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Basic nutrients and UPLC- ZenoTOF-MS/MS based lipomics analysis of *Chenopodium quinoa* Willd. varieties

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Abstract

This study conducted a comparison of the nutritional content and lipid composition of five different varieties of quinoa (QL-1, SJ-1, SJ-2, KL-1, and KL-2) from Qinghai Province, China. Each of the five varieties exhibited varying levels of essential nutrients, including crude protein, dietary fiber, and crude fat. The QL-1 variety has the highest concentration of phytic acid, measuring 1.66 g/100 g. A non-targeted lipomics analysis discovered a total of 16 lipid categories and 383 individual lipids in quinoa. Out of the several substances, glyceride had the highest concentration, exceeding 70%, with phospholipids coming next. The percentage of fatty acids and fatty acid esters was between 5 and 11%. The glycerides in all five kinds exhibited a similar composition, with unsaturated glycerides constituting over 99% of the total glycerides. Phospholipids constituted over 11% of the overall lipid content, with lecithin comprising more than 80% and cephalin ranging from 16.70 to 18.61%. The results establish a solid basis for the utilization of quinoa in processing, particularly in lipid processing.

Keywords Quinoa, Nutrients, Lipomics, Phospholipid, Fatty acid

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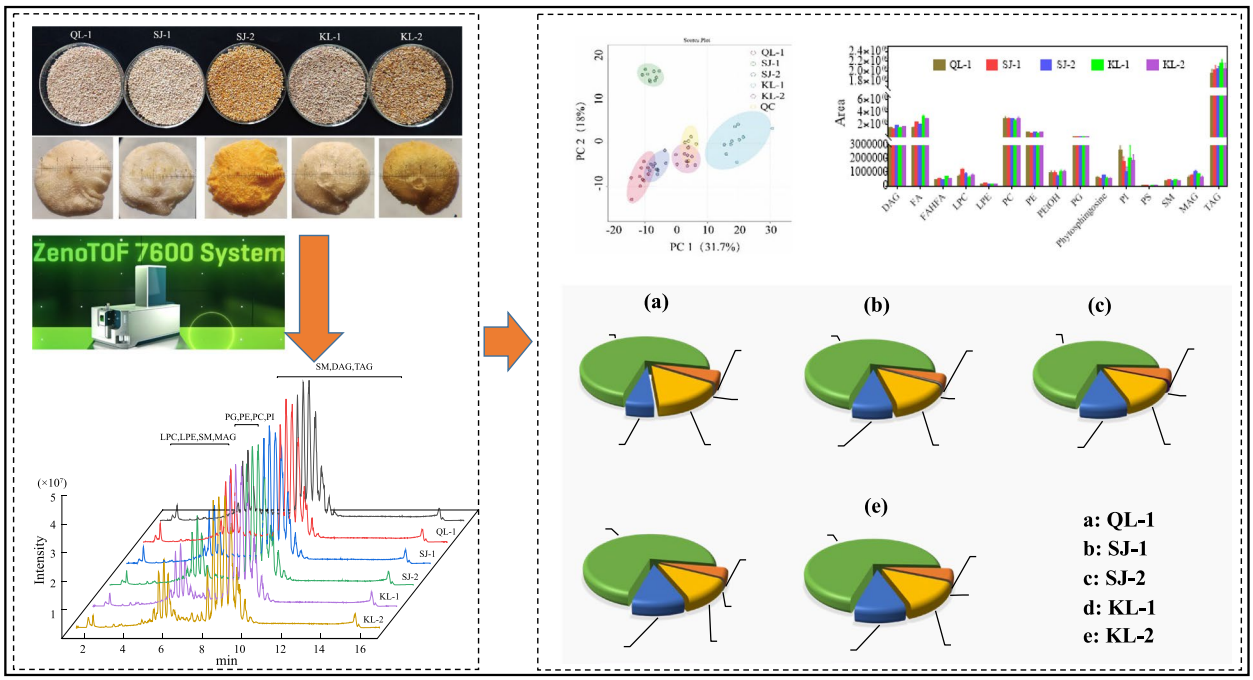
Graphical Abstract



Background

Quinoa (*Chenopodium quinoa* Willd) has gained recognition as functional and nutritious food source owing to its substantial protein content (Tavano et al. 2022), slow digestible starch (Ma et al. 2021), dietary fiber (Zhu 2020) and phytochemicals (Pereira et al. 2020). Quinoa proteins are regarded as superior to those of other cereal proteins on account of their well-balanced composition of essential amino acids and their high lysine content, which is deficient in conventional cereals (Tavano et al. 2022). Consequently, individuals with celiac disease and wheat allergies have been advised to incorporate it into their gluten-free dietary regimen (Jacinto et al. 2020).

