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Potential health-related phytoconstituents in leaves of *Chenopodium quinoa*

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Abstract

Background: *Chenopodium quinoa* Willd. or quinoa is an important food crop, having many pharmacological properties. It is recently introduced in Pakistan. In the present study, a phytochemical profile of its leaf extract was assessed through GC-MS analysis, and the health-related compounds were identified through a literature survey.

Methods: Quinoa was grown in Lahore, Pakistan, and its leaves were collected at maturity, dried, ground, and extracted in methanol. GC-MS analysis of this extract was done that showed the presence of 30 compounds.

Results: The most abundant compound was α-linolenic acid (12.13%), followed by *n*-hexadecanoic acid (11.51%), ergosta-5,7-dien-3-ol, (3β)- (10.99%), phytol (10.25%), and stigmast-7-en-3-ol, (3.beta.,5.alpha.,24S)- (7.33%). Moderately occurring compounds included DL-proline, 5-oxo-, methyl ester (6.01%), hydroxylamine, O-pentyl- (5.38%), neophytadiene (4.36%), 2-methoxy-4-vinylphenol (3.96%), 2-isopropoxyethyl propionate (3.84%), vitamin E (2.52%), and linolenic acid, methyl ester (2.46%). The remaining compounds were less abundant, having peak areas of less than 2%.

Conclusion: Literature survey revealed that α-linolenic acid; *n*-hexadecanoic acid; phytol; squalene, vitamin E and linolenic acid, and methyl ester; present in leaf extract of quinoa possess various health-related properties such as antibacterial, antifungal, cardio-protective, anti-inflammatory, hypocholesterolemic, antihistaminic, antiandrogenic and antieczemic.

Introduction

Plants are the basis of both traditional and modern drug discoveries [1]. These are a supply of secondary metabolites having exciting biological properties that continue to play a significant role to provide mankind with remedies against ailments [2-4]. These metabolites have a wide variety of structural arrangements and properties. Information on phytochemicals is needed for the discovery of therapeutic compounds as well as for identifying new sources for the preparation of complex molecules [1]. Several reports on green plants represent that these are easily biodegradable and are a reservoir of effective chemotherapeutics while most of them remain neglected, undocumented, and are becoming rare [5]. In different cultures, the majority of higher plant species are well documented in the healthcare system by producing essential oils, biocides, agrochemicals, and pharmaceuticals [6-8]. The introduction of natural-originated novel drugs has drawn attention to identifying, exploring, and preserving various plants for the preparation of drug formulations [9].

Chenopodium quinoa Willd. stress-tolerant food crop that has been grown in the Andean region for several thousand years. Recently, it has been introduced in various countries in Europe, Asia, Africa, and North and South America [10]. It grows well under adverse conditions like wind, hail, frost, drought, and saline soils [11]. It is an important source of vitamins, essential nutrients, amino acids, and minerals. It also contains compounds like saponins, phytosterols, polyphenols, and flavonoids [12,13]. It is a gluten-free crop that has many positive characteristics, including dietary fibers help in the lowering of cholesterol in the blood to reduce cardiovascular diseases, diabetes, anemia, and obesity [14,15]. Moreover, recent investigations have focused on the therapeutic properties and chemical constituents of quinoa which is rapidly gaining recognition as a nutraceutical and functional food [16]. It different parts contain excellent antifungal, antioxidant, antiviral, anticancer, hypoglycemic, hypocholesterolemic, anti-inflammatory, antithrombotic, and diuretic activities effective against a wide range of human diseases [17-19]. This study was undertaken to explore the phytochemical profile of *C. quinoa* methanolic leaf extract through GC-MS analysis.

Methods

Sample collections

Mature *C. quinoa* plants cultivated at Punjab University, Lahore, Pakistan were selected for experimentation. Young plant leaves were collected, washed under running tap water, and kept under shade. After ten days, dried leaves were collected, placed in paper bags, and kept in a dry heat oven for two days at 35 °C for complete removal of moisture contents. Thereafter, leaves were crushed using a pestle and mortar.

Extract preparation

The methanolic extract was prepared by using 50 g of *C. quinoa* dried plant leaves. The material was dipped in high-grade methanol 100 mL for fifteen days at room temperature. After that, it was passed through two layers of a Whatman filter, and the resultant was collected in a glass vial (5 mL) for GC-MS analysis.

