Identification of Pharmaceutically Important Constituents of Quinoa Root

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ABSTRACT

The present investigation was carried out to explore the bioactive compounds from the *n*-hexane fraction of methanolic extract of quinoa (*Chenopodium quinoa* Willd.) roots. For this purpose, *C. quinoa* roots were collected, shade dried, and crushed into a fine powder. The powdered material was extracted in methanol, filtered, and the filtrate was partitioned with *n*-hexane, followed by GC-MS analysis of the *n*-hexane fraction. The quantitative determination of this fraction revealed the presence of 15 phytochemical constituents of diverse nature. Among these, octadec-9-enoic acid (44.18%); *n*-hexadecanoic acid (18.87%); methyl (Z)-octadec-9-enoate (12.87%); methyl hexadecanoate (4.30%); 2,3-dihydroxypropyl elaidate (3.63%); phthalic acid (3.08%); methyl octadecanoate (2.27%) and 1,12-tridecadiene (2.00%) were prevailing as the most abundant to moderately occurring compounds. A thorough literature survey was carried out to collect information regarding the pharmaceutical properties of the identified compounds. It showed some of the identified compounds namely dodecanoic acid; tetradecanoic acid; 2-benzoyl-d-galactosan; *n*-hexadecanoic acid; methyl octadecanoate; octadec-9-enoic acid; and 2,3-dihydroxypropyl elaidate possess antifungal, antibacterial, antioxidant, antiviral, anti-inflammatory, and/or anti-cancer properties.

Keywords: Bioactive constituents, *Chenopodium quinoa*, n-hexane extract, GC-MS analysis, root.

INTRODUCTION

The plant kingdom represents an extraordinary reservoir of natural bioactive compounds across the globe. These natural products have been exploited to prepare traditional, folk, and modern medical systems.[1,2] Several plant genera have been screened in search of alternatives to reduce the dependency on synthetic substances.[3,4] Many plant species produce organic compounds such as phenolic acid, phenols, flavones, eugenol, epicatechin, carvacrol, quinones, thymol, myricetin, flavonoids, coumarins, tannins, and flavanols.[5,6] Natural plant-based products are gaining importance worldwide because of their non-toxic behavior, fast action, efficiency even at lower concentrations, pleasant odor, and cost-effective properties.[7] In addition, they presumed a preventive role to indicate their diverse beneficial functions against soil-borne fungal pathogens, human pathogens and food-borne diseases.[8-10]

Quinoa (*Chenopodium quinoa* Willd.) is an ancient crop grown widely in South America, Chile, China, Argentina, Bolivia, Ecuador, Colombia, Peru, Canada and France.[11] Recently, it has evoked interest in Asia, especially in Pakistan, because of its richness in protein contents, amino acids, lipids, fibers, minerals (Zn, Cu, Fe, Mg, Ca), and vitamins A and E.[12] It is considered a multipurpose agro-industrial crop consumed in the form of flour, grain, cereals, and cookies.[13] It is cultivated as a potential crop in salt, saline, drought and frost-affected areas.[14] Moreover, it is a disease-resistant, early-maturing plant commonly used as a break crop in a crop rotation system. Quinoa is rich in saponins and other important

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compounds exhibiting various biological activities.[15,16] The present investigation was undertaken to determine the pharmaceutically important compounds from quinoa's n-hexane soluble fraction of methanolic root extract.

MATERIALS AND METHODS

Cultivation of Quinoa

Seeds of Quinoa var. Colorado 407D, with origin from Colorado, USA was sown in autumn 2017 under agro-ecological conditions in Lahore, Pakistan. After the crop matured, the plant roots (2 kg) were carefully collected and washed thoroughly under tap water to remove physical contaminants and then shade dried. After that, the roots were cut into small pieces and completely dried at 40 ºC in an electric oven.

