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Exploring the Chemical Composition and Antioxidant Properties of Apricot Kernel Oil

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Abstract: Apricot kernels are known to be rich in bioactive compounds such as polyphenols, which have applications in various fields such as cosmetology and the food industry. However, the extraction of these compounds has not been extensively studied. In this study, we aimed to extract oil from apricot kernels and investigate its composition and antioxidant properties. Samples from two years of apricot cannery by-products were used in the study. We employed a common extraction procedure using hexane as a solvent, followed by an analysis of the oil's fatty acid composition and determination of its antioxidant properties using several methods. Our results indicated that the oil extracted from apricot kernels is rich in oleic and palmitoleic acids, which exhibit health benefits. As regards the volatile compounds of the oil, 2-methyl propanal, benzaldehyde, and benzyl alcohol were detected as the main compounds. Benzaldehyde was also found to be the main component of the essential oil of the kernel. Furthermore, the oil exhibited low antioxidant activity, as demonstrated by its ability to scavenge free radicals. Overall, our findings suggest that apricot kernels are a valuable source of oil with potential applications in the food and cosmetic industries.

Keywords: antioxidants; apricot kernel oil; essential oil; extraction; fatty acids; GC-MS; LC-MS/MS; polyphenols; volatile compounds

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1. Introduction

The apricot (*Prunus armeniaca*) is a fruit tree that is cultivated worldwide due to its tasty and nutritious fruit [1]. Due to their sweet and juicy flesh, apricots are widely used for the production of jams, and they are also consumed either dried or canned [2]. During the cannery process, a significant amount of waste is generated, which consists mainly of pits and peels [3]. The pit consists of about 10% of the total weight of the fruit. An apricot pit is about 1.5–2 cm long and weighs approximately 0.5 g [4]. About one-third of its weight is due to the apricot kernel (AK) that is contained within. AK is a valuable source of bioactive compounds, such as polyphenols, tocopherols, phytosterols, etc., that bestow their beneficial properties on human health. It is noteworthy that AK also contains a significant amount of oil, with its oil content reaching up to 50% [5].

AK oil (AKO) has drawn more and more attention in recent years due to its potential health effects [6]. AKO is rich in unsaturated fatty acids, such as oleic acid (18:1, ω-9) and linoleic acid (18:2, ω-6), which have been shown to have various health benefits [7]. Oleic acid, a monounsaturated fatty acid has been found to possess anti-inflammatory properties, improve insulin sensitivity, and decrease the risk of heart disease [8]. Linoleic acid is a polyunsaturated fatty acid, that has been shown to have anti-inflammatory and antioxidant

properties and may help reduce the risk of chronic diseases such as cancer, heart disease, and diabetes [9]. In addition, AKO also contains compounds such as polyphenols that exhibit antioxidant activity. Owing to them, AKO may exhibit health-promoting activity by scavenging the free radicals within an organism, thus protecting it from oxidative stress [10]. Due to the above, AKO is a valuable ingredient that is being used in the cosmetics industry. In addition, AKO is being used in the food industry due to its mild, nutty flavor, making it a suitable ingredient for many dishes [5].

Given the growing interest in AKO and its applications in various industries, it is important to explore its chemical composition and evaluate its antioxidant properties. The aim of this study is to examine the chemical composition and antioxidant properties of AKO. AKO was extracted from kernels obtained from the pit waste of cannery by-products using apricots harvested for two consecutive years. The composition of the oil in terms of volatile compounds and fatty acids was analyzed. In addition, the content of AKO in polyphenols and flavonoids was assessed. Finally, the composition of the apricot kernel essential oil was also evaluated.

2. Materials and Methods

2.1. Chemicals and Reagents

Methanol, 2-propanol, petroleum ether, acetone, L-ascorbic acid, hydrochloric acid, 2,4,6-tris(2-pyridyl)-*s*-triazine (TPTZ), and 2,2-diphenylpicrylhydrazyl (DPPH) were purchased from Sigma-Aldrich (Darmstadt, Germany). Gallic acid, ethanol, *n*-hexane, and the Folin-Ciocalteu reagent were purchased from Panreac Co. (Barcelona, Spain). Anhydrous sodium carbonate was purchased from Penta (Prague, Czech Republic). Iron chloride (hexahydrate) was purchased from Merck (Darmstadt, Germany).

