

UNIVERSITÉ DU QUÉBEC À TROIS-RIVIÈRES

LA COMPARAISON DES PROFILS DES COMPOSÉS ORGANIQUES VOLATILES  
PROVENANT DE CADAVRES HUMAINS ET ANIMAUX AFIN D'ÉtudIER LA  
RÉPONSE OLFACTIVE DES CHIENS DÉTECTEURS DE CADAVRES

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LIST OF ABBREVIATIONS AND SYMBOLS

1D	One dimension
2D	Two dimension
ADD	Accumulated degree days
ATP	Adenosine triphosphate
DIC	Deconvoluted ion current
GC-MS	Gas chromatography-mass spectrometry
GCxGC	Comprehensive two-dimensional gas chromatography
HRD	Human remains detection
m/z	Mass-to-charge ratio
ODORS	OPP Decomposition Odor Research Site
OPP	Ontario Provincial Police
PCA	Principal Component Analysis
REST[ES]	Recherches en Sciences Thanatologies [Expérimentales et Sociales]
SPME	Solid-phase microextraction
TOFMS	time-of-flight mass spectrometer
TRACES	Taphonomic Research in Anthropology - Center for Experimental Study
UQTR	Université du Québec à Trois-Rivières
VOC	Volatile organic compound

## RÉSUMÉ

La décomposition humaine est un processus complexe et variable influencé par divers facteurs. À chaque étape du processus de décomposition, une diversité de composés organiques volatils (COV) est émise dans l'environnement, souvent appelée odeur de décomposition. La compréhension de cette odeur cible a été au centre de nombreuses études en taphonomie médico-légale, car elle contribue largement au travail de l'unité canine de la police. Les chiens détecteurs de cadavres sont spécifiquement dressés pour aider les forces de l'ordre dans les opérations de recherche de victimes décédées. Des études antérieures ont montré que des chiens spécialement dressés sont capables de différencier les restes animaux des restes humains, mettant en évidence leur sensibilité et leur spécificité aux odeurs. En conséquence, le choix des sources d'odeurs pour la formation des chiens détecteurs de cadavre est une considération majeure. Bien qu'ils s'appuient sur des signaux olfactifs lors de la recherche de restes humains, il est important de reconnaître quels composés sont détectés dans les odeurs de décomposition. Dans cette étude, les profils de COV provenant de divers os d'animaux ont été collectés et analysés par désorption thermique couplée à une spectrométrie de masse à temps de vol par chromatographie en phase gazeuse bidimensionnelle (TD-GC × GC-TOFMS). Les profils de COV de décomposition animale ont ensuite été comparés aux profils de COV obtenus à partir d'outils de formation des chiens détecteurs de cadavres constitués de membres humains amputés utilisés par la police provinciale de l'Ontario. Les réponses olfactives des chiens cadavres en présence de ces outils de formation et des restes d'animaux ont ensuite été étudiées. Au cours de l'entraînement, les chiens HRD ont reçu pour instruction de localiser et d'alerter sur les restes humains en présence de restes d'animaux et d'autres odeurs de distraction. Les résultats ont démontré que les chiens HRD étaient capables de distinguer les restes humains en présence de restes de pores, de cerfs et/ou d'originaux de manière cohérente dans les séries d'entraînement. Mettre en évidence les différences dans les profils de COV entre la décomposition animale et humaine peut contribuer à améliorer la sensibilité des chiens détecteurs de cadavres aux restes humains tout en reconnaissant l'importance d'utiliser du matériel cadavérique humain à des fins de dressage.

ABSTRACT

Human decomposition is a complex and variable process with a variety of influencing factors. During each stage of the decomposition process, a diversity of volatile organic compounds (VOCs) is emitted into the environment, often referred to as decomposition odor. Understanding this target odor has been a main focus in numerous studies in forensic taphonomy as it contributes largely to police canine work. Human Remains Detection (HRD) dogs are specifically trained to aid law enforcement agencies in search operations for deceased victims. Previous studies have shown that specially trained canines are able to differentiate between animal and human remains, highlighting their odor sensitivity and specificity. Accordingly, the choice of odor sources for HRD training is a major consideration. While they rely on olfactory cues when searching for human remains, it is important to recognize which compounds are being detected in the decomposition odors. In this study, VOC profiles from a variety of animal bones were collected and analyzed using thermal desorption coupled to comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry (TD-GC×GC-TOFMS). The animal decomposition VOC profiles were subsequently compared to VOC profiles obtained from HRD training aids consisting of amputated human limbs used by the Ontario Provincial Police. The olfactory responses of cadaver dogs in the presence of these training aids and animal remains were subsequently investigated. During training, HRD dogs were instructed to locate and alert to human remains in the presence of the animal remains and other distraction odors. Results have demonstrated that HRD dogs were able to distinguish human remains in the presence of pig, deer, and/or moose remains consistently throughout all series of single-blind scenarios. Highlighting the differences in VOC profiles between animal and human decomposition may help to enhance the sensitivity of HRD dogs to human remains while recognizing the importance of using human cadaveric material for training purposes.

# **CHAPTER 1: INTRODUCTION**

### **1.1. Forensic Taphonomy**

The term taphonomy is derived from the Greek word *'taphos'* which means burial and *'nomos'* meaning laws.<sup>1</sup> The first definition of taphonomy was the 'study of the transition, in all details, of organics from the biosphere into the lithosphere of the geological record' proposed by Russian paleontologist Ivan Efremov.<sup>2</sup> In simple terms, taphonomy is defined as the 'laws of embedding'.<sup>3</sup> From the development of the field of taphonomy in the 1940s until the late 1980s, the concept of taphonomy related to vertebrate paleontology and prehistoric archaeozoology, ergo strictly considering animal remains.<sup>4</sup> Understanding the processes contributing to fossil preservation and investigating their influence on the fossil record was a major goal for this new branch of paleontology.<sup>1,5</sup>

The introduction of taphonomy involving humans in a forensic setting began in the late 1980s with a study conducted by Haglund et al.<sup>6</sup> This study aimed to provide insight on animal scavenging of human remains and its application in law enforcement agencies' search operations.<sup>4,6</sup> Analyzing skeletal damages from animal scavenging assisted in recognizing certain behavioral patterns as well as identifying unnatural and natural disarticulation of the bodies.<sup>6</sup> Results from this study highlighted the importance of considering animal scavenging patterns while estimating the postmortem interval.<sup>6</sup>

Today, one of the main research foci of the field of forensic taphonomy is understanding the process and rate of human decomposition and the factors that influence it.<sup>7,8</sup> Current studies in this field investigate human decomposition in soil and water environments, a variety of climate conditions, animal scavenging in different contexts, and many other taphonomic factors.<sup>9-11</sup> As the scope of taphonomy broadens, the call for different forensic experts increases.

### **1.2. Decomposition Process**

Within minutes following death, the human body experiences postmortem changes driven by two destructive processes: autolysis and putrefaction.<sup>2</sup> Autolysis occurs as a result of intrinsic enzymes that are released following the breakdown of cell membranes.<sup>2</sup> This self-destructive process is independent of bacterial activity. By contrast, the process of putrefaction is driven largely by bacterial enzyme activity and begins within an hour following death.<sup>2</sup>

Several physical postmortem changes can be observed as decomposition progresses. Once the circulatory system loses its function, blood pools to the lowest parts of the body due to gravity, resulting in skin discoloration.<sup>12,13</sup> This physical process is referred to as livor mortis. Visual indications of livor mortis typically appear within an hour following death and continue to develop between two to four hours postmortem. Subsequently, the muscles of the body begin to stiffen.<sup>2,13</sup> This occurs as a result of a chemical change and is typically observed two to six hours following death. More specifically, the cessation of adenosine triphosphate (ATP) activity leads to the inability of actin and myosin filaments to separate.<sup>12,13</sup> Once muscle proteins begin to deteriorate, about 15 to 25 hours later, the body returns to its relaxed state.<sup>14</sup> Algor mortis describes the third early characteristic of death during which the body cools to the ambient temperature. In most cases, this cooling period lasts between 18 to 20 hours.<sup>13</sup> The occurrence and timeline of livor, rigor, and algor mortis are predictable to a reasonable degree, thus being useful in postmortem interval estimation.<sup>12,13</sup>

#### 1.2.1. Stages of decomposition

Human decomposition is a continuum.<sup>2</sup> It is a complex and variable process that has been divided into five stages: fresh, bloat, active decay, advanced decay, and dry remains/skeletonization.<sup>2</sup> These stages are characterized by physical and chemical changes and insect activity.<sup>13</sup>

*Fresh* – This stage begins moments after the heart stops.<sup>15</sup> Postmortem changes include livor, rigor, and algor mortis. Minimal macroscopic changes, such as greenish discoloration of the skin, are associated with this stage.<sup>13,16</sup> The conclusion of this stage is noted when the body begins to bloat.<sup>13</sup>

*Bloat* – This stage, also known as the distension phase, is characterized by autolysis and putrefaction.<sup>2</sup> Physical evidence of autolysis is seen with skin slippage.<sup>3,13</sup> Hydrolytic enzymes are released between the epidermis and the underlying dermis, causing both layers to detach from one another.<sup>7,13</sup> Distension of the abdomen is caused by anaerobic bacteria activity.<sup>3,17</sup> Tissue digestion leads to gas production and ultimately, abdomen distension.<sup>13</sup> Marbling of the skin occurs also as a result of anaerobic bacteria activity.<sup>13,16</sup>

*Active Decay* – The physical changes associated with this stage are skin ruptures due to the increased pressure caused by the gasses within the abdomen and advanced insect activity.<sup>7,13</sup> With the release of gasses comes a persisting and strong decomposition odor.<sup>13</sup> At this stage, the body loses most of its mass due to maggot feeding and expulsion of decomposition fluids.<sup>13,16</sup> Putrefaction is still on going as cadaveric material continues to breakdown.<sup>16</sup>

*Advanced Decay* – At this stage, the majority of soft tissue has decomposed. Accordingly, maggot activity has decreased, thus reducing the rate of decomposition.<sup>16</sup> Cadaveric material is still visibly moist with minimal bone exposure.<sup>13</sup>

*Dry Remains/Skeletonization* – The stage of dry remains is reached when more than half of the body's bones have been exposed and contain little to no moisture.<sup>16,18</sup> Skeletonization is the final stage of the human decomposition process where any remaining tissues have been consumed by insects and/or bacteria.<sup>16</sup>

The categorization of the decomposition process aids in its understanding and facilitates postmortem estimation. However, the postmortem process of human decomposition involves numerous and overlapping chemical and biological processes that are readily influenced by external environmental factors as well as internal bodily changes.<sup>16</sup>

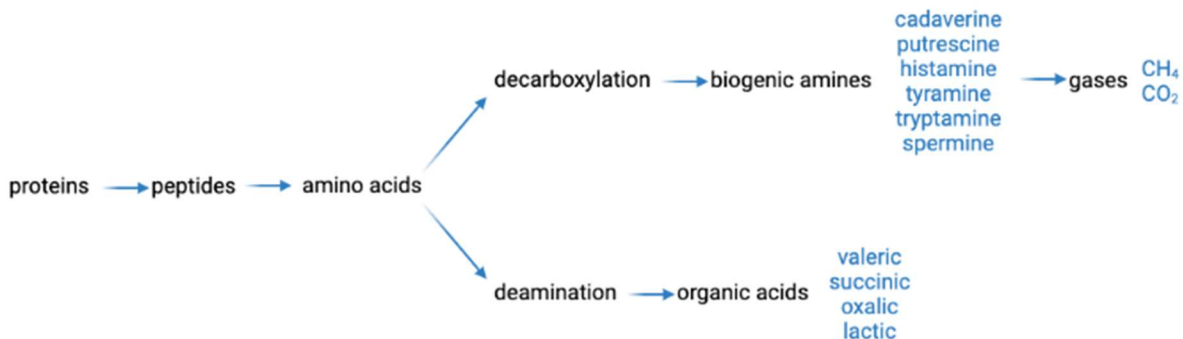
#### 1.2.2. Chemical and biological pathways

The postmortem changes associated with each stage of decomposition are driven by chemical and biological pathways. Two main processes are associated with decomposition: autolysis and putrefaction.<sup>19</sup> The lack of oxygen to the body's cells provokes both of these processes. The decomposition of soft tissue, which is composed of skin, adipose tissue, and muscle, is the outcome of protein, carbohydrate, and fat breakdown. The progressive deterioration of these compounds leads to tissue liquefaction.<sup>2</sup> The release of compounds during human decomposition can be associated with different stages of this process.<sup>19</sup>

Protein decomposition, or proteolysis, is when protein molecules are broken down into smaller peptides and/or amino acids by proteolytic enzymes.<sup>2,20</sup> The rate of protein decomposition varies

with moisture content, bacterial activity, and temperature.<sup>2</sup> Soft tissue proteins found in the epithelial tissues of the gastrointestinal tract and neuronal membranes begin to degrade at an early decomposition stage.<sup>2,19</sup> Less easily susceptible to proteolysis are epidermis, reticulin, and muscle proteins, degrading at later decomposition stages.<sup>7,19</sup>

Proteins are initially broken down into proteoses, peptones, polypeptides, and amino acids.<sup>19,21</sup> This ultimately leads to the production of organic and inorganic gasses, such as ammonia, methane, hydrogen sulfide, and carbon dioxide. The distinct smell associated with decomposition odor is a result of the toxic diamines, cadaverine, derived from lysine, and putrescine, derived from ornithine.<sup>19,22</sup> Amines can further decompose by oxidative decarboxylation to produce volatile organic compounds, including dimethylamine and trimethylamine.<sup>23</sup> Sulfur-containing amino acids can be decomposed into thiols, sulfides, and inorganic sulfurous gasses by desulfhydralation and subsequent oxidative reactions. Produced VOCs known to be the cause of pungent decomposition odors include dimethyl disulfide, dimethyl trisulfide, and dimethyl tetrasulfide.<sup>19,21,23</sup> Under aerobic conditions, these VOCs will oxidize to produce elemental sulfur.<sup>23</sup> Skatole and indole are produced as a result of the breakdown of aromatic amino acids with by-products that include benzonitrile, benzaldehyde, ethylbenzene, and phenol.<sup>23,24</sup>

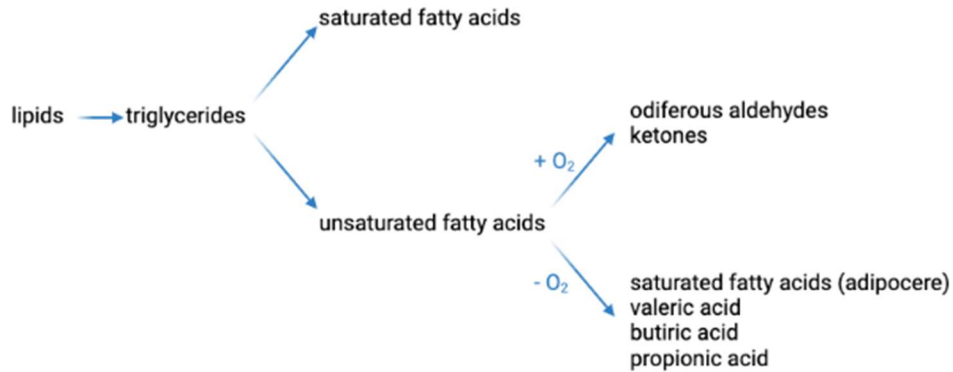


**Figure 1.1** Schematic representation of postmortem decomposition of proteins

Adipose tissue in the body is made up of approximately 60-85% lipids, while the remainder 40-15% consists of water.<sup>7</sup> For the most part, 90-99%, lipids are formed of triglycerides.<sup>19,21</sup> Lipids are degraded into hydrocarbons, nitrogen, phosphorus, and oxygenated compounds, palmitic acid and oleic acid. The initial breakdown of lipids into triglycerides is catalyzed by lipase activity.<sup>19</sup> Triglycerides, which are esters composed of glycerol and three fatty acids, are then decomposed into saturated and unsaturated fatty acids through hydrolytic activity by lipases. In aerobic

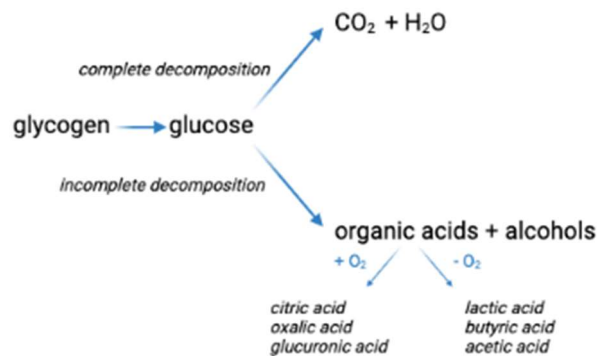


conditions, oxidation will drive the decomposition of unsaturated fatty acids into aldehydes and ketones, contributing to foul odor.<sup>19</sup> In anaerobic conditions, hydrogenation will drive the decomposition of unsaturated fatty acids into saturated fatty acids, leading to the formation of adipocere.<sup>19,21</sup>



**Figure 1.2** Schematic representation of postmortem decomposition of lipids

Carbohydrates present in the soft tissue will decompose into oxygenated compounds, such as alcohols, aldehydes, ketones, acids, ethers, and esters. Microorganism activity leads to the conversion of glycogen into glucose monomers.<sup>19,21</sup> Glucose can break down further via two pathways; through oxidation to form carbon dioxide and water, or incomplete decomposition yielding organic acids, such as citric, oxalic, or glucuronic acids, and alcohols.<sup>19,21,23</sup> In anaerobic conditions, bacteria will yield lactic, butyric, and acetic acids along with ethanol and butanol.<sup>19,21</sup> Alternatively in an aerobic environment, fungi will break down sugars leading to the production of glucuronic, citric, and oxalic acids.<sup>19,21</sup> Methane, hydrogen gas, and hydrogen sulfide are formed as a result of bacterial fermentation.<sup>19,21</sup>



**Figure 1.3** Schematic representation of postmortem decomposition of carbohydrates

Bone can experience postmortem changes known as diagenesis.<sup>25</sup> This phenomenon describes the chemical and physical changes to bones following death.<sup>25,26</sup> Bone consists of organic components, mainly fat and proteins, and mineral components.<sup>27</sup> Therefore, fat, also a major component of marrow, can further decompose at later stages of decomposition allowing the release of VOCs. The degradation of fat produces ketones and aldehydes.<sup>23,28</sup> Collagen proteins make up roughly 90% to 95% of bone protein.<sup>23,26</sup> Their degradation leading to the production of peptides is a result of bacterial collagenases.<sup>23</sup> The breakdown of hydroxyapatite, a mineral component of bone, is caused by physical weathering.<sup>23</sup>

### **1.3. Animal Decomposition**

The decomposition of animal carrion in terrestrial environments is divided into five stages: fresh, bloat, active decay, advanced decay and dry remains.<sup>29</sup> Animal carcasses experience similar postmortem microscopic and macroscopic changes to human cadavers. After death, either human or animal, the body's cells are deprived of oxygen and nutrients causing loss of function. The lack of oxygen results in enzymatic and biochemical activity leading to autolysis and putrefaction.<sup>30</sup> Carrion decomposition is largely driven by microorganism activity in the digestive tract and on an animal's skin surface. The enzymes released by these microbes enable the breakdown of cells. During the early stages of carrion decomposition, a large number of gasses, including methane, hydrogen sulfide, and carbon dioxide, are released by decaying tissues causing the carcass to bloat.<sup>29,30</sup> These gasses attract a diversity of insects who rely on carrion as a food source. Insect activity ultimately leads to the animal carcasses physical breakdown. Vertebrate scavengers will also contribute largely to the physical decomposition by ingesting sizeable amounts of tissue while potentially disarticulating the animal carcass.<sup>30</sup> Consequently, animal carcasses are often found in smaller and scattered pieces due to scavenging. Depending on the environment, several parts of the carcass, such as the fur, nails, and skeleton, will persist for longer periods of time.

#### **1.3.1. Human versus Animal**

Insect succession, decomposition chemistry, microbial activity, and overall decomposition processes are research areas involving animal models. Decomposition studies involve a variety of mammalian cadavers as human analogues. These include pigs, rats, dog, deer, bison, and rabbits.<sup>31-</sup>  
<sup>35</sup> Domestic pig carcasses (*Sus scrofa domesticus L.*) are routinely used when investigating human

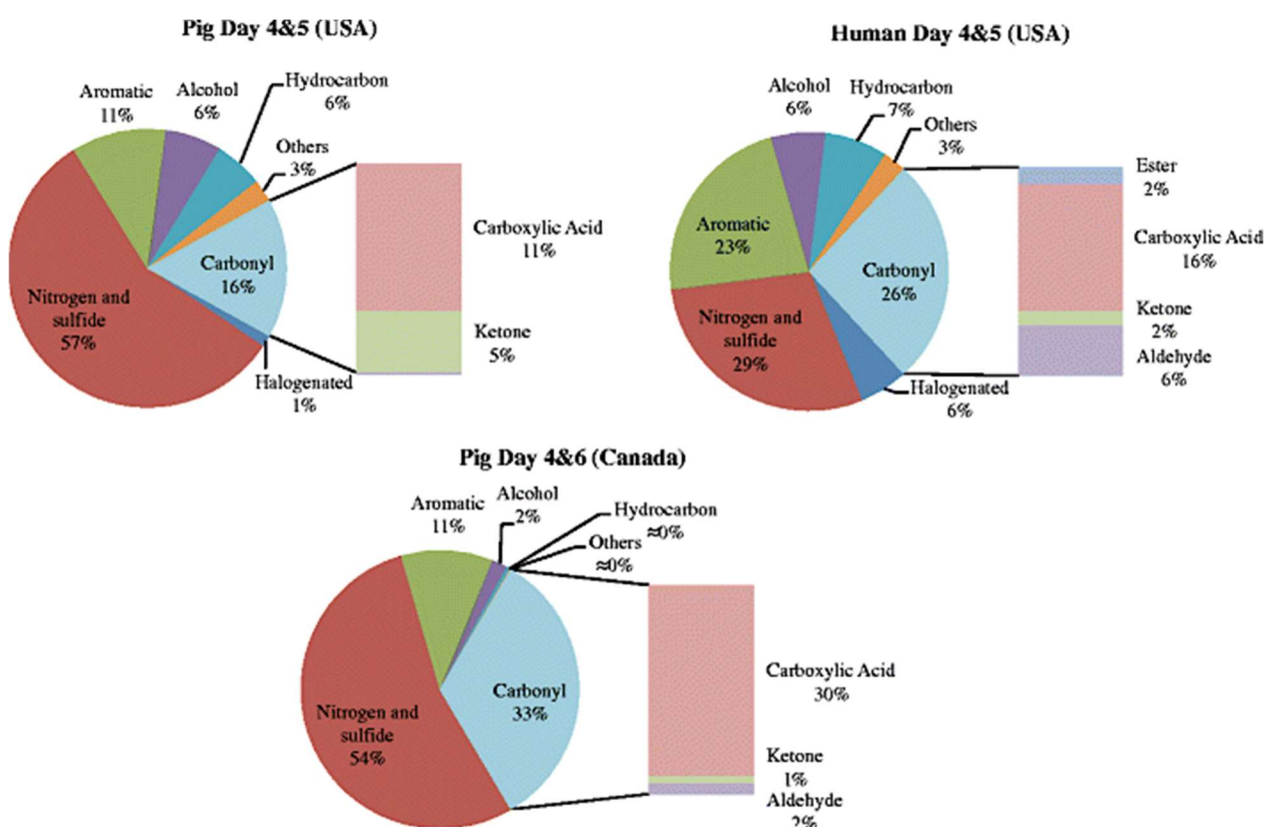
decomposition processes under varying conditions.<sup>36</sup> Pigs present similar internal organ anatomy and gut microbiota to that of humans suggesting their suitability as human analogues.

