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Correlation of SPME-GC-MS Volatile Compounds with Descriptive Sensory Odor Analysis of Whole Wheat and Quinoa Flours in Accelerated Storage

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A thesis submitted to the faculty of
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Master of Science

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ABSTRACT

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The acceptability of whole grain flours during storage varies widely, as does the estimated shelf life of such flours, in part because acceptability is typically determined using subjective human sensory testing. Research is needed to establish more objective measures of acceptability. This study correlated the quantitative results of a descriptive odor sensory panel with volatile compounds determined by solid-phase microextraction-gas chromatograph-mass spectrometry (SPME-GC-MS). Whole wheat flour and quinoa flour were held at 40°C for up to 24 weeks to accelerate changes occurring during storage. Samples were collected every 4 weeks and placed in frozen storage. Thawed samples were then evaluated using SPME-GC-MS and descriptive sensory odor analysis. Significant correlations were found between 1-hexanol, 2-pentylfuran, phenol, hexanoic acid, and hexanal volatiles of whole wheat flour and the odor descriptor cardboard/stale. This indicates that SPME-GC-MS can be used as a less expensive, less time-consuming, more precise method to determine the acceptability of whole wheat flour during storage. Significant correlations were not present in the quinoa flour data, suggesting that SPME-GC-MS may not be preferable to human sensory odor analysis in determining acceptability of stored quinoa flour.

Keywords: wheat flour, quinoa flour, sensory, volatiles, SPME, shelf life

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Abstract

The acceptability of whole grain flours during storage varies widely, as does the estimated shelf life of such flours, in part because acceptability is typically determined using subjective human sensory testing. Research is needed to establish more objective measures of acceptability. This study correlated the quantitative results of a descriptive odor sensory panel with volatile compounds determined by solid-phase microextraction-gas chromatograph-mass spectrometry (SPME-GC-MS). Whole wheat flour and quinoa flour were held at 40°C for up to 24 weeks to accelerate changes occurring during storage. Samples were collected every 4 weeks and placed in frozen storage. Thawed samples were then evaluated using SPME-GC-MS and descriptive sensory odor analysis. Significant correlations were found between 1-hexanol, 2-pentylfuran, phenol, hexanoic acid, and hexanal volatiles of whole wheat flour and the odor descriptor cardboard/stale. This indicates that SPME-GC-MS can be used as a less expensive, less time-consuming, more precise method to determine the acceptability of whole wheat flour during storage. Significant correlations were not present in the quinoa flour data, suggesting that SPME-GC-MS may not be preferable to human sensory odor analysis in determining acceptability of stored quinoa flour.

1. Introduction

The USDA's informational website ChooseMyPlate.org states that half of all grains consumed should be whole grains. Whole grains provide many nutrients, including vitamins, minerals, and dietary fiber (ChooseMyPlate, 2017). Studies have shown that increasing fiber intake can lower blood cholesterol levels and help lower the risk of heart disease, obesity, and type II diabetes (Khan et al., 2009; Seal and Brownlee, 2015). An increased demand for whole grain foods has spurred food manufacturers to develop innovative foods that contain a variety of whole grains and their corresponding flours. These flours are often milled in one location, shipped to a food processing plant, incorporated into a food, and then shipped to grocery stores. Each of these steps takes time and affects the shelf life of whole grain flours and their blends. However, the sensory shelf life remaining for a given whole grain flour at any given time is hard to define. Even whole wheat flour, which has been used in the industry for decades, has an ill-defined shelf life range of 3 to 15 months.

In addition to the subjectivity of the determination, this wide range in shelf life for whole wheat flour is attributable to a variety factors (Doblado-Maldonado et al., 2012). The cultivar of grain being milled, the time of harvest, the amount of time between harvest and milling, and the moisture of the grain when milled all affect flour shelf life. Additionally, the type of milling performed and the particle size can affect shelf life (Doblado-Maldonado et al., 2012). Although these factors have been described in relation to whole wheat flour, the same issues could pertain to other milled grains as well.

Of the various reactions occurring during storage, lipid degradation most affects the shelf life of whole wheat flour (Pomeranz, 1988). Lipid degradation is often the result of lipid oxidation, which creates off-flavor and off-odor compounds that are characterized as being rancid. Most of the rancid flavors in foods are caused by the breakdown of the unsaturated fatty acids present in a given food. This is because unsaturated fatty acids are very susceptible to oxidation, even when the amount of unsaturated fatty acids is very low (Labuza, 1971). Whole grain cereals have fat contents ranging between 2% and 6%; whole wheat contains 1.95% fat and quinoa contains 6.07% fat (USDA Nutrient Database, 2017).

While rancidity can be determined by using off-odors, it is difficult to evaluate those off-odors. For quality control purposes during production, acceptability is often determined subjectively by a few employees smelling the flour, which results in large variation (Doblado-Maldonado et al., 2012). Consumer and descriptive sensory analyses can reduce the variance from subjectivity and are considered the most reliable indications of rancidity (Robards et al., 1988). However, consumer sensory panels are costly, and descriptive sensory work is time consuming due to the extensive and lengthy training of panelists. Because each whole grain flour has different rancidity odors, each flour would require a separately trained set of descriptive analysis panelists.

Another method used to evaluate rancidity in food products is solid-phase microextraction-gas chromatography (SPME-GC) (Kataoka et al., 2000; Xu et al., 2016; Zhou et al., 1999). SPME-GC is a rapid method for identifying the volatile compounds that are present in the headspace of a sample. Previous studies have investigated the volatiles present in various bread formulas stored under a variety of conditions but did not evaluate wheat flour itself (Licciardello et al., 2016; Marti et al., 2014; Purcaro et al., 2008). Recent studies have looked at the volatiles present in fresh whole wheat flour (Yuan et al., 2016) and in ozone treated wheat flour (Li et al., 2013). However, these studies did not investigate the change in whole wheat flour volatiles over storage time.

Previous studies have looked at volatiles formed in quinoa wine (Liu et al., 2015), quinoa malt (Dezelak et al., 2014), quinoa bread (Pico et al., 2017), and sausages made with quinoa as a fat replacer (Fernandez-Diez et al., 2016). While these studies did measure volatiles of the final products, they did not identify the volatiles present in the quinoa flour before incorporation into the products. One study found increasing levels of hexanal present in ground quinoa during accelerated storage but did not identify other compounds present (Ng et al., 2006). While the increasing presence of hexanal is well documented, there might be other compounds that better represent the changes occurring in stored quinoa flour.

A correlation of SPME-GC headspace volatiles with descriptive sensory analysis scores would allow for faster, more cost-effective determinations of flour shelf-life. The purpose of this study was to correlate SPME-GC-MS analysis of headspace volatile concentrations with descriptive sensory odor analysis scores for whole wheat flour and quinoa flour during accelerated storage conditions.

2. Materials and Methods

2.1 Flour preparation and storage

Whole wheat flour milled from hard red winter wheat was purchased from a local mill (Lehi Roller Mills, Lehi, Utah) within two weeks of milling. The wheat was milled from the same lot within 6 months of harvest. The whole wheat flour was then homogenized by blending in a one-speed ribbon blender (Model IMB5, Aaron Process Equipment, Bensenville, Illinois) for 15 minutes. The homogenized whole wheat flour was then weighed out in 1.05 kg samples and placed in double-layer kraft bags (Abugoch et al., 2009).

White quinoa was purchased from a local health foods store. The quinoa was milled in a Quadrumat Junior II Mill (C.W. Brabender Instruments, South Hackensack, New Jersey) with a 200 μm mesh screen. The mill feed gate was opened completely to allow maximum grain flow. After milling, the quinoa endosperm and bran were recombined and homogenized by blending for 15 minutes in the ribbon blender. The homogenized quinoa flour was then weighed out in 0.55 kg samples and placed in double-layer kraft bags. The samples were placed in double-layer kraft bags to simulate the types of bags used for flour storage in the industry. The whole wheat and quinoa flours were then placed in storage.

Immediately after milling and homogenization, three bags of each type of flour were transferred to mylar bags (Uline, Pleasant Prairie, Wisconsin) and placed in a -30°C freezer (Model BTQ50FSHD, Kelvinator, Detroit, Michigan) for preservation as Week 0 samples. The remainder of the whole wheat flour bags and the quinoa flour bags were placed in an atmosphere-controlled chamber (Environmental Growth Chambers, Chagrin Falls, Ohio) at 40°C and 40% relative humidity. This is the temperature used by Singh et al. (2012), and a lower relative humidity was used to reduce the formation of mold. The samples were placed at this temperature and relative humidity to accelerate the degradation process in order to more quickly evaluate the changes that occurred in the flours over time. Every 4 weeks up to 24 weeks, three bags of each type of flour were removed from the atmosphere-controlled chamber, transferred to mylar bags, and placed in the -30°C freezer to halt potential degradation until analyzed.

2.2 SPME-GC-MS

Volatiles were analyzed using the extraction method of Kaseleht et al. (2011), and the GC analysis method modified from Cramer et al. (2005). Clear glass 20 mL headspace vials and magnetic screw caps with a 1.3 mm polytetrafluoroethylene/silicone septum (SAFC, Sigma Aldrich, St. Louis, Missouri) were baked in a forced draft oven (1600 HAFO Series, Sheldon Manufacturing, Cornelius, Oregon) overnight at 120°C to remove volatile contaminants. Flour (1.50 g) was placed in the headspace vials along with 8 µL internal standard (80 mg/L 2-methyl-3-heptanone in methanol; Supelco, Sigma Aldrich, St. Louis, Missouri). Each sample was prepared in triplicate.

Volatile extraction, separation, and detection was performed by solid phase microextraction-gas chromatography-mass spectroscopy (SPME-GC-MS) using a divinylbenzene/carboxen/polydimethylsiloxane StableFlex SPME fiber (Supelco, Sigma Aldrich, St. Louis, MO). Extraction was automated using an MPS 2XL Multipurpose Sampler (Gerstel, Mülheim, Germany). Vials were incubated at 40°C for 30 min. while being shaken at 250 rpm. The SPME fiber was then injected and volatiles were extracted at 40°C for 30 min. while being shaken at 250 rpm.

Volatiles were thermally desorbed at 200°C in the injector port of a HP6890 gas chromatograph (Agilent Technologies Inc., Santa Clara, CA) with a DB-5ms column (30.0m × 0.25mm with 0.5µm film thickness; Agilent Technologies Inc., Santa Clara, CA). Helium (0.8 mL/min) was used as the carrier gas. The oven temperature was programmed with an initial temperature of 33°C for 5 min., a ramp of 2°C/min up to 50°C, followed by a ramp of 5°C/min up to 77°C and 7 minute holding time, followed by another ramp of 5°C/min up to 125°C, and a final ramp of 10°C/min up to 225°C. The total run time was 59.5 min.

Volatiles were detected using an HP5973 mass selective detector (Agilent Technologies Inc., Santa Clara, CA) and then identified by spectra comparison to a library using ChemStation software (Agilent Technologies Inc., Santa Clara, CA). Semi-quantitative analysis was used for determination of volatile compounds, where concentrations were calculated relative to the internal standard, assuming a 1:1 response ratio, and were reported as relative abundance.

2.3 Descriptive odor analysis

Descriptive odor analysis was completed using a group of trained panelists (n=8, 4 females, 4 males, ages 23 to 59), in compliance with the Brigham Young University Institutional Review Board. Flour samples (7.00 g) were placed in 59 mL plastic soufflé cups with lids (Solo

Cup Company, Lake Forest, Illinois). The cups were labeled with randomly assigned three digit numbers. The panelists had over ten hours of training for each of the two panels. The training consisted of presenting panelists with flour samples of various ages. As part of the training, panelists determined three descriptors for whole wheat flour odor: fresh flour, cardboard/stale, and musty. In a subsequent panel, panelists determined three descriptors for quinoa flour odor: grassy, cardboard/stale, and musty. Once an odor lexicon was established, additional training focused on properly distinguishing intensity of the various descriptors. The scale for intensity ranged from 0 to 15. Scale guidelines were provided where 0 was defined as “not detected,” 1-5 was “slight,” 6-10 was “moderate,” and 11-15 was “extreme.” Reference samples for each descriptor with panelist-determined intensities were provided for each session. Evaluations consisted of smelling 2 sets of references and samples with a 10 minute break between the 2 sets. Panelists recorded their evaluation on paper ballots. Panelists were instructed to sniff their arms, shake their cups, and immediately open the lid and smell the samples. The mean of each descriptor for each sample was reported.

2.4 Statistical analysis

Data was analyzed using SAS software (Version 9.4, SAS Institute Inc., Cary, North Carolina). Significance was set at $p<0.05$. Mixed models were constructed to look at significant differences within the each volatile compound over time using the Tukey-Kramer test. A Pearson Correlation model was constructed to evaluate possible correlations of volatile compound amounts with sensory descriptor scores.

3. Results and Discussion

3.1 SPME-GC-MS

Representative gas chromatograms of headspace volatiles at Week 0 and Week 24 are shown in Figure 1 for whole wheat flour and Figure 2 for quinoa flour. Tables 1 and 2 list volatile compounds identified in whole wheat flour and quinoa flour, respectively. The values in Table 1 are the amounts of volatile compounds in whole wheat flour that were consistently present during storage, either in increasing or decreasing concentrations. The results are reported as relative abundance in mg/L, compared to the known concentration of the internal standard.

The data in Table 1 indicate that 1-hexanol is present in all samples and significantly increases over time. The compounds 2-pentylfuran, phenol, hexanoic acid, hexanal, and 1-pentanol also significantly increase over time, after they appear in the samples. These compounds are consistent with the compounds in fresh whole wheat flour identified by Xu et al. (2017), who identified pentanol, hexanal, 1-hexanol, 2-pentylfuran, and other compounds. A study by Yuan et al. (2016) also identified 1-hexanol as one of the main volatile compounds in fresh whole wheat flour. Yuan et al. additionally identified hexanoic acid and other compounds. A study conducted by Li et al. (2013) found hexanal, furan, and phenol in whole wheat flour.

The differences in identified compounds among the three previous studies and this research could be due to the differences in the wheat, sensitivity of the instruments used, and variations in preparation of the whole wheat flour samples, i.e. milling method. None of the previous studies looked at whole wheat flour over time, at room temperature or higher temperatures of accelerated storage. The increase of 1-hexanol, 2-pentyl furan, phenol, hexanoic acid, hexanal, and 1-pentanol during storage in this study suggests they may be good indicators of flour age.

Table 2 shows the data for the SPME-GC-MS for quinoa flour. The compound 1-hexanol is present in all samples and significantly increases between Week 0 Week 16. Phenol significantly increases after appearing in Week 8 and then decreases at Week 24. Hexanal, 1-pentanol, and 1-octanol all appear at Week 12 and significantly increase by Week 16. Nonanal, decanal, and 2-undecenal appear at Week 16 and significantly increase through Week 24. 2,4-nonadienal did not significantly increase.

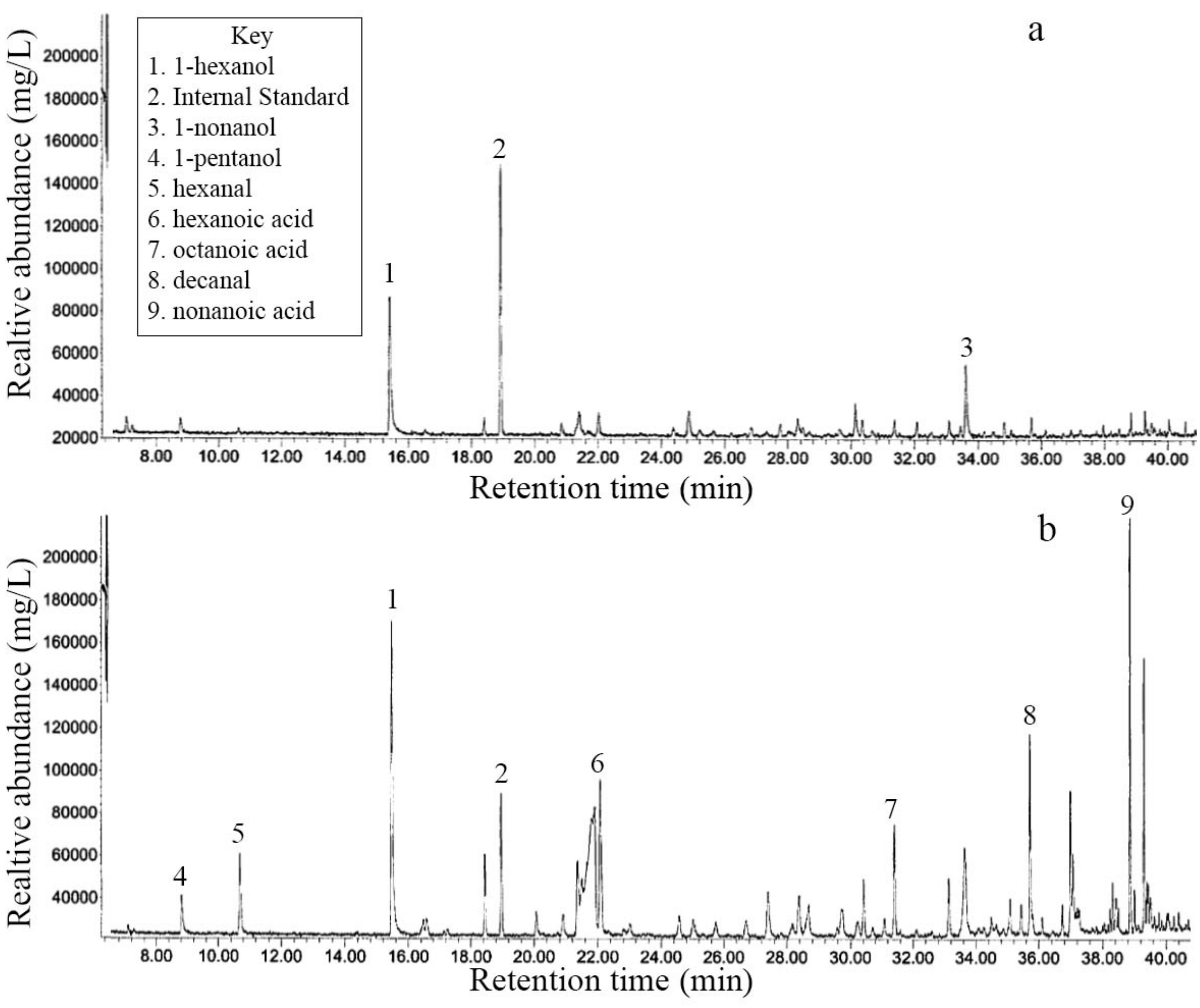

Figure 1: Gas chromatogram of headspace volatiles in whole wheat flour at Week 0 (a) and Week 24 (b).