Extract preparation

The dried roots were pulverized into a fine powder by using a mechanical grinder and exhaustively macerated with methanol (6 L) for 15 days at room temperature. The material was then filtered through Whatman No. 1 filter paper. The methanol was evaporated on a rotary evaporator at 45 °C to get a gummy residue (98 g) remaining stirred in 150 mL of distilled water. The resultant mixture was mixed with *n*-hexane (500 mL), thoroughly shaken, put in a separating funnel and left for 2 hours to separate the *n*-hexane layer.[17]

GC-MS analysis

The *n*-hexane fraction was subjected to GC-MS analysis to identify compounds following Khan and Javaid.[18] Analysis was done on a Shimadzu GC-2010plus system coupled with autosampler AOC-20s, an auto-injector AOC-20i, and a gas chromatograph. A capillary column of 0.25 µm × 0.25 mm × 30 m was used in this study. Helium was used as a carrier gas. Turbo mass 5.2 gold Perkin Elmer was used as the mass detector. A 1.0 µl volume of sample was injected by setting the injector at 250 °C. The interface temperature was set at 320 °C. The initial column temperature was 100 °C for 60 s after injection of the sample and enhanced from 100 to 200 °C at 20 °C min^{-1}, and finally from 200 °C to 300 °C at 40 °C min^{-1}. The total run time of the sample was 11 min. Compounds were identified by NIST (National Institute of Standards and Technology) Library.

Literature survey

A thorough survey of the literature was done to search for bioactivities of the various compounds identified through GC-MS. Structures of pharmaceutically important compounds were drawn by using the software ChemDraw.

RESULTS AND DISCUSSION

The GC-MS chromatogram for the quinoa's *n*-hexane soluble fraction of methanolic root extract is given in Figure 1. Results reveal the presence of 15 constituents belonging to diverse groups of natural compounds. Details of the identified compounds with their molecular weight, peak area percentages and retention time are shown in Table 1, whereas the structures of these compounds are given in Figure 2. The most prevailing chemical constituents were octadec-9-enoic acid (**12**); *n*-hexadecanoic acid (**9**); and methyl (Z)-octadec-9-enoate (**10**) with peak areas of 44.18%, 18.87% and 12.87%, respectively. The moderately occurring compounds namely methyl hexadecanoate (**7**); 2,3-dihydroxypropyl elaidate (**14**); phthalic acid (**15**); methyl octadecanoate (**11**) and 1,12-tridecadiene (**8**) were showing 4.30%, 3.63%, 3.08%, 2.27% and 2.00% peak areas, respectively. The compounds present in less concentrations were ar-tumerone, 2-methyl-6-(4-methylphenyl)-2-hepten-4-one (**3**); tetradecanoic acid (**4**); 2-benzoyl-d-galactosan (**6**); pentadecane (**5**); 10,13-eicosadienoic acid, methyl ester (**13**); dodecanoic acid (**1**) and hexadecane (**2**) with peak areas ranging from 1.68 to 0.77%.

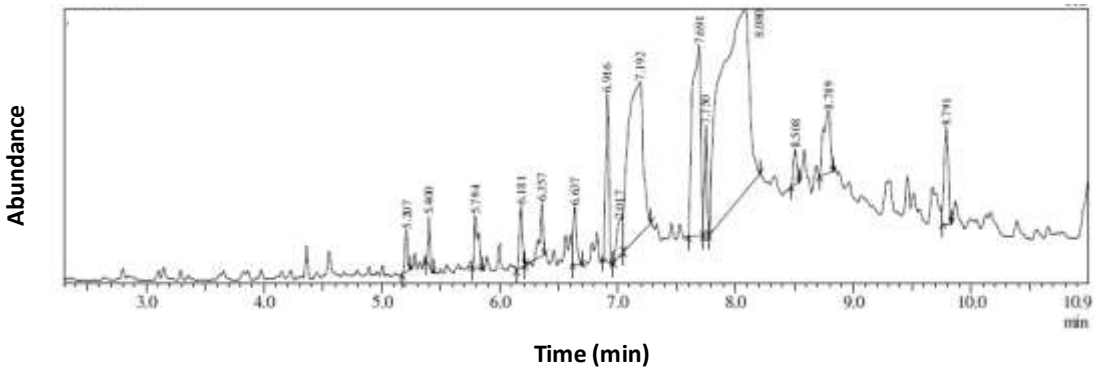

Figure 1: GC-MS chromatogram of *n*-hexane fraction of methanolic extract of *Chenopodium quinoa* roots

Table 1: Compounds identified in *n*-hexane fraction of methanolic extract of quinoa roots through GC-MS analysis.

