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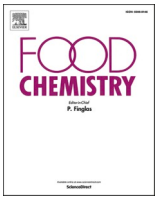

Lipid and volatile profiles of Finnish oat batches of pure cultivars: Effect of storage on the volatile formation

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ABSTRACT

Recent data showing the compositional variation and storage behavior among different oat batches for the purpose of food remains limited. Lipids of twenty oat flour samples of pure cultivars grown in Finland during 2019 were extracted and fractionated into neutral and polar-rich lipids. Flour was stored for nine months, and profiles of volatiles and tocols were analyzed to reveal oxidative stability. The lipid content was 5.9–8.9 g per 100 g of flour [DW] and consisted of 78.7 ± 2.5 % neutral and 21.3 ± 2.5 % polar lipids. Palmitic (16 %), oleic (36 %), and linoleic (39 %) acids were the most abundant fatty acids. Neutral lipids had more oleic and less linoleic and palmitic acids than polar lipids. The fresh samples correlated with tocols, pentanal, 2-pentylfuran, 2-heptanone, nonanal, 2-butanone, and heptanal, while stored samples were associated with 3-octen-2-one, 2-octenal, hexanal, and octanal. Lipid composition and oxidative stability are essential factors for selecting oat batches for food applications.

1. Introduction

Recently, the use of oats (*Avena Sativa*) for food has increased extensively. Associated with a plant-based diet and known for its nutritional value and proven health effects, oats have become a popular part of a diet and food ingredient as products supporting healthy, vegan, and gluten-free diets. In addition to being rich in carbohydrates, lipids, dietary fiber, proteins, minerals, and phytochemicals (Holopainen-Mantila et al., 2023; Zwer, 2017), oats have several health benefits. The European Food Safety Agency (EFSA) and the European Union have approved four health claims for oats for which oat fibers support intestinal function, and oat beta-glucan lowers cholesterol and balances postprandial blood glycemia (EFSA, 2010, 2011a, 2011b).

Oats have the highest lipid content (3–12 %) among grains (Brown & Craddock, 1972). Yet, only a few studies exist on the influence of the variety, growing conditions, or processing methods on oat lipids (Brown & Craddock, 1972; Doehlert et al., 2010; Lampi et al., 2015; Lapveteläinen et al., 2001; Leonova et al., 2008). Oats' chemical and physical properties largely determine the behavior of lipids in food processing. The type of lipids in a food system significantly impacts its processing characteristics, including stability, texture, and sensory properties. For instance, polar lipids have emulsification properties that improve loaf volume and delay staling in breadmaking (Erazo-Castrejón et al., 2001). The neutral lipids, mostly triacylglycerols (TAGs), account for 50–85 % of the total lipid content in oats, and polar lipids, such as phospholipids (PLs) and glycolipids (GLs), account for 20–40 % of the lipids (Lehtinen & Kaukovirta-Norja, 2011). In addition, oats are a rich source of unsaturated fatty acids, mainly oleic and linoleic, which are associated with health benefits and are valuable for the nutritional properties of oat-based products. However, unsaturated fatty acids are prone to oxidation and thus can affect sensory quality and reduce nutritional value.

Lipid oxidation results in various volatile and non-volatile oxidation products. The most common volatiles in oats include aldehydes, ketones, alcohols, esters, and pyrazines (Li et al., 2023; McGorrin, 2019) and occur during processing or storage. Harvested and unprocessed oat grains are stable once dried and have low levels of aroma compounds (Zhou et al., 1999a). The mechanical treatment on grain structure in milling, grinding, and flaking activates lipid degradation and can cause the formation of bitter off-flavors (Decker et al., 2014; Sides et al., 2001). Heat treatment is needed to inactivate the endogenous lipolytic enzyme system. At the same time, lipid degradation produces a range of

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volatile compounds that give oats their characteristic nutty, toasty, or caramel-like aroma and flavor (Heydanek & McGorrin, 1981). While some oxidation products may be desirable and contribute to the overall aroma of oats, others negatively impact the flavor quality. For example, hexanal is a well-known oxidation product associated with a grassy and green flavor and contributes to an unpleasant taste in oats (McGorrin, 2019). In general, the formation of rancid flavors in oat products occurs during storage and is related to the oxidation of unsaturated fatty acids (Lehtinen & Kaukovirta-Norja, 2011).

Considering the positive effects of oats on health and recent dietary trends, the consumption of oats in Finland has increased to an annual 10.2 kg per capita (Natural Resources Institute Finland, Statistical Database). The variety of oat-based products available in Finland is wide. From rolled oats to bread, granola, oat milk-like drinks, oat chocolate, oat licorice, pulled oats®, oat beer, and liqueur, there are many different types of oat-derived products. However, most use, domestically, of oats (69 %) ends up in feed use and only 21 % goes into the food industry, while the remaining amount is used for seeds and farm energy use (Natural Resources Institute Finland, Statistical Database). Several factors, including a lack of knowledge regarding the variation in the properties of different oat cultivars and batches and the impact of compositional differences on the perceived quality of oats, hinder the utilization of oats in foods. Hence, more scientific data on the variation of batches and the nature of the cultivar constituents are needed to shift the use of oats from fodder to food.

To our knowledge, there are no previous scientific data on lipids and volatiles that compares batches of oats from pure cultivars from the same crop year. This study hypothesized that the composition of lipids and volatiles vary between oat flours of different cultivars and growing locations, and that lipid and tocopherol composition affects volatile formation during storage. Therefore, the present study aimed to determine the lipid profiles of different Finnish oat batches representing pure cultivars and investigate their relation to volatile compounds. Storage of flours for nine months, on a trial basis, was conducted at room temperature to identify changes in volatile compounds and to reveal lipid-related oxidation products. In addition, the loss of tocols (i.e., tocopherols and tocotrienols) was measured to connect possible antioxidant interactions on lipid oxidation and the formation of volatiles during storage. The lipids were extracted using a four-stage extraction method and fractionated into neutral and polar-rich lipids with solid phase columns. Gas chromatography with flame-ionization detection (GC-FID) was used to analyze the fatty acid compositions of isolated neutral and polar-rich lipid fractions, and solid phase microextraction gas chromatography-mass spectrometry (SPME-GC–MS) was used to analyze oat volatiles. Additionally, the loss of tocols was measured by normal-phase liquid chromatography with fluorescence detection (NP-HPLC-FLD).

2. Materials and methods

2.1. Reagents

For all analyses, commercial analytical grade solvents and reagents were used. HPLC-grade *tert*-butyl methyl ether (MTBE) was purchased from Sigma–Aldrich (Steinheim, Germany) for the lipid extraction. Triheptadecanoin (TAG 17:0) and 1,2-dipentadecanoyl-*sn*-glycero-3-phosphatidylcholine (PL 15:0) from Larodan (Solna, Sweden) were used as internal standards. Extra dry, stabilized AcroSeal® diethyl ether from Acros Organics (Thermo Fisher Scientific, NJ, USA) was used in the lipid fractionation. Acetyl chloride and sodium hydroxide were obtained from Sigma–Aldrich (Steinheim, Germany) for the fatty acid analyses. Supelco 37 Component FAME mix from Supelco (Sant Louis, MO, USA) and GLC-68D standard mixture from Nu-Check-Prep (Elysian, MN, USA) were used as external standards. Acetone was used for the extraction of tocols, and heptane and 1,4-dioxane used for tocol HPLC analysis were of Chromasolv quality and purchased from Honeywell Riedel-de Haën (Seelze, Germany). α- and β-tocopherols from the Tocopherol Set (Merck KGaA, Darmstadt, Germany) were used as external standards. HPLC-grade hexane and HPLC-grade methanol from Honeywell (Seelze, Germany) and chloroform from Fisher Scientific (Loughborough, England) were used in several analyses.

2.2. Sample materials and the storage trial

The study samples consisted of 20 heat-treated oat flour batches representing different Finnish oat cultivars from the crop year 2019. The oat grains were obtained from Boreal Plant Breeding Ltd. (Jokioinen, Finland), Lantmännen Agro Ltd. (Vantaa, Finland), Peltosiemen Ltd. (Forssa, Finland), Plantanova Ltd. (Ruukki, Finland), Raisio plc (Raisio, Finland), and Vääksyn Mylly Ltd. (Vääksy, Finland). All native, hulled oat grains were milled at Vääksyn Mylly Ltd. (Asikkala, Finland) to produce the heated oat groats for enzyme deactivation. Process completion was confirmed with lipase activity measurements, and flakes were milled to flour. The processing details as well as the composition of batches are described in Jokinen et al., 2021. The milling process included drying, de-hulling, kilning, flaking, and milling. While the pure cultivar batches were obtained all from the crop year 2019 and were processed and analyzed equally, factors such as soil, fertilization, or threshing time were not controlled for in this study. Therefore, the samples are referred to as batches of pure cultivars and not as cultivars.

The portions of fresh flour (t = 0) were immediately frozen and kept at −20 °C until analysis. Aliquots for the lipid and volatile compound analysis were frozen in borosilicate glass laboratory bottles, and aliquots for the tocopherol analysis were stored in plastic bags. For the storage trial, freshly milled oat flours were sorted into paper bags and stored at room temperature (22 °C) in a storage room cabinet. The samples were collected at six (t = 6) and nine (t = 9) months and frozen (−20 °C) in glass bottles or plastic bags until used. The basic physical and chemical properties of oat cultivar samples were published in the study by Jokinen et al. (2021), and the same oat sample codes are used in the current study.

2.3. Dry matter determination

The dry matter and moisture content of oat flour samples were determined according to the one-stage AACC 44-15A method (2000). Two grams of oat flour were dried at 103 ± 1 °C for 60 min in a Memmert UF110 lab oven (Büchenbach, Germany) with an air fan of 70 % and flap settings of 30 %. Aluminum moisture dishes were used for the drying. Analysis was performed in triplicate.