2.2. Apricot Seeds

The apricot seeds came from the 2020 and 2021 harvests of the *Prunus armeniaca* 'Bebeco' variety. The sample was taken from the byproducts of an industrial fruit cannery (ELBAK S.A., Falani, Larissa, Greece). The apricot seeds were collected and flash-frozen using liquid nitrogen. A Biobase BK-FD10P freeze-dryer (Jinan, Shandong, China) was used to freeze-dry the sample. The moisture of the AK was determined to be 7.1 $\pm$ 0.4%. Finally, a blender was used to grind the dried apricot kernels into a fine powder.

2.3. Apricot Kernel Oil Extraction

In an amber-colored glass bottle, 100 g of AK was added along with 0.5 L of petroleum ether. The mixture was stirred for two hours at 500rpm at room temperature (~22 °C) and then centrifuged for 10 min at 4500 rpm using a NEYA 16R centrifuge (Remi Elektrotechnik Ltd., Palghar, India). The supernatant was retracted (extraction yield: 33.2%), and the solid residue was re-extracted with the abovementioned conditions (extraction yield: 1.4%). A rotary evaporator (Laborota 4000 efficient, Heidolph Instruments GmbH and Co. KG, Schwabach, Germany) was then used to mix the supernatants and evaporate the solvent. The yield of the AKO extraction was calculated to be 34.6 $\pm$ 2.2% of the AK dry weight.

2.4. Volatile Compound Analysis by HS-SPME/GC-MS

The headspace solid-phase microextraction (HS-SPME) method used was a modification of the method described by Sarolic et al. [11]. For further information please see the Supplementary material.

2.5. Essential Oil

2.5.1. Extraction of Apricot Kernel Essential Oil

The essential oil from AK was extracted via hydrodistillation with a Clevenger apparatus. More specifically, 100 g of AK were added to a round-bottom flask along with 900 mL of water, and the mixture was heated for 3 h. Finally, the essential oil was collected from the apparatus. The essential oil yield was calculated to be 0.17% *w/w*.

2.5.2. Essential Oil Analysis by GC-MS

For the analysis of the essential oil, 0.1 g of the sample was transferred into a vial and diluted with 1 mL of *n*-hexane. A modified approach described by Daferera et al. [12] was used. Further details are provided in the Supplementary material.

2.6. Quality Indicators for AKO Samples

2.6.1. Fatty Acid Composition by GC-FID

The appropriate fatty acid methyl esters (FAMEs) were made in accordance with Commission Regulation (EC) No 796/2002 (Annex XB) in order to determine the fatty acids [13]. In brief, 0.1 g of the AKO sample was transferred to a screw-capped glass vial along with 2 mL of *n*-hexane. After thorough mixing, 0.2 mL of 2 N methanolic potassium hydroxide solution was added, and the mixture was vortexed for 1 min. Finally, the mixture was left, until the phases were separated. A modified approach described by Lalas et al. [14] was used for the analysis. Further details can be found in the Supplementary material.

2.6.2. Untargeted profiling by LC-MS/MS

In a test tube with 10 µL of the AKO sample, 990 µL of isopropanol was added. The solution was filtered using a filter (Chromafil RC 0.20 µm, 25 mm), and 400 µL of isopropanol and 500 µL of water were added to 100 µL of it. The final solution was further analyzed according to Mantzourani et al. [15]. Further details can be found in the Supplementary material.

2.6.3. Extraction Procedure of Water-Soluble Components

The extraction of water-soluble components from the AKO samples was carried out according to a modified method previously described [16]. 1 g of AKO sample was diluted with 2 mL of *n*-hexane, and water-soluble components were extracted with 2 mL of a 60:40 (*v*/*v*) methanol/water solution. After vortexing for 2 min, the mixture was centrifuged at 4500 rpm for 5 min. The aqueous phase was retracted and further analyzed. Based on preliminary experiments, a single extraction step was adequate to extract the water-soluble components.

2.6.4. Total Polyphenol Content (TPC)

An analysis of TPC was carried out based on a previous study [17]. Detailed information is given in the Supplementary material.