Quinoa is extensively cultivated worldwide due to its high stress tolerance. It was first introduced to China in the 1990s and is now widely grown in Tibet. After nearly 30 years of breeding and cultivation technology development, it has been gradually extended to Qinghai, Gansu, Shanxi and other arid regions (Shah et al. 2020). The research on quinoa mainly focused on the analysis of nutritional components (Zapana et al. 2020), anti-nutritional factors such as phytic acid (Demir & Bilgicli 2020) and saponins (Navarro del Hierro et al. 2020), and functional components such as phenolics and flavonoids (Pereira et al. 2020). Meanwhile, some researchers have also focused on the effects of different processing methods such as milling (Sciarini et al. 2020) and heat processing on the nutritional, anti-nutritional and functional components of quinoa (Dong et al. 2021; Yang et al. 2022). In addition, many studies concentrated on the improvement of quinoa nutritional and functional quality by germination in recent years (He et al. 2022; Ma et al. 2021). However, few studies have compared the nutritional quality of different varieties of quinoa. The genotype of plant-based food materials has an impact on their quality (Miranda et al. 2011; Shah et al. 2020). The composition and nature of nutrients vary considerably among distinct varieties. The same variety grown under different environmental circumstances has distinct nutritional properties. The protein content averaged 14.2%, whereas the starch amount ranged from 47.22 to 59.72% (Diaz-Valencia et al. 2018), and the lipid content was between 5.94 and 10.71% (Pachari Vera et al. 2019). Quinoa fat has a high content of linoleic (C18:2) and linolenic (C18:3), which represent 52–63% of lipids (Tang et al. 2016), while oleic acid content is up to 33% (Pereira et al. 2019). The fatty acid profile is of great significance for evaluating the nutritional value of the oil, especially the content of polyunsaturated fatty acids (PUFAs). The recommended intake of PUFAs (European Food Safety Authority, 2010) was established as 2 g alpha-linolenic acid (ALA, ω-3) per day, 250 mg eicosapentaenoic (EPA)

plus docosahexaenoic (DHA) fatty acids (long-chain ω-3) per day and 10 g linoleic acid (LA, ω-6) per day for adult. To better understand and utilize the nutritional potential of quinoa, it's vital to analyze its basic nutrient content and lipomics across various variations.

China is a significant region for cultivating quinoa in Asia. Qinghai province is the main production area of quinoa in China. This study analyzed the basic nutrients composition and lipomics of five quinoa varieties mainly produced in Qinghai, providing theoretical and data support for the development of quinoa processing and the breeding of high-quality quinoa varieties. Moreover, the research results can provide data support for other countries to import quinoa produced in China.

Methodology

Materials and reagents

Five quinoa varieties (Qingli-1, QL-1; Sanjiang-1, SJ-1; Sanjiang-2, SJ-2; Keli-1, KL-1 and Keli-2, KL-2) were purchased from Qinghai province in 2021. The dried seeds were stored at -20 °C for use. The morphology of the seeds is shown in Fig. S1. Five varieties of quinoa were ground and screened through 80 mesh sieve (Mesh size: 180 μm), and 3 portions were prepared for each variety. LC–MS grade absolute methanol (MeOH) and acetonitrile (ACN), isopropyl alcohol (IPA) was purchased from VWR International (Zaventem, Belgium). Ammonium acetate (99%, chromatographic purity) was from Sigma–Aldrich (Shanghai, China). Ultrafree®-MC centrifugal filter devices (Mesh size: 0.22 μm) were obtained from Millipore (Bredford, MA, USA). All other chemicals and reagents used were of analytical grade.

Moisture, protein, and amino acid content assay

The moisture content was calculated from the weight difference before and after drying at 105 °C in a convection oven for 6 h. According to (Joint 1973), the crude protein content was determined using the Kjeldahl method with a conversion factor of 6.25. Protein content was expressed as the percentage of edible portion on a dry weight basis. The coomassie bright blue G-250 staining method was used to determine soluble protein (Lin et al. 2013). The content of amino acids was determined according to the method of Yoon et al. (2017) with minor modifications. Samples (0.03 g) were mixed with a 3 mL of 6 M HCl. After filling with nitrogen, they were hydrolyzed in an oven at 110 °C for 23 h, then cooled and put into a 25 mL volumetric flask for constant volume. The 2 mL sample was taken and dried with nitrogen, and dissolved with 0.02 M HCl. After that, the mixtures were centrifuged (3000 × g, 15 min) and the supernatants were filtered through a syringe filter (0.22 μm). The content of the amino acids was measured by an amino acid analyzer (L − 8800, Hitachi, Japan).

Dietary fiber, phytic acid, minerals and crude fat content assay

Dietary fiber content was determined according to the "Determination of Dietary Fiber in National Food Safety Standards of China (GB 5009.88–2014)". Phytic acid content was determined according to the instructions of a standard kit (SAP-2-Y, Suzhou Comin Biotechnology Co. Lid, Suzhou, China). Minerals content was determined according to "Determination of Minerals in Food in National Food Safety Standards of China (GB 5009.268–2016)". The standard samples were purchased from Agilent Technologies (Shanghai, China). Crude fat content was determined by quantification of ether extracts in acid medium (GB 5009.6–2016).

Lipomics analysis

Sample preparation

Samples were extracted using a modified QuEChERS (Quick, Easy, Cheap, Effective, Rugged, Safe) based approach. 20 mg quinoa flour and 200 μL methanol were put into a 1.5 mL centrifuge tube, vortexed for 30 s, and then 540 μL Methyl tertbutyl ether (MTBE) was added. After vortexing for 3 min, added 360 μL water, vortexed briefly and stand for 10 min, then centrifuge at 4 °C for 10 min (15000 rpm/min). The extract was divided into organic phase and aqueous phase. The upper layer (organic phase) was collected and put on a N-EVAP nitrogen drying instrument for drying at 30 °C. The residue was redissolved with 1 mL mixed solution ofACN/IPA/water (65/30/5, v/v/v) by vortexing for 30 s. After centrifuging at 15,000 r/min, the supernatant was transferred into the sample bottle for analyses.

