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ORIGINAL PAPER

NMR fingerprinting in apricot (*Prunus Armeniaca* L.) kernels and fruits concerning its different cultivars and soil type as analyzed using chemometrics

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Abstract

Prunus armeniaca L. (apricot) is an economical tree widely cultivated for its nutritive and health benefits. Herein, we standardized apricot fruits and kernels for the first time in context to different cultivars and soil type using 1D and 2D NMR metabolomics leading to the identification of 23 metabolites belonging to sugars, amino acids, organic, phenolic, and fatty acids, flavonoids, sterols, vitamins, cyanogenic glycosides, and carotenoids accounting for apricot nutritive and sensory attributes. Multivariate data analysis revealed distinct metabolic differences between the fruits and kernels, with the fruits being higher in sugars, organic acids, and flavonoids, whereas kernels were richer in fatty acids, phytosterols, and amygdalin. OPLS-DA plot revealed apricots from sandy soil to be high in organic acids however those from muddy soil were rich in sugars. This study underscores the influence of soil type on the chemical composition of apricot fruits and kernels, of value for standardization and quality control purposes.

Keywords 1D and 2D NMR · Apricot fruits · Apricot seeds · Multivariate analysis · Muddy *vs* sandy soil · Bitter *vs* sweet cultivar

Introduction

Apricot is a major edible fruit belonging to family Rosaceae widely cultivated for its nutritive value, tasty flavor, and huge market development potential [1]. It grows in different regions worldwide, especially in the Mediterranean climate, and is closely related to peaches [1, 2]. There are 3 to 12 species of apricot of which six are distinct and are well recognized including *P. holosericeae* Batal (Tibetan apricot), *P. brigantina* Vill. (Briancon apricot or Alpine plum), *P. sibirica* L. (Siberian apricot), *P. armeniaca* L. (common apricot), *P. mandshurica* (Maxim) (Manchurian apricot), and *P. mume* (Sieb.) Sieb. & Succ. (Japanese apricot) [2, 3]. However, the majority of cultivars grown for its edible fruits belong to *P. armeniaca* L that is the commercial taxa used in agriculture as a fruit yielding tree [2]. The post-harvest increased respiration rate of climacteric fruits like apricots fasten their ripening, triggers texture softening, causes weight reduction, and converts stored starch to sugars leading to their quick decay [4, 5]. The short shelf life of apricots causes fluctuation and irregular market supply beside their susceptibility to diseases compared to other summer fruits [2]. Nevertheless, the World production has increased over the last two decades reaching up to 85% due to increased cultivation specially in several Asian and African countries [1, 2], where Turkey is by far the World top apricot producer of both fresh (22.9% of total production) and dried (68% of total production) fruits [6]. Italy is also the leading country in Europe, with a production around 275.000 tonnes (*FAOSTAT*, https://www.fao.org/faostat/en/#data/QCL) [7].

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Egypt is also among the major producers of apricot in the region with production yield exceeding 98,000 tons in 2019 based on FAO stats (https://www.fao.org/faostat/en/#home). Some of the local Egyptian Apricot cultivars include Balady, Amar, and Hamawy, whose trees vary in size, fruit yield, fruit quality, and fruit maturity date. Because of the short marketing ability (short shelf life up to two weeks) of apricots, many attempts are made by the Egyptian ministry of Agriculture and the private sector to prolong the marketing period of apricots through introducing new varieties such as Canino, Beliana, Solitaire, Charisma, and Feriana to be evaluated under the Egyptian climatic conditions [8, 9]. However, the local Egyptian strains are distinguished by their excellent quality characteristics that suit the taste of the Egyptian consumer, compared to imported apricot varieties. Owing to the limited supply in the market, the cultivated area in Al-Amar region is decreasing.

Apricots have high nutritional value remarkably beneficial to human health owing to their richness in organic acids, carotenoids, minerals, and phenolic compounds, reducing the risk of chronic diseases like cancer, hypertension, and cardiovascular disorders [1, 10]. Aside from its nutritional value, this stone fruit exhibits diverse pharmacological properties including antioxidant, antimicrobial, and anti-inflammatory effects making it of particular use as a functional food [1, 11]. Even the kernel exhibits a nutritive value due to its content of vitamins (primarily ascorbic acid and ɣ-tocopherol), carotenoids (especially for β-carotene), amino acids (mainly alanine, glutamic acid, arginine, and leucine), organic acids (predominantly malic acid), unsaturated fatty acids (mainly oleic and linoleic acids), and sugars (mostly sucrose, glucose, and fructose) [1, 12]. The rich chemical composition and potential economic value of apricot fruits warrant for the development of analytical techniques for quality control purposes, or to account for its health and nutritive values [12].

Nuclear magnetic resonance (NMR)-based metabolomic fingerprinting is one of the sophisticated analytical tools to evaluate the quality of food [13], detect adulteration, and authenticate the geographical origin of food matrices [14–16]. NMR foodomics showed advantage over hyphenated techniques coupled to mass detectors (i.e., LC-MS and GC-MS) owing to its reproducibility, non-destructive nature (allowing the sample to be used for other analysis), no need for derivatization, and the increase in NMR sensitivity through the use of superconducting magnetic coils and cryogenically-cooled probes [15, 17–19]. Advances in NMR processing, the growing list of 2D NMR experiments (i.e., HSQC (Heteronuclear Single Quantum Coherence), HMBC (Heteronuclear Multiple Bond Correlation), NOESY (Nuclear Overhauser Effect Spectroscopy), TOCSY (Total Correlation Spectroscopy), COSY (Correlation Spectroscopy)), the online coupling of NMR with HPLC, made it possible for NMR to be increasingly employed in foods metabolites profiling [16, 17, 20, 21]. Despite being less sensitive than mass analyzers [22], NMR is a universal detector that can differentiate between isomers [15, 17], aside from its potential quantitative nature suiting it for quality control purposes [23]. Considering the complexity of NMR data measurements, chemical shifts and signal integration values are used to create a data set which could be later analyzed using chemometric unsupervised (i.e., hierarchical cluster analysis-HCA and principal component analysis-PCA), or supervised (i.e., orthogonal projections to latent structures-OPLS) tools to group similar components while segregating the dissimilar ones based on identifying spectral features that define group segregation [17, 24].

We have previously reported on the application of mass spectroscopy based chemometrics for the classification of apricot fruits targeting its aroma and primary metabolites using gas chromatography mass spectroscopy [12]. Herein, we present the first report on NMR profiling of apricot fruits and kernels from Egypt targeting both primary and secondary metabolites using combined 1D and 2D NMR experiments. Since the attributes of the soil could impact the productivity of the unit land and the abundance of plant nutrients, we evaluated the effect of soil type (muddy/clay such as Manshiet Al-Ammar and Al-Amar Al-Kubra vs. sandy desert soil such as Nubaria mountain) and cultivar type (the bitter vs. sweet varieties of apricots) on the chemical composition of apricots that reflects their nutritive value. Samples were classified using chemometric tools and were further standardized for their major bioactives using quantitative NMR.

Materials and methods

Plant material

Fruits and seed kernels of *Prunus armeniaca* L. were cultivated in different soil types. The collected samples include bitter apricots (the bitter varieties have their kernels enriched with cyanogenic glycosides hence contributing to their bitter taste) of Manshiet Al-Ammar (AP-B_1-F, AP-B_1-S) (Qalyubia, Egypt, 30°20’28"N 31°08’23"E) (Fig. S1) and Al-Amar Al-Kubra (AP-B_2-F, AP-B_2-S) (Qalyubia, Egypt, 30°20’37"N 31°07’40"E) as well as sweet apricots (varieties whose kernels contain less cyanogenic glycosides) of Al-Amar Al-Kubra (AP-S_2-F, AP-S_2-S), all growing in a Muddy soil along with bitter apricots of Nubaria mountain (AP-M_3-F, AP-M_3-S) (Al-Behera, Egypt, 31°09’24"N 29°51’50"E), which grows in sandy soil (sample codes interpretation is illustrated in Table 1S). All trees were around

Table 1 Assignment of major phytochemical classes in apricot fruits and kernels using 1D and 2D NMR measurements on their respective total methanol extracts

