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Latvia University of Life Sciences and Technologies

Faculty of Food Technology

Mg. sc. sal. **Ilze Laukalēja**

doctoral thesis

VOLATILE AND BIOACTIVE COMPOUNDS IN DIFFERENT ROAST LEVEL SPECIALTY COFFEE

GAISTOŠIE UN BIOLOĢISKI AKTĪVIE SAVIENOJUMI DAŽĀDA GRAUZDĒJUMA PAKĀPES *SPECIALTY* KAFIJĀ

for acquiring a Doctor of Science (**PhD***)* in Food and Beverage Technologies

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2022

ANNOTATION

Doctoral thesis by Ilze Laukalēja "Volatile and bioactive compounds in different roast level specialty coffee" was developed from 2017 to 2022 in the scientific laboratories of the Department of Food Technology, Latvia University of Life Sciences and Technologies, and Center for Sensory Analysis and Consumer Behavior, Kansas State University (USA). The **object** of the doctoral thesis is *Coffea arabica* L. coffee beans at different roast levels.

The **hypothesis** of the doctoral thesis – coffee consumers would preffer specialty coffee due to increased bioactive compound contet by adjusted roast level.

The hypothesis was confirmed by the following **theses**.

1. Solid-phase microextraction (SPME) fibre coating affects volatile compound extraction and detection in specialty coffee brew.
2. Specialty coffee origin and roasting parameters impact phenolic compound content and sensory quality.
3. Light roast level has a positive effect on phenolic and volatile compound content in specialty coffee.
4. Initial gas chromatography-olfactometry vocabulary allows to detect and describe aroma-active compounds in specialty coffee.
5. Consumer perception of specialty coffee brews can be affected by sensory attributes and potentially increased bioactive compound content.

The **aim** of the doctoral thesis was to evaluate the impact of the roast level on the composition of bioactive compounds and sensory quality in specialty coffee.

To achieve the aim of the doctoral thesis, the following **objectives** have been established.

1. To evaluate different solid-phase microextraction (SPME) fibre influence on specialty coffee brew volatile compound extraction and detection.
2. To analyse phenolic compound content and cup quality profile in different origin and roast specialty coffees.
3. To determinate roasting process influence on volatile compound profile.
4. To evaluate non-volatile compound content changes during the roasting process.
5. To develop an initial gas chromatography-olfactometry vocabulary for specialty coffee.

To assess consumer perception of specialty coffee brews with potentially increased bioactive compound content.

The doctoral thesis consists of three chapters.

Chapter 1 summaries previous literature about coffee's chemical composition, sensory properties, and possible changes during roasting and brewing processes; provides information about the biologically active compound composition and their impact on health; defines specialty coffee and coffee quality standards.

Chapter 2 describes the coffee roasting process and summarises the materials and methods of analysis.

Chapter 3 summarises the results obtained in this study with a discussion to achieve the conclusions according to the hypothesis and established objectives. The chapter describes the evaluation of different SPME fibre influence on specialty coffee brew volatile compound extraction and detection; the chemical and sensory profile changes under the influence of roasting process; aroma-active compound perception in coffee by gas chromatography-olfactometry; analysis of consumer perception of specialty coffee brews.

The **novelty** of the doctoral thesis.

1. A complex volatile and biologically active compound comparison has been developed for different roast level specialty coffee.
2. Solid-phase microextraction fibre evaluation for improved volatile compound detection in specialty coffee.
3. Volatile and aroma-active compound profile analysis in different roast level specialty coffee;
4. Developed gas chromatography-olfactometry vocabulary allows to analyse aroma-active compound perception in differently roasted and brewed specialty.

The **economic significance** of the doctoral thesis: the completed analysis about the roast level impact on coffee quality and bioactive compound content in specialty coffee provides the coffee roasters with an opportunity to adjust roast parameters.

During the PhD studies, the author had an internship at the Center for Sensory Analysis and Consumer Behavior in Kansas State University (United States of America), where experimental work was done. The internship was provided by the Baltic-American Freedom Foundation (BAFF) and the Council on International Education Exchange (CIEE).

The study was partly **financed** by:

- the LLU programme "Strengthening Research Capacity at the Latvia University of Agriculture" grant contract No. 3.2-10/2018/LLU/74 “The changes of biologically active compounds of specialty coffee under the influence of technological processes”;
- the "8th European PhD Flavour Research Awards Programme";
- the doctoral studies grant "Transition to the new doctoral funding model at the Latvia University of Life Sciences and Technologies" Contract No. 8.2.2.0/20/I/001.

The thesis is written in English (United Kingdom); it consists of 108 pages, 27 tables, 16 figures, four appendixes, and 190 bibliographic sources.

ANOTĀCIJA

Ilzes Laukalējas promocijas darbs “Gaistošie un bioloģiski aktīvie savienojumi dažāda grauzdējuma pakāpes *specialty* kafijā” izstrādāts no 2017. gada līdz 2022. gadam Latvijas Lauksaimniecības universitātes Pārtikas tehnoloģijas fakultātē un Patērētāju uzvedības un sensorās zinātnes centrā, Kanzasas štata universitātē (ASV).

Promocijas darba **hipotēze** – pielāgojot grauzdēšanas pakāpi, kafijas patērētāji dotu priekšroku *specialty* kafijai tās palielināto bioloģiski aktīvo savienojumu satura dēļ.

Promocijas darba hipotēze tika pierādīta ar piecām **tēzēm**.

1. Cietās fāzes mikroekstrakcijas šķiedras pārklājums ietekmē gaistošo savienojumu ekstrakciju specialty kafijas dzērienos.
2. Specialty kafijas izcelsmes valsts un grauzdēšanas parametri ietekmē fenola savienojumu saturu un sensoro kvalitāti.
3. Viegla grauzdēšanas pakāpe pozitīvi ietekmē fenolu un gaistošo savienojumu sastāvu specialty kafijā.
4. Gāzu hromatogrāfijas-olfaktometrijas vārdnīca ļauj noteikt un aprakstīt aromātu veidojošo savienojumus *specialty* kafijai.

Patērētāju uztveri par *specialty* kafijas pagatavošanas veidiem var ietekmēt sensorās īpašības un informācija par potenciāli palielinātu bioloģiski aktīvo savienojumu saturu kafijā.

Darba **mērķis** – izvērtēt grauzdēšanas pakāpes ietekmi uz bioloģiski aktīvo savienojumu sastāvu un sensoro kvalitāti specialty kafijā.

Darba mērķa sasniegšanai izvirzīti šādi **uzdevumi**.

1. Novērtēt cietās fāzes mikroekstrakcijas šķiedru ietekmi uz *specialty* kafijas dzērienu gaistošo savienojumu ekstrakciju un noteikšanu.
2. Analizēt fenolu savienojumu sastāvu un sensoro kvalitāti dāžadas izcelsmes un grauzdējuma specialty kafijā.
3. Noteikt grauzdēšanas procesa ietekmi uz gaistošo savienojumu sastāvu.
4. Analizēt negaistošo savienojumu sastāva izmaiņas grauzdēšanas procesā.
5. Izveidot gāzu hromatogrāfijas-olfaktometrijas vārdnīcu *specialty* kafijai.

Analizēt patērētāju novērtējumu par specialty kafijas dzērieniem ar potenciāli palielinātu bioloģiski aktīvo savienojumu koncentrāciju.

Promocijas darbs apkopots **trīs nodaļās**.

1. nodaļā aprakstīts kafijas ķīmiskais sastāvs, sensorās īpašības un iespējamās to izmaiņas grauzdēšanas procesā; izvērtēta informācijapar bioloģiski aktīvo savienojumu sastāvu kafijā un to ietekmi uz veselību; sniegta informāciju par *specialty* kafijas kvalitātes standartiem.

2. nodaļā sniegts kafijas grauzdēšanas procesa apraksts un apkopotas izmantotās metodes, materiāli promocijas darbā.

3. nodaļā sniegts apkopojums par promocijas darbā iegūtajiem rezultātiem ar to diskusiju, lai iegūtu secinājumus atbilstoši izvirzītajai hipotēzei un uzdevumiem. Nodaļā izvērtēta dažādu cietās fāzes mikroekstrakciju (CFME) šķiedru spēja ekstrahēt *specialty* kafijā nozīmīgus gaistošos savienojumus; aprakstītas ķīmisko un sensoro rādītāju izmaiņas grauzdēšanas procesu ietekmē; analizēta aromātu veidojošo savienojumu uztvere dažādi grauzdētā un pagatavotā kafijā ar gāzu hromatogrāfijas-olfaktometrijas metodi; izvērtēts kafijas patērētāju viedoklis par specialty kafiju.

Promocijas darba **novitāte.**

1. Veikts komplekss gaistošo savienojumu un bioloģiski aktīvo savienojumu salīdzinājums dažāda grauzdējuma pakāpes *specialty* kafijā.
2. Cietās fāzes mikroekstrakcijas šķiedru izvērtējums uzlabotai gaistošo savienojumu noteikšanai *specialty* kafijā.
3. Gaistošo savienojumu un aromātu veidojošo savienojumu profila noteikšana dažāda grauzdējuma un pagatavošanas metožu kafijās.
4. Gāzu hromatogrāfijas-olfaktometrijas vārdnīcas izveide, kas ļauj analizēt aromātveidojošo savienojumu uztveri dažāda grauzdējuma pakāpes un pagatavošanas veida kafijā.

Tautsaimniecības nozīme.

Analīze par grauzdēšanas pakāpes ietekmi uz kafijas kvalitāti un bioloģiski aktīvo savienojumu saturu specialty kafijā, sniedz kafijas grauzdētājiem iespēju pielāgot grauzdēšanas procesu.

Doktorantūras studiju laikā promocijas darba autore praktizējās Kanzasas štata universitātes "Patērētāju uzvedības un sensorās zinātnes" centrā (Amerikas Savienotajās Valstīs), kurā tika veikta pētnieciskā darba izstrāde. Prakses vietu un iespēju veikt pētniecisko darbību nodrošināja Baltijas Amerikas Brīvības fonda (BAFF) un Starptautiskās izglītības apmaiņas padomes (CIEE) piešķirtā **stipendija**.

Promocijas darba izstrāde tika veikta pateicoties sekojošiem **līdzfinansējumiem**:

- pētījuma programmas "Zinātniskās kapacitātes stiprināšana LLU" (2018.–2020.) projekta Nr. 3.2-10/2018/LLU/74 "Specialty kafijas bioloģiski aktīvo savienojumu izmaiņas tehnoloģisko procesu ietekmē" (Z22);
- "8th European PhD Flavour Research Awards" programma;
- ES32 "LLU pāreja uz jauno doktorantūras finansēšanas modeli" projekts Nr. 8.2.2.0/20/I/001.

Promocijas darbs ir rakstīts angļu valodā (Apvienotās Karalistes) 108 lapās, ieskaitot 27 tabulas, 16 attēlus, četri pielikumi, un 190 zinātniskās literatūras atsauces.

Approbation of the scientific work / *Zinātniskā darba aprobācija*

The research results are published in six scientific issues, including five publications indexed in the international citation databases SCOPUS and Web of Science, and reported at nine international conferences. / *Pētījuma rezultāti ir publicēti septiņos zinātniskajos izdevumos, ieskaitot sešas publikācijas, kas indeksētas starptautiskās citēšanas datubāzēs SCOPUS un Web of Science, un par tiem ziņots deviņās starptautiskajās konferencēs.*

Publication indexed in international citation databases SCOPUS or Web of Science / *Publikācijas, kas indeksētas starptautiskajā datu bāzē SCOPUS vai Web of Science*.

1. Laukaleja, I., & Koppel, K. (2021). Aroma-active compound perception in differently roasted and brewed coffees by gas chromatography-olfactometry. *Journal of Sensory Studies*, 36(6), e12708. DOI:10.1111/joss.12708
2. Laukaleja, I., & Kruma, Z. (2019). Evaluation of a headspace solid-phase microextraction with different fibres for volatile compound determination in specialty coffee brews. *Research for Rural Development 2019*, 1, 215–221. DOI:10.22616/rrd.25.2019.032
3. Laukaleja, I., & Kruma, Z. (2019). Phenolic and volatile compound composition influence specialty coffee cup quality. *Agronomy Research*, 17(S2), 1367–1379. DOI:10.15159/ar.19.074
4. Laukaleja, I., & Kruma, Z. (2019). Influence of the roasting process on bioactive compounds and aroma profile in specialty coffee: a review. *Proceedings of 13th Baltic Conference on Food Science and Technology "Food. Nutrition. Well-Being" and NEEFOOD 2019 5th North and East European Congress on Food*, Jelgava: LLU, 7–12. DOI:10.22616/FoodBalt.2019.002.
5. Laukaleja, I., & Kruma, Z. (2018). Quality of Specialty Coffee: Balance between aroma, flavour, and biologically active compound composition: Review. *Research for Rural Development 2018*, 1, 240–247. DOI:10.22616/rrd.24.2018.038.

Publications in peer reviewed scientific issues / *Publikācijas recenzētā zinātniskajā izdevumā*.

Laukaleja, I., Kruma, Z., & Cinkmanis, I. (2022). The impact of the roast level on chemical composition in coffee from Colombia. *Proceedings of the Latvian Academy of Sciences, Section B: Natural, Exact, and Applied Sciences*, 76(1), DOI:20–26. 10.2478/prolas-2022-0022

Laukaleja, I., & Koppel, K. (2022). Consumer's perception of specialty coffee brews with potentially increased bioactive compound content. *Foods*, 11 (submitted / *iesniegts*).

Results have been presented at nine international conferences in Latvia, Estonia, Germany, Portugal, United States of America / *Par rezultātiem ziņots deviņās starptautiskajās konferencēs Latvijā, Igaunijā, Vācijā, Portugālē un Amerikas Savienotajās Valstīts.*

1. Laukaleja, I., Koppel, K. (2021) Consumer's perception of different roast degree coffee brews with potentially increased bioactive compound content. The 14th Pangborn Sensory Science Symposium, United States of America (online), August 9–12 (Poster presentation / *Stenda referāts*).

2. Kruma Z., Laukaleja, I., Cinkmanis, I. (2019) The impact of the roasting process on chemical composition and sensory profile in specialty coffee from Colombia. EuroFoodChem XX Conference, Porto, Portugal, June 17–19 (Poster presentation / *Stenda referāts*).
3. Laukaleja, I., Kruma Z., Cinkmanis, I. (2019) Sensory profile and phenolic compound composition of specialty coffees from three different regions. EuroFoodChem XX Conference, Porto, Portugal, 2019, June 17–19 (Poster presentation / *Stenda referāts*).
4. Laukaleja, I., Kruma Z. (2019) Evaluation of a headspace solid-phase microextraction with different fibres for volatile compound determination in specialty coffee brews. 25th Annual International Scientific Conference "Research for Rural Development 2019", Jelgava, Latvia, May 15–16 (Oral presentation / Mutiskā prezentācija).
5. Laukaleja, I., Kruma Z. (2019) Phenolic and volatile compound composition influence on specialty coffee cup quality. International Conference on Biosystems Engineering 2019 "BSE 2019", Tartu, Estonia, May 8–10 (Oral presentation / Mutiskā prezentācija).
6. Laukaleja, I., Kruma Z. (2019) Influence of the roasting process on bioactive compounds and aroma profile in specialty coffee. 13th Baltic Conference on Food Science and Technology "Food. Nutrition. Well-being", Jelgava, Latvia, May 2–3 (Oral presentation / Mutiskā prezentācija).
7. Laukaleja, I., Kruma Z. (2018) Biologically active compound influence on specialty coffee cup quality. 12th World Congress "Polyphenols Application 2018", Bonn, Germany, September 26–28 (Poster presentation / *Stenda referāts*).
8. Laukaleja, I., Kruma Z. (2018) Quality of specialty coffee: balance between aroma, flavour and biologically active compound composition: a review. 24th Annual International Scientific Conference "Research for Rural Development 2018", Jelgava, Latvia, 2018, May 14–16 (Oral presentation / Mutiskā prezentācija).
9. Laukaleja, I., Kruma Z. (2017) Influence of brewing method to phenolic composition in specialty coffees. 4th North and East European Congress on Food "NEEFood," Kaunas, Lithuania, September 11–13 (Poster presentation / *Stenda referāts*).

CONTENT / *SATURS*

List of included tables / *Darbā iekļauto tabulu saraksts*

List of included figures / *Darbā iekļauto attēlu saraksts*

List of designations and abbreviations used in the doctoral thesis /
Promocijas darbā lietoto apzīmējumu un saīsinājumu skaidrojums

VC	volatile compounds / *gaistošie savienojumi*
AAC	aroma active compounds / *aromātveidojošie savienojumi*
GAE	gallic acid equvalient / *gallu skābes ekvivalents*
CE	catechin equvalient / *katehīna ekvivalents*
ABTS˙+	2,2-azinobis (3-ethylbenzothiazoline-6-sulfonic acid) antiradical activity / *2,2'-azino-bis 3-etilbenzotiazolīn-6-sulfoskābes mono-katjonu antiradikālā aktivitāte*
DPPH˙	2,2-diphenyl-1-picrylhydrazyl antiradical activity / *2,2-difenil-1pikrilhidrazil antiradikālā aktivitāte*
AEDA	aroma extract dilution analysis / *aromātu ekstraktu atšķaidījuma analīze*
AHC	agglomerative hierarchical clustering / *aglomeratīvā hierarhisko klasteru analīze*
ANOVA	analysis of variance / *dispersijas analīzebn*
BAC	biologically active compounds / *bioloģiski aktīvi savienojumi*
BAFF / BABF	Baltic-American Freedom Foundation / *Baltijas-Amerikas Brīvības Fonds*
CAR/PDMS	carboxen/polydimethylsiloxane / *karboksēns/polidimetilsiloksāns*
CIEE / SIAP	council on international education exchange / *starptautiskās izglītības apmaiņas padomes*
CQA	coffee quality organization / *kafijas kvalitātes organizācija*
CW/DVB	carbowax/ divinylbenzene / *karbovasks/ divinilbenzēns*
DHA	dynamic headspace analysis / *dinamiskā tvaika fāzes analīze*
DVB/CAR/PDMS	divinylbenzene/ carboxen/polydimethylsiloxane / *divinilbenzols/karboksēns/polidimetilsiloksāns*
EFSA	European Food Safety Authority / *Eiropas Pārtikas nekaitīguma iestāde*
GC-MS	gas chromatography mass spectrometry / *gāzu hromatogrāfijas masas spektrometrija*
GC-O	gas chromatography-olfactometry / *gāzu hromatogrāfijas-olfaktometrija*
ICO	International Coffee Organization / *Starptautiskā Kafijas Organizācija*
NCAA	National Coffee Association of America / *Amerikas Nacionālā Kafijas Asociācija*
NIF / NIB	nasal impact frequency method / *nazālās ietekmes biežuma metode*
PA	polyacrylate / *poliakrilāts*
PCA	principal component analysis / *galveno komponentu analīze*
PDMS	polydimethylsiloxane / *polidimetilsiloksāns*
PDMS/DVB	polydimethylsiloxane/divinylbenzene / *polidimetilsiloksāns/ divinilbenzols*
pH	negative logarithm of hydrogen ions concentration / *negatīvais logaritms no ūdeņraža jonu koncentrācijas*

SCA	Specialty Coffee Association / *Specialty Kafijas Asociācija*
SD	standard deviations / *standarta novirze*
SDE	simultaneous distillation-extraction / *vienlaicīgā destilācija-ekstrakcija*
SHA	static headspace analysis / *statiskā tvaika fāzes analīze*
SPME / CFME	solid-phase microextraction / *cietās fāzes mikroekstrakcija*
WCR	World Coffee Research / *Pasaules Kafijas Pētniecības Organizācija*

INTRODUCTION / *IEVADS*

Coffee consumption increases each year significantly. The demand for ethical and sustainably produced coffee is the main reason for specialty coffee segment growth. Specialty coffee can be defined as coffee with high-quality standards from the green coffee beans until brewing the coffee. By applying these standards, it is possible to highlight the high-quality sensory characteristics of coffee brew (Urwin, Kesa, & Joao 2019).

Meanwhile, consumers not only pay more attention to the quality of the coffee but are willing to learn more about potential health benefits. The coffee health benefits are associated with the wide range of biologically active compounds in coffee (Nuhu 2014; Laukaleja & Kruma 2018). Coffee has also been recorded as one of the primary polyphenol sources in Eastern European individual diets (Moskal et al. 2015).

Significant physical and chemical changes of coffee bean occur during the roasting process. The complex chemical reactions in roasting process are responsible for volatile, including aroma-active compound formation. In has been reported that coffee defects have negative impact on the coffee aroma (Moon & Shibamoto 2009; Laukaleja & Kruma 2018).

Previous studies have reported polyphenol compound content decrease during the coffee roasting process (Mojica et al. 2018). Specialty coffee is mainly roasted at a light level to highlight specific sensory characteristics. However, light roasted coffee has higher organic acid content and tend to highlight sensory attributes which are not expected for the regular coffee consumer(Poltronieri & Rossi 2016; Laukaleja & Kruma 2019a).

The **object** of the doctoral thesis is *Coffea arabica* L. coffee beans at different roast levels.

Research hypothesises that it is possible to obtain a higher biologically active compound content and improve speciality coffee brew's sensory quality by adjusting roasting processes.

The **aim** of the doctoral thesis was to evaluate the impact of the roast level on the composition of biologically active compounds and sensory quality in specialty coffee. To achieve the aim of the doctoral thesis, the following **objectives** have been established.

1. To evaluate different solid–phase microextraction (SPME) fibre influence on specialty coffee brew volatile compound extraction and detection.
2. To analyse phenolic compound content and cup quality profile in different origin and roast specialty coffees.
3. To determinate roasting process influence on volatile compound profile.
4. To evaluate non–volatile compound content changes during the roasting process.
5. To develop an initial gas chromatography-olfactometry vocabulary for specialty coffee brews.
6. To assess consumer perception of specialty coffee brews with potentially increased bioactive compound content.

The doctoral thesis consists of three chapters.

Chapter 1 describes coffee's chemical composition, sensory properties, and possible changes during roasting and brewing processes; provides information about the biologically active compound composition and their impact on health; defines specialty coffee and coffee quality standards.

Chapter 2 describes the coffee roasting process and summarises the materials and methods of analysis.

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The **novelty** of the doctoral thesis.

1. A complex volatile and biologically active compound comparison has been developed for different roast level specialty coffee.
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The **economic significance** of the doctoral thesis: the completed analysis about the roast level impact on coffee quality and bioactive compound content in specialty coffee provides the coffee roasters with an opportunity to adjust roast parameters.

During the PhD studies, the author had an internship at the Human Behaviour and Sensory Science Centre in Kansas State University (United States of America), where experimental work was done. The internship was provided by the Baltic–American Freedom Foundation (BAFF) and the Council on International Education Exchange (CIEE).

The study was partly **financed** by:

- the LLU programme “Strengthening Research Capacity at the Latvia University of Agriculture” grant contract No. 3.2.-10/2018/LLU/74 “The changes of biologically active compounds of specialty coffee under the influence of technological processes” (Z22);
- the “8th European PhD Flavour Research Awards Programme”;
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The thesis is written in English (United Kingdom); it consists of 108 pages, 27 tables, 16 figures, four appendixes, and 190 bibliographic sources.

1. PROBLEM STATEMENT / *PROBLEMĀTIKAS RAKSTUROJUMS*

1.1. Coffee production steps and quality standards / *Kafijas ražošanas posmi un kvalitātes standarti*

Coffee beans are the seeds from the *Coffea* tree (*genus Caffea* L.), which belongs to the *Rubiaceae* family. *The Coffea* tree has naturally grown in African forests and is cultivated in tropical areas around the equator, such as India, Indonesia, Central and South America (Preedy 2015). *The Coffea* tree has more than 100 species, however, only two of them are commercialized – *Coffea arabica* and *Coffea canephora* (Adepoju et al. 2017; Ferreira et al. 2019).

Several studies have reported that *Coffea arabica* was created from natural hybridization between *Coffea canephora* and *Coffea eugenioides*. As a result of natural hybridization, *Coffea arabica* is the only *genus Caffea* species with 44 chromosomes (Geleta et al. 2012; Ferreira et al. 2019). The uniqueness of *Coffea arabica* chromosome status could be one of the reasons for the pleasant flavour and aroma profile formation, which is respected among coffee consumers. *Coffea arabica* makes approximately 70% and *Coffea canephora* 30% of coffee production. For example, International Coffee Organization (ICO) reported that from December 2020 to November 2021, 79.67 million bags of *Coffea arabica,* while 47.37 million bags of *Coffea canephora* were exported[1]. However, *Coffea arabica* is highly sensitive to climate changes, pesticides, and diseases that have a strong negative effect on the sensory quality (Fassio et al. 2016; Farah 2019). If the safety measurements during coffee production are not monitored, it could increase the possible risks related to consumer health and safety. The high demand and potential environmental and production risks of *Coffea arabica* are the main reasons for strong quality standards implemented in each step from planting *Coffea* trees until brewing roasted coffee.

1.1.1. Coffee production steps / Kafijas ražošanas posmi

Coffee production is based by multiple steps from planting the *Coffea* trees till serving or selling the coffee product. The coffee fruit harvesting and processing can be carried out at the same *Coffea* tree plantation site. After green coffee bean quality evaluation, the coffee is shipped to storage facilities or specific roaster.

The growing conditions are essential to monitor and take preventive actions, if threats are observed. Coffee, especially *Coffea arabica*, is sensitive to direct sunlight, increased temperature, humidity, strong winds, pesticides, and diseases (Preedy 2015; Martins et al. 2020). Preventative actions such as creating an artificial shade environment could potentially improve the plant's growing conditions and improve the sensory attributes of coffee (Geromel et al. 2008; Odeny et al. 2015; Tassew et al. 2021).

Harvesting is the critical step that determines the further quality of coffee. Harvesting can be done by two methods – strip or selective coffee harvesting. The strip coffee harvesting method strip the coffee fruits from the branches of the tree by machines or by hands. By selective coffee harvesting method coffee fruits are handpicked only when the coffee fruits are mature. Mechanical harvesting is less time consuming and less expensive compared to hand-picked and selected methods. However, the selective method has proven to yield better quality coffee (Sridevi & Giridhar 2016; Kazama et al.

[1] ICO, (2021) Exports of all forms of coffee by exporting countries to all destinations [online] [viewed on 13. March 2022] Retrieved from https://www.ico.org/prices/m1-exports.pdf

2021). By only picking matured fruits, it is possible to limit further coffee defects such as black beans (overripe) with a strong bitter flavour and immature beans with strong sour flavour (Franca & Oliveira 2008; Yang et al. 2016). Also, picking coffee from ground could cause greater risk associated with quality, for example. The moulded coffee could not only significantly decrease the sensory quality of the coffee but also increasing the risks of ochratoxin A presence.

Sorting and processing of coffee fruits. After harvesting, the fruits are sorted by size, shape, coffee defects and other physical objects before they are processed. Coffee processing is the step when the pulp of coffee fruits outer layers and pulp is removed, and the coffee seed is collected. There are several post-harvest methods, although two are the most popular and the most studied - natural (dry) method and wet method. The entire coffee processing methods are illustrated in Figure 1.1.

Fig. 1.1. Coffee processing scheme / *1.1. att. Kafijas pārstrādes shēma* (Preedy, 2015)

The natural (dry) method is the oldest treatment method, which is based on drying the soft part of the fruit until the moisture content of the coffee beans is in the range of 10–12% (to avoid bacteria and mould growth). Coffee fruits are kept on cloth nets, pruned regularly for several weeks. The duration of the method depends on the weather (Taveira et al. 2015).

The wet processing method has gained popularity among coffee producers because of the higher quality of the product. The wet method only uses matured fruits, while natural method can be done with fruits form all maturation stages. The mature fruits can be selected by hand, machines, or floating tanks. The next step is to separate the coffee seeds from outer layers, including pulp, the process is called pulping. After pulping the coffee seeds with removed pulps are stored in fermentation tanks for 12 to 36 hours. The fermentation can be done naturally or with added enzymes, microorganisms. While the remaining silverskins of coffee and pulp are removed by microorganisms, the pH decreases to 4.5 and acidity increases. After fermentation the coffee seeds are washed with fresh water and sun dried until moisture content is in the range of 10–12% (Taveira et al. 2015; Poltronieri & Rossi 2016).

After drying the coffee seeds, the dried outer layers of coffee seeds are mechanically removed, this process is called dehusking (natural method) or dehulling (wet method). Coffee has more sweetness, overall texture if the natural method is used, while wet method can highlight acidity. The quality standards for coffee processing are crucial, the coffee is at risks of mould, fungus, bacteria, and insects (Preedy, 2015). The ICO recommends several guidelines and procedures to avoid coffee contamination[2;3].

Coffee roasting is the process of modifying the chemical and physical properties of green coffee beans and creating a roasted coffee product. Green coffee beans are higher in acidity, protein, sugar, and caffeine, but don't have the desired flavour. The roasting process is the main stage in the coffee production which is responsible for the coffee's characteristic taste and aroma. The roasting process can be divided into four stages:

- Drying stage (up to 150 °C).
- First stage of roasting (150 °C to 180 °C).
- Second stage of roasting (180° to 230 °C).
- Third stage of roasting (above 230 °C) (Farah 2019).

In the drying stage the green coffee beans have just been placed in the roaster, the temperature drops immediately, as the coffee beans absorb the energy of the environment, so the first phase of roasting is endothermic. As the temperature rises from 50 °C to 100 °C, changes in the structure of the coffee cells are observed, and as the temperature approaches or slightly exceeds 100 °C, the water in the coffee bean begins to form steam and pressure. The created pressure increases the initial bean temperature. With increasing temperature, the colour components in the beans, such as chlorophylls and anthocyanins, decompose and thus the green colour of the beans changes to yellow-golden tones (Petisca et al. 2012; Toci, Azevedo, & Farah 2020).

The first roasting stage is responsible for the most chemical and physical changes of coffee bean. Maillard reaction between amino acids and reducing sugars starts when the bean temperature increases to 150 °C, and the aroma of coffee beans changes from earthy notes to roasted nuts and baked bread aroma (Oestreich-Janzen 2014; Mojica et al. 2018). The generated steam starts to create pressure inside the beans. As the pressure rises temperature to a certain threshold (approximately 180–205 °C), a rupture occurs at the cellular level, called the "first crack". With the "first crack", the size of the coffee bean doubles and the moisture content of the coffee decreases from the initial 10–12% to 3–5% (Petisca et al. 2012; Preedy 2014). The coffee beans cell expansion and rupture allow the inner soluble compounds to be more easily extracted during brewing process.

When the third stage is reached (225 to 230 °C or above), internal pressure begins to form from CO_2, CO and NO_2 and other gases. Under the influence of pressure, cells rupture. This is called the "second crack", at which the coffee oils start to cover the outer surface of the coffee bean, obtaining a glossy visual image (Gloess et al. 2014). At the second stage the coffee oils are still "trapped" in the coffee bean cells, and with increasing

[2] ICO, (2006) Guidelines for the Prevention of Mould Formation in Coffee [online] [viewed on 20. March 2022] Retrieved from http://dev.ico.org/documents/ed1988e.pdf

[3] ICO, (2002). Code of practice - Guidelines for the Prevention of Mould Formation in Coffee [online] [viewed on 20. March 2022] Retrieved from https://www.ico.org/documents/pscb36.pdf

temperature and "second crack", undesirable oxidation processes of aromatic substances have been observed (Mojica et al. 2018; Giacalone et al. 2019).

During the roasting process coffee defects can be created. For example, "light" or "underdeveloped" defects are the results of two low roasting temperature at the beginning of the roasting process. If the starting temperature is slightly too high or the roasting process is too long, the "dark" defect can occur with phenolic, ash-like flavour, aroma notes. If the roasting process was too long and the starting temperature was too high, the "scorched "defect can be created with unpleasant bitterness, astringency and burnt aroma notes. In order to avoid possible defects in roasted coffee, quality evaluation is necessary before and after roasting process. Despite that there are no specific roasting standards, only guidelines by countries or organizations such as Specialty Coffee association (SCA), National Coffee Association of America (NCAA). Coffee roasting profile can be divided in several levels – light, medium and dark, although it is crucial to base these levels on roasting parameters and/or colour standards (Agtron) (Oliveira et al. 2013; Vignoli et al. 2014). Melo (2004) study presented Agtron roast profile stages, which are used in scientific studies as measurement of roast level.

The green coffee beans physical parameters such as density, moisture content can impact the roasting time and the expected roast level. Beans with lower density or high moisture content have shown to increase the roasting time, while beans with high density or low moisture content can decrease the roast time (Ramalakshmi, Kubra, & Rao 2007; Kipkorir, Muliro, & Muhoho 2015). To ensure the roasting process repeatability, it is important to adjust the roasting variables according to green coffee beans physical parameters. In the scientific studies mostly four roasting variabales are considered – the roast temperature when coffee beans are inserted in the roaster (charge temperature), the roast temperature when the coffee beans are removed from the roaster (drop temperature), the airflow inside the roaster and the roasting time (Fuller & Rao 2017; Kwak, Ji, & Jeong 2017; Garcia et al. 2018).

1.1.2. Coffee quality standards and specialty coffee definition / *Kafijas kvalitātes standarti un specialty kafijas definējums*

Coffee quality standards are defined by each producing and exporting country. The ICO collects and summarises the standards and guidelines from all coffee producing countries, an example, in 2018 ICO reported "National Quality Standards" with detailed information about every coffee producing country grading and certification standards[4]. Organizations like Coffee Quality organization (CQA), NCAA and World Coffee Research (WCR) are non-profit agricultural research organizations, which provide information about coffee market trends, latest academic studies or created guidelines to improve the quality of coffee.

The definition of quality changes, with increasing coffee consumption, production rates and awareness of situation in coffee producing countries. The quality of coffee can be affected in every coffee producing step. To minimize the risks of potential threats, educational guidelines are set with clear cup quality evaluation protocols. Specialty coffee can be defined as coffee with high-quality standards from the coffee plantation process until delivery to the consumer. By applying these standards, it is possible to highlight the high-quality sensory characteristics of coffee brew (Urwin, Kesa, & Joao 2019). Specialty coffee standards are regulated by SCA. The SCA provides protocols and best practices, for example "Green Coffee Grading Protocols" and "Brewing Best Practices". The protocols have been used in scientific studies as coffee sample, preparation guidelines or

[4] ICO (2018) National Quality Standards [online] [viewed on 20. March 2022] Retrieved from https://www.ico.org/documents/cy2017-18/icc-122-12e-national-quality-standards.pdf

as coffee sample quality evaluation method (Carvalho & Spence 2018; Cotter et al. 2021). The most widely used protocols are “Cupping protocols”.

SCA cup quality assessment method is applied to analyse the quality of coffee beans. Certified coffee assessors (Q-graders) perform cup quality assessment using specialty coffee cupping protocol[5]. Coffees are measured by ten specialty cup quality attributes and for each attribute 10 points are given. (Fig. 1.2).