2.4. Lipid extraction

The oat flour samples were extracted in duplicates by four-stage lipid extraction: double extraction with MTBE/methanol, extraction with hexane, and extraction with methanol (Supplementary Fig. 1). The extraction method was modified further from the double-stage extraction method of Multari et al. (2018). Stock solutions (500 μL) of internal lipid standards of 1 mg/mL TAG 17:0 in hexane and 1 mg/mL PL 15:0 in chloroform–methanol (2:1, *v/v*) were added to a glass test tube and evaporated under nitrogen flow, after which, an oat sample (0.5 g) was added to the test tube. In the first extraction, 1.25 mL of methanol was pipetted into a glass tube with an oat sample and standards and stirred with an Ultra Turrax homogenizer (Ika, Staufen, Germany) with a speed of 8000 rpm for 1 min. Then, 3.75 mL of MTBE (methyl *tert*-butyl ether) solvent was added, and the mixture was stirred again with the Ultra Turrax (8000 rpm) for 1 min. After the homogenization, samples were centrifuged at 700 x g for 15 min, and the supernatant (extract 1) was collected into a new glass tube. For the second extraction, 1.68 mL of MTBE-methanol (10:3, *v/v*) was added to the solid oat residue, vortexed for 1 min, then 0.32 mL of Milli-Q water was added, vortexed for 1 min, and centrifuged (700 x g, 5 min). The supernatant (extract 2) was

collected and added to the first extract. 1.5 mL of Milli-Q water was added to the combined extracts (extract 1 + extract 2), vortexed (1 min), and centrifuged (700 x g, 5 min). The upper layer was collected into a new and tared test tube. In the third extraction, 2 mL of hexane was added to the solid residue left after the second extraction, vortexed (1 min), and centrifuged (700 x g, 5 min). The supernatant (extract 3) was collected and placed into the tared test tube containing the upper layer phase from the combined extracts 1 and 2. In the fourth extraction, 2 mL of methanol was added to the solid oat residue left after the third extraction, vortexed (1 min), and centrifuged (700 x g, 5 min). After the centrifugation, the supernatant (extract 4) was collected and pipetted into a test tube with the previous three extracts. The solvent was evaporated from the test tube containing four extracts under the nitrogen flow (37 °C). The tubes were weighed, and the yield of extracted lipids was calculated. Extracted lipids were dissolved into 3 mL (1 x 1 mL + 4 x 0.5 mL) of chloroform, transferred to an autosampler vial, and stored at −80 °C until analysis.

2.5. Fractionation

An elution chamber with a vacuum, faucets, and 200 mg Sep-Pak Vac3 cc silica cartridges (Waters, England) was used for the fractionation with some modifications of Christie's (2003) method. The sample amount corresponding to 6 mg of lipids was pipetted into an autosampler vial and evaporated under nitrogen flow, after which, it was dissolved with 1 mL of chloroform. The silica column was conditioned with 5 mL of extra dry diethyl ether. To collect a neutral fraction, the samples in chloroform (1 mL) were transferred to the silica columns, washed twice with 1 mL of diethyl ether, and then eluted with 9 mL of diethyl ether. The polar fraction was eluted with 10 mL of methanol and collected into a separate disposable glass tube. The elution solvents were evaporated to dryness under nitrogen flow, glass tubes were weighed, and the fractionation yields were calculated. The neutral-rich fraction was dissolved with methanol, and the polar-rich fraction was dissolved with chloroform–methanol (2:1, *v/v*). All samples were stored at −80 °C.

2.6. Fatty acid composition

The extracted lipids were transformed into fatty acid methyl esters (FAMEs) using an acid-catalyzed method and analyzed by Shimadzu Nexis GC-2030 gas chromatograph with an AOC-20i auto-injector and flame ionization detector (FID) (Shimadzu Corporation, Japan) equipped with an Agilent JandW GC column DB-23 (60 m x 0.25 mm i.d., liquid film 0.25 μm; Santa Clara, CA, USA) (Damerau et al., 2020). Briefly, unfractionated and fractionated lipid samples, which already contained the internal standards of TAG 17:0 and PL 15:0 from the extraction phase, were methylated overnight at 50 °C with a portion of acetyl chloride/methanol (1:10, *v/v*). After adding 1 M potassium carbonate and hexane, samples were vortexed and centrifuged at 1000 x g for 3 min. The upper layer containing FAMEs in hexane was collected. GC-FID analysis was performed as described by Damerau et al. (2020). The peaks were identified using external standards being the Supelco 37 Component FAME mix and GLC-68D standard mix and quantified using internal standards and correction factors.

2.7. Tocol content

Tocols were extracted from the oat flours in triplicate by accelerated solvent extraction (ASE, Dionex ASE-200, Dionex Corporation, Sunnyvale, CA, USA) with acetone according to the method of Lampi et al. (2015). Tocol content (α- and β-tocopherols and α- and β-tocotrienols) of the ASE extracts was measured by normal-phase high-performance liquid chromatography (NP-HPLC) with fluorescence detection (FLD) according to Pöysä et al. (2024). The calibration curves of commercial α- and β-tocopherol standards from the Tocopherol Set were used to quantitate both α- and β-tocopherols and the corresponding α- and β-tocotrienols. Other tocols were not reported because they were absent in the samples. Contents of individual tocols (μg/g, on a dry weight basis [DW]) of oat samples were used in statistical analysis. Proportions of individual tocols and total tocols remaining (%) in the storage experiment are presented in Supplementary Table 1. The tocol concentrations of fresh oat samples are reported in detail in the publication of Pöysä et al. (2024).

2.8. Volatile oxidation products

The volatile profile of fresh and stored oat flour samples was analyzed with a headspace solid-phase microextraction (HS-SPME) injector and the GC–MS instrument Thermo Scientific Trace 1300 GC, TSQ 8000 Evo triple quadrupole MS and TriPlus RSH autosampler (Waltham, MA, USA) with a DB-624 Ultra Inert (UI) capillary column (60 m × 0.25 mm i.d., 1.4 μm film thickness; Supelco, Bellefonte, PA, USA). Before the analysis, oat flours were transferred from −20 °C to 4 °C. The flour sample (1 g of dry flour) was weighed in a 20 mL SPME vial and incubated for 20 min at 50 °C. The extraction of volatiles was conducted at 50 °C for 30 min using divinylbenzene/carboxy/polydimethylsiloxane (DVB/CAR/PDMS) fiber (50/30 μm film thickness; Supelco, Bellefonte, PA, USA). The incubation and extraction temperatures were chosen and tested based on the previous study by Lampi et al. (2015). The temperature for 5-min desorption in the GC-injector port was 240 °C (splitless injection), and the column oven temperature program was as follows: 40 °C held for 6 min, 5 °C/min to 145 °C, 3 °C/min to 185 °C, 6 °C/min to 210 °C held for 7 min. Helium (1.4 mL/min) was used as a carrier gas. Electron ionization at 250 °C and 70 eV was employed for the MS, and mass-to-charge ratios were scanned between 40 and 300 amu. Analyses were performed in triplicates. The compounds were identified using the NIST MS Search library (version 2.3, National Institute of Standards and Technology, Gaithersburg, Maryland, USA). Only compounds with a match ≥ 850 with the reference spectra of the NIST20 library were considered for identification. The data were processed with Chromeleon 7.2.10 ES software (Thermo Fisher Scientific, Waltham, MA, USA).

2.9. Statistical analysis

The differences in moisture, extractable oil amount, neutral and polar lipid content, and fatty acid composition between the cultivars were analyzed with a one-way analysis of variance (ANOVA) and Tukey's HSD test (IBM SPSS Statistics, version 27.0.1.0, IBM, New York, USA). The linear regression and correlation test between the total oil content and fatty acid variables was performed with Origin 2016 Sr2 b9.3.2.303 (Originlab Corporation, Northampton, MS, USA). The principal component analysis (PCA) was applied using the Unscrambler® X version 11.0 (Camo Process AS, Oslo, Norway) for the sample grouping and differentiation of volatiles and tocols.

3. Results and discussion

3.1. Moisture and oat oil content

Lower moisture content improves the microbiological quality and shelf-life of grain products. However, the optimal water capacity of flour is an essential parameter in its baking quality (Sammalisto et al., 2021). The moisture content of the twenty investigated oat samples significantly differed ($p < 0.05$) and varied from 9.8 % to 12.1 % (Table 1) confirming earlier results (Jokinen et al., 2021) on the same samples determined by a slightly different drying method. The results were also comparable to the results of Multari et al. (2018) for eight Finnish oat cultivars with moisture ranging from 8.5 % to 11.8 %. In addition, the flour samples investigated in this study have been successfully used for baking in the parallel study by Sammalisto et al. (2021).

Since various solvents have different lipid group extraction

Table 1
Moisture, extracted oil yield (as grams per 100 g of oat flour of dry weight (DW)), and neutral and polar lipids ratio of 20 investigated oat flour samples. Different letters within the same column indicate a statistically significant difference ($p < 0.05$) between samples.

Sample code [1)]	Moisture, %	Oat oil, g/100 g flour DW	Neural lipids, %	Polar lipids, %
F11	10.6 ± 0.0^{de}	6.77 ± 0.03^{cd}	71.5 ± 0.1^{a}	28.5 ± 0.1^{e}
F12	10.7 ± 0.0^{ef}	7.15 ± 0.05^{de}	79.6 ± 0.1^{bcde}	20.4 ± 0.1^{abcd}
F13	10.9 ± 0.0^{ghi}	6.70 ± 0.13^{cd}	78.0 ± 1.2^{bcde}	22.0 ± 1.2^{abcd}
F14	10.2 ± 0.0^{b}	7.67 ± 0.09^{fg}	77.8 ± 0.6^{bcde}	22.2 ± 0.6^{abcd}
F15	10.8 ± 0.1^{fg}	8.50 ± 0.02^{h}	80.7 ± 2.5^{cde}	19.3 ± 2.5^{abc}
F16	10.9 ± 0.0^{gh}	6.76 ± 0.02^{cd}	76.3 ± 0.1^{bc}	23.7 ± 0.2^{cd}
F17	11.0 ± 0.1^{hi}	8.85 ± 0.08^{h}	81.0 ± 0.0^{de}	19.0 ± 0.0^{ab}
F18	10.8 ± 0.0^{fg}	8.47 ± 0.27^{h}	82.0 ± 0.3^{e}	18.0 ± 0.3^{a}
F19	10.4 ± 0.1^{c}	7.87 ± 0.13^{g}	80.3 ± 0.2^{cde}	19.7 ± 0.2^{abc}
F20	10.6 ± 0.0^{d}	6.21 ± 0.06^{ab}	76.5 ± 0.1^{bcd}	23.5 ± 0.1^{bcd}
F21	9.8 ± 0.1^{a}	7.65 ± 0.02^{fg}	79.1 ± 0.6^{bcde}	20.9 ± 0.6^{abcd}
F22	10.6 ± 0.0^{d}	6.49 ± 0.08^{bc}	79.6 ± 0.0^{bcde}	20.4 ± 0.0^{abcd}
F23	11.8 ± 0.0^{l}	6.79 ± 0.22^{cd}	80.2 ± 2.0^{bcde}	19.8 ± 2.0^{abcd}
F24	12.1 ± 0.0^{m}	6.41 ± 0.22^{bc}	79.6 ± 1.1^{bcde}	20.4 ± 1.1^{abcd}
F25	11.7 ± 0.1^{kl}	5.89 ± 0.05^{a}	75.6 ± 2.5^{b}	24.4 ± 2.5^{d}
F26	12.0 ± 0.1^{m}	6.83 ± 0.16^{cd}	78.6 ± 0.2^{bcde}	21.4 ± 0.2^{abcd}
F27	11.4 ± 0.0^{j}	6.82 ± 0.05^{cd}	78.8 ± 0.1^{bcde}	21.2 ± 0.1^{abcd}
F28	11.7 ± 0.0^{kl}	7.84 ± 0.21^{g}	81.2 ± 2.7^{de}	18.8 ± 2.7^{ab}
F29	11.0 ± 0.0^{i}	7.33 ± 0.21^{ef}	78.1 ± 0.3^{bcde}	21.9 ± 0.3^{abcd}
F30	11.7 ± 0.0^{k}	6.10 ± 0.10^{ab}	79.0 ± 0.2^{bcde}	21.0 ± 0.2^{abcd}
mean	11.0 ± 0.6	7.16 ± 0.83	78.7 ± 2.5	21.3 ± 2.5

