Journal of King Saud University – Science 32 (2020) 1884–1888

Contents lists available at ScienceDirect

Journal of King Saud University – Science

journal homepage: www.sciencedirect.com

Original article

Molecular characteristics and function of elliptical Kiwifruit

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ARTICLE INFO

Article history:
Received 22 September 2019
Revised 17 December 2019
Accepted 16 January 2020
Available online 28 January 2020

Keywords:
Elliptical Kiwifruit
FT-IR
GC–MS
Chemical composition
Application

ABSTRACT

Elliptical Kiwifruit (Actinidia chinensis Planch) is a popular fruit among consumers. It has abundant nutrition. And it also has medicinal value and economic value. In our research, we detected and analyzed the chemical components by Fourier transform infrared spectroscopy (FT-IR) and gas chromatography mass spectrometry (GC–MS) technologies. In FT-IR analysis, we known that there it main had O-H stretching vibration, C-H stretching vibration, C=C stretching vibration, benzene ring stretching vibration, C-H C-O stretching vibration and anomeric carbon vibrational frequency absorption peak attribution. The types of compound that may be in this band is cellulose, carboxylic acid, alcohol, phenol, amine and ester. In GC–MS analysis, we known that the main chemical compounds were 5-hydroxymethylfurfural, 1,2,3,5-cyclohexanetetrol, quinic acid, D-alanine, N-propargyloxycarbonyl-, isohexyl ester, 4H-Pyran-4-one, cyclotetrasiloxane, octamethyl- and furfural. And these organic components can be used at food processing, medical treatment and light industry fields.

1. Introduction

Elliptical Kiwifruit (Actinidia chinensis Planch) belongs actinidiaceae, actinidia. Originally, it was a wild fruit produced in Yichang, Hubei Province (Takeoka et al., 1986). At the beginning of the last century, Kiwifruit was taken away from Yichang by New Zealanders and was artificially planted. Until now, many varieties have been developed. Kiwifruit is not only rich in water, soft, fragrant and tasty, but also rich in nutritional value. It has a high vitamin C content and also contains a lot of sugar, amino acids and minerals, for example: calcium, selenium, zinc, potassium, tellurium, fructose, malic acid, citric acid, antioxidants, flavonoids, carotenoids, anthocyanins, folate, and melatonin (Selman, 1983; Liu, 2001).

Kiwi has a very prominent medicinal value. It has the functions of heat-clearing and detoxifying, improving appetite, promoting digestion and anticancerous, etc. (Nødtvedt et al., 2017) reported that it may have some sleep improvement effect. Chan et al. (2007) reported that increase dietary fiber intake can effectively relieve chronic constipation and Kiwifruit had abundant in dietary fiber. Lim (2016) reported that hardy elliptical Kiwifruit contained high amount of ascorbic acid. Kiwifruit has clinical effect in atopic dermatitis and its fruit extracts have anticancer effect (Al-zaqri et al., 2017; Boussaid et al., 2018; Li et al., 2018; Maddi et al., 2018; Qadir et al., 2018; Yang et al., 2018). Hunter (2012) reported that gold Kiwifruit contains vitamins C and vitamins E, folate, carotenoids and polyphenols. These nutrients play an important role in enhancing immune function and alleviating symptoms of infection (Ge et al., 2017a). Kiwifruit can also reduce the duration and severity of upper respiratory infections in elderly patients. Kiwifruit was used as a medicine and it has been a long time in the history of China. Motohashi et al. (2002) reported that in the records of some ancient book, such as 'neijing', 'Jin-shu', 'zhu-bingyuan-hou-lun' and'san yin-fang' and so on, the ancients used kiwifruit as a prescription to treat many diseases that may be cancer, such as skin cancer, breast cancer and the cancer of digestive system.

In our study, we used FT-IR and GC–MS technology to analyze the chemical components and types of compounds for providing

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Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.jksus.2020.01.029
1018-3647/

reference to other scholars and follow-up studies of our research group.

2. Material and methods

2.1. Experimental material

The material used for this study was the entire elliptical Kiwifruit. This elliptical Kiwifruit was produced in Xixia County, Nanyang City, Henan Province. Xixia County is located between longitude 111°48′ E, latitude 33°28′ N. It is rich in fruit resources, it is known as the hometown of kiwi. Kiwi varieties used in this experiment are shown in the following Fig. 1.