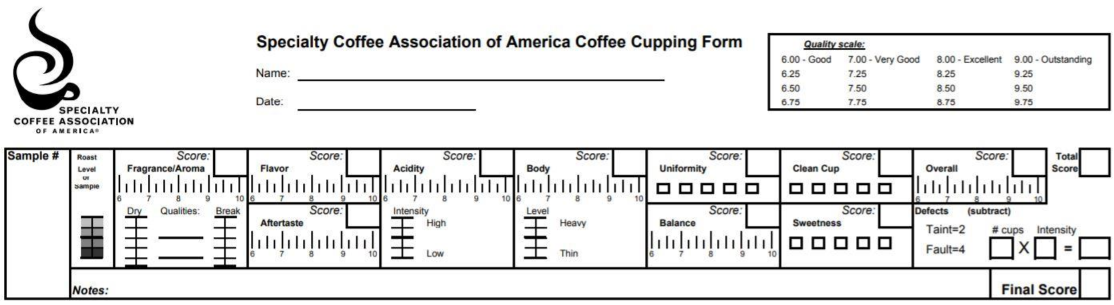


Fig. 1.2. Specialty Coffee Association cupping form /
1.2. att. Specialty kafijas asociācijas kafijas vērtēšanas lapa[5]

The coffee evaluation process is divided in three steps:

1) aroma evaluation of dry ground samples (15 minutes after the coffee sample was ground);
2) aroma evaluation of coffee brew after 3 minutes from extraction (coffee brew temperature 93 °C);
3) evaluation of coffee brew flavour after 8–10 minutes from extraction (flavour, aftertaste at 71 °C; acidity, body, and balance at 71 to 60 °C).

The panellists also can give a description of specific flavour, aroma perceived according to Chambers IV et al. (2016) statements. Each attribute is evaluated in scale from six to ten with quarter point increment (Table 1.1).

Table 1.1 / *1.1. tabula*

Attribute evaluation scale for cupping / *Kafijas sensoro īpašību vērtējuma skala*

Quality Scale / *Kvalitātes vērtējumu skala*			
Good / *Labi* (6.00)	**Very Good /** *Ļoti labi* (7.00)	**Excellent /** *Teicami* (8.00)	**Outstanding /** *Izcili* (9.00)
6.00	7.00	8.00	9.00
6.25	7.25	8.25	9.25
6.50	7.50	8.50	9.50
6.75	7.75	8.75	9.75

The final cup quality score is in a range from 60 to 100 points (by summing all ten attribute scores). Coffee is classified as a specialty only if the final cupping score is at least 80 points (Tolessa et al. 2016; Velásquez et al. 2019).

SCA cup quality assessment method has been used in several scientific studies. Kwak, Ji, & Jeong (2017) have evaluated the airflow influence on coffee quality in

[5]Specialty Coffee Association of America (2015) Cupping Specialty Coffee [online] [viewed on 20. March 2022] Retrieved from https://www.scaa.org/PDF/resources/cupping-protocols.pdf >

roasting process. Piccino et al. (2014) analysed specific coffee odorant role on overall coffee cup quality.

1.1.3. Sensory analysis role in coffee quality and liking determination / *Sensorās analīzes nozīme kafijas kvalitātes un patērētāju patikšanas novērtējumā*

Sensory analysis allows to better understand coffee characteristics. To analyse the intensity of specific attribute in coffee descriptive analysis is applied. Hedonic liking score tests are applied to understand consumer opinion, preference or acceptance of coffee (Kim, Lee, & Kim 2016; Cotter et al. 2021; Caporaso, Whitworth, & Fisk 2022). For better understanding sensory attributes of product, sensory lexicons are developed. Lexicons are objectively described vocabularies for specific food products (Lawless & Civille 2013). Lexicon development creates enlightenment between industries participants and academic researchers to better evaluate sensory characteristics of the products (Xia et al. 2015; Chambers IV et al. 2016; Echeverria-Beirute et al. 2017). Lexicon development and implementation allow to avoid misconception of attributes, example, "green" attribute in Bueno de Godoy, Chambers IV, & Yang (2020) study mate tea lexicon was defined as "slightly sweet fresh aromatics associated with cut grasses", while in Chambers IV et al. (2016) research of coffee lexicon it's defined as "aromatics commonly associated with cooked green vegetables such as spinach, kale, green beans that may include bitter, sweet, dusty, musty, earthy, and may have a dark heavy impression".

1.2. Chemical composition in different roast level coffee / *Kafijas ķīmiskais sastāvs dažāda grauzdējuma pakāpes kafijā*

1.2.1. Chemical composition of coffee / *Kafijas ķīmiskais sastāvs*

The basic chemical composition of coffee is lipids, proteins, carbohydrates, chlorogenic acid, caffeine. Lipids, proteins, and carbohydrates in coffee are the aroma, flavour precursors. Table 1.2 illustrates the chemical composition of coffee.

Table 1.2 / *1.2. tabula*

Chemical composition of green and roasted coffee /
Zaļās un grauzdētās kafijas ķīmiskais sastāvs (Preedy, 2014)

Chemical compounds / *Ķīmiskie savienojumi*	**Chemical compound content** / *Ķīmisko savienojumu sastāvs, %*			
	C.arabica		***C.canephora***	
	Green coffee / *Zaļā kafija*	**Roasted coffee** / *Grauzdēta kafija*	**Green coffee** / *Zaļā kafija*	**Roasted coffee** / *Grauzdēta kafija*
Polysaccharides / *Polisaharīdi*	50.0–55.0	24.0–39.0	37.0–47.0	-
Oligosaccharides / *Oligosaharīdi*	6.0–8.0	0–3.5.0	5.0–7.0	0.0–3.5
Lipids / *Lipīdi*	12.0–18.0	14.5–20.0	9.0–13.0	11.0–16.0
Free amino acids / *Brīvās aminoskābes*	2.0	0.0	2.0	0.0
Protein / *Proteīni*	11.0–13.0	13.0–15.0	11.0–13.0	13.0–15.0

Continued Table 1.2 / *1.2. tabulas turpinājums*

Chemical compounds / *Ķīmiskie savienojumi*	Chemical compound content / *Ķīmisko savienojumu sastāvs, %*			
	C.arabica		***C.arabica***	
	Green coffee / *Zaļā kafija*	**Roasted coffee** / *Grauzdēta kafija*	**Green coffee** / *Zaļā kafija*	**Roasted coffee** / *Grauzdēta kafija*
Chlorogenic acid / *Hlorogēnskābe*	5.5–8.0	1.2–2.3	7.0–10.0	3.9–4.6
Caffeine / *Kofeīns*	0.9–1.2	0–1.0	0.6–0.8	0.3–0.6
Trigonelline / *Trigonelīni*	1.0–1.2	0.5–1.0	0.6–0.8	0.3–0.6
Fatty acids / *Taukskābes*	1.5–2.0	1.0–1.5	1.5–2.0	1.0–1.5
Minerals / *Minerālvielas*	3.0–4.2	3.5–4.5	4.0–4.5	4.6–5.6
Melanoidins / *Melanoīdi*	-	16.0–17.0	-	16.0–17.0

Coffee lipids can be formed from triglycerides, diterpenes and esterified sterols. Diterpene kahweol and cafestol are the main coffee lipids. *Coffea arabica* L. has higher concentration of both coffee lipids compared to *C. canephora*. Kahweol and cafestol are esterified with fatty acids. Linoleic and palmitic acid are the main fatty acids linked to diterpenes (Sridevi, Giridhar, & Ravishankar 2011; Kitzberger et al. 2013).

Figueiredo et al. (2015) reported that saturated fatty acids can have a positive correlation with sensory quality scores of specialty coffee. Coffee with higher stearic and arachidic fatty acid content are associated with more pleasant sensory attributes like texture and body of coffee drink. While unsaturated fatty acids tend to have a negative correlation with sensory attributes such as aroma, flavour of coffee brews (Figueiredo et al. 2015; Laukaleja & Kruma 2018).

Carbohydrates account for about 40–50% of green coffees chemical composition and can be divided into soluble and insoluble carbohydrates. Insoluble carbohydrates in coffee are polysaccharides such as arabinogalactans and galactomannans. They are responsible for the strength of coffee beans cell walls (Fischer et al. 2001; Coelho et al. 2014). Polysaccharides degrade to reducing sugars such as mannose, arabinose, and glucose during the roasting process. The reducing sugars are one of the most essential aroma and flavour precursors in coffee. At the first stage of roasting Maillard reaction occurs between amino acids and reducing sugars. As the result of Maillard reaction, complex volatile compounds are formed (Moon & Shibamoto 2009; Ludwig et al. 2013).

Sucrose content in green coffee is associated with improvement of roasted coffee brew sensory quality. Borém et al. (2016) has stated that sucrose content in green coffee has a positive correlation on acidity and sweetness of roasted coffee. The coffee fruit maturation has been reported as one of the factors impacting sucrose content in green coffee. Geromel et al. (2008) have found significant importance in creating and monitoring coffee tree and their fruit exposure to direct sunlight. A more controlled shade environment slows down the coffee fruit maturation, which improves reducing sugar formation. These findings can explain specialty coffee standard importance for the harvesting and post-harvesting processes.

Coffee proteins. Proteins in green coffee account for about 10–12% of the chemical composition. Coffee proteins can be divided into amino acids and peptides (Oestreich-Janzen 2014). The amino acids are largely transformed during the roasting process via several chemical reactions such as Maillard reaction, Strecker degradation. In reaction with reducing sugars, sulphur-containing amino acids (cysteine and methionine) can form important volatile compounds like furfurylthiol (Ribeiro et al. 2009; Laukaleja, Kruma, & Cinkmanis 2022). Proline and hydroxyproline via Maillard reaction are reported to form pyrroles, pyrrolizines, and pyridines. From Strecker degradation, aldehydes are formed, which are crucial in aroma profile formation. The most common Strecker aldehydes in coffee are 3-methylbutanal with malt, nutty notes and phenylacetaldehyde with honey notes (Franca & Oliveira 2008; Lee, Kim, & Lee 2017; Laukaleja & Kruma 2019a).

1.2.2. Characterization of coffee biologically active compounds / *Bioloģiski aktīvo savienojumu raksturojums kafijā*

Biologically active compounds could be explained as compounds that can interact with one or more living cells or tissues positively or negatively affecting their function. Moderate coffee consumption has proven to have several health benefits. Moderate coffee consumption is associated with reduced mortality, risk of cardiovascular disease, depression, and migraine. For example, a prospective cohort study conducted in 2016 confirmed that regular coffee consumption reduces mortality among Eastern Europeans. More specifically, consuming 3–4 cups of coffee per day reduces mortality from cardiovascular disease in men and mortality from malignancies in women

(Grosso et al. 2015). Meta-analysis data, including eight cohort studies with a total of 3153 participants, show that taking 1–3 cups of coffee a day reduces the risk of developing liver cancer by 50%. Still, by taking more than 4 cups of coffee a day, mortality from liver cancer is reduced by 90% (Cavalli & Tavani 2016).

The biologically active compound composition in coffee is one of the main reasons for the beneficial effects on human health. The main biologically active compounds in coffee are caffeine, trigonelline, diterpenes and phenolic compounds such as chlorogenic acid and catechin.

Studies on coffee consumption and a specific health problem include a general conclusion about coffee and its components. To avoid contradicting situations, the effects of biologically active compounds in the disease should be considered separately. Mainly because biologically active compounds are not always defined by positive health effects alone. Several factors influence their interaction with living tissues:

- chemical structure, bioavailability;
- the living cell itself, with which it interacts;
- application of the component (the dose: used alone or in a mixture with other substances) (Guaadaoui et al. 2014).

The expression of bioactive compounds in coffee per serving is not the most accurate unit. However, it is the most precise measure of the daily intake of biologically active compounds in epidemiology studies (Carman et al. 2014). The most important biologically active compounds in coffee for human health are expressed per serving – espresso coffee (30 mL coffee drink), French press coffee and filtered coffee (200 mL coffee drink).

Phenolic compounds are one of the main bioactive compound groups found in plant-based products as pomegranate, blueberries, green tea, wine, and coffee. Coffee is considered the main polyphenol source in Eastern European countries living people's diets (Zamora-Ros et al. 2018). The main phenolic acids in the coffee brew are chlorogenic acid, caffeic acid, ferulic and q-coumaric acid. The presence of the phenolic hydroxyl group in the benzene ring has crucial role for antiradical activity of the compound, which is one of the reasons why chlorogenic, caffeic and ferulic acid have significantly higher antiradical activity then cinnamic acid in coffee (Sova 2012). Flavonoid concentration is higher in leaves or the outer layer of coffee fruit than in coffee beans. For example, rutin is mainly found in *Coffea* tree leaves or the pulp. Higher rutin concentration could be found in roasted coffee and coffee brews if the wet processing method was applied (Farah 2019).

Chlorogenic acid is mainly obtained from tobacco, mulberry leaves, coffee beans and hard dicotyledonous fruits. With increasing roast level, the concentration of chlorogenic acid decreases significantly. Chlorogenic acid with increasing roast level transform to chlorogenic acid lactones (Moreira et al. 2012). The chlorogenic acid lactones can transform to phenylindanes if the roasting process continues after medium roast level. In coffee brew, chlorogenic acid can give sour or an astringent taste, chlorogenic acid lactones are associated with pleasant bitterness, while phenylindanes have bitter, burnt taste (Tolessa et al. 2016; Yang et al. 2016). Several studies have confirmed that it is possible to provide high sensory quality coffee without losing significant levels of chlorogenic acid (Moon & Shibamoto 2009; Somporn et al. 2011; Coelho et al. 2014). Chlorogenic acid content in coffee brew can vary between 5 mg mL^{-1} to 200 mg mL^{-1} (Jeon et al. 2017). A person who regularly drinks coffee consumes more than 1 g of chlorogenic acid per day (Ludwig et al. 2014).

Caffeine is one of the most potent bioactive compounds in coffee. Caffeine is twice as much in *C. canephora* (1.5–2.5 g 100^{-1} g dry weight) as in *Coffea arabica* L. beans (0.9–1.3 g 100 g^{-1} dry weight). The caffeine content of coffee can be influenced by genetic factors and environmental factors such as coffee roasting and brewing. Caffeine is an alkaloid that dissolves well in water; therefore, the brewing technique can influence caffeine extraction in the coffee brew. Phuoc & Phu (2014) states that caffeine extraction increases until the water temperature reaches 96 °C, afterwards caffeine extraction reaches a plateau. Caffeine is burned during the long-term roasting process (roasting temperature above 230 °C). Several studies confirm that light roasted coffee will contain significantly more caffeine than dark roast coffee (Dias & Benassi 2015).

According to a scientific report by the European Food Safety Authority (EFSA) on the safety standards for caffeine[6], the dose of caffeine can be 200 mg per intake. Still, the total daily dose can be 400 mg. According to several scientific reports, Europeans consume 40–94% of their coffee caffeine. Citizens of seven out of thirteen European countries exceed their daily caffeine intake by almost 32%. The highest caffeine consumption from coffee is in Sweden (the average daily dose of caffeine is 690 mg) (Martini et al. 2016).

Melanoidins are formed as Maillard reaction final products. Several studies have mentioned that also chlorogenic acid could be involved in melanoidin formation (Moreira et al. 2012; Coelho et al. 2014). Melanoidin concentration is higher in *Coffea arabica* L. coffee than in *C. canephora.* It could indicate that the sugar composition has a higher impact on melanoidin formation than chlorogenic acid since *Coffea arabica* L. has lower chlorogenic acid content and higher carbohydrate content than *C. canephora* (Ciaramelli, Palmioli, & Airoldi 2019). Melanoidins have also been shown to prevent linoleic acid peroxidation, which is more pronounced for dark-roasted coffee than light-roasted coffee (Labbe et al. 2016).

[6] European Food Safety Authority (2015) Scientific Opinion on the safety of caffeine [online] [viewed on 20. January 2022] Retrieved from https://www.efsa.europa.eu/sites/default/files/consultation/150115.pdf

1.2.3. Volatile and aroma-active compound composition of coffee / *Gaistošo un aromātu veidojošo savienojumu sastāvs kafijā*

The aroma of coffee is one of the most crucial sensory attributes for predicting the quality of the product. The volatile compounds and their composition strongly affect the aroma of coffee (Ribeiro et al. 2012). The volatile compound formation occurs in the roasting process through complex chemical reactions, however it is possible to predict specific compound formation by understanding the precursors and their reactions. The amino acids, sugars, lipids and phenolic compounds in green coffee act as aroma, volatile compound precursors during roasting process (Yeretzian et al. 2002).

Although the coffee aroma is generated from volatile compounds, not all volatile compounds impact the coffee aroma. A compound can be called aroma-active if a human assessor can detect an odour in minimum concentration (odour threshold) or in concentration at which the odour can be described (odour recognition threshold) (Tamura et al. 2011; Paravisini et al. 2015; Song & Liu 2018; Laukaleja & Koppel 2021).

Previous studies have confirmed more than 800 volatile compounds detected in roasted coffee (Franca & Oliveira 2002; Yang et al. 2016; Jeon et al. 2017), although only about 20-30 of them can potentially impact the aroma profile of coffee (Mahattanatawee, Goodner, & Baldwin 2005; Laukaleja & Koppel 2021). For example, Deibler & Delwiche (2004) reported that freshly brewed coffee had 66 volatile compounds, and only 20 had potent aroma characteristics.

Volatile compound associated aromas can be impacted by roasting process. Volatiles detected in light roast coffee can present aromas attributes such as fruity, floral, citrusy, while dark roasted coffees have volatiles associated with coffee-like, roasted and burnt aroma attributes (Yeretzian et al. 2002; Laukaleja & Kruma 2018).

Table 1.3 shows the aroma-active compound effect on sensory quality under influence of coffee roasting process. The main chemical classes of volatile compounds detected in coffee are furans, ketones, aldehydes, organic acids, esters, pyridines, phenolic, and sulphur-containing compounds.

Table 1.3 / *1.3. tabula*

Aroma-active compound effect on cup quality under influence of coffee roasting process / *Aromātu veidojošo savienojumu ietekme uz sensoro kafijas kvalitāti grauzdēšanas procesa ietekmē* (Laukaleja & Kruma 2018)

Effect on cup quality / *Ietekme uz sensoro kafijas kvalitāti**	**Roast level** / *Grauzdēšanas pakāpe***	**Compounds** / *Savienojumi*	**Aroma attributes** / *Aromāta īpašības*
Positive / *Pozitīva*	light / *viegls*	(e)-β-damascenone / *(e)-β-damascenons*	cooked apple, sweet / *salds, cepts ābola*[a]
		2-phenylacetaldehyde/ *2-fenilacetaldehīds*	floral, fruit / *ziedu, augļu*[b]
		2-methylpyrazine / *2-metilpirazīns*	chocolate, nutty/ *šokolādes, riekstu*[c]
		2-pentanone / *2-pentanons*	sweet, fruity / *salds, augļu*[d]
	medium / *vidējs*	3-methylbutanal / *3-metilbutanāls*	malt / *iesala*[e]
		2,3-butanedione / *2,3-butāndions*	buttery / *sviesta*[f]
		methanethiol / *metāntiols*	fresh / *svaiguma*[g]

Continued Table 1.3 / *1.3. tabulas turpinājums*

Effect on cup quality / *Ietekme uz sensoro kafijas kvalitāti**	**Roast level /** *Grauzdēšanas pakāpe***	**Compounds /** *Savienojumi*	**Aroma attributes /** *Aromāta īpašības*
Negative / *Negatīva*	dark / *tumšs*	2- methyl-3-furanthiol / *2-metil-3-furantiols*	sulphury, vegetable / *sēra, dārzeņu*[g]
		2-methylpyrazine / *2-metilpirazīns*	overripe fruit / *pārgatavojušos augļu*[h]

*Sensory quality of coffee brew (flavor, aroma, texture) / *Kafijas sensorās kvalitāte (aromāts, garša, tekstūra)* (Donnet, Weatherspoon, & Hoehn 2008; Suslick, Feng, & Suslick 2010; Cheong et al. 2013)
**The roast level parameters adjusted according to Moon & Shibamoto (2009) / *Grauzdēšanas parametri ir saskaņā ar Moon, Shibamoto (2009) pētījumu.*
[a]Mestdagh et al. (2014); [b]Piccino et al. (2014); [c]Wei et al. (2017a); [d]Majcher, Ławrowski, & Jeleń (2010); [e]Yang et al. (2016); [f]Sunarharum, Williams, & Smyth (2014); [g]Quintanilla-Casas et al. (2015); [h]Haile, Bae, & Kang (2020).

Furans and their compounds, according to research data, are the largest chemical class by their concentration in roasted coffee (Petisca et al. 2012). Most of furans have high odour threshold level, however their high content in roasted coffee makes them an important role for sensory quality and aroma composition (Cordoba et al. 2019). Some of the most important furans in coffee are 2-furfurylthiol (chocolate, roasted aroma notes), furaneol (caramel, sweet aroma notes). While furans have the highest concentration aldehydes, ketones and pyrazines have lower odour threshold level and higher count of aroma-active compounds (Moon & Shibamoto 2009; Steen et al. 2017).

Ketones and aldehydes concentration and possible aroma can be significantly impacted by the roast level. Their sensitivity is one of the reasons why they are used as a sensory quality markers for roasted coffee (Poltronieri & Rossi 2016). For example, the 2,3-pentanedione is associated with higher cup quality scores (Ribeiro et al. 2009; Toledo et al. 2016). Ketones and aldehydes such as (e,e)-nona-2,4-dienal, 3-methylbutanal and 2-phenylacetaldehyde in light roast coffee can bring aroma notes like citrus, rose, chocolate (Mestdagh et al. 2014; Cordoba et al. 2019). Also, (e)-β-damascenone and benzaldehyde are aroma-active compounds with sweet almond or cooked apple, fruit tea aroma notes (Mayer, Czerny, & Grosch 1999). With increasing roast level 2,3-pentanedione concentration decreases and in lower concentration its aroma is associated with buttery notes (Sunarharum, Williams, & Smyth 2014).

Pyrazine compounds are formed mostly in Maillard reaction and are associated with roasted, nutty, or smoky aroma attributes. Pyrazine concentration is higher in *C. canephora* than in *Coffea arabica* L. coffee. Some studies suggest that in *Coffea arabica* L. pyrazines can bring floral aroma notes (Sunarharum, Williams, & Smyth 2014). Similar to ketones and aldehydes pyrazines have low threshold level and are used as roasting quality markers. Some of the most important pyrazines are 2-ethyl-3,5-dimethylpyrazine with hazelnut aroma notes and 2,3-dimethyl-5-ethylpyrazine with cacao, nutty aroma notes (Piccino et al. 2014; Steen et al. 2017). With increasing roast level pyrazine concentration increases and the associated aroma notes become unpleasant. For example, 2-methylpyrazine and 2-ethyl-6-methylpyrazine associates overripe, harsh, fermented aroma in dark roast level coffee (Parenti et al. 2014; Sunarharum, Williams, & Smyth 2014).

Organic acids in coffee are formed during coffee fruit maturation and can be maintained in higher concentration with natural post-harvesting method. The main organic acids are malic, citric, and phosphoric. Malic acid aroma and flavour can be associated with apples, pears, while citric acid with lime and lemon and phosphoric acid with grapefruit (Borém et al. 2016). Lactic acid and hexanoic acid have buttery, creamy flavour, and provide pleasant acidity (Galli & Barbas 2004; Jham et al. 2007). Acidity for organic acids have shown positive correlation with the final cup quality scores during coffee sensory evaluation (Borém et al. 2016; Fassio et al. 2017). Organic acid content is rapidly decreasing with increasing roast level (Ginz et al. 2000).

Suphur containing compounds in coffee are in minimal concentration, however they have crucial role in aroma profile formation (Toledo et al. 2016). The sulphur compounds transform during coffee roasting, for example methanethiol concentration increases with the roasting process till the dark roast level, and then by the oxidation process, it converts to dimethyl disulfide (Wei et al. 2017b).

In low concentration 2-furfurylthiol has been mentioned as the coffee freshness indicator with aroma associated with pleasant roast, coffee like notes. While in dark roast level 2-methyl-3-furanthiol and dimethyl disulphide are associated with sulphury/ cabbage aroma (Mayer, Czerny, & Grosch 1999; Cheong et al. 2013; Kim et al. 2018).

1.3. Gas chromatography-olfactometry importance in specialty coffee brew studies / *Gāzu hromotaogrāfijas-olfaktometrijas nozīme specialty kafijas dzērienu pētījumos*

1.3.1. Solid-phase microextraction fibre analysis for coffee brew volatile compound extraction / *Cietās fāzes mikroekstrakcijas šķiedru analīze kafijas gaistošo savienojumu ekstrakcijai*

Volatile compounds extraction methods suitability can vary based on the analysing product, volatiles, and technical parameters such as extraction time. Three methods have been reported as the most suitable for coffee volatile compound extraction – simultaneous distillation extraction (SDE), static headspace analysis (SHA), dynamic headspace analysis (DHA) and solid-phase microextraction (SPME).

The advantages of the SPME method: it is a simple and fast volatile compound extraction while providing high sensitivity and extraction rates. The disadvantage of SPME is the ability to be effective only for freshly prepared samples, which means the samples must be prepared right before extraction and cannot be stored. The SPME method has been reported as the most common and reliable method for freshly brewed coffee sample volatile compound extraction and analysis (Chen, Chiang, & Chung 2019).

Choosing the extraction technique is not the only crucial step for volatile extraction, it is also important to select the most appropriate SPME fibre coating. Seven types of SPME fibres have been reported commercially for volatile compound extraction – polyacrylate (PA), polydimethylsiloxane (PDMS), polydimethylsiloxane/divinylbenzene (PDMS/DVB), carbowax/ divinylbenzene (CW/DVB), carboxen/polydimethylsiloxane (CAR/PDMS) and divinylbenzene/ carboxen/polydimethylsiloxane (DVB/CAR/PDMS) (Risticevic, Carasek, & Pawliszyn 2008; Spietelun et al. 2010; Rubio et al. 2014).

Four of them have been reported as the most suitable for coffee volatile compound extraction and analysis. The DVB/CAR/PDMS fibre is one of the most common choices for coffee sample aroma profile analysis. For example, the DVB/CAR/PDMS fibre was selected by Mestdagh et al. (2014) for analysing the kinetics of coffee aroma extraction and could extract volatiles with different polarities. While, Lee, Kim, & Lee (2017) used DVB/CAR/PDMS fibre for volatile compound profile analysis of coffee by reversed grinding and roasting process. Roberts, Pollien, & Milo (2000) suggested the

PDMS/DVB fibre for comprehensive coffee volatile compound extraction. The CAR/PDMS fibre showed the best results for extracting the most common coffee volatile chemical classes such as furans and ketones (Petisca et al. 2012; Kim et al. 2018).

The commercial coffees and specialty coffee aroma profiles can significantly differ due to coffee production steps and roasting process. In previous literature main focus was on commercial coffee, and limited research has been done about specialty coffee volatile compound profile analysis and evaluation of SPME fibres suitability for volatile extraction (Akiyama et al. 2007; Risticevic, Carasek, & Pawliszyn 2008; Ribeiro et al. 2012).

1.3.2. Gas chromatography-olfactometry vocabulary application for specialty coffee brew aroma-active compound analysis / *Gāzu hromatogrāfijas-olfaktometrijas vārdnīcas pielietojums speciality kafijas dzērienu aromātveidojošo savienojumu analīzei*

For quality purposes descriptive sensory studies are carried out, usually creating or using lexicons for specific food product sensory attribute description (Lawless & Civille 2013). Meanwhile, gas chromatography-mass spectrometry (GC-MS) is one of the most common and effective methods used for volatile compound detection in order to analyse the aroma profile and possible off-flavours of food products (Ribeiro et al. 2009; Yang et al. 2016). However, GC-MS cannot identify and describe the volatile compound aroma. With gas chromatography-olfactometry (GC-O) method it is possible to identify aroma-active compounds (Song & Liu 2018). GC-O lexicons and vocabularies have shown to improve the food product sensory characteristic evaluation and understand the aroma profile formation (Xia et al. 2015; Tang et al. 2019).

While coffee aroma and volatile compounds are studied in roasted and brewed coffee samples separately, there are limited in-depth olfactory analysis of aroma-active compounds and their changes during roasting and brewing process (López-Galilea et al. 2006; Laukaleja & Koppel 2021). The limitations of previous GC-MS studies are that analysed coffee volatile compounds are associated with other GC-O studies results or completed coffee GC-O studies focus only specific roast or brew not the complex analysis between roast levels. It is crucial to consider volatile compound concentration impact on aroma perception. Both the volatile compound concentration and the chemical composition of the food can affect the aroma active compound perception (Koppel, Adhikari, & Di Donfrancesco 2013; Adhikari, Chambers, & Koppel 2019).

The most common methods used for GC-O studies are:

- the detection frequency method;
- direct intensity method;
- combined hedonic aroma response measurement (CharmAnalysis™) method;
- aroma extract dilution analysis (AEDA).

Each method has different advantages. While CharmAnalysis™ and AEDA are more focused on analysis of samples with high dilution, the detection frequency method has shown repeatability and sensitivity between different concentrations (Van Ruth 2004; Delahunty, Eyres, & Dufour 2006; Laukaleja & Koppel 2021).

Summary / *Kopsavilkums*

Specialty coffee stands for coffee with high-quality standards and guidelines to highlight specific sensory characteristics of coffee with limited defects during production stages. The specialty coffee market rapid growth in the past decade confirms consumer's interest in high-quality products. While volatile compounds are comprehensively analysed in commercial coffee, limited research has been published about volatiles, including aroma-active compounds, in specialty coffee. More in-depth gas chromatography and olfactometry analysis about aroma-active compounds in different roast level specialty coffee would provide insights about aroma perception changes during the roasting process.

With increased coffee consumption coffee consumers are not only interested in the quality of coffee but also the possible health effects. Studies have proven that moderate coffee consumption is associated with a reduced risk of cardiovascular and neurological diseases. Additionally, coffee could be one of the main polyphenol sources in Eastern European individual diets.

The roasting process is the main production step that impacts the chemical composition of the coffee including both bioactive compound content and volatile compound profile. There are limited studies carried out about complex volatile and bioactive compound analysis in different roast level coffee.

For the adjusted roast level to be practically applied in the specialty coffee market, it is necessary to analyse consumer perception about specialty coffee and consumer purchase intent, if information about potentially increased bioactive compound content was provided. The aim of the research was to evaluate the impact of the roast level on the composition of biologically active compounds and sensory quality in specialty coffee.

Specialty kafijas apzīmē kafiju ar augstiem kvalitātes standartiem un vadlīnijām, lai izceltu noteiktas sensorās īpašības kafijā un mazinātu defektu attīstību ražošanas posmos. Specialty kafijas tirgus straujā izaugsme pēdējā desmitgadē apstiprina patērētāju interesi pēc augstas kvalitātes produktiem. Kamēr plaši tiek analizēti gaistošie savienojumi komerciālās kafijās, ir limitēts pētījumu skaits par gaistošo un aromātveidojošo savienojumu profilu specialty kafijā. Padziļināti gāzu hromatogrāfijas un olfaktometrijas pētījumi par aromātveidojošiem savienojumiem dažāda grauzdējuma pakāpes specialty kafijā sniegtu informāciju par grauzdēšanas procesa ietekmi uz aromātu uztveres izmaiņām.

Līdz ar palielinātu kafijas patēriņu kafijas patērētāji ne tikai interesējas par kafijas kvalitāti, bet arī par tās ietekmi uz veselību. Pētījumi apliecina, ka mērens kafijas patēriņš var samazināt sirds un asinsvadu un neiroloģisko slimību riskus. Kafija var būt, kā viens no galvenajiem polifenolu avotiem austrumeiropiešu iedzīvotāju uzturā.

Grauzdēšanas process ir viens no galvenajiem ražošanas posmiem, kas ietekmē kafijas ķīmisko sastāvu, ieskaitot bioloģiski aktīvo savienojumu saturu un gaistošo savienojumu profilu. Kompleksa gaistošo un bioloģiski aktīvo savienojumu analīze dažāda grauzdējuma pakāpes kafijās nav plaši pētīta.

Lai nodrošinātu pielāgotu grauzdēšanas pakāpju praktisku pielietojumu specialty kafijas tirgū, būtiski ir analizēt patērētāju uztveri par specialty kafiju un vēlmi iegādāties produktu, ja tiktu sniegta informācija par potenciāli palielinātu bioloģiski aktīvo savienojumu saturu kafijā. Darba mērķis ir izvērtēt grauzdēšanas procesu pakāpes ietekmi uz bioloģiski aktīvo savienojumu sastāvu un sensoro kvalitāti specialty kafijā.

2. MATERIALS AND METHODS / *MATERIĀLI UN METODES*

2.1. Time and location of the research / *Pētījuma laiks un vieta*

Experimental work was conducted in the period from 2017 to 2022 in the following scientific laboratories.

1. Latvia University of Life Sciences and Technologies:
   - total and individual phenolic, flavonoid compound analysis;
   - radical scavenging activity analysis;
   - moisture content and pH evaluation;
   - volatile compound analysis.
2. Center for Sensory Analysis and Consumer Behavior, Kansas State University (USA):
   - coffee sample roasting;
   - initial olfactometry vocabulary development;
   - consumer analysis.
3. J.S. Hamilton Baltic Ltd. Laboratory (outsource): acrylamide concentration, amino acid, and fatty acid profile detection.

2.2. Description of used materials / *Materiālu raksturojums*

Green and roasted *Coffea arabica* L. beans were purchased from local specialty coffee roasteries or roasted at the site. By SCA standards and protocols, all coffee samples were qualified as specialty coffee with >80 points. The roasting parameters and sample preparation steps are presented in each research stage.

2.3. The structure of the research / *Pētījuma struktūra*

The research work consists of 5 stages (Table 2.1).

Table 2.1 / *2.1. tabula*

Description of the research stages / *Pētījuma posmu raksturojums*

Stage / *Posms*	**Description** / *Raksturojums*
Stage I / *I posms*	Evaluation of headspace solid-phase microextraction with different fibres for volatile compound determination in specialty coffee / Gaistošo savienojumu analīze, izmantojot četras dažādas cietās fāzes mikroekstrakcijas šķiedras
Stage II / *II posms*	Influence of phenolic and volatile compound composition on specialty coffee cup quality / *Fenolu un gaistošo savienojumu satura ietekme uz specialty kafijas sensoro kvalitāti*
Stage III / *III posms*	The impact of the roasting process on chemical composition and sensory profile in specialty coffee / *Grauzdēšanas procesa ietekme uz ķīmisko sastāvu specialty kafijā*
Stage IV / *IV posms*	Aroma-active compound perception in different roast and brew coffee by gas chromatography-olfactometry / *Dažādi grauzdētas un pagatavotas kafijas aromātveidojošo savienojumu uztveres izvērtējums, izmantojot gāzu hromatogrāfiju olfaktometriju*
Stage V / *V posms*	Consumer's perception of specialty coffee with potentially increased bioactive compound content / *Patērētāju sensorais novērtējums par dažāda grauzdējuma kafijām ar iespējami lielāku bioloģiski aktīvo savienojumu koncentrāciju*

2.4. Stage I of the research / *I pētījuma posms*

In Stage I the volatile compound composition of specialty coffee was evaluated using different SPME fibres. Selecting the most appropriate fibre for coffee brews volatile and aroma-active compound detection could improve the volatile compound profile analysis and further application in coffee sensory assessmentor coffee quality standard development.