[1)] Sample codes of extracted oat flours (crop 2019) equal those in Jokinen et al., 2021. The values are mean ± SD of three replicates for moisture analysis and two replicates for extraction and fractionation.

properties (Doehlert et al., 2010; Sahasrabudhe, 1979), a four-step lipid extraction containing a double extraction with MTBE-methanol, extraction with hexane, and extraction with methanol was chosen based on a pretest (data not shown). Moreover, the total lipid content determined using a SoxCap TM 2047 combined with a Soxtec TM 2050 extraction system, published previously by Jokinen et al., 2021, supports the functionality of the method used in this study. The extractable oat oil varied from 5.9 to 8.9 g per 100 g of flour DW (Table 1). The flour samples 15, 17, 18, 19, 25, and 28 were statistically different ($p < 0.05$) from the other flour samples regarding the extractable oat oil amount. The lowest oat oil content was measured in flour 25, and the highest was in flour 17 followed by samples 15 and 18. Samples 11, 12, 13, 14, 16, 20, 21, 22, 23, 24, 26, 27, and 30 did not significantly differ from each other in terms of oat oil content.

In an early and comprehensive study, Brown and Craddock (1972) reported that over 90 % of the studied 4533 oat groat samples analyzed by NMR contained 5–9 % oat oil with some exception of higher lipid-containing oat groats (up to 11.6 %). Our results align with these oat oil amounts. In addition, similar quantities analyzed by NMR were found in a study by Saastamoinen et al. (1989) on Finnish oats, which were considered whole oats, including hull and bran. They consisted of 6.1–7.8 % oat oil. According to recent results by Multari et al. (2018), the oil content of eight Finnish cultivars, as milled oat kernels, varied from 3.9 % to 5.9 %. Thus far, over 70 cultivars are approved for cultivation in Finland with new ones coming to the agricultural market and old ones falling out of use. Wild oats generally contain more oil than cultivated oats resulting from genetic differences (Leonova et al., 2008). Selectively breeding oats with wild species can achieve high-oil varieties with a lipid content of 18 % in the groat (Frey & Holland, 1999). High oil content is desired in feed applications due to its nutritional value (Zhou et al., 1999b), but the food industry prefers varieties with low to medium oil content for food processing applications. The oat batches reviewed in this study have low to medium oil content making them suitable for industrial food production.

Solid phase extraction was used to divide extracted oat oil into neutral-rich and polar-rich lipid fractions. On average, the lipid mass composition was 78.7 ± 2.5 % from neutral lipids and 21.3 ± 2.5 % from polar lipids (Table 1). A significant difference ($p < 0.05$) in neutral and polar lipids content was found in samples 11, 18, and 25. Flour sample 11 contained the smallest amount of neutral lipids (71.5 %) and the largest amount of polar lipids (28.5 %) among the samples. Conversely, flour sample 18 was richer in neutral lipids (82.0 %) but contained less polar lipids (18.0 %) than other samples. Sample 25 differed from the group with an average amount of neutral lipids (75.6 %) and polar lipids (24.4 %). Presently, scientific knowledge on oat lipids of modern cultivars remains scarce. Still, the proportion of neutral and polar lipids detected in this study corresponds with those investigated in the late 1970s and are reviewed by Lehtinen and Kaukovirta-Norja (2011). However, as reviewed by Zhou et al., (1999b), the extraction method and the solvent choice affect how much of each lipid class is extracted. This study's four-step lipid extraction was designed to ensure a quantitative lipid extraction of all lipid classes.

Findings by Doehlert et al. (2010) suggested that genotypes with the lowest total oil concentration had the highest polar lipid concentration in oat flour. The data in this study showed a similar trend. For example, flour 25, with the lowest total lipid content of 5.9 %, had the highest percentage of polar lipids (24.4 %) (Table 1). This could be explained because neutral lipids are mainly comprised of TAGs (Lampi et al., 2015), which are storage lipids affecting the overall lipid content, while polar lipids primarily originate from structural lipids like PLs and GLs, which are mainly constant and affected by grain size. Both neutral and polar lipids have their applications in the food industry. Neutral lipids, in the form of TAGs, are widely used for bulk oils, e.g., in margarine production. Polar lipids, instead, are valuable emulsifier agents in baking and promote loaf volume properties in breadmaking. With industrial features in mind, flour sample 11 would be a good choice for breadmaking. A correlation between the fat content of the investigated flour samples and the "bread-specific volume" baking quality parameter was found in the parallel study conducted by Sammalisto et al. (2021). This association may be linked to the presence of polar lipids.

3.2. Fatty acid composition

Fourteen fatty acids were identified and quantified as the percentage of total fatty acids. The most abundant fatty acids in unfractionated and fractionated lipid extracts were palmitic (C16:0), oleic (C18:1(n-9)), and linoleic (C18:2(n-6)) acids (Tables 2 and 3) as reported previously on primary oat fatty acids (Lehtinen & Kaukovirta-Norja, 2011; Leonova et al., 2008; Saastamoinen et al., 1989; Sahasrabudhe, 1979; Zhou et al., 1999b). On average, palmitic acid accounted for 15.74 ± 0.66 %, oleic acid for 35.71 ± 2.57 %, and linoleic acid for 39.03 ± 2.06 % of unfractionated lipid extracts (Table 2). The content of stearic acid (C18:0) was 1.77 ± 0.35 %, α-linolenic acid (C18:3(n-3)) was 1.40 ± 0.15 %, *cis*-vaccenic acid (C18:1(n-7)) was 0.74 ± 0.10 %, and gondoic acid (20:1(n-9)) was 0.68 ± 0.05 %. The fatty acids C14:0, C16:1(n-7), C20:0, C20:2(n-6), 22:0, 22:1(n-9), and 24:1(n-9) accounted for less than 1 % of the fatty acid composition. There was significant variation in the fatty acid composition of the oat samples. According to the ANOVA test results, almost all twenty samples were significantly different from each other. The samples were more similar in total saturated fatty acid (SAFA) composition (Table 2), where nine flours (samples 11, 14, 16, 17, 18, 19, 20, 22, 26) were not significantly different. Meanwhile, eleven flours (samples 12, 13, 15, 21, 23, 24, 25, 27, 28, 29, 30) differed significantly from each other.

The fractionating of lipid extract revealed that the polar fraction included a higher palmitic acid (on average, 19.20 ± 0.74 %) and linoleic acid content (on average, 44.07 ± 1.86 %) than the neutral fraction (Table 3B). In contrast, the neutral fraction contained higher quantities of oleic acid (on average, 38.01 ± 2.03 %) than the polar fraction (Table 3A). The mean composition of the neutral fraction was similar to the unfractionated lipid oat extract, while the polar fraction

Table 2
Fatty acid composition (percentage of total FAs) of unfractionated oat oil. Different letters within the same column indicate a statistically significant difference ($p < 0.005$) between samples.

