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Changes in phenolic content, antioxidant activity and volatile compounds during processing of fermented sorghum grain tea

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Abstract:

Background and objective: Sorghum is an important cereal crop with abundant content of polyphenols and may be used to develop nutraceutical sorghum grain tea. This study investigated the changes of phenolic content, antioxidant capacity and volatile compounds in sorghum grain during the production of fermented sorghum grain tea using *Lactobacillus plantarum* subsp. *Argentoratensis* (LAB) and *Saccharomyces cerevisiae*.

Findings: Significant ($P < 0.05$) changes in total phenolic content (TPC), total flavonoids content (TFC) and condensed tannins content (CTC) were observed during the soaking, fermentation, steaming and roasting process. TPC, TFC and CTC were significantly decreased after soaking, steaming and fermentation stages, whereas roasting led to a significant increase. A total of 53 volatile compounds were recorded from raw and processed sorghum. Pyrazines, phenols and esters were the most abundant volatile compounds. Alcohols, carboxylic acids, ketones and alkanes decreased during processing. Esters increased during soaking, steaming and fermentation but decreased during roasting.

Conclusions: Processing affected the phenolic content significantly ($P < 0.05$) and changed the volatile profiles of sorghum grain. Fermented sorghum grain tea by *Saccharomyces cerevisiae* showed a higher possibility of being developed as sorghum grain tea.

Significance and novelty: The study developed a practical method to process novel sorghum grain tea products.

Keywords: Antioxidant capacity; Fermented sorghum tea; Phenolic compounds; Volatile compounds

1. Introduction

Sorghum (*Sorghum bicolor* (L.) Moench), the fifth primary cereal crop in the world, has been attracting much attention because of its high content of phytochemicals (Ragaei et al. 2006). Sorghum grains contains high portion of bioactive phytochemicals such as phenolic acids, procyanidins, 3-deoxyanthocyanidins and condensed tannins (Vanamala., 2017; Xiong et al.,

2019a). Epidemiological studies have consistently shown that the consumption of sorghum products is associated with reduced risk of chronic diseases, including type II diabetes, cardiovascular diseases and cancer owing to the phenolic profile (Awika and Rooney, 2004). Recently, a large variety of cereal grain tea emerged in the market due to their unique flavor and function, such as Tartary buckwheat tea, barley tea and wheat bran tea (Guo et al., 2011; Wang et al., 2019). Therefore, sorghum grain may be used to produce a novel nutraceutical tea beverage.

Processing is a prerequisite to produce grain-based food. Different processing methods (soaking, fermentation and thermal processing) may significantly affect physical characteristics and chemical compositions of grains (Wu et al., 2013). For example, microorganisms have the ability to assimilate condensed tannins by producing tannase which catalyzes the biodegradation of large tannin molecules during fermentation (Chávez-González et al., 2011). Additionally, aroma and flavor are important quality indicators of the fermented sorghum tea, which are primarily affected by the composition of volatile substances. Xiong et al. (2019b) identified a total of 63 aromatic compounds, mainly alcohols, aldehydes and esters in processed sorghum grain tea, which were highly influenced by the processing methods.

However, limited information is available on the effects of processing methods on the phytochemicals and volatile compounds in fermented sorghum. The present study used *Lactobacillus plantarum* subsp. *argentoratensis* and *Saccharomyces cerevisiae* to ferment sorghum grain and examined the effect of fermentation together with other processing methods (soaking, steaming and roasting) on the phenolic content, antioxidant and volatile compounds of the fermented sorghum tea. This study may have provided a practical method to produce fermented sorghum tea as a novel value-added grain beverage product.

2. Materials and methods

2.1 Materials and chemicals

Sorghum sample (MR-Buster) was obtained from Pacific Seeds, Toowoomba, QLD, Australia. It is a red color, medium maturity hybrid sorghum cultivar well established in Australia. Methanol, Folin & Ciocalteu's phenol reagent, sodium carbonate, sodium nitrite, aluminum chloride, sodium hydroxide, vanillin, hydrochloric acid, 2,2'-Azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) diammonium salt (ABTS), potassium persulfate, 2,2-Diphenyl-1-picrylhydrazyl (DPPH), (±)-6-Hydroxy-2,5,7,8-tetramethylchromane-2-carboxylic acid (Trolox), gallic acid, (+)-catechin hydrate, n-alkanes (C8–C22), 4-octanol, de Man, Rogosa and Sharpe (MRS) broth and yeast extract peptone- dextrose (YEPD) broth were all purchased from Sigma-Aldrich (Castle Hill, NSW, Australia). All chemicals were of analytical or HPLC grade.

2.2 Microorganisms and Media

Lactobacillus plantarum subsp. *argenteratensis* (DSM-16365) was obtained from German Collection of Microorganisms and Cell Cultures (DSMZ, Braunschweig, Germany) and cultivated in MRS broth at 30 °C under anaerobic conditions without shaking. *Saccharomyces cerevisiae* was collected from the Microbiology Laboratory of Faculty of Agricultural and Veterinary Sciences, University of Melbourne, Australia and cultured aerobically at 25 °C in YEPD broth.

2.3 Preparation of starter cultures

Activation of LAB or yeast was conducted by mixing 1.0 g of freeze-dried strain pellet with 0.5 mL of MRS broth. The pellet was allowed to rehydrate for up to 30 min and aseptically transferred to a 10 mL centrifuge tube containing 9 mL MRS broth. Then the liquid culture

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was incubated at 30 °C anaerobically to obtain inoculums with a cell concentration of approximate 10⁷ CFU/mL, which was determined by standard curves between optical densities (OD) and CFU/mL. The total counts for both lactic acid bacteria and yeast were performed using a spread plate technic following the methods of Bhatia et al. (1989). The correlation between CFU/ml and optical densities (OD) was also established by measuring the OD of various serially diluted solution using M501 Single Beam Scanning UV-Vis spectrophotometer (Camspec, Leeds, UK) at 600 nm (Emamifar 2011).

