



Data Article

LC-MS/MS-QTOF dataset of chemical compounds detected in honey samples from Bali and Lombok, Indonesia

Fahrul Huyop^{a,c,*}, Saeed ullah^a, Huszalina Hussin^a,
Razauden Mohamed Zulkifli^a, Nurul Huda^b,
Nyoman Semadi Antara^c, Roswanira Abdul Wahab^d,
Satrijo Saloko^e, Anak Agung Sagung Putri Risa Andriani^f,
Che Muhammad Khairul Hisyam Ismail^g,
Azzmer Azzar Abdul Hamid^g, I. Nyoman Suarsana^h,
Ida Bagus Wayan Gunam^{c,*}

^a Department of Biosciences, Faculty of Science, Universiti Teknologi Malaysia, UTM Johor Bahru 81310, Malaysia

^b Faculty of Sustainable Agriculture, Universiti Malaysia Sabah, Sandakan, Sabah 90509, Malaysia

^c Bioindustry Laboratory, Department of Agro-Industrial Technology, Udayana University, Denpasar, Indonesia

^d Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, UTM Johor Bahru 81310, Malaysia

^e Faculty of Food Technology and Agro Industry, University of Mataram, Nusa Tenggara Barat, 83126, Indonesia

^f Program Studi Agroteknologi, Fakultas Pertanian, Universitas Warmadewa, Denpasar, Indonesia

^g Department of Biotechnology, Kulliyah of Science, International Islamic University Malaysia, Kuantan, Pahang 25200, Malaysia

^h Biochemical Laboratory, Faculty of Veterinary Medicine, Udayana University, Denpasar, Indonesia

ARTICLE INFO

Article history:

Received 15 March 2024

Revised 14 August 2024

Accepted 23 August 2024

Available online 5 September 2024

Dataset link: [LC-MS/MS-QTOF dataset of chemical compounds detected in honey samples from Bali and Lombok, Indonesia. \(Original data\)](#)

ABSTRACT

Honey production is susceptible to manipulation by unscrupulous sellers, making honey authentication crucial to prevent fraud. The process of authenticating honey often necessitates the use of various analytical techniques, such as identifying the chemicals present in honey by means of hyphenated mass spectrometry. Here, we report on the investigation of the chemical composition of three honey samples collected at two locations in Lombok and Bali by liquid chromatography mass spectrometry (LC-MS). The three datasets include information regarding compound name, mass,

* Corresponding authors at: Bioindustry Laboratory, Department of Agro-Industrial Technology, Udayana University, Denpasar, Indonesia.

E-mail addresses: fahrul@utm.my (F. Huyop), ibwgunam@unud.ac.id (I.B.W. Gunam).

Keywords:

Honey
Bali
Lombok
Mass spectrometry
LC-MS/MS QTOF

retention times, as well as findings from database searches. Collectively, these data afford first insights into the compositional profile of honey samples from this specific geographical area.

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Specifications Table

Subject	Chemistry
Specific subject area	Phytochemical, Natural product research, Spectrometry
Type of data	Table, and Figure
Data collection	The chemical composition of honey obtained from Lombok and Bali, Indonesia were analysed using an LC MS/MS QTOF system equipped with a Zorbax Extend C18 (2.1×50 mm/1.8 microns) column. For sample preparation, honeys were dissolved into ionized water and filtrated using a 0.045 µm nylon filter. The chromatographic separation process utilized a gradient mobile phase containing formic acid in water and formic acid in acetonitrile with a flowrate of 0.2 mL/min for 20 min, and eluate detection by monitoring the absorbance in the visual spectrum at 660 nm.
Sample information	The honey samples were obtained from Madu Lombok Utara, Desa Sukadana, North of Lombok (-8.22134 116.39950) and Desa Kuwum, Badung Regency, in Bali (-8.45512 115.18728) in the month of August 2023.
Data accessibility	The complete dataset is accessible at the Mendeley Repository: 10.17632/8wtn82v7wg.3 .

1. Value of the Data

- The data article provides a baseline dataset of chemical components in honeys from Lombok and Bali, Indonesia.
- These data provide comparative insights with respect to the variation of chemical composition of honeys from different geographical locations
- These data could aid the investigation of honeys in the context of potential medicinal benefits.