	Unfractionated oat oil										
Sample code [1]	**16:0**	**18:0**	**18:1 (n-9)**	**18:1 (n-7)**	**18:2 (n-6)**	**18:3 (n-3)**	**20:1 (n-9)**	**Others** [2]	**Σ SAFA**	**Σ MUFA**	**Σ PUFA**
F11	15.54 ± 0.00^{d}	1.71 ± 0.01^{e}	34.21 ± 0.05^{ef}	0.83 ± 0.00^{hi}	40.37 ± 0.03^{j}	1.53 ± 0.01^{h}	0.72 ± 0.00^{i}	0.92 ± 0.01^{fg}	17.77 ± 0.01^{de}	36.11 ± 0.04^{ef}	41.95 ± 0.04^{i}
F12	15.94 ± 0.00^{fg}	1.79 ± 0.00^{f}	36.09 ± 0.04^{k}	0.76 ± 0.01^{ef}	38.70 ± 0.01^{e}	1.41 ± 0.00^{de}	0.69 ± 0.00^{fg}	0.79 ± 0.00^{ab}	18.19 ± 0.02^{i}	37.83 ± 0.06^{j}	40.15 ± 0.02^{f}
F13	16.47 ± 0.02^{i}	1.86 ± 0.01^{g}	35.37 ± 0.02^{j}	0.74 ± 0.01^{cde}	38.24 ± 0.03^{d}	1.46 ± 0.00^{f}	0.74 ± 0.00^{j}	0.94 ± 0.01^{gh}	18.91 ± 0.01^{l}	37.16 ± 0.01^{i}	39.75 ± 0.03^{e}
F14	15.53 ± 0.01^{d}	1.94 ± 0.00^{i}	38.23 ± 0.04^{n}	0.58 ± 0.01^{a}	37.16 ± 0.06^{c}	1.26 ± 0.00^{b}	0.68 ± 0.00^{efg}	0.83 ± 0.03^{bc}	18.02 ± 0.00^{gh}	39.73 ± 0.04^{m}	38.44 ± 0.05^{c}
F15	15.54 ± 0.02^{d}	2.26 ± 0.01^{m}	40.27 ± 0.06^{p}	0.59 ± 0.01^{a}	35.36 ± 0.07^{a}	1.24 ± 0.00^{b}	0.62 ± 0.00^{bc}	0.79 ± 0.00^{ab}	18.35 ± 0.01^{j}	41.71 ± 0.07^{o}	36.62 ± 0.07^{a}
F16	16.96 ± 0.03^{k}	1.45 ± 0.01^{c}	33.54 ± 0.01^{c}	0.79 ± 0.00^{gh}	39.94 ± 0.01^{i}	1.47 ± 0.00^{fg}	0.74 ± 0.00^{j}	0.91 ± 0.02^{fg}	18.95 ± 0.04^{lm}	35.39 ± 0.03^{c}	41.46 ± 0.02^{h}
F17	15.05 ± 0.02^{b}	2.55 ± 0.00^{n}	40.84 ± 0.03^{q}	0.56 ± 0.01^{a}	35.22 ± 0.08^{a}	1.28 ± 0.00^{b}	0.60 ± 0.00^{a}	0.75 ± 0.01^{a}	18.11 ± 0.02^{hi}	42.23 ± 0.05^{p}	36.52 ± 0.08^{a}
F18	15.89 ± 0.01^{f}	1.53 ± 0.01^{d}	39.67 ± 0.03^{o}	0.70 ± 0.01^{c}	36.31 ± 0.02^{b}	1.08 ± 0.01^{a}	0.75 ± 0.00^{jk}	0.82 ± 0.01^{bc}	17.93 ± 0.02^{fg}	41.41 ± 0.03^{n}	37.43 ± 0.02^{b}
F19	15.46 ± 0.00^{d}	1.89 ± 0.01^{gh}	37.69 ± 0.04^{m}	0.66 ± 0.00^{b}	38.06 ± 0.01^{d}	1.11 ± 0.00^{a}	0.67 ± 0.00^{e}	0.85 ± 0.01^{cde}	17.85 ± 0.01^{ef}	39.33 ± 0.03 ^{l}	39.20 ± 0.00^{d}
F20	15.95 ± 0.01^{fg}	1.58 ± 0.00^{d}	34.24 ± 0.03^{fg}	0.67 ± 0.00^{b}	39.56 ± 0.03^{h}	1.65 ± 0.01^{i}	0.78 ± 0.00^{l}	0.98 ± 0.01^{hi}	18.13 ± 0.00^{hi}	36.02 ± 0.04^{e}	41.27 ± 0.02^{h}
F21	15.27 ± 0.01^{c}	1.92 ± 0.00^{hi}	36.52 ± 0.01^{l}	0.67 ± 0.00^{b}	39.21 ± 0.00^{f}	1.39 ± 0.01^{de}	0.61 ± 0.00^{ab}	0.84 ± 0.00^{bcde}	17.72 ± 0.02^{d}	38.09 ± 0.01^{k}	40.63 ± 0.01^{g}
F22	16.38 ± 0.02^{h}	2.00 ± 0.01^{j}	34.04 ± 0.05^{de}	0.72 ± 0.01^{cd}	39.52 ± 0.01^{gh}	1.62 ± 0.01^{i}	0.62 ± 0.00^{bc}	0.93 ± 0.00^{g}	18.98 ± 0.04^{lm}	35.67 ± 0.07^{d}	41.18 ± 0.01^{h}
F23	14.52 ± 0.00^{a}	1.39 ± 0.01^{b}	35.02 ± 0.02^{i}	0.81 ± 0.00^{ghi}	41.20 ± 0.00^{k}	1.38 ± 0.00^{d}	0.69 ± 0.00^{gh}	0.85 ± 0.00^{bcde}	16.39 ± 0.00^{b}	36.85 ± 0.02^{h}	42.62 ± 0.00^{j}
F24	14.46 ± 0.02^{a}	1.22 ± 0.01^{a}	34.40 ± 0.05^{g}	0.79 ± 0.00^{fg}	41.68 ± 0.10^{l}	1.47 ± 0.01^{fg}	0.76 ± 0.00^{k}	0.83 ± 0.01^{bc}	16.13 ± 0.03^{a}	36.27 ± 0.04^{fg}	43.20 ± 0.11^{k}
F25	15.71 ± 0.02^{e}	1.44 ± 0.01^{bc}	31.48 ± 0.05^{a}	0.84 ± 0.01^{ij}	42.34 ± 0.02^{m}	1.50 ± 0.00^{g}	0.67 ± 0.00^{ef}	0.89 ± 0.01^{defg}	17.64 ± 0.03^{d}	33.32 ± 0.03^{a}	43.90 ± 0.02^{l}
F26	15.97 ± 0.01^{fg}	1.44 ± 0.00^{c}	33.71 ± 0.01^{c}	0.86 ± 0.01^{j}	40.47 ± 0.04^{j}	1.55 ± 0.00^{h}	0.68 ± 0.00^{efg}	0.92 ± 0.02^{fg}	17.93 ± 0.01^{fg}	35.61 ± 0.03^{d}	42.07 ± 0.04^{i}
F27	16.60 ± 0.00^{j}	1.86 ± 0.01^{g}	33.90 ± 0.01^{d}	0.84 ± 0.01^{ij}	39.25 ± 0.02^{fg}	1.47 ± 0.00^{fg}	0.64 ± 0.00^{d}	0.99 ± 0.01^{i}	19.06 ± 0.00^{m}	35.73 ± 0.01^{d}	40.75 ± 0.04^{g}
F28	16.00 ± 0.04^{g}	2.06 ± 0.03^{k}	37.80 ± 0.05^{m}	0.64 ± 0.01^{b}	36.97 ± 0.04^{c}	1.31 ± 0.01^{c}	0.65 ± 0.00^{d}	0.84 ± 0.00^{bcd}	18.60 ± 0.06^{k}	39.35 ± 0.04^{l}	38.32 ± 0.05^{c}
F29	16.46 ± 0.05^{hi}	2.19 ± 0.02^{l}	34.74 ± 0.09^{h}	0.74 ± 0.01^{de}	38.84 ± 0.24^{e}	1.32 ± 0.03^{c}	0.63 ± 0.01^{c}	0.90 ± 0.02^{efg}	19.19 ± 0.07^{n}	36.42 ± 0.10^{g}	40.21 ± 0.26^{f}
F30	15.06 ± 0.00^{b}	1.25 ± 0.00^{a}	32.48 ± 0.01^{b}	0.97 ± 0.00^{k}	42.22 ± 0.00^{m}	1.42 ± 0.00^{e}	0.70 ± 0.00^{h}	0.86 ± 0.01^{cdef}	16.76 ± 0.00^{c}	34.52 ± 0.01^{b}	43.69 ± 0.02^{l}
mean	15.74 ± 0.66	1.77 ± 0.35	35.71 ± 2.57	0.74 ± 0.10	39.03 ± 2.06	1.40 ± 0.15	0.68 ± 0.05	0.87 ± 0.06	18.03 ± 0.84	37.44 ± 2.44	40.47 ± 2.17

[1] Sample codes of extracted oat flours (crop 2019) equal those in Jokinen et al., 2021. The values are mean ± SD of two extract replicates.
[2] Others include 14:0, 16:1(n-7), 20:0, 20:2(n-6), 22:0, 22:1(n-9) and 24:1(n-9).

was more abundant in total polyunsaturated fatty acids (PUFA). In addition, the amount of α-linolenic acid in the polar fraction (C18:3(n-3), 1.83 ± 0.13 %) was higher than in the neutral fraction (C18:3(n-3), 1.33 ± 0.15 %) (Table 3). Polar lipids commonly contain higher quantities of α-linolenic acid, in the matter of PLs and GLs, than neutral lipids. The separation of polar-rich lipid fractions with better α-linolenic concentration could be a possible industrial application for foods with health claims for omega-3 fatty acids.

Compared with unfractionated oat oil (Table 2), fractionated samples had less significant differences between the samples in fatty acid composition (Table 3). For palmitic acid, the flour samples 13, 16, 17, 21, 23, 24, 25, 27, 29, and 30 were significantly different ($p < 0.005$) from each other in the neutral fraction, while in the polar fraction, a significant difference was observed in samples 11, 13, 16, 17, 18, 19, 22, 25, 26, and 27. For oleic acid, significant differences were found in samples 15, 17, 25, and 30 for the neutral fraction and in samples 14, 15, 17, 18, 22, 28, and 30 for the polar fraction. In terms of linoleic acid concentration, significantly different samples were found in only three flour samples (15, 23, and 25) in the neutral fraction, while in the polar fraction, differences were identified in seven flour samples (12, 14, 15, 17, 18, 25, and 29).

Earlier studies (Holland et al., 2001; Leonova et al., 2008; Sahasrabudhe, 1979) found a correlation between the total oil content and palmitic, oleic, and linoleic acids. For example, Sahasrabudhe (1979) and Holland et al. (2001) described a positive correlation between oil content and oleic acid and a negative correlation of oil content with palmitic and linoleic acid. In addition, Leonova et al. (2008) reported a positive correlation between lipid content and oleic acid and a negative correlation between lipid content with linoleic and α-linolenic acid. Our results support previously described associations between the total lipid content and oleic, linoleic, and α-linolenic acid. In contrast, we found no correlations between total lipid content and palmitic acid (Supplementary Table 2).

The fat content and fatty acid composition vary in the different parts of the oat grain and change during the oat maturation period (Banaś et al., 2007). Moreover, the cultivar origin, the growth location, the growth condition, the milling process, and further handling affect the fat and fatty acid content. In our study case, the milling process did not affect the fat and general fatty acid contents of the studied oat flour samples, as revealed previously by Jokinen et al., 2021. No significant difference in protein, fat, and fatty acid content (e.g., total SAFA, MUFA, and PUFA) was found between dehulled and ground native grains and

Table 3
Fatty acid composition (percentage of total FAs) of neutral (**A**) and polar fraction (**B**) of oat oil. Different letters within the same column indicate a statistically significant difference ($p < 0.005$) between samples.

