*, 45, 703–714. <https://doi.org/10.1002/jms.1777>

- Hughes-Formella, B., Wunderlich, O., & Williams, R. (2006). Anti-inflammatory and skin-hydrating properties of a dietary supplement and topical formulations containing oligomeric proanthocyanidins. *Skin Pharmacology and Physiology*, 20(1), 43–49. <https://doi.org/10.1159/000096171>
- Ito, T., Okabe, S., Satoh, H., & Watanabe, Y. (2002). Successional development of sulphate-reducing bacterial populations and their activities in a wastewater biofilm growing under microaerophilic conditions. *Applied and Environmental Microbiology*, 68(3), 1392–1402. <https://doi.org/10.1128/aem.68.3.1392-1402.2002>
- Jingfu, W., Liu, G., Wang, G., Zhang, J., Li, C., & Li, F. (2016). Sulfur speciation in the surface sediments of lakes from different regions, China: Characterization by S K-edge XANES spectroscopy. *Journal of Chemistry*, 2016, 3672348. <https://doi.org/10.1155/2016/3672348>
- Karimi, E., Jaafar, H.Z.E., Ghasemzadeh, A., & Ebrahimi, M. (2015). Fatty acid composition, antioxidant, and antibacterial properties of the microwave aqueous extract of three varieties of *Labisia pumila* Benth. *Biological Research*, 48(1), 9. <https://doi.org/10.1186/0717-6287-48-9>
- Li, M., Lin, X.F., Lu, J., Zhou, B.R., & Luo, D. (2016). Hesperidin ameliorates UV radiation-induced skin damage by abrogation of oxidative stress and inflammation in HaCaT cells. *Journal of Photochemistry and Photobiology B: Biology*, 165, 240–245. <https://doi.org/10.1016/j.jphotobiol.2016.10.037>
- Mao, J., Ma, X., Zhu, J., & Zhang, H. (2022). Ginsenoside Rg1 ameliorates psoriasis-like skin lesions by suppressing proliferation and NLRP3 inflammasomes in keratinocytes. *Journal of Food Biochemistry*, 46(5), e14053. <https://doi.org/10.1111/jfbc.14053>
- Margalef-Martí, R., Sebilo, M., Thibault de Chanvalon, A., Anschutz, P., Charbonnier, C., Lauga, B., ... Amouroux, D. (2023). Upside down sulphate dynamics in a saline inland lake. *Scientific Reports*, 13(1), 1–11. <https://doi.org/10.1038/s41598-022-27355-9>
- Merfort, I., Heilmann, J., Hagedorn-Leweke, U., & Lippold, B.C. (1994). In vivo skin penetration studies of camomile flavones. *Die Pharmazie*, 49(7), 509–511.
- Ministry of the Environment. (2019). *The ABCs for the safe and secure use of onsen: What should we be aware of when bathing in onsen (hot springs) and drinking onsen mineral water?*. <https://www.env.go.jp/content/900492871.pdf>
- Mourelle, M.L., Gómez, C.P., & Legido, J.L. (2024). Unveiling the role of minerals and trace elements of thermal waters in skin health. *Applied Sciences*, 14(14), 6291. <https://doi.org/10.3390/app14146291>
- National Center for Biotechnology Information. (2022). *Bioproject: PRJNA905208: Metagenomic analysis of Gandhak-ki-Baoli for assessing microbial diversity* [Data set]. U.S. National Library of Medicine. <https://www.ncbi.nlm.nih.gov/bioproject/PRJNA905208/>
- Ncube, S., Beevers, L., & Momblanch, A. (2021). Towards intangible freshwater cultural ecosystem services: Informing sustainable water resources management. *Water*, 13(4), 535. <https://doi.org/10.3390/w13040535>
- Parai, D., Islam, E., Mitra, J., & Mukherjee, S.K. (2017). Effect of bacoside A on growth and biofilm formation by *Staphylococcus aureus* and *Pseudomonas aeruginosa*. *Canadian Journal of Microbiology*, 63(2), 169–178. <https://doi.org/10.1139/cjm-2016-0365>
- Park, S., Lee, J.B., & Kang, S. (2012). Topical application of *Chrysanthemum indicum* L. attenuates the development of atopic dermatitis-like skin lesions by suppressing serum IgE levels, IFN- γ , and IL-4 in NC/Nga mice. *Evidence-Based Complementary and Alternative Medicine*, 2012, 821967. <https://doi.org/10.1155/2012/821967>
- Patil, U.K., & Saraogi, R. (2014). Natural products as potential drug permeation enhancers in transdermal drug delivery systems. *Archives of Dermatological Research*, 306(5), 419–426. <https://doi.org/10.1007/s00403-014-1445-y>
- Protano, C., Vitali, M., De Giorgi, A., Marotta, D., Crucianelli, S., & Fontana, M. (2024). Balneotherapy using thermal mineral water baths and dermatological diseases: A systematic review. *International Journal of Biometeorology*, 68, 1005–1013. <https://doi.org/10.1007/s00484-024-02649-x>
- Sachdeva, S., & Sarethy, I.P. (2024). Diving into freshwater microbial metabolites: Pioneering research and future prospects. *Environmental Technology*, 45(3), 282–300. <https://doi.org/10.1080/09603123.2024.2351153>
- Sachdeva, S., & Sarethy, I.P. (2025). Actinomycetes from sulphur-rich reservoirs: Pioneering healthcare innovations. *Applied Biochemistry and Microbiology*, 61(2), 312–320.