2.6.5. Total Flavonoid Content (TFC)

An analysis of TFC was carried out based on a previous study [17]. Detailed information is given in the Supplementary material.

2.6.6. Reducing Power (P_R, FRAP Assay)

The FRAP assay was carried out based on a previous study [18]. Detailed information is given in the Supplementary material.

2.6.7. Antiradical Activity (A_{AR}, DPPH Assay)

The DPPH assay was carried out based on a previous study [18]. Detailed information is given in Supplementary material.

2.7. Statistical Analysis

All analyses were carried out in triplicate. Results express the mean values of the three replicate analyses, and standard deviation (SD) results are provided. Using the statistical program IBM SPSS Statistics (Version 29) (SPSS Inc., Chicago, IL, USA), a one-way ANOVA was performed to evaluate statistically significant differences for $p < 0.05$.

3. Results and Discussion

Extraction of AKO can be achieved via various techniques and processing conditions. Hao et al. [19] examined the use of pressing, ultrasound-assisted extraction, and Soxhlet extraction for AKO extraction. Although ultrasound-assisted extraction was found to be the most effective in terms of extraction yield, the fact that the extraction was carried out for up to 70 min with an additional 12 min needed to leave the sample standing renders the technique less appealing for extraction. In our case, we chose to use a simple extraction technique. The extraction was carried out at room temperature. This is because it was found that although elevated temperatures may result in increased extraction yields, the composition in terms of fatty acids remains almost unaltered. However, the acid value of the AKO increases at elevated temperatures, resulting in a lower AKO value. Therefore, since AKO can be used in the cosmetics and food industries, extraction was carried out without temperature to better preserve the AKO.

3.1. Volatile Compounds (VCs) and Essential Oil Characterization

Analyzing the VCs of oil is of high significance. VCs are responsible for the sensory properties (either positive or negative) of a product, including its aroma and flavor, which are valuable criteria for the acceptance of a product by consumers [20,21]. Since AKO is becoming more popular, data are needed for the VCs to gain a better overview of how agronomic and climatic conditions (such as ripeness of fruits upon harvesting, climate, etc.), as well as processing techniques, affect the sensory attributes [21]. However, studies on this topic are scanty and sparse. What is even more important is to obtain data from several years so as to gain a better overview. To the best of our knowledge, there are no previous reports examining the composition of AKO over multiple years.

A total of 38 VCs were identified in the AKO from apricots harvested in 2020 and 2021, while 34 VCs were identified in each AKO (Table 1 and Figure S1). In the AKO of 2020, butyl-cyclohexane, 6-methyl-undecane, 2-methyl-undecane, and tridecane were detected, which were not detected in the AKO of 2021. Likewise, in the AKO of 2021, ethyl benzoate, 2,4-diethyl-1-methyl-benzene, 1-methyl-4-(1-methylpropyl)-benzene, and benzoin were detected, which were not detected in AKO of 2020. However, in both cases, the abovementioned compounds accounted for less than 1% of the total identified VCs. As such, their contribution to the overall sensory attributes of AKO may not be significant. In both cases, the main VCs were 2-methyl propanal, benzaldehyde, and benzyl alcohol. The presence of benzaldehyde was somewhat expected. This is because it is a VC well known for its almond aroma and is widely used in the food industry. Approximately 20 tons of benzaldehyde are extracted annually from apricot kernels to be used in natural fruit flavors [22]. Therefore, its presence in AKO can be attributed to its lipophilic nature, which made its co-extraction with AKO feasible. Benzaldehyde occurs during the degradation process of amygdalin. Amygdalin is a natural cyanogenic glycoside present in the seeds of some edible plants [23]. Among others things, apricot kernels contain a high amount of amygdalin. Upon degradation, amygdalin is broken down into hydrogen cyanide, benzaldehyde, and glucose [24]. Benzaldehyde can then be further oxidized to yield benzyl alcohol. The above results are in accordance with a previous report on the AKO of Longwangmo apricots [20]. In this study, it was reported that benzaldehyde, 2-methyl-propanal, 2-methyl-butylaldehyde, furfural, nonanal, methylpyrazine, 2,5-dimethyl-pyrazine, methoxy pyrazine, and 3-ethyl-2,5-dimethyl-pyrazine were the main VCs of AKO from Longwangmo apricots. Finally, according to the results, no statistically significant ($p > 0.05$) differences in the concentration of these compounds in the AKO produced from apricots harvested in two years were recorded. This was also the case with most of the identified VCs, suggesting consistent sensory properties.