2.4 Processing of fermented sorghum tea

The fermented sorghum tea was prepared through four main processing procedures including: soaking, fermenting, steaming and roasting (**Fig. 1**). About 50 g of materials were collected from each processing step, packed separately in plastic bags and stored at -20°C for further analyses. The processing was performed in triplicates.

2.4.1 Soaking

Raw red sorghum (350 g) was soaked in reverse osmosis (RO) water (1:4 w/v) for 24 h at room temperature (25 °C). Then the soaked grains were drained through paper towels and dried to constant weight at room temperature (25 °C). About 50 g dried grains were stored at -20 °C for analyses and the rest were subjected to further processing steps (Xiong et al., 2019b).

2.4.2 Fermenting

The remaining soaked sorghum (300 g) was divided into two equal amounts. Each portion (150 g) was weighted into 500 mL Erlenmeyer flask, mixed with 150 mL sterilized water (1:1 w/v), and then autoclaved at 121 °C for 20 min. After cooling to room temperature (25 °C),

the two samples were inoculated with 30 mL *Lactobacillus plantarum* subsp. *argentoratensis* and *Saccharomyces cerevisiae* active cultures, respectively. These inoculated samples were incubated anaerobically for 5 days at optimal temperature (*Lactobacillus plantarum* at 30 °C; *Saccharomyces cerevisiae* at 25 °C). The fermented grains were drained, dried and stored as described (section 2.4.1). The remaining fermented samples were subjected to steaming.

2.4.3 Steaming

Each type of fermented sample (100g) was steamed at 100 °C for 55 min (steam mode, fan level 1) using the Convotherm 4 easyDial 10.10 multifunctional oven (Convotherm Elektrogeräte GmbH, Eglfing, Germany). The sample was cooled to room temperature (25 °C) and drained on paper towel. A proportion of the steamed grain (50 g) was stored at -20 °C for analyses, and the remaining was subjected to roasting.

2.4.4 Roasting

Roasting was performed at 150 °C for 60 min in a Convotherm 4 easyDial 10.10 multifunctional oven (Wolfratshausen, Germany) to produce the final fermented sorghum grain tea. After cooled to room temperature (25 °C), the samples were vacuum packed in high density polyethylene bags and stored in a fridge at -20 °C for further analysis. This product is ready for consumption by infusing into hot water, just like traditional leaf tea.

2.5 Total polyphenol and antioxidant capacity assay

2.5.1 Extraction of phenolic compounds

Phenolic compounds in various treated sorghum grains were extracted following the method of Wu et al. (2013). Briefly, 5 g of sorghum sample was ground into power in liquid nitrogen using a FCML2012 coffee grinder (Home & Co., Mulgrave, Australia), and all ground

samples were sieved through a 500 μm sieve. About 1 g of sieved sorghum powder was extracted with 45 mL 80% (v/v) aqueous methanol for 2 h in 50 °C water bath and then centrifuged at 5,400 rpm at 4 °C for 10 mins. The supernatant was moved into a new container and the residue was extracted and centrifuged again following the same procedures. The supernatant of two extract were combined and evaporated to dryness at 60 °C using a Hei-vap rotary evaporator (Heidolph, Schwabach, Germany). Solids were reconstituted in 10 mL methanol and stored at -20 °C in the dark until analysis. All extraction and following measurements were repeated in triplicates.

2.5.2 Determination of total phenolic content (TPC)

The TPC of each extract was determined using a modified Folin–Ciocalteu method (de la Rosa et al., 2011). The absorbance was determined at 760 nm using the M501 Single Beam Scanning UV-Vis spectrophotometer. Gallic acid was used as a standard and the results were expressed as mg gallic acid equivalents (GAE)/g dried sample basis (db).

2.5.3 Determination of total flavonoid content (TFC)

The TFC was determined following an established method (de la Rosa et al. 2011). Briefly, the extracts (0.2 mL) were mixed with 0.8 mL of water and 0.06 mL of 5% NaNO_2 solution (w/v). After 5 mins of reaction, 0.06 mL 10 AlCl_3 solution (w/v) was added to the mixture and incubated for another 3 min. 0.5 mL of 0.5 M NaOH was then added and the mixture was incubated in the dark for 30 min at room temperature. The absorbance was read immediately at 510 nm. Catechin was used as standard and the results were expressed as mg catechin equivalents (CE)/g db.

2.5.4 Determination of condensed tannins content (CTC)

The CTC was determined by the vanillin assay (Price, Van Scoyoc and Butler, 1978). The absorbance was measured at 500 nm. Catechin was used as standard and the results were expressed as mg catechin equivalents (CE)/g db.

2.5.5 Determination of ABTS radical scavenging activity

ABTS assay was performed following the protocol of Thaipong et al. (2006). The stock solution was prepared by mixing the 7mM ABTS⁺ and 2.6 mM potassium persulfate in equal amounts and allowed to react in the dark for 12 h at room temperature. The stock solution of 1 mL was diluted with 50 mL of methanol to obtain an absorbance of 1.1 ± 0.02 units at 734 nm. Each sample extract (1 mL) was diluted with 10 ml of 80% methanol, and 0.2 mL of the diluted extracts were mixed with 1 mL of fresh ABTS⁺ working solution. After incubation at room temperature for 2 h in dark, the absorbance was measured at 734 nm. Trolox was used as standard and the results were expressed as mg Trolox equivalents (TE)/g db.