2. Background

Honey, a traditional food substance, primarily comprises sugars along with additional components. These include enzymes, amino acids, organic acids, carotenoids, vitamins, minerals, and aromatic compounds [1–4]. The composition, flavor, color, and aroma of honey exhibit considerable variability, primarily attributed to its floral source. Furthermore, external factors, such as seasonal and environmental influences, as well as processing methods, also contribute to this variation [1–3]. The analytical verification of the authenticity of individual honey is challenging owing to the complex composition of this food, remains a vital aspect for further exploration. In Indonesia, the predominant bee species namely *Apis mellifera*, *Apis cerana*, *Apis dorsata*, and *Trigona* species (stingless bee), are known for their high honey production throughout the country. In Particular, Lombok and Bali are renowned for its rich biodiversity, providing abundant opportunities for these bee species to forage for nectar. This abundance of diverse plant species contributes to the high-quality honey they produce. In this present study, the chemical compositions of wild honey samples collected from Lombok and Bali were analysed. The primary objective is to identify the specific chemical compounds in honey samples obtained from dis-

Table 1

An overview of data files.

Label	Name of data file/data	types (file extension)	Data repository and identifier (DOI or accession number)
Data file 1	Chemical compound identified in B1 (Lombok)	pdf	Mendeley Data repository Doi: 10.17632/8wtn82v7wg.3
Data file 2	Chemical compound identified in B2 (Bali)	pdf	Mendeley Data repository Doi: 10.17632/8wtn82v7wg.3
Data file 3	Chemical compound identified in B3 (Bali)	pdf	Mendeley Data repository Doi: 10.17632/8wtn82v7wg.3

tinct regions of Lombok and Bali. In this study, two honey samples were collected from different regions in Bali, and one sample was collected from Lombok.

3. Data Description

Table 1 provides an overview of the data files used in this study. Each data file contains information on the chemical compounds identified in specific locations. The data files are stored in the Mendeley Data repository and can be accessed using the provided DOIs.

Tables 2–4 present the chemical composition of honey samples collected from Lombok Island (B1) and two distinct locations on Bali Island (B2 and B3). The compounds were analyzed using an LC-MS/MS-QTOF-based untargeted technique. The tabulated data encompasses tentatively identified compounds, their corresponding retention times (RT), molecular formulas, molecular masses, and similarity scores derived from spectral matching against online databases.

Data analysis in B1 unveiled 16 known chemical compounds and 75 unknown compounds. Additionally, 23 chemical compounds were identified as undefined in the honey sample. The 16 known chemical compounds were subjected to further scrutiny and their physical properties were obtained from the respective compound entries in the database PubChem (Table 2). The analysis of Lombok (B1) honey indicates the existence of many different bioactive compounds that have potential anthelmintic properties. These include Ophiopogonin C' (glycoside) [5], 5 β -Cyprinolsulfate, and Petromyzonol (both steroid sulfates), as well as OH-Spheroidenone, a terpenoid renowned for its anticancer effects [6].

In addition, honey contains various chemicals such as phospholipids and amino alcohol (Halaminol A) that could potentially enhance immunological function, hence increasing its overall therapeutic value [7]. Although honey is largely a sugar derivative, it can also contain compounds like 3-Deoxyarabinohexonic acid that enhance its nutritional value. The complex mixture of compounds in Lombok honey (B1) indicates its potential value in traditional medicine, namely for the treatment of parasite illnesses. However, additional research is necessary to validate these effects.

Data analysis of honey sample B2 (Table 3) revealed a total of 18 known, 60 unknown, and 39 undefined chemical compounds. The 18 known chemical compounds underwent comprehensive scrutiny, with their physical properties validated through PubChem (Table 3). Bali honey (B2) has a diverse range of bioactive chemicals that have potential medicinal properties, including some that may have anthelmintic effects. Halaminol A is an amino alcohol that possesses antibacterial characteristics, and it may also have anthelmintic activity [7]. Austrobailignan 7 is a lignan that has antioxidant properties and the potential to fight against microbes [8]. This suggests that it may contribute to the honey's ability to treat parasitic illnesses. The presence of Isorhamnetin 3-O- $[\beta$ -D-glucopyranosyl-(1 \rightarrow 2)]- α -L-rhamnopyranoside, a compound that is a combination of a sugar molecule and Isorhamnetin, suggests that the honey may have antioxidant and anti-inflammatory properties that could contribute to its overall health advantages [9]. Ceanothine E is an organic compound that potentially exhibits several biological activities that makes it a substance that is worthy of further investigation. Phosphatidylcholines (PCs) like PC(O-16:0/0:0)

Table 2
The identified compounds from B1 (Lombok) extract.