2.4.1. Coffee samples for stage I / *I pētījuma posma kafijas paraugi*

Five roasted coffee bean (*Coffea arabica* L.) samples were purchased from two different roasteries in Latvia. Table 2.2 shows the main characteristics of the coffee samples. The roast settings were adjusted to fit the light-medium roast level regarding the used roasting machine. All coffees were rated as specialty coffees (total cup quality score was 80 points or above) (Silveira et al. 2016; Laukaleja & Kruma 2019b; Pereira et al. 2019).

Table 2.2 / *2.2. tabula*

Coffee samples for stage I description / *I pētījuma posma kafijas paraugu raksturojums*

Sample code / *Parauga kods*	**Origin /** *Izcelsmes valsts*	**Roast settings /** *Grauzdēšanas parametri*	**Roaster /** *Grauzdēšanas iekārta*
H_1*	Honduras / *Hondurasa*	193 °C; 11 min	Besca BSC-01, Turkey
K_1	Kenya / *Kenija*		
C_1	Columbia / *Kolumbija*		
E_1	Ethiopia / *Etiopija*	205 °C; 11 min	Loring Smart Roast Kestrel 35, USA
H_2*	Honduras / *Hondurasa*		

*For H_1 sample coffee was processed using natural post-harvest method, H_2 sample coffee was processed using anaerobic post-harvest method / *H_1 paraugam tika izmantota dabīgā (sausā) pārstrādes metode, H_2 paraugam tika izmantota anaerobā pārstrādes metode*

Coffee brew preparation. The coffee samples were ground in a coffee grinder (DeLonghi KG79, Italy) at a coarse grind level 20 minutes before the brewing process. French press (Bodum, Switzerland) brewing technique was used according to the Specialty Coffee Association (SCA)[7]. Samples were brewed in duplicate.

2.4.2. Description of the materials and methods of analysis used in the stage I / *I pētījuma posmā izmantoto meteriālu un analīžu metožu raksturojums*

Headspace volatile compound extraction was carried out by solid-phase micro-extraction (SPME). Four different solid-phase microextraction fibres were purchased from Supelco (Bellefonte, USA):

- carboxen/polydimethylsiloxane (CAR/PDMS);
- divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMA);
- polyacrylate (PA);
- polydimethylsiloxane/divinylbenzene (PDMS/DVB).

After sample brewing, five mL of sample were immediately transferred in preheated 20 mL glass vial and immediately caped with screw-cap vial equipped with a polytetrafluoroethylene/silicone septum. The vial was transferred to a 50 ±1°C heated surface for four minutes of incubation. After the incubation period, the fibre was inserted into the sample headspace for seven min volatile compound absorption.

The parameters **for gas chromatography method** with adjustments were chosen according to Gloess et al. (2013) and Steen et al. (2017). A Clarus 500 gas chromatograph

[7] Specialty Coffee Association (2016). Guidelines for Brewing with French Press [online] [viewed on 20. January 2022] Retrieved from https://sca.coffee/s/best-practices-three-cup-french-press.pdf

(Perkin Elmer, USA) was used. The GC injection port was heated up to 250 °C, the compounds were desorbed in 15 minutes and further separated in Elite-Waw ETR column (60 mx 0.25 mm internal diameter; DF 0.25 column). The oven starts temperature was 40 °C, at which volatiles was held for 7 minutes. Then the initial temperature was programmed from 40 to 160 °C at a speed of 6 °C min^{-1}, at which column was held for 10 minutes. The further temperature was set from 160 to 210°C at a speed of 10 °C min^{-1}, at which column was held for 15 minutes. Helium was used as the carrier gas with the column initial flow rate of 1 mL min^{-1}. The outlet split ratio was set to 1:2. The compounds were scanned between 40 and 300 mass to charge ratios. The GC transfer line to the mass spectrometer was programmed at 260 °C. The compounds were identified using the mass spectral database Nist98. GC peak area means for each compound was given as a quantitative measure (Laukaleja & Kruma 2019b).

2.4.3. Statistical analysis for stage I of research / *I pētījuma posma datu statistiskā analīze*

To compare differences between extraction rates received by different SPME fibres, analysis of variance (ANOVA) was used, and significant differences were stated if $p<0.05$. All samples were analysed in triplicate. The volatile compound peak areas were expressed as means with standard deviations (SD). Data analyses were performed using XLSTAT software (vs. 2020.2.3.65347, XLSTAT, New York, NY, USA).

2.5. Stage II of the research / *II pētījuma posms*

Stage II evaluated the influence of phenolic and volatile compound composition on specialty coffee cup quality. The volatile and phenolic compound analysis could help determine if coffee can have good cup quality without losing health beneficial phenolic compounds.

2.5.1. Coffee samples for stage II / *II pētījuma posma Kafijas paraugi*

Seven roasted coffee bean (*Coffea arabica* L.) samples were purchased from two different roasteries in Latvia. Table 2.3. shows the main characteristics of the coffee samples.

Table 2.3 / *2.3. tabula*

Coffee samples of stage II description / *II pētījuma posma kafijas paraugu raksturojums*

Sample code / *Parauga kods*	**Origin /** *Izcelsmes valsts*	**Roast settings /** *Grauzdēšanas parametri*	**Roaster /** *Grauzdēšanas iekārta*
H_1*	Honduras / *Hondurasa*	light-medium / *viegli/vidēji* (193 °C; 11 min)	Besca BSC-01, Turkey
K_1	Kenya / *Kenija*		
C_1	Columbia / *Kolumbija*		
H_2*	Honduras / *Hondurasa*	light-medium / *viegli/vidēji* (205 °C; 11 min)	Loring Smart Roast Kestrel35, USA
E_1	Ethiopia / *Etiopija*		
H_3*	Honduras / *Hondura*sa		
E_2	El Salvador / *Salvadora*		

* For H_1 sample coffee was processed using natural post-harvest method, H_2 sample coffee was processed using anaerobic post-harvest method, H_3 – wet post-harvest method / *H_1 paraugam tika izmantota dabīgā (sausā) pārstrādes metode, H_2 paraugam tika izmantota anaerobā pārstrādes metode un H_3 – mazgātā pārstrādes metode*

The roast settings were adjusted to fit the light-medium roast level regarding the used roasting machine.

Sample preparation for chemical analysis: The coffee samples brewing process is described at Stage I in 2.4.2. chapter. For total phenolic and flavonoid content and DPPH and

ABTS radical scavenging activity analysis, samples were diluted in ratio 1:33 with distilled water. Samples were brewed in triplicate.

Sample preparation for sensory analysis: Six trained coffee specialists prepared and evaluated coffee samples according to the SCA cupping protocol (SCA 2015). Samples were brewed in quintuplicate.

2.5.2. Materials and chemicals for stage II / *II pētījuma posma materiāli un reaģenti*

The divinylbenzene/carboxen/poly (dimethylsiloxane) (DVB/CAR/PDMS) fibre was used for volatile compounds extraction by solid-phase microextraction (SPME).

The following chemicals were purchased from Sigma-Aldrich Chemie (Steinheim, Germany):

- ABTS$^{\cdot+}$ (2,2-azinobis (3-ethylbenzothiazoline-6-sulfonic acid));
- $AlCl_3H_{12}O_6$ (aluminium chloride hexahydrate);
- $C_{15}H_{14}O_6$ ((+)-catechin);
- $C_7H_6O_5$ (gallic acid);
- DPPH $^{\cdot}$ (2,2-diphenyl-1-picrylhydrazyl);
- Folin-Ciocalteu reagent;
- $K_2S_2O_8$ (potassium persulfate);
- KCl (potassium chloride);
- KH_2PO_4 (potassium dihydrogen phosphate);
- Na_2CO_3 (sodium carbonate);
- Na_2HPO_4 (disodium phosphate);
- NaCl (sodium chloride);
- $NaNO_2$ (sodium nitrite);
- NaOH (sodium hydroxide);
- Trolox (6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid).

2.5.3. Methods of sample analysis in stage II / *II pētījuma posma* **paraugu** *analīzēšanas metodes*

Table 2.4 illustrates a summary of the applied methods for each parameter in research Stage II. Metadologies will be briefly described further in this chapter.

Table 2.4 / *2.4. tabula*

Applied methods in stage II of the research / *II pētījuma posmā pielietotās metodes*

Parameters / *Parameteri*	**Standards and methods** / *Standarti un metodes*
Total phenolic content / *Kopējais fenolu saturs*	Zhishen, Mengcheng, & Jianming (1999)
Total flavonoid content / *Kopējais flavonoīdu saturs*	Zhishen, Mengcheng, & Jianming (1999)
ABTS$^{\cdot+}$ radical scavenging activity / ABTS + *antiradikālā aktivitāte*	Re et al. (1999)
DPPH$^{\cdot}$ radical scavenging activity / DPPH$^{\cdot}$ *antiradikālā aktivitāte*	Brand-Willieams, Cuvelier, & Berset (1995)
Volatile compounds / *Gaistošie savienojumi*	Gas chromatography method (GC) / *Gāzes hromatogrāfijas metode*
Cup quality assessment / *Kafijas kvalitātes novērtējums*	Specialty coffee cupping protocol / *Specialty kafijas kvalitātes novērtēšanas protokols* (SCA 2015)

Headspace volatile compound extraction was carried out by solid-phase micro-extraction (SPME). After sample brewing, 5 mL of sample were immediately transferred in preheated 20 mL glass vial and immediately caped with screw-cap vial equipped with a polytetrafluoroethylene/silicone septum. The vial was transferred to a 50±1 °C heated surface for four minutes of incubation. After the incubation period, DVB/CAR/PDMS fibre was inserted into the sample headspace for 7 minutes volatile absorption.

The gas chromatography methods parameters with adjustments are described in chapter 2.4.2.

Cup quality assessment was performed according to the SCA protocols for cupping specialty coffee. The coffee evaluation process was divided into three steps shown in Table 2.5.

Table 2.5 / *2.5. tabula*

Cup quality assessment process / *Kafijas kvalitātes novērtēšanas process*

Step No / *Posma Nr.*	**Step** / *Posms*	**Eveluation conditions** / *Vērtēšanas nosacījumi*
1	Evaluating the aroma of dry ground samples / *Maltas kafijas aromāta vērtēšana*	15 minutes after the coffee samples were ground / *15 minūtes pēc kafijas pupiņu samalšanas*
2	Evaluating the aroma of coffee / *Kafijas aromāta vērtēšana*	brew temperature 93 °C, evaluate 3 minutes after extraction of coffee / *dzēriena temperatūra 93 °C, novērtēts 3 minūtes pēc kafijas ekstrakcijas*
3	Evaluation of coffee flavour / *Kafijas garšas vērtēšana*	flavour, aftertaste evaluated when the brew temperature is 71 °C (~8 min after extraction); acidity, body and balance are evaluated when the brew temperature is between 70 and 60 °C (~10 min after extraction) / *garša, pēcgarša novērtēta, kad dzēriena temperatūra ir 71 °C (~8 min pēc ekstrakcijas); skābums, balanss novērtēts, kad dzēriena temperatūra ir starp 70 and 60 °C (~10 min pēc ekstrakcijas)*

Coffee quality was measured by ten specialty cup quality attributes: cup cleanness, acidity, body, flavour, aroma, after taste, uniformity, sweetness, balance, and overall cup preference. The panellists also described a specific flavour, aroma perceived according to The World Coffee Research Sensory Lexicon[8] statements. Each attribute was evaluated on a scale from 1 to 10, with the final cup quality score of 100 points. The specialty coffee grade only applies if the total specialty cup quality score is 80 points or above (Figueiredo et al. 2013; Tolessa et al. 2016; Bressanello et al. 2017).

Total phenolic content (TPC) was determined by a spectrophotometric method using Folin-Ciocalteu reagent by Singleton, Orthofer, & Lamuela-Raventós (1999) using gallic acid as a standard. A 2.5 mL of Folin-Ciocalteu reagent (Sigma-Aldrich Chemie, Steinheim, Germany) (diluted in proportion 1:10 with distilled water) was added to 0.5 mL diluted coffee. After 5 minutes, 2.0 mL of 7.5% Na_2CO_3 solution was added. After 30 minutes of incubation at room temperature, the absorbance of samples was measured at 765 nm using a Spectrophotometer Jenway 6300 (Barloworld Scientific Ltd., UK). TPC was expressed as gallic acid equivalents (mg GAE 100 mL^{-1}) using a standard curve of gallic acid ($y = 0.1069x–0.0107$; $R^2 = 0.9991$).

Total flavonoid content (TF) was determined by the spectrophotometric method reported by Zhishen, Mengcheng, & Jianming (1999) with some modifications. To 2.0 mL of distilled water and 0.5 mL diluted coffee extract was added 0.15 mL 5% $NaNO_2$ solution. After 5 minutes, 0.15 mL of 10% $AlCl_3{*}_6H_2O$ solution was added. After 5 minutes, 1.0 mL of 1M NaOH solution was added. Each coffee sample flask was mixed and incubated at room temperature for 15 minutes. The absorbance of samples was measured at 415 nm with a

[8]WCR, (2017) World Coffee Research Sensory Lexicon [online] [viewed on 9. March 2022] Retrieved from https://worldcoffeeresearch.org/download/5806d8c7-cd7c-4882-a81a-2850bd6fbd36

Spectrophotometer Jenway 6300 (Barloworld Scientific Ltd., UK). Total flavonoid content was expressed as catechin equivalent (mg CE 100 mL^{-1}) using standard curve of catechin (y = 2.7592x+0.0244; R^2 = 0.9982).

$ABTS^{\cdot+}$ radical scavenging activity was determined by the Re et al. (1999) method with some modifications. To prepare ABTS radical, 2,2-azinobis(3-ethylbenzothiazoline- 6-sulfonic acid was dissolved in phosphate buffer (PBS) solution and oxidised with potassium persulfate. The solution was kept in the dark at room temperature for 16 h before further use. The $ABTS^{\bullet+}$ solution was diluted with PBS solution to an absorbance of 0.70 ABS (± 0.02) at 734 nm. To 0.05 mL of diluted coffee extract, 5 mL of diluted $ABTS^{\bullet+}$ solution was added. The samples were stored in darkness for 12 h; the absorbance was measured at 734 nm using a Spectrophotometer (Jenway 6300). The Trolox (6-hydroxy-2,5,7,8-tetramethylchromane-2-carboxylic acid) was used as standard and the results were expressed as Trolox equivalents (µmol Trolox mL^{-1}), using standard curve of Trolox (y = –0.9755x + 0.7604; R^2 = 0.9948).

$DPPH^{\cdot}$ radical scavenging activity was assessed by Brand-Willieams, Cuvelier, & Berset (1995) with some modifications. The 2,2-diphenyl-1-picrylhydrazyl (DPPH) was dissolved in ethanol, and the $DPPH^{\cdot}$ solution was diluted to an absorbance of 1.00 ABS (± 0.02) at 517 nm. To 0.5 mL of diluted coffee extract (diluted in proportion 1:33 with distilled water), 3.5 mL of diluted $DPPH^{\cdot}$ solution was added. After 30 minutes of incubation in darkness, the absorbance of samples was measured at 517 nm using a Spectrophotometer Jenway 6300 (Barloworld Scientific Ltd., UK). Trolox (6-hydroxy-2,5,7,8-tetramethylchromane-2-carboxylic acid) (Sigma-Aldrich Chemie, Steinheim, Germany) was used as standard, and the DPPH radical scavenging activity was expressed as Trolox equivalent (µmol Trolox mL^{-1}), using a standard curve of Trolox (y = –11.579x + 0.8931; R^2 = 0.9985).

2.5.4. Statistical analysis for stage II of research / *II pētījuma posma datu statistiskā analīze*

To evaluate the differences between total phenolic, flavonoid content, antiradical activity and final cup quality scores, one-way ANOVA was used. The sensory assessment was carried out in five replicates, and all chemical analysis measures were carried out in triplicate. The data were expressed as means. Statistical analysis was performed using Microsoft Office Excel 2013. A linear correlation analysis was performed to determine the relationship between TPC, TF, antioxidant activity such as $DPPH^{\cdot}$ and $ABTS^{\cdot}$+, volatile compounds and final cup quality score.

2.6. Stage III of the research / *III pētījuma posms*

In Stage III, the chemical composition of different roast level coffee was evaluated. The results can provide positive and negative bioactive compound changes in different roast level coffee.

2.6.1. Coffee samples for stage III / *III pētījuma posma Kafijas paraugi*

The roasting parameters are described in Table 2.6. (the batch size – 2.2 kg). The coffee qualifies as a specialty with 89.0 points. Green *Coffea arabica* L. coffee beans from Colombia were roasted in a local roastery in Latvia at three different roast levels using a Diedrich IR-2.5 roasters (Diedrich Roasters, Ponderay, ID, USA). Roasting parameters were adjusted according to green coffee bean density and moisture content and the roaster parameters.

For one week, the roasted coffee beans were degassed in a dry, cool place and then sealed in vacuum bags. All roasted samples were analysed within two to three weeks after roasting.

Table 2.6 / *2.6. tabula*

Roasting parameters for research stage III / III pētījuma posma *grauzdēšanas parametri*

Parameters / *Parametri*		**Roast level** / *Grauzdējuma pakāpe*		
		Light / *Viegls*	**Medium** / *Vidējs*	**Dark** / *Tumšs*
Roast temperature / *Grauzdēšanas temperatūra*, °C		195	200	210
Roast time / *Grauzdēšanas laiks*, min		10	11	12
Colour parameters / *Krāsas parametri**	L*	37.01 ± 0.02	33.94 ± 0.03	27.67 ± 0.02
	a*	4.9 ± 0.04	8.57 ± 0.05	5.4 ± 0.05
	b*	5.05 ± 0.01	6.16 ± 0.01	4.04 ± 0.01

*Colour was measured in CIE L*a*b* colour system using colorimeter (ColorTec-PCM, USA) / *Krāsas mērījumi tika noteikti izmantojot CIE L*a*b* krāsu sistēmu.*

Table 2.7 illustrates the coffee sample preparation for each physical and chemical parameter analysis. Samples were immediately analysed after preparation. All brewed coffee samples were prepared and analysed in triplicate.

Table 2.7 / *2.7. tabula*

Coffee sample preparation for each parameter analyses /
Kafijas paraugu sagatavošana katra parametra analīzei

Parameters / *Parametri*	**Coffee sample preparation /** *Kafijas paraugu pagatavošana*
Proteinogenic amino acids, fatty acids profile, acrylamide / *Proteinogēnās aminoskābes, taukskābju profils, akrilamīds*	roasted coffee beans sealed in 200 g vacuumed bags / *grauzdētas kafijas pupiņas iesaiņotas 200 g vakuuma maisos*
Moisture content Volatile compound profile / *Mitruma saturs, Gaistošo savienojumu profils*	roasted coffee beans ground* to a fine grind size / *grauzdētas kafijas pupiņas, kas samaltas* līdz smalkam malumam*
pH Total phenolic content, Total flavonoid content, Individual phenolic content / *pH Kopējais fenola saturs, Kopējais flavonoīdu saturs, Atsevišķs fenola saturs*	roasted coffee beans ground* to a coarse grind level 20 minutes before the brewing process. the french press brewing technique was used according to the specialty coffee association guidelines / *grauzdētas kafijas pupiņas, kas samaltas* līdz rupjai maluma pakāpei 20 minūtes pirms pagatavošanas procesa. Tika izmantota Franču preses brūvēšanas tehnika tika izmantota saskaņā ar specialty coffee association vadlīnijām* [9]

* KG79 Coffee grinder (DeLonghi, Italy) / *KG79 kafijas dzirnaviņas (DeLonghi, Italy)*

2.6.2. Materials and chemicals for stage III / *III pētījuma posma materiāli un ķīmiskās vielas*

For volatile compounds extraction by solid–phase microextraction (SPME), the carboxen/ polydimethylsiloxane (CAR/PDMS) fibre was purchased from Supelco (Bellefonte, USA). The following chemicals were purchased from Sigma–Aldrich Chemie (Steinheim, Germany):

- Folin–Ciocalteu reagent;
- sodium carbonate;
- gallic acid;

[9] Specialty Coffee Association (2016). Guidelines for Brewing with French Press, viewed January 4th, 2022 https://sca.coffee/s/best-practices-three-cup-french-press.pdf

- (+)-catechin;
- sodium nitrate;
- aluminium chloride hexahydrate;
- sodium hydroxide.

2.6.3. Methods of sample analysis in stage III / *III pētījuma posma Paraugu analīzēšanas metodes*

The summary of applied methods for each parameter is illustrated in Table 2.8. Roasted coffee bean samples, for the analysis of proteinogenic amino acids, fatty acid profile, acrylamide content, were shipped to Hamilton laboratory (outsource service).

The moisture content was determined by ISO 6673:2003 standard for green coffee and ISO 11294:1994 for roasted coffee. **The pH** was analysed after cooling the coffee brew to room temperature (±18 °C) and measuring the pH with a "Jenway™ 351101" pH meter (Jenway™, UK).

Table 2.8 */ 2.8. tabula*

Applied methods in stage III of research */ III pētījuma posmā pielietotās metodes*

Parameters / *Parametri*	**Applied methods** / *Pielietotās metodes*	**Laboratory** / *Laboratorija*
Moisture in green and roasted coffee / *Mitrums zaļā un grauzdētā kafijā %*	ISO 6673:2003 (green coffee) ISO 11294:1994 (roasted coffee)	At the scientific laboratory, Latvia University of Life Science and Technologies / *Latvijas Lauksaimniecības universitātes zinātniskajās laboratorijās*
Total phenolic content / *Kopējais fenolu saturs*	Singleton, Orthofer, & Lamuela-Raventós (1999)	
Total flavonoid content / *Kopējais flavonoīdu saturs*	Zhishen, Mengcheng, & Jianming (1999)	
Individual phenolics / *Atsevišķie fenolu savienojumi*	Liquid chromatography method (HPLC) / *Augstefektīvo šķidruma hromatogrāfijas metode (AEŠH)*	
Volatile compounds / *Gaistošie savienojumi*	Gas chromatography method (GC)/ *Gāzes hromatogrāfijas metode (GH)*	
Proteinogenic amino acids / *Proteinogēnās aminoskābes*	PB-53/HPLC ed. II of 30.12.2008	J.S. Hamilton Baltic Ltd. Laboratory */ J.S. Hamilton Baltic Ltd. laboratorija*
Fatty acids profile / *Taukskābju profils*	PN-EN ISO 12966-1:2015-01, PN-EN ISO 12966-2:2017-05 except p.5.3 and 5.5, PN-EN ISO 12966-4:2015-07	
Acrylamide */ Akrilamīds*	PB-39/GC ed. IV of 12.01.2018	

Methods used for total phenolic content (TPC) and total flavonoid content (TF) analysis are described in chapter 2.5.3.

Analysis of individual phenolic compounds was conducted using the high-performance liquid chromatography (HPLC) method described by Augšpole *et al.* (2018). The HPLC analysis was performed using an "LC–20 Prominence" chromatograph (Shimadzu USA Manufacturing Inc., USA) with a "Perkin Elmer C18" column (4.6 mm, 250 mm, 5 µm). Diode array detector gradient system (PDA-SPD-M10A) and the column was maintained at 30 °C. The mobile phase consisted of methanol (A, 20%), water (B, 78.4%) and acetic acid (C, 1.6%). The starting flow rate was 1 mL min^{-1}. The retention times of samples were compared with standards to determine the individual phenolic compounds in coffee samples.

Headspace volatile compound extraction was carried out by solid-phase micro-extraction (SPME). After sample brewing, five grams of sample was immediately transferred in preheated 20 mL glass vial and immediately caped with screw-cap vial equipped with a polytetrafluoroethylene/silicone septum. The vial was transferred to a 50±1 °C heated surface for four minutes of incubation. After the incubation period, carboxen/ polydimethylsiloxane (CAR/PDMS) fibre was inserted into the sample headspace for 7 minutes of absorption time.

The gas chromatography method is described in chapter 2.5.3.

2.6.4. Statistical analysis for stage III of research / *III pētījuma posma datu statistiskā analīze*

One-way ANOVA was conducted to determine significant differences between coffee samples and chemical parameters. The data were expressed as means reported as means with standard deviation (SD). Principal Components Analysis (PCA) and correlation biplot PCA was chosen to analyse possible variable patterns. The data statistical analyses were performed using XLSTAT software (vs. 2020.2.3.65347, XLSTAT, New York, NY, USA).

2.7. Stage IV of research / *IV pētījuma posms*

In this stage IV, aroma-active compound perception in different roast and brew coffee was evaluated and gas chromatography-olfactometry vocabulary was developed.

2.7.1. Coffee samples for stage IV / *IV pētījuma posma kafijas paraugi*

Green *Coffea arabica* L. beans from Colombia was used in this study. The post-harvesting method used was natural. The coffee qualifies as a specialty with 86.75–87.25 points following Specialty Coffee Association (SCA) standards and protocols.

The green coffee beans were sealed into 2.2 kg vacuum bags. The frozen green coffee beans were stored in a freezer at –18 °C and returned to room temperature (20±2 °C) 2 hours before roasting.

Roasting process. Green coffee beans were roasted two weeks before the start of the instrumental evaluation using a Diedrich IR- 2.5 roasters (Diedrich Roasters, Ponderay, ID, USA) (Table 2.9). Three roast levels were selected (light, medium, dark), and the roasting parameters were adjusted according to the green coffee bean density and moisture content and the roaster parameters.

Table 2.9 / *2.9. tabula*

Roasting parameters for stage IVof research /
IV pētījuma posma grauzdēšanas parametric (Laukaleja & Koppel 2021)

Parameters / *Parametri*		**Roast level** / *Grauzdēšanas pakāpe*		
		Light /*Viegls*	**Medium** / *Vidējs*	**Dark** / *Tumšs*
Roast Temperature / *Grauzdēšanas temperatūra*, °C		205	210	215
Roast Time / *Grauzdēšanas laiks, min*		11	12	13
Colour values / *Krāsas parametri**	*L**	40.01±0.02	31.94±0.03	29.67±0.06
	*a**	4.99±0.04	4.07±0.05	3.90±0.02
	*b**	15.05±0.01	9.11±0.04	8.16±0.01

* Colour was measured in CIE L*a*b* colour system using colorimeter measured with (ColorTec-PCM, USA) / *Krāsas mērījumi tika noteikti izmantojot CIE L*a*b* krāsu sistēmu.*

The samples were cooled to room temperature (18°C) and were degassed in a dry, cool place for one week, and then sealed in vacuum bags. All roasted samples were analysed within two weeks after roasting.

Grinding and brewing process. The roasted coffee samples were ground 20 minutes before brewing, using a Baratza Forte Brew Grinder (Baratza LLC, Bellevue, WA, USA). The grind level was adjusted according to the manufacturer instructions both brewing methods[10].The coffee samples were brewed fallowing SCA Brewing Best Practices guidelines for French press coffee and automatic drip coffee[11] with adjustments from Laukaleja & Koppel (2021). Before instrumental analysis, all brewed coffee samples were poured into a preheated beaker, maintaining a temperature of 70 °C. Samples were prepared in duplicate for each panellist.

2.7.2. Headspace solid-phase microextraction (HS-SPME) gas chromatography-olfactometry (GC-O) method for research stage IV / *IV pētījuma posma cietās fazes mikroekstrakcijas (CFME) gāzu hromatogrāfijas-olfaktometrijas (GH-O) metode*

Headspace volatile compound extraction was carried out by solid-phase microextraction (HS-SPME) with divinylbenzene/ carboxen/ poly(dimethylsiloxane) (DVB/CAR/PDMS) fibre (50/30 µm thickness and 1 cm coating phase). The DVB/CAR/PDMS fibre has been recommended as one of the most efficient and effective fibres for volatile compound extraction from brewed coffee (López-Galilea et al. 2006; Laukaleja & Kruma 2019b). The fibre was conditioned at 150 °C for 5 min before and after each run. After brewing, 2.5 mL of sample was immediately transferred in preheated 10 mL screw-cap vial with a polytetrafluoroethylene/silicone septum. The vials with sample were incubated for 2 min at 70 °C at 250 rpm using the autosampler. The SPME fibre was inserted into the vial and exposed to the sample head space for 7 min at 70 °C for volatiles extraction. The fibre was removed from the vial and the analytes were desorbed from the SPME fibre to the injection port of gas chromatography for 2 minutes at 240 °C in splitless mode.

The parameters for **gas chromatography-olfactometry** with adjustments were chosen according to Koppel, Adhikari, & Di Donfrancesco (2013) and Laukaleja & Koppel (2021). The chromatographic analyses were performed with Shimadzu GCMS-QP2020 gas chromatograph-mass spectrometer (Shimadzu Corporation, Kyoto, Japan) equipped with an SH-Rxi-5Sil MS column (30.0 m long, 0.25 µm thickness, 0.25 mm diameter) (Restek, State College, PA, USA). The initial temperature of the column was 60 °C and was ramped to 120 °C with a 7 °C min^{-1} rate, and from 120 to 250 °C with an 11 °C min^{-1} rate. Helium gas was used as a carrier. Mass spectrometry was performed using electron-impact ionisation at 70 eV (200 °C). The 18.39 min run time was recorded in full scan mode (35–350 m/z mass range). The volatile compounds were resolute from an average of six replicate chromatograms, calculated and expressed as the area percentage of their abundance (total area %). The volatiles were identified based on a) NIST library (vs2.2, 2014), b) Kovats Indices were calculated based on hydrocarbon mixture (C7-C30 saturated alkanes, Supelco, Bellafonte, PA, USA) retention times and compared to values in the literature and c) several volatiles were confirmed against pure standards (2-methyl propanol, hexanal, nonanal, 2-furan methanol acetate, furfural, 6-methyl-5-heptane-2-one, methyl pyrazine, pyridine, linalool). These compounds were acquired from Sigma Aldrich (St. Louis, MO, USA). GC effluent was combined with a stream of humidified olfactometer air (7 L min^{-1}, 1 cm in diameter) and presented to the panellists through a glass nosepiece using a Shimadzu Sniffport (Shimadzu Corporation, Kyoto, Japan).

2.7.3. Olfactometry vocabulary development for research stage IV / *IV pētījuma posma olfaktometrijas vārdnīcas izveide*

Three panellists from the Center for Sensory Analysis and Consumer Behavior (Manhattan, KS, USA) were screened for smell sensitivity and could recognise common volatile compound odours using an aroma palette with 19 common coffee aroma attributes from previous GC-O studies (Deibler, Acree, & Lavin 1998; López-Galilea et al. 2006; Chin, Eyres, & Marriott 2011). Two orientation sessions with randomly selected coffee samples were

[10] Baratza (2017). Grinding Tips, viewed June 10th, 2021 https://baratza.com/grinding-tips/

[11] Specialty Coffee Association (2016). Brewing Best Practices [online] [viewed on 20. January 2022] Retrieved from https://sca.coffee/research/protocols-best-practices

completed before sample evaluation. The nasal impact frequency method (NIF) was selected as one of the most efficient and rapid method for volatile compound odour detection (Brattoli et al. 2013; Lawless & Civille 2013). For the first orientation, each panellist evaluated three randomised, coded samples of different roast and brew coffee. After the first orientation session, panellists were introduced to reference materials for the most common aroma attributes detected in the session by all panellists. The panellists calibrated themselves and analysed the suitability of each reference materials. From the calibration The initial vocabulary was developed with 17 attributes (berry, burnt, caramelised, floral, grainy, nutty, roasted, sharp, smoky, spice, sweet, toast, plastic, bread, green/floral, cotton candy, wine). The aroma palette in software program (Olfactory Voicegram V2.2.17 Voice recorder, Shimadzu Corporation, Kyoto, Japan) was adjusted according to the initial vocabulary. In the second orientation session, the panellists had a chance to calibrate themselves with adjusted reference materials and an aroma attribute list. GC-O data was analysed, the aroma palette was aligned with the final 23 aroma attributes, and the reference material list was finalised after the second session (Table 2.10).