2.5.6 Determination of DPPH radical scavenging activity

DPPH assay was performed following the method of Thaipong et al. (2006). Briefly, 24 mg of DPPH was dissolved in 100 ml of 80% methanol to prepare the stocking solution, then stored at -20 °C in the dark until analysis. The working solution was prepared by diluting 10 mL of the stock solution with 45 mL of 80% methanol to obtain an absorbance of 1.1 ± 0.02 units at 515 nm. Then 0.2 mL of sample extract was mixed with 3.8 mL of DPPH working solution and allowed to react at room temperature for 8 h at dark. The final absorbance was determined at 515 nm. Trolox was used as standard and the results were expressed as mg Trolox equivalents (TE)/g db.

2.6 Headspace solid phase microextraction and gas chromatography mass spectrometry (HS-SPME-GC-MS) for volatile compounds analyses

The extraction of volatile compounds was modified from our previous experimental conditions (Xiong et al. 2019b). Each sorghum sample (5 g) was ground into powder in liquid nitrogen using a FCML2012 coffee grinder (Home & Co., Mulgrave, Australia). Sorghum powder (2 g) were transferred into a 20 mL vial with 20 μ L of internal standard (4-octanol, 0.01 g/100 mL) and sealed with a magnetic PTFE silicon cap. Vial was equilibrated at room temperature for 20 min. A 65 μ m PDMS/DVB SPME fibre (Agilent, Palo Alto, USA) was then exposed to the headspace for 35 min at 80 $^{\circ}$ C for adsorption. The fibre was then desorbed in the GC injector at 250 $^{\circ}$ C for 30 min in splitless mode.

The analysis of volatile compounds was performed using a 6850 series II gas chromatograph connected to a 5973 mass selective detector and coupled with a PAL 3 multi-purpose automated sampler (Agilent Technologies, Palo Alto, USA). Volatiles were separated on a J&W DB-5MS capillary column (30 m x 250 μ m x 0.25 μ m, Agilent Technologies, Palo Alto, USA). Helium (99.999%) was used as the carrier gas under a constant flow rate at 1 mL/min. The oven temperature was programmed as follows: an initial temperature of 50 $^{\circ}$ C for 5 mins, 3 $^{\circ}$ C/min to 125 $^{\circ}$ C and held for 3 mins, 2 $^{\circ}$ C/min to 180 $^{\circ}$ C with 3 mins holding, 15 $^{\circ}$ C/min to 230 $^{\circ}$ C without holding, 20 $^{\circ}$ C/min to a final temperature of 280 $^{\circ}$ C with 5 mins holding. The MS interface temperature, ion source and quadrupole temperature were set at 280 $^{\circ}$ C, 230 $^{\circ}$ C and 150 $^{\circ}$ C, respectively. MS was operated in scan mode from m/z 35 to 400. Blank and internal standard were analyzed using the same sample program and performed at the beginning and end of each sample analysis.

Volatile compounds were identified by comparing their mass spectra and linear retention indices (RIs), with those reported in the NIST reference database (NIST 11.0) and NIST Chemistry Webbook (NIST 2018). The RIs were calculated from the retention time of a series

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of n-alkanes (C7-C30) (Sigma-Aldrich, Germany). For quantification, 15 external standards diluted with methanol were analyzed as samples to establish standard curves. Volatiles without standards were semi-quantified by comparing the peak areas of target compounds to the peak area of internal standard.

2.7 Statistical analysis

One-way ANOVA was used to investigate the differences in TPC, TFC, CTC, ABTS, DPPH among samples from each process steps using Minitab Express software (Version 1.2.0, Minitab Pty Ltd, Sydney, Australia). Principal component analysis (PCA) was conducted for TPC, TFC, CTC, ABTS, DPPH and volatile compounds using Matlab® (Version 9.3, Mathwork Inc, Natick, MA, USA).

3. Results and discussion

3.1 Effects of processing on the phenolic compounds in sorghum grain tea

The influences of processing treatments on the phenolic compounds and antioxidant capacity of the sorghum grain tea are summarized in **Table 1**. Soaking process significantly decreased TPC, TFC and CTC compared to untreated sorghum, which was likely due to the rupture of sorghum cell wall and accelerated the leaching of conjugated water-soluble polyphenols into soaking water during the process (Xiong et al., 2019b).

Fermentation significantly ($P < 0.05$) decreased TFC and CTC but not TPC when compared with the soaked sorghum (**Table 1**). No significant differences ($P > 0.05$) were observed between the two types of fermentations in sorghum polyphenol content and antioxidant capacity. The significant losses of flavonoids and condensed tannins during fermentation may due to the degradation of phenolic compounds (Adebo et al., 2018). *Lactobacillus plantarum*

can decompose condensed tannins into oligomeric tannins and other derivatives through the action of tannase and gallate decarboxylase (Jiménez et al., 2014). In addition, oxidation of diffused phenolic compounds may also lead to reduced TPC. Towo et al., (2006) reported that oxidation induced by polyphenol oxidase (PPO) in red sorghum varieties might also reduce TPC. On the contrary, fermentation may also lead to the release of bound polyphenols from cell walls, and therefore leading to an increase in the detectable phenolic content (Đorđević et al., 2010). Enzymes such as amylases and proteases produced by starter culture could hydrolyze phenolic conjugates with one or more bounded sugar into free polyphenols (Shrestha et al., 2013). Kadiri (2017) reported that *Saccharomyces cerevisiae* could synthesize some enzymes, including β -glucosidase, cellulase and xylanase, which have the capability to hydrolyze the β -glucosidic bonds of certain polyphenols. Therefore, the significant decrease in TFC and CTC but limited change of TPC were the result of the combined effects of enzymatic, physical and biochemical activities during the fermenting process.