Sample code [1)]	(A) Neutral fraction of oat oil										
	16:0	18:0	18:1 (n-9)	18:1 (n-7)	18:2 (n-6)	18:3 (n-3)	20:1 (n-9)	Others [2)]	Σ SAFA	Σ MUFA	Σ PUFA
F11	15.20 ± 0.01^{def}	1.82 ± 0.01^{cdefg}	36.57 ± 0.01^{abc}	0.77 ± 0.02^{hij}	38.95 ± 0.03^{def}	1.44 ± 0.01^{def}	0.80 ± 0.00^{abc}	1.09 ± 0.01^{ab}	17.59 ± 0.00^{de}	38.61 ± 0.01^{abc}	40.44 ± 0.04^{defgh}
F12	15.47 ± 0.00^{gh}	1.88 ± 0.01^{defg}	38.50 ± 0.01^{bcde}	0.71 ± 0.02^{efgh}	37.36 ± 0.03^{cd}	1.32 ± 0.01^{bcdef}	0.75 ± 0.00^{abc}	0.94 ± 0.00^{ab}	17.88 ± 0.01^{ef}	40.34 ± 0.01^{cde}	38.72 ± 0.03^{bcde}
F13	15.81 ± 0.05^{j}	1.94 ± 0.00^{efgh}	37.87 ± 0.16^{bcd}	0.69 ± 0.02^{defg}	37.07 ± 0.10^{cd}	1.37 ± 0.01^{cdef}	0.82 ± 0.00^{abc}	1.08 ± 0.00^{ab}	18.38 ± 0.06^{fgh}	39.78 ± 0.13^{bcd}	38.48 ± 0.11^{bcde}
F14	15.04 ± 0.01^{cd}	2.04 ± 0.00^{ghi}	40.61 ± 0.14^{ef}	0.52 ± 0.01^{a}	35.91 ± 0.01^{abc}	1.17 ± 0.00^{abcd}	0.75 ± 0.00^{abc}	0.92 ± 0.01^{ab}	17.69 ± 0.02^{de}	42.16 ± 0.12^{def}	37.11 ± 0.01^{abc}
F15	14.95^{cd}	2.36^{ij}	42.74^{f}	0.54^{ab}	34.11^{a}	1.15^{abc}	0.68^{ab}	0.91^{ab}	17.90^{efg}	44.23^{f}	35.29^{a}
F16	16.29 ± 0.00^{k}	1.54 ± 0.00^{abcd}	36.35 ± 0.01^{ab}	0.75 ± 0.01^{fghi}	38.58 ± 0.00^{de}	1.38 ± 0.00^{cdef}	0.82 ± 0.00^{bc}	1.01 ± 0.01^{ab}	18.41 ± 0.01^{fgh}	38.30 ± 0.00^{abc}	40.01 ± 0.00^{cdefgh}
F17	14.60 ± 0.01^{b}	2.65 ± 0.00^{j}	42.78 ± 0.02^{f}	0.50 ± 0.00^{a}	34.29 ± 0.03^{ab}	1.18 ± 0.00^{abcd}	0.65 ± 0.00^{a}	0.85 ± 0.02^{a}	17.80 ± 0.00^{e}	44.20 ± 0.02^{f}	35.50 ± 0.04^{a}
F18	15.44 ± 0.02^{fgh}	1.61 ± 0.02^{abcde}	41.07 ± 0.95^{ef}	0.67 ± 0.01^{de}	35.83 ± 0.76^{abc}	1.07 ± 0.08^{ab}	0.78 ± 0.05^{abc}	0.96 ± 0.04^{ab}	17.64 ± 0.08^{de}	42.86 ± 1.00^{ef}	36.95 ± 0.84^{ab}
F19	14.98 ± 0.00^{cd}	1.97 ± 0.00^{fgh}	40.11 ± 0.01^{de}	0.61 ± 0.00^{cd}	36.71 ± 0.00^{bcd}	1.03 ± 0.00^{a}	0.74 ± 0.00^{abc}	0.95 ± 0.02^{ab}	17.50 ± 0.01^{de}	41.82 ± 0.01^{def}	37.77 ± 0.01^{abcd}
F20	15.19 ± 0.00^{de}	1.66 ± 0.01^{bcdef}	37.70 ± 0.07^{bcd}	0.62 ± 0.01^{cd}	37.74 ± 0.01^{cd}	1.53 ± 0.00^{f}	0.88 ± 0.00^{c}	1.07 ± 0.03^{ab}	17.49 ± 0.02^{de}	39.58 ± 0.05^{bcd}	39.32 ± 0.02^{bcdef}
F21	14.52 ± 0.05^{b}	2.02 ± 0.01^{ghi}	39.25 ± 0.01^{cde}	0.63 ± 0.02^{cd}	37.77 ± 0.02^{cd}	1.28 ± 0.00^{abcdef}	0.68 ± 0.00^{ab}	0.95 ± 0.02^{ab}	17.11 ± 0.08^{bcd}	40.90 ± 0.03^{cde}	39.10 ± 0.02^{bcde}
F22	15.79 ± 0.01^{ij}	2.11 ± 0.01^{ghi}	36.72 ± 0.01^{abc}	0.68 ± 0.02^{def}	38.13 ± 0.00^{cd}	1.55 ± 0.00^{f}	0.69 ± 0.00^{ab}	1.06 ± 0.02^{av}	18.55 ± 0.02^{h}	38.45 ± 0.05^{abc}	39.72 ± 0.00^{bcdefg}
*F*23	13.82 ± 0.09^{a}	1.37 ± 0.15^{ab}	36.29 ± 1.53^{ab}	0.75 ± 0.01^{ghi}	41.30 ± 1.75^{f}	1.43 ± 0.16^{def}	0.72 ± 0.10^{ab}	0.97 ± 0.01^{ab}	15.71 ± 0.22^{a}	38.17 ± 1.66^{abc}	42.77 ± 1.93^{h}
F24	13.79 ± 0.02^{a}	1.28 ± 0.02^{a}	36.87 ± 0.01^{abc}	0.75 ± 0.01^{fghi}	40.67 ± 0.13^{ef}	1.41 ± 0.01^{cdef}	0.83 ± 0.00^{bc}	0.94 ± 0.01^{ab}	15.57 ± 0.01^{a}	38.82 ± 0.02^{abc}	42.12 ± 0.14^{fgh}
F25	14.83 ± 0.00^{c}	1.49 ± 0.02^{abc}	34.39 ± 0.07^{a}	0.79 ± 0.01^{ij}	41.11 ± 0.04^{f}	1.44 ± 0.00^{def}	0.75 ± 0.00^{abc}	1.01 ± 0.01^{ab}	16.86 ± 0.02^{bc}	36.35 ± 0.04^{a}	42.60 ± 0.05^{h}
F26	15.29 ± 0.04^{efg}	1.51 ± 0.01^{abc}	36.16 ± 0.01^{ab}	0.82 ± 0.01^{j}	39.32 ± 0.08^{def}	1.47 ± 0.02^{ef}	0.75 ± 0.00^{abc}	1.05 ± 0.01^{ab}	17.37 ± 0.05^{cde}	38.16 ± 0.00^{abc}	40.83 ± 0.09^{efgh}
F27	15.97 ± 0.01^{j}	1.96 ± 0.01^{fgh}	36.29 ± 0.01^{ab}	0.79 ± 0.01^{ij}	38.15 ± 0.01^{cd}	1.40 ± 0.00^{cdef}	0.71 ± 0.00^{ab}	1.15 ± 0.01^{b}	18.60 ± 0.01^{h}	38.23 ± 0.00^{abc}	39.59 ± 0.01^{bcdefg}
F28	15.56 ± 0.01^{hi}	2.11 ± 0.14^{ghi}	38.76 ± 1.74^{bcde}	0.59 ± 0.00^{bc}	36.67 ± 1.45^{bcd}	1.35 ± 0.17^{cdef}	0.65 ± 0.09^{a}	1.14 ± 0.22^{b}	18.46 ± 0.14^{gh}	40.32 ± 1.87^{cde}	38.05 ± 1.61^{abcde}
F29	15.99 ± 0.05^{j}	2.28 ± 0.03^{hi}	36.93 ± 0.09^{abc}	0.70 ± 0.03^{efgh}	37.62 ± 0.12^{cd}	1.21 ± 0.01^{abcde}	0.69 ± 0.00^{ab}	1.02 ± 0.01^{ab}	18.87 ± 0.08^{h}	38.72 ± 0.13^{abc}	38.87 ± 0.13^{bcde}
F30	14.58 ± 0.21^{b}	1.49 ± 0.26^{abc}	34.83 ± 0.25^{a}	0.92 ± 0.02^{k}	41.02 ± 0.12^{ef}	1.33 ± 0.00^{bcdef}	0.76 ± 0.01^{abc}	0.95 ± 0.04^{ab}	16.56 ± 0.48^{b}	36.92 ± 0.33^{ab}	42.40 ± 0.11^{gh}
mean	15.16 ± 0.68	1.84 ± 0.35	37.92 ± 2.31	0.69 ± 0.11	38.01 ± 2.03	1.33 ± 0.15	0.75 ± 0.07	1.00 ± 0.09	17.59 ± 0.90	39.74 ± 2.17	39.38 ± 2.13
	(B) Polar fraction of oat oil										
F11	17.78 ± 0.04^{a}	1.80 ± 0.01^{de}	19.22 ± 0.01^{cde}	0.81 ± 0.10^{fgh}	45.83 ± 0.02^{lmn}	1.98 ± 0.02^{i}	0.28 ± 0.01^{bcde}	1.17 ± 0.05^{fgh}	20.11 ± 0.04^{a}	20.89 ± 0.05^{de}	47.88 ± 0.01^{jk}
F12	18.95 ± 0.00^{de}	1.86 ± 0.00^{de}	20.16 ± 0.14^{ef}	0.80 ± 0.00^{fg}	44.44 ± 0.09^{h}	1.86 ± 0.00^{fg}	0.29 ± 0.00^{cdef}	1.03 ± 0.00^{bcd}	21.30 ± 0.00^{ffg}	21.72 ± 0.14^{ef}	46.36 ± 0.10^{gh}
F13	20.17 ± 0.03^{i}	1.91 ± 0.07^{e}	20.23 ± 0.56^{ef}	0.75 ± 0.01^{de}	43.04 ± 0.29^{ef}	1.94 ± 0.02^{hi}	0.31 ± 0.02^{efg}	1.20 ± 0.03^{ghi}	22.74 ± 0.12^{i}	21.78 ± 0.58^{ef}	45.04 ± 0.31^{de}
F14	18.35 ± 0.03^{bc}	1.75 ± 0.01^{d}	24.33 ± 0.12^{i}	0.57 ± 0.00^{a}	42.42 ± 0.09^{d}	1.70 ± 0.00^{b}	0.31 ± 0.00^{efg}	0.99 ± 0.02^{abc}	20.70 ± 0.03^{cd}	25.59 ± 0.10^{h}	44.14 ± 0.12^{c}
F15	19.39 ± 0.12^{fg}	2.04 ± 0.01^{f}	24.93 ± 0.21^{i}	0.60 ± 0.01^{a}	41.12 ± 0.01^{b}	1.74 ± 0.01^{bc}	0.29 ± 0.00^{cdef}	0.99 ± 0.05^{abc}	22.03 ± 0.13^{ij}	26.17 ± 0.19^{h}	42.90 ± 0.02^{b}
F16	20.18 ± 0.05^{i}	1.39 ± 0.01^{ab}	19.78 ± 0.08^{def}	0.81 ± 0.00^{fg}	44.96 ± 0.08^{hij}	1.85 ± 0.00^{efg}	0.32 ± 0.00^{efg}	1.09 ± 0.00^{bcdefg}	22.22 ± 0.05^{jk}	21.30 ± 0.08^{de}	46.86 ± 0.07^{ghi}
F17	18.27 ± 0.04^{b}	2.28 ± 0.00^{g}	27.01 ± 0.02^{j}	0.56 ± 0.00^{a}	39.41 ± 0.11^{a}	1.87 ± 0.01^{fg}	0.26 ± 0.00^{abcd}	0.97 ± 0.01^{ab}	21.07 ± 0.03^{ef}	28.24 ± 0.01^{i}	41.31 ± 0.09^{a}
F18	19.22 ± 0.06^{f}	1.53 ± 0.04^{c}	24.27 ± 0.13^{i}	0.70 ± 0.02^{cd}	41.70 ± 0.12^{c}	1.57 ± 0.01^{a}	0.30 ± 0.00^{defg}	1.05 ± 0.01^{bcdef}	21.35 ± 0.03^{fgh}	25.67 ± 0.09^{h}	43.33 ± 0.12^{b}
F19	18.57 ± 0.04^{c}	1.81 ± 0.03^{de}	21.41 ± 0.15^{gh}	0.66 ± 0.01^{b}	44.65 ± 0.16^{hi}	1.56 ± 0.02^{a}	0.25 ± 0.00^{abc}	1.03 ± 0.00^{bcde}	20.92 ± 0.08^{de}	22.75 ± 0.15^{fg}	46.27 ± 0.18^{fg}
F20	19.46 ± 0.00^{fg}	1.54 ± 0.01^{c}	18.18 ± 0.10^{bc}	0.66 ± 0.00^{bc}	46.06 ± 0.05^{mno}	2.12 ± 0.02^{j}	0.35 ± 0.01 ^{g}	1.16 ± 0.00^{efgh}	21.71 ± 0.00^{hi}	19.56 ± 0.08^{bc}	48.26 ± 0.07^{k}
F21	19.64 ± 0.03^{gh}	1.85 ± 0.02^{de}	20.31 ± 0.08^{ef}	0.72 ± 0.01^{d}	45.06 ± 0.02^{hijk}	1.88 ± 0.02^{gh}	0.25 ± 0.00^{abc}	1.09 ± 0.00^{bcdefg}	22.11 ± 0.02^{jk}	21.72 ± 0.08^{ef}	46.98 ± 0.04^{hi}
F22	19.81 ± 0.01^{h}	1.91 ± 0.00^{e}	17.99 ± 0.06^{b}	0.72 ± 0.00^{d}	45.28 ± 0.00^{ijkl}	1.96 ± 0.01^{i}	0.24 ± 0.00^{ab}	1.20 ± 0.01^{ghi}	22.44 ± 0.01^{kl}	19.36 ± 0.05^{bc}	47.30 ± 0.01^{ij}
*F*23	18.39 ± 0.00^{bc}	1.50 ± 0.01^{bc}	19.58 ± 0.42^{def}	0.81 ± 0.01^{fgh}	45.63 ± 0.12^{klm}	1.84 ± 0.01^{efg}	0.29 ± 0.01^{bcde}	1.16 ± 0.04^{efgh}	20.48 ± 0.01^{bc}	21.19 ± 0.39^{de}	47.54 ± 0.12^{ij}
F24	18.35 ± 0.02^{bc}	1.30 ± 0.01^{a}	19.35 ± 0.08^{de}	0.79 ± 0.02^{ef}	45.39 ± 0.04^{jkl}	1.80 ± 0.00^{cdef}	0.33 ± 0.00^{fg}	1.15 ± 0.03^{defgh}	20.23 ± 0.00^{ab}	20.96 ± 0.12^{de}	47.27 ± 0.04^{ij}
F25	19.86^{h}	1.55^{c}	16.90^{a}	0.84^{ghi}	46.48^{o}	1.76^{bcd}	0.31^{efg}	1.17^{fgh}	22.00^{ij}	18.56^{ab}	48.31^{k}