- Sharifi-Rad, J., Cruz-Martins, N., López-Jornet, P., Pons-Fuster Lopez, E., Harun, N., Yeskaliyeva, B., ... Cho, W.C. (2021). Natural coumarins: Exploring the pharmacological complexity and underlying molecular mechanisms. *Oxidative Medicine and Cellular Longevity*, 2021, 6492346. <https://doi.org/10.1155/2021/6492346>
- Shen, X., Guo, M., Yu, H., Liu, D., Lu, Z., & Lu, Y. (2019). *Propionibacterium acnes*-related anti-inflammation and skin hydration activities of madecassoside, a pentacyclic triterpene saponin from *Centella asiatica*. *Bioscience, Biotechnology, and Biochemistry*, 83(3), 561–568. <https://doi.org/10.1080/09168451.2018.1547627>
- Silva, L.F.O., Fdez-Ortiz de Vallejuelo, S., Martínez-Arkarazo, I., Castro, K., Oliveira, M.L.S., & Sampaio, C.H. (2013). Study of environmental pollution and mineralogical characterization of sediment rivers from Brazilian coal mining acid drainage. *Science of the Total Environment*, 447(1), 169–178. <https://doi.org/10.1016/j.scitotenv.2012.12.013>

- Sudji, I.R., Subburaj, Y., Frenkel, N., García-Sáez, A.J., & Wink, M. (2015). Membrane disintegration caused by the steroid saponin digitonin is related to the presence of cholesterol. *Molecules*, 20(11), 20146–20160. <https://doi.org/10.3390/molecules201119682>
- Taevernier, L., Veryser, L., Roche, N., Peremans, K., Burvenich, C., Delesalle, C., & De Spiegeleer, B. (2015). Human skin permeation of emerging mycotoxins (beauvericin and enniatins). *Journal of Exposure Science & Environmental Epidemiology*, 26(3), 277–287. <https://doi.org/10.1038/jes.2015.10>
- Tallar, R., & Suen, J.P. (2017). Measuring the aesthetic value of multifunctional lakes using an enhanced visual quality method. *Water*, 9(3), 233. <https://doi.org/10.3390/w9030233>
- Vári, Á., Podschun, S.A., Erős, T., Hein, T., Pataki, B., Iojă, I.C., ... Báldi, A. (2021). Freshwater systems and ecosystem services: Challenges and chances for cross-fertilization of disciplines. *Ambio*, 51(1), 135–151. <https://doi.org/10.1007/s13280-021-01547-y>
- Verleur, N., & Wanders, R.J.A. (1993). Permeability properties of peroxisomes in digitonin-permeabilized rat hepatocytes: Evidence for free permeability towards a variety of substrates. *European Journal of Biochemistry*, 218(1), 75–82. <https://doi.org/10.1111/j.1432-1033.1993.tb18353.x>
- Vessichelli, M., Mariggio, S., Varone, A., Zizza, P., Di Santo, A., Amore, C., ... Corda, D. (2017). The natural phosphoinositide derivative glycerophosphoinositol inhibits the lipopolysaccharide-induced inflammatory and thrombotic responses. *Journal of Biological Chemistry*, 292(31), 12828–12841. <https://doi.org/10.1074/jbc.m116.773861>
- Wang, L., Xian, Y.F., Loo, S.K.F., Ip, S.P., Yang, W., Chan, W.Y., ... Wu, J.C.Y. (2022). Baicalin ameliorates 2,4-dinitrochlorobenzene-induced atopic dermatitis-like skin lesions in mice through modulating skin barrier function, gut microbiota, and JAK/STAT pathway. *Bioorganic Chemistry*, 119, 105538. <https://doi.org/10.1016/j.bioorg.2021.105538>
- Wang, Q., & Xu, L. (2012). Beauvericin, a bioactive compound produced by fungi: A short review. *Molecules*, 17(3), 2367–2377. <https://doi.org/10.3390/molecules17032367>
- Wu, X.F., Xu, R., Ouyang, Z.J., Qian, C., Shen, Y., Wu, X.D., ... Sun, Y. (2013). Beauvericin ameliorates experimental colitis by inhibiting activated T cells via downregulation of the PI3K/Akt signaling pathway. *PLoS ONE*, 8(12), e83013. <https://doi.org/10.1371/journal.pone.0083013>
- Yang, G., Lee, K., Lee, M.H., Kim, S.H., Ham, I.H., & Choi, H.Y. (2011). Inhibitory effects of Chelidonium majus extract on atopic dermatitis-like skin lesions in NC/NGA mice. *Journal of Ethnopharmacology*, 138(2), 398–403. <https://doi.org/10.1016/j.jep.2011.09.028>
- Yang, Y., & Ling, W. (2025). Health benefits and future research of phytochemicals: A literature review. *The Journal of Nutrition*, 155(1), 87–101. <https://doi.org/10.1016/j.tjnut.2024.11.007>