Pig carcasses have been used in research activities as an alternative to human cadavers in decomposition studies since the 1960s.<sup>37-39</sup> Early decomposition studies focused on establishing statistical models and field activities by studying arthropod succession on pigs.<sup>37</sup> Payne conducted a carrion study over the summers of 1962 and 1963 investigating the impact of arthropods on decomposition.<sup>39</sup> Payne had recognized six stages (fresh, bloated, active decay, advanced decay, dry, and remains) of decomposition for carrion exposed to arthropods.<sup>39</sup> These stages have become the most widely recognized classification for human decomposition. Later, pigs became the animal of choice for forensic entomologists and experimental research in taphonomy.<sup>37</sup>

A review conducted by Matuszewski et al. further supported the use of pig carcasses as analogues for human cadavers. Among the many advantages stated, the use of pig carcasses provided a greater replicability at a low expense without being confined to human decomposition facilities and medical examiner offices.<sup>37</sup> Despite the challenges associated with using human cadavers in decomposition studies, a major advantage includes the absence of species-related differences.<sup>37,40</sup> Additionally, the utilization of both human and animal cadavers provides the opportunity to compare decomposition processes between the two.<sup>40</sup>

While some studies reveal similarities between pig and human decomposition, others highlight their differences.<sup>35,41</sup> A study conducted by Notter et al. suggested that fatty acid proportions and distribution between pig and human tissues affected the process of adipocere formation. Pigs having higher levels of total saturated fatty acids experienced quicker adipose tissue decomposition.<sup>41</sup> A recent study compared decomposition rates and odor profiles of pig and human remains.<sup>32</sup> Visual observations reported during this study undermine the use of pigs as human analogues due to significant variation in decomposition patterns between the two species. Additionally, ratio and abundance of VOCs showed significant differences suggesting distinct odor profiles.<sup>32</sup>

One study revealed similar trends in early decomposition stages for pig and human decomposition.<sup>38</sup> VOC profiles from human and pig decomposition were compared. Figure 1.4 illustrates similarities in identified chemical families for each VOC profile. Specifically considering the carbonyl compound class, carboxylic acids reported the highest amount with similar percentages observed in Pig Day 4 & 5 (11%) and Human Day 4 & 5 (16%). Overall, the abundant presence of nitrogen and sulfide compounds is seen in both pigs and humans. The similarities in abundances of specific compounds supported a robust VOC profile obtained from the bloat stage of decomposition.<sup>38</sup>

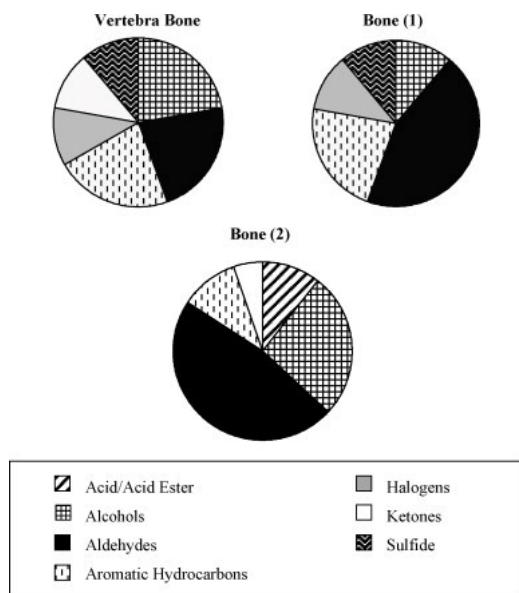


**Figure 1.4** Comparison of decomposition VOC profiles recorded during two separate studies on pig carcasses (USA and Canada) and one study using a human cadaver (insect included)<sup>38</sup>

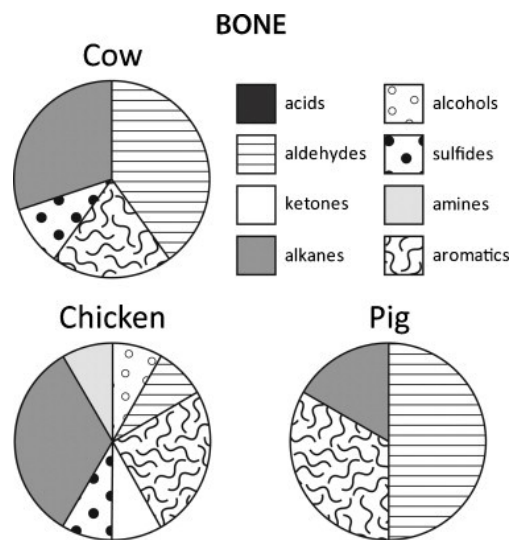
Conversely, a study conducted by Cablk et al. reported significantly different VOC signatures between decomposing animal remains and human remains.<sup>42</sup> This study aimed to compare VOCs from animal remains to those of human remains studied by Hoffman et al.<sup>43</sup> While Hoffman et al. focused on identifying potential signature compounds from human remains for their implementation in Human Remains Detection (HRD) dog training, Cablk et al. investigated

compounds that may be uniquely associated to human remains by comparing animal and human samples.<sup>42,43</sup>

Figure 1.5 depicts the distribution of chemical classes among human bone samples while Figure 1.6 depicts that of cow, chicken, and pig bone samples. Unlike in the chicken and cow bone samples, the compound classes in the pig bone varied the least.<sup>42</sup> Following the comparison of VOC profiles from animal and human remains, Cablk et al. determined humans and pigs to be the least similar.<sup>42</sup>



**Figure 1.5** Distribution of chemical classes among human bone samples<sup>43</sup>



**Figure 1.6** Distribution of chemical classes in animal bone samples<sup>42</sup>

Several taphonomy research facilities rely on animal models due to the lack of accessibility to facilities that would allow the use of human cadavers. TRACES (Taphonomic Research in Anthropology – Centre for Experimental Study) is a facility established by the University of Central Lancashire in the United Kingdom.<sup>44</sup> This facility strictly involves the use of animal models for forensic taphonomy research.<sup>44</sup> Since 2009, TRACES has been successful in conducting numerous experimental decomposition studies.<sup>4,45–48</sup> For instance, wild rabbits were used in an experimental study on the impacts of adipocere on the decomposition rate of submerged remains.<sup>47</sup>

Widya, et al. successfully demonstrated a direct correlation between accumulated degree days (ADD) and the likelihood of adipocere formation in wild rabbit remains.<sup>47</sup> Additionally, this study revealed influencing factors in the formation of adipocere, providing new research areas. Another study conducted by Gruenthal, et al. investigated decomposition patterns in charred remains using pig carcasses.<sup>46</sup> This study aimed to test the applicability of traditional postmortem interval techniques on charred remains.<sup>46</sup> Despite reporting no significant differences in overall decomposition rates between charred and uncharred remains, it was noted that certain body regions in the charred remains, such as the head, neck, and limb regions, decomposed at a slower rate.<sup>46</sup> A notable limitation is the applicability of the derived decomposition rate equations from this study to human remains due to their significant size difference.<sup>46</sup> Lastly, Cross and Simmons investigated the effects of gunshot wounds on decomposition rates using pig carcasses.<sup>48</sup> Visual observations supported an increase in decomposition patterns in wounded pigs, however quantitative data obtained from this study revealed no significant differences in decomposition rates between non-wounded pigs and wounded pigs.<sup>48</sup> The authors concluded that small wound trauma had no effect on decomposition rates in pigs.<sup>48</sup>

In essence, the application of animal models for human decomposition studies has yielded tremendous research output and has broadened the scope of taphonomic studies. Animal models enable large-scale replicable experimental studies and are essential to the development of novel practices.<sup>4,49</sup> However, these techniques should be employed in decomposition studies using human cadavers for further validation.<sup>4</sup>

#### **1.4. Chemical Detection of VOCs**

Odor analysis generally involves sample collection and/or extraction of VOCs and subsequent analyses. The type of samples chosen for VOC characterization influences the analytical method employed.<sup>50</sup> Headspace analysis is a commonly used sampling technique for trapping volatiles to prepare them for separation.<sup>51</sup> Gas chromatography coupled with mass spectrometry (GC-MS) is typically used for the detection and characterization of VOC profile analysis.<sup>50</sup>

#### 1.4.1. Sample Types

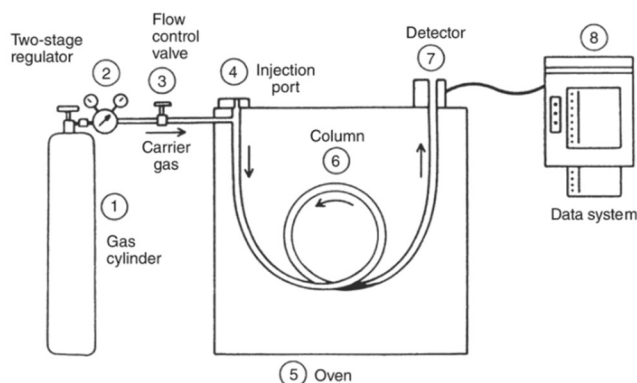
In decomposition studies, VOCs can be collected from a variety of sample types and environments. Human cadavers, human analogues, human tissue, blood, fat, and bones are primary odor sources. VOCs persist in their surrounding environment creating additional sampling sources. Accordingly, air, soil, water, and textiles are routinely investigated in decomposition studies.<sup>24,52,53</sup>

#### 1.4.2. VOC Collection

A variety of sampling devices, such as gas tight syringes, adsorbent filters, solid-phase microextraction (SPME) fibers, and sorbent tubes, have been used for the collection of VOCs.<sup>54</sup> Among these, SPME fibers and sorbent tubes, both sorbent-based methods, are most commonly implemented in VOC studies relating to decomposition odor.<sup>54,55</sup> The sample matrix ultimately influences which collection method is to be employed. In most cases, SPME is limited to tissue samples placed in vials, whereas sorbent tubes can be used in the collection of VOCs from larger sample types, such as animal carcasses and human remains in outdoor environments.<sup>54</sup> Additionally, the choice of sorbent material varies with manufacturing specifications.<sup>55</sup> Studies have shown that a combination of TenaxTA and Carbograph 5TD provides optimal results when collecting VOCs from decomposition odors. Once volatiles are adsorbed onto the sorbent tubes, thermal desorption is used for desorbing the VOCs into the injection port of a gas chromatograph column for subsequent analysis.<sup>55</sup>

#### 1.4.3. Analytical Instrumentation

Gas chromatography is an analytical technique used for the separation of volatile or semi-volatile compounds.<sup>56</sup> The foundation of this technique is the partitioning of sample components between a stationary phase and a mobile phase.<sup>56</sup> The basic components of a GC system are shown in Figure 1.7. A gaseous or liquid sample is introduced into the injection port and carried through the column via an inert carrier gas (helium, nitrogen, hydrogen, or argon) acting as the mobile phase. Compound separation occurs within the column and the rate at which compounds reach the detector is determined by their interaction with the stationary phase.<sup>56</sup>

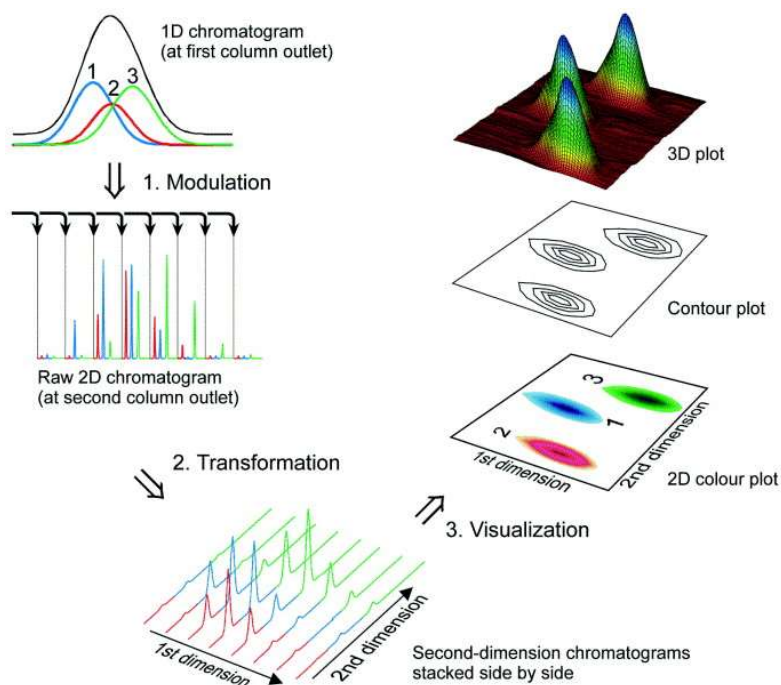


**Figure 1.7** Schematic representation of a gas chromatograph<sup>56</sup>

Limitations associated with GC include its restriction to small volatile compounds, unsuitability for thermally labile samples, and necessity for spectroscopy for peak characterization.<sup>56</sup> However, GC presents numerous advantages that include high specificity and sensitivity, compound separation capacity, detector compatibility, low sample concentration, and speed of analysis, making GC the preferred method for the separation of volatile compounds.<sup>56</sup>

Comprehensive two dimensional gas chromatography (GCxGC) has become the analytical method of choice for trace-level analyses of complex mixtures.<sup>57</sup> The addition of a secondary column allows for a second GC separation based on a separation mechanism different from the first column.<sup>57</sup> The differing separation mechanisms produce orthogonal separation conditions. In other words, retention times obtained in the first dimension are independent of those from the second dimension.<sup>57,58</sup> The resulting chromatogram displays the retention time of the first column on one axis (first dimension) and the retention time of the second column on a second axis (second dimension) (Figure 1.8).<sup>57</sup> This chromatogram is obtained by stacking second-dimension chromatograms side by side.



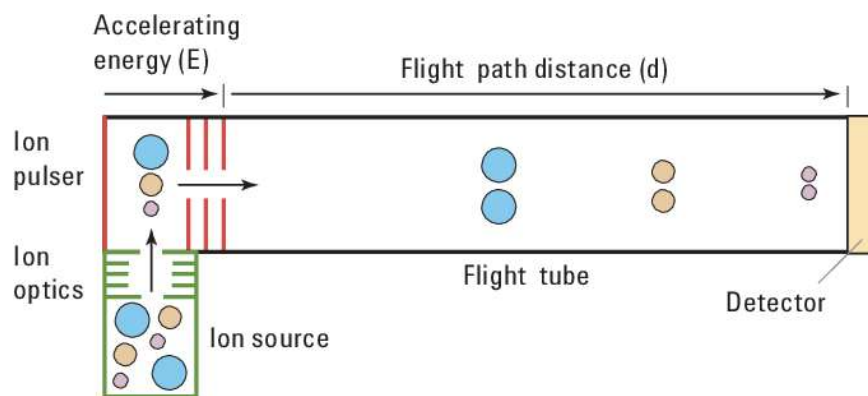


**Figure 1.8** Generation and visualization of a GCxGC chromatogram<sup>59</sup>

Numerous advantages are associated with utilizing GCxGC over conventional GC. Firstly, GCxGC provides an enhanced analyte separation due to higher peak capacity.<sup>57</sup> Secondly, lower limits of detection are attainable with GCxGC.<sup>57</sup> Lastly, group-type analyses and classification of unknown compounds are enabled.<sup>57</sup> Compared to a one-dimensional GC system, a more complex approach is needed when configuring and optimizing a GCxGC system.<sup>57</sup> Parameters, such as temperature and carrier gas flow, affect separation capacity in both dimensions, therefore must be considered during optimization. A 2008 study compared one-dimensional and comprehensive two-dimensional separations by gas chromatography.<sup>60</sup> Results from this study suggest that the peak capacity of GCxGC is not significantly greater than that of conventional GC when using typical 1D-GC parameters. However, following parameter optimization, the peak capacity of GCxGC is significantly greater than that of conventional GC. It was determined that GCxGC peak capacity can exceed an order of magnitude than that of 1D-GC.<sup>60</sup>

Mass spectrometry is an analytical technique used in measuring the mass-to-charge ratio ( $m/z$ ) of molecules present in a sample.<sup>61</sup> A mass spectrometer, consisting of an ionization source, a mass analyzer, and an ion detection system, is used in the identification and quantification of unknown compounds.<sup>61</sup> A time-of-flight mass spectrometer (TOFMS) is a mass analyzer which separates

ions based on their travel time from the ion source to the detector within the flight tube (Figure 1.9).<sup>61-63</sup> An ion's trajectory will depend on its momentum and kinetic energy. Ions with lower mass-to-charge ratios will travel quicker and attain the detector first, while ions with higher mass-to-charge ratios will travel slower and attain the detector last.<sup>61</sup>



**Figure 1.9** Schematic representation of a time-of-flight analysis of ions of various masses<sup>63</sup>

TOFMS is often coupled with two dimensional gas chromatography as it provides greater mass resolution, sensitivity, acquisition rate and linear dynamic range.<sup>64</sup> A TOFMS instrument has the capability to resolve coeluting chromatographic peaks due to its fast acquisition rates.<sup>64</sup> The application of a deconvoluted ion current (DIC) acts as a third dimension when coupled to a GCxGC system.<sup>64</sup> The combination of the optimized chromatographic resolution of a GCxGC system and resolving power of the TOFMS enables the analysis of complex mixtures.

### 1.5. Biological Detection of VOCs

Despite recent advances in chemical detection systems, an animal's olfactory sensitivity remains superior.<sup>65</sup> The integration of canines (*Canis lupus familiaris*) in forensic investigations dates as early as 1888 in the search for Jack the Ripper in Britain.<sup>66,67</sup> In 1893, the Supreme Court of Alabama in the United States of America recognized that 'dogs may be trained to follow the tracks of a human being with considerable certainty and accuracy'.<sup>66,68</sup> Since then, canines have continued to aid law enforcement agencies in the detection of narcotics and explosives and in search operations. Canine olfaction accounts for their reliability and efficiency. Like humans, canines possess receptor cells and olfactory nerves responsible for the detection of compounds and signal transmission to the brain.<sup>66,69</sup> Unlike humans, olfactory sensory cells constitute half of a canine's

internal nasal area.<sup>66</sup> As a result, a canine's olfactory abilities are much superior to that of humans. A canine's odor sensitivity and discriminating power stems from their olfactory repertoire consisting of 1300 genes, a value 20 times greater than that of humans.<sup>66,70</sup>

Studies have demonstrated dogs' capacities in detecting a diversity of odors.<sup>65</sup> Dogs can be used as non-biological or biological scent-detection devices. Non-biological scents can include explosives, land mines, accelerants, hazardous chemicals, and drugs.<sup>71</sup> Mine-detection dogs represent the most reliable and cost-efficient detection methods for explosives.<sup>71,72</sup> These dogs are trained to locate buried landmines by recognizing the scent of explosive chemicals. Accelerant-detection dogs are employed in fire scene investigation to locate ignitable liquid residues.<sup>71,73</sup> Trained to locate the residual scent of flammable products, they can detect volumes as low as 0.005 $\mu$ L.<sup>71,74</sup> Similarly, dogs trained to confirm the presence of hazardous chemicals, are able to detect small quantities of toxins over large areas.<sup>71</sup> Drug-detection dogs are routinely used by law enforcement and border services agencies to search for illicit substances.<sup>71</sup>

Instances in which dogs have been used as biological scent detectors involve animal and human scents.<sup>71</sup> Dogs have been employed for the basis of biosecurity.<sup>71</sup> For example, snake-detection dogs have been used by border services agencies to prevent accidental infestation.<sup>71,75</sup> Dogs have also been used to locate invasive insect species.<sup>71</sup> Dogs are often used for wildlife conservation. These dogs are trained to locate scat for the study of rare animal populations.<sup>71,76</sup> Alternatively, dogs have also contributed to cancer diagnostics and the prevention of health related attacks, such as epileptic and hypoglycaemic attacks.<sup>77-79</sup> Other cases in which scent-detection dogs rely on human scent include search and rescue operations. This includes searching for missing people, avalanche victims, disaster survivors, and drowning victims.<sup>71</sup> In cases where an individual is presumed dead and/or a significant period of time has passed, cadaver-detection dogs, also referred to as human remains detection dogs, are employed.<sup>71</sup>

#### 1.5.1. Human Remains Detection Dogs

Human Remains Detection (HRD) dogs are specially trained to locate and alert to human decomposition odor in order to recover human cadavers and/or human body parts.<sup>80,81</sup> A well trained scent-detection dog will possess the ability to detect target odors while ignoring non-target

odors present during each search operation. This demonstrates their capabilities and ultimately their reliability as highly specialized biosensors. HRD dog training procedures will vary between agencies, countries, and canine handlers.<sup>82</sup> HRD dogs are trained with a large variety of training aids. Those explored include blood, human remains (exposed or buried), decomposition fluid, soil, textiles, synthetic materials, and human analogues.<sup>81</sup> While the use of human cadavers presents the most realistic training scenarios, it is impractical for training purposes.<sup>81</sup> Accordingly, many alternatives to entire cadavers have been investigated. Tissue samples from human remains, namely skin, muscle, body fat, teeth, bone, etc., have been proposed as training aids with studies reporting successful dog responses.<sup>43,81,83</sup> Blood is most commonly used in the training of blood-detection dogs who are trained to locate blood evidence.<sup>84</sup> Due to compound similarity found in blood and decomposition fluid, blood has been accepted as one of several training aids for HRD canine training.<sup>43,81</sup> Both fresh and aged blood should be incorporated in canine trainings as differences in VOC patterns have been reported.<sup>81,84</sup> Soil contaminated by a decomposing body has previously been studied as a potential odor source for HRD canine training.<sup>53,80</sup> As a body decomposes, fluids and gasses released become embedded in the soil. Soil porosity will determine the retention capacity of the compounds responsible for any residual odor and should be considered during collection for training purposes.<sup>53,80</sup> Decomposition fluid itself has been considered as a training aid. Studies have shown that HRD dogs are able to detect decomposition fluid with a concentration as low as 0.1 mL of 1-part-per-trillion ( $10^{-12}$ ).<sup>84</sup> As with soil, decomposition fluid can adhere to textiles depending on their composition alluding to their suitability as training material.<sup>52,80</sup> The manner in which biological training aids are integrated into training may present ethical and biohazard issues. To address these issues, synthetic training aids have been developed and investigated. Studies have reported the lack of reliability and efficiency of synthetic training aids when compared to biological training aids due to oversimplified odor profiles.<sup>80,85</sup>

Recently, the use of amputated limbs as HRD training aids has been validated.<sup>85</sup> The Ontario Provincial Police (OPP) Canine Unit located in Orillia, Ontario utilizes amputated limbs provided by the Anatomy Learning Centre and Teaching Laboratories at Queen's University, Kingston, Ontario, as HRD training aids.<sup>85</sup> In the study conducted by Dargan et al., the VOC composition of these training aids were investigated. The confirmed presence of decomposition VOCs in the

amputated limbs along with HRD dog performance measurements supported the validity of amputated limbs as training aids.<sup>85</sup>

The manner in which training aids are integrated in training procedures can vary greatly which in turn, may influence dog performances. The basics of training incorporate patience, perseverance, and praise.<sup>86</sup> Despite methods differing from canine handler to canine handler and canine to canine, training should consist of consistent rewards, marking desired behavior, exercise repetitions, diverse scent sources, regular exposure to scent sources, etc. Factors such as duration and frequency of training have been demonstrated to influence detection performance and should be considered when wanting to improve detection accuracy.<sup>82,86</sup> Reward systems that include toys, balls, and/or any positive reinforcement other than food have equally shown to influence dog performances.<sup>82</sup> The limitations of cadaver detection dogs do not strictly lie within the quality of their training. In real-life scenarios, external factors such as the actual presence of human remains, wind speed and direction, and a canine handler's ability to properly interpret their dog's behavior, play a role in successfully locating human remains.<sup>82,86</sup>

## **1.6. Objectives**

It has been proven through analytical testing that animal and human decomposition differ in chemical composition. However, are these differences significant enough for HRD dogs to differentiate the scent of animal decomposition from the scent of human decomposition?

This research aims to establish volatile profiles for various animal bones and compare them to human bone volatile profiles to determine and highlight their similarities or differences. The ratios of certain VOCs will be studied and their role in enabling scent differentiation will be investigated. Canine trials will be performed to study HRD dog olfactory responses to animal and human bones in the presence of other distractor odor sources.

To detect and identify compounds found in complex VOC mixtures released from decomposing remains, GCxGC-TOFMS will be implemented as the analytical method of choice.

The goals of this study are to:

- (1) establish and compare VOC decomposition profiles for pig, deer, moose, and bear bones, with human bones,
- (2) perform canine trials to study HRD dog olfactory responses to pig, deer, moose, and bear, and human bones.

Highlighting the differences in VOC profiles between animal and human decomposition may help to enhance the sensitivity of HRD dogs to human remains while recognizing the importance of using human cadaveric material for training purposes.

## **CHAPTER 2: DECOMPOSITION VOC PROFILING OF BONES USING GC<sub>x</sub>GC-TOFMS**

**2.1. Samples for VOC collection**

2.1.1. Ethics

The human research ethics approval for working with human remains in the form of HRD training aids was obtained from *le comité d'éthique de la recherche avec des êtres humains* at Université du Québec à Trois-Rivières (UQTR) with the certificate number SCELERA-22-06.

2.1.2. HRD Training Aids

The HRD training aids used by the Ontario Provincial Police (OPP) Canine Unit consist of donated human limbs. The donors were individuals who required amputation surgery due to diabetes. Surgeries were performed at Kingston General Hospital, Kingston, Ontario. The Anatomical Department of Queen’s University, Kingston, Ontario was responsible for the collection and storage of amputated limbs. The amputated limbs were stored in PVC pipes or Mason glass jars to be used as training aids for the OPP Canine Unit. Between training sessions, HRD training aids were stored at room temperature. This study focused on training aids categorized as foot bones and ankle, tibia and fibula bones with little to no tissue remaining. The training aids used in this study are summarized in Table 2.1. Foot bone samples are denoted by ‘FB’, leg bone samples by ‘LB’, and ankle bone samples by ‘AB’. In cases where exact dates samples were obtained are unknown, month and day are denoted by ‘XX’.

**Table 2.1** OPP training aid descriptions and their respective sample collection dates.

Sample ID	Date of surgery/tissue donation/sample collection	Date sample was obtained as training aids by OPP	Sample Type and Storage	Date of VOC sample collection		
				02/22	05/22	10/22
FB1	09/29/17	10/02/17	Heel and foot bones stored in a glass jar at room temperature	✓	✓	✓
FB2	12/08/17	12/11/17	Foot without toes stored in a glass jar at room temperature	✓	✓	✓



FB3	-	XX/XX/17	Small foot bones stored in glass jar at room temperature	✓		✓
FB4	-	XX/XX/17	Small foot bones stored in glass jar at room temperature	✓		✓
FB5.1	-	01/24/19	Right foot with 5 toes stored in glass jar at room temperature	✓	✓	✓
FB5.2	-		Right foot without toes stored in glass jar at room temperature	✓	✓	✓
FB11	-	XX/XX/19	Foot bone stored in Mason jar at room temperature		✓	✓
FB6	-	07/08/20	Left foot stored in a Mason jar at room temperature	✓	✓	✓
LB7	-	07/08/20	Leg section of tibia/fibula stored in a Mason jar at room temperature	✓	✓	✓
AB8	-	XX/XX/20	Small ankle bones stored in a glass jar at room temperature	✓	✓	✓
LB9	-	XX/XX/20	Left section of tibia/fibula stored in a Mason jar at room temperature	✓	✓	✓
FB10	-	XX/XX/20	Left foot stored in a Mason jar at room temperature	✓	✓	✓
FB12	-	XX/XX/20	Small ankle bones stored in a glass jar at room temperature		✓	✓

### 2.1.3. Animal Bones

This study involved the use of animal bones from various species (pig, moose, deer, and bear). Pig carcasses were allowed to decompose at the Université du Québec à Trois- Rivières (UQTR) site for Research in Experimental and Social Thanatology/*Recherche en Sciences Thanatologiques [Expérimentales et Sociales (REST[ES])* located in Bécancour, Québec. These pig carcasses had previously been used for other experimental studies the year prior to the commencement of this study. Moose skeletal remains were located near the facility and collected for experimental purposes. It is assumed a calf was allowed to decompose during the summer season and its remains collected in the fall. This assumption stems from video footage of a moose with twin offspring roaming near the facility. Deer and bear remains were collected from the OPP Decomposing Odor Research Site (ODORS). It is unknown how long the deer and bear remains were allowed to decompose prior to collection as their carcasses were not purposely planted on site. The animal bones chosen for VOC profile characterization and their descriptions are summarized in Table 2.2. A controlled environment was not a necessity for the decomposition of the animal bones as it would not provide the most realistic scenario in cases involving HRD dogs. As previously discussed, HRD dogs are trained to locate and alert to human remains. During search operations, it is likely that HRD dogs will encounter animal carcasses they are expected to ignore. The state in which these animal carcasses are found can vary from intact to disarticulated due to vertebrate scavengers. Hence, the importance of a random decomposition process and the advantages associated with obtaining different bone types from varying animal species.

**Table 2.2** Animal bone descriptions and their respective VOC sample collection dates.

Sample ID	Animal species	Sample Type and Storage	Date of VOC sample collection							
			02/22	05/22	07/22	08/22	09/22	11/22	01/23	03/23
P1	Pig	long bone stored in Mason jar at room temperature	✓	✓				✓	✓	✓
P2	Pig	stored in Mason jar at room temperature	✓	✓				✓	✓	✓
P3	Pig	stored in metal can at room temperature	✓	✓		✓	✓	✓	✓	✓
P4	Pig	rib stored in biohazard bag at room temperature			✓	✓	✓	✓	✓	✓
M1	Moose	long bone stored in Mason jar at room temperature	✓	✓		✓	✓	✓	✓	✓
M2	Moose	stored in metal can at room temperature	✓	✓		✓	✓	✓	✓	✓
M3	Moose	vertebrae stored in biohazard bag at room temperature			✓	✓	✓	✓	✓	✓
M4	Moose	rib stored in biohazard bag at room temperature			✓	✓	✓	✓	✓	✓
D1	Deer	stored in Mason jar at room temperature		✓				✓	✓	✓
B1	Bear	stored in Mason jar at room temperature		✓				✓	✓	✓

## 2.2. VOC collection

Sample collection procedures for both animal remains and OPP training aids were identical. Similar to previous odor decomposition studies, VOCs were collected on a sorbent tube following accumulation in the headspace above the remains.<sup>32,55,87</sup> Stainless steel hoods were used to create the headspace above the remains (Figure 2.1). The hood was placed over the remains to allow accumulation of VOCs for a period of 15 minutes.



**Figure 2.1** Stainless steel hood used to create headspace above samples

Following the accumulation period, 500 mL of headspace was collected through a sorbent tube via an ACTI-VOC low flow air sampling pump (Markes international Ltd., Llantrisant, UK). The dual Thermal desorption tube consisted of Tenax TA and Carboxograph 5TD (Markes international Ltd.). One end of the sorbent tube was linked to the sampling port located on the top of the stainless steel hood, and the other end attached to the sampling pump. VOCs were collected at a flow rate of 100 mL/min over 5 minutes. VOCs were collected in triplicates. Additionally, control samples were collected to ensure proper sample collection and to monitor any possibility of contamination. Three types of control samples were collected from: (1) a clean empty Mason jar placed on aluminum foil, (2) a clean empty metal can placed on aluminum foil, and (3) aluminum foil. After odor collection, sorbent tubes were sealed with brass storage caps and enveloped with aluminum foil. Sorbent tubes were then placed in Mason jars for transportation. Once at the laboratory, the tubes were stored in a refrigerator at 4°C.