Instrumental conditions

An ExionLC AD ultra-performance liquid chromatography (UPLC, AB Sciex Analytical Instrument Trading Co., Ltd., Shanghai, China) system was used for samples separation. The analytical column used was Kinetex C18, 100 × 2.1 mm, 2.6 μm (Waters; Zellik, Belgium), with a flow rate of 0.3 mL/min. The 5 μL aliquot sample extract was injected into a chromatographic system. The column temperature was maintained at 50 °C. Mobile phase A was MeOH/ACN/water (1/1/1, v/v/v) containing 5 mmol/L of ammonium acetate. Mobile phase B was IPA containing 5 mmol/L of ammonium acetate. A gradient elution program starting with 20% B was maintained for 0.5 min. From 0.5 to 1.5 min, it linearly increased to 40%. From 1.5 to 3.0 min, it increased to 60%, and from 3 to 13 min, it increased to 98% and maintained for 1.5 min. At the last 2.5 min, it decreased

to 20%. The whole process was lasting for 17 min. The detailed information is shown in Table S1.

The UPLC system was coupled to a ZenoTOF7600 mass spectrometer equipped with an electrospray ionization (ESI) source (AB Sciex, Shanghai, China). The ESI source conditions were set as follows: spray voltage (5.5 kV), curtain gas (N2, 99.999%, 35 psi, Domnik Hunter), temperature (550 °C), ion source gas1 (nebulizer gas, 55 psi), and ion source gas 2 (turbo gas, 55 psi). Data were collected in both positive and negative ionization modes over a mass range between 100 ~ 1250 m/z. The MS/MS experiments were performed using collision energy of 35 eV in negative mode. Mass range was set between 200–1250 m/z for the fragmentation products.

Statistical analysis

GraphPad Prism 7 was used for data elaboration and statistical analysis using a level of significance set at 95%. One-way analysis of variance (ANOVA) was used to assess the difference in nutrient content in different quinoa varieties. Differences were considered statistically significant at $p < 0.05$. Lipomics analysis was carried out using the online tool Metaboanalyst 5.0 (https://www.metaboanalyst.ca/).

Results

Basic chemicals of different varieties of quinoa

The moisture content of the five quinoa varieties was concentrated at about 10%, and the content in SJ-2 was relatively high, reaching 10.07% (Fig. 1A). There was no

