Norwegian University of Life Sciences

**Master's Thesis 2023 60 ECTS**

Faculty of Chemistry, Biotechnology and Food Science

# Determination of volatile emissions from indoor wood surfaces

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Chemistry

# Acknowledgement

This master project was a collaboration between the Norwegian University of Life Sciences (NMBU) and the Climate and Environmental Research Institute (NILU). The analytical method development, chemical analysis and statistical data evaluation were conducted at NILU. The master thesis was carried out from November 2022 until August 2023, and it represents 60 ECTS of a 120 ECTS master's degree in chemistry.

I would like to express my sincere gratitude to my supervisors, Professor Roland Kallenborn and Pawel Rostkowski, for your support and guidance during the process. Thank you for the opportunity to work with this challenging and rewarding thesis and for providing me with all the necessary resources to finish the project.

I am grateful to my co-supervisor, PhD Candidate Ingrid Bakke, for providing laboratory samples, guiding through the sampling process, and motivating me throughout the project. I greatly appreciate all your help.

My greatest appreciation also goes to Alexander Håland, who always found time to help me if I struggled with GC-instrument or had any questions about the theoretical parts of my thesis. I would also like to thank Anders Røsrud Borgen, Hans Gundersen and Norbert Schmidbauer for helpful feedback and suggestions during the analytical method development phase.

Lastly, I am deeply thankful to my friends and family. Thank you for all your support and patience during this period. Without your encouragement and love, I would not have been able to achieve my goals.

August 2023, Ås

Indre Tarvydaite

# Abstract

Wood is an important material widely utilised in construction, furniture manufacturing as well as for floor and wall coating in indoor environments. To improve material durability and for preservation purposes, wood materials are often modified with different additives and coatings that can affect indoor air quality (IAQ). Therefore, there was an interest in uncovering if treated wood surfaces emit anthropogenic volatile organic compounds (VOCs) such as xylene, toluene, and ethylbenzene, commonly found in different wood finishes. At the same time, wood naturally emits diverse groups of fatty acid derivatives, aldehydes or/and terpenes that can elevate VOC levels in indoor environments. Hence, the biogenic VOCs such as α-pinene, β-pinene, hexanal, d-limonene, and 3-carene, were quantified to determine the magnitude of the biogenic emissions.

The object of this project was to develop and validate an analytical method suited for the GC-HR-QTOF-TDU system. Acknowledging that VOC emissions from wood are not sufficiently characterised, the project aimed to determine emission profiles based on targeted compound quantification and non-targeted screening of unknown compounds. The project analysed three different Norway spruce samples (*Picea abies*): untreated interior panel (USP), cross-laminated timber (CLT) and stained interior panel (SSP). The test parameters utilised for this project were based on European Standard NS-EN 16516:2017+A1. The climate chamber method was used to determine the VOCs emitted from the laboratory samples, and the air samples were collected three days after the test specimens were placed in the chambers.

Results for three laboratory samples demonstrated that hexanal had the highest emissions (80.07-3.00µg/$m^3$) followed by α-pinene (45.4-1.9µg/$m^3$), β-pinene (15.4-0.32µg/$m^3$), 3-carene (7.3-0.04µg/$m^3$) and d-limonene (3.9-0.007µg/$m^3$). The concentration of the compounds was highest in the USP and CLT samples. Concentrations of the VOCs were noticeably variating between the duplicates of the same laboratory sample, demonstrating that chambers used for the analysis could have had contamination issues or that variations were caused by the loss of analyte due to insufficient vacuum chamber sealing. Lower concentrations of hexanal and α-pinene were determined in the SSP, suggesting that treating the wood surface can contribute to lower biogenic monoterpene and aldehyde emissions. However, further investigation should be conducted to confirm the assumption.

The Suspect and Non-target screening (SUS and NTS) revealed that alkanes were the most dominant chemical group identified in SSP (29%), CLT (31%) and USP (37%). The most abundant alkanes identified were 2,3-dimethylpentane, 2-methylhexane, methylcyclohexane, 3-metylhexane and heptane. The compounds were not identified in chamber blanks implying that the alkane emissions could be caused by contamination of the sample surface from anthropogenic sources. Terpenes contributed to 7-10% of VOC emissions, and the most abundant terpenes identified were the targeted β-pinene, α-pinene, d-limonene, 3-carene, and non-targeted β-myrcene and o-cymene. Aldehydes contained 5-8% of total VOC emissions in laboratory samples. The most abundant aldehydes identified by the unknown analysis were heptanal, nonanal, decanal, pentanal and targeted hexanal.

# Sammendrag

Trematerialе er mye brukt i konstuksjon, møbelproduksjon samt til gulv- og veggklednings meteriale innendørs. For å forbedre materialets holdbarhet og for konserveringsformål, behandles ofte trevirke med forskjellige tilsetningstoffer og belegg som kan føre til endring av inneluftkvaliteten (IAQ). Derfor var det ønske å definere om behandlet treoverflater slipper ut antropogene flyktige organiske forbindelser (VOCs) som xylen, toluen og etylbenzen, siden stoffene er en vanlig ingredient i f.eks. maling eller beis som brukes for å behandle trevirke. Samtidig, tre emitterer forskjellige grupper av fettsyrederivater, aldehyder eller/og terpener som kan øke VOC-nivået i innemiljø. Derfor ble biogene VOC-ene som f.eks. α-pinen, β-pinen, heksanal, d-limonen og 3-carene, kvantifisert for å definere mengden av biogene utslippene.

Målet med dette prosjektet var å utvikle og validere en analysemetode for GC-HR-QTOF-TDU-systemet. Siden VOC-utslippene fra tre ikke er tilstrekkelig karakterisert, hadde prosjektet som mål å bestemme kjemiske utslippsprofiler basert på «targeted» og «non-targeted» analyser av VOC-er. Prosjektet fokuserte på å analysere tre ulike granprøver (*Picea abies*): ubehandlet interiørpanel (USP), krysslimt tre (CLT) og beiset interiørpanel (SSP). Testparameterne som ble brukt i dette prosjektet var basert på europeisk standard NS-EN 16516:2017+A1. Klimakammermetoden ble brukt for å bestemme VOC-utslippene fra trevirke, og luftprøvene ble samlet tre dager etter at prøvene ble plassert i klimakamrene.

Etter analysen av tre laboratorieprøver, ble det avklart at heksanal hadde de høyeste utslippene (80,07-3,00 µg/m$^3$) etterfulgt av α-pinen (45,4-1,9 µg/m$^3$), β-pinen (15,4-0,32 µg/m$^3$), 3-carene (7,3-0,04 µg/m$^3$) og d-limonen (3,9-0,007µg/m$^3$). Høyest konsentrasjon av VOC-ene ble funnet i ubehandlet granpanel og krysslimt tre. Konsentrasjonene av VOC-ene hadde en stor variasjon mellom duplikatene av den samme laboratorieprøven, noe som kan antyde at kamrene som ble brukt til analysen hadde kontamineringsproblemer eller at variasjonen ble forårsaket av analytt tap på grunn av utilstrekkelig vakuumkammerforsegling. Lavere konsentrasjoner av heksanal og α-pinen ble identifisert i det beisede granpanelet, noe som kan tyde på at behandling av treoverflaten kan bidra til lavere emisjoner av biogene monoterpener og aldehyder. Allikevel, mer omfattende utslippsanalyser av behandlede treoverflater burde gjennomføres for å bekrefte antagelsen.

«Suspect» og «Non-targeted»- screeningen (SUS og NTS) identifiserte alkaner som den mest dominerende gruppen funnet i SSP (29 %), CLT (31 %) og USP (37 %). De hyppigst forekommende alkanene som ble identifisert var 2,3-dimetylpentan, 2-metylheksan,

metylcykloheksan, 3-metylheksan og heptan. Forbindelsene ble ikke identifisert i blindprøver, noe som kan tyde på at alkanutslippene kan være forårsaket av kontaminering av prøveoverflaten fra antropogene kilder. Terpener bidro til 7-10% av VOC-utslippene, og de mest dominerende terpenene som ble identifisert var «tageted» β-pinen, α-pinen, d-limonen, 3-carene og «non-targeted» β-myrcen og o-cymen. Aldehyder inneholdt rundt 5-8% av de totale VOC-utslippene i laboratorieprøver. De hyppigst forekommende aldehyder identifisert av NTS og SUS var heptanal, nonanal, decanal, pentanal og hexanal.

# Abbreviations

BREEAM - Building Research Establishment Environmental Assessment Methodology

BTEX - Benzene, toluene, ethylbenzene and xylene

CI - Chemical Ionisation

CMR - Carcinogenic, Mutagenic, Reprotoxic

CTL - Cross-laminated tree

DAMPP - Dimethylallyl pyrophosphate

EI - Electron Ionisation

EU - LCI- European Union-Lowest Concentration of Interest

eV - Electron Volt

GC - Gas Chromatography

HR - High Resolution

IPP - Isopentenyl pyrophosphate

ISO - International Organisation for Standardization

M/z - Mass over charge ratio

MEP- Methylerythritol phosphate

MS - Mass Spectrometry

MVA - Mevalonic acid

NIST - National Institute of Standards and Technology

NTS - Non-target screening

PCDL - Personal Component Database and Library

QTOF - Quadrupole Time of Flight

RH - Relative Humidity

RI - Retention Index

SBS - Sick building syndrome

SD - Standard deviation

SOA- Secondary organic aerosols

SSP - Stained spruce panel

SUS - Suspect screening

SVOC - Semi -volatile organic compound

USP - Untreated spruce panel

VOC - Volatile organic compounds

VVOC - Very volatile organic compounds

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# 1 Introduction

## 1.1 Volatile organic compounds

Based on the definition given by US-EPA, volatile organic compounds (VOCs) are carbon-based organic compounds, excluding CO, $CO_2$, $H_2CO_3$, $(NH_4)_2CO_3$, and metallic carbines or carbonates, that can easily evaporate under normal indoor temperature and pressure conditions (EPA, 2022). The overview written by US-EPA divides VOCs into three main groups based on their boiling point range: very volatile organic compounds (VVOCs) have a boiling point <0-50°C to 100°C, VOCs between 50-100°C to 260°C and semi-volatile organic compounds (SVOCs) over 240°C to 400°C (EPA, 2022). However, the European Standard EN 16516:2017+A1 has a different approach when defining the VOCs. The standard defines VOCs as compounds eluting between n-hexane and n-hexadecane when separated by a capillary GC-column consisting of 5% phenyl 95% methyl polysiloxane phase (European Committee For Standardization, 2017).

VOCs are found in both biogenic and anthropogenic sources. Biogenic VOCs originate mainly from green vegetation and are essential for plant-to-plant or plant-to-animal /microorganism interactions (Peñuelas et al., 2014). Biogenic VOCs serve communication or signalling purposes in ecosystems or act as bioactive growth-promoting or growth-inhibiting agents (Peñuelas et al., 2014).

Biogenic VOC emissions from wood depend on different abiotic factors such as temperature, humidity, soil, or geographic location. Additionally, the VOC emission levels differ based on age and the wood species. Generally, wood emits VOCs as terpenes, terpenoids, benzenoids, fatty acid derivatives, aliphatic aldehydes, and ketones (Adamová et al., 2020; Holopainen & Gershenzon, 2010). Softwood emits higher amounts of VOC (compared to hardwood) and contains mainly mono- and tetraterpenes; most common terpenes are α-, β-pinene and limonene, δ-carene, camphene, myrcene and β-phellandrene (Hyttinen et al., 2010).

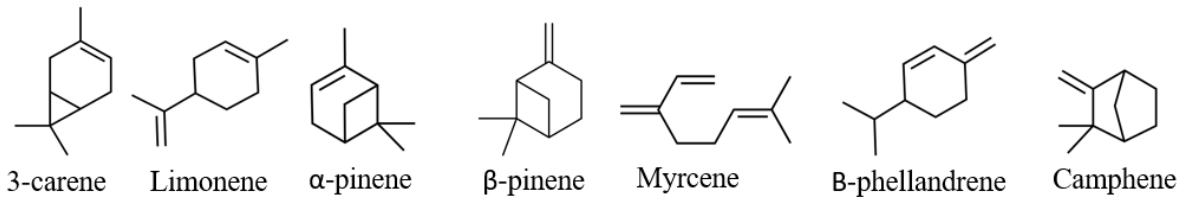



*Figure 1.1 Chemical structure of most common terpenes found in softwood.*

The highest VOC emissions are found in freshly cut trees, and emission from a wood surface decreases during the drying and storage of the wood materials (Hyttinen et al., 2010). Parts of tree correlating to the highest VOC emissions are resin, resin canals and conifers in softwood (Pohleven et al., 2019). Therefore, softwood accommodates significantly higher terpenoid emissions compared to hardwood that does not contain resin ducts.

Human activities, such as manufacturing, refining petroleum, transportation, or fuel combustion, are the primary sources of anthropogenic VOCs. Generally, anthropogenic VOCs consist mainly of aromatic compounds and alkanes (Rissanen, 2021). BTEX are one of the anthropogenic VOCs commonly observed in ambient air and indoor environments. These aromatic hydrocarbons can be extracted and isolated by liquid-liquid extraction with the organic solvent like sulfolane and polyglycols or synthesised by aromatisation of light olefins (e.g., ethylene or propylene) (Ke et al., 2022; Larriba et al., 2014). BTEX have many applications and is an additive in different coatings, adhesives, dyes, paints, solvent, pesticides, and rubber cement. Moreover, BTEX are widely used in the synthesis of other chemical product in pharmaceutical and chemical industries and fuel formulations (Bolden et al., 2015). These aromatic compounds are also identified in heated tobacco products and have highly negative health effects in humans.

### 1.2 Terpenes and the formation of secondary organic aerosols

Terpenes are one of the most common VOCs found in ambient air and softwood like pine and spruce. Terpenes are derived from $C_5$ isoprene units, and the $C_5$ units are derived from either mevalonic acid (MVA) or methylerythritol phosphate (MEP) (Dewick, 2009). The MEP pathway is more common in plants than the MVA pathway. Pyruvic acid and glyceraldehyde 3-phosphate are intermediates for MEP and, with the assistance of various enzymatic reactions, are converted to isopentenyl pyrophosphate (IPP) and a dimethylallyl pyrophosphate (DAMPP) $C_5$ units (Dewick, 2009). The phosphate group on the IPP and DAMPP is a good leaving group, resulting in easier biosynthesis of various terpenoids.

Mono ($C_{10}H_{16}$) and sesquiterpenes ($C_{15}H_{24}$) are the most abundant terpenes in plants. These compounds contain double bonds that make mono and sesquiterpenes reactive with oxidative agents like $NO_3$, ozone or OH radicals and form secondary organic aerosols (SOA) (Król et al., 2014). Naturally emitted terpenes contribute to around 70% of SOA emissions (Wu et al., 2020).

Human activities can also result in the formation of SOA. Anthropogenic sesquiterpenes contribute to around 30% formation of SOA; however, in some countries, the contribution can be as high as 50% (Granström, 2010; Wu et al., 2020). The primary anthropogenic sources of terpenes are biofuels, paints, glues, adhesives, and additives used to treat wooden building materials, walls, or furniture.

Oxidative reactions of terpenes contribute to the formation of Photo-oxidants (Granström, 2007). Oxidants like aldehydes, peroxides and other radicals can form ground-level ozone, which can cause forest and crop damage (Granström, 2007). Ground-level ozone can negatively affect human health and cause respiratory tract irritation. The impact of VOC is usually determined by the reactivity of the compound and not necessarily by the emission levels. Since terpenes are highly reactive, they have a higher environmental impact. Secondary aerosols formed from terpenes contribute to cloud formation and affect climate (Granström, 2007).

### 1.3 Aldehydes

Aldehydes are the second most abundant VOCs emitted from plants and trees. Aldehydes are organic compounds with at least one hydrogen bonded to the carbon of the carbonyl group at the end of the carbon chain (Hart et al., 2012). Aldehydes are formed during autoxidation and photo-oxidation of unsaturated fatty acids (Granström, 2010). Auto-oxidation is a self-catalysing, free-radical chain reaction (Granström, 2010). The chemical reaction starts after cutting since the damaged wood surface is more accessible to oxygen that can oxidise fatty acids. During oxidation, fatty acid-free radicals are formed, which can easily react with oxygen and form fatty acid hydroperoxides. During homolytic cleavage, hydroperoxides lose the OH group, forming alkoxy radicals that can form aldehydes. The autoxidation reaction continues until all radicals have been neutralised (Granström, 2010).

Large amounts of aldehydes found in softwood are the results of the oxidation of unsaturated lipid compounds like oleic acid (18:0, n-9), linoleic acid (18:2, n-6) or α- linoleic acid (18:3, n-3) (Granström, 2010). Investigation of biogenic VOCs carried out by Müller et al. (2006) states that the most common aldehydes emitted from Norway spruce in German forests are acetone, formaldehyde and acetaldehyde (Müller et al., 2006). The emissions of aldehydes depended on the temperature and humidity level, and higher levels of aldehyde emissions were generally determined in higher temperatures with daylight. Higher levels of aldehydes were determined in the canopy region, while lower levels are stated to be above the crown of the Norway spruce (Müller et al., 2006).

## 1.4 Health effects of volatile organic compounds

A survey from 2010 conducted by Statistics Norway revealed that Norwegians spend around 21 hours indoors (Vaage, 2012). Different pollutants tend to accumulate in poorly ventilated indoor environments, and as a result, compounds such as formaldehyde, toluene, benzene or styrene could be up to 5 times higher compared to outdoor concentrations (EPA, 2023). Consequentially, indoor air quality (IAQ) directly correlates to residents' health and well-being.

In the last decade, more emphasis has been put on reducing negative environmental impact by replacing concrete and metal with more sustainable building materials (Sandoli et al., 2021). Subsequently, wood-framed buildings have become more popular since wood is a renewable material and contributes to reducing the carbon footprint (Sandoli et al., 2021). Moreover, the scent of wood often has positive associations and evokes a feeling of comfort and relaxation. Analysis conducted by Zhang et al. (2017) on human physiological response to a wooden indoor environment observed that participants exposed to a wooden environment had lower blood pressure. Furthermore, lower stress levels and a positive effect on eye fatigue regulation were observed in participants staying in wooden rooms compared to test participants in non-wooden environments (Zhang et al., 2017). An investigation on rats conducted by Akutsu et al. (2002) discovered that α-pinene had elongated nocturnal resting periods and suppressed stress-induced hyperthermia. Some wood species were identified to contain antimicrobial properties. A study conducted by Kotradyova et al. (2019) on wood's impact on healthcare facilities concluded that wood positively influenced patients' physiological function. Moreover, a test of microbiological activity on wood surfaces showed that after 20h, untreated oak had less microbiological activity compared to laminate surface, revealing the antimicrobial effects of some wood species (Kotradyova et al., 2019).

On the other hand, people living in poorly ventilated indoor spaces can experience more noticeable adverse health effects. Consumer products such as personal care products and fragrances can elevate indoor VOC levels (Adamová et al., 2020). Furniture coated with formaldehyde-based resins, treated building materials, mould and wood rot is one of the primary sources of VOCs (Adamová et al., 2020). If paints, glues, coatings and additives used to alter wood and other building materials are not selected cautiously, they can negatively affect the health of the occupants (Adamová et al., 2020). Above-average VOC levels are one of the reasons that cause "Sick building syndrome" (SBS) (Brinke et al., 1998). Typical symptoms of SBS are fatigue, headache, eye and nose irritations, skin itchiness, and difficulty breathing

(Brinke et al., 1998). This results in reduced productivity or concentration problems, and extreme cases can cause long-term health problems (Brinke et al., 1998).

Formaldehyde is a frequent compound in wood coatings, paints, and glues. In addition, formaldehyde is naturally emitted from softwood and is a well-known irritant and carcinogen. Secondary formaldehyde emissions occurring from oxidation between ozone and terpenes can also contribute to hazardous levels of VOCs (World Health Organization, 2010). Formaldehyde concentrations between 0.94mg/$m^3$ and 1.25mg/$m^3$ can cause eye and upper airway irritation (World Health Organization, 2010). A long-term-exposure experiment on rats revealed that formaldehyde concentrations above 2.5mg/$m^3$ caused nasal cancer (World Health Organization, 2010). Due to evidence of adverse effects on test animals, formaldehyde has been classified as a carcinogenic compound to humans, and the emissions in indoor environments are regulated.

Compounds such as BTXS (benzene, toluene, xylene, styrene), naphthalene, ammonia, pinenes and limonene are other types of VOCs commonly identified indoor air due to their wide application in cleaning products, varnishes, paints or solvents (Sarigiannis et al., 2011). Benzene and naphthalene are anthropogenic VOCs found in tobacco products, building materials, furniture and vehicle exhaust (World Health Organization, 2010). Benzene is a carcinogenic compound, and based on World Health Organization (2010), no safe exposure level of benzene exists. Naphthalene is another carcinogenic aromatic hydrocarbon that, based on evidence from animal testing, is classified as a suspected human carcinogen (World Health Organization, 2010). A Literature review by Adamová et al. (2020) revealed that high concentrations of VOCs such as α-pinene, β-pinene, limonene, hexanal and decanal cause respiratory system, eye and skin irritation. VOC concentrations up to 25,000µg/$m^3$ may cause negative health effects such as headaches and discomfort (Adamová et al., 2020). However, research on monoterpene exposure and health effects are conflicting since monoterpenes have known physiological and psychological benefits (Alapieti et al., 2020). Therefore, the health effects purely depend on the compound concentrations and the complete chemical composition of the VOCs found indoors.

## 1.5 VOC emission regulations in wooden building materials

Wood-based construction materials are widely utilised in Norway and the rest of Europe. The EU have established No 305/2011 regulation stating that construction material manufacturers need to consider indoor air emission; however, no particular concentration of VOC emissions is provided in the document. Even though the EU provides general guidelines, different countries may have specific regulations considering VOC emissions, making the export of more sustainable building materials challenging. In Germany, manufacturers must provide a complete chemical composition of the building material, which must be approved by *Deutsches Institut für Bautechnik* (Bulian, 2016). The VOC emissions are required to be expressed as total volatile organic compounds (TVOCs), excluding carcinogenic compounds. Concentrations of carcinogenic compounds are obligatory to define individually. France has adopted mandatory labelling of VOC emissions from building materials (Bulian, 2016). The legislation highlights emission limits of ten individual substances and TVOC emissions. The regulation state that products can be placed on the market if emissions of carcinogenic, mutagenic and reprotoxic (CMR) compounds after 28 days are lower than 1µg/$m^3$ (Bulian, 2016). A list of the regulated VOC emissions in France are provided in Table 1.5.1.

*Table 1.1 VOC emission limits of selected compounds in France (Bulian, 2016).*

| **Compound** | **Class A+ µg/$m^3$** | **Class A µg/$m^3$** | **Class B µg/$m^3$** | **Class C µg/$m^3$** |
|---|---|---|---|---|
| **Formaldehyde** | <10 | <60 | <120 | >120 |
| **Acetaldehyde** | <200 | <300 | <400 | >400 |
| **Toluene** | <300 | <450 | <600 | >600 |
| **Tetrachloroethylene** | <150 | <350 | <500 | >500 |
| **Xylene** | <200 | <300 | <400 | >400 |
| **Trimethyl benzene** | <1000 | <1500 | <2000 | >2000 |
| **Dichloro benzene** | <60 | <90 | <120 | >120 |
| **Ethyl benzene** | <750 | <1000 | <1500 | >1500 |
| **Butoxy ethanol** | <1000 | <1500 | <2000 | >2000 |
| **Styrene** | <250 | <350 | <500 | >500 |
| **TVOC** | <1000 | <1500 | <2000 | >2000 |

Buildings with environmentally sustainable materials are gaining more attention; therefore, certification systems like BREEAM have become common. BREEAM certification is internationally recognised and defines limits for TVOC emissions after 28 days. Formaldehyde and other carcinogenic compound limits are defined for emissions after 3 or 28 days (BREEAM-NOR, 2016). The certificate describes requirements for products like wooden flooring, timber structures and wood panels, and the certification is based on various standards such as ISO16000-9, EN 161516 or/and EN 717:2004.

European Union's lowest concentration of interest (EU-LCI) reference values provide general thresholds for the concentration of VOC emissions after 28 days of exposure. The reference values provided in the EU-LCI were obtained by the test chamber procedure based on the EN161516 standard (European Commission, 2021).

*Table 1.2 Agreed EU-LCI values of VOCs commonly identified in softwood (European Commission, 2021).*

| Compound | EU-LCI values (µg/m$^3$) |
|---|---|
| **3-Carene** | 1500 |
| **A-Pinene** | 2500 |
| **B-Pinene** | 1400 |
| **Limonene** | 5000 |
| **Other terpene hydrocarbons** | 1400 |
| **Pentanal** | 800 |
| **Hexanal** | 900 |
| **Furfural** | 10 |

Establishing legislation suitable for wood emissions is essential to achieve more environmentally sustainable buildings. Several compounds that are relevant for wood emissions have insufficient data. Therefore, more focus should be on compound identification and analysis for wooden materials.

## 1.6 Gas Chromatography and Mass Spectrometry

Gas Chromatography is an analytical technique that involves sample vaporisation in the heated GC instrument and analyte separation by the suitable stationary phase. Separation is based on analyte distribution between the mobile and stationary phases (Sparkman et al., 2011). A carrier gas (mobile phase) such as helium or hydrogen is utilised to introduce and force analytes through the CG column, where analytes are separated from each other and eluted from the column. Most GC utilises capillary columns with a stationary phase coating the inner wall (Sparkman et al., 2011). Capillary columns can be purchased with different lengths and stationary phase characteristics that separate compounds based on their physicochemical properties, such as boiling point and polarity. Compounds with high vapour pressure and no extensive interactions with the stationary phase will elute first from the column, resulting in low retention time (RT). After elution, carrier gas forces the compound to a detector that converts the analytical signals into chromatographic data that can be interpreted. GC instruments achieve results in a wide temperature range (<0$^o$C to <400$^o$C); therefore, the separation technique is widely utilised in fields such as environmental analysis, food safety, biotechnology, pharmaceutical chemistry, forensic science or/and geoscience (Sparkman et al., 2011).

The configuration of the GC instrument varies and depends on which type of results are desired. Detectors such as thermal conductivity (TCD), flame ionisation (FID), electron capture (ECD), flame photometric (FPD), and nitrogen-phosphorus detector (NPD) are specifically designed for the GC system (Sparkman et al., 2011). However, Triple Quadrupole (QqQ) or Time-of-Flight (TOF) are becoming more common mass selective detectors coupled together with the GC instrument.

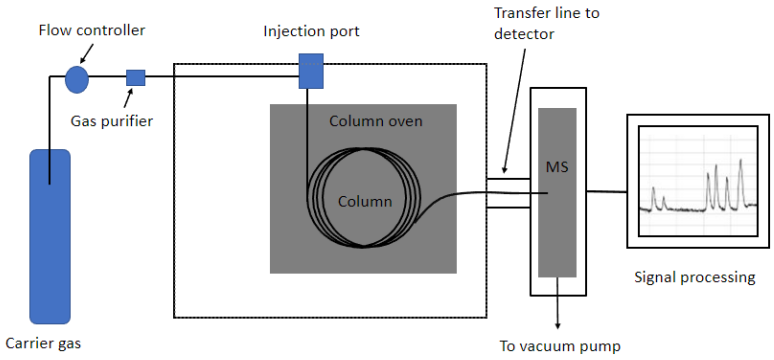



*Figure 1.2. Simplified schematic diagram of GC-MS system. A schematic diagram was produced based on information adapted from Sparkman et al. (2011).*

## 1.7 Mass spectrometry

A mass spectrometer (MS) is a type of detector that provides structural identification of separated components (Sparkman et al., 2011). Data obtained can be utilised for qualitative and quantitative purposes since the MS produce fragment patterns unique for each compound (Sparkman et al., 2011). In order to obtain spectral information, compounds are ionised before entering the MS detector. The most common ionisation techniques in GCMS are electron impact (EI) and chemical ionisation (CI).

MS separate the fragmented ions according to their mass-to-charge ratio (m/z). The m/z ratio of one charge ions represents the molecular mass of the fragments produced in the ionisation source (Sparkman et al., 2011). The most common mass analysers used in MS are TOF and quadrupole. These analysers can be used individually or in a union, called tandem MS, to achieve better mass selectivity and greater resolution data (Sparkman et al., 2011).

### 1.7.1 Ionisation techniques

Electron impact (EI) is one of the most common ionisation techniques used in GC-MS. EI is defined as a "hard" ionisation technique since it results in extensive fragmentation of molecules. EI source consists of a filament heated by a high-energy electric current (Usually 70eV) (Sparkman et al., 2011).

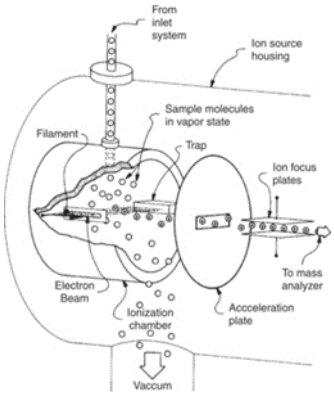



*Figure 1.3 Schematic presentation of EI ion source. The figure was adapted from Sparkman et al. (2011).*

The analyte vapour (M) is introduced into an ionisation source where high energy filament results in the loss of an electron, creating a molecular ion ($M^{+\cdot}$) (E. de Hoffmann & V. Stroobant, 2007). The filament is made of a metal such as tungsten to withstand high temperatures in the ion source. The molecular ions accelerate towards the anode and collide with other gaseous molecules in the ion source (E. de Hoffmann & V. Stroobant, 2007). Loss of the electron results in an ion with an unpaired electron high in internal energy. High-energy ions are unstable and, as a result, break into smaller, more stable fragments to lower their energy state, creating a pattern that can be converted into MS data (Harris, 2016).

$$M + e^-_{70eV} \rightarrow M^{+\cdot} + e^-_{\sim 55eV} + e^-_{0.1eV} \quad (1)$$

An ionisation energy of 70eV is commonly applied in EI since the maximum amount of ions is produced at this voltage. As a result, more fragmentation and greater molecular information can be achieved at 70eV (Sparkman et al., 2011). On the other hand, extensive fragmentation can often result in the loss of molecular ion, making structural annotation of the compound challenging. Sparkman et al. (2011) state that 10eV is enough to ionise most organic molecules. However, operating RI below 70eV reduces the ion efficiency and the ability to lead the electrons to the ionisation chamber. Some solutions exist to circumvent the extensive fragmentation issue. The first solution is the high-efficiency ion source that allows the fragmentation at lower ionisation energy. Agilent Technologies has developed a modified lens

geometry with a filament position in-line with the ion beam (Kranenburg et al., 2020). The modification enables efficient fragmentation in low eV and improves molecular ion intensity (Kranenburg et al., 2020).

Another option is to utilise Chemical ionisation (CI) to obtain additional spectral information. The CI produces less fragmentation and can be a complementary technique in cases where EI cannot obtain the molecular ion. In CI, reagent gases like methane, ammonia or isobutane are introduced into the reaction chamber, undergo electron ionisation, and generate molecular ions (Smith, 2013). The molecular ions then will continue colliding with other reagent gas molecules, resulting in further fragmentation (E. de Hoffmann & V. Stroobant, 2007). Constant pressure must be maintained inside the ion source to ensure proper fragmentation.

Different fragmentation results can be achieved depending on the type of chemical reaction used in CI and the type of reagent gas. Molecules protonated by $CH_5^+$ reagent ion result in more fragmentation because of the high difference in proton affinity between methane and the analyte molecule (Sparkman et al., 2011). Using $NH_4^+$ protons produced by ammonia results in less fragmentation since the difference between proton affinity is reduced (Sparkman et al., 2011).

### 1.7.2 Time-of-Flight

Ions produced by EI or CI can be separated and detected by TOF based on their travel time in the TOF tube. Externally produced ions are directed to the source, where ~20 000V energy is applied to the backplate repeller to accelerate the ions towards the drift region (Harris, 2016). After ions reach a drift region, no electric field and further hastening of ions are applied. Theoretically, all ions have approximately the same kinetic energy and can be separated based on their m/z ratio. Lighter ions will travel through TOF faster and be detected before the heavier ions (Harris, 2016). Modern TOF analysers have reflectrons (electrostatic mirrors) to improve the resolving power. The reflectron slows down the ions and reflects them to the other side of the tube where the detector is installed (Allen & McWhinney, 2019). The reflectron corrects for the small dispersion in kinetic energy; therefore, all ions with the same m/z will reach the detector simultaneously despite the difference in kinetic energy. The reflectron increases the flight path length; thus, a higher mass resolution can be achieved (Allen & McWhinney, 2019).

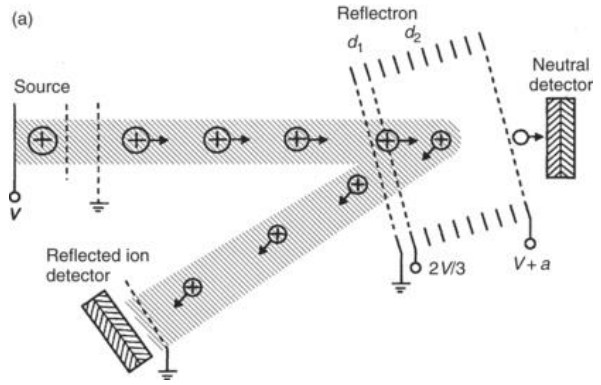



*Figure 1.4 Schematic representation of TOF mass analyser. The figure was adapted from Sparkman et al. (2011).*

TOF can be modified by adding quadrupole before the ions are sent to the TOF analyser. Tanden MS delivers the advantage of targeted ion separation provided by quadrupole, fast analysis, and high mass resolution provided by TOF (Allen & McWhinney, 2019).

Quadrupoles consist of four parallel rods, two of which have opposite charges. Rods are arranged so that negatively charged rods are on the y-axis and positive ones are on the x-axis (Sparkman et al., 2011).

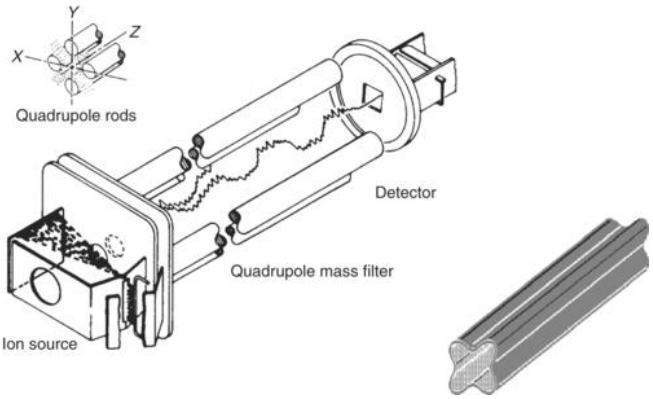



*Figure 1.5 Schematic presentation of the quadrupole. The figure was adapted from (Sparkman et al., 2011)*

The direct current (DC) and radio frequency (RF) electric field applied to the rods result in an oscillating electric field that separates ions based on their m/z (Sparkman et al., 2011). A wide range of m/z ions can travel through the quadrupole if only RF voltage is applied (Dunn, 2011). The combination of RF and DC allows a tuneable electric field where only stable ions with a specific m/z can travel through the quadrupole to the detector (Dunn, 2011; Harris, 2016). Ions that do not match the frequency of the applied electric field will be lost due to unstable trajectories in the quadrupole (Dunn, 2011).