GC-MS analysis

Gas chromatography (GC) machine model 7890B, Agilent Technologies (USA) was used for the evaluation of the phytochemical profile of *C. quinoa* leaf methanolic extract. Helium, an inert gas was used as a carrier. The column DB-5ms was selected having 0.25 µm × 30 m × 0.25 µm dimensions with an injection volume of 1 µL. The initial oven temperature was 80 °C, which raised up to 300 °C with an interval of 10 °C min^{-1}. MS analysis was carried out on machine model 5977A, Agilent Technologies (USA). The scan ranged between 50-500 m/z with a solvent delay time of 5 min. The sample run for 50 min, and the source temperature was 230 °C. For the characterization of the phytochemical profile, the obtained spectrum was analyzed with NIST library version 2017. Compounds' relative abundance was analyzed by using chromatogram peak heights, and their structures were drawn in ChemDraw software [8].

Literature survey

A comprehensive literature survey was performed on the basis of previously reported biological activities of the identified compounds.

Results

GC-MS chromatogram shows the presence of 30 compounds in the leaf extract of quinoa (Fig. 1), with their details in Table 1. α-Linolenic acid was the most abundant compound. Other frequently occurring compounds were *n*-hexadecanoic acid (11.51%), ergosta-5,7-dien-3-ol, (3β)- (10.99%), phytol (10.25%), and stigmast-7-en-3-ol, (3.beta.,5.alpha.,24S)- (7.33%). Compounds with peak areas between 2 and 7, namely DL-proline, 5-oxo-, methyl ester (6.01%), hydroxylamine, O-pentyl- (5.38%), neophytadiene (4.36%), 2-methoxy-4-vinylphenol (3.96%), 2-isopropoxyethyl propionate (3.84%), vitamin E (2.52%), and linolenic acid, methyl ester (2.46%), were categorized as moderately occurring ones. Compounds showing peak areas smaller than 2% were named as less abundant. These included 3-methylene-7,11-dimethyl-1-dodecene (1.64%), linolelaidic acid (1.59%), pentadecanoic acid, methyl ester (1.45%), pelletierine (1.36%), phenol, 4-(ethoxymethyl)-2-methoxy- (1.23%), 11,13-dimethyl-12-tetradecen-1-ol acetate (1.16%),

Names of compounds	Molecular formula	Molecular weight	Retention time (min)	Peak area (%)
Hydroxylamine, O-pentyl-	$C_5H_{13}NO$	103.16	4.743	5.38
Benzofuran, 2,3-dihydro-	C_8H_8O	120.15	6.453	0.86
2-Methoxy-4-vinylphenol	$C_9H_{10}O_2$	150.17	7.443	3.96
2-Ethoxy-3,5-hexadiene	$C_8H_{14}O$	126.20	8.262	0.82
DL-Proline, 5-oxo-, methyl ester	$C_6H_9NO_5$	143.14	8.410	6.01
Pelletierine	$C_8H_{15}NO$	141.21	8.696	1.36
2-Isopropoxyethyl propionate	$C_8H_{16}O_3$	160.21	9.286	3.84
Nonanoic acid	$C_9H_{18}O_2$	158.24	9.972	0.95
Octanoic acid, 4-tridecyl ester	$C_{21}H_{42}O_2$	326.6	10.648	0.62
1,3-Diphenylpropane	$C_{15}H_{16}$	196.28	11.643	2.07
Isoaromadendrene epoxide	$C_{15}H_{24}O$	220.35	12.576	0.72
Phenol, 4-(ethoxymethyl)-2-methoxy-	$C_{10}H_{14}O_3$	182.22	13.005	1.23
Neophytadiene	$C_{20}H_{38}$	278.5	13.451	4.36
11,13-Dimethyl-12-tetradecen-1-ol acetate	$C_{18}H_{38}O_2$	282.5	13.514	1.16
Cyclopentane, decyl-	$C_{15}H_{30}$	210.40	13.703	0.93
3-Methylene-7,11-dimethyl-1-dodecene	$C_{15}H_{28}$	208.38	13.898	1.64
Pentadecanoic acid, methyl ester	$C_{16}H_{32}O_2$	256.42	14.367	1.45
n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256.42	14.768	11.51
9,12-Octadecadienoic acid (Z, Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	16.004	0.61
Linolenic acid, methyl ester	$C_{19}H_{32}O_2$	292.45	16.066	2.46
Phytol	$C_{20}H_{40}O$	296.5	16.152	10.25
Linolelaidic acid	$C_{18}H_{38}O_2$	282.5	16.421	1.59
α-Linolenic acid	$C_{18}H_{30}O_2$	278.42	16.467	12.13
Dimethylaminoethyl palmitate	$C_{20}H_{41}NO_2$	327.5	17.703	0.60
Cyclopropaneoctanal, 2-octyl	$C_{19}H_{36}O$	280.5	17.817	0.85
Squalene	$C_{30}H_{50}$	410.7	21.829	1.08
1,1,1,3,5,5,5-Heptamethyltrisiloxane	$C_7H_{21}O_2Si_3$	221.50	22.653	0.68
Vitamin E	$C_{29}H_{50}O_2$	430.7	23.997	2.52
Ergosta-5,7-dien-3-ol,(3β)-	$C_{28}H_{46}O$	398.7	25.428	10.99
Stigmast-7-en-3-ol, (3.beta.,5.alpha.,24S)-	$C_{29}H_{50}O$	414.7	25.931	7.33