TPC, TFC and CTC of the extracts were significantly ($P < 0.05$) decreased after steaming process. Wu et al., (2013) suggested that steaming could degrade phenolic compounds such as vanillic and *p*-coumaric acids. Similar phenomenon was also observed by Xiong et al., (2019b), who indicated that the losses of phenolic compounds may due to the breakdown and oxidation of heat-labile phenolic compounds.

However, different to the steaming effect, roasting process significantly ($P < 0.05$) increased TPC, TFC and CTC, which may be the result of depolymerization of conjugated phenolic compounds (Wu et al., 2013). High temperature could lead to breakdown of high molecular weight polyphenols, such as condensed tannins, and convert into lower molecular weight and more extractable compounds (Xiong et al., 2019b). Additionally, Randhir et al., (2008) demonstrated that roasting treatment led to the release of bound phenolic compounds originally combined to macromolecules such as structural proteins, cellulose and pectin in the

cell wall matrix, which could have contributed to the increase of phenolic compounds as well.

3.2 Effects of processing on the antioxidant capacity in sorghum grain tea

Compared with the processed samples, the raw sorghum grain showed the highest antioxidant capacity (**Table 1**). The soaking process significantly ($P < 0.05$) decreased the DPPH and ABTS levels, which could be attributed to the lower TPC as discussed in section 3.1. However, the antioxidant capacity of sorghum was significantly enhanced after the roasting process. Wu et al., (2013) suggested that the increase may be attributed to the formation of Maillard reaction products such as melanoidins. Rufián-Henares & Morales (2007) reported the antioxidant ability of melanoidins through scavenging oxygen radicals or chelating metals. TPC and CTC were correlated directly to antioxidant capacity, and significant positive correlation were observed between polyphenols and antioxidant capacity (**Table 2**). TPC in both yeast-fermented and LAB-fermented sorghum tea was positively related to the DPPH and ABTS assays, which reflected the contribution of TPC to the antioxidant capacity in sorghum tea. On the other hand, CTC was also found to weakly but significantly correlated with DPPH and ABTS in both yeast-fermented and LAB-fermented sorghum tea. However, large amounts of condensed tannins may be degraded and modified as previous studies have reported that tannin content in sorghum grain was reduced by 36%-80% after high temperature treatment (Dlamini et al., 2007; Babiker et al., 2008). This may be the result of the formation of insoluble complexes by reacting between phenolic hydroxyl groups of tannin and proteins, minerals (Wu et al., 2016) or heat induced degradation of condensed tannin molecules (Xiong et al., 2019b). Therefore, the total phenolic acids affected the major antioxidant capacity, which explained that TPC has stronger correlation with antioxidant capacity than condensed tannins.

3.3 Volatile compounds in sorghum grain tea

A total of 53 volatile compounds were detected in all sorghum samples. Among these compounds, 51 were identified, including 4 alcohols, 5 alkanes, 4 aldehydes, 3 phenols, 3 ketones, 2 carboxylic acids, 4 pyrazines, 2 pyrroles and 25 esters (**Table 3**). However, another 2 isolated compounds were unable to be identified. The total volatile content (TVC) did not change after soaking. Only LAB fermentation significantly ($P < 0.05$) increased TVC, but not yeast fermentation. A significant ($P < 0.05$) decrease in the TVC after the steaming process was observed in all samples followed by an increment of TVC in roasted sample of yeast fermented sorghum, but not in that of LAB fermented sorghum. Another important finding is that different fermentation influenced the volatile compounds significantly. *S. cerevisiae* fermented sorghum tea showed a higher content of pyrazine, pyrrole and aldehyde than LAB fermented sorghum tea. Both fermentation lead to a high content of esters (**Table 3**).

3.3.1 Effects of processing on volatile compounds in sorghum tea

In raw sorghum, esters and alcohols are the major volatiles followed by alkanes, which was consistent to a previous study (Xiong et al., 2019b). The major alcohol and ester observed were 1-hexanol, 1-nonaol and methyl hexanoate, while hexanal and nonanal were detected in low concentrations, as in consistent to past studies. The two detected ketones of 4-octanone and 2(3H)-furanone, 5-pentyl-, were previously reported in literature (Xiong et al., 2019b). Two carboxylic acids, nonanoic acid and 6-Octadecenoic acid, were firstly detected in sorghum in the current study, which may give a waxy, green and fatty flavor (The Good Scents Company, 2019).

The soaking process decreased the total alcohol, ketone and carboxylic acid content in sorghum (**Table 3**), likely due to the leaching effect (Lucas, Le Ray and Mariette, 2007). However, the content of aldehyde and ester were increased significantly. Two main factors may have contributed to this increment i) soaking disrupted the physical structure, and

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released more volatile compounds; ii) soaking increased the activity of lipoxygenase, which accelerate lipid oxidation and formation of aldehyde (Lucas, Le Ray and Mariette, 2007;).

Both yeast and LAB fermentation resulted in the increment of phenols and esters, and reduction of aldehyde and alkanes (**Table 3**). Alcohols were disappeared in yeast fermented samples but remained consist in LAB samples. The change of phenols during both fermentations has been reported by previous studies, which might be due to decarboxylation of ferulic acid (Zhu and Cui, 2013). The abundant fatty acids content in sorghum and the esterase activity of microorganisms were responsible for the elevated esters in fermented sorghum (Mehmood et al., 2008). Among all esters, butanoic acid, butyl ester and hexadecenoic acid, and methyl ester had the highest concentration, which could be formed by lipase-catalyzed esterification (Mamede, 2005).