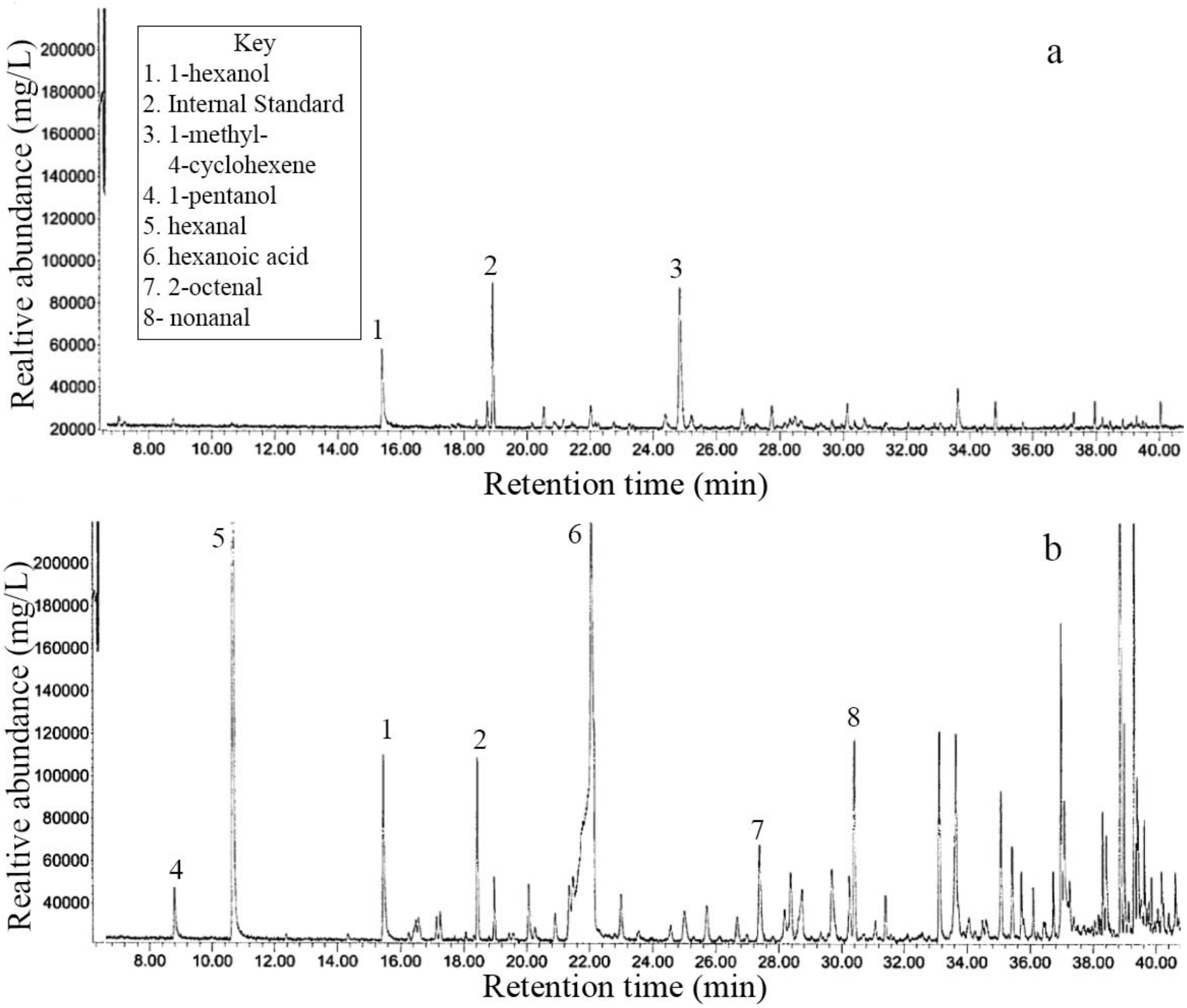

Figure 2: Gas chromatogram of headspace volatiles in quinoa flour at Week 0 (a) and Week 24 (b).

Table 1: Whole wheat flour volatiles and their relative abundances (mg/L) during storage at 40°C as determined by SPME-GC-MS*

Compound	Week 0	Week 4	Week 8	Week 12	Week 16	Week 20	Week 24
1-hexanol	49.7 ±5.4^{a}	56.66 ±8.52^{a}	115.20 ±17.71^{b}	135.33 ±18.24^{b}	174.84 ±12.29^{cd}	136.04 ±6.35^{bc}	215.22 ±6.25^{d}
2-pentylfuran	ND**	15.10 ±2.51^{a}	35.68 ±6.30^{ab}	58.51 ±9.83^{bc}	94.59 ±11.28^{de}	83.10 ±2.74^{cd}	120.20 ±2.74^{e}
Phenol	ND	ND	34.85 ±8.56^{a}	80.72 ±17.95^{ac}	116.62 ±12.29^{c}	101.95 ±8.15^{bc}	63.20 ±0.28^{ab}
Hexanoic acid	ND	ND	62.32 ±6.41^{a}	129.72 ±12.12^{a}	336.02 ±51.99^{b}	343.64 ±26.88^{b}	399.95 ±31.94^{b}
Hexanal	ND	ND	ND	19.38 ±3.93^{a}	51.42 ±10.28^{b}	45.98 ±3.78^{ab}	53.32 ±3.80^{b}
1-pentanol	ND	ND	ND	ND	25.98 ±156^{ab}	22.25 ±0.68^{a}	28.17 ±1.08^{b}

*Mean values are reported with the standard error of the means, n=3

**ND- none detected for that sample

$^{a-e}$ Means with different superscript letters within a row indicate significant differences ($P<0.05$)

Table 2: Quinoa flour volatiles and their relative abundances (mg/L) during storage at 40°C as determined by SPME-GC-MS*

Compound	Week 0	Week 4	Week 8	Week 12	Week 16	Week 20	Week 24
1-hexanol	53.16 ±4.05^{a}	34.45 ±1.62^{a}	164.66 ±7.89^{ac}	329.70 ±72.47^{b}	311.22 ±17.55^{b}	193.10 ±10.11^{bc}	252.58 ±2.50^{bc}
2-pentylfuran	ND**	ND	37.25 ±7.42^{a}	142.26 ±36.86^{b}	ND	ND	ND
Phenol	ND	ND	105.16 ±20.41^{a}	105.33 ±6.99^{a}	152.68 ±7.06^{ab}	185.49 ±4.65^{b}	103.86 ±6.35^{a}
Hexanal	ND	ND	ND	175.41 ±3.45^{a}	1062.56 ±48.42^{b}	1677.45 ±63.16^{c}	1132.14±74.96^{b}
1-pentanol	ND	ND	ND	39.49 ±4.99^{a}	98.96 ±9.55^{bc}	114.13 ±4.27^{c}	81.70 ±1.17^{b}
1-octanol	ND	ND	ND	68.08 ±11.27^{a}	146.98 ±8.57^{b}	187.34 ±10.58^{b}	146.33 ±9.59^{b}
1-nonanol	35.81 ±0.56^{a}	ND	ND	67.27 ±8.73^{b}	173.08 ±3.75^{c}	ND	ND
Nonanal	ND	ND	ND	ND	237.55 ±10.78^{a}	422.17 ±14.72^{c}	307.02 ±19.71^{b}
Decanal	ND	ND	ND	ND	93.21 ±1.47^{a}	202.44 ±5.12^{b}	195.73 ±17.15^{b}
2,4-nonadienal	ND	ND	ND	ND	119.45 ±2.12^{a}	183.32 ±12.00^{b}	113.08 ±5.98^{a}
2-undecenal	ND	ND	ND	ND	127.09 ±6.14^{a}	221.64 ±12.11^{b}	212.60 ±10.26^{b}

*Mean values are reported with the standard error of the means, n=3

**ND- none detected for that sample

$^{a-c}$ Means with different superscript letters within a row indicate significant differences ($P<0.05$)

3.2 Sensory

Figure 3 represents the data from the descriptive odor analysis sensory panel for whole wheat flour. The values on the chart represent the averaged results from duplicate panels. Figure 3 indicates that the intensity of fresh flour steadily decreased over time. Cardboard/stale increased during storage up to Week 16, plateaued at Week 20, and then declined. Musty intensity was low until an increase at Week 16 that dramatically rose at Week 24. It is probable that any presence of cardboard/stale odor after Week 16 was obscured by the musty odor detected at Weeks 20 and 24.

These findings seem to correspond with previous sensory analysis relating to wheat germ and whole wheat bread. Work by Sjovall et al. (2000) used sensory paired-comparison tests to detect differences in samples of wheat germ and found significant differences in samples stored for three weeks compared to one week. Jensen et al. (2011) used descriptive sensory analysis to determine that the scores for aroma descriptors of bran and dough of whole wheat bread decreased after storage. The aroma descriptors of dust, fatty, and rancid increased over the same storage period. Licciardello et al. (2017) evaluated how packaging affects the sensory aspects of whole wheat bread stored in plastic bags for consumers. They observed that the odors of semolina and toast decreased during storage, while the odors of stale and sour increased during storage.

Results of the descriptive panel on quinoa flour is represented in Figure 4, which indicates that the intensity of grassy drops drastically after Week 0 and then steadily declines. Cardboard/stale rose steadily until Week 16, plateaued, and then declined. Musty intensity was low until Week 16 where it increased gradually before rising quickly at Week 24. Like whole wheat flour, it is probable that any presence cardboard/stale after Week 16 was obscured by the musty odor detected at Weeks 20 and 24. The initial presence of the descriptor grassy appears to match the results of a study by Hager et al. (2012) that compared bread made with various flours to bread made from wheat flour. The aroma profile analysis for the crumb of bread from quinoa showed a medium to high intensity for the descriptor pea-like. Since the bread samples were only evaluated shortly after preparation, it is not possible to compare the results presented by Hager et al. (2012) to the descriptors that developed over time in this study.

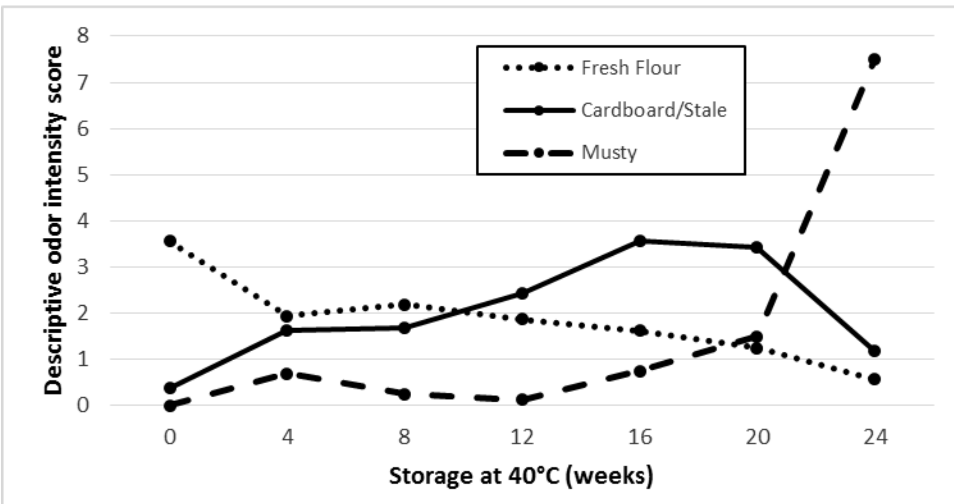

Figure 3: Whole wheat flour odor descriptor intensity scores on a scale of 0 to 15 during storage at 40°C (n=8)

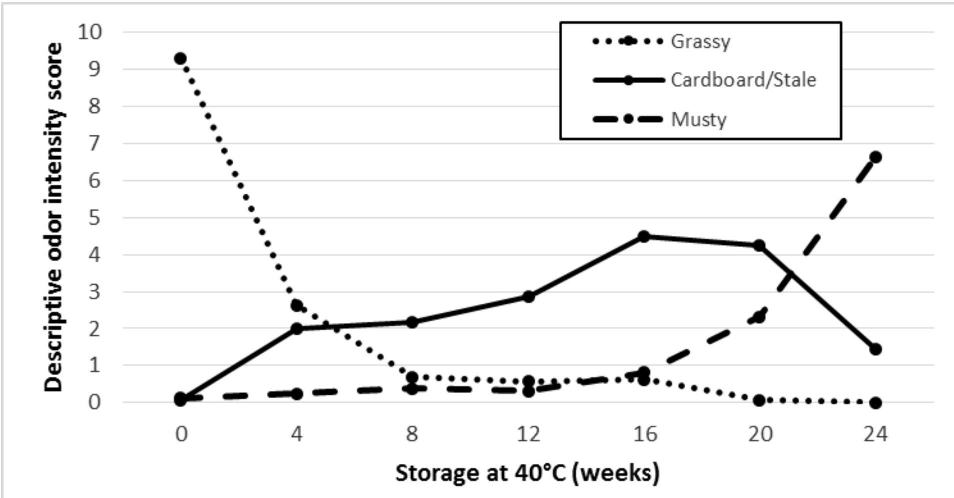

Figure 4: Quinoa flour odor descriptor intensity scores on a scale of 0 to 15 during storage at 40°C (n=8)

3.3 Correlation of GC Volatiles and Sensory

Several significant correlations were observed between GC volatiles and odor scores across the 6 months of storage. In whole wheat flour, the scores for the descriptor fresh flour were negatively correlated with 1-hexanol (r=-0.82), 2-pentylfuran (r=-0.86), and hexanoic acid (r=-0.88). These negative correlations indicate that as whole wheat flour ages, it loses its fresh flour odor in a rate similar to its increase in these volatiles. Additionally, the descriptor cardboard/stale was positively correlated with 1-hexanol (r=0.89), 2-pentylfuran (r=0.97), phenol (r=0.97), hexanoic acid (r=0.98), and hexanal (r=0.99). This suggests that it is possible to evaluate rancidity using compounds other than hexanal. The correlations with the descriptors fresh flour and cardboard/stale show that SPME-GC-MS can effectively identify and quantitate at least some aspects of whole wheat flour odor changes.

In quinoa flour, only one significant correlation was observed between volatiles and odor descriptors ($P<0.05$). The descriptor musty was positively correlated with the compound 1-

nonanol (r=.99). The rise and fall of the compounds in quinoa flour prevent more significant correlations between the volatile compounds and descriptive sensory analysis scores.

4. Conclusions

Volatile compounds, as measured by SPME-GC-MS, present in whole wheat and quinoa flours change over time in accelerated storage. Descriptive sensory analysis of odors also indicates that accelerated storage alters the human-perceptible volatiles. The positive correlations that 1-hexanol, 2-pentylfuran, phenol, hexanoic acid, and hexanal have with the descriptor cardboard/stale indicate that SPME-GC-MS analyses can be used as a rapid and less expensive means of determining whole wheat flour age and acceptability. The SPME-GC-MS data could potentially be included on a certificate of analysis (COA) originating from a mill, similar to how oil companies include peroxide values on COAs. Future studies should be conducted with flours stored at ambient temperatures in real time to determine if the same correlations exist. In contrast, the absence of multiple correlations between instrumental quantitation of volatiles and descriptive sensory analysis scores in quinoa flour suggest that SPME-GC-MS analyses may not be preferable to human sensory determination of quinoa flour age and acceptability.

References

Abugoch, L., Castro, E., Tapia, C., Cristina Anon, M., Gajardo, P., Villarroel, A., 2009. Stability of quinoa flour proteins (*Chenopodium quinoa Willd*.) during storage. International Journal of Food Science and Technology 44, 2013-2020.

ChooseMyPlate. Grains. Available at http://www.choosemyplate.gov/food-groups/grains.html. Accessed June 6, 2017.

Cramer, A., Mattinson, D., Fellman, J., Baik, B., 2005. Analysis of volatile compounds from various types of barley cultivars. Journal of Agricultural and Food Chemistry 53, 7526-7531.

Dezelak, M., Zarnkow, M., Becker, T., Kosir, I.J., 2014. Processing of bottom-fermented gluten-free beer-like beverages based on buckwheat and quinoa malt with chemical and sensory characterization. Journal of the Institute of Brewing 120, 360-370.

Doblado-Maldonado, A.F., Pike, O.A., Sweley, J.C., Rose, D.J., 2012. Key issues and challenges in whole wheat flour milling and storage. Journal of cereal science 56, 119-126.

Fernandez-Diez, A., Caro, I., Castro, A., Salva, B.K., Ramos, D.D., Mateo, J., 2016. Partial fat replacement by boiled quinoa on the quality characteristics of a dry-cured sausage. Journal of Food Science 81, C1891-C1898.

Hager, A., Wolter, A., Czerny, M., Bez, J., Zannini, E., Arendt, E.K., Czerny, M., 2012. Investigation of product quality, sensory profile and ultrastructure of breads made from a range of commercial gluten-free flours compared to their wheat counterparts. European Food Research and Technology 235, 333-344.

Jensen, S., Oestdal, H., Skibsted, L.H., Larsen, E., Thybo, A.K., 2011. Chemical changes in wheat pan bread during storage and how it affects the sensory perception of aroma, flavour, and taste. Journal of Cereal Science 53, 259-268.

Kaseleht, K., Leitner, E., Paalme, T., 2011. Determining aroma-active compounds in Kama flour using SPME-GC/MS and GC-olfactometry. Flavour and Fragrance Journal 26, 122-128.