- Yourick, J.J., & Bronaugh, R.L. (1997). Percutaneous absorption and metabolism of coumarin in human and rat skin. *Journal of Applied Toxicology*, 17(3), 153–158. [https://doi.org/10.1002/\(sici\)1099-1263\(199705\)17:3<153::aid-jat426>3.0.co;2-e](https://doi.org/10.1002/(sici)1099-1263(199705)17:3<153::aid-jat426>3.0.co;2-e)
- Zhang, C., Wang, K., Yang, L., Liu, R., Chu, Y., Qin, X., ... Yu, H. (2018). Lipid metabolism in inflammation-related diseases. *The Analyst*, 143(19), 4526–4536. <https://doi.org/10.1039/c8an01046c>
- Zhou, W., Hu, M., Zang, X., Liu, Q., Du, J., Hu, J., ... Xiang, Z. (2020). Luteolin attenuates imiquimod-induced psoriasis-like skin lesions in BALB/c mice via suppression of the inflammatory response. *Biomedicine & Pharmacotherapy*, 131, 110696. <https://doi.org/10.1016/j.biopha.2020.110696>

Supplementary Table 1 Compounds identified through MassBank

M/Z ratio	Adduct type	Tolerance	Compounds from MassBank database		
			Compound name	Compound formula	MassBank class
116.9796	[M+H] ⁺	0.02	Chloridazon	C ₁₀ H ₈ ClN ₃ O	Environmental standard
127.0266		0.01	Asiaticoside	C ₄₈ H ₇₈ O ₁₉	Triterpene saponins
128.9961	[M+H] ⁺	0.01	Oxadiazone	C ₁₅ H ₁₈ Cl ₂ N ₂ O ₅	Environmental standard
132.9712	[M+H] ⁺	0.01	Clothianidin	C ₆ H ₆ ClN ₃ O ₂ S	Environmental standard
133.0837	[M+H] ⁺	0.01	2,6-Cycloycopene-1,5-diol	C ₄₀ H ₅₈ O ₂	Natural product: Sesquiterpenoids
136.9199	[M+H] ⁺	0.1	Methylchloroisothiazolinone	C ₄ H ₄ ClNOS	Environmental standard
149.0154	[M+H] ⁺	0.001	Thiophanate-methyl	C ₁₂ H ₁₄ N ₄ O ₄ S ₂	Environmental standard
166.947	[M+H] ⁺	0.04	2-(Methylthio)benzothiazole	C ₈ H ₇ NS ₂	Environmental standard
171.0775	[M+H] ⁺	0.001	Triamcinolone	C ₂₁ H ₂₇ FO ₆	Environmental standard
189.0811	[M+H] ⁺	0.01	Chelidonin	C ₂₀ H ₁₉ NO ₅	Hexahydrobenzophenanthridine alkaloids
190.0836	[M+H] ⁺	0.001	Tetrandrine	C ₃₈ H ₄₂ N ₂ O ₆	Lignans
194.0946	[M+H] ⁺	0.001	5(S)-5-carboxystroictosidine	C ₂₈ H ₃₄ N ₂ O ₁₁	Terpene glycosides
203.0554	[M+H] ⁺	0.01	Procyanidin	C ₃₀ H ₂₆ O ₁₂	Biflavonoids
218.1794	[M+H] ⁺	0.01	Ginsenoside	C ₄₂ H ₇₀ O ₁₂	Triterpene saponins
219.0813	[M+H] ⁺	0.01	19S-Methoxytubotaiwine	C ₂₁ H ₂₆ N ₂ O ₃	Strychnos alkaloids
246.2002	[M+H] ⁺	0.01	Phantolide	C ₁₇ H ₂₄ O	Environmental standard
250.1366	[M+H] ⁺	0.01	4-Coumaroylcholine	C ₁₄ H ₂₀ NO ₃ ⁺	Natural product; Phenolic choline ester
274.2209	[M+H] ⁺	0.05	Ginsenoside	C ₄₂ H ₇₀ O ₁₂	Triterpene saponins
275.2234	[M+H] ⁺	0.01	Madecassoside	C ₄₈ H ₇₈ O ₂₀	Triterpene saponins
279.0391	[M+H] ⁺	0.01	Amidosulfuron	C ₈ H ₁₅ N ₃ O ₇ S ₂	Environmental standard
301.0765	[M+H] ⁺	0.001	Eriodictyol-7-O-neohesperidoside	C ₂₇ H ₃₂ O ₁₅	Flavonoid-7-O-glycosides
318.2293	[M+H] ⁺	0.1	Bupirimate	C ₁₅ H ₂₄ N ₄ O ₃ S	Environmental standard
319.1227	[M+H] ⁺	0.01	Perrottetin	C ₂₈ H ₂₆ O ₄	Natural product; Lignane
398.1277, 399.1305	[M+H] ⁺	0.01	Flecainide	C ₁₇ H ₂₀ F ₆ N ₂ O ₃	Environmental standard
429.2544	[M+H] ⁺	0.01	Irbesartan	C ₂₅ H ₂₈ N ₆ O	Environmental standard
522.1959	[M+H] ⁺	1	Lycopene	C ₄₀ H ₅₆	Natural product; Carotenoids, carotene
615.2955	[M+H] ⁺	0.1	Soyasapogenol B base+O-HexA-Hex-Pen	C ₅₄ H ₈₄ O ₂₁	Triterpene saponins
714.3149–714.649	[M+H] ⁺	2	Ginsenoside	C ₄₂ H ₇₀ O ₁₂	Triterpene saponins
740.2629	[M+H] ⁺	1	Kaempferol-3-O-robinoside-7-O-rhamnoside	C ₃₃ H ₄₀ O ₁₉	Natural product
756.2875	[M+H] ⁺	0.1	Rifaximin	C ₄₃ H ₅₁ N ₃ O ₁₁	Environmental standard
757.29, 760.3234	[M+H] ⁺	0.1, 2	Cyanidin 3-(2G-glucosylrutinoside)	C ₃₃ H ₄₁ O ₂₀ ⁺	Anthocyanidin-3-O-glycosides
779.0623–780.2749	[M+H] ⁺	0.5	Bacoside A3	C ₄₇ H ₇₆ O ₁₈	Natural product; Terpenoids
781.2772	[M+H] ⁺	0.1	Digitonin	C ₅₆ H ₉₂ O ₂₉	Steroidal saponins
782.2904	[M+H] ⁺	0.1	Coumarin	C ₉ H ₆ O ₂	Natural product
783.2927		0.1	Digitonin	C ₅₆ H ₉₂ O ₂₉	Steroidal saponins
784.2958	[M+H] ⁺	0.2	Beauvericin	C ₄₅ H ₅₇ N ₃ O ₉	Natural product; Peptide derivatives