Fig. 1. Experimental Materials.

2.2. Experimental methods

The elliptical Kiwifruit of this study used sample should clean by deionized water. Then crushed entire fruit flesh together with pericarp. Divided pulp into two parts, respectively added methanol and ethanol as solvents to perform extraction experiments (Ge et al., 2017b). In order to acquire more accurate experimental data, we put the leaching liquor into rotator evaporator to evaporate the water and redundant solvents. Finally, send the sample to do FT-IR and GC–MS detections.

2.2.1. FT-IR analysis

The study uses infrared spectroscopy to analyze the structure and chemical bonds of molecules, and can identify the type of compound by the characteristic wave number of the chemical bond (Ge et al., 2017c). In this study, we used the polished KBr slice as the salt slice of infrared spectrometer. The recorded range of FT-IR spectra was all in 4000 cm^{-1}-400 cm^{-1} (Sherazi, 2009; Li, 2015) (see Fig. 2).

2.2.2. GC–MS analysis

Gas chromatograph has an effective separation ability for organic compounds. Under the control of the computer, it let compounds into the mass spectrometer ion source one by one, and satisfy the requirements of mass spectrometry for sample unity (Dauner and Sauer, 2000). In our study, the GC–MS analysis used 7890B-5977A (Agilent). Chromatographic column was HP-5MS (30 m × 250 μm × 0.25 μm). Capillary column of this experiment was elastic quartz. Carrier gas was high purity He, the flow rate was 1 mL/min and using shunting mode, the split ratio was 20:1. The temperature of GC program started at 50 , Firstly rose to 250 at 8 /min, secondly rose to 300 at 5 /min (Peng et al., 2017). The temperature of ion source and quadrupole respectively were 230 and 150 . Ionization voltage was 70 eV, ionization current (EI) was 150μA. MS program scanning quality range was 30–600 amu (Proestos et al., 2006; Ma et al., 2007; Wang et al., 2009a).

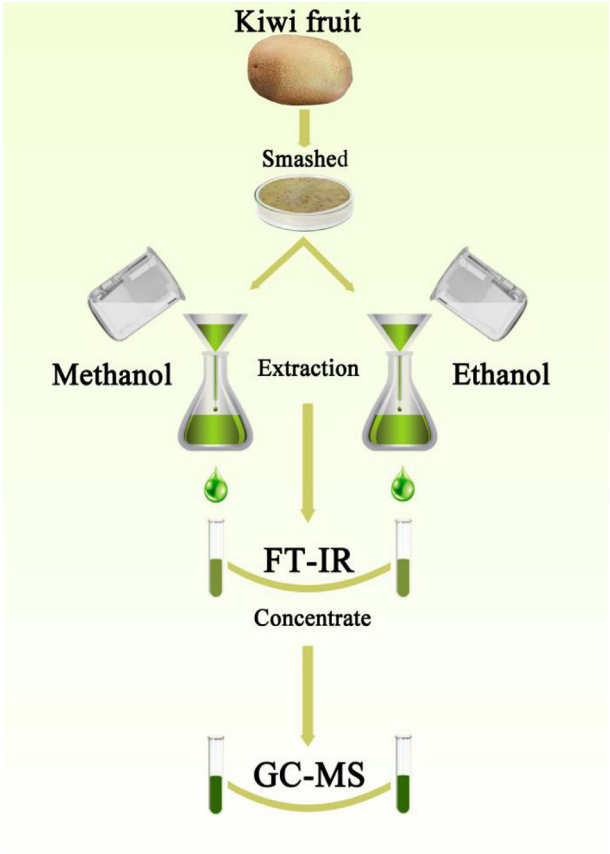

Fig. 2. The diagram of experimental process.