Q-TOF can be operated in two different scan modes. The first mode is single MS (TOF) mode, where after the fragmentation in the source, all ions travel through the quadrupole into TOF

without being filtered in the quadrupole. The MS mode is especially advantageous in non-target-suspect screening, where full spectrum measurements are needed. However, the amount of data generated in MS mode can be extensive; consequentially, good mass profiling software and databases are required for data acquisition (Imma Ferrer et al., 2018). The second mode that can be applied is MS/MS, where quadrupole is utilised as a mass filter, and only ions with targeted masses enter the TOF (Allen & McWhinney, 2019). This mode provides higher sensitivity and better ion fragment information. However, the MS/MS mode is only applicable to soft ionisation. MS/MS is not compatible together with EI; therefore, the quadrupole was not utilised in this project.

## 1.8 High-Resolution Mass Spectrometry

The number of environmental pollutants is increasing every year, and at the same time, new compounds with novel chemical structures are emerging. While conventional MS is still widely used to identify various unknown compounds, high-resolution MS (HRMS) is gaining popularity for accurate mass determination and annotation of unknowns.

Several types of mass analysers can be used for HRMS data acquisition; however, the most common ones are QTOF and Orbitrap detectors. As mentioned in section 1.8, QTOF measures the travel time of the ions in the TOF tube. The m/z ratio is directly proportional to the flight time in the tube, allowing high-accuracy mass determination of ions. Therefore, developers are continuously optimising the path length of QTOF to achieve even greater accurate mass data. Orbitrap uses electrostatic trapping to measure the mass of the ions. Ions are trapped and oscillate in an electrostatic field between the central electrode and the surrounding outer electrode (Harris, 2016). The oscillation frequency is proportional to m/z rations and allows the determination of accurate mass and high chromatographic resolution.

HRMS can distinguish the ions with similar masses allowing precise compound identification in complex matrices where low-resolution (LR) MS would result in identical masses (Koelmel et al., 2022). The advantage of HRMS is that it allows more reliable identification and annotation of compounds without the necessity of prior structural information (Koelmel et al., 2022). Applying HRMS in an analytical workflow can significantly increase confidence of the identification of novel compounds. Moreover, the prediction of low-mass fragments and unique isotopic patterns obtained by HR mass analysers can provide additional information for compound annotation (Koelmel et al., 2022). Therefore, HRMS is gaining significance in Suspect and Non-target data acquisition. Important to note that structural annotation of

compounds is still a challenge with HRMS. Consequently, additional tools such as Kovats RI, HRMS databases and suitable software for data processing are essential for the correct structural annotation of compounds.

## 1.9 Suspect and Non-target chemical analysis

Three main approaches are considered for the identification and annotation of compounds. The first part is targeted analysis. Targeted analysis utilises reference standards for the annotation and quantification of compounds. Information such as RT and MS are known before the analysis. An article written by Schymanski et al. (2015) categorises targeted compounds as identification level 1 since the structure can be confirmed by reference standards. The possibility of incorrect annotation of the compound is usually implausible. The identification of confidence levels is defined in Figure 1.6.

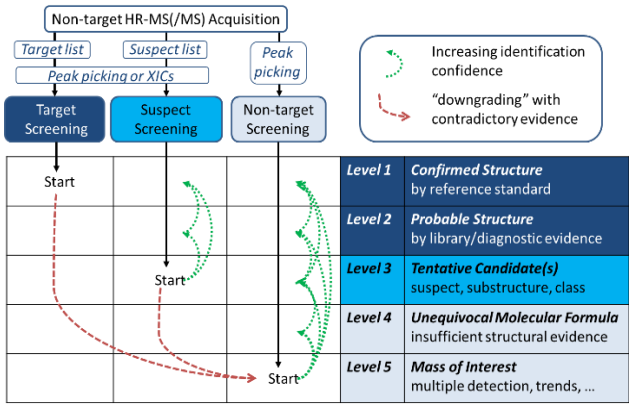



*Figure 1.6 Definition of confidence levels used in HR suspect and non-target data acquisition. The figure was adapted from an article written by Schymanski et al. (2015).*

The second approach of the analysis is Suspect screening (SUS). SUS involves identifying compounds that are expected (known unknowns) to be found in the laboratory sample. No reference standard is usually available in SUS. However, prior knowledge of expected compounds, such as accurate mass or isotopic pattern, is utilised for confirmation (Schymanski et al., 2015). The structure can be confirmed by libraries such as NIST (National Institute of Standards and Technology) or PCDL (Personal Component Database and Library). Kovats RI can be utilised as additional diagnostic evidence for confirmation. The confirmed compounds are classified with confidence level 2. Compound hits with insufficient MS evidence (e.g. low library match score) or poor RI values ($\geq \pm 100$) are labelled as "non-target of interest" (Schymanski et al., 2015).

The third approach is a non-target screening (NTS), where no structural information before analysis is available. NTS starts at confidence level 5, and identified structure gains a higher

confidence level every time more structural information about the compound is established (Schymanski et al., 2015). Information products like mass spectra libraries, chemical databases or software algorithms that can predict mass spectra are essential for conducting the NTS. Mass spectra prediction *in silico* is standard practice for NTS, and because of rapid technological development, prediction accuracy is increasing (Milman & Zhurkovich, 2022). Data processing software such as MassHunter Unknown Analysis provides automated data deconvolution and simultaneous Suspect and Non-target identification of compounds. Automated workflows allow extensive data processing, making *in silico* prediction approaches more accurate and less time-consuming.

### 1.10 Kovats retention index

Kovats retention index (RI) is commonly utilised in gas chromatography to improve the confidence level of the identification of annotated compounds. The retention time (RT) of the molecule is affected by the type of GC column, molecular interactions, carrier gas flow and temperature program (Sparkman et al., 2011). The type of stationary phase interactions and temperature effects result in relations that are unique for each molecule and can be expressed mathematically (Goel et al., 2015). Separated compounds of interest can be identified by comparison of retention times and retention indices of homogenous alkane series (e.g., $C_7$-$C_{30}$). Alkane series and analytes must be analysed under the same chromatographic conditions for the results to be compatible. RI normalises variables in the GC system and allows the obtained values to be compared between different systems (Goel et al., 2015).

Calculated RI values can be compared with the reference RI found in NIST or Wiley libraries. Originally Kovats RI was developed for the calculation of isothermal conditions. However, most of the chromatographic methods are established with temperature programming. Therefore, the equation by van den Dool and Kratz is utilised for the determination of RI in linear temperature programming ($I_{DK}$) (Battaloglu, 2021):

$$I_{DK} = 100\left[\frac{t_{Rp(x)} - t_{Rp(z)}}{t_{Rp(z+1)} - t_{Rp(z)}} + z\right] \quad (2)$$

$t_{Rp(x)}$is the retention time of a compound of interest. $t_{Rp(z)}$ is expected as the retention time of an n-alkane eluting before the compound of interest. $t_{Rp(z+1)}$ is the retention time of an n-

alkane eluting after the compound of interest, and *z* represents the carbon number of n-alkane eluting before the peak of a compound of interest (Battaloglu, 2021).

An article by Koelmel et al. (2022) explains that RI helps identify isomers with similar EI spectra, reducing the probability of false positive compounds. Furthermore, RI prediction applied to the GC system is relatively consistent between laboratories compared to the LC systems (Koelmel et al., 2022). The interlaboratory RI value consistency between GC systems increases the reliability of confirmation of unknown compounds (Koelmel et al., 2022).

### 1.11 Thermal desorption unit

Thermal desorption (TD) is a widely used sample introduction technique used in GC that has become a standard technique in the analysis of VOCs. During sampling, VOCs are directly adsorbed on the sorbent bed; consequentially, no solvent or sample preparation is necessary prior to the analysis (Poole, 2012). Sample desorption is usually a two-stage operation. In the first stage, inert carrier gas flow (e.g., helium or nitrogen) and high temperature are applied to desorb the analytes from the sorbent tube and introduce it into the focusing trap (cold trap). The second stage is focusing trap desorption. Focusing trap preconcentrates and focuses the sample for simultaneous introduction to the GC system (Poole, 2012). Multiple application stages minimise the chromatographic peak broadening and increase the sensitivity/detection limits of the analysis.

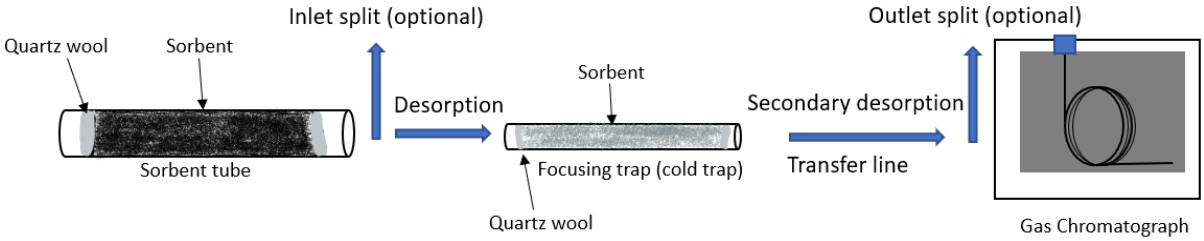



*Figure 1.7 Simplified schematic diagram of thermal desorption unit (TDU). The diagram was created based on information from Poole (2012).*

The cold traps are usually manufactured from inert materials such as quartz to withstand radical temperature changes. During primary desorption, a focusing trap (up to -30$^{o}$C) is held cold to efficiently retain and refocus all the analytes desorbed from the sorbent tube. After refocusing, the trap is rapidly heated to release the compound into the analytical system (Poole, 2012).

In traditional TD, samples are completely desorbed and deteriorated during the analysis, making TD a "one-shot" sample introduction technique (Poole, 2012). However, modern TD systems can be utilised with a quantitative recollection function. During the recollection, the sample is desorbed in a known split ratio; consequentially, a known amount of sample is redirected back to the sorbent tube. Sample recollection enables repeat testing and quantification of the sample and overcomes "one-shot" limitations that the old TD system encounters (Poole, 2012). Due to time constraints, sample recollection was not utilised in this project, and all samples were analysed single time.

Tenax TA is one of the most widely used sorbent for sampling gaseous VOCs. The sorbent is a poly-2,6-dipheyl-p-phenylene oxide polymer that has hydrophobic properties and does not retain water (Chu et al., 2016). It is primarily used for the identification of VOCs in the $C_6$-$C_{30}$ range. Tenax TA is most suitable for retaining non-polar molecules with higher molecular weight (Chu et al., 2016). Small, polar molecules such as methanol, acetone or n-butanol are poorly retained by the Tenax TA sorbent (Chu et al., 2016). Therefore, compounds that have low molecular weight and are polar (e.g., methanol) can be suitable as solvents.

A combination of multiple sorbents can be applied to increase the range of VOCs adsorbed on sorbent tubes. Sorbents are usually arranged in increasing sorbent strength to prevent less volatile compounds from being irreversibly retained in the strongest sorbent (Ras et al., 2009). Weaker sorbents are generally more hydrophobic and are suitable for the adsorption of heavier and more reactive molecules (Noorden, 2020). Stronger sorbents are usually hydrophilic and are utilised to analyse small, highly volatile compounds (Noorden, 2020). Because of physicochemical properties, choosing the correct combination of sorbents is essential.

## 1.12 Aim of Study

Wood is rapidly increasing in popularity as a construction material in Norway. Simultaneously, wood is widely used as an indoor wall coating material and furniture. For preservation purposes and to improve durability, wood materials are often treated with different coatings, additives, or glues. Therefore, there was an interest in uncovering if coated wood surfaces emit anthropogenic VOCs such as xylene, toluene, and ethylbenzene, commonly found in paints and coatings. At the same time, wood naturally emits diverse types of ketones, aldehydes, fatty acids, and terpenes that can elevate VOC levels in indoor environments. Therefore, the most common biogenic VOCs emitted from softwood, such as α-pinene, β-pinene, hexanal, d-limonene, and 3-carene, were quantified.

This project aimed to develop and validate the GC-QTOF-TDU analytical method that was applied for the identification and quantitation of VOCs emitted from untreated and coated wood surfaces. Acknowledging that VOC emission profiles from untreated and coated wood materials are not sufficiently characterised, the project focused on targeted and non-targeted screening evaluation to obtain the complete emission profiles. Moreover, two different sorbents (Tenax TA and Universal) were utilised for the collection of air samples. The sorbent comparison was carried out to determine if the sorbents were able to retain different VOCs emitted from softwood surfaces. Lastly, the Personal Compound Database and Library (PCDL) development and its application in the Agilent MassHunter Unknown analysis was also emphasised.

# 2 Methods and Materials

The analysis of VOC emissions from the wood surfaces was conducted at NILU-Climate and Environmental Research Institute at the Department of Environmental Chemistry in Kjeller, Norway. Air sample introduction to the GC system was carried out with Markes Centri 360 Thermal Desorption Unit (TDU). Sample analysis was performed on an Agilent 8890 GC system connected to the Agilent 7250 Quadrupole Time-of-Flight (Q-TOF) mass analyser. EI technique was utilised for ionisation and fragmentation of the analytes.

A low/mid polarity capillary column DB-1701 (J&W DB-1701, 60m x ID 0.32mm, 1.00µm, Agilent Technologies, Santa Clara, USA) with stationary phase composition of (14% cyanopropyl-phenyl)-methylpolysiloxane was used to separate targeted and non-targeted VOCs. Helium (Grade 5, Nippon Gases Norway AS, Oslo) was used for carrying analytes in the GC system. Prepacked stainless steel Tenax TA tubes (C1-AXXX-5005, Tenax TA, (35/60), Markes International, Bridgend, UK) were utilised for the active sampling of VOCs emitted from untreated and treated wood samples. In addition, multi-sorbent tubes Universal from Markes (C3-AXXX-5266, Universal, Markes International, Bridgend, UK) were used in this project. Different sorbent types were utilised to compare analytical results and provide additional information on the sample emission profiles. Markes did not provide information on the chemical composition of the multi-sorbent bed. However, universal tubes have been packed with a proprietary recipe of weak, medium, and strong sorbents, allowing the adsorption of $C_{2/3}$ to n-$C_{30}$ compounds.

The sampling of VOC was carried out at the University of Life Sciences (NMBU). Active air sampling was performed by utilising a climate chamber method, suggested by EN16516:2017+A1, the European standard for the determination of emissions into indoor air. Wood sample specimens were placed in environmental chambers Termaks (KB 8000 F series). Temperature and humidity were held constant throughout the sampling period. Active sampling was carried out with SCK pocket pumps at 100mL/min sampling flow. Detailed information on analytical instruments, chemical standards and materials used in this project can be found in Appendix A.

## 2.1 Test samples

Three types of Norway spruce (*Picea abies*) samples were analysed to determine VOC emission profiles. Each wood specimen consisted of four duplicates to define the variance between the duplicate values. The first batch of test specimens analysed in this project was an untreated spruce interior panel (USP). The spruce panel (Glattpanel Nat) was produced by Bergene Holm AS and cut into 10x20cm pieces at the company's workshop. Another sample batch analysed in this project was a stained spruce interior panel (SSP). The panel (Sprekkpanel Nat Lysne) was produced by Bergene Holm AS five months prior to the analysis. The water-based wood stain (Lacroma, Clear Lysne- Light white) was supplied by Sherwin-Williams Sweden AB. For a complete chemical overview of Lysne wood stain, refer to Appendix A. USP and SSP provided by Bergene Holm AS were dried in closed chambers between 60-80$^{o}$C until 12% moisture content was achieved.

The third sample batch of interest was cross-laminated timber (CLT). The one larger piece of CLT was supplied by Splitkon AS and transported to the NMBU. The piece was cut into four smaller 10x20x8cm pieces at the NMBU wood laboratory. Melanin-urea-formaldehyde (MUF) adhesive provided by Dynea was utilised to bond the inner and outer lamellas of CLT.

*Stained spruce panel* *Untreated spruce panel* *Cross-laminated timber*

*Figure 2.1 Test specimens analysed in this project. Pictures of wood samples were provided by Ingrid Bakke.*

All sample specimens analysed in this project were individually packed in aluminium foil, followed by tight wrapping with polyethylene film before transportation and storage at the NMBU campus. Test specimens were stored at room temperature for approximately two months at the NMBU wood laboratory before the sampling and analysis were conducted. Additional information for sample specimens can be obtained in Appendix A.

## 2.2 Method development

Analytical parameters utilised in GC and TDU systems were based on an analytical method developed by Brown et al. (2014). The study aimed to validate the storage performance of the various sorbents loaded with a VOC mixture relevant for indoor air emission testing (Brown et al., 2014). Sorbents examined in the study were Tenax TA, quartz wool/Tenax TA/Carbograph 5T and quartz wool/Tenax TA/Carbopack X. Based on the information and the results provided in the article, the method developed by Brown et al. (2014) was a good candidate for adaptation. Specific changes in analytical method needed to be implemented to complement GC and TDU systems that were utilised for this project.

Markes TC-20 conditioning unit was utilised for conditioning Tenax TA and Universal sorbent tubes. The article written by Brown et al. (2014) suggested conditioning the tubes at 320$^{o}$C for one hour, followed by 335$^{o}$C for 30min in a helium flow of 60ml/min. This project applied conditioning recommendations from Markes International to achieve optimally cleaned tubes. Freshly packed tubes were conditioned for 2 hours at 320$^{o}$C and 4 hours at 330$^{o}$C. Before conducting the sampling procedure of VOC emissions, sorbent tubes were reconditioned for 1 hour at 320$^{o}$C. Oxygen-free nitrogen (Grade 5, Nippon Gases Norway AS, Oslo) was utilised for the conditioning of the tubes because of the lower cost compared to helium. Gas flow was set to 50mL/min to save the amount of nitrogen used for the conditioning. All reconditioned tubes were analysed before the sampling to ensure the sorbents were contaminant-free.

Pre-purge of the TDU system was set to 40mL/min to fill the tubes with a carrier gas (nitrogen, grade 5) to remove air and potential humidity from the sorbent tubes. The primary desorption time was increased to 10min instead of 8min to ensure complete analyte elution from the sorbent tubes. Uncoated deactivated fused silica (0.25mm ID) by Markes International was used for transferring the desorbed analytes to GC-oven. In the analysis conducted by Brown et al. (2014), the transfer line temperature was set to 210$^{o}$C. In this project, recommendations from Markes International were adopted; therefore, the transfer line temperature was set to 150$^{o}$C. Detailed information on the instruments utilised in the analysis can be obtained in Appendix A.

Liquid standard solutions were utilised for method validation and calibration of targeted VOC emissions. Standard solutions were prepared with distilled methanol, which corresponds to Absolute grade (99.98% purity). Information on the standard solutions used in this project can be obtained in Appendix A. In order to load a standard solution on the sorbent, tubes were

mounted onto Markes International Calibration Solution Loading Rig (CSLR). 1µL of the standard solution was loaded with a 10µL Hamilton syringe. The solvent was purged using a 100mL/min nitrogen gas (5N purity grade) flow for 2 min.

The targeted and untargeted analysis was carried out in scan mode. The scan mode mass range was set between 35-300m/z. Detailed information on the final analytical method parameters used for GC and TDU systems is provided in Appendix B.

### 2.3 Development of Personal Compound Database and Library

PCDL manager is an Agilent MassHunter software that allows the establishment of in-house MS libraries for faster and more accurate identification of unknown analytes. PCDL is utilised together with other software packages in MassHunter Suite. In this project, the HRMS library was developed through the acquisition of a variety of VOC reference standards with known chemical content. The library was built based on compounds of interest and compounds that are commonly detected in indoor air. Eleven individual reference standards were analysed to obtain HRMS data and build the PCDL. Analytical HRMS data was also collected from two different VOC mixes containing a total of 200 reference standards. The list of all the standards used for the establishment of the PCDL is provided in Appendix A.

In-house PCDL was developed by utilising MassHunter Qualitative analysis. In the first part of the development, the TIC of the analytical run was investigated to determine if chromatographic data possess good peak resolution. Coeluting peaks were discarded from further analysis. In the second part, the EIC of the reference standard was extracted by utilising the monoisotopic mass of the compound acquired from ChemCalc. To narrow down the EIC extraction window, a maximum monoisotopic mass deviation of ±20ppm was defined in MassHunter Qualitative analysis. The area inside the EIC was chosen to extract the MS of the compound. The extracted MS data was cleaned for background noise to obtain ion fragments that only belong to the compound. The deviation between monoisotopic mass and molecular ion mass was calculated. Ppm of $\leq \pm 5$ was defined as an acceptable deviation window. It was essential to determine mass deviation because PCDL containing MS with inaccurate masses could cause a false compound annotation in suspect and non-targeted analysis. The formula used for calculating mass deviation is provided in Equation 3.

$$\frac{Monoisotopic\ mass - mass\ of\ molecular\ ion}{molecular\ weight} * 1000\ 000 \quad (3)$$

Moreover, it was important to export HRMS data that did not contain saturated ion fragments. Saturated fragments usually contain inaccurate masses and incorrect abundance that would result in the false annotation of the compound. If the MS data matched the criteria, the compounds were annotated with the IUPAC name and CAS number, and HRMS data was exported to the PCDL manager.

### 2.4 Kovats retention indices

To increase confidence of the identification of the unknown compounds, Kovats RI was utilised. 1µl standard alkane mix $C_7$-$C_{30}$ (conc. 10ng/µL diluted in methanol) was loaded with a 10µL Hamilton syringe on the sorbent tube and analysed under the same analytical conditions as the test samples. Obtained analytical data was used to develop a CSV file that could be uploaded to MassHunter Unknown Analysis. The CSV file contained information such as the IUPAC compound name, CAS number, retention index of specific alkane, and the RT obtained from the analytical run. Information in the CSV file was used for automatic RI calculation, and the values were compared with standard RI obtained from the NIST20 library. Unknown compounds with 70% library match and RI with a standard deviation ≥±100 were given the confidence level 2 (Figure 1.6). Compounds with RI match over ±100 were given the confidence level 3. RI calculation was also applied when building the in-house PCDL because it provided a quality control step for the correct annotation of compounds.

### 2.5 Suspect and Non-target screening

The suspect and non-target screening (SUS and NTS) was conducted to obtain complete emission profiles from the laboratory samples analysed in this project. The SUS and NTS was carried out by Agilent MassHunter Unknown Analysis. All chromatographic data obtained was converted to SureMass format before the SUS and NTS.

SureMass is a deconvolution algorithm designed for the GC-QTOF system. The algorithm processes TIC data in a continuous 3-dimensional array (Agilent Technologies, 2017). The m/z inconsistencies caused by changing experimental conditions are minimized, allowing better m/z accuracy and better use of high-resolution data (Agilent Technologies, 2017). The algorithm allows to obtain data in low abundance levels and gives a greater sensitivity for trace-

level components (Agilent Technologies, 2017). Moreover, SureMass significantly reduces signal processing time, resulting in faster analysis of a large amount of analytical data.

After converting chromatographic data to SureMass, a customised method was developed to ensure that the method conditions were optimised for the unknown analysis. For the compound annotation NIST20 library and in-house PCDL were utilised. As a quality assurance, only compounds with a match factor of ≥70% were considered.

Two conditioned blank tubes were analysed together with each sample batch to distinguish the compounds identified in sample form compounds found in the blank. Compounds identified in blank samples were subtracted from the VOC samples to reduce the possibility of false positives. The obtained data from the SUS and NTS was converted to a pivot table in Excel to ensure a comprehensible statistical overview of the identified compounds.

### 2.6 Development of volatile organic compounds sampling method

Sample sizes, climate conditions and air sampling were based on European standard NS-EN-16516:2017+A1: "Construction products. Assessment of release of dangerous substances. Determination of emissions into indoor air". The method for determination of VOC described in the standard was developed for test chambers where temperature, humidity and airflow rate could be kept constant under the testing period. For the result to be representative, the sample size had to be suited for the loading capacity of the test chamber. In this project, five 20L vacuum chambers (VC3028AC, Ignatki-Osiedle, Poland) were used to place the test samples. One 20L vacuum chamber was kept empty for the air collection of chamber blanks. Based on the NS-EN-16516:2017+A1, the recommended sample size should not exceed 30% of the empty test chamber volume. The proper product loading factor ensures that air in the chamber can be adequately mixed during emission sampling (European Committee For Standardization, 2017). The temperature was suggested to be kept at 23±1$^{o}$C and the relative humidity (RH) at 50±5% (European Committee For Standardization, 2017).

The vacuum chambers used in the project were not established to provide constant temperature and humidity conditions. As a workaround, vacuum chambers were placed in climate chambers KB 8182 from Termaks AS. The climate chambers only provided constant temperature. To increase the humidity in the vacuum chamber, a beaker with 200mL distilled water was placed in each chamber. Based on NS-EN-16516:2017+A1, test chambers should be manufactured from stainless steel or glass to avoid undesirable chamber emissions and possible reactivity

between chamber materials and analytes of interest (European Committee For Standardization, 2017). This project had limited funding and obtaining chambers with recommended materials was not feasible. Test chambers available for this project were made from aluminium with a tempered glass lid. Aluminium is generally a reactive metal; however, exposure to oxygen forms an $Al_2O_3$ layer that does not react with other materials.

Clean air to the chambers was provided by Big Trap Gas $^1/_8$"- Hydrocarbon filter from Trajan attached to the air supply system installed in the laboratory. The hose connected directly to the filter was split into five hoses by attaching stainless steel splitting brass to the main air hose (Figure 2.2, picture a).


a) Stainless steel splitting brass b) Set up of the vacuum chambers c) Rotameter

*Figure 2.2 The set-up of the test chamber model.*

Each hose was connected to the rotameter from Aalborg, which was connected to the bottom ball valve of the vacuum chamber. Finally, a separate air hose was installed to the top ball valve of the vacuum chamber, and the second end was attached to the reducer bushing for coupling a smaller diameter air hose (Figure 2.2, picture b). The air hoses were placed outside the climate chamber and utilised to collect VOC emissions from wood specimens.

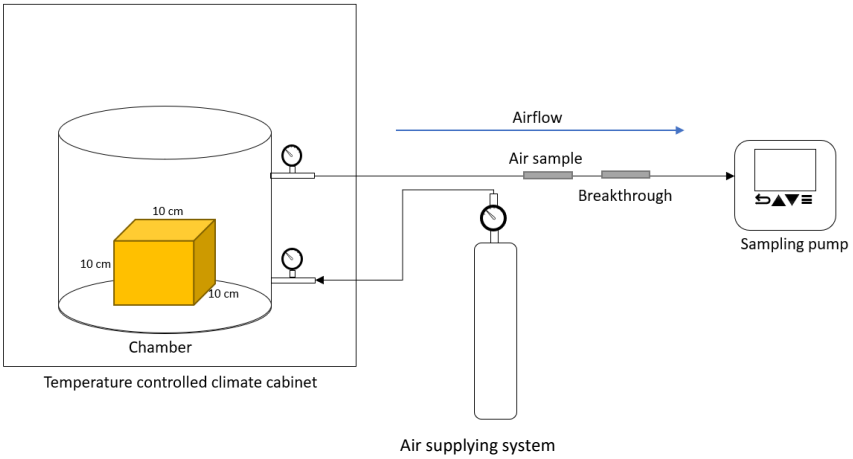


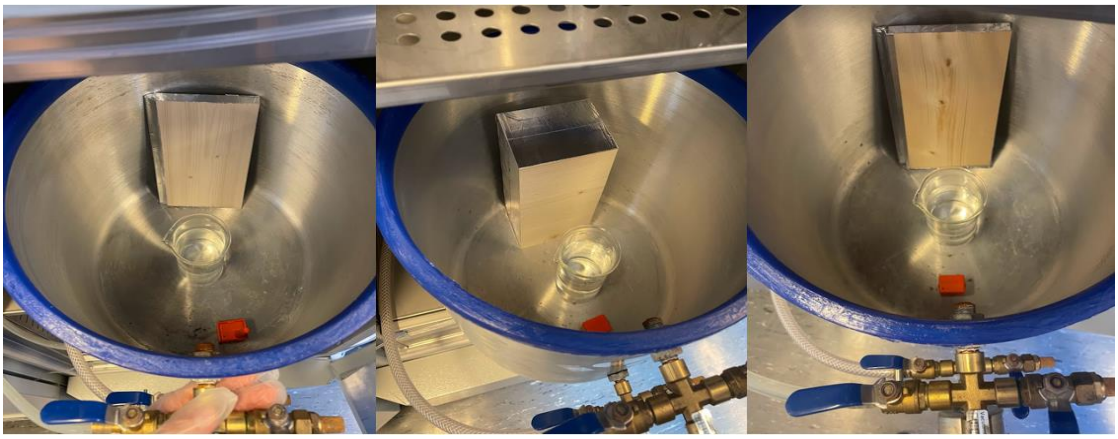

*Figure 2.3 Simplified schematic diagram of the VOCs emission sampling system.*

## 2.7 Sample preparation and sampling of volatile organic compounds

Four duplicates of three different spruce samples were analysed. Sample type, size and storage conditions are already described in section 2.1. One day before sampling, vacuum chambers were washed with distilled water. Beakers with 200mL distilled water were placed in the vacuum chamber to increase the humidity. Moreover, data loggers (SenseAnywhere Airo sensor 20-20-24/00, Oud Gastel, Netherlands) were positioned for temperature and humidity monitoring. Glass lids were cleaned with distilled water, and vacuum chamber rims were lubricated with vacuum grease (Grease for laboratories, suitable for vacuum, Glisseal N, Borer) to create a seal that prevents from air leaks. After placing glass lids on the chambers, 1kg weight was placed on the top to secure the lids from movement. The rotameters were set to 400mL/min, and the temperature of the climate cabinets was set to 23$^{o}$C.

*Figure 2.4 Emission sampling system used for identification of VOC emissions from different wood materials.*

Sample preparation was based on European Standard NS-EN-16516:2017+A1. Aluminium tape with low emitting acrylic adhesive (10mx50mm, tesa®, Germany) was utilised to tape the rear surface and edges of wood specimens so that only one side of the sample was left exposed. One side was left uncovered, given that it represented the exposed material surface in an indoor environment. The 200cm$^2$ surface area was utilised to identify and quantify VOC emissions in wood sample specimens. Four sample duplicates were placed in four different chambers, and the fifth chamber was left empty for a sampling of chamber blanks.



a) Stained spruce panel b) Cross-laminated timber c) Untreated spruce panel

*Figure 2.5 Sample specimens analysed in this project. Each sample batch contained four duplicate samples.*

Samples were placed in chambers that had a continuous clean air supply. Chamber climate and airflow conditions were discussed in section 2.6. Due to time limitations, the determination of long-term emissions 28d after sample installation was not feasible to achieve. Therefore, the project focused on identifying short-term emissions, determined three days after sample installation in the climate chambers. After the collection of the air samples, the former batch of wood samples was removed from the chambers, and the procedure prior to sampling was repeated before placing the new bath of sample specimens.

Replicate air samples were collected using different time intervals to obtain different sample volumes. Sample replicates were collected immediately after each other at 5L and 3L air volumes. The compound breakthrough was tested by placing two sorbent tubes in series to assess the breakthrough volume of the sorbent bed. Breakthrough sampling was performed for 5L duplicate samples. Active air sampling was carried out with a pocket pump from SKC Inc. (SKC Pocket Pump 210-1002, SKC, Blandford, Dorset, UK). Air sampling parameters are

shown in Table 2.1, and more information on the equipment used in sampling refer to Appendix A.

*Table 2.1 Air sample volume and sampling rate used for sampling VOCs from the SSP, USP and CLT.*

| | |
|---|---|
| **Sampling rate** | 100 mL/min |
| **Sample volume** | 5 L |
| **Sampling time** | 50 min |
| **Sampling rate of replicates** | 100 ml/min |
| **Sample volume of replicates** | 3L |
| **Sampling time of replicates** | 30 min |

## 2.8 Quantification of the volatile organic compounds

Calibration curves of targeted VOCs were developed by loading Tenax TA sorbent tubes with 1µL standard solution that covered the concentration range of interest: 1ng/µl, 5ng/µl, 10ng/µl, 50ng/µl, 100ng/µl and 150ng/µl. Toluene-d8 (Toluene-d8, Chiron As, Trondheim, Norway) was utilised as an internal standard. Calibration mixtures, blanks and samples were spiked with 1µL of 10ng/µl internal standard. All liquid standard solutions and internal standards used in this analysis were solved in methanol. After loading the liquid standard on a sorbent tube, a 100mL/min flow of nitrogen gas was applied for 2 min to purge the solvent from the sorbent tube. The sample loading procedure is explained in section 2.2. New stock solutions were prepared before every analysis to minimise the possibility of unwanted chemical reactions due to prolonged storage time. Information on standard solutions used in this project can be obtained in Appendix A.

*Table 2.2 List of targeted VOC calibration standards and their quantifier, qualifier ions chosen for the quantification.*

| Name | Quantifier ion | Qualifier ion |
|---|---|---|
| Toluene-D8 | 98.0982 | 100.1123 |
| Toluene | 65.0386 | 62.0227 |
| Hexanal | 56.0621 | 44.0257 |
| Ethylbenzene | 77.0386 | 65.0386 |
| m-xylene | 79.0542 | 77.0386 |
| Furfural | 96.0206 | 39.0229 |
| α-pinene | 77.0386 | 121.1012 |
| β-pinene | 69.0699 | 136.1247 |
| 3-carene | 91.0542 | 79.0542 |
| D-limonene | 79.0542 | 136.1247 |
| Benzaldehyde | 51.0229 | 50.0151 |

Quantification of targeted compounds was based on quantifier and qualifier ions after integration of EIC. In general, qualifiers and quantifiers are chosen to be fragments with higher

abundance because they are less affected by the matrix. In this project, saturation of the most abundant ion peaks was an issue when working with more concentrated analytes. Saturated fragments should not be used for quantification since the abundance of these ions does not correspond to the correct concentration. Therefore, only unsaturated fragments with the highest abundance were chosen as qualifier and quantifier ions. The quantifier and qualifier ions utilised in this project can be obtained in Table 2.2.

The analysis was executed in full scan mode. Each calibration level was created by analysis of three calibration replicates. Two conditioned Tenax TA tubes were analysed at the start of the sample batch to account for the background noise and possible contamination of the blank.

## 2.9 Data-analysis

Mass Hunter Qualitative Analysis 10.0 was utilised to interpret mass spectrophotometric data and develop the in-house PCDL. Quantification of the targeted compounds was carried out by MassHunter TOF Quantitative Analysis 12.0. The suspect and non-target screening of analytical compounds was performed by MassHunter Unknown Analysis 12.0. Mass Hunter Unknown analysis was also used for the RI calculations of the non-targeted compounds. NIST20 library and personal PCDL were utilised to identify the non-targeted compounds. The list of the type of software utilised in this project can be obtained in Appendix A.