856.959, 857.0596	[M+H] ⁺	1	Paclitaxel	C ₄₇ H ₅₄ NO ₁₄	Natural product; Terpenoid
857.1595–857.3598	[M+H] ⁺	0.5	Ginsenoside	C ₃₃ H ₄₄ O ₁₉	Triterpene saponins
952.0541, 952.277	[M+H] ⁺	1	Hyperoside	C ₂₁ H ₂₀ O ₁₂	Natural product
952.1652, 952.3884	[M+H] ⁺	1	Myricitrin	C ₂₁ H ₂₀ O ₁₂	Natural product
116.9841	[M-H] ⁻	0.05	Epicatechin	C ₁₅ H ₁₄ O ₆	Catechins
116.9841	[M-H] ⁻	0.04	Apigeninidin	C ₁₅ H ₁₁ ClO ₄	Catechins
131.0248	[M-H] ⁻	0.01	Chrysanthelein A	C ₅₈ H ₉₄ O ₂₅	7-hydroxyflavonoids
136.9853	[M-H] ⁻	0.01	6-Methoxyluteolin	C ₁₆ H ₁₂ O ₇	Triterpene saponins
160.9056	[M-H] ⁻	0.1	Hesperetin	C ₁₆ H ₁₄ O ₆	Natural product
162.9028	[M-H] ⁻	0.01	L-(+)-Rhamnose	C ₆ H ₁₂ O ₅	Natural product; Flavanoid
164.9006	[M-H] ⁻	0.01	Rhamnetin	C ₁₆ H ₁₂ O ₇	Monosaccharide
164.9952	[M-H] ⁻	0.01	Methyl Dihydrojasmonate	C ₁₃ H ₂₂ O ₃	Flavanoid
170.9487	[M-H] ⁻	0.1	Baicalcin	C ₁₅ H ₁₀ O ₅	—
175.0215	[M-H] ⁻	0.01	Isomajdine	C ₂₃ H ₂₈ N ₂ O ₆	Flavones
180.9788	[M-H] ⁻	0.01	Bacosine	C ₃₀ H ₄₈ O ₃	Indolizidines
195.8796	[M-H] ⁻	0.1	Cyanidin-3-O-galactoside	C ₂₁ H ₂₁ O ₁₁ ⁺	Natural product; Terpenoids
197.8768	[M-H] ⁻	0.05	Lagocholic acid	C ₂₄ H ₄₆ O ₅	Natural product; Anthocyanidin-3-O-glycosides
199.8741	[M-H] ⁻	0.1	Folic acid	C ₁₉ H ₁₉ N ₇ O ₆	Natural product
201.9041	[M-H] ⁻	0.1	3-Nitrobenzenesulfonic acid	C ₆ H ₅ NO ₃ S	Amino acids
219.9169	[M-H] ⁻	0.1	Mitragynine	C ₂₃ H ₃₀ N ₂ O ₄	Environmental standard
221.9138	[M-H] ⁻	0.1	2-Amido-3,5,6-trichloro-4-cyanobenzenesulfonic acid	C ₈ H ₃ Cl ₃ N ₂ O ₄ S	Corynanthean-type alkaloids
232.9477	[M-H] ⁻	0.1	Climbazol	C ₁₅ H ₁₇ ClN ₂ O ₂	Environmental standard

Supplementary Table 2 Compound identified from LipidMaps

Input mass	Ion	Delta	Compounds from LipidMaps database		Name	Formula
127.0266	[M+H] ⁺	0.0488	3-heptynoic acid	4-Methyl-3Z,5-hexadienoic acid	FA 7:2	C ₇ H ₁₀ O ₂
127.0266	[M+H] ⁺	0.0488	Methyl sorbate	–	SFE 7:2	C ₇ H ₁₀ O ₂
127.0266	[M+Na] ⁺	0.0264	Malonic acid	–	FA 3:1;O2	C ₃ H ₄ O ₄ Na
127.0266	[M+Na] ⁺	0.01	2S-Hydroxybutanoic acid	alpha-hydroxy-isobutyric acid	FA 4:0;O	C ₄ H ₈ O ₃ Na
127.0266	[M+K] ⁺	0.0474	Pyruvic acid	–	FA 3:1;O	C ₃ H ₄ O ₃ K
127.0266	[M+K] ⁺	0.011	Butyric acid	–	FA 4:0	C ₄ H ₈ O ₂ K
127.0266	[M+K] ⁺	0.011	Methyl propionate	–	SFE 4:0	C ₄ H ₈ O ₂ K
128.9961	[M+H] ⁺	0.0221	Glutinic acid	–	FA 5:3;O2	C ₅ H ₈ O ₄
132.9712	[M+H] ⁺	0.0419	2-hydroxy-2-butenedioic acid	Oxalacetic acid	FA 4:2;O3	C ₄ H ₄ O ₅
133.0837	[M+H] ⁺	0.0342	3-hydroxy-3-methyl-2-oxo-butanoic acid	2-Acetolactate	FA 5:1;O2	C ₅ H ₈ O ₄
133.0837	[M+H] ⁺	0.0022	2-hydroxy-3-methyl-pentanoic acid	5-hydroxy caproic acid	FA 6:0;O	C ₆ H ₁₂ O ₃
149.0154	[M+H] ⁺	0.0073	dihydroxy-fumaric acid	–	FA 4:2;O4	C ₄ H ₄ O ₆
149.0154	[M+H] ⁺	0.029	2-dehydro-3-deoxy-D-arabinonic acid	2-hydroxyglutaric acid	FA 5:1;O3	C ₅ H ₈ O ₅
149.0154	[M+Na] ⁺	0.0419	3-heptynoic acid	–	FA 7:2	C ₇ H ₁₀ O ₂ Na
149.0154	[M+Na] ⁺	0.0419	R-Lavender lactone	–	FA 7:2	C ₇ H ₁₀ O ₂ Na
149.0154	[M+Na] ⁺	0.0419	Methyl sorbate	–	SFE 7:2	C ₇ H ₁₀ O ₂ Na
166.947	[M+K] ⁺	0.0271	Glutinic acid	–	FA 5:3;O2	C ₅ H ₈ O ₄ K
171.0775	[M+H] ⁺	0.0241	Dendryphielllic acid B	4-oxo-2E-nonenic acid	FA 9:2;O	C ₉ H ₁₄ O ₃
171.0775	[M+H] ⁺	0.0147	2,3-Dihydroxy-3-methylpentanoic acid	Mevalonic acid	FA 6:0;O2	C ₆ H ₁₂ O ₄ Na
171.0775	[M+K] ⁺	0.0357	3R-hydroxy-hexanoic acid	L-Isoleucic acid	FA 6:0;O	C ₆ H ₁₂ O ₃ K
189.0811	[M+H] ⁺	0.0417	(2E)-2-(methoxycarbonylmethyl)but-2-enedioic acid	–	FA 7:3;O4	C ₇ H ₈ O ₆
189.0811	[M+H] ⁺	0.0417	(2E)-3-(methoxycarbonyl)pent-2-enedioic acid	–	WE 7:3;O4	C ₇ H ₈ O ₆
189.0811	[M+H] ⁺	0.0099	5,8,11-dodecatriynoic acid	–	FA 12:6	C ₁₂ H ₁₂ O ₃
189.0811	[M+H] ⁺	0.031	Azelaic acid	3-Methylsubericacid	FA 9:1;O2	C ₉ H ₁₆ O ₄
189.0811	[M+H] ⁺	0.031	cis- and trans-Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	–	SFE 9:1;O2	C ₉ H ₁₆ O ₄
189.0811	[M+Na] ⁺	0.0075	2,4,7-Decatrienoic acid	–	FA 10:3	C ₁₀ H ₁₄ O ₂ Na