Table 2.10 / *2.10. tabula*

Attribute list, reference materials, and preparation of references /
Aromātu referenču materiālu saraksts ar pagatavošanas norādēm

No / Nr.*	**Aroma Attribute /** *Aromāti*	**Reference /** *References materiāls***	**Preparation /** *Pagatvošana* ***
1	Boiled potato / *Vārītu kartupeļu*	methionyl acetate / *metionilacetāts*	100,000 ppm in propylene glycol, one drop placed on a strip in a sealed tube / *100 000 ppm propilēnglikolā no kura vienu pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē*
2	Berry / *Ogu*	damascene / *damaskons*	10,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *10 000 ppm propilēnglikolā no kura trīs pilienus uzpilina uz sloksnes un ievieto noslēgtā mēģenē*
3	Burnt / *Deguma*	benzyl disulfide / *benzildisulfīds*	1,000 ppm in propylene glycol, one drop placed on a strip in a sealed tube / *1000 ppm propilēnglikolā no kura vienu pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē*
4	Buttery / *Sviesta*	Land O'Lakes Unsalted butter / *sviests*	Serve 4, 1/2 inch cubes in a medium snifter with a watch glass / *četrus ½ collu kubiņus novietot vidēja izmēra brendija glāzē*
5	Caramelised / *Karamelizēts*	5-methyl furfural / *5-metilfurfurols*	100,000 ppm in propylene glycol, one drop placed on a strip in a sealed tube / *100 000 ppm propilēnglikolā no kura vienu pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē*
6	Chemical / *Ķīmisks*	trans-2-Hexen-1-ol / *trans-2-heksēn-1-ols*	100,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *100 000 ppm propilēnglikolā no kura trīs pilienus uzpilina uz sloksnes un ievieto noslēgtā mēģenētrīs pilienus 10 000 ppm propilēnglikola uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
7	Floral / *Ziedu*	decen-2-one / *decen-2-one*	100,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *100 000 ppm propilēnglikolā no kura trīs pilienus uzpilina uz sloksnes un ievieto noslēgtā mēģenē*
8	Garlic / *Ķiploka*	dimethyl sulphide / *dimetilsulfīds*	1,000 ppm in propylene glycol, one drop placed on a strip in a sealed tube / *1000 ppm propilēnglikolā no kura vienu pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē*

Continued Table 2.10 / *2.10. tabulas turpinājums*

No / Nr.*	**Aroma Attribute /** *Aromāti*	**Reference /** *Atsauces materiāls***	**Preparation /** *Pagatvošana ****
9	Grainy / *Graudu*	2-acethylpyridine / *2-acetilpiridīns*	10,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / trīs pilienus references materiāla šķīduma ar 10 000 ppm propilēnglikolu uzpilina uz sloksnes un ievieot noslēgtā mēģenē
10	Green / *Zaļas zāles*	3,7-dimethyl-6-octenoic acid / *3,7-dimetil-6-oktēnskābe*	100,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *trīs pilienus references materiāla šķīduma ar 100 000 ppm propilēnglikolu uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
11	Leather / *Ādas*	leather glove / ā*das cimdi*	2-inch strip of leather placed in a medium snifter / *2 collu ādas sloksne, kas ievietota vidēja izmēra brendija glāzē*
12	Mushroom / *Sēņu*	1-octen-3-ol / *1-okten-3-ols*	100,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *trīs pilienus references materiāla šķīduma ar 100 000 ppm propilēnglikolu uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
13	Musty / *Mitra pagraba/ pelējuma*	2-methoxy phenol / *2-metoksifenols*	100,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *trīs pilienus references materiāla šķīduma ar 10 000 ppm propilēnglikolu uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
14	Nutty / *Riekstu*	2,5 dimethyl pyrazine / *2,5 dimetilpirazīns*	1,000 ppm in propylene glycol, one drop placed on a strip in a sealed tube / *1000 ppm propilēnglikolā no kura vienu pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē*
15	Roasted / *Grauzdēts*	2-ethyl 3,5(or 6) dimethyl pyrazine / *2-etil-3,5(vai 6) dimetilpirazīns*	1,000 ppm in propylene glycol, one drop placed on a strip in a sealed tube / 1000 ppm propilēnglikolā no kura vienu pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē
16	Sharp / *Ass*	propionic acid / *propionskābe*	100 ppm in deionised water, three drops placed on a strip in a sealed tube / *trīs pilienus references materiāla šķīduma ar 100 ppm propilēnglikolu uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
17	Skunky / *Skunksa*	Methanethiol / *metāntiols*	100 ppm in propylene glycol, one drop placed on a strip in a sealed tube / *100 ppm propilēnglikolā no kura vienu pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē*
18	Smoky / *Dūmu*	4-ethyl-2-methoxyphenyl / *4-etil-2-metoksifenils*	100,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *trīs pilienus references materiāla šķīduma ar 100 000 ppm propilēnglikolu uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
19	Spice / *Pikants*	(E)-cinnamaldehyde / *(E)-kanēļamaldehīds*	100,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *trīs pilienus 100 000 ppm propilēnglikola uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
20	Sweat / *Sviedru*	Parmesan cheese / *Parmezāna siers*	cut the cheeses into 1inch size cubes, place five pieces in a medium snifter / *sagrieziet sieru2 cm kubiņos, ievietot piecus gabaliņus vidēja izmēra brendija glāzē*
21	Sweet / *Salds*	Lyramre / *Lirama*	One drop placed on a strip in a sealed tube / vienu *pilienu uzpilina uz sloksnes un ievieto noslēgtā mēģenē*

Continued Table 2.10 / *2.10. tabulas turpinājums*

No / Nr.*	**Aroma Attribute /** *Aromāti*	**Reference /** *Atsauces materiāls***	**Preparation** / *Pagatvošana ****
22	Boiled vegetable / *Vārītu dārzeņu*	2-isobutylthiazole / *2-izobutiltiazols*	10,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *trīs pilienus 10 000 ppm propilēnglikola uzpilina uz sloksnes un ievieot noslēgtā mēģenē*
23	Waxy / *Vaska*	1-nonanal / *1-nonanāls*	10,000 ppm in propylene glycol, three drops placed on a strip in a sealed tube / *trīs pilienus references materiāla šķīduma ar 10 000 ppm propilēnglikolu uzpilina uz sloksnes un ievieot noslēgtā mēģenē*

*Chemical references were acquired from / ķīmiskie referenču materiāli tika iegūti no Sigma Aldrich (St. Louis, MO, USA), Lyrame Super from International Flavors & Fragrances (New York, New York, USA); **The chemical references were prepared according to recommended smelling concentration http://www.thegoodscentscompany.com/ / *Atsauces materiāli tika pagatavoti pēc ieteiktajām koncentrācijam no The good scents company datu bāzes.*

A total of 6 points from the initial list (toast, plastic, bread, green/floral, cotton candy, and wine) were replaced with baked potato, buttery, chemical, garlic, green, leather, mushroom, musty, sharp, sweat, vegetable, and waxy aroma.

Sample evaluation. Panellists evaluated samples by smelling the effluent from the column, and recorded each aroma by clicking on the aroma palette attributes. One sample analysis was 18.39 min and each panellist evaluated six samples with two replicates over 1–2 sessions per day. The serving order was randomised, and the registered name of the sample was coded. The sample evaluation was conducted in a temperature-controlled room (20 ±2 °C).

2.7.4. Statistical analysis for research stage IV / *IV pētījuma posma datu statistiskā analīze*

Aroma peaks that were detected more than four times during GC-O analysis (i.e., nasal impact frequency (NIF) >60 %) were selected as highly potent odorants for further analysis (Mayuoni-Kirshinbaum et al. 2012). The volatile compounds were identified as aroma-active if:

1) the GC-O retention times matched with GC-MS retention times of potent volatile compounds with ±0.01 min deviation;
2) aroma peaks that were detected more than four times during GC-O analysis were selected as impact potent odorants for further analysis;
3) using mass spectral database ‘Nist98’ compounds were identified if their probability rate was 90% or above;
4) the experimental KI was compared using the National Institute of Standards and Technology (NIST) library with strict column parameters (30 m; 0.25 mm, 0.5 µg) temperature range: 320/350 °C.

Volatile compounds detected at least in four out of six repetition samples were selected for further consideration for the vocabulary.

Analysis of Variance (ANOVA) was performed based on peak area per cent values using XLSTAT software (vs. 2020.2.3.65347, XLSTAT, New York, NY, USA). Least squares means were used to understand significantly different roast levels and preparation methods at the 5% significance level. Average peak area values of volatile compounds were used for Principal Component Analysis (PCA) correlation biplot using XLSTAT software (vs. 2020.2.3.65347, XLSTAT, New York, NY, USA).

2.8. Stage V of research / *V pētījuma* posms

In stage V consumer's perception of specialty coffee brews was analysed.

2.8.1. Coffee samples for research stage V / *V pētījuma posma kafijas paraugi*

Green *Coffea arabica* L. coffee from Colombia was used in the study. The post-harvesting method used was natural Selected coffee qualifies as a specialty with 86.75–87.25 points following Specialty Coffee Association (SCA) standards and protocols. Green coffee bean storage before roasting is described at Stage IV in 2.7.1. chapter.

Roasting process. Diedrich IR- 2.5 roaster (Diedrich Roasters, Ponderay, ID, USA) was used with a 2.2 kg batch size. Green coffee beans were roasted in two roast levels (Light roast at 205°C for 11 min; Medium roast at 210°C for 12 min). The colour values of the roast level were analysed using a ColorTec-PCM colorimeter (Color-Tec Associates, Inc., Clinton, NJ, USA). Colour values: L* indicates white/black coordinate (light roast 40.01±0.02; medium roast 31.94±0.03), the a* indicates red/green coordinate (light roast 4.99±0.04; medium roast 4.07±0.05), and b* – yellow/blue coordinate (light roast 15.0±0.01; medium roast 9.11±0.04). Roasted coffee beans were stored in a dry, airtight container until the grinding/brewing process.

Brewing process. The roasted coffee beans were ground 10–15 minutes before brewing, using a Baratza Forte Brew Grinder (Baratza LLC, Bellevue, WA, USA). Two brewing techniques were used - French Press (Bodum, Triengen, Switzerland) and Automatic drip coffee (Newell Brand, Cleveland, Ohio, USA). For both techniques coffee: water ratio was 55 g : 100 mL. Deionized water was used heated to 93 *°C*. For French press coffee: water was poured over ground coffee and extracted for 4 min. Automatic drip coffee was brewed following manufacturer guidelines.

Brewed coffee was poured in a pre-heated air-pot (Zojirushi AASB-22SB Air Pot, Zojirushi Corp, Osaka, Japan. To maintain a 70 ◦C serving temperature (Adhikari, Chambers, & Koppel 2019), the coffee samples were served in 4 oz Styrofoam cups (with lids) to participants right before the sample evaluation.

2.8.2. Consumer study for stage V of research / *V pētījuma posma patērētāju pētījuma gaita*

Participants. From 301 screened people, 188 were qualified to participate in this study. The recruitment goal was to include only regular coffee consumers (consume black coffee at least 2–3 times per week) over 18 and who do not work for a restaurant or coffee shop companies. After giving their written consent, 90 participants took part in this study.

Study location and set up. The consumer study was conducted at the Center for Sensory Analysis and Consumer Behavior at Kansas State University (Manhattan, Kansas). The tests were conducted in a single session (~30 min.) in a panel room with a maximum of 10 consumers per session. Consumers were asked to answer nine demographic and coffee consumption-related questions and to perform evaluation of four coffee samples. Four coffee samples (LD – light roast/drip coffee; LF – light roast/ French Press coffee; MD – medium roast/ drip coffee; MF – medium roast/ French press coffee) were labelled with 3-digit codes, presented monadically in randomised order. After each sample evaluation, participants had a 1-minute break with unsalted crackers and water provided as a cleanout.

Questionnaire. The questionnaire included four questions about sensory attributes in the following order: overall like overall aroma, overall flavour, overall texture. This study used a 9-point hedonic scale (from 1 - dislike significantly to 9 - like extremely) for sensory attribute liking. Consumers were asked to evaluate the sourness and bitterness of coffee samples using the "Just-About-Right" scale (where 1=Not Sour; 2=Not Sour Enough; 3=Just About Right; 4=Slight Too Sour; 5=Much Too Sour). Consumers were asked to answer the last question about how likely they would purchase the coffee sample, knowing it has high antioxidants. This study used a 5-point scale (from 1=Definitely not; 2=Probably not; 3=Possibly; 4=Probably; 5=Definitely) for purchase intent.

2.8.3. Statistical analysis for stage V of research / *V pētījuma posma datu statistiskā analīze*

Shapiro-Wilk test was used for normality test at a significance level of 0.05, and histograms visualised data distribution. To examine coffee consumers based on four different coffee brew sensory attribute liking scores, agglomerative hierarchical clustering (AHC) was carried out using Euclidean distance and Ward's method. To determine consumer sample effect on sensory attribute liking scores and purchase intent, a two-way Analysis of Variance (ANOVA) was performed following pairwise comparison by Tukey's Honestly Significant Difference (HSD) test. The correlation between purchase intent and sensory attribute was tested using Kendall's tau coefficient (τ) at 5% probability levels. Penalty analysis, Just-About-Right (JAR) data was applied to determine how much the overall liking and acceptance of the coffee samples were impacted by their flavour attributes (sourness and bitterness). The consumer recruiting electronic questionnaire results were collected by RedJade Sensory Software (Martinez, CA, USA). All statistical analyses were performed using the software program XLSTAT (Addinsoft, New York, NY, USA).

3. RESULTS AND DISCUSSION / *REZULTĀTI UN DISKUSIJA*

3.1. Evaluation of a headspace solid-phase microextraction with different fibres for volatile compound determination in specialty coffee / *Specialty kafijas gaistošo savienojumu analīze, izmantojot četras dažādas cietās fāzes mikroekstrakcijas šķiedras*

The SPME is a frequently applied method for volatile compound extraction, although there is a limited research disclosed about different SPME fibre suitability for volatile compound extraction from specialty coffee brews. The aim of research stage I was to evaluate the volatile composition of specialty coffee brews using different SPME fibres.

3.1.1. Evaluation of coffee volatile compound chemical groups, detected with four different SPME fibres / *Kafijas gaistošo savienojumu ķīmisko klašu novērtējums, izmantojot četras dažādas cietās fazes mikroekstrakcijas šķiedras*

In total 76 compounds from 16 chemical classes were extracted from coffee samples. A significant relationship between SPME fibres and chemical compound classes have been detected by Chi-Square test ($p<0.05$). The CAR/PDMS fibre could extract volatile compounds from all chemical classes while PA fibre could extract only from eight classes (Table 3.1).

Table 3.1 / *3.1. tabula*

Contingency table indicating the percentage (%) of extracted volatile compounds with each SPME fibre / *Ekstrahēto gaistošo savienojumu procentuāls sadalījums pēc to ķīmiskajām klasēm un CFME šķiedrām*

Chemical classes / *Ķīmiskās klases*	**Volatile compound content** / *Gaistošo savienojumu sastāvs, %*			
	CAR/PDMS	DVB/CAR/PDMS	PA	PDMS/DVB
Alcohols / *Spirti*	1.34	-	-	1.63
Aldehydes / *Aldehīdi*	1.79	-	11.43	4.07
Alkanes / *Alkāni*	16.52	19.57	18.57	24.39
Amides /*Amīdi*	1.34	1.09	-	-
Esters / *Esteri*	2.68	-	-	-
Furans / *Furāni*	7.59	7.61	35.71	1.63
Ketones / *Kertoni*	17.86	25.00	35.71	21.95
Organic acids / *Organiskās skābes*	13.84	13.04	1.43	9.76
Oxides / *Oksīdi*	7.59	6.52	12.86	4.07
Phenolic compounds / *Fenolu savienojumi*	4.02	3.26	14.29	2.44
Pyrazines / *Pirazīni*	0.45	-	4.29	1.63
Pyridines / *Piridīni*	10.71	4.35	-	18.70
Pyrimidines / *Pirimidīni*	3.57	5.43	-	0.81
Pyrroles / *Piroli*	2.23	6.52	1.43	0.81
Sulphur-containing compounds / *Sēru saturoši savienojumi*	7.14	7.61	-	7.32
Terpenes / *Terpēni*	1.34	-	-	0.81

These are in accordance with previous studies indicating that bipolar fibres such as DVB/CAR/PDMS, CAR/PDMS and PDMS/DVB have the ability to extract a wide range of volatile compounds from coffee (Risticevic, Carasek, & Pawliszyn 2008; Viegas et al. 2009; Spietelun et al. 2010). Additionally, Salum et al. (2017) and Chen, Chiang, & Chung (2019) reported that fibres with carboxen (CAR) coating allow extracting smaller size molecules. It could be explained by CAR large surface area with micro and macropores structure. The results align with Roberts, Pollien, & Milo (2000) study, where CAR/PDM fibre could extract small molecules like acetaldehyde and organic acids more than other fibres.

The PA fibre could extract the most phenolic compounds compared to bipolar fibres. Contrarily the PA fibre could only extract 17 compounds from 8 chemical compound classes with the lowest total compound peak areas. The possible explanation could be the polar compound coating material, which has shown a disadvantage to extracting nonpolar compounds (Spietelun et al. 2010). The PA could be benefitial for coffee defect analysis toger with one of the bipolar fibres, because the majority of phenolic compounds in coffee are found in green or burnt coffee (Yang et al. 2016). However, for specialty coffee volatile compound analysis it is important to focus on chemical classes such as aldehydes, ketones, pyrazines, sulphur-containing compounds. The results are consistent with Chen, Chiang, & Chung (2019) study where PA fibre could not extract sulphur-containing compounds and pyrazines.

3.1.2. Important volatile compounds in specialty coffee brew / *Nozīmīgākie gaistošie savienojumi speacialty kafijas dzērienos*

Previous studies have confirmed that from all volatile compounds (more than 800), only 20–25 can significantly impact the aroma and flavour of coffee, which are particularly detected in specialty coffees (Sobreira et al. 2015; Laukaleja & Kruma 2018; Zamora-Ros et al. 2018). Consistent with the literature, this research found that CAR/PDMS fibre was able to extract 17, DVB/CAR/PDMS – 15, PDMS/DVB – 13; PA – 6 important specialty coffee volatile compounds. From 17 compound peak areas, 8 showed significant differences between SPME fibres (Table 3.2.). Only the CAR/PDMS fibre could extract acetaldehyde, this finding was also reported by Caprioli et al. (2012). A possible explanation for this might be the low boiling point of aldehydes. The PDMS/DVB fibre showed significantly higher peak area for 1-(2-furanylmethyl)-1H-pyrrole compound (savoury, vegetable aroma notes) extraction. The PDMS/DVB fibre was selected by Ribeiro et al. (2009) to predict sensory chracteristics of roasted *Coffea arabica* L. coffee from Brazil. Although in this study the PDMS/DVB fibre was not able to extract four important volatile compounds in specialty coffee.

Table 3.2 / *3.2. tabula*

Identified important volatile compounds in specialty coffee brews using four different SPME fibres /
Identificēti sensorai kvalitātei nozīmīgākie gaistošie savienojumi specialty kafijā, izmantojot četras dažādas cietās fāzes mikroekstrakcijas šķiedras (Laukaleja & Kruma 2019b)

No. / Nr	**Compounds** / *Savienojumi*	**Coffee volatile peak area** / *Kafijas gaistošo savienojumu snaiļu laukums (x10^8)*				***p* value** / *p vērtība**	**Compound sensory description** / *Savienojumu sensorās īpašības***
		CAR/PDMS	DVB/CAR/PDMS	PDMS/DVB	PA		
1.	1-(2-Furanylmethyl)-1h-pyrrole / *1-(2-Furanilmetil)-1h-pirols*	3.53	2.97	6.38	-	*0.008*	vegetables / *dārzeņu*
2.	2,3-Pentanedione / *2,3-Pentāndions*	48.81	19.64	6.75	-	*<0.000*	buttery / *sviesta*
3.	2,6-Dimethyl-4-thiopyrone / *2,6-Dimetil-4-tiopirons*	-	5.00	-	-	-	caramel / *karameles*
4.	5-Methyl-2-furancarboxaldehyde / *5-Metil-2-furānkarboksaldehīds*	127.43	56.01	31.18	5.04	*0.032*	caramel / *karameles*
5.	2-Furanmethanol / *2 - Furānmetanols*	73.31	35.85	19.71	10.25	*<0.000*	floral / *ziedu*
6.	Furfuryl acetate / *Furfurilacetāts*	55.82	48.37	41.75	2.23	*0.005*	floral, fruity / *ziedu, augļu*
7.	3-Methyl-butanal / *3-Metil-butanāls*	27.43	5.47	13.87	0.61	*0.043*	fruity / *augļu*
8.	1-(2-Furanyl), ethenone / *1-(2-Furanil), etanons*	9.91	4.48	2.59	0.17	*0.125*	nutty / *riekstu*
9.	2-(Methoxymethyl)furan / *2-(Metoksimetil)furāns*	0.57	0.99	-	-	*0.565*	nutty, ground coffee–like / *riekstu, maltas kafijas*
10.	2-Methylfuran / *2-Metilfurāns*	32.20	4.82	0.59	-	*0.000*	roasted almond, coffee / *grauzdētas kafijas*
11.	Furfural / *Furfurols*	164.31	73.77	26.17	6.86	*<0.000*	caramel / *karameles*
12.	2-Methylpropanal / *2-Metilpropanāls*	3.37	5.83	3.17	-	*0.522*	roasted sweet almond / *grauzdētu saldu mandeļu*
13.	2.5-Dimethylpyrazine / *2,5-Dimetilpirazīns*	3.48	-	3.16	-	*0.979*	roasted / *greuzdēts*
14.	Ethyl-pyrazine / *Etilpirazīns*	3.35	3.19	2.30	-	*0.402*	chocolate–peanut, nutty / *šokolādes-zemesriekstu, riekstu*
15.	4-Methyl-pyrimidine / *4-Metil-pirimidīns*	20.18	13.30	1.87	-	*0.041*	popcorn / *popkorna*
16.	Acetaldehyde / *Acetaldehīds*	2.63	-	-	-	-	fruity / *augļu*
17.	Furfurylformate / *Furfurilformiāts*	2.46	-	-	-	-	malt, fruity / *iesala, augļu*

* Significance differences between SPME fibres at *p*<0.05 / *Būtiskas atšķirības starp CFME šķiedrām (p<0.05)* **According to previous studies / *Atsaucoties uz iepriekšejiem pētījumiem:* Mondello et al. (2005); Somporn et al. (2011); Mestdagh et al. (2014); Piccino et al. (2014); Yang et al. (2016).

Previous studies have shown that the CAR/PDMS fibre can better extract compounds with low boiling points compared to other SPME fibres (Salum et al. 2017; Dadalı & Elmacı 2019). The CAR/PDMS fibre shows the highest peak areas for eight volatile compounds. All these compounds are associated with fruity, caramel, floral aroma notes. Comparison of the findings with those of other studies confirms that CAR/PDMS fibre is the most suitable for furan compound extraction (Mayuoni-Kirshinbaum et al. 2012; Petisca et al. 2012).

3.1.3. Principal component and agglomerative hierarchical clustering analysis of the specialty coffee brews with different SPME fibres / *Specialty kafijas dzērienu galveno komponentu un aglomeratīvās hierarhisko klasteru analīze, izmantojot četras dažādas cietās fāzes mikroekstrakcijas šķiedras*

Principal Component Analysis (PCA) illustrates (Fig. 3.1) the SPME fibre coating impact on volatile compound extraction from specialty coffee samples. The first two principal components explained 57.12 % of total variance. Axes (F1 and F2 factors-the first and second principal component) refer to the ordination scores obtained from the samples. Axis F1 (first principal component) accounts for 41.94% and F2 (second principal component) accounts for a further 15.19% of the total variance.

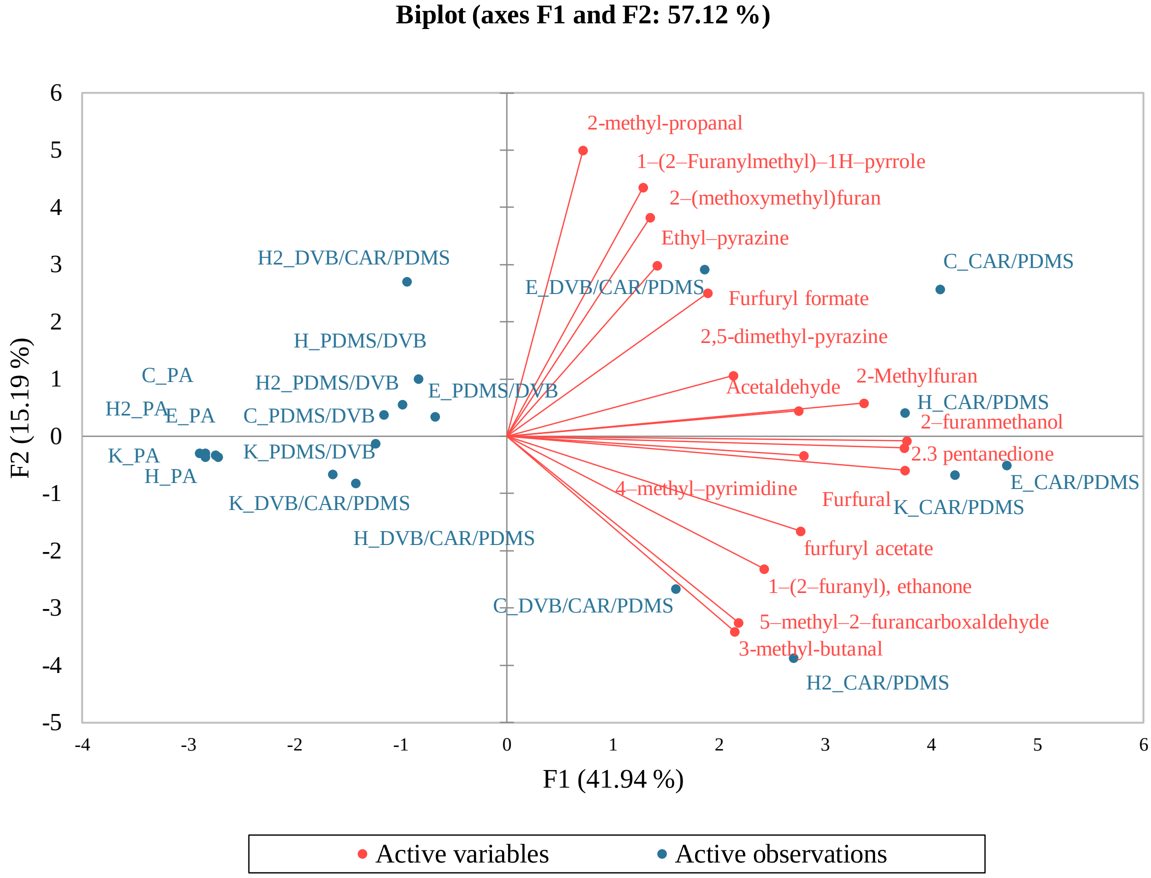


Fig. 3.1. Biplot diagram by principal component analysis of five coffee brew samples with four different SPME fibres /
3.1. att. Galveno komponentu analīzes biplot diagramma, analizējot piecu kafijas dzērienu paraugu gaistošo savienojumu ekstrakciju, izmantojot četras dažādas CFME šķiedras

In the biplot, Kenya (K_) and Honduras (H_) sample volatiles extracted with all four fibres and Colombia (C_), Ethiopia (E_) extracted with CAR/PDMS, PDMS/DVB and PA were classified in the first principal component, while the second principal component presented Honduras_2, Colombia, Ethiopia sample volatiles extracted with DVB/CAR/PDMS fiber.

A positive correlation was found between CAR/PDMS fibers and majority of volatile compound peak areas, while PDMS/DVB and PA showed strong negative correlation with the same volatile compounds.

Agglomerative hierarchical clustering (AHC) was performed to evaluate if the volatile compounds are grouped by the coffee samples or by SPME fibres. The results of AHC analysis were illustrated by dendrogram (Fig. 3.2).

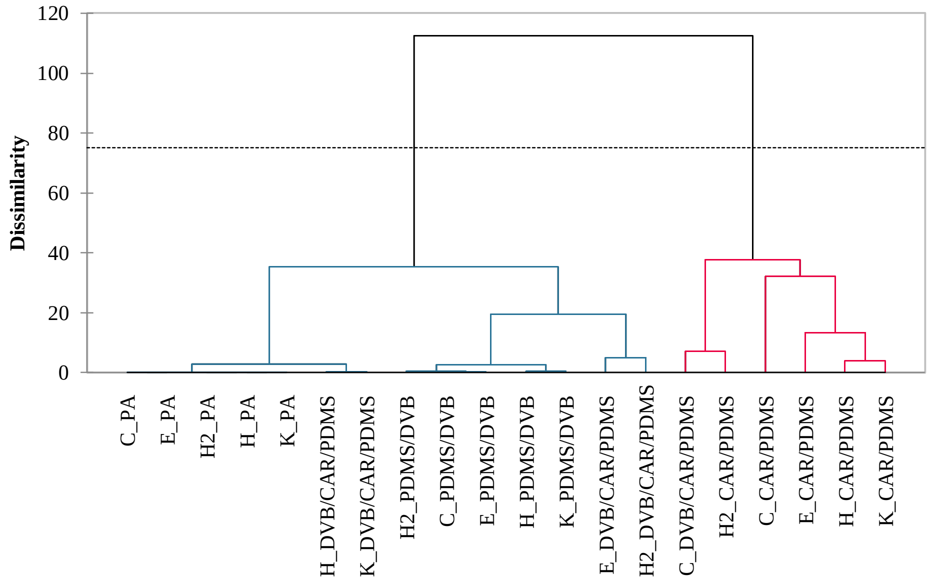


Fig. 3.2 Dendrogram (AHC analysis) representing volatile compound dissimilarity relationships of coffee samples and SPME fibres / *3.2. att. Aglomeratīvās hierarhisko klasteru analīzes dendrogramma, illtustrējot gaistošo savienojumu atšķirīguma attiecības starp kafijas paraugiem un CFME šķiedrām*

The AHC analysis grouped the coffee volatiles into two clusters. First cluster is more homogeneous and represents DVB/CAR/PDMS, PDMS/DVB, PA fibres and the second cluster represents CAR/PDMS fibre. Only C_DVB/CAR/PDMS was grouped with CAR/PDMS fibre. The given data could indicate that the DVB/CAR/PDMS fibre only from Colombia coffee could extract volatile compounds as efficient as CAR/PDMS fibre. The AHC and PCA analysis confirmed the importance of SPME fibre coating selection for analysis of coffee volatile profile, because samples were classified based on fibre coating, not the coffee origin.

Summary of Chapter 3.1. Evaluation of a headspace solid - phase microextraction with different fibers for volatile compound determination in specialty coffee brews / *Kopsavilkums par 3.1. posmu Gaistošo savienojumu analīze, izmantojot četras dažādas cietās fazes mikroekstrakcijas škiedras*

Consistent with the literature, this research found that bipolar fibres such as DVB/CAR/PDMS, CAR/PDMS and PDMS/DVB have ability to extract more polar and non-polar volatiles form coffee samples.

The findings contradict with previous studies, showing that CAR/PDMS fibre could detect and extract broader range of volatile compounds from different origin specialty coffee samples. The AHC and PCA confirmed that SPME fibre could significantly impact the volatile compound extraction from specialty coffee, because the analysed samples were clustered by the selected SPME fibres. The CAR/PDMS fibre would be the preferable choice for volatile compound extraction from specialty coffee brew, although DVB/CAR/PDMS fibre can be a reliable alternative for volatile compound extraction from specialty coffee brew from Colombia.

Saskaņā ar literatūru, bipolārās šķiedras, kā DVB/CAR/PDMS, CAR/PDMS un PDMS/DVB, pierāda spēju no kafijas paraugiem ekstrahēt polāros un nepolāros gaistošos savienojumus. Rezultāti ir pretrunā ar iepriekšējiem pētījumiem, kas parāda, ka PDMS/DVB šķiedra spēj iegūt plašāku gaistošo savienojumu saturu un lielāku to koncentrāciju kafijā nekā CAR/PDMS šķiedra. Pētījumā CAR/PDMS šķiedra spēja uzrādīt ievērojami vairāk gaistošo savienojumu ar lielākiem smaiļu laukumiem no visām ķīmiskajām klasēm, izņemot fenolu savienojumus. AHK un GKA analīze apstiprina CFME šķiedru pārklājuma izvēles nozīmi kafijas gaistošos savienojumu sastāva analīzē, jo paraugi tika klasificēti, pamatojoties uz šķiedru pārklājumu, nevis kafijas izcelsmi. CAR/PDMS šķiedra būtu ieteicama specialty kafijas gaistošo savienojumu ekstrakcijai, taču DVB/CAR/PDMS šķiedra var būt, kā atbilstoša alternatīva CAR/PDMS šķiedrai, ka specialty kafija ir no Kolumbijas.

3.2. Influence of phenolic and volatile compound composition on specialty coffee cup quality / *Fenolu un gaistošo savienojumu satura ietekme uz specialty kafijas sensoro kvalitāti*

During the roasting process compounds such as chlorogenic acid and ferulic acid degrades and create different volatile compounds including phenolic compounds. Phenolic compounds can increase the harsh bitter taste and smoky aroma. It is important to know phenolic and volatile compound profile composition in coffee and their influence on cup quality. The aim of research stage II was to evaluate the influence of phenolic and volatile compound composition on specialty coffee cup quality.

3.2.1. Cup quality assessment / *Kafijas kvalitātes novērtējums*

The cup quality assessment showed that all coffees scored in the range 83.00–90.25 (Table 3.3). The lowest score (83 points) had SAL_1, and the highest score was for the HON_2 coffee sample (90.25). These results could be explained by the acidity and sweetness balance in coffee.

It has been suggested that the balance between acidity and sweetness is correlated with a higher final cup quality score, as shown in Mendonça de Carvalho et al. (2016) study that analysed the relationship between coffee plantation regions in Brazil and cup quality attributes. The SAL_1 coffee was associated with higher acidity, which can disbalance the overall cup preference. From another point of view, the HON_2 sample shows a balance between the acidity and sweetness of the coffee brew.

A positive correlation was found between the frequency of fruit, caramel flavour notes and a pleasant acidity with coffees whose quality standards was the most in accordance with the SCAA standard guidelines.

Borém et al. (2016) reported that final cup quality scores could be influenced by sucrose content in green coffee and sourness level in the roasted coffee brew. The higher sucrose content in green coffee has shown positive correlation with acidity, sweetness in final cup quality.

Table 3.3 / *3.3. tabula*

Final cup quality scores with sensory description /
Kafijas paraugu kvalitātes novērtējums (Laukaleja & Kruma 2019c)

Roastery / *Grauzdētava*	**Coffee sample** / *Kafijas paraugs*	**Final cup quality score** / *Kopējais kvalitātes vērtējums*	**Sensory description** / *Sensorais raksturojums*
R_1	HON_1	86.50	plum, grapes, red pepper, toffee (caramel) / *plūme, vīnogas, sarkanie pipari, īriss (karamele)*
	KEN_1	88.75	blackberry, red pepper, roses, dark chocolate / *kazenes, sarkanie pipari, rozes, tumšā šokolāde*
	COL_1	89.00	pineapple, dried apricot, elderflower / *ananāsi, žāvēti aprikozes, plūškoks*
R_2	HON_2	90.25	dried fruits, passion fruit, melon, kombucha / *žāvēti augļi, marakujas augļi, melone, kombucha*
	ETH_1	88.25	lime, jasmine, chocolate cream, cherry brandy / *laims, jasmīns, šokolādes krēms, ķiršu brendijs*
	HON_3	85.00	cacao, red apples, dried fruits / *kakao, sarkanie āboli, žāvēti augļi*
	SAL_1	83.00	nutty and creamy notes / *riekstu un krēmveida notis*

Pleasant acidity mostly is associated with dry fruit taste (Poltronieri & Rossi 2016), and this could be the reason why HON_2 with dry fruits and melon characteristics showed the highest final cup quality score.

3.2.2. Volatile compound profile in different origin and differently roasted coffee brews / *Gaistošo savienojumu kompozīcija dažādu izcelsmes valstu un grauzdējuma kafijas dzērienos*

The major volatile compounds in coffee brew samples were furans, pyrazines, aldehydes, and ketones (Table 3.4). Volatiles from furan chemical class set the highest concentration in coffee, although aldehydes, ketones and pyrazines can crucially impact the aroma profile of coffee brew (Gruczyńska et al. 2018; Cordoba et al. 2019). More studies approve the positive correlation between coffee cup quality and volatile compound concentration with floral, fruity aroma notes (Piccino et al. 2014; Poltronieri & Rossi 2016). Chemical classes such as ketones and aldehydes are associated with a floral, fruity aroma and pleasant acidity in coffee.