During the steaming process, the alkanes content was increased while the esters content decreased (**Table 3**). Decrease in aldehydes were only observed in yeast-steamed sorghum, while the alcohols content was only reduced in LAB-steamed sorghum. The increment of aldehyde was due to the appearance of benzeneacetaldehyde, which was formed with amino acids during the Strecker degradation (Ji et al., 2015). However, no aldehydes were detected in lactic fermented samples, which may due to the synthesis of amino acid in yeast fermentation but biodegradation of amino acid in LAB fermentation (Fernández and Zúñiga, 2006). The increment of alkanes may due to the thermal damage of sorghum structure during steaming, which released more alkanes (Wu et al., 2013). Reduction in alcohols and esters content post steaming was also reported in previous study, mainly due to the leaching effect and thermal evaporation (Xiong et al., 2019b).

During the roasting process, pyrrole and pyrazine were formed and became the major volatile compounds in yeast-fermented sorghum, but not in LAB fermented sorghum (**Table 3**). These compounds formed during the Strecker degradation with amino acids and therefore contributed to the nutty and roasted flavor in final product (Arkadaş, 2018). It can be deduced that the absence of pyrazine and pyrrole in LAB-roasted samples was the result of low amino acids concentrations present in LAB fermented sorghum. It has been suggested that amino acids were generally in low concentrations after fermentation due to LAB growth (Pozo-Bayón et al., 2005). However, some studies mentioned the fact that the release of amino acids post-fermentation of *Saccharomyces cerevisiae* (Valero et al., 2003). Therefore, the difference of amino acids concentrations affected Maillard reaction. Roasting process also increased total aldehydes content in yeast-fermented sorghum due to the formation of 2,4-decadienal, (E,E)-. 2,4-decadienal, (E,E)-, which could be formed by autoxidation and lipoxygenase action on linoleic acid, and giving a fatty, cucumber and melon flavor to final sorghum tea product (Gassenmeier and Schieberle, 1994). The roasting process further reduced the alcohol contents in LAB-roasted samples and the esters contents in both type of fermented tea, which were likely due to the evaporation caused by high roasting temperature. Alkanes are relatively heat-resistant, which explained their stable contents during processing.

3.4 Principal components analysis of sorghum grains during processing

Principal component analysis was performed to illustrate the differences in sorghum grain samples subjected to different fermentation and processing treatments in phenolic content, antioxidant capacity and volatiles profile (**Figure 2**). The first (48.14%) and second (25.82%) component explained 73.96% of total variance. Total alkanes and ketones are the major contributors to the positive aspect of PC1, while the total pyrazine, pyrrole and phenol are the major contributors to the positive aspect of PC2. The total ester is the major contributor to the negative aspect of PC1 and total aldehyde contributes to the positive aspect of PC1 and PC2; and total alcohol contributed to the positive aspect of PC1 and the negative aspect of PC2.

Phenolics, ketones, alkanes, carboxylic acids and alcohols are the key compounds in raw sorghum, which gradually decreased during processing steps. Ester becomes the key volatile after fermentation process, while phenol, pyrrole and pyrazine are the major volatiles in yeast-roasted samples. Most processing steps, soaking, fermenting and roasting resulted in dramatic changes on sorghum chemical profile, while the influences of steaming were less than that of other steps.

4. Conclusion

In summary, the present study produced novel fermented sorghum tea with *Saccharomyces cerevisiae* or *Lactobacillus plantarum* and demonstrated that soaking, fermenting, steaming and roasting significantly changed its phenolic content, antioxidant capacity and volatile compounds. No significant differences in TPC were observed between the two types of fermentation whereas significant changes in aroma profiles were detected. Processing treatments, soaking, fermenting and steaming led to significant decreases in the concentration of phenolic compounds, while roasting significantly enhanced the TPC and antioxidant capacity. Significant ($P < 0.05$) positive correlations were observed between total phenolic compounds, condensed tannins content and antioxidant capacity. A total of 53 volatile compounds were detected. The abundance and composition of these volatiles were significantly influenced by each processing step, especially the two types of fermentation. Yeast fermentation showed a better performance regarding volatile profiles with esters, phenols and pyrazines being predominant. However, further studies are required to evaluate the sensory characteristics of the fermented sorghum grain tea and optimize the processing methods.

Conflict of interest

The authors declare no conflict of interest.

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Figure 1. Flow chart of processing procedures for fermented sorghum tea with two different species of microorganisms

Figure 2. Principal component analysis biplots of wheat bran tea processing. PC1 (48.14%) and PC2 (25.82%) explained 73.96% of total variance. Left and bottom axes represent loading plot, right and top axes represent score plot.