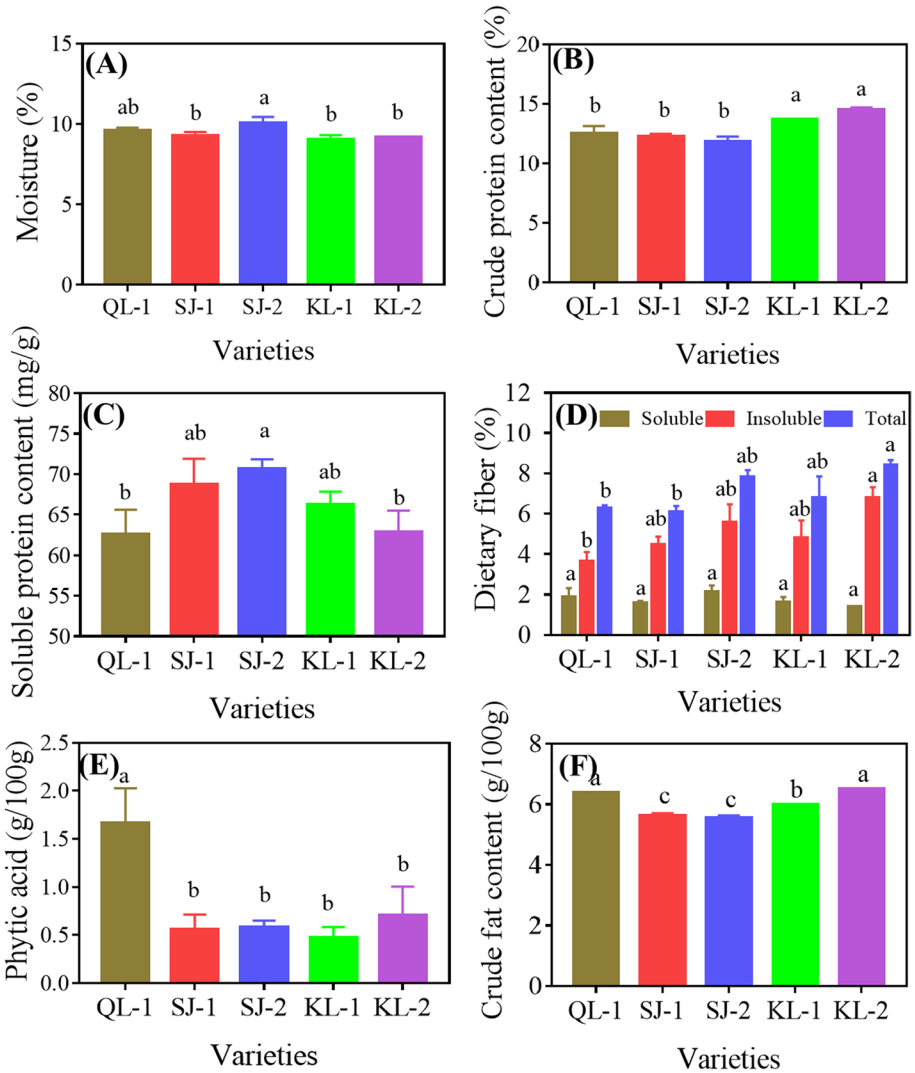


Fig. 1 Moisture (**A**), protein (**B**, **C**), dietary fiber (**D**), phytic acid (**E**) and crude fat (**F**) content of five quinoa varieties. Values are expressed as mean ± SD. Lowercase letters represent significant differences among the five quinoa varieties ($p < 0.05$)

significant difference in the crude protein content among the QL-1, SJ-1 and SJ-2, while the KL-1 and KL-2 were significantly higher than those of other varieties (Fig. 1B). Although the total protein content in SJ-1 and SJ-2 varieties was low, the soluble protein content was relatively high (Fig. 1C). The results of dietary fiber content showed that the total dietary fiber content was 6.0–8.5%, and the insoluble dietary fiber content was 3.6–6.8%. Among the five varieties, there was no significant difference in the content of soluble dietary fiber, except for the KL-2 variety, which had the highest insoluble dietary fiber content, and there was no significant difference in other varieties (Fig. 1D). Phytic acid is one of the anti-nutritional factors in quinoa. Among the five varieties, the content of phytic acid in QL-1 was the highest, reaching 1.66%, which was significantly higher than the other four varieties that had no significant difference (Fig. 1E). Crude fat content of the five varieties of quinoa is about 6%. There was no significant difference in crude fat content between SJ-1 and SJ-2, and no significant difference in crude fat content between QL-1 and KL-2 (Fig. 1F).

In the present study, 17 amino acids were detected, and of which Asp, Glu, Phe, Lys and Arg showed relatively higher content. Their content ranged from 40.72% to 55.67% of the total amino acid content (Table 1). Essential amino acid content accounted for a high proportion of total amino acid content, reaching 35.69–47.03%. Especially, the lysine (Lys) content in other grains was 0.67 g/100 g—1.15 g/100 g. Among five quinoa varieties, total amino acid content was higher in KL-1 and KL-2, and the lowest in QL-1. Asp, Phe, Lys, Arg, and Pro content were higher in QL-1 and SJ-1, while Glu and Tyr content were higher in the other three varieties. Overall, the amino acid composition of five varieties was balanced, but there were differences in each amino acid among these varieties.

From Table 2, it could be seen that K content is higher compared with other minerals, but there was no significant difference among five quinoa varieties. The content of Mg in SJ-1 was the lowest, and there was no significant difference among other varieties. The Na content in SJ-1 and SJ-2 was significantly lower than that in the other three varieties, was about 30–40% of that in the other varieties. The Ca content in KL-1 and KL-2 was significantly higher than that in the other three varieties. The content of Fe was significantly different among five quinoa varieties, and the content of SJ-1 was relatively low. Al content was the highest in QL-1, and its content was 56.6% higher than in SJ-1. The contents of some heavy metals in five quinoa varieties were also measured. Except for Cu, Cr and As, the contents of other heavy metals in the five varieties were significantly different. Ni and Cd were the lowest in SJ-1 and Pb was the lowest in KL-2. Overall, minerals were low in SJ-1.

Table 1 Amino acid content in 5 varieties of quinoa investigated in this study (g/100 g)

Amino acid	Variety				
	QL-1	SJ-1	SJ-2	KL-1	KL-2
Asp	1.01 ± 0.08a	0.84 ± 0.11b	0.51 ± 0.12d	0.71 ± 0.06c	0.45 ± 0.03d
Thr	0.24 ± 0.02d	0.33 ± 0.09c	0.37 ± 0.06b	0.50 ± 0.04a	0.39 ± 0.06b
Ser	0.29 ± 0.10c	0.36 ± 0.04c	0.46 ± 0.03b	0.59 ± 0.01a	0.48 ± 0.04b
Glu	0.47 ± 0.11c	0.55 ± 0.05c	0.93 ± 0.05b	1.31 ± 0.02a	0.96 ± 0.08b
Gly	0.35 ± 0.09c	0.20 ± 0.06d	0.61 ± 0.04b	0.74 ± 0.04a	0.66 ± 0.02a
Ala	0.39 ± 0.05b	0.40 ± 0.03b	0.46 ± 0.03b	0.58 ± 0.05a	0.45 ± 0.05b
Cys	0.20 ± 0.01a	0.12 ± 0.05b	0.25 ± 0.01a	0.22 ± 0.06a	0.23 ± 0.03a
Val	0.32 ± 0.01c	0.32 ± 0.06c	0.39 ± 0.02b	0.54 ± 0.07a	0.46 ± 0.06ab
Met	0.06 ± 0.02b	0.11 ± 0.07a	0.12 ± 0.04a	0.13 ± 0.03a	0.12 ± 0.01a
Ile	0.14 ± 0.03c	0.20 ± 0.05b	0.19 ± 0.05b	0.32 ± 0.06a	0.25 ± 0.04b
Leu	0.27 ± 0.01c	0.60 ± 0.08a	0.45 ± 0.06b	0.63 ± 0.05a	0.45 ± 0.03b
Tyr	0.78 ± 0.06d	1.05 ± 0.13c	1.46 ± 0.18b	1.67 ± 0.07a	1.78 ± 0.05a
Phe	1.32 ± 0.04b	1.63 ± 0.12a	0.84 ± 0.06c	0.93 ± 0.08c	0.98 ± 0.06c
Lys	0.88 ± 0.05b	1.15 ± 0.21a	0.67 ± 0.09c	0.80 ± 0.07b	0.69 ± 0.07c
His	0.18 ± 0.02b	0.36 ± 0.05a	0.31 ± 0.09a	0.41 ± 0.03a	0.39 ± 0.05a
Arg	1.05 ± 0.08a	0.92 ± 0.03b	0.87 ± 0.06b	1.06 ± 0.02a	1.07 ± 0.03a
Pro	1.95 ± 0.11a	2.02 ± 0.02a	0.46 ± 0.05b	0.44 ± 0.05b	0.37 ± 0.06b
Total	8.47	9.42	9.34	11.55	10.18