In Caporaso et al. (2018) study a positive correlation was detected between aldehydes and ketones, but a negative correlation between aldehydes and pyrazines. Ribeiro et al. (2009) study stated that a higher concentration of 5-methyl-2-furancarboxaldehyde and furfural increased the overall quality of Brazilian *Coffea arabica* L. coffee samples. The present study found correlation between final cup quality scores and 2-furanmethanol (r=0.616; p=0.036) and strong correlations between 2-furanmethanol and 5-methyl-2-furancarboxaldehyde (r=0.920; p=0.003) and furfuryl acetate (r=0.879; p=0.009).

It has been suggested that the fermentation process during coffee fruit harvesting could have a critical role in coffee brew sensory quality. In that case, where the fermentation process is not maintained during the coffee bean and post-harvesting step, the desired aldehyde and ketone compounds can quickly transform into alcohols. As a result, it can imbalance the coffee volatile compound composition (Preedy 2015). Isoamyl acetate, detected in HON_2 coffee sample has a specific fermented aroma and flavour, with potential brandy, overripe fruit notes (Toledo et al. 2016). In sensory analyses, panellists detected kombucha (non–alcoholic fermented fruit beverage) notes. Fermented flavour notes are associated with positive cup quality characteristics in this situation. The high final cup quality score was in line with the trend in specialty market – exploring the fermented and specific aroma notes (Sepúlveda et al. 2016).

Four compounds were only detected in specific coffee samples. The dihydro-2-methyl-3-furanone was only detected in the KEN_1 coffee sample, while 2-methoxy-4-vinylphenol was detected in HON_1 coffee sample. In coffee sample from Ethiopia 2-(methoxymethyl)furan and in coffee sample from Colombia 1-(2-furanyl)-ethenone was detected.

Toledo et al. (2016) confirmed that coffee furanone (dihydro-2-methyl-3-furanone) concentration has a strong association with final cup quality scores. All detected volatile compounds in KEN_1 is associated with positive specialty coffee characteristics (Steen et al. 2017). The ETH_1 coffee with the final cup quality score of 88.25 showed the highest concentration of furfuryl acetate, 2-furan methanol (fruity, floral aroma notes) and 2-methyl butyraldehyde,2-methyl-propanal (coffee-like, roasted aroma notes). None of the coffee samples had compounds associated with defective coffee quality attributes (phenolic, pungent, ashy aroma notes).

This approves that the specialty coffee high standards for green coffee beans limit the risk of damaged or unripe beans. Limiting coffee defects also excludes possible defective/unpleasant volatile phenolic compounds presence in the coffee brew, for example, 4-ethyl-2-methoxyphenol, 2-methylphenol (Steen et al. 2017; Giacalone et al. 2019).

Table 3.4 / 3*.4. tabula*

Volatile compounds mean area in different origin and differently roasted coffee brews / *Gaistošo savienojumu kompozīcija dažādu izcelsmes valstu un grauzdējuma kafijas dzērienos* (Laukaleja & Kruma 2019c)

Compounds / *Savienojumi*	**GC–MS peak area** / *GH-MS smaiļu laukums (x10⁶)*							**Aroma description** / *Aromāta īpašības*
	HON_1	KEN_1	COL_1	HON_2	ETH_1	HON_3	SAL_1	
1-(2-Furanylmethyl)-1h-pyrrole / *1-(2-Furanilmetil)-1h-pirols*	-	-	-	7.03a	7.85b	8.54c	7.60b	savoury, vegetables/ *dārzeņu*[a]
2.3 Pentanedione / *2,3 Pentanedions*	17.45 b	20.99c	23.37d	12.77a	26.01e	30.19f	26.27e	buttery/ *sviesta*[b]
5-Methyl-2-furancarboxaldehyde / *5-Metil-2-furānkarboksaldehīds*	48.05 b	40.48a	76.43e	51.62c	63.47d	97.23e	76.85f	red pepper/ *sarkanā pipara*[c]
2-Furanmethanol / *Furfurilspirts*	39.03c	37.86b	55.16 e	32.84a	49.48d	72.41 e	70.25f	floral/ *ziedu*[b]
Furfuryl acetate / *Furfurilacetāts*	38.76b	31.60a	93.11 e	-	78.38c	98.54f	83.26d	floral, fruity/ *ziedu, augļu*[e]
2-Methylbutanal / *2-Metilbutanāls*	14.94a	21.14b	36.07c	93.31 e	36.94c	93.31 e	39.43d	cacao, coffee–like/ *kakao, kafijas*[e]
2-Methylfuran / *2-Metilfurāns*	-	-	-	-	24.12	18.56	-	caramel/ *karameles*[b]
Furfural / *Furfurols*	**-**	10.80a	102.1e	64.53b	95.72c	133.03f	99.56d	sweet, almond/ *salds, mandeļu*[a]
2-Methylpropanal / *2-Metilpropanāls*	-	-	-	19.24	9.89	-	-	chocolate/ *šokolādes*[e]
Ethylpyrazine / *Etilpirazīns*	-	-	-	8.47	7.46	11.15	-	chocolate, nutty/ *šokolādes, riekstu*[a]
4-Methylpyrimidine / *4-Metilpirimidīns*	14.17	-	26.27	1.43	24.66	32.69	2.71	popcorn/ *popkorna*[c]

[a] Bressanello et al. (2017), [b]Lee, Kim, & Lee (2017), [c]Toledo et al. (2016), [d]Steen et al. (2017), [e]Piccino et al. (2014).
Different letters indicate statistically significant ($p<0.05$) differences between samples / *Vērtības atzīmētas ar atšķirīgiem burtiem rindās norāda uz būtiskām atšķirībām starp kafijas paraugiem (p<0.05)*

3.2.3. Assessment of phenolic compound composition and free radical scavenging activity in different origin and differently roasted coffee brews / *Fenolu savienojumu un antiradikālās aktivitātes novērtējums dažādu izcelsmes valstu un grauzdējuma kafijas dzērienos*

Significant differences for phenolic compounds were detected between different coffee roasteries (Fig. 3.3). It can be associated with different technical conditions in the roasting process and with the specific characteristics of each origin. The coffee samples from Roastery_1 was roasted at a lower temperature and for a shorter roasting time, which could confirm the phenolic compound sensitivity to temperature.

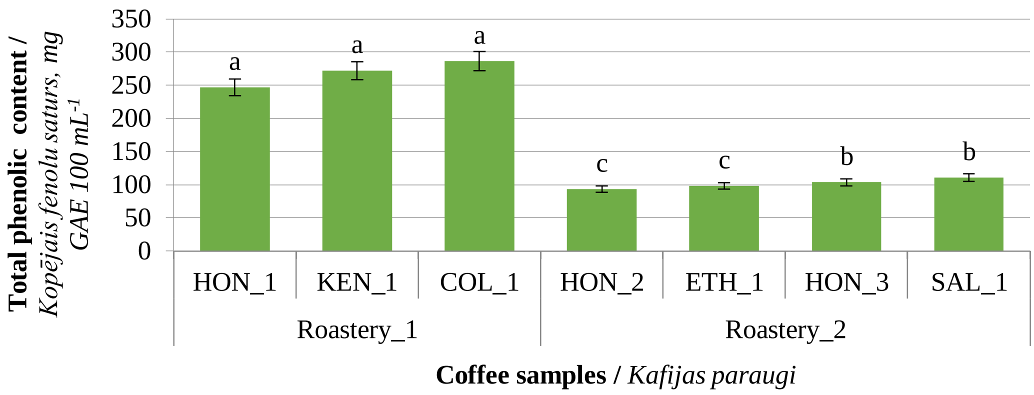


Fig. 3.3 Total phenolic content in different origin and differently roasted coffee brews / *3.3. att. Kopējais fenolu saturs dažādu izcelsmes valstu un grauzdējuma kafijas dzērienos*

Total flavonoid content in coffee brews showed a similar pattern (Fig. 3.4). The highest phenolic and flavonoid content were detected in COL_1, KEN_1 and HON_1 and the lowest in HON_2 and ETH_1.

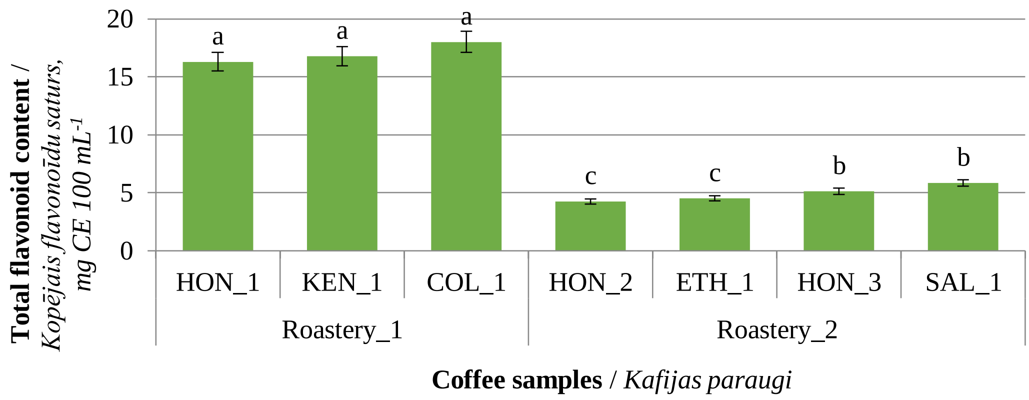


Fig. 3.4 Total flavonoid content in different origin and differently roasted coffee brews / *3.4. att. Kopējais flavonoīdu saturs dažādu izcelsmes valstu un grauzdējuma kafijas dzērienos*

From the volatile compounds profile, COL_1 showed a more balanced composition than HON_2. COL_1 volatile compound profile had a fruity and floral aroma, flavour notes from organic acids and phenolic acids. However, HON_2 dominated in higher nutty, chocolate flavour notes from furans.

It has been proven that between green coffee samples, the compositions of phenolic compounds are similar, but between roasted coffee samples, the phenolic compound composition can change significantly for various reasons, for example, roasting temperature, time, storage etc. (Somporn et al. 2011; Cheong et al. 2013), this can be one of the main reasons why results for high-quality coffees have significant differences between roasteries.

$ABTS^{•+}$ and $DPPH^{•}$ radical scavenging activity was significantly different between almost all coffee samples (Fig. 3.5). Interestingly, the data showed significant difference between COL_1 and HON_2 samples for $DPPH^{•}$ antiradical activity, while the same samples showed no significant differences for $ABTS^{•+}$ antiradical activity.

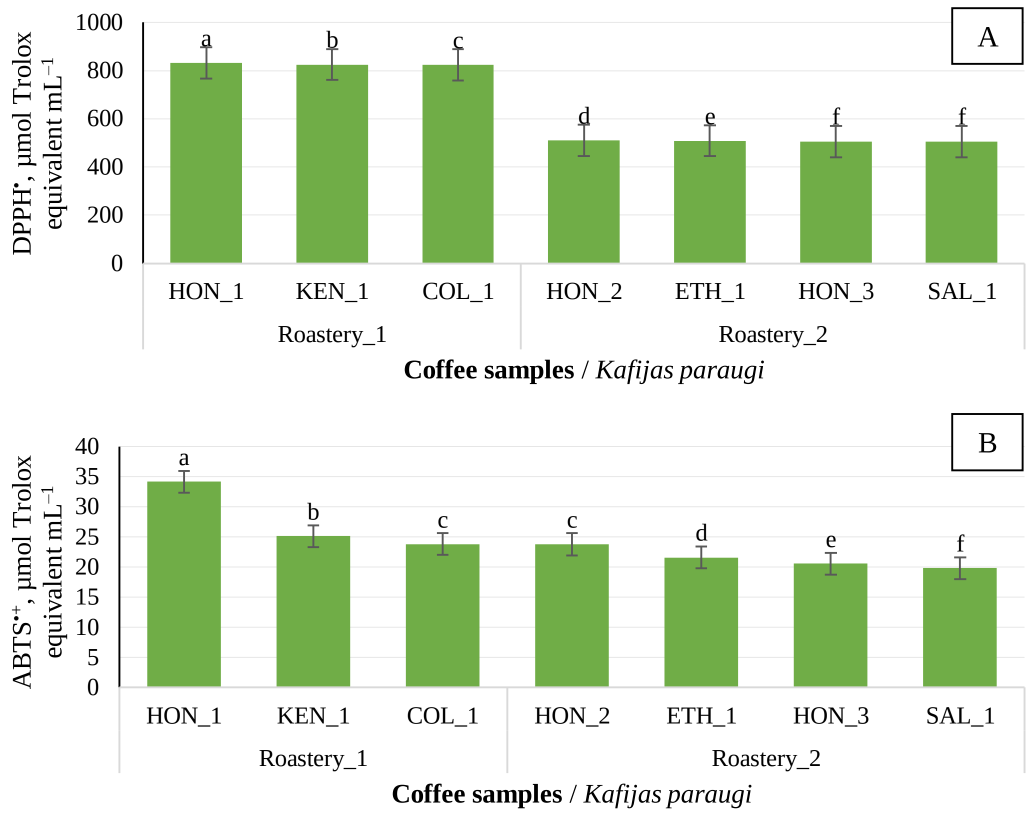


Fig. 3.5. $ABTS^{•+}$ (A) and $DPPH^{•}$ (B) radical scavenging activity in different origin and differently roasted coffee / *3.5. att. Dažādu izcelsmes valstu un grauzdējuma kafijas dzērienu antiradikālā aktivitāte pēc $ABTS^{•+}$ (A) un $DPPH^{•}$ (B)*

The HON_1 sample showed the highest $DPPH^{•}$ (832.44 µmol Trolox equivalent mL^{-1}) and $ABTS^{•+}$ (34.13 µmol Trolox equivalent mL^{-1}) values. The $ABTS^{•+}$ value was detected in SAL_1 sample (34.13 µmol Trolox equivalent mL^{-1}). Meanwhile both SAL_1 and HON_3 samples showed the lowest $DPPH^{•}$ value (505.20 µmol Trolox equivalent mL^{-1}).

3.2.4. Correlation between total phenolic content and cup quality in different origin and different roast level coffee / *Korelācija starp kafijas sensorās kvalitātes novērtējumu un kopējo fenolu saturu dažādu grauzdētavu kafijas dzērienos*

Surprisingly, when grouping coffee brews by roasteries, strong positive correlation was detected between final cup quality scores and total phenolic and flavonoid content in coffee brews from Roastery_1, and strong negative correlation was detected in coffee brews from Roastery_2 (Table 3.5). Only for Roastery_2 coffee brews significant negative correlation was detected between final cup quality scores and $ABTS^{\bullet+}$, $DPPH^{\bullet}$ radical scavenging activity.

Table 3.5 / *3.5. tabula*

Correlation between final cup quality scores and phenolic compound content in different roastery coffee brews / *Korelācija starp kafijas sensorās kvalitātes novērtējumu un kopējo fenolu saturu dažādu grauzdētavu kafijas dzērienos*

Roastery / *Grauzdētava*	**Pearson correlation** / *Pīrsona korelācija*	TPC	TF	$ABTS^{\bullet+}$	$DPPH^{\bullet}$
R_1_Final cup quality score / *R_1 Kafijas kvalitātes vērtējums*	coefficient (r) / *koeficients* (r)	**0.959**	**0.745**	0.464	0.464
	*Sig.2-tailed**	**<0.000**	**0.021**	0.208	0.208
R_2_Final cup quality score / *R_2 Kafijas kvalitātes vērtējums*	coefficient (r) / *koeficients* (r)	**-0.851**	**-0.879**	**-0.825**	**-0.951**
	*Sig.2-tailed**	**0.000**	**0.000**	**0.001**	**<0.000**

*Numbers in **bold** are significant at p<0.05 / *Vērtības* ***treknrakstā,*** *norādā uz būtisku korelāciju (p<0.05)*

The opposite correlations between two roasteries could suggest that roasting process parameters influence important chemical compound content in coffee brews differently. Roastery_1 coffee volatile compound profile is more balanced and focused on fruity and floral compounds, like furfuryl acetate, 2–furanmethanol, while Roastery_2 coffee volatile compounds profiles have a higher number of volatile compounds with roasted, chocolate notes, for example, 2–methylpropanal, 4-methylpyrimidine. The sensory results for Roastery_1 coffee sample showed minimal final cup quality score differences, while Roastery_2 had wider amplitude from 83 points to 90.25 points. These two results could suggest that it is possible to maintain high phenolic compound content in coffee brew if the composition of the volatile compounds is focused on specific aroma attributes like sweet and pleasant acidity of fruity, floral aroma, flavour notes.

The analysis of other studies about the phenolic content correlation with sensory results in coffee shows opposite results about cup quality and phenolic compound composition. In some research studies, phenolic compounds like 5-caffeoylquinic acid (5-CQA) and feruloylquinic acid (5-FQA) is associated with lower cup quality because of the bitterness (Fujioka & Shibamoto 2008). Frank et al. (2007) analysis of bitter-tasting compounds in roasted coffee states that 5-CQA is associated with coffee-like bitterness, caffeic acid with strong roasted coffee bitterness and only ferulic acid and trigonelline has an association with harshly strong bitterness. The phenolic compounds such as 2-methoxy-4-vinylphenol brings pleasant spicy, floral notes to coffee brew in low concentrations (Piccino et al. 2014). In low concentrations, 2-methoxy-4-vinylphenol was detected in Roastery_1 Kenya_1 coffee brew and its volatile compounds sensory descriptions match with the panellists compound sensory description. Moon & Shibamoto (2009) research states that phenolic compounds with a pleasant and fresh aroma, flavour notes as 2-methoxyphenol, chlorogenic acids and 2-methoxy-4-vinylphenol rapidly decreases after light roasting level. Still, caffeic acid, catechol increases with the roasting level bringing harsh bitterness to the coffee brew. Zanin et al. (2016) proved that it is possible to contain good cup quality without losing the valuable chlorogenic acid content. These studies suggest that individual phenolic compounds could affect the overall sensory characteristics of the coffee differently. These findings indicate that it is essential to determine individual phenolic content and analyse its correlation with the sensory assessment results.

Summary of 3.2. Phenolic and volatile compound composition influence on specialty coffee cup quality / *Kopsavilkums par 3.2. Fenolu un gaistošo savienojumu satura ietekme uz specialty kafijas sensoro kavlitāti*

The final cup quality score in sensory analysis varied from 83–90.25 points, with the highest score for HON_2 and the lowest for SAL_1. The volatile compound profile in Roastery_1 coffee was more balanced with compounds associated with fruity and floral notes, while Roastery_2 coffee volatile compounds profile had more compounds associated with chocolate, nutty, roasted aroma notes. The difference between the total phenolic, flavonoid content and antiradical scavenging activity in the roastery coffee sample also showed significant differences. A positive correlation was found between final cup quality scores and total phenolic, flavonoid content for Roastery_1 coffee brews and a negative correlation between final cup quality scores and total phenolic, flavonoid content and $ABTS^{\bullet+}$, $DPPH^{\bullet}$ radical scavenging activity for Roastery_2 coffee brews. The different correlations could be associated with specific phenolic compound presence in the coffee brew. These results indicate that the roastery-specific roasting process parameters could influence volatile compounds profile and the total and individual phenolic compound content. To better predict the roasting process's influence on the phenolic compound composition, it is crucial to analyse the specific roasting parameters and individual phenolic compounds with a correlation between volatile compounds.

Specialty kafijas sensorās kvalitātes novērtējuma rezultāti bija amplitūdā no 83 līdz 90.25 punktiem, ar lielāko punktu skaitu HON_2 un mazāko – SAL_1. Roastery_1 grauzdētavas kafijas paraugu gaistošo savienojumu profils uzrādīja pārsvarā savienojumus, kas asociējas ar augļu un ziedu aromātu, savukārt Roastery_2 grauzdētavas kafijas paraugu gaistošo savienojumu profilā bija vairāk savienojumu, kas asociēti ar šokolādes, riekstu, grauzdētu aromātu. Būtiskas atšķirības tika konstatētas starp kopējo fenolu, flavonoīdu saturu un antitradikālas aktivitātes rādītājiem abu grauzdētavu kafijas paraugos. Tika konstatēta pozitīva korelācija starp sensorās kvalitātes novērtējuma rādītājiem un kopējo fenolu, flavonoīdu saturu Roastery_1 kafijas paraugos un negatīva korelācija starp sensorās kvalitātes novērtējuma rādītājiem un kopējo fenola, flavonoīdu saturu un ABTS+•, DPPH• antitradikālo aktivitāti Roastery_2 kafijas paraugos. Pretējie korelācijas rādītāji var būt saistīti ar specifiskiem fenolu savienojumiem, kas atrodas kafijas dzērienos. Rezultāti apliecina, ka grauzdētavu izvēlētie grauzdēšanas parametri var ietekmēt gaistošo savienojumu profilu un kopējo, individuālo fenolu savienojumu saturu. Lai labāk izvērtētu grauzdēšanas procesa ietekmi uz fenolu savienojumu sastāvu un tā izmaiņām, ir būtiski izvērtēt konkrētu grauzdēšanas parametru un individuālo fenolu savienojumu sastāva korelācijas ar gaistošajiem savienojumiem.

3.3. The impact of the roasting process on chemical composition and sensory profile in specialty coffee / *Grauzdēšanas procesa ietekme uz ķīmisko sastāvu specialty kafijā*

The roasting process significantly impacts the sensory characteristics and biologically active compound content in coffee. It is crucial to understand the positive and negative effects of the roasting process on coffee's bioactive compound composition and sensory quality. The aim of research stage III was to evaluate the chemical composition changes in different roast level coffee samples.

3.3.1. Physical parameter analyses / *Fizikālo parametru analīze*

Moisture content ranged from 10.7% in green coffee and rapidly decreased to 3.0% in light roasted coffee, 2.2% in medium roasted, and 2.0% in dark roasted coffee (Table 3.6).

Table 3.6 / *3.6. tabula*

Moisture content and pH in different roast level coffee /
Mitruma saturs un pH dažāda grauzdējuma pakāpes kafijā

Parameters / *Parametri*	**Roast level** / *Grauzdējuma pakāpe*			
	Green coffee / *Zaļā kafija*	**Light** / *Viegls*	**Medium** / *Vidējs*	**Dark** / *Tumšs*
pH	5.58±0.04	5.00±0.03	5.17±0.02	5.30±0.02
Moisture / *Mitrums, %*	10.70±0.00	3.00±0.00	2.20±0.00	2.10±0.01

Moisture content in green coffee beans was in line with other studies and was under 11%, which is suggested to maintain the quality standards for specialty coffee (Borém et al. 2016; Tolessa et al. 2016). Some studies have linked moisture content with pH in coffee (Lee, Kim, & Lee 2017). **The pH** increased with the increased roast level, and these findings are consistent with Rao, Fuller, & Grim (2020) study. Tassew et al. (2021) suggest that the pH strongly correlates with acidity, body, and overall score of coffee quality. The aliphatic acid formation could determine the changes in pH from carbohydrate degradation during the roasting process. For example, formic acid and acetic acid are associated with lower pH in light roasted coffee (Ginz et al. 2000; Rao, Fuller, & Grim 2020).

3.3.2. Amino acid and fatty acid profile / *Aminoskābju un taukskābju kompozīcija kafijā*

The amino acid content in different roast levels of coffee is shown in Table 3.7. Among 17 amino acids, 13 showed the highest concentration in medium roasted coffee. Only serine and cysteine concentration decreased with increased roast level. Glutamic acid showed the highest concentration in all roast levels compared to other amino acids. There were no associations found between roast levels and amino acid concentration with Fisher's exact test. Although between several amino acids, strong correlations were observed, especially in medium roast level coffee. Arginine had a strong correlation with cysteine ($r=0.999$; $p<0.05$), glutamic acid with glycine ($r=1.000$; $p<0.05$).

Table 3.7 / *3.7. tabula*

Amino acid content in different roast level coffee beans /
Aminoskābju saturs dažāda grauzdējuma pakāpes kafijas pupiņas

Amino acids / *Aminoskābes*	**Amino acid content** / *Aminoskābju saturs, g 100 g^{-1}*			
	Green coffee / *Zaļā kafija*	**Light** / *Viegls*	**Medium** / *Vidējs*	**Dark** / *Tumšs*
Aspartic acid / *Asparagīnskābe*	0.85	0.68	**0.75**	0.69
Glutamic acid / *Glutamīnskābe*	1.99	1.84	**2.15**	2.11
Serine / *Serīns*	0.52	**0.31**	0.3	0.2
Glycine / *Glicīns*	0.65	0.58	**0.68**	0.67
Histidine / Histidīns	0.22	0.17	**0.19**	0.18
Arginine / *Arginīns*	0.6	0.1	**0.08**	0.06
Threonine / *Treonīns*	0.61	0.53	**0.59**	0.55
Alanine / *Alanīns*	0.46	0.43	**0.51**	**0.51**
Proline / *Prolīns*	0.57	0.51	0.59	**0.61**
Tyrosine / *Tirozīns*	0.32	0.28	**0.33**	**0.33**
Valine / *Valīns*	0.52	0.47	**0.53**	**0.53**
Methionine / *Metionīns*	0.14	0.14	**0.15**	**0.15**
Cysteine / *Cisteīns*	0.15	**0.06**	0.05	0.03
Isoleucine / *Izoleicīns*	0.34	0.31	**0.35**	**0.35**
Leucine / *Leicīns*	0.85	0.78	0.91	**0.92**
Phenylalanine / *Fenilalanīns*	0.52	0.47	**0.55**	**0.55**
Lysine / *Lizīns*	0.58	0.08	**0.09**	0.08

Numbers in **bold** indicate significant correlation between amino acid and roast level by Pearson correlation coefficient at significance level $p<0.05$ / *Vērtības, izceltas **treknrakstā,** norāda uz būtisku saistību starp aminoskābes saturu un grauzdešanas pakāpi pēc Pīrsona korelācijas pie būtiskuma līmeņa p<0.05*

Leucine strongly correlated with alanine, tyrosine, valine, methionine, isoleucine, and phenylalanine ($r=0.998$; $p<0.05$). Strong correlations were also detected between alanine, tyrosine, valine, methionine, isoleucine, phenylalanine ($r=1.000$; $p<0.05$). The roasting process did not show direct associations with the amino acid profile. In line with previous studies, glutamic and aspartic acids are the dominant amino acids in roasted coffee (Bressanello et al. 2017). However, the present study did not confirm the previously reported rapid degradation of amino acids with increased roast levels (Guenther et al. 2007; Wei et al. 2017a). Only arginine and serine showed a high decrease during the roasting process, according to Moreira et al. (2012).

Fatty acid content was significantly affected by roast level. It can be seen in Fig. 3.6. that saturated fatty acid, monounsaturated fatty acid, and polyunsaturated fatty acid content were the highest in medium roasted coffee and the lowest in the light roasted coffee. This outcome is contrary to Speer & Kölling-Speer (2006) and Oestreich-Janzen (2014) who found that no significant differences have been detected between fatty acid content and roast levels. However, the changes in fatty acid profile are in line with Lee, Kim & Lee (2017). As a result of pressure change inside coffee bean cell walls, the fatty acids shift with increased roast level to the outer layer of coffee bean (Sridevi, Giridhar, & Ravishankar 2011).

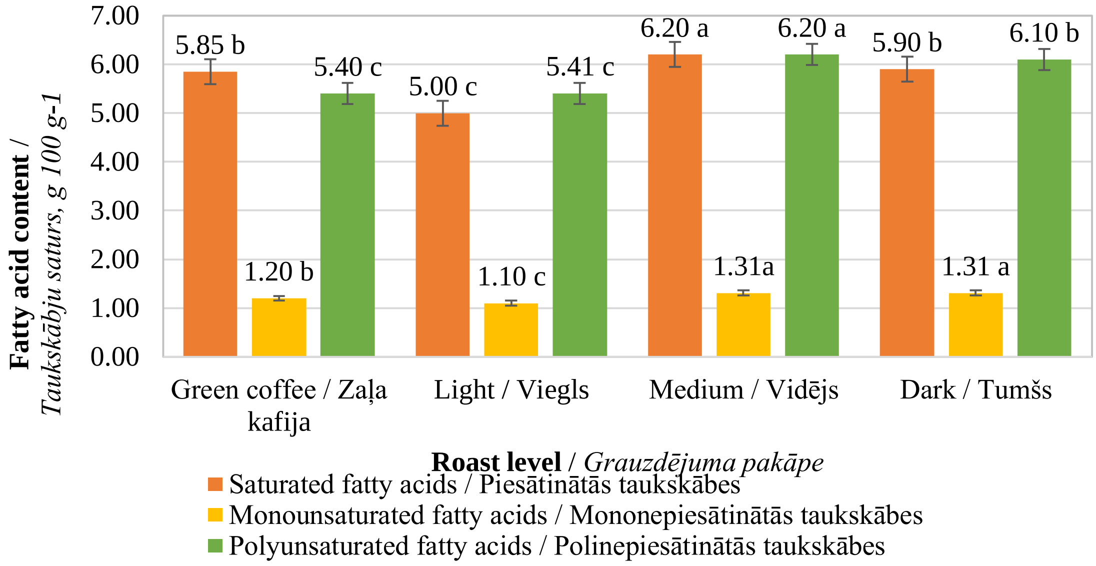


Fig 3.6. Fatty acid content in different roast level coffee beans /
3.6. att. Taukskābju sastāvs dažāda grauzdējuma pakāpes kafijas pupiņās

Different letters (a, b, c) within each fatty acid group indicate the statistically significant difference between roast levels ($p<0.05$) / *Vērtības, atzīmētas ar atšķirīgiem burtiem (a,b,c) pie katras taukskābes, norāda būtiskas atšķirības starp grauzdēšanas pakāpēm ($p<0.05$)*

These reports could explain why the fatty acid content changes have been only detected 2-3 months after the roasting. The fatty acids on the outer layer of coffee beans are exposed to oxidation, which is the leading cause of decreasing fatty acid content in roasted coffee (Toci et al. 2013).

3.3.3. Phenolic compound content analysis in different roast level coffee brew / *Fenolu savienojumu sastāva analīze dažāda grauzdējuma pakāpes kafijas dzērienā*

The highest **total phenolic and flavonoid content** was found in light roasted coffee (292.85 mg GAE 100 mL^{-1} and 18.26 mg CE 100 mL^{-1} respectively) and the lowest in dark roast coffee (246.17 mg GAE 100 mL^{-1}; 15.79 mg CE 100 mL^{-1}) (Table 3.8).

Table 3.8 / *3.8. tabula*

Total phenolic and flavonoid content in different roast level coffee brew /
Kopējo fenolu un flavonoīdu sastāvs dažāda grauzdējuma pakāpes kafijas dzērienā

Roast Level / *Grauzdējuma pakāpe*	**TPC (mg GAE 100 mL^{-1}) ±SD**	**TF (mg CE 100 mL^{-1}) ±SD**
Light / *Viegls*	292.85±0.04 a	18.26±0.21 a
Medium / *Vidējs*	265.30±0.08 b	16.69±0.23 b
Dark / *Tumšs*	246.17±0.02 c	15.79±0.25 c
p value / *p vērtība*	<0.0001	<0.0001

Different letters in column indicate statistically significant differences between roast levels / *Vērtības, atzīmētas ar atšķirīgiem burtiem kolonās, norāda uz būtiskām atšķirībām starp grauzdēšanas pakāpēm ($p<0.05$)*

Individual phenolic compound content is illustrated in Table 3.9. The highest concentration irrespective of the roast level showed 3.5-dihydroxybenzoic acid and chlorogenic acid, although their concentration decreased most rapidly. For example, the chlorogenic acid concentration decreased from 117.54 mg mL^{-1} in the light roasted coffee to 53.0 mg mL^{-1} in the dark roasted coffee. Only sinapic and 4-hydroxybenzoic acid increased with the increased roast level.

Table 3.9 */ 3.9 tabula*

Individual phenolic compound concentration in different roast level coffee brew / *Atsevišķo fenolu savienojumu koncentrācija dažāda grauzdējuma pakāpes kafijas dzērienā*

Coffee sample / *Kafijas paraugi*	**Individual phenol concentration ± standard deviations** / *Atsevišķo fenolu koncentrācija un ± standarda novirze, mg 100 mL^{-1}*		
	Light / *Viegls*	**Medium** / *Vidējs*	**Dark** / *Tumšs*
Gallic acid / *Gallu skābe*	0.02±0.03b	0.07±0.00a	0.07±0.00a
3,5-Dihydroxybenzoic acid / *3,5-Dihidroksibenzoskābe*	217.24±0.96a	182.68±0.63b	114.81±0.45c
Catechin / Katehīns	2.54±0.19a	2.62±0.10a	1.91±0.14b
4-hydroxybenzoic acid / *4-Hidroksibenzoskābe*	1.95±0.04c	2.92±0.02b	3.66±0.08a
Chlorogenic acid / *Hlorogēnskābe*	117.54±3.41a	96.00±1.12b	53.50±1.62c
Caffeic acid / *Kafijskābe*	1.34±0.88c	2.14±0.09a	1.82±0.00b
Epicatechin / *Epikatehīns*	0.19±0.00	-	-
Vanillin / *Vanilīns*	0.18±0.03a	0.15±0.00b	0.08±0.00b
P-coumaric acid / p-*kumarskābe*	0.04±0.01a	0.01±0.00b	0.01±0.00b
Sinapic acid / *Sinapīnskābe*	0.85±1.21b	2.07±0.02ab	2.46±0.01a
Ferulic acid / *Ferulīnskābe*	0.05±0.00b	0.06±0.00a	0.06±0.00a
2-Hydroxycinnamic acid / *2-Hidroksikanēļskābe*	0.06±0.02a	0.03±0.00b	0.02±0.00b
Rutin / *Rutīns*	9.70±0.32a	7.40±0.22b	3.37±0.31c
Luteolin / *Luteolīns*	0.72±0.50a	0.36±0.00b	0.34±0.01b

Different letters (a, b, c) within a row indicate the statistically significant difference between coffee samples ($p < 0.05$) / *Vērtības, atzīmētas ar atšķirīgiem burtiem (a,b,c) rindās, norāda būtiskas atšķirības starp kafijas paraugiem (p < 0.05)*

The decreasing individual phenolic acid and flavonoid compound content with increasing roast level confirmed the phenolic compound degradation process with increasing roast temperature and time (Coelho et al. 2014; Kwak, Ji, & Jeong 2017). According to previous literature the most abundant phenolic compounds in coffee are chlorogenic and 3.5-dihydroxybenzoic acids. Moreira et al. (2012) have suggested that these two compounds could be responsible for coffee melanoidin formation. Although only chlorogenic acid has been associated with potential antioxidative activity in coffee, even if 3.5-dihydroxybenzoic acid content is higher Alcalde, Granados, & Saurina (2019).

The rapid chlorogenic acid content decrease with increasing roast level could be explained by several chemical reactions during roasting process. From chlorogenic acid thermal degradation caffeic acid is slowly released. The caffeic acid content increases with chlorogenic acid decrement and it is in line with previous studies (Frank et al. 2007; Kamiyama et al. 2015). Budryn et al. (2015) and Farah et al. (2005) reported rapid degradation of chlorogenic acid after light roast level and increased chlorogenic acid lactone concentration.