(*continued on next page*)

Table 3 (*continued*)

Sample code [1]	(A) Neutral fraction of oat oil										
	16:0	18:0	18:1 (n-9)	18:1 (n-7)	18:2 (n-6)	18:3 (n-3)	20:1 (n-9)	Others [2]	Σ SAFA	Σ MUFA	Σ PUFA
F26	20.12 ± 0.02^{i}	1.54 ± 0.04^{c}	18.64 ± 0.01^{bcd}	0.88 ± 0.01^{i}	44.54 ± 0.03^{h}	1.86 ± 0.01^{efg}	0.28 ± 0.00^{bcde}	1.24 ± 0.00^{hi}	22.31 ± 0.06^{jk}	20.33 ± 0.03^{cd}	46.45 ± 0.01^{gh}
F27	20.30 ± 0.06^{i}	1.75 ± 0.01^{d}	19.23 ± 0.03^{cde}	0.86 ± 0.00^{hi}	43.52 ± 0.09^{fg}	1.81 ± 0.00^{cdef}	0.25 ± 0.00^{abc}	1.31 ± 0.06^{i}	22.72 ± 0.08^{l}	20.95 ± 0.08^{de}	45.38 ± 0.10^{e}
F28	19.20 ± 0.19^{ef}	1.80 ± 0.07^{de}	22.04 ± 0.78^{h}	0.65 ± 0.03^{b}	42.87 ± 0.40^{de}	1.78 ± 0.02^{cde}	0.25 ± 0.02^{abc}	1.10 ± 0.00^{cdefg}	21.54 ± 0.27^{gh}	23.48 ± 0.77^{g}	44.69 ± 0.42^{cd}
F29	19.36 ± 0.03^{f}	1.80 ± 0.03^{de}	20.61 ± 0.03^{fg}	0.80 ± 0.01^{fg}	43.80 ± 0.22^{g}	1.82 ± 0.01^{defg}	0.23 ± 0.00^{a}	0.91 ± 0.02^{a}	21.62 ± 0.06^{gh}	22.05 ± 0.02^{ef}	45.67 ± 0.21^{ef}
F30	18.89 ± 0.05^{d}	1.31 ± 0.00^{a}	16.13 ± 0.01^{a}	1.05 ± 0.00^{j}	46.43 ± 0.01^{no}	1.94 ± 0.03^{hi}	0.28 ± 0.02^{bcde}	1.05 ± 0.02^{bcdef}	20.72 ± 0.04^{cde}	17.92 ± 0.01^{a}	48.45 ± 0.04^{k}
mean	19.20 ± 0.74	1.72 ± 0.25	20.61 ± 2.73	0.75 ± 0.12	44.07 ± 1.86	1.83 ± 0.13	0.28 ± 0.03	1.10 ± 0.10	21.50 ± 0.81	22.10 ± 2.60	45.96 ± 1.93

[1] Sample codes of extracted oat flours (crop 2019) equal those in Jokinen et al., 2021. The values are mean ± SD of two extract replicates. The data of one replicate of sample 19 in the neutral fraction and sample 29 in the polar fraction was excluded.
[2] Others include 14:0, 16:1(n-7), 20:0, 20:2(n-6), 22:0, 22:1(n-9) and 24:1(n-9).

heat-treated oat flours industrially produced from the same grains. Instead, some correlations existed between oat grain's chemical and physical properties. For example, the thousand seed weight of the native grains showed a significant positive correlation ($p < 0.01$) with starch and total PUFA content (unfractionated extracts), and a negative correlation ($p < 0.01$) with grain color value a*, fat, and total MUFA content

Table 4
Volatile compounds identified in stored oat flour samples by HS-SPME-GC–MS using semipolar column DB-624.

Compound	RT (min)	Match with NIST20	0 month*	6 months*	9 months*	Chemical group
Pentane	7.1	884	4.99	3.72	1.34	Alkane
1-Hydroxy-2-propanone	9.4	898	7.34	5.32	4.09	Ketone
2-Methylpropanal	10.9	930	6.33	4.77	0.91	Aldehyde
1-Propanol	11.8	936	6.55	4.38	n.d.**	Alcohol
Butanal	12.6	937	0.94	7.37	4.43	Aldehyde
2-Butanone	13.1	943	8.42	7.67	16.29	Ketone
3-Methylbutanal	15.6	925	8.57	6.13	1.10	Aldehyde
Acetic acid	15.8	932	40.92	40.35	8.89	Acid
2-Methybutanal	16.0	868	27.52	21.45	5.92	Aldehyde
1-Butanol	16.8	927	20.03	25.75	9.38	Alcohol
2-Pentanone	17.4	874	0.91	2.68	1.77	Ketone
Pentanal	17.6	948	6.02	116.47	71.00	Aldehyde
4-Methyl-2-pentanone	19.8	902	2.50	3.29	n.d.**	Ketone
1-Pentanol	22.0	885	1.54	8.56	6.11	Alcohol
Hexanal	22.3	979	48.23	1481.63	996.37	Aldehyde
4-Methyloctane	23.5	926	5.95	9.16	1.90	Alkane
3-Methyl-1-butyl acetate	25.0	897	1.96	n.d.**	n.d.**	Ester
(*E*)-2-Hexenal	25.2	924	n.q.***	4.58	4.17	Aldehyde
2-Butylfuran	25.3	929	n.d.**	6.28	4.90	Furan
4-Hydroxy-4-methyl-2-pentanone	25.4	959	5.27	4.14	n.d.**	Ketone
1-Hexanol	25.7	892	7.66	95.92	27.54	Alcohol
2-Heptanone	26.2	909	2.32	17.57	8.03	Ketone
Heptanal	26.6	893	2.24$^{\#}$	29.50	19.58	Aldehyde
α-Pinene	27.0	948	625.83	24.66	13.17	Terpene
2-Pentylfuran	29.2	927	7.22	84.12	50.83	Furan
1-Octen-3-ol	29.8	921	n.q.***	27.43	11.58	Alcohol
Benzaldehyde	29.9	921	63.11	11.75	4.47	Aldehyde
3-Carene	30.1	947	362.47	13.24	6.41	Terpene
Octanal	30.5	982	1.43	30.63	31.55	Aldehyde
D-Limonene	30.8	924	33.51	18.39	5.01	Terpene
p-Cymene	31.0	949	13.82	n.q.***	6.91	Terpene
β-Phellandrene	31.1	939	35.23$^{\#\#}$	n.d.**	n.d.**	Terpene
Dihydro-5-methyl-2(*3H*)-furanone	31.3	875	3.83$^{\#\#\#}$	n.d.**	n.d.**	Furanone
γ-Terpinene	31.9	902	7.99$^{\#\#\#\#}$	n.d.**	n.d.**	Terpene
(*E*)-3-Octen-2-one	32.5	926	n.d.**	12.78	8.51	Ketone
(*E*)-2-Octenal	33.5	964	n.d.**	14.25	7.48	Aldehyde
(*E,E* or *E,Z*)-3,5-Octadien-2-one	34.0	928	1.74	5.14	2.49	Ketone
Nonanal	34.7	912	25.31	124.64	94.23	Aldehyde
(*E,E* or *E,Z*)-3,5-Octadien-2-one	35.1	937	0.70	2.95	1.34	Ketone
5-Ethyldihydro-2(*3H*)-furanone	35.5	933	1.05	3.20	2.93	Furanone
(*E* or *Z*)-2-Nonenal	37.7	945	1.49	5.04	1.90	Aldehyde
Decanal	38.9	926	1.36	4.34	4.23	Aldehyde