Sr. No.	Names of compounds	Molecular formula	Molecular weight	Retention time (min)	Peak area (%)
1	Dodecanoic acid	$C_{12}H_{24}O_2$	200	5.207	0.92
2	Hexadecane	$C_{16}H_{34}$	226	5.400	0.77
3	Ar-tumerone, 2-Methyl-6-(4-methylphenyl)-2-hepten-4-One	$C_{15}H_{20}O$	216	5.794	1.68
4	Tetradecanoic acid	$C_{14}H_{28}O_2$	228	6.181	1.53
5	Pentadecane	$C_{15}H_{32}$	212	6.357	1.41
6	2-Benzoyl-d-galactosan	$C_{13}H_{14}O_6$	266	6.637	1.51
7	Methyl hexadecanoate	$C_{17}H_{34}O_2$	270	6.916	4.30
8	1,12-Tridecadiene	$C_{13}H_{24}$	180	7.017	2.00
9	*n*-Hexadecanoic acid	$C_{16}H_{32}O_2$	256	7.192	18.87
10	Methyl (Z)-octadec-9-enoate	$C_{19}H_{36}O_2$	296	7.691	12.87
11	Methyl octadecanoate	$C_{19}H_{38}O_2$	298	7.750	2.27
12	Octadec-9-enoic acid	$C_{18}H_{34}O_2$	282	8.080	44.18
13	10,13-Eicosadienoic acid, methyl ester	$C_{21}H_{38}O_2$	322	8.508	0.98
14	2,3-Dihydroxypropyl elaidate	$C_{21}H_{40}O_4$	356	8.789	3.63
15	Phthalic acid	$C_{24}H_{38}O_4$	390	9.791	3.08

Table 2: Bioactivity of components of *n*-hexaane fraction of methanolic extract of quinoa roots.

Comp. No.	Names of compounds	Bioactivity	Reference
1	Dodecanoic acid	Antibacterial, antiviral, antioxidant	[34,35]
2	Hexadecane	Antidiarrheal, antioxidant antimicrobial	[2]
3	Ar-tumerone, 2-Methyl-6-(4-methylphenyl)-2-hepten-4-one	Pharmaceutical and medicinal properties	[32]

Comp. No.	Names of compounds	Bioactivity	Reference
4	Tetradecanoic acid	Anti-inflammatory, antimicrobial	[31]
5	Pentadecane	Antiulcer, antitussive and antioxidant	[20,33]
6	2-Benzoyl-d-galactosan	Antioxidant	[30]
7	Methyl hexadecanoate	Anti-inflammatory, antioxidant, antibacterial	[22]
8	1,12-Tridecadiene	No activity reported	-
9	*n*-Hexadecanoic acid	Antioxidant, antimicrobial	[21]
10	Methyl (Z)-octadec-9-enoate	Antibacterial, antifungal	[27]
11	Methyl octadecanoate	Antibacterial, antiviral	[26]
12	Octadec-9-enoic acid	Anti-inflammatory, cancer preventive, antioxidant	[19,20]
13	10,13-Eicosadienoic acid, methyl ester	Antioxidant	[31]
14	2,3-Dihydroxypropyl elaidate	Anticancer, antimicrobial, antioxidant	[23]
15	Phthalic acid	Antibacterial and antifungal	[28,29]