3.3.4. Volatile compound profile in different roast level coffee / *Gaistošo savienojumu sastāvs dažāda grauzdējuma pakāpes kafijā*

All roast levels, 41 compounds from eight chemical classes were detected. Furan compounds in all roast levels had the highest mean peak area percentage, compared to other chemical classes (Fig. 3.7).

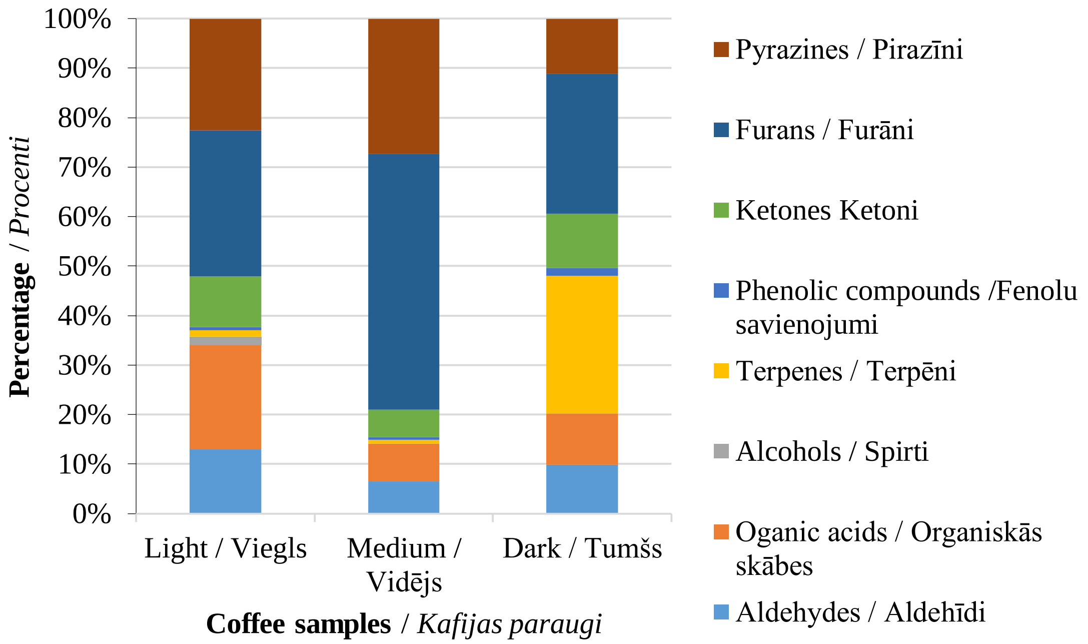


Fig. 3.7. Profile of the volatile compound chemical classes in different roast level coffee / *3.7. att. Gaistošo savienojumu sastāvs pēc to ķīmiskajām klasēm dažāda grauzdējuma pakāpes kafijā*

Light roast coffee showed the highest aldehyde, organic acid, and alcohol content. In contrast, medium roasted coffee showed the highest pyrazine and furan content, and dark roast coffee – the highest terpene, phenolic acid, and ketone content. Furans are the main volatile compounds in roasted coffee and are formed from Maillard reaction (Petisca et al. 2012; Cordoba et al. 2019), which can explain the high percentage of furans in all roasted levels.

The volatile phenolic compound content increased in dark roast level can be due to phenolic compound degradation. For example, caffeic acid due to degradation in dark roasted coffee transforms into volatile phenolic compounds such as 2-methoxy-4-vinylphenol.

Organic acids are sensitive to roasting process and their concentration decreases rapidly with increasing roast level. Ginz et al. (2000) suggest that organic acids content is significantly lost, after roasting temperature reach 210 °C (Jham et al. 2007; Wan Kamarul Zaman, Loh, & Mohd Esa 2019).

3.3.5. Acrylamide content in different roast level coffee / *Akrilamīda koncentrācija dažāda grauzdējuma pakāpes kafijā*

The acrylamide content at first showed increasing trend with roast level (Fig.3.8.), although it reached the peak value in medium roasted coffee (310 µg kg^{-1}) and then rapidly decreased in dark roasted coffee (260 µg kg^{-1}). In this study acrylamide content was lower than Regulation (EU) No 2158/2017 benchmark levels for the presence of acrylamide in roasted coffee (400 µg kg^{-1}).[12]

It has been suggested that acrylamide is formed from reducing carbohydrates and asparagine during Maillard reaction. However, there was no correlation found between aspartic acid (asparagine) and acrylamide content in coffee (Bagdonaite, Derler, & Murkovic 2008; Bertuzzi et al. 2020).

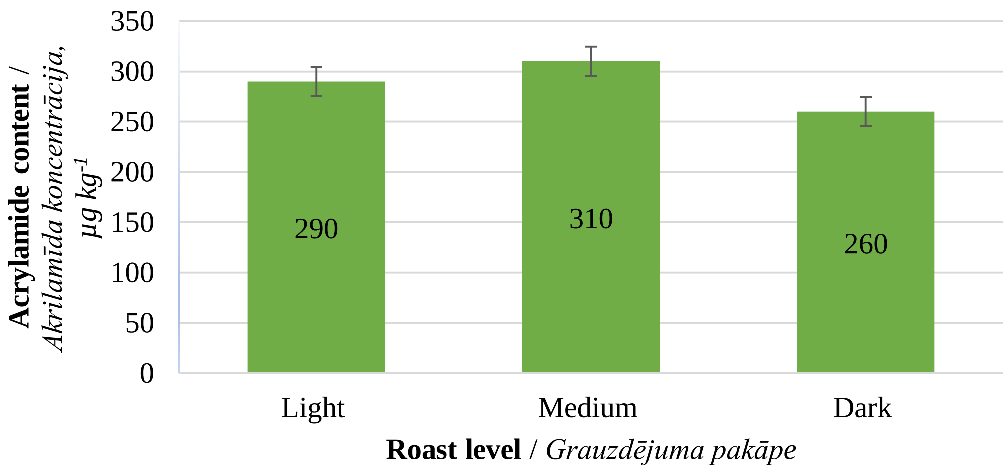


Fig. 3.8. Acrylamide content in different roast level coffee /
3.8. att. Akrilamīda koncentrācija dažāda grauzdējuma pakāpes kafijā

Alternative acrylamide formation has been reported by Guenther et al. (2007). Acrylamide could be formed through amino-dihydroxylation or pyrolytic reactions. Serine and cysteine could convert pyruvic acid to lactic acid and generate acrylamide in these reactions. This could be one of the possible explanations for acrylamide formation in the present study, because the serine and cysteine content has negative correlation with acrylamide content. Scientific opinions vary about the peak point of acrylamide content decrease, whereas roasting temperature parameters varies by the used roasting machine in specific studies and the batch size. The time and temperature ratio could be the potential markers for detecting the peak point. For example, Bagdonaite & Murkovic (2004) reported the highest acrylamide content at 220 °C for five minutes and 240 °C for five minutes of roasting while roasting at the same temperature for the same temperature 10 to 15 minutes, the acrylamide content decreased. Another study showed the highest acrylamide peak point after 10 minutes of roasting at 175–177 °C and a rapid decrease after 14 minutes of roasting at 203–205 °C (Bertuzzi et al. 2020). It can be seen from the previous studies that the highest acrylamide content was detected after the "first crack" when the deeper bean cells with potential acrylamide precursors are exposed to the heat

[12] Official Journal of the European Union (2017) Commission Regulation (EU) 2158/2017 [online] [viewed on 20. January 2022] Retrieved from https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32017R2158&from=EN

(Bagdonaite & Murkovic 2004; Oestreich-Janzen 2014; Bertuzzi et al. 2020; Endeshaw & Belay 2020).

Summary of 3.3. The impact of the roasting process on chemical composition and sensory profile in specialty coffee from Colombia / *Kopsavilkums par 3.3. Grauzdēšanas procesa ietekme uz ķīmisko sastāvu specialty kafijā no Kolumbijas*

The highest total and individual phenolic and flavonoid content was found in light roasted coffee (291.85 mg GAE 100 mL^{-1}; 18.26 mg CE 100 mL^{-1}) and it decreased with increased roast level. From volatile compound point of view, the light roasted coffee had higher content of volatiles associated with fruity, creamy, and caramelised aroma, flavour characteristics, while the dark roast coffee had higher content of volatiles such as phenolic acids which are associated with smoky, burnt aroma and flavour characteristics. Dark roast coffee had the lowest acrylamide concentration, organic acid content, and the highest pH in coffee brew, which would be more suitable for coffee consumers with gastro esophageal reflux symptoms.

Vislielākais kopējo un individuālo fenola un flavonoīdu saturs tika konstatēts viegli grauzdētā kafijā (291,85 mg GAE 100 mL^{-1}; 18,26 mg 100 mL^{-1}), un to saturs samazinājās palielinoties grauzdējuma pakāpei. Viegli grauzdētā kafijā bija būtiski vairāk gaistošo savienojumu, kuriem raksturīgas augļu, karameles aromāta un garšas īpašības. Savukārt tumši grauzdētajā kafijā bija vairāk gaistošo savienojumu, piemēram, 2-metoksifenols, kas saistīts ar dūmu, piedeguma aromātu. Tumši grauzdētajā kafijai bija zemākā akrilamīda koncentrācija, organisko skābju un lielāks pH. Viegli grauzdēta kafija būtu piemērota specialty kafijas patērētājiem, kuri novērtē sensorās īpašības, kas tiek izceltas grauzdēšanas laikā, taču kafijas patērētājiem ar gastroezofageālā refluksa simptomiem piemērotāka būtu tumši grauzdēta kafija.

3.4. Aroma-active compound perception in different roast and brew coffee by gas chromatography-olfactometry / *Dažādi grauzdētas un pagatavotas kafijas aromātveidojošo savienojumu uztveres izvērtējums, izmantojot gāzu hromatogrāfiju-olfaktometriju*

Gas-chromatography-olfactometry (GC-O) method allows detecting and describing volatile compound associated aromas. Although coffee has been studied profusely by GC-O, there is a limited research on aroma-active compound perception in different roast and brew coffee. The aim of research stage IV was to form a chromatography-olfactometry vocabulary and evaluate aroma-active compound perception in differently roasted and brewed coffee samples.

3.4.1. Gas chromatography-olfactometry (GC-O) vocabulary / *Gāzu hromatogrāfijas-olfaktometrijas (GC-O) vārdnīcas izveide*

From detected 56 volatile compounds (Appendix 1), 30 were reported as aroma-active compounds. The olfactory panellists could identify 23 different aromas. Aroma profile, frequency of detection, and associated volatiles for different roast and brew coffee samples is summarised in Appendix 2.

The aroma attribute frequencies within coffee samples is illustrated in Fig. 3.9, the most frequent attributes were sweet, musty, leather, skunky, burnt, and nutty (identified 7–15 times).

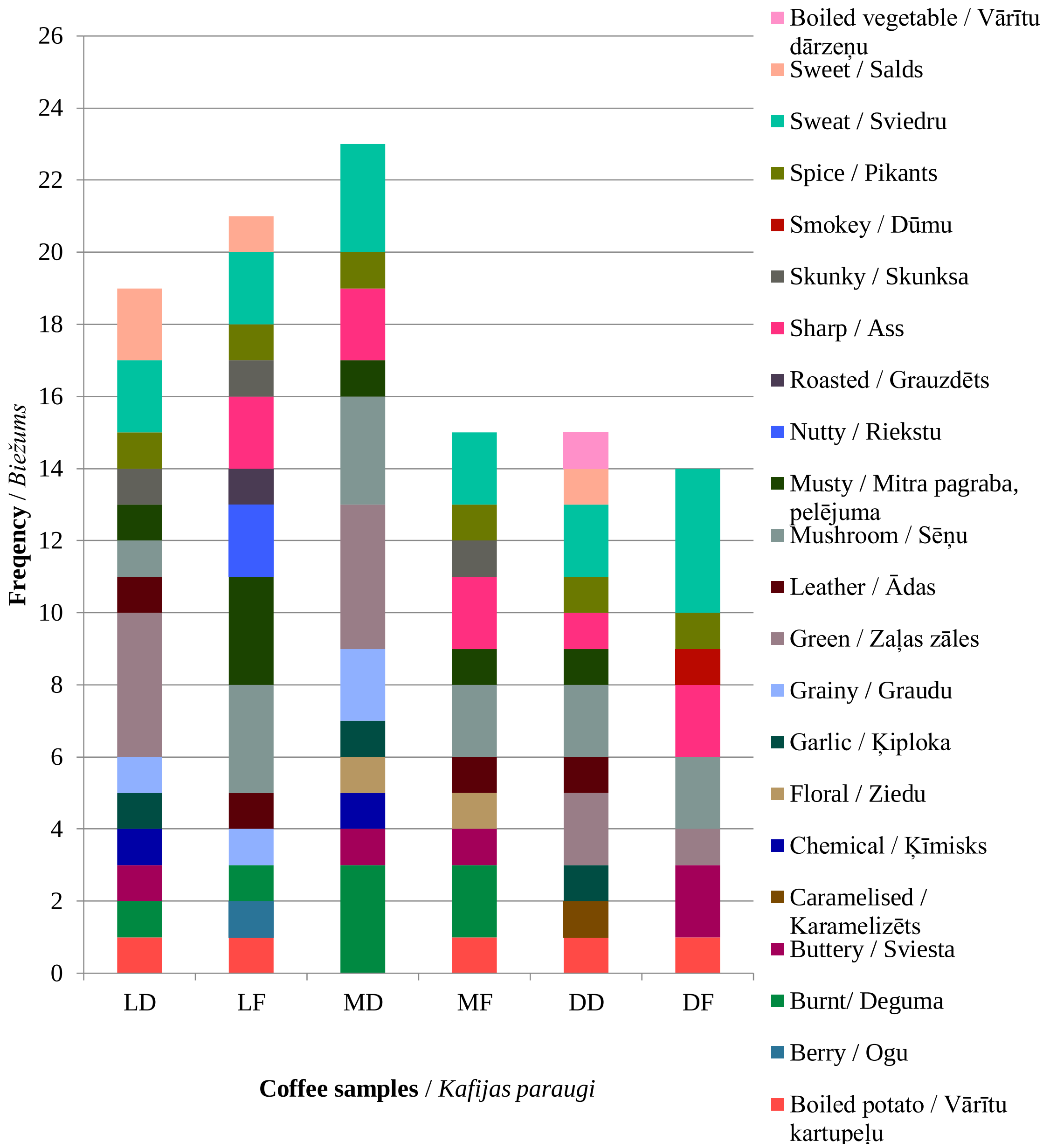


Fig. 3.9. Aroma attribute frequency within coffee samples /
3.9. att. Aromātu īpašību biežums kafijas paraugos

Sample codes: The first letter represents the roast level (L–light; M–medium; D–dark); the second letter represents the brewing technique (D–automatic drip; F–French press) / *Kafijas paraugu kodi: Pirmais burts apzīmē grauzdēšanas pakāpi (L–viegls; M–vidējs; D–tumšs); otrs burts apzīmē pagatavošanas metodi (D–automātiskā filtra; F–franču preses).*

By Pearson's chi-squared test no significant differences between aroma attribute frequencies and coffee samples were found, although significant differences were detected between aroma-active compounds and aroma attributes.

Most frequent aroma attributes associated with volatiles in differently roast level and brew coffee samples are described in olfactometry vocabulary in Table 3.10. Sweet, the most frequent attribute, was linked with six different volatile compounds.

Benzene acetaldehyde (**7**) was associated with sweet aroma in all roast levels samples, except in the light French sample, where it was associated with a sharp, sweet aroma.

Table 3.10 */ 3.10 tabula*

Olfactometry vocabulary of aroma-active compound perception in different roast and brew coffee / *Dažādi grauzdētas un pagatavotas kafijas aromātveidojošo savienojumu uztveres olfaktometrijas vārdnīca* (Laukaleja & Koppel 2021)

Aroma Attribute / *Aromātu īpašības*	**Coffee sample** / *Kafijas paraugi**	**Volatile compounds associated with the aroma /** *Gaistošie savienojumi*
Sweet / *Salds*	LD	3-furanmethanol / *3-furānmetanols* (**23**); benzeneacetaldehyde / *fenilacetaldehīds* (**7**)
	LF	benzeneacetaldehyde / *fenilacetaldehīds* (**7**); 1-(6-methyl-2-pyrazinyl)-1-ethanone / *1-(6-metil-2-pirazinil)-1-etanons* (**37**)
	MD	3-furanmethanol / *3-furānmetanols* (**23**); 2-ethyl-6-methylpyrazine / *2-etil-6-metilpirazīns* (**42**); benzeneacetaldehyde / *fenilacetaldehīds* (**7**)
	MF	3-furanmethanol / *3-furānmetanols* (**23**); 1-(2-furanyl)-2-butanone / *1-(2-furanil)-2-butanons* (**29**)
	DD	benzeneacetaldehyde / *fenilacetaldehīds* (**7**); nonanal / *nonanāls* (**11**)
	DF	3-furanmethanol / *3-furānmetanols* (**23**); benzeneacetaldehyde / *fenilacetaldehīds* (**7**); 1,2-dihydrolinalool / *1,2-dihidrolinalols* (**53**); 4-ethyl-2-methoxyphenol / *4-etilguaiacols* (**35**)
Musty / *Mitra pagraba, pelējuma*	LD	methylpyrazine / *metilpirazīns* (**44**)
	LF	2,6-dimethylprazine / *2,6-dimetilprazīns* (**39**); 2-ethyl-3-methylpyrazine / *2-etil-3-metilpirazīns* (**40**); 2,3-diethyl-5-methylpyrazine / *2,3-dietil-5-metilpirazīns* (**38**)
	MD	2,2'-methylenebisfuran / *2,2'-metilēnbisfurāns* (**18**); nonanal / *nonanāls* (**11**); tetradecane / *tetradekāns* (**12**)
	MF	3-ethyl-2,5-dimethylpyrazine / *3-etil-2,5-dimetilpirazīns* (**45**); tetradecane / *tetradekāns* (**12**)
	DD	methylpyrazine / *metilpirazīns* (**44**); 2-(2-furanylmethyl)-5-methylfuran / *2-(2-furanilmetil)-5-metilfurāns* (**16**)
	DF	1-(2-Furanyl)-ethanone / *1-(2-Furanil)-etanons* (**30**); 2,2'-methylenebisfuran / *2,2'-metilēnbisfurāns* (**18**)
Leather / *Ādas*	LD	2,3-diethyl-5-methylpyrazine / *2,3-dietil-5-metilpirazīns* (**38**); 2-n-heptylfuran / *2-n-heptilfurāns* (**22**); 4-hydroxy-2-methylacetophenone / *4-hidroksi-2-metilacetofenons* (**36**); 1-dodecanol / *1-dodekanols* (**56**)
	MD	3-ethyl-2,5-dimethylpyrazine / *3-etil-2,5-dimetilpirazīns* (**45**); 1-(1H-pyrrol-2-yl)-ethanone / *1-(1H-pirol-2-il)-etanons* (**28**); 2-n-heptylfuran (**22**); 1-dodecanol / *1-dodekanols* (**56**)
	DD	1-(1H-pyrrol-2-yl)-ethanone / *1-(1H-pirol-2-il)-etanons* (**28**); 2-n-heptylfuran / *2-n-heptilfurāns* (**22**)
	DF	1-(1H-pyrrol-2-yl)-ethanone / *1-(1H-pirol-2-il)-etanons* (**28**)

Continued Table 3.10 / *3.10. tabulas turpinājums*

Aroma Attribute / *Aromātu īpašības*	**Coffee sample /** *Kafijas paraugi**	**Volatile compounds associated with the aroma /** *Gaistošie savienojumi*
Skunky / *Skunksa*	LF	methylpyrazine / *metilpirazīns* (**44**); n-(2-cyanoethyl)-pyrrole / *n-(2-ciānetil)-pirols* (**51**)
	MD	2-methylbutanal / *2-metilbutanāls* (**2**); methylpyrazine / *metilpirazīns* (**44**)
	MF	
	DD	methylpyrazine / *metilpirazīns* (**44**)
	DF	2-methylbutanal / *2-metilbutanāls* (**2**); methylpyrazine / *metilpirazīns* (**44**)
Burnt / *Deguma*	LD	tetradecane / *tetradekāns* (**12**)
	LF	2-methylbutanal / *2-metilbutanāls* (**2**)
	MD	2-methylbutanal / *2-metilbutanāls* (**2**); nonanal / *nonanāls* (**11**); 4-hydroxy-2-methylacetophenone / *4-hidroksi-2-metilacetofenons* (**36**)
	MF	2-methylbutanal / *2-metilbutanāls* (**2**); 4-hydroxy-2-methylacetophenone / *4-hidroksi-2-metilacetofenons* (**36**)
Nutty / *Riekstu*	LD	1-(2-furanylmethyl)-1H-pyrrole / *1-(2-furanilmetil)-1H-pirols* (**48**)
	LF	1-butanol, 3-methyl-acetate / *izoamilacetāts* (**13**); 2,6-dimethylprazine / *2,6-dimetilprazīns* (**39**); 2-ethyl-3-methylpyrazine / *2-etil-3-metilpirazīns* (**40**)
	MD	2-(2-furanylmethyl)-5-methylfuran / *2-(2-furanilmetil)-5-metilfurāns* (**16**)
	MF	nonanal / *nonanāls* (**11**)
	DD	1-(2-furanylmethyl)-1H-pyrrole / *1-(2-furanilmetil)-1H-pirols* (**48**)

* Sample codes: The first letter represents the roast level (L–light; M–medium; D–dark); the second letter represents the brewing technique (D–automatic drip; F–French press) / *Kafijas paraugu kodi: Pirmais burts apzīmē grauzdēšanas pakāpi (L–viegls; M–vidējs; D–tumšs); otrs burts apzīmē pagatavošanas metodi (D–automātiskā filtra; F–franču preses).*

*** The numbers in bold represent volatile compound in line with Appendix 1 / Skaitļi izcelti treknrakstā apzīmē gaistošo savienojumu saskaņā ar 1. pielikumu.*

The benzeneacetaldehyde (**7**) has been associated with sweet, fruity aroma in previous publications, (Qin et al. 2011; Chen, Chiang, & Chung 2019). In light, medium drip coffee and medium, dark French press coffee samples 3-furanmethanol (**23**) was associated with sweet aroma, while in previous studies 3-furanmethanol (**23**) has not been identified as an aroma-active compound. In dark French coffee two different aroma-active compounds were detected, apart from benzeneacetaldehyde (**7**) and 3-furanmethanol (**23**), (1,2-dihydrolinalool (**53**); 4-ethyl-2-methoxyphenol (**35**)).

Musty aroma attribute was associated with ten different volatile compounds. Interestingly, musty aroma has been linked with ketones and sulphur containing compounds, while in the present study they are associated with pyrazines (Mayuoni-Kirshinbaum et al. 2012; Laukaleja & Koppel 2021; Pinsuwan et al. 2022). Methylpyrazine (**44**) was detected and associated with musty aroma in light and dark drip coffee. Musty aroma in Light French coffee was associated with 2,3-diethyl-5-methylpyrazine (**38**) 2,6-dimethylprazine (**39**), 2-ethyl-3-methylpyrazine (**40**), while medium French coffee associated 2,3-diethyl-5-methylpyrazine (**45**) with musty aroma.

The leather aroma was detected 11 times in coffee samples and was associated with 7 aroma-active compounds.

In dark roast coffee samples 1-(1H-pyrrol-2-yl)-ethanone (**28**) was associated with leather aroma, while in drip coffee samples – 2-n-heptylfuran (**22**) and 4-hydroxy-2-methylacetophenone (**36**). In previous studies leather aroma has been associated with volatile compounds in wines or herbs but rarely in coffee (Falcão et al. 2008; Sánchez-Palomo et al. 2017). The 2-n-heptylfuran (**22**) has been identified in espresso coffee samples as a coffee aroma quality marker (Greco et al. 2021) and 3-ethyl-2,5-dimethylpyrazine (**32**) has been reported to have chocolate and nutty aroma in roasted coffee samples (López-Galilea et al. 2006).

Skunky aroma was detected nine times by the panellists and were associated with four aroma-active compounds. The methylpyrazine (**44**) and 2-methylbutanal (**2**) volatiles were associated with skunky aroma in almost all samples. In previous studies skunky aroma has been associated with thiols, for example, 3-methyl-2-butene-1-thiol (Fors 1983; Delahunty, Eyres, & Dufour 2006; Dulsat-Serra, Quintanilla-Casas, & Vichi 2016).

Burnt and Nutty aroma attributes were detected seven times. The burnt aroma was associated with four aroma-active compounds. The nutty aroma was associated with six aroma-active compounds. In light French coffee the nutty aroma was to most frequent and associated with three different aroma-active compounds (2,6-dimethylprazine (**39**), 2-ethyl-3-methylpyrazine (**40**), 1-butanol, 3-methyl-acetate (**13**)). These volatiles have associated with nutty and roasted aroma in Caporaso et al. (2018) study.

Aroma attributes such as floral, berry were only detected 1–2 times and only in light medium coffee samples. It is important to understand that volatile compound associated aroma can be impacted by the concentration of it and it could be one of the reasons why in this study perceived volatile compound aromas are different with previous studies. Nonanal (**11**) has been associated with nutty, musty smoky aroma, while in previous studies nonanal (**11**) was described with waxy and smoky aroma (Akiyama et al. 2007; Piccino et al. 2014). Laukaleja & Koppel (2021) has mentioned that not only the concentration and roast level but also the specific food product could impact the aroma-active compound perception. For example, Chin, Eyres, & Marriott (2011) in their study about Merlot wine volatile profile associated nonanal with strong fatty aroma, meanwhile Xia et al. (2015) in soymilk aromatic lexicon linked nonanal with peanut, beany aroma.

3.4.2. Principal component analysis / *Galveno komponentu analīze*

Principal Component Analysis (PCA) illustrates (Fig. 3.10) the roasting and brewing process impact on the volatile and aroma active compound content, and GC-O aroma frequencies. The first two principal components explained 59.19 % (36.49 % and 22.69 %, respectively) variation in the data. The first principal component separated the samples by the roast levels, while the second component separated the samples based on the brewing technique. The first principal component samples were characterised by volatile such as 5-methyl-2-furancarboxaldehyde **(5)**, dodecanal **(9)**, 2,2’-methylenebisfuran acetate **(21)**, 1-(2-furanyl)-2-butanone **(29)**, 2,6-dimethylprazine **(39)**, methylpyrazine **(44)**, 4-amino-2-methoxypyrimidine **(47)**, and also with GC-O aromas such as sweet, nutty, vegetable, waxy, spice, smoky.

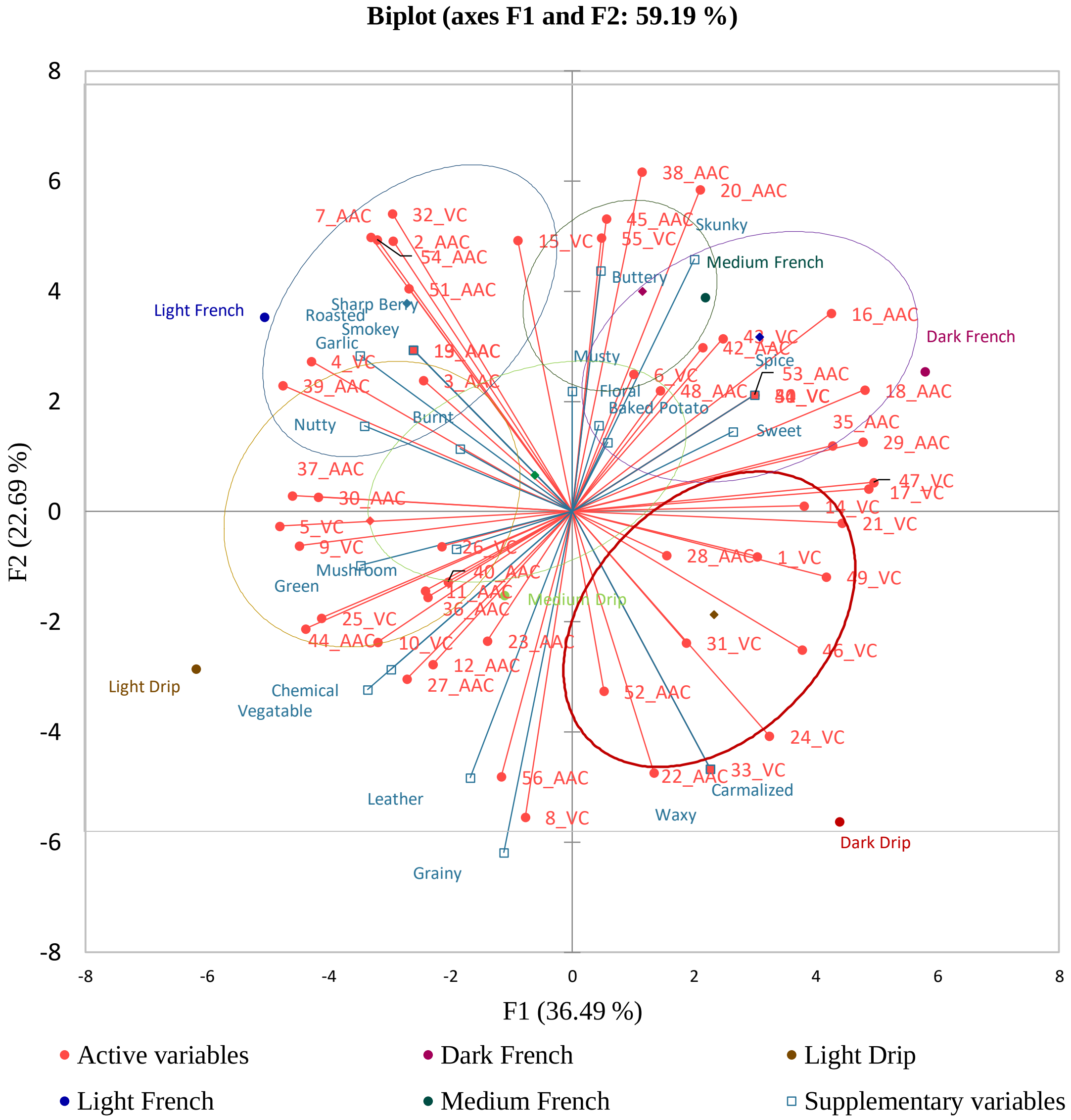


Fig. 3.10. Scatter plot of PCA scores associated with volatile compounds (VC), aroma-active compounds (AAC) and aroma attributes /
3.10. att. Izkliedes diagramma, kas ilustrē galveno komponenšu analīzes vērtējumu asociācijas ar gaistošajiems avienojumiem (VC), aromātu veidojošiem savienojumiem (AAC) un aromāta īpašībām

The second principal component samples were characterised by 2-[(methyldithio)methyl]-furan (**20**), 2,3-diethyl-5-methylpyrazine (**38**), dimethyl trisulfide (**52**), 1-dodecanol (**56**) volatile compounds and GC-O aromas such as grainy, leather, musty, skunky, buttery aromas.

Dark roast drip coffee had a stronger correlation with volatile compounds that were not found aroma-active. Compounds such as 2,2'-[oxybis(methylene)] bisfuran (**17**), 2-furanmethanol, acetate (**21**), 4-amino-2-methoxypyrimidine (**47**) were not identified as aroma-active, although, they have proven a positive correlation with roast level and a negative correlation with sensory quality. In the present study 2'-[oxybis(methylene)]bisfuran (**17**) concentration increases with the roast level, and in previous studies showed that higher 2'-[oxybis(methylene)]bisfuran (**17**) concentration associated with common roast defects (Yang et al. 2016; Laukaleja & Kruma 2019b).

Studies report that the sharp aroma attributes found in dark roasted coffees are associated with pyrrole compounds (Moon & Shibamoto 2009; Cordoba et al. 2019). Both pyrolles and pyridines are formed in pyroline thermal degradation process (Laukaleja & Koppel 2021). Meanwhile, the light roast French press coffee showed strong association with the majority of aroma-active compounds. For example, aroma-active compounds such as 2,2'-bifuran (**19**), 2,6-dimethylprazine (**39**), 1-(6-methyl-2-pyrazinyl)-1-ethanone (**37**) where only found in French press coffee. Also, the light roast French press coffee was associated with several GC-O aroma frequencies (roasted, smoky, nutty, sharp, berry).

The PCA confirms that the aroma-active compounds and volatile compounds with GC-O aroma frequencies divide the samples by their roast levels the brewing technique.

Summary of 3.4. Aroma-active compound perception in differently roasted and brewed coffees by gas chromatography-olfactometry / *Kopsavilkums par 3.4. Aromātu veidojošo savienojumu uztvere ar gāzu hromatogrāfiju-olfaktometriju dažādi grauzdētā un dažādi pagatavotā kafijā*

The olfactory vocabulary for coffee brews was developed by evaluating coffee samples with three different roast profiles and two different brewing techniques by nasal impact frequency method. From detected 56 volatile compounds, 30 were identified as aroma-active. The olfactory panellists detected 23 aromas linked to aroma-active compounds. The most frequent aroma attributes were sweet, musty, leather, skunky, burnt, and nutty, which were identified 7–15 times in all samples. Light French coffee showed the widest aroma attribute profile (including attributes as sharp, garlic berry). In dark roasted coffee samples most frequent aroma attributes were sweet and musty (identified 4–6 times). Both roasting, brewing process as well as the concentration of the volatile compound had significant impact on the aroma-active compound perception. The PCA analysis confirmed that samples were clustered by roast levels and brewing techniques. The future research could apply this olfactory vocabulary to create more objective lexicons for differently roasted coffee brews.

Kafijas dzērienu gāzu hromatogrāfijas-olfaktometrijas vārdnīca tika izstrādāta, novērtējot trīs dažādas grauzdēšanas pakāpes un divas kafijas pagatavošanas metodes, izmantojot "nasal impact frequency" metodi. No 56 gaistošajiem savienojumiem, 30 tika izvirzīti kā aromātveidojoši, un vērtētāji spēja identificēt 23 dažādus aromātus. Biežākie aromāti bija salds, mitra pagraba, ādas, skunska, dedzināts un riekstu. Šie aromāti tika identificēti visos paraugos 7–15 reizes. Viegli grauzdētā franču preses kafijā tika konstatēts visplašākais aromāta īpašību profils (ieskaitot tādus aromātus kā ass, ķiploku, ogu). Tumši grauzdētā kafijā visbiežāk gaistošie savienojumi tika identificēti ar aromātu notīm, kā salds un mitra pagraba (biežums: 4–6 reizes). Gan grauzdēšanas pakāpe, gan pagatavošanas metode būtiski ietekmēja aromātveidojošo savienojumu uztveri. Galveno komponenšu analīze apstiprināja šo secinājumu, vizuāli ilustrējot datu sadalījumu pēc grauzdēšanas pakāpēm un pagatavošanas metodēm. Iegūtos datus var pielietot kafijas aromātu leksikona izveidei.