Compound	Name	Formula	RT	Mass	CAS ID	Source	Score (DB)	Score (MFG)	Class compound
1	3-Deoxyarabinohexonic acid	C ₆ H ₁₂ O ₆	0.706	180.064	29625-79-4	DBSearch-MFG	85.11	45.67	Carbohydrate
3	5β-Cyprinolsulfate	C ₂₇ H ₄₈ O ₈ S	7.347	532.3072	-	DBSearch-MFG	65.43	47.56	Steroid sulphate
16	Ophiopogonin C'	C ₃₉ H ₆₂ O ₁₂	8.098	722.4274	19057-67-1	DBSearch	56.58	-	Glycosides
17	Pitheduloside A	C ₄₁ H ₆₆ O ₁₃	8.221	766.454	78285-89-9	DBSearch	67.68	-	Organic compound
18	PE (16:1(9Z)/22:6(4Z,7Z,13Z,16Z,19Z))	C ₄₃ H ₇₂ NO ₈ P	8.224	761.4987	-	DBSearch	93.83	-	Phosphatidyle thanolamine (PE)
22	PS (19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C ₄₇ H ₈₀ NO ₁₀ P	8.436	849.5505	-	DBSearch	77.23	-	Phosphatidylserine (PS)
26	Hebevinoside XIII	C ₄₉ H ₇₆ O ₁₆	8.513	920.5123	138995-52- 5	DBSearch	57.33	-	Organic compound
27	Chondrillasterol 3-[glucosyl-(1->2)- glucosyl-(1->2)-glucoside]	C ₄₇ H ₇₈ O ₁₆	8.534	898.5303	-	DBSearch	62.47	-	Lipid
31	1-(8-[5]-ladderaneoctanoyl)-2-(8-[3]- ladderane-octanyl)-sn- glycerophosphocholine	C ₄₈ H ₈₁ NO ₇ P	8.79	814.5751	-	DBSearch	98.53	-	Lipid
32	Halaminol A	C ₁₄ H ₂₉ NO	9.513	227.2242	-	DBSearch-MFG	82.69	82.72	Amino alcohol
51	Austrobailignan 7	C ₂₀ H ₂₂ O ₅	11.701	342.1456	55890-25-0	DBSearch	79.18	-	Organic molecule
69	Petromyzonol	C ₂₄ H ₄₂ O ₄	12.885	394.3068	28979-29-5	DBSearch	68.32	-	Steroid sulphate.
70	PC (O-16:0/0:0) [U]	C ₂₄ H ₅₃ NO ₆ P	12.887	482.3595	-	DBSearch	70.29	-	Phosphatidylcholine (PC)
71	27-Nor-5b-cholestane3a,7a,12a,24,25- pento	C ₂₆ H ₄₆ O ₅	12.895	438.3324	78648-95-0	DBSearch	64.9	-	Sterol lipid
76	35S-Methylkodaic acid 7-hexadecanoate	C ₆₁ H ₁₀₀ O ₁₄	13.474	1056.7104	-	DBSearch	92.96	-	Fatty acid esters
109	OH-Spheroidenone	C ₄₁ H ₆₀ O ₃	14.093	600.4546	-	DBSearch-MFG	94.64	94.64	Terpenoid

Table 3
The identified compounds from B2 (Bali) extract.