203.0554	[M+H] ⁺	0.0368	4-carboxy-2-hydroxy-cis,cis-muconic acid	–	FA 7:4;O5	C ₇ H ₈ O ₇
203.0554	[M+Na] ⁺	0.0028	Fuconic acid	–	FA 6:0;O4	C ₆ H ₁₂ O ₆ Na
203.0554	[M+Na] ⁺	0.0125	Propyl 2-furanacrylate	–	SFE 10:4;O	C ₁₀ H ₁₂ O ₃ Na
203.0554	[M+Na] ⁺	0.0488	7E,10-undecadien-4-olide	–	FA 11:3	C ₁₁ H ₁₆ O ₂ Na
203.0554	[M+Na] ⁺	0.0488	Methyl 2E,4E,6Z-decatrienoate	–	SFE 11:3	C ₁₁ H ₁₆ O ₂ Na
203.0554	[M+K] ⁺	0.0449	Methyl 2E,4E,6Z-decatrienoate	–	FA 9:5;O	C ₉ H ₈ O ₃ K
203.0554	[M+K] ⁺	0.0238	Digitoxic acid	–	FA 6:0;O3	C ₆ H ₁₀ O ₃ K
203.0554	[M+K] ⁺	0.0085	2,4-decadiynoic acid	–	FA 10:4	C ₁₀ H ₁₂ O ₂ K
203.0554	[M+K] ⁺	0.0085	Methyl 3-phenylpropanoate	–	SFE 10:4	C ₁₀ H ₁₂ O ₂ K
203.0554	[M+K] ⁺	0.0279	11-oxo-undeca-5,8-dienoic acid	Alutacenoic acid B	FA 11:3;O	C ₁₁ H ₁₆ OK
218.1794	[M+H] ⁺	0.0407	O-propanoyl-carnitine	Propionylcarnitine	CAR 3:0	C ₁₀ H ₁₉ NO ₄
219.0813	[M+H] ⁺	0.0203	6-hydroxytrideca-7,8-dien-10,12-diynoic acid	–	FA 14:6;O	C ₁₃ H ₁₄ O ₃
219.0813	[M+H] ⁺	0.0414	2-hydroxy-decanedioic acid	3-hydroxy-sebacic acid	FA 10:1;O3	C ₁₀ H ₁₈ O ₅
219.0813	[M+Na] ⁺	0.0179	cis-Jasmone	–	FA 11:3;O	C ₁₁ H ₁₆ O ₃ Na
219.0813	[M+Na] ⁺	0.0179	11-oxo-undeca-5,8-dienoic acid	5S,6S-epoxy-7-undecynoic acid	FA 11:3;O	C ₁₁ H ₁₆ O ₃ Na
219.0813	[M+Na] ⁺	0.0179	Isobutyl 2-furanpropionate	–	WE 11:3;O	C ₁₁ H ₁₆ O ₃ Na
219.0813	[M+K] ⁺	0.0395	Propyl 2-furanacrylate	–	SFE 10:4;O	C ₁₀ H ₁₂ O ₃ K
219.0813	[M+K] ⁺	0.0031	7E,10-undecadien-4-olide	–	FA 11:3	C ₁₁ H ₁₆ O ₂ K
219.0813	[M+K] ⁺	0.0031	Methyl 2E,4E,6Z-decatrienoate	Methyl 2E,4Z,6Z-decatrienoate	SFE 11:3	C ₁₁ H ₁₆ O ₂ K
246.2002	[M+H] ⁺	0.0302	2-Methylbutyrylcarnitine	Valeryl carnitine	CAR 5:0	C ₁₂ H ₂₃ NO ₄
274.2209	[M+H] ⁺	0.0196	Heptanoylcarnitine	–	CAR 7:0	C ₁₄ H ₂₇ NO ₄
275.2234	[M+H] ⁺	0.0381	3-hydroxy-tetradecanedioic acid	–	FA 14:1;O3	C ₁₄ H ₂₆ O ₅
275.2234	[M+H] ⁺	0.0229	3,6,9,12,15-octadecapentaenoic acid	Dicranin	FA 18:5	C ₁₈ H ₂₆ O ₂
275.2234	[M+H] ⁺	0.0229	Rhodinyl phenylacetate	–	SFE 18:5	C ₁₈ H ₂₆ O ₂
275.2234	[M+H] ⁺	0.0229	mandrolone	–	ST 18:2;O2	C ₁₈ H ₂₆ O ₂
275.2234	[M+H] ⁺	0.0229	Citronellyl alpha-toluate	–	WE 18:5	C ₁₈ H ₂₆ O ₂
275.2234	[M+H] ⁺	0.0017	2,15-dihydroxy-pentadecylic acid	Turpetholic acid A	FA 15:0;O2	C ₁₅ H ₃₀ O ₄
275.2234	[M+H] ⁺	0.0135	alpha-androstenol	–	ST 19:1;O	C ₁₉ H ₃₀ O
275.2234	[M+Na] ⁺	0.0253	2E,4E-hexadecadienoic acid	Hydnocarpic acid	FA 16:2	C ₁₆ H ₂₈ O ₂ Na
275.2234	[M+Na] ⁺	0.0253	10E,12E-Tetradecadienyl acetate	–	SFE 16:2	C ₁₆ H ₂₈ O ₂ Na
275.2234	[M+Na] ⁺	0.0253	(E)-3,7-Dimethyl-2,6-octadienyl hexanoate	–	WE 16:2	C ₁₆ H ₂₈ O ₂ Na
279.0391	[M+Na] ⁺	0.0448	3-carboxy-4-methyl-5-(1-hydroxypropyl)-2-furanpropionic acid	–	FA 12:4;O4	C ₁₂ H ₁₆ O ₆ Na
279.0391	[M+K] ⁺	0.0238	2-carboxyethyl-5-furanpentanoic acid	–	FA 12:4;O3	C ₁₂ H ₁₆ O ₃ K
301.0765	[M+K] ⁺	0.0283	Phaseolic acid	–	FA 12:1;O4	C ₁₂ H ₂₂ O ₆ K

Supplementary Table 2 Compound identified from LipidMaps

Input mass	Ion	Delta	Compounds from LipidMaps database	Name	Formula
318.2293	[M+Na] ⁺	0.011	(4E,8E,10E-d18:3) sphingosine	SPB 18:3;O2	C ₁₈ H ₃₃ NO ₂ Na
319.1227	[M+Na] ⁺	0.0289	3,4-dimethyl-5-carboxybutyl-2-furanpentanoic acid	FA 16:4;O3	C ₁₆ H ₂₄ O ₃ Na
319.1227	[M+Na] ⁺	0.0441	4,8,11,14-Eicosatetraynoic acid	FA 20:8	C ₂₀ H ₃₄ O ₂ Na
319.1227	[M+Na] ⁺	0.0441	17alpha-Ethinyl estradiol	ST 20:5;O2	C ₂₀ H ₂₄ O ₂ Na
319.1227	[M+K] ⁺	0.0496	6-hydroxy-7E,9E-Octadecadiene-11,13,15,17-tetraynoic acid	Caryoyneincin A	C ₁₈ H ₁₆ O ₃ K
319.1227	[M+K] ⁺	0.0079	5-Acetoxy-tetradeca-2E,4E,6E-trienoic acid	FA 16:4;O2	C ₁₆ H ₂₄ O ₄ K
319.1227	[M+K] ⁺	0.0443	12S-HHTrE	FA 17:3;O	C ₁₇ H ₂₈ O ₃ K
399.1305	[M+Na] ⁺	0.0473	18-oxo-cortisol	ST 21:4;O6	C ₂₁ H ₂₈ O ₆ Na
399.1305	[M+K] ⁺	0.0263	Aldosterone	ST 21:4;O5	C ₂₁ H ₂₈ O ₅ K
429.2544	[M+H] ⁺	0.0296	PG(12:0/0:0)	LPG 12:0	C ₁₈ H ₃₇ O ₉ P
429.2544	[M+H] ⁺	0.0303	1(3)-glyceryl-PGF2alpha	FA 23:3;O5	C ₂₃ H ₄₀ O ₇
429.2544	[M+H] ⁺	0.0455	17(20)-Dehydrocryptogenin	Bufospirostenin A	C ₂₇ H ₄₀ O ₄