Table 1. Percentage volatile compounds (VCs) identified in the AKO 2020 and 2021 harvests.

A/A	VCs (%)	RT (min)	2020	2021
1	Toluene	4.329	1.02 ± 0.07	1.01 ± 0.04
2	2,3-Butanediol	4.8	0.54 ± 0.02	0.53 ± 0.01
3	Ethylbenzene	8.845	3.23 ± 0.21	3.58 ± 0.15
4	2-methyl-propanal	9.569	15.09 ± 0.62	15.03 ± 0.41
5	1,3-Dimethyl-benzene	11.333	5.12 ± 0.19	5.18 ± 0.15
6	Nonane	14.755	0.18 ± 0.01	0.18 ± 0.01
7	Benzaldehyde	17.713	22.85 ± 1.33	22.23 ± 0.49
8	1,2,4-Trimethyl-benzene	27.268	0.94 ± 0.07	0.9 ± 0.03
9	1,2,3-Trimethyl-Benzene	33.125	0.84 ± 0.06	0.8 ± 0.04
10	Decane	35.078	0.44 ± 0.03	0.44 ± 0.02
11	Benzyl alcohol	36.379	15.35 ± 1.14	15.13 ± 0.73
12	Butyl-cyclohexane	37.948	0.12 ± 0	nd
13	1,2-Diethyl-benzene	39.132	0.54 ± 0.02	0.57 ± 0.02
14	1-Methyl-3-propyl-benzene	39.534	1.3 ± 0.05	1.27 ± 0.04
15	1-Methyl-2-propyl-benzene	39.922	1.08 ± 0.02	1.15 ± 0.08
16	1-Ethyl-3,5-dimethyl-benzene	40.606	1.47 ± 0.04	1.49 ± 0.1
17	2-Ethyl-1,3-dimethyl-benzene	42.835	3.16 ± 0.21 *	3.53 ± 0.07
18	*o*-Cymene	43.598	0.37 ± 0.01 *	2.91 ± 0.09
19	2-Ethyl-1,4-dimethyl-benzene	45.493	0.73 ± 0.04	0.69 ± 0.04
20	Decahydro-2-methyl-naphthalene	46.433	0.29 ± 0.01	0.29 ± 0.01
21	1,2,3,5-tetramethyl-benzene	46.945	2.47 ± 0.13	2.46 ± 0.13
22	1,2,4,5-tetramethyl-benzene	47.252	3.26 ± 0.07	3.55 ± 0.25
23	Undecane	48.315	1.2 ± 0.08	1.2 ± 0.09
24	2,3-Dihydro-4-methyl-1H-indene	48.46	0.55 ± 0.04	0.54 ± 0.03
25	1-Phenyl-1-butene	49.29	0.64 ± 0.03	0.7 ± 0.04
26	1,2,3,4-Tetramethyl-5-methylene-1,3-cyclopentadiene	49.978	0.82 ± 0.02	0.83 ± 0.06
27	1-Phenyl-1,2-propanedione	50.308	2.23 ± 0.07	2.2 ± 0.04
28	Benzyl acetate	50.903	0.53 ± 0.02	0.5 ± 0.02
29	Azulene	51.367	0.29 ± 0.02	0.29 ± 0.02
30	Ethyl benzoate	51.547	nd	0.29 ± 0.01
31	2,4-Diethyl-1-methyl-benzene	52.145	nd	0.1 ± 0.01
32	1-Methyl-4-(1-methylpropyl)-benzene	52.728	nd	0.12 ± 0
33	6-Methyl-undecane	53.436	0.1 ± 0	nd
34	2-Methyl-undecane	54.202	0.2 ± 0.01	nd
35	Benzoin	55.174	nd	0.1 ± 0.01
36	Dodecane	57.111	0.93 ± 0	0.95 ± 0.04
37	2,6-Dimethyl-undecane	58.311	0.19 ± 0.01	0.19 ± 0.01
38	Tridecane	64.438	0.11 ± 0.01	nd

Data represent mean values ± standard deviation of three replicates; within each line, statistically significant differences ($p < 0.05$) are denoted with (*) asterisks; nd: not detected.