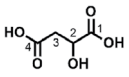
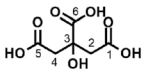
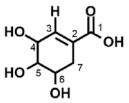
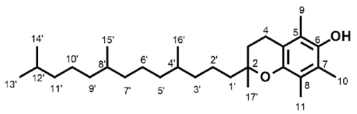
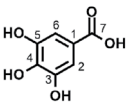
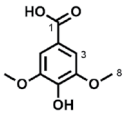
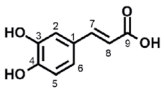
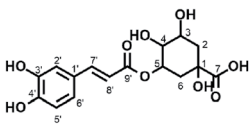
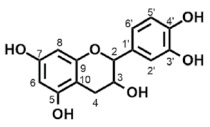
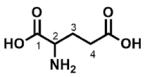
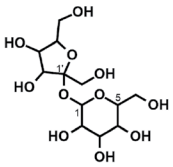
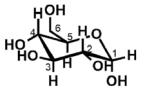
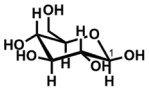
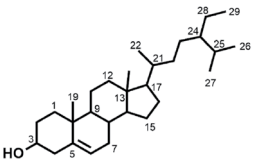
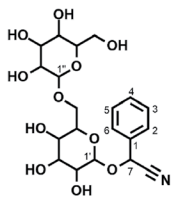
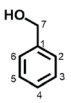
No.	Metabolite	Position	δ_H (ppm)	HSQC	HMBC	TOCSY	Structure	Fruits	Kernels
	Organic acids								
1	Malic acid	CH_2-3_a	2.57* (dd, 16.1, 7.6)	40.3	68.6 (C-2), 177.3 (C-1), 174.6 (C-4)	4.38 (H-2)		+	n.d.
		CH_2-3_b	2.75 (dd, 16.1, 4.6)			-----			
		H-2	4.38* (dd, 7.6, 4.6)	68.6	40.3 (C-3), 177.3 (C-1), 174.6 (C-4)	2.57 (H-3)			
2	Citric acid	CH_2-2/4	2.88* (d, 15.5) and 2.89* (d, 15.5)	44.3	44.3 (C-4/2), 74.6 (C-3), 171.5 (C-1/5), 174.2 (C-6)	-----		+	n.d.
3	Shikimic acid	CH_2-7_a	1.99-2.04, ov.	28.0	172.9 (C-1), 130.6 (C-3), 76.7 (C-5)	3.37		+	n.d.
		CH_2-7_b	2.70-2.74, ov.	-----		3.94 (H-6 and H-5)			
		H-3	6.22* (d, 15.8)	-----	-----	-----			
	Vitamins								
4	Tocopherol	CH_3-9/10/11	2.03-2.07, ov.	28.0	-----	-----		n.d.	+
		CH_3-13'/14'/15'/16'/17'	0.89-0.94, ov. 1.30, ov.	14.8-15.1 23.5					
	Phenolic acids								
5	Gallic acid	H-2/6	6.68*, s	114.8	114.8 (C-2/6), 145.8 (C-4), 169.2 (C-7)	-----		+	n.d.
6	Syringic acid	OCH_3-8	3.17*, s (fruits) 3.20*, s (kernels)	54.6 (fruits) 54.5 (kernels)	-----	-----		+	+
7	Caffeic acid	H-7	7.53 (d, 15.6)	146.4	115.3 (C-2), 122.6 (C-6), 169.1 (C-9)	6.27 (H-8)		+	n.d.
		H-8	6.26 (d, 15.6)	-----	127.8 (C-1)	7.53 (H-7)			
		H-5	6.73 (d, 8.0)	116.2	127.8 (C-1), 146.0 (C-3)	7.20 (H-6)			
		H-6	6.84* (d, 8.0)	-----	-----	-----			
8	Chlorogenic acid	H-5	4.24, m	79.1	68.6 (C-3), 70.3 (C-1), 175.0 (C-9')	1.38 (H-6) 2.31 (H-6) 4.03 (H-4)		+	n.d.
		H-7'	7.51* (d, 15.7)	146.7	115.2 (C-2'), 122.6 (C-6'), 168.9 (C-9')	-----			
		H-8'	6.26* (d, 15.7)	-----	127.4 (C-1')	7.51			
		H-5'	6.73 (d, 8.0)	116.2	127.8 (C-1), 146.0 (C-3)	7.20 (H-6)			
		H-6'	6.84* (d, 8.0)	-----	-----	-----			
		H-2'	7.22, s	129.4	-----	-----			
		$H\text{-}2_{ax}$	1.81 (dd, 13.2, 10.4)	41.8	38.3 (C-6), 73.1 (C-4), 179.0 (C-7)	2.05 ($H\text{-}2_{eq}$), 3.37 (H-3), 3.93 (H-4)			
		$H\text{-}2_{eq}$	2.05 (dd, 13.2, 4.5)			1.81 ($H\text{-}2_{ax}$), 3.37 (H-3), 3.93 (H-4)			
		$H\text{-}6_a$	1.97 (dd, ov.)	38.3	41.8 (C-2), 73.1 (C-4), 179.0 (C-7)	2.00, 1.81, 2.05			
		$H\text{-}6_b$	2.00 (dd, ov.)			1.97, 1.81, 2.05			
	Flavonoids								
9	(epi)Catechin	H-5'	6.71 (d, 8.3)	116.0	132.0 (C-1'), 145.8 (C-3')	6.91 (H-6')		+	n.d.
		H-6'	6.91 (dd, 8.3, 1.8)	119.3	115.1 (C-2'), 149.2 (C-4')	6.71 (H-5')			
		H-2'	6.78* (d, 1.9)	115.1	119.3 (C-6'), 149.2 (C-4')	-----			
		H-6	6.88 (d, 1.82)	-----	-----	-----			
		H-8	6.92 (d, 1.82)	-----	-----	-----			

Table 1 (continued)

		H-1"	5.28 (d, 7.5)	102.1	129.6 (C-3) 74.4 (C-5" and/or C-3")	3.58, 3.91 (H-2" and/or H-5" and/or H-3")			
		H-1"'	5.04, ov.	98.0	Region covering 72.8-74.6	3.29, 3.42, 3.48, 3.58, 3.66 (Sugar protons)		+	n.d.
10	Rutin (Quercetin-3-rutinoside)	CH_3-6"'	1.06* (d, 6.6)	17.4	73.3 (C-4"')	3.29, 3.42, 3.48 (Sugar protons)			
		H-6	6.17* (d, 2.0)	99.7	105.5 (C-8 or C-6)	6.38 (H-8)			
		H-8	6.37 (d, 2.0)	-----	-----	6.17 (H-6)			
		H-5' H-6'	7.09 (d, 6.9) 7.32, ov.	-----	-----	-----			
		CH_2-2'/6'	7.37 (d, 7.1)	129.0	129.0 (C-2'/6')	7.27 (CH_2-3'/5')			
11	Kaempferol-3-rutinoside*	CH_2-3'/5'	7.27 (d, 7.6)	128.8	128.8 (C-3'/5'), 138.8 (C-1')	7.37 (CH_2-2'/6')		+	n.d.
		CH_3-6"'	1.17* (d, 6.7)	-----	72.9 (C-4"')	-----			
	Carotenoids and their degradation products								
		CH_3-16/17	1.30, ov. (fruits) 1.33, ov. (kernels)	30.2 (fruits) 30.0 (kernels)	30.2 (CH_3-16/17), 32.5 (C-2), 130.9 (C-6)	2.01, 1.55 (CH_2-2)			
		CH_3-18	1.96, s (fruits) 1.97, s (kernels)	20.7 (fruits) 21.1 (kernels)	30.3 (C-4), 130.9 (C-6)	-----	refers to structure symmetry	+	+
12	β-carotene	CH_3-19/20	2.05, ov. (kernels)	12.0 (kernels)	-----	-----			
		H-7/8/10/11/12/14/15	7.29-7.43, ov. (kernels) 7.21-7.41, ov. (fruits)	128.9-129.2 (kernels) 128.6-129.0 (fruits)	-----	-----			
		CH_3-1	2.04, ov.	27.9	212.8 (C-2), 130.5 (C-3)	5.32 (H-3)			
		H-3	5.32, ov.	130.5	27.9 (CH_3-1)	2.04 (CH_3-1)			
13	β-ionone	CH_3-13	1.96, s	20.7	30.3 (C-7), 130.7 (C-5)	1.28		+	n.d.
	Fatty acids								
		H-9/10	5.30, t (fruits) 5.31, ov. (kernels)	130.8 (fruits) 130.6 (kernels)	26.2 (C-7), 28.0 (C-11)	H-7/12: 1.28 H-8/11: 2.00			
14	Oleic acid (ω-9)	CH_2-3	1.55, ov. (fruits) 1.58, ov. (kernels)	25.8 (fruits) 25.9 (kernels)	29.7 (C-5), 174.7 (C-1)	H-2: 2.29 H-4: 1.27		+	+
		CH_2-2	2.25-2.27, ov. (kernels) 2.22-2.27, ov. (fruits)	35.4 (kernels) 34.7 (fruits)	-----	-----			
15	Palmitic acid	CH_3-16	0.89-0.94, ov.	14.8-15.1	-----	-----		n.d.	+
		CH_2-2	2.25-2.27, ov.	35.4	-----	-----			
	Amino acids								
		CH_3-3	1.42* (d, 7.2) (fruits) 1.46* (d, 7.2) (kernels)	17.0 (fruits) 17.0 (kernels)	50.9 (C-2), 175.0 (C-1)	3.65 (H-2)		+	+

Table 1 (continued)