# 3 Quality assurance and quality control

Validation of the method is an essential step for assuring the quality of the analysis. Drug quality assurance is especially important in pharmaceutical laboratories since there is a risk of products being unsafe and harmful for human consumption. Therefore, properly established analytical methods are essential to ensure the pharmaceuticals' stability, purity, and shelf life and to determine the intermediates and physiochemical properties of the product.

Using the poorly validated method in environmental analysis is less consequential compared to pharmaceutical analysis. However, without a validated method, there is a risk of higher identification uncertainty and bias, poor method selectivity or ambiguous quantification of the analytes. Correct compound quantification is essential where the specific levels of targeted environmental compounds can be noxious. Properly documented and validated analytical methods also ensure confidence in the quality of the laboratory work performed (Barwick, 2016).

The laboratory is responsible for ensuring that the analytical method produces sufficient results. However, standard guidelines exist that can be followed in other to validate the analytical method. Eurachem guidelines state that it is important to determine whether the developed method fits its purpose (Barwick, 2016). Method efficiency can be experimentally demonstrated by the determination of selectivity, working range and linearity, LOQ, LOD, bias, ruggedness, and measurement uncertainty.

## 3.1 Selectivity

Based on Eurachem's definition, selectivity is the ability to identify the analytes of interest in the mixture of matrices without interferences of compounds with similar characteristics (Barwick, 2016). Selectivity is a part of qualitative analysis, and different procedures can be used to establish how selective the method is (Barwick, 2016).

Selectivity can be determined by analysis of reference standards of interest. The method selectivity can also be determined by comparison of spectral data utilising different analytical parameters. Different temperature programs or mobile phases can be used for GC systems to achieve desirable chromatographic peak resolution (Reichenbächer & Einax, 2011). Selectivity is also established by analysing analytes in different matrices, from pure reference materials to

RM in complicated matrices and determining interferences between the analytes and matrices (Reichenbächer & Einax, 2011).

### 3.2 Quantification

Quantification is an important part of method development and validation to statistically evaluate compounds of interest. Quantifying analytical measurement is essential when large amounts of specific compounds can negatively affect human health or the environment.

The amount of compound can be determined by establishing a calibration curve. IUPAC defines calibration as the set of operations that are established under specified conditions and gives a relationship between values indicated by the analytical instrument and the known value of the analyte (IUPAC, 1997). Calibration is carried out by repeated measurements of suitable calibration standards (Barwick, 2016). A calibration curve is typically established by plotting the y-axis that represents the signal response from analytical instruments against x-values that correlate to the concentration of the analyte (Marwa, 2017).

The calibration curve can be established using different techniques, such as external, internal and standard addition methods. In this project, an internal standard was applied to establish calibration curves. An internal standard is a compound that is added in constant concentration to all samples, calibration standards and blanks in an analysis (Skoog, 2018). Internal standards are advantageous for samples containing complex matrices because they can compensate for random and systematic errors and analytical signal changes due to matrix effects (Skoog, 2018).

The calibration curve for the internal standard method can be developed by calculating the relative response factor for concentration and the signal response and expressing the values in linear regression (Harris, 2016):

$$y = \frac{A_x}{A_s} \qquad x = \left(\frac{[X]}{[S]}\right) \qquad b = constant \tag{4}$$

$$y = ax + b \tag{5}$$

$A_x$ is a signal from the analyte, and $A_s$ is the signal from the internal standard. $[X]$ is the concentration of the analyte, and $[S]$ is the concentration of the internal standard (Harris, 2016). In linear regression, $a$ express the slope of a calibration curve, and $b$ is the intercept. The

equation can also be utilised for determination of LoD and LoQ (Marwa, 2017). The most common method for developing a calibration curve is multi-point calibration. In this type of calibration, different concentrations of standards are established in the range of interest. The concentrations directly represent the response to a signal of the compound of interest. The amount of calibration points that are chosen depends on the type of method and the analyte that is determined. However, it is recommended that a calibration curve would consist of five to eight calibration points (Marwa, 2017). It is also important that the calibration curve would cover the concentration range where the analyte of interest can be expected. The lowest concentration should be LLoQ (lower LoQ), and the highest concentration should be ULoQ (upper LoQ) (McMillan, 2016).

### 3.3 Working range and Linear range

Working range and linearity define the response of signal directly corresponding to analyte concentration with acceptable uncertainty (Barwick, 2016). The working range is more extensive than the linear range; however, both properties can be expressed by the linear equation described in section 3.2. Linearity is determined by analysing reference standards and laboratory samples at different concentrations and determining the range at which results can be achieved with acceptable uncertainty (Barwick, 2016). For the determination, it is necessary to analyse a series of at least five different concentrations in the range of 50-150% of the expected working range (Tentu Nageswara, 2018).

### 3.4 Recovery

Recovery is defined as the true value of the analyte that was identified by an analytical instrument (Burns et al., 2002). In analytical analysis, the amount of laboratory sample that is analysed and the amount of the sample identified by an instrument can differentiate; therefore, it is important to determine the recovery of an analytical method (Burns et al., 2002). Recovery can be determined by spiking the laboratory sample with an internal standard of a known concentration and calculating the apparent recovery. ($R'_A$). Apparent recovery is used when the information is obtained from a calibration graph (Burns et al., 2002).

$$R'_A = \frac{x_A(exp)}{x_A(theor)} * 100 \quad (6)$$

where $x_A(exp)$ is the value of the analyte obtained from the calibration graph and $x_A(theor)$ is a known amount of the spike (Burns et al., 2002).

### 3.5 Limit of detection and quantification

The limit of detection (LoD) is defined as the smallest amount of analyte that can be identified with an acceptable level of uncertainty (IUPAC, 1997). LoD depends on the instrument's sensitivity, injection technique, and analytical method parameters. LoD can vary for individual analytes; therefore, it must be determined for each compound of interest individually. Based on a book published by Skoog (2018), LoD can be determined in two steps. The first step is to determine a minimum distinguishable signal ($S_m$) by calculating the standard deviation ($s_{bl}$) of the signal in blank samples and the mean value of the blank signal:

$$S_m = \overline{S_{bl}} + ks_{bl} \tag{7}$$

*k* is a factor usually expressed as 3 for the determination of LoD and 10 for the calculation of LoQ. The second step is to utilise the slope ($m$) from equation 5 to convert $S_m$ to LoD:

$$LoD = \frac{S_m - \overline{S_{bl}}}{m} \tag{8}$$

The limit of quantification (LoQ) is defined as the smallest concentration of analyte that can be quantified at an acceptable level of uncertainty (Barwick, 2016). LoQ can be determined from the linear calibration similar to the LoD. At least ten repetitive measurements of blank samples are recommended for better precision and accuracy of calculated standard deviation (Barwick, 2016).

### 3.6 Intermediate precision

Precision is often divided into three subgroups: repeatability, intermediate precision, and reproducibility. In this project, only intermediate precision was considered. Intermediate prescription is determined as closeness in repeated analytical values within the same method but in different conditions, such as a longer time scale, different days, different analytical equipment, or different analysts (Barwick, 2016). Intermediate precisions can be expressed by considering any of the mentioned operation conditions. The laboratory itself determines the acceptable SD and RSD limits of intermediate precision. The acceptable RSD limits can variate from 5% to 20%. For this project, the acceptable RSD value for intermediate precision was set to 10%.

Eurachem guidelines encourage developing warning and action limits for interpreting intermediate precision. For the warning values, it is advisable to set ±2SD of the mean value, and the action limit should be set at ±3SD of the mean value (Barwick, 2016). Acceptable values of the intermediate precision should not exceed the ±2SD of the mean value. The ±3SD indicates that the method is not fully optimised and must be adjusted.

### 3.7 Breakthrough

Breakthrough is defined by the concentration of compounds that the sorbent cannot retain. The breakthrough is determined by placing a non-sampling tube that contains the same sorbent type in series with a sampling (primary) tube (EPA, 1999). The breakthrough can be calculated with an equation:

$$Breakthrough = \frac{Amount\ in\ second\ tube}{Amount\ in\ the\ firt\ tube} * 100\% \quad (9)$$

The breakthrough is identified when more than 5% of analyte concentration is identified in the non-sampling tube. The breakthrough amount can depend on the sorbent type, the sampling flow, or/and the temperature. EPA guidelines assert that breakthroughs can be reduced by increasing the sorbent bed-length. Consequentially doubling the sorbent bed-length would double the safe sampling volume (EPA, 1999). Moreover, efficient airflow is also a significant factor in reducing the breakthrough. Insufficient airflow will not allow proper interaction between the analyte and the sorbent, resulting in an increased breakthrough of the analyte (Dettmer & Engewald, 2002). Tenax TA can efficiently adsorb analytes with a sampling flow between 50-500mL/min. Therefore, sampling outside the ranges should be avoided (Dettmer & Engewald, 2002).

# 4 Results

## 4.1 Method validation results

Method validation was performed for ten targeted VOC compounds in full scan EI mode. Five calibration points were selected for the quantification of VOC emissions, and two orders of magnitude were chosen for the working range. The acceptable recovery range was set between 70-130%, with an RSD of ±20%, based on International Council for Harmonisation (ICH, 1995). The acceptable RSD value for intermediate precision was set to 10%.

### 4.1.1 Selectivity

Method selectivity was determined based on the standard NS-EN 16516:2017+A1. The method was developed for the VOCs eluting between hexane and hexadecane. The selectivity was determined by VOC standard mixture analysis and observing the chromatographic peak resolution. GC temperature programme was adjusted to achieve optimal resolution.

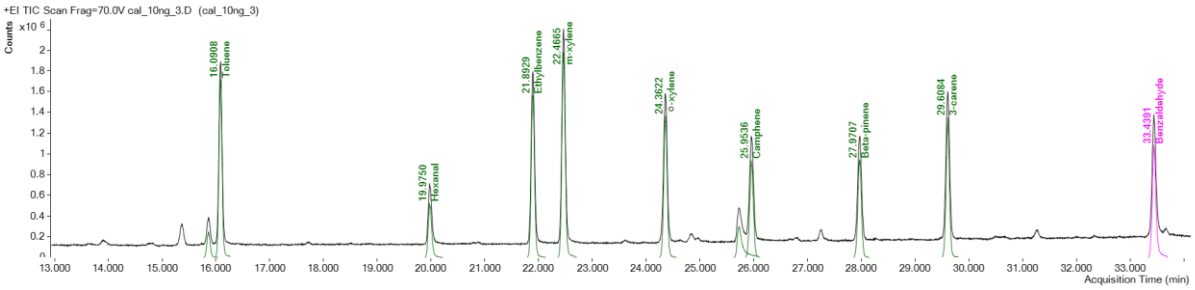



*Figure 4.1 TIC of targeted VOC standards used to determine the selectivity of the analytical method.*

The first experiment was conducted on ten reference standards and internal standard (IS) toluene d-8, with the first GC temperature ramp set to 140°C to 3°C/min. The analysis showed good resolution between 9 of 10 targeted compounds. Co-elution between furfural and camphene peaks was observed; therefore, the first temperature ramp was adjusted to 2.5°C/min to improve the resolution between co-eluting compounds. Changes made on the GC-temperature ramp improved the separation between toluene-d8 and toluene. The co-elution issue between furfural and camphene was not utterly resolved.

Experimental analysis was conducted on a low/medium polarity GC column that could have contributed to stationary phase interactions between non-polar compounds. Camphene is a non-polar monoterpene, while furfural is an aldehyde with an electron-donating hydroxyl group. The non-polar stationary phase could have interacted with non-polar analytes and retained the compound longer. Stationary phase and analyte interactions could explain why camphene

(159ºC) is retained longer by the column compared to furfural, despite having a lower boing point than furfural (162ºC). During the method validation stage, the reference standard of camphene was exhausted, and due to time limitations was not reordered from the manufacturer. Consequentially, camphene was excluded from the further determination.

A new standard mixture was prepared by adding α-pinene and d-limonene. The solution was analysed a second time for a more extensive determination of selectivity. The TIC of targeted VOC standards can be seen in Figure 4.2.

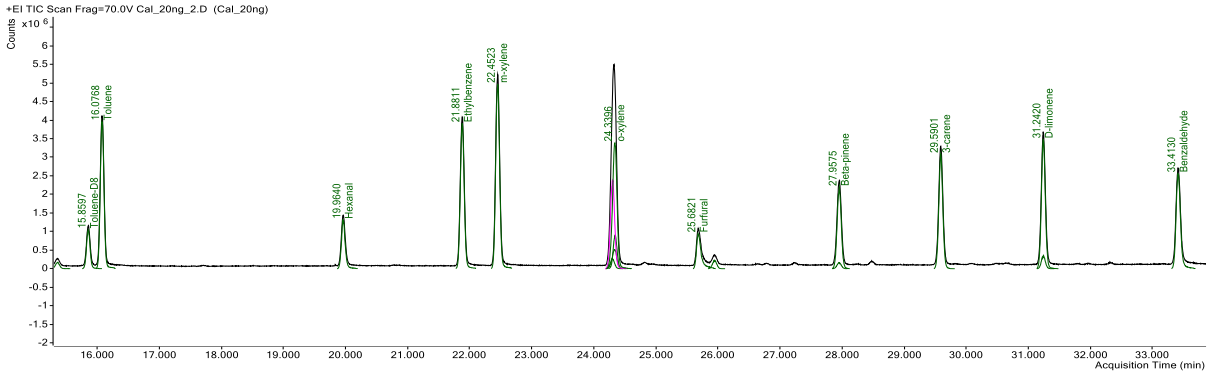



*Figure 4.2 Determination of analytical method selectivity. TIC of targeted VOC compounds.*

Good peak resolution was observed between the standards; however, α-pinene and o-xylene were fully co-eluting. Knowing the origin of the test samples, it was more likely to observe α-pinene; therefore, o-xylene was excluded from the analysis. The list of the targeted compounds used for validation of the analytical method selectivity is presented in Table 4.1.

*Table 4.1 Information of targeted compounds utilised for determination of VOC emissions.*

| Compound of interest | CAS number | Retention time (min) |
|---|---|---|
| Toluene | 108-88-3 | 14.827 |
| Hexanal | 66-25-1 | 18.827 |
| Ethylbenzene | 100-41-4 | 20.292 |
| m-xylene | 108-38-3 | 20.621 |
| Alpha-pinene | 7785-26-4 | 22.621 |
| Furfural | 98-01-1 | 23.925 |
| Beta-pinene | 127-91-3 | 26.167 |
| 3-carene | 13466-78-9 | 27.763 |
| D-limonene | 138-86-3 | 29.380 |
| Benzaldehyde | 100-52-7 | 31.521 |

### 4.1.2 Calibration

The optimal coefficient of determination ($R^2$) was achieved by excluding outliers from all five calibration points and by selecting data points that were closest to the value of expected

concentration. The internal and external standard quantification methods were compared to determine which method resulted in the $R^2$ value being closer to the unity.

The external standard method revealed that residual values between replicates were more extensive at higher concentrations. To achieve the $R^2$ of 0.999, more outliers were necessary to exclude compared to the IS. Furfural had the poorest linearity using external standard (R=0.998). In addition, only four concentration points could be utilised to attain greater linearity. Four calibration points were also utilised for toluene, β-pinene, ethylbenzene, m-xylene, d-limonene due to outliers. The extensive deviation between replicate values could be explained by inaccuracies when spiking the standards on the sorbent tubes. Liquid standards were manually loaded with a 10µL Hamilton syringe, and systematic errors between the replicates are highly probable. In addition, replicates were analysed over an extended period which could contribute to the deviation between the replicates. Calibration curves and linear regression equations based on the external standard method can be obtained in Appendix C.

Calibration curves developed with IS method revealed better linearity and lower deviation between replicate values. In addition, fewer outliers were necessary to exclude compared to the external standard. An optimal $R^2$ of 0.999 with five concentration points was achieved for toluene, ethylbenzene, m-xylene, β-pinene, α-pinene, 3-carene and d-limonene.

Calibration issues were observed for hexanal, benzaldehyde and furfural. Deficient recoveries for hexanal and furfural were observed at the lowest calibration level (1ng/µL). To establish a 0.999 coefficient of determination, the lowest concentration point was discarded from the linear range. Benzaldehyde had an RSD of 24.1% between the replicates at 100ng/µL; hence, the calibration point was excluded from the analysis. After excluding outliers, a linearity of 0.999 was achieved for all targeted VOCs. The calibration curves based on IS method are acquired in Appendix D.

*Table 4.2 Linear regression equation and coefficient of determination of targeted compounds using IS method.*

| Name | Linear range | Slope | Intercept | Type | Origin | Weight | $R^2$ |
|---|---|---|---|---|---|---|---|
| Toluene | 1-150 | 9.52e-03 | 2.45e-03 | Linear | Ignore | None | 0.9997 |
| Hexanal | 10-150 | 1.79e-02 | 1.69e-02 | Linear | Ignore | None | 0.9999 |
| Ethylbenzene | 1-150 | 7.79e-03 | 5.51e-04 | Linear | Ignore | None | 0.9996 |
| m-xylene | 1-150 | 1.14e-02 | 8.73e-04 | Linear | Ignore | None | 0.9999 |
| Alpha-pinene | 1-150 | 1.42e-02 | 1.83e-03 | Linear | Ignore | None | 0.9996 |
| Beta-pinene | 1-150 | 1.60e-02 | 5.65e-03 | Linear | Ignore | None | 0.9992 |
| Furfural | 10-150 | 3.79e-02 | 0.116 | Linear | Ignore | None | 0.9999 |
| 3-carene | 1-150 | 2.67e-02 | 6.04e-03 | Linear | Ignore | None | 0.9994 |
| D-limonene | 1-150 | 1.27e-02 | 3.36e-03 | Linear | Ignore | None | 0.9996 |
| Benzaldehyde | 1-150 | 1.06e-02 | 2.94e-03 | Linear | Ignore | None | 0.9999 |

After integrating EIC, examination of HRMS ion peaks revealed that most abundant ion fragments were saturated at the concentration between 50ng/µL to 150ng/µL. Saturated ions can cause an incorrect representation of the ion abundance and mass inaccuracies resulting in high quantification uncertainty of targeted analytes (Bilbao et al., 2018). Extensive ion saturation is a known phenomenon for TOF analysers, limiting the detector's dynamic range. As a workaround, unsaturated ions with lower abundance were utilised as quantifiers and qualifiers (Table 2.2). Applying lower abundance ions resulted in good recovery and acceptable linearity at higher concentrations. Different algorithms can be applied to correct the abundance of saturated ions *in silico*. However, the application of the algorithm was not in the scope of this project. The linear regression for targeted compounds can be observed in Table 4.2.

## 4.2 Intermediate precision

Three replicates of five calibration points were analysed in a two-week time frame. Due to time limitations and technical issues of the TD unit, it was not feasible to determine the repeatability of the replicate values. Therefore, intermediate precision was established for the targeted VOCs. The intermediate precision was expressed in SD and present RSD between the replicates, and the results are provided in Table 4.3.

*Table 4.3 Expected concentration, average calculated concentration, SD, and RSD values of the targeted compounds used to determine intermediate precision.*

| **Expect. Conc. (ng/µL)** | **Toluene** | | | **Ethylbenzene** | | | **Hexanal** | | | **m-xylene** | | | **Furfural** | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** |
| **1** | 1.38 | 0.53 | 38.4 | 1.25 | 0.10 | 8.10 | 2.36 | 0.23 | 9.72 | 1.18 | 0.07 | 6.01 | 3.69 | 0.09 | 2.34 |
| **10** | 10.4 | 0.69 | 6.63 | 10.4 | 0.29 | 2.86 | 10.6 | 0.88 | 8.29 | 10.0 | 0.31 | 3.08 | 10.04 | 0.32 | 3.17 |
| **50** | 48.5 | 1.33 | 2.74 | 48.9 | 1.08 | 2.21 | 49.1 | 1.42 | 2.90 | 49.6 | 0.21 | 0.43 | 48.1 | 2.70 | 5.63 |
| **100** | 98.7 | 2.74 | 2.82 | 98.8 | 2.41 | 2.44 | 100.1 | 3.35 | 3.25 | 97.8 | 2.58 | 2.64 | 95.6 | 6.85 | 7.17 |
| **150** | 148.1 | 3.54 | 2.39 | 148.5 | 3.54 | 2.39 | 151.2 | 4.04 | 2.67 | 145.5 | 4.57 | 3.14 | 144.2 | 5.89 | 4.09 |
| | **B-pinene** | | | **A-pinene** | | | **3-carene** | | | **Benzaldehyde** | | | **D-limonene** | | |
| | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** | **Av. Con.** | **SD** | **RSD (%)** |
| **1** | 1.28 | 0.19 | 15.2 | 1.23 | 0.07 | 5.78 | 0.80 | 0.05 | 5.96 | 0.34 | 0.59 | 169.4 | 1.32 | 0.12 | 9.09 |
| **10** | 9.88 | 1.15 | 11.6 | 10.2 | 0.32 | 3.17 | 9.51 | 0.23 | 2.43 | 9.08 | 1.59 | 17.5 | 9.14 | 0.35 | 3.81 |
| **50** | 37.6 | 7.50 | 19.9 | 46.6 | 4.22 | 9.05 | 53.2 | 1.55 | 2.91 | 51.3 | 2.17 | 4.23 | 51.78 | 1.67 | 3.23 |
| **100** | 84.6 | 16.4 | 19.4 | 97.8 | 6.03 | 6.17 | 102.1 | 4.08 | 3.99 | 93.78 | 22.6 | 24.1 | 94.4 | 10.3 | 10.9 |
| **150** | 129.2 | 35.1 | 27.2 | 138.6 | 9.35 | 6.75 | 147.6 | 5.41 | 3.66 | 150.1 | 14.8 | 9.92 | 141.9 | 7.18 | 5.06 |

Acceptable intermediate precision can be observed for ethylbenzene, hexanal, m-xylene, furfural, α-pinene, and 3-carene. The RSD for those compounds were calculated under 10% in the range of 1ng/µL to 150ng/µL. D-limonene had acceptable RSD values except at 100ng/µL (RSD=10.9%), which indicates a sizeable deviation between the replicates. Toluene had RSD at 38,4% for the lowest calibration point, revealing undesirable deviation between the values. Extensive RSD (169,4%) at the lowest concentration point was also calculated for benzaldehyde. Poor RSD for toluene and benzaldehyde at 1ng/µL could be caused by random errors such as spiking inaccuracy, resulting in a high deviation between the values. Another explanation for the extensive deviation between the replicates could be that benzaldehyde and toluene are artefacts that can accumulate in the sorbent tubes. Tenax TA is a polymer that has a proclivity to produce artefacts such as benzaldehyde and toluene when exposed to high temperatures and ozone that accumulate in the sorbent tube (Chu et al., 2016). During the analysis, the artefacts are desorbed together with analytes of interest, such as benzaldehyde and toluene; consequently, the artefact accumulation result in elevated analyte concentrations and higher deviation between the replicates that are more noticeable at lower concentrations.

Hexanal and furfural had acceptable SD and RSD values at 1ng/µL (Table 4.3). However, the average calculated concentration for these compounds was 2.36ng/µL and 3.69ng/µL, respectively. The high concentration calculated for hexanal could be explained by the contamination of the sorbent tube. Analysis of blank tubes (Appendix E) identified approximately 1.4ng/µL of hexanal in all blank samples, which could explain the elevated hexanal concentration at 1ng/µL. The contamination could be caused by the passive adsorption of hexanal that can occur in laboratory air. The possible air contamination could also explain why furfural had elevated concentration in blank samples (3.07ng/µL).

The highest RSD values were calculated for β-pinene. RSD for the compound was calculated over 10% at all concentration levels. As mentioned earlier, high RSD could be explained by systematic spiking errors. Nonetheless, optimal linear regression for β-pinene was achieved by choosing concentrations closest to the expected values instead of utilising average values. Thus, poor SD and RSD values between the replicated did not affect the quantification accuracy.

### 4.3 LoD and LoQ

The S/N ratio is a common approach when determining the LoD and LoQ. However, it was not feasible to achieve linear regression by utilising values obtained from S/N. Therefore, LoD and LoQ were determined by calculating the standard deviation of the analytical signal (peak area)

in the blank sample and plotting the value against the slope of the calibration curve of targeted compounds (section 3.5).

*Table 4.4 Limit of detection and limit of quantification for the targeted compounds.*

| Targeted compound | LoD (ng/µL) | LoQ (ng/µL) |
|---|---|---|
| Toluene | 0.63 | 2.11 |
| Hexanal | 0.52 | 1.72 |
| Ethylbenzene | 0.06 | 0.20 |
| m-xylene | 0.07 | 0.23 |
| Alpha-pinene | 0.09 | 0.31 |
| Furfural | 0.06 | 0.21 |
| Beta-pinene | 0.02 | 0.07 |
| 3-carene | 0.04 | 0.12 |
| D-limonene | 0.05 | 0.18 |
| Benzaldehyde | 1.50 | 5.00 |

The highest LoD and LoQ values were calculated for benzaldehyde. The LoD for benzaldehyde was calculated at 1.5ng/µL and LoQ at 5.00ng/µL. Benzaldehyde is a common Tenax TA sorbent artefact. As mentioned earlier, artefacts are formed by oxidation of the Tenax TA polymer causing higher concentrations of benzaldehyde in the blank samples (Chu et al., 2016). This could explain the high LoD and LoQ values. Toluene and hexanal also had higher LoD and LoQ values than other targeted compounds. Toluene is another artefact produced by the degradation of Tenax TA and thus has the exact reasoning behind the results of calculated values. Higher LoD (0.52ng/µL) and LoQ (1.72ng/µL) values for hexanal could be caused by sorbent tube contamination. The LoD and LoQ values for all targeted compounds can be observed in Table 4.4.

## 4.4 Recovery

Recovery at 1ng/µL, 10ng/µL, 50ng/µL, 100ng/µL and 150ng/µL was automatically calculated by utilising MassHunter Quantitative analysis. The raw data for the apparent recovery can be observed in Appendix E. The software annotated recovery as accuracy; however, values are closely related. Accuracy is defined by the closeness of the expected concentration value in particular samples and is reported as recovery (ICH, 1995). Therefore, apparent recovery is equivalent to the accuracy calculated by MassHunter, and the defined values are based on Equation 6. The average apparent recovery was calculated based on data acquisition from three replicates. The calculation results are represented in Table 4.5.

*Table 4.5 Calculated average recovery and RSD (%) of targeted VOC compounds.*

| | **Avg. Recov. (%)** | **RSD (%)** | **Avg. Recov. (%)** | **RSD (%)** | **Avg. Recov. (%)** | **RSD (%)** | **Avg. Recov. (%)** | **RSD (%)** | **Avg. Recov. (%)** | **RSD (%)** |
|---|---|---|---|---|---|---|---|---|---|---|
| **Conc. / Name** | **1ng/µL** | | **10ng/µL** | | **50ng/µL** | | **100ng/µL** | | **150ng/µL** | |
| Toluene | 138.2 | 38.4 | 103.5 | 6.62 | 96.9 | 2.74 | 98.6 | 2.81 | 98.7 | 2.36 |
| Hexanal | 235.9 | 9.72 | 105.7 | 8.24 | 98.1 | 2.91 | 100.1 | 3.25 | 100.8 | 2.67 |
| Ethylbenzene | 125.4 | 8.09 | 104.3 | 2.89 | 98.0 | 2.22 | 98.8 | 2.42 | 98.9 | 2.53 |
| m-xylene | 117.6 | 6.03 | 100.4 | 3.06 | 99.2 | 0.40 | 97. | 2.57 | 96.9 | 3.15 |
| α-pinene | 122.3 | 5.78 | 101.9 | 3.17 | 93.3 | 9.07 | 97.8 | 6.14 | 92.4 | 6.76 |
| Furfural | 369.5 | 2.33 | 100.4 | 3.18 | 96.1 | 5.61 | 95.6 | 7.22 | 96.1 | 4.09 |
| β-pinene | 128.9 | 15.2 | 98.73 | 11.5 | 75.1 | 19.9 | 84.6 | 19.4 | 86.2 | 27.2 |
| 3-carene | 80.8 | 6.01 | 95.1 | 2.45 | 106.4 | 2.92 | 102.0 | 4.03 | 98.43 | 3.67 |
| D-limonene | 131.5 | 9.08 | 91.43 | 3.76 | 103.6 | 3.23 | 94.4 | 10.9 | 94.63 | 5.07 |
| Benzaldehyde | 34.8 | 169.5 | 90.8 | 17.5 | 102.6 | 4.23 | 93.8 | 24.1 | 100.1 | 9.94 |

Recovery calculations were based on IS method, and the matrix effects were considered for all targeted concentrations. The calculation revealed optimal recoveries for all targeted compounds at 10ng/µL and 50ng/µL. The poor average recovery and RSD at 1ng/µL were calculated for benzaldehyde, toluene, hexanal, furfural and d-limonene. Benzaldehyde had an average apparent recovery of 34,8% with an RSD of 169.5%, while toluene had an average recovery of 138,2% and an RSD of 38,4%. A low RSD value for hexanal (9.72%) and furfural (2.33%) at 1ng/µL indicates that the concentration loaded on the sorbent tube was constant; nevertheless, recovery of >200% was indicated for both compounds that could be caused by systematic errors. Dilution errors in preparing standard solutions or spiking errors when loading the standards on the tube can contribute to higher recoveries. The other possibility is sorbent tube contamination due to the passive adsorption of laboratory air.

The trend can be seen for recovery at lower concentrations. Five targeted compounds had average recoveries above 130% or under 70% (Table 4.5). The results can indicate that minor errors during the spiking of liquid samples or preparing standard solutions cause significant deviation and uncertainty at low concentrations. In addition, artefact accumulation for compounds such as toluene and benzaldehyde potentially contribute to the higher recovery that is more noticeable at low concentrations. Large RSD of toluene (41,9%) and benzaldehyde (86.9%) in blank samples (Appendix E) reveals that not all sorbent tubes possess equal amounts of artefacts, resulting in an extensive deviation between the replicates and higher apparent recovery.

## 4.5 Quantification of targeted VOC

VOC emissions were determined for three different wood materials: untreated spruce panel (USP), stained spruce panel (SSP) and cross-laminated three (CLT). The emissions were quantified for ten targeted compounds. Air samples were collected from four duplicate samples of each sample batch. Sampling was based on the 16516: 2017+A1 standard, and the sampling procedure is explained in section 2.6. The air samples were collected three days after placing the samples in climate chambers.

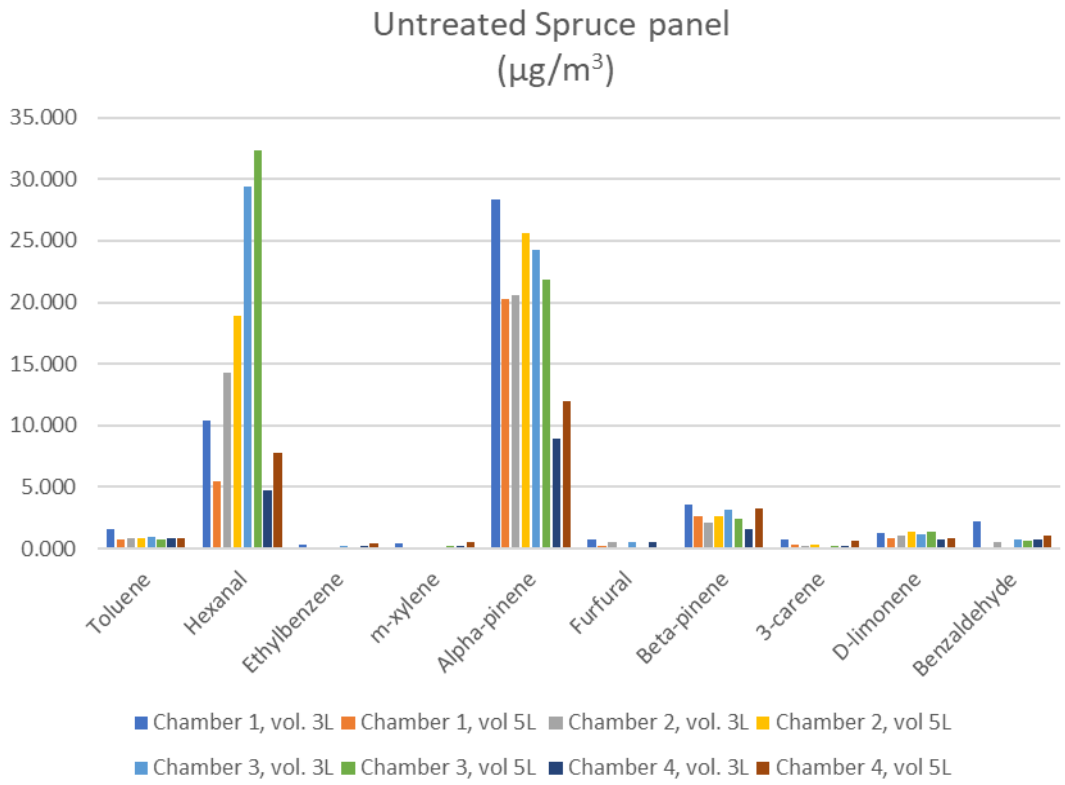



*Figure 4.3. Quantification results of targeted VOC emissions form the untreated spruce panel.*

Targeted VOC emissions from USP were quantified with an external standard method, and the matrix effects were not considered for this sample batch. The external standard method was used because of an error during spiking sorbent tubes with the IS. The error made the application of IS method not achievable, and due to time limitations repeating the sampling procedure for USP was not feasible.

VOC emissions identified in the blank chamber were subtracted from concentrations identified in sample duplicates to determine the actual value of targeted VOC emissions. Quantification results revealed that hexanal and α-pinene were the most dominant VOCs emitted from USP. Hexanal had significant concentration variations between climate chambers, with the highest

concentration of 32.32µg/$m^3$ in chamber three (5L sample) and the lowest 4.75µg/$m^3$ in chamber four (3L sample). Significantly lower hexanal concentration in chambers one and four could suggest that chambers were not sufficiently sealed and potentially caused a loss of analyte. The concentration variation between the duplicates can be observed in Appendix F.

The concentration of α-pinene was highest in chamber one, at 28.38µg/$m^3$, which contradicts the chamber having a sealing issue. The lower concentration in chamber four was observed for all targeted compounds in both 3L and 5L air samples and could verify the possible loss of analyte. Low amounts of m-xylene (0.09-0.53µg/$m^3$) and ethylbenzene (N.A.-0.19µg/$m^3$) were also identified in the USP samples. Ethylbenzene concentrations in all replicates were below the working range, and emissions for the compound could only be semi-quantified. Benzaldehyde concentration varied from 0.06µg/$m^3$ to 2.21µg/$m^3$, considering both 3L and 5L air samples. The raw data of calculated VOC emissions can be observed in Appendix F. As mentioned in previous sections, benzaldehyde is an artefact commonly found in Tenax TA sorbent, and there is a possibility that the concentration calculated in the samples does not represent the true value of emissions. Due to time constraints, further investigation of benzaldehyde emissions was unattainable.