3.5. Consumer's perception of specialty coffee with potentially increased bioactive compound content / *Patērētāju sensorais novērtējums par dažāda grauzdējuma kafijām ar iespējami lielāku bioloģiski aktīvo savienojumu koncentrāciju*

Bioactive compounds in coffee are present in higher concentrations in light roast coffee. With a light roast level, it is possible to maintain higher biologically active compound content and highlight specialty coffee sensory characteristics such as pleasant acidity, fruity and sweet aroma notes (Laukaleja, Kruma, & Cinkmanis 2022). However, most coffee consumers associate coffee with darker roast sensory attributes. The aim of the research stage V was to analyse regular coffee consumer's perception of specialty coffee brews and their purchase interest, knowing it has potentially increased antioxidant level.

3.5.1. Consumer coffee consumption habits / *Patērētāju kafijas patēriņa ieradumi*

A dendrogram illustrated by agglomerative hierarchical clustering (AHC) of coffee consumers (Fig. 3.11), shows that based on the dissimilarity of overall liking scores and purchase intent 90 consumers were classified into two groups (Cluster 1 (n=45) and Cluster 2 (n=45).

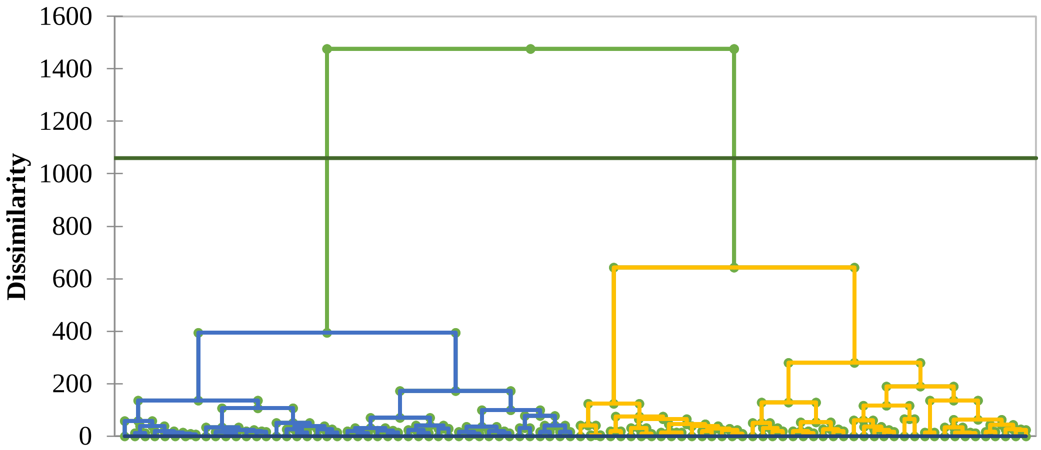


Fig. 3.11. A dendrogram of agglomerative hierarchical clustering (AHC) illustrating coffee consumers based on overall liking scores and purchase intent /
3.11. att. Patērētāju aglomeratīvā hierarhisko klasteru analīzes (AHC) dendrogramma pēc kafijas patikšanas novērtējuma un vēlmes iegādāties kafiju

Data further was analysed regarding consumer group (Cluster_1 and Cluster_2). The Table 3.11 illustrates frequency distribution of coffee consumer groups by gender and age. In this study, the dominant were fem ale coffee consumers (n=33 Cluster_1 and 30=n Cluster_2). Cluster 1 had younger consumers from 18–24 and 25–34 age groups, while cluster 2 had more consumers from 35–44 and 55–64 age groups.

By Fisher's exact test there was no association between gender and consumer groups (p=0.646) and age and consumer groups (p=0.734). Also, ANOVA with pairwise comparison by Tukey’s HSD test did not a show significant association between age and purchase intent.

Previous studies reported no association between gender and willingness to buy products with potential health benefits (Urala & Lähteenmäki 2007; Corso, Kalschne, & Benassi 2018). However, some studies have found an association between age and overall liking or purchase intent. The main statement is that with increasing age there is a positive correlation with purchase intent of food products with health benefits (Verbeke 2005; Mikołajczyk-Stecyna et al. 2021).

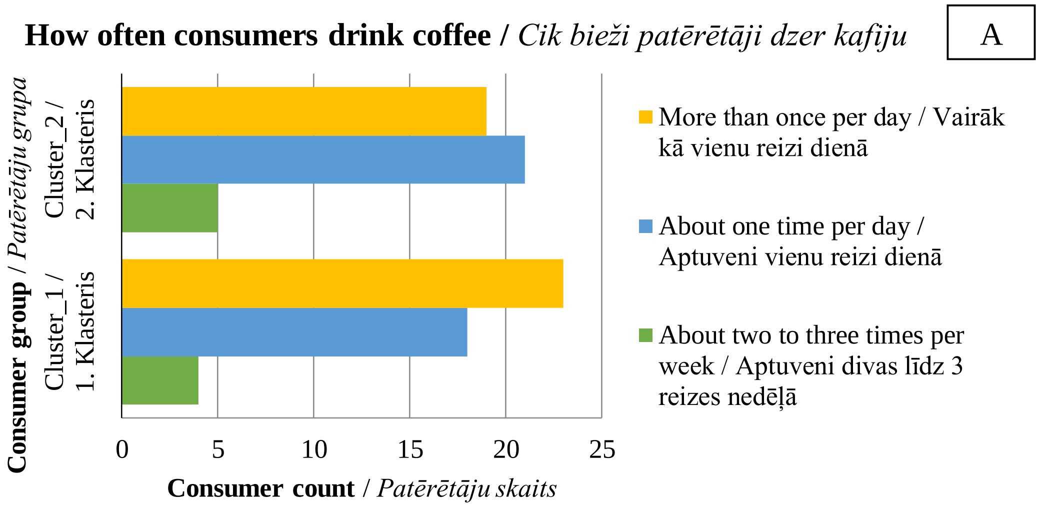
Table 3.11 / *3.11. tabula*

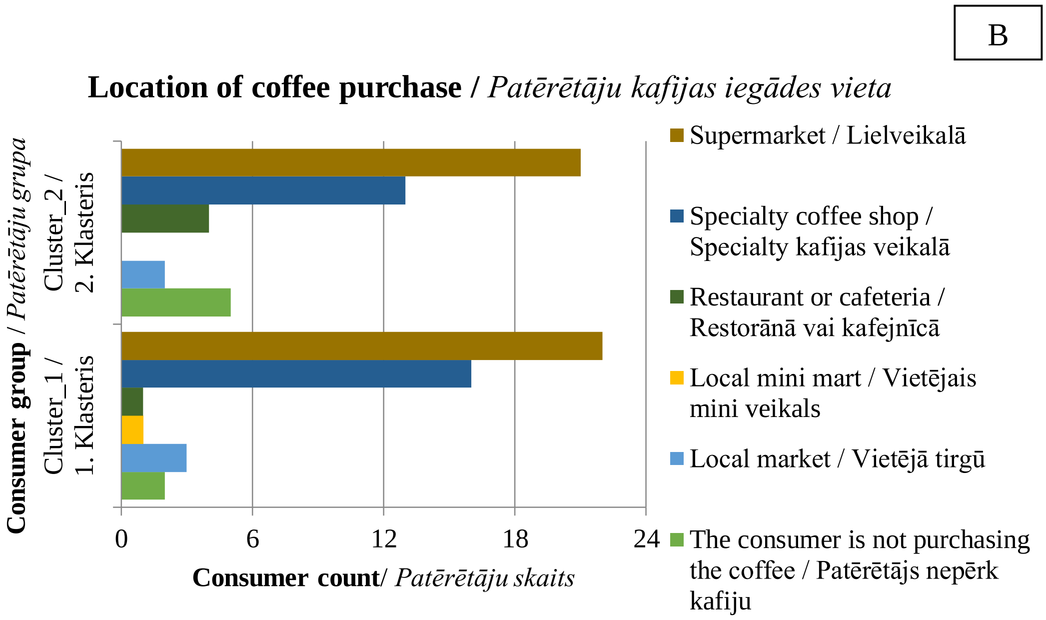
Demographic characteristics of consumers by Consumer groups /
Patērētāju demogrāfiskie rādītāji pēc patērētāju grupu sadalījuma

Demographic characteristics / *Demogrāfiskie rādītāji*	**Consumer group** / *Patērētāju grupa*	
	Cluster 1 / *1. Klasteris*	**Cluster 2** / *2. Klasteris*
Gender / *Dzimums*		
Female / *Sieviete*	33	30
Male / *Vīrietis*	12	15
Age group / *Vecuma grupa*		
18–24	8	4
25–34	16	13
35–44	4	6
45–*54*	4	4
55–64	9	13
64+	4	5

From the data in Appendix 3, it is apparent that most of the consumer's drink coffee at least once a day, and 54% of them chose automatic drip coffee (25.6% Cluster_1 and 28.9% Cluster_2). Similar to Czarniecka-Skubina et al. (2021) study majority of Polish consumers drink coffee at home (42.2%) and at work (34.4%). In contrast with this study, the location where consumers drink coffee had a significant difference between different consumer cluster groups in Poland.

Fig. 3.12 illustrates that from 90 consumers, 70% believe coffee effect on health depends on how much is consumed (33.3% Cluster_1 and 36.7% Cluster_2). Both consumer groups believe that coffee has more positive than negative effects on health (16.6% Cluster_1 and 8.9% Cluster_2).





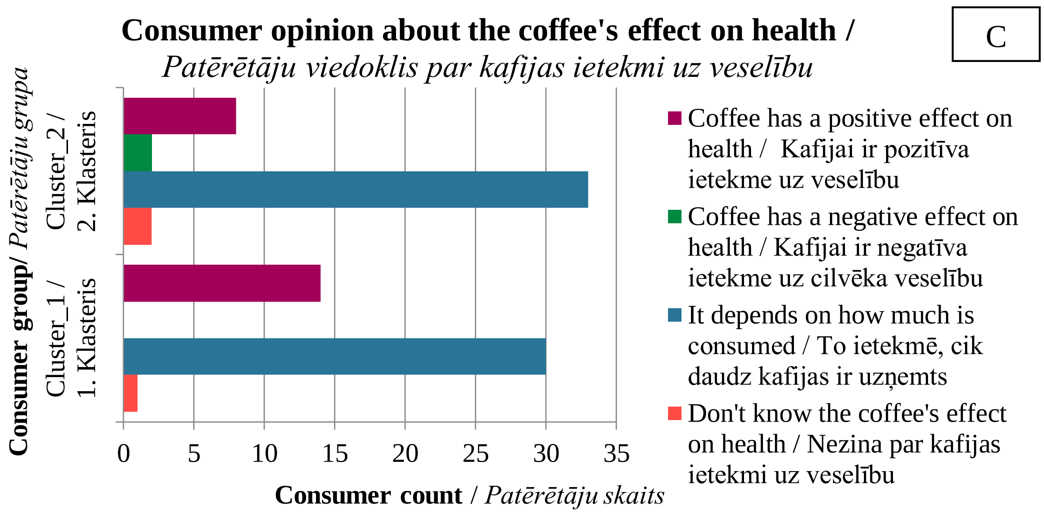


Fig. 3.12. Consumer coffee consumption habits /
3.12. att. Patērētāju kafijas patēriņa ieradumi

It is apparent that some of the consumer habits are more dominant than others, although by Fisher's exact test there was no association between cluster groups and coffee consumption habits. To determine consumer consumption habit's possible impact on overall liking scores ANOVA was performed following pairwise comparison by Tukey's HSD test. No significant differences were detected between consumer consumption habits and coffee sample liking scores. What is striking about the data, the coffee consumers from both groups had opposite liking scores of automatic drip coffee samples and no correlation or significant impact was found between consumer preferred coffee brew method and cluster group or liking scores.

Kalschne et al. (2018) propose that age, schooling, income, and understanding about functional food health benefits had a positive correlation with acceptance of functional foods (including coffee). Other previous studies indicate that knowledge about the quality standards and nutritional value of specific food products increase the possibility to purchase the product regardless of sensory factors (Bech-Larsen & Grunert 2003; Lee, Bonn, & Cho 2013; Sepúlveda et al. 2016)

3.5.2. Coffee sensory attribute liking scores and purchase intent / Kafijas sensoro īpašību patikšanas novērējums un vēlme iegādāties

It can be seen in Table 3.12 that consumers from cluster 1 showed significantly higher liking scores for all sensory attributes (mean scores between 5.87–6.76), while cluster 2 consumers showed significantly lower liking scores for all sensory attributes (mean scores between 3.22–5.84). Overall like, aroma and flavour attribute liking scores between consumer group*sample interaction are significantly different, except overall texture (*p*=0.20).

Tabula 3.12 */ 3.12. tabula*

Consumer mean liking scores (9-point Hedonic scale) for sensory attributes of coffee samples */ Patērētāju kafijas paraugu sensoro īpašību novērtējums, izmantojot 9 punku hēdonisko skalu*

Consumer group / *Patērētāju grupa*	**Sample** / *Paraugs*	**Sensory attributes** /*Sensorās īpašības*			
		Overall like / *Patikšana*	**Overall aroma** / *Aromāts*	**Overall flavour** / *Garša*	**Overall texture** / *Tekstūra*
Cluster 1 / *1. Klasteris*	LD	6.38 a	6.42 a	6.44 a	6.51 a
	LF	6.69 a	6.49 a	6.76 a	6.31 ab
	MD	6.22 a	6.16 ab	6.18 a	6.42 a
	MF	5.87 ab	5.89 abc	5.89 a	6.18 ab
Cluster 2 / *2. Klasteris*	LD	3.93 cd	5.02 cd	3.91 bc	5.13 c
	LF	3.22 d	4.56 d	3.24 c	4.47 c
	MD	4.38 cd	5.84 abc	4.33 bc	5.31 bc
	MF	4.69 bc	5.20 bcd	4.68 b	5.33 bc

Within columns, numbers followed by a different letter are significantly different (p<0.05), following pairwise comparison by Tukey HSD test */ Vērtības, atzīmētas ar atšķirīgiem burtiem kolonās, norāda uz būtiskām atšķirībām starp kafijas paraugiem (p<0.05)*

Even though no significant differences were detected between four sample liking scores for sensory attributes, light roast coffee samples were more liked by consumers from Cluster_1 and medium roast coffee samples by consumers from Cluster_2. LF (light roast French press) coffee sample was scored the highest for overall like, aroma, flavour by cluster 1 and the lowest by Cluster_2. By the present results, previous studies have demonstrated that overall aroma and flavour have a positive correlation to overall acceptance while evaluating C.arabica and C.canephora coffee samples (Kalschne et al. 2018; Donfrancesco, Gutierrez Guzman, & Chambers 2019). It is interesting to notice, that consumers from Cluster_2 gave lower liking scores after tasting the coffee, while consumers from Cluster_1 scored coffee samples slightly higher after tasting. Fig. 3.13 demonstrates Cluster_1 consumer's likeliness to purchase different roast and brew coffee, knowing it has a high antioxidant content is significantly higher than Cluster_2 consumers. Consumer group* sample interaction have a significant effect on purchase intent ($p<0.001$), following a similar pattern as overall like and flavour scores.

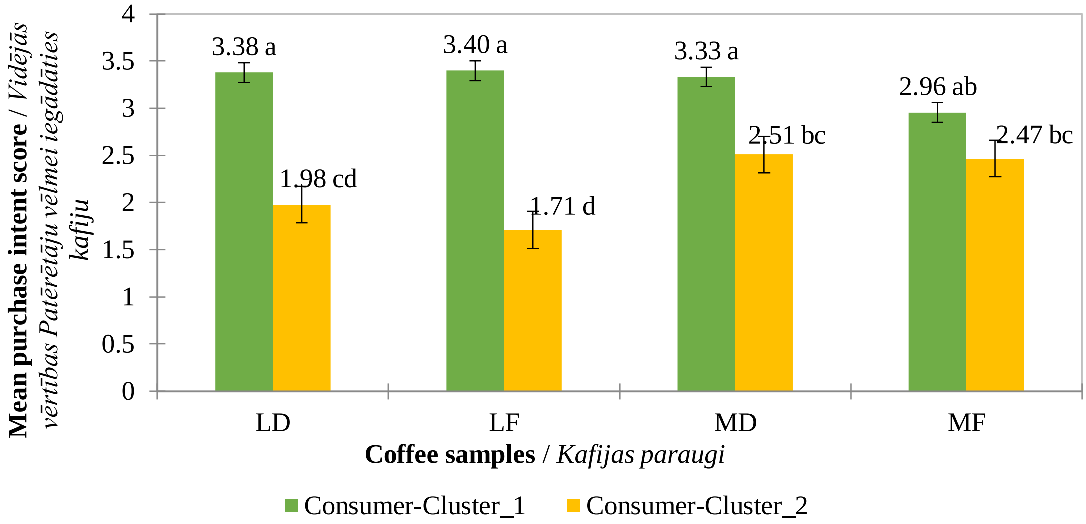


Fig 3.13. Consumer purchase intent / *3.13. att. Patērētāju vēlme iegādāties kafiju*
Numbers followed by a different letter are significantly different ($p<0.05$), following pairwise comparison by Tukey HSD test / *Vērtības atzīmētas ar atšķirīgiem burtiem norāda uz būtiskām atšķirībām starp kafijas paraugiem ($p<0.05$)*

Sensory attribute liking scores by both consumer groups had a positive correlation to purchase intent (Table 3.13). Overall aroma and texture of coffee samples showed the weakest correlation with purchase intent for both clusters.

Tabula 3.13 / *3.13. tabula*

Kendall correlations between consumers' sensory attribute liking scores and consumer's likeliness to purchase coffee, knowing it has a high antioxidant content / *Kendāla τ korelācija starp patērētāju sensoro īpašību novērtējumu un patērētāju vēlmi pirkt kafiju*

Correlation τ / *Korelācija (tau)*	**Consumer group** / *Patērētāju grupa*	**Sensory attributes** / *Sensorās īpašības*			
		Overall like / *Patikšana*	**Overall aroma** / *Aromāts*	**Overall flavour** / *Garša*	**Overall texture** / *Tekstūra*
Purchase intent / *Vēlme iegādāties*	Cluster 1 / *1. Klasteris*	**0.618**	**0.435**	**0.595**	**0.476**
	Cluster 2 / *2. Klasteris*	**0.650**	**0.354**	**0.657**	**0.420**

Values in bold are different from 0 with a significance level alpha=0.05 / *Vērtības treknrakstā norāda uz būtisku korelāciju starp sensoro īpašību un patērētāju vēlmi pirkt kafiju ($p<0.05$)*

The strongest correlation to purchase intent for cluster 1 consumers was overall liking of coffee samples and for Cluster_2 the overall flavour of coffee samples. This could indicate that for Cluster_2 consumers purchase intent and overall liking of coffee samples could be impacted by unpleasant flavour or taste aspects.

From the correlation and penalty analysis this study supports Verbeke (2005) statement that consumers are not willing to choose healthier products if they don't prefer the taste of it. Previous studies have insisted to analyse consumer beliefs about antioxidants and coffee quality factors to better understand their willingness to purchase coffee as a functional food (Urala & Lähteenmäki 2007; Cavalli & Tavani 2016; Corso, Kalschne, & Benassi 2018).

3.5.3. Just-about-right (JAR) data and penalty analysis of coffee consumer groups and coffee samples / *Kafijas patērētāju grupu un kafijas paraugu "Penalty" analīze*

Penalty analysis with Just-About-Right (JAR) frequencies and mean drops are shown in Appendix 4.

The data indicate that bitterness and sourness significantly affect the overall liking of coffee samples, especially for Cluster_2 consumers. The consumers from Cluster_2 evaluated all coffee samples as too bitter and too sour. Cluster_1 LF coffee sample had the highest selection of JAR for sourness (69%) and bitterness (69%) of coffee (Fig.3.14). Meanwhile, 73% of cluster 2 consumers evaluated the LF sample sourness as "Too much" and 56% bitterness as "Too much".

The findings are in accordance with overall flavour liking scores presented in Table 3.14, where cluster 1 liked the flavour of the LF sample the most and Cluster_2 the least from all four coffee samples. This table also illustrates that Cluster_2 customers strongly penalize the French press coffee (LF and MF) when they consider it too sour, and automatic drip coffee (LD and MD) when they consider it too sour and bitter. Also, the mean drops are significantly different from 0, including overall penalty, which indicates the significant impact of flavour attributes to overall like of coffee sample. Only bitterness of French press coffee did not have a significant impact or concerning mean drop on cluster 2 consumer liking of coffee sample.

For Cluster_1 automatic drip coffee (LD and MD) sample bitterness, the overall penalties are slight significant, including "too much" mean drops, while the bitterness of French press (LF and MF) coffee samples did not have a significant impact on Cluster_1 consumer overall liking scores. On the contrary, sourness had a significant impact on overall liking scores for all four samples by Cluster_1 consumer, even though Cluster_1 consumers mostly selected JAR (44–69%) for the sourness of coffee samples.

Comparing the Table 3.13 correlation coefficients with the Appendix 4, the significance of the penalties confirms the possibility that sourness and bitterness is the key factors for Cluster_2 consumers overall like and purchase intent of coffee.

This study supports evidence from previous observations of (Cotter et al. 2021) where the sourness of coffee samples was strongly penalized by consumers who were more conservative with coffee flavour attributes. Bhumiratana et al. (2019) study about coffee drinking experience and emotions concluded that coffees with higher acidity consumers associated with "guilt", "off-balance", and "bored" emotions.

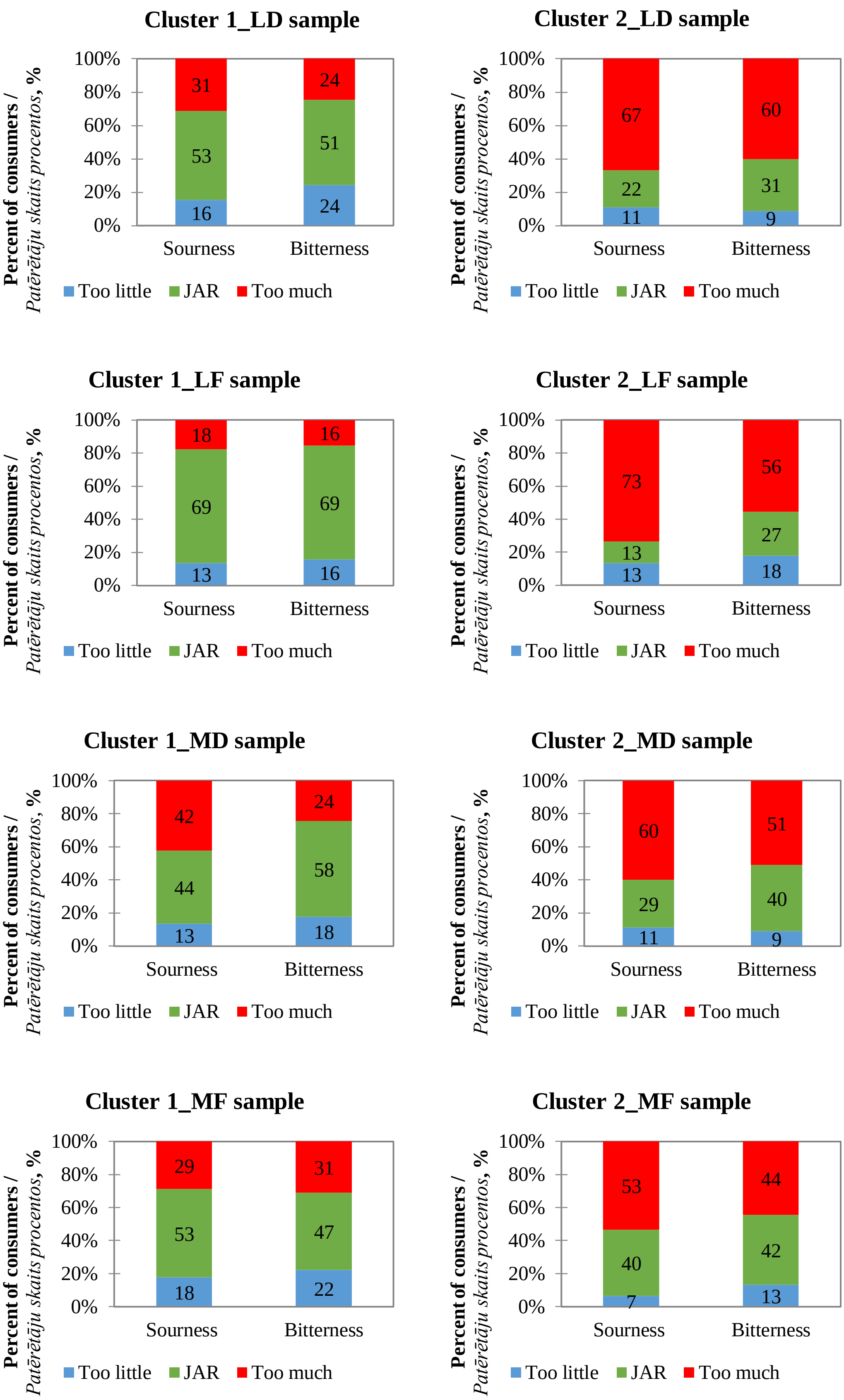


Fig. 3.14. Just-about-right (JAR) scale of coffee sample sensory attributes /
3.14. att. Kafijas paraugu sensoro īpašību novērtējums, izmantojot Just-about-right (JAR) skalu

Cocoa, burnt and bitter notes were associated with positive emotions. A possible explanation for acidic taste dislike among coffee consumers could be the unfamiliar association with regular coffee flavour.

Summary of 3.5. Consumer's perception of different roast level coffee brews with potentially increased bioactive compound content / *Kopsavilkums par 3.5. Patērētāju sensorais novērtējums par dažāda grauzdējuma kafijām ar iespējami lielāku bioloģiski aktīvo savienojumu koncentrāciju*

The findings of this study suggest that there is an association between sensory attribute liking scores and purchase intent among black coffee consumers. Consumer gender, age, and coffee consumption habits had no significant impact on the overall liking scores of coffee samples.

There was a significant difference between the two consumer groups' sensory attribute liking scores of all four coffee samples (Cluster_1 most frequent liking score 6 and 7 ("like slight" and "like moderately"). Cluster_1 consumers selected all coffee sample sourness and bitterness "just-about-right", while a majority of Cluster_2 consumers evaluated all coffee sample sourness and bitterness as "too much". Penalty analysis confirms that coffee sample sourness and bitterness could significantly impact both consumer group liking scores and purchase intent. A strong positive correlation was found between consumers, who evaluated coffee bitterness and sourness as "too much", overall flavour liking scores, and purchase intent. Information about possible high antioxidant content in coffee did not influence consumers' willingness to purchase coffee.

Taken together, these results propose that consumer sensitivity to sour and bitter taste of coffee should be evaluated when analysing overall sensory attribute liking and purchase intent. A greater focus on consumer education about coffee, nutrition science, rural/urban divide could produce interesting findings that could help understand the preferable coffee flavour triggers. Further investigation is required to accurately understand the role of health effect information about coffee on purchase intent.

Pētījuma rezultāti pierāda, ka pastāv saistība starp sensoro īpašību patikšanas rādītājiem un melnas kafijas patērētāju pirkšanas nodomu. Patērētāju demogrāfiskie rādītāji un kafijas patēriņa paradumi būtiski neietekmēja kopējos kafijas paraugu patikšanas rādītājus.

Būtiskas atšķirības tika konstatētas starp abu patērētāju grupu kafijas paraugu sensoro īpašību novērtēšanas rādītājiem. "Penalty" analīzes rezultāti norādīja, ka 1. klāstera patērētāji lielākoties novērtēja visu kafijas parauga skābumu un rūgtumu ar "JAR" rezultātu. Savukārt lielākā daļa 2. klāstera patērētāju novērtēja visu kafijas paraugu skābumu un rūgtumu ar atzīmi "pārāk daudz". "Penlaty" analīze apstiprina, ka kafijas parauga skābums un rūgtums var būtiski ietekmēt gan patērētāju grupu patikšanas rādītājus, gan vēlmi iegādāties kafiju. Izteikti pozitīva korelācija tika konstatēta starp patērētājiem, kuri kafijas rūgtumu un skābumu novērtēja kā "pārāk daudz", garšas patikšanas rādītājiem un pirkšanas vēlmi.

Rezultāti norāda, ka, informācija par iespējami palielinātu antioksidantu saturu kafijā neietekmēja patērētāju vēlmi iegādāties kafiju. Analizējot sensorās īpašības, patikšanas slieksni un pirkšanas vēlmi, ir būtiski ņemt vērā patērētāju jutību pret skābu un rūgtu kafijas garšu. Padziļināti pētījumi ir nepieciešami, lai izvērtētu, vai informācija par kafijas ietekmi uz veselību ietekmē patērētāja vēlmi iegādāties produktu.

CONCLUSIONS

1. The selected SPME fibre coating significantly effects the specialty coffee volatile compound detection. The CAR/PDMS was the only fibre which extracted significantly more important volatile compounds in specialty coffee brew with higher peak areas in all chemical compound groups, except phenolic compounds.
2. A positive correlation was found between final cup quality scores and total phenolic, flavonoid content for Roastery_1 coffee brews and a negative correlation between final cup quality scores and total phenolic, flavonoid content and $ABTS^{\bullet+}$, DPPH• radical scavenging activity for Roastery_2 coffee brews. These results indicate that the roastery-specific roasting process parameters could influence volatile compounds profile and the total and individual phenolic compound content.
3. The total phenolic, flavonoid content (291.85 mg GAE mL^{-1}; 18.26 mg CE mL^{-1}) and individual phenolic such as 3,5-dihydroxybenzoic acid (217.24 mg 100 mL^{-1}), chlorogenic acid (117.54 mg 100 mL^{-1}) and rutin (9.70 mg 100 mL^{-1}) content was the highest in light roast coffee, and their content degreased with increasing roast level.
4. The roasting levels did not show direct associations with the amino acid profile, although strong correlations were observed between several amino acids in medium roast level coffee. While the fatty acid content was the highest in medium roast and the lowest in the light roast coffee.
5. With olfactory vocabulary of specialty coffee brews, 23 aromas and 30 aroma-active compounds were identified.
6. The most frequent aromas of specialty coffee volatiles were associated with sweet, musty, leather, skunky, burnt, and nutty aromas.
7. Penalty analysis confirmed that sourness and bitterness of coffee brew could significantly impact both consumer group liking scores and purchase intent.
8. A significant correlation was detected between sensory attribute liking scores and purchase intent among black coffee consumers. Information about possible high antioxidant content in coffee did not influence consumers' willingness to purchase coffee.
9. The results of the research rejects the hypothesis that coffee consumers would prefer specialty coffee due to increased bioactive compound content by adjusted roast level.

SECINĀJUMI

1. Cietās fāzes mikro ekstrakcijas šķiedras izvēle būtiski ietekmē gaistošo savienojumu noteikšanu *specialty* kafijā. CAR/PDMS bija vienīgā šķiedra, kas spēja uzrādīt ievērojami vairāk nozīmīgo gaistošu savienojumu ar lielākiem smaiļu laukumiem no visām ķīmiskajām klasēm, izņemot fenolu savienojumus.
2. Tika konstatēta pozitīva korelācija starp sensorās kvalitātes novērtējuma rādītājiem un kopējo fenolu, flavonoīdu saturu Roastery_1 kafijas paraugos un negatīva korelācija starp sensorās kvalitātes novērtējuma rādītājiem un kopējo fenola, flavonoīdu saturu un $ABTS^{\bullet+}$, DPPH• antitradikālo aktivitāti Roastery_2 kafijas paraugos. Rezultāti apliecina, ka grauzdētājiem raksturīgie grauzdēšanas parametri var ietekmēt gaistošo savienojumu profilu un kopējo, individuālo fenola savienojumu saturu.
3.
4. Vislielākais kopējo fenolu, flavonoīdu saturs (291.85 mg GAE 100 mL^{-1}; 18.26 mg CE 100 mL^{-1}) un atsevišķo fenolu kā, 3,5-dihidroksibenzoskābes (217.24 mg 100 mL^{-1}), hlorogēnskābes (117.54 mg 100 mL^{-1}) un rutīna (9.70 mg 100 mL^{-1}) tika konstatēts gaiši grauzdētā kafijā un to saturs samazinājās palielinoties grauzdējuma pakāpei.
5. Grauzdēšanas pakāpes neuzrādīja tiešu saistību ar aminoskābju profilu, lai gan starp vairākām aminoskābēm tika novērotas spēcīgas korelācijas vidēja grauzdējuma pakāpes kafijā. Savukārt, taukskābju saturs bija vislielākais vidēji grauzdētā kafijā un vismazākais viegli grauzdētā kafijā.
6. Izmantojot olfaktorisko specialty kafijas dzērienu vārdnīcu, tika noteikti 23 aromāti un 30 aromātu veidojoši savienojumi.
7. Biežākie aromāti *specialty* kafijas gaistošajiem savienojumiem tika asociēti ar saldumu, pelējumu/mitru pagrabu, ādu, skunksu, degumu un riekstiem.
8. "Penlaty" analīze apstiprina, ka kafijas parauga skābums un rūgtums var būtiski ietekmēt gan patērētāju grupu patikšanas rādītājus, gan vēlmi iegādāties kafiju.
9. Pētījuma rezultāti pierāda, ka pastāv saistība starp sensoro īpašību patikšanas rādītājiem un melnas kafijas patērētāju pirkšanas nodomu. Informācija par iespējami palielinātu antioksidantu saturu kafijā neietekmēja patērētāju vēlmi iegādāties kafiju.
10. Pētījumu iegūtie rezultāti noraida hipotēzi, ka pielāgojot grauzdēšanas pakāpi, kafijas patērētāji dotu priekšroku *specialty* kafijai tās palielināto bioloģiski aktīvo savienojumu satura dēļ.