Values are expressed as mean ± SD. Lowercase letters represent significant differences among the five quinoa varieties for each amino acid ($p < 0.05$)

Table 2 Minerals content in the different varieties of quinoa

Minerals	Variety				
	QL-1	SJ-1	SJ-2	KL-1	KL-2
K (mg/g)	8.76 ± 0.82a	9.84 ± 0.65a	8.47 ± 0.27a	8.45 ± 0.79a	9.13 ± 0.13a
Mg (mg/g)	1.70 ± 0.13a	1.36 ± 0.08b	1.66 ± 0.04a	1.60 ± 0.15ab	1.66 ± 0.05a
Na (μg/g)	100.94 ± 12.19a	37.14 ± 4.49b	23.80 ± 3.92b	107.35 ± 4.27a	122.45 ± 18.64a
Ca (μg/g)	67.39 ± 6.74b	53.82 ± 3.31c	59.70 ± 1.73b	80.52 ± 4.64a	74.52 ± 2.85a
Fe (μg/g)	48.09 ± 0.64ab	37.63 ± 7.87c	42.65 ± 1.17bc	59.02 ± 5.05a	53.74 ± 2.03ab
Al (μg/g)	16.49 ± 1.38a	10.43 ± 1.94b	10.53 ± 1.13b	11.59 ± 1.98b	12.39 ± 1.19ab
Cu (μg/g)	3.97 ± 0.23a	4.04 ± 0.20a	4.44 ± 0.06a	3.75 ± 0.47a	4.12 ± 0.11a
Ni (μg/g)	1.01 ± 0.03ab	0.91 ± 0.03b	1.00 ± 0.02ab	1.01 ± 0.03ab	1.06 ± 0.09a
Cr (μg/g)	1.21 ± 0.02a	1.16 ± 0.03a	1.18 ± 0.04a	1.16 ± 0.02a	1.16 ± 0.01a
Pb (ng/g)	153.88 ± 37.89a	127.65 ± 5.92ab	130.24 ± 14.91ab	132.66 ± 29.79ab	85.63 ± 3.87b
Cd (ng/g)	19.64 ± 1.51ab	12.51 ± 3.54b	17.17 ± 0.92ab	25.74 ± 6.03a	25.00 ± 6.76a
As (ng/g)	22.38 ± 1.33a	17.87 ± 0.77a	14.89 ± 0.15a	17.43 ± 2.92a	20.05 ± 5.67a

Values are expressed as mean ± SD. Different letters represent significant differences among the five quinoa varieties ($p < 0.05$)

Difference of lipid composition in quinoa

Lipid composition analysis

The lipid composition of five quinoa varieties was identified by UPLC-TOF–MS/MS. A quality control (QC) sample was used to verify the repeatability and stability of the established method. The total ion chromatograms of QC and 5 samples for 10 injections were given in the supplementary documents (Fig. S2A and B). Various quinoa lipids were separated under the ESI source in the positive ion mode and negative ion mode. There were significant differences in the lipid content of five varieties of quinoa, which could be accurately distinguished by mass spectrometry (Fig. S2C and Fig. S3A). A total of 383 lipid components were identified by non-targeted lipomics, including 16 types of lipids, glycerides (186), free fatty acids (65) and phospholipids (117) were the dominant components (Fig. S3B). The principal component analysis (PCA) screened 154 differential lipid molecules (Fig. 2A), and glycerides, free fatty acids and phospholipids were the main types of differential lipids (Fig. 2B). Among five quinoa varieties, glyceride accounted for the largest proportion of lipids (Fig. 2C), in which triacylglycerol (TAG) was 71.10–73.82% and diacylglycerol (DAG) was 4.96–5.72%. The second was phospholipid, which was the highest in QL-1 and lowest in KL-1, but accounted for more than 11% of five varieties. Free fatty acids and fatty acid esters were the least abundant in QL-1, while that in SJ-2, KL-1 and KL-2 accounted for more than 10% of total lipids.