429.2544	[M+H] ⁺	0.0455	Fomentarol A	Stoloniferone H	C ₂₇ H ₄₀ O ₄
429.2544	[M+Na] ⁺	0.0296	antiogenin	bipindogenin	C ₂₃ H ₃₄ O ₆ Na
429.2544	[M+Na] ⁺	0.0067	3-Oxocholeic acid	-	C ₂₄ H ₃₈ O ₃ Na
429.2544	[M+Na] ⁺	0.0431	Homochenodeoxycholeic acid	-	C ₂₅ H ₄₂ O ₄ Na
429.2544	[M+K] ⁺	0.0142	7-oxolithocholic acid	-	C ₂₄ H ₃₈ O ₄ K
429.2544	[M+K] ⁺	0.0221	Homolithocholic acid	-	C ₂₅ H ₄₂ O ₃ K
522.1959	[M+K] ⁺	0.027	PS(15:0/0:0)	LPS 15:0	C ₂₁ H ₄₂ NO ₉ PK
522.1959	[M+K] ⁺	0.027	1-(2-methoxy-6Z-tetradecenyl)-sn-glycero-3-phosphoserine	LPS O-15:1;O	C ₂₁ H ₄₂ NO ₉ PK
615.2955	[M+H] ⁺	0.0361	1,2-(8R,9R-epoxy-octadec-13Z,15Z-dien-4,6-diynoyl)-sn-glycerol	TG 35:13;O	C ₃₈ H ₄₆ O ₇
615.2955	[M+Na] ⁺	0.0414	PI(18:4(6Z,9Z,12Z,15Z)/0:0)	-	C ₂₇ H ₄₈ O ₁₂ PNa
615.2955	[M+Na] ⁺	0.005	OHHDiA-PA	PA 25:3;O3	C ₂₈ H ₄₉ O ₁₁ PNa
615.2955	[M+K] ⁺	0.026	OHOHA-PA	PA 25:3;O2	C ₂₈ H ₄₉ O ₁₀ PK
615.2955	[M+K] ⁺	0.0468	PA(12:0/15:1(9Z))	PA 27:1	C ₃₀ H ₅₇ O ₈ PK
714.3149	[M+Na] ⁺	0.0076	OKODiA-PS	PS 26:4;O3	C ₃₂ H ₅₄ NO ₁₃ PNa
714.3149	[M+K] ⁺	0.0134	OKOOA-PS	PS 26:4;O2	C ₃₂ H ₅₄ NO ₁₂ PK
714.3149	[M+K] ⁺	0.023	OKHdiA-PC	PC 25:4;O3	C ₃₃ H ₅₈ NO ₁₁ PK
714.3985	[M+H] ⁺	0.0356	PS(13:0/18:4(6Z,9Z,12Z,15Z))	PS 31:4	C ₃₇ H ₆₄ NO ₁₀ P
714.3985	[M+Na] ⁺	0.0032	OHODiA-PC	PC 26:3;O3	C ₃₄ H ₆₂ NO ₁₁ PNa
714.3985	[M+Na] ⁺	0.0332	OA-PC	PC 27:2;O2	C ₃₅ H ₆₆ NO ₁₀ PNa
714.3985	[M+Na] ⁺	0.0332	PS(12:0/17:1(9Z))	PS 29:1	C ₃₅ H ₆₆ NO ₁₀ PNa
714.3985	[M+K] ⁺	0.0242	OHOOA-PC	PC 26:3;O2	C ₃₄ H ₆₂ NO ₁₀ PK
714.3985	[M+K] ⁺	0.0242	PKDdiA-PE	PE 29:3;O2	C ₃₄ H ₆₂ NO ₁₀ PK
714.3985	[M+K] ⁺	0.0242	PS(14:1(9Z)/14:1(9Z))	PS 28:2	C ₃₄ H ₆₂ NO ₁₀ PK
714.3985	[M+K] ⁺	0.0122	OON-PC	PC 27:2;O	C ₃₅ H ₆₆ NO ₉ PK
714.3985	[M+K] ⁺	0.0486	PC(10:0/18:1(9Z))	PC 28:1	C ₃₆ H ₇₀ NO ₈ PK
714.3985	[M+K] ⁺	0.0486	PE(12:0/19:1(9Z))	PE 31:1	C ₃₆ H ₇₀ NO ₈ PK
714.4822	[M+H] ⁺	0.0481	PS(13:0/18:4(6Z,9Z,12Z,15Z))	PS 31:4	C ₃₇ H ₆₄ NO ₁₀ P
714.4822	[M+H] ⁺	0.0246	PC(13:0/18:3(6Z,9Z,12Z))	PC 31:3	C ₃₉ H ₇₂ NO ₈ P
714.4822	[M+H] ⁺	0.0246	PE(14:0/20:3(8Z,11Z,14Z))	PE 34:3	C ₃₉ H ₇₂ NO ₈ P
714.4822	[M+Na] ⁺	0.0142	PS(O-16:0/14:1(9Z))	PS O-35:3	C ₃₆ H ₇₀ NO ₉ PNa
714.4822	[M+Na] ⁺	0.0222	PC(10:0/19:0)	PC 29:0	C ₃₇ H ₇₄ NO ₈ PNa
714.4822	[M+Na] ⁺	0.0222	PE(12:0/20:0)	PE 32:0	C ₃₇ H ₇₄ NO ₈ PNa
714.4822	[M+K] ⁺	0.0351	PC(10:0/18:1(9Z))	PC 28:1	C ₃₆ H ₇₀ NO ₈ PK
714.4822	[M+K] ⁺	0.0351	PE(12:0/19:1(9Z))	PE 31:1	C ₃₆ H ₇₀ NO ₈ PK
714.4822	[M+K] ⁺	0.0012	PC(P-16:0/13:0)	PC O-29:1	C ₃₇ H ₇₄ NO ₇ PK
714.4822	[M+K] ⁺	0.0012	PE(O-16:0/16:1(9Z))	PE O-32:1	C ₃₇ H ₇₄ NO ₇ PK
714.5657	[M+H] ⁺	0.0225	PC(O-14:0/18:3(9Z,12Z,15Z))	PC O-32:3	C ₄₀ H ₇₆ NO ₇ P
714.5657	[M+H] ⁺	0.0225	PE(P-18:0/17:2(9Z,12Z))	PE O-35:3	C ₄₀ H ₇₆ NO ₇ P
714.5657	[M+H] ⁺	0.0142	Cerebroside E	GlcCer(d14:2(4E,6E)/20:0(2OH))	HexCer 34:2;O3
714.5657	[M+H] ⁺	0.0221	GlcCer(d15:1/20:0)	HexCer 35:1;O2	C ₄₁ H ₇₉ NO ₈
714.5657	[M+Na] ⁺	0.0249	PC(O-14:0/16:0)	PC O-30:0	C ₃₈ H ₇₈ NO ₇ PNa
714.5657	[M+Na] ⁺	0.0249	PE(O-16:0/17:0)	PE O-33:0	C ₃₈ H ₇₈ NO ₇ PNa
714.649	[M+K] ⁺	0.0329	Cer(d18:1/26:1(17Z))	Cer 44:2;O2	C ₄₄ H ₈₅ NO ₃ K
760.3234	[M+K] ⁺	0.02	PKDdiA-PS	PS 28:3;O3	C ₃₄ H ₆₀ NO ₁₃ PK
779.3361	[M+K] ⁺	0.0345	PKODiA-PI	PI 24:3;O2	C ₃₃ H ₅₇ O ₁₆ PK
779.4273	[M+H] ⁺	0.0432	PI(12:0/18:2(9Z,12Z))	PI 30:2	C ₃₅ H ₇₁ O ₁₃ P
779.4273	[M+K] ⁺	0.0224	PA(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	PA 40:10	C ₄₃ H ₆₅ O ₈ PK
779.4273	[M+K] ⁺	0.0166	PI(12:0/15:0)	PI 27:0	C ₃₆ H ₆₉ O ₁₃ PK

Supplementary Table 2 Compound identified from LipidMaps

Input mass	Ion	Delta	Compounds from LipidMaps database		Name	Formula
779.4273	[M+K] ⁺	0.0013	PG(14:0/20:5(5Z,8Z,11Z,14Z,17Z))	—	PG 34:5	C ₄₀ H ₆₉ O ₁₀ PK
779.4273	[M+K] ⁺	0.0198	PI(O-16:0/12:0)	—	PI O-28:0	C ₃₇ H ₇₃ O ₁₂ PK
779.5179	[M+H] ⁺	0.0474	PI(12:0/18:2(9Z,12Z))	—	PI 30:2	C ₃₉ H ₇₁ O ₁₃ P
779.5179	[M+H] ⁺	0.0321	PG(15:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	—	PG 37:7	C ₄₃ H ₇₁ O ₁₀ P