*Average peak area of volatile compound of all quantifiable samples in counts per s per 10^5 analyzed by headspace solid-phase microextraction with gas chromatography with mass spectrometer detection (HS-SPME-GC–MS).
** n.d. = not detected, ***n.q. = detected but not quantifiable.
n.d. in F11, F12, F14, F15 and F18; $^{\#\#}$ only in F11, F12, F14 and F18; $^{\#\#\#}$ only in F11, F17, F22 and F24-27; $^{\#\#\#\#}$only in F12 and F18.

(unfractionated extracts) (Jokinen et al., 2021). Hence, this data could be valuable in agriculture, wherein the "thousand seed weight" parameter could be used to estimate grains characterized by a high PUFA content and select them for specific industrial uses requiring increased omega-3 and omega-6 fatty acids.

3.3. The storage trial, volatiles, and tocols

Over 160 compounds (peaks) were detected by using the SPME-GC–MS method. From these, 42 volatile compounds were identified (Table 4). The volatiles included aldehydes (14), ketones (9), alcohols (5), terpenes (6), alkanes (2), furans (2), furanones (2), acids (1) and esters (1). Similar to earlier studies on oat volatiles, aldehydes were the most abundant group of volatiles followed by ketones (Klensporf & Jeleń, 2008; Lampi et al., 2015; Li et al., 2023). No pyrazines were found in this study against some previous reports (Dach & Schieberle, 2021; Li et al., 2023). The lack of pyrazines as Maillard reaction products in this study suggests a milder heat treatment in the industrial production of oat flours than oat flakes where pyrazines were detected (Li et al., 2023). A similar conclusion on the effect of heat treatment was also drawn by Klensporf & Jeleń (2008) in their study on the flavor of oat flake. Furthermore, the terpenes, such as α-pinene, 3-carene, and D-limonene, natural organic compounds of unprocessed plants, which are sensitive to elevated temperatures, were present in fresh flours in high concentrations. α-Pinene was the predominant volatile in the profile of fresh oat samples followed by the 3-carene peak. The terpene levels significantly changed after six months of storage with some minor amounts still detectable in the nine-month stored samples. The volatiles with medium-sized peaks in fresh oat flours included 2-butanone, acetic acid, hexanal, D-limonene, and other terpenes, 2-pentylfuran, and nonanal. These volatile compounds showed variability among samples. Other volatiles were present at a minor intensity. From two identified furanone peaks, 5-methyl-dihydro-2(3*H*)-furanone occurred only in a few fresh flour samples and was not detected later, while 5-ethyl-dihydro-2(3*H*)-furanone appeared in all samples during the whole storage period. Furanons are interesting compounds known for their sweet and fruity aroma and flavor and, in this study case, most likely originated from heat treatment.

In stored samples, hexanal was the most abundant volatile compound followed by pentanal, 2-pentylfuran and nonanal (Table 4). Hexanal was also detected as the main volatile in previous studies (Heiniö et al., 2002; Klensporf & Jeleń, 2008; Lampi et al., 2015; Li et al., 2023). Typical volatiles related to lipid oxidation, like aldehydes (e.g., hexanal, octanal, and nonanal), ketones (e.g., 2-butanone, 2-heptanone and (*E*)-3-octen-2-one), and alcohols (e.g., 1-pentanol, 1-hexanol, 1-octen-3-ol) increased during storage. A similar behavior during storage at room temperature or accelerated shelf-life testing was also seen by Heiniö et al. (2002) for native and processed oats, Molteberg et al. (1996) for raw and heat-treated flour samples, Lampi et al. (2015) for oat flours and extrudates, and Li et al. (2023) for oat flakes. According to existing literature, the presence and significant increase of hexanal and 2-pentylfuran were most noticed during the storage of oat samples. Thereby, a higher content of 2-pentylfuran than hexanal indicates oat lipoxygenase activity rather than autoxidation (Lampi et al., 2015). In the current study, hexanal was the most abundant volatile further confirming the full inactivation of enzymes in oat flours. In addition to the hexanal and 2-pentylfuran compounds, an increase in the contents of pentanal, heptanal, octanal, and nonanal was reported earlier (Heiniö et al., 2002; Klensporf & Jeleń, 2008; Molteberg et al., 1996; Sjövall et al., 1997). In our study, ten volatile oxidation indicator compounds, being 2-butanone, 2-heptanone, pentanal, hexanal, heptanal, octanal, nonanal, 2-pentylfuran, 3-octen-2-one, and 2-octenal, were selected for the principal component analysis (PCA) based on earlier findings and abundance in the samples. The volatile data were combined with the tocol content measured from the same storage samples (0, 6, and 9 months) to get an overview of oxidation behavior including consumption of tocols.

In general, tocol content decreased during storage. The initial tocol contents, as presented by Pöysä et al. (2024), were on average with a range of 6.0 (4.1–7.9) μg/g DW, 25.9 (21.1–32.0) μg/g DW, 0.7 (0.5–1.3) μg/g DW, and 3.2 (2.2–5.2) μg/g DW, for α-tocopherol, α-tocotrienol, β-tocopherol, and β-tocotrienol, respectively. During storage, α-tocols were less stable than β-tocols, which aligns with their high reactivity (Barouh et al., 2022) (Supplementary Table 1). Losses of β-tocopherol seemed to be greater than those of other tocols after nine months of storage, but low remaining values were due to its low initial content, which were close to the limit of determination. In most samples, trends of tocol losses were similar, except in sample 28, where tocols degraded much faster. After six months, less than 23 % of its original tocol content was left, and after nine months, it dropped to under 7 %. In contrast, after 6 and 9 months of storage, 57 % and 46 % of initial tocols remained in other samples, respectively (Supplementary Table 1).

In the PCA model of the selected volatile compounds and tocols of the stored oat flours (Fig. 1A and 1B), PC-1 accounted for 57 % and PC-2 for 12 % of the variation. All fresh samples (0 months) are located on the positive side of PC-1, while all stored samples (6 and 9 months) are located on the negative side of PC-1 (Fig. 1A). The fresh oat flours 11, 12, 13, 14, 18, and 20 are found in the right upper quadrant of the PCA. They are associated with tocols, pentanal, and 2-pentylfuran (Fig. 1B), which reflects their high tocol content (Pöysä et al., 2024) and a low range of volatile secondary oxidation compounds. The other fresh samples are located in the lower right corner of the PCA and correlated with 2-heptanone, nonanal, 2-butanone, and heptanal. The fresh samples are generally associated with volatile compounds formed early and did not increase drastically during storage time. Simultaneously, the stored samples are related to volatile compounds, which significantly increased during the storage period.

The oat flours stored for six months are all located in the left upper quadrant of the PCA (Fig. 1A), except samples 21 and 28, and are associated with 3-octen-2-one, 2-octenal, and hexanal (Fig. 1B). Samples 21 and 28 at six months and most samples stored for nine months are situated in the lower left quadrant of the PCA. They correlate positively with octanal, formed later in the oxidation process from C18:1(n-9), and negatively with remaining tocols and early formed volatiles. Oat flour samples 12, 14, 17, 18, 19, and 20 are still found in the left upper quadrant at nine months with most six-month samples (Fig. 1A). These oat flours can be considered the most stable over the storage period of nine months at room temperature. Interestingly, either the remaining tocol content at nine months (Supplementary Table 1) or the initial lipid content or neutral to polar lipid ratio (Table 1) could explain this higher stability, as the samples were not significantly different from others more oxidized at nine months (samples 21, 22, 23, 24, 25, 26, 27, 29, and 30). Also, the fatty acid composition, especially the content of α-linolenic acid (Table 2), could not describe this behavior as only samples 18 and 19 had a significantly lower content of α-linolenic acid than other samples.