A similar emission trend can be observed for CLT sample duplicates. The most profound compound quantified was hexanal at 80.07µg/$m^3$ in chamber three. The concentration calculated for hexanal in chamber three was above the method working range; hence, it was semi-quantified. The hexanal concentration in chamber three was distinctively higher compared to the concentration calculated for other duplicate samples. The results could suggest that chamber three had a source of contamination. Contamination could be caused by insufficient chamber cleaning practices before placing a new sample batch. Elevated concentration in chamber three can also be observed for α-pinene, β-pinene and 3-carene (see Figure 4.4). This trend could conclude that chamber three had contamination from an unknown source.

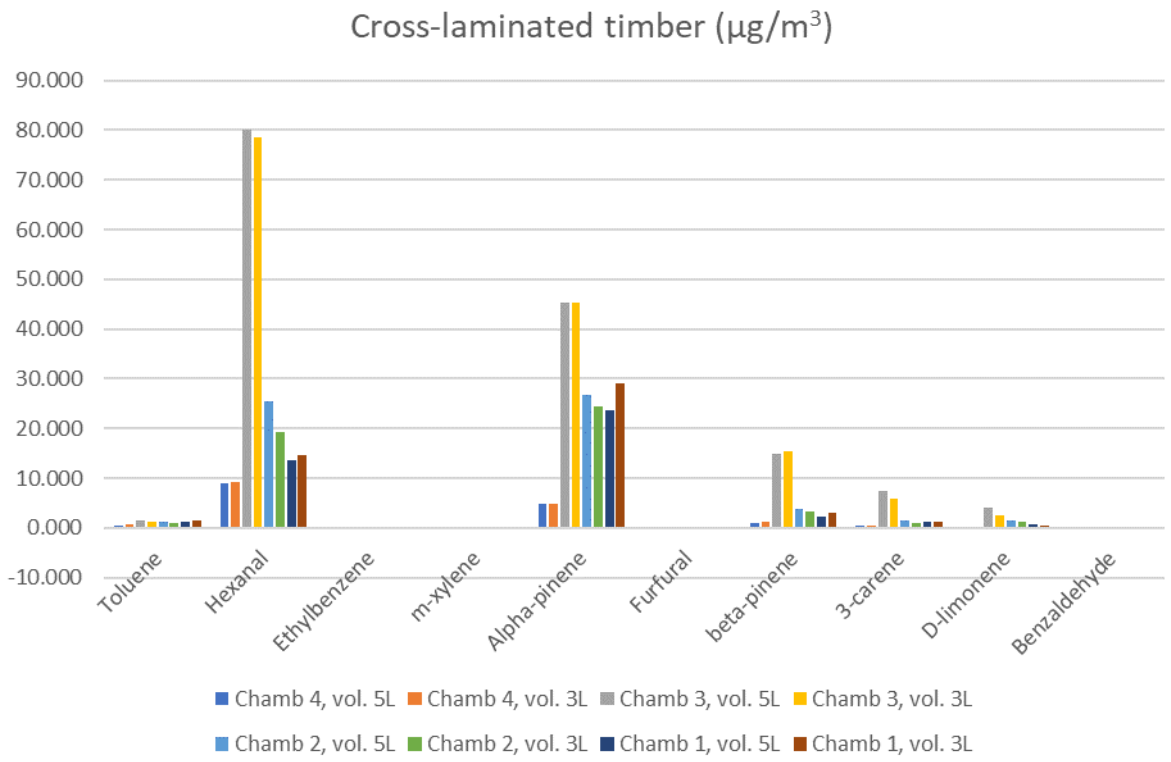



*Figure 4.4 Quantification results of targeted VOC emissions from the cross-laminated timber.*

A-pinene was the second most dominant compound quantified in CLT sample replicates. The highest concentration was identified in chamber three at 25.51µg/m$^3$, and the lowest concentration was calculated in chamber four at 4.77µg/m$^3$. Lower targeted compound concentrations in chamber four were observed for both CTL, USP and SSP samples, which could imply that chamber four had a leak issue that potentially resulted in the loss of targeted analytes. Low levels of toluene were observed in both CLT to USP samples (0.40-1.58µg/m$^3$). Identification of toluene could indicate contamination of the sample surface or contamination in chamber air. Moreover, a possible artefact accumulation in sorbent tubes should also be considered as a source of contamination.

The last emission analysis carried out in this project was on SSP duplicates. Lower emissions of α-pinene hexanal, d-limonene and β-pinene were observed in the SSP compared to CLT and USP samples. The concentration of hexanal was calculated to be slightly higher than α-pinene. Hexanal concentration was highest in chamber three at 16.55µg/m$^3$. The lowest concentration was found in chamber four at 3.11µg/m$^3$.

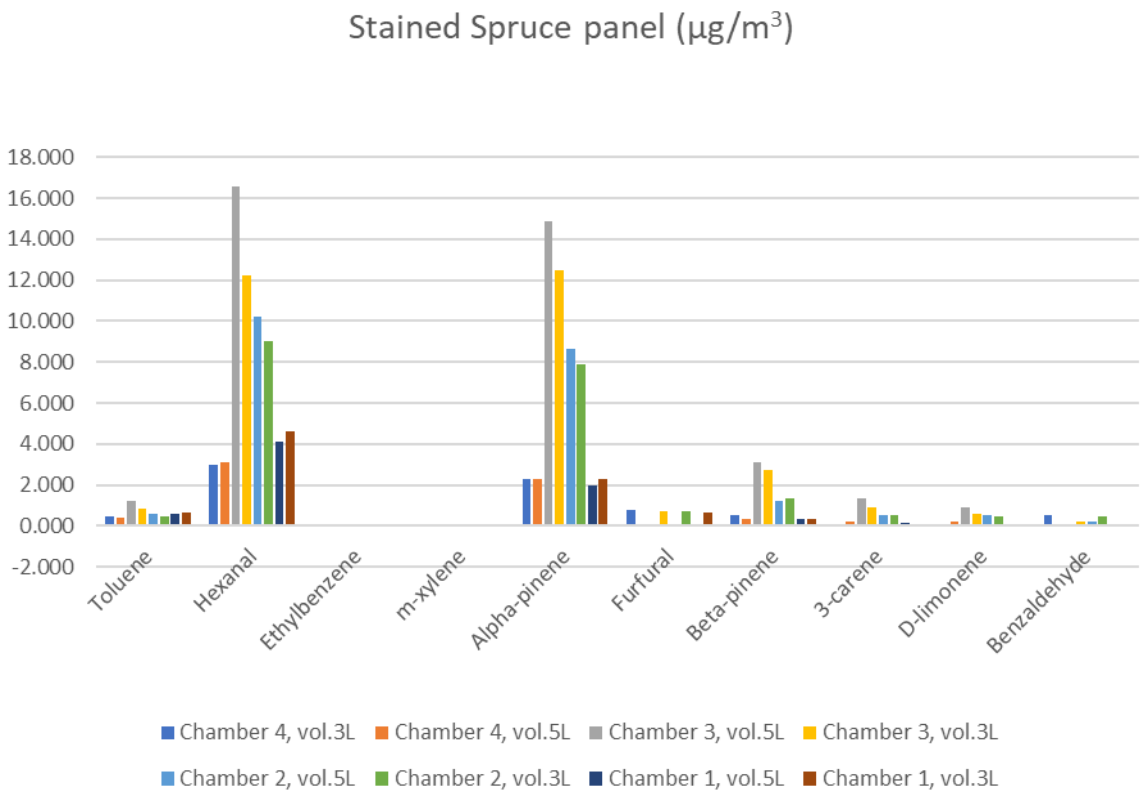



*Figure 4.5. Quantification results of targeted VOC emissions from stained spruce panel.*

The highest concentration of α-pinene was found in chamber three at 14.87µg/m$^3$ in the 5L volume sample and 12.85µg/m$^3$ in the 3L volume sample. Slightly higher emissions of furfural (0.69-0.77µg/m$^3$) were identified in SSP samples compared to other spruce samples analysed in this project (USP: 0.12-0.70 µg/m$^3$, CLT:0.04-0.22 µg/m$^3$). The furfural was semi-quantified since all determined values were under the working range of calibration. Interestingly, only 3L air sample volumes had detectable concentrations of furfural, while furfural in 5L volumes either were not identified or had negative values. Negative values indicate that the chamber blank had a higher concentration of furfural than the sample itself. This could occur by the contamination of the blank chamber or the sorbent tubes. Another cause could be incorrect sorbent tube mounting on the air hose when collecting 5L air samples. However, these assumptions cannot explain why only 3L samples had a detectable amount of furfural.

As mentioned in section 2.6, constant temperature and RH conditions were important factors for achieving representative results. These conditions were continuously monitored with SenseAnywhere sensors. The sensor calculated the average temperature in all four climate chambers at 22.4±0.01ºC, which complied with the temperature norms established by NS-EN 16516:2017+A1 standard. However, RH 50±5% was not possible to achieve. The average

monitored humidity in chambers was 32.2±4% during the sampling period. A study conducted by Akutsu et al. (2002) on acetaldehyde emissions in wood-based materials concluded that higher humidity increased acetaldehyde emissions and had a greater significance in emission rates than the temperature. The study was conducted at constant humidity with variating temperatures and in fixed temperature conditions and variating humidity at 20, 50 and 80%. Another emission evaluation on wood pellets conducted by Wang et al. (2016) concluded that aldehyde emissions significantly increase between 30-50% RH. Hence, it is possible that RH at 32% could have resulted in lower hexanal emissions in Norway spruce samples analysed in this project. Due to time limitations, further investigation of the hypothesis was not feasible.

### 4.6 Breakthrough of targeted VOCs.

A breakthrough test was carried out to determine if a part of the analyte is eluted through the non-sampling end of Tenax TA sorbent during sample collection. The test was conducted by joining two identical tubes in the series with a union. The breakthrough is considered when ≥5% of the analyte is identified in the non-sampling tube (EPA, 1999). The amount of breakthrough was calculated by Equation 9.

Analysis for SSP revealed a 517% breakthrough of d-limonene in chamber one and 132% in chamber four. Breakthrough greater than 100% implies that the non-sampling tube had a higher amount of d-limonene than the sampling tube. This can occur if the non-sampling tube was contaminated with d-limonene. Moreover, >100% breakthrough values were calculated for chamber one (287%) and chamber two (152%) in the analysis of USP samples. Other breakthrough values of d-limonene varied between 9.4-44% in both USP and SSP sample analysis. A less extreme amount of breakthrough of d-limonene was calculated for CLT samples at 7.2% breakthrough in chamber one and 54% in chamber three. The only compound with no breakthrough was d-limonene (4.5%) in chamber two. During breakthrough analysis, TDU malfunctioning caused the loss of CLT analytical data in chamber four; hence the breakthrough was not determined for this chamber.

Analytical data evaluation of USP duplicates in chambers one and two revealed that 3-carene and benzaldehyde possessed a breakthrough significantly above 100%. Breakthrough of 3-carene was determined at 245% in chamber one and 184% in chamber two. Benzaldehyde had a breakthrough of 179% in chamber one and 197% in chamber two. The extensive breakthrough could be caused by prolonged storage time with unsuitable storage caps. The storage caps utilised to seal the sorbent tubes were designed for in-lab, short-term storage. Markes

International asserts that the storage caps are only suitable for up to 3-day storage. Due to the malfunctioning of TDU, sorbent tubes were stored longer than three days before conducting the analysis. Furthermore, sample sorbent tubes were transported between NILU and NMBU locations, while the storage caps utilised were not suited for the transportation of sample tubes. PTFE O-rings used in short-term storage caps potentially were not able to provide a tight enough seal for all sorbent tubes and resulted in passive sampling of laboratory air. The prolonged storage time and an insufficient tube seal could rationalise why some of the non-sampling tubes had immense breakthroughs.

The accumulation of Tenax TA sorbent artefacts could also cause elevated breakthrough values of benzaldehyde. Toluene is also described as a compound of issue; nonetheless, the breakthrough varied between 5.5%-33%, which is significantly lower than benzaldehyde. However, the possibility of accumulating toluene artefacts resulting in a higher amount of breakthroughs should not be overlooked. The same argumentation for calculated toluene and benzaldehyde breakthrough values could be applied to SSP and CLT duplicates.

Determination of breakthrough for CLT replicates detected no breakthrough for m-xylene. Hexanal also had no breakthrough identified, except in chamber four, where the breakthrough was determined at 6,9%. No breakthrough for 3-carene (4.9%), toluene (4.2%) and d-limonene (4.5%) were identified in chamber two. The rest of the non-sampling tubes in the CLT sample batch possessed breakthroughs with amounts highly varying between each replicate. The raw breakthrough data for each compound can be obtained in Appendix F. High ethylbenzene breakthrough was identified in chamber one (11.25%) and chamber three (77.5%) during the analysis of CLT duplicates. Chambers two and four did not possess any ethylbenzene breakthrough. Ethylbenzene is a common pollutant found in urban areas and other anthropogenic sources. High breakthrough levels in sampling tubes could suggest that laboratory air was contaminated with ethylbenzene and resulted in the contamination of non-sampling tubes.

Furfural had a breakthrough between 83-87% in CLT, USP, and SSP sample replicates. Breakthrough values could indicate that furfural is poorly retained by a Tenax TA sorbent or that the non-sampling tube was contaminated during analysis. Analysis of blank samples (Appendix E) revealed relatively high levels of furfural that could contribute to high breakthrough levels. Furfural is not determined as compounds that could be accumulated by

degradation of Tenax TA. Therefore, the reason for high furfural levels in blank samples is unknown.

### 4.7 Non-target and Suspect screening

The NTS and SUS were carried out for USP, SSP and CLT samples to determine the complete composition of VOC emissions. The screening was carried out by Agilent MassHunter Unknown analysis. NIST20 and in-house HR-PCDL were utilised for the MS identification and annotation of non-targeted VOCs. RT, CAS number, monoisotopic mass, MS spectra matching, and RI were utilised as identities in a SUS and NTS. Statistical evaluation of laboratory samples was conducted for 5L and 3L air sample replicates; the breakthrough samples were not considered for the SUS and NTS.

*Table 4.6 Statistical evaluation of compound hits identified by MassHunter Unknown Analysis.*

| | **Untreated spruce panel** | | **CLT** | | **Stained wood panel** | |
|---|---|---|---|---|---|---|
| | **Components** | **Hits** | **Components** | **Hits** | **Components** | **Hits** |
| **Chamber 1, 5L** | 574 | 106 | 588 | 102 | 1376 | 137 |
| **Chamber 1, 3L** | 1720 | 245 | 673 | 95 | 1573 | 111 |
| **Chamber 2, 5L** | 1008 | 163 | 758 | 122 | 1737 | 197 |
| **Chamber 2, 3L** | 1273 | 189 | 824 | 119 | 1791 | 144 |
| **Chamber 3, 5L** | 1445 | 239 | 580 | 115 | 1051 | 127 |
| **Chamber 3, 3L** | 1205 | 189 | 603 | 106 | 1297 | 118 |
| **Chamber 4, 5L** | 1568 | 262 | 568 | 103 | 1310 | 115 |
| **Chamber 4, 3L** | 1253 | 208 | 689 | 98 | 1707 | 129 |
| **Chamber 5, 5L** | 1199 | 210 | 1536 | 140 | 1783 | 138 |
| **Sum** | 11245 | 1811 | 6819 | 1000 | 13625 | 1216 |
| **Total hits** | **4027** | | | | | |
| **Total components** | **31 689** | | | | | |

The screening identified 31 689 hits in three laboratory samples and their duplicates. The number includes both VOCs annotated by the library and the compounds that only mass spectra were identified. A total of 4027 hits were annotated by the PCDL and NIST libraries with a match factor above 70%. Hits were calculated for air samples adsorbed on Tenax TA sorbent, and blank sample hit subtraction was not considered at this stage. After the blank sample subtraction and RI calculation, 1498 hits were determined with an identification confidence level 2. Non-targeted VOCs annotated by the library but having RI values outside the accepted range (>±100) were classified with an identification confidence level 3. After the statistical data evaluation, 2504 hits were determined with a confidence level of 3. Unknowns identified with

retention time and signal response, but no library match were determined with identification confidence level 5. A total of 19 249 hits were identified with confidence level 5. A detailed statistical overview of hits identified in the laboratory samples and their replicates can be found in Appendix H. The project focused on the compounds with an identification level 1 and 2; therefore, further discussion was designated for compounds determined at these confidence levels.

The pie diagram was used to classify the most dominant VOC groups identified in CLT, UPS and SSP sample duplicates.

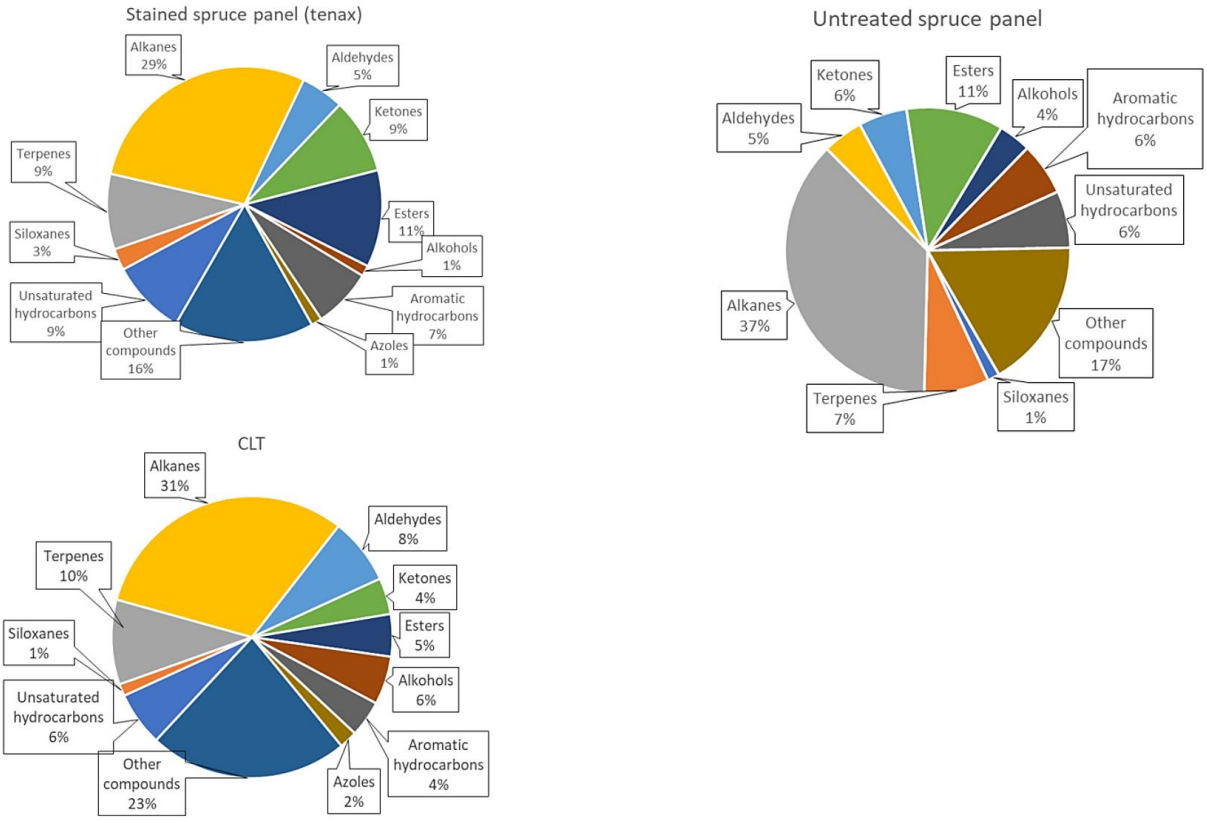



*Figure 4.6 Pie charts of major compounds group identified in CLT, SSP and USP samples and their replicates.*

Important to note that the classification was carried out manually; therefore, fluctuations from the true compound distribution are highly probable. Pie charts revealed that the most dominant compound group was alkanes. SSP contained around 29% of alkanes, CLT 31% and USP 37%. 2,3-dimetylpentane, 2-methylhexane, methylcyclohexane, 3-methylhexane and heptane were the most abundant alkanes identified in CLT, USP, and SSP samples and their duplicates (Appendix I). Based on information obtained from PubChem, these types of alkanes are common ingredients in gasoline and can be a product of biomaterial combustion. The compounds were not identified in chamber blanks, implying that these alkanes are emitted from

the wood sample surface. Alkanes are not biogenically emitted from Norway spruce, implying a potential source of alkanes could be contamination. After the wood specimens were manufactured, samples were stored in the exposed storage before transporting the samples specimens to NMBU. Long pallets are usually transported by vehicles, and contaminants could be a result of exhaust emissions. However, further investigation should be undertaken to confirm this statement. Based on visual observations of peak response in TIC, alkanes were found in trace amounts, while aldehydes and terpenes had dominating emissions.

The second abundant chemical group was terpenes. The USP sample contained approximately 7%, CLT 10% and SSP 9% of terpenes. SUS and NTS correctly annotated targeted terpenes: β-pinene, α-pinene, d-limonene and 3-carene. Since the compounds could be confirmed with a reference standard, they were categorised as identification confidence level 1. The most abundant non-targeted monoterpenes identified by screening were camphene, β-myrcene and o-cymene. O-cymene is an oxidation product of 3-carene (Hyttinen et al., 2010). Based on the article published by Hyttinen et al. (2010), air-dried samples were found to contain a higher amount of o-cymene compared to heat-treated wood samples. The spruce panels provided for this project were kiln-dried between 60-80$^{o}$C. The temperature was not high enough to start a rapid terpenes degradation, which could explain why terpenes, including o-cymene, were abundant in all three wood samples. β-phellandrene is a monoterpene commonly found in spruce. After the screening, β-phellandrene was identified in USP and CLT samples. However, no compound match was found in SSP sample duplicates. No β-phellandrene match in SSP could imply that the wood stain used on the panel hinders biogenic terpene emissions.

The pie chart revealed that aldehydes contributed to 5-8% of total VOC emissions in SSP, USP and CLT samples. The most abundant aldehydes identified by NTS and SUS were heptanal, nonanal, decanal, pentanal and targeted hexanal. The compounds were identified in all CLT, SSP and USP duplicates. Aldehydes are commonly found in thermally unmodified wood and are products of the oxidation of unsaturated fatty acids (Pohleven et al., 2019). Cleaved wood samples were stored exposed before transporting them to the NMBU campus. Wood cleaving damages the physical structure of the wood by exposing resin channels. This could accelerate fatty acid oxidation since air could penetrate the panel surface more easily. The oxidation of unsaturated fatty acids could explain why different aldehydes were identified in all the wood samples, and hexanal had the most dominant emissions.

Aromatic hydrocarbons styrene and naphthalene were identified in USP and SSP sample duplicates after SUS and NTS. Naphthalene and styrene were identified in all four USP sample duplicates, including chamber blank. A compound match in the chamber blank could suggest that the compound emissions were caused by air contamination in the chamber. CLT samples did not contain naphthalene while styrene was found in duplicates placed in chambers four and two. Naphthalene was identified in SSP samples except the duplicate placed in chamber three, while styrene was identified in all four duplicates. Naphthalene was not identified in the chamber blank during the identification of SSP emissions, indicating that the compound could be a result of sample surface contamination. Styrene was identified in the chamber blank; therefore, the compound could be identified due to camber air contamination. For a complete list of the VOCs identified by NTS and SUS in samples analysed in this project, refer to Appendix I.

### 4.8 In-House Personal Compound Database and Library

Custom PCDL manager was utilised with the NIST20 library for NTS and SUS analysis. In the method editor, the PCDL library was prioritised so that the MassHunter Unknown Analysis would first find a match in PCDL, and if no matches were found, the software would search for a match in the NIST library. After the analysis, 18 compounds were annotated by the in-house PCDL. The most abundant compounds found by the PCDL manager were 3-carene, β-pinene, hexanal, d-limonene, decanal, camphene, benzaldehyde, and m-xylene. The match factor for these compounds varied between 84.6% to 98.7%. Utilising PCDL, however, resulted in incorrect annotation of α-pinene. The PCDL manager annotated the peak as 3-carene for all samples. A-pinene was a targeted compound in this project; therefore, the peak was confirmed with the reference standard and annotation was corrected with a revised compound. Compounds identified by in-house PCDL can be acquired in Appendix J.

Utilising custom PCDL had an advantage over the NIST library because of the application of HRMS data during NTS and SUS. Moreover, retention time matching could also give an advantage when annotating chemical structures since the library could be customised for a specific analytical method. However, some disadvantages were observed after the custom PCDL was developed. For PCDL to work efficiently, a large amount of analytical data is required. The in-house PCDL contained HRMS data of 47 compounds; thus, the PCDL could only be applicable as a supplement to the NIST library and not as an independent library. The list of compounds added to PCDL can be found in Appendix G.

The second disadvantage was that most HRMS data utilised for building the PCDL came from a cocktail of standard mixtures. In this project, two standard mixtures containing in total over 200 VOC were utilised. Many of the compounds in standard mixtures contained isomers with identical MS data, and even with the advantage of HR, it was challenging to confirm the correct compound annotation. Therefore, individual reference standards should be prioritised for the development of PCDL. The compound list used to build the in-house library can be obtained in Appendix A.

Lastly, automatic calculation of RI is not possible when utilising the PCDL manager. PCDL does not contain RI standard database values; hence, MassHunter Unknown Analysis cannot automatically calculate RI values during NTS and SUS. The values can be calculated manually; however, the process would be time-consuming and ineffective when working with large analytical data. On the other hand, efficiently developed PCDL would provide a high level of identification of confidence without the necessity of RI. Therefore, it is essential to establish PCDL with a fully developed analytical method and by utilising HRMS data of individual reference standards.

### 4.9 Comparison of Universal and Tenax TA sorbents

Universal and Tenax TA sorbents were compared when analysing SSP samples. The comparison was made to define if Universal sorbent was capable of a broader range of compound absorption compared to Tenax TA. The comparison was made only with stained wood samples due to manufacturing and dispatching delays of Universal sorbent tubes.

*Table 4.7 Total amount of compounds identified in Tenax and Universal sorbents. The sixth and seventh rows represent identical compounds found in both sorbents.*

| | **Tenax** | | **Universal** | | **Tenax and Universal** | |
|---|---|---|---|---|---|---|
| | **Confidence level 2** | **Conf. level 2 and 3** | **Confidence level 2** | **Conf. level 2 and 3** | **Confidence level 2** | **Conf. level 2 and 3** |
| **Chamber 1, 5L** | 57 | 137 | 56 | 141 | 31 | 62 |
| **Chamber 2, 5L** | 74 | 197 | 63 | 163 | 38 | 64 |
| **Chamber 3, 5L** | 49 | 127 | 48 | 134 | 28 | 56 |
| **Chamber 4, 5L** | 50 | 115 | 61 | 164 | 39 | 67 |

In general, the Universal sorbent was able to adsorb more compounds than Tenax TA; however, some exceptions can be observed (Table 4.7). More compound hits in chamber two were adsorbed by Tenax TA (197 hits) compared to Universal (163 hits). When comparing compound data with confidence levels 2 and 3, approximately 43% of compounds were found in both Tenax TA and Universal sorbents. Compounds identified with confidence level 3 are

more likely to be annotated as false positives, which could be a reason why a higher amount of hits were unique to either Tenax TA or Universal sorbent.

The method implemented in this project was developed for VOCs eluting between n-hexane and hexadecane. N-hexane was eluting in 9min window. Therefore, an 8min solvent delay was utilised when analysing the samples adsorbed on Tenax TA. During the analysis of samples collected on Universal sorbent, the solvent delay was not utilised. Solvent delay is a significant reason why more compounds were identified by Universal sorbent.

Different trends can be observed when comparing hits for compounds characterised with confidence level 2. A lower amount of compound hits was identified with a confidence level 2 that were adsorbed on Universal. The exception can be observed in chamber four, where 61 compounds were identified with confidence level 2 (Table 4.7), while only 50 hits were identified for Tenax TA sorbent. It can also be detected that, on average, 59% of the compounds identified with a confidence level 2 were found in both Tenax TA and Universal. When evaluating compounds only adsorbed by the Tenax TA (Table 8.16, Appendix I), it was observed that the most dominant compounds were 2,2-dimethylhoxybutane, heptane and octane. The compounds were identified in all four SSP sample duplicates. The 2,2-dimethylhoxybutane match in the chamber blank could suggest that the compound is identified due to chamber air contamination.

Universal sorbent chromatographic data collected in the first 10 minutes revealed an extensive compound coelution between 8min and 9min. The identical coelution can also be observed for the compounds adsorbed on Tenax TA sorbent. Coelution could be caused by poor method selectivity in the first 9min of an analytical run. As mentioned earlier, the method was developed for VOCs eluting between n-hexane and hexadecane; therefore, the identification of VVOCs and SVOCs was outside of the analytical method scope. Consequentially, compound coelution at the start of the analytical run was expected.

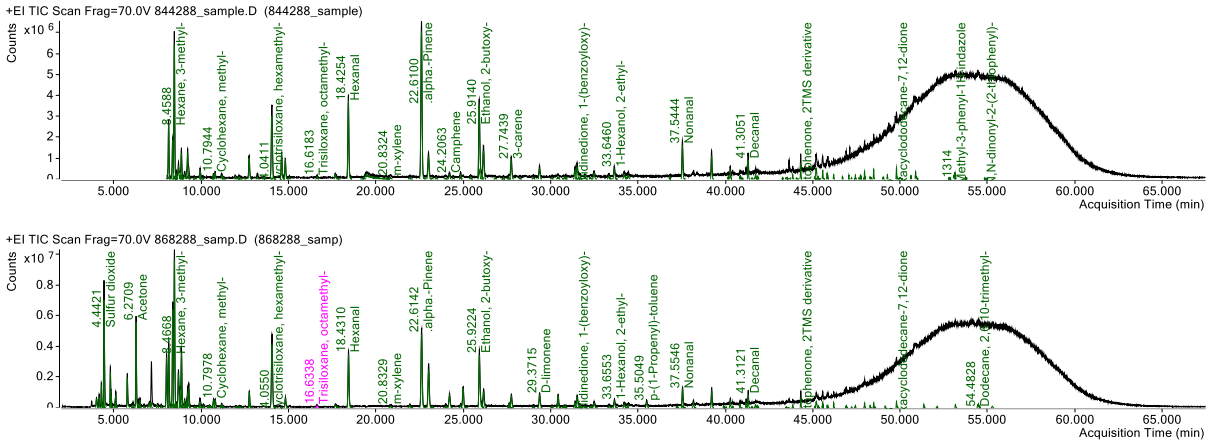



*Figure 4.7 TIC of sample analysis. The TIC above identifies analytes collected on the Tenax TA sorbent tube and below is the TIC of analytes adsorbed on the Universal multi-sorbent tube. The results observed in the TICs were collected from the SSP duplicate in chamber three.*

Examination of TIC samples adsorbed by Universal sorbent showed no peaks in the first 4 minutes of the analytical run. This implies that Universal sorbent had a 4min data acquisition advantage over Tenax TA. A large peak of sulphur dioxide can be observed in the TIC of Universal sorbent. Sulphur dioxide is an artefact found in all blank Universal tubes; hence compound is not emitted from the laboratory samples. The most abundant VOCs identified with confidence level 2 between 4min to 8min were 2,2-dimethylpentane, acetone, n-hexane, 2,4-dimenthylpentane and formic acid ethenyl ester (Table 8.15, Appendix I). An article published by Pohleven et al. (2019) explained that different ketones, such as acetone, are commonly emitted from untreated softwood. Since acetone had a significant peak abundance in TIC this could imply that water-based wood stain does not hinder acetone emissions. Due to time limitations, quantification of acetone in different spruce samples was not carried out. Therefore, it was impossible to conclude if acetone emissions would variate in other softwood samples analysed in this project.

Moreover, Pohleven et al. (2019) explained that different alkanes can be formed in wood components during cellulose, lignin and hemicellulose degradation. Therefore, thermally modified wood usually has higher alkane emissions. The decomposition of hemicellulose starts at 200$^{o}$C, while cellulose degrades at around 300$^{o}$C. Lignin has the lowest degradation temperature at 160$^{o}$C. The SSP duplicates analysed in this project were kiln-dried between 60-80$^{o}$C. The temperature applied during the drying process was too low to initiate the decomposition of wood components. Alkane emissions identified in Universal sorbent could imply that the compounds are the result of sample surface contamination. The possible contamination sources were already discussed in section 4.5.

The most abundant compounds with confidence level 3 identified in the first 8 minutes of analysis were dichlorofluoromethane, methylene chloride, trichloromonofluoromethane and 1-chloro-1,1-difluoro-ethane. Chlorofluorocarbons (CFCs) are compound of anthropogenic origin. The CFCs identified in the samples are bioaccumulating molecules that form halogen radicals in the stratosphere and contribute to ozone layer depletion (Rhoderick & Dorko, 2004). The compounds are commonly used in air conditioners, aerosol propellants, solvents or refrigerators (Adcock et al., 2018). After the literature review, it can be concluded that the CFCs adsorbed by Universal sorbent are sourced from contamination of the sample surface or chamber air. Since the compounds are identified with confidence level 3, incorrect compound annotation is plausible. To confirm if compounds were annotated correctly, further investigation should be carried out.

Monoterpenes such as d-limonene, β-pinene, camphene and α-pinene were identified when analysing compounds adsorbed on both Tenax TA and Universal. The most abundant aldehydes identified in all samples were nonanal, hexanal, octanal and pentanal. As discussed earlier, these VOCs are typical biogenic emissions from wood. Based on a visual comparison of TIC data of Universal and Tenax TA, the most abundant analytes eluting between n-hexane and hexadecane were identical for both sorbents (Figure 4.7). Higher peak abundance can be seen for compounds adsorbed by Universal between 8min to 10min analytical run, indicating that VOCs with lower molecular weight are more efficiently absorbed by Universal sorbent than Tenax TA. The complete list of compounds identified in both Universal and Tenax TA can be found in Appendix I.

# 5 Instrumental challenges

## 5.1 Sinusoidal baseline pattern

A completely new Agilent 8890 GC system with Markes Centri 360 Thermal Desorption Unit was utilised for the targeted and non-targeted analysis of VOCs. Consequentially several challenges were encountered when developing analytical method on the instrument.

The first significant challenge endured was a sinusoidal wave pattern in the chromatographic baseline between 8min and 16min. The pattern can be observed in Figure 5.1.

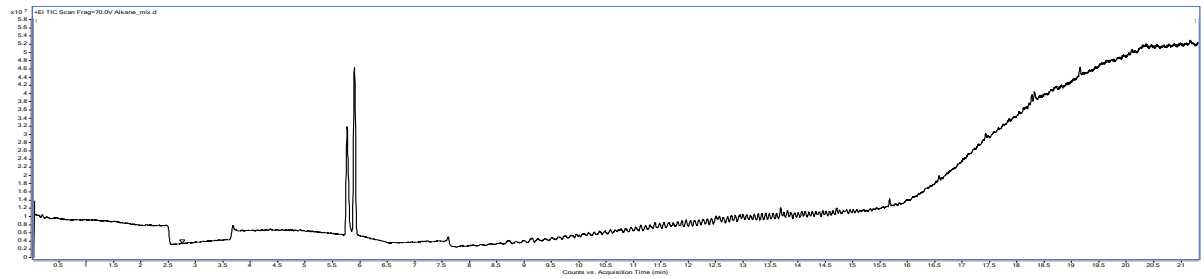


*Figure 5.1 Chromatographic baseline with a sinusoidal peak pattern.*

The workaround for the problem was discovered in a blog published by Rattray (2020), where the writer described this type of baseline as an issue occurring from uncontrolled cooling at the end of the GC temperature program. Rattray (2020) explained that when the GC column is cooled down too rapidly, parts of the stationary phase can be cooled non-homogenously, resulting in condensed column bleeds that enter the sequential run. The column bleed products will be focused on the start of the GC temperature program, and as the temperature increases, their products will be chromatographically separated as any other analyte resulting in sinusoidal waves in the baseline (Rattray, 2020). This problem is more commonly observed in GC columns with a ticker stationary phase and a higher phenyl group content. Rattray (2020) also explained that the sinusoidal waves are not a concern when analysing analytical compounds in high concentrations; however, the waves can cause interferences and integration challenges in trace analysis.