The most abundant compound **12** is also known as oleic acid, an unsaturated fatty acid previously isolated from a medicinally important plant Tectaria coadunata leaves that possess strong pharmaceutical, anti-inflammatory, cancer preventive, and antioxidant properties.[19,20] Likewise, compounds **2**, **4**, **7**, **9** and **14** have also been reported to possess strong antioxidant, anti-inflammatory, antibacterial, nematicide, antimicrobial and pesticide properties.[21-25] Similarly, in previous studies, compounds **10** and **11** were found effective against pathogenic bacterial strains, including *Staphylococcus epidermidis, Escherichia coli, Staphylococcus aureus, Proteus mirabilis, Klebsiella pneumoniae, Citrobacter freundi, Salmonella typhi* and *Enterobacter aerogenes*.[26,27] Moreover, compound **15** was identified from a medicinal plant *Hibiscus rosa-sinensis* flower extract. It was tested against gram-positive bacterial strains, namely *Bacillus subtilis* and *Staphylococcus aureus*, and against phytopathogenic fungi *viz. Aspergillus flavus, Drechslera australiensis, Fusarium oxysporum, Alternaria alternata* and *Macrophomina phaseolina*. The compound was very effective in completely inhibiting the tested bacterial and fungal pathogens.[28,29] Similarly, compounds **6** and **13** have been reported from *Homalium zeylanicum* and *Actinidia deliciosa* plant extracts with potent antioxidant activities.[30,31] Likewise, many scientists worked on compounds **1**, **3** and **5** to evaluate their antioxidant, antiviral, antibacterial, pharmaceutical and medicinal efficacy against human diseases, including cancer, ulcer and tussive.[32-35] Therefore, the present study concludes that the *n*-hexane fraction of root extract of *C. quinoa* is enriched with various bioactive substances having antioxidant, antiviral, antifungal, antibacterial, pharmaceutical, pesticidal and anti-inflammatory activities justifying quinoa root as a major source of compounds of pharmaceutical and pesticidal importance.

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تحديد المكونات المهمة صيدلانياً لجذر الكينوا

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ملخص

تم إجراء الدراسة الحالية لاستكشاف المركبات النشطة بيولوجيًا من الجزء hexan-n من المستخلص الميثانولي لجذور الكينوا. (Chenopodium quinoa Willd) لهذا الغرض، تم جمع جذور C. quinoa وتجفيف الظل وسحقها إلى مسحوق ناعم. تم استخلاص مادة المسحوق في ميثانول، وترشيحه، وتم تقسيم المرشح باستخدام hexan-n، متبوعًا بتحليل GC-MS لجزء hexan-n. كشف التحديد الكمي لهذا الجزء عن وجود 15 مكونًا كيميائيًا نباتيًا ذات طبيعة متنوعة. ومن بين هؤلاء octadec-9-enoic acid (44.18٪؛ n-hexadecanoic acid (18.87٪؛ methyl (Z)-octadec-9-enoate (12.87٪؛ methyl hexadecanoate (4.30٪؛ dihydroxypropyl elaidate (3.63–2,3٪؛ phthalic acid (3.08٪؛ methyl octadecanoate (2.27٪؛ و tridecadiene (2.00–1,12٪ (باعتبارها الأكثر وفرة للمركبات المتوسطة التكوّن. تم إجراء مسح شامل للأدبيات لجمع المعلومات المتعلقة بالخصائص الصيدلانية للمركبات المحددة. أظهرت بعض المركبات المحددة وهي n-dodecanoic acid; tetradecanoic acid; 2-benzoyl-d-galactosan; hexadecanoic acid; methyl octadecanoate; octadec-9-enoic acid؛ و dihydroxypropyl elaidate–2،3 يمتلكان خصائص مضادة للفطريات، ومضادة للبكتيريا، ومضادة للأكسدة، ومضادة للفيروسات، ومضادة للالتهابات، و / أو مضادة للسرطان.

الكلمات الدالة: المكونات النشطة بيولوجيًا، تشينوبوديوم كينوا، مستخلص ن–هكسان، تحليل GC-MS، الجذر.

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