Kataoka, H., Lord, H.L., Pawliszyn, J., 2000. Applications of solid-phase microextraction in food analysis. Journal of Chromatography A 880, 35-62.

Khan, N.A., Hernmelgarn, B., Herman, R.J., Bell, C.M., Mahon, J.L., Leiter, L.A., Rahkin, S.W., Hill, M.D., Padwal, R., Touyz, R.M., Larochelle, P., Feldman, R.D., Schiffrin, E.L., Campbell, N.R.C., Moe, G., Prasad, R., Arnold, M.O., Campbell, T.S., Milot, A., Stone, J.A., Jones, C., Ogilvie, R.I., Hamet, P., Fodor, G., Carruthers, G., Burns, K.D., Ruzicka, M., deChamplain, J., Pylypchuk, G., Petrella, R., Boulanger, J., Trudeau, L., Hegele, R.A., Woo, V., McFarlane, P., Vallee, M., Howlett, J., Bacon, S.L., Lindsay, P., Gilbert, R.E., Lewanczuk, R.Z., Tobe, S., Canadian Hypertension Educ Program, 2009. The 2009 Canadian hypertension education program recommendations for the management of hypertension: Part 2-therapy. Canadian Journal of Cardiology 25, 287-298.

Labuza, T.P., 1971. Kinetics of lipid oxidation in foods. CRC Critical Reviews in Food Technology 2, 355-405.

Li, M., Peng, J., Zhu, K., Guo, X., Zhang, M., Peng, W., Zhou, H., 2013. Delineating the microbial and physical-chemical changes during storage of ozone treated wheat flour. Innovative Food Science & Emerging Technologies 20, 223-229.

Licciardello, F., Giannone, V., Del Nobile, M.A., Muratore, G., Summo, C., Giarnetti, M., Caponio, F., Paradiso, V.M., Pasqualone, A., 2017. Shelf life assessment of industrial durum wheat bread as a function of packaging system. Food Chemistry 224, 181-190.

Liu, H., Liu, X., Ren, G., 2015. Analysis of volatile composition of Chinese oat wine and Chinese quinoa wine by headspace solid phase micro-extraction and gas chromatography-mass spectrometry. Science and Technology of Food Industry 4, 61-66.

Marti, A., Torri, L., Casiraghi, M.C., Franzetti, L., Limbo, S., Morandin, F., Quaglia, L., Pagani, M.A., 2014. Wheat germ stabilization by heat-treatment or sourdough fermentation: Effects on dough rheology and bread properties. LWT - Food Science and Technology 59, 1100-1106.

Ng, S., Anderson, A., Coker, J., Ondrus, M., 2007. Characterization of lipid oxidation products in quinoa (*Chenopodium quinoa*). Food Chemistry 101, 185-192.

Pico, J., Luis Bernal, J., Gomez, M., 2017. Influence of different flours and starches on gluten-free bread aroma. Journal of Food Science and Technology 54, 1433-1441.

Pomeranz, Y., 1988. Composition and functionality of wheat flour components. In: Pomeranz, Y. (Ed.), Wheat: Chemistry and Technology, third ed., vol. 2. American Association of Cereal Chemists, St. Paul, MN, pp. 219-370.

Robards, K., Kerr, A., Patsalides, E., 1988. Rancidity and its measurement in edible oils and snack foods - a review. Analyst 113, 213-224.

Seal, C.J., Brownlee, I.A., 2015. Whole-grain foods and chronic disease: evidence from epidemiological and intervention studies. Proceedings of the Nutrition Society 74, 313-319.

Sjovall, O., Virtalaine, T., Lapvetelainen, A., Kallio, H., 2000. Development of rancidity in wheat germ analyzed by headspace gas chromatography and sensory analysis. Journal of Agricultural and Food Chemistry 48, 3522-3527.

United States Department of Agriculture. National Nutrient Database for Standard Reference. http://ndb.nal.usda.gov/ndb/foods. Accessed June 6, 2017.

Xu, C., Chen, G., Xiong, Z., Fan, Y., Wang, X., Liu, Y., 2016. Applications of solid-phase microextraction in food analysis. Trends in Analytical Chemistry 80, 12-29.

Xu, J., Zhang, W., Adhikari, K., Shi, Y., 2017. Determination of volatile compounds in heat-treated straight-grade flours from normal and waxy wheats. Journal of Cereal Science 75, 77-83.

Yuan, Z., Zhang, Q., Ren, C., Zhu, Y., Yu, W., Wang, Q., 2016. Analysis of volatile compounds from whole wheat flour by headspace solid-phase microextraction-gas-chromatography-mass spectrometry. Journal of Chinese Institute of Food Science and Technology 16, 240-245.

Zhou, M., Robards, K., Glennie-Holmes, M., Helliwell, S., 1999. Analysis of volatile compounds and their contribution to flavor in cereals. Journal of Agricultural and Food Chemistry 47, 3941-3953.

APPENDIX A: EXPANDED LITERATURE REVIEW

The initial objective of this research was to develop a rapid method for predicting the shelf life of whole grain flours. The following research and method development sections include the information related to the initial objective.

USDA Guidelines Regarding Whole Grain Consumption

Current USDA guidelines recommend that at least half of all grains consumed should be whole grains (ChooseMyPlate). These government regulations come from many recent studies about the health effects of dietary fiber, which is found in whole grains. Fiber has been found to reduce blood cholesterol, to reduce the risk of heart disease, obesity and type II diabetes, and to give a feeling of fullness. The Adequate Intake value for fiber corresponds with the median value of fiber intake shown to lower the risk of coronary heart disease. The results published in the *Handbook of Dietary Fiber*, as mentioned by Slavin, affirmed that soluble fibers help lower blood cholesterol, which can have heart-healthy benefits. The same report also mentioned that an increased intake of dietary fiber could increase the levels of satiety, potentially helping with weight loss (Slavin, 2008). These desirable outcomes were also discussed by Khan (2009) in an article developed for the Canadian Hypertension Education Program which recommends "to prevent and treat hypertension … follow a diet that emphasizes dietary and soluble fiber, whole grains and protein from plant sources."

Factors Influencing Whole Wheat Flour Shelf Life

Variation in flour shelf life can be due to grain conditions prior to milling. The type of grain being milled, the time of harvest, amount of time between harvest and milling, and the moisture of the grain when milled all affect the flour. Additionally, the form of milling used and the particle size can effect shelf life. With all the factors that can affect shelf life, it is important to know which influence plays the largest role in the shelf life of whole wheat flour. Galliard (1986) indicated that the lipid oxidation occurs rapidly in stored whole wheat flour. Lipid oxidation is the most unstable factor affecting the shelf life of whole wheat flour and is the main reason flour loses functionality during storage (Doblado-Maldonado et al., 2012).

Whole-grain and Other Flour Product Storage Studies

Many studies have looked at the effect of storage on the chemical, physical, and/or sensory changes in different types of flour, including whole wheat, quinoa, fufu, oat, sorghum, walnut, cassava, einkorn, and pregerminated breadwheat (Abugoch et al., 2009; Becker and Hanners, 1990; Brandolini et al., 2009; Doblado-Maldonado et al., 2012; Labuckas et al., 2011; Meera et al., 2011; Molteberg et al., 1996; Nielsen and Hansen, 2008; Ng et al., 2007; Obadina et al., 2007; Ogungbenle, 2003). These studies provide useful information and entailed either an ambient condition shelf life study or an accelerated shelf life study. Many studies have looked at different flours including wheat, quinoa, amaranth, kaniwa, buckwheat, teff, sorghum, and millet, and mixtures of these flours in basic food matrices (Alvarez-Jubete et al., 2001; Bell et al., 1979; Chlopicka et al., 2012; Collar and Angioloni, 2014; Demir, 2014; Diaz et al., 2015; Elgeti et al., 2013; Hozova et al., 1997; Lee et al., 2006; Robin et al., 2015; Schoenlechner et al., 2010; Tait and Galliard, 1988). The studies looked at the physiological, sensory, and flavor changes to these products initially and after storage. Studies have also been done looking at how pretreating flours can increase the shelf life of various grain flours, including wheat, corn masa, millet, and quinoa (Brady et al., 2005; Marathe et al., 2002; Marquez-Castillo and Vidal-Quintanar, 2011; Nantanga et al., 2008; Rose et al., 2008). Grains have varying levels of unsaturated fatty acids and iron, which can greatly affect the shelf life of the whole grain flours.

Table 3 shows the lipid and iron levels of several traditional and "ancient" grains, as reported in the USDA National Nutrient Database (2017).

Table 3: Lipid and iron content of whole grains.

Grain	**Total Lipid (%)**	**Saturated Fatty Acids (%)**	**Monounsaturated Fatty Acids (%)**	**Polyunsaturated Fatty Acids (%)**	**Iron (mg/100 g)**
Quinoa	6.07	1.20	2.74	5.60	4.57
Amaranth	7.02	1.46	1.69	2.78	7.61
Whole Wheat	1.95	0.43	0.28	1.17	3.71
Spelt	2.43	0.41	0.45	1.26	4.44
Teff	2.38	0.45	0.59	1.07	7.63
Kamut	2.13	0.20	0.21	0.62	3.77
Chia	30.74	3.33	2.31	23.67	7.72
Millet	4.22	0.72	0.77	2.13	3.01
Sorghum	3.46	0.61	1.13	1.56	3.36

Correlation of OSI with Sensory Shelf Life

Previous studies have correlated sensory results with OSI values. In a study reported by Broadbent and Pike (2003), canola oil samples stored for an increasing number of days at 60°C were evaluated for nine days. The sensory scores were then correlated to the induction time found using a fresh sample and OSI. A similar study conducted by Coppin and Pike (2001) correlated sensory results with OSI of light-exposed soybean oil.

Use of Rancimat to Determine Stability of Whole Foods

Metrohm Inc. has published an application bulletin (Metrohm, 2015) that lists several solid foodstuffs that were evaluated using the Rancimat. Table 4 states the induction time for several such foodstuffs. The bulletin includes the method parameters and suggested sample size.

Table 4: Induction times for solid foodstuffs (Metrohm, 2015)

Sample	Induction time / h
Butter cookies	24.25
Muffins (Magdalenas)	10.23
Potato chips (crackers)	28.47
Peanut curls	8.19
Almonds	7.56
Peanuts	3.10
Instant noodles	16.81
Kitsune Udon noodles	15.12
Yakisoba noodles	21.02
Soup pearls	8.31
Hazelnuts	20.60
Potato chips (crackers, 140 °C)	9.20

Proposed Methods

Oil Stability Index is determined using a two vessel system (See Figure 5). One of the vessels contains the sample and is heated to a specific temperature. The other vessel contains a water trap. This water trap collects the volatiles formed in the first vessel and measures the changing conductivity. When the conductivity begins to change rapidly, this indicates the endpoint (See Figure 6). Once the endpoint has been determined, the induction time can then be calculated (Pike, 2001).

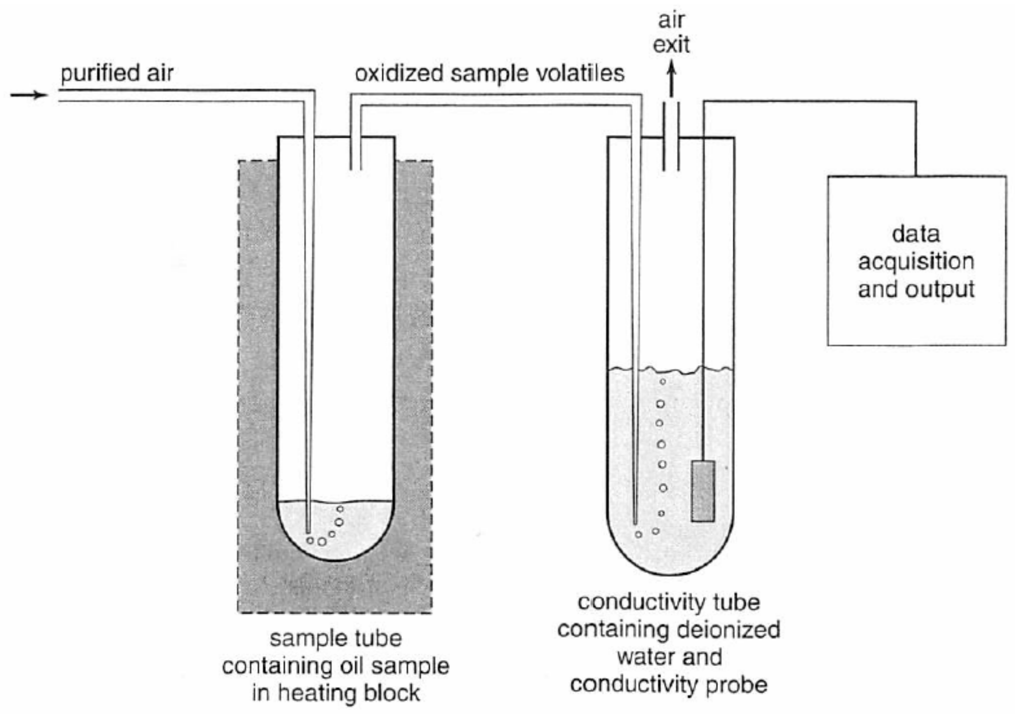

Figure 5: Schematic of Oil Stability Index apparatus

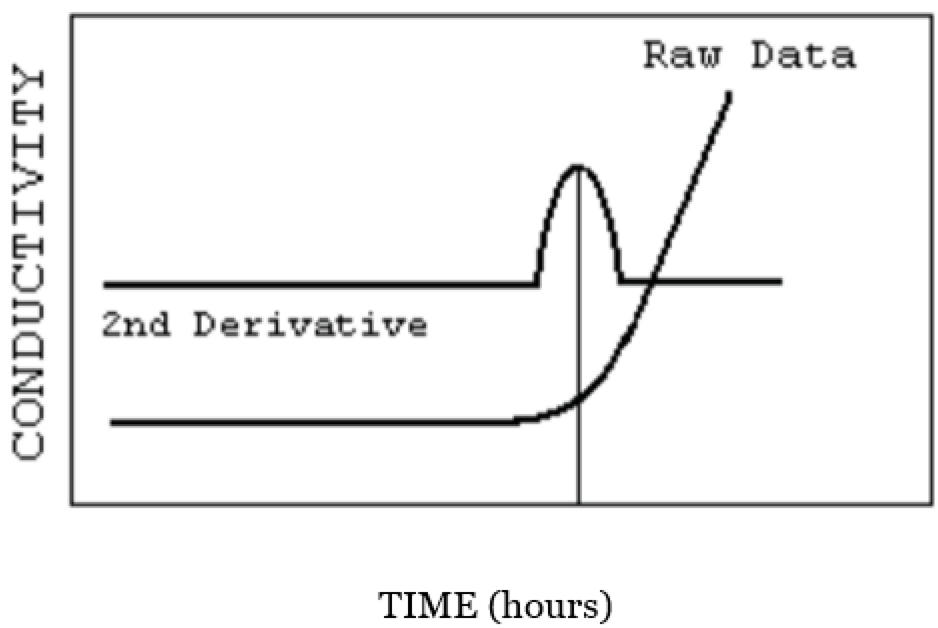

Figure 6: Determination of induction period

Gas Chromatography of Grain Products

Recent reviews have looked at the increasing number of studies done using solid-phase microextraction (SPME) to evaluate food (Kataoka et al., 2000; Xu et al., 2016). There have been many studies looking at the headspace volatiles present in cereal products baked with flours stored for various amounts of time (Ruiz et al., 2003; Jensen et al., 2011; Jensen and Risbo, 2005). There have also been studies identifying volatiles in millet powder (Wang et al., 2014), barley flour (Cramer et al., 2005), semolina (Beleggia et al., 2009), oat flour (Moltederg et al., 1996), and oat flakes (Klensporf and Jelen, 2008). One study investigated the volatiles present in whole wheat flour, but it did not look at correlation the volatile compounds to sensory data (Yuan 2016). An additional study looked at the volatile compounds in heat-treated wheat flour (Xu 2017).

Correlations Between Gas Chromatography and Descriptive Sensory

Studies have looked at the correlations between SPME-GC-MS data and descriptive sensory analysis for various products, including sour cream (Shepard et al., 2013), milk powder (Park and Drake, 2017), and extruded oats (Lampi et al., 2015).

Fatty Acid Profiles and Oxidation Mechanisms

Tables 5 and 6 show fatty acid profiles for wheat flour and quinoa, respectively, as reported in the USDA National Nutrient Database (2017).

Table 5: Wheat lipid fatty acid profile

Fatty Acid		Amount (g per 100 g of flour)
16:0	Hexadecanoic acid	0.410
18:0	Octadecanoic acid	0.020
18:1	9-octadecenoic acid	0.273
18:2	9,12-octadecadienoic acid	1.093
18:3	6,9,12-octadecenoic acid	0.073
20:1	9-eicosenoic acid	0.010

Table 6: Quinoa lipid fatty acid profile

Fatty Acid		Amount (g per 100 g of flour)
16:0	Hexadecanoic acid	0.600
18:0	Octadecanoic acid	0.037
18:1	9-octadecenoic acid	1.420
18:2	9,12-octadecadienoic acid	2.977
18:3	6,9,12-octadecenoic acid	0.260
20:0	Eicosanoic acid	0.030
20:1	9-eicosenoic acid	0.093
22:0	Docosanoic acid	0.030
22:1	13-docosenoic acid	0.083
22:6	DHA	0.047
24:0	Tetracosanoic acid	0.010
24:1	Nervonic acid	0.017

APPENDIX B: EXPANDED MATERIALS AND METHODS

Oil Stability Index

Whole wheat flour samples were evaluated using the Rancimat (Metrohm Inc.) instrument. The parameters used were based on application bulletins published by Metrohm (2015) and personal modifications determined from laboratory experiments.

Lipids were extracted from whole wheat flour using a modified version of the method described by Bekes et al. (1983). The solvent of hexane:isopropanol (3:2) was determined through experiment and the information from Bahrami et al. (2013). The effectiveness of the different methods and solvents was determined by comparing the fatty acid profiles determined using the sodium methoxide method (AOAC Method 969.33) with the profile from a Soxhlet extraction (AOAC Method 920.39C).