For the utilisation of NTS and SUS, it was critical to ensure a minimal amount of matrix and background noise interferences during the sample analysis; hence, it was important to resolve the sinusoidal baseline issue. As a solution, a controlled cooling ramp (20$^{o}$C/min to 50$^{o}$C) was applied at the end of the GC temperature program. A blank sample was tested to ensure that the problem was resolved.

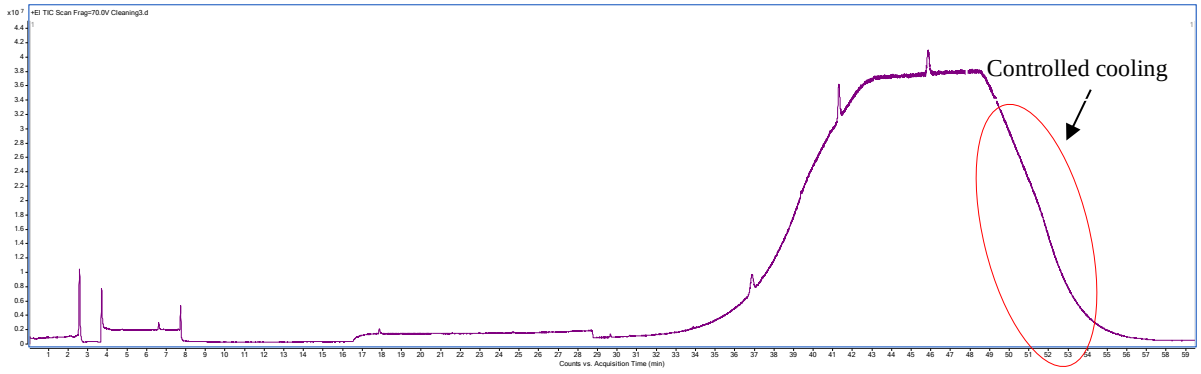



*Figure 5.2 Chromatographic baseline after controlled cooling is applied at the end of the temperature program.*

Analysis of the blank sample disclosed that no sinusoidal waves were occurring in the chromatographic baseline. The analysis, therefore, confirmed that the issue for the sinusoidal baseline pattern resulted from uncontrolled cooling at the end of the GC temperature program. The downside of the solution is a prolonged analytical run. Controlled cooling added 10.5min to the analytical run resulting in a 67.5min run time. Regardless, the added controlled cooling ramp helped minimise background noise interference and was kept as a part of the analytical run.

## 5.2 Background noise

The high chromatographic background noise was a considerable issue when developing the analytical method for identifying and quantifying VOCs. One source of the chromatographic background was the siloxane polymer particles such as hexamethylcyclotrisiloxane or octamethylcyclotetrasiloxane, coming from a thick stationary phase in the GC column. Moreover, extensive background noise, in addition to degradation of the stationary phase, was caused by the oxidation of Tenax TA sorbent.

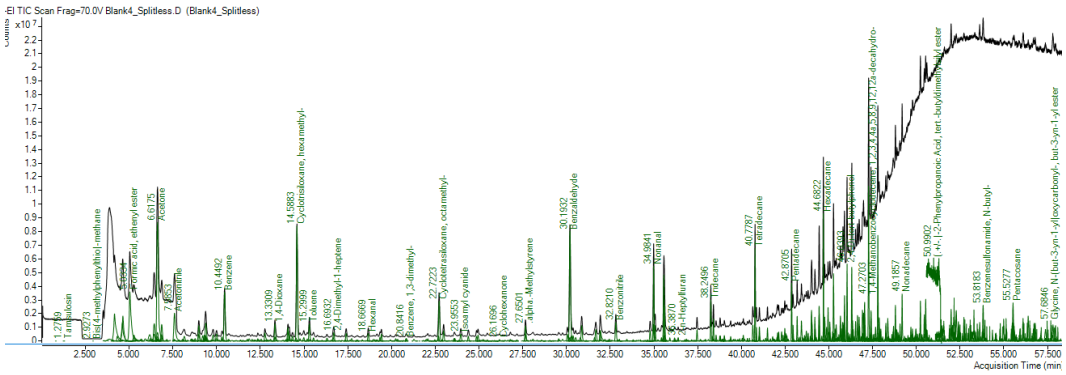


*Figure 5.3 Chromatographic background noise observed in splitless mode.*

Most extensive background noise was observed when the analysis ran in spitless mode. Many of the matrix peaks observed were Tenax TA degradation products such as toluene, benzene,

and benzaldehyde. At the same time, hexanal, nonanal, benzonitrile and higher alkanes were identified. The degradation products are commonly observed in newly packed sorbent tubes, and the background noise goes down as the sorbent goes through several conditioning and desorption cycles. In this project, brand new Tenax TA tubes were utilised; therefore, the matrix peaks observed in Figure 5.3 were expected. At the start of the method development, tubes were conditioned at 300ºC for 60min to avoid degradation of Tenax TA sorbent. After each conditioning cycle, tubes were analysed for the background noise. No lowering of the background noise was observed after the tubes were conditioned 5 times. This concluded that quantitative and non-targeted analysis would be problematic in the splitless mode. Background compounds would most likely interfere with analytes and, in non-targeted analysis, would result in false positive compounds, while in quantitative analysis, the matrix would result in inadequate quantification of targeted compounds. For this reason, a split mode test was carried out to determine which split ratio would produce less background noise but would not interfere with method sensitivity. The test was performed at 5mL/min, 10mL/min, and 20mL/min split ratios, splitting the sample after secondary desorption (outlet).

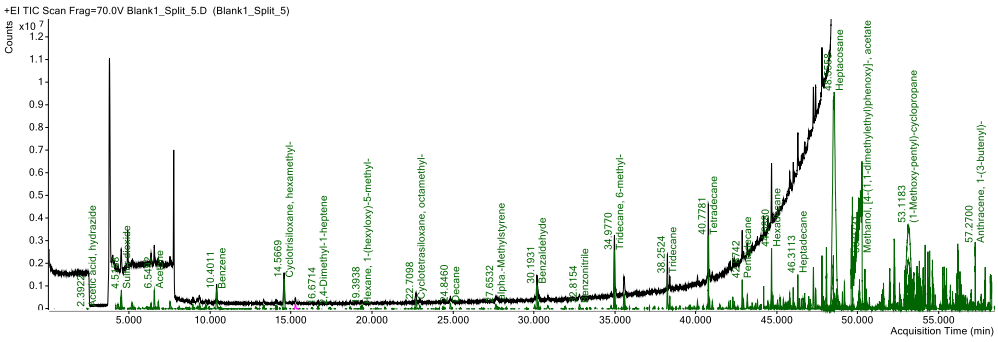



*Figure 5.4 Chromatographic background noise after analysis of the blank sample in the split of 5mL/min.*

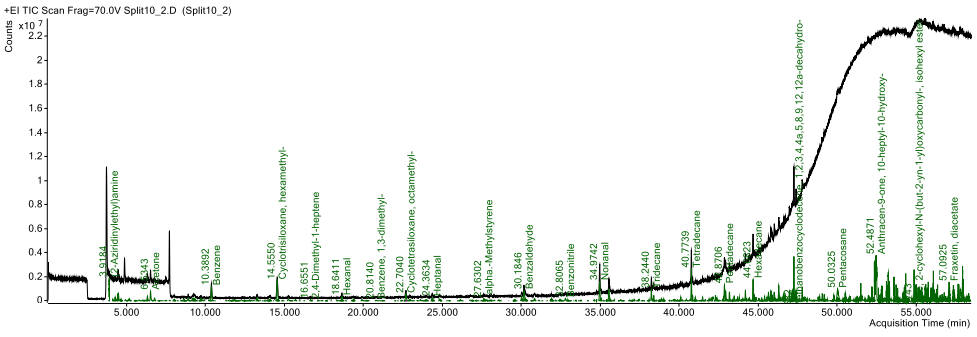



*Figure 5.5 Chromatographic background noise after analysis of the blank sample in the split of 10mL/min*

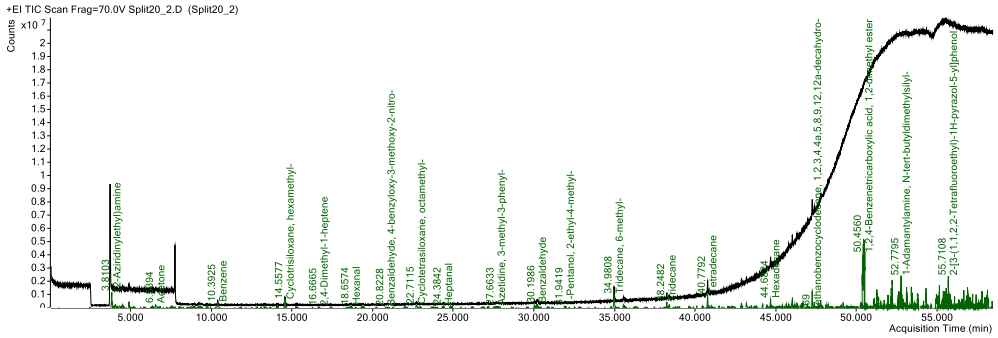



*Figure 5.6 Chromatographic background noise after analysis of the blank sample in the split of 20mL/min*

At a split ratio of 5mL/min, the background noise was still too expensive for the split to be used in the final method. The lowest background noise was observed at a split ratio of 20mL/min. At this slit ratio, the part of the Tenax TA degradation products were vented out through the split vent, resulting in a lower signal response of the matrix. The disadvantage of the 20mL/min split mode was that a larger part of the analyte would be vented together with the degradation products, making the method less sensitive and potentially losing low trace analytes. Therefore, a 10mL/min split was applied to the final method, and after the application of the conditioning procedure provided by Markes International (section 2.2), the background noise was minimised.

# 6 Conclusion

This project aimed to develop and validate an analytical method for the GC-HRMS-QTOF-TDU system for identifying and quantifying VOCs emitted from wood surfaces. The project was divided into four parts. The first part was the development and validation of the analytical method. The second part was the development of an in-house HRMS library by utilising Agilent MassHunter Qualitative analysis and Agilent MassHunter PCDL manager. The third part was the quantification of targeted VOCs. In the last part, SUS and NTS was carried out by Agilent MassHunter Unknown Analysis to obtain complete VOC emission profiles for USP, SSP and CLT samples.

Results from analytical method development and validation revealed that the method was suitable for quantifying ten targeted VOCs. Due to the coelution issue, camphene and o-xylene were excluded from the validation. The analytical method was able to quantify α-pinene, β-pinene, toluene, benzaldehyde, d-limonene, ethylbenzene, 3-carene and m-xylene in the 1ng/µL to 150ng/µL working range. Hexanal and furfural had a poor signal response at 1ng/µL and had compound recoveries outside the accepted range (recovery of furfural 369.5% and hexanal 235.9%); therefore, the lowest concentration point was excluded from further validation.

Quantitative analysis of targeted compounds revealed that the most abundant compounds in USP, CLT and SSP were hexanal, with a concentration between 80.1-3.00µg/$m^3$, followed by α-pinene (45.4-1.9µg/$m^3$), β-pinene (15.4-0.32µg/$m^3$), 3-carene (7.3-0.04µg/$m^3$) and d-limonene (3.9-0.01µg/$m^3$). Hexanal and α-pinene were identified in all three samples and their four duplicates. Significant concentration variations between the duplicate samples could imply contamination of the vacuum chamber or possible sample loss due to insufficient vacuum chamber sealing. Lower VOC emissions were identified in SSP samples. The hexanal concentration from SSP was determined between 16.55-3.01µg/$m^3$ and α-pinene at 14.87-1.95µg/$m^3$. The results could suggest that treating wood surfaces with water-based wood stain reduces biogenic VOC emissions. However, further analysis should be carried out to confirm the statement.

The SUS and NTS identified a total of 31 689 compound hits in CLT, SSP and USP samples. From these, 1498 were identified with identification confidence 2. Three hundred eight compound hits were identified with identification confidence 1 since the annotated compounds could be confirmed by a reference standard. Alkanes were the most abundant chemical group identified in SSP (29%), CLT (31%) and USP (37%) by NTS and SUS. The most dominating

alkanes identified were 2,3-dimethylpentane, 2-methylhexane, methylcyclohexane, 3-metylhexane and heptane which are compounds identified in various anthropogenic sources. These alkanes were not identified in chamber blanks implying that the emissions could be caused by contamination of the sample surface. Various terpenes were identified and annotated with identification levels 1 and 2. The most abundant terpenes identified by SUS and NTS were targeted VOCs, such as β-pinene, α-pinene, d-limonene and 3-carene, and non-targeted β-myrcene and o-cymene. Aldehydes contributed to 5-8% of total VOC emissions in SSP, USP and CLT samples. The most abundant aldehydes identified and annotated by NTS and SUS were heptanal, nonanal, decanal, pentanal and hexanal. These aldehydes were identified in all three spruce samples and their duplicates.

During the development of in-house PCDL, HRMS of 47 compounds were successfully exported to the PCDL manager. PCDL annotated 18 compounds with a match factor between 84,6% to 98,7%. The most abundant compounds annotated by PCDL were 3-carene, β-pinene, hexanal, d-limonene, decanal, camphene, benzaldehyde, and m-xylene. The analysis concluded that PCDL is a valuable tool for the annotation of unknown compounds; however, it can only be used as a supplement to the NIST library due to the limited amount of HRMS data that PCDL contains.

SSP samples were collected on Universal and Tenax TA to compare the adsorption range between these two sorbents. The analysis revealed that approximately 59% of the compounds identified with a confidence level 2 were adsorbed by both Universal and Tenax TA. The most abundant compounds identified only by Universal sorbent were acetone, 3,3-dimethylpentane, formic acid ethenyl ester, 2,4-dimethylpenatne, n-hexane and 2,2-dimethylester. Important to note that the compound adsorption range between these two sorbents was not entirely comparable since compounds adsorbed by Universal sorbent were analysed with no sorbent delay and had a 4-minute advantage over Tenax TA tubes that had an 8-minute solvent delay at the start of an analytical run.

## 6.1 Future perspectives

Further optimisation of the analytical method should be conducted for the determination of VOC emissions from wood surfaces. The liquid standard loading on the sorbent tube should be replaced by gas standards for better apparent recovery and lower standard deviation between calibration replicates. For targeted analysis, a higher number of VOC standards should be considered for a greater overview of VOC emissions. Compounds such as nonanal, decanal, pentanal, heptanal, ammonia and camphene should be contemplated for the quantification. Moreover, semi-quantification based on toluene equivalent should be utilised for compounds identified during SUS and NTS.

In-house PCDL should be optimised for increased identification and annotation accuracy of unknown compounds. A larger amount of HRMS data should be added, and the HRMS data should be acquired from a single reference standard instead of a standard mixture. PCDL should also be developed after the analytical method is utterly developed and validated.

To determine how VOC emissions from wood surfaces are affected by temperature and RH changes, analysis of wood samples based on different RH and temperature conditions could be considered. Lastly, additional wood samples should be analysed. Analysis revealed lower VOC emissions in the SSP samples, therefore different types of coated wood materials and wood finishes should be analysed to determine if the results are consistent.

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# 8 Appendices

# A. Materials and Chemical standards

**Carier gas**

- Helium, 5.0 grade Ultra, 50L, Nippon gasses Norge AS, Oslo
- Nitrogen 5.0 grade Ultra, 50L, Nippon gasses Norge AS, Oslo

**Materials**

- Hamilton® syringe 10µL, fixed needle, Perkin-Elmer, Norwalk USA
- SureSTART™ 2mL Glass Screw Top Vials, Level 1 Everyday analysis, catalogue number: CHSV9-10P, Thermo Fisher Scientific, USA.
- Micro weight model: XPR204, Mettler Toledo, Philippines.
- Micropipettes of various volumes, Blaubrand® intraMARK, Brand®, Germany.
- Micro pipette controller for pipettes up to 1mL, Art.-Nr.: 25800, Brand®, Germany
- Erlenmeyer flasks and beakers of various volumes
- Stainless steel TD tubes, prepacked with Tenax TA (35/60), product code C1-AXXX-5003, Markes International, England.
- Stainless steel TD tubes, prepacked with Universal sorbent, product code C3-AXXX-5266, Makes International, England.
- Capillary GC column, DB-1701, low/mid polarity with a stationary phase composed of 14% cyanopropyl-phenyl-methylpolysiloxane, length 60m, diameter (mm) 0.320, film (µm) 1.00, part number 123-0763, Agilent Technologies, Santa Clara, USA
- Transfer line insert fused silica (0.25 mm ID) and PTFE sleeve- 2m, product code SERUTE-5099, Markes International, England
- Focusing trap- Material Emissions, product code U-T12ME-2S, Markes International, England.

**Instrumentation**

- 8890 GC system, Agilent Technologies, Santa Clara, CA, USA
- 7250 GC/ Quadrupole-Time-of-Flight, Agilent Technologies, Santa Clara, USA
- Thermal Desorption Unit Centri 360, Makes International, England
- Calibration Solution Loading Rig (CSLR), product code C-CSLR, Markes International, England.

## Computer software

- Agilent MassHunter Qualitative Analysis 10.0
- Agilent MassHunter Quantitative Analysi5 (TOF) (Quant-My-Way) 12.0
- Agilent MassHunter Unknown Analysis (Quant-May-Way) 12.0
- Agilent MassHunter PCDL manager B.08.00
- Microsoft Excel, Office 365

## Instrumentation and materials for specimen sampling

- Vacuum Chamber VC3028AC, Ignatki-Osiedle, Poland
- Data logger (temperature, humidity, motion) AiroSensor Sense Anywhere, model 20-20-25, Oud Gastel, the Netherlands.
- Single flow tube meter 800ml/min, Aalborg Instruments, Orangeburg, NY, USA
- Hydrocarbon filter Big Trap Gas $^{1}/_{8}$, 250 psig, Trajan, Australia
- Climate chamber KB8182, Termaks AS, Bergen, Norway
- Pocket pump SKC Inc., model 210-1002, Blandford, Dorset, UK
- Aluminium tape, 10mx50mm, tesa®, Germany
- Grease for laboratories, suitable for vacuum, Glisseal N, Borer Chemie AS, Switzerland

## Calibration standards

| Compound | IUPAC | Concentration/ Purity | Producer | Product code |
|---|---|---|---|---|
| m-xylene | 1,3-Dimethylbenzene | 99.5% | Sigma-Aldrich | 95670-5ML |
| Furfural | 2-Furalalgehyde | 98.5% | Sigma-Aldrich | 04623-1ML |
| Ethylbenzene | | ≥99.5% | Sigma-Aldrich | 03079-5ML |
| β-pinene | 6,6-Dimethyl-2-methylidenebicyclo[3.1.1]heptane | ≥98.5% | Sigma-Aldrich | 80607-1ML |
| o-xylene | 1,2-Dimethylbenzene | ≤100% | Sigma-Aldrich | 95660-5ML |
| Benzaldehyde | | ≥99.5% | Sigma-Aldrich | 09143-5ML-F |
| Toluene | Methylbenzene | ≥99.9% | Sigma-Aldrich | 89680-5ML |
| n-Hexanal | | Neat | Chiron AS | 10010.6-1ML |
| Toluene-D8 | Benzene-d5, methyl-d3- | Neat | Chiron AS | C2253.7-1ML |

| Compound | IUPAC | Concentration/ Purity | Producer | Product code |
|---|---|---|---|---|
| 3-Carene | 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane | 1000µg/mL | Chiron AS | |
| d-(+)-Limonene | (4R)-4-Isopropenyl-1-methylcyclohexene | ≥98% | Rotichrom® GC | UN 2052 |
| A-pinene | 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene | 2000µg/mL | Sigma-Aldrich | CRM40339 |

## Chemical standards used to build Personal Compound Database and Library

| Standard | Concentration (ng/µl) | | Producer | Product code |
|---|---|---|---|---|
| VOC mixture 154 | 100ng/µl in methanol | | Dr. Ehrenstorfer™ | DRE-GA09000154ME |
| **Analyte:** | **Concentration (ng/µl)** | **Purity%** | **CAS Number** | **Lot Number** |
| Dichlorodifluoromethane | 105 | 99 | 75-71-8 | 142.158.5P |
| Chloromethane | 105 | 99 | 74-87-3 | 140.158.2.2P |
| Vinyl chloride | 104 | 99 | 75-01-4 | 143.158.5.2P |
| Bromomethane | 105 | 99.5 | 74-83-9 | 139.158.1.1P |
| Chloroethane | 105 | 99.94 | 75-00-3 | 141.2.3P |
| Trichlorofluoromethane | 105 | 99 | 75-69-4 | 144.1.3P |
| 1,1-dichloroethylene | 105 | 99.98 | 75-35-4 | 165.1.4P |
| Carbon Disulfide | 105 | 99.9 | 75-15-0 | 200.24.1P |
| Methylene Chloride | 105 | 99.99 | 75-09-2 | 178.271.1P |
| Methyl T-butyl Ether | 105 | 99.97 | 1634-04-4 | 208.24.4P |
| Trans-1,2-dichloroethylene | 105 | 99.7 | 156-60-5 | 167.9.1P |
| 1,1-dichloroethane | 105 | 98.1 | 75-34-3 | 163.247.3.2P |
| Cis-1,2-dichloroethylene | 105 | 98.5 | 156-59-2 | 166.1.7.1P |
| 2,2-dichloropropane | 104 | 99 | 594-20-7 | 170.158.1.1P |
| Bromochloromethane | 106 | 99.7 | 74-97-5 | 148.1.3P |
| Chloroform | 105 | 99.8 | 67-66-3 | 156.7.1P |
| 1,1,1-Trichlororethane | 106 | 99.6 | 71-55-6 | 187.247.11P |
| 1,1-dichloropropylene | 105 | 99 | 563-58-6 | 171.158.2.2P |
| Carbon Tetrachloride | 105 | 100 | 56-23-5 | 154.9.1P |
| Benzene | 105 | 99.99 | 71-43-2 | 146.1.9P |
| 1,2-dichloroethane | 104 | 99.9 | 107-06-2 | 164.158.8.1P |
| Trichloroethylene | 105 | 98.1 | 79-01-6 | 188.29.1P |
| 1,2-dichloropropane | 105 | 99.7 | 78-87-5 | 168.8.1P |
| Dibromomethane | 106 | 99.8 | 74-95-3 | 162.1.2P |
| Bromodichloromethane | 105 | 98.7 | 75-27-4 | 149.1.11P |

| Analyte: | Concentration (ng/µl) | Purity% | CAS number | Lot number |
|---|---|---|---|---|
| Cis-1,3-dichloropropylene | 105 | 99.5 | 10061-01-5 | 172.7.6P |
| Toluene | 105 | 100 | 108-88-3 | 184.48.1P |
| Trans-1,3-dichloropropylene | 105 | 99 | 10061-01-5 | 173.7.11P |
| 1,1,2-trichloroethylene | 104 | 99.6 | 79-00-5 | 195.7.1.6P |
| Tetrachloroethylene | 106 | 100 | 127-18-4 | 183.1.2P |
| 1,3-dichloropropane | 106 | 99.8 | 142-28-9 | 169.7.2.1P |
| Dibromochloromethane | 105 | 98.6 | 124-48-1 | 159.1.8P |
| 1,2-dibromoethane | 105 | 99.9 | 106-93-4 | 161.9.1P |
| Chlorobenzene | 105 | 99.9 | 108-90-7 | 155.29.1P |
| Ethylbenzene | 105 | 100 | 100-41-4 | 174.7.1P |
| 1,1,1,2-tetrachloroethane | 104 | 99.8 | 630-20-6 | 181.7.2.9P |
| M-xylene | 105 | 99.7 | 108-38-3 | 193.7.1.2P |
| P-Xylene | 105 | 99.9 | 106-42-3 | 194.7.1P |
| O-Xylene | 105 | 99 | 95-47-6 | 192.29.3P |
| Styrene | 105 | 99.5 | 100-42-5 | 180.9.4P |
| Bromoform | 105 | 99.3 | 75-25-2 | 150.7.2P |
| Isopropylbenzene | 105 | 99.9 | 98-82-8 | 176.9.3P |
| 1,1,2,2-tetrachloroethane | 104 | 99.4 | 79-34-5 | 182.8.2P |
| 1,2,3-trichloropropane | 105 | 99.5 | 96-18-4 | 189.1.3P |
| Bromobenzene | 105 | 100 | 108-86-1 | 147.7.1P |
| N-Propylbenzene | 105 | 99.7 | 103-65-1 | 179.7.2.2P |
| 2-chlorotoluene | 105 | 99.5 | 95-49-8 | 157.7.1P |
| 1,3,5-trimethylbenzene | 105 | 99.5 | 108-67-8 | 191.7.1P |
| 4-chlorotoluene | 105 | 99.9 | 106-43-6 | 158.9.3P |
| Tert-butylbenzene | 105 | 99.9 | 98-06-6 | 153.29.1P |
| 1,2,4-trimethylbenzene | 105 | 98.7 | 95-63-6 | 190.7.1P |
| Sec-butylbenzene | 105 | 99.6 | 135-98-8 | 152.1.2P |
| 4-isopropylbenzene | 105 | 99.7 | 99-87-6 | 177.9.2P |
| 1,3-dichlorobenzene | 105 | 99.8 | 541-73-1 | 44.1.2P |
| 1,4-dichlorobenzene | 106 | 99.9 | 106-46-7 | 45.29.1P |
| N-butylbenzene | 105 | 99.2 | 104-51-8 | 151.7.3.2P |
| 1,2-dichlorobenzene | 105 | 99.8 | 95-50-1 | 43.7.1P |
| 1,2-dibromo-3-chloropropane | 105 | 98.6 | 96-12-8 | 160.7.2.3P |
| 1,2,4-trichlorobenzene | 105 | 99.6 | 120-82-1 | 54.29.1P |
| Hexachlorobutadiene | 105 | 98 | 87-68-3 | 47.158.3.1P |
| Naphthalene | 105 | 99.8 | 91-20-3 | 26.9.2P |
| 1,2,3-trichlorobenzene | 105 | 99 | 87-61-6 | 185.1.1.6P |

| **Standard** | **Concentration (ng/µl)** | **Producer** | | **Product code** |
|---|---|---|---|---|
| 50 components, Indoor Air Standard | 100µg/mL in methanol | Supelco® | | 49148-U |
| **Analyte:** | **Lot Number** | **CAS number** | **Purity %** | **Analytical conc. (µg/mL)** |
| Ethanol, Absolute | LC20779 | 64-17-5 | 99.9 | 99.4 |
| 2-Propanol | LC09276 | 67-63-0 | 99.9 | 98.9 |
| Acetone | LC12737 | 67-64-1 | 99.9 | 98.4 |
| Dichloromethane | LC17906 | 75-09-2 | 99.9 | 98.1 |
| 1-Propanol | LC09485 | 71-23-8 | 99.9 | 86.6 |
| Hexane | LC17823 | 110-54-3 | 99.9 | 102.5 |
| 2,4-Dimethylpentane | LC07929 | 108-08-7 | 99.9 | 95.2 |
| 2-Butanone | LB97056 | 78-93-3 | 99.9 | 99.2 |
| Ethyl acetate | LB91404 | 141-78-6 | 99.7 | 98.9 |
| Chloroform | LB97804 | 67-66-3 | 98.2 | 98.3 |
| Isooctane | LB90728 | 540-84-1 | 99.9 | 94.5 |
| n-Heptane | LC07614 | 142-82-5 | 99.7 | 94.9 |
| n-Butanol | LC03116 | 71-36-3 | 99.9 | 101.9 |
| Benzene* | LC03683 | 71-43-2 | 99.9 | 97.1 |
| 1,2-Dichloroethane* | LB74294 | 107-06-2 | 99.9 | 98.5 |
| Trichloroethene | LB56674 | 79-01-6 | 98.4 | 98.1 |
| 1,2-Dichloropropane | LC14320 | 78-87-5 | 99.9 | 98.6 |
| Bromodichloromethane | LC08591 | 75-27-4 | 98.3 | 98.3 |
| 4-Methyl-2-Pentanone | LC05179 | 108-10-1 | 99.9 | 101.6 |
| n-Octane | LB63797 | 111-65-9 | 99.4 | 99.9 |
| Toluene | LC14689 | 108-88-3 | 99.9 | 98.6 |
| Internal Standard | N/A | N/A | N/A | N/A |
| Butyl Acetate | LC07239 | 123-86-4 | 99.9 | 100.2 |
| Tetrachloroethene | LB67182 | 127-18-4 | 99.9 | 98.5 |
| Dibromochloromethane | LB89245 | 124-48-1 | 95.2 | 101.4 |
| n-Nonane | LC00219 | 111-84-2 | 99.9 | 99.5 |
| Ethylbenzene | LB69556 | 100-41-4 | 99.9 | 100.2 |
| m-Xylene* | LB87531 | 108-38-3 | 99.9 | 200 |
| p-Xylene** | LB73203 | 106-42-3 | 99.9 | |
| o-Xylene | LB63785 | 95-47-6 | 99.9 | 101.4 |
| Styrene | LC17632 | 100-42-5 | 99.9 | 100.2 |
| (1S)-(-) Alpha-Pinene, Synthetic | LB48082 | 7785-26-4 | 99.4 | 99.9 |
| n-Decane | LC07947 | 124-18-5 | 99.9 | 100.9 |
| 3-Ethyltoluene** | LC10656 | 620-14-4 | 99.8 | 199.9 |
| 4-Ethyltoluene** | LB27098 | 622-96-8 | 99.2 | |
| 1,3,5-Trimethylbenzene | LB82157 | 108-67-8 | 99.3 | 100.1 |
| (-)-Beta-Pinene | LC12016 | 18172-67-3 | 99.6 | 102.6 |
| 2-Ethyltoluene | LB69440 | 611-14-3 | 99.9 | 100.7 |
| 1,2,4-Trimethylbenzene | LB97224 | 95-63-6 | 98.8 | 99.6 |
| R-(+)-Limonene | LC07591 | 5989-27-5 | 98.7 | 103.7 |
| 1,2,3-Trimethylbenzene | LC20115 | 526-73-8 | 97.7 | 103.9 |
| n-Undecane | LC08959 | 1120-21-4 | 99.6 | 100.4 |
| 1,4-Dichlorobenzene | LB90630 | 106-46-7 | 99.9 | 101.1 |
| Nonanal | LC21819 | 124-19-6 | 99.1 | 101.1 |

| Analyte: | Lot Number | CAS number | Purity % | Analytical conc. (µg/mL) |
|---|---|---|---|---|
| n-Dodecane | LC08158 | 112-40-3 | 99.6 | 100.5 |
| 1,2,4,5-Tetramethylbenzene | LB93477 | 95-93-2 | 99.9 | 101.3 |
| Decanal, Synthetic | LB99839 | 112-31-2 | 93.4 | 101.7 |
| n-Tridecane | LC14314 | 629-50-5 | 99.9 | 101.7 |
| n-Tetradecane | LC15053 | 629-59-4 | 99.5 | 100.9 |
| n-Pentadecane | LC08640 | 629-62-9 | 99.6 | 101.9 |
| n-Hexadecane | LC02125 | 544-76-3 | 99.9 | 102.5 |

*Coelute
**Coelute-certified as sum

## Sample information

| Sample type | Stained Spruce panel | Untreated spruce panel | Cross-laminated timber |
|---|---|---|---|
| **Product name** | Sprekkpanel Nat Lysne | Glattpanel Nat | Splitkon AS |
| **Manufacturer** | Bergene Holm AS | Bergene Holm AS | Splitkon AS |
| **Date of packing** | 25.01.2023 | 23.03.2023 | 29.03.2023 |
| **Packaging number** | 2047505-37 | 1106006-28 | - |
| **Treatment** | Water based wood stain Lacroma Clear Lysne | Untreated | Cleaving, gluing of lamelles Adhesive: Melamine urea-formaldehyde (MUF) |
| **Sample size (cm)** | 10x20 | 10x20 | 10x20x8 |
| **Sample placing in the climate chamber date** | 22.05.2023 | 08.05.2023 | 15.05.2023 |
| **Air sampling date** | 25.05.2023 | 11.05.2023 | 18.05.23 |

## Chemical composition of Lacroma Clear Lysne-Light White wood stain

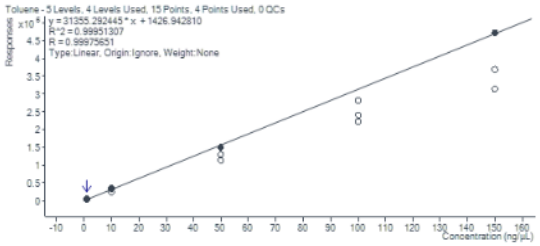
| Compound | CAS number | % |
|---|---|---|
| 2-butoxyethanol | 111-76-2 | ≤3 |
| Di(propylene glycol)methyl ether | 34590-94-8 | ≤3 |
| Adipohydrazide | 1071-93-8 | ≤0.3 |
| 3:1 mix of: | | |
| 5-Chloro-2-methyl-3(2H)-isothiazolone | 55965-84-9 | <0.001 |
| 2-methyl-3(2H)-isothiazolone | | |

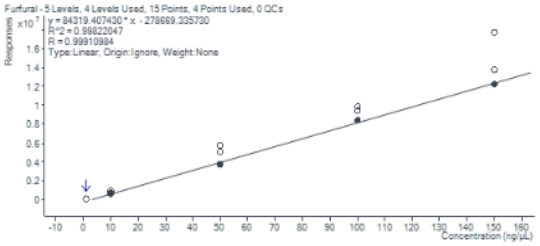
# B. Analytical method parameters

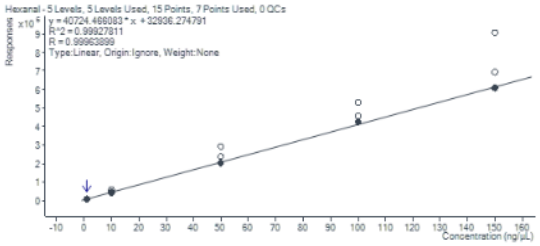
Table 8.1 Comparison of Brown et al. (2014) analytical conditions and final analytical conditions used for this project.