Glyceride and fat acids composition

The glyceride composition of five quinoa varieties was similar. TAG content accounted for more than 90% of total glyceride content in each group of samples, which was the most important glyceride. Secondly, DAG accounted for 5–10%. The proportion of MAG was the smallest (Fig. 3A). The total glyceride content of KL-1 was the highest, and there was no significant difference between SJ-2 and KL-2. The content of QL-1 was the lowest (Fig. 3B). The proportion of unsaturated glycerides in quinoa accounted for more than 99%, and there was no significant difference among the varieties (Fig. 3C).

The fatty acids in five quinoa varieties were composed of saturated fatty acids (SFA), monounsaturated fatty acids (MUFA) and polyunsaturated fatty acids (PUFA), among which the content of MUFA was the highest, followed by PUFA, and the content of SFA was the lowest. The unsaturated fatty acids in KL-1 and KL-2 were relatively high compared with other varieties (Fig. 3D). Specifically, MUFA accounted for more than 50% of the five varieties, which accounted for 56.77% of SJ-2. PUFA content was about half of MUFA, and accounted for 28.66% in SJ-1 (Fig. S4). Linoleic acid (18:2, ω-6) and linolenic acid (18:3, ω-3) are the essential fatty acids for the human body. The proportion of linoleic acid and linolenic acid was close to 50% of total free fatty acids, and there was no significant difference among the five quinoa varieties (Fig. 3E). Among unsaturated fatty acids, linoleic acid content was about 40% and linolenic acid accounted for 5–8%, of which QL-1 had the least and KL-1 had the highest content (Fig. S5).

Phospholipid composition

Among five quinoa varieties, nine phospholipids were detected, of which phosphatidylcholine (PC), phosphatidylethanolamine (PE) and phosphatidylglycerol (PG)

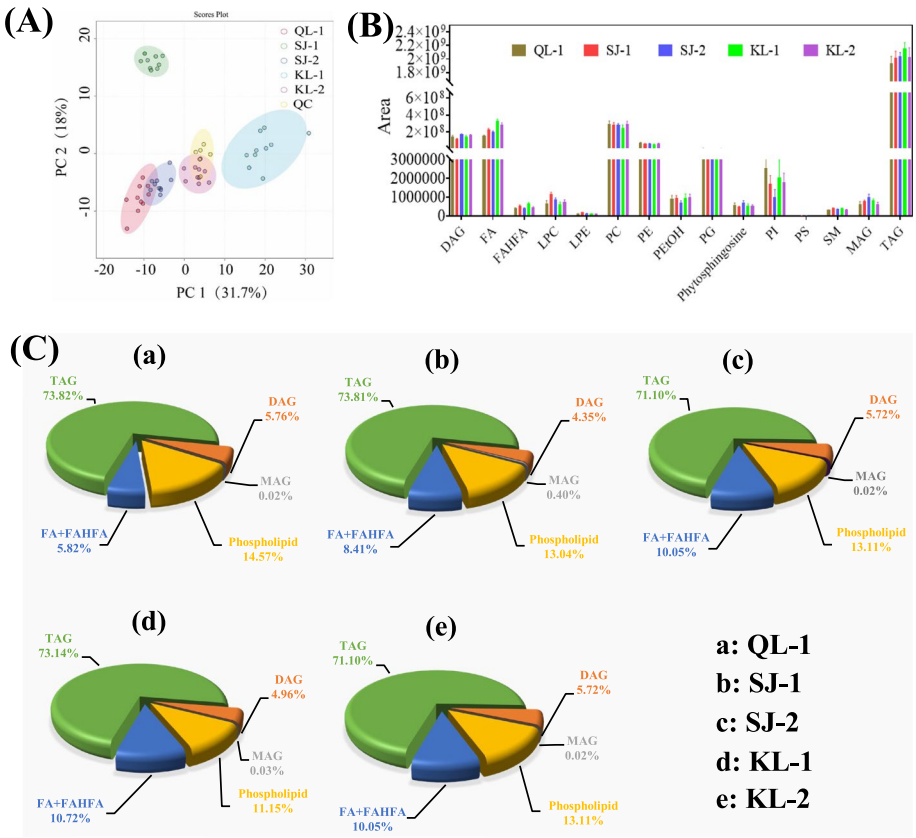


Fig. 2 Lipid identification and composition analysis. 20 μL of each sample was mixed to prepare quality control (QC) samples for quality control at the time of data collection and inserted one QC every 5–10 samples during the data collection process

were the main phospholipids. PC accounted for the highest proportion and phosphatidylserine (PS) accounted for the least (Fig. 4A). KL-1 and SJ-1 had low total phospholipid content and no significant difference, while those in the other three varieties had a significant difference (Fig. 4B). The contents of PC, PE, and PG in QL-1 and KL-2 had no significantly difference, but they were significantly higher than those in KL-1. The content of PC, PE, and PG in KL-1 was significantly lower than that of the other four varieties (Fig. 4C, D, and E). Among five varieties, the PC content was close to 80% of total phospholipids, and the PE proportion was 16.70–18.61%. PG only accounted for about 2.0% of total phospholipids, while other phospholipids were all below 1% (Fig. S6).