16	Alanine	H-2	3.31, ov. (fruits) 3.32, ov. (kernels)	50.0 (fruits) 50.2 (kernels)	-----	-----			
17	Glutamic acid	H-2	3.30, ov. (kernels) 3.30, ov. (fruits)	49.3 (kernels) 49.7 (fruits)	-----	-----		+	+
		CH_2-4	2.25-2.27, ov. (kernels) 2.25-2.31, ov. (fruits)	35.4 (kernels) 34.7 (fruits)					
	Sugars								
18	Sucrose	H-1	5.34* (d, 3.7) (fruits) 5.10* (d, 3.6) (kernels)	93.4 (fruits) 93.9 (kernels)	74.1 (C-5), 105.5 (C-1')	3.39, 3.68, 3.78 (Sugar protons)		+	+
19	α-Glucose	H-1	5.48* (d, 3.7) (fruits) 5.38, ov. (kernels)	93.4 (fruits and kernels)	-----	3.39, 3.68, 3.78 (Sugar protons)		+	+
20	β-Glucose	H-1	4.47* (d, 7.8) (kernels) 4.43* (d, 7.8) (fruits)	97.9 (kernels) 97.7 (fruits)	76.2, 77.8	3.09, 3.28		+	+
	Sterols								
21	β-sitosterol	CH_2-1	1.94-1.96, ov.	38.4	41.6 (C-9), 76.4 (C-3), 130.7 (C-5)	0.96 (CH_3-19) 1.27 (H-2) 1.82 (H-2) 3.39 (H-3)		+	+
		H-3	3.57, ov. (fruits) 3.59, ov. (kernels)	73.8 (fruits) 74.0 (kernels)	-----	-----			
		H-6	5.29, ov. (fruits) 5.31, ov. (kernels)	129.1 (fruits) 129.0 (kernels)	28.6 (C-8)	-----			
		CH_3-18	0.66	12.1	40.6 (C-12), 43.0 (C-13), 57.3 (C-17)	-----			
		CH_3-22/29	0.83	19.9	-----	-----			
		CH_3-26	0.84	14.2	23.4 (C-25), 32.1 (C-24)	1.24 (H-25)			
		CH_3-27	0.85	14.2	23.4 (C-25), 32.1 (C-24)	1.24 (H-25)			
		CH_3-19	0.96	19.6	38.4 (C-1), 51.3 (C-9), 142.1 (C-5)	-----			
	Cyanogenic glycosides and their hydrolysis products								
22	Amygdalin	H-7	5.89*, s	68.9	-----	-----		n.d.	+
		H-1'	4.47 (d, 7.8)	97.9					
		H-1"	4.55 (d, 7.8)	104.7					
		H-2"/3"/ 4"/ 5"/6" H-2'/3'/ 4'/ 5'/6'	3.11-4.38, ov.	62.7-84.1		-----			
23	Benzyl alcohol	H-2/6 H-3/5 H-4	7.45-7.46, ov.	130.2	-----	-----		n.d.	+
		H-2/6 H-3/5 H-4	7.60-7.62, ov.	128.7					

"ov." refers to overlapped signals. "n.d." means not detected * refer to signals used for quantification

10–12 years old and they attain an average height of 5–6 m (in Manshiet Al-Ammar and Al-Amar Al-Kubra), yet only 2 m in Nubaria mountain. Al-Amar strains are soft fruits with low firmness. They are characterized by their high total soluble solid (TSS) content and their distinctive taste [25, 26]. The pomological characteristics of the samples are described in Fig. S2. Samples were collected from Menoufia governorate in Egypt in June 2020 during the harvest

period. Stones were separated from fruits, and kernels were removed, and both fruits and kernels were lyophilized till complete dryness and kept at -20°C till further analysis. For assessment of biological replicates, pooled samples of 3 to 6 fruits were collected from three different apricot trees and subjected to extraction and analysis under the same conditions.

Chemicals and reagents

Methanol-d_4 and hexamethyldisiloxane (HMDS – the internal standard) were provided from Deutero GmbH (Kastellaun, Germany).

Extraction procedure and sample Preparation for NMR analysis

Around 120 mg of ground plant materials (fruits and kernels) were individually homogenized with 5 ml of 100% methanol using a Turrax mixer (11,000 RPM, IKA, Staufen, Germany) for 20 s (5 times) and were further processed using the methodology previously described by Farag et al. 2021 [27].

NMR analysis and processing

Agilent VNMRS 600 NMR spectrometer was employed for recording all NMR spectra using the parameters previously described by Farag et al. 2021 [27]. NMR spectra were processed using MestReNova 15.0.1 (Santiago de Compostela, Spain).

NMR quantification

For NMR based metabolites quantification, the peak areas of selected proton signals of the target compounds were calculated relative to the internal standard (HMDS) through manual integration of all samples. The absolute metabolite level calculation was implemented adopting the equation previously reported by Farag et al. 2021 [27]. One-way ANOVA followed by post hoc Tukey's test was carried out using Minitab version 17 (Minitab Inc., State College, PA, USA) to determine significant differences among groups. Differences were considered statistically significant at $p<0.05$.

Fig. 1 **A** ^{1}H-NMR spectrum of apricot fruit extract showing aliphatic methyl groups resonating in the range of 0.9–1.7 ppm and aliphatic methylenes at 1.5-3.0 ppm, oxygenated methine protons at 3.2-4.0 ppm, anomeric sugar protons and alkene protons at 4.5–5.7 ppm, and aromatic protons of phenolic compounds at 6.0-7.8 ppm and **B** ^{1}H-NMR spectrum of the kernels extract of apricots showing the aliphatic methyl groups (0.89–1.30 ppm), oxygenated methine protons (3.11–4.21 ppm), anomeric and alkene protons (4.34–5.40 ppm), and aromatic region (7.29-8.0 ppm)

Results

NMR-based profiling of metabolites in Prunus armeniaca fruits and kernels extracts

A multiplex of 1D (Fig. 1A and B for ^{1}H) and 2D (HSQC, HMBC, and TOCSY) NMR were implemented to characterize the main primary and secondary metabolites in apricot fruits and kernels resulting in the identification of 23 compounds belonging to organic acids, phenolics, fatty acids, flavonoids, sterols, amino acids, saccharides, ionones, vitamins, cyanogenic glycosides, and carotenoids (Table 1) to allover account for the nutritive, health and sensory attributes in apricot, as detailed in the next subsections for each class.