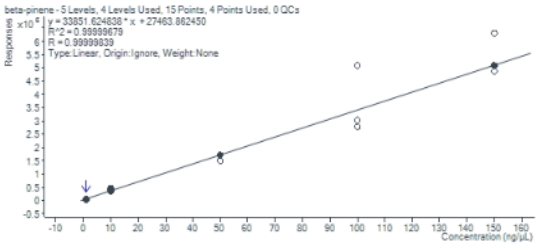
| | | **Analytical conditions developed by Brown et al. (2014)** | **Final analytical conditions used in this project** |
|---|---|---|---|
| **TD system** | **TD sorbent type** | Tenax TA<br>Quartz wool/Tenax TA/Carbograph 5T<br>Quartz wool/Tenax TA/Carbopack X | Tenax TA<br>Universal |
| | **Pre-purge** | 1min at 30ml/min | 1min 40ml/min |
| | **Primary desorption** | 280ºC for 8min<br>Helium flow 50ml/min | 280 for 10min<br>Nitrogen flow 50ml/min |
| | **Inlet Split**<br>**Outlet Split** | No split<br>10ml/min | No split<br>10ml/min |
| | **Cold trap/ secondary desorption** | Low temp.: -10ºC<br>High temp.: 300ºC for 3min | Low temp.: -10<br>High temp.: 300ºC for 3min |
| | **Trap heating rate** | max | max |
| | **Flow path** | 210ºC | 150ºC |
| **GC system** | **Flow of Helium gas** | Constant flow 1,3 ml/min | Constant flow 1,2ml/min |
| | **GC-column** | DB5 60m, 0.25mm I.D., 0.5µm | DB-1701 60m, 0.32mm I.D., 1.00µm |
| | **Temperature programming** | Initial temp 35ºC, hold 1 min.<br>Ramp 1: 2ºC/min to 75ºC<br>Ramp 2: 5ºC/min 140ºC<br>Ramp 3: 10ºC/min to 250, hold 5min.<br>(Runtime: 50 min) | Initial temp: 50ºC<br>Ramp 1: 2.5ºC/min 140ºC<br>Ramp 2: 10ºC/min to 280, hold 6min.<br>Ram 3: 20ºC/min to 50ºC<br>(Runtime: 67.5 min) |
| **MS system** | **Source temperature** | 230ºC | 200ºC |
| | **Quadrupole temperature** | 150ºC | 150ºC |
| | **Ionisation mode** | Not Defined | EI |
| | **Ionisation energy** | Not Defined | 70eV |
| | **Mode** | Full scan mode | MS mode (full scan mode) |
| | **Scan mode mass range** | 20-450m/z | 35-300m/z |

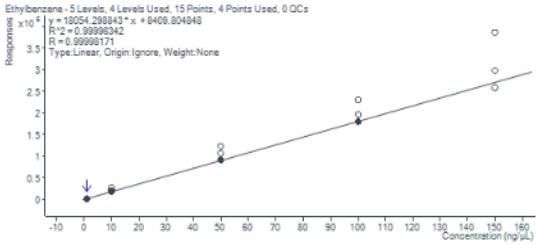
# C. External standard calibration curves of three replicants. Split flow 10mL/min

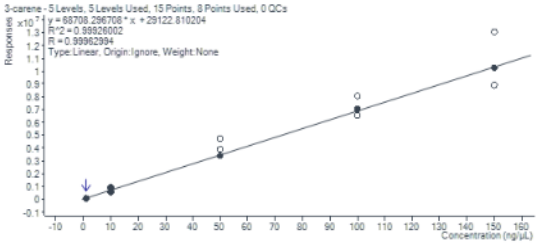


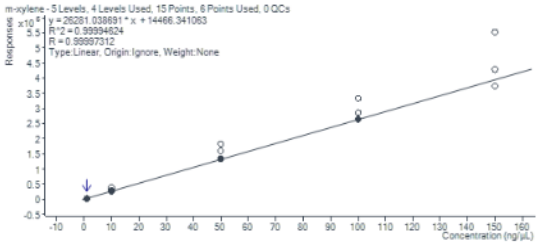



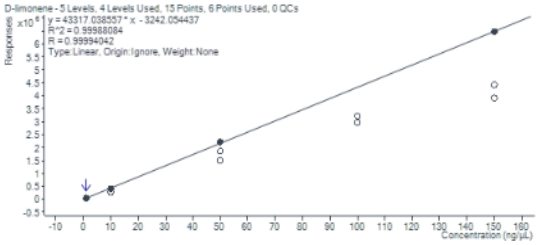



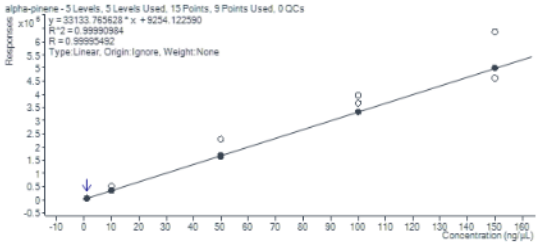



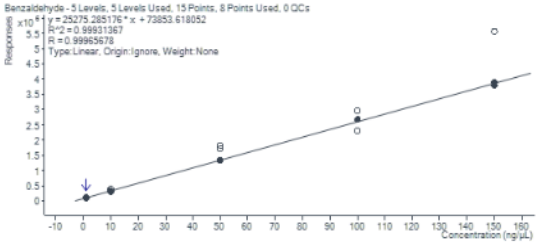
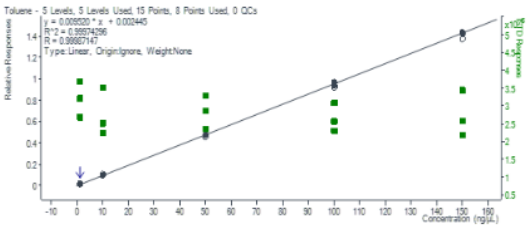
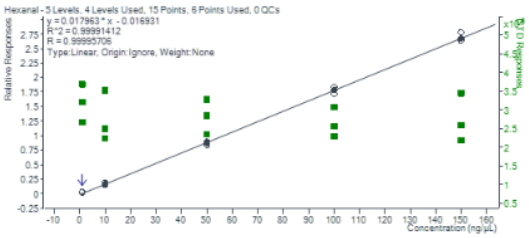



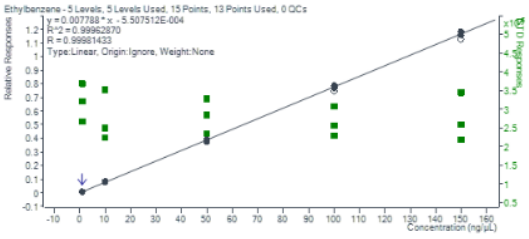
Table 8.2 Linear regression equation and coefficient of determination of targeted compounds using an external standard method.

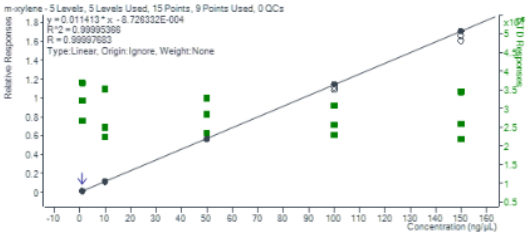
| Name | Linear range | Slope | Intercept | Type | Origin | Weight | $R^2$ |
|---|---|---|---|---|---|---|---|
| **Toluene** | 1-150 | 31355.29 | 1426.94 | Linear | Ignore | None | 0.9995 |
| **Hexanal** | 1-150 | 40724.47 | 32936.27 | Linear | Ignore | None | 0.9992 |
| **Ethylbenzene** | 1-100 | 18054.29 | 8409.80 | Linear | Ignore | None | 0.9999 |
| **m-xylene** | 1-100 | 26281.04 | 14466.34 | Linear | Ignore | None | 0.9999 |
| **Alpha-pinene** | 1-150 | 33133.77 | 9254.12 | Linear | Ignore | None | 0.9996 |
| **Beta-pinene** | 1-150 | 33851.62 | 27463.86 | Linear | Ignore | None | 0.9999 |
| **Furfural** | 10-150 | 84319.41 | 278669.36 | Linear | Ignore | None | 0.9982 |
| **3-carene** | 1-150 | 68708.29 | 29122.81 | Linear | Ignore | None | 0.9992 |
| **D-limonene** | 1-150 | 43317.04 | 3242.05 | Linear | Ignore | None | 0.9998 |
| **Benzaldehyde** | 1-150 | 25275.29 | 73853.62 | Linear | Ignore | None | 0.9993 |

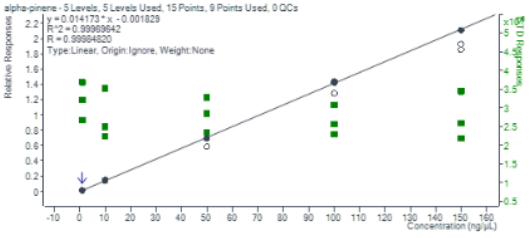
# D. Calibration curves of three replicants based on the Internal Standard method. Split flow 10ml/min

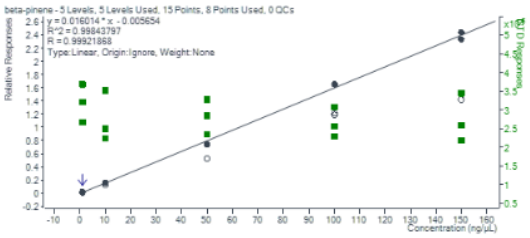


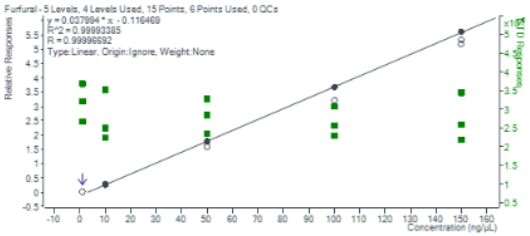



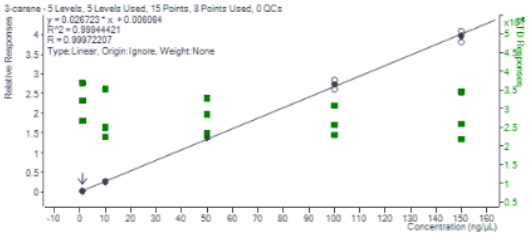



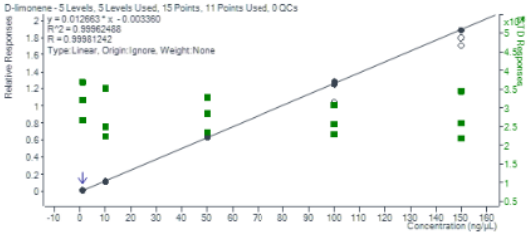



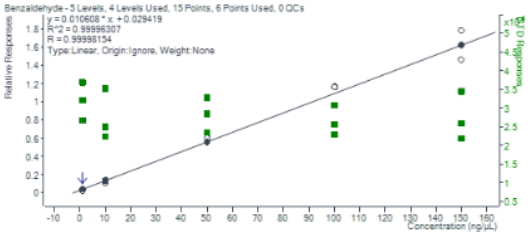



# E. Raw data of targeted compound calibration and blank sample results

Table 8.3 Raw data of blank sample results.

| | | | | Furfural Results | | | | beta-pinene Results | | | | 3-carene Results | | | | D-limonene Results | | | | Benzaldehyde Results | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Data File** | **Type** | **Level** | **Acq. Date-T** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** |
| blank1.D | Blank | | 6/6/2023 | 23.96 | 3.07 | 52 | 18.07 | 26.15 | 0.36 | 278 | 5.26 | 27.75 | 0.00 | 387 | 8.85 | 29.36 | 0.35 | 1679 | 18.11 | 31.52 | 1.72 | 73324 | 117.98 |
| blank2.D | Blank | | 6/6/2023 | 24.01 | 3.07 | 40 | 127.46 | 26.16 | 0.39 | 979 | 22.78 | 27.76 | 0.00 | 2889 | 71.02 | 29.37 | 0.33 | 1300 | 17.24 | 31.51 | 0.00 | 42566 | 240.51 |
| blank3.D | Blank | | 6/6/2023 | 24.02 | 3.08 | 992 | 127.52 | 26.21 | 0.38 | 557 | 8.98 | 27.72 | 0.00 | 453 | 60.73 | 29.36 | 0.34 | 1342 | 590.21 | 31.51 | 1.33 | 66115 | 132.91 |
| blank4.D | Blank | | 6/6/2023 | 24.02 | 3.07 | 255 | 243.23 | 26.16 | 0.36 | 233 | 29.94 | 27.76 | 0.00 | 664 | 9.18 | 29.37 | 0.36 | 1918 | 7.46 | 31.52 | 0.18 | 48763 | 179.08 |
| blank5.D | Blank | | 6/6/2023 | 24.03 | 3.16 | 5905 | 656.82 | 26.21 | 0.36 | 231 | 2.59 | 27.80 | 0.00 | 393 | 3.93 | 29.38 | 0.28 | 221 | 7.23 | 31.51 | 1.05 | 69956 | 184.82 |
| blank6.D | Blank | | 6/6/2023 | 24.07 | 3.08 | 695 | 157.06 | 26.19 | 0.38 | 529 | 6.97 | 27.78 | 0.00 | 312 | 2.37 | 29.38 | 0.29 | 473 | 27.63 | 31.52 | 2.68 | 80910 | 135.94 |
| blank7.D | Blank | | 6/6/2023 | 24.08 | 3.07 | 575 | 733.64 | 26.19 | 0.37 | 473 | 9.38 | 27.74 | 0.00 | 1057 | 10.83 | 29.36 | 0.40 | 2722 | 6.71 | 31.51 | 0.44 | 55987 | 100.46 |
| blank8.D | Blank | | 6/6/2023 | 23.96 | 3.07 | 52 | 74.58 | 25.99 | 0.37 | 480 | 20.76 | 27.84 | 0.00 | 454 | 8.34 | 29.35 | 0.32 | 1011 | 34.19 | 31.52 | 2.16 | 74038 | 200.02 |
| blank9.D | Blank | | 6/6/2023 | 24.05 | 3.07 | 69 | 77.65 | 26.10 | 0.38 | 689 | 8.05 | 27.74 | 0.00 | 234 | 8.20 | 29.40 | 0.28 | 379 | 353.21 | 31.52 | 0.33 | 59088 | 64.06 |
| blank10.D | Blank | | 6/6/2023 | 23.83 | 3.07 | 29 | 22.29 | 26.54 | 0.37 | 397 | 4.27 | 28.00 | 0.00 | 217 | 3.23 | 29.44 | 0.33 | 1119 | 73.36 | 31.57 | 0.54 | 50546 | 75.70 |
| **Average** | | | | | **3.08** | | | | **0.37** | | | | **0.00** | | | | **0.33** | | | | **1.04** | | |
| **SD** | | | | | **0.03** | | | | **0.01** | | | | **0.00** | | | | **0.04** | | | | **0.91** | | |
| **RSD%** | | | | | **0.89** | | | | **2.42** | | | | **0.00** | | | | **11.46** | | | | **86.96** | | |

| | | | | Toluene Results | | | | Hexanal Results | | | | Ethylbenzene Results | | | | m-xylene Results | | | | alpha-pinene Results | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Data File** | **Type** | **Level** | **Acq. Date-T** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** | **RT** | **Final Conc** | **Area** | **S/N** |
| blank1.D | Blank | | 6/6/2023 | 14.82 | 1.1659 | 20840 | 516.17 | 18.45 | 1.4047 | 12773 | 29.37 | 20.225 | 0.0914 | 248 | 3.82 | 20.87 | 0.2108 | 2359 | 4.08 | 23.239 | 0.2969 | 3661 | 4.95 |
| blank2.D | Blank | | 6/6/2023 | 14.818 | 0.6733 | 13944 | 36.04 | 18.434 | 1.204 | 7396 | 9.63 | 20.31 | 0.0888 | 222 | 6.02 | 20.854 | 0.1402 | 1146 | 6.03 | 22.615 | 0.1647 | 797 | 67.67 |
| blank3.D | Blank | | 6/6/2023 | 14.812 | 0.8949 | 16645 | 47.7 | 18.449 | 1.4776 | 14591 | 36.77 | 20.26 | 0.126 | 654 | 19.81 | 20.828 | 0.1399 | 1099 | 2.28 | 22.66 | 0.2067 | 1672 | 3.41 |
| blank4.D | Blank | | 6/6/2023 | 14.824 | 0.8563 | 16498 | 47.17 | 18.44 | 1.3783 | 12187 | 43.3 | 20.208 | 0.0883 | 213 | 4.36 | 20.82 | 0.2437 | 2972 | 1759.24 | 22.585 | 0.1591 | 663 | 4.2 |
| blank5.D | Blank | | 6/6/2023 | 14.815 | 1.0763 | 21875 | 115.67 | 18.435 | 2.0105 | 33062 | 75.83 | 20.31 | 0.1201 | 663 | 6.23 | 20.882 | 0.1899 | 2232 | 1.59 | 22.602 | 0.1425 | 328 | 8.01 |
| blank6.D | Blank | | 6/6/2023 | 14.825 | 1.0568 | 17482 | 52.39 | 18.455 | 1.4398 | 12487 | 33.57 | 20.841 | 0.2012 | 1421 | 23.17 | 20.841 | 0.1748 | 1568 | 2.82 | 22.653 | 0.2077 | 1559 | 18.34 |
| blank7.D | Blank | | 6/6/2023 | 14.819 | 1.9945 | 35164 | 138.03 | 18.456 | 1.4323 | 14432 | 46.47 | 20.56 | 0.0824 | 150 | 8.45 | 20.839 | 0.1716 | 1782 | 22.35 | 22.654 | 0.1754 | 1078 | 26.68 |
| blank8.D | Blank | | 6/6/2023 | 14.811 | 0.9675 | 16484 | 80.18 | 18.435 | 1.4268 | 12302 | 4140.88 | 20.434 | 0.1359 | 718 | 2.65 | 20.838 | 0.2024 | 2033 | 55.39 | 22.659 | 0.1457 | 334 | 7.73 |
| blank9.D | Blank | | 6/6/2023 | 14.815 | 0.3952 | 11127 | 65.78 | 18.452 | 1.2546 | 10048 | 11.99 | 20.28 | 0.0902 | 273 | 14.09 | 20.821 | 0.1346 | 1190 | 14.44 | 22.609 | 0.1461 | 433 | 5.25 |
| blank10.D | Blank | | 6/6/2023 | 14.833 | 0.8313 | 14888 | 64.04 | 18.473 | 1.3674 | 10968 | 14.67 | 20.341 | 0.1213 | 567 | 17.72 | 20.889 | 0.1805 | 1706 | 56.58 | 22.644 | 0.1457 | 340 | 5.1 |
| **Average** | | | | | **0.9912** | | | | **1.4396** | | | | **0.11456** | | | | **0.17884** | | | | **0.17905** | | |
| **SD** | | | | | **0.41614** | | | | **0.217947** | | | | **0.036034** | | | | **0.034871** | | | | **0.048001** | | |
| **RSD%** | | | | | **41.98348** | | | | **15.13943** | | | | **31.45434** | | | | **19.49828** | | | | **26.80897** | | |

Table 8.4 Raw data of standard calibration results based on the Internal Standard method. The outlier values are highlighted in red, and the accuracy (%) represents the apparent recovery.

| | | | | Furfural Results | | | | | Beta-pinene Results | | | | | 3-carene Results | | | | | D-limonene Results | | | | | Benzaldehyde Results | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Data File | Type | Level | Acq. Date-Time | RT | Final Conc. | Accuracy (%) | Area | S/N | RT | Final Conc. | Accuracy (%) | Area | S/N | RT | Final Conc | Accuracy (%) | Area | S/N | RT | Final Conc | Accuracy (%) | Area | S/N | RT | Final Conc | Accuracy (%) | Area | S/N |
| 844419_150ng_1.D | Cal | 5 | 5/19/2023 | 23.93 | 139.11 | 92.70 | 17776246 | 585299.93 | 26.17 | 88.83 | 59.20 | 4872985 | 6476.33 | 27.76 | 142.01 | 94.70 | 13072048 | 11528.24 | 29.38 | 149.08 | 99.40 | 6481307 | 6256.75 | 31.52 | 149.98 | 100.00 | 5572605 | 5130.52 |
| 844403_150ng_2.D | Cal | 5 | 5/21/2023 | 23.92 | 142.86 | 95.20 | 13758858 | 473557.83 | 26.17 | 152.53 | 101.70 | 6312951 | 9162.51 | 27.76 | 148.08 | 98.70 | 10266384 | 20408.15 | 29.37 | 134.73 | 89.80 | 4410963 | 6529.98 | 31.51 | 135.30 | 90.20 | 3794158 | 5138.71 |
| 844281_cal150ng.D | Cal | 5 | 5/28/2023 | 23.92 | 150.66 | 100.40 | 12240309 | 202240.52 | 26.17 | 146.35 | 97.60 | 5103276 | 12802.40 | 27.75 | 152.79 | 101.90 | 8925046 | 19793.25 | 29.37 | 142.01 | 94.70 | 3917941 | 7090.92 | 31.51 | 165.09 | 110.10 | 3886547 | 7890.92 |
| 844376_100ng_1.D | Cal | 4 | 5/19/2023 | 23.93 | 87.65 | 87.60 | 9891599 | 171136.11 | 26.17 | 103.46 | 103.50 | 5082677 | 8660.36 | 27.76 | 97.83 | 97.80 | 8065862 | 13090.24 | 29.38 | 82.59 | 82.60 | 3208800 | 7258.80 | 31.52 | 67.68 | 67.70 | 2300419 | 3462.70 |
| 844291_100ng_2.D | Cal | 4 | 5/21/2023 | 23.93 | 99.56 | 99.60 | 9398524 | 247889.02 | 26.17 | 74.31 | 74.30 | 3036243 | 4026.99 | 27.76 | 102.33 | 102.30 | 7026179 | 8939.95 | 29.37 | 99.09 | 99.10 | 3208348 | 13122.69 | 31.52 | 106.57 | 106.60 | 2973490 | 4394.76 |
| 844245_cal100ng.D | Cal | 4 | 5/28/2023 | 23.92 | 99.47 | 99.50 | 8441707 | 333957.00 | 26.16 | 75.93 | 75.90 | 2789732 | 6453.93 | 27.75 | 105.98 | 106.00 | 6541127 | 5100.98 | 29.37 | 101.61 | 101.60 | 2957924 | 6358.86 | 31.51 | 107.08 | 107.10 | 2685827 | 5287.91 |
| 844404_50ng_1.D | Cal | 3 | 5/19/2023 | 23.93 | 49.33 | 98.70 | 5763557 | 259338.76 | 26.17 | 33.11 | 66.20 | 1720047 | 1535.66 | 27.76 | 53.88 | 107.80 | 4740848 | 4058.05 | 29.38 | 53.48 | 107.00 | 2209373 | 4453.13 | 31.52 | 49.90 | 99.80 | 1832108 | 1213.62 |
| 844402_50ng_2.D | Cal | 3 | 5/21/2023 | 23.93 | 49.87 | 99.70 | 5061611 | 149918.60 | 26.17 | 33.33 | 66.70 | 1502935 | 2346.26 | 27.76 | 51.40 | 102.80 | 3926413 | 2376.93 | 29.38 | 51.71 | 103.40 | 1854226 | 2943.73 | 31.51 | 53.79 | 107.60 | 1707861 | 1594.35 |
| 844418_cal_50ng.D | Cal | 3 | 5/28/2023 | 23.92 | 44.94 | 89.90 | 3739584 | 618739.72 | 26.16 | 46.21 | 92.40 | 1726236 | 1963.56 | 27.75 | 54.23 | 108.50 | 3420346 | 7576.47 | 29.37 | 50.13 | 100.30 | 1484260 | 1967.34 | 31.51 | 50.19 | 100.40 | 1320446 | 1747.99 |
| 844204_10ng_1.D | Cal | 2 | 5/19/2023 | 23.96 | 9.68 | 96.80 | 884926 | 47904.38 | 26.17 | 8.55 | 85.50 | 462184 | 383.46 | 27.76 | 9.33 | 93.30 | 899454 | 1040.56 | 29.38 | 9.03 | 90.30 | 390668 | 227.36 | 31.53 | 7.34 | 73.40 | 377669 | 829.85 |
| 844279_10ng_2.D | Cal | 2 | 5/21/2023 | 23.95 | 10.29 | 102.90 | 687169 | 18485.56 | 26.17 | 10.56 | 105.60 | 409369 | 404.10 | 27.76 | 9.42 | 94.20 | 645193 | 968.36 | 29.38 | 8.87 | 88.70 | 272650 | 305.82 | 31.53 | 9.44 | 94.40 | 324379 | 859.30 |
| 844342_cal_10ng.D | Cal | 2 | 5/28/2023 | 23.94 | 10.15 | 101.50 | 602739 | 25192.83 | 26.17 | 10.51 | 105.10 | 364248 | 613.53 | 27.75 | 9.77 | 97.70 | 598137 | 1129.34 | 29.37 | 9.53 | 95.30 | 262790 | 796.47 | 31.52 | 10.46 | 104.60 | 314362 | 366.55 |
| 844347_1ng_1.D | Cal | 1 | 5/19/2023 | 24.01 | 3.74 | 374.20 | 94907 | 4925.34 | 26.17 | 1.26 | 125.80 | 53492 | 93.84 | 27.76 | 0.75 | 75.30 | 96725 | 329.37 | 29.38 | 1.23 | 122.90 | 45067 | 123.03 | 31.53 | 0.00 | 0.00 | 100291 | 258.89 |
| 844271_1ng_2.D | Cal | 1 | 5/21/2023 | 24.00 | 3.59 | 359.50 | 64400 | 5044.28 | 26.17 | 1.50 | 149.90 | 58788 | 110.52 | 27.76 | 0.84 | 84.50 | 91720 | 157.36 | 29.39 | 1.26 | 126.40 | 40503 | 81.40 | 31.53 | 0.02 | 1.50 | 94752 | 187.40 |
| 844416_cal1ng.D | Cal | 1 | 5/28/2023 | 23.99 | 3.75 | 374.70 | 69277 | 13245.99 | 26.17 | 1.11 | 111.10 | 32467 | 71.06 | 27.75 | 0.83 | 82.60 | 75271 | 55.74 | 29.37 | 1.45 | 145.10 | 40159 | 86.08 | 31.53 | 1.03 | 103.00 | 107867 | 382.91 |

| | | | | Toluene Results | | | | | Hexanal Results | | | | | Ethylbenzene Results | | | | | m-xylene Results | | | | | Alpha-pinene Results | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Data File | Type | Level | Acq. Date-Time | RT | Final Conc. | Accuracy (%) | Area | S/N | RT | Final Conc. | Accuracy (%) | Area | S/N | RT | Final Conc | Accuracy (%) | Area | S/N | RT | Final Conc | Accuracy (%) | Area | S/N | RT | Final Conc | Accuracy | Area | S/N |
| 844419_150ng_1.D | Cal | 5 | 5/19/2023 | 14.83 | 144.10 | 96.10 | 4726530 | 11677.06 | 18.44 | 147.91 | 98.60 | 9079274 | 19259.56 | 20.29 | 144.66 | 96.40 | 3872996 | 4868.45 | 20.84 | 140.92 | 93.90 | 5528161 | 4703.90 | 22.62 | 130.76 | 87.20 | 6367694 | 6194.92 |
| 844403_150ng_2.D | Cal | 5 | 5/21/2023 | 14.82 | 149.15 | 99.40 | 3684329 | 6732.70 | 18.43 | 149.94 | 100.00 | 6933174 | 16612.31 | 20.29 | 148.71 | 99.10 | 2998823 | 3478.33 | 20.83 | 145.54 | 97.00 | 4300408 | 2246.41 | 22.62 | 135.97 | 90.60 | 4987318 | 3512.93 |
| 844281_cal150ng.D | Cal | 5 | 5/28/2023 | 14.82 | 150.93 | 100.60 | 3141519 | 6131.21 | 18.43 | 155.69 | 103.80 | 6067344 | 11585.94 | 20.28 | 152.07 | 101.40 | 2583896 | 6676.09 | 20.82 | 150.06 | 100.00 | 3736139 | 8015.20 | 22.61 | 148.93 | 99.30 | 4603199 | 6422.90 |
| 844376_100ng_1.D | Cal | 4 | 5/19/2023 | 14.83 | 96.10 | 96.10 | 2823467 | 11944.19 | 18.44 | 96.78 | 96.80 | 5299025 | 3834.04 | 20.29 | 96.18 | 96.20 | 2303993 | 4320.04 | 20.83 | 95.30 | 95.30 | 3345039 | 5578.29 | 22.62 | 90.86 | 90.90 | 3958233 | 5928.94 |
| 844291_100ng_2.D | Cal | 4 | 5/21/2023 | 14.82 | 98.27 | 98.30 | 2404701 | 6647.15 | 18.43 | 100.27 | 100.30 | 4574216 | 3609.88 | 20.29 | 99.27 | 99.30 | 1980586 | 2451.34 | 20.83 | 97.77 | 97.80 | 2858309 | 4060.20 | 22.62 | 100.64 | 100.60 | 3651957 | 3188.72 |
| 844245_cal100ng.D | Cal | 4 | 5/28/2023 | 14.82 | 101.62 | 101.60 | 2235353 | 6194.20 | 18.43 | 103.28 | 103.30 | 4236784 | 3584.17 | 20.28 | 100.94 | 100.90 | 1810625 | 3622.51 | 20.82 | 100.46 | 100.50 | 2640458 | 4987.63 | 22.61 | 101.89 | 101.90 | 3324087 | 5180.61 |
| 844404_50ng_1.D | Cal | 3 | 5/19/2023 | 14.83 | 47.75 | 95.50 | 1498376 | 4071.71 | 18.44 | 50.44 | 100.90 | 2915441 | 5992.94 | 20.29 | 48.48 | 97.00 | 1236283 | 1699.54 | 20.83 | 49.39 | 98.80 | 1845241 | 1239.01 | 22.62 | 49.21 | 98.40 | 2280949 | 2068.07 |
| 844402_50ng_2.D | Cal | 3 | 5/21/2023 | 14.82 | 47.66 | 95.30 | 1298450 | 4974.75 | 18.44 | 47.60 | 95.20 | 2385370 | 1884.53 | 20.29 | 48.25 | 96.50 | 1067973 | 1465.33 | 20.83 | 49.62 | 99.20 | 1609296 | 1147.83 | 22.62 | 41.76 | 83.50 | 1679483 | 1917.48 |
| 844418_cal_50ng.D | Cal | 3 | 5/28/2023 | 14.82 | 50.01 | 100.00 | 1124633 | 5155.94 | 18.43 | 49.14 | 98.30 | 2034750 | 2297.98 | 20.29 | 50.23 | 100.50 | 918248 | 1895.20 | 20.83 | 49.82 | 99.60 | 1334241 | 1365.16 | 22.62 | 48.93 | 97.90 | 1625683 | 1421.22 |
| 844204_10ng_1.D | Cal | 2 | 5/19/2023 | 14.83 | 9.87 | 98.70 | 339468 | 1005.10 | 18.44 | 9.76 | 97.60 | 557315 | 1081.01 | 20.29 | 10.11 | 101.10 | 275383 | 241.64 | 20.84 | 9.76 | 97.60 | 388889 | 705.83 | 22.62 | 10.11 | 101.10 | 498149 | 882.54 |
| 844279_10ng_2.D | Cal | 2 | 5/21/2023 | 14.83 | 10.05 | 100.50 | 245695 | 917.82 | 18.44 | 10.45 | 104.50 | 427335 | 2152.85 | 20.29 | 10.46 | 104.60 | 202507 | 504.20 | 20.83 | 10.00 | 100.00 | 283577 | 552.29 | 22.62 | 9.92 | 99.20 | 347453 | 380.83 |
| 844342_cal_10ng.D | Cal | 2 | 5/28/2023 | 14.82 | 11.14 | 111.40 | 242987 | 782.90 | 18.44 | 11.49 | 114.90 | 424406 | 491.31 | 20.29 | 10.71 | 107.10 | 185538 | 281.19 | 20.83 | 10.37 | 103.70 | 263057 | 524.23 | 22.61 | 10.55 | 105.50 | 330759 | 858.39 |
| 844347_1ng_1.D | Cal | 1 | 5/19/2023 | 14.83 | 1.09 | 109.30 | 47433 | 149.08 | 18.45 | 2.25 | 225.10 | 86803 | 89.29 | 20.30 | 1.14 | 113.70 | 30657 | 37.75 | 20.84 | 1.10 | 110.10 | 43187 | 47.16 | 22.63 | 1.17 | 117.20 | 54552 | 79.82 |
| 844271_1ng_2.D | Cal | 1 | 5/21/2023 | 14.83 | 1.06 | 105.90 | 40124 | 305.93 | 18.45 | 2.20 | 220.30 | 72538 | 94.87 | 20.29 | 1.31 | 130.70 | 30854 | 30.97 | 20.85 | 1.24 | 124.20 | 42617 | 75.14 | 22.62 | 1.19 | 119.40 | 48330 | 63.62 |
| 844416_cal1ng.D | Cal | 1 | 5/28/2023 | 14.83 | 1.99 | 199.40 | 57301 | 211.22 | 18.44 | 2.62 | 262.20 | 80676 | 162.25 | 20.28 | 1.32 | 131.80 | 25971 | 65.10 | 20.82 | 1.18 | 118.40 | 33785 | 72.33 | 22.61 | 1.30 | 130.40 | 44517 | 35.15 |

# F. Quantification and breakthrough results identified in USP, CLT and SSP

Table 8.5 Quantification results of targeted VOCs in USP sample duplicates. N.A. is abbreviation for not applicable.

| Untreated spruce panel | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Toluene | Hexanal | Ethylbenzene | m-xylene | Alpha-pinene | Furfural | Beta-pinene | 3-carene | D-limonene | Benzaldehyde |
| Type | Chamber | Sample Vol. L | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 |
| Sample | Chamber 1, vol. 3L | 2.924 | 1.58 | 10.38 | 0.33 (<LoQ) | 0.38 | 28.38 | 0.69 | 3.62 | 0.70 | 1.24 | 2.21 |
| Sample | Chamber 1, vol 5L | 4.886 | 0.73 | 5.50 | 0.04 (<LoD) | 0.15 | 20.21 | 0.18 | 2.63 | 0.34 | 0.81 | 0.06 (<LOQ) |
| **RSD%** | | | **51.88** | **43.48** | **108.90** | **63.02** | **23.78** | **84.40** | **22.32** | **48.48** | **29.28** | **133.99** |
| Sample | Chamber 2, vol. 3L | 2.921 | 0.86 | 14.31 | 0.11 | 0.15 | 20.60 | 0.58 | 2.09 | 0.20 | 1.04 | 0.51 (<LOQ) |
| Sample | Chamber 2, vol 5L | 4.878 | 0.85 | 18.95 | N.A. | 0.09 | 25.61 | 0.12 | 2.66 | 0.32 | 1.40 | 0.14 (<LOQ) |
| **RSD%** | | | **1.18** | **19.74** | **-** | **37.28** | **15.33** | **91.93** | **16.90** | **32.67** | **20.90** | **79.73** |
| Sample | Chamber 3, vol. 3L | 2.914 | 0.93 | 29.41 | 0.18(<LoQ) | 0.14 | 24.29 | 0.56 | 3.19 | 0.13 | 1.12 | 0.75 (<LOQ) |
| Sample | Chamber 3, vol 5L | 4.873 | 0.77 | 32.32 | 0.16 (<LoQ) | 0.21 | 21.85 | 0.12 | 2.39 | 0.17 | 1.35 | 0.62 (<LOQ) |
| **RSD%** | | | **13.04** | **6.67** | **6.33** | **26.52** | **7.49** | **90.80** | **20.03** | **21.84** | **13.06** | **13.69** |
| Sample | Chamber 4, vol. 3L | 2.928 | 0.85 | 4.75 | 0.19 (<LoQ) | 0.23 | 8.92 | 0.55 | 1.60 | 0.25 | 0.79 | 0.77 (<LOQ) |
| Sample | Chamber 4, vol 5L | 4.891 | 0.89 | 7.82 | 0.48 (<LoQ) | 0.53 | 12.01 | 0.15 | 3.30 | 0.62 | 0.84 | 1.10 |
| **RSD%** | | | **3.35** | **34.54** | **60.91** | **56.36** | **20.83** | **79.85** | **49.05** | **59.92** | **3.94** | **24.91** |
| **RSD% between all sample duplicates** | | | **28.53** | **64.33** | **107.63** | **77.01** | **31.09** | **61.52** | **25.73** | **69.19** | **22.01** | **93.06** |