Rancimat Results for Whole Wheat Flour

Different parameters of the Rancimat method were altered to test the results using whole wheat flour. Figures 7 and 8 show the results from various tests. Despite several attempts to find a working method, none of the whole wheat flour samples produced typical oil stability index curves.

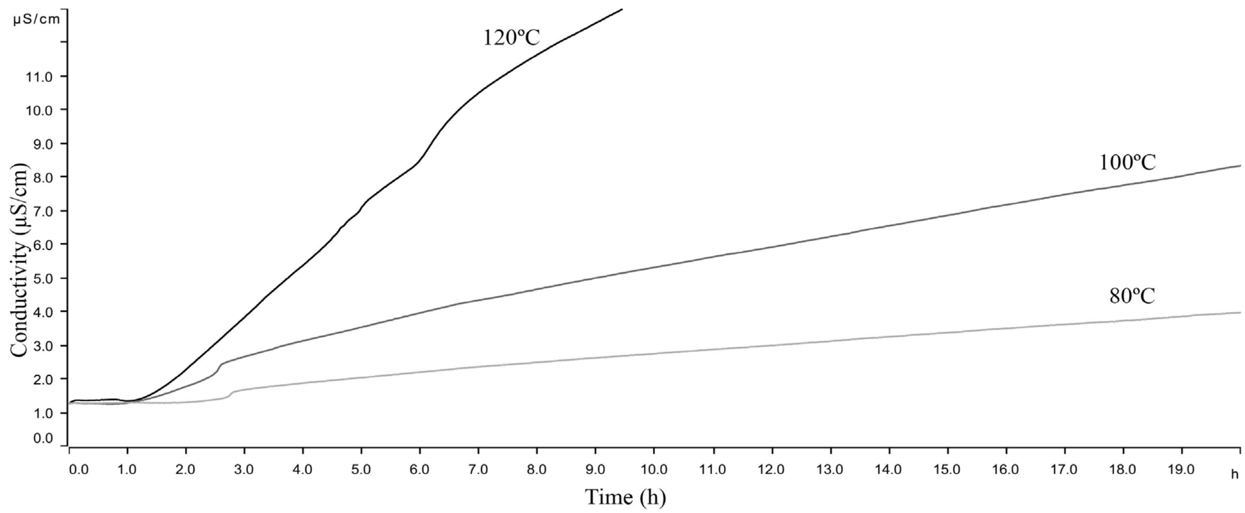

Figure 7: OSI plots of whole wheat flour at different Rancimat temperatures

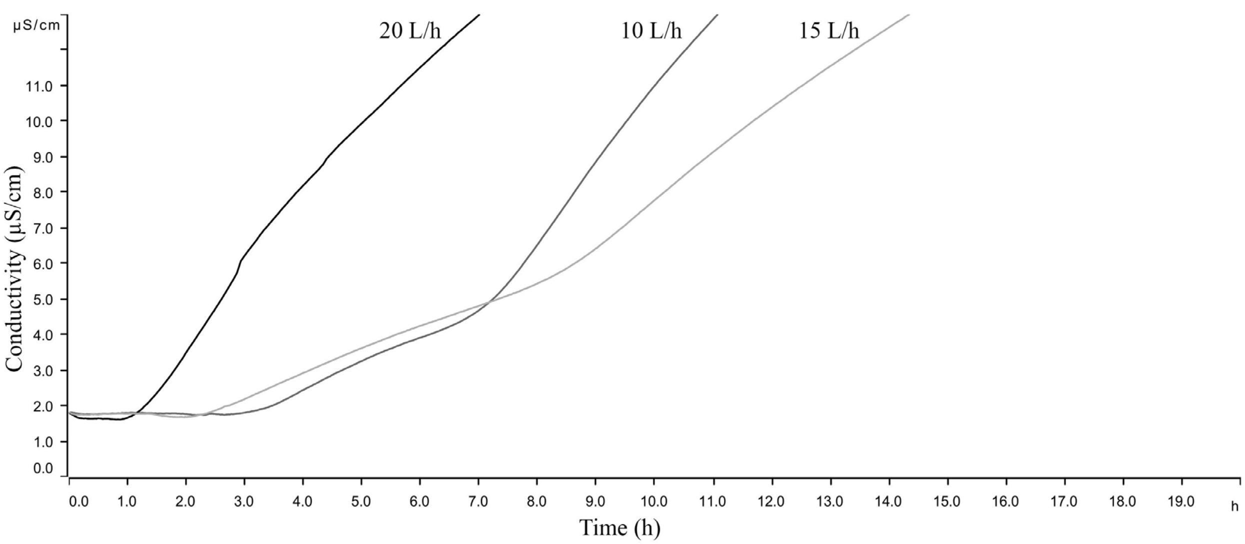

Figure 8: OSI plots of whole wheat flour at different Rancimat flow rates

Extraction Method

After determining that whole wheat flour could not be tested in the Rancimat, an attempt was made to determine the OIS of extracted wheat flour lipids. The lipid extraction method used was a modified version of Bekes et al. (1983). Since the method was modified, fatty acid profiles were run on the samples to determine if the results were the same as those from a Soxhlet extraction. These results are presented in Table 7.

Table 7: Fatty acid profiles for different lipid extraction methods

	Fatty Acid in Percentage							
Solvent	14:0	15:0	16:0	18:0	18:1	18:2	18:3	Total
USDA	0.00	0.00	21.94	1.07	14.61	58.48	3.91	100.00
Soxhlet 1	0.20	0.00	18.12	0.88	18.08	59.53	3.19	100.00
Soxhlet 2	0.18	0.19	17.64	0.89	19.25	58.61	3.25	100.00
Water-Saturated Butanol 1	0.19	0.00	20.90	0.72	13.55	61.47	3.16	100.00
Water-Saturated Butanol 2	0.25	0.20	19.94	0.73	14.53	61.22	3.14	100.00
Hexane:Isopropanol 1	0.17	0.00	16.58	0.73	16.58	62.54	3.40	100.00
Hexane:Isopropanol 2	0.13	0.00	16.71	0.76	16.64	62.43	3.33	100.00
Hexane:Isopropanol 12.5:1 3 hour 1	0.00	0.00	16.75	0.00	17.17	62.74	3.34	100.00
Hexane:Isopropanol 12.5:1 3 hour 2	0.20	0.00	16.91	0.71	16.30	62.53	3.34	100.00
Hexane:Isopropanol 6:1 3 hour 1	0.00	0.00	16.29	0.00	18.69	61.61	3.42	100.00
Hexane:Isopropanol 6:1 3 hour 2	0.00	0.00	15.95	0.00	19.34	61.23	3.47	100.00
Hexane:Isopropanol 6:1 .5 hour 2	0.00	0.00	16.76	0.00	18.70	61.22	3.32	100.00

Rancimat Results for Extraction Method

After the extraction method was established with a 6:1 solvent to flour ratio, oil was extracted from wheat flour. The results at different Rancimat parameters are shown in Figures 9 and 10.

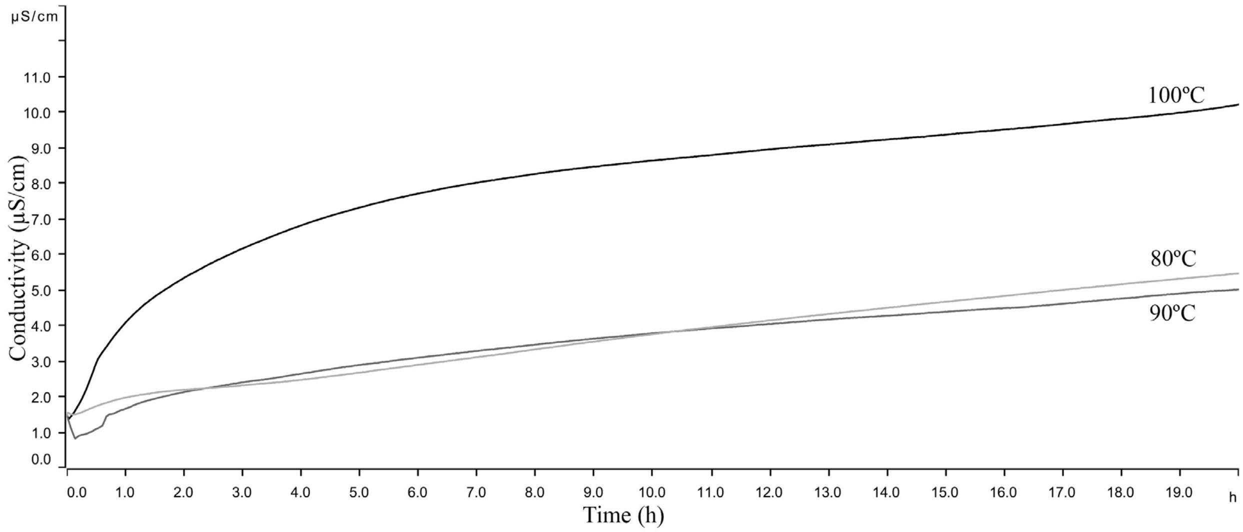

Figure 9: OSI plots of extracted whole wheat flour oil at different temperatures

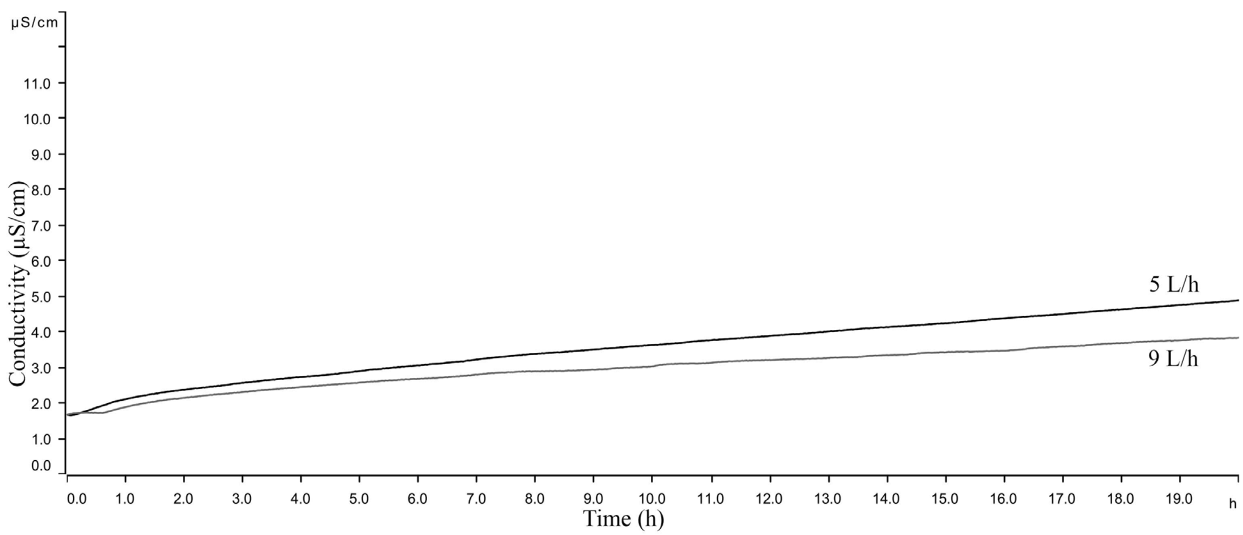

Figure 10: OSI plots of extracted whole wheat flour oil at different Rancimat flow rates

Even with extracting the lipids from the flours, no clear endpoint was observed. This led to the conclusion that an alternative instrumental method would be necessary to evaluate the flour samples.

APPENDIX C: EXPANDED REFERENCES

Abugoch, L., Castro, E., Tapia, C., Cristina Anon, M., Gajardo, P., Villarroel, A., 2009. Stability of quinoa flour proteins (*Chenopodium quinoa Willd*.) during storage. International Journal of Food Science and Technology 44, 2013-2020.

Alvarez-Jubete, L., Auty, M., Arendt, E.K., Gallagher, E., 2010. Baking properties and microstructure of pseudocereal flours in gluten-free bread formulations. European Food Research and Technology 230, 437-445.

AOCS. 2013. Official Methods and Recommended Practices of the American Oil Chemists' Society. Sampling and Analysis of Commercial Fats and Oils.

Arya, S., Parihar, D., 1981. Effect of moisture and temperature on storage changes in lipids and carotenoids of *Atta* (wheat-flour). Nahrung-Food 25, 121-126.

Bahrami, N., Yonekura, L., Linforth, R., Carbalho da Silva, M., Hill, S., Penson, S., Chope, G., Fisk, I.D., 2014. Comparison of ambient solvent extraction methods for the analysis of fatty acids in non-starch lipids of flour and starch. Journal of the Science of Food and Agriculture 94 (3), 415-423.

Becker, R., Hanners, G., 1990. Compositional and nutritional-evaluation of quinoa whole grain flour and mill fractions. LWT-Food Science and Technology 23, 441-444.

Bekes, F., Zawistowska, U., Bushuk, W., 1983. Protein-lipid complexes in the gliadin fraction. Cereal Chemistry 60(5), 371-378.

Beleggia, R., Platani, C., Spano, G., Monteleone, M., Cattivelli, L., 2009. Metabolic profiling and analysis of volatile composition of durum wheat semolina and pasta. Journal of Cereal Science 49, 301-309.

Bell, B.M., Chamberlain, N., Collins, T.H., Daniels, D.G.H., Fisher, N., 1979. The composition, rheological properties and breadmaking behaviour of stored flours. Journal of the Science of Food and Agriculture 30, 1111-1122.

Brady, K., Ho, C., Rosen, R.T., Sang, S., Karwe, M.V., 2007. Effects of processing on the nutraceutical profile of quinoa. Food Chemistry 100, 1209-1216.

Brandolini, A., Hidalgo, A., Plizzari, L., 2010. Storage-induced changes in einkorn (*Triticum monococcum L.*) and breadwheat (*Triticum aestivum L. ssp aestivum*) flours. Journal of Cereal Science 51, 205-212.

Broadbent, C., Pike, O., 2003. Oil Stability Index correlated with sensory determination of oxidative stability in canola oil. Journal of the American Oil Chemists Society 80, 59-63.

Chlopicka, J., Pasko, P., Gorinstein, S., Jedryas, A., Zagrodzki, P., 2012. Total phenolic and total flavonoid content, antioxidant activity and sensory evaluation of pseudocereal breads. LWT-Food Science and Technology 46, 548-555.

ChooseMyPlate. Grains. Available at http://www.choosemyplate.gov/food-groups/grains.html. Accessed March 30, 2015.

Collar, C., Angioloni, A., 2014. Pseudocereals and teff in complex breadmaking matrices: Impact on lipid dynamics. Journal of Cereal Science 59, 145-154.

Coppin, E., Pike, O., 2001. Oil stability index correlated with sensory determination of oxidative stability in light-exposed soybean oil. Journal of the American Oil Chemists Society 78, 13-18.

Cramer, A., Mattinson, D., Fellman, J., Baik, B., 2005. Analysis of volatile compounds from various types of barley cultivars. Journal of Agricultural and Food Chemistry 53, 7526-7531.

Demir, M.K., 2014. Use of quinoa Flour in the production of gluten-free tarhana. Food Science and Technology Research 20, 1087-1092.

Diaz, J.M.R., Suuronen, J., Deegan, K.C., Serimaa, R., Tuorila, H., Jouppila, K., 2015. Physical and sensory characteristics of corn-based extruded snacks containing amaranth, quinoa and kaniwa flour. LWT-Food Science and Technology 64, 1047-1056.

Doblado-Maldonado, A.F., Pike, O.A., Sweley, J.C., Rose, D.J., 2012. Key issues and challenges in whole wheat flour milling and storage. Journal of Cereal Science 56, 119-126.

Elgeti, D., Nordlohne, S.D., Foeste, M., Besl, M., Linden, M.H., Heinz, V., Jekle, M., Becker, T., 2014. Volume and texture improvement of gluten-free bread using quinoa white flour. Journal of Cereal Science 59, 41-47.

Galliard, T., 1986. Hydrolytic and oxidative-degradation of lipids during storage of wholemeal flour - effects of bran and germ components. Journal of Cereal Science 4, 179-192.

Hozova, B., Buchtova, V., Dodok, L., Zemanovic, J., 1997. Microbiological, nutritional and sensory aspects of stored amaranth biscuits and amaranth crackers. Nahrung-Food 41, 155-158.

Jensen, S., Ostdal, H., Skibsted, L.H., Thybo, A.K., 2011. Antioxidants and shelf life of whole wheat bread. Journal of Cereal Science 53, 291-297.

Jensen, P.N., Risbo, J., 2007. Oxidative stability of snack and cereal products in relation to moisture sorption. Food Chemistry 103, 717-724.

Kataoka, H., Lord, H.L., Pawliszyn, J., 2000. Applications of solid-phase microextraction in food analysis. Journal of Chromatography A 880, 35-62.

Khan, N.A., Hernmelgarn, B., Herman, R.J., Bell, C.M., Mahon, J.L., Leiter, L.A., Rahkin, S.W., Hill, M.D., Padwal, R., Touyz, R.M., Larochelle, P., Feldman, R.D., Schiffrin, E.L., Campbell, N.R.C., Moe, G., Prasad, R., Arnold, M.O., Campbell, T.S., Milot, A., Stone, J.A., Jones, C., Ogilvie, R.I., Hamet, P., Fodor, G., Carruthers, G., Burns, K.D., Ruzicka, M., deChamplain, J., Pylypchuk, G., Petrella, R., Boulanger, J., Trudeau, L., Hegele, R.A., Woo, V., McFarlane, P., Vallee, M., Howlett, J., Bacon, S.L., Lindsay, P., Gilbert, R.E., Lewanczuk, R.Z., Tobe, S., Canadian Hypertension Educ Program, 2009. The 2009 Canadian hypertension education program recommendations for the management of hypertension: Part 2-therapy. Canadian Journal of Cardiology 25, 287-298.