	Yeast					LAB				
	Raw	Soak	Fermentation	Steam	Roast	Raw	Soak	Fermentation	Steam	Roast
TPC (mg	6.93 ±	3.92 ±	3.80 ± 0.12 ^{cA}	3.23 ±	4.61 ±	6.93 ±	3.92 ±	3.87 ± 0.39 ^{cA}	3.02 ± 0.25 ^{dA}	4.49 ±
GAE/g)	0.62 ^{aA}	0.26 ^{cA}		0.10 ^{dA}	0.14 ^{bA}	0.62 ^{aA}	0.26 ^{aA}			0.38 ^{bA}
TFC (mg	1.07 ±	0.83 ±	0.63 ± 0.05 ^{cA}	0.39 ±	0.80 ±	1.07 ±	0.83 ±	0.61 ± 0.08 ^{cA}	0.44 ± 0.09 ^{dA}	0.85 ±
CAE/g)	0.02 ^{aA}	0.11 ^{bA}		0.12 ^{dA}	0.08 ^{bA}	0.02 ^{aA}	0.11 ^{bA}			0.06 ^{bA}
CTC (mg	38.02 ±	29.85 ±	19.55 ± 2.22 ^{cA}	9.95 ±	18.12 ±	38.02 ±	29.85 ±	21.68 ± 1.63 ^{cA}	11.02 ± 2.68 ^{dA}	20.26 ±
CAE/g)	1.63 ^{aA}	2.13 ^{bA}		2.46 ^{dA}	2.82 ^{cA}	1.63 ^{aA}	2.13 ^{bA}			1.85 ^{cA}
DPPH (mg	1.37 ±	1.10 ±	0.97 ± 0.20 ^{cA}	0.93 ±	1.17 ±	1.37 ±	1.10 ±	0.96 ± 0.05 ^{cA}	0.93 ± 0.08 ^{cA}	1.20 ±
TEAC/g)	0.05 ^{aA}	0.09 ^{bA}		0.17 ^{dA}	0.04 ^{bA}	0.05 ^{aA}	0.09 ^{bcA}			0.05 ^{bA}
ABTS (mg	12.62 ±	7.07 ±	6.06 ± 0.30 ^{cdA}	5.80 ±	9.54 ±	12.62 ±	7.07 ±	6.63 ± 1.11 ^{cdA}	6.36 ± 0.58 ^{dA}	10.31 ±
TEAC/g)	0.68 ^{aA}	0.53 ^{cA}		0.09 ^{dA}	0.11 ^{bA}	0.68 ^{aA}	0.53 ^{cA}			0.52 ^{bA}

511 **Table 1. Changes of phenolic compounds and antioxidant activity during fermented sorghum grain tea processing (mg/g)**

512 Data were displayed as mean $\pm$ standard deviation (n=3) on a dry basis.

513 a-d indicate significant difference within each pretreatment group, while A, B indicate the significant difference between two types of fermentation (p<0.05)

514 Abbreviation: LAB, fermented by *Lactobacillus plantarum subsp. argenteratensis*; Yeast, fermented by *Saccharomyces cerevisia*; TPC, Total phenolic content; TFC, Total
515 flavonoid content; CTC, Condensed tannins content.

516 **Table 2.** Pearson's correlation coefficients of TPC, CTC and antioxidant activities after fermentation with different starter cultures.

Correlation coefficient (r)	Treatment	DPPH	ABTS
TPC	Yeast-treated	0.96	0.97
	LAB-treated	0.93	0.92
CTC	Yeast-treated	0.83	0.72
	LAB-treated	0.80	0.66

517 Correlation is significant at P < 0.05 (two-tailed)

518 Abbreviation: TPC, total phenolic content; CTC, condensed tannins content; N/A, Not applicable; LAB, Lactic acid bacteria

519 **Table 3.** Identification and quantification of volatile compounds (ng/g dried sample basis) in raw and processed sorghum grains.

RI	RI NIST	Compound	Quantification	Yeast					LAB					Odor description									
			method	Raw	Soaked	Fermentation	Steaming	Roasting	Raw	Soaked	Fermentation	Steaming	Roasting										
1	874	871	1-Hexanol	ES	1062.0 [±]	280.2 [±] ±35.4	ND	ND	ND	1062.0 [±] ± 590.4	280.2 [±] ±35.4	ND	ND	ND	Ethereal, fruity, alcoholic								
					590.4																		
2	1070	1070	1-Octanol	ES	631.3 [±] ±78.9	ND	ND	ND	ND	631.3 [±] ±78.9	ND	ND	ND	ND	Waxy, green, citrus, aldehydic								
3	1107	1103	Phenylethyl Alcohol	IS	ND	ND	ND	ND	ND	ND	ND	1029.9 [±] ± 290.1	428.8 [±] ± 144.6	164.9 [±] ± 41.7	Sweet, flora, fresh, honey								
4	1169	1172	1-Nonanol	ES	1080.1 [±] ± 72.6	741.6 [±] ±8.1	ND	ND	ND	1080.1 [±] ± 72.6	741.6 [±] ±8.1	ND	ND	ND	Fresh, fatty, citrus, floral								
					2773.4 [±] ±											2773.4 [±] ±							
					Alcohol											1021.8 [±] ± 35.7	ND	ND	ND	1021.8 [±] ± 35.7	1029.9 [±] ± 290.1	428.8 [±] ± 144.6	164.9 [±] ± 41.7
					741.9											741.9							
5	1099	N/A	Undecane	IS	74.5 [±] ±14.3	40.3 [±] ± 4.3	ND	ND	ND	74.5 [±] ±14.3	40.3 [±] ± 4.3	ND	ND	ND	N/A								
6	1197	N/A	Dodecane	IS	58.2 [±] ± 14.4	106.1 [±] ± 10.6	ND	ND	28.2 [±] ± 1.1	58.2 [±] ± 14.4	106.1 [±] ± 10.6	ND	ND	ND	Alkane								
7	1297	N/A	Tridecane	IS	367.7 [±] ± 82.7	396.1 [±] ± 30.0	186.7 [±] ± 12.5	252.9 [±] ± 39.6	270.2 [±] ± 69.6	367.7 [±] ± 82.7	396.1 [±] ± 30.0	57.0 [±] ± 19.4	194.6 [±] ± 59.2	150.9 [±] ± 59.7	N/A								
8	1396	N/A	Tetradecane	IS	76.0 [±] ± 20.0	35.2 [±] ± 7.5	85.7 [±] ± 4.9	55.9 [±] ± 0.9	48.8 [±] ± 5.9	76.0 [±] ± 20.0	35.2 [±] ± 7.5	ND	58.9 [±] ± 7.3	51.7 [±] ± 18.8	Mild waxy								
9	1497	N/A	Heptadecane	IS	13.2 [±] ±2.64	ND	ND	ND	ND	13.2 [±] ±2.64	ND	ND	ND	ND	N/A								
		Alkane		589.6 [±] ± 133.7	577.9 [±] ± 41.7	242.6 [±] ± 27.4	307.6 [±] ± 34.2	347.1 [±] ± 64.1	589.6 [±] ± 133.7	577.9 [±] ± 41.7	57.0 [±] ± 19.4	253.6 [±] ± 54.2	202.6 [±] ± 78.4										