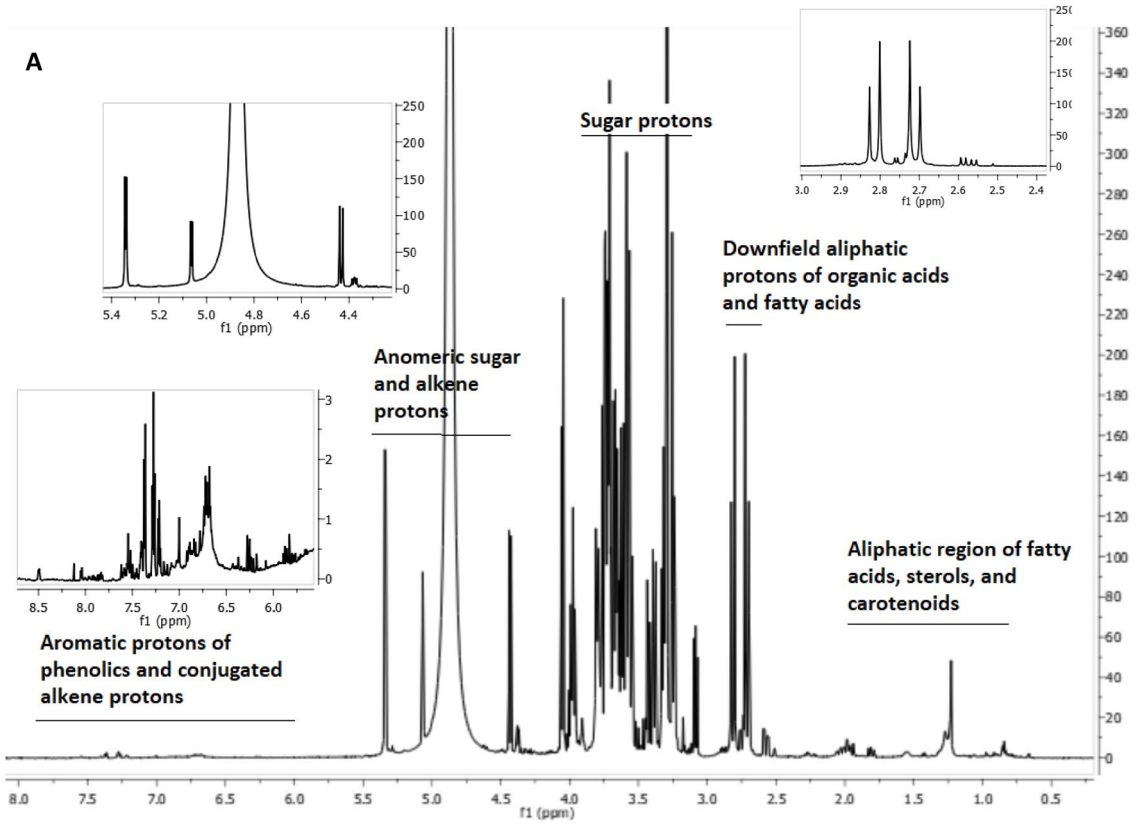
Primary metabolites

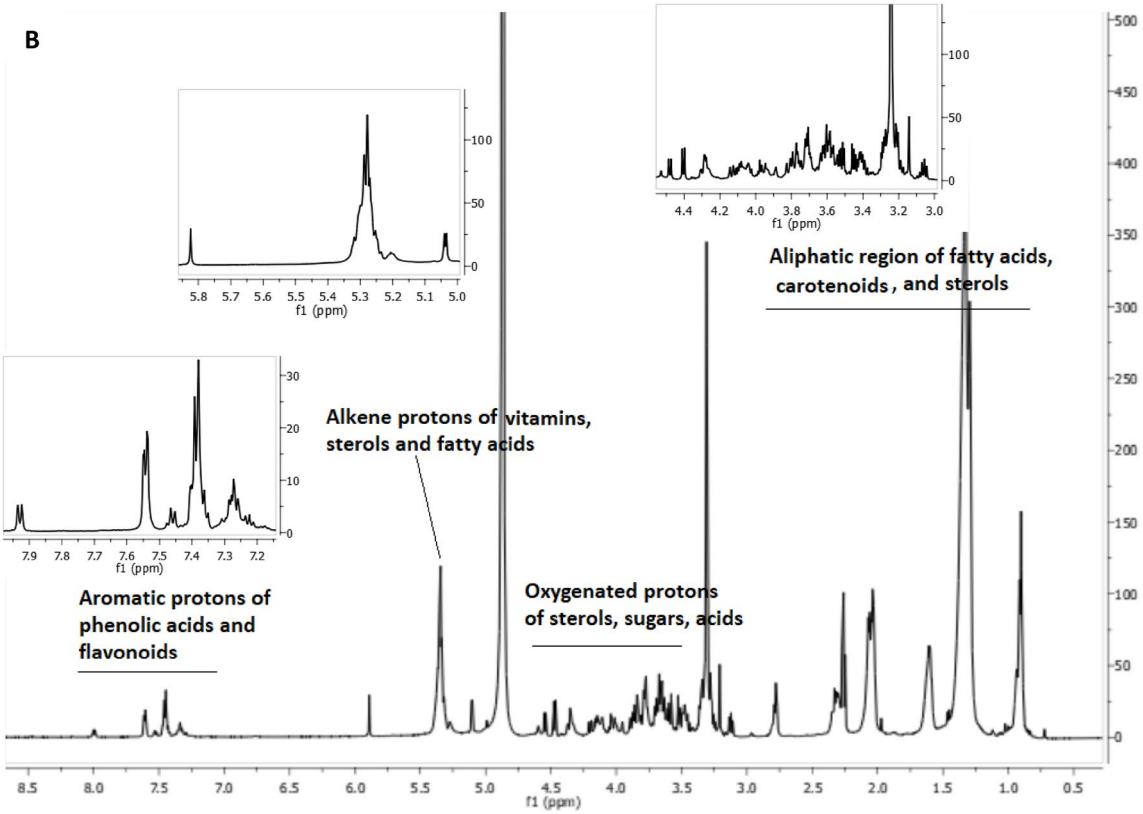
Sugars

Sugars represented the most abundant metabolite class identified in apricot fruits, albeit at much lower levels in kernels (Fig. 2) represented mostly by di- and mono-sugars i.e., sucrose and glucose. Sugars content in fruits increases during ripening due to the conversion of starch to saccharides which affects consumer satisfaction [28–30]. Sucrose and α-glucose were detected from their anomeric protons at 5.34 and 5.10 ppm for sucrose in fruits and kernels, respectively, and 5.48 ppm and 5.38 ppm for α-glucose in fruits and kernels, respectively (Fig. 1A, B). Their downshifted carbon appeared at ca. 93 ppm displaying TOCSY and HMBC interactions with neighboring sugar protons and carbons (Table 1 and Supplementary Figs. S3 and S4). Similarly, β-glucose signals were confirmed from its anomeric proton at 4.47 and 4.43 ppm in kernels and fruits, respectively (Table 1) with a typical J value of 7.8 Hz (Fig. S5).

Amino acids

Amino acids are among the primary metabolites needed for plant growth and functions. Like sugars and organic acids, amino acids´ level is known to change during fruit ripening and development [31, 32]. Alanine was identified as


A
Sugar protons
Downfield aliphatic protons of organic acids and fatty acids
Anomeric sugar and alkene protons
Aliphatic region of fatty acids, sterols, and carotenoids
Aromatic protons of phenolics and conjugated alkene protons
f1 (ppm)


B
Aliphatic region of fatty acids, carotenoids, and sterols
Alkene protons of vitamins, sterols and fatty acids
Oxygenated protons of sterols, sugars, acids
Aromatic protons of phenolic acids and flavonoids
f1 (ppm)

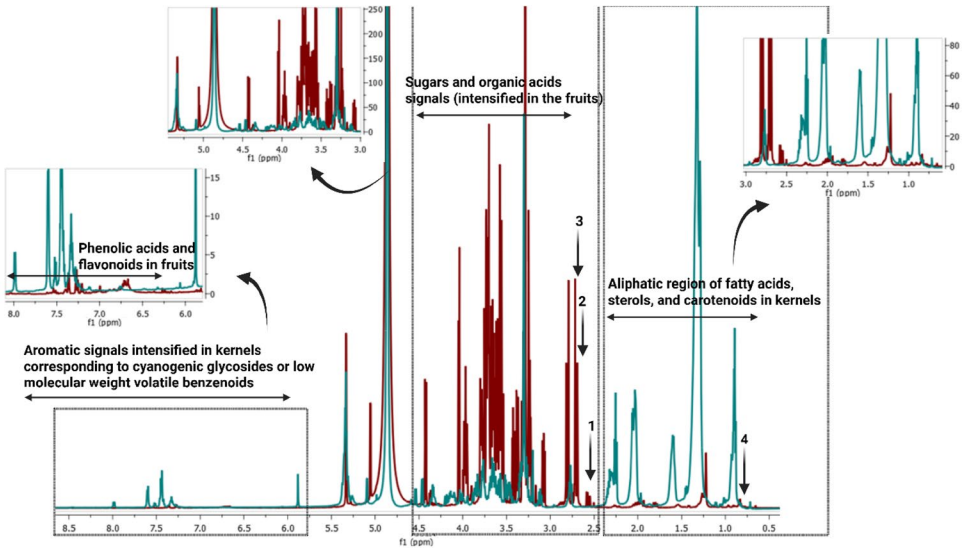


Fig. 2 The overlapped ^{1}H NMR spectra of fruits (in red) and kernels (in green)

the major amino acid in apricot based on resonance of its methyl group (at 1.42 ppm in fruits and 1.46 ppm in kernels; Fig. 1A, B) showing HMBC cross peaks to carboxylic carbon atom at 175.0 ppm (C-1) and carbon 2 (50.9 ppm) (supplementary Fig. S6). Alanine level in kernels seemed to be higher than that in fruits as observed from NMR signal intensity. Glutamic acid is another amino acid whose signals were detected in both fruits and kernels, especially for H-2 resonating at 3.99 and 3.89 ppm in fruits and kernels, respectively (supplementary Fig. S7).

Fatty acids

Based on the intensity of their ^{1}H NMR signals in the aliphatic region, fatty acids constituted around 10–14% of kernel extract versus 1–3% in fruit extract as expected in storage organs such as kernels. Signals of alkene protons in the ω-9 fatty acid, oleic acid (a major fatty acid in apricots [1, 6, 33]), appeared at 5.30 ppm in the ^{1}H-NMR spectrum of fruits (5.31 ppm) and corresponding to 130 ppm as revealed from HSQC experiment, and showing TOCSY correlations to its allylic protons at C-8/11 resonating around 2.00 ppm and HMBC correlation to the nearby aliphatic methylene (26.2 and 28.0 ppm) (supplementary Fig. S8), confirming Egyptian apricot richness in omega-9 fatty acid to add for its health benefits such as anti-inflammatory and anti-cancer effects, asides from being considered a healthier alternative to saturated animal fats [34]. The two protons at the β-position to the carboxylate (resonating at ca. 1.55 ppm) displayed HMBC cross peaks to the carbonyl carbon (C-1 at 174.7 ppm) and TOCSY correlations to the neighboring α-CH_2 at C-2 resonating at ca. 2.29 ppm (Table 1). Apricot kernels showed also characteristic signals for saturated fatty acids (i.e., palmitic acid) based on its deshielded CH_2 protons at a- position to the carboxylate, which resonated between 2.25 and 2.27 ppm, and the terminal methyl group (at ca. 0.89–0.94 ppm) (Fig. 1B, supplementary Fig. S9).

Organic acids

Organic acids are among the predominant classes in apricot fruits (3–5% of the total fruit extract), yet their NMR signals were not detected in kernels (Fig. 2). Many organic acids predominate in the fleshy parts of several fruits [35], and contribute to the taste and flavor of these fruits [35, 36]. Organic acids also affect the nutritional quality of the fruit by causing chemical stabilization of water-soluble vitamins (i.e., vitamin B and C), enhancing digestion, and increasing minerals' bioavailability [35, 37]. In apricot, acids were represented by citric, malic, and shikimic acids which are likely to impart the slightly acidic taste in apricots. Malic acid is the major acid in both kernels and fruits and to account for fruit sourness [38]. Additionally, malic and citric acids have been widely used in food industries owing to their preservative action against food spoilage bacteria along with their antioxidant properties [39–41]. The ^{1}H NMR signals of its methylene protons at C-3 appeared in the fruit sample as a dd at 2.57 ppm (H-3a) and 2.75 ppm (H-3b) (Fig. 1A) with a *J* value at 16.1 Hz typical for geminal-coupled protons, and is splitted by the neighboring oxygenated methine proton at 4.38 ppm (H-2) (as revealed from the TOCSY experiment) with *J* values of 4.6 Hz and 7.6 Hz for H-3a and H-3b, respectively (Table 1). Cross peaks of these methylene protons to the dicarboxylate carbons at 177.3 (C-1) and 174.6 (C-4) were further observed in the HMBC spectrum (supplementary Fig. S10). ^{1}H NMR signals for citric acid were likewise detected based (supplementary Fig. S11). The methylene protons at C-2 and C-4 in citric acid (2.88 and 2.89 ppm), and showing geminal coupling constant of 15.5 Hz, and further confirmed from HMBC cross peaks to

the dicarboxylate carbons at 171.5 ppm (C-1/5) and 174.2 ppm (C-6). Citric acid [42] exhibits antioxidant effect to reduce oxidative damage in the cells asides from its preservative action as an acidulant [43, 44]. Levels of citrate in apricot fruits are known to increase during maturation in the ripening stage [28] where its levels (together with sucrose) are the key flavors contributing to consumer preferences [28]. Shikimic acid is a key precursor to flavonoids and other phenolics in apricot [45] that was assigned from its methylene protons at C-7 in the aliphatic region between 1.99 and 2.04 ppm (H-7a) and 2.70–2.74 ppm (H-7b) (Fig. 1A, supplementary Fig. S12), however confirmation of the structure was based on key TOCSY cross peaks to the neighboring oxygenated methine protons at C-6 (3.37 ppm) and C-5 (3.94 ppm) (Table 1), and further HMBC correlations to the carbonyl group of the acid (172.9 ppm), the oxygenated C-5 (76.7 ppm), and to the alkene carbon C-3 (130.6 ppm).