In addition to the VCs of the AKO, the essential oil of the AK was also examined. As can be seen in Table 2 and Figure S2, the essential oil consists, almost exclusively, of benzaldehyde. Its high concentration is justified based on the above discussion. Furthermore, a significant (~10%) amount of mandelonitrile was detected. Mandelonitrile is a precursor compound for the synthesis of amygdalin [25]. In both AK essential oil samples analyzed, no differences in their content were recorded.

Table 2. Apricot kernel essential oils from the 2020 and 2021 harvests identified by GC-MS.

A/A	Compounds (%)	RT (min)	2020	2021
1	Benzaldehyde	7.223	87.25 ± 5.41	86.52 ± 2.51
2	Benzyl alcohol	11.096	1.59 ± 0.04	1.53 ± 0.06
3	Benzoic acid	20.868	0.67 ± 0.03	0.64 ± 0.03
4	Mandelonitrile	28.59	10.49 ± 0.49	11.31 ± 0.76

Data represent mean values ± standard deviation of three replicates; no statistically significant differences ($p > 0.05$) were found between the samples using Student's *t*-test.

3.2. Fatty Acid Profile

Fatty acids are essential components of food and play an important role in maintaining human health. The fatty acid composition of the two AKOs was examined. Results can be seen in Table 3 and Figure S3. The results showed that the major fatty acid in both AKOs was oleic acid (C18:1, ω-9), followed by linoleic acid (C18:2, ω-6) and palmitic acid (C16:0). A minor (3%), yet statistically significant ($p < 0.05$) decrease in the percentage of oleic acid in the AKO of 2021 was found compared to the AKO of 2020. This difference can be attributed to the maturation stage of the apricots upon harvesting [26]. Upon maturation of apricots, the content of AKO in oleic acid increases, whereas the content in palmitic acid and linoleic acid may either remain constant or slightly decrease. Zhou et al. [20] reported that AKO from Longwangmo apricots contained 4.71% palmitic acid, 0.7% palmitoleic acid, 0.91% stearic acid, 70.47% oleic acid, and 0.17% linolenic acid. Likewise, Pavlovic et al. [7] reported that AKO contained 5.48%, 62.73%, and 29.18% palmitic, oleic, and linoleic acids, respectively.

Table 3. Percentage fatty acid content in the AKO 2020 and 2021 harvests determined using GC-FID.

Fatty Acid	2020	2021
Palmitic (C16:0)	4.74 ± 0.27	4.91 ± 0.12
Stearic (C18:0)	1.28 ± 0.04	1.24 ± 0.03
∑*Saturated (SFA)*	6.02 ± 0.3	6.15 ± 0.15
Palmitoleic (C16:1)	0.84 ± 0.03	0.9 ± 0.05
Oleic (C18:1, ω-9)	65.71 ± 1.64	62.31 ± 1.24 *
∑*Monounsaturated (MUFA)*	66.55 ± 1.67	63.21 ± 1.29
Linoleic (C18:2, ω-6)	28.16 ± 1.66	28.61 ± 0.94
∑*Polyunsaturated (PUFA)*	28.16 ± 1.66	28.61 ± 0.94
PUFA:SFA ratio	4.68 ± 0.04	4.65 ± 0.04
MUFA:PUFA ratio	2.37 ± 0.08	2.21 ± 0.04 *

Data represent mean values ± standard deviation of three replicates; within each line, statistically significant differences ($p < 0.05$) are denoted with (*) asterisks.

As can be seen from the results, the AKO had a PUFA:SFA ratio of approximately 4.6. The PUFA:SFA ratio is a commonly employed index used to evaluate the effect of a food product on cardiovascular health. Since PUFAs are known to decrease the levels of cholesterol in human serum and low-density lipoprotein cholesterol, while SFAs increase serum cholesterol levels, the higher the PUFA:SFA ratio, the better the product for cardiovascular health. The PUFA:SFA ratio of AKO is four times higher than that of olive oil, while it is similar to that of sunflower oil [27]. With regards to the MUFA:PUFA ratio, it can be seen that AKO had a value of 2.2–2.4, which is close to the recommended ratio of 1.5 [28].