Discussions

Protein is an important nutrient component of quinoa, with a content of 10–18% and an average balance of amino acids (Abugoch James 2009; Mufari et al. 2018). This work evaluated five quinoa varieties, with three white (QL-1, SJ-1, and KL-1) and two red (SJ-2 and KL-2) (Fig. S1). The reports demonstrated a correlation between the pigmentation of quinoa and its nutrient content (He et al. 2022). Black quinoa contains more crude protein than red quinoa. This study found that KL-1 and KL-2 of the five quinoa varieties have high crude protein content, indicating a correlation between color and genotype. In this investigation, KL-2 had a high total protein content but a low soluble protein level (Fig. 1C). The amino acid content varied across five varieties, but was generally reasonable (Table 1). This might be related to the protein composition in different varieties of quinoa. Dietary fiber content is an important indicator to reflect the nutritional quality of quinoa, and the total dietary fiber content in quinoa has been reported to range from 7.0% to 9.7% (Abugoch James 2009). In this study, the dietary fiber content in five quinoa varieties were 6.2–8.4% (Fig. 1C). Only insoluble dietary fiber content showed a significant difference among varieties. Phytic acid is one of the recognized anti-nutritional factors. It combines with divalent cation to reduce the absorption and bioavailability of minerals (Wang et al. 2015). Among five quinoa varieties studied in this study, the phytic acid content of QL-1 was more than 2 times higher than that of other varieties (Fig. 1E). In addition, phytic acid can also combine with proteins and other macromolecules to reduce

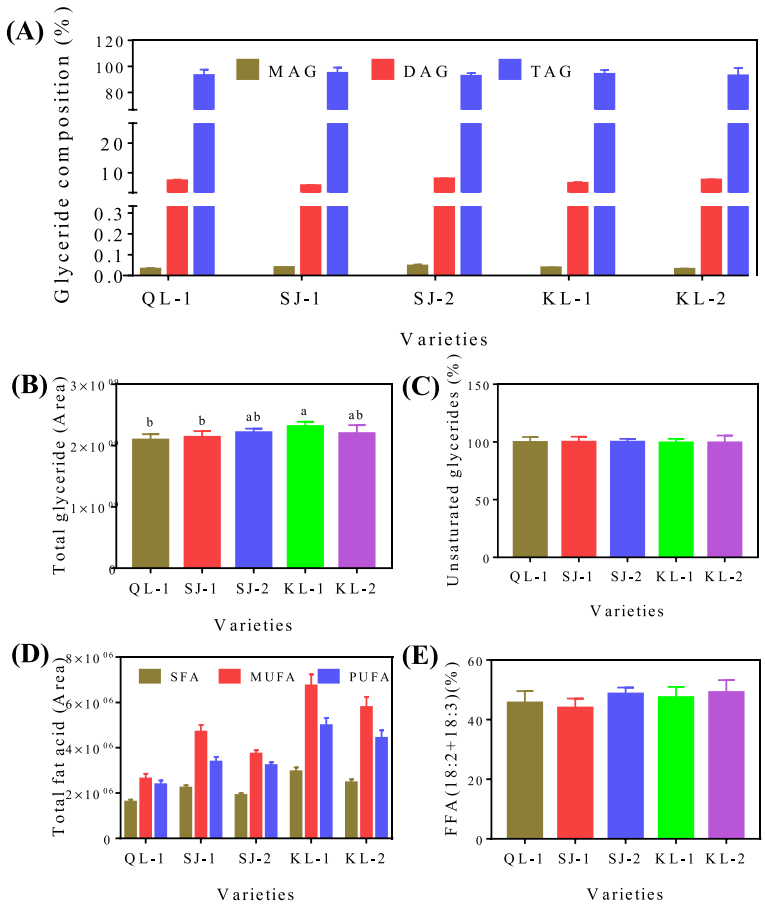


Fig. 3 Glyceride and fat acids composition analysis of five quinoa varieties. Values are expressed as mean ± SD. Lowercase letters represent significant differences among the five quinoa varieties ($p < 0.05$)

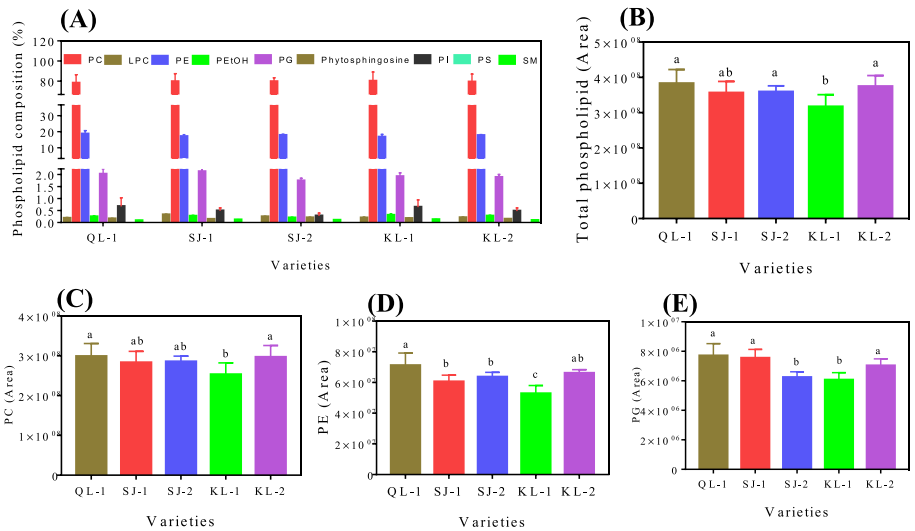


Fig. 4 Phospholipid composition of five quinoa varieties. PC: Phosphatidylcholine; PE: Phosphatidylethanolamine; PG: Phosphatidylglycerol; PI: Phosphatidylinositol; PS: Phosphatidylserine; SM: Sphingomyelin; PEtOH: Phosphatidylethanol. Values are expressed as mean ± SD. Lowercase letters represent significant differences among the five quinoa varieties ($p < 0.05$)