### 2.3. VOC profile analysis by GCxGC-TOFMS

#### 2.3.1. Sample Preparation and Instrument Parameters

Sample preparation consisted of injecting an internal standard onto the sorbent tubes prior to analysis by GCxGC-TOFMS. The internal standard consisted of 0.2  $\mu\text{L}$  of 50 ppm bromobenzene (GC grade, Sigma-Aldrich) in methanol (HPLC Grade, Sigma-Aldrich). An eVol® XR handheld automated analytical syringe (SGE Analytical Science, Weatherill Park BC, NSW, Australia) was used for injection of the internal standard.

Thermal desorption (TD) was carried out using a Markes TD 100-xr multi-tube autosampler (Markes International Ltd.). Thermal desorption of VOCs from the sorbent tubes was achieved by heating the sorbent tubes to 300°C for 5 minutes. The desorbed compounds were then collected onto a general purpose cold trap at -10°C. At a desorption flow rate of 20 mL/min and a 10:1 split ratio, the trap was desorbed at 300°C for 5 minutes.

A transfer line was used to link the Markes TD to a Pegasus® BT 4D GCxGC-TOFMS (LECO, Mississauga, Ontario, Canada). The first dimension (1D) column consisted of a 30 m Rxi®-624Sil MS column (Restek Corporation) with an inner diameter of 0.250 mm and a film thickness of 1.40  $\mu\text{m}$ . The second dimension (2D) column consisted of a 2 m Stabilwax® column (Restek Corporation) with an inner diameter of 0.250 mm and a film thickness of 0.25  $\mu\text{m}$ . A helium carrier gas (high purity, Praxair Canada Inc., Trois-Rivieres, Québec, Canada) was used at a constant pressure of 17.8 psi. The first dimension oven temperature was held at 35°C for 7 minutes, then increased to 230°C at a rate of 4°C/min and held for an additional 5 minutes. The second dimension oven temperature was set at 15°C while the modulator oven temperature was at 5°C. The modulation period was 4 seconds with hot pulses every 1.2 seconds and a cool time of 0.8 seconds between stages. An acquisition rate of 250 spectra per second was set to target a mass acquisition range of 29 to 450 amu. The emission current for the ion source was set at 1mA, while the source temperature was held at 250°C with an electron ionization energy at 70 eV.

#### 2.3.2. Data Analysis

Data acquisition and analysis was performed using ChromaTOF® (version 5.51, LECO). Data were processed in two steps: (1) non-targeted deconvolution (NTD®) peak finding with integration

baseline, (2) GC×GC subpeak combining; and library searching. A minimum signal to noise ratio of 100 was applied for peak finding along with an ‘auto-calculated’ setting selected for integration baseline. A minimum threshold of 650 spectral matches was set for GCxGC subpeak combining with a minimum similarity set to 600 spectral matches. Library matches were established using the National Institute of Standards and Technology (NIST) Mass Spectral Library with a mass spectral match threshold of 75% and first-dimension linear temperature-programmed retention indices (LTPRI; ±10 required) matches. Processed data for each sample were copied into Excel worksheets with the following columns: “Peak Number”, “Sample”, “Name”, “Formula”, “1<sup>st</sup> Dimension”, “2<sup>nd</sup> Dimension”, “Similarity”, “Area”, “Height”, “Quant Masses”, “Base Mass”, “Quant S/N”, and “Peak S/N”.

Further statistical analysis was performed using custom R programming scripts with R Studio® (version 2023.03.0+386; R Studio®). The exported Excel sheets were loaded and processed into .rda objects in R Studio®. Sample classes were created with each class representing a group of replicate samples. This allowed the comparison between different sample classes. Control samples were compared to each class of experiment samples independently. Peak areas were normalized with a bromobenzene reference standard. Compounds were retained if they were unique to the samples and/or had a signal-to-noise ratio of at least two times that of control samples. Compounds such as bromobenzene, oxygen, acetone, methanol, and silica-containing were removed along with unidentified peaks following NIST library matches. Following this process, all individual animal and human sample data frames were merged into respective files comprising a list of compounds identified across each animal sample and across all human samples. Files were exported as .csv files then converted to .xlsx files via Microsoft® Excel.

Data visualization was achieved using Principal Component Analysis (PCA) using the The Unscrambler® (Version 11 CAMO software) for the final list of analytes established. This multivariate data analysis is used dimensionality of the data is high and where the possibility of replication is low.<sup>88,89</sup> Data is visualized across multiple principal components (PC). Each principal component is accompanied with a loading depicting its significance. The abundance of information available decreases as the PCs increase i.e. PC-1 provides more information than PC-2. The explained variance of the scores is provided in percentage values.

## **2.4. Dog Trials**

### 2.4.1. Ethics

The animal ethics approval for conducting an observational study with working dogs was obtained from *le comité de bons soins aux animaux* at UQTR with the certificate number 2022-S.F.3.

### 2.4.2. Human Remains Detection Dogs and Training Sessions

Two series of dog trials were conducted at the OPP headquarters in Orillia, Ontario. The first series of dog trials took place in February 2022, and the second in May 2022. The first series of dog trials involved two OPP handlers and their certified HRD dogs. The second series of dog trials involved 5 canine handlers from various law enforcement agencies and their certified police dogs. HRD dog and canine handler information and training session attendance is summarized in Table 2.3. Trials of all series consisted of single-blind indoor scenarios. In this setting, only the individual conducting the experiment was aware of the training aid and/or animal bone location. The first indoor scenarios were set up in an OPP ‘Imprint Room’ (Figure 2.2a), and the second scenarios in a carousel room (Figure 2.2b). Distracting odors such as dog food, treats, kongs, candy, etc. were used and placed in either boxes or metal cans depending on the scenario. One scenario consisted of placing one HRD training aid and one animal bone in the room. A second scenario consisted of placing one HRD training aid and two animal bones in the room. A final scenario consisted of placing an animal bone only in the room. During each trial and for every scenario, canine handlers had the choice between allowing their canine to search off-leash with their handler monitoring from the doorway or working on-leash with their handler entering the room. Once a final response was given by the canine, the canine handler would request HRD target confirmation prior to rewarding the canine.

**Table 2.3** Participating HRD dogs in OPP Canine Unit training trials performed in February 2022 and May 2022.

<b>Dog ID#</b>	<b>Dog 1</b>	<b>Dog 2</b>	<b>Dog 3</b>	<b>Dog 4</b>	<b>Dog 5</b>
Canine Handler Agency	OPP	OPP	Durham Regional Police	MetroLinx	MetroLinx
Age at the time of their first training session	2 yo	6 yo	6 yo	3 yo	2 yo
Gender	Male	Male	Male	Male	Male
Breed	Labrador	Labrador	Belgian Malinois	Belgian Malinois	Labrador
Years of experience in HRD work	1	5	1.5	2	<1
Training	HRD	HRD	HRD	HRD	HRD
Final response	Sit	Sit	Sit	Freeze	Sit
Training trial attendance	02/22, 05/22	02/22, 05/22	05/22	05/22	05/22



Dog responses were recorded as follows:

**True Positive** Dog alerted to exact location of the hide

**Partial Positive** Behavioral change noted, dog did not alert to exact location of the hide

**False Positive** Dog alerted to a location without a hide

**False Negative** Dog did not alert to a hide location

The purpose of the dog trials was to investigate dog responses and/or behavioral changes when presented with animal remains in the presence of human remains. Dog responses were observed and noted along with the bone sample used in the training session.

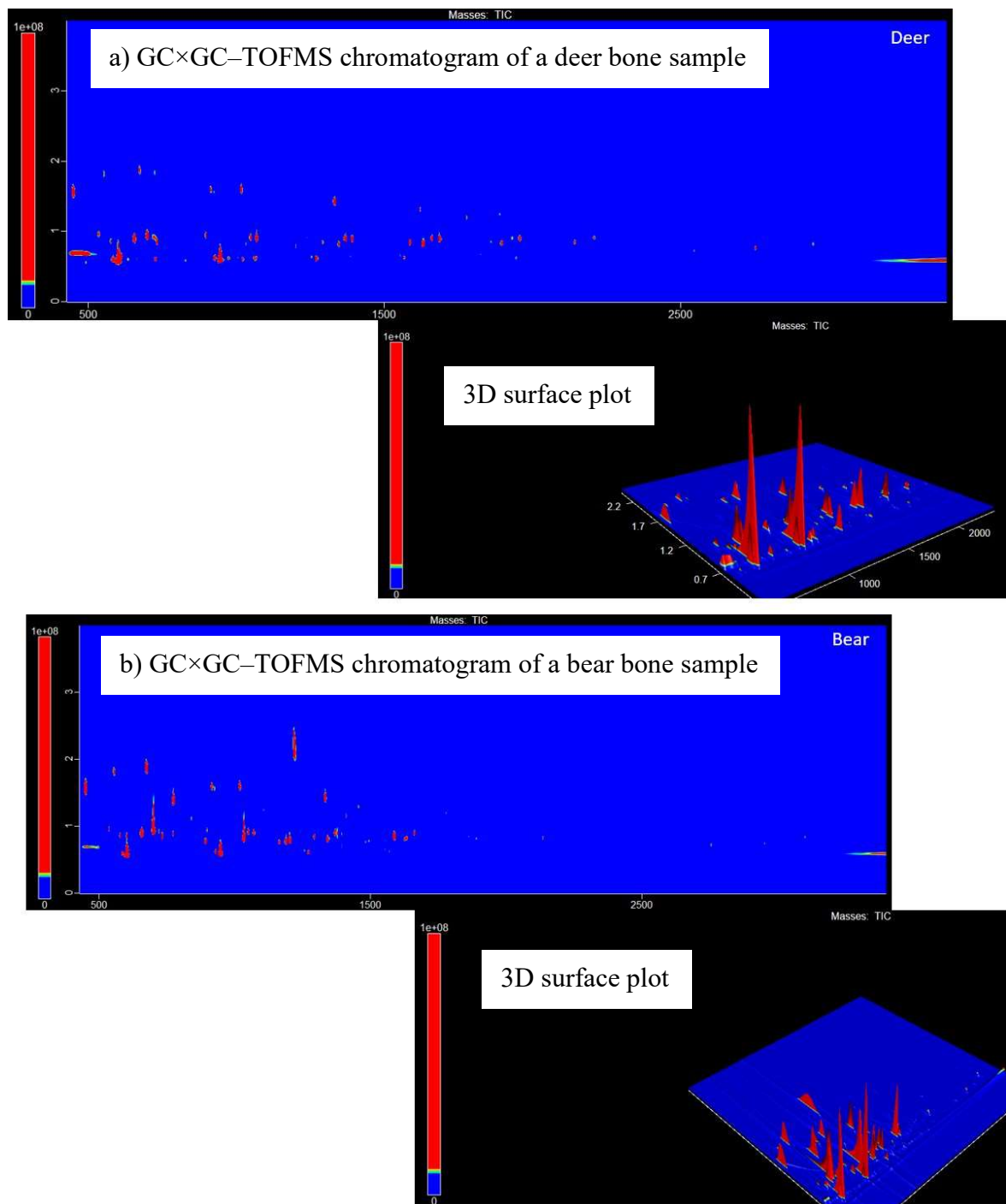


**Figure 2.2** (a) Indoor scenario set up in the ‘Imprint Room’, (b) Indoor scenario set up in the carousel room.

## **CHAPTER 3: RESULTS AND DISCUSSION**

### 3.1. Analytical Output

The output of a GCxGC-TOFMS run is illustrated in Figure 3.1. The separation of analytes on two columns results in two retention times along the X-axis plotted against the peak intensity along the Y-axis. The Z-axis can be seen in the 3D surface plot representing peak intensity with peak height reflecting analyte concentration. The second dimension column reveals analytes with identical and/or similar retention times allowing the identification of more than one compound for a specific retention time. This results in a more detailed VOC profile in comparison to a VOC profile established with conventional GC. The GCxGC chromatograms observed in Figure 3.1a and Figure 3.1b show the VOC profiles produced by a deer bone and a bear bone, respectively. In the case of the deer VOC profile, compounds were detected at various retention times throughout the entirety of the GCxGC-TOFMS chromatogram with a select few compounds displaying high concentrations. Meanwhile in the case of the bear VOC profile, most of the compounds were detected within the first 20 minutes of the GCxGC-TOFMS chromatogram with significantly fewer variations in analyte concentrations. The identification of VOCs relevant to advanced stages of decomposition was achieved with further data processing such as library and retention indices-based matches.



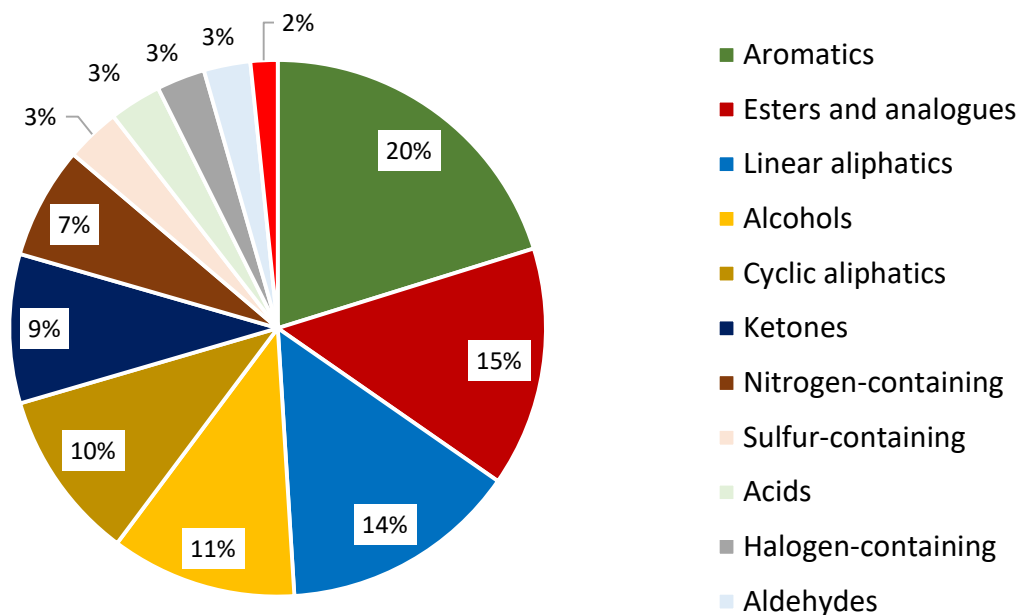
**Figure 3.1** Analytical output of GC×GC–TOFMS chromatograms of a) deer bone and b) bear bone showing the retention times plotted against the peak intensity and 3D surface plot (inserts) with peaks.

### 3.2. VOC profiles for HRD training aids

Thirteen HRD training aids, categorized as foot, ankle, and leg bones with little to no tissue remaining, used by the OPP Canine Unit were analyzed over a span of 8 months. This resulted in the odor analysis of 35 samples. Analysis of the samples resulted in the detection and identification of 857 VOCs, with the total number of VOCs varying for each sample. The lowest number of total VOCs for a single sample was 27 (ID# LB7 February 2022) and the highest number of total VOCs for a single sample was 268 (ID# FB6 October 2022). VOCs were classified into one of the following compound classes following detection: acids, alcohols, aldehydes, aromatics, cyclic aliphatics, esters and analogues, ethers, halogen-containing, ketones, linear aliphatics, nitrogen-containing, and sulfur-containing VOCs.

#### 3.2.1. Compound class abundance and prominent VOCs

This section discusses compound class abundance and prominent VOCs detected in all HRD training aids used in the dog trials for this study and by the OPP Canine Unit. Figure 3.2 illustrates the compound class abundance of the 857 VOCs detected across all HRD training aids sampled for this study. Aromatics were the most abundant class ( $n = 173$ ; 20%), followed by esters and analogues ( $n = 124$ ; 14%), linear aliphatics ( $n = 123$ ; 14%), alcohols ( $n = 96$ ; 11%), cyclic aliphatics ( $n = 88$ ; 10%), ketones ( $n = 77$ ; 9%), nitrogen-containing ( $n = 58$ ; 7%), sulfur-containing ( $n = 28$ ; 3%), acids ( $n = 27$ ; 3%), halogen-containing ( $n = 25$ ; 3%), aldehydes ( $n = 24$ ; 3%), and ethers ( $n = 14$ ; 2%).



**Figure 3.2** VOC abundance per compound class for HRD training aids.

Table 3.1 describes the 21 most prominent VOCs detected across all HRD training aid samples. These VOCs were detected in 18 or more samples (more than 50%) and are classified as acids, alcohols, aromatics, aldehydes, esters and analogues, ketones, linear aliphatics, sulfur-containing, and nitrogen-containing VOCs. Ethers and cyclic aliphatic VOCs comprised the least prominent compounds among HRD training aid samples. The five most frequently detected VOCs were 2-methyl-1-propanol, dimethyl disulfide, 3-methyl-1-butanol, 2-pentanol, and 2,6-lutidine. The role of specific prominent VOCs in human decomposition odour will be discussed in section 3.1.3.

**Table 3.1** 21 prominent VOCs detected in over 50% of HRD training aid samples analyzed between February 2022 and October 2022.

<b>Volatile organic compound</b>	<b>Compound class</b>	<b>Percentage of samples in which the VOC was detected</b>
1-Propanol, 2-methyl <sup>90</sup>	Alcohols	80.65%
Disulfide, dimethyl <sup>43,90</sup>	Sulfur-containing	74.19%
1-Butanol, 3-methyl <sup>90</sup>	Alcohols	67.74%
2-Pentanol <sup>90</sup>	Alcohols	67.74%
2,6-Lutidine	Aromatics	67.74%
1-Butanol, 3-methyl <sup>90</sup>	Alcohols	64.52%
Propanoic acid, 2-methyl <sup>90</sup>	Acids	64.52%
Dimethyl trisulfide <sup>43,90</sup>	Sulfur-containing	61.29%
Pyridine, 2,4-dimethyl-	Aromatics	61.29%
2-Hexanol <sup>43</sup>	Alcohols	58.06%
2-Pentanone, 3-methyl	Ketones	58.06%
1-Pentanol	Alcohols	54.84%
1-Butanol <sup>90</sup>	Alcohols	54.84%
Isopropyl acetate	Esters and analogues	54.85%
Propanoic acid <sup>43,90</sup>	Acids	54.84%
Pyridine, 2-methyl	Aromatics	54.84%
2-n-Butyl furan <sup>90</sup>	Aromatics	51.61%
4-Cyanocyclohexene	Nitrogen-containing	51.61%
Butanal, 3-methyl <sup>90</sup>	Aldehydes	51.61%
Butanoic acid <sup>90</sup>	Acids	51.61%
Hexane, 2,5-dimethyl-	Linear aliphatics	51.61%

### 3.2.1.1. Foot bones

Among the 35 HRD training aid samples, 24 were categorized as foot bones. The VOC profile of foot bone samples consisted of 800 VOCs. The total number of VOCs detected in the foot bone samples was significantly higher compared to the leg and ankle bone samples. The lowest number of total VOCs for a single foot bone sample was 28 (ID# FB12 May 2022) and the highest number of total VOCs for a single sample was 268 (ID# FB6 October 2022). Aromatics were the most abundant class ( $n = 162$ ; 20%), followed by esters and analogues ( $n = 120$ ; 15%), linear aliphatics ( $n = 118$ ; 15%), alcohols ( $n = 85$ ; 11%), cyclic aliphatics ( $n = 84$ ; 11%), ketones ( $n = 68$ ; 9%), nitrogen-containing ( $n = 57$ ; 7%), sulfur-containing ( $n = 25$ ; 3%), acids ( $n = 24$ ; 3%), halogen-containing ( $n = 21$ ; 3%), aldehydes ( $n = 19$ ; 2%), and ethers ( $n = 14$ ; 2%).

### 3.2.1.2. Leg bones

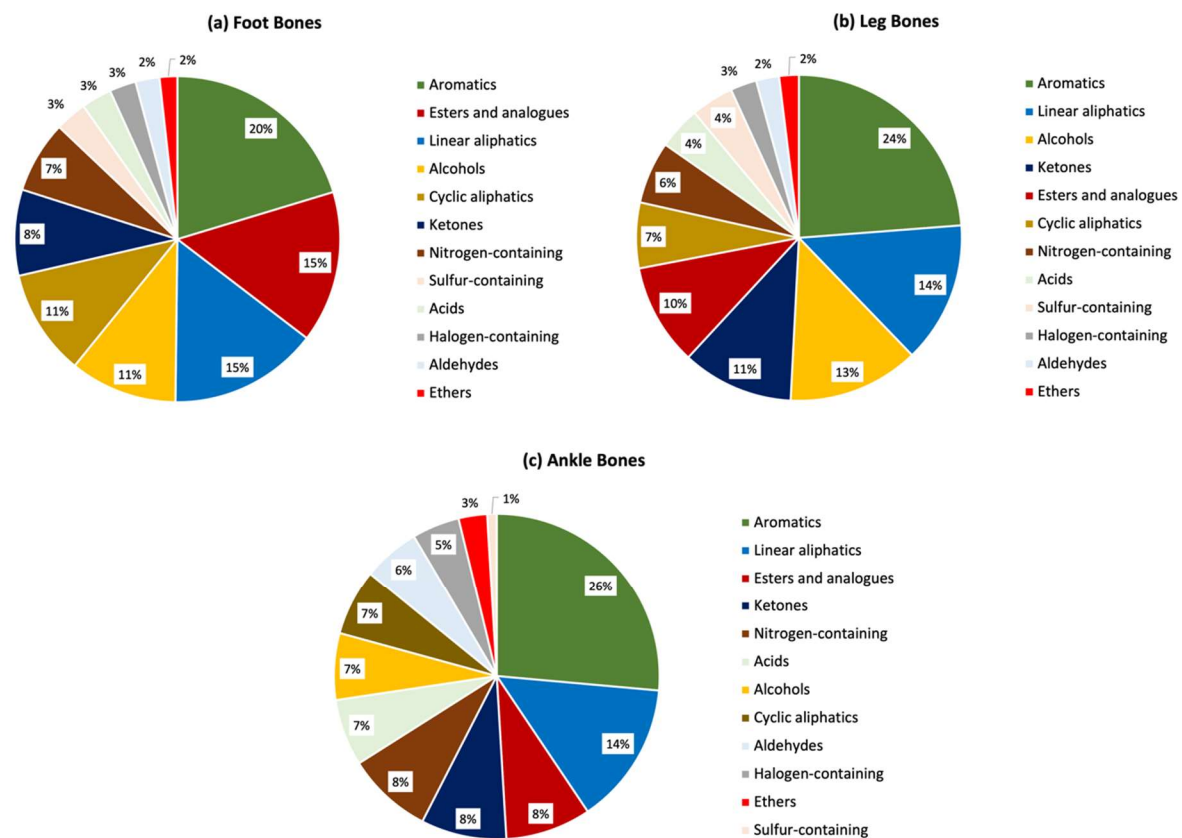
Among the 35 HRD training aid samples, five were categorized as leg bones. The VOC profile of leg bone samples consisted of 308 VOCs. The lowest number of total VOCs for a single leg bone sample was 27 (ID# LB7 February 2022) and the highest number of total VOCs for a single sample was 186 (ID# LB7 November 2022). Aromatics were the most abundant class ( $n = 73$ ; 24%), followed by linear aliphatics ( $n = 43$ ; 14%), alcohols ( $n = 40$ ; 13%), ketones ( $n = 34$ ; 11%), esters and analogues ( $n = 31$ ; 10%), cyclic aliphatics ( $n = 20$ ; 6%), nitrogen containing ( $n = 19$ ; 6%), acids ( $n = 13$ ; 4%), sulfur-containing ( $n = 13$ ; 4%), halogen-containing ( $n = 8$ ; 3%), aldehydes ( $n = 7$ ; 2%), and ethers ( $n = 6$ ; 2%).

### 3.2.1.3. Ankle bones

Among the 35 HRD training aid samples, two were categorized as ankle bones. The VOC profile of ankle bone samples consisted of 107 VOCs, the lowest number of total VOCs detected compared to the foot and leg bone samples. The lowest number of total VOCs for a single ankle bone sample was 54 (ID# AB8 May 2022) and the highest number of total VOCs for a single sample was 59 (ID# AB8 November 2022). Aromatics were the most abundant class ( $n = 28$ ; 26%), followed by linear aliphatics ( $n = 15$ ; 14%), esters and analogues ( $n = 9$ ; 8%), ketones ( $n = 9$ ; 8%), nitrogen-containing ( $n = 9$ ; 8%), acids ( $n = 7$ ; 7%), alcohols ( $n = 7$ ; 7%), cyclic



aliphatics ( $n = 7$ ; 7%), aldehydes ( $n = 6$ ; 6%), halogen-containing ( $n = 5$ ; 5%), ethers ( $n = 3$ ; 3%), and sulfur-containing ( $n = 1$ ; 1%). Figure 3.3. illustrates the compound class abundance of the VOCs detected in each HRD training aid category sampled for this study.



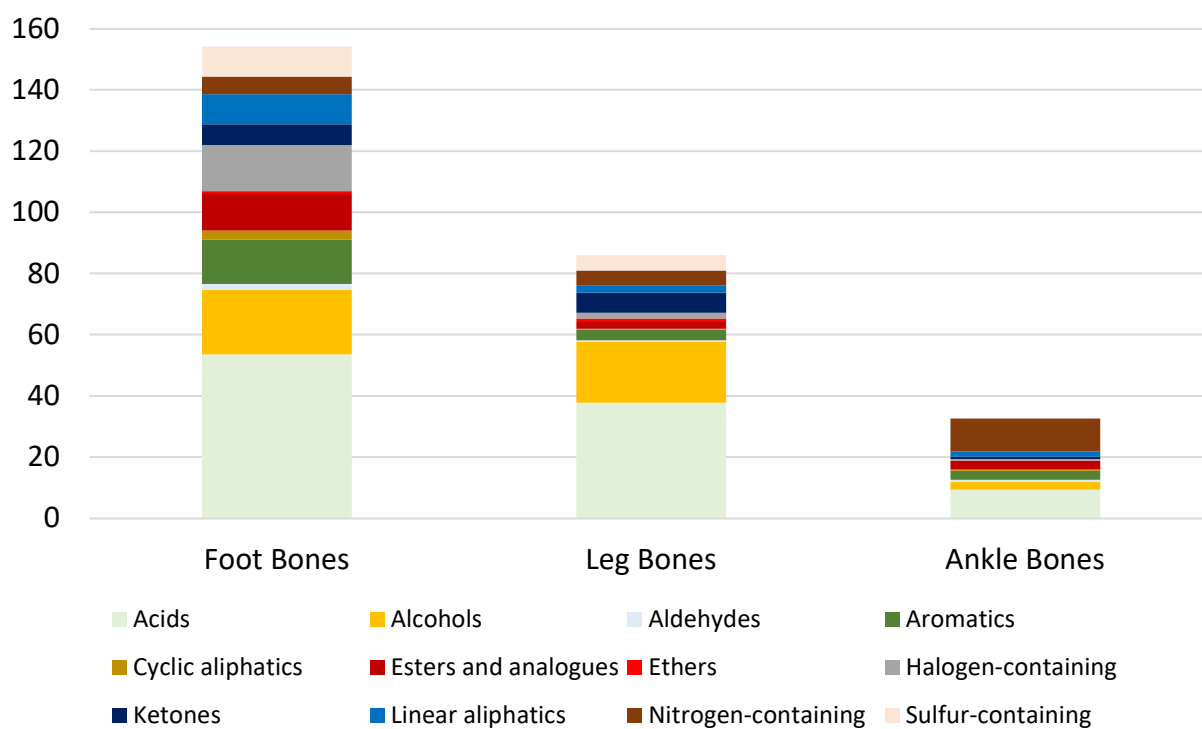
**Figure 3.3.** VOC abundance per compound class for each HRD training aid category (a) foot bones, (b) leg bones, and (c) ankle bones.