3. Results and discussion

3.1. Analysis of FT-IR

Based on the data obtained from FT-IR analysis, we can make a chart as Fig. 3, and referenced to existing books and other scholars' research results, we made Table 1. According Fig. 4 we can find that as a whole, the absorption peaks of leaching liquor extracted by methanol (M) was stronger than the absorption peaks of leaching liquor extracted by ethanol (E). The phenomenon was because it extracted more chemical components by methanol solvent. According Table 1 and Fig. 3, we can know that in the range of 3650 cm^{-1} to 3200 cm^{-1} wave number, shown a wide and strong absorption peak of O-H stretching vibration. The types of compound that may be in this band was carboxylic acid, alcohol, phenol. In the range of 2975 cm^{-1} to 2840 cm^{-1} wave number, shown several absorption peak of C-H stretching vibration. At 1648 cm^{-1}, the absorption peak was C=C Stretching vibration. At 1450 cm^{-1}, the absorption peak was benzene ring stretching vibration. At 1420 cm^{-1}, 1412 cm^{-1} and 1329 cm^{-1}, the absorption peak was C-N stretching vibration. At 1383 cm^{-1}, the absorption peak was C-H flexural vibration. In the range of 1110–1018 cm^{-1} wave number, shown several absorption peak of C-O stretching vibration. At 881 cm^{-1}, the absorption peak was benzene ring stretching vibration. Some scholars reported that the characteristic absorption peak of cellulose was 2900 cm^{-1}, 1425 cm^{-1}, 1370 cm^{-1} and

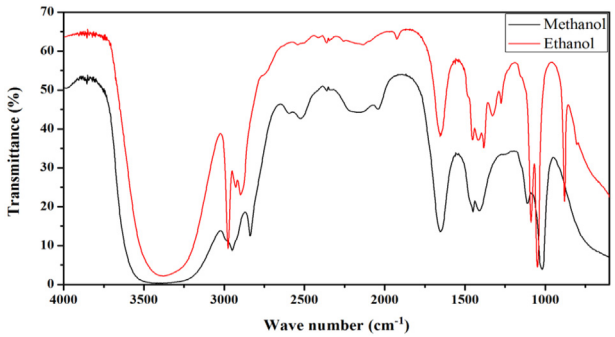

Fig. 3. FT-IR curves of methanol extractives and ethanol extractives.

Table 1
Analytical result of FT-IR of elliptical Kiwifruit leaching liquor.

Absorption peak (cm^{-1})		Absorption peak attribution	Chemical composition
Methanol	Ethanol		
3375	3375	O-H Stretching vibration	Carboxylic acid, alcohol, phenol
2950, 2840	2975, 2930	C-H Stretching vibration	Cellulose
1648	1648	C=C Stretching vibration	Alkene
1450	1450	Benzene ring stretching vibration	Aromatic hydrocarbon
1412	1420	C-N Stretching vibration	Cellulose, amine
	1383	C-H Flexural vibration	Cellulose
	1329	C-N Stretching vibration	Amine
1110, 1018	1088, 1049	C-O Stretching vibration	Acid, phenol, carboxylic acid, ester
	881	Anomeric carbon vibrational frequency	Cellulose

895 cm^{-1}. In our study, we can find absorption peak at 2930 cm^{-1}, 1420 cm^{-1}, 1383 cm^{-1} and 881 cm^{-1} in E. We can consider that these were characteristic absorption peak of cellulose and this kind of elliptical Kiwifruit has abundant cellulose (Schwanninger et al., 2004; Szymańska-Chargot et al., 2011) (see Table 2).

3.2. Analysis of GC–MS

The result was shown that in GC–MS analysis, the leaching liquor of methanol solvent was detected 25 peaks and indentified 18 types chemical components. The main chemical compositions were 5-hydroxymethylfurfural (37.58%; PubChem CID: 237332), 1,2,3,5-cyclohexanetetrol (12.60%; PubChem CID: 548226), quinic acid (12.29%; PubChem CID: 6508), D-alanine, N-propargyloxycarbonyl-, isohexyl ester (6.59%), 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- (6.52%), cyclotetrasiloxane, octamethyl- (6.40%; PubChem CID:121111), furfural (4.07%; PubChem CID: 7362), *cis*-aconitic anhydride (1.81%; PubChem CID: 65163), cyclobutanecarboxylic acid, nonyl ester (1.76%; PubChem CID: 568107) and ethyl propionylacetate (1.42%; PubChem CID: 78656) and so on (see Table 3).