Klensporf, D., Jeleń, H.H., 2008. Effect of heat treatment on the flavor of oat flakes. Journal of Cereal Science 48, 656-661.

Labuckas, D., Maestri, D., Lamarque, A., 2011. Lipid and protein stability of partially defatted walnut flour (Juglans regia L.) during storage. International Journal of Food Science and Technology 46, 1388-1397.

Lee, Y., Lee, J., Choe, E., 2006. Effects of flour storage conditions on the lipid oxidation of fried products during storage in the dark. Food Science and Biotechnology 15, 399-403.

Marathe, S., Machaiah, J., Rao, B., Pednekar, M., Rao, V., 2002. Extension of shelf life of whole-wheat flour by gamma radiation. International Journal of Food Science and Technology 37, 163-168.

Marquez-Castillo, A., Vidal-Quintanar, R.L., 2011. Improvements in the shelf life of commercial corn dry masa flour (CMF) by reducing lipid oxidation. Journal of Food Science 76, C236-C241.

Meera, M.S., Bhashyam, M.K., Ali, S.Z., 2011. Effect of heat treatment of sorghum grains on storage stability of flour. LWT-Food Science and Technology 44, 2199-2204.

Metrohm, 2015. Oxidation stability of fats and oils in solid foodstuffs – Rancimat method. Accessed online 6 Nov 2015. http://partners.metrohm.com/GetDocument?action=get_dms_document&docid=1669519

Molteberg, E., Magnus, E., Bjorge, J., Nilsson, A., 1996. Sensory and chemical studies of lipid oxidation in raw and heat-treated oat flours. Cereal Chemistry 73, 579-587.

Nantanga, K.K.M., Seetharaman, K., de Kock, H.L., Taylor, J.R.N., 2008. Thermal treatments to partially pre-cook and improve the shelf life of whole pearl millet flour. Journal of the Science of Food and Agriculture 88, 1892-1899.

Ng, S., Anderson, A., Coker, J., Ondrus, M., 2007. Characterization of lipid oxidation products in quinoa (*Chenopodium quinoa*). Food Chemistry 101, 185-192.

Nielsen, M.M., Hansen, A., 2008. Stability of vitamin E in wheat flour and whole wheat flour During storage. Cereal Chemistry 85, 716-720.

Obadina, A.O., Oyewole, O.B., Odubay, M.O., 2007. Effect of storage on the safety and quality of fufu flour. Journal of Food Safety 27, 148-156.

Ogungbenle, H., 2003. Nutritional evaluation and functional properties of quinoa (*Chenopodium quinoa*) flour. International journal of food sciences and nutrition 54, 153-158.

Park, C.W., Drake, M., The effect of homogenization pressure on the flavor and flavor stability of whole milk powder. Journal of Dairy Science, in press.

Pike, Oscar A., 2001. Assessment of Oxidative Stability of Lipids. Current Protocols in Food Analytical Chemistry. Editors John Wiley & Sons, Inc.

Robin, F., Théoduloz, C., Srichuwong, S., 2015. Properties of extruded whole grain cereals and pseudocereals flours. International Journal of Food Science & Technology 50, 2152-2159.

Rose, D.J., Ogden, L.V., Dunn, M.L., Pike, O.A., 2008. Enhanced lipid stability in whole wheat flour by lipase inactivation and antioxidant retention. Cereal Chemistry 85, 218-223.

Ruiz, J., Quilez, J., Mestres, M., Guasch, J., 2003. Solid-phase microextraction method for headspace analysis of volatile compounds in bread crumb. Cereal Chemistry 80, 255-259.

Schoenlechner, R., Wendner, M., Siebenhandl-Ehn, S., Berghofer, E., 2010. Pseudocereals as alternative sources for high folate content in staple foods. Journal of cereal science 52, 475-479.

Shepard, L., Miracle, R.E., Leksrisompong, P., Drake, M.A., 2013. Relating sensory and chemical properties of sour cream to consumer acceptance. Journal of Dairy Science 96, 5435-5454.

Slavin, J.L., 2008. Position of the American Dietetic Association: health implications of dietary fiber. Journal of the American Dietetic Association 108, 1716-1731.

Tait, S., Galliard, T., 1988. Oxidation of linoleic-acid in doughs and aqueous suspensions of wholemeal flours - effects of storage. Journal of Cereal Science 8, 55-67.

United States Department of Agriculture. National Nutrient Database for Standard Reference. http://ndb.nal.usda.gov/ndb/foods.

Wang, R., Chen, Y., Ren, J., Guo, S., 2014. Aroma stability of millet powder during storage and effects of cooking methods and antioxidant treatment. Cereal Chemistry 91, 262-269.

Xu, C., Chen, G., Xiong, Z., Fan, Y., Wang, X., Liu, Y., 2016. Applications of solid-phase microextraction in food analysis. Trends in Analytical Chemistry 80, 12-29.

Xu, J., Zhang, W., Adhikari, K., Shi, Y., 2017. Determination of volatile compounds in heat-treated straight-grade flours from normal and waxy wheats. Journal of Cereal Science 75, 77-83.

Yuan, Z., Zhang, Q., Ren, C., Zhu, Y., Yu, W., Wang, Q., 2016. Analysis of volatile compounds from whole wheat flour by headspace solid-phase microextraction-gas-chromatography-mass spectrometry. Journal of Chinese Institute of Food Science and Technology 16, 240-245.

APPENDIX D: SAMPLE BALLOT

Name ____________________

Date __May 17____________

Descriptive Analysis of Quinoa Flour Odor, Final

Scale:

0 = None detected	6-10 = Moderate	
1-5 = Slight	11-15 = Extreme	

1. Sniff arm
2. Shake cup
3. Open lid partway
4. Thorough initial sniff

Quinoa Flour

Reference Samples	Grassy - 10 (G10)	Cardboard - 5 (C5)	Musty - 8 (M8)
Sample	Grassy	Cardboard/Stale	Musty
925	___________	___________	___________
630	___________	___________	___________
356	___________	___________	___________
294	___________	___________	___________

APPENDIX E: ADDITIONAL GAS CHROMATOGRAM DATA

Table 8: Sample printout of MS library search of chromatographic data

```
Library Search Report
Data Path : C:\msdchem\1\DATA\
Data File : WHOLEWHEAT-33.D
Acq On : 29 Mar 2017 21:00
Operator :
Sample : WT00C
Misc :
ALS Vial : 8 Sample Multiplier: 1
Search Libraries: C:\Database\W8N08.L Minimum Quality: 0
Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - flavor.e
Pk# RT Area% Library/ID Ref# CAS# Qual
_____________________________________________________________________________
1 1.249 2.21 C:\Database\W8N08.L
No name... 5740 000000-00-0 2
3-(3-OXO-3H-BENZO[F]CHROMEN-2-YL)- 7476 999007-47-7 2
2,4(1H,3H)-QUINOLINEDIONE $$ 4-HYD
ROXY-3-(2-OXO-2H-1-OXA-3-PHENANTHR
YL)-2(1H)-QUINOLINONE
[1,1'-BIBICYCLO[2.2.2]OCTANE]-4-CA 7416 074467-50-8 1
RBOXYLIC ACID $$ 1,1'-BIBICYCLO(2.
2.2)OCTYL-4-CARBOXYLIC ACID
2 1.327 17.71 C:\Database\W8N08.L
AMMONIA $$ AM-FOL $$ AMMONEMIA $$ 197 007664-41-7 2
AMMONIA (8CI,9CI)
METHANE-D1 $$ MONODEUTEROMETHANE 195 000676-49-3 2
AMMONIA $$ AM-FOL $$ AMMONEMIA $$ 196 007664-41-7 2
AMMONIA (8CI,9CI)
3 1.400 72.89 C:\Database\W8N08.L
.ALPHA.,.BETA.-D3-ETHYLENE $$ CD2= 5068 002680-01-5 5
CDH $$ ETHENE-D3 $$ ETHYLENE-D3
2-AMINO-1-PROPANOL $$ 1-PROPANOL, 5205 006168-72-5 4
2-AMINO- $$ 1-PROPANOL, 2-AMINO-,
(.+-.)- $$ 2-AMINOPROPAN-1-OL
Methyl Alcohol $$ Methanol $$ Carb 5072 000067-56-1 4
inol $$ Methyl hydroxide
4 15.418 1.10 C:\Database\W8N08.L
1-HEXANOL $$ HEXAN-1-OL $$ 1-HEXAN 62406 000111-27-3 83
O $$ 1-HEXANOL, ALUMINUM SALT
1-Hexanol $$ Hexyl alcohol $$ n-He 62395 000111-27-3 83
xan-1-ol $$ n-Hexanol
FORMIC ACID, HEXYL ESTER $$ HEXYL 62941 000629-33-4 83
FORMATE $$ HEXYL METHANOATE $$ N-H
EXYL FORMATE
5 18.915 1.46 C:\Database\W8N08.L
3-Hexanone, 2,5-dimethyl- $$ Isobu 66287 001888-57-9 91
tyl isopropyl ketone $$ 2,5-Dimeth
yl-3-hexanone
3-HEPTANONE, 2-METHYL- $$ 2-METHYL 66384 013019-20-0 91
HEPTAN-3-ONE $$ 2-METHYL-3-HEPTANO
NE $$ 2-METHYL-HEPTAN-3-ONE
```

3-Heptanone, 2-methyl- $$ 2-Methyl 66285 013019-20-0 91
-3-heptanone $$ 2-Methylheptanone-
(3)
6 30.131 0.25 C:\Database\W8N08.L
UNDECANE $$ HENDECANE $$ N-C11H24 23743 001120-21-4 72
$$ N-UNDECANE
DODECANE $$ ACETIC ACID 3-HYDROXY- 25222 000112-40-3 64
7-ISOPROPENYL-1,4A-DIMETHYL-2,3,4,
4A,5,6,7,8-OCTAHYDRO-NAP $$ ADAKAN
E 12 $$ BA 51-090453
PENTADECANE $$ CH3(CH2)13CH3 $$ N- 29073 000629-62-9 64
PENTADECANE
7 33.616 0.61 C:\Database\W8N08.L
1-NONANOL $$ NONANOL $$ NONAN-1-OL 63202 000143-08-8 91
$$ 1-HYDROXYNONANE
1-NONANOL $$ NONANOL $$ NONAN-1-OL 63211 000143-08-8 90
$$ 1-HYDROXYNONANE
1-NONANOL $$ NONANOL $$ NONAN-1-OL 9799 000143-08-8 86
$$ 1-HYDROXYNONANE
8 43.198 2.02 C:\Database\W8N08.L
Hexadecanoic acid, methyl ester $$ 121184 000112-39-0 97
Palmitic acid, methyl ester $$ n-
Hexadecanoic acid methyl ester $$
Metholene 2216
HEXADECANOIC ACID, METHYL ESTER $$ 121192 000112-39-0 97
METHYL HEXADECANOATE $$ PALMITIC
ACID METHYL ESTER $$ EMERY 2216
Hexadecanoic acid, methyl ester $$ 121186 000112-39-0 97
Palmitic acid, methyl ester $$ n-
Hexadecanoic acid methyl ester $$
Metholene 2216
9 43.813 1.01 C:\Database\W8N08.L
METHYL (9E,12E)-9,12-OCTADECADIENO 92651 002566-97-4 83
ATE $$ 9,12-OCTADECADIENOIC ACID,
METHYL ESTER, (E,E)- $$ LINOLELAID
IC ACID, METHYL ESTER $$ METHYL (9
E,12E)-OCTADECA-9,12-DIENOATE
9,12-Octadecadienoic acid, methyl 92605 002566-97-4 83
ester, (E,E)- $$ Linolelaidic acid
, methyl ester $$ Methyl linolelai
date $$ Methyl trans,trans-9,12-oc
tadecadienoate
METHYL (9E,12E)-9,12-OCTADECADIENO 92652 002566-97-4 81
ATE $$ 9,12-OCTADECADIENOIC ACID,
METHYL ESTER, (E,E)- $$ LINOLELAID
IC ACID, METHYL ESTER $$ METHYL (9
E,12E)-OCTADECA-9,12-DIENOATE
10 44.132 0.61 C:\Database\W8N08.L
2-HYDROXYCYCLOPENTADECANONE $$ CYC 58886 004727-18-8 45
LOPENTADECANONE, 2-HYDROXYCyclopentadecanone,
2-hydroxy- $$ 58836 004727-18-8 45
2-Hydroxycyclopentadecanone #
9-OCTADECEN-1-OL, (Z)- $$ OCTADEC- 59505 000143-28-2 22
9-EN-1-OL $$ (9Z)-9-OCTADECEN-1-OL
$$ (Z)-9-OCTADECEN-1-OL

11 44.636 0.14 C:\Database\W8N08.L
OCTADECANOIC ACID, METHYL ESTER $$ 121372 000112-61-8 90
METHYL OCTADECANOATE $$ STEARIC A
CID METHYL ESTER $$ EMERY 2218
METHYL ICOSANOATE $$ EICOSANOIC AC 121518 001120-28-1 90
ID, METHYL ESTER $$ ARACHIDIC ACID
METHYL ESTER $$ EICOSANOIC ACID M
ETHYL ESTER
UNDECANOIC ACID, METHYL ESTER $$ M 120836 001731-86-8 86
ETHYL UNDECANOATE $$ METHYL ESTER
OF UNDECANOIC ACID $$ METHYL HENDE
CANOATE

flavor-7.M Tue Apr 11 12:55:09 2017

Table 9: Sample printout of GC results from chromatographic data

Name= C:\MSDCHEM\1\DATA\WHOLEWHEAT-33.D
1= INT TIC: WHOLEWHEAT-33.D\data.ms
[INT TIC: WHOLEWHEAT-33.D\data.ms]
Time= Wed Mar 29 21:44:39 2017

Header=	Peak	R.T.	First	Max	Last	PK TY	Height	Area	Pct Max	Pct Total
1=	1	1.251	13	30	35	BV	593006	5747201	3.03	2.206
2=	2	1.326	35	44	54	PV	1650692	46149576	24.3	17.712
3=	3	1.4	54	57	542	VB	3694481	1.9E+08	100	72.888
4=	4	15.418	2537	2563	2606	BB 3	64333	2868194	1.51	1.101
5=	5	18.918	3159	3189	3214	BB	127084	3797830	2	1.458
6=	6	30.133	5138	5193	5218	BB 8	15232	639116	0.34	0.245
7=	7	33.614	5800	5816	5858	BV 7	33108	1592287	0.84	0.611
8=	8	43.199	7486	7529	7577	BB 3	123270	5257453	2.77	2.018
9=	9	43.816	7603	7639	7673	BV 3	33696	2633340	1.39	1.011
10=	10	44.132	7673	7696	7728	VV 3	22179	1601632	0.84	0.615
11=	11	44.634	7764	7786	7809	BB 4	15509	355015	0.19	0.136

Table 10: Relative abundances of whole wheat flour volatiles – raw data

	1-hexanol	2-pentyl furan	Phenol	Hexanoic acid	Hexanal	1-pentanol
WT00A	45.37	ND	ND	ND	ND	ND
WT00B	43.18	ND	ND	ND	ND	ND
WT00C	60.42	ND	ND	ND	ND	ND
WT04A	45.35	12.60	ND	ND	ND	ND
WT04B	51.26	12.58	ND	ND	ND	ND
WT04C	73.36	20.12	ND	ND	ND	ND
WT08A	90.45	29.32	35.55	52.23	ND	ND
WT08B	105.64	29.42	19.69	60.50	ND	ND
WT08C	149.50	48.29	49.30	74.22	ND	ND
WT12A	114.73	46.83	67.89	133.72	16.53	ND
WT12B	119.56	50.66	58.11	107.01	14.46	ND
WT12C	171.69	78.05	116.17	148.42	27.16	ND
WT16A	164.71	93.25	124.82	297.06	47.30	25.55
WT16B	160.95	75.76	92.46	272.02	36.03	23.53
WT16C	198.86	114.76	132.59	439.00	70.91	28.87
WT20A	148.53	88.19	100.07	395.89	53.20	22.05
WT20B	127.76	78.80	88.87	328.45	40.40	23.51
WT20C	131.84	82.32	116.90	306.58	44.35	21.19
WT24A	215.45	121.45	62.96	459.26	57.13	28.83
WT24B	204.28	114.95	62.88	349.75	45.72	26.06
WT24C	225.91	124.19	63.76	390.83	57.11	29.62

Table 11: Relative abundances of quinoa flour volatiles – raw data

	1-hexanol	2-pentyl furan	Phenol	Hexanal	1-pentanol	1-octanol	1-nonanol	Nonanal	Decanal	2,4-nonadienal	2-undecenal
QT00A	48.96	ND	ND	ND	ND	ND	34.71	ND	ND	ND	ND
QT00B	49.26	ND	ND	ND	ND	ND	36.24	ND	ND	ND	ND
QT00C	61.26	ND	ND	ND	ND	ND	36.49	ND	ND	ND	ND
QT04A	34.14	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
QT04B	31.80	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
QT04C	37.39	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
QT08A	151.51	27.68	86.91	ND	ND	ND	ND	ND	ND	ND	ND
QT08B	163.69	32.22	82.68	ND	ND	ND	ND	ND	ND	ND	ND
QT08C	178.78	51.85	145.90	ND	ND	ND	ND	ND	ND	ND	ND
QT12A	270.13	105.00	114.82	171.41	35.38	55.71	58.62	ND	ND	ND	ND
QT12B	245.05	105.80	109.46	172.55	33.68	57.96	58.47	ND	ND	ND	ND
QT12C	473.90	215.97	91.70	182.27	49.43	90.58	84.74	ND	ND	ND	ND
QT16A	315.66	ND	159.38	1068.96	91.20	147.21	165.78	245.56	95.26	122.77	135.12
QT16B	339.14	ND	138.57	1143.05	117.95	161.70	178.23	250.88	94.00	115.49	115.03
QT16C	278.85	ND	160.09	975.67	87.73	132.02	175.24	216.22	90.36	120.07	131.14
QT20A	190.89	ND	176.20	1554.82	105.82	166.29	ND	395.81	192.74	159.32	197.45
QT20B	176.81	ND	189.90	1764.98	116.57	199.73	ND	446.71	210.14	195.26	232.79
QT20C	211.61	ND	190.38	1712.56	120.01	195.99	ND	423.98	204.42	195.37	234.68
QT24A	247.68	ND	115.19	1224.09	81.22	147.11	ND	323.81	226.65	107.82	207.14
QT24B	254.18	ND	103.16	1188.72	83.93	162.53	ND	329.49	193.15	125.01	232.45
QT24C	255.87	ND	93.23	983.60	79.96	129.34	ND	267.75	167.40	106.41	198.20