Table 1: Compounds identified in methanolic leaf extract of quinoa through GC-MS analysis

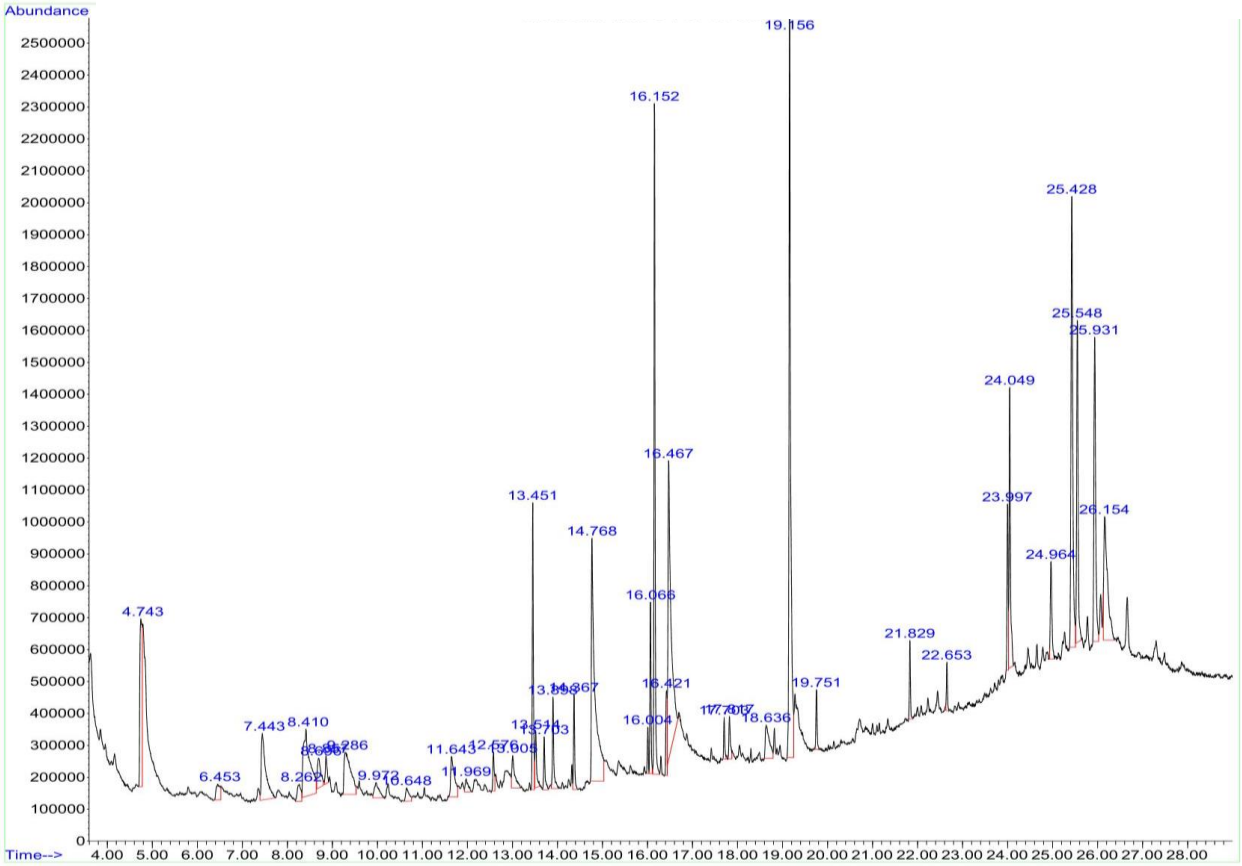

Figure 1: GC-MS chromatogram of methanolic leaf extract of quinoa.