### 3.2.2. Normalized area based concentrations

To study the relative class concentration of compound classes present in each sample, a semi-quantitative approach was used. The normalization of VOCs detected in each sample was accomplished using bromobenzene as an internal standard.

The sum of average normalized areas indicating the relative class concentrations for all compound classes in each type of HRD training aids analyzed between February 2022 to October 2022 are illustrated in Figure 3.4. HRD training aids were categorized as foot bones, ankle bones, and leg

bones. The foot bone samples showed the highest relative class concentration of all compound classes in comparison to the ankle and leg bones. Acid VOCs had the highest relative class concentration for each sample, followed by alcohol VOCs for leg bones and foot bones only. Aromatic VOCs showed the second highest relative class concentration in the ankle bone samples. Aldehyde, halogen-containing, and nitrogen-containing VOCs were not present in the ankle bone samples. Aldehyde, cyclic aliphatic, and nitrogen-containing VOCs had the lowest relative class concentration in the foot bone samples. For the leg bone samples, aldehyde, cyclic aliphatic, ether, halogen-containing, and nitrogen-containing VOCs had the lowest relative class concentration.



**Figure 3.4** Sum of average normalized areas indicating the relative class concentrations for all compound classes in all HRD training aids.

### 3.2.3. Discussion

The purpose of this part of the study was to establish a VOC profile for HRD training aids routinely used by the OPP Canine Unit. The analysis of thirteen HRD training aids over a period of eight months resulted in the detection and identification of 857 VOCs. No significant variation was

observed in the presence of compounds as well as their relative class concentrations over the sampling period. As such, the effects of ageing on VOC profiles are not reported herein.

When comparing VOC profiles for each category (foot, leg, and ankle bones) of HRD training aids (see Figure 3.3), the trends in compound class abundance were similar despite variations in the number of VOCs detected for each category. Aromatics and linear aliphatic VOCs consisted of high abundance compounds while low abundance compounds belonged to ethers, aldehydes, sulfur-containing, and halogen-containing VOCs. Subtle variations are observed in alcohols and acids. Alcohols were less abundant and acids were more abundant in HRD training aids categorized as ankle bones in comparison to foot and leg bones.

The HRD training aids categorized as foot bones had the highest class concentration while the HRD training aids categorized as ankle bones had the lowest class concentration. This occurrence can also be observed for compound class abundances. A greater number of total VOCs detected (800 VOCs detected in foot bones samples vs. 107 VOCs detected in ankle bone samples) can impact relative VOC concentration. In addition, only three HRD training aids were categorized as ankle bones, whereas 26 were categorized as foot bones. Leg bones made up six out of the 35 HRD training aid samples leading to the detection of 308 VOCs. The number of total VOCs detected increased more than two-fold when the number of samples doubled.

Each HRD training aid sample had similar storage conditions in which they were placed in glass containers at room temperature. Samples containing more soft tissue on the bone(s) may result in a greater release of VOCs leading to higher relative class concentrations. In this study, foot bones identified as FB2, FB5.1, FB5.2, and FB6 had significant amounts of tissue remaining and/or decomposition fluid present in their storage containers. This is consistent with the higher values in abundances and relative class concentrations obtained for the foot bone samples. Conversely, the ankle bone identified as AB8 with no tissue remaining and free of decomposition fluid produced the least number of VOCs and had a lower relative class concentration. These results demonstrate the impact of soft tissue and decomposition fluid on VOC production.

A study conducted by Hoffman et al., investigated the presence of VOCs in the headspace of different tissue types of decomposing human remains.<sup>43</sup> A greater number of VOCs was detected

in fat tissue (22 VOCs) in comparison to muscle and bone. None of the 33 key VOCs measured were detected in the bone sample known to come from vertebrae. In the second bone sample, nine out of the 33 key VOCs were detected. Among the key VOCs measured, four compounds (dimethyl disulfide, 2-hexanol, 1-pentanol, and propanoic acid) were also reported in the current study and listed as some of the most prominent compounds detected across all HRD training aids.

The five most frequently detected VOCs were 2-methyl-1-propanol, dimethyl disulfide, 3-methyl-1-butanol, 2-pentanol, and 2,6-lutidine. Like other pyridine derivatives, 2,6-lutidine has previously been reported in odor decomposition studies.<sup>90</sup> Sulfur-containing VOCs, such as dimethyl disulfide, are repeatedly reported in odor decomposition studies as they significantly contribute to the potent smell associated with human decomposition.<sup>90</sup> The presence of 2-methyl-1-propanol may be due to the location in which the amputated limbs were placed to decompose. Studies have reported 2-methyl-1-propanol in the headspace and soil surrounding decomposing human remains.<sup>22,31,55</sup> Carbohydrate degradation combined with bacterial activity leads to the production of particular alcohols, such as 2-methyl-1-propanol, 3-methyl-1-butanol, and 2-pentanol.<sup>21,22,87</sup>

The use of amputated limbs as HRD training aids by the OPP Canine Unit has recently been validated.<sup>85</sup> Dargan et al. discussed non-decomposition-related compounds present in the headspace of HRD training aids potentially due to the administration of anesthesia prior to amputation surgery. Sevoflurane, an anesthetic agent, was identified in 55% of bone samples in their study.<sup>85,91</sup> The authors suggested storing samples at room temperature to decrease the concentration of sevoflurane. HRD training aids used in the current study, some of which were also sampled in the previously mentioned study, were stored at room temperature. Sevoflurane was not detected in any of the HRD training aids following odor analysis. Results from this study support the suggested storage conditions. The presence of VOCs related to surgical procedures and/or medical treatments should continue to be considered in future decomposition studies.

### **3.3. VOC profiles for animal bones**

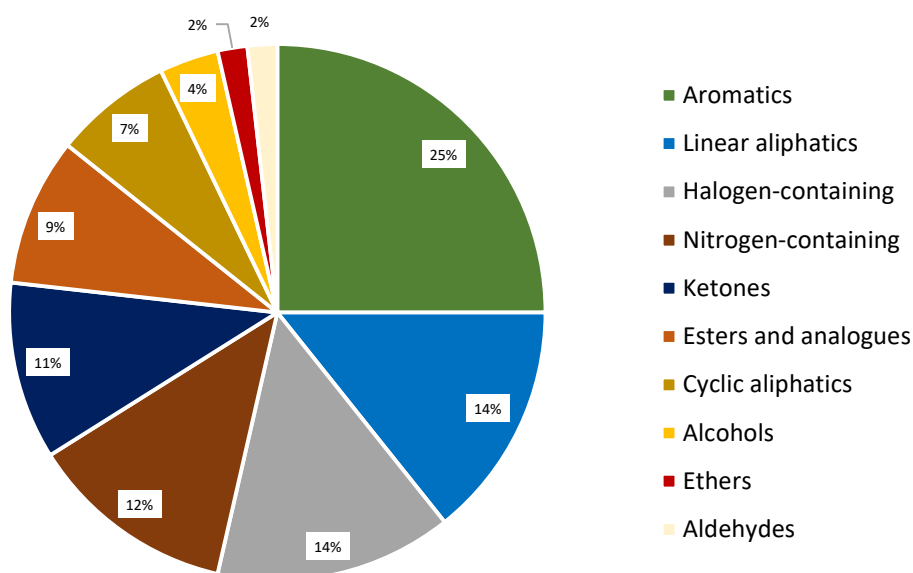
Four pig bones, four moose bones, one deer bone, and one bear bone were analyzed over a span of 8 months (Table 2.1). This resulted in the odor analysis of 43 samples. VOCs were classified into of the following compound classes following detection: acids, alcohols, aldehydes, aromatics,

cyclic aliphatics, esters and analogues, ethers, halogen-containing, ketones, linear aliphatics, nitrogen-containing, and sulfur-containing VOCs.

### 3.3.1. Compound class abundance

#### 3.3.1.1. Pig bone samples

Figure 3.5 illustrates the compound class abundance of the 56 VOCs detected in at least 30% of pig bone samples analyzed in this study. Aromatics were the most abundant class ( $n = 14$ ; 28%), followed by linear aliphatics ( $n = 8$ ; 16%), halogen-containing ( $n = 8$ ; 16%), nitrogen-containing ( $n = 7$ ; 14%), ketones ( $n = 6$ ; 12%), esters and analogues ( $n = 5$ ; 10%), cyclic aliphatics ( $n = 4$ ; 8%), alcohols ( $n = 2$ ; 4%), ethers ( $n = 1$ ; 2%), and aldehydes ( $n = 1$ ; 2%).

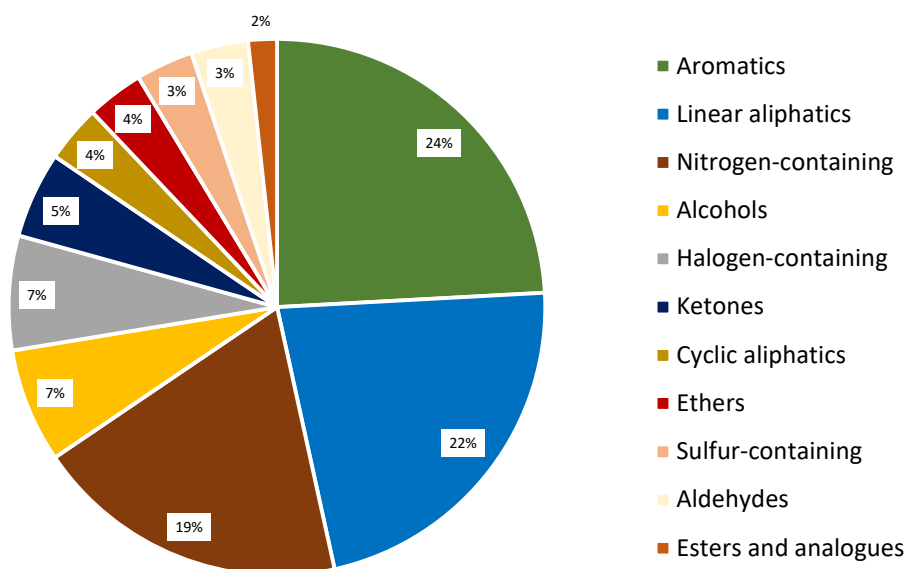


**Figure 3.5** VOC abundance per compound class for pig bone samples.

#### 3.3.1.2. Moose bone samples

Figure 3.6 illustrates the compound class abundance of the 58 VOCs detected in at least 30% of moose bone samples analyzed in this study. Aromatics were the most abundant class ( $n = 14$ ; 24%), followed by linear aliphatics ( $n = 13$ ; 18%), nitrogen-containing ( $n = 11$ ; 22%), alcohols

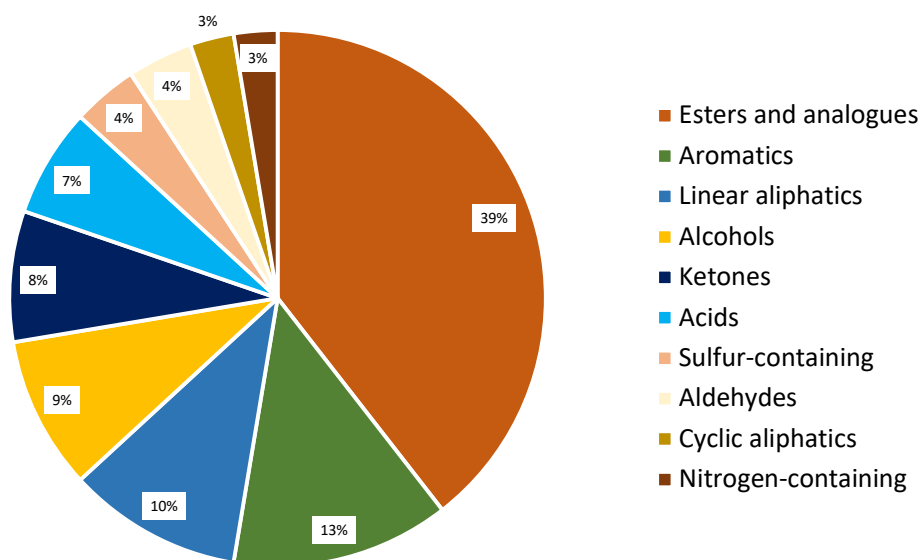
( $n = 4$ ; 19%), halogen-containing ( $n = 4$ ; 7%), ketones ( $n = 3$ ; 7%), cyclic aliphatics ( $n = 2$ ; 3%), ethers ( $n = 2$ ; 3%), sulfur-containing ( $n = 2$ ; 3%), aldehydes ( $n = 2$ ; 3%), and esters and analogues ( $n = 1$ ; 2%).



**Figure 3.6** VOC abundance per compound class for moose bone samples.

### 3.3.1.3. Bear bone samples

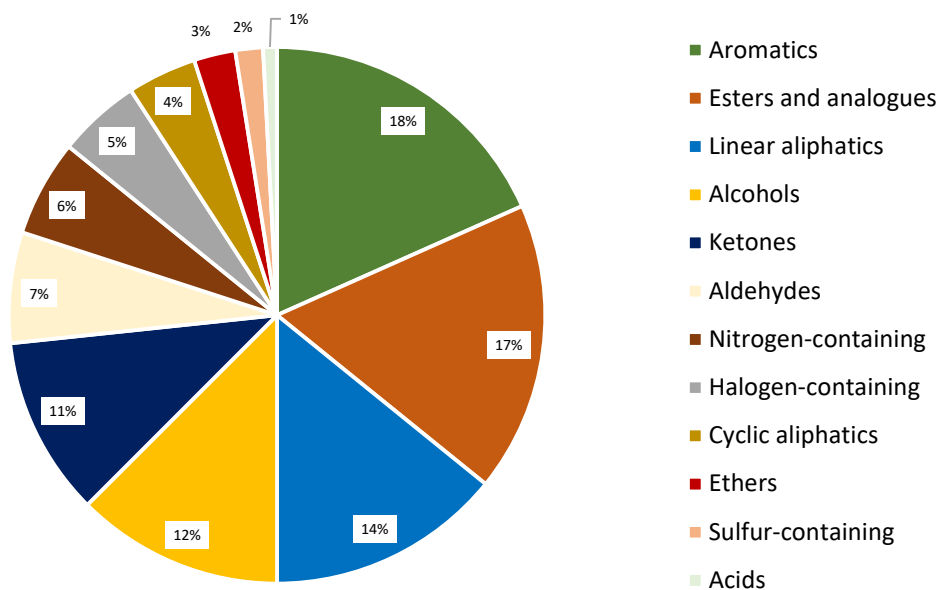
Figure 3.7 illustrates the compound class abundance of the 76 VOCs detected in at least 30% of bear bone samples analyzed in this study. Esters and analogues were the most abundant class ( $n = 30$ ; 39%), followed by aromatics ( $n = 10$ ; 13%), linear aliphatics ( $n = 8$ ; 11%), alcohols ( $n = 7$ ; 9%), ketones ( $n = 6$ ; 8%), acids ( $n = 5$ ; 7%), sulfur-containing ( $n = 3$ ; 4%), aldehydes ( $n = 3$ ; 4%), cyclic aliphatics ( $n = 2$ ; 3%), and nitrogen-containing ( $n = 2$ ; 3%) VOCs.



**Figure 3.7** VOC abundance per compound class for bear bone samples.

#### 3.3.1.4. Deer bone samples

Figure 3.8 illustrates the compound class abundance of the 120 VOCs detected in at least 30% of deer bone samples analyzed in this study. Aromatics were the most abundant class ( $n = 22$ ; 18%), followed by esters and analogues ( $n = 21$ ; 18%), linear aliphatics ( $n = 17$ ; 14%), alcohols ( $n = 15$ ; 13%), ketones ( $n = 13$ ; 11%), aldehydes ( $n = 8$ ; 7%), nitrogen-containing ( $n = 7$ ; 6%), halogen-containing ( $n = 6$ ; 5%), cyclic aliphatics ( $n = 5$ ; 4%), ethers ( $n = 3$ ; 3%), sulfur-containing ( $n = 2$ ; 2%), and acids ( $n = 1$ ; 1%).



**Figure 3.8** VOC abundance per compound class for deer bone samples.

### 3.3.2. Normalized area based concentrations

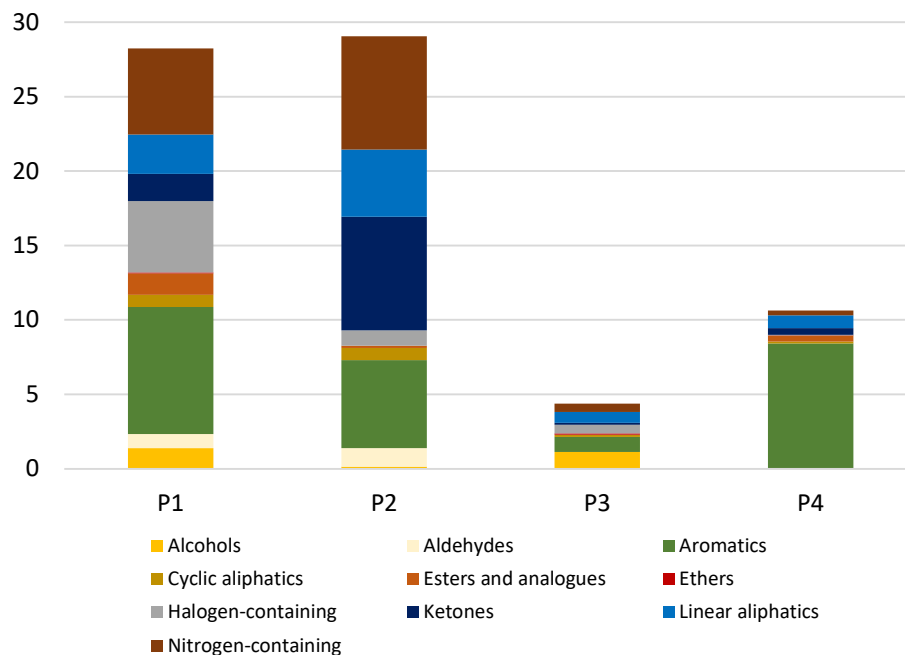
To study the relative class concentration of compound classes present in each sample, a semi-quantitative approach was used. The normalization of VOCs detected in each sample was accomplished using bromobenzene as an internal standard.

#### 3.3.2.1. Pig bone samples

The sum of average normalized areas indicating the relative class concentrations for all compound classes in each pig bone sample are illustrated in Figure 3.9. P1 and P2 samples presented with the highest relative class concentration of all compound classes in comparison to P3 and P4 samples. P1, P2, P3, and P4 are categorized as leg bone, rib, rib, and vertebrae, respectively. Aromatics, nitrogen-containing VOCs and halogen-containing VOCs showed the highest relative class concentration in P1 samples. Ketones, nitrogen-containing VOCs, and aromatics showed the highest relative class concentration in P2 samples. Ethers, acids, and sulfur-containing VOCs were not detected in P2 samples. Alcohols and aromatics showed the highest relative concentration in P3 samples. Aldehydes, acids, and sulfur-containing VOCs were not detected in P3 samples.



Aromatics showed the highest relative concentration in P4 samples. Alcohols, acids, aldehydes, and sulfur-containing VOCs were not detected in P4 samples.

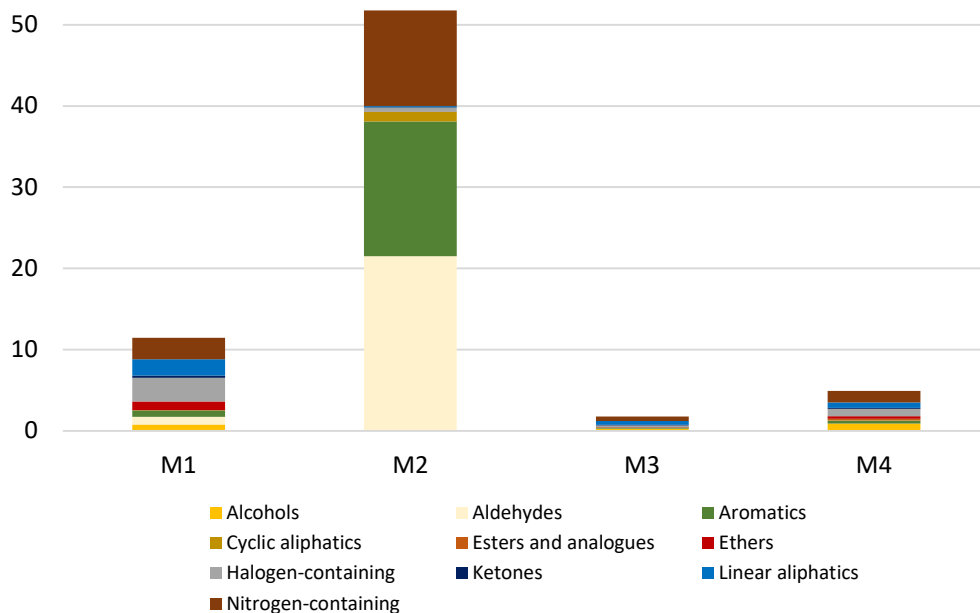


**Figure 3.9** Sum of average normalized areas indicating the relative class concentrations for all compound classes in all pig bone samples

### 3.3.2.2. Moose bone samples

The sum of average normalized areas indicating the relative class concentrations for all compound classes in each moose bone sample are illustrated in Figure 3.10. M2 samples showed the highest relative class concentration of all compound classes in comparison to M1, M3, and M4 samples. M1, M2, M3, and M4 are categorized as long bone, vertebrae, vertebrae, and rib, respectively. Halogen-containing VOCs, linear aliphatics, and nitrogen-containing VOCs showed the highest relative class concentration in M1 samples. Aldehydes, aromatics, and nitrogen-containing VOCs showed the highest relative class concentration in M2 samples. Alcohols, ethers, ketones, acids, and sulfur-containing VOCs were not detected in M2 samples. Nitrogen-containing VOCs and linear aliphatics showed the highest relative class concentration in M3 samples. Aldehydes, acids, and sulfur-containing VOCs were not detected in M3 samples. Nitrogen-containing VOCs,

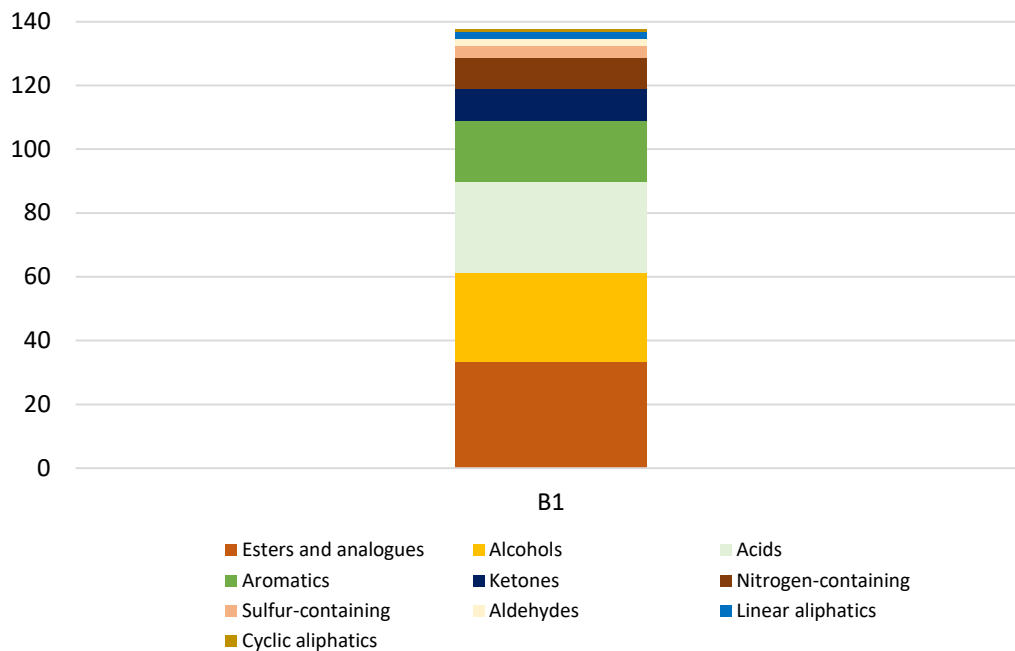
halogen-containing VOCs, and alcohols showed the highest relative class concentration in M4 samples. Aldehydes, acids, and sulfur-containing VOCs were not detected in M4 samples.



**Figure 3.10** Sum of average normalized areas indicating the relative class concentrations for all compound classes in all moose samples

### 3.3.2.3. Bear bone samples

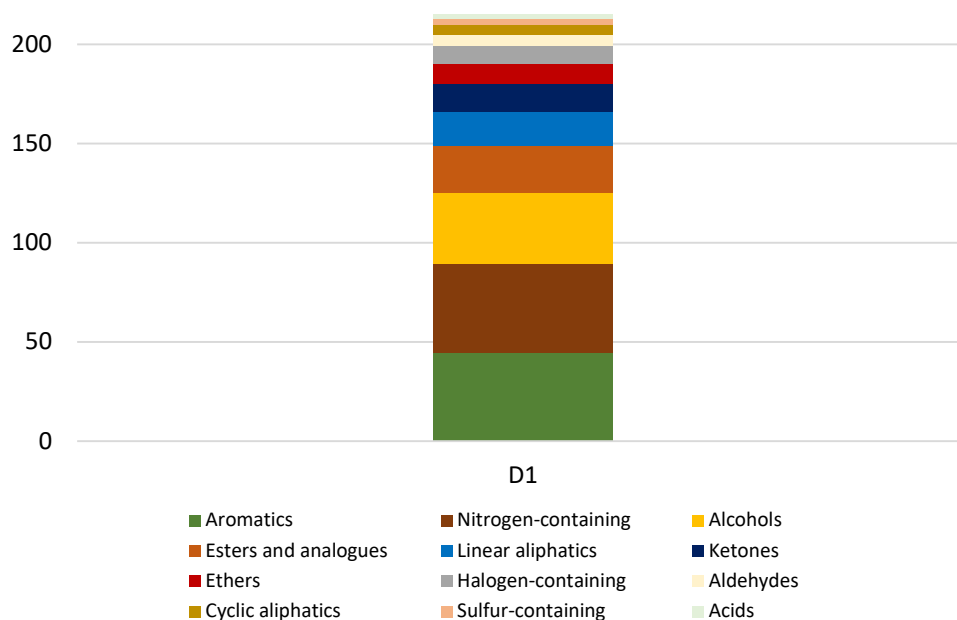
The sum of average normalized areas indicating the relative class concentrations for all compound classes in the bear bone sample are illustrated in Figure 3.11. The bear bone sample (ID# B1) is categorized as long bone. Esters and analogues, alcohols, and acids showed the highest relative class concentration, whereas aldehydes, linear and cyclic aliphatics showed the lowest relative class concentration. Ethers and halogen-containing VOCs were not detected.



**Figure 3.11** Sum of average normalized areas indicating the relative class concentrations for all compound classes in all bear bone samples

#### 3.3.2.4. Deer bone samples

The sum of average normalized areas indicating the relative class concentrations for all compound classes in the deer bone sample are illustrated in Figure 3.12. The deer bone sample (ID# D1) is categorized as long bone. Aromatics, nitrogen-containing VOCs and alcohols showed the highest relative class concentration, whereas cyclic aliphatics, sulfur-containing VOCs, and acids showed the lowest relative class concentration.