Compound	Name	Formula	RT	Mass	CAS ID	Source	Score (DB)	Score (MFG)	Class compound
1	3-Deoxyarabinoheonic acid	C ₆ H ₁₂ O ₆	0.748	180.0635	29625-79-4	DBSearch-MFG	94.55	47.58	Carbohydrate
6	Arg Gln Arg	C ₁₇ H ₃₄ N ₁₀ O ₅	6.961	458.2707	-	DBSearch	76.76	-	Amino Acids
10	Isorhamnetin 3-O-[β-Dglucopyranosyl-(1->2)-α-L-rhamnopyranoside]	C ₂₈ H ₃₂ O ₁₆	7.424	624.1679	-	DBSearch	60.31	-	Flavonoids
12	Ceanothine E	C ₃₄ H ₄₀ N ₄ O ₄	7.457	568.3052	23926-98-9	DBSearch-MFG	75.35	75.3	Organic compound
23	GalCer(d18:0/26:0)	C ₅₀ H ₉₉ NO ₈	8.451	841.734	-	DBSearch	79.42	-	Lipid
25	1-(8-[5]-ladderaneoctanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	C ₄₈ H ₈₁ NO ₇ P	8.773	814.5753	-	DBSearch	99.4	-	Lipid
29	Halaminol A	C ₁₄ H ₂₉ NO	9.267	227.2243	-	DBSearch-MFG	83.8	83.82	Amino alcohol
35	(±)-2-methyl 5,8,11,14-all-cistricosatetraenoyl-2'-fluoroethylamine	C ₂₆ H ₄₄ FNO	9.608	405.3421	-	DBSearch	74	-	Fatty amides
39	Palmitic amide	C ₁₆ H ₃₃ NO	10.419	255.2555	629-54-9	DBSearch	97.74	-	Organic compound
43	Austrobailignan 7	C ₂₀ H ₂₂ O ₅	11.707	342.1458	55890-25-0	DBSearch	97.17	-	Organic compound
50	PC(O-16:0/0:0) [U]	C ₂₄ H ₅₃ NO ₆ P	12.884	482.3591	-	DBSearch	54.81	-	Phosphatidylcholine (PC)
52	27-Nor-5b-cholestane3a,7a,12a,24,25-pento	C ₂₆ H ₄₆ O ₅	12.885	438.3327	78648-95-0	DBSearch	66.5	-	Lipid
65	35S-Methylokadaic acid 7-hexadecanoate	C ₆₁ H ₁₀₀ O ₁₄	13.459	1056.709	-	DBSearch	92.04	-	fatty acid ester
71	PC (15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C ₄₅ H ₇₉ NO ₈ P	13.531	792.5544	-	DBSearch	96.6	-	Phosphatidylcholine (PC)
100	PC (17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C ₄₇ H ₈₃ NO ₈ P	13.958	820.5845	-	DBSearch	97.43	-	Phosphatidylcholine (PC)
101	PC (O15:0/20:4(5Z,8Z,11Z,14Z)) [U]	C ₄₃ H ₈₁ NO ₇ P	13.984	754.5779	-	DBSearch	89.13	-	Phosphatidylcholine (PC)
110	Retinoyl CoA	C ₄₁ H ₆₂ N ₇ O ₁₇ P ₃ S	14.338	1049.312	81295-48-9	DBSearch	58.49	-	Organic compound
111	TG (10:0/10:0/10:0)	C ₃₃ H ₆₂ O ₆	14.376	554.4519	621-71-6	DBSearch	56.11	-	Triacylglycerol (TG)

Table 4
The identified compounds from B3 (Bali) extract.

Compound	Name	Formula	RT	Mass	CAS ID	Source	Score (DB)	Score (MFG)	Class compound
3	3-Deoxyarabinohexonic acid	C ₆ H ₁₂ O ₆	0.724	180.0633	29625-79-4	DBSearch-MFG	86.87	47.61	Carbohydrates
5	Cordycepin	C ₁₀ H ₁₃ N ₅ O ₃	1.105	251.1016	73-03-0	DBSearch-MFG	68.6	47.43	Carbohydrates
6	Trifluoperazine	C ₂₁ H ₂₄ F ₃ N ₃ S	3.974	407.1654	117-89-5	DBSearch	82.72	-	Phenothiazines
7	Cyflufenamid	C ₂₀ H ₁₇ F ₅ N ₂ O ₂	4.172	412.1202	-	DBSearch	65.65	-	benzenes
14	PS (18:3(9Z,12Z,15Z)/0:0)	C ₂₄ H ₄₂ NO ₉ P	7.447	519.2602	-	DBSearch	77.87	-	Phosphatidylserine (PS)
19	16-dimethyl Prostaglandin E2 p-(pacetamidobenzamido) phenyl ester	C ₃₇ H ₄₈ N ₂ O ₇	8.037	632.3453	62873-55-6	DBSearch	85.25	-	Prostanoid
20	Posaconazole	C ₃₇ H ₄₂ F ₂ N ₈ O ₄	8.038	700.3312	171228-49-2	DBSearch	66.89	-	Antifungal compound
23	Calendulose G methyl ester	C ₄₃ H ₆₈ O ₁₄	8.472	808.46	155740-15-1	DBSearch	65.86	-	Terpenoids
25	Antanapeptin C	C ₄₁ H ₆₄ N ₄ O ₈	8.476	740.4728	-	DBSearch	95.74	-	Peptides
27	C18 Sulfatide	C ₄₂ H ₈₁ NO ₁₁ S	8.778	807.556	-	DBSearch	50.86	-	Glycosphingolipid.
36	27-Nor-5b-cholestane3a,7a,12a,24,25-pentol	C ₂₆ H ₄₆ O ₅	12.886	438.3327	78648-95-0	DBSearch	73.5	-	Lipid
41	PC (15:0/20:3(5Z,8Z,11Z))	C ₄₃ H ₈₁ NO ₈ P	13.542	770.5707	-	DBSearch	62.92	-	Phosphatidylcholine (PC)
54	Germanicol cinnamate	C ₃₉ H ₅₆ O ₂	14.105	556.4276	65883-48-9	DBSearch-MFG	60.32	60.77	Triterpenoids