To evaluate the oxidative stability in more detail, the data of the leading volatile oxidation indicators, such as 3-octen-2-one, 2-octenal, hexanal, and octanal, were plotted into column chart graphs and their changes during the storage period are shown in Fig. 2. The statistical results of Fig. 2 are presented in Supplementary Table 3. The volatile compounds 3-octen-2-one and 2-octenal were not detected in any samples at 0 months (Fig. 2A and 2B). The oxidation pathways of fatty acid breakdown previously described in Frankel (1982) support our findings. The volatile oxidation product, 3-octen-2-one, generates from linoleate hydroperoxides (9-hydroperoxy-10,12-cyclic peroxide) by autooxidation or photosensitized oxidation and 2-octenal from linoleate hydroperoxides (9-hydroperoxy) or 2,4-decadienal (Frankel, 1982). Consequently, no 3-octen-2-one and 2-octenal should be present in fresh samples. Moreover, hexanal and octanal content was low in all samples at 0 months (Fig. 2C and 2D) confirming that all samples had low oxidation levels at the start of the storage trial. As the PCA shows

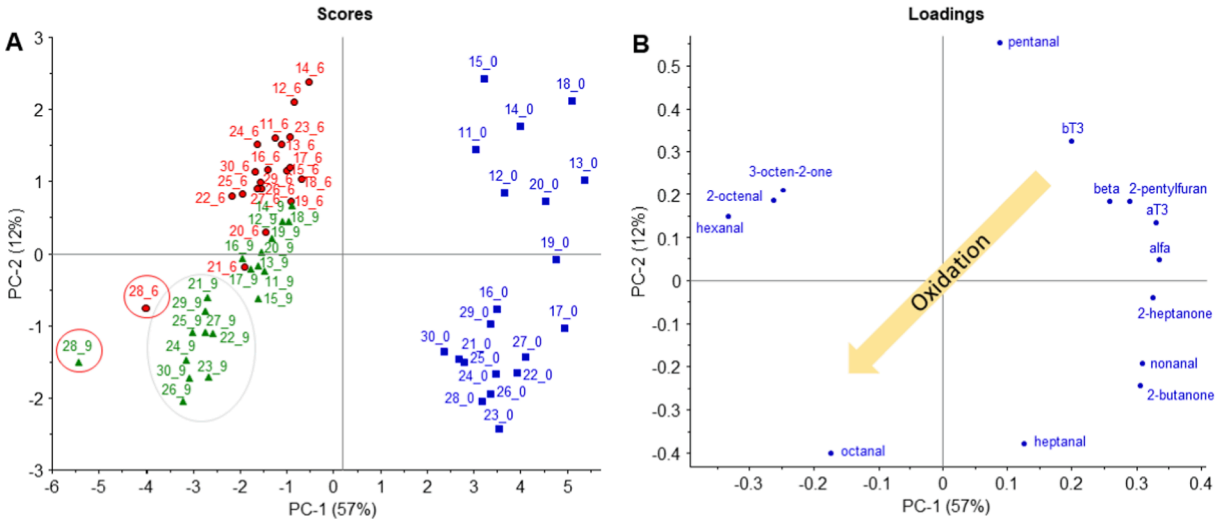

Fig. 1. Principle component analysis (PCA) of lipid oxidation indicators. (A) PCA scores plot showing oat flours of different oat cultivars during storage (blue ■ = 0 months, red ● = 6 months, and green▲ = 9 months). (B) PCA loading plot showing selected volatile compounds and tocols (alfa = α-tocopherol, aT3 = α-tocotrienol, beta = β-tocopherol, bT3 = β-tocotrienol) variables. The volatile data was area normalized, and all data was mean-centered and weighed (1/sdev). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

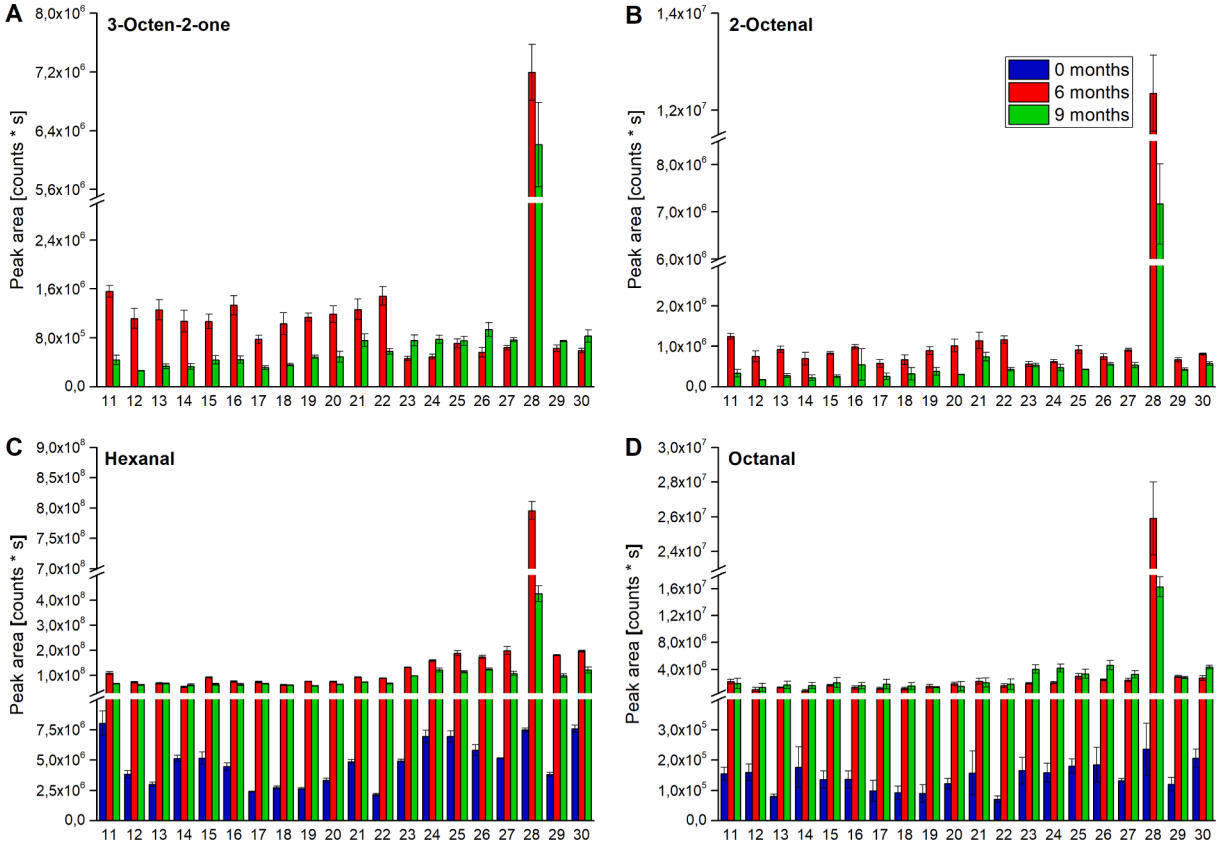

Fig. 2. Changes in the total peak area of 3-octen-2-one, 2-octenal, hexanal, and octanal of 20 investigated flour samples during the storage period of three-time points (0, 6, and 9 months). No peaks of 3-octen-2-one and 2-octenal are detected at the zero time point in fresh samples. The statistical differences between the samples are presented in the Supplementary Table 2. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

(Fig. 1), sample 28 significantly differed from the others. The content of the main volatile oxidation indicators was 4 to 6 times higher in 28 than for other samples at six months. Further, the content of all indicators went down at nine months (Fig. 2) indicating further oxidation of 3-octen-2-one, 2-octenal, hexanal, and octanal. A reduction in intensity at nine months was also seen for almost all samples for 2-octenal and hexanal and from samples 11 to 22 for 3-octen-2-one. In the case of octanal, the content was either higher at nine compared to six months or comparable at both time points except for sample 28 (Fig. 2D). Octanal is formed from oleic acid (Frankel, 1982), which is more oxidatively

stable than linoleic acid and α-linolenic acid and thus oxidizes later. Similar as seen in the PCA (Fig. 1), samples 11 to 22 behaved differently than samples 23 to 30 at a nine-month storage point.

A similar observation, in terms of nonanal, was made by Sjövall et al. (1997) in storing extruded flours at 32 °C for 18 weeks. The induction time of nonanal, another volatile product derived from oleic acid, was longer than that of hexanal. In our study, nonanal was not strongly associated with the stored samples (Fig. 1) supporting milder heat treatment and lower storage temperature. While several storage studies on different oat samples reported gradual changes in pentanal, hexanal, heptanal, octanal, nonanal, decanal, and 2-pentylfuran during storage, currently, only hexanal and 2-pentylfuran were suggested for the indicators of oxidation (Heiniö et al., 2002; Heydanek & McGorrin, 1981; Klensporf & Jeleń, 2008; Lampi et al., 2015; Li et al., 2023; Molteberg et al., 1996; Sjövall et al., 1997). In our storage trial, 2-pentylfuran was associated mainly with the variability between the fresh samples. According to the current study results, 3-octen-2-one, 2-octenal, and octanal could be potential oxidation indicators besides hexanal in storing oat flour at room temperature.

4. Conclusion

In this study, batches of pure cultivars from the same crop year were processed identically at the same mill and by a controlled kiln treatment to prevent the activity of lipolytic enzymes. The storage trial was designed to mimic the real-life situation of storing oat flour by a consumer and thus conducted in normal shelf-life scenarios, not as accelerated. In this study, while the crop year, purity of cultivar, and equal milling and processing were carefully controlled, factors such as soil properties or fertilization could not be equalized. As hypothesized, the composition of lipids and volatiles varied between the studied oat batches. The fresh oat samples had a low content of volatile oxidation products. In general, the volatile profile of six- and nine-month storage samples was similar with a few exceptions. The loss of tocols during the storage was noticeable. In some cases, some minor correlations between lipid and tocol composition and the formation of volatile oxidation compounds during storage could be found. However, overall, the oxidation behavior could not be predicted based on lipid and tocol content or composition, which is contrary to our hypothesis. The main lipid-related oxidation products for oat samples indicated in this study were hexanal, 3-octen-2-one, 2-octenal, and octanal, from which 3-octen-2-one and 2-octen were not reported previously. These compounds can potentially be used as oxidation indicators for oat products. Most oxidation products can be linked to compounds formed from heat treatment or autoxidation and further deterioration of fatty acids being mainly oleic and linoleic acid. As recent knowledge of lipids and volatiles of currently available oats is limited, this study provides valuable information on how their properties affect the use of oat crops for food applications.

CRediT authorship contribution statement

Anna Puganen: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Annelie Damerau:** Writing – review & editing, Writing – original draft, Visualization, Supervision, Formal analysis, Conceptualization. **Marjo Pöysä:** Methodology, Investigation, Formal analysis. **Anna-Maija Lampi:** Writing – review & editing, Supervision, Methodology. **Vieno Piironen:** Funding acquisition, Conceptualization, Resources, Supervision, Writing – review & editing. **Baoru Yang:** Resources, Writing – review & editing. **Kaisa M. Linderborg:** Conceptualization, Formal analysis, Project administration, Resources, Supervision, Writing – original draft, Writing – review & editing.

Declaration of competing interest

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

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodchem.2024.139448.

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