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APPENDIXES/ *PIELIKUMI*

Appendix 1 / *1. Pielikums*

Volatile compound profile in differently roasted and brewed coffee /
Gaistošo savienojumu sastāvs dažādi grauzdētā un pagatavotā kafijā (Laukaleja & Koppel 2021)

Code / Kods	**KI exp.**	**KI ref.** **	**Volatile compounds** / *Gaistošie savienojumi*	**Volatile compound peak area means** / *Gaistošo savienojumu pīķa laukuma vidējās vērtības, % ± SD*					
				LD	LF	MD	MF	DD	DF
Aldehydes / *Aldehīdi*									
1_VC	1104	1010[4]	1-methyl-1H-pyrrole-2-carboxaldehyde / *1-metil-1H-pirol-2-karboksaldehīds*	n/a	n/a	n/a	2.8±0.49a	2.68±0.14a	0.34±0.02b
2_AAC	n/a	653[3]	2-methylbutanal / *2-metilbutanāls****	3.88±1.94bc	6.55±0.50a	3.44±0.54bc	4.71±0.37b	2.44±0.39c	3.5±0.20bc
3_AAC	n/a	537[3]	2-methylpropanal / *2-metilpropanāls****	2.33±0.65ab	2.36±0.72a	0.57±0.26d	1.92±0.30abc	1.34±0.13cd	1.56±0.26bc
4_VC	n/a	655[3]	3-methylbutanal / *3-metilpropanāls****	3.34±0.84ab	4.11±0.55a	2.19±0.34bc	2.21±1.12bc	1.54±0.15c	2.3±0.42bc
5_VC	1043	963[5]	5-methyl-2-furancarboxaldehyde / *5-metil-2-furānkarboksaldehīds****	13.15±0.80a	10.24±0.96b	9.37±0.87b	9.32±0.59b	7.07±0.55c	6.7±0.21c
6_VC	912	960[3]	Benzaldehyde / *Benzaldehīds****	n/a	1.21±0.16a	n/a	1.12±0.11ab	0.97±0.10b	0.36±0.03c
7_AAC	1088	1051[3]	Benzeneacetaldehyde / *Fenilacetaldehīds****	1.01±0.28b	1.28±0.12a	0.90±0.12bc	1.07±0.11ab	0.69±0.08c	0.91±0.06bc
8_VC	1285	1209[3]	Decanal / *Dekanāls*	0.51±0.07a	n/a	n/a	n/a	0.50±0.06a	n/a
9_VC	1212	1385[1]	Dodecanal / *Dodekanāls*	0.12±0.09a	0.07±0.02a	n/a	n/a	n/a	n/a
10_VC	836	812[3]	Hexanal / *Heksanāls*	0.81±0.29	n/a	n/a	n/a	n/a	n/a
11_AAC	1094	1071[3]	Nonanal / *Nonanāls**	1.25±0.12ab	1.2±0.13ab	1.5±0.46a	1.25±0.29ab	1.16±0.11ab	1.00±0.06b
Total Aldehydes / *Kopējie aldehīdi*				26.40	27.02	17.97	24.40	18.39	16.67
Alkanes / *Alkāni*									
12_AAC	1407	1400[5]	Tetradecane / *Tetradekāns*	0.34±0.09a	0.24±0.14a	0.33±0.18a	0.35±0.18a	0.33±0.09a	n/a
Esters / *Esteri*									
13_AAC	832	864[3]	1-Butanol, 3-methyl-acetate / *Izoamilacetāts*	n/a	1.12±0.55	n/a	n/a	n/a	n/a

Continued appendix 1 / *1. Pielikuma turpinājums*

Code / *Kods*	KI exp.	KI ref. **	**Volatile compounds** / *Gaistošie savienojumi*	**Volatile compound peak area mean /** *Gaistošo savienojumu pīķa laukuma vidējās vērtības, % ± SD*					
				LD	LF	MD	MF	DD	DF
14_VC	1200	1228[8]	Butanoic acid, 3-methyl-, 2-furanylmethyl ester / *Butānskābes 3-metil-, 2-furanilmetilesteris*	n/a	n/a	n/a	1.07±0a	0.91±0.08b	0.43±0.03c
15_VC	1228	1200[5]	Methyl salicylate / *Metilsalicilāts****	1.19±0.11ab	1.14±0.10abc	1.12±0.17bc	1.35±0.16a	0.93±0.05c	0.17±0.15ab
Total Esters / *Kopējie Esteri*				1.19	1.69	1.12	2.42	1.84	1.60
Furans / Furāni									
16_AAC	1164	1184[8]	2-(2-Furanylmethyl)-5-methylfuran / *2-(2-Furanilmetil)-5-metilfurāns* ***	0.75±0.26d	1.05±0.08c	1.19±0.17c	1.54±0.08b	1.14±0.13c	1.81±0.10a
17_VC	1237	1292[8]	2,2’-[Oxybis(methylene)]bisfuran / *2,2’-[Oksibis(metilēn)]bisfurāns****	0.64±0.16c	0.59±0.10c	1.02±0.15b	1.09±0.05ab	1.04±0.15b	1.26±0.10a
18_AAC	1077	1061[1]	2,2’-Methylenebisfuran / *2,2'-Metilēnbisfurāns* ***	0.89±0.50e	1.55±0.27d	2.4±0.63c	3.12±0.11ab	2.52±0.25bc	3.61±0.07a
19_AAC	1082	1047[8]	2,2'-Bifuran / *2,2'-Bifurāns*	n/a	1.27 ±0.15	n/a	n/a	n/a	n/a
20_AAC	1459	1472[1]	2-[(Methyldithio)methyl]-furan / *2-[(Metilditio)metil]-furāns*	n/a	0.03±0.03b	n/a	0.05±0.04a	n/a	0.05±0.04a
21_VC	930	998[5]	2-Furanmethanol, acetate / *2-Furānmetanola acetāts****	9.36±4.65c	9.93±0.75bc	13.79±2.05a	13.87±0.36a	13.68±0.94ab	13.34±0.38 ab
22_AAC	1170	1177[8]	2-n-Heptylfuran / *2-n-Heptilfurāns*	0.75±0.38a	n/a	0.99±0.06a	n/a	0.85±0.07a	0.84±0.42a
23_AAC	n/a	835	3-Furanmethanol / *3-Furānmetanols****	11.65±7.20a	13.57±2.33a	15.22±0.98 a	5.39±0.65b	11.97±1.15a	12.31±1.21 a
24_VC	1207	1238[5]	3-Phenylfuran / *3-Fenilfurāns*	n/a	n/a	n/a	n/a	2.00±1.42a	0.62±0.03b
25_VC	n/a	776[1]	Dihydro-2-methyl-3(2H)-furanone / *Dihidro-2-metil-3(2H)-furanons****	1.17±0.55a	1.15±0.19a	1.11±0.13a	0.36±0.15b	0.72±0.39ab	0.67±0.05a b
26_VC	n/a	828[5]	Furfural / *Furfurols*	8.71±9.13a	6.97±7.64a	9.89±1.98a	9.27±0.65a	6.88±1.077a	5.7±0.13a
27_AAC	958	875[8]	Furfuryl formate / *Furfurilformiāts*	3.56±7.15a	n/a	n/a	n/a	0.55±0.19a	0.26±0.04a
Total Furans / *Kopējie furāni*				49.12	49.41	64.08	54.31	59.77	60.56

Continued appendix 1 / *1. Pielikuma turpinājums*

Code / *Kods*	**KI exp.**	**KI ref. ****	**Volatile compounds** / *Gaistošie savienojumi*	**Volatile compound peak area mean /** *Gaistošo savienojumu pīķa laukuma vidējās vērtības, % ± SD*					
				LD	LF	MD	MF	DD	LD
Ketones / *Ketoni*									
28_AAC	1171	1064[6]	1-(1H-pyrrol-2-yl)-ethanone / *1-(1H-pirol-2-il)-etanons* ***	0.91±0.45b	0.95±0.23b	1.19±0.10b	n/a	1.04±0.08b	2.09±0.24a
29_AAC	1092	1078[3]	1-(2-Furanyl)-2-butanone / *1-(2-Furanil)-2-butanons*	n/a	n/a	n/a	0.73±0.21a	0.62±0.20a	0.85±0.39a
30_AAC	970	882[1]	1-(2-Furanyl)-ethanone / *1-(2-Furanil)-etanons****	1.96±0.23a	1.82±0.20ab	1.88±0.17ab	1.88±0.05ab	1.65±0.09b	1.61±0.09b
31_VC	1036	985[8]	1-(Acetyloxy)-2-butanone / *1-(Acetiloksi)-2-butanons*	0.2±0.06b	n/a	n/a	0.49±0.24a	0.56±0.05a	n/a
32_VC	788	786[1]	2,3-hexanedione / *2,3-heksāndions* ***	1.08±0.26ab	1.23±0.18a	1.03±0.14ab	1.12±0.14ab	0.88±0.10b	1.06±0.16ab
33_VC	937	987[5]	6-methyl-5-hepten-2-one / *6-metil-5-hepten-2-ons*	n/a	n/a	n/a	n/a	0.15±0.08	n/a
Total Ketones / Kopējie ketoni				4.15	4.00	4.10	4.22	4.91	5.61
Phenolic compounds / *Fenolu savienojumi*									
34_VC	1050	1086[5]	2-Methoxy-phenol / *2-Metoksifenols*	n/a	n/a	n/a	n/a	n/a	2.33±0.18
35_AAC	1311	1299[3]	4-Ethyl-2-methoxyphenol / *4-Etilguaiacols****	0.4±0.04c	0.37±0.03c	0.25±0.0d	0.66±0.03b	0.65±0.11b	0.80±0.07a
36_AAC	1213	n/a	4-Hydroxy-2-methylacetophenone / *4-Hidroksi-2-metilacetofenons****	3.29±0.60ab	4.08±0.96a	3.2±1.74ab	1.57±0.31b	3.18±0.62ab	3.11±0.46ab
Total Phenolic compounds / *Kopējie fenolu savienojumi*				3.69	4.45	3.54	2.23	3.83	6.24
Pyrazines / *Pirazīni*									
37_AAC	1074	1083[1]	1-(6-Methyl-2-pyrazinyl)-1-ethanone / *1-(6-Metil-2-pirazinil)-1-etanons*	0.7±0.07a	0.65±0.13a	n/a	n/a	n/a	n/a
38_AAC	1128	1153[3]	2,3-Diethyl-5-methylpyrazine / *2,3-Dietil-5-metilpirazīns****	0.34±0.04cd	0.3±0.03bc	0.35±0.01c	0.43±0.03a	0.30±0.02d	0.42±0.03ab
39_AAC	976	906[7]	2,6-Dimethylprazine / *2,6-Dimetilprazīns*	5.26±0.33a	5.2±0.99a	4.68±1.45a	4.65±1.23a	4.02±1.25a	4.4±1.32a
40_AAC	978	1004[5]	2-Ethyl-3-methylpyrazine / *2-Etil-3-metilpirazīns*	3.11±1.69a	3.44±1.71a	4.14±0.25a	4.46±0.24a	3.64±0.14a	n/a
41_VC	942	973[7]	2-Ethyl-5-methylpyrazine / *2-Etil-5-metilpirazīns*	n/a	n/a	n/a	n/a	n/a	2.9±1.17
42_AAC	974	969[7]	2-Ethyl-6-methylpyrazine / *2-Etil-6-metilpirazīns****	n/a	2.28±0.22a	2.09±0.04a	2.13±0.12a	1.8±0.07b	1.71±0.06b
43_VC	1130	1184[3]	3,5-Diethyl-2-methylpyrazine / *3,5-Dietil-2-metilpirazīns*	n/a	0.61±0.04a	0.61±0.03a	0.67±0.03a	0.51±0.04a	0.51±0.25a
44_AAC	n/a	794[1]	Methylpyrazine / *Metilpirazīns*	4.36±0.42a	3.39±1.77	3.47±0.16b	2.92±1.44c	2.97±0.19c	2.96±0.14c
45_AAC	1017	1078[5]	3-Ethyl-2,5-dimethylpyrazine / *3-Etil-2,5-dimetilpirazīns*	2.63±1.07a	3.17 ±0.25a	3.12±0.15a	3.33±0.16a	2.73±0.13a	2.98±0.20a
Total Pyrazines / *Kopējie pirazīni*				16.4	18.55	17.88	17.95	15.5	15.66

Continued appendix 1 / *1. Pielikuma turpinājums*

Code / *Kods*	KI exp.	KI ref. **	**Volatile compounds /** *Gaistošie savienojumi*	***Volatile compound peak area*** **mean /** *Gaistošo savienojumu pīķa laukuma vidējās vērtības, % ± SD*					
				LD	LD	LD	LD	LD	LD
Pyridines / *Piridīni*									
46_VC	n/a	717[1]	Pyridine / *Piridīns**	3.74±0.26b	n/a	4.92±0.97a	5.25±0.36a	5.61±0.59a	5.29±0.26a
Pyrimidine / *Pirimidīni*									
47_VC			4-amino-2-methoxypyrimidine / *4-amino-2-metoksipirimidīns****	n/a	n/a	0.16±0.17b	0.34±0.02a	0.29±0.02a	0.31±0.03a
Pyrroles / *Piroli*									
48_AAC	1146	1149[1]	1-(2-furanylmethyl)-1H-pyrrole / *1-(2-furanilmetil)-1H-pirols****	2.79±0.22b	2.86±0.11b	n/a	3.55±0.15a	2.91±0.16a	3.49±0.19a
49_VC	1053	1059[5]	1-pentyl-1H-pyrrole / *1-pentil-1H-pirols*	n/a	n/a	n/a	n/a	0.25±0.10b	0.34±0.02a
50_VC	1389	1387[2]	3-methylindole / *3-metilindols*	n/a	n/a	n/a	n/a	n/a	0.08±0.01
51_AAC	953	n/a	N-(2-Cyanoethyl)-pyrrole / *N-(2-Ciānetil)-pirols****	1.19±0.15a	1.17±0.10ab	1.16±0.06ab	1.24±0.08a	1.03±0.04b	1.11±0.02ab
Total Pyrroles / *Kopējie piroli*				3.98	4.03	1.32	5.13	1.57	5.33
Sulphur compounds / *Sēru saturoši savienojumi*									
52_AAC	n/a	967[2]	Dimethyl trisulfide / *Dimetiltrisulfīds****	0.57±0.41c	0.92±0.07b	n/a	0.62±0.31c	1.96±0.75a	n/a
Terpenes / *Terpēni*									
53_AAC	1128	1121[1]	1,2-Dihydrolinalool / *1,2-Dihidrolinalols*	n/a	n/a	n/a	n/a	n/a	0.76±0.04
54_VC	1105	1104[3]	Linalool / *Linalols****	1.13±0.06ab	1.28±0.09a	1.17±0.15ab	1.17±0.08a b	0.91±0.06c	1.1±0.07b
55_VC	1226	1106[3]	Maltol / *Maltols****	0.48±0.43b	0.45±0.33b	0.70±0.17a	0.96±0.32a	n/a	0.81±0.53a
56_AAC	1433	1476[5]	1-Dodecanol / *1-Dodekanols****	0.46±0.18b	0.14±0.03c	0.77±0.41a	n/a	0.43±0.16b	0.17±0.10c
Total Terpenes / *Kopējie terpēni*				2.64	2.79	2.64	2.75	3.3	2.84
Total Volatiles / *Kopējie gaistošie savienojumi*				107.57	111.94	112.65	113.4	109.11	114.51

n/a – not available

*The volatile compounds (VC-number of the compound), aroma-active compounds (AAC-number of the compound).

**Kovats retention index compared using the National Institute of Standards and Technology (NIST) library of compounds (NIST/EPA/NIH mass spectral library, version 2.2, 2014) and literature [1]DB-1 column (Blanco Tirado et al. 1995; Takeoka, Perrino, & Buttery 1996; Lin & Rouseff 2001; Odri et al. 2007; Lee, Kim, & Lee 2017); [2]DB-5 column (Angeloni et al. 2020); [3]DB-5 MS column (Gómez & Ledbetter 1994; Lee, Suriyaphan, & Cadwallader 2001; Schirack et al. 2006; Whetstine et al. 2006; Cho et al. 2008; Majcher, Ławrowski, & Jeleń 2010; Paravisini et al. 2015); [4]HP-5 column (Lef & Dalrymple-Alford 2005); [5]HP-5 MS column (Juliani et al. 2004; Kim et al. 2006; Radulovic, Blagojevic, & Palic 2010; Qin et al. 2011); [6]OV-101 column (Shibamoto, Kamiya, & Mihara 1981); [7]SPB-5 column (Piccino et al. 2014); [8]SLB-5MS column (Risticevic, Carasek, & Pawliszyn 2008).

***Different letters (a, b, c) indicate the statistically significant difference between samples of a compound at $p<0.05$

Appendix 2 / *2. Pielikums*

Aroma profile, frequency of detection, and associated volatiles for differently roasted and brewed coffee samples / *Aromātu sastāvs, noteiktās frekvences un saistītie gaistošie savienojumi dažāda grauzdējuma un pagatavošanas metodes kafijās* (Laukaleja & Koppel 2021)

<table>
<tr><th>Aroma Attribute / Aromāta īpašība</th><th>Aroma detection frequency / Aromāta noteikšanas biežums</th><th>Coffee sample / Kafijas paraugs*</th><th>Volatile compounds associated with the aroma / Gaistošie savienojumi saistīti ar aromātu**</th></tr>
<tr><td rowspan="6">Sweet / Salds</td><td rowspan="6">15</td><td>LD</td><td>3-furanmethanol / 3-furānmetanols (23); benzeneacetaldehyde / fenilacetaldehīds (7)</td></tr>
<tr><td>LF</td><td>benzeneacetaldehyde / fenilacetaldehīds (7); 1-(6-methyl-2-pyrazinyl)-1-ethanone / 1-(6-metil-2-pirazinil)-1-etanons (37)</td></tr>
<tr><td>MD</td><td>3-furanmethanol / 3-furānmetanols (23); 2-ethyl-6-methylpyrazine / 2-etil-6-metilpirazīns (42); benzeneacetaldehyde / fenilacetaldehīds (7)</td></tr>
<tr><td>MF</td><td>3-furanmethanol / 3-furānmetanols (23); 1-(2-furanyl)-2-butanone / 1-(2-furanil)-2-butanons (29)</td></tr>
<tr><td>DD</td><td>benzeneacetaldehyde / fenilacetaldehīds (7);
nonanal / nonanāls (11)</td></tr>
<tr><td>DF</td><td>3-furanmethanol / 3-furānmetanols (23); benzeneacetaldehyde / fenilacetaldehīds (7);
1,2-dihydrolinalool / 1,2-dihidrolinalols (53);
4-ethyl-2-methoxyphenol / 4-etilguaiacols (35)</td></tr>
<tr><td rowspan="6">Musty / Mitra pagraba/ pelējuma</td><td rowspan="6">13</td><td>LD</td><td>methylpyrazine / metilpirazīns (44)</td></tr>
<tr><td>LF</td><td>2,6-dimethylprazine / 2,6-dimetilprazīns (39); 2-ethyl-3-methylpyrazine / 2-etil-3-metilpirazīns (40); 2,3-diethyl-5-methylpyrazine / 2,3-dietil-5-metilpirazīns (38)</td></tr>
<tr><td>MD</td><td>2,2'-methylenebisfuran / 2,2'-metilēnbisfurāns (18); nonanal / nonanāls (11); tetradecane / tetradekāns (12)</td></tr>
<tr><td>MF</td><td>3-ethyl-2,5-dimethylpyrazine / 3-etil-2,5-dimetilpirazīns (45); tetradecane / tetradekāns (12)</td></tr>
<tr><td>DD</td><td>methylpyrazine / metilpirazīns (44); 2-(2-furanylmethyl)-5-methylfuran / 2-(2-furanilmetil)-5-metilfurāns (16)</td></tr>
<tr><td>DF</td><td>1-(2-Furanyl)-ethanone / 1-(2-Furanil)-etanons (30); 2,2'-methylenebisfuran / 2,2'-metilēnbisfurāns (18)</td></tr>
<tr><td rowspan="4">Leather / Ādas</td><td rowspan="4">11</td><td>LD</td><td>2,3-diethyl-5-methylpyrazine / 2,3-dietil-5-metilpirazīns (38); 2-n-heptylfuran / 2-n-heptilfurāns (22); 4-hydroxy-2-methylacetophenone / 4-hidroksi-2-metilacetofenons (36); 1-dodecanol / 1-dodekanols (56)</td></tr>
<tr><td>MD</td><td>3-ethyl-2,5-dimethylpyrazine / 3-etil-2,5-dimetilpirazīns (45); 1-(1H-pyrrol-2-yl)-ethanone / 1-(1H-pirol-2-il)-etanons (28); 2-n-heptylfuran (22); 1-dodecanol / 1-dodekanols (56)</td></tr>
<tr><td>DD</td><td>1-(1H-pyrrol-2-yl)-ethanone / 1-(1H-pirol-2-il)-etanons (28); 2-n-heptylfuran / 2-n-heptilfurāns (22)</td></tr>
<tr><td>DF</td><td>1-(1H-pyrrol-2-yl)-ethanone / 1-(1H-pirol-2-il)-etanons (28)</td></tr>
<tr><td rowspan="5">Skunky / Skunska</td><td rowspan="5">9</td><td>LF</td><td>methylpyrazine / metilpirazīns (44);
n-(2-cyanoethyl)-pyrrole / n-(2-ciānetil)-pirols (51)</td></tr>
<tr><td>MD</td><td>2-methylbutanal / 2-metilbutanāls (2);
methylpyrazine / metilpirazīns (44)</td></tr>
<tr><td>MF</td><td>2-methylbutanal / 2-metilbutanāls (2);
methylpyrazine / metilpirazīns (44)</td></tr>
<tr><td>DD</td><td>methylpyrazine / metilpirazīns (44)</td></tr>
<tr><td>DF</td><td>2-methylbutanal / 2-metilbutanāls (2);
methylpyrazine / metilpirazīns (44)</td></tr>
</table>

Continued appendix 2 / *2. Pielikuma turpinājums*

Aroma Attribute / *Aromāta īpašība*	**Aroma detection frequency** / *Aromāta noteikšanas biežums*	**Coffee sample** / *Kafijas paraugs**	**Volatile compounds associated with the aroma** / *Gaistošie savienojumi saistīti ar aromātu***
Burnt / *Deguma*	7	LD	tetradecane / *tetradekāns* (**12**)
		LF	2-methylbutanal / *2-metilbutanāls* (**2**)
		MD	2-methylbutanal / *2-metilbutanāls* (**2**); nonanal / *nonanāls* (**11**); 4-hydroxy-2-methylacetophenone / *4-hidroksi-2-metilacetofenons* (**36**)
		MF	2-methylbutanal / *2-metilbutanāls* (**2**); 4-hydroxy-2-methylacetophenone / *4-hidroksi-2-metilacetofenons* (**36**)
Nutty / *Riekstu*	7	LD	1-(2-furanylmethyl)-1H-pyrrole / *1-(2-furanilmetil)-1H-pirols* (**48**)
		LF	1-butanol, 3-methyl-acetate / *izoamilacetāts* (**13**); 2,6-dimethylprazine / *2,6-dimetilprazīns* (**39**); 2-ethyl-3-methylpyrazine / *2-etil-3-metilpirazīns* (**40**)
		MD	2-(2-furanylmethyl)-5-methylfuran / *2-(2-furanilmetil)-5-metilfurāns* (**16**)
		MF	nonanal / *nonanāls* (**11**)
		DD	1-(2-furanylmethyl)-1H-pyrrole / *1-(2-furanilmetil)-1H-pirols* (**48**)
Buttery / *Sviesta*	6	LD	2-methylpropanal / *2-metilpropanāls* (**3**)
		LF	
		MD	
		MF	
		DF	2-methylpropanal / *2-metilpropanāls* (**3**); 2-methylbutanal / *2-metilbutanāls* (**2**)
Sweat / *Sviedru*	6	LD	n-(2-cyanoethyl)-pyrrole / *n-(2-ciānetil)-pirols* (**51**)
		LF	
		MD	
		MF	
		DD	
		DF	
Boiled potato / *Vārtītu kartupeļu*	5	LD	1-(2-furanyl)-ethanone / *1-(2-furanil)-etanons* (**30**)
		LF	
		MF	
		DD	
		DF	
Green / *Zaļas zāles*	4	LD	1-dodecanol / *1-dodekanols* (**56**)
		LF	2,3-diethyl-5-methylpyrazine / *2,3-dietil-5-metilpirazīns* (**38**)
		MD	2,2'-methylenebisfuran / *2,2'-metilēnbisfurāns* (**18**); 2,3-diethyl-5-methylpyrazine / *2,3-dietil-5-metilpirazīns* (**38**)
Mushroom / *Sēņu*	4	LD	dimethyl trisulfide / *dimetiltrisulfīds* (**52**)
		LF	
		MF	
		DD	

Aroma Attribute / *Aromāta īpašība*	**Aroma detection frequency** / *Aromāta noteikšanas biežums*	**Coffee sample** / *Kafijas paraugs**	**Volatile compounds associated with the aroma** / *Gaistošie savienojumi saistīti ar aromātu***
Vegetable / *Dārzeņu*	4	LD	1-(2-furanylmethyl)-1H-pyrrole / *1-(2-furanilmetil)-1H-pirols* (**48**); 1-dodecanol / *1-dodekanols* (**56**)
		LF	2,2'-bifuran / *2,2'-bifurāns* (**19**)
		DD	1-(2-furanylmethyl)-1H-pyrrole / *1-(2-furanilmetil)-1H-pirols* (**48**)
Grainy / *Graudu*	3	LF	1-butanol, 3-methyl-acetate / *izoamilacetāts* (**13**)
		MD	tetradecane / *tetradekāns* (**12**)
		DD	2-methylbutanal / *2-metilbutanāls* (**2**)
Smoky / *Dūmu*	3	LD	2-methylbutanal / *2-metilbutanāls* (**2**)
		LF	2-[(methyldithio)methyl]-furan / *2-[(metilditio)metil]-furāns* (**20**)
		MF	nonanal / *nonanāls* (**11**)
Roasted / *Grauzdēts*	2	LF	2-[(methyldithio)methyl]-furan / *2-[(metilditio)metil]-furāns* (**20**); 2-methylbutanal / *2-metilbutanāls* (**2**)
Chemical / *Ķīmisks*	2	LD	2-ethyl-3-methylpyrazine / *2-etil-3-metilpirazīns* (**40**)
		MD	2-ethyl-6-methylpyrazine / *2-etil-6-metilpirazīns* (**42**)
Floral / *Ziedu*	2	MD	benzeneacetaldehyde / *fenilacetaldehīds* (**7**)
		MF	1-(2-furanyl)-2-butanone / *1-(2-furanil)-2-butanons* (**29**)
Caramelised / *Karamelizēts*	1	DD	1-(2-furanyl)-2-butanone / *1-(2-furanil)-2-butanons* (**29**)
Spice / *Pikants*	1	DF	4-ethyl-2-methoxyphenol / *4-etilguaiacols* (**35**)
Sharp / *Asa*	1	LF	benzeneacetaldehyde / *fenilacetaldehīds* (**7**)
Garlic / *Ķiploku*	1	LF	2,2'-bifuran / *2,2'-bifurāns* (**19**)
Waxy / *Vaska*	1	DD	2-ethyl-3-methylpyrazine / *2-etil-3-metilpirazīns* (**40**)
Berry / *Ogu*	1	LF	3-furanmethanol / *3-furānmetanols* (**23**)

[*] The first letter represents the roast level (L–light; M–medium; D–dark); the second letter represents the brewing technique (D–automatic drip; F–French press) / *Pirmais burts apzīmē grauzdēšanas pakāpi (L–viegls; M–vidējs; D–tumšs); otrs burts apzīmē pagatavošanas metodi (D–automātiskā filtra; F–franču preses).*

[**](**n**) represents the number of the compound in line with Appendix 1 / *(n) – kārtas numurs savienojumiem, saskaņā ar 1. pielikumu*

Appendix 3 / *3. Pielikums*

Frequency distribution of consumer coffee consumption habit answers /
Patērētāju atbildes par kafijas patēriņa ieradumiem (frekvences sadalījums)

Coffee consumption habits / *Kafijas patēriņa ieradumi* (%)	**Consumer group** / *Patērētāju grupa* (%)	
	Cluster 1 / *1. Klāsteris*	**Cluster 2** / *2. Klāsteris*
How often do you usually drink coffee? / *Cik bieži Jūs dzeriet kafiju?*		
About 2-3 times per week / *Aptuveni 2-3 reizes nedēļā* (10)	4.4	5.6
About one time per day / *Aptuvei vienu reizi dienā* (43.3)	20	23.3
More than once per day / *Biežāk, kā vienu reizi dienā* (46.7)	25.6	21.1
Where do you usually purchase coffee? / *Kur Jūs viesbiežāk iegādājieties kafiju?*		
I am not purchasing the coffee / *Es neiegādājos kafiju* (7.8)	2.2	5.6
Local market / *Vietējā tirgū* (5.6)	3.3	2.2
Local mini mart / *Vietējā mini veikalā* (1.1)	1.1	0
Restaurant/cafeteria / *Restorānā/kafejnīcā* (5.6)	1.1	4.4
Specialty coffee shop / *Specialty kafijas veikalā* (32.2)	17.8	14.4
Supermarket / *Lielveikalā* (47.8)	24.4	23.3
Where do you usually drink coffee? / *Kur Jūs visbiežāk dzeriet kafiju?*		
At home / *Mājās* (42.2)	22.2	20
At work / *Darbā* (34.4)	13.3	21.1
In a coffee shop / *Kafejnīcā* (10)	7.8	2.2
On my way to work/home / *Ceļā uz darbu/mājām* (12.2)	5.6	6.7
Other / *Citur* (1.1)	1.1	0
In your opinion, what specialty coffee means? / *Jūsuprāt, ko nozīmē specialty kafija?*		
Coffee with a cup score of 80+ points / *Kafija ar kvalitātes novērtējumu 80+ punktiem* (3.3)	2.2	1.1
Flavored coffee drinks which usually can buy in coffee shops / *Kafijas dzērienu kokteiļi, kurus pagatavo kafejnīcās* (26.7)	16.7	10
I don't know / *Es nezinu* (6.7)	2.2	4.4
Organic/ Fair trade coffee (5.6)	4.4	1.1
Other / *Cits* (4.4)	0	4.4
"Gourmet" high-quality coffee / *Gurmentu augstas kvalitātes kafija* (53.3)	24.4	28.9
What kind of coffee do you usually drink? / *Kā kafiju Jūs visbiežāk dzeiriet?*		
Automatic drip / *Filtra kafijas automata* (54.4)	25.6	28.9
Cold brew / *Auksti brūvēta kafija* (4.4)	2.2	2.2
Espresso / *Espresso* (3.3)	2.2	1.1
Frappuccino or blended drink / *Frapučino un miksēti kafijas dzērieni* (3.3)	0	3.3
French press / *Franču preses kafija* (10)	6.7	3.3
Latte or Cappuccino / *Espresso bāzes, piena dzērieni* (20)	10	10
Other / *Cits* (2.2)	1.1	1.1
Pour over / *Filtra kafija* (2.2)	2.2	0
In your opinion, what kind of effect coffee has on health? / Jūsuprāt, kāda ir kafijas ietekme uz veselību?		
I don't know / *Es nezinu* (3.3)	1.1	2.2
It depends on how much is consumed / *Tas ir atkarīgs no uzņemtā kafijas daudzuma* (70)	33.3	36.7
Negative / *Negatīva* (2.2)	0	2.2
Positive / *Pozitīva* (24.4)	15.6	8.9

Appendix 4 / *4. Pielikums*

Penalty analysis of coffee brew penalty analysis / *Penalty analīze kafijas dzērienu sensorajām īpašībām* (Laukaleja & Koppel 2021)

Sample / *Paraugs*	**Consumer group** / *Patērētāju grupa*	**Taste** / *Garša*	**Level** / *Līmenis*	**Frequencies** / *Biežums, %*	**Overall like score** / *Patikšanas novērtējums*	*"Mean drops"*	*"Penalties"*	**p-value** / *p-vērtība*
LD	Cluster 1 / *1. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	15.56	7.00	-0.04	-	-
			JAR	53.33	6.96	-	1.24	0.01
			Too sour / *Pārāk skābs*	31.11	5.07	1.89	-	0.00
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	24.44	6.18	0.99	-	0.15
			JAR	51.11	7.17	-	1.63	0.00
			Too bitter / *Pārāk rūgts*	24.44	4.91	2.27	-	0.00
	Cluster 2 / *2. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	11.11	4.60	1.20	-	-
			JAR	22.22	5.80	-	2.40	0.00
			Too sour / *Pārāk skābs*	66.67	3.20	2.60	-	0.00
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	8.89	5.75	-0.11	-	-
			JAR	31.11	5.64	-	2.48	< 0.00
			Too bitter / *Pārāk rūgts*	60.00	2.78	2.87	-	< 0.00
LF	Cluster 1 / *1. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	13.33	6.67	0.30	-	-
			JAR	68.89	6.97	-	0.90	0.01
			Too sour / *Pārāk skābs*	17.78	5.63	1.34	-	-
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	15.56	6.714	0.12	-	-
			JAR	68.89	6.84	-	0.48	0.16
			Too bitter / *Pārāk rūgts*	15.56	6.00	0.84	-	-
	Cluster 2 / *2. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	13.33	3.50	1.50	-	-
			JAR	13.33	5.00	-	2.05	0.00
			Too sour / *Pārāk skābs*	73.33	2.85	2.15	-	0.00
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	17.78	3.75	0.08	-	-
			JAR	26.67	3.83	-	0.83	0.11
			Too bitter / *Pārāk rūgts*	55.56	2.76	1.07	-	0.05

Continued appendix 4 / *4. Pielikuma turpinājums*

Sample / *Paraugs*	**Consumer group** / *Patērētāju grupa*	**Taste** / *Garša*	**Level** / *Līmenis*	**Frequencies** / *Biežums, %*	**Overall like score** / *Patikšanas novērtējums*	*"Mean drops"*	*"Penalties"*	**p-value** / *p-vērtība*
MD	Cluster 1 / *1. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	13.33	5.83	1.12	-	-
			JAR	44.44	6.95	-	1.31	0.01
			Too sour / *Pārāk skābs*	42.22	5.58	1.37	-	0.01
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	17.78	6.38	0.36	-	-
			JAR	57.78	6.73	-	1.20	0.03
			Too bitter / *Pārāk rūgts*	24.44	4.91	1.82	-	0.00
MD	Cluster 2 / *2. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	11.11	3.40	2.99	-	-
			JAR	28.89	6.39	-	2.82	< 0.00
			Too sour / *Pārāk skābs*	60.00	3.59	2.79	-	< 0.0001
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	8.89	5.50	0.11	-	-
			JAR	40.00	5.61	-	2.06	0.00
			Too bitter / *Pārāk rūgts*	51.11	3.22	2.39	-	0.00
MF	Cluster 1 / *1. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	17.78	5.88	0.54	-	-
			JAR	53.33	6.42	-	1.18	0.03
			Too sour / *Pārāk skābs*	28.89	4.85	1.57	-	0.01
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	22.22	6.50	-0.12	-	0.98
			JAR	46.67	6.38	-	0.96	0.08
			Too bitter / *Pārāk rūgts*	31.11	4.64	1.74	-	0.01
	Cluster 2 / *2. Klāsteris*	Sourness / *Skābums*	Not sour enough / *Nav pietiekams skābs*	13.33	3.50	1.50	-	-
			JAR	13.33	5.00	-	2.05	0.00
			Too sour / *Pārāk skābs*	73.33	2.85	2.15	-	0.00
		Bitterness / *Rūgtums*	Not bitter enough / *Nav pietiekams rūgts*	17.78	3.75	0.08	-	-
			JAR	26.67	3.83	-	0.83	0.11
			Too bitter / *Pārāk rūgts*	55.56	2.76	1.07	-	0.05