Secondary metabolites

Phenolic acids

Aromatic signals were generally weak in intensity compared to the aliphatic region in both fruits (0.6–0.8%) and kernels (yet more intense in apricot kernels reaching 1.5-2%, Fig. 2), and to constitute a minor percentage of the total identified metabolites. Gallic acid is a trihydroxy benzoic acid and is one of the naturally occurring polyphenols that exist in fruits and vegetables [46]. Besides its use, along with its ester derivatives, in several food applications as flavors and preservative agents [47], it exhibits several pharmacological activities [46]. Aromatic signals of the two symmetric protons at C-2 and C-6 in gallic acid resonated at 6.68 ppm and 114.8 ppm for protons and carbons, respectively. HMBC cross-peaks were observed to the carbonyl at 169.2 ppm and to C-4 at 145.8 ppm which confirmed its assignment (supplementary Fig. S13). Caffeic acid is a hydroxycinnamic acid that imparts resistance of many fruits to microbial pathogens [48] found either free in plants or in the form of quinate ester forming chlorogenic acid. Signals of caffeic acid were assigned mostly based on its olefinic protons detected at 7.53 (H-7) and 6.26 (H-8) ppm, as doublets with a *trans* coupling of 15.6 Hz (Tables 1 and Fig. 1A). 2D-NMR further confirmed its assignment from key TOCSY cross peak to its neighboring alkene (H-8 at 6.27 ppm) and the HMBC correlations to C-2 (115.3 ppm), C-6 (122.6 ppm), and carboxylic carbon at 169.1 ppm (supplementary Fig. S14). In apricot fruits, the oxygenated proton at C-5 (4.24 ppm) of chlorogenic acid displayed TOCSY correlations to the methylene protons at C-6 (1.38 and 2.31 ppm) and H-4 (4.03 ppm) as well as HMBC interactions to the oxygenated methine C-1 (70.3 ppm) and C-3 (68.6 ppm) (supplementary Fig. S15). TOCSY and HMBC cross peaks of the alkene proton at C-7' (7.51 ppm) and the methylene protons at C-2 (1.81 and 2.05 ppm) and C-6 (1.97 and 2.00 ppm) further confirmed its structure (Table 1). On the other hand, signals for chlorogenic acid were not typically observed in apricot kernels. Levels of syringic acid, a dimethoxy derivative of gallic acid was likewise reported to show similar changes during fruit development, and to play a defensive role in the plant against pathogens [49, 50]. NMR signals of the methoxy groups in syringic acid were found to resonate as singlets at 3.17 and 3.20 ppm in fruits and kernels, respectively (supplementary Fig. S16). Its percentage was higher in kernels than in fruits (Fig. 2).

Flavonoids

Flavonoids belong to the major class of polyphenols, widely distributed in the plant kingdom [51], with a wide spectrum of biological activities [51]. Flavonoids were detected in apricot fruits (0.5–0.8% of total extract) represented by flavonols i.e., quercetin and kaempferol in addition to the flavanone (epi)catechin. Identification of flavonols was based on the *meta*-coupled protons ($J=2$ Hz) at C-6 and C-8 of ring "A" resonating at 6.17 and 6.37 for H-6 and H-8, respectively, in rutin (Fig. 1A). Sugar moiety in flavonol glycosides were identified from methyl group in the case of rhamnose appearing as (d) at 1.06 ppm with J value at 6.6 Hz showing TOCSY correlations to the surrounding sugar protons (Tables 1 and supplementary Fig. S17). Signals of anomeric protons in glucose (H-1'') and rhamnose (H-1''') resonated at 5.28 and 5.04, respectively. The attachment of the disaccharide part to the flavonol aglycone was confirmed from HMBC cross peak of the anomeric proton H-1'' to the alkene C-3 in aglycone at 129.6 ppm. In kaempferol-3-rutinoside, signals of the *ortho*-coupled protons 2' and 3' as well as 5' and 6' were observed at 7.37 ppm (for H-2'/6') and at 7.27 ppm (for H-3'/5') (Fig. 1A, supplementary Fig. S18). Signals for (epi)catechin (supplementary Fig. S19) were recognized from the *ortho*-coupled aromatic protons H-5' and H-6' ($J=8$ Hz) of ring-B which appeared at 6.71 and 6.91 ppm, respectively, and displayed TOCSY correlations to each other (Table 1). Further, protons 2' and 6' showed HMBC interactions to quaternary carbon (C-4') at 149.2 ppm. In-ring A, *meta*-coupled protons H-6 and H-8 (J value <2 Hz) resonated at 6.88 and 6.92 ppm, respectively. Flavonoids were detected in apricot fruits, yet their signals were not detected in kernels using NMR and suggestive that flavonoids are more activated in fruits considering their role as UV protectant [52] or antioxidants [53, 54].

Carotenoids and their degradation products

Aside from flavonoids, dark yellow to orange color of apricot fruit is attributed mainly for its richness in carotenoids viz., β-carotene with powerful antioxidant capacity [55, 56]. Carotenoids are reported to concentrate more in apricot peels than in the flesh [57], therefore peeling of apricots reduces its carotenoid content [58]. Signals for β-carotene were identified from its methyl groups at C-16 and C-17, which overlapped around 1.30 and 1.33 ppm in fruits and kernels, respectively (Table 1; Fig. 1A and B). They showed TOCSY correlations to the nearby methylene protons at C-2 (1.55 and 2.01 ppm) and HMBC cross peaks to C-2 (32.5 ppm) and the alkene carbon at C-6 (130.9 ppm) (supplementary Fig. S20). Signals of the methyl group at C-5 (CH_3-18) appeared as singlet at 1.96 ppm, while the methyl groups localized on the long olefinic chain (CH_3-19/20) were overlapped around 2.05 ppm. The richness of apricot in β-carotene impart its distinct color, and further to its aroma post degradation yielding ionone compounds which were likewise detected using NMR (Table 1) and suggests that this technique can provide insight on sensory attributes i.e., color and aroma in apricot. The apocarotenoid β-ionone, was recognized from its methyl group at C-1 a-to the carbonyl which appeared at 2.04 ppm, and showing HMBC correlations to a carbonyl carbon at 212.8 ppm (C-2) and an alkene C-3 at 130.5 ppm (supplementary Fig. S21).

Sterols

A common phytosterol in many plants is β-sitosterol which was detected in both fruits and kernels, yet at higher levels in kernels considering its richness in lipids, and suggestive for its potential antidiabetic, cardio- and hepato-protective properties [59]. The similarity in the structure of β-sitosterol and cholesterol made it useful in the treatment of hyperlipidemia without notable toxicity [60]. It was identified based on its methylene protons at C-1 resonating between 1.94 and 1.96 ppm and showing HMBC correlation to C-5 alkene carbon (130.7 ppm) and the oxygenated carbon at C-3 (76.4 ppm). Further, TOCSY correlations were observed to the nearby methyl group (CH_3-19 at 0.96 ppm) and aliphatic protons at C-2 (1.27 and 1.82 ppm) (supplementary Fig. S22). The methyl groups (CH_3-18, 19, 22, 26, 27, and 29) in β-sitosterol mostly resonate in the region between 0.66 and 0.96 ppm in ^{1}H NMR, and between 12.1 and 19.9 ppm in ^{13}C-NMR (Table 1) aiding in its assignment considering their higher intensities for these signals.

Cyanogenic glycosides and their degradation products

The bitterness of apricot kernel is attributed to cyanogenic glycosides such as amygdalin accounting for several of apricot kernel health [6, 61, 62]. Bitter apricot kernels contained considerably higher levels of cyanogenic glycosides as expected than the sweet varieties making them unsafe for human consumption due to risk of cyanide poisoning [63, 64]. Amygdalin (whose concentration averaged between 14 and 19% of the total kernel extract) was detected from the deshielded H-7 appearing as a singlet at 5.89 ppm and 68.9 in ^{1}H NMR (Fig. 1B) and HSQC, respectively (supplementary Fig. S23). Hydrolysis product of amygdalin was likewise detected by benzyl alcohol showing its aromatic protons overlapped in the region between 7.60 and 7.62 ppm (supplementary Fig. S24). Amygdalin signals were not detected, as expected, in apricot fruits [64–67].