Sample Chromatograms (B1)

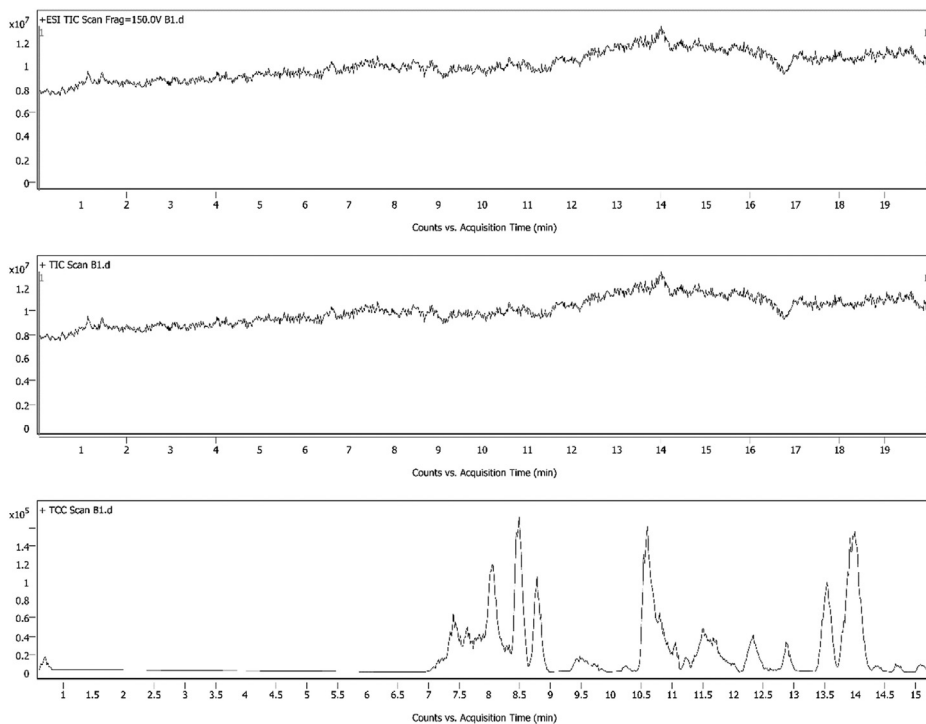


Fig. 1. The LC- MS/MS-QTOF chromatogram of honey sample from Lombok Island (B1).

[U], PC (15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)), and PC(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) and fatty acid esters like 3S-Methylokadaic acid 7-hexadecanoate contribute to membrane stability and may support immune function [10,11].

These chemicals improve honey's therapeutic capabilities, suggesting a complex bioactivities interaction that may include anthelmintic effects.

Analysis of honey sample B3 (Table 4) revealed the presence of 13 known, 35 unknown, and 7 undefined chemical compounds. The 13 known compounds underwent detailed examination, and their physical properties were verified through PubChem (Table 4). Analysis of the Bali honey sample (B3) reveals the presence of various significant chemicals with potential therapeutic effects. Cordycepin is notable for its established antibacterial and antiparasitic characteristics and also antidiabetic [12]. Calenduloside G methyl ester and Antanapeptin C exhibit potential due to their antioxidant and antifungal properties, which could enhance the honey's overall medicinal profile [13,14]. Moreover, the phospholipid PS (18:3(9Z,12Z,15Z)/0:0) and the sterol 27-Nor-5b-cholestane3a,7a,12a,24,25-pentol have the potential to improve immunological function and maintain the integrity of cell membranes. Posaconazole and Trifluoperazine are other chemicals that show promise in their ability to combat fungal infections and have a wider range of antimicrobial properties [15].