APPENDIX F: STATISTICAL ANALYSIS

The SAS System
Wheat analysis for _1_pentanol

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	_1_pentanol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System
Wheat analysis for _1_pentanol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	4.0522

Fit Statistics	
-2 Res Log Likelihood	28.7
AIC (Smaller is Better)	30.7
AICC (Smaller is Better)	31.7
BIC (Smaller is Better)	30.5

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	6.63	0.0302

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	25.9848	1.1622	6	22.36	<.0001
Week	20	22.2533	1.1622	6	19.15	<.0001
Week	24	28.1708	1.1622	6	24.24	<.0001

The SAS System

Wheat analysis for _1_pentanol

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	3.7315	1.6436	6	2.27	0.0636	Tukey	0.1368
Week	16	24	-2.1860	1.6436	6	-1.33	0.2318	Tukey	0.4310
Week	20	24	-5.9174	1.6436	6	-3.60	0.0114	Tukey	0.0264

The SAS System
Wheat analysis for hexanal

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	hexanal
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	5
Columns in Z	0
Subjects	1
Max Obs per Subject	12

Number of Observations	
Number of Observations Read	21
Number of Observations Used	12
Number of Observations Not Used	9

The SAS System
Wheat analysis for hexanal

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	112.40

Fit Statistics	
-2 Res Log Likelihood	64.9
AIC (Smaller is Better)	66.9
AICC (Smaller is Better)	67.5
BIC (Smaller is Better)	67.0

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	3	8	6.61	0.0147

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	12	19.3829	6.1209	8	3.17	0.0133
Week	16	51.4153	6.1209	8	8.40	<.0001
Week	20	45.9832	6.1209	8	7.51	<.0001
Week	24	53.3208	6.1209	8	8.71	<.0001

The SAS System
Wheat analysis for hexanal

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	12	16	-32.0324	8.6563	8	-3.70	0.0060	Tukey	0.0250
Week	12	20	-26.6003	8.6563	8	-3.07	0.0153	Tukey	0.0600
Week	12	24	-33.9379	8.6563	8	-3.92	0.0044	Tukey	0.0185
Week	16	20	5.4321	8.6563	8	0.63	0.5478	Tukey	0.9203
Week	16	24	-1.9055	8.6563	8	-0.22	0.8313	Tukey	0.9959
Week	20	24	-7.3376	8.6563	8	-0.85	0.4213	Tukey	0.8307

The SAS System
Wheat analysis for _1_hexanol

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	_1_hexanol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	8
Columns in Z	0
Subjects	1
Max Obs per Subject	21

Number of Observations	
Number of Observations Read	21
Number of Observations Used	21
Number of Observations Not Used	0

The SAS System
Wheat analysis for _1_hexanol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	416.85

Fit Statistics	
-2 Res Log Likelihood	131.9
AIC (Smaller is Better)	133.9
AICC (Smaller is Better)	134.2
BIC (Smaller is Better)	134.5

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	6	14	25.53	<.0001

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	0	49.6569	11.7877	14	4.21	0.0009
Week	4	56.6558	11.7877	14	4.81	0.0003
Week	8	115.20	11.7877	14	9.77	<.0001

The SAS System
Wheat analysis for _1_hexanol

The Mixed Procedure

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	12	135.33	11.7877	14	11.48	<.0001
Week	16	174.84	11.7877	14	14.83	<.0001
Week	20	136.04	11.7877	14	11.54	<.0001
Week	24	215.22	11.7877	14	18.26	<.0001

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	0	4	-6.9989	16.6703	14	-0.42	0.6810	Tukey	0.9994
Week	0	8	-65.5394	16.6703	14	-3.93	0.0015	Tukey	0.0197
Week	0	12	-85.6689	16.6703	14	-5.14	0.0002	Tukey	0.0022
Week	0	16	-125.18	16.6703	14	-7.51	<.0001	Tukey	<.0001
Week	0	20	-86.3866	16.6703	14	-5.18	0.0001	Tukey	0.0021
Week	0	24	-165.56	16.6703	14	-9.93	<.0001	Tukey	<.0001
Week	4	8	-58.5405	16.6703	14	-3.51	0.0035	Tukey	0.0420
Week	4	12	-78.6700	16.6703	14	-4.72	0.0003	Tukey	0.0047
Week	4	16	-118.18	16.6703	14	-7.09	<.0001	Tukey	<.0001

The SAS System

Wheat analysis for _1_hexanol

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	4	20	-79.3877	16.6703	14	-4.76	0.0003	Tukey	0.0043
Week	4	24	-158.56	16.6703	14	-9.51	<.0001	Tukey	<.0001
Week	8	12	-20.1295	16.6703	14	-1.21	0.2472	Tukey	0.8801
Week	8	16	-59.6436	16.6703	14	-3.58	0.0030	Tukey	0.0373
Week	8	20	-20.8472	16.6703	14	-1.25	0.2316	Tukey	0.8627
Week	8	24	-100.02	16.6703	14	-6.00	<.0001	Tukey	0.0005
Week	12	16	-39.5141	16.6703	14	-2.37	0.0327	Tukey	0.2791
Week	12	20	-0.7177	16.6703	14	-0.04	0.9663	Tukey	1.0000
Week	12	24	-79.8897	16.6703	14	-4.79	0.0003	Tukey	0.0041
Week	16	20	38.7964	16.6703	14	2.33	0.0355	Tukey	0.2967
Week	16	24	-40.3756	16.6703	14	-2.42	0.0296	Tukey	0.2589
Week	20	24	-79.1720	16.6703	14	-4.75	0.0003	Tukey	0.0045

The SAS System

Wheat analysis for hexanoic_acid__methyl_ester

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	hexanoic_acid__methyl_ester
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	5
Columns in Z	0
Subjects	1
Max Obs per Subject	12

Number of Observations	
Number of Observations Read	21
Number of Observations Used	12
Number of Observations Not Used	9

The SAS System

Wheat analysis for hexanoic_acid__methyl_ester

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	19.8777

Fit Statistics	
-2 Res Log Likelihood	51.0
AIC (Smaller is Better)	53.0
AICC (Smaller is Better)	53.7
BIC (Smaller is Better)	53.1

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	3	8	21.79	0.0003

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	12	20.3303	2.5741	8	7.90	<.0001
Week	16	40.7931	2.5741	8	15.85	<.0001
Week	20	44.0059	2.5741	8	17.10	<.0001
Week	24	46.7758	2.5741	8	18.17	<.0001

The SAS System

Wheat analysis for hexanoic_acid__methyl_ester

The Mixed Procedure

Differences of Least Squares Means									
Effect	Week	Week	Estimate	Standard Error	DF	t Value	Pr > |t|	Adjustment	Adj P
Week	12	16	-20.4628	3.6403	8	-5.62	0.0005	Tukey	0.0022
Week	12	20	-23.6756	3.6403	8	-6.50	0.0002	Tukey	0.0008
Week	12	24	-26.4455	3.6403	8	-7.26	<.0001	Tukey	0.0004
Week	16	20	-3.2128	3.6403	8	-0.88	0.4032	Tukey	0.8140
Week	16	24	-5.9827	3.6403	8	-1.64	0.1389	Tukey	0.4091
Week	20	24	-2.7699	3.6403	8	-0.76	0.4686	Tukey	0.8697

The SAS System

Wheat analysis for phenol

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	phenol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	6
Columns in Z	0
Subjects	1
Max Obs per Subject	15

Number of Observations	
Number of Observations Read	21
Number of Observations Used	15
Number of Observations Not Used	6

The SAS System
Wheat analysis for phenol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	367.62

Fit Statistics	
-2 Res Log Likelihood	92.9
AIC (Smaller is Better)	94.9
AICC (Smaller is Better)	95.4
BIC (Smaller is Better)	95.2

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	4	10	8.45	0.0030

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	8	34.8474	11.0698	10	3.15	0.0104
Week	12	80.7238	11.0698	10	7.29	<.0001
Week	16	116.62	11.0698	10	10.53	<.0001
Week	20	101.95	11.0698	10	9.21	<.0001
Week	24	63.1985	11.0698	10	5.71	0.0002

The SAS System
Wheat analysis for phenol

The Mixed Procedure

Differences of Least Squares Means									
Effect	Week	Week	Estimate	Standard Error	DF	t Value	Pr > |t|	Adjustment	Adj P
Week	8	12	-45.8764	15.6551	10	-2.93	0.0150	Tukey	0.0873
Week	8	16	-81.7733	15.6551	10	-5.22	0.0004	Tukey	0.0028
Week	8	20	-67.0991	15.6551	10	-4.29	0.0016	Tukey	0.0108
Week	8	24	-28.3511	15.6551	10	-1.81	0.1002	Tukey	0.4184
Week	12	16	-35.8969	15.6551	10	-2.29	0.0448	Tukey	0.2238
Week	12	20	-21.2227	15.6551	10	-1.36	0.2050	Tukey	0.6662
Week	12	24	17.5253	15.6551	10	1.12	0.2891	Tukey	0.7933
Week	16	20	14.6742	15.6551	10	0.94	0.3707	Tukey	0.8760
Week	16	24	53.4222	15.6551	10	3.41	0.0066	Tukey	0.0414
Week	20	24	38.7480	15.6551	10	2.48	0.0328	Tukey	0.1726

The SAS System
Wheat analysis for hexanoic_acid

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	hexanoic_acid
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	6
Columns in Z	0
Subjects	1
Max Obs per Subject	15

Number of Observations	
Number of Observations Read	21
Number of Observations Used	15
Number of Observations Not Used	6

The SAS System
Wheat analysis for hexanoic_acid

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	Estimate
Residual	2780.10

Fit Statistics	
-2 Res Log Likelihood	113.2
AIC (Smaller is Better)	115.2
AICC (Smaller is Better)	115.7
BIC (Smaller is Better)	115.5

Type 3 Tests of Fixed Effects				
Effect	Num DF	Den DF	F Value	Pr > F
Week	4	10	23.81	<.0001

Least Squares Means						
Effect	Week	Estimate	Standard Error	DF	t Value	Pr > |t|
Week	8	62.3184	30.4417	10	2.05	0.0678
Week	12	129.72	30.4417	10	4.26	0.0017
Week	16	336.02	30.4417	10	11.04	<.0001

The SAS System

Wheat analysis for hexanoic_acid

The Mixed Procedure

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	20	343.64	30.4417	10	11.29	<.0001
Week	24	399.95	30.4417	10	13.14	<.0001

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	8	12	-67.3970	43.0511	10	-1.57	0.1485	Tukey	0.5479
Week	8	16	-273.71	43.0511	10	-6.36	<.0001	Tukey	0.0006
Week	8	20	-281.32	43.0511	10	-6.53	<.0001	Tukey	0.0005
Week	8	24	-337.63	43.0511	10	-7.84	<.0001	Tukey	0.0001
Week	12	16	-206.31	43.0511	10	-4.79	0.0007	Tukey	0.0051
Week	12	20	-213.92	43.0511	10	-4.97	0.0006	Tukey	0.0040
Week	12	24	-270.23	43.0511	10	-6.28	<.0001	Tukey	0.0007
Week	16	20	-7.6154	43.0511	10	-0.18	0.8631	Tukey	0.9997
Week	16	24	-63.9242	43.0511	10	-1.48	0.1684	Tukey	0.5931
Week	20	24	-56.3088	43.0511	10	-1.31	0.2202	Tukey	0.6929

The SAS System
Wheat analysis for _2_pentylfuran

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	_2_pentylfuran
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	7
Columns in Z	0
Subjects	1
Max Obs per Subject	18

Number of Observations	
Number of Observations Read	21
Number of Observations Used	18
Number of Observations Not Used	3

The SAS System

Wheat analysis for _2_pentylfuran

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	142.45

Fit Statistics	
-2 Res Log Likelihood	100.2
AIC (Smaller is Better)	102.2
AICC (Smaller is Better)	102.6
BIC (Smaller is Better)	102.6

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	5	12	31.98	<.0001

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	4	15.0982	6.8907	12	2.19	0.0489
Week	8	35.6759	6.8907	12	5.18	0.0002
Week	12	58.5135	6.8907	12	8.49	<.0001

Wheat analysis for _2_pentylfuran

The Mixed Procedure

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	94.5933	6.8907	12	13.73	<.0001
Week	20	83.1034	6.8907	12	12.06	<.0001
Week	24	120.20	6.8907	12	17.44	<.0001

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	4	8	-20.5777	9.7450	12	-2.11	0.0564	Tukey	0.3430
Week	4	12	-43.4152	9.7450	12	-4.46	0.0008	Tukey	0.0079
Week	4	16	-79.4950	9.7450	12	-8.16	<.0001	Tukey	<.0001
Week	4	20	-68.0052	9.7450	12	-6.98	<.0001	Tukey	0.0002
Week	4	24	-105.10	9.7450	12	-10.78	<.0001	Tukey	<.0001
Week	8	12	-22.8375	9.7450	12	-2.34	0.0371	Tukey	0.2495
Week	8	16	-58.9173	9.7450	12	-6.05	<.0001	Tukey	0.0006
Week	8	20	-47.4275	9.7450	12	-4.87	0.0004	Tukey	0.0040
Week	8	24	-84.5203	9.7450	12	-8.67	<.0001	Tukey	<.0001
Week	12	16	-36.0798	9.7450	12	-3.70	0.0030	Tukey	0.0280

The SAS System
Wheat analysis for _2_pentylfuran

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	12	20	-24.5900	9.7450	12	-2.52	0.0267	Tukey	0.1917
Week	12	24	-61.6828	9.7450	12	-6.33	<.0001	Tukey	0.0004
Week	16	20	11.4898	9.7450	12	1.18	0.2612	Tukey	0.8384
Week	16	24	-25.6030	9.7450	12	-2.63	0.0221	Tukey	0.1636
Week	20	24	-37.0928	9.7450	12	-3.81	0.0025	Tukey	0.0235

The SAS System
Wheat analysis for octanoic_acid__methyl_ester

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	octanoic_acid__methyl_ester
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System

Wheat analysis for octanoic_acid__methyl_ester

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	75.2661

Fit Statistics	
-2 Res Log Likelihood	46.2
AIC (Smaller is Better)	48.2
AICC (Smaller is Better)	49.2
BIC (Smaller is Better)	48.0

Type 3 Tests of Fixed Effects

Effect	Num DF	Den DF	F Value	Pr > F
Week	2	6	0.63	0.5623

Least Squares Means

Effect	Week	Estimate	Standard Error	DF	t Value	Pr > |t|
Week	16	56.4024	5.0089	6	11.26	<.0001
Week	20	56.6486	5.0089	6	11.31	<.0001
Week	24	63.4332	5.0089	6	12.66	<.0001

The SAS System

Wheat analysis for octanoic_acid__methyl_ester

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-0.2463	7.0836	6	-0.03	0.9734	Tukey	0.9993
Week	16	24	-7.0308	7.0836	6	-0.99	0.3593	Tukey	0.6077
Week	20	24	-6.7845	7.0836	6	-0.96	0.3752	Tukey	0.6272

The SAS System

Wheat analysis for nonanoic_acid__methyl_ester

The Mixed Procedure

Model Information	
Data Set	WORK.WGOOD
Dependent Variable	nonanoic_acid__methyl_ester
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	Levels	Values
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System

Wheat analysis for nonanoic_acid__methyl_ester

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	614.53

Fit Statistics	
-2 Res Log Likelihood	58.8
AIC (Smaller is Better)	60.8
AICC (Smaller is Better)	61.8
BIC (Smaller is Better)	60.6

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	0.38	0.7021

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	90.0841	14.3124	6	6.29	0.0007
Week	20	91.2000	14.3124	6	6.37	0.0007
Week	24	75.4848	14.3124	6	5.27	0.0019

The SAS System

Wheat analysis for nonanoic_acid__methyl_ester

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-1.1159	20.2408	6	-0.06	0.9578	Tukey	0.9983
Week	16	24	14.5992	20.2408	6	0.72	0.4979	Tukey	0.7606
Week	20	24	15.7152	20.2408	6	0.78	0.4670	Tukey	0.7300

The SAS System
Quinoa analysis for _1_pentanol

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	_1_pentanol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	5
Columns in Z	0
Subjects	1
Max Obs per Subject	12

Number of Observations	
Number of Observations Read	21
Number of Observations Used	12
Number of Observations Not Used	9

The SAS System
Quinoa analysis for _1_pentanol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	101.79

Fit Statistics	
-2 Res Log Likelihood	64.1
AIC (Smaller is Better)	66.1
AICC (Smaller is Better)	66.7
BIC (Smaller is Better)	66.2

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	3	8	30.62	<.0001

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	12	39.4953	5.8251	8	6.78	0.0001
Week	16	98.9614	5.8251	8	16.99	<.0001
Week	20	114.13	5.8251	8	19.59	<.0001
Week	24	81.7044	5.8251	8	14.03	<.0001

The SAS System

Quinoa analysis for _1_pentanol

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	12	16	-59.4661	8.2379	8	-7.22	<.0001	Tukey	0.0004
Week	12	20	-74.6363	8.2379	8	-9.06	<.0001	Tukey	<.0001
Week	12	24	-42.2091	8.2379	8	-5.12	0.0009	Tukey	0.0040
Week	16	20	-15.1703	8.2379	8	-1.84	0.1028	Tukey	0.3228
Week	16	24	17.2570	8.2379	8	2.09	0.0695	Tukey	0.2333
Week	20	24	32.4272	8.2379	8	3.94	0.0043	Tukey	0.0181