**Figure 3.12** Sum of average normalized areas indicating the relative class concentrations for all compound classes in all deer bone samples.

### 3.3.3. Discussion

The purpose of this part of the study was to establish VOC profiles for a variety of animal species, namely pig, moose, deer, and bear. The analysis of four pig bones, four moose bones, one deer bone, and one bear bone over a span of 8 months resulted in the detection and identification of a combined 1,332 VOCs. No significant variation was observed in the presence of compounds as well as their relative class concentrations over the sampling period. Therefore, the effects of ageing on VOC profiles are not reported herein.

The pig bone samples produced the greatest number of VOCs (515 VOCs), followed by moose bone samples (309 VOCs), deer bone samples (285 VOCs), and bear bone samples (223 VOCs). With the exception of the bear bone samples, aromatics were the most abundant compound class across the animal bone samples (see Figures 3.4-3.7). Low abundance compounds varied for each odor profile. Similarly, the general trend for relative class concentration varied for each odor profile. While some compound classes showed high abundance, they had a low relative class concentration, and vice versa. A variation in relative class concentration is also observed in

different sample types for the same animal species. For example, pig samples labelled as P1 and P2 showed the highest relative class concentration of all compound classes in comparison to P3 and P4 samples. P1, P2, P3, and P4 are categorized as leg bone, rib, rib, and vertebrae, respectively. A similar variation can be observed in moose bone samples where samples labelled as M2 showed the highest relative class concentration of all compound classes among the moose bone samples. M1, M2, M3, and M4 are categorized as long bone, vertebrae, vertebrae, and rib, respectively. Variations in carrion decomposition processes may explain these differences. Additionally, body mass has been reported to affect the rate of decomposition.<sup>92-94</sup> Evidently, smaller carcasses tend to decompose at a faster rate than larger carcasses. Variations in the length of each stage of decomposition have also been reported. For example, larger carcasses may remain in the stage of active decay for a longer period in comparison to smaller carcasses.<sup>93</sup> Bear, pig, moose, and deer all vary in size. Therefore, differences in their respective odor profiles are to be expected.

Different storage sample containers may have effects on the analysis of volatile organic compounds. Animal bones used in this study were either stored in Mason jars, metal cans, or biohazard bags at room temperature. Of the four moose bone samples, half were stored in separate biohazard bags, one in a metal can, and the fourth sample in a Mason jar. It has been previously reported that polymer bags, such as biohazard bags, do not guarantee the absence of possible contaminating substances nor the proper confinement of VOCs.<sup>95</sup> Moose samples labelled as M3 and M4 were stored in biohazard bags and reported the least amount of VOCs when compared to M1 and M2 samples. Additionally, metal canisters have been shown to release VOCs from the container material itself.<sup>96</sup> This may explain the increased relative class concentration of all compound classes reported in M2 samples in comparison to all other moose samples.

The following eight compounds were identified in each animal sample set: 1-tetradecene, 2-octanone, 4-hydroxy-4-methyl-2-pentanone, 4-cyanocyclohexene, 2-pentyl-furan, 2,2,4-trimethyl-hexane, nonanal, and 2,3-dimethyl pentane (Appendix A). Aldehydes, such as nonanal, and hydrocarbons have been reported in skeletal material of pig, deer, and dog.<sup>97,98</sup> The presence of these compounds along with furans increases as decomposition progresses.<sup>97</sup> Nonanal has previously been reported in decomposition studies using chicken, cow, and pig bone samples.<sup>42</sup> The nitrogen-containing compound 4-cyanocyclohexene was detected across both the HRD training

aids and animal bone samples. Its presence should not be associated to decomposition odor as it has been reported to be a possible contaminant from nitrile gloves.<sup>99,100</sup>

It is important to note the absence of specific compound classes for each animal sample set. The pig and moose bone samples lacked acids and sulfur-containing VOCs overall. Previous decomposition studies using human analogues have also reported the lack of acids in pig and cow bones.<sup>83</sup> The moose bone samples also lacked aldehydes while bear bone samples lacked ethers and halogen-containing VOCs. However, compounds belonging to each compound class were identified in the deer bone samples. The presence and/or absence of specific compound classes may have been influenced by several factors such as: storage conditions, age of bone, primary location of decomposition, and animal nutrition.

Studies have shown that the release of VOCs from both animal and human remains changes over time.<sup>101,102</sup> In a study investigating the impact of different biotopes on VOCs released by decaying pigs, variations in decomposition processes and VOC production were due to different surrounding environments.<sup>101</sup> The pig bones used in this current study were allowed to decompose at the REST[ES] facility located in Bécancour, Québec, while the moose bones were found at a different location within the same facility. The deer and bear bones were acquired in Orillia, Ontario, at a later time. Thus, differences in environment as well as time spent outdoors may have impacted the presence and/or concentration of cadaveric VOCs.

### **3.4. Human vs. Animal**

One of the main objectives of this study was to compare VOC profiles of HRD training aids and animal remains. The previous sections reported VOC profiles for HRD training aids and pig, moose, deer, and bear bones. This section aims to compare these reported results in order to highlight the similarities and differences between the VOC profiles of HRD training aids and selected animal bones.

### 3.4.1. VOC profiles of HRD training aids and animal bones

A total of 857 VOCs were detected across all HRD training aids (800 VOCs detected in foot bone samples, 308 VOCs in leg bone samples, 107 VOCs detected in ankle bone samples), while 515 VOCs were detected in the pig bone samples, 309 VOCs in the moose bone samples, 223 VOCs in the bear bone samples, and 285 VOCs in the deer bone samples. The significant difference in VOC production from the HRD training aids in comparison to the animal bone samples may be a result of differences in bone type and variability in processes of decomposition. Of the 800 VOCs detected in the HRD training aids categorized as foot bones, 268 VOCs were in common with the pig bone samples, 226 VOCs were in common with the moose bone samples, 215 VOCs were in common with the deer bone sample, and 202 VOCs were in common with the bear bone sample. Of the 308 VOCs detected in the HRD training aids categorized as leg bones, 148 VOCs were in common with the pig bone samples, 126 VOCs were in common with the moose bone samples, 124 VOCs were in common with the deer bone sample, and 114 VOCs were in common with the bear bone sample. Of the 107 VOCs detected in the HRD training aids categorized as ankle bones, 74 VOCs were in common with the pig bone samples, 61 VOCs were in common with the moose bone samples, 58 VOCs were in common with the deer bone sample, and 52 VOCs were in common with the bear bone sample.

676 VOCs were strictly detected in HRD training aids only. These compounds have the potential of being associated exclusively to human decomposition VOCs with further investigation. Table 3.2 lists the compounds present exclusively in HRD training aids and which were detected in at least 40% of HRD training aid samples ranging up to 55% and belong to the following classes: acids, aromatics, linear aliphatics, ethers, esters and analogues, ketones, and halogen-containing VOCs. Compounds present in over 55% of HRD training aid samples were also detected in at least one animal bone sample and were not included in Table 3.2. The purpose of Table 3.2 is to highlight prominent compounds exclusively detected in the HRD training aids.

**Table 3.2** Unique VOCs detected in over 40% of HRD training aids

Compound name	Compound class	Percentage of samples in which the VOC was detected
Propanoic acid <sup>90</sup>	Acids	54.84
Butanoic acid <sup>90</sup>	Acids	51.61
1-Pentanol, 4-methyl-	Alcohols	48.39
Butanoic acid, 2-methyl-	Acids	48.39
Butanoic acid, 2-methyl-, 1-methylethyl ester	Esters and analogues	48.39
Cyclopentane, 1-ethyl-3-methyl-, trans-	Cyclic aliphatics	48.39
Propanoic acid, 2-methyl-, 1-methylethyl ester <sup>90</sup>	Esters and analogues	48.39
2-Hexanone, 5-methyl-	Ketones	45.16
Benzene, 1,2,4,5-tetramethyl-	Aromatics	45.16
Butanoic acid, 3-methyl-	Acids	45.16
Naphthalene, 1,2,3,4-tetrahydro-	Aromatics	45.16
1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl-	Ethers	41.94
1H-Indene, 2,3-dihydro-4-methyl-	Aromatics	41.94
5,9-Undecadien-2-one, 6,10-dimethyl-	Ketones	41.94
Ethane, hexachloro-	Halogen-containing	41.94
Hexane, 3,4-dimethyl-	Linear aliphatics	41.94
Propane, 2,2-dimethoxy-	Ethers	41.94

Table 3.3 lists the compounds present in HRD training aids, each animal sample set, and reference compounds previously reported in both human and animal decomposition studies. These compounds were detected in at least 40% of HRD training aids and at least 10% of animal bone samples. The 14 VOCs listed belong to the following classes: aromatics, cyclic aliphatics, linear aliphatics, ketones, nitrogen-containing VOCs, and sulfur-containing VOCs.

**Table 3.3** Most prominent VOCs detected in HRD training aids and animal bone samples.

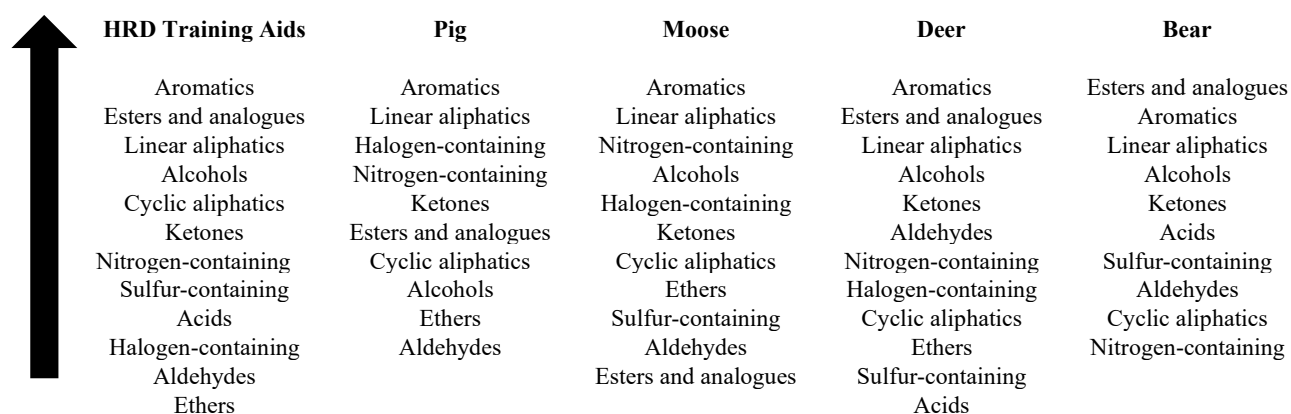
Compound	Compound class	Percentage of samples in which the VOC was detected (%)					Previously reported in literature as human and animal decomposition odour-related [31; 90; 102]
		HRD training aids	Pig	Moose	Bear	Deer	
Disulfide, dimethyl <sup>31,90,102</sup>	Sulfur-containing	71.19	14.29	19.05	100	100	[31; 90; 102]
4-cyanocyclohexene	Nitrogen-containing	51.61	28.57	28.57	100	75	
Hexane, 2,5-dimethyl-	Linear aliphatics	51.61	21.43	9.52	33.33	25	
Cyclopentane, ethyl-	Cyclic aliphatics	48.39	21.43	4.76	100	100	



Cyclopentanone, 2-methyl	Ketones	48.39	21.43	14.29	33.33	75	
Nonadecane <sup>31</sup>	Linear aliphatics	48.39	21.43	23.81	66.67	75	[31]
Pentane, 2,3,4-trimethyl- <sup>90</sup>	Linear aliphatics	48.39	21.43	9.52	33.33	25	[90]
Hexane, 2,4-dimethyl-	Linear aliphatics	45.16	21.43	9.52	33.33	25	
Indan, 1-methyl	Aromatics	45.16	21.43	4.76	33.33	25	
Indane	Aromatics	45.16	21.43	14.29	66.67	100	
Pentane, 2,3,3-trimethyl-	Linear aliphatics	45.16	21.43	9.52	33.33	25	
Cyclohexane, ethyl	Cyclic aliphatics	41.94	21.43	9.52	66.67	75	
Methanesulfonic anhydride	Sulfur-containing	41.94	21.43	14.29	66.67	100	
o-Xylene <sup>42,90,103</sup>	Aromatics	41.94	28.57	14.29	33.33	25	[42; 90; 103]

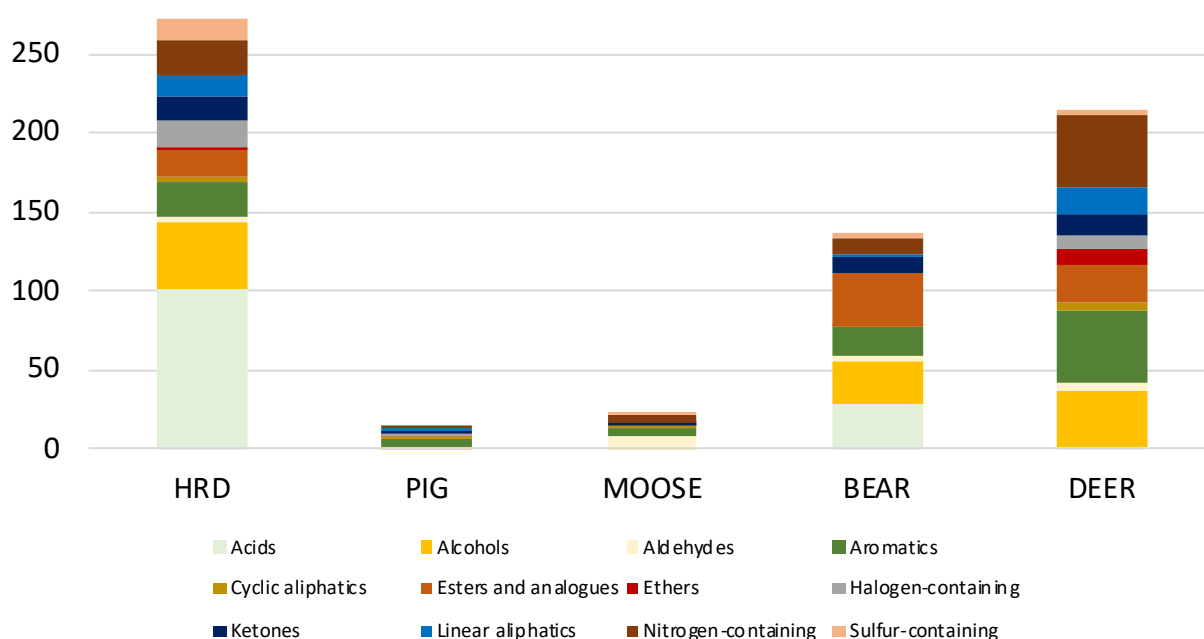
3.4.2. Trends in VOC profiles of HRD training aids and animal bones

The trend for compound class abundance of each VOC profile in increasing order of abundance is illustrated in Figure 3.13. High abundance compounds made up at least 10% of total VOCs, average abundance compounds made up between 5 to 10% of total VOCs, and low abundance compounds made up less than 5% of total VOCs. Overall, high abundance compounds belonged to aromatics, esters and analogues, linear aliphatics, and alcohols. Average abundance compounds belonged to ketones and nitrogen-containing VOCs. Low abundance compounds belonged to acids, aldehydes, sulfur-containing VOCs, and ethers. The most similar trend in compound class abundance is observed between three sample sets: HRD training aids, the deer bone samples, and the bear bone samples. The greatest variation in class abundance is observed between HRD training aids and moose bone samples. Esters and analogues had high abundance in HRD training aids, while they had low abundance in moose bone samples. Halogen-containing VOCs had low abundance in HRD training aids, while they had average abundance in moose bone samples and high abundance in pig bone samples. Pig bone samples showed little variation in class abundance when compared to HRD training aids. A significant variation is seen where alcohols had high abundance in HRD training aids, while they had low abundance in pig bone samples.



**Figure 3.13.** Summary of class abundance trends in HRD training aids and animal bone samples.

The trend for relative class concentration for each VOC profile is illustrated in Figure 3.14. The highest relative class concentrations can be seen for HRD training aids, followed by deer bone samples and bear bone samples. Acids, alcohols, and esters and analogues had the highest relative class concentration for both HRD training aids and bear bone samples, while nitrogen-containing VOCs and aromatics had the highest relative class concentration for deer bone samples. The lowest relative class concentrations can be seen for pig bone samples and moose bone samples. Similar to the trends observed in compound class abundance, both bear and deer bone samples showed the greatest similarity to the HRD training aids in terms of relative class concentration.

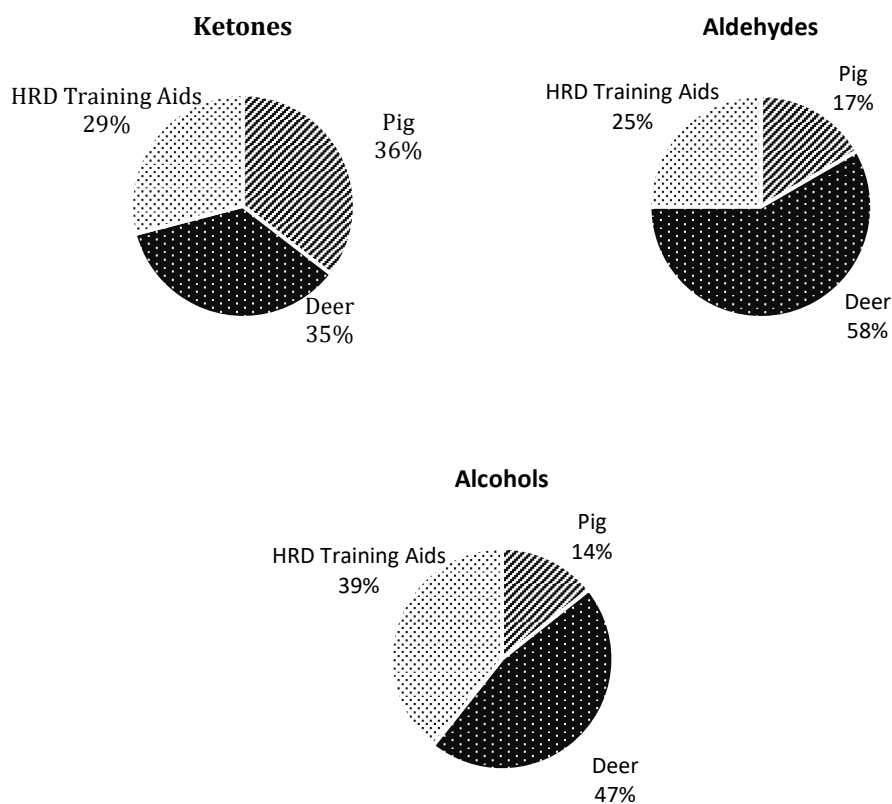


**Figure 3.14** Sum of average normalized areas indicating the relative class concentrations for all compound classes in HRD training aids and animal bone samples.

A study conducted by Cablk et al. aimed to compare VOCs from animal remains to human remains reported in a study by Hoffman et al.<sup>42,43</sup> The aromatic compound *o*-xylene was not detected in any animal bone samples, however, in the current study, it was identified in pig, moose, deer, and bear bone samples. Furthermore, the sulfur-containing compound dimethyl disulfide was not detected in pig bones in the Cablk study, whereas it was detected in 14% of all pig samples analyzed in this current study. Based on the study conducted by Cablk et al., pig remains were the least similar to human remains. Results from this study support the significant variation in both

compound class abundance and relative class concentration between pig bone samples and HRD training aids. Another study conducted by Rosier et al., investigated time-dependent VOCs of human and animal remains.<sup>102</sup> Among the eight human and pig specific compounds reported, only pyridine was detected in the HRD training aid sample set. Of the five pig specific compounds reported, none were detected in the pig bone samples analyzed in this study.

In a study conducted by Vass et al., the differences in bone odor composition among human, dog, deer, and pig were presented.<sup>34</sup> Vass et al. compared the composition of ketones, aldehydes, and alcohols among all samples. For the purpose of direct comparison, Figure 3.15 illustrates the difference in compound class abundance for ketones, alcohols, and aldehydes in HRD training aids, deer, and pig bone samples used in this study.



**Figure 3.15** Difference in compound class abundance for ketones, aldehydes, and alcohols in HRD training aids, pig, and deer bone samples.

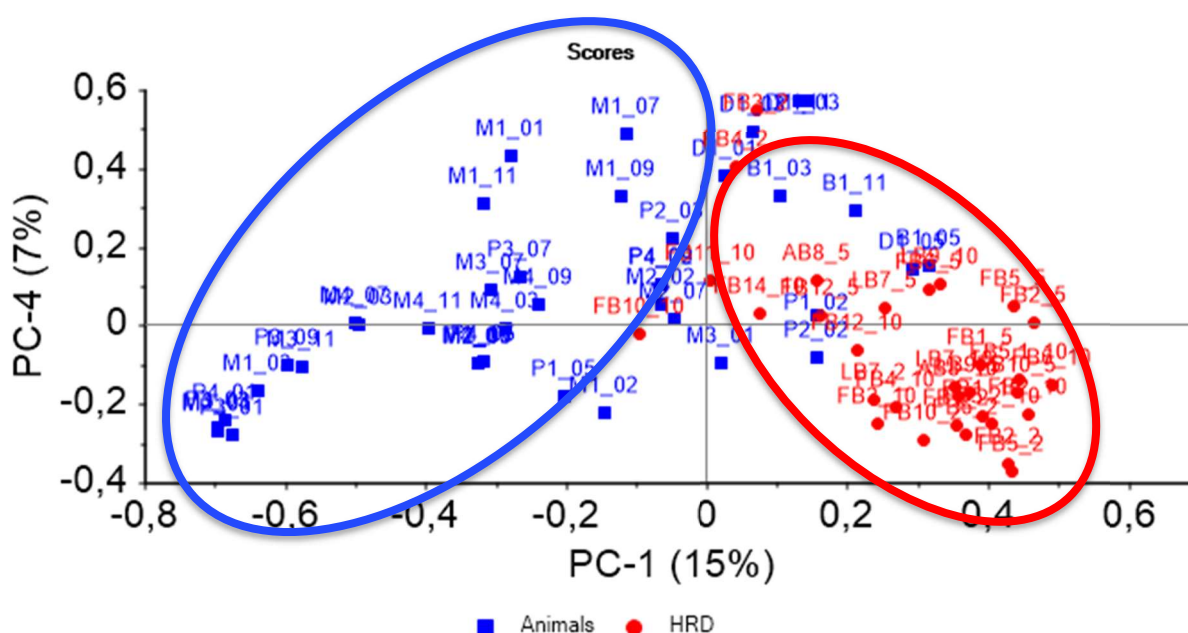
Similar to the study conducted by Vass et al., ketones and aldehydes were most abundant in deer. While alcohols consisted of only 5% of human bone odor composition in the Vass study, alcohols were most abundant in the HRD training aids in comparison to the animal bones. The reduced alcohol composition in the Vass et al. study may be due to the fact the studied samples were allowed to decompose in shallow burial sites. The samples used in the current study were allowed to decompose on the surface. Numerous studies have reported the effects of burial environments on human decomposition.<sup>2,21</sup> The rate of human decomposition is accelerated at the ground surface.<sup>2</sup> With buried remains, there is a reduced presence of insect activity and scavenging which, in turn, reduces the rate of decomposition.<sup>2,104</sup> Shallow burial sites provide anaerobic conditions favoring the production of sulfur-containing compounds.<sup>21</sup> Nitrogen-containing compounds derived from the decomposition of proteins are consumed by soil microbes as an energy source.<sup>21</sup> Glucose monomers, decomposition products of carbohydrates, may further decompose into alcohols depending on the availability of oxygen.<sup>21</sup>

Numerous studies have investigated the volatile profile of pig carcasses to further support their use as analogues in human decomposition studies.<sup>31,87,103</sup> Among the 21 most prominent VOCs identified across all HRD training aids, nearly 50% of compounds were identified in decomposition studies using human surrogate models.<sup>31</sup> These studies focused on the volatile profile during the early postmortem period, whereas the HRD training aids used in the current study are considered to be at advanced stages of decomposition. When comparing the volatile profiles of pig bone samples to the HRD training aids, only six compounds (2-methyl-propanoic acid, dimethyl trisulfide, 1-pentanol, propanoic acid, 3-methyl-butanol, and butanoic acid) were listed among the 21 most prominent VOCs identified across all HRD training aids.

#### 3.4.3. Principal Component Analysis

Principal component analysis (PCA) was performed to understand the variability between VOC profiles of HRD training aids and animal bone samples. Data were merged into a single Excel sheet prior to uploading in The Unscrambler<sup>®</sup>. Samples and compounds were displayed as headers and rows, respectively. To facilitate data manipulation, headers and rows were transposed. The ‘Center and Scale’ task option was performed followed by ‘Unit Vector Normalization’.

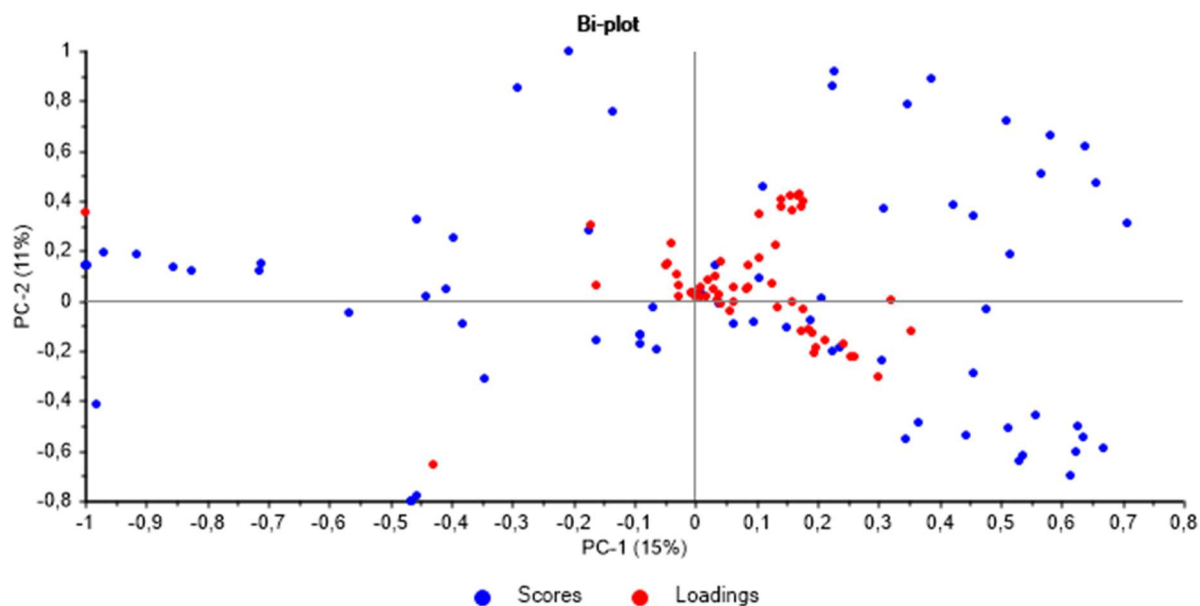
To investigate two sample sets, data obtained from the animal bone samples were grouped and used as a single sample set while HRD training aid samples were grouped as another (Figure 3.16). Both sample sets consisted of compounds identified in at least 30% of all samples, whether human or animal. Thus, the PCA was based on a total of 57 compounds. The resulting PCA highlighted 15%, 11%, 11%, 7%, 6%, 5%, 5% of the explained variance along PC-1, PC-2, PC-3, PC-4, PC-5, PC-6, and PC-7 respectively (cumulative: 60%). Evident clustering was present across all PCs (PC-1– PC-7) highlighting the separation of both sample sets.