Vitamins

Vitamin E (α- and ɣ-tocopherol) is characteristic for apricot kernels to account for antioxidant effect [68–70]. Tocopherol (α- and/or ɣ) was primarily detected in kernels where the signals of its benzylic methyl groups aided mostly in its assignment at 2.05 and 2.07 ppm, while its aliphatic methyl groups resonated between 0.89 and 1.30 ppm (Fig. 1B, supplementary Fig. S25).

^{1}H-NMR multivariate data analysis of apricot fruits and kernels

Unsupervised multivariate PCA analysis of full range ^{1}H-NMR dataset

Principal component analysis (PCA) was employed to the full range of the ^{1}H-NMR spectrum (δ 11.0–0.0 ppm) to assess metabolite heterogeneity among apricot fruit and kernel samples collected from Manshiet Al-Ammar, Al-Amar Al-Kubra, and Nubaria (Fig. 3), exhibiting differences in soil types (muddy versus sandy soil). A total of 6 samples, comprising three fruits and three kernels, each represented by three biological replicates to assess for natural variance. The first principal component (PC1) accounted for 69.6% of the total variance, while the second principal component (PC2) accounted for 61.3% (Fig. 3A).

The PCA score plot revealed two distinct clusters corresponding to the different apricot specimens (Fig. 3A). Importantly, kernels exhibited negative scores along PC1, segregated clearly from fruit samples. This separation was attributed to the high content of specific metabolites in kernels, including palmitic acid (δ 0.887 ppm), oleic acid (δ 1.290 ppm), and amygdalin (δ 7.459 ppm), as illustrated in

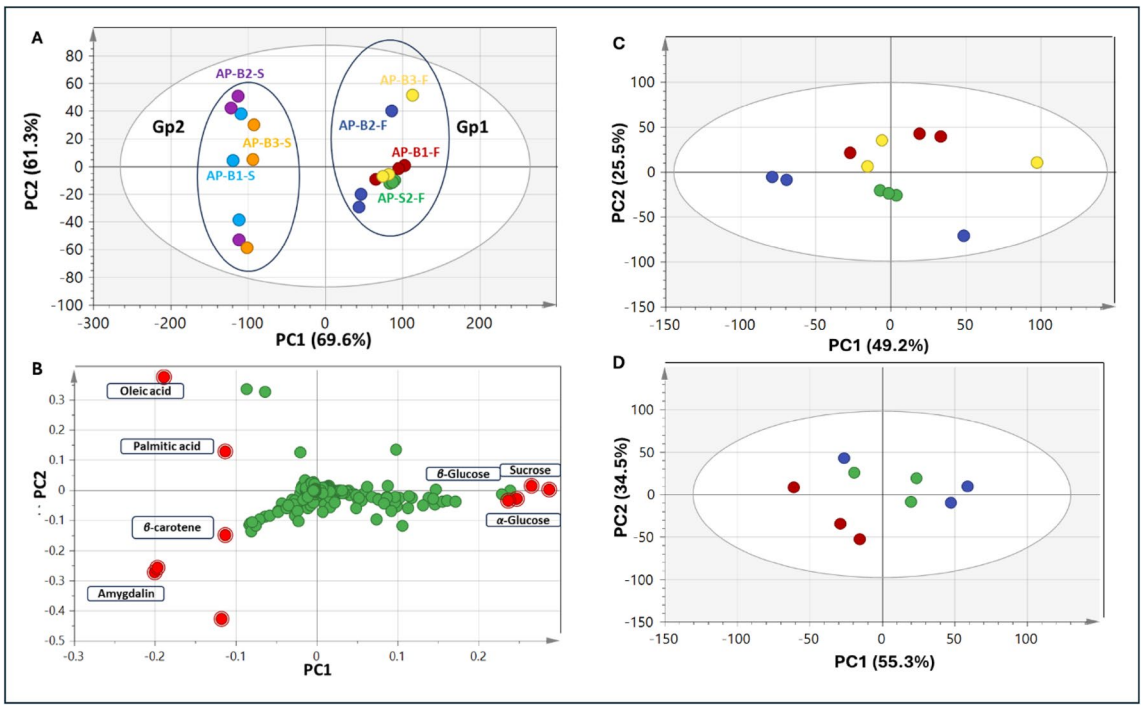


Fig. 3 ^{1}H-NMR peak-based principal component analysis (PCA) of the 6 apricot samples represented by fruit and kernel: AP-B_3-F (Nubaria fruit), AP-B_1-F and AP-B_2-F (Manshiet Al-Ammar and Al-Amar Al-Kubra fruits, respectively), AP-B_1-S and AP-B_2-S (Manshiet Al-Ammar and Al-Amar Al-Kubra kernels, respectively), and AP-B_3-S (Nubaria kernel). In the full spectrum (δ 11.0–0.0 ppm), clusters were located at distinct positions in the two-dimensional space described by principal component PC1 (69.6%) and PC2 (30.4%). **A** Score plot of PC1 vs. PC2 scores demonstrating clustering of apricot samples. **B** Loading plot for PC1 and PC2 with contributing ^{1}H-NMR signals and their assignments, highlighting metabolites like palmitic acid, oleic acid, β-carotene, amygdalin, sucrose, α-glucose, and β-glucose to the differentiation of fruit samples. **C** Score plot of fruits samples with no separation occur. **D** Kernel score plot with no separation occur

Fig. 3B. In contrast, apricot fruits were clustered all together on the opposite positive side of PC1, suggesting of a distinct metabolic profile. Fruits were abundant in sugars based on NMR signals for sucrose (δ 3.66–3.7–3.75 ppm), α-glucose (δ 3.62–3.79 ppm), β-glucose (δ 3.83 ppm), as depicted in Fig. 3B. Upon modelling fruits and kernels using PCA, no clear separation was observed among the samples within these groups based on origin or soil type with overlap among replicates belonging to different specimens (Fig. 3C and D). This lack of distinction suggests that the metabolic variations within fruits or kernels were not significant enough to be distinguished using PCA analysis. Overall, these findings underscore the distinct metabolic profiles of apricot fruits and kernels, where sugars and flavonoids predominantly influence fruits' metabolome, while fatty acids, β-carotene, and amygdalin serve as markers for kernels.

Supervised multivariate OPLS-DA analysis of apricot fruits using the full region ^{1}H-NMR dataset (δ 11.0–0.0 ppm)

To aid in classification among apricot fruit samples that failed using PCA analysis, a supervised orthogonal partial least squares discriminant analysis (OPLS-DA) was employed to the ^{1}H-NMR full spectral region (δ 11.0–0.0 ppm). As illustrated in Fig. 4A and B of the score plot and loading plot, the analysis revealed a distinct clustering pattern among fruit samples from different regions. Specifically, apricot fruits from Nubaria (AP-B_3-F) in sandy soil were clearly separated from those grown in muddy soil regions (AP-B_1-F and AP-B_2-F) as shown at (Fig. 4A). Separation appeared to be mostly influenced by soil type on the metabolic composition of apricot fruits. The loading plot revealed higher levels of citric acid (δ 2.823 ppm) and shikimic acid (δ 2.742 ppm) in Nubaria fruits. In contrast, apricot fruit samples grown in muddy soil were enriched in sugars viz. sucrose (δ 3.669–3.790 ppm), α-glucose (Fig. 4B). The OPLS-DA model for fruit samples demonstrated rather low predictive accuracy, with an R_2 value of 0.32, and a Q_2 value of 0.19, indicating limited predictive power and reliability of classification. This suggests that the model requires further refinement to improve its validation metrics or by inclusion of more samples from other origins to strengthen the model.

Similarly, for apricot kernel samples, OPLS-DA was conducted in the full region of the ^{1}H-NMR spectrum, as depicted in Fig. 4C and D. Although the score plot displayed a less distinct separation compared to the fruit samples, partial clustering was observed among kernel samples from