The SAS System
Quinoa analysis for hexanal

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	hexanal
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	5
Columns in Z	0
Subjects	1
Max Obs per Subject	12

Number of Observations	
Number of Observations Read	21
Number of Observations Used	12
Number of Observations Not Used	9

The SAS System
Quinoa analysis for hexanal

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	Estimate
Residual	8973.95

Fit Statistics	
-2 Res Log Likelihood	99.9
AIC (Smaller is Better)	101.9
AICC (Smaller is Better)	102.6
BIC (Smaller is Better)	102.0

Type 3 Tests of Fixed Effects				
Effect	Num DF	Den DF	F Value	Pr > F
Week	3	8	129.23	<.0001

Least Squares Means						
Effect	Week	Estimate	Standard Error	DF	t Value	Pr > |t|
Week	12	175.41	54.6929	8	3.21	0.0125
Week	16	1062.56	54.6929	8	19.43	<.0001
Week	20	1677.45	54.6929	8	30.67	<.0001
Week	24	1132.14	54.6929	8	20.70	<.0001

The SAS System
Quinoa analysis for hexanal

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	12	16	-887.14	77.3475	8	-11.47	<.0001	Tukey	<.0001
Week	12	20	-1502.04	77.3475	8	-19.42	<.0001	Tukey	<.0001
Week	12	24	-956.72	77.3475	8	-12.37	<.0001	Tukey	<.0001
Week	16	20	-614.89	77.3475	8	-7.95	<.0001	Tukey	0.0002
Week	16	24	-69.5785	77.3475	8	-0.90	0.3946	Tukey	0.8056
Week	20	24	545.32	77.3475	8	7.05	0.0001	Tukey	0.0005

The SAS System

Quinoa analysis for _1_hexanol

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	_1_hexanol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	8
Columns in Z	0
Subjects	1
Max Obs per Subject	21

Number of Observations	
Number of Observations Read	21
Number of Observations Used	21
Number of Observations Not Used	0

The SAS System

Quinoa analysis for _1_hexanol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	Estimate
Residual	2463.72

Fit Statistics	
-2 Res Log Likelihood	156.8
AIC (Smaller is Better)	158.8
AICC (Smaller is Better)	159.1
BIC (Smaller is Better)	159.4

Type 3 Tests of Fixed Effects				
Effect	Num DF	Den DF	F Value	Pr > F
Week	6	14	16.58	<.0001

Least Squares Means						
Effect	Week	Estimate	Standard Error	DF	t Value	Pr > |t|
Week	0	53.1600	28.6573	14	1.86	0.0848
Week	4	34.4455	28.6573	14	1.20	0.2493
Week	8	164.66	28.6573	14	5.75	<.0001

The SAS System
Quinoa analysis for _1_hexanol

The Mixed Procedure

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	12	329.70	28.6573	14	11.50	<.0001
Week	16	311.22	28.6573	14	10.86	<.0001
Week	20	193.10	28.6573	14	6.74	<.0001
Week	24	252.58	28.6573	14	8.81	<.0001

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	0	4	18.7146	40.5275	14	0.46	0.6513	Tukey	0.9990
Week	0	8	-111.50	40.5275	14	-2.75	0.0156	Tukey	0.1556
Week	0	12	-276.54	40.5275	14	-6.82	<.0001	Tukey	0.0001
Week	0	16	-258.06	40.5275	14	-6.37	<.0001	Tukey	0.0003
Week	0	20	-139.94	40.5275	14	-3.45	0.0039	Tukey	0.0467
Week	0	24	-199.42	40.5275	14	-4.92	0.0002	Tukey	0.0033
Week	4	8	-130.22	40.5275	14	-3.21	0.0063	Tukey	0.0713
Week	4	12	-295.25	40.5275	14	-7.29	<.0001	Tukey	<.0001
Week	4	16	-276.77	40.5275	14	-6.83	<.0001	Tukey	0.0001

The SAS System
Quinoa analysis for _1_hexanol

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	4	20	-158.66	40.5275	14	-3.91	0.0016	Tukey	0.0203
Week	4	24	-218.13	40.5275	14	-5.38	<.0001	Tukey	0.0014
Week	8	12	-165.03	40.5275	14	-4.07	0.0011	Tukey	0.0152
Week	8	16	-146.56	40.5275	14	-3.62	0.0028	Tukey	0.0348
Week	8	20	-28.4396	40.5275	14	-0.70	0.4943	Tukey	0.9903
Week	8	24	-87.9151	40.5275	14	-2.17	0.0478	Tukey	0.3682
Week	12	16	18.4772	40.5275	14	0.46	0.6554	Tukey	0.9991
Week	12	20	136.60	40.5275	14	3.37	0.0046	Tukey	0.0541
Week	12	24	77.1199	40.5275	14	1.90	0.0778	Tukey	0.5092
Week	16	20	118.12	40.5275	14	2.91	0.0113	Tukey	0.1189
Week	16	24	58.6426	40.5275	14	1.45	0.1699	Tukey	0.7692
Week	20	24	-59.4755	40.5275	14	-1.47	0.1643	Tukey	0.7583

The SAS System
Quinoa analysis for hexanoic_acid__methyl_ester

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	hexanoic_acid__methyl_ester
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	Levels	Values
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System

Quinoa analysis for hexanoic_acid__methyl_ester

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	148.97

Fit Statistics	
-2 Res Log Likelihood	50.3
AIC (Smaller is Better)	52.3
AICC (Smaller is Better)	53.3
BIC (Smaller is Better)	52.1

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	47.37	0.0002

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	104.19	7.0466	6	14.79	<.0001
Week	20	182.26	7.0466	6	25.86	<.0001
Week	24	193.08	7.0466	6	27.40	<.0001

The SAS System

Quinoa analysis for hexanoic_acid__methyl_ester

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-78.0670	9.9654	6	-7.83	0.0002	Tukey	0.0006
Week	16	24	-88.8862	9.9654	6	-8.92	0.0001	Tukey	0.0003
Week	20	24	-10.8192	9.9654	6	-1.09	0.3193	Tukey	0.5561

The SAS System

Quinoa analysis for phenol

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	phenol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	6
Columns in Z	0
Subjects	1
Max Obs per Subject	15

Number of Observations	
Number of Observations Read	21
Number of Observations Used	15
Number of Observations Not Used	6

The SAS System
Quinoa analysis for phenol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	Estimate
Residual	346.16

Fit Statistics	
-2 Res Log Likelihood	92.3
AIC (Smaller is Better)	94.3
AICC (Smaller is Better)	94.8
BIC (Smaller is Better)	94.6

Type 3 Tests of Fixed Effects				
Effect	Num DF	Den DF	F Value	Pr > F
Week	4	10	11.92	0.0008

Least Squares Means						
Effect	Week	Estimate	Standard Error	DF	t Value	Pr > |t|
Week	8	105.16	10.7419	10	9.79	<.0001
Week	12	105.33	10.7419	10	9.81	<.0001
Week	16	152.68	10.7419	10	14.21	<.0001
Week	20	185.49	10.7419	10	17.27	<.0001
Week	24	103.86	10.7419	10	9.67	<.0001

The SAS System
Quinoa analysis for phenol

The Mixed Procedure

Differences of Least Squares Means									
Effect	Week	Week	Estimate	Standard Error	DF	t Value	Pr > |t|	Adjustment	Adj P
Week	8	12	-0.1635	15.1913	10	-0.01	0.9916	Tukey	1.0000
Week	8	16	-47.5175	15.1913	10	-3.13	0.0107	Tukey	0.0644
Week	8	20	-80.3296	15.1913	10	-5.29	0.0004	Tukey	0.0025
Week	8	24	1.3028	15.1913	10	0.09	0.9333	Tukey	1.0000
Week	12	16	-47.3540	15.1913	10	-3.12	0.0109	Tukey	0.0655
Week	12	20	-80.1661	15.1913	10	-5.28	0.0004	Tukey	0.0026
Week	12	24	1.4663	15.1913	10	0.10	0.9250	Tukey	1.0000
Week	16	20	-32.8121	15.1913	10	-2.16	0.0561	Tukey	0.2687
Week	16	24	48.8204	15.1913	10	3.21	0.0093	Tukey	0.0564
Week	20	24	81.6324	15.1913	10	5.37	0.0003	Tukey	0.0022

The SAS System
Quinoa analysis for _2_pentylfuran

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	_2_pentylfuran
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	3
Columns in Z	0
Subjects	1
Max Obs per Subject	6

Number of Observations	
Number of Observations Read	21
Number of Observations Used	6
Number of Observations Not Used	15

The SAS System

Quinoa analysis for _2_pentylfuran

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	2120.21

Fit Statistics	
-2 Res Log Likelihood	44.2
AIC (Smaller is Better)	46.2
AICC (Smaller is Better)	48.2
BIC (Smaller is Better)	45.6

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	1	4	7.80	0.0492

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	8	37.2476	26.5845	4	1.40	0.2338
Week	12	142.26	26.5845	4	5.35	0.0059

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	8	12	-105.01	37.5962	4	-2.79	0.0492	Tukey	0.0492

The SAS System
Quinoa analysis for _1_octanol

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	_1_octanol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	5
Columns in Z	0
Subjects	1
Max Obs per Subject	12

Number of Observations	
Number of Observations Read	21
Number of Observations Used	12
Number of Observations Not Used	9

The SAS System

Quinoa analysis for _1_octanol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	Estimate
Residual	303.20

Fit Statistics	
-2 Res Log Likelihood	72.8
AIC (Smaller is Better)	74.8
AICC (Smaller is Better)	75.5
BIC (Smaller is Better)	74.9

Type 3 Tests of Fixed Effects				
Effect	Num DF	Den DF	F Value	Pr > F
Week	3	8	24.64	0.0002

Least Squares Means						
Effect	Week	Estimate	Standard Error	DF	t Value	Pr > |t|
Week	12	68.0839	10.0532	8	6.77	0.0001
Week	16	146.98	10.0532	8	14.62	<.0001
Week	20	187.34	10.0532	8	18.63	<.0001
Week	24	146.33	10.0532	8	14.56	<.0001

The SAS System
Quinoa analysis for _1_octanol

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	12	16	-78.8927	14.2173	8	-5.55	0.0005	Tukey	0.0024
Week	12	20	-119.25	14.2173	8	-8.39	<.0001	Tukey	0.0001
Week	12	24	-78.2413	14.2173	8	-5.50	0.0006	Tukey	0.0025
Week	16	20	-40.3602	14.2173	8	-2.84	0.0219	Tukey	0.0835
Week	16	24	0.6514	14.2173	8	0.05	0.9646	Tukey	1.0000
Week	20	24	41.0116	14.2173	8	2.88	0.0204	Tukey	0.0783

The SAS System

Quinoa analysis for nonanal

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	nonanal
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System

Quinoa analysis for nonanal

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	721.05

Fit Statistics	
-2 Res Log Likelihood	59.8
AIC (Smaller is Better)	61.8
AICC (Smaller is Better)	62.8
BIC (Smaller is Better)	61.6

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	36.18	0.0004

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	237.55	15.5032	6	15.32	<.0001
Week	20	422.17	15.5032	6	27.23	<.0001
Week	24	307.02	15.5032	6	19.80	<.0001

The SAS System
Quinoa analysis for nonanal

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-184.62	21.9249	6	-8.42	0.0002	Tukey	0.0004
Week	16	24	-69.4670	21.9249	6	-3.17	0.0194	Tukey	0.0442
Week	20	24	115.15	21.9249	6	5.25	0.0019	Tukey	0.0046

The SAS System
Quinoa analysis for _1_nonanol

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	_1_nonanol
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System
Quinoa analysis for _1_nonanol

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	Estimate
Residual	90.6459

Fit Statistics	
-2 Res Log Likelihood	47.4
AIC (Smaller is Better)	49.4
AICC (Smaller is Better)	50.4
BIC (Smaller is Better)	49.2

Type 3 Tests of Fixed Effects				
Effect	Num DF	Den DF	F Value	Pr > F
Week	2	6	171.16	<.0001

Least Squares Means						
Effect	Week	Estimate	Standard Error	DF	t Value	Pr > |t|
Week	0	35.8108	5.4968	6	6.51	0.0006
Week	12	67.2749	5.4968	6	12.24	<.0001
Week	16	173.08	5.4968	6	31.49	<.0001

The SAS System
Quinoa analysis for _1_nonanol

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	0	12	-31.4641	7.7737	6	-4.05	0.0067	Tukey	0.0159
Week	0	16	-137.27	7.7737	6	-17.66	<.0001	Tukey	<.0001
Week	12	16	-105.81	7.7737	6	-13.61	<.0001	Tukey	<.0001

The SAS System

Quinoa analysis for decanal

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	decanal
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System
Quinoa analysis for decanal

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	322.67

Fit Statistics	
-2 Res Log Likelihood	55.0
AIC (Smaller is Better)	57.0
AICC (Smaller is Better)	58.0
BIC (Smaller is Better)	56.8

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	34.85	0.0005

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	93.2077	10.3710	6	8.99	0.0001
Week	20	202.44	10.3710	6	19.52	<.0001
Week	24	195.73	10.3710	6	18.87	<.0001

The SAS System

Quinoa analysis for decanal

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-109.23	14.6668	6	-7.45	0.0003	Tukey	0.0007
Week	16	24	-102.53	14.6668	6	-6.99	0.0004	Tukey	0.0010
Week	20	24	6.7020	14.6668	6	0.46	0.6638	Tukey	0.8932

The SAS System
Quinoa analysis for _2_4_nonadienal

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	_2_4_nonadienal
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System
Quinoa analysis for _2_4_nonadienal

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	184.24

Fit Statistics	
-2 Res Log Likelihood	51.6
AIC (Smaller is Better)	53.6
AICC (Smaller is Better)	54.6
BIC (Smaller is Better)	53.4

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	24.57	0.0013

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	119.45	7.8367	6	15.24	<.0001
Week	20	183.32	7.8367	6	23.39	<.0001
Week	24	113.08	7.8367	6	14.43	<.0001

The SAS System

Quinoa analysis for _2_4_nonadienal

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-63.8716	11.0827	6	-5.76	0.0012	Tukey	0.0029
Week	16	24	6.3686	11.0827	6	0.57	0.5864	Tukey	0.8381
Week	20	24	70.2403	11.0827	6	6.34	0.0007	Tukey	0.0018

The SAS System

Quinoa analysis for dihydro_5_pentyl_2_3h__furanone

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	dihydro_5_pentyl_2_3h__furanone
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	Levels	Values
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System

Quinoa analysis for dihydro_5_pentyl_2_3h__furanone

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	1323.01

Fit Statistics	
-2 Res Log Likelihood	63.4
AIC (Smaller is Better)	65.4
AICC (Smaller is Better)	66.4
BIC (Smaller is Better)	65.2

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	99.98	<.0001

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	232.17	21.0001	6	11.06	<.0001
Week	20	439.84	21.0001	6	20.94	<.0001
Week	24	652.12	21.0001	6	31.05	<.0001

The SAS System

Quinoa analysis for dihydro_5_pentyl_2_3h__furanone

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-207.66	29.6986	6	-6.99	0.0004	Tukey	0.0010
Week	16	24	-419.95	29.6986	6	-14.14	<.0001	Tukey	<.0001
Week	20	24	-212.29	29.6986	6	-7.15	0.0004	Tukey	0.0009

The SAS System

Quinoa analysis for _2_undecenal

The Mixed Procedure

Model Information	
Data Set	WORK.QGOOD
Dependent Variable	_2_undecenal
Covariance Structure	Diagonal
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Class Level Information		
Class	**Levels**	**Values**
Week	7	0 4 8 12 16 20 24

Dimensions	
Covariance Parameters	1
Columns in X	4
Columns in Z	0
Subjects	1
Max Obs per Subject	9

Number of Observations	
Number of Observations Read	21
Number of Observations Used	9
Number of Observations Not Used	12

The SAS System
Quinoa analysis for _2_undecenal

The Mixed Procedure

Covariance Parameter Estimates	
Cov Parm	**Estimate**
Residual	289.50

Fit Statistics	
-2 Res Log Likelihood	54.3
AIC (Smaller is Better)	56.3
AICC (Smaller is Better)	57.3
BIC (Smaller is Better)	56.1

Type 3 Tests of Fixed Effects				
Effect	**Num DF**	**Den DF**	**F Value**	**Pr > F**
Week	2	6	28.21	0.0009

Least Squares Means						
Effect	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**
Week	16	127.09	9.8234	6	12.94	<.0001
Week	20	221.64	9.8234	6	22.56	<.0001
Week	24	212.60	9.8234	6	21.64	<.0001

The SAS System
Quinoa analysis for _2_undecenal

The Mixed Procedure

Differences of Least Squares Means									
Effect	**Week**	**Week**	**Estimate**	**Standard Error**	**DF**	**t Value**	**Pr > |t|**	**Adjustment**	**Adj P**
Week	16	20	-94.5434	13.8924	6	-6.81	0.0005	Tukey	0.0012
Week	16	24	-85.5034	13.8924	6	-6.15	0.0008	Tukey	0.0020
Week	20	24	9.0400	13.8924	6	0.65	0.5393	Tukey	0.7989

The SAS System
correlations for Quinoa

The CORR Procedure

13 With Variables:	_1_hexanol _1_pentanol hexanal hexanoic_acid__methyl_ester phenol _1_octanol nonanal decanal _2_4_nonadienal dihydro_5_pentyl_2_3h__furanone _2_undecenal _2_pentylfuran _1_nonanol
3 Variables:	Grassy Cardboard_Stale Musty