The result was shown that the leaching liquor of ethanol solvent was detected 29 peaks and indentified 21 types chemical components. The main chemical compositions were 5-hydroxymethylfurfural (42.26%; PubChem CID: 237332), quinic acid (26.17%; PubChem CID: 6508), cyclotetrasiloxane, octamethyl- (7.50%; PubChem CID:121111), 4H-pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- (6.21%), pyrazole-4-carboxaldehyde, 1-methyl- (4.73%), 3-methoxycarbonylpyrazole (2.99%; PubChem CID: 565662), 2,5-furandione, 3-methyl- (1.75%; PubChem CID: 12012), 1,3-dioxepane, 2-pentadecyl- (1.36%) and 3,5-dimethylpyrazole (1.10%; PubChem CID: 6210).

These organic components can be used at food processing, medical treatment and light industry fields. For example: 5-

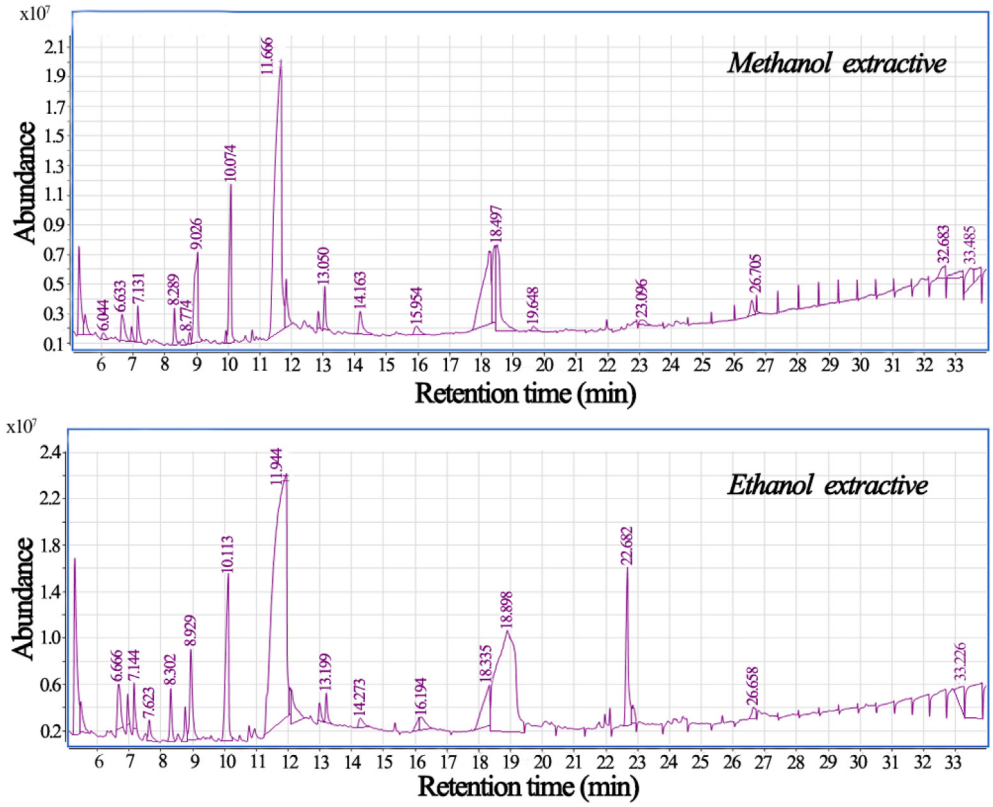

Fig. 4. The total ion chromatogram of methanol and ethanol extractives by GC–MS.

Table 2
The analysis results of methanol extractives.

No.	RT (min)	Peak area (%)	Compound	PubChem CID	Molecular formula
1	5.27	4.07	Furfural	7362	$C_5H_4O_2$
2	5.46	1.06	Levoglucosenone	699486	$C_6H_6O_3$
3	6.63	1.81	*cis*-Aconitic anhydride	65163	$C_6H_4O_5$
4	7.13	1.24	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one		$C_6H_8O_4$
5	8.29	1.21	1,3-Dioxane-5-methanol, 4,5-dimethyl-		$C_7H_{14}O_3$
6	9.03	6.59	D-alanine, N-propargyloxycarbonyl-, isohexyl ester		$C_{13}H_{21}NO_4$
7	10.07	6.52	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-		$C_6H_8O_4$
8	11.67	34.93	5-Hydroxymethylfurfural	237332	$C_6H_6O_3$
	11.83	2.13			
	12.84	0.52			
9	13.05	1.42	Ethyl propionylacetate	78656	$C_7H_{12}O_3$
10	14.16	1.76	Cyclobutanecarboxylic acid, nonyl ester	568107	$C_{14}H_{26}O_2$
11	15.95	0.91	Lactose		$C_{12}H_{22}O_{11}$
12	18.26	12.29	Quinic acid	6508	$C_7H_{12}O_6$
13	18.42	4.68	1,2,3,5-Cyclohexanetetrol	548226	$C_6H_{12}O_4$
	18.50	7.92			
13	32.68	1.16	Cyclotetrasiloxane, octamethyl-	121111	$C_8H_{24}O_4Si_4$
	33.24	1.26			
	33.49	2.68			
	33.80	1.30			