1	810	812	Hexanal	ES	144.4 ^{ab} ±9.8	255.4 ^{ab} ±64.4	ND	ND	ND	144.4 ^{ab} ±9.8	255.4 ^{ab} ±64.4	ND	ND	ND	Fresh, green, fatty
0															
1	1041	1044	Benzeneacetaldehyde	ES	ND	ND	ND	186.7 [±] 4.9	164.3 ^b ±4.4	ND	ND	ND	ND	ND	Green, honey, flora
1															
1	1103	1102	Nonanal	IS	31.9 ^{ab} ±10.4	66.9 ^{ab} ±21.0	22.2 ^{ab} ±1.7	27.4 ^{ab} ±11.9	37.4 ^{ab} ±8.3	31.9 ^{ab} ±10.4	66.9 ^{ab} ±21.0	ND	ND	ND	Waxy, aldehydic, citrus, fresh
2															
1	1313	1314	2,4-Decadienal, (E,E)-	ES	ND	ND	ND	ND	375.5 [±] 19.9	ND	ND	ND	ND	ND	Fatty, cucumber, melon,
3															
			Aldehyde		176.3 ^{ab} ±4.7	322.3 ^{ab} ±63.2	22.2 ^{ab} ±1.7	214.4 ^{ab} ±16.0	577.2 ^{ab} ±31.3	176.3 ^{ab} ±4.7	322.3 ^{ab} ±63.2	ND	ND	ND	
1	1160	1163	Phenol, 4-ethyl-	IS	ND	ND	56.3 ^{ab} ±21.6	112.8 ^{ab} ±40.4	58.1 ^{ab} ±7.7	ND	ND	254.9 ^{ab} ±73.4	399.2 ^{ab} ±80.0	128.2 ^{ab} ±63.8	Phenolic, castoreum, smoky
4															
1	1266	1268	Phenol, 4-ethyl-2-methoxy-	IS	ND	ND	693.1 ^{ab} ±237.6	671.4 ^{ab} ±	570.5 ^{ab} ±65.8	ND	ND	524.7 ^{ab} ±168.4	246.7 ^{ab} ±77.5	130.4 ^{ab} ±20.9	Spicy, clove, woody, sweet
5								188.0							
1															
6	1302	1301	2-Methoxy-4-vinylphenol	ES	ND	ND	1468.9 ^{ab} ±37.7	1621.2 ^{ab} ±20.8	7277.0 ^{ab} ±1186.6	ND	ND	1456.5 ^{ab} ±20.4	1663.0 ^{ab} ±30.2	7405.0 ^{ab} ±285.7	Woody, fresh, amber

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2	1173	1172	1H-Pyrrole,	IS	ND	ND	ND	ND	54.2 ^{ab} ± 2.0	ND	ND	ND	ND	ND	Burnt, roasted, smoky
7			1-(2-furanylmethyl)-												
			Pyrrole		ND	ND	ND	ND	122.3 ^{ab} ± 16.4	ND	ND	ND	ND	ND	
2					1204.3 ^{ab} ±	360.0 ^{ab} ±				1204.3 ^{ab} ±	360.0 ^{ab} ±				
937	938		Hexanoic acid methyl ester	ES			ND	ND	ND			ND	ND	ND	Fruity, pineapple, ethereal
8					128.5	107.9				128.5	107.9				
2								4795.9 ^{ab} ±	2719.8 ^{ab} ±			83799.8 ^{ab} ±	20076.4 ^{ab} ±	19725.1 ^{ab} ±	
998	995		Butanoic acid, butyl ester	ES	ND	ND	3074.3 ^{ab} ± 308.2			ND	ND				Fruity, sweet, banana, green
9								751.8	1279.8			12787.1	6770.1	10219.9	
3	1035	N/A	Pantolactone	IS	ND	ND	ND	ND	146.8 ^a ± 28.7	ND	ND	ND	ND	ND	Cotton, candy
0															
3	1056	1056	Butanoic acid, 3-methylbutyl ester	IS	ND	ND	57.2 ^{ab} ± 4.4	70.1 ^{ab} ± 6.1	99.8 ^{ab} ± 34.3	ND	ND	378.3 ^{ab} ± 106.7	491.3 ^{ab} ± 197.4	358.9 ^a ± 145.9	Fruity, sweet, estery, green,
1															
3	1090	1094	Benzoic acid, methyl ester	IS	264.0 ^{ab} ± 74.2	413.9 ^{ab} ± 28.7	142.5 ^{ab} ± 17.2	ND	ND	264.0 ^{ab} ± 74.2	413.9 ^{ab} ± 28.7	ND	ND	ND	Phenolic, wintergreen, almond
2															
3															Waxy, green, sweet, orange,
1122	1120		Octanoic acid methyl ester	ES	228.0 ^{ab} ± 17.3	171.4 ^{ab} ± 19.1	ND	ND	ND	228.0 ^{ab} ± 17.3	171.4 ^{ab} ± 19.1	ND	ND	ND	
3															aldehydic