779.5179	[M+H] ⁺	0.011	PI(P-16:0/15:1(9Z))	—	PI O-31:2	C ₄₀ H ₇₅ O ₁₂ P
779.5179	[M+H] ⁺	0.0042	PG(P-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	—	PG O-38:7	C ₄₄ H ₇₅ O ₉ P
779.5179	[M+H] ⁺	0.0406	PA(20:1(11Z)/22:4(7Z,10Z,13Z,16Z))	—	PA 42:5	C ₄₅ H ₇₉ O ₈ P
779.5179	[M+H] ⁺	0.0489	MGDG(18:2(9Z,12Z)/18:2(9Z,12Z))	—	MGDG 36:4	C ₄₅ H ₇₈ O ₁₀
779.5179	[M+Na] ⁺	0.0345	PG(13:0/22:4(7Z,10Z,13Z,16Z))	—	PG 35:4	C ₄₁ H ₇₃ O ₁₀ PNa
779.5179	[M+Na] ⁺	0.0018	PG(O-16:0/20:4(5Z,8Z,11Z,14Z))	—	PG O-36:4	C ₄₂ H ₇₇ O ₉ PNa
779.5179	[M+Na] ⁺	0.0382	PA(18:0/22:2(13Z,16Z))	—	PA 40:2	C ₄₃ H ₈₁ O ₈ PNa
779.5179	[M+Na] ⁺	0.0465	MGDG(16:0/18:1(9Z))	—	MGDG 34:1	C ₄₃ H ₈₀ O ₁₀ Na
779.5179	[M+Na] ⁺	0.0495	CerPE(d16:2(4E,6E)/24:1(15Z)(2OH))	—	CerPE 40:3;O3	C ₄₂ H ₈₁ N ₂ O ₇ PNa
779.5179	[M+K] ⁺	0.0191	PA(17:1(9Z)/22:2(13Z,16Z))	—	PA 39:3	C ₄₂ H ₇₇ O ₈ PK
779.5179	[M+K] ⁺	0.0172	PA(O-20:0/20:3(8Z,11Z,14Z))	—	PA O-40:3	C ₄₃ H ₈₁ O ₇ PK
779.5179	[M+K] ⁺	0.0285	CerPE(d16:2(4E,6E)/24:1(15Z))	—	CerPE 40:3;O2	C ₄₂ H ₈₁ N ₂ O ₆ PK
779.5179	[M+K] ⁺	0.0407	TG(12:0/12:0/20:5(5Z,8Z,11Z,14Z,17Z))[iso3]	—	TG 44:5	C ₄₇ H ₈₀ O ₆ K
779.6082	[M+H] ⁺	0.0497	PA(20:1(11Z)/22:4(7Z,10Z,13Z,16Z))	—	PA 42:5	C ₄₅ H ₇₉ O ₈ P
779.6082	[M+H] ⁺	0.0414	MGDG(18:2(9Z,12Z)/18:2(9Z,12Z))	—	MGDG 36:4	C ₄₅ H ₇₈ O ₁₀
779.6082	[M+H] ⁺	0.0285	PG(14:0/22:0)	—	PG 36:0	C ₄₂ H ₈₃ O ₁₀ P
779.6082	[M+H] ⁺	0.0078	PG(O-16:0/21:0)	—	PG O-37:0	C ₄₃ H ₈₇ O ₉ P
779.6082	[M+Na] ⁺	0.0438	MGDG(16:0/18:1(9Z))	—	MGDG 34:1	C ₄₃ H ₈₀ O ₁₀ Na
779.6082	[M+Na] ⁺	0.0408	CerPE(d16:2(4E,6E)/24:1(15Z)(2OH))	—	CerPE 40:3;O3	C ₄₂ H ₈₁ N ₂ O ₇ PNa
779.6082	[M+Na] ⁺	0.0045	SM(d16:1/22:1)	—	SM 38:2;O2	C ₄₃ H ₈₅ N ₂ O ₆ PNa
779.6082	[M+Na] ⁺	0.0078	TG(12:0/13:0/20:4(5Z,8Z,11Z,14Z))[iso6]	—	TG 45:4	C ₄₈ H ₈₀ O ₆ Na
779.6082	[M+K] ⁺	0.0496	TG(12:0/12:0/20:5(5Z,8Z,11Z,14Z,17Z))[iso3]	—	TG 44:5	C ₄₇ H ₈₀ O ₆ K
781.2772	[M+K] ⁺	0.04	PHODiA-PI	—	PI 24:2;O3	C ₃₃ H ₅₉ O ₁₆ PK
952.1652	[M+Na] ⁺	0.0291	caffeoyl-CoA	—	CoA 9:5;O2	C ₃₀ H ₄₂ N ₇ O ₁₉ P ₃ SNa
116.9841	[M-H] ⁻	0.0352	xi-3-Hydroxy-2-oxobutanoic acid	Methylmalonic acid	FA 4:1;O2	C ₄ H ₆ O ₄
131.0248	[M-H] ⁻	0.0262	2-hydroxy-2-butenedioic acid	Oxalacetic acid	FA 4:2;O3	C ₄ H ₄ O ₅
131.0248	[M-H] ⁻	0.0109	2,4,6-Octatriynoic acid	—	FA 8:6	C ₈ H ₄ O ₂
131.0248	[M-H] ⁻	0.0102	3-hydroxy-3-methyl-2-oxo-butanoic acid	Ethylmalonic acid	FA 5:1;O2	C ₅ H ₈ O ₄
131.0248	[M-H] ⁻	0.0466	L-Isoleucic acid	5-hydroxy caproic acid	FA 6:0;O	C ₆ H ₁₂ O ₃
175.0215	[M-H] ⁻	0.0033	2-hydroxy-3-oxoadipic acid	(4S,5S)-4,5-dihydroxy-2,6-dioxohexanoic acid	FA 6:2;O4	C ₆ H ₈ O ₆
175.0215	[M-H] ⁻	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diynoic acid	—	FA 10:6;O	C ₁₀ H ₈ O ₃
175.0215	[M-H] ⁻	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	2-isopropyl-malic acid	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl] ⁻	0.0316	2E,7-Octadienoic acid	Alepramic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	2E,4E-Hexadienyl acetate	Ethyl sorbate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	Allyl tiglate	—	WE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M-H] ⁻	0.0033	3-deoxy-D-glycero-hexo-2,5-diulosonic acid	2-hydroxy-3-oxoadipic acid	FA 6:2;O4	C ₆ H ₈ O ₆
175.0215	[M-H] ⁻	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diynoic acid	10-hydroxy-8E-Decene-2,4,6-triynoic acid	FA 10:6;O	C ₁₀ H ₈ O ₃
175.0215	[M-H] ⁻	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	3-propylmalic acid	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl] ⁻	0.0316	2E,7-Octadienoic acid	Alepramic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	2E,4E-Hexadienyl acetate	Ethyl sorbate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	Allyl tiglate	—	WE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M-H] ⁻	0.0033	2-hydroxy-3-oxoadipic acid	3-deoxy-D-glycero-hexo-2,5-diulosonic acid	FA 6:2;O4	C ₆ H ₈ O ₆
175.0215	[M-H] ⁻	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diynoic acid	—	FA 10:6;O	C ₁₀ H ₈ O ₃