**Figure 3.16** PCA scores plot for PC-1, PC-4. PCA scores were calculated using the pre-processed GC×GC-TOFMS normalized peak area of 58 prominent VOCs in over 30% of HRD training aids (represented by red circles) and animal bone samples (represented by blue squares) collected in the current study.

PCA loadings plots aid in the identification of VOCs contributing to the separation of points over the scores plots. Figure 3.17 consists of a PCA biplot in which the scores are made up of the HRD training aid and animal bone samples while the loadings are made up of the 57 compounds identified in at least 30% of all samples. From the loadings (Figure 3.17), 2,2,4-trimethyl-hexane, decyl-benzene, and methanesulfonic anhydride were identified as extreme loadings. 2,2,4-trimethyl-hexane, previously identified as one of the eight compounds detected across all animal bone samples, dominated in pig and moose samples. Decyl-benzene dominated in pig bones

labelled as P4 resulting in their separation from other samples. Methanesulfonic anhydride, listed as one of the most prominent VOCs detected across HRD training aids and animal bone samples, dominated in foot bones from the February 2022 trials as well as in the deer bone.

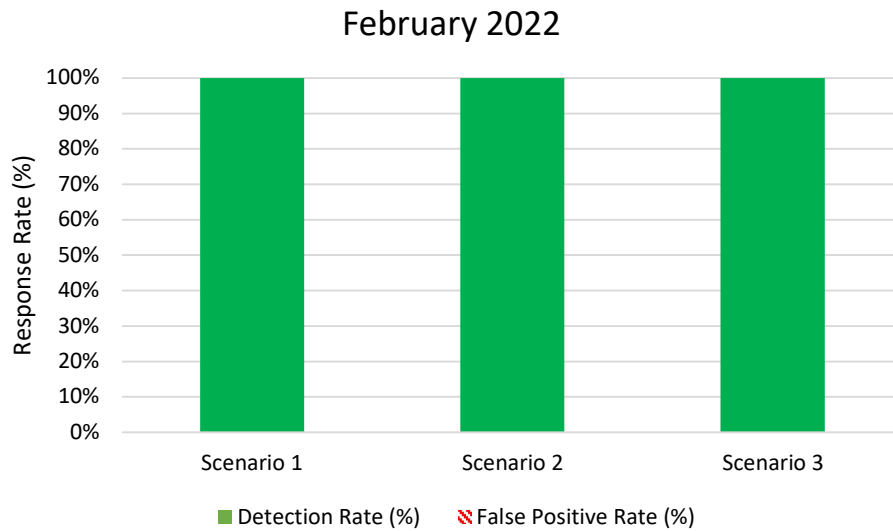


**Figure 3.17** PCA biplot for PC-1, PC-4 for HRD training aids and animal bone samples collected in the current study. Scores for HRD training aids and animal bone samples are represented by blue circles while loadings are represented by red circles.

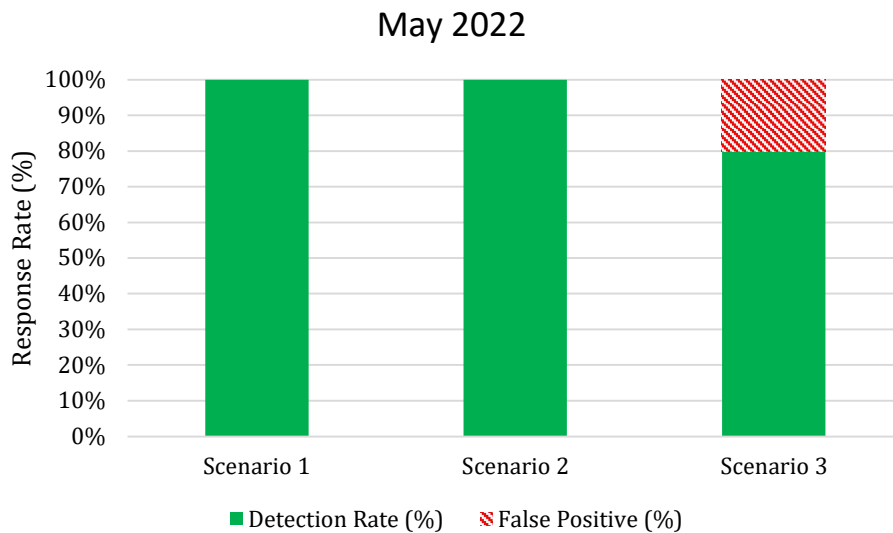
### 3.5. Human Remain Detection Dog Performance

Two series of dog trials were conducted at the OPP headquarters in Orillia, Ontario. The first series of dog trials took place in February 2022 and involved two OPP handlers and their certified HRD dogs. The second series of dog trials took place in May 2022 and involved 5 canine handlers from different law enforcement agencies and their certified HRD dogs. For each series of dog trials, three scenarios were set up in an OPP ‘Imprint Room’ and/or carousel room: (1) one HRD training aid and one animal bone, (2) one HRD training aid and two animal bones, and (3) one animal bone only. HRD dog responses from trials conducted in February 2022 and May 2022 are summarized in Table B.1 and B.2 (Appendix B) and are visualized in Figures 3.17 and 3.18. Figure 3.18

indicates a 100% detection rate for each HRD training aid used in Scenarios 1 and 2. No false positives were recorded in Scenario 3 involving strictly animal remains. Both dogs during the trial conducted in February 2022 were successful in detecting and alerting to HRD training aids in the presence of animal remains. Figure 3.19 indicates a 97% detection rate. Dog 2 falsely alerted to a deer bone sample during dog trials conducted in May 2022. This represents the only false positive event recorded.



**Figure 3.18** Detection rates of two HRD dogs for each scenario of the dog trials conducted in February 2022.



**Figure 3.19** Detection rates of five HRD dogs for each scenario of the dog trials conducted in May 2022.



The main objective of performing dog trials was to investigate the response rate of HRD dogs on human remains training aids in the presence of animal remains. This study primarily focused on evaluating HRD dogs' abilities to discriminate and differentiate the odor of human decomposition from that of animal decomposition. The detection rate and false response rate of participating dogs in three different scenarios were recorded. The detection rate for the first dog trial conducted in February 2022 was 100%, while that of the second dog trial conducted in May 2022 was 97% with a single false response event. A false positive occurred in a search scenario in which a deer bone was used along with distractor odors. It is not uncommon for scent-detection dogs to engage in positive alert responses when novel non-target odors are introduced.<sup>105,106</sup> The first exposure to the deer bone was during the first series of dog trials in February 2022. Between the first and second series of dog trials, participating HRD dogs were not exposed to the animal bones used in this study. The false positive event occurred when the dog was exposed to the deer bone a second time. It should also be noted that the introduction of animal bones resulted in a change in behavior in some HRD dogs in the scenarios. Changes of behavior included spending more time sniffing the boxes and/or metal cans, licking and/or biting the boxes and/or metal cans, returning to boxes and/or metal cans before giving a final confirmed response on the HRD training aid. Changes of behavior were mainly observed when either deer or bear bones were present in the search scenario. These particular bones possessed a more pungent odor in comparison to the pig and moose bones used in the trials. Sulfur-containing compounds such as dimethyl disulfide and methanesulfonic anhydride were identified in higher percentages of deer and bear bone samples in comparison to pig and moose bone samples as well as HRD training aids (Table 3.4). Similarly, indane, an aromatic hydrocarbon, was identified in 100% and 67% in deer and bear bone samples, respectively, in comparison to 45% in HRD training aids. Like some of the HRD training aids, the bear bone had remaining soft tissue. While the deer bone did not have remaining soft tissue, its storage container was visibly moist. Pig and moose bone samples were completely dry with no tissue remaining and no noticeable odor which may have resulted in a dog's disinterest.

Another false positive event occurred in a search scenario in which a bear bone was used in the presence of an HRD training aid and distractor odors. This particular event was not recorded as the specific HRD training aid had been treated differently than the HRD training aids used for this

study. The training aid in question had previously been submerged in water for an extended period. Studies using human analogues have reported a difference in the detection and frequency of VOCs in decomposition odor profiles from surface-deposited and submerged remains.<sup>24</sup> Moreover, the process of human decomposition in aquatic environments differs from that of terrestrial environments.<sup>10,107,108</sup> Submerged skeletal remains are prone to abrasion, encrustation, and erosion.<sup>107</sup> These factors along with the presence of strong odors should be considered when attempting to understand HRD dogs' behavior and false positive alerts. During a second attempt with a different HRD training aid in the presence of the bear bone, a confirmed final response was obtained for the HRD target. Thus, it can be assumed that submerging the HRD training aid caused a variation in its VOC profile.

The purpose of conducting two separate dog trials over the course of seven months was to study any variation in HRD dog response rates. Any variation would be indicative of changes in VOC odor profiles. No variation in HRD dog response rates were noted over the course of seven months. This suggests no significant variation in odor profiles as reported in previous sections. The results of the dog trials support HRD dogs' abilities to discriminate and differentiate the odor of human decomposition and the odor of animal decomposition. HRD dogs gave a confirmed final response to human remains during all trials, with the exception of dog 2.

## **CHAPTER 4: CONCLUSIONS AND FUTURE WORK**

#### 4.1. Summary of research outcomes

This two-part study firstly aimed to establish VOC profiles from HRD training aids and select animal species for their direct comparison. Secondly, the ability of certified HRD dogs from a variety of law enforcement agencies to differentiate human decomposition odor and animal decomposition odor was evaluated. Certain law enforcement agencies, specifically in the UK, use pig remains as training aids for their HRD dogs.<sup>109</sup> Decomposition studies have revealed inconsistencies in decomposition odor profiles from animal remains when compared to those of human remains.<sup>32,42</sup>

A primary objective of this study was to analyze the VOC profiles of HRD training aids used by the OPP canine unit. The odor analysis of 35 HRD training aid samples over the span of 8 months resulted in the detection and identification of 857 VOCs. This study reported no significant variation in VOC profiles over time. HRD training aids were categorized as foot bones ( $n = 26$ ), leg bones ( $n = 6$ ), or ankle bones ( $n = 3$ ). Foot bones produced the greatest number of VOCs (800), followed by leg bones (308) and ankle bones (107). The quantity of VOCs detected and their relative class concentrations were determined to be predominantly influenced by the presence of remaining soft tissue. When comparing VOC profiles for each category (foot, leg, and ankle bones) of HRD training aids (Figure 3.3), high abundance compounds belonged to aromatics, linear aliphatics, esters and analogues, alcohols, and ketones, while low abundance compounds belonged to aldehydes, ethers, halogen-containing VOCs, and sulfur-containing VOCs. The remaining compound classes showed average abundance. Similarly, the general trend for relative class concentration across all HRD training aids was acids followed by alcohols, nitrogen-containing VOCs, aromatics, halogen-containing VOCs, esters and analogues, sulfur-containing VOCs, ketones, linear aliphatics, cyclic aliphatics, aldehydes, and ethers.

To compare VOC profiles of HRD training aids to VOC profiles of animal remains, pig ( $n = 4$ ), moose ( $n = 4$ ), deer ( $n = 1$ ), and bear ( $n = 1$ ) bones were analyzed using the same analytical method. The pig bone samples produced the greatest number of VOCs (515 VOCs), followed by moose bone samples (309 VOCs), deer bone samples (285 VOCs), and bear bone samples (223 VOCs). Like the HRD training aids, no significant variation in VOC profiles over time were reported. The most abundant compound class consisted of aromatics while low abundance

compounds varied for each animal odor profile. Likewise, the general trend for relative class concentration varied for each odor profile.

A direct comparison of VOC profiles of HRD training aids and select animal species was discussed in section 3.3. Compound class abundance, relative class concentration, and prominent VOCs were compared. One prominent non-decomposition-related VOC, 4-cyanocyclohexene, was detected across all HRD training aids and animal bone samples. This nitrogen-containing compound has previously been reported as a contaminant originating from nitrile gloves and therefore, should not be associated with human decomposition odor. In terms of compound class abundance trends, deer and bear bone samples showed the most similar trend to the HRD training aids. Conversely, the greatest variation in class abundance was observed between HRD training aids and moose bone samples. Of the 857 VOCs detected across all HRD training aids, 676 VOCs were exclusive to HRD training aids.

The performance of HRD dogs was assessed during trial sessions conducted in February 2022 and May 2022 with 2 and 5 certified police dogs, respectively. The purpose of these trials was to evaluate HRD dogs' abilities to discriminate and differentiate the odor of human decomposition from that of animal decomposition. During indoor search scenarios, HRD dogs were exposed to HRD training aids routinely used by the OPP canine unit, animal bone, and distractor odors. Results of these trial sessions concluded that HRD dogs were able to successfully locate HRD training aids in the presence of animal remains with an overall detection rate ranging between 97% – 100%. One false positive event was recorded on a bear bone. No false positives were recorded on distractor odors. No variation in HRD dog responses was observed between trials conducted in February 2022 and May 2022.

The similarities and differences between VOC profiles of HRD training aids and select animal species have been highlighted by this study and HRD dogs were determined to have the ability to successfully locate HRD targets in the presence of animal bones.

#### **4.2. Future Works**

A significantly greater number of VOCs was detected and identified in the HRD training aids in comparison to the animal bones analyzed in this study. This is assumed to be due to the presence

of some remaining soft tissue on the HRD training aids. As it has been witnessed by the author that dry human remains are increasingly difficult to locate for HRD dogs, further research should be conducted in establishing decomposition odor biomarkers from dry human remains. This could potentially reveal which compounds are detected by HRD dogs when giving a final confirmed response to human remains. Additionally, the use of dry human remains in HRD dog training may provide more realistic scenarios for search operations involving aged human remains.

This study reported only one false positive event during a dog trial session involving both human and animal bones. It has been stated that the HRD training aid initially used in the scenario had been submerged in water. It is unclear whether the HRD dog positively alerted to the bear bone in the room due to it having a strong odor, as noted by the author. As such, further investigation is recommended into the impact of submerged human remains on decomposition odor profiles.

What constitutes an adequate HRD training aid is its accurate representation of human decomposition odor. Recently, the use of amputated lower limbs has been validated as HRD training aids.<sup>85</sup> Studies have determined that the frequency of exposure to human cadavers and/or human cadaveric material, such as amputated lower limbs, as well as the frequency of training can be directly correlated to HRD dogs' performance. This study performed two separate dog trials involving at most five certified HRD dogs over the span of three months. HRD dog performance should be evaluated at consistent intervals over a longer period. The addition of participating certified canines of varying breeds may highlight a particular breed's sensitivity and specificity to human remains.

This study has identified a large number of decomposition VOCs not found in animal remains, however which compounds are exclusively detected by HRD dogs eliciting a confirmed final response cannot be established. Further investigating VOCs at various stages of human decomposition will greatly narrow this list of compounds. The search for human specific markers can not only aid in the training of HRD dogs but contribute to the understanding of the mechanisms behind canine behaviour. Physiological and neurological pathways can be evaluated by introducing target odors that elicit a confirmed final response.

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APPENDIX A

**Table A.1** VOCs detected in HRD training aids and animal bone samples

	Compound	Compound class	Percentage HRD training aid samples in which VOC was detected	Percentage pig bone samples in which VOC was detected	Percentage deer bone samples in which VOC was detected	Percentage moose bone samples in which VOC was detected	Percentage bear bone samples in which VOC was detected
1	(3-Methylphenyl) methanol, 1-methylpropyl ether	Alcohols				4.76	
2	(7a-Isopropenyl-4,5-dimethyloctahydroinden-4-yl)methanol	Alcohols	3.23	14.29		4.76	
3	(R)-(-)-3-Methyl-2-butanol	Alcohols	6.45				
4	(R)-(+)-3-Methylcyclopentanone	Ketones	3.23				
5	(R)-9-[(S)-2-(Hydroxymethyl)pyrrolidin-1-yl]-3-methyl-3,4-dihydro-2H-benzo[b][1,4,5]oxathiazepine 1,1-dioxide	Aromatics	3.23			4.76	
6	(S)-(+)-1-Cyclohexylethylamine	Nitrogen-containing	6.45	7.14			
7	(S)-9-[(S)-2-(Hydroxymethyl)pyrrolidin-1-yl]-3-methyl-3,4-dihydro-2H-benzo[b][1,4,5]oxathiazepine 1,1-dioxide	Aromatics	3.23	7.14			
8	(Z)-3-Heptene	Linear aliphatics	3.23				
9	1-(2,4-Dihydroxyphenyl)-2-(4-methoxy-3-nitrophenyl)ethanone	Ketones				9.52	
10	1-[2-Pyridyl]-2,2-dimethyl-2-morpholino ethanol	Alcohols		7.14			
11	1-[6,8-Dichloro-2-phenyl-4-quinolyl]hexahydro-3H-oxazol[3,4-a]pyridine	Aromatics	3.23				
12	1-acenaphthenol, trifluoroacetate ester	Esters and analogues		7.14			
13	1-Butanamine, N-methyl-	Nitrogen-containing		7.14			
14	1-Butanol	Alcohols	6.45	7.14	25		
15	1-Butanol, 2-methyl-	Alcohols	64.52		100		
16	1-Butanol, 2-methyl-, acetate	Esters and analogues	3.23				
17	1-Butanol, 2,3-dimethyl-	Alcohols	6.45				
18	1-Butanol, 3-methyl-	Alcohols	67.74		100		100
19	1-Butanol, 3-methyl-, acetate	Esters and analogues	12.9				33.33
20	1-Butanol, 3-methyl-, propanoate	Esters and analogues	12.9				
21	1-Butylpyrrolidine	Nitrogen-containing		7.14			
22	1-Decene	Linear aliphatics				9.52	
23	1-Docosene	Linear aliphatics	3.23				
24	1-Dodecanol	Alcohols	6.45	21.43	25		
25	1-Ethyl-3-methylcyclohexane (c,t)	Cyclic aliphatics	3.23		25		
26	1-Ethyl-4-methylcyclohexane	Cyclic aliphatics	9.68	7.14		4.76	
27	1-Ethylcyclopentene	Cyclic aliphatics	19.35				
28	1-Heptanamine	Nitrogen-containing	16.13				
29	1-Heptanol	Alcohols	25.81		25		33.33
30	1-Heptanol, 6-methyl-	Alcohols		7.14			
31	1-Hepten-3-ol	Alcohols	3.23				
32	1-Hepten-3-one	Ketones	3.23				
33	1-Heptene	Linear aliphatics	16.13	7.14	25	4.76	33.33
34	1-Hexadecanol	Alcohols	3.23	14.29			
35	1-Hexanol	Alcohols	48.39	7.14	100		100
36	1-Hexanol, 2-ethyl-	Alcohols	6.45	7.14	25	4.76	
37	1-Hexene, 3,3-dimethyl-	Linear aliphatics	3.23				
38	1-Hexene, 5,5-dimethyl-	Linear aliphatics		7.14			
39	1-Iodo-2-methylundecane	Halogen-containing	6.45				
40	1-Methyldecahydronaphthalene	Aromatics	6.45			4.76	
41	1-Methyldodecylamine	Nitrogen-containing	3.23	21.43	25	4.76	

42	1-Nonanol	Alcohols			25		
43	1-Nonene	Linear aliphatics	6.45	21.43		14.29	
44	1-Octadecanamine, N-methyl-	Nitrogen-containing		7.14	25	23.81	
45	1-Octanamine, N-methyl-	Nitrogen-containing			25	4.76	
46	1-Octanol	Alcohols	9.68	7.14	75		
47	1-Octanol, 2-butyl-	Alcohols	16.13	14.29		14.29	
48	1-Octen-3-ol	Alcohols	16.13		25		33.33
49	1-Octen-3-one	Ketones	3.23				
50	1-Octene	Linear aliphatics	6.45			9.52	
51	1-Octene, 3,7-dimethyl-	Linear aliphatics	3.23				
52	1-Pentanol	Alcohols	54.84		100		100
53	1-Pentanol, 2-ethyl-4-methyl-	Alcohols	6.45				
54	1-Pentanol, 2-methyl-	Alcohols	3.23				
55	1-Pentanol, 4-methyl-	Alcohols	48.39				
56	1-Penten-3-ol	Alcohols	16.13				33.33
57	1-Penten-3-one	Ketones	3.23				
58	1-Pentene, 2,4-dimethyl-	Linear aliphatics	3.23				
59	1-Pentene, 2,4,4-trimethyl-	Linear aliphatics	16.13		25		
60	1-Propanol, 2-(2-hydroxypropoxy)-	Alcohols	3.23				
61	1-Propanol, 2-amino-	Alcohols				4.76	
62	1-Propanol, 2-amino-, (±)-	Alcohols	6.45				
63	1-Propanol, 2-methyl-	Alcohols	80.65		100		100
64	1-Propanol, 2,2'-oxybis-	Alcohols	3.23				
65	1-Propanone, 1-(2-furanyl)-	Alcohols	3.23		75		
66	1-Propanone, 1-(5-methyl-2-furanyl)-	Alcohols	3.23				
67	1-Propen-2-ol, acetate	Esters and analogues		7.14	25	9.52	
68	1-Tetradecanol	Alcohols		7.14			
69	1-Tetradecene	Linear aliphatics	3.23	35.71	100	23.81	66.67
70	1-Undecene	Linear aliphatics			25		
71	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	Aromatics	19.35	21.43		9.52	
72	1,1'-Biphenyl, 3-methyl-	Aromatics		7.14			
73	1,1'-Biphenyl, 3,4-diethyl-	Aromatics		7.14			
74	1,1'-Biphenyl, 4-methyl-	Aromatics	3.23	7.14			
75	1,1'-Biphenyl, 4,4'-difluoro-	Halogen-containing		7.14			
76	1,1'-Biphenyl,3,3'-difluoro-	Halogen-containing		7.14			
77	1,2-Benzenedicarboxylic acid	Acids	3.23			4.76	
78	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	Esters and analogues		7.14			
79	1,2-Benzenediol, O-(4-methoxybenzoyl)-O'-(2-furoyl)-	Alcohols		7.14			
80	1,2-Benzenediol, o-(4-methoxybenzoyl)-o'-(2,2,3,3,4,4,4-heptafluorobutyryl)-	Halogen-containing		7.14			
81	1,2-Benzisothiazole	Aromatics	3.23	7.14			
82	1,2-Bis(p-acetoxyphenyl)ethanedione	Ketones		7.14			
83	1,2-Dimethyl-5-nitroadamantane	Nitrogen-containing		7.14			
84	1,2-Ethanediol	Alcohols				4.76	
85	1,2-Ethanediol, 1,2-diphenyl-, (R*,R*)-(±)-	Alcohols		7.14			
86	1,2-Ethanediol, 1,2-diphenyl-, [R-(R*,R*)]-	Alcohols	3.23				
87	1,2,3-Trifluoro-4-trifluoromethylbenzene	Halogen-containing		21.43	25		
88	1,2,3-Trifluorobenzene	Halogen-containing		14.29			



89	1,2,3,3a,4,5,6,10b-Octahydrofluoranthene	Halogen-containing		7.14			
90	1,2,4-Metheno-1H-cyclobuta[cd]pentalene, octahydro-	Cyclic aliphatics	3.23	14.29			
91	1,2,4-Trithiolane	Sulfur-containing	6.45				
92	1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl-	Ethers	41.94	7.14	25		
93	1,2,5-Thiadiazole, 3-methyl-	Aromatics	3.23				
94	1,3-Benzenediol, O,O'-di(2-methoxybenzoyl)-	Alcohols		7.14			
95	1,3-di-iso-propylnaphthalene	Aromatics		7.14			
96	1,3-Diazine	Nitrogen-containing	3.23				
97	1,3-Dioxane, 2-methyl-	Ethers			25		
98	1,3-Dioxolane, 2-methyl-	Ethers		7.14			
99	1,3-Dioxolane, 2,2-dimethyl-	Ethers	3.23	14.29	25	9.52	
100	1,3-Hexadiene, 3-ethyl-2-methyl-	Linear aliphatics	3.23				
101	1,3-Oxathiane	Sulfur-containing	3.23				
102	1,3-Pentadiene, 2,3-dimethyl-	Linear aliphatics	3.23				
103	1,3,5-Trifluorobenzene	Halogen-containing	6.45		25	4.76	
104	1,3,5,7-Cyclooctatetraene	Cyclic aliphatics		7.14			
105	1,3,6-Trioxocane	Ethers	3.23	7.14			
106	1,4-Cyclohexadiene, 1-methyl-	Cyclic aliphatics	3.23				
107	1,4-Dioxane	Ethers	19.35	14.29	50	19.05	
108	1,4-Dioxin, 2,3-dihydro-	Ethers	6.45	7.14	25		
109	1,4-Heptadiene	Linear aliphatics	3.23				
110	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	Cyclic aliphatics	3.23				
111	1(3H)-Isobenzofuranone	Esters and analogues		7.14			
112	12-Methylaminolauric acid	Acids	3.23	28.57		4.76	
113	1H-Indene, 1-ethylidene-	Aromatics	6.45				
114	1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl-	Aromatics		7.14			
115	1H-Indene, 2,3-dihydro-1,6-dimethyl-	Aromatics	29.03	7.14		4.76	
116	1H-Indene, 2,3-dihydro-4-methyl-	Aromatics	41.94	21.43	25	4.76	
117	1H-Indene, 2,3-dihydro-4,7-dimethyl-	Aromatics	22.58				
118	1H-Indene, 2,3-dihydro-5-methyl-	Aromatics	3.23				
119	1H-Indene, octahydro-	Aromatics	9.68	14.29		4.76	
120	1H-Indene, octahydro-, cis-	Aromatics	6.45				
121	1H-Indene, octahydro-, trans-	Aromatics	6.45				
122	1H-Indene, octahydro-5-methyl-	Aromatics	6.45			4.76	
123	1H-Pyrazole, 4,5-dihydro-5-propyl-	Aromatics				4.76	
124	1H-Pyrrole, 1-methyl-	Aromatics	6.45			4.76	
125	1H-Pyrrole, 2-methyl-	Aromatics	12.9				
126	1H-Pyrrole, 3-methyl-	Aromatics	22.58	14.29			
127	2-(E)-Pentenoic acid, (4S)-amino-5-phenyl-	Acids		7.14			
128	2-(Methylmercapto)benzothiazole	Aromatics		7.14			
129	2-Amino-1,3-propanediol	Alcohols	6.45		25	9.52	
130	2-Benzothiazolamine, N-ethyl-	Aromatics		7.14			
131	2-Butanamine, 3,3-dimethyl-	Nitrogen-containing		14.29		4.76	33.33
132	2-Butanamine, N,N-dimethyl-	Nitrogen-containing		7.14			
133	2-Butanol	Alcohols	54.84	7.14	50		33.33
134	2-Butanone	Ketones	19.35		50		
135	2-Butanone, 1-bromo-3,3-dimethyl-	Ketones		7.14			