Table 8.6 Quantification results of targeted VOCs in CLT sample duplicates. N.A. is abbreviation for not applicable.

| Cross-laminated tree | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Toluene | Hexanal | Ethylbenzene | m-xylene | Alpha-pinene | Furfural | beta-pinene | 3-carene | D-limonene | Benzaldehyde |
| Type | Sample Vol. L | Chamber nr. | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 |
| Sample | 4.919 | Chamb 4, vol 5L | 0.52 (<LoQ) | 8.91 | 0.02 (<LoD) | 0.01 (<LoD) | 4.77 | 0.06 | 1.09 | 0.36 | 0.18 | -0.03 |
| Sample | 2.943 | Chamb 4, vol. 3L | 0.61 (<LoQ) | 9.14 | 0.10 (<LOQ) | N.A. | 4.94 | 0.19 | 1.29 | 0.38 | 0.13 | 0.13 (<LOQ) |
| **RSD%** | | | **11.39** | **1.80** | **95.52** | **-** | **2.54** | **72.21** | **11.95** | **3.52** | **25.19** | **207.59** |
| Sample | 4.934 | Chamb 3, vol 5L | 1.54 | 80.07 | 0.02 (<LoD) | 0.02 (<LoQ) | 45.38 | 0.06 | 15.03 | 7.32 | 4.00 | 0.10 (<LOQ) |
| Sample | 2.948 | Chamb 3, vol. 3L | 1.36 | 95.52 | N.A. | N.A. | 45.30 | 0.17 | 15.44 | 5.97 | 2.49 | 0.27 (<LOQ) |
| **RSD%** | | | **8.93** | **12.44** | **-** | **-** | **0.14** | **71.37** | **1.90** | **14.39** | **32.85** | **63.25** |
| Sample | 4.917 | Chamb 2, vol 5L | 1.23 | 25.55 | 0.01 (<LOD) | 0.01 (<LoD) | 26.69 | 0.04 | 3.93 | 1.39 | 1.56 | 0.31 (<LOQ) |
| Sample | 2.941 | Chamb 2, vol. 3L | 0.88 | 19.24 | N.A. | N.A. | 24.51 | 0.15 | 3.30 | 1.07 | 1.22 | 0.13 (<LOQ) |
| **RSD%** | | | **22.95** | **19.92** | **-** | **-** | **6.03** | **84.44** | **12.35** | **18.54** | **17.49** | **58.35** |
| Sample | 4.929 | Chamb 1, vol 5L | 1.32 | 13.49 | 0.01 (<LoD) | 0.02 (<LoQ) | 23.58 | 0.03 | 2.25 | 1.12 | 0.67 | -0.05 |
| Sample | 2.945 | Chamb 1, vol. 3L | 1.46 | 14.58 | 0.01 (<LoD) | N.A. | 29.15 | 0.22 | 3.15 | 1.32 | 0.53 | 0.03 (<LOD) |
| **RSD%** | | | **6.84** | **5.47** | **27.67** | **-** | **14.93** | **103.16** | **23.70** | **11.29** | **16.17** | **-413.64** |
| **RSD% between all sample duplicates** | | | **36.91** | **89.93** | **140.07** | **99.45** | **61.52** | **74.31** | **98.78** | **106.97** | **90.83** | **104.63** |

Table 8.7 Quantification results of targeted VOCs in SSP duplicates. N.A. is abbreviation for not applicable.

| Stained spruce panel | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Toluene | Hexanal | Ethylbenzene | m-xylene | Alpha-pinene | Furfural | Beta-pinene | 3-carene | D-limonene | Benzaldehyde |
| Type | Chamber nr | Sample Vol. L | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 | conc.µg/m^3 |
| Sample | Chamber 4, vol. 3L | 2.919 | 0.49 | 3.01 | N.A. | 0.04 | 2.31 | 0.77 | 0.53 | 0.04 | 0.01 (<LoQ) | 0.50 (<LoQ) |
| Sample | Chamber 4, vol.5L | 4.893 | 0.40 | 3.11 | 0.03 (<LoQ) | 0.04 | 2.28 | 0.00 | 0.32 | 0.19 | 0.18 | -0.01 |
| **RSD%** | | | **14.72** | **2.42** | **-** | **8.18** | **1.12** | **141.53** | **35.40** | **96.24** | **130.30** | **148.09** |
| Sample | Chamber 3, vol.5L | 4.912 | 1.25 | 16.54 | 0.11 | 0.02 | 14.87 | -0.02 | 3.13 | 1.33 | 0.93 | 0.07 (<LoQ) |
| Sample | Chamber 3, vol.3L | 2.934 | 0.87 | 12.25 | 0.05 (<LoQ) | 0.00 | 12.47 | 0.69 | 2.75 | 0.90 | 0.60 | 0.24 (<LoQ) |
| **RSD%** | | | **25.24** | **21.08** | **51.17** | **116.07** | **12.44** | **148.19** | **9.04** | **27.37** | **30.68** | **81.38** |
| Sample | Chamber 2, vol.5L | 4.909 | 0.57 | 10.24 | 0.01 (<LoQ) | -0.01 | 8.64 | -0.03 | 1.20 | 0.54 | 0.51 | 0.24 (<LoQ) |
| Sample | Chamber 2, vol.3L | 2.933 | 0.49 | 9.01 | -0.01 | 0.01 | 7.86 | 0.72 | 1.36 | 0.50 | 0.45 | 0.49(<LoQ) |
| **RSD%** | | | **10.25** | **9.03** | **-** | **-494.64** | **6.68** | **153.39** | **8.93** | **5.17** | **8.51** | **49.72** |
| Sample | Chamber 1, vol.5L | 4.901 | 0.58 | 4.14 | 0.02 (<LOQ) | 0.02 | 1.95 | -0.05 | 0.33 | 0.13 | 0.04 | 0.03 (<LoQ) |
| Sample | Chamber 1, vol.3L | 2.932 | 0.68 | 4.63 | -0.01 | 0.00 | 2.30 | 0.68 | 0.36 | -0.02 | 0.03 | 0.09 (<LoQ) |
| **RSD%** | | | **10.83** | **7.88** | **378.95** | **212.70** | **11.60** | **165.59** | **6.04** | **184.54** | **23.14** | **74.40** |
| **RSD% between all sample duplicates** | | | **41.27** | **59.51** | **137.86** | **118.10** | **71.56** | **133.65** | **81.79** | **90.39** | **85.55** | **90.68** |

Table 8.8 Calculated breakthrough in non-sampling tubes. Breakthrough values ≥100% are highlighted in red.

| | | Toluene | | Hexanal | | Ethylbenzene | | m-xylene | | Alpha-pinene | | Furfural | | b-pinene | | 3-carene | | D-limonene | | Benzaldehyde | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Chamber nr. | Conc. ng/µL | Breaktr % | Conc. ng/µL | Breaktr % | Conc. ng/µL | Breaktr % | Conc. ng/µL | Breaktr % | Conc. ng/µL | Breaktr % | Conc. ng/µL | Breaktr % | Conc. ng/ | Breaktr % | Conc. ng/µL | Breaktr % | Conc. ng/µL | Breaktr % | Conc. ng/µL | Breaktr % |
| Stained spruce panel | Chamb. 1, vol 5L | 0.313 | 8.380 | 5.143 | 18.179 | 0.000 | 0.000 | 0.045 | 7.633 | 4.138 | 34.191 | 5.381 | 88.455 | 1.666 | 54.556 | 1.244 | 74.371 | 1.389 | 517.393 | 2.846 | 80.088 |
| | Chamb. 2, vol 5L | 0.968 | 26.226 | 5.664 | 9.719 | 0.000 | 0.000 | 0.001 | 0.287 | 11.308 | 25.153 | 5.478 | 88.142 | 2.438 | 33.450 | 1.104 | 29.917 | 1.144 | 44.666 | 3.732 | 81.495 |
| | Chamb. 3, vol 5L | 0.388 | 5.532 | 5.125 | 5.739 | 0.000 | 0.000 | 0.000 | 0.000 | 12.848 | 16.998 | 5.390 | 85.783 | 2.789 | 16.613 | 0.781 | 10.332 | 0.464 | 10.029 | 2.088 | 55.780 |
| | Chamb. 4, vol 5L | 0.591 | 20.700 | 4.587 | 19.753 | 0.000 | 0.000 | 0.000 | 0.000 | 3.586 | 26.217 | 5.374 | 84.814 | 1.468 | 49.563 | 0.956 | 48.385 | 1.265 | 132.868 | 2.465 | 73.515 |
| Untreated spruce panel | Chamb.1, vol 5L | 1.735 | 32.052 | 14.960 | 43.644 | 0.000 | 0.000 | 0.000 | 0.000 | 22.216 | 20.090 | 4.032 | 87.145 | 4.797 | 30.406 | 9.361 | 245.114 | 15.588 | 287.811 | 7.137 | 179.116 |
| | Chamb. 2, vol 5L | 1.876 | 31.446 | 14.962 | 14.989 | 0.000 | 0.000 | 0.026 | 4.593 | 24.484 | 17.904 | 3.841 | 87.987 | 5.163 | 32.572 | 6.890 | 184.703 | 12.618 | 152.459 | 8.631 | 197.181 |
| | Chamb. 3, vol 5L | 1.411 | 25.179 | 7.871 | 4.774 | 0.165 | 103.125 | 0.659 | 57.681 | 24.711 | 20.895 | 3.632 | 83.418 | 2.328 | 15.982 | 0.000 | 0.000 | 0.755 | 9.446 | 5.335 | 79.545 |
| CLT | Chamb. 1, vol 5L | 0.562 | 8.090 | 2.177 | 3.021 | 0.006 | 11.359 | 0.000 | 0.000 | 24.963 | 20.594 | 0.962 | 74.499 | 1.177 | 9.552 | 0.407 | 5.329 | 0.826 | 19.748 | 1.686 | 108.408 |
| | Chamb. 2, vol 5L | 0.269 | 4.163 | 2.111 | 1.609 | 0.000 | 0.000 | 0.000 | 0.000 | 23.867 | 17.525 | 0.931 | 71.070 | 2.537 | 12.320 | 0.445 | 4.993 | 0.387 | 4.510 | 1.172 | 35.410 |
| | Chamb. 3, vol 5L | 0.577 | 7.188 | 4.514 | 1.127 | 0.100 | 77.510 | 0.000 | 0.000 | 90.069 | 39.350 | 1.072 | 76.240 | 19.690 | 26.114 | 2.200 | 5.754 | 1.317 | 6.388 | 1.563 | 67.577 |
| | Chamb. 4, vol 5L | 0.289 | 9.719 | 3.424 | 6.937 | 0.000 | 0.000 | 0.000 | 0.000 | 4.517 | 15.904 | 0.954 | 66.790 | 0.507 | 7.664 | 0.695 | 17.922 | 0.979 | 54.240 | 1.024 | 60.934 |

# G. MassHunter PCDL manager list of compounds used in the identification of unknown.

Compound Results: 47 hits

| Name | Formula | Mass | Retention Time | CAS | NumSpectra | Cation | Anion | CCS Count |
|---|---|---|---|---|---|---|---|---|
| 1,2,3-trichlorobenzene | C6H3Cl3 | 179.93003 | 39.1827 | 87-61-6 | 1 | ☐ | ☐ | 0 |
| 1,2,3-trimethylbenzene | C9H12 | 120.0939 | 29.92321666666... | 526-73-8 | 1 | ☐ | ☐ | 0 |
| 1,2,4,5-tetramethylbenzene | C10H14 | 134.10955 | 34.42776666666... | 95-93-2 | 1 | ☐ | ☐ | 0 |
| 1,2,4-dichlorobenzene | C6H3Cl3 | 179.93003 | 37.62201666666... | 120-82-1 | 1 | ☐ | ☐ | 0 |
| 1,2,4-trichlorobutadiene | C6H3Cl3 | 179.93003 | 15.33833333333... | 87-68-3 | 1 | ☐ | ☐ | 0 |
| 1,2,4-trimethylbenzene | C9H12 | 120.0939 | 28.00751666666... | 95-63-6 | 1 | ☐ | ☐ | 0 |
| 1,2-dichlorobenzene | C6H4Cl2 | 145.96901 | 32.02898333333... | 95-50-1 | 1 | ☐ | ☐ | 0 |
| 1,2-dichloropropane | C3H6Cl2 | 111.98466 | 13.0671 | 78-87-5 | 1 | ☐ | ☐ | 0 |
| 1,3,5-trimethylbenzene | C9H12 | 120.0939 | 26.30951666666... | 108-67-8 | 1 | ☐ | ☐ | 0 |
| 1,3-dichlorobenzene | C6H4Cl2 | 145.96901 | 10.52938333333... | 541-73-1 | 1 | ☐ | ☐ | 0 |
| 1,4-dichlorobenzene | C6H4Cl2 | 145.96901 | 10.79471666666... | 106-46-7 | 1 | ☐ | ☐ | 0 |
| 2-chlorotoluene | C7H7Cl | 126.02363 | 8.8844 | 95-49-8 | 1 | ☐ | ☐ | 0 |
| 2-ethyltoluene | C9H12 | 120.0939 | 27.17358333333... | 611-14-3 | 1 | ☐ | ☐ | 0 |
| 3-carene | C10H16 | 136.1252 | 26.97893333333... | 13466-78-9 | 1 | ☐ | ☐ | 0 |
| 3-Ethyltoluene | C9H12 | 120.0939 | 25.87413333333... | 620-14-4 | 1 | ☐ | ☐ | 0 |
| 4-chlorotoluene | C7H7Cl | 126.0234 | 9.11655 | 106-43-4 | 1 | ☐ | ☐ | 0 |
| 4-Ethyltoluene | C9H12 | 120.0939 | 26.03155 | 622-96-8 | 1 | ☐ | ☐ | 0 |
| Acetone | C3H6O | 58.04186 | 6.549716666666... | 67-64-1 | 1 | ☐ | ☐ | 0 |
| Benzaldehyde | C7H6O | 106.04171 | 30.24226666666... | 100-52-7 | 1 | ☐ | ☐ | 0 |
| Benzene | C6H6 | 78.04695 | 10.3803 | 71-43-2 | 1 | ☐ | ☐ | 0 |
| Beta-pinene | C10H16 | 136.12508 | 25.52 | 127-91-3 | 1 | ☐ | ☐ | 0 |
| Camphene | C10H16 | 136.1252 | 23.89105 | 79-92-5 | 1 | ☐ | ☐ | 0 |
| Decanal | C10H20O | 156.15142 | 6.593783333333... | 112-31-2 | 1 | ☐ | ☐ | 0 |
| Decane | C10H22 | 142.17215 | 24.8493 | 124-18-5 | 1 | ☐ | ☐ | 0 |
| D-limonene | C10H16 | 136.12636 | 4.589283333333... | 5989-27-5 | 1 | ☐ | ☐ | 0 |
| Dodecane | C12H26 | 170.20345 | 34.96028333333... | 112-40-3 | 1 | ☐ | ☐ | 0 |
| Ethylbenzene | C8H10 | 106.07825 | 20.33135 | 95-47-6 | 1 | ☐ | ☐ | 0 |
| Furfural | C5H4O2 | 96.02088 | 23.64785 | 98-01-1 | 1 | ☐ | ☐ | 0 |
| Hexachlorobutadiene | C4Cl6 | 257.81312 | 37.23686666666... | 87-68-3 | 1 | ☐ | ☐ | 0 |
| Hexadecane | C16H34 | 226.26605 | 44.68611666666... | 544-76-3 | 1 | ☐ | ☐ | 0 |
| Hexanal | C6H12O | 100.08882 | 18.64426666666... | 66-25-1 | 1 | ☐ | ☐ | 0 |
| Isopropylbenzene | C9H12 | 120.0939 | 8.11165 | 98-82-8 | 1 | ☐ | ☐ | 0 |
| Mesitylene | C9H12 | 120.0939 | 9.441583333333... | 108-67-8 | 1 | ☐ | ☐ | 0 |
| m-xylene | C8H10 | 106.07821 | 18.40781666666... | 108-38-3 | 1 | ☐ | ☐ | 0 |
| Naphtalene | C10H8 | 128.0626 | 38.75736666666... | 91-20-3 | 1 | ☐ | ☐ | 0 |
| N-butylbenzene | C10H14 | 134.10955 | 12.05498333333... | 104-51-8 | 1 | ☐ | ☐ | 0 |
| Nonane | C9H20 | 128.15674 | 19.31656666666... | 111-84-2 | 1 | ☐ | ☐ | 0 |
| N-propylbenzene | C9H12 | 120.0939 | 8.960683333333... | 103-65-1 | 1 | ☐ | ☐ | 0 |
| Octane | C8H18 | 114.14085 | 14.07183333333... | 111-65-9 | 1 | ☐ | ☐ | 0 |
| o-xylene | C8H10 | 106.07825 | 19.70126666666... | 95-47-6 | 1 | ☐ | ☐ | 0 |
| Pentadecane | C15H32 | 212.2504 | 42.87425 | 629-62-9 | 1 | ☐ | ☐ | 0 |
| Styrene | C8H8 | 104.0626 | 22.93361666666... | 100-42-5 | 1 | ☐ | ☐ | 0 |
| Tert-butylbenzene | C10H14 | 134.10955 | 11.10978333333... | 98-06-6 | 1 | ☐ | ☐ | 0 |
| Tetrachloroethylene | C2Cl4 | 163.87541 | 16.15833333333... | 127-18-4 | 1 | ☐ | ☐ | 0 |
| Tetradecane | C14H30 | 198.23475 | 40.78105 | 629-59-4 | 1 | ☐ | ☐ | 0 |
| Toluene | C7H8 | 92.0626 | 15.3575 | 108-88-3 | 1 | ☐ | ☐ | 0 |
| Tridecane | C13H28 | 184.2191 | 38.25246666666... | 629-50-5 | 1 | ☐ | ☐ | 0 |

# H. Statistical evaluation of SUS and NTS

Table 8.9 Compound hit classification based on the confidence level. Evaluated hits were absorbed on Tenax TA sorbent.

| | Untreated spruce | | | | | | | | | CLT | | | | | | | | | Stained spruce | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Chamb. Volume L** | **C1, 5L** | **C1, 3L** | **C2, 5L** | **C2, 3L** | **C3, 5L** | **C3, 3L** | **C4, 5L** | **C4, 3L** | **C5, 5L** | **C1, 5L** | **C1, 3L** | **C2, 5L** | **C2, 3L** | **C3, 5L** | **C3, 3L** | **C4, 5L** | **C4, 3L** | **C5, 5L** | **C1, 5L** | **C1, 3L** | **C2, 5L** | **C2, 3L** | **C3, 5L** | **C3, 3L** | **C4, 5L** | **C4, 3L** | **C5, 5L** | **Total** |
| **Conf. Level 1** | 7 | 14 | 10 | 10 | 13 | 12 | 14 | 13 | 14 | 8 | 8 | 9 | 8 | 8 | 8 | 6 | 9 | 15 | 14 | 13 | 18 | 13 | 10 | 12 | 15 | 14 | 13 | **308** |
| **Conf. level 2** | 36 | 85 | 59 | 66 | 82 | 73 | 93 | 73 | 64 | 36 | 35 | 45 | 46 | 45 | 41 | 41 | 42 | 54 | 57 | 40 | 74 | 53 | 49 | 50 | 50 | 54 | 55 | **1498** |
| **Conf. level 3** | 70 | 160 | 77 | 123 | 157 | 116 | 169 | 135 | 146 | 66 | 60 | 77 | 73 | 70 | 65 | 62 | 56 | 86 | 80 | 71 | 123 | 91 | 78 | 68 | 65 | 77 | 83 | **2504** |
| **Conf. level 4** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | **N.A.** |
| **Conf. level 5** | 271 | 1065 | 541 | 748 | 757 | 649 | 816 | 659 | 615 | 281 | 380 | 383 | 468 | 244 | 282 | 274 | 383 | 1150 | 972 | 1220 | 1199 | 1387 | 661 | 923 | 957 | 1341 | 1381 | **19 259** |

# I. Volatile organic compounds identified by SUS and NTS

Table 8.10 Pivot table VOC emissions from CLT duplicates. VOCs identified in the table were absorbed on Tenax TA sorbent. The compounds represented in the table are classified with identification levels 1 and 2.

| Cross-laminated timber | Sample | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Compound name | Chamber 1, 3L | Chamber 1, 5L | Chamber 2, 3L | Chamber 2, 5L | Chamber 3, 3L | Chamber 3, 5L | Chamber 4, 3L | Chamber 4, 5L | Chamber 5, 5L | Grand Total |
| Cyclotrisiloxane, hexamethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Nonanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| .alpha.-Pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Pentanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 1,6-Dioxacyclododecane-7,12-dione | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| D-limonene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 2-Pentanone | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexane, 3-methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 3-carene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| o-Cymene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Decanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Pentane, 3-ethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Octanal | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Hexane, 2-methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Cyclotetrasiloxane, octamethyl- | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Pentane, 2,3-dimethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Heptanal | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 8 |
| Tetradecanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Heptane | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Octane | 1 | 1 | 1 | 1 | 1 | 1 | | | 1 | 7 |
| Cyclohexane, methyl- | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | | 7 |
| Hexadecanoic acid, methyl ester | | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | 7 |
| Cyclohexane | 1 | | 1 | | 1 | 1 | 1 | 1 | | 6 |
| .beta.-Phellandrene | 1 | 1 | 1 | 1 | 1 | 1 | | | | 6 |
| Ethyl Acetate | 1 | 1 | 1 | 1 | | | 1 | 1 | | 6 |
| 1-Methyl-1H-1,2,4-triazole | 1 | 1 | 1 | 1 | | | | 1 | | 5 |
| Bicyclo[2.2.1]heptane, 7,7-dimethyl-2-methylene- | 1 | 1 | 1 | 1 | | 1 | | | | 5 |
| Cyclopentane, 1,3-dimethyl- | | 1 | | 1 | 1 | 1 | | 1 | | 5 |
| Hexadecane, 2-methyl- | | | 1 | | | 1 | 1 | 1 | | 4 |
| Butanal, 3-methyl- | 1 | | | | 1 | 1 | | 1 | | 4 |
| 4-Methyl-2-hexene,c&t | | | 1 | | 1 | 1 | | | | 3 |
| Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-trimethyl- | 1 | | 1 | | | 1 | | | | 3 |
| Pentane, 3,3-dimethyl- | | 1 | | | | 1 | | 1 | | 3 |
| Phthalic acid, hept-4-yl isobutyl ester | | | 1 | 1 | | | 1 | | | 3 |
| .beta.-Myrcene | | | 1 | | 1 | 1 | | | | 3 |
| Methyl Isobutyl Ketone | | | | | | | 1 | 1 | 1 | 3 |
| Tridecane, 3-methyl- | | | | | | | 1 | 1 | 1 | 3 |
| m-xylene | | | | 1 | | | 1 | | 1 | 3 |
| Longifolene | | | | 1 | | | | 1 | 1 | 3 |
| 2-Ethylhexyl acrylate | | | 1 | 1 | | | | | | 2 |
| Cyclohexene, 4-methylene-1-(1-methylethyl)- | | 1 | | | 1 | | | | | 2 |
| Undecane | | | | 1 | | | | | 1 | 2 |
| Heptadecane, 2-methyl- | | | | 1 | | | | | 1 | 2 |
| Styrene | | | 1 | | | | 1 | | | 2 |
| Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]- | 1 | | 1 | | | | | | | 2 |
| Cyclopentane, ethyl- | 1 | | | 1 | | | | | | 2 |
| Naphthalene, 2-ethyldecahydro- | | 1 | | 1 | | | | | | 2 |
| 2-Ethylacrolein | | | | | | 1 | 1 | | | 2 |
| 2-Heptanone | | | | | | 1 | | | 1 | 2 |
| Hexanal, 4-methyl- | | | | | 1 | 1 | | | | 2 |
| .alpha.-Phellandrene | | | | | | | | 1 | 1 | 2 |
| 2-Butenal, 2-methyl- | | | | | 1 | | | | 1 | 2 |
| 5-Hepten-2-one, 6-methyl- | | | 1 | | | | 1 | | | 2 |
| Cyclopentane, 1,3-dimethyl-, cis- | 1 | | 1 | | | | | | | 2 |
| 2-Hexene, 4-methyl-, (E)- | | | | | | | 1 | 1 | | 2 |
| 2,2-Dimethoxybutane | 1 | | | | | | 1 | | | 2 |
| (1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene | | | | 1 | 1 | | | | | 2 |

Table 8.11 Pivot table of VOC emissions from USP duplicates. VOCs identified in the table were absorbed on Tenax TA sorbent. The compounds represented in the table are classified with identification levels 1 and 2.

| Untreated spruce panel | Sample | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Compound name | Chamber 1, 3L | Chamber 1, 5L | Chamber 2, 3L | Chamber 2, 5L | Chamber 3, 3L | Chamber 3, 5L | Chamber 4, 3L | Chamber 4, 5L | Chamber 5, 5L | Grand Total |
| Nonanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| D-Limonene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Decanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 3-carene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Pentanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Heptanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| m-xylene | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Toluene-D8 | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| o-Cymene | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| .beta.-Phellandrene | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Hexane, 2-methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Cyclohexane, methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Octanal | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 8 |
| Ethylbenzene | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| .alpha.-Pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Heptadecane | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 8 |
| Heptane | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 8 |
| Hexane, 3-methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Octane, 4-methyl- | 1 | | 1 | | 1 | 1 | 1 | 1 | 1 | 7 |
| 1,6-Dioxacyclododecane-7,12-dione | 1 | | 1 | | 1 | 1 | 1 | 1 | 1 | 7 |
| Ethyl Acetate | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | | 7 |
| Undecane, 3-methyl- | 1 | 1 | | | 1 | 1 | 1 | 1 | 1 | 7 |
| Naphthalene | 1 | | 1 | | 1 | 1 | 1 | 1 | 1 | 7 |
| Cyclotetrasiloxane, octamethyl- | | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 7 |
| Styrene | 1 | | | 1 | 1 | 1 | 1 | 1 | 1 | 7 |
| Benzene, 1,3-bis(1-methylethenyl)- | 1 | | 1 | | 1 | 1 | 1 | 1 | 1 | 7 |
| Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-trimethyl- | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | | 7 |
| Methyl Isobutyl Ketone | 1 | | | 1 | 1 | 1 | 1 | 1 | 1 | 7 |
| Cyclotrisiloxane, hexamethyl- | | | | 1 | 1 | 1 | 1 | 1 | 1 | 6 |
| Undecane, 3,4-dimethyl- | 1 | | 1 | | | 1 | 1 | 1 | 1 | 6 |
| Methyl methacrylate | 1 | | 1 | | | 1 | 1 | 1 | 1 | 6 |
| Naphthalene, 2-ethyldecahydro- | 1 | 1 | 1 | | 1 | 1 | 1 | | | 6 |
| Silane, methyldiethoxyisopropoxy- | 1 | | | 1 | 1 | 1 | | | 1 | 5 |
| 2-Pentanone | 1 | | | 1 | 1 | 1 | | 1 | | 5 |
| Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]- | | | 1 | 1 | | 1 | | 1 | 1 | 5 |
| Nonane, 5-butyl- | 1 | | | | 1 | | 1 | 1 | 1 | 5 |
| Phthalic acid, hept-4-yl isobutyl ester | | 1 | 1 | | 1 | | 1 | | 1 | 5 |
| Decane | | 1 | | 1 | 1 | | | 1 | 1 | 5 |
| 2,2-Dimethoxybutane | 1 | 1 | 1 | | 1 | | | 1 | | 5 |
| Beta-Myrcene | | 1 | 1 | | 1 | | | 1 | 1 | 5 |
| 1,2,4-trimethylbenzene | 1 | | 1 | | | | 1 | 1 | 1 | 5 |
| 1-Methyl-1H-1,2,4-triazole | 1 | | 1 | 1 | | 1 | | 1 | | 5 |
| Nonane | 1 | | | | | 1 | 1 | 1 | 1 | 5 |
| Dodecane, 5-methyl- | 1 | | | | 1 | 1 | | 1 | 1 | 5 |
| Decane, 5-methyl- | | | 1 | | 1 | 1 | | 1 | 1 | 5 |
| 2-Butanone | | | 1 | 1 | 1 | | 1 | | | 4 |
| Tetradecanal | 1 | | 1 | | 1 | | | | 1 | 4 |
| Pentadecane, 7-methyl- | 1 | | | | | 1 | 1 | 1 | | 4 |
| 1,4-Benzenedicarboxaldehyde, 2-methyl- | 1 | | 1 | | 1 | | 1 | | | 4 |
| Undecane, 2,4-dimethyl- | | | | | | 1 | 1 | 1 | 1 | 4 |
| Cyclohexene, 4-ethenyl- | 1 | | | | | 1 | | 1 | 1 | 4 |
| 2-Heptanone | | | | | 1 | 1 | | 1 | 1 | 4 |
| .beta.-Myrcene | 1 | | | 1 | | 1 | 1 | | | 4 |
| Pentane, 3-ethyl- | 1 | 1 | | 1 | | 1 | | | | 4 |
| Dodecane, 6-methyl- | 1 | | 1 | | | | 1 | 1 | | 4 |
| Tetradecane, 4-methyl- | | | | | | 1 | 1 | 1 | 1 | 4 |
| Eicosane | | 1 | | 1 | | | 1 | | 1 | 4 |
| Undecane, 2,6-dimethyl- | 1 | 1 | 1 | 1 | | | | | | 4 |
| Heptadecane, 3-methyl- | 1 | | | 1 | | | 1 | | 1 | 4 |
| Pentadecane, 3-methyl- | | | 1 | | | | | 1 | 1 | 3 |
| Tridecane, 3-methyl- | | | 1 | | | 1 | | 1 | | 3 |
| Tetradecane, 3-methyl- | 1 | | | 1 | | | 1 | | | 3 |
| Cyclobutane, 1,1,2,3,3-pentamethyl- | | | | | 1 | 1 | 1 | | | 3 |
| Nonane, 5-(2-methylpropyl)- | | | 1 | | 1 | 1 | | | | 3 |
| .alpha.-Methylstyrene | 1 | | | | | | | 1 | 1 | 3 |
| Cyclopentane, 1,3-dimethyl-, cis- | 1 | | | 1 | | | 1 | | | 3 |
| Formic acid, octyl ester | | | | 1 | | | | 1 | 1 | 3 |
| 1,3,5-trimethylbenzene | | | | 1 | 1 | 1 | | | | 3 |
| Furan, 2,3-dihydro-4-methyl- | | | | | 1 | 1 | 1 | | | 3 |
| Dodecane | 1 | | | | 1 | | 1 | | | 3 |
| Cyclododecanol | | 1 | | | | 1 | 1 | | | 3 |
| Nonane, 5-methyl-5-propyl- | 1 | | 1 | | | | | | 1 | 3 |
| Undecane, 3,7-dimethyl- | | | 1 | | 1 | | | | 1 | 3 |

Table 8.12 Pivot table of VOC emissions form SSP duplicates. VOCs identified in the table were absorbed on Tenax TA sorbent. The compounds represented in the table are classified with identification levels 1 and 2.

| Stained spruce panel (Tenax) | Sample | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Compound name | Chamber 4, 3L | Chamber 1, 3L | Chamber 2, 3L | Chamber 2, 5L | Chamber 3, 3L | Chamber 3, 5L | Chamber 4, 5L | Chamber 5, 5L | Chamber1, 5L | Total |
| Pentanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Toluene-D8 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 1,6-Dioxacyclododecane-7,12-dione | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Nonanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 2-Pentanone | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Decane | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 3-carene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Furfural | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Methyl Isobutyl Ketone | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Octanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Cyclotetrasiloxane, octamethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Cyclotrisiloxane, hexamethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| D-limonene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| m-xylene | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Styrene | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Pentane, 2,3-dimethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 8 |
| .alpha.-Pinene | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | 8 |
| Cyclohexane | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 8 |
| Ethylbenzene | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 8 |
| o-Cymene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Heptanal | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 8 |
| Pentane, 3-ethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 8 |
| Hexane, 2-methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 8 |
| Decanal | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 8 |
| Hexane, 3-methyl- | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Ethyl Acetate | 1 | | | 1 | 1 | 1 | 1 | | 1 | 6 |
| 2-Heptanone | 1 | | 1 | 1 | 1 | 1 | | | 1 | 6 |
| 2,2-Dimethoxybutane | 1 | | 1 | 1 | 1 | | | 1 | 1 | 6 |
| Heptane | | 1 | | 1 | 1 | 1 | 1 | | 1 | 6 |
| 1,2,4-trimethylbenzene | 1 | | 1 | | 1 | | 1 | 1 | 1 | 6 |
| Cyclohexane, methyl- | 1 | 1 | | 1 | 1 | 1 | | | 1 | 6 |
| Octane | 1 | | 1 | 1 | 1 | 1 | | | 1 | 6 |
| 2-Butanone | 1 | 1 | 1 | | | | 1 | | 1 | 5 |
| Isopropylcyclobutane | | | 1 | 1 | 1 | | 1 | | 1 | 5 |
| .alpha.-Phellandrene | 1 | | 1 | 1 | 1 | 1 | | | | 5 |
| Undecane | 1 | | | 1 | | | 1 | 1 | 1 | 5 |
| Nonadecane | | | 1 | 1 | 1 | | | 1 | | 4 |
| Naphthalene | 1 | | | 1 | | | 1 | | 1 | 4 |
| Hexadecanoic acid, methyl ester | | | | 1 | | | 1 | 1 | 1 | 4 |
| 3-Heptanone | 1 | 1 | | | | | 1 | | 1 | 4 |
| Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]- | | 1 | | | 1 | 1 | | 1 | | 4 |
| 1-Methyl-1H-1,2,4-triazole | 1 | 1 | | | | 1 | | | 1 | 4 |
| 2-Hexanone | 1 | | | 1 | | | | 1 | 1 | 4 |
| Tetrasiloxane, decamethyl- | | | 1 | 1 | 1 | 1 | | | | 4 |
| Hexadecane, 2-methyl- | | | 1 | | 1 | | 1 | | 1 | 4 |
| Phthalic acid, hept-4-yl isobutyl ester | | | | 1 | | | 1 | 1 | | 3 |
| 1,3,5-trimethylbenzene | | 1 | | 1 | | 1 | | | | 3 |
| 4-Undecene, 4-methyl- | | 1 | 1 | | | | | | 1 | 3 |
| Cyclohexene, 4-methylene-1-(1-methylethyl)- | | | 1 | | 1 | 1 | | | | 3 |
| Heptadecane | | | 1 | | | 1 | | 1 | | 3 |
| Nonane | | | | 1 | | | | 1 | | 2 |
| 3-Methylcyclopentyl acetate | 1 | | | | | | | 1 | | 2 |
| 2-Hexene, 5,5-dimethyl-, (Z)- | 1 | | | | | | | 1 | | 2 |
| 1-Octen-3-one | | | | 1 | | 1 | | | | 2 |
| Butane, 1,1'-[oxybis(2,1-ethanediyloxy)]bis- | | | | | | 1 | | | 1 | 2 |
| Eicosane | | | | 1 | | | | 1 | | 2 |
| Octadecane | | | | | | | | 1 | 1 | 2 |
| Furan, 2,3-dihydro-4-methyl- | 1 | | | | | | | | 1 | 2 |
| 2-Pentene, 2,4-dimethyl- | | | 1 | | | | 1 | | | 2 |
| 2-Pentene, 3,4-dimethyl-, (Z)- | | | | | 1 | | | | 1 | 2 |
| Benzene, (1-butylheptyl)- | | | | 1 | | | | 1 | | 2 |
| Hexadecane | | | | 1 | | | | 1 | | 2 |
| Butane, 2-cyclopropyl- | | | | | | 1 | | | 1 | 2 |
| 5-Hepten-2-one, 6-methyl- | | | | | | 1 | | 1 | | 2 |
| Nonane, 2,2,4,4,6,8,8-heptamethyl- | 1 | | | | | | | 1 | | 2 |
| Benzaldehyde, 2,4-dichloro- | | | | 1 | | | | 1 | | 2 |
| Valeric anhydride | | | | 1 | | | | 1 | | 2 |
| Hexanal, 4-methyl- | | | | 1 | | 1 | | | | 2 |
| Cyclobutane, 1,1,2,3,3-pentamethyl- | | | | | 1 | | 1 | | | 2 |
| Hexane, 2,3-dimethyl- | 1 | | | | | | | | 1 | 2 |
| 4,4-Dimethyl octane | | | | | 1 | | | | 1 | 2 |
| 2-Butenal, 2-methyl- | | | | | 1 | | | 1 | | 2 |
| Longifolene | | 1 | | 1 | | | | | | 2 |