In summary, these findings highlight the intricate bioactive composition of this honey, suggesting its potential therapeutic applications. In this study, the identified compounds are those successfully matched to known entries in reference databases using techniques such as LC-MS-QTOF. Conversely, unknown compounds are those detected but not matched to any entries in the current databases. Non-identified compounds lack sufficient data for accurate classification. The prevalence of unidentified or uncharacterized compounds is common in natural product research, largely due to the complex nature of substances like honey, limitations of existing ref-

Table 5

The comparison of identified compounds from honey obtained from Lombok Island (B1) and Bali Island (B2 and B3).

No	Bioactive Compound Identified through LC-MS-QTOF	Honey		
		B1	B2	B3
1	1-(8-[5]-ladderaneoctanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	✓	✓	
2	35S-Methylokadaic acid 7-hexadecanoate	✓	✓	
3	3-Deoxyarabinohexonic acid	✓	✓	✓
4	Antanapeptin C			✓
5	Arg Gln Arg		✓	
6	Austrobailignan 7	✓	✓	
7	C18 Sulfatide			✓
8	Calendulose G methyl ester			✓
9	Ceanothine E		✓	
10	Chondrillasterol 3-[glucosyl-(1->2)-glucosyl-(1->2)-glucoside]	✓		
11	Cordycepin			✓
12	Cyflufenamid			✓
13	GalCer(d18:0/26:0)		✓	
14	Germanicol cinnamate			✓
15	Halaminol A	✓	✓	
16	Hebevinoside XIII	✓		
17	Isorhamnetin 3-O-[β-D-glucopyranosyl-(1->2)-α-L-rhamnopyranoside]		✓	
18	Ophiopogonin C	✓		
19	Palmitic amide		✓	
20	PC(O-16:0/0:0)[U]	✓	✓	
21	PE (16:1(9Z)/22:6(4Z,7Z,13Z,16Z,19Z))	✓	✓	
22	Petromyzonol	✓		
23	Pithedulose A	✓		
24	Posaconazole			✓
25	PS (19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	✓		
26	Retinoyl CoA		✓	
27	TG (10:0/10:0/10:0)		✓	
28	Trifluoperazine			✓
29	(±)-2-methyl 5,8,11,14-all-cistriscosatetraenoyl-2'-fluoroethylamine		✓	
30	16-dimethyl Prostaglandin E2 p-(pacetamidobenzamido) phenyl ester			✓
31	27-Nor-5b-cholestane3a,7a,12a,24,25-pentol	✓	✓	✓
32	5β-Cyprinolsulfate	✓		
33	OH-Spheroidenone	✓		
34	PC (15:0/20:3(5Z,8Z,11Z))			✓
35	PC (15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))		✓	
36	PC (17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))		✓	
37	PC (O15:0/20:4(5Z,8Z,11Z,14Z))[U]		✓	
38	PS (18:3(9Z,12Z,15Z)/0:0)			✓

erence databases, and the presence of unique or geographically specific chemicals. Addressing this challenge in future research will require the expansion of reference databases, the use of advanced analytical techniques, the application of bioinformatics tools, and the promotion of collaborative research to improve the identification of these compounds.

Table 5 presents a comparison of the presence of distinct bioactive chemicals in three types of honey samples: B1 from Lombok, B2 from Bali, and B3 from a different site in Bali. Each row displays a diverse compound found using LC-MS-QTOF analysis, with checkmarks showing its existence in the corresponding honey sample. This comparison provides valuable insights into the variations in composition across the honey samples. Figs 1–3 depict the total ion chromatograms obtained from the analysis of Lombok honey samples (B1) and Bali honey samples (B2 & B3) using LC MSMS QTOF.