175.0215	[M-H] ⁻	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	—	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl] ⁻	0.0316	2E,7-Octadienoic acid	Alepramic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	2E,4E-Hexadienyl acetate	Ethyl sorbate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	Allyl tiglate	—	WE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M-H] ⁻	0.0033	(4S,5S)-4,5-dihydroxy-2,6-dioxohexanoic acid	2-hydroxy-3-oxoadipic acid	FA 6:2;O4	C ₆ H ₈ O ₆
175.0215	[M-H] ⁻	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diynoic acid	—	FA 10:6;O	C ₁₀ H ₈ O ₃
175.0215	[M-H] ⁻	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	2-isopropyl-malic acid	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl] ⁻	0.0316	2E,7-Octadienoic acid	2-octynoic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	2E,4E-Hexadienyl acetate	Ethyl 2-methyl-3,4-pentadienoate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl] ⁻	0.0316	Allyl tiglate	—	WE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M-H] ⁻	0.0033	(4S,5S)-4,5-dihydroxy-2,6-dioxohexanoic acid	2-hydroxy-3-oxoadipic acid	FA 6:2;O4	C ₆ H ₈ O ₆

Supplementary Table 2 Compound identified from LipidMaps

Input mass	Ion	Delta	Compounds from LipidMaps database		Name	Formula
175.0215	[M-H]–	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diyonic acid	–	FA 10:6;O	C ₁₀ H ₁₈ O ₃
175.0215	[M-H]–	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	2-isopropyl-malic acid	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl]–	0.0316	2-octynoic acid	2E,7-Octadienoic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	2E,4E-Hexadienyl acetate	Ethyl 2-methyl-3,4-pentadienoate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	Allyl tiglate	–	WE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M-H]–	0.0033	(4S,5S)-4,5-dihydroxy-2,6-dioxohexanoic acid	2-hydroxy-3-oxoadipic acid	FA 6:2;O4	C ₆ H ₈ O ₆
175.0215	[M-H]–	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diyonic acid	–	FA 10:6;O	C ₁₀ H ₁₈ O ₃
175.0215	[M-H]–	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	2-isopropyl-malic acid	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl]–	0.0316	2-octynoic acid	2E,7-Octadienoic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	2E,4E-Hexadienyl acetate	Ethyl 2-methyl-3,4-pentadienoate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	Allyl tiglate	–	WE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M-H]–	0.0033	(4S,5S)-4,5-dihydroxy-2,6-dioxohexanoic acid	2-hydroxy-3-oxoadipic acid	FA 6:2;O4	C ₆ H ₈ O ₆
175.0215	[M-H]–	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diyonic acid	–	FA 10:6;O	C ₁₀ H ₁₈ O ₃
175.0215	[M-H]–	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	2-isopropyl-malic acid	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl]–	0.0316	2-octynoic acid	2E,7-Octadienoic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	2E,4E-Hexadienyl acetate	Ethyl 2-methyl-3,4-pentadienoate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	Allyl tiglate	–	WE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M-H]–	0.0033	(4S,5S)-4,5-dihydroxy-2,6-dioxohexanoic acid	2-hydroxy-3-oxoadipic acid	FA 6:2;O4	C ₆ H ₁₀ O ₄
175.0215	[M-H]–	0.0186	10-hydroxy-2E,8E-Decadiene-4,6-diyonic acid	–	FA 10:6;O	C ₆ H ₁₀ O ₄
175.0215	[M-H]–	0.0397	2,3-dimethyl-3-hydroxy-glutaric acid	2-isopropyl-malic acid	FA 7:1;O3	C ₇ H ₁₂ O ₅
175.0215	[M+Cl]–	0.0316	2-octynoic acid	2E,7-Octadienoic acid	FA 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	2E,4E-Hexadienyl acetate	Ethyl 2-methyl-3,4-pentadienoate	SFE 8:2	C ₈ H ₁₂ O ₂
175.0215	[M+Cl]–	0.0316	prop-2-en-1-yl (2Z)-2-methylbut-2-enoate	–	WE 8:2	C ₈ H ₁₂ O ₂
180.9788	[M+Cl]–	0.0485	3-hydroxy-3-methyl-2-oxo-pentanoic acid	(R)-4-Dehydropantoate	FA 6:1;O2	C ₆ H ₁₀ O ₄
180.9788	[M+Cl]–	0.0485	3-hydroxy-3-methyl-2-oxo-pentanoic acid	Acetohydroxybutyrate	FA 6:1;O2	C ₆ H ₁₀ O ₄