136	2-Butanone, 3-methyl-	Ketones	32.26	14.29		14.29	
137	2-Butanone, 3,3-dimethyl-	Ketones	6.45				
138	2-Butenal, 2-methyl-	Aldehydes	16.13		75		
139	2-Butoxyethyl nonanoate	Esters and analogues		7.14			
140	2-Butyl-1-decene	Linear aliphatics		14.29		9.52	
141	2-Butylcyclopentanone	Ketones	3.23				
142	2-Butynedinitrile	Nitrogen-containing	6.45	7.14			
143	2-Chloroethanol	Alcohols	3.23	14.29	50	9.52	33.33
144	2-Cyano-2-O-fluorosulfatofluoropropane	Halogen-containing	3.23				
145	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-	Ketones	3.23				
146	2-Cyclohexen-1-one, 3-methyl-6-(1-methylethylidene)-	Ketones	3.23				
147	2-Cyclopenten-1-one	Ketones	9.68	7.14		4.76	
148	2-Cyclopenten-1-one, 2,3-dimethyl-	Ketones			25		
149	2-Decanone	Ketones	25.81	14.29	100		100
150	2-Decenal	Aldehydes		7.14			
151	2-Decene, 5-methyl-	Linear aliphatics		7.14		9.52	
152	2-Dodecanol	Alcohols	3.23				
153	2-Dodecanone	Ketones		7.14			
154	2-Dodecene	Linear aliphatics		7.14	25		
155	2-Ethyl-1-hexanol, trifluoroacetate	Halogen-containing				4.76	
156	2-Ethyl-2,3-dihydro-1H-indene	Aromatics	19.35				
157	2-Ethyl-trans-2-butenal	Aldehydes	3.23				
158	2-Ethylacrolein	Aldehydes	22.58	14.29	50	14.29	
159	2-Ethylhexyl 2-ethylhexanoate	Esters and analogues	3.23	7.14			
160	2-Heptanol	Alcohols	9.68				
161	2-Heptanol, 6-methyl-	Alcohols	12.9		75		
162	2-Heptanone	Ketones		7.14			
163	2-Heptanone, 3-methyl-	Ketones	3.23				
164	2-Heptanone, 4,6-dimethyl-	Ketones	9.68				
165	2-Heptanone, 6-methyl-	Ketones	16.13		75	14.29	33.33
166	2-Heptanone, 7,7,7-trichloro-	Ketones	9.68				
167	2-Hepten-4-one, 2-methyl-	Ketones	3.23				
168	2-Heptenal	Aldehydes	3.23				
169	2-Heptenal, 2-methyl-	Aldehydes	3.23				
170	2-Heptene	Linear aliphatics	29.03		100	4.76	33.33
171	2-Hexanamine, 4-methyl-	Nitrogen-containing	22.58	21.43		9.52	
172	2-Hexanol	Alcohols	58.06		100		100
173	2-Hexanol, 5-methyl-	Alcohols	3.23				
174	2-Hexanone	Ketones	3.23	7.14		9.52	
175	2-Hexanone, 3-methyl-	Ketones	3.23				
176	2-Hexanone, 3,4-dimethyl-	Ketones	3.23				
177	2-Hexanone, 4-methyl-	Ketones	9.68				
178	2-Hexanone, 5-methyl-	Ketones	45.16			4.76	
179	2-Hexene, 2,5,5-trimethyl-	Linear aliphatics		7.14	50	19.05	33.33
180	2-Hexene, 3-methyl-	Linear aliphatics	35.48	7.14	25	4.76	
181	2-Hexene, 3,5,5-trimethyl-	Linear aliphatics				4.76	
182	2-Isopropylpymazine	Aromatics	3.23				

183	2-Methyl-1-hexanol	Alcohols	3.23				
184	2-Methyl-6-(p-tolyl)hept-2-en-4-ol	Alcohols	3.23				
185	2-Methylheptanoic acid	Acids				4.76	
186	2-Methylthiolane, S,S-dioxide	Sulfur-containing		7.14			
187	2-n-Butyl furan	Aromatics	51.61		100	4.76	100
188	2-n-Heptylfuran	Aromatics	3.23		100		33.33
189	2-n-Octylfuran	Aromatics			75		33.33
190	2-Nitro-2-methyl-1,3-propanediol	Alcohols	3.23				
191	2-Nonanol	Alcohols	25.81				
192	2-Nonanone	Ketones	25.81	35.71	100	4.76	100
193	2-Nonenal	Aldehydes		7.14			
194	2-Octanol	Alcohols	19.35		25		33.33
195	2-Octanone	Ketones	25.81	50	100	19.05	66.67
196	2-Octene	Linear aliphatics	16.13		75		66.67
197	2-Octene, 4-ethyl-	Linear aliphatics	6.45				
198	2-Pentadecanol	Alcohols		7.14			
199	2-Pentanol	Alcohols	67.74	7.14	100		100
200	2-Pentanol, 2-methyl-	Alcohols	3.23				
201	2-Pentanol, 3-methyl-	Alcohols	16.13		75		
202	2-Pentanol, 4-methyl-	Alcohols	29.03				
203	2-Pentanol, acetate	Esters and analogues	3.23				
204	2-Pentanone	Ketones	9.68	7.14			
205	2-Pentanone, 3-methyl-	Ketones	58.06				
206	2-Pentanone, 4-hydroxy-4-methyl-	Ketones	32.26	35.71	100	19.05	100
207	2-Pentanone, 5-hydroxy-	Ketones	3.23	7.14	25		
208	2-Penten-1-ol	Alcohols	3.23				
209	2-Phenyl-2H-1,2,3-benzotriazole	Aromatics		7.14			
210	2-Piperidinone	Ketones	9.68				
211	2-Propanamine, N,N'-methanetetraylbis-	Nitrogen-containing	3.23				
212	2-Propanol, 1-butoxy-	Alcohols	6.45				
213	2-Propanol, 1-methoxy-	Alcohols	16.13		25	4.76	
214	2-Propanone, 1-(acetyloxy)-	Ketones			25		
215	2-Propanone, 1-chloro-	Ketones		21.43	75	4.76	66.67
216	2-Propanone, 1-hydroxy-	Ketones			25		
217	2-Propenoic acid, 2-methyl-	Acids	3.23				
218	2-Propenoic acid, 2-methyl-, 2-ethyl-2-[[[2-methyl-1-oxo-2-propenyl]oxy]methyl]-1,3-propanediyl ester	Esters and analogues				4.76	
219	2-Propenoic acid, 2-methyl-, octyl ester	Esters and analogues		14.29			
220	2-Propynenitrile, 3-fluoro-	Nitrogen-containing				4.76	
221	2-Pyrazoline, 1-isobutyl-3-methyl-	Nitrogen-containing	3.23				
222	2-t-Butyl-5-methyl-[1,3]dioxolane-4-carboxylic acid	Acids		7.14			
223	2-Tetradecanol	Alcohols		7.14			
224	2-Tetradecanone	Ketones		7.14			
225	2-Thiophenecarboxylic acid, 4-nitrophenyl ester	Esters and analogues	3.23				
226	2-Trifluoroacetoxypentadecane	Halogen-containing		7.14	25	19.05	33.33
227	2-Undecanethiol, 2-methyl-	Alcohols	3.23	7.14	75		33.33
228	2-Undecanone	Ketones	16.13	7.14	25		
229	2-Undecen-4-ol	Alcohols			25		

230	2-Vinylfuran	Aromatics			50		33.33
231	2,2-Dimethoxybutane	Ethers	6.45				
232	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	Esters and analogues	3.23	7.14			
233	2,2,4,4-Tetramethyloctane	Linear aliphatics			25		
234	2,2'-Difluorobiphenyl	Halogen-containing		7.14			
235	2,3-Butanediol, [S-(R*,R*)]-	Alcohols	3.23				
236	2,3-Butanedione	Ketones			25		
237	2,3-Dehydro-1,8-cineole	Ethers	9.68				
238	2,3-Dimethyl-1-hexene	Linear aliphatics	3.23				
239	2,3-Hexanedione	Ketones	3.23				
240	2,3-Pentanedione	Ketones	3.23		25		
241	2,3,5-Trimethyl-6-ethylpyrazine	Nitrogen-containing	3.23				
242	2,4-Di-tert-butylphenol	Alcohols	32.26	35.71	50	47.62	33.33
243	2,4-Dimethyl 1,4-pentadiene	Linear aliphatics		7.14	25		
244	2,4-Dimethyl-1-heptene	Linear aliphatics	19.35	7.14			
245	2,4-Dimethyl-4-penten-2-ol	Alcohols	6.45			4.76	
246	2,4-Dimethylfuran	Aromatics	3.23				
247	2,4-Dithiapentane	Sulfur-containing	25.81				
248	2,4,4-Trimethyl-1-pentanol, trifluoroacetate	Halogen-containing		7.14			
249	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	Alcohols		7.14			
250	2,5-Difluorobenzaldehyde	Halogen-containing		7.14			
251	2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dien-1-one	Ketones	9.68	7.14		4.76	
252	2,6-Diisopropyl-naphthalene	Aromatics		14.29			
253	2,6-Dimethylbicyclo[3.2.1]octane	Cyclic aliphatics	6.45			4.76	
254	2,6-Lutidine	Aromatics	67.74	7.14	75		66.67
255	2(3H)-Furanone, 5-butylidihydro-	Esters and analogues	3.23		100	9.52	
256	2(3H)-Furanone, 5-ethylidihydro-	Esters and analogues	29.03	28.57	100	9.52	66.67
257	2(3H)-Furanone, 5-ethylidihydro-3-methyl-	Esters and analogues	3.23				
258	2(3H)-Furanone, 5-ethylidihydro-5-methyl-	Esters and analogues	6.45		25		
259	2(3H)-Furanone, 5-heptyldihydro-	Esters and analogues		7.14			
260	2(3H)-Furanone, 5-hexylidihydro-	Esters and analogues	12.9	14.29			
261	2(3H)-Furanone, dihydro-4,4,5,5-tetramethyl-	Esters and analogues		7.14			
262	2(3H)-Furanone, dihydro-4,5-dimethyl-	Esters and analogues	3.23				
263	2(3H)-Furanone, dihydro-5-methyl-	Esters and analogues	22.58	14.29	75		66.67
264	2(3H)-Furanone, dihydro-5-pentyl-	Esters and analogues	22.58	7.14	50	4.76	33.33
265	2(3H)-Furanone, dihydro-5-propyl-	Esters and analogues	9.68	28.57	100	4.76	33.33
266	2H-1,2-Oxazine, 6-(4-chlorophenyl)tetrahydro-2-methyl-	Aromatics			25		33.33
267	2H-Indol-2-one, 1,3-dihydro-1,3,3-trimethyl-	Ketones		7.14			
268	2H-Pyran-2-one, tetrahydro-	Ethers	9.68				
269	3-(6-Methylpyridin-2-yl)prop-2-enoic acid	Acids	3.23				
270	3-Amino-2-oxazolidinone	Ketones				4.76	
271	3-Buten-1-ol, 3-methyl-	Alcohols	3.23				
272	3-Buten-2-ol, 2-methyl-	Alcohols	3.23				
273	3-Decanone	Ketones	12.9				
274	3-Decene, 2,2-dimethyl-	Linear aliphatics	3.23				
275	3-Ethoxy-2-bromo-1-propanol	Alcohols	3.23				
276	3-Ethyl-3-methylheptane	Linear aliphatics	3.23				

277	3-Ethylcyclopentanone	Ketones	19.35				
278	3-Furaldehyde	Aldehydes	3.23				
279	3-Heptanone	Ketones	9.68	14.29	25	9.52	
280	3-Heptene	Linear aliphatics	16.13		75		
281	3-Heptene, 3-ethyl-	Linear aliphatics		7.14			
282	3-Heptene, 4-ethyl-	Linear aliphatics		14.29			
283	3-Hexanol	Alcohols	9.68				
284	3-Hexanol, 5-methyl-	Alcohols	3.23				
285	3-Hexanone	Ketones	29.03		100		
286	3-Hexanone, 2-methyl-	Ketones	6.45				
287	3-Hexanone, 2,5-dimethyl-4-nitro-	Ketones		7.14		4.76	
288	3-Hexanone, 4-methyl-	Ketones	9.68				
289	3-Hexen-2-one	Ketones	9.68				
290	3-Methoxyamphetamine	Aromatics	3.23	7.14		4.76	
291	3-Methoxybenzoic acid, 2,4,6-trichlorophenyl ester	Esters and analogues	3.23				
292	3-Methyl-2-(2-methyl-2-butenyl)-furan	Aromatics	38.71				
293	3-Methylbenzidine	aromatics		7.14			
294	3-Methylcyclopentyl acetate	Esters and analogues	3.23				
295	3-Methylheptyl acetate	Esters and analogues	25.81				
296	3-Octanol	Alcohols	22.58				
297	3-Octanol, 3,7-dimethyl-	Alcohols	6.45				
298	3-Octanone	Ketones	38.71		25		33.33
299	3-Octen-2-one	Ketones	16.13				
300	3-Octene	Linear aliphatics			25		
301	3-Pentadecanol	Alcohols		7.14			
302	3-Pentanol	Alcohols	22.58	7.14	25		33.33
303	3-Pentanone	Ketones	22.58	7.14	25		
304	3-Pentanone, 2,2,4,4-tetramethyl-	Ketones	3.23				
305	3-Penten-2-ol	Alcohols	12.9				33.33
306	3-Penten-2-one	Ketones	3.23		25		
307	3-Penten-2-one, 4-methyl-	Ketones	3.23	14.29			
308	3-Pentenoic acid, 4-methyl-	Acids	38.71				33.33
309	3-Trifluoroacetoxy-6-ethyldecane	Halogen-containing		7.14			
310	3-Trifluoroacetoxydodecane	Halogen-containing		7.14			
311	3-Undecene	Linear aliphatics		7.14			
312	3,3'-Dimethylbiphenyl	Linear aliphatics		7.14			
313	3,4-Difluorobenzaldehyde	Halogen-containing				4.76	
314	3,4-dimethylfuran	Aromatics	6.45				
315	3,4-Hexanedione, 2,2,5-trimethyl-	Ketones	6.45				
316	3,4-Methylenedioxy-N-ethylamphetamine	Aromatics		7.14			
317	3,5-Difluorophenol	Halogen-containing		7.14			
318	3,5-Dimethylcyclopentene	Cyclic aliphatics	12.9			4.76	33.33
319	3,5-Dimethyldihydropyran-2,6-dione	Ketones		7.14			
320	3,5-Dithiahexanol 5,5-dioxide	Alcohols	3.23				
321	3,5-O-Furylidene-d-xylofuranose	Aromatics		7.14			
322	3H-1,2,4-Triazol-3-one, 1,2-dihydro-	Ketones		7.14			
323	3H-Purin-6-amine, N,N,3-trimethyl-	Aromatics		7.14			

324	4-Cyano-4-methylthio-tetracyclo(6,2,1,1(3,6),0(2,7)dodec-9-ene	Nitrogen-containing		7.14			
325	4-Cyanocyclohexene	Nitrogen-containing	51.61	28.57	75	28.57	100
326	4-Dodecene	Linear aliphatics	6.45				
327	4-Ethoxycarbonyl-1-methyl-4-phenyl-1,2,3,4-tetrahydropyridine	Nitrogen-containing		7.14			
328	4-Ethyl-4-methyl-5-methylene-[1,3]dioxolan-2-one	Ketones		7.14			
329	4-Heptanol	Alcohols	3.23				
330	4-Heptanone	Ketones	9.68				
331	4-Heptanone, 3-methyl-	Ketones	3.23				
332	4-Hexyn-3-ol	Alcohols	3.23				
333	4-Methoxycarbonyl-4-butanolide	Esters and analogues			25		
334	4-Methyl-2-hexanol	Alcohols	3.23				
335	4-Methyl-2-tert-octylphenol	Alcohols		7.14			
336	4-Methyl-3-(methylamino)pentan-2-one	Ketones			25		
337	4-Methylpentyl 4-methylpentanoate	Esters and analogues	9.68				
338	4-Methylthiazole	Aromatics	25.81				
339	4-Nonanone	Ketones	6.45				
340	4-Nonene	Linear aliphatics	3.23	7.14			
341	4-Oxohept-2-enal	Aldehydes	3.23		25		
342	4-Penten-1-ol, 2-methyl-	Alcohols			25		
343	4-Penten-2-one, 4-methyl-	Ketones	3.23	35.71	25	9.52	
344	4-Pentenal, 2-methyl-	Aldehydes	3.23				
345	4-Propylcyclohexylamine	Nitrogen-containing		7.14			
346	4-Undecene	Linear aliphatics					33.33
347	4-Undecene, 3-methyl-	Linear aliphatics		7.14		4.76	
348	4,4-Dimethyl-2-cyclopenten-1-one	Ketones	3.23				
349	4,4'-Dimethylbiphenyl	Linear aliphatics		7.14			
350	4,7-Methano-1H-inden-6-ol, 3a,4,5,6,7,7a-hexahydro-, acetate	Esters and analogues		7.14		4.76	
351	4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-, endo-	Cyclic aliphatics		7.14			
352	4,9:5,8-Dimethano-1H-benz[ <i>f</i> ]indene, 3a,4,4a,5,8,8a,9,9a-octahydro-	Cyclic aliphatics		7.14			
353	4a,8a-(Methaniminomethano)naphthalene-9,11-dione, 10-phenyl-	Ketones		7.14			
354	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	Cyclic aliphatics	3.23	14.29		4.76	
355	5-Decanone	Ketones	3.23				
356	5-Eicosene	Linear aliphatics		7.14			
357	5-Ethyl-1-nonene	Linear aliphatics		7.14		4.76	
358	5-Hepten-2-ol, 6-methyl-	Alcohols	12.9				
359	5-Hepten-2-one, 6-methyl-	Ketones	3.23	35.71			33.33
360	5-Methyl-1-phenyloctane	Linear aliphatics					
361	5-Methyl-2-thiophenecarboxaldehyde	Aldehydes		7.14		4.76	
362	5-Methyl-2,4-diisopropylphenol	Alcohols		7.14			
363	5-Oxotetrahydrofuran-2-carboxylic acid, ethyl ester	Esters and analogues				4.76	
364	5-Undecene	Linear aliphatics	19.35				
365	5-Undecene, 4-methyl-	Linear aliphatics				4.76	
366	5,6,7,8,9,10-Hexahydrobenzocyclooctene	Aromatics	3.23				
367	5,9-Undecadien-2-one, 6,10-dimethyl-	Ketones	41.94	14.29	25	4.76	
368	6-Ethoxy-1,2,3,4-tetrahydro-2,2,4-trimethylquinoline	Aromatics		7.14			
369	6-Methyl-3,5-heptadiene-2-one	Ketones	6.45				
370	6-Methyl-bicyclo[4.2.0]octan-7-one	Ketones	3.23				

371	6-Thiopyrazolo[3,4-d]pyrimidin-4,6(5H,7H)-dione-3-carboxamide	Aromatics	6.45		75	14.29	
372	6H-1,2,5-Oxadiazine-6-thione, 4,5-dihydro-3-phenyl-	Ketones					33.33
373	7-Octen-2-ol, 2,6-dimethyl-	Alcohols	29.03	7.14	25	28.57	
374	7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(1-methylethyl)-	Esters and analogues		7.14			
375	9-Octadecenoic acid (Z)-, methyl ester	Esters and analogues	3.23	7.14			
376	9-Oxabicyclo[6.1.0]nonane, 1-methyl-, cis-	Esters and analogues			25		
377	9H-Fluoren-9-ol	Alcohols		7.14			
378	Ä±-Ï±,Ï±-Dimethyl-Ï±-(hydroxy-methyl)-Ï±-butyrolactone	Ketones	3.23				
379	Acenaphthylene	Aromatics		7.14			
380	Acetamide, 2,2-dichloro-	Halogen-containing	3.23				
381	Acetamide, 2,2,2-trifluoro-	Halogen-containing	12.9	7.14		14.29	33.33
382	Acetic acid	Acids	3.23	21.43		9.52	
383	Acetic acid, [(1,1-dimethylethyl)thio]-	sulfur-containing		7.14			
384	Acetic acid, anhydride with formic acid	Esters and analogues	6.45				
385	Acetic acid, butyl ester	Esters and analogues	38.71				
386	Acetic acid, hexyl ester	Esters and analogues	9.68				33.33
387	Acetic acid, hydrazide	Nitrogen-containing	19.35	28.57	100	19.05	33.33
388	Acetic acid, hydroxy-	Acids			25		
389	Acetic acid, hydroxy-, ethyl ester	Esters and analogues	3.23				
390	Acetic acid, methoxy-, anhydride	Esters and analogues	3.23				
391	Acetic acid, phenylmethyl ester	Esters and analogues	3.23				
392	Acetic acid, rubidium salt	Esters and analogues		7.14			
393	Acetic acid, trifluoro-, anhydride	Esters and analogues			25		
394	Acetic acid, trifluoro-, ethyl ester	Esters and analogues		14.29		4.76	
395	Acetic anhydride	Esters and analogues	3.23				
396	Acetoin	Ketones	6.45		25		66.67
397	Acetone	Ketones	9.68		25		33.33
398	Acetonitrile	Nitrogen-containing	12.9	14.29		19.05	
399	Acetonitrile, hydroxy-	Nitrogen-containing	6.45	7.14		19.05	33.33
400	Acetophenone	Ketones	19.35	14.29			
401	Adamantane	Cyclic aliphatics	3.23				
402	Alanine	Nitrogen-containing	3.23				
403	Allantoic acid	Acids	3.23	7.14			33.33
404	Allophanic acid, phenyl ester	Esters and analogues		7.14			
405	Ammonium acetate	Esters and analogues	22.58				
406	Amylene hydrate	Alcohols	3.23				
407	Androsta-1,4-dien-3-one, 6E±,17E±-dihydroxy-, 17-acetate	Esters and analogues		7.14			
408	Aniline	Aromatics	3.23				
409	Anisole	Ethers	22.58				33.33
410	Azulene	Aromatics		7.14			
411	Benzaldehyde	Aldehydes	3.23	7.14	25		
412	Benzenamine, 2-(2,4,5-trichlorophenylsulfonylamino)-5-methyl-	Aromatics	3.23				
413	Benzenamine, 2-iodo-	Halogen-containing		21.43		4.76	
414	Benzene	Aromatics	12.9				33.33
415	Benzene, (1-butylheptyl)-	Aromatics	22.58	14.29		33.33	33.33
416	Benzene, (1-butylhexyl)-	Aromatics	6.45	7.14			
417	Benzene, (1-butylonyl)-	Aromatics	12.9				

418	Benzene, (1-butyloctyl)-	Aromatics	29.03	28.57	50	28.57	33.33
419	Benzene, (1-ethyldecyl)-	Aromatics	25.81	21.43		19.05	
420	Benzene, (1-ethylnonyl)-	Aromatics	16.13	7.14		9.52	
421	Benzene, (1-methyldecyl)-	Aromatics	16.13	14.29	25	4.76	
422	Benzene, (1-methyldodecyl)-	Aromatics		7.14			
423	Benzene, (1-methylethyl)-	Aromatics	12.9	7.14	25		
424	Benzene, (1-methylnonyl)-	Aromatics	9.68	7.14			
425	Benzene, (1-methylpropyl)-	Aromatics	22.58				33.33
426	Benzene, (1-methylundecyl)-	Aromatics	3.23	14.29		4.76	
427	Benzene, (1-pentylheptyl)-	Aromatics	25.81	35.71	25	23.81	33.33
428	Benzene, (1-pentylhexyl)-	Aromatics	6.45				
429	Benzene, (1-pentylloctyl)-	Aromatics	6.45	14.29	25	14.29	
430	Benzene, (1-propylnonyl)-	Aromatics	19.35	35.71		28.57	
431	Benzene, (1-propyloctyl)-	Aromatics	9.68	7.14	25	14.29	
432	Benzene, (1,1-dimethyldecyl)-	Aromatics		7.14			
433	Benzene, (1,2-dimethoxyethyl)-	Ethers		7.14			
434	Benzene, (2-methyl-1-propenyl)-	Aromatics		7.14			
435	Benzene, (2-methyl-2-propenyl)-	Aromatics	3.23				
436	Benzene, (2-methylpropyl)-	Aromatics	25.81				
437	Benzene, 1-chloro-4-(trifluoromethyl)-	Aromatics	9.68	7.14			
438	Benzene, 1-ethyl-2-methyl-	Aromatics				4.76	
439	Benzene, 1-ethyl-2,4-dimethyl-	Aromatics	22.58	14.29		4.76	33.33
440	Benzene, 1-ethyl-2,4,5-trimethyl-	Aromatics	29.03	7.14			
441	Benzene, 1-ethyl-3-methyl-	Aromatics	9.68	21.43	25	4.76	66.67
442	Benzene, 1-ethyl-3,5-dimethyl-	Aromatics	6.45	7.14			
443	Benzene, 1-ethyl-4-(1-methylethyl)-	Aromatics		7.14			
444	Benzene, 1-ethyl-4-methyl-	Aromatics	3.23	7.14	25	4.76	
445	Benzene, 1-ethynyl-4-methyl-	Aromatics	3.23				
446	Benzene, 1-methoxy-4-methyl-	Aromatics	16.13				33.33
447	Benzene, 1-methyl-2-propyl-	Aromatics	16.13	7.14	25	4.76	
448	Benzene, 1-methyl-3-(1-methylethyl)-	Aromatics	19.35	21.43	25	19.05	
449	Benzene, 1-methyl-3-propyl-	Aromatics	29.03	28.57	25	9.52	33.33
450	Benzene, 1-methyl-4-(1-methylethenyl)-	Aromatics	3.23				
451	Benzene, 1-methyl-4-(1-methylpropyl)-	Aromatics	35.48			4.76	33.33
452	Benzene, 1-methyl-4-(2-methylpropyl)-	Aromatics	3.23	21.43			
453	Benzene, 1-methyl-4-butyl	Aromatics	38.71	7.14		4.76	33.33
454	Benzene, 1-methyl-4-propyl-	Aromatics	35.48	21.43		4.76	33.33
455	benzene, 1,1'-(1-methylethylidene)bis[4-methyl-	Aromatics		14.29			
456	Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, cis-	Aromatics	3.23				
457	Benzene, 1,1'-(1,2-cyclobutanediyl)bis-, trans-	Aromatics		7.14			
458	Benzene, 1,1'-(3-methyl-1-propene-1,3-diyl)bis-	Aromatics		7.14			
459	Benzene, 1,2-diethyl-	Aromatics	3.23				
460	Benzene, 1,2-difluoro-	Halogen-containing	12.9			14.29	
461	Benzene, 1,2,3-trimethyl-	Aromatics	6.45				
462	Benzene, 1,2,3,5-tetrafluoro-	Halogen-containing	3.23				
463	Benzene, 1,2,3,5-tetramethyl-	Aromatics	6.45				
464	Benzene, 1,2,4-trimethyl-	Aromatics		7.14			