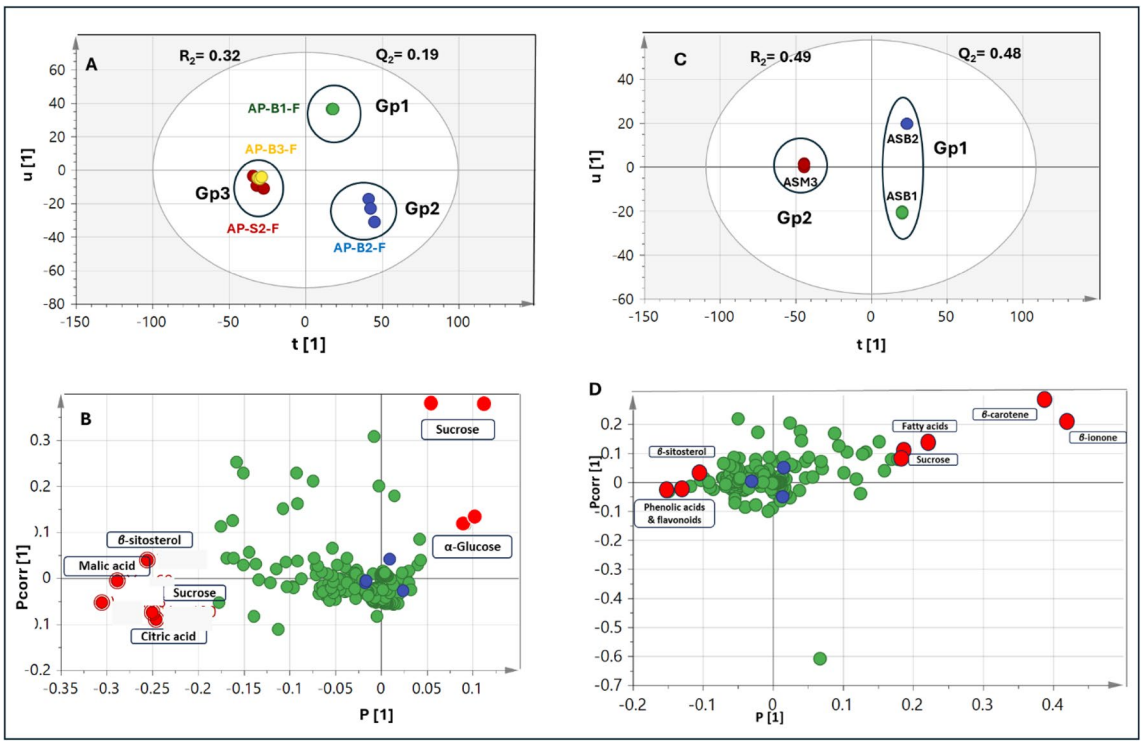


Fig. 4 OPLS-DA analysis of the full ^{1}H-NMR spectra (δ 11.0–0.0 ppm) for apricot fruit and kernel samples. **A** OPLS-DA score **B** Loading plot highlighting key metabolites like citric acid, shikimic acid, and sucrose that contribute to the differentiation among fruit samples. **C** OPLS-DA score plot of kernel samples. **D** Kernel loading plot displaying the distribution of fatty acids, β-carotene, and β-ionone as key differentiating metabolites

different soil types. The metabolites driving such segregation were primarily β-sitosterol (δ 3.508 ppm), β-ionone (δ 1.29–2.05 ppm), oleic acid (δ 1.25ppm), and β-carotene (δ 1.330 ppm), which were more abundant in the Al-Amar Al-Kubra kernel samples (AP-B_2-S) grown in muddy soil, as illustrated in Fig. 4D. In contrast hand, kernel samples from Nubaria (sandy soil) (AP-B_3-S), displayed higher levels of polyphenols viz. syringic acid (δ 3.18 ppm) and flavonoids such as rutin (δ 1.04 ppm), in addition to β-sitosterol (δ 0.96–1.00 ppm), as shown in Fig. 4D. These compounds play a significant role in improving tree fitness to the likely more harsh sandy soil type in desert than in muddy type [71, 72]. Whether such hypothesis is generalized for trees from other origins to prove richness of sandy derived kernels in phenolics should be considered. The kernel OPLS-DA model showed strong model performance compared to that of fruits, with an R_2 value of 0.49 and a Q_2 value of 0.48, indicating a more reliable predictive capability than in the fruit model.

These findings conclusively demonstrate that supervised OPLS-DA analysis more effectively classified apricot fruit and kernel samples. The fruit samples showed a broader metabolic composition, significantly influenced by their growing conditions. Organic acids (such as citric acid and shikimic acid) and sugars (including sucrose) were key factors in distinguishing fruit profiles. Variation in metabolites level reflects the diverse environmental impact on fruit samples from different regions and soil types. In contrast, the kernel samples displayed a more uniform metabolic composition, primarily characterized by sterols and flavonoids and β-carotene. The kernel composition, being less affected by environmental variability, appeared more consistent across regions, resulting in a more homogeneous profile.

While OPLS-DA analysis revealed clustering trends that suggest an influence of soil type on the metabolite composition of apricot fruits and kernels, these observations should be interpreted with caution. Given the limited number of biological samples analyzed, the current findings remain preliminary and exploratory. Although trends such as increased organic acid content in fruits grown in sandy soils and higher sugar levels in those from muddy soils were observed, the statistical power is insufficient to support definitive conclusions regarding soil–metabolite associations. To enhance the reliability of our findings, we conducted permutation tests (N=20 permutations) for the OPLS-DA models of both apricot fruits and seeds derived from different cultivation regions. The fruit model yielded a high R^2 value (0.94) and a Q^2 value of 0.48, while the seed model demonstrated even stronger metrics with an R^2 of 0.996 and Q^2 of 0.897 (Fig. S26). In both cases, all

permuted Q^2 values were significantly lower than the originals, and the regression lines for Q^2 showed negative intercepts, confirming the models are statistically valid and not overfitted. These results, along with the corresponding permutation test figures and explanatory legends, have been included in the revised manuscript to underscore the robustness and interpretive value of the multivariate statistical analyses. Nonetheless, we emphasize the need for future studies incorporating larger sample sizes, multiple cultivars, and replicated environmental variables to validate these preliminary trends and establish statistically significant soil–metabolite correlations in apricot metabolomics.

Quantification of major metabolites detected via ^{1}H-NMR

^{1}H-NMR analysis was employed to comprehensively quantify major metabolites in *P. armeniaca* fruits and kernels, providing detailed insights into their metabolic profiles and to aid in standardization of apricot extracts to be included in nutraceuticals. Sugars represented the most abundant class in apricot fruits, with notably much lower concentrations in kernels. Sucrose and glucose were the major forms, with the highest sucrose level found in fruit from Manshiet Al-Ammar (AP-B_1-F) at 710.17 µg/mg, followed by Al-Amar Al-Kubra fruit (AP-B_2-F) at 513.9 µg/mg. Glucose followed a similar trend, with *β*-glucose being more prevalent in apricot fruits at highest levels in Nubaria apricots (AP-B_3-F) of 256.73 µg/mg, compared with much lower levels in kernels such as (AP-B_1-S) to encompass only 21.2 µg/mg. *α*-Glucose was also detected, though at much lower levels than *β*-glucose in all samples, found at highest level in fruits from Manshiet Al-Ammar (AP-B_1-F) at 2.1 µg/mg. These results reveal for sugar richness in apricot fruits compared to kernels, which act as storage organs richer in fatty acids [73]. Fatty acids, particularly oleic acid (ω-9), were predominantly found at higher levels in apricot kernels compared to fruits. Specifically, kernels from Manshiet Al-Ammar (AP-B_1-S) exhibited the highest oleic acid levels, ca. 3-fold higher than those found in the fruit samples, making it the richest sample in (ω-9) fatty acid content. This was followed by the AP-B_3-S kernels, which showed a 2.7-fold increase compared to fruits. In contrast, the highest oleic acid level in fruit samples (AP-B_3-F) was significantly lower than kernels, underscoring the relative scarcity of omega-9 fatty acids in apricot fruits compared to kernels. This analysis indicates apricot kernels, particularly from Manshiet Al-Ammar (AP-B_1-S) is considerably richer in omega-9 fatty acids, which might contributes to potential health benefits, including anti-inflammatory effects [74, 75].

Amino acids, essential for plant growth and development, were represented by alanine as a prominent amino acid with highest level in apricot fruits (AP-B_1-F) and (AP-S_2-F) at 0.7 µg/mg. In contrast, the lowest level was detected in apricot kernels (AP-B_1-S and AP-B_3-S) at 0.3 µg/mg. Such difference in alanine levels between fruits and kernels indicates its critical role in energy storage and nitrogen transport during fruit maturation [76]. Organic acids, including malic, citric, and shikimic acids, represented another significant class of metabolites identified in apricot samples. Malic acid was the major form detected at highest level in apricot fruit (AP-B_3-F) at 4.0 µg/mg, compared to much lower levels in kernels. Citric acid also showed a similar pattern, being more enriched in fruits at ca. 17 times higher than those found in kernels. Shikimic acid, another key organic acid, was also detected, primarily in apricot fruits at highest levels likewise in (AP-S_2-F) at 3.21 µg/mg and posing (AP-S_2-F) as the richest in organic acids. Shikimic acid plays a crucial role in the biosynthesis of aromatic compounds, which may contribute to the sensory attributes of apricots [77], and to be confirmed using headspace analysis.