squalene (1.08%), nonanoic acid (0.95%), cyclopentane, decyl- (0.93%), benzofuran, 2,3-dihydro- (0.86%), cyclopropaneoctanal, 2-octyl (0.85%), 2-ethoxy-3,5-hexadiene (0.82%), isoaromadendrene epoxide (0.72%), 1,1,1,3,5,5,5-heptamethyltrisiloxane (0.68%), octanoic acid, 4-tridecyl ester (0.62%), 9,12-octadecadienoic acid (Z,Z)-, methyl ester (0.61%), dimethylaminoethyl palmitate (0.60%).

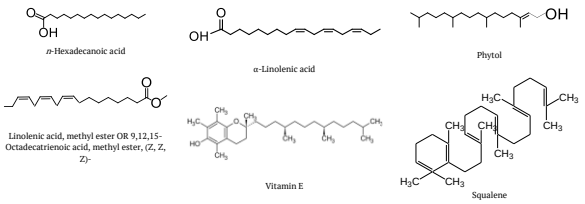

Figure 2: Structures of major bioactive compounds in methanolic leaf extract of quinoa.

Discussion

The most abundant compound linolenic acid, a polyunsaturated fatty acid, has a number of biological activities including antibacterial activity against *Bacillus subtilis* and *Staphylococcus aureus* [20]. It can act as a potential anti-inflammatory molecule in eye inflammation [21]. Moreover, it also has other important functions, such as improving cardiovascular health, and brain development, and is an anti-tumor agent [22]. Likewise, *n*-hexadecanoic acid or palmitic acid, is an important biologically active molecule also found in *Coronopus didymus* [23] and *Chenopodium murale* [24], and has antioxidant, antimicrobial, anti-inflammatory, hypocholesterolemic, and pesticidal properties [25,26]. Phytol has been identified in *Euphorbia prostrata* [27], *Ageratum conyzoides* flowers [28], and various other plant species. It exhibited antibacterial activity against *Pseudomonas aeruginosa* and *Bacillus licheniformis* [29,30], and antifungal activity against *Aspergillus niger* and *Candida albicans* [31].

Among the moderately occurring compounds, linolenic acid, methyl ester has earlier been identified in many other plants, including quinoa roots [32] and *Vinca major* flowers [33]. It has many biological properties such as anticancer, antiarthritic, anti-inflammatory, antihistaminic, antiandrogenic, antieczemic, nematicidal, cardio-protective, and hypocholesterolemia [34,35] (Akpuaka *et al.,* 2013; Devi and Muthu, 2014). Vitamin E, obtained from the diet, is an important fat-soluble molecule in the antioxidant defense system of the cell. It is effective against cancer, cataracts, and arthritis, and also reduces the formation of prostaglandins that causes platelet clumping [36].

Among less abundant compounds, 9,12-octadecadienoic acid (Z,Z)-, methyl ester has many biological properties, including zinc bioavailability enhancer, urine acidifier, and uric acid inhibitor [37]. Likewise, squalene belongs to triterpenes, and mostly occurs in adequate quantity in various oils such as olive and palm oils. It has antioxidant as well as antitumor properties [38].

This study concludes that leaves of quinoa contain a number of bioactive molecules such as α-linolenic acid; phytol; linolenic acid, methyl ester, squalene, *n*-hexadecanoic acid; and vitamin E. These compounds possess a number of health-related properties including antibacterial, antifungal, anti-inflammatory, cardio-protective, antihistaminic, hypocholesterolemic, antieczemic and antiandrogenic.

Competing Interest

Authors declare that they have no conflict of interest.

Author Contributions

AJ conceived idea and wrote most part of this manuscript; IHK did experimental work, contributed in paper writing and draw structures of the compounds; FAC did final editing; and MFHF monitored GC-MS analysis.

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