Aside from the fatty acid profile determined by GC, an untargeted LC-MS/MS approach was employed in an effort to identify other compounds present in the AKO. A list of the tentatively annotated and detected compounds is given in Table 4, while a heatmap with the chromatographic area of the peaks in the two samples is given in Figure 1. In addition, a total ion chromatogram of the untargeted fatty acids is represented in Figure S4. As can be seen, the high oleic content of the AKO samples was further validated. In addition to the abovementioned fatty acids, myristic acid, isopalmitic acid, margaric acid, and caprylic acid were also detected in both samples, along with 4-cyclopropylcarbonyloxytridecane and 2-hexyl-1,3-dioxolane. Further research is needed to elaborate on the bioactivities and the health benefits of the two abovementioned compounds and examine whether the consumption of AKO is accompanied by further benefits.

Table 4. LC-MS/MS detected ion peaks for fatty acids present in the AKO.

A/A	Compounds	Exact Mass	[M-H]-
1	Methyl palmitate	270.2559	269.2486
2	Methyl myristate	242.2246	241.2173

Table 4. *Cont.*

A/A	Compounds	Exact Mass	[M-H]-
3	Methyl palmitoleate	268.2402	267.2329
4	12-Methyl-tetradecanoic acid	242.2246	241.2173
5	Heptadecanoic acid	270.2559	269.2486
6	9-Octadecenoic acid	282.2559	281.2486
7	Caprylic acid	172.1463	171.1390
8	9,12-Octadecadienoic acid	280.2402	279.2329
9	4-Cyclopropylcarbonyloxytridecane	268.2402	267.2329
10	2-Hexyl-1,3-dioxolane	158.1307	157.1234