3	1142	1145	Methyl nicotinate	IS	11.6 [±] 3.8	42.9 [±] 11.7	13.2 [±] 4.2	ND	ND	11.6 [±] 3.8	42.9 [±] 11.7	ND	ND	ND	Warm, herbal, tobacco
4															
3	1166	1168	Benzoic acid, ethyl ester	ES	ND	ND	ND	ND	ND	ND	ND	405.8 [±] 31.6	151.5 [±] 14.3	75 [±] 5.2	Fruity, sweet, wintergreen
5															
3	1189	1186	Hexanoic acid, butyl ester	IS	ND	ND	ND	ND	ND	ND	ND	143.8 [±] 22.2	117.9 [±] 59.4	88.8 [±] 9.1	Fruity, berry, pineapple
6															
3	1223	N/A	Nonanoic acid methyl ester	IS	145.3 [±] 48.1	27.8 [±] 7.1	ND	ND	ND	145.3 [±] 48.1	27.8 [±] 7.1	ND	ND	ND	Sweet, fruity, pear, waxy
7															
3	1365	N/A	Butyl benzoate	IS	92.6 [±] 15.6	34.9 [±] 7.8	125.3 [±] 21.7	46.9 [±] 7.5	47.9 [±] 6.0	92.6 [±] 15.6	34.9 [±] 7.8	356.5 [±] 97.0	463.0 [±] 123.2	199.5 [±] 35.8	Amber, balsamic, fruity
8															
3	1375	1373	Butyl caprylate	IS	ND	ND	ND	ND	ND	ND	ND	83.0 [±] 13.3	67.8 [±] 24.7	81.0 [±] 20.6	Buttery, ethereal, herbal
9															
4	1431	N/A	Benzoic acid, 2-methylbutyl ester	IS	72.7 [±] 12.3	136.7 [±] 11.0	93.5 [±] 33.7	70.6 [±] 17.6	46.8 [±] 4.3	72.7 [±] 12.3	136.7 [±] 11.0	ND	ND	ND	N/A
0															
4	1432	1439	.beta.-Phenylethyl butyrate	IS	ND	ND	ND	ND	ND	ND	ND	292.3 [±] 99.5	415.8 [±] 152.1	183.5 [±] 31.2	Fruity, sweet, berry, juice
1															

4	1520	1521	Dodecanoic acid, methyl ester	IS	20.4 [±] 9.0	22.4 [±] 4.2	ND	ND	ND	20.4 [±] 9.0	22.4 [±] 4.2	ND	ND	ND	Waxy, creamy, coconut, mushroom
2															
4			Hexadecanoic acid, methyl			2892.1 [±]				2892.1 [±]	11176.1 [±]				
	1921	1921		IS	656.5 [±] 195.2		3871.9 [±] 1027.2	38.7 [±] 4.0	ND	656.5 [±] 195.2			ND	ND	Oily, waxy, fatty, orris
3			ester			497.5				497.5	1998.2				
4						363.7 [±]				363.7 [±]					Waxy, fruity, creamy, milky,
	1993	1994	Hexadecanoic acid, ethyl ester	ES	25.1 [±] 4.0		151.5 [±] 88.7	17.2 [±] 2.4	13.1 [±] 0.9	25.1 [±] 4.0		1051.9 [±] 238.8	119.1 [±] 12.5	91.6 [±] 39.7	
4						149.7					149.7				balsamic
4			9,12-Octadecadienoic acid												
	2089	2087		IS	337.4 [±] 98.2	402.5 [±] 61.9	801.3 [±] 530.9	26.8 [±] 6.6	ND	337.4 [±] 98.2	402.5 [±] 61.9	690.0 [±] 82.0	ND	ND	Bland
5			(Z,Z)-, methyl ester												
4			9-Octadecenoic acid, methyl			583.4 [±]					583.4 [±]				
	2095	N/A		IS	223.4 [±] 54.9		554.2 [±] 327.8	23.6 [±] 6.6	ND	223.4 [±] 54.9		386.1 [±] 49.2	ND	ND	N/A
6			ester, (E)-			209.1					209.1				
4															
	2128	2128	Methyl stearate	IS	18.3 [±] 3.1	26.0 [±] 5.9	71.3 [±] 40.4	ND	ND	18.3 [±] 3.1	26.0 [±] 5.9	59.1 [±] 11.6	ND	ND	Oily, waxy
7															
4															
	2159	2155	Linoleic acid ethyl ester	IS	39.3 [±] 10.8	51.4 [±] 29.3	172.5 [±] 52.0	14.2 [±] 0.6	ND	39.3 [±] 10.8	51.4 [±] 29.3	256.4 [±] 46.4	100.6 [±] 17.9	47.1 [±] 14.6	Fatty, fruity
8															
4															
	2180	2180	Ethyl Oleate	IS	27.5 [±] 7.8	36.5 [±] 14.0	105.6 [±] 52.0	11.4 [±] 0.7	ND	27.5 [±] 7.8	36.5 [±] 14.0	147.8 [±] 36.5	86.4 [±] 26.9	27.3 [±] 4.2	N/A
9															

520 a-d indicate significant difference within each pretreatment group, while A, B indicate significant difference between two types of fermentation ($p<0.05$)

521 Odor description were obtained from The Good Scents Company (2018).

522 Volatile compounds were identified by mass spectra (NIST library 11.0) and retention index from NIST Webbook (NIST 2018).

523 Semi-quantified was used by comparing the peak areas of target compounds to the peak area of internal standard, external quantification method was used by calculation of

524 standard curve

525 Abbreviation: RI = Retention index; RI NIST = Retention indices obtained from NIST Webbook; N/A = Not Applicable; ND = Not Detected; IS=internal standard;

526 ES=external standard

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