Simple Statistics						
Variable	**N**	**Mean**	**Std Dev**	**Sum**	**Minimum**	**Maximum**
_1_hexanol	7	191.26573	116.68178	1339	34.44546	329.69639
_1_pentanol	4	83.57318	32.23335	334.29271	39.49530	114.13163
hexanal	4	1012	621.74291	4048	175.41341	1677
hexanoic_acid__methyl_ester	3	159.84434	48.49787	479.53303	104.19329	193.07947
phenol	3	147.34475	41.07700	442.03425	103.86048	185.49293
_1_octanol	3	160.21288	23.49229	480.63864	146.32520	187.33683
nonanal	3	322.24619	93.24627	966.73857	237.55119	422.16915
decanal	3	163.79204	61.21962	491.37613	93.20770	202.43522
_2_4_nonadienal	3	138.61331	38.84551	415.83994	113.07702	183.31728
dihydro_5_pentyl_2_3h__furanone	3	441.37664	209.97856	1324	232.17281	652.12145
_2_undecenal	3	187.10952	52.17120	561.32855	127.09393	221.63732
_2_pentylfuran	2	89.75212	74.25256	179.50425	37.24763	142.25661

The SAS System

correlations for Quinoa

The CORR Procedure

Simple Statistics						
Variable	**N**	**Mean**	**Std Dev**	**Sum**	**Minimum**	**Maximum**
_1_nonanol	3	92.05669	71.91393	276.17007	35.81080	173.08439
Grassy	7	1.98214	3.34900	13.87500	0	9.31250
Cardboard_Stale	7	2.47321	1.56077	17.31250	0.06250	4.50000
Musty	7	1.54464	2.36338	10.81250	0.12500	6.62500

Simple Statistics	
Variable	**Label**
_1_hexanol	_1-hexanol
_1_pentanol	_1-pentanol
hexanal	hexanal
hexanoic_acid__methyl_ester	hexanoic acid, methyl ester
phenol	phenol
_1_octanol	_1-octanol
nonanal	nonanal
decanal	decanal
_2_4_nonadienal	_2,4-nonadienal
dihydro_5_pentyl_2_3h__furanone	dihydro-5-pentyl-2(3h)-furanone
_2_undecenal	_2-undecenal
_2_pentylfuran	_2-pentylfuran
_1_nonanol	_1-nonanol
Grassy	Grassy
Cardboard_Stale	Cardboard/Stale
Musty	Musty

The SAS System

correlations for Quinoa

The CORR Procedure

Pearson Correlation Coefficients Prob > |r| under H0: Rho=0 Number of Observations			
	Grassy	**Cardboard_Stale**	**Musty**
_1_hexanol _1-hexanol	-0.66668 0.1019 7	0.59784 0.1563 7	0.29295 0.5237 7
_1_pentanol _1-pentanol	-0.41985 0.5801 4	0.51029 0.4897 4	0.20555 0.7944 4
hexanal hexanal	-0.65179 0.3482 4	0.31295 0.6871 4	0.39541 0.6046 4
hexanoic_acid__methyl_ester hexanoic acid, methyl ester	-0.99978 0.0133 3	-0.65103 0.5487 3	0.77490 0.4356 3
phenol phenol	0.20224 0.8704 3	0.88494 0.3084 3	-0.78874 0.4215 3
_1_octanol _1-octanol	-0.40669 0.7334 3	0.44743 0.7047 3	-0.28239 0.8177 3
nonanal nonanal	-0.72730 0.4815 3	0.06828 0.9565 3	0.10906 0.9304 3

The SAS System
correlations for Quinoa

The CORR Procedure

Pearson Correlation Coefficients Prob > |r| under H0: Rho=0 Number of Observations			
	Grassy	**Cardboard_Stale**	**Musty**
decanal decanal	- 0.98941 0.0927 3	-0.51620 0.6547 3	0.65940 0.5416 3
_2_4_nonadienal _2,4-nonadienal	- 0.34348 0.7768 3	0.50734 0.6613 3	- 0.34711 0.7743 3
dihydro_5_pentyl_2_3h__furanone dihydro-5-pentyl-2(3h)-furanone	- 0.90516 0.2795 3	-0.90318 0.2825 3	0.96481 0.1694 3
_2_undecenal _2-undecenal	- 0.98426 0.1131 3	-0.48855 0.6751 3	0.63502 0.5620 3
_2_pentylfuran _2-pentylfuran	- 1.00000 . 2	1.00000 . 2	- 1.00000 . 2
_1_nonanol _1-nonanol	- 0.67276 0.5302 3	0.89767 0.2905 3	0.99892 0.0295 3

9 With Variables:	_1_hexanol _2_pentylfuran phenol hexanoic_acid hexanal _1_pentanol hexanoic_acid__methyl_ester octanoic_acid__methyl_ester nonanoic_acid__methyl_ester
3 Variables:	Fresh_Flour Cardboard_Stale Musty

Simple Statistics							
Variable	**N**	**Mean**	**Std Dev**	**Sum**	**Minimum**	**Maximum**	**Label**
_1_hexanol	7	126.13342	59.56239	882.93392	49.65691	215.21555	_1-hexanol
_2_pentylfuran	6	67.86343	38.96945	407.18059	15.09823	120.19628	_2-pentylfuran
phenol	5	79.46735	32.18259	397.33673	34.84737	116.62065	phenol
hexanoic_acid	5	254.32955	148.53659	1272	62.31842	399.94899	hexanoic acid
hexanal	4	42.52555	15.73853	170.10221	19.38288	53.32080	hexanal
_1_pentanol	3	25.46963	2.99217	76.40890	22.25332	28.17077	_1-pentanol
hexanoic_acid__methyl_ester	4	37.97627	12.01529	151.90509	20.33032	46.77578	hexanoic acid, methyl ester
octanoic_acid__methyl_ester	3	58.82806	3.99006	176.48419	56.40236	63.43319	octanoic acid, methyl ester
nonanoic_acid__methyl_ester	3	85.58966	8.76879	256.76897	75.48485	91.20003	nonanoic acid, methyl ester
Fresh_Flour	7	1.85714	0.92401	13.00000	0.56250	3.56250	Fresh Flour
Cardboard_Stale	7	2.04464	1.17078	14.31250	0.37500	3.56250	Cardboard/Stale
Musty	7	1.54464	2.67432	10.81250	0	7.50000	Musty

Pearson Correlation Coefficients Prob > |r| under H0: Rho=0 Number of Observations			
	Fresh_Flour	**Cardboard_Stale**	**Musty**
_1_hexanol _1-hexanol	-0.82402 0.0226 7	0.42002 0.3481 7	0.70120 0.0792 7
_2_pentylfuran _2-pentylfuran	-0.85729 0.0291 6	0.24142 0.6449 6	0.70637 0.1167 6
phenol phenol	-0.19749 0.7502 5	0.87581 0.0515 5	- 0.17854 0.7739 5
hexanoic_acid hexanoic acid	-0.87940 0.0494 5	0.23013 0.7096 5	0.66274 0.2228 5
hexanal hexanal	-0.68766 0.3123 4	-0.00068 0.9993 4	0.56001 0.4400 4
_1_pentanol _1-pentanol	-0.51597 0.6549 3	-0.75178 0.4584 3	0.71456 0.4933 3
hexanoic_acid__methyl_ester hexanoic acid, methyl ester	-0.77790 0.2221 4	-0.04538 0.9546 4	0.61137 0.3886 4
octanoic_acid__methyl_ester octanoic acid, methyl ester	-0.94780 0.2066 3	-0.99987 0.0101 3	0.99750 0.0450 3
nonanoic_acid__methyl_ester nonanoic acid, methyl ester	0.91347 0.2668 3	0.99391 0.0703 3	- 0.98638 0.1052 3

correlations for Quinoa

Obs	week	Grassy	Cardboard_ Stale	Musty	_1_hexanol	_1_pentanol	hexanal	hexanoic_ acid__methyl_ ester	phenol
1	Week 0	9.3125	0.0625	0.1250	53.160	.	.	.	.
2	Week 4	2.6250	2.0000	0.2500	34.445	.	.	.	.
3	Week 8	0.6875	2.1875	0.3750	164.661	.	.	.	.
4	Week 12	0.5625	2.8750	0.3125	329.696	39.495	175.41	.	.
5	Week 16	0.6250	4.5000	0.8125	311.219	98.961	1062.56	104.193	152.681
6	Week 20	0.0625	4.2500	2.3125	193.101	114.132	1677.45	182.260	185.493
7	Week 24	0.0000	.	6.6250	252.577	81.704	1132.14	193.079	103.860

Obs	_1_octanol	nonanal	decanal	_2_4_ nonadienal	dihydro_5_ pentyl_2_3h__ furanone	_2_undecenal	_2_pentylfuran	_1_nonanol
1	.	.	.	.	.	.	.	35.811
2	.	.	.	.	.	.	.	.
3	.	.	.	.	.	.	37.248	.
4	.	.	.	.	.	.	142.257	67.275
5	146.977	237.551	93.208	119.446	232.173	127.094	.	173.084
6	187.337	422.169	202.435	183.317	439.836	221.637	.	.
7	146.325	307.018	195.733	113.077	652.121	212.597	.	.

correlations for Quinoa

The CORR Procedure

13 With Variables:	_1_hexanol	_1_pentanol	hexanal
	hexanoic_acid__methyl_ester	phenol	_1_octanol
	nonanal	decanal	
	_2_4_nonadienal	dihydro_5_pentyl_2_3h__furanone	
	_2_undecenal	_2_pentylfuran	_1_nonanol
3 Variables:	Grassy	Cardboard_Stale	Musty

Simple Statistics

Variable	N	Mean	Std Dev	Sum
_1_hexanol	7	191.26573	116.68178	1339
_1_pentanol	4	83.57318	32.23335	334.29271
hexanal	4	1012	621.74291	4048
hexanoic_acid__methyl_ester	3	159.84434	48.49787	479.53303
phenol	3	147.34475	41.07700	442.03425
_1_octanol	3	160.21288	23.49229	480.63864
nonanal	3	322.24619	93.24627	966.73857
decanal	3	163.79204	61.21962	491.37613
_2_4_nonadienal	3	138.61331	38.84551	415.83994
dihydro_5_pentyl_2_3h__furanone	3	441.37664	209.97856	1324
_2_undecenal	3	187.10952	52.17120	561.32855
_2_pentylfuran	2	89.75212	74.25256	179.50425
_1_nonanol	3	92.05669	71.91393	276.17007
Grassy	7	1.98214	3.34900	13.87500
Cardboard_Stale	6	2.64583	1.63491	15.87500
Musty	7	1.54464	2.36338	10.81250

Simple Statistics

Variable	Minimum	Maximum	Label

_1_hexanol	34.44546	329.69639	_1-hexanol
_1_pentanol	39.49530	114.13163	_1-pentanol
hexanal	175.41341	1677	hexanal
hexanoic_acid__methyl_ester	104.19329	193.07947	hexanoic acid, methyl ester
phenol	103.86048	185.49293	phenol
_1_octanol	146.32520	187.33683	_1-octanol
nonanal	237.55119	422.16915	nonanal
decanal	93.20770	202.43522	decanal
_2_4_nonadienal	113.07702	183.31728	_2,4-nonadienal
dihydro_5_pentyl_2_3h__furanone	232.17281	652.12145	dihydro-5-pentyl-2(3h)-furanone
_2_undecenal	127.09393	221.63732	_2-undecenal
_2_pentylfuran	37.24763	142.25661	_2-pentylfuran
_1_nonanol	35.81080	173.08439	_1-nonanol
Grassy	0	9.31250	Grassy
Cardboard_Stale	0.06250	4.50000	Cardboard/Stale
Musty	0.12500	6.62500	Musty

correlations for Quinoa

The CORR Procedure

Pearson Correlation Coefficients
Prob > |r| under H0: Rho=0
Number of Observations

	Grassy	Cardboard_ Stale	Musty
_1_hexanol	-0.66668	0.71558	0.29295
_1-hexanol	0.1019	0.1098	0.5237
	7	6	7
_1_pentanol	-0.41985	0.94381	0.20555
_1-pentanol	0.5801	0.2144	0.7944
	4	3	4
hexanal	-0.65179	0.84583	0.39541
hexanal	0.3482	0.3582	0.6046
	4	3	4
hexanoic_acid__methyl_ester	-0.99978	-1.00000	0.77490
hexanoic acid, methyl ester	0.0133	.	0.4356
	3	2	3
phenol	0.20224	-1.00000	-0.78874
phenol	0.8704	.	0.4215
	3	2	3
_1_octanol	-0.40669	-1.00000	-0.28239
_1-octanol	0.7334	.	0.8177
	3	2	3
nonanal	-0.72730	-1.00000	0.10906

nonanal	0.4815	.	0.9304
	3	2	3
decanal	-0.98941	-1.00000	0.65940
decanal	0.0927	.	0.5416
	3	2	3
_2_4_nonadienal	-0.34348	-1.00000	-0.34711
_2,4-nonadienal	0.7768	.	0.7743
	3	2	3
dihydro_5_pentyl_2_3h__furanone	-0.90516	-1.00000	0.96481
dihydro-5-pentyl-2(3h)-furanone	0.2795	.	0.1694
	3	2	3
_2_undecenal	-0.98426	-1.00000	0.63502
_2-undecenal	0.1131	.	0.5620
	3	2	3

correlations for Quinoa

The CORR Procedure

Pearson Correlation Coefficients
Prob > |r| under H0: Rho=0
Number of Observations

	Grassy	Cardboard_ Stale	Musty
_2_pentylfuran _2-pentylfuran	-1.00000 . 2	1.00000 . 2	-1.00000 . 2
_1_nonanol _1-nonanol	-0.67276 0.5302 3	0.89767 0.2905 3	0.99892 0.0295 3

correlations for Wheat

Obs	week	Fresh_ Flour	Cardboard_ Stale	Musty	_1_hexanol	_2_pentylfuran	phenol	hexanoic_ acid
1	Week 0	3.5625	0.3750	0.0000	49.657	.	.	.
2	Week 4	1.9375	1.6250	0.6875	56.656	15.098	.	.
3	Week 8	2.1875	1.6875	0.2500	115.196	35.676	34.847	62.318
4	Week 12	1.8750	2.4375	0.1250	135.326	58.513	80.724	129.715
5	Week 16	1.6250	3.5625	0.7500	174.840	94.593	116.621	336.025
6	Week 20	1.2500	3.4375	1.5000	136.044	83.103	101.946	343.640
7	Week 24	0.5625	.	7.5000	215.216	120.196	63.198	399.949

Obs	hexanal	_1_pentanol	hexanoic_ acid__methyl_ ester	octanoic_ acid__methyl_ ester	nonanoic_ acid__methyl_ ester
1	.	.	.	.	.
2	.	.	.	.	.
3	.	.	.	.	.
4	19.3829	.	20.3303	.	.
5	51.4153	25.9848	40.7931	56.4024	90.0841
6	45.9832	22.2533	44.0059	56.6486	91.2000
7	53.3208	28.1708	46.7758	63.4332	75.4848

correlations for Wheat

The CORR Procedure

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9 With Variables:    _1_hexanol                       _2_pentylfuran              phenol
                     hexanoic_acid                    hexanal                     _1_pentanol
                     hexanoic_acid__methyl_ester      octanoic_acid__methyl_ester
                     nonanoic_acid__methyl_ester
3      Variables:    Fresh_Flour                      Cardboard_Stale             Musty
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Simple Statistics

Variable	N	Mean	Std Dev	Sum	Minimum	Maximum
_1_hexanol	7	126.13342	59.56239	882.93392	49.65691	215.21555
_2_pentylfuran	6	67.86343	38.96945	407.18059	15.09823	120.19628
phenol	5	79.46735	32.18259	397.33673	34.84737	116.62065
hexanoic_acid	5	254.32955	148.53659	1272	62.31842	399.94899
hexanal	4	42.52555	15.73853	170.10221	19.38288	53.32080
_1_pentanol	3	25.46963	2.99217	76.40890	22.25332	28.17077
hexanoic_acid__methyl_ester	4	37.97627	12.01529	151.90509	20.33032	46.77578
octanoic_acid__methyl_ester	3	58.82806	3.99006	176.48419	56.40236	63.43319
nonanoic_acid__methyl_ester	3	85.58966	8.76879	256.76897	75.48485	91.20003
Fresh_Flour	7	1.85714	0.92401	13.00000	0.56250	3.56250
Cardboard_Stale	6	2.18750	1.21385	13.12500	0.37500	3.56250
Musty	7	1.54464	2.67432	10.81250	0	7.50000

Simple Statistics

Variable	Label
_1_hexanol	_1-hexanol
_2_pentylfuran	_2-pentylfuran
phenol	phenol
hexanoic_acid	hexanoic acid

hexanal	hexanal
_1_pentanol	_1-pentanol
hexanoic_acid__methyl_ester	hexanoic acid, methyl ester
octanoic_acid__methyl_ester	octanoic acid, methyl ester
nonanoic_acid__methyl_ester	nonanoic acid, methyl ester
Fresh_Flour	Fresh Flour
Cardboard_Stale	Cardboard/Stale
Musty	Musty

correlations for Wheat

The CORR Procedure

Pearson Correlation Coefficients
Prob > |r| under H0: Rho=0
Number of Observations

	Fresh_ Flour	Cardboard_ Stale	Musty
_1_hexanol	-0.82402	0.88963	0.70120
_1-hexanol	0.0226	0.0176	0.0792
	7	6	7
_2_pentylfuran	-0.85729	0.97333	0.70637
_2-pentylfuran	0.0291	0.0052	0.1167
	6	5	6
phenol	-0.19749	0.97247	-0.17854
phenol	0.7502	0.0275	0.7739
	5	4	5
hexanoic_acid	-0.87940	0.98404	0.66274
hexanoic acid	0.0494	0.0160	0.2228
	5	4	5
hexanal	-0.68766	0.99834	0.56001
hexanal	0.3123	0.0367	0.4400
	4	3	4
_1_pentanol	-0.51597	1.00000	0.71456
_1-pentanol	0.6549	.	0.4933
	3	2	3
hexanoic_acid__methyl_ester	-0.77790	0.97436	0.61137

hexanoic acid, methyl ester	0.2221	0.1445	0.3886
	4	3	4
octanoic_acid__methyl_ester	-0.94780	-1.00000	0.99750
octanoic acid, methyl ester	0.2066	.	0.0450
	3	2	3
nonanoic_acid__methyl_ester	0.91347	-1.00000	-0.98638
nonanoic acid, methyl ester	0.2668	.	0.1052
	3	2	3