The presence of 3-deoxyarabinohexonic acid in all samples is essential for providing important carbohydrates. The honey samples from Lombok (B1) and Bali (B2) have five chemical compounds in common. However, despite both being from Bali, B2 and B3 only share two chemical compounds. These findings indicate that the chemical makeup of honey is greatly affected by its

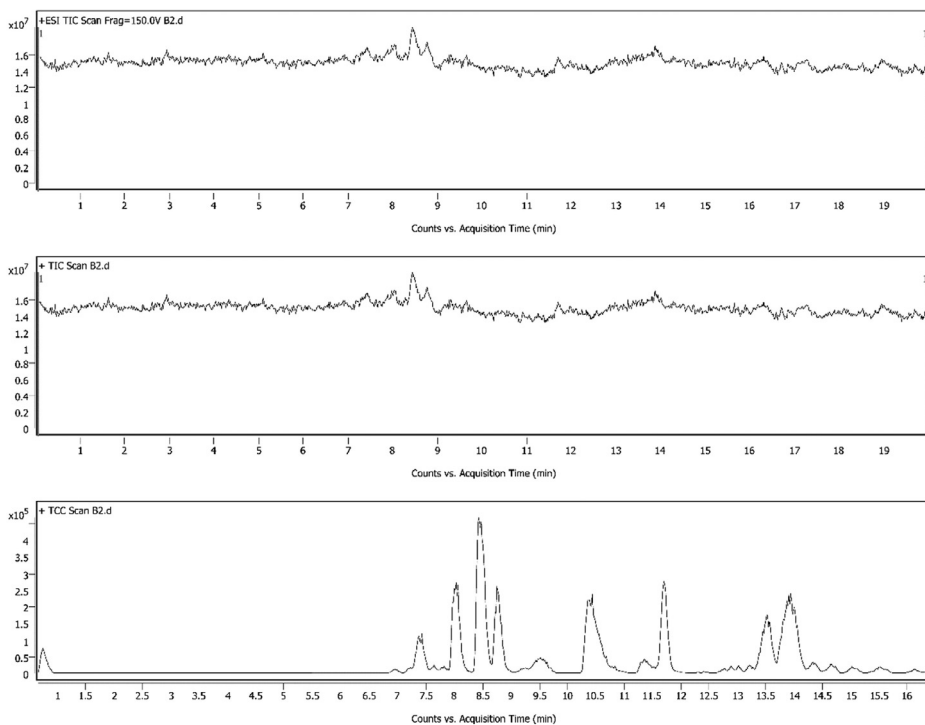
Sample Chromatograms (B2)

Fig. 2. The LC- MS/MS-QTOF chromatogram of honey sample from Bali Island (B2).

precise geographical location. Local flora, climate, and environmental circumstances can affect honey's chemical composition, even within the same region (Table 5).

4. Experimental Design, Materials and Methods

4.1. Sample Collection

The honey sample was supplied for research purposes by private suppliers at Desa Kuwum, Badung Regency, in Bali (-8.45512 115.18728) and Madu Lombok Utara, Desa Sukadana, North of Lombok (-8.22134 116.39950) in the month of August 2023.

4.2. Sample Preparation

The honey samples from Lombok Island (B1) and Bali Island (B2 and B3) were prepared using a standard procedure as described by Alghamdi et al. [4]. A total of 2.5 g of the corresponding honey sample was dissolved in 25 ml of de-ionized water in a beaker. The resulting solution was then filtered through a 0.045 μ m nylon filter into a 50 ml volumetric flask.

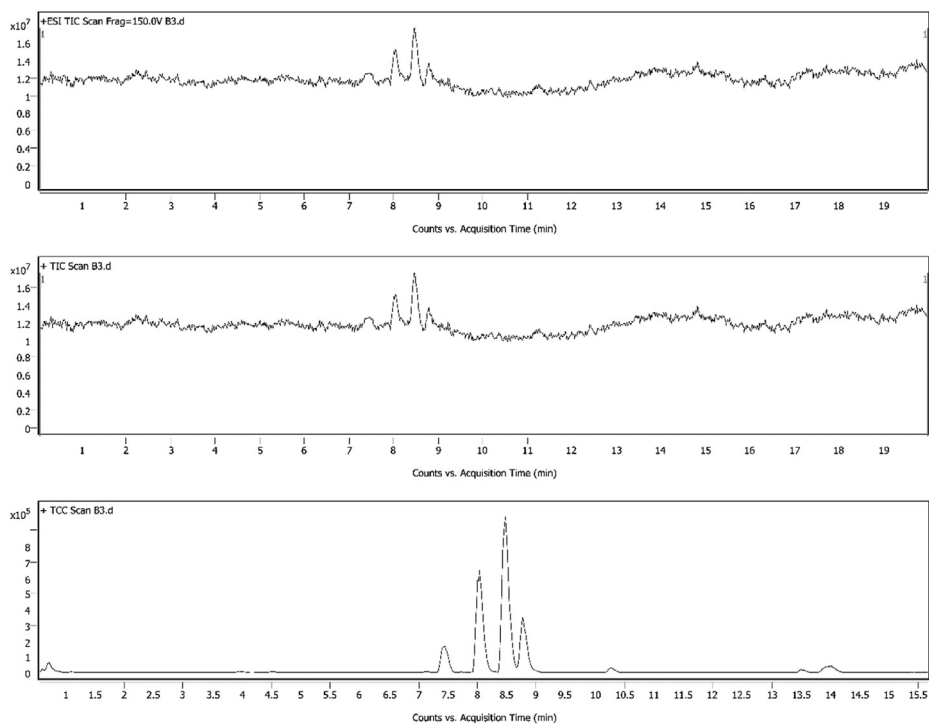
Sample Chromatograms (B3)