the solubility and digestibility. Therefore, the low content of soluble protein in QL-1 might be related to the chelation by phytic acid. SJ-1 contained relatively low minerals (Table 2), and except for Cr, the content of other heavy metals was lower than the limit specified in the National Standard of the People's Republic of China "Limit of Pollutants in Food" (GB 2762–2017). This standard requires that Cr in cereals should be less than 1.0 mg/kg, but the present study found that Cr content in five quinoa varieties was 16–21% higher than the requirement. However, the safety standards for quinoa raw materials have not been formulated at present.

The researchers reported that crude fat content in quinoa was about 7%, which was significantly higher than other cereals (Abugoch James 2009). It was also reported that crude fat content of quinoa was about 5% (cv. Pasankalla) (Ludena Urquizo et al. 2017). The present study revealed that there was no significant difference in lipid content in colored quinoa (white and red) of different varieties. The differences of various lipids among five quinoa varieties were not particularly significant in the lipomics analysis (Fig. 2B). It is possible that QL-1 and KL-2 contain high content of other fat soluble substances except lipids. And different agronomic, genotypic and climatic factors also played a role in lipid content of seeds in different species, even within the same variety (Chappell et al. 2017; Curti et al. 2018). None of these authors indicated the year in which they made the conclusions, but it could be indicated that seed storage time should be considered even when comparing results of seeds from the same season and variety.

It was found that the lipid compositions of five quinoa varieties were different with each other (Fig. S2C, Fig. S3A), implying more differences in the metabolite composition among the varieties. Therefore, PCA model showed well-separated clusters and could successfully discriminate different samples (Fig. 2A). The content of unsaturated fatty acids in lipids is an important index to evaluate the quality of lipids. In this study, the unsaturated fatty acids of five quinoa varieties accounted for more than 80% of total fatty acids. The unsaturated fatty acids content of KL-1 and KL-2 was higher than that of the other varieties (Fig. 3D), indicating that these two varieties had higher lipids nutritional value. Although there was no significant difference in total linoleic acid and linolenic acid content among five varieties, linoleic acid content of SJ-2 and KL-2 reached 42.2%, which was higher than that of other varieties. It has been reported that lipid content in rice bran from different varieties of rice was significantly different. The content of linoleic acid (18:2) was 31–42%, but the content of linolenic acid (18:3) was less than 2% (Goffman et al. 2003), significantly lower than quinoa (Pellegrini et al. 2018). In addition, phospholipid is an important functional lipid, which has significant antioxidant property and other functions (Pachari Vera et al. 2019). Studies on phospholipid composition analysis have mainly focused on soybean (Lee et al. 2011; Park et al. 2013), mushroom (Yang et al. 2021). There were few reports on cereal phospholipids have been published. Quinoa is recognized as a functional grain. Phospholipids account for 11—15% of total lipids (Fig. 2), in which lecithin accounted for about 80% and cephalin accounted for about 17% of total phospholipids (Fig. S6). The research showed that the proportion of lecithin and cephalin in soybean phospholipids was similar, accounting for about 40% of total phospholipids (Park et al. 2013). However, the proportion of lecithin in quinoa was relatively high. Hence, quinoa is an important source of functional lipids. Compared with the five quinoa varieties, SJ-2, KL-1 and KL-2 have more functional lipids.

Conclusion

Color may be indicative of the higher concentrations of crude protein and insoluble dietary fiber in KL-1 and KL-2 quinoa varieties relative to the other varieties. The phytic acid content of QL-1 was high. SJ-1 contained relatively low minerals. Lipomics analysis showed that the lipid composition of five varieties of quinoa was similar, but triacylglycerol was still the main lipid. Unsaturated fatty acids accounted for more than 80% of total fatty acids, among which linoleic acid and linolenic acid accounted for more than 50%. Phospholipids accounted for 11–15% of total lipids, and PC and PE accounted for about 97% of total phospholipids. Therefore, quinoa is rich in nutrients and functional lipids, and the content and properties depend on the variety.

Supplementary Information

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Supplementary Material 1.

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Authors' contributions

Shufang Wang, Mian Wang, You Zhou and Runqiang Yang were involved in the study conceptualisation and writing of the original manuscript draft. Jianhong Xu, Kang Tu and Jianrong Shi were responsible for funding acquisition for the study. All the authors were involved in developing data collection tools, data collection, reviewing and editing, and approving the final manuscript.

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Availability of data and materials
The datasets used and/or analyzed during the current study are available from the corresponding author upon reasonable request.

Declarations

Ethics approval and consent to participate
Not applicable.

Consent for publication
Not applicable.

Competing interests
Dr. Jianrong Shi is a member of Editorial Board of *Food Production, Processing and Nutrition* and he was not involved in the journal's review of, or decisions related to this manuscript.

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