Table 3
The analysis results of ethanol extractives.

No.	RT (min)	Peak area (%)	Compound	PubChem CID	Molecular formula
1	5.47	1.10	3,5-Dimethylpyrazole	6210	$C_5H_8N_2$
2	6.67	1.75	2,5-Furandione, 3-methyl-	12012	C5H4O3
3	8.30	1.36	1,3-Dioxepane, 2-pentadecyl-		$C_{20}H_{40}O_2$
4	8.93	2.99	3-Methoxycarbonylpyrazole	565662	$C_5H_6N_2O_2$
5	10.11	6.21	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-		$C_6H_8O_4$
6	11.94	38.82	5-Hydroxymethylfurfural	237332	$C_6H_6O_3$
	12.06	0.48			
	12.11	1.74			
	12.98	0.51			
	13.20	0.71			
7	18.34	3.45	Quinic acid	6508	$C_7H_{12}O_6$
	18.90	22.72			
8	22.68	4.73	Pyrazole-4-carboxaldehyde, 1-methyl-		$C_5H_6N_2O$
9	33.23	1.63	Cyclotetrasiloxane, octamethyl-	121111	$C_8H_{24}O_4Si_4$
	33.84	5.87			

hydroxymethylfurfural has rich chemical property, and it can potential be acquired from carbohydrates, like inulin, cellulose, sucrose, fructose and glucose. It's a kind of important chemical intermediate (Rosatella et al., 2011). For a long time, quinic acid has been used as antioxidant, and might have anticarcinogenic properties (Wang et al., 2009b). Cyclotetrasiloxane, octamethyl-(octamethylcyclotetrasiloxane) has been used in industrial applications, personal care consumer products and other industries for more than 40 years. It has thermal stability, chemical stability, UV radiation resistance and low surface tension (Zareba et al., 2002). Furfural is a raw material for preparing many medicine and industrial products. The chemical properties of furfural are active, numerous derivatives can be prepared by condensation reaction and oxidation reaction. And it is widely used in the synthesis of organic products such as resins, pharmaceuticals, varnishes, rubbers, coatings and pesticides. Its derivatives also are potential bio-fuel components worthy attention (Lange et al., 2012). Ethyl propionylacetate can be used in the essences and spices industry with a mild fruity fragrance. It is also used as a solvent for paints, varnishes, nitro spray paints and various resins.

According this study, we learned from books, literature, and experiments that Kiwifruit has rich nutritional, medicinal, and industrial value. In the report of FT-IR, we known that there were O-H stretching vibration, C-H stretching vibration, C=C stretching vibration, benzene ring stretching vibration, C-N stretching vibration, C-H flexural vibration, C-O stretching vibration and anomeric carbon vibrational frequency in our sample. The types of compound that may be in this band is cellulose, carboxylic acid, alcohol, phenol, amine and ester. In the report of GC–MS, we known that 25 peaks and indentified 18 types chemical components were detected in M and 29 peaks and indentified 21 types chemical components were detected in E. The main chemical compounds were 5-hydroxymethylfurfural (PubChem CID: 237332), 1,2,3,5-cyclohexanetetrol (PubChem CID: 548226), quinic acid (PubChem CID: 6508), D-alanine, N-propargyloxycarbonyl-, isohexyl ester, 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-, cyclotetrasiloxane, octamethyl- (PubChem CID:121111) and furfural (PubChem CID: 7362). And these organic components can be used at food processing, medical treatment and light industry fields.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This work was financially supported by the National Natural Science Foundation of China (31872697). The Hunan Science Fund for Distinguished Young Scholars (16JJ1028).

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