Fig. 3. The LC- MS/MS-QTOF chromatogram of honey sample from Bali Island (B3).

4.3. Chemical profiling analysis using LC-MS QTOF

A suitable volume of the filtered solution was then transferred into a Liquid Chromatography-Mass Spectrometry (LC-MS/MS) instrument for further analysis. The analysis of chemical compounds in honey samples was conducted using an LC MS/MS QTOF system equipped with a Zorbax Extend C18 column (2.1×50 mm/1.8 microns). The separation process employed a gradient mobile phase composed of formic acid in water and formic acid in acetonitrile, allowing for the separation of compounds within 20 min at a flow rate of 0.2 ml/min. Detection was carried out at A660 nm, and the identification of compounds relied on factors such as retention time and mass [16].

Limitations

- The study employed LC-MS/MS QTOF for the identification of chemical compounds in the honey samples. It is important to note that this method provides identification only and does not offer information on concentration (quantitative).
- The chemical compound composition of honey samples can also vary depending on their age and geographical origin.
- It is important to consider that a small sample size may not be representative of the larger population, potentially limiting the generalizability of the findings.

Ethics Statement

This research under title: **AUTHENTICATION & ESTABLISHMENT OF THE PROVENANCE OF HONEY USING A METAGENOMIC APPROACH** has been awarded: "Letter of Clearance Ethic Approval" by "Badan Riset dan Inovasi Nasional" (BRIN), address at Gedung B.J. Habibie, Jl. M.H. Thamrin No. 8, Jakarta Pusat 10340. (Phone +62811-1933-3639) Email: ppid@brin.go.id.

Data Availability

LC-MS/MS-QTOF dataset of chemical compounds detected in honey samples from Bali and Lombok, Indonesia. (Original data) (Mendeley Data).

CRediT Author Statement

Fahrul Huyop: Conceptualization, Methodology, Data curation, Supervision, Formal analysis; **Saeed ullah:** Conceptualization, Methodology, Data curation, Formal analysis, Validation, Writing – original draft; **Huszalina Hussin:** Conceptualization, Methodology, Data curation; **Razauden Mohamed Zulkifli:** Conceptualization, Methodology, Data curation, Validation, Writing – original draft; **Nurul Huda:** Conceptualization, Methodology, Data curation; **Nyoman Semadi Antara:** Formal analysis, Methodology; **Roswanira Abdul Wahab:** Conceptualization, Methodology, Data curation, Validation; **Satrijo Saloko:** Writing – original draft; **Anak Agung Sagung Putri Risa Andriani:** Writing – original draft; **Che Muhammad Khairul Hisyam Ismail:** Writing – review & editing, Visualization; **Azmer Azzar Abdul Hamid:** Conceptualization, Methodology, Data curation, Validation; **I. Nyoman Suarsana:** Conceptualization, Methodology, Data curation, Validation; **Ida Bagus Wayan Gunam:** Conceptualization, Methodology, Data curation, Supervision.

Acknowledgments

The authors wish to express their sincere appreciation to the private suppliers, Balangan Bee Farm in Desa Kuwum, Badung Regency, Bali, and Madu Lombok Utara in Desa Sukadana, North Lombok. Furthermore, we would like to extend our gratitude to Udayana University for their support through the UNISERF Program and providing research funding (No. B/775-4/UN14.4A/PT.01.03/2023). Additionally, we would like to acknowledge the Mass Spectrometry Lab at Universiti Teknologi Malaysia for their essential role in conducting the LCMS analysis. Their invaluable assistance and support significantly contributed to the successful completion of this research.

Declaration of Competing Interest

The authors declare that they have no competing interests.

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