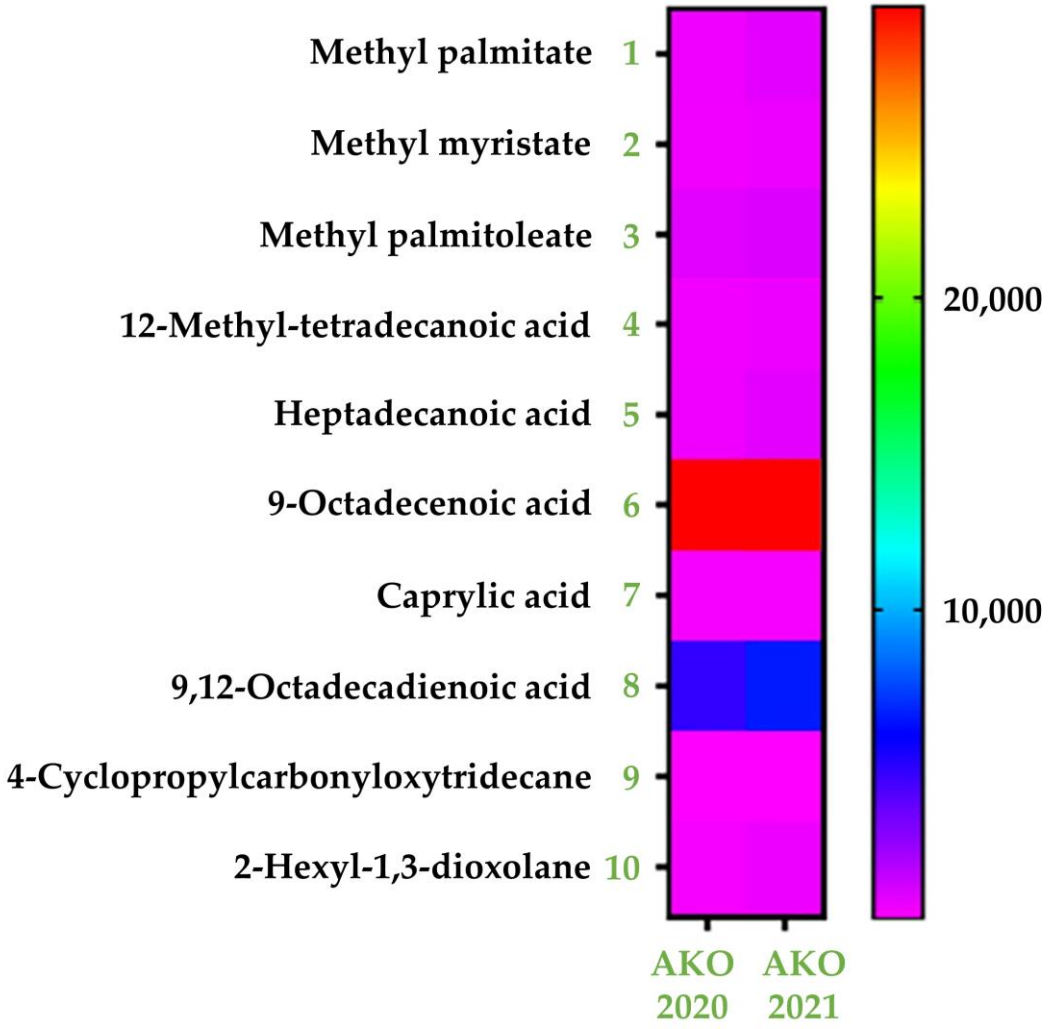

Figure 1. Heat map of AKO samples 2020 and 2021 harvest by LC-MS/MS.

3.3. Content of Polyphenols, Flavonoids, and Antioxidant Activity

Lately, antioxidant compounds are gaining more and more interest as a vital part of a healthy diet, aiming to prevent damage caused by oxidative stress. In addition to their health benefits, antioxidant compounds can also protect a food product against oxidation [29]. More specifically, antioxidant compounds such as butylated hydroxytoluene (BHT) are added to food products to prevent oxidative degradation. However, plant-derived products are rich in polyphenols, a naturally occurring class of compounds with exceptional antioxidant properties [30]. Polyphenols and their subclass, flavonoids, are present in high amounts in apricots [31]. However, polyphenols are compounds of variable polarity, and as such, their presence in AKO should not be taken for granted. To this end,

we evaluated the content of AKO in polyphenols and flavonoids, while their antioxidant potential was further examined. Results can be seen in Table 5. A relatively low polyphenol and flavonoid content was recorded for both examined AKO samples. The polyphenol content is higher than that of grapeseed oil (5.1 mg GAE/kg) and lower than that of sunflower oil (12 mg GAE/kg) [32]. The low content of AKOs in the above compounds barely bestows antioxidant properties on them, as evidenced by the DPPH and FRAP assays. Therefore, it is not expected that AKO would exhibit high stability against oxidation (and consequently, a short shelf life), and the addition of an antioxidant compound as an additive would prove beneficial.

Table 5. Content of polyphenols and flavonoids, as well as antioxidant assays, of AKO samples from the 2020 and 2021 harvests.

Assays	2020	2021
TPC (mg GAE/kg dw)	8.18 ± 0.41	7.94 ± 0.23
TFC (mg RtE/kg dw)	3.08 ± 0.06	2.57 ± 0.09 *
P_R (μmoL AAE/kg dw)	90.47 ± 2.17	86.58 ± 1.82
A_{AR} (μmoL DPPH/kg dw)	42.1 ± 2.11	40.02 ± 2.16

Data represent mean values ± standard deviation of three replicates; within each line, statistically significant differences ($p < 0.05$) are denoted with (*) asterisks.

4. Conclusions

In conclusion, this study examined the volatile compounds and fatty acid profile of apricot kernel oil (AKO) from the Bebeko variety over two consecutive years. The results indicated that 2-methyl propanal, benzaldehyde, and benzyl alcohol were the main VCs in AKO, while oleic acid was the main fatty acid. No significant differences were recorded in the chemical composition of the AKO during the two years, indicating a product with a relatively stable composition. Although the content of AKO in antioxidant compounds is low, its antioxidant activity is counterbalanced by the high content of unsaturated fatty acids, which exhibit many advantages for human health. Overall, AKO is a highly promising material with potential health benefits, and its chemical composition does not vary significantly from year to year, making it easier for industries to capitalize on its properties.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/separations10060332/s1, Figure S1: A TIC (total ion chromatogram) of the volatile compounds by HS-SPME/GC-MS; Figure S2: A TIC of the essential oil of AK by GC-MS; Figure S3: A GC-FID chromatogram of the fatty acid profile; Figure S4: A TIC of the fatty acid content by LC-MS/MS.

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