Table 8.13 Pivot table VOC emissions from SSP duplicates. VOCs identified in the table were absorbed on Universal sorbent. The compounds represented in the table are classified with identification levels 1 and 2.

| Stained spruce panel (Universal) | Sample | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Compound name | Chamber 1, 3L | Chamber 1, 5L | Chamber 2, 3L | Chamber 2, 5L | Chamber 3, 3L | Chamber 3, 5L | Chamber 4, 3L | Chamber 4, 5L | Chamber 5, 5L | Grand Total |
| Disiloxane, hexamethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Nonanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| .alpha.-Pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Pentanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Heptanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexane, 3-methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Cyclotetrasiloxane, octamethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Octanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Cyclotrisiloxane, hexamethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Decanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| D-limonene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 1,6-Dioxacyclododecane-7,12-dione | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 8 |
| Styrene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| 3-carene | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 8 |
| Hexane, 2-methyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| o-Cymene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Acetone | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Pentane, 2,3-dimethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| m-xylene | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 8 |
| Pentane, 3,3-dimethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Formic acid, ethenyl ester | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 8 |
| Cyclohexane | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 7 |
| 3-Hexanone | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | | 7 |
| Pentane, 2,4-dimethyl- | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | | 7 |
| n-Hexane | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | | 7 |
| Pentane, 3-ethyl- | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | | 7 |
| Pentane, 2,2-dimethyl- | 1 | 1 | | 1 | 1 | 1 | | 2 | | 7 |
| Heptadecane | 1 | 1 | 1 | 1 | | 1 | | 1 | 1 | 7 |
| Ethylbenzene | 1 | 1 | | 1 | | | 1 | 1 | 1 | 6 |
| Tetradecanal | 1 | | 1 | 1 | | | 1 | 1 | | 5 |
| Cyclopentane, 1,1-dimethyl- | 1 | 1 | | | 1 | 1 | 1 | | | 5 |
| Cyclohexane, methyl- | 1 | 1 | 1 | | | 1 | 1 | | | 5 |
| Ethyl Acetate | 1 | | | 1 | | 1 | 1 | 1 | | 5 |
| Phthalic acid, hept-4-yl isobutyl ester | 1 | | 1 | | | 1 | | 1 | 1 | 5 |
| Furan, 2,5-dihydro- | | 1 | 1 | 1 | 1 | | 1 | | | 5 |
| 2-Heptanone | | | | 1 | 1 | | 1 | 1 | 1 | 5 |
| Methyl Isobutyl Ketone | 1 | 1 | | 1 | | | 1 | 1 | | 5 |
| Hexadecanoic acid, methyl ester | | 1 | 1 | | | | 1 | | 1 | 4 |
| Tridecane | 1 | 1 | | 1 | | 1 | | | | 4 |
| Naphthalene | | 1 | | | | | 1 | 1 | 1 | 4 |
| 1,3,5-trimethylbenzene | | 1 | | | 1 | 1 | | 1 | | 4 |
| Furfural | | 1 | | 1 | | | | 1 | 1 | 4 |
| Naphthalene, 2-ethyldecahydro- | 1 | 1 | | 1 | 1 | | | | | 4 |
| p-(1-Propenyl)-toluene | | | | 1 | 1 | 1 | | | | 3 |
| Undecane | | | | 1 | | | | 1 | 1 | 3 |
| Cyclohexene, 4-methylene-1-(1-methylethyl)- | | 1 | 1 | 1 | | | | | | 3 |
| Aciphyllene | | | | 1 | | | 1 | 1 | | 3 |
| Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]- | | 1 | | | 1 | | | | 1 | 3 |
| Hexane, 2,3,4-trimethyl- | | | 1 | | | | | 1 | 1 | 3 |
| 2-Propenoic acid, 6-methylheptyl ester | | | 1 | | 1 | 1 | | | | 3 |
| Isopropylcyclobutane | 1 | | | 1 | | | 1 | | | 3 |
| 1,2,4-trimethylbenzene | 1 | | | 1 | | | | | 1 | 3 |
| Longifolene | 1 | | | 1 | | 1 | | | | 3 |

Table 8.14 Compounds identified in Tenax TA and Universal sorbent. tubes. Number two indicates that the compounds were identified in both sorbents. The compounds represented in the table are classified with identification levels 1 and 2.

| Compound name | Chamber 4, 3L | Chamber 1, 3L | Chamber1, 5L | Chamber 2, 3L | Chamber 2, 5L | Chamber 3, 3L | Chamber 3, 5L | Chamber 4, 5L | Chamber 5, 5L | Total |
|---|---|---|---|---|---|---|---|---|---|---|
| Octanal | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Hexanal | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Cyclotrisiloxane, hexamethyl- | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Beta-pinene | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Nonanal | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Camphene | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Pentanal | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Cyclotetrasiloxane, octamethyl- | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| D-limonene | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 18 |
| Hexane, 3-methyl- | 2 | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 17 |
| 1,6-Dioxacyclododecane-7,12-dione | 2 | 2 | 2 | 2 | 1 | 2 | 2 | 2 | 2 | 17 |
| .alpha.-Pinene | 2 | 2 | 2 | 2 | 1 | 2 | 2 | 2 | 2 | 17 |
| Decanal | 2 | 2 | 2 | 2 | 2 | 2 | 1 | 2 | 2 | 17 |
| Heptanal | 2 | 2 | 2 | 2 | 2 | 1 | 2 | 2 | 2 | 17 |
| 3-carene | 2 | 2 | 2 | 2 | 2 | 1 | 2 | 2 | 2 | 17 |
| Styrene | 2 | 2 | 2 | 1 | 2 | 2 | 2 | 2 | 1 | 16 |
| Pentane, 2,3-dimethyl- | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |  | 16 |
| o-Cymene | 2 | 2 | 1 | 2 | 2 | 2 | 2 | 2 | 1 | 16 |
| Hexane, 2-methyl- | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |  | 16 |
| m-xylene | 1 | 2 | 2 | 2 | 2 | 2 | 1 | 2 | 2 | 16 |
| Cyclohexane | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |  | 15 |
| Pentane, 3-ethyl- | 2 | 1 | 2 | 2 | 2 | 2 | 2 | 2 |  | 15 |
| Ethylbenzene | 2 | 2 | 1 | 2 | 1 | 1 | 1 | 2 | 2 | 14 |
| Methyl Isobutyl Ketone | 2 | 2 | 1 | 2 | 1 | 1 | 2 | 2 | 1 | 14 |
| Furfural | 1 | 2 | 1 | 2 | 1 | 1 | 1 | 2 | 2 | 13 |
| Cyclohexane, methyl- | 2 | 2 | 2 |  | 1 | 2 | 2 |  |  | 11 |
| 2-Heptanone | 1 |  | 1 | 2 | 2 | 1 | 2 | 1 | 1 | 11 |
| 2-Pentanone | 1 | 1 | 1 | 2 | 1 | 1 | 1 | 2 | 1 | 11 |
| Ethyl Acetate | 2 |  | 1 | 1 | 1 | 2 | 2 | 2 |  | 11 |
| Heptadecane | 1 | 1 | 1 | 2 |  | 1 | 1 | 1 | 2 | 10 |
| Disiloxane, hexamethyl- | 1 | 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 10 |
| Decane | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 10 |
| 1,2,4-trimethylbenzene | 2 |  | 1 | 2 |  | 1 |  | 1 | 2 | 9 |
| Isopropylcyclobutane | 1 |  | 1 | 2 | 1 | 1 | 1 | 1 |  | 8 |
| Phthalic acid, hept-4-yl isobutyl ester | 1 |  | 1 |  | 1 | 1 |  | 2 | 2 | 8 |
| Naphthalene | 1 | 1 | 1 |  | 1 |  | 1 | 2 | 1 | 8 |
| 2-Butanone | 1 | 1 | 1 | 2 |  |  | 1 | 2 |  | 8 |
| 3-Hexanone | 2 | 1 | 1 | 1 |  | 1 | 1 | 1 |  | 8 |
| Undecane | 1 |  | 1 | 1 | 1 |  |  | 2 | 2 | 8 |
| Hexadecanoic acid, methyl ester |  | 1 | 2 |  | 1 |  | 1 | 1 | 2 | 8 |
| .alpha.-Phellandrene | 1 |  |  | 1 | 2 | 2 | 1 |  |  | 7 |
| 1,3,5-trimethylbenzene |  | 2 |  |  | 2 | 1 | 1 | 1 |  | 7 |
| Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,7.beta.,8a.alpha.)]- |  | 2 |  |  | 1 | 1 | 1 |  | 2 | 7 |
| Tetrasiloxane, decamethyl- |  |  |  | 2 | 2 | 1 | 1 |  |  | 6 |
| Tetradecanal | 1 |  | 1 | 1 |  |  | 1 | 2 |  | 6 |
| Hexadecane, 2-methyl- |  |  | 1 | 2 |  | 1 |  | 2 |  | 6 |
| Cyclohexene, 4-methylene-1-(1-methylethyl)- |  | 1 | 1 | 2 |  | 1 | 1 |  |  | 6 |
| 2-Propenoic acid, 6-methylheptyl ester |  |  | 1 | 1 | 2 | 1 |  |  |  | 5 |
| 3-Heptanone | 1 | 1 | 1 |  |  |  |  | 2 |  | 5 |
| Longifolene | 1 | 1 |  | 1 | 1 | 1 |  |  |  | 5 |
| Tridecane | 1 | 1 |  | 1 |  | 1 |  | 1 |  | 5 |
| Butane, 1,1'-[oxybis(2,1-ethanediyloxy)]bis- |  |  | 2 |  |  | 1 | 1 |  |  | 4 |
| 2-Pentene, 2,4-dimethyl- |  |  |  | 2 |  |  |  | 2 |  | 4 |
| Nonane, 2,2,4,4,6,8,8-heptamethyl- | 1 |  |  |  |  |  |  | 1 | 2 | 4 |
| Furan, 2,3-dihydro-4-methyl- | 1 |  | 1 |  |  |  | 1 | 1 |  | 4 |
| 2-Butenal, 2-methyl- |  |  |  |  |  | 2 |  |  | 2 | 4 |
| Hexane, 2,3,4-trimethyl- |  |  | 1 |  |  |  |  | 1 | 2 | 4 |
| Cyclobutane, 1,1,2,3,3-pentamethyl- |  | 1 | 1 |  |  | 1 |  | 1 |  | 4 |
| 5-Hepten-2-one, 6-methyl- | 1 |  |  |  |  |  | 1 |  | 2 | 4 |
| 2-Pentene, 3,4-dimethyl-, (Z)- |  |  | 1 |  |  | 1 |  |  | 1 | 3 |
| Benzaldehyde, 2,4-dichloro- |  |  |  |  | 1 |  |  |  | 2 | 3 |
| Eicosane |  |  |  |  | 1 |  |  |  | 2 | 3 |
| Cyclopentane, ethyl- | 1 |  | 1 |  |  | 1 |  |  |  | 3 |
| 2-Hexene, 5,5-dimethyl-, (Z)- | 1 |  |  |  |  |  | 1 |  | 1 | 3 |
| Butane, 2,2,3,3-tetramethyl- | 1 |  |  |  | 1 |  | 1 |  |  | 3 |
| Eucalyptol |  | 1 | 1 |  |  | 1 |  |  |  | 3 |
| Hexane, 2,3-dimethyl- | 1 | 1 | 1 |  |  |  |  |  |  | 3 |
| 1-Propanone, 1-cyclopropyl- |  |  | 1 |  |  | 1 |  |  |  | 2 |
| 2-Propenoic acid, octyl ester |  |  |  | 1 | 1 |  |  |  |  | 2 |
| Pentadecane, 2,6,10-trimethyl- |  |  |  | 1 |  |  |  |  | 1 | 2 |
| 1,3,5-Trifluorobenzene |  |  |  |  | 1 |  |  | 1 |  | 2 |
| Benzenemethanol, .alpha.-methyl-.alpha.-(1-methyl-2-propenyl)- |  |  |  | 1 | 1 |  |  |  |  | 2 |
| 4-Methyl-2-hexene,c&t |  | 1 |  |  |  |  | 1 |  |  | 2 |
| Cyclobutanecarbohydrazide |  |  |  |  | 2 |  |  |  |  | 2 |
| 2-Ethylacrolein |  |  |  |  | 1 |  | 1 |  |  | 2 |

Table 8.15 List of compounds identified only by Universal sorbent tubes. The compounds represented in the figure are of the confidence identification level 2.

| Compound name | Chamber 4, 3L | Chamber 1, 3L | Chamber1, 5L | Chamber 2, 3L | Chamber 2, 5L | Chamber 3, 3L | Chamber 3, 5L | Chamber 4, 5L | Chamber 5, 5L | Total |
|---|---|---|---|---|---|---|---|---|---|---|
| Acetone | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Pentane, 3,3-dimethyl- | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Formic acid, ethenyl ester | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 8 |
| Pentane, 2,4-dimethyl- | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | | 7 |
| n-Hexane | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | | 7 |
| Pentane, 2,2-dimethyl- | 1 | 1 | | 1 | 1 | 1 | | 2 | | 7 |
| Cyclopentane, 1,1-dimethyl- | 1 | 1 | | | 1 | 1 | 1 | | | 5 |
| Furan, 2,5-dihydro- | | 1 | 1 | 1 | 1 | | 1 | | | 5 |
| Naphthalene, 2-ethyldecahydro- | 1 | 1 | | 1 | 1 | | | | | 4 |
| p-(1-Propenyl)-toluene | | | | 1 | 1 | 1 | | | | 3 |
| Aciphyllene | | | | 1 | | | 1 | 1 | | 3 |
| Bicyclo[2.2.1]heptane, 7,7-dimethyl-2-methylene- | | | | 1 | 1 | 1 | | | | 3 |
| 2-Propenoic acid, ethenyl ester | | 1 | | 1 | | | | | | 2 |
| Benzene, 1-methyl-3-(1-methylethenyl)- | 1 | | | | | | | 1 | | 2 |
| Tetradecane, 1-chloro- | | | | | | | 1 | 1 | | 2 |
| Undecane, 6,6-dimethyl- | | | | | | | 1 | 1 | | 2 |
| Cyclopentane, 1,2-dimethyl-, cis- | | | 1 | | 1 | | | | | 2 |
| Cyclopentane, 1,3-dimethyl-, cis- | | | 1 | | 1 | | | | | 2 |
| Oxirane, 2,3-dimethyl-, cis- | | | | | | | | 1 | 1 | 2 |
| Benzene, 4-ethenyl-1,2-dimethyl- | | 1 | 1 | | | | | | | 2 |
| Cyclohexane, (4-methylpentyl)- | | | | | | 1 | | | | 1 |
| Cyclopropane, propyl- | | | | | | | | | 1 | 1 |
| 2,3-Dimethyl-1-hexene | | | | | | | 1 | | | 1 |
| 5-Ethyl-5-methylnonadecane | | | | | | | | 1 | | 1 |
| 1,2,4,5-tetramethylbenzene | | | | | | | | | 1 | 1 |
| Acenaphthene | | | | | | | | 1 | | 1 |
| Cyclopentane, 1-butyl-2-propyl- | | | | | | | | 1 | | 1 |
| 3-Heptene, 2,2,4,6,6-pentamethyl- | | | | | | | | | 1 | 1 |
| 1,4-Pentadien-3-one | | | | | 1 | | | | | 1 |
| Undecane, 3-methyl- | | | | | 1 | | | | | 1 |
| N-Methyl-L-prolinol | 1 | | | | | | | | | 1 |
| Benzene, 1,3-dimethyl- | | | | | | | 1 | | | 1 |
| 3-Amino-s-triazole | | | | | 1 | | | | | 1 |
| Heptadecanal | | | | 1 | | | | | | 1 |
| .alpha.-Aminoisobutanoic acid | | | 1 | | | | | | | 1 |
| 2-Oxa-1,3-disilacyclohexane, 1,1,3,3-tetramethyl- | | | | 1 | | | | | | 1 |
| Phthalic acid, 2-chloropropyl ethyl ester | | | | 1 | | | | | | 1 |
| Heptane, 2,4-dimethyl- | | 1 | | | | | | | | 1 |
| 3-Methylpentyl methacrylate | | | | | 1 | | | | | 1 |
| Dodecane, 4,6-dimethyl- | | 1 | | | | | | | | 1 |
| Hexadecane, 7-methyl- | | | 1 | | | | | | | 1 |
| 1H-Pyrimido[1,2-a]quinoline-2-acetic acid, 1-oxo-, ethyl ester | | 1 | | | | | | | | 1 |
| 1,1-Dodecanediol, diacetate | | | 1 | | | | | | | 1 |
| Cyclohexane, hexyl- | | 1 | | | | | | | | 1 |
| 2-Pentene, 2,4,4-trimethyl- | | | | | | | 1 | | | 1 |
| Hexanal, 2,2-dimethyl- | | | | | 1 | | | | | 1 |
| Cyclopentane, 1,1,3-trimethyl- | | | | | 1 | | | | | 1 |
| Hexane, 2,2-dimethyl- | | | | | 1 | | | | | 1 |
| Oxirane, 2-(1,1-dimethylethyl)-3-ethyl-, cis- | | | | | | | | 1 | | 1 |
| Butanal | | 1 | | | | | | | | 1 |
| Cyclopentane, 1,2-dimethyl-, trans- | | | | 1 | | | | | | 1 |
| 3-Formyl-2-buten-1-yl acetate | | | | | | | 1 | | | 1 |
| 1-Hexene, 5,5-dimethyl- | 1 | | | | | | | | | 1 |
| Cyclopropane, pentyl- | | | | 1 | | | | | | 1 |
| 2-Pentene, 4,4-dimethyl-, (Z)- | | | 1 | | | | | | | 1 |
| Pentane, 3-methyl- | | | | | | | 1 | | | 1 |
| Carbon Tetrachloride | | | | | | 1 | | | | 1 |
| Phthalic acid, butyl 2-pentyl ester | | | | | | | 1 | | | 1 |
| Mesitylene | | | | | 1 | | | | | 1 |
| Methacrolein | | | | | | | | | 1 | 1 |
| 2-Propanone, 1-methoxy- | | 1 | | | | | | | | 1 |
| 5-Dodecene, (E)- | | | | | | | | 1 | | 1 |
| Undecane, 2,6-dimethyl- | | | | 1 | | | | | | 1 |
| N-(2,6-Dimethylphenyl)-N-[(2E)-3-methyl-1,3-thiazin | 1 | | | | | | | | | 1 |
| Cyclododecanol | | | | | | | | | 1 | 1 |
| Cyclopropane, pentamethyl- | | 1 | | | | | | | | 1 |

Table 8.16 List of compounds identified only by Tenax Ta sorbent emitted from SSP. The compounds represented in the figure are of the confidence identification level 2.

| Compound name | Chamber 4, 3L | Chamber 1, 3L | Chamber1, 5L | Chamber 2, 3L | Chamber 2, 5L | Chamber 3, 3L | Chamber 3, 5L | Chamber 4, 5L | Chamber 5, 5L | Total |
|---|---|---|---|---|---|---|---|---|---|---|
| Toluene-D8 (IS) | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 2,2-Dimethoxybutane | 1 | | 1 | 1 | 1 | 1 | | | 1 | 6 |
| Heptane | | 1 | 1 | | 1 | 1 | 1 | 1 | | 6 |
| Octane | 1 | | 1 | 1 | 1 | 1 | 1 | | | 6 |
| Nonadecane | | | | 1 | 1 | 1 | | | 1 | 4 |
| 1-Methyl-1H-1,2,4-triazole | 1 | 1 | 1 | | | | 1 | | | 4 |
| 2-Hexanone | 1 | | 1 | | 1 | | | | 1 | 4 |
| 4-Undecene, 4-methyl- | | 1 | 1 | 1 | | | | | | 3 |
| Nonane | | | | | 1 | | | | 1 | 2 |
| 3-Methylcyclopentyl acetate | 1 | | | | | | | | 1 | 2 |
| 1-Octen-3-one | | | | | 1 | | 1 | | | 2 |
| Octadecane | | | 1 | | | | | | 1 | 2 |
| Benzene, (1-butylheptyl)- | | | | | 1 | | | | 1 | 2 |
| Hexadecane | | | | | 1 | | | | 1 | 2 |
| Butane, 2-cyclopropyl- | | | 1 | | | | 1 | | | 2 |
| Valeric anhydride | | | | | 1 | | | | 1 | 2 |
| Hexanal, 4-methyl- | | | | | 1 | | 1 | | | 2 |
| 4,4-Dimethyl octane | | | 1 | | | 1 | | | | 2 |
| Pentadecane, 2,6,10,14-tetramethyl- | | | | | 1 | | | | | 1 |
| 5-Tetradecene, (E)- | 1 | | | | | | | | | 1 |
| 3,3-Dimethyl-1,2-epoxybutane | | | | | | | | | 1 | 1 |
| Benzene, ethylpentamethyl- | | 1 | | | | | | | | 1 |
| 3-Pentanone | | | | | | | | | 1 | 1 |
| Propanamide, N-acetyl- | | | | | 1 | | | | | 1 |
| Hexane, 3-ethyl- | | | | | | | | 1 | | 1 |
| Cyclobutanecarboxylic acid, 4-methylpentyl ester | | | | | 1 | | | | | 1 |
| 2-Fluoro-6-trifluoromethylbenzoic acid, 4-nitrophenyl ester | | | | | | | | 1 | | 1 |
| Cyclobutanone, 2,2,3-trimethyl- | | | | 1 | | | | | | 1 |
| 1,3-Cyclohexadiene, 1,5,5,6-tetramethyl- | | | | | | | | | 1 | 1 |
| 1,6-Heptadiene, 2-methyl- | 1 | | | | | | | | | 1 |
| 2-Pentenal, (E)- | | | | | | | | 1 | | 1 |
| 1,7-Dimethyl-4-(1-methylethyl)cyclodecane | | | | | | | | 1 | | 1 |
| Thiophene, 3-methyl- | | | | 1 | | | | | | 1 |
| Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate | 1 | | | | | | | | | 1 |
| Acetyl valeryl | 1 | | | | | | | | | 1 |
| 3,4-Dimethyldihydrofuran-2,5-dione | | | | 1 | | | | | | 1 |
| Isopropyl myristate | | | | | 1 | | | | | 1 |
| Cyclopentane, 1,3-dimethyl- | | 1 | | | | | | | | 1 |
| 2-Ethylbutyric acid, tetrahydrofurfuryl ester | | | | | | | | | 1 | 1 |
| Cyclopentane, 1-methyl-2-propyl- | | | | | 1 | | | | | 1 |
| Benzene, (1-propyloctyl)- | | | | 1 | | | | | | 1 |
| 1-Butene, 2,3,3-trimethyl- | | | | | | | | 1 | | 1 |
| 1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, [1aR-(1a.alpha.,7.alpha. | | | 1 | | | | | | | 1 |
| 2-Oxepanone, 7-methyl- | | | | | | 1 | | | | 1 |
| 1-Hexene, 4-methyl- | | | | | | | 1 | | | 1 |
| Phthalic acid, cyclobutyl ethyl ester | 1 | | | | | | | | | 1 |
| 4-Ethyltoluene | | | | 1 | | | | | | 1 |
| 4-Formyl-3,5-dimethyl-1H-pyrrole-2-carbonitrile | | | | 1 | | | | | | 1 |
| Tricyclo[2.2.1.0(2,6)]heptane, 1,3,3-trimethyl- | | | | | 1 | | | | | 1 |
| (Z)-4-Methyl-2-hexene | | | | | | 1 | | | | 1 |
| Dodecanoic acid, 1-methylethyl ester | | | | | | | | | 1 | 1 |
| Azetidine, 3-methyl-3-phenyl- | | | | 1 | | | | | | 1 |
| Isopropylbenzene | | | | | 1 | | | | | 1 |
| 1-Oxa-3,4-diazacyclopentadiene | | | 1 | | | | | | | 1 |
| Methyl n-hexyl ketone-1-phenyl-1,2-ethanediol ketal 2 | | | | | | 1 | | | | 1 |
| Ethylene glycol monoisobutyl ether | | | | | 1 | | | | | 1 |
| 3,3-Dimethoxy-2-butanone | | | | | | 1 | | | | 1 |
| n-Butyl ether | | | | | | | 1 | | | 1 |
| 3-Acetoxypentadecane | | | | | | | 1 | | | 1 |
| 1,3,5-Triazine | | | | | 1 | | | | | 1 |
| Furan, 2-ethyl- | | | | | | | | | 1 | 1 |
| Benzofuran | | | | | | | | | 1 | 1 |
| 1-Undecene, 10-methyl- | | | | | 1 | | | | | 1 |
| Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, (1R)- | | | | | 1 | | | | | 1 |
| Germacrene D | | | | | | | | 1 | | 1 |
| 2-n-Butyl furan | | | | | | | | | 1 | 1 |
| Heneicosane | | | | | 1 | | | | | 1 |
| 5,5-Dibutylnonane | | | | 1 | | | | | | 1 |
| Heptadecane, 2-methyl- | | | | | 1 | | | | | 1 |
| Phthalic acid, butyl cyclobutyl ester | 1 | | | | | | | | | 1 |
| 1,2,3-Triphenyl-3-methyl-cyclopropene | | | 1 | | | | | | | 1 |
| 2,3-Butanedione | | | | | | 1 | | | | 1 |
| 3-Hexanone, 2,5-dimethyl- | | 1 | | | | | | | | 1 |
| 3-Butenenitrile | | | | 1 | | | | | | 1 |
| Butylated Hydroxytoluene | | | | | 1 | | | | | 1 |
| 5-Methyl-3-phenyl-1H-indazole | | | | | | | 1 | | | 1 |
| .alpha.-Methylstyrene | | | | | 1 | | | | | 1 |
| 5-Oxotetrahydrofuran-2-carboxylic acid, ethyl ester | 1 | | | | | | | | | 1 |
| 2,3-Pentanedione | | | | 1 | | | | | | 1 |
| D-Norleucine, N-ethoxycarbonyl-, ethyl ester | | | | | 1 | | | | | 1 |
| Carbonochloridic acid, decyl ester | | | | 1 | | | | | | 1 |
| (S)-(+)-1,2-Propanediol | 1 | | | | | | | | | 1 |
| cis-11-Tetradecen-1-ol | | | | | | | | 1 | | 1 |

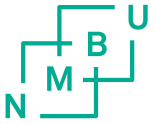
# J. Compounds identified and annotated by Personal Compound Database and Library

| Library | PCDL | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Stained spruce panel (Universal)** | **Sample** | | | | | | | | | |
| **Compound name** | **Chamber 1, 3L** | **Chamber 1, 5L** | **Chamber 2, 3L** | **Chamber 2, 5L** | **Chamber 3, 3L** | **Chamber 3, 5L** | **Chamber 4, 3L** | **Chamber 4, 5L** | **Chamber 5, 5L** | **Grand Total** |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Acetone | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| m-xylene | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 8 |
| D-limonene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 8 |
| Decanal | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Styrene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | | 7 |
| 3-carene | 1 | 1 | 1 | | 1 | | 1 | 1 | 1 | 7 |
| Ethylbenzene | 1 | 1 | | 1 | | | 1 | 1 | 1 | 6 |
| Tridecane | 1 | 1 | | 1 | | 1 | | | | 4 |
| Naphthalene | | 1 | | | | | 1 | 1 | 1 | 4 |
| 1,3,5-trimethylbenzene | | 1 | | | 1 | 1 | | 1 | | 4 |
| Furfural | | 1 | | 1 | | | | 1 | 1 | 4 |
| 1,2,4-trimethylbenzene | 1 | | | 1 | | | | | 1 | 3 |
| Mesitylene | | | | | 1 | | | | | 1 |
| 1,2,4,5-tetramethylbenzene | | | | | | | | | 1 | 1 |
| Decane | | | | | | | | | 1 | 1 |
| **Grand Total** | **12** | **13** | **9** | **12** | **11** | **10** | **10** | **12** | **12** | **101** |

| **Untreated spruce panel** | **Sample** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Compound name** | **Chamber 1, 3L** | **Chamber 1, 5L** | **Chamber 2, 3L** | **Chamber 2, 5L** | **Chamber 3, 3L** | **Chamber 3, 5L** | **Chamber 4, 3L** | **Chamber 4, 5L** | **Chamber 5, 5L** | **Grand Total** |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 3-carene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Decanal | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | 8 |
| m-xylene | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Ethylbenzene | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| Naphthalene | 1 | | 1 | | 1 | 1 | 1 | 1 | 1 | 7 |
| Styrene | 1 | | | 1 | 1 | 1 | 1 | 1 | 1 | 7 |
| D-Limonene | 1 | 1 | | 1 | | | 1 | | 1 | 5 |
| Nonane | 1 | | | | | 1 | 1 | 1 | 1 | 5 |
| 1,2,4-trimethylbenzene | 1 | | 1 | | | | 1 | 1 | 1 | 5 |
| Decane | | 1 | | 1 | 1 | | | 1 | 1 | 5 |
| 1,3,5-trimethylbenzene | | | | 1 | 1 | 1 | | | | 3 |
| Isopropylbenzene | | | | | | 1 | | 1 | | 2 |
| 3-Ethyltoluene | 1 | | | | | | | | | 1 |
| **Grand Total** | **13** | **7** | **9** | **10** | **11** | **12** | **12** | **13** | **13** | **100** |

| Library | PCDL | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Stained spruce panel (Tenax)** | **Sample** | | | | | | | | |
| **Compound name** | **Chamber4, 3L** | **Chamber 1, 3L** | **Chamber2, 3L** | **Chamber2, 5L** | **Chamber3, 3L** | **Chamber 3, 5L** | **Chamber 4, 5L** | **Chamber5, 5L** | **Chamber1, 5L** | **Total** |
| Decane | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Furfural | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| m-xylene | | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 8 |
| 3-carene | 1 | 1 | 1 | 1 | | 1 | 1 | | 1 | 7 |
| D-limonene | 1 | 1 | | 1 | 1 | | 1 | 1 | 1 | 7 |
| Styrene | 1 | 1 | | 1 | 1 | | 1 | 1 | 1 | 7 |
| Decanal | 1 | 1 | 1 | 1 | 1 | | 1 | | 1 | 7 |
| Ethylbenzene | 1 | 1 | 1 | 1 | | | 1 | 1 | 1 | 7 |
| 1,2,4-trimethylbenzene | 1 | | 1 | | 1 | | 1 | 1 | 1 | 6 |
| Octane | 1 | | 1 | 1 | 1 | 1 | | | 1 | 6 |
| Naphthalene | 1 | | | 1 | | | 1 | | 1 | 4 |
| 1,3,5-trimethylbenzene | | 1 | | 1 | | 1 | | | | 3 |
| Hexadecane | | | | 1 | | | | 1 | | 2 |
| Nonane | | | | 1 | | | | 1 | | 2 |
| Isopropylbenzene | | | | 1 | | | | | | 1 |
| Tridecane | | | | | | | 1 | | | 1 |
| 4-Ethyltoluene | | | 1 | | | | | | | 1 |
| **Total** | **13** | **12** | **12** | **17** | **11** | **9** | **14** | **12** | **14** | **114** |

| **Cross-laminated tree** | **Sample** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **Compound name** | **Chamber 1, 3L** | **Chamber 1, 5L** | **Chamber 2, 3L** | **Chamber 2, 5L** | **Chamber 3, 3L** | **Chamber 3, 5L** | **Chamber 4, 3L** | **Chamber 4, 5L** | **Chamber 5, 5L** | **Grand Total** |
| Decanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Tert-butylbenzene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Hexanal | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Beta-pinene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| Camphene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| D-limonene | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 9 |
| 3-carene | 1 | 1 | | 1 | 1 | 1 | 1 | | 1 | 7 |
| Octane | 1 | 1 | 1 | 1 | 1 | 1 | | | 1 | 7 |
| m-xylene | | | | 1 | | | 1 | | 1 | 3 |
| Styrene | | | 1 | | | | 1 | | | 2 |
| Ethylbenzene | | | | | | | | | 1 | 1 |
| Naphtalene | | | | | | | | | 1 | 1 |
| 1,2,3-trimethylbenzene | | | | | | | | | 1 | 1 |
| Furfural | | | | | | | | | 1 | 1 |
| 3-Ethyltoluene | | | | | | | | | 1 | 1 |
| 1,3,5-trimethylbenzene | | | | | | | | | 1 | 1 |
| **Grand Total** | **8** | **8** | **8** | **9** | **8** | **8** | **9** | **6** | **15** | **79** |

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