With regards to secondary metabolites, phenolic acids were identified as a significant class in both apricot fruits and kernels. Notably, chlorogenic acid was the most abundant phenolic acid, being highly abundant in Nubaria apricot (AP-B_3-F) at 11.2 µg/mg, followed by sweet fruits from Al-Amar Al-Kubra (AP-S_2-F) at 8.8 µg/mg. On the other hand, the lowest level of chlorogenic acid was observed in kernels from Manshiet Al-Ammar (AP-B_2-S) at 4 µg/mg, indicating a substantial difference between its presence in fruits and kernels. In contrast, caffeic acid, although present at lower levels, reached its peak level in Al-Amar Al-Kubra fruit (AP-B_2-F) at 0.68 µg/mg and was mostly absent in kernels. Furthermore, gallic acid exhibited the highest level in Al-Amar Al-Kubra sweet fruit (AP-S_2-F) at 2.75 µg/mg highlighting the pronounced phenolic acids' richness in fruits compared to kernels. Similarly, syringic acid was predominantly found in fruits at highest level in (AP-B_1-F) at 3.01 µg/mg (Table 2). Flavonoids were likewise distributed in both apricot fruits and kernels. Importantly, rutin was the major form reaching its peak in sweet apricot fruit (AP-S_2-F) at 4.82 µg/mg, compared to a significantly lower level in kernels at 1.45 µg/mg. Moreover, (epi)catechin was highest in Al-Amar Al-Kubra fruit (AP-B_2-F) at 2.07 µg/mg, with minimal levels in Nubaria apricots (AP-B_3-F) at 0.55 µg/mg, and was largely absent in kernels, indicating a strong association with fruit tissues. Similarly, kaempferol-3-rutinoside peaked in Al-Amar Al-Kubra fruit (AP-B_2-F) at 0.6 µg/mg, with lower levels in kernels (AP-B_1-S at 0.3 µg/mg), underscoring its limited presence in kernels compared to fruits (Table 2). Altogether, these findings demonstrate variation in phenolic acids and flavonoids between apricot fruits and kernels, with fruits more abundant in phenolics,

Table 2 ^{1}H-NMR quantification of major primary and secondary metabolites in different samples of methanol extracts (Manshiet Al-Ammar apricots (Muddy soil); fruits (AP-B1-F) and kernels (AP-B1-S), Al-Amar Al-Kubra apricots (Muddy soil), fruits (AP-B2-F) and kernels (AP-B2-S); Al-Amar Al-Kubra apricots (Muddy soil) fruits (AP-S2-F); Nubaria mountain apricots (Sandy soil) fruits (AP-B3-F) and kernels (AP-B3-S)

ID	Compound	Protons used in quantification	Amount µg/mg dry matter						
			AP-B1-F	AP-B2-F	AP-S2-F	AP-B3-F	AP-B1-S	AP-B2-S	AP-B3-S
1	Malic acid	CH_2-3_a	3.02±0.2^{a}	1.46±0.13 ^{b}	2.82±0.31 ^{a}	3.98±0.21 ^{a}	0.45±0.07 $^{b, c}$	0.5±0.01 $^{b, c}$	0.66±0.03 ^{c}
2	Citric acid	CH_2-2/4	1.05±0.1 ^{b}	0.72±0.07 ^{b}	1.75±0.27 ^{a}	1.59±0.15 ^{a}	0.05±0.001 ^{c}	0.09±0.003 ^{c}	0.07±0.001 ^{c}
3	Shikimic acid	CH/3	1.64±0.11 ^{b}	0.98±0.09 ^{c}	3.21±0.67 ^{a}	0.65±0.07 ^{c}	-	-	-
4	Gallic acid	H-2/6	0.8±0.05 ^{c}	1.5±0.24 ^{b}	2.75±0.29 ^{a}	0.64±0.03 ^{c}	0.16±0.01 ^{c}	0.19±0.03 ^{c}	0.1±0.009 ^{c}
5	Syringic acid	OCH_3-8	3.01±0.25 ^{a}	2.58±0.42 ^{a}	2.53±0.17 ^{a}	2.71±0.28 ^{a}	1.54±0.09 ^{b}	1.61±0.09 ^{b}	0.52±0.03 ^{c}
6	Caffeic acid	CH/6	0.54±0.02 ^{b}	0.68±0.04 ^{a}	0.27±0.02 ^{d}	-	-	-	0.41±0.04 ^{c}
7	Chlorogenic acid	H-2_{ax}	6.93±0.51 ^{c}	5.33±0.75 ^{d}	8.79±0.18 ^{b}	11.19±0.72 ^{a}	8.79±0.23 ^{b}	4±0.42 ^{e}	9.73±0.95 ^{b}
8	(epi)Catechin	H-2’	2.07±0.24 ^{a}	0.87±0.07 ^{b}	0.76±0.04 ^{c}	0.55±0.07 ^{d}	-	-	0.98±0.07 ^{b}
9	Rutin	CH_3-6"’	2.83±0.29 ^{c}	2.45±0.34 ^{c}	1.22±0.14 ^{e}	4.82±0.26 ^{a}	2.14±0.17 ^{d}	1.45±0.1 ^{e}	3.44±0.29 ^{b}
10	Kaempferol- 3-rutinoside*	CH_3-6’’’	0.3±0.07 ^{b}	0.6±0.03 ^{a}	0.3±0.09 ^{b}	0.67±0.06 ^{a}	-	-	-
11	Oleic acid (ω-9)	CH3	3.61±0.39 ^{c}	2.55±0.21 ^{d}	4.83±0.29 ^{c}	2.34±0.18 ^{d}	15.45±1.72 ^{a}	7.59±0.75 ^{b}	13.12±0.43 ^{a}
12	Alanine	H-9/10	0.68±0.03 ^{a}	0.38±0.08 ^{c}	0.66±0.11 ^{a}	0.49±0.03 ^{b}	0.3±0.03 ^{c}	0.6±0.07 ^{a}	0.3±0.01 ^{c}
13	Sucrose	CH_3-3	710.17±4.91 ^{a}	513.9±3.89 ^{b}	454.7±2.54 ^{b}	462.04±3.81 ^{b}	43.76±1.91 ^{c}	39.51±1.42 ^{d}	51.61±2.01 ^{c}
14	α-Glucose	H-1	2.1±0.34 ^{a}	1.49±0.18 ^{b}	1.29±0.23 ^{b}	1.49±0.24 ^{b}	0.14±0.02 ^{d}	0.2±0.03 ^{d}	0.61±0.07 ^{c}
15	β-Glucose	H-1	208.64±2.58 ^{a}	117.66±1.61 ^{b}	256.73±3.44 ^{a}	199.35±2.75 ^{a}	21.2±0.7 ^{d}	19.64±0.43 ^{d}	35.7±1.07 ^{c}
16	Amygdalin	H-1	-	-	-	-	1.72±0.23 ^{a}	1.03±0.14 ^{c}	1.55±0.19 ^{b}

“-“: Indicates the compound could not be detected using NMR

Values are expressed as µg/mg dry powder± s.d (n=3). Chemical shifts used for metabolite quantification were determined in methanol-d6 and were expressed as values relative to HDMS (0.94 mM final concentration). Post hoc tukey’s test was performed based on one-way ANOVA. Different superscript letters indicate statistically significant differences at $p<0.05$

contributing to their antioxidant properties against UV, and further potential health benefits in animals [78, 79].

Amygdalin, a cyanogenic glycoside responsible for the bitterness in apricot kernels [80], was detected at high levels in apricot kernel from Manshiet Al-Ammar (AP-B_1-S) at 1.72 ug/mg. NMR quantification suggests that amygdalin is more concentrated in apricot kernels compared to fruits, emphasizing its role in plant defense mechanisms, especially in seed tissues where it may act as a deterrent against herbivores [63]. The detailed ^{1}H-NMR analysis of *P. armeniaca* fruits and kernels revealed a clear metabolic distinction between these two components. Apricot fruits are notably rich in sugars, organic acids, phenolic acids, and flavonoids, which collectively contribute to flavor, antioxidant activity, and nutritional value in fruits. On the other hand, apricot kernels as storage organs are more rich in fatty acids, particularly oleic acid, along with amygdalin, emphasizing their roles in energy storage and plant defense [81]. Such comprehensive metabolite fingerprinting not only enhances our understanding of apricot composition but also guides the development of targeted nutraceutical and food products, optimizing the use of both fruits and kernels for their distinct metabolite profiles.

Conclusion

This study presents the first comprehensive NMR-based metabolomic analysis of apricot fruits and kernels from three localities in Egypt, differing in both cultivar type and soil conditions, offering novel insights into the metabolic fingerprint of locally grown apricots in Egypt. Utilizing 1D and 2D NMR techniques, a total of 23 primary and secondary metabolites, including sugars, organic acids, amino acids, fatty acids, cyanogenic glycosides, and phenolic compounds were identified. Multivariate data analysis highlighted qualitative differences in metabolic profiles of fruits versus kernels, with fruits being rich in sugars (sucrose, α and β-glucose), flavonoids, and organic acids (specially for malic and citric acids) which are crucial for their flavor and nutritive value, whereas kernels were richer in sterols (β-sitosterol), fatty acids (palmitic and oleic acids), and cyanogenic glycosides (amygdalin). Supervised multivariate analysis showed discrimination between samples based on soil type and geographical origin, with stronger models being observed in the case of kernels than fruits. Markers in fruits included citric acid and sucrose, while *β*-sitosterol and oleic acid were dominant in kernels. Quantification results revealed highest sucrose levels in Manshiet Al-Amar fruits, highest β-glucose and chlorogenic acid levels in Nubaria fruits, highest oleic acid and amygdalin levels in Manshiet Al-Amar seeds, and highest caffeic acid and rutin levels in Al-Amar Al-Kubra fruits. These findings underscore the potential of apricot fruits as nutritionally valuable components and further suggests the potential uses and valorization purposes of kernels in food and health applications. The findings highlight the potential for apricot kernels to be valorized as functional ingredients in food and nutraceutical applications due to their richness in sterols and fatty acids. This study is limited by the small number of samples, which restricts the ability to definitively distinguish whether the observed metabolomic differences are primarily driven by cultivar type or by soil type. Further studies involving a larger and more diverse set of samples, representing multiple cultivars, agricultural environments, and harvest seasons, are required to disentangle the individual contributions of genetic and environmental variables to apricot metabolome variation. The same metabolomic platform could be used to assess the effect of processing steps in the apricot industry such as drying, juice, puree, and paste preparation on the final quality of the product.

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Data availability Data is provided within the manuscript and supplementary information files.

Declarations

Conflict of interest The authors report no declarations of interest.

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