465	Benzene, 1,2,4,5-tetramethyl-	Aromatics	45.16	21.43	25	4.76	33.33
466	Benzene, 1,3-diethyl-	Aromatics	25.81	7.14		4.76	
467	Benzene, 1,3-diethyl-5-methyl-	Aromatics	19.35	14.29		4.76	
468	Benzene, 1,3-difluoro-	Halogen-containing	12.9	14.29	25	9.52	33.33
469	Benzene, 1,3-dimethyl-	Aromatics	6.45	7.14	25		
470	Benzene, 1,3,5-tri-tert-butyl-	Aromatics	32.26	35.71	25	28.57	33.33
471	Benzene, 1,4-dichloro-	Aromatics	3.23				
472	Benzene, 1,4-diethyl-	Aromatics	3.23				
473	Benzene, 1,4-dimethyl-2,5-bis(1-methylethyl)-	Aromatics		7.14			
474	Benzene, 2-ethyl-1,4-dimethyl-	Aromatics	22.58	14.29		4.76	
475	Benzene, 3-cyclohexen-1-yl-	Aromatics	3.23				
476	Benzene, 4-ethenyl-1,2-dimethyl-	Aromatics	6.45			4.76	
477	Benzene, 4-ethyl-1,2-dimethyl-	Aromatics	16.13		25	4.76	
478	Benzene, chloro-	Aromatics					33.33
479	Benzene, decyl-	Aromatics	25.81	42.86	50	38.1	
480	Benzene, fluoro-	Halogen-containing	3.23	21.43		23.81	
481	Benzene, n-butyl-	Aromatics	16.13	14.29	50	9.52	
482	Benzene, pentafluoro-	Halogen-containing				4.76	
483	Benzene, pentyl-	Aromatics	16.13			4.76	
484	Benzene, propyl-	Aromatics	16.13		25		
485	Benzene, tert-butyl-	Aromatics	6.45				
486	Benzeneacetaldehyde	Aldehydes	6.45	14.29	75	4.76	
487	Benzeneethanamine, 2-fluoro- $\beta$ ,3-dihydroxy-N-methyl-	Halogen-containing	3.23				
488	Benzeneethanamine, 3-fluoro- $\alpha$ ,5-dihydroxy-N-methyl-	Halogen-containing		14.29			
489	Benzeneethanamine, 4-fluoro- $\alpha$ ,3-dihydroxy-N-methyl-	Halogen-containing		7.14			
490	Benzenemethanol, $\beta$ -methyl-	Alcohols	19.35				
491	Benzenemethanol, $\beta$ , $\beta$ -dimethyl-	Alcohols	9.68				
492	Benzenemethanol, $\beta$ , $\beta$ ,4-trimethyl-	Alcohols	3.23				
493	Benzenemethanol, $\alpha$ , $\alpha$ -dimethyl-	Alcohols		7.14	25	4.76	
494	Benzenesulfonamide, N-ethyl-2-methyl-	Nitrogen-containing		7.14			
495	Benzestrol	Alcohols		7.14			
496	Benzofuran	Aromatics			25		33.33
497	Benzoic acid, 2-ethylhexyl ester	Esters and analogues	19.35	14.29			
498	Benzoic acid, 4-ethoxy-, ethyl ester	Esters and analogues	6.45				
499	Benzoic acid, methyl ester	Esters and analogues	3.23			4.76	
500	Benzonitrile	Nitrogen-containing	9.68	14.29	25	4.76	
501	Benzophenone	Ketones	38.71	35.71	25	42.86	33.33
502	Benzothiazole	Aromatics	6.45	7.14	50	4.76	
503	Benzyl alcohol	Alcohols	6.45	21.43	50	4.76	
504	Benzyl methyl sulfide	Sulfur-containing	12.9			4.76	
505	Benzyl-diseryl phosphate	Esters and analogues					
506	Betaxolol	Alcohols		7.14			
507	Bicyclo[2.2.1]heptane, 2-chloro-2,3,3-trimethyl-	Cyclic aliphatics	3.23				
508	Bicyclo[2.2.1]heptane, 2-ethyl-	Cyclic aliphatics	3.23			4.76	
509	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, (1R)-	Cyclic aliphatics	3.23				
510	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-methylene-, (1S)-	Cyclic aliphatics	3.23				33.33
511	Bicyclo[3.1.0]hex-2-ene, 4-methylene-1-(1-methylethyl)-	Cyclic aliphatics	3.23				

512	Bicyclo[3.1.0]hexane	Cyclic aliphatics		7.14			
513	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	Cyclic aliphatics	12.9				
514	Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde, 6,6-dimethyl-	Cyclic aliphatics	3.23				
515	Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-, (1R)-	Ketones				4.76	
516	Bicyclo[3.1.1]heptan-3-ol, 6,6-dimethyl-2-methylene-, [1S-(1i±,3i±,5i±)]-	Alcohols	3.23			23.81	
517	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-	Cyclic aliphatics	12.9	14.29			33.33
518	Bicyclo[4.2.0]octa-1,3,5-triene	Cyclic aliphatics		7.14			
519	Biphenyl	Aromatics		7.14	25	9.52	
520	Bis-(ethoxycarbonyl)methoxymethoxyiminomethane	Nitrogen-containing	9.68				
521	Borane, diethyl(decyloxy)-	Linear aliphatics		7.14			
522	Butanal, 2-methyl-	Aldehydes	16.13				66.67
523	Butanal, 3-methyl-	Aldehydes	51.61		100	4.76	100
524	Butanamide, N-(3-methylphenyl)-	Nitrogen-containing		7.14			
525	Butane, 1-methoxy-3-methyl-	Ethers	9.68		100		33.33
526	Butane, 1,1,3,4-tetrachloro-1,2,2,3,4,4-hexafluoro-	Halogen-containing	32.26	35.71	50	52.38	33.33
527	Butane, 2,2,3,3-tetramethyl-	Linear aliphatics	3.23		25		33.33
528	Butane, 1,2,4-trichloro-heptafluoro-	Halogen-containing	35.48	21.43	50	23.81	33.33
529	Butanenitrile	Nitrogen-containing	22.58		50	23.81	
530	Butanenitrile, 2-methyl-	Nitrogen-containing	35.48				33.33
531	Butanenitrile, 2,3-dioxo-, dioxime, O,O'-diacetyl-	Nitrogen-containing		7.14		4.76	
532	Butanenitrile, 3-methyl-	Nitrogen-containing	38.71			28.57	33.33
533	Butanoic acid	Acids	51.61				66.67
534	Butanoic acid, 1-methylbutyl ester	Esters and analogues	19.35				
535	Butanoic acid, 1-methylhexyl ester	Esters and analogues	3.23				
536	Butanoic acid, 1-methylpropyl ester	Esters and analogues	9.68				
537	Butanoic acid, 2-hydroxy-, methyl ester	Esters and analogues	16.13		25		
538	Butanoic acid, 2-methyl-	Acids	48.39				66.67
539	Butanoic acid, 2-methyl-, 1-methylethyl ester	Esters and analogues	48.39				33.33
540	Butanoic acid, 2-methyl-, 2-methylpropyl ester	Esters and analogues	19.35				
541	Butanoic acid, 2-methyl-, 3-methylbutyl ester	Esters and analogues	6.45				
542	Butanoic acid, 2-methyl-, ethyl ester	Esters and analogues	35.48		75		100
543	Butanoic acid, 2-methyl-, methyl ester	Esters and analogues					33.33
544	Butanoic acid, 2-methyl-, propyl ester	Esters and analogues	19.35				66.67
545	Butanoic acid, 2-methylbutyl ester	Esters and analogues	3.23				33.33
546	Butanoic acid, 2-methylpropyl ester	Esters and analogues	32.26				
547	Butanoic acid, 3-amino-2-methyl-	Acids		7.14			
548	Butanoic acid, 3-methyl-	Acids	45.16				66.67
549	Butanoic acid, 3-methyl-, 1-methylethyl ester	Esters and analogues	35.48				66.67
550	Butanoic acid, 3-methyl-, 2-methylbutyl ester	Esters and analogues	6.45				
551	Butanoic acid, 3-methyl-, 3-methylbutyl ester	Esters and analogues	6.45				
552	Butanoic acid, 3-methyl-, butyl ester	Esters and analogues	25.81				33.33
553	Butanoic acid, 3-methyl-, ethyl ester	Esters and analogues	29.03		76		100
554	Butanoic acid, 3-methyl-, propyl ester	Esters and analogues	22.58				66.67
555	Butanoic acid, 3-methylbutyl ester	Esters and analogues	19.35				33.33
556	Butanoic acid, 4-chloro-	Acids	9.68				
557	Butanoic acid, butyl ester	Esters and analogues	48.39	7.14			66.67
558	Butanoic acid, ethyl ester	Esters and analogues	35.48		75		100

559	Butanoic acid, heptyl ester	Esters and analogues	3.23				
560	Butanoic acid, hexyl ester	Esters and analogues					66.67
561	Butanoic acid, methyl ester	Esters and analogues	3.23				
562	Butanoic acid, pentyl ester	Esters and analogues	35.48				66.67
563	Butanoic acid, propyl ester	Esters and analogues	29.03				66.67
564	Butyl 2-methylbutanoate	Esters and analogues	29.03				
565	Butyl benzoate	Esters and analogues	3.23				
566	Butyrolactone	Esters and analogues	12.9	7.14	50		
567	Camphene	Aromatics	29.03	28.57	25	28.57	33.33
568	Caprolactam	Nitrogen-containing	12.9	7.14			
569	Carbamic acid, monoammonium salt	Acids	38.71				
570	Carbamic acid, N-[1,1-bis(trifluoromethyl)ethyl]-, 4-(1,1,3,3-tetramethylbutyl)phenyl ester	Halogen-containing	6.45	28.57			
571	Carbamimidioic acid, methyl ester	Esters and analogues					33.33
572	Carbohydrazide	Nitrogen-containing	3.23				
573	Carbon disulfide	Sulfur-containing	3.23				
574	Carbonic acid, dimethyl ester	Esters and analogues	12.9	7.14			66.67
575	Carbonic acid, octadecyl phenyl ester	Esters and analogues		7.14			
576	Carbonyl sulfide	Sulfur-containing	6.45				
577	Cetene	Linear aliphatics		7.14			4.76
578	Chloromethylmethyl sulfide	Sulfur-containing	3.23				
579	cis-1-Ethyl-3-methyl-cyclohexane	Cyclic aliphatics	3.23				
580	cis-2-Nonene	Linear aliphatics			50		
581	cis-3-Methylcyclohexanol	Alcohols	6.45				
582	cis-Decalin, 2-syn-methyl-	Cyclic aliphatics	6.45				
583	Cyanamide, dimethyl-	Nitrogen-containing		7.14			
584	Cyclobuta[1,2:3,4]dicyclopentene, 1,3a,3b,4,6a,6b-hexahydro-	Cyclic aliphatics	3.23				
585	Cyclobutane, (1-methylethylidene)-	Cyclic aliphatics	16.13				
586	Cyclobutane, ethenyl-	Cyclic aliphatics		7.14			
587	Cyclobutanol	Alcohols	16.13	14.29		9.52	
588	Cyclodocosane, ethyl-	Cyclic aliphatics	3.23				
589	Cyclododecane	Cyclic aliphatics		7.14			
590	Cycloheptane	Cyclic aliphatics		7.14			
591	Cyclohexanamine, N-cyclohexyl-	Cyclic aliphatics		7.14			
592	Cyclohexane	Cyclic aliphatics		7.14	25		
593	Cyclohexane, (1-methylethyl)-	Cyclic aliphatics	3.23				
594	Cyclohexane, (1-methylpropyl)-	Cyclic aliphatics	6.45			9.52	
595	Cyclohexane, [6-cyclopentyl-3-(3-cyclopentylpropyl)hexyl]-	Cyclic aliphatics	3.23				
596	Cyclohexane, 1-ethyl-1-methyl-	Cyclic aliphatics	3.23				
597	Cyclohexane, 1-ethyl-2-methyl-	Cyclic aliphatics	6.45			4.76	33.33
598	Cyclohexane, 1-ethyl-2-propyl-	Cyclic aliphatics				4.76	
599	Cyclohexane, 1-ethyl-2,3-dimethyl-	Cyclic aliphatics					
600	Cyclohexane, 1-ethyl-4-methyl-, cis-	Cyclic aliphatics	6.45			4.76	
601	Cyclohexane, 1-methyl-2-propyl-	Cyclic aliphatics	12.9	7.14		4.76	
602	Cyclohexane, 1,1,2,3-tetramethyl-	Cyclic aliphatics		7.14		4.76	
603	Cyclohexane, 1,1,3-trimethyl-	Cyclic aliphatics	9.68	28.57		4.76	
604	Cyclohexane, 1,2-diethyl-, cis-	Cyclic aliphatics	12.9			4.76	
605	Cyclohexane, 1,2-dimethyl- (cis/trans)	Cyclic aliphatics	3.23				

606	Cyclohexane, 1,2-dimethyl-, cis-	Cyclic aliphatics	3.23				
607	Cyclohexane, 1,2,3-trimethyl-	Cyclic aliphatics	3.23				
608	Cyclohexane, 1,2,3-trimethyl-, (1 $\dot{\pm}$ ,2 $\dot{\mp}$ ,3 $\dot{\pm}$ )-	Cyclic aliphatics	3.23				
609	Cyclohexane, 1,2,4-trimethyl-	Cyclic aliphatics	35.48	14.29		4.76	
610	Cyclohexane, 1,2,4-trimethyl-, (1 $\dot{\pm}$ ,2 $\dot{\mp}$ ,4 $\dot{\mp}$ )-	Cyclic aliphatics	6.45				
611	Cyclohexane, 1,3-dimethyl-	Cyclic aliphatics	3.23				
612	Cyclohexane, 1,3-dimethyl-, cis-	Cyclic aliphatics	22.58	28.57	50	4.76	33.33
613	Cyclohexane, 1,3-dimethyl-, trans-	Cyclic aliphatics	6.45	7.14		4.76	
614	Cyclohexane, 1,3,5-trimethyl-	Cyclic aliphatics	16.13			4.76	
615	Cyclohexane, 1,4-dimethyl-	Cyclic aliphatics	6.45				
616	Cyclohexane, 1,4-dimethyl-, cis-	Cyclic aliphatics	3.23				
617	Cyclohexane, 2-propenyl-	Cyclic aliphatics	3.23				
618	Cyclohexane, 2,4-diethyl-1-methyl-	Cyclic aliphatics	3.23				
619	Cyclohexane, 3-ethyl-5-methyl-1-propyl-	Cyclic aliphatics	3.23				
620	Cyclohexane, butyl-	Cyclic aliphatics	6.45				
621	Cyclohexane, ethyl-	Cyclic aliphatics	41.94	21.43	75	9.52	66.67
622	Cyclohexane, isocyanato-	Nitrogen-containing	9.68		50		
623	Cyclohexane, isothiocyanato-	Nitrogen-containing	9.68		25		33.33
624	Cyclohexane, methyl-	Cyclic aliphatics	12.9	14.29	25		33.33
625	Cyclohexane, methylene-	Cyclic aliphatics	6.45				
626	Cyclohexane, octyl-	Cyclic aliphatics		7.14		4.76	
627	Cyclohexane, pentyl-	Cyclic aliphatics	6.45				
628	Cyclohexane, propyl-	Cyclic aliphatics	6.45	21.43	25		33.33
629	Cyclohexanol	Alcohols	3.23				
630	Cyclohexanol, 2-methyl-, cis-	Ketones	6.45				
631	Cyclohexanone, 2-methyl-	Ketones	9.68				
632	Cyclohexanone, 3-methyl-	Ketones	3.23				
633	Cyclohexanone, 4-ethyl-	Ketones	6.45				
634	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, (2R-cis)-	Ketones		7.14			
635	Cyclohexene	Cyclic aliphatics	16.13		25	4.76	33.33
636	Cyclohexene, 1-methyl-	Cyclic aliphatics	12.9	50	25	9.52	33.33
637	Cyclohexene, 3-methyl-	Cyclic aliphatics	3.23				
638	Cyclohexene, 3,3,5-trimethyl-	Cyclic aliphatics		7.14			
639	Cyclohexene, 4-(1,1-dimethylethyl)-	Cyclic aliphatics	6.45			4.76	
640	Cyclohexene, 4-methyl-1-(1-methylethyl)-	Cyclic aliphatics	3.23				
641	Cyclohexylamine	Nitrogen-containing	6.45	7.14			
642	Cyclooctane, 1,4-dimethyl-, trans-	Cyclic aliphatics	6.45				
643	Cyclooctane, ethyl-	Cyclic aliphatics	3.23				
644	Cyclooctane, methyl-	Cyclic aliphatics	3.23				
645	Cyclopentane, (1-methylethyl)-	Cyclic aliphatics				4.76	
646	Cyclopentane, 1-ethyl-2-methyl-, cis-	Cyclic aliphatics	6.45			4.76	
647	Cyclopentane, 1-ethyl-3-methyl-, trans-	Cyclic aliphatics	48.39	21.43	25	4.76	
648	Cyclopentane, 1-methyl-2-(2-propenyl)-, trans-	Cyclic aliphatics				4.76	
649	Cyclopentane, 1-methyl-2-propyl-	Cyclic aliphatics	25.81	14.29			
650	Cyclopentane, 1-methyl-3-(1-methylethyl)-	Cyclic aliphatics	3.23				
651	Cyclopentane, 1,1'-[4-(3-cyclopentylpropyl)-1,7-heptanediy]bis-	Cyclic aliphatics		7.14			
652	Cyclopentane, 1,2-dimethyl-, trans-	Cyclic aliphatics	9.68				

653	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	Cyclic aliphatics	6.45			4.76	
654	Cyclopentane, 1,2,4-trimethyl-	Cyclic aliphatics	19.35	7.14		4.76	33.33
655	Cyclopentane, 1,2,4-trimethyl-, (1Ī±,2Ī±,4Ī±)-	Cyclic aliphatics	3.23				
656	Cyclopentane, 1,2,4-trimethyl-, (1Ē±,2Ē±,4Ē±)-	Cyclic aliphatics			25		
657	Cyclopentane, 1,3-dimethyl-	Cyclic aliphatics	9.68				
658	Cyclopentane, 1,3-dimethyl-, cis-	Cyclic aliphatics	29.03	28.57		9.52	33.33
659	Cyclopentane, 2-isopropyl-1,3-dimethyl-	Cyclic aliphatics	3.23				
660	Cyclopentane, butyl-	Cyclic aliphatics	3.23		75		
661	Cyclopentane, ethyl-	Cyclic aliphatics	48.39	21.43	100	4.76	100
662	Cyclopentane, propyl-	Cyclic aliphatics			100		
663	Cyclopentanecetic acid, 3-oxo-2-pentyl-, methyl ester	Esters and analogues		7.14			
664	Cyclopentanol	Alcohols	9.68				
665	Cyclopentanone	Ketones			25		
666	Cyclopentanone, 2-ethyl-	Ketones	6.45		100		33.33
667	Cyclopentanone, 2-methyl-	Ketones	48.39	21.43	75	14.29	33.33
668	Cyclopentanone, 3-butyl-	Ketones	3.23				
669	Cyclopentanone, 3-methyl-	Ketones	19.35				
670	Cyclopentene, 1-methyl-	Cyclic aliphatics	32.26	21.43		4.76	33.33
671	Cyclopentene, 1,2,3-trimethyl-	Cyclic aliphatics	25.81			4.76	
672	Cyclopentene, 3-ethyl-	Cyclic aliphatics	9.68				
673	Cyclopentene, 4,4-dimethyl-	Cyclic aliphatics	6.45				
674	Cyclopropane	Cyclic aliphatics		7.14			
675	Cyclopropane, 1-butyl-1-methyl-2-propyl-	Cyclic aliphatics		7.14			
676	Cyclopropane, 1,1,2,2-tetramethyl-	Cyclic aliphatics			25	4.76	
677	Cyclopropane, 1,2-dimethyl-3-pentyl-, (1Ī±,2Ī±,3Ī±)-	Cyclic aliphatics	3.23				
678	Cyclopropane, propyl-	Cyclic aliphatics		7.14			
679	Cyclotetradecane	Cyclic aliphatics		7.14			
680	Cycluron	Aromatics	12.9	7.14			
681	D-Limonene	Cyclic aliphatics		7.14		4.76	
682	Decanal	Aldehydes	6.45		50	4.76	33.33
683	Decane	Linear aliphatics		7.14		9.52	
684	Decane, 2-methyl-	Linear aliphatics	35.48	7.14		4.76	
685	Decane, 2,5-dimethyl-	Linear aliphatics				9.52	
686	Decane, 2,5,9-trimethyl-	Linear aliphatics	3.23				
687	Decane, 2,6,7-trimethyl-	Linear aliphatics	19.35	7.14			
688	Decane, 2,6,8-trimethyl-	Linear aliphatics	3.23	7.14	25		
689	Decane, 2,9-dimethyl-	Linear aliphatics	6.45				
690	Decane, 3-methyl-	Linear aliphatics	22.58			9.52	
691	Decane, 3,6-dimethyl-	Linear aliphatics	3.23	7.14			
692	Decane, 3,7-dimethyl-	Linear aliphatics	6.45	7.14			
693	Decane, 3,8-dimethyl-	Linear aliphatics	3.23				
694	Decane, 4-methyl-	Linear aliphatics	6.45			4.76	
695	Decane, 5-methyl-	Linear aliphatics	12.9		25		
696	Desmethyldoxepin	Aromatics	9.68	28.57	50	9.52	
697	di-tert-Butyl dicarbonate	Esters and analogues		7.14			
698	Diacetyl sulphide	Sulfur-containing		7.14			
699	Diazene, dimethyl-	Nitrogen-containing	16.13	7.14	25	14.29	33.33

700	Dibenzofuran	Aromatics	12.9	21.43	25	4.76	
701	Dibutyl phthalate	Esters and analogues	16.13	14.29		19.05	
702	Dicyclopentadiene	Cyclic aliphatics	6.45				
703	Dicyclopropyl carbinol	Alcohols		7.14			
704	Diethyl azodicarboxylate	Nitrogen-containing	3.23	21.43		4.76	
705	Diethyl Phthalate	Esters and analogues	9.68	28.57	25	4.76	
706	Diethyltoluamide	Nitrogen-containing	9.68	21.43	25		
707	Diisobutyl cellosolve	Linear aliphatics				4.76	
708	Dimethyl phthalate	Esters and analogues	12.9		25		
709	Dimethyl sulfide	Sulfur-containing	3.23				
710	Dimethyl sulfone	Sulfur-containing	38.71				
711	Dimethyl Sulfoxide	Sulfur-containing	12.9				
712	Dimethyl trisulfide	Sulfur-containing	61.29				100
713	Dimethylamine	Nitrogen-containing	3.23	7.14			
714	Dinocap	Nitrogen-containing	6.45	28.57		14.29	33.33
715	Diphenyl ether	Ethers	6.45	7.14			
716	Diphenyl sulfide	Sulfur-containing		7.14			
717	Disulfide, dimethyl	Sulfur-containing	74.19	14.29	100	19.05	100
718	Disulfide, isopentyl methyl	Sulfur-containing	3.23				
719	Disulfide, methyl (methylthio)methyl	Sulfur-containing	29.03				
720	Disulfide, methyl propyl	Sulfur-containing	9.68				
721	dl-3-Aminoisobutyric acid, N-methyl-, methyl ester	Esters and analogues	22.58	28.57		4.76	
722	dl-7-Azatryptophan	Nitrogen-containing				4.76	
723	dl-Alanine	Nitrogen-containing		7.14			
724	dl-Alanyl-dl-leucine	Nitrogen-containing	9.68	14.29		14.29	33.33
725	dl-Alanyl-dl-serine	Nitrogen-containing		7.14			
726	dl-Alanyl-dl-valine	Nitrogen-containing		7.14			
727	dl-Alanyl-l-alanine	Nitrogen-containing	9.68	28.57	25	14.29	33.33
728	dl-Phenylephrine	Aromatics	3.23	7.14			
729	Dodecanal	Aldehydes	9.68	7.14	25	4.76	
730	Dodecane	Linear aliphatics	32.26	42.86	75	14.29	33.33
731	Dodecane, 1-iodo-	Halogen-containing	9.68				33.33
732	Dodecane, 2-methyl-	Linear aliphatics	6.45	7.14			
733	Dodecane, 2,6,10-trimethyl-	Linear aliphatics	6.45	14.29			
734	Dodecane, 2,6,11-trimethyl-	Linear aliphatics	22.58	21.43			
735	Dodecane, 2,7,10-trimethyl-	Linear aliphatics	22.58		25	9.52	
736	Dodecane, 4,6-dimethyl-	Linear aliphatics	12.9	21.43			
737	Dodecane, 6-methyl-	Linear aliphatics	3.23				
738	Dotriacontane	Linear aliphatics			25	19.05	
739	Eicosane	Linear aliphatics	35.48	28.57	50	19.05	33.33
740	EMDP	Nitrogen-containing		7.14			
741	Erythro-2-methyl-3,4-dibromo-2-butanol	Alcohols	3.23				
742	Ethane, 1-(o-ethylphenyl)-1-phenyl-	Linear aliphatics		7.14			
743	Ethane, 1,1,1-trifluoro-	Halogen-containing	3.23				
744	Ethane, 1,2-dichloro-	Halogen-containing	12.9		25	14.29	33.33
745	Ethane, hexachloro-	Halogen-containing	41.94	7.14	25		33.33
746	Ethane, nitro-	Nitrogen-containing	6.45	7.14		4.76	

747	Ethanediamide	Nitrogen-containing	3.23				
748	Ethanol	Alcohols	3.23		50		33.33
749	Ethanol, 2-(2-butoxyethoxy)-	Alcohols	3.23	7.14	25		
750	Ethanol, 2-(methylthio)-	Alcohols	3.23				
751	Ethanol, 2-butoxy-	Alcohols	31.26	7.14	25		33.33
752	Ethanol, 2-ethoxy-	Alcohols			25		
753	Ethanol, 2-fluoro-	Alcohols	3.23	7.14			
754	Ethanol, 2-methoxy-	Alcohols			25		
755	Ethanol, 2-methoxy-, acetate	Esters and analogues			25		
756	Ethanol, 2,2-dichloro-	Alcohols	6.45			23.81	33.33
757	Ethanone, 1-(1-methylcyclohexyl)-	Ketones	3.23				
758	Ethanone, 1-(2-furanyl)-	Ketones			75		33.33
759	Ethanone, 1,1'-(1,4-phenylene)bis-	Ketones	3.23				
760	Ethanone, 2-(1-methylethoxy)-1,2-diphenyl-	Ketones		14.29			
761	Ethyl Acetate	Esters and analogues	6.45		25		
762	Ethyl acetoacetate ethylene acetal	Esters and analogues				4.76	
763	Ethyl methanesulfinate	Sulfur-containing	3.23				
764	Ethylbenzene	Aromatics		21.43	25		
765	Ethylene glycol adipate	Esters and analogues		7.14			
766	Ethylidenecyclobutane	Cyclic aliphatics				4.76	
767	Ethyne, fluoro-	Halogen-containing		7.14			
768	Eucalyptol	Ethers	6.45				
769	Fenchone	Ketones	6.45				
770	Fluorene	Aromatics		14.29			
771	Formaldehyde	Aldehydes	6.45			19.05	
772	Formamide, N-cyclohexyl-	Nitrogen-containing		7.14			
773	Formic acid	Acids	3.23				
774	Formic acid, 2-methylpropyl ester	Esters and analogues	3.23				
775	Formic acid, butyl ester	Esters and analogues				4.76	
776	Formic acid, heptyl ester	Esters and analogues	12.9				
777	Formic acid, hexyl ester	Esters and analogues	3.23				
778	Formic acid, octyl ester	Esters and analogues	6.45				
779	Formic acid, pentyl ester	Esters and analogues	12.9				
780	Formic acid, propyl ester	Esters and analogues	6.45				
781	Furan, 2-(dichloromethyl)-tetrahydro-	Aromatics	3.23				
782	Furan, 2-butyltetrahydro-	Aromatics			25		
783	Furan, 2-ethyl-	Aromatics	25.81		50		33.33
784	Furan, 2-ethyl-5-methyl-	Aromatics	6.45		75		66.67
785	Furan, 2-hexyl-	Aromatics	29.03		75		100
786	Furan, 2-pentyl-	Aromatics	38.71	50	100	23.81	100
787	Furan, 2-propyl-	Aromatics	12.9		75		66.67
788	Furan, 2,3-dihydro-	Aromatics	3.23				
789	Furan, 2,3-dihydro-5-methyl-	Aromatics	9.68	7.14		4.76	
790	Furan, 2,3,5-trimethyl-	Aromatics	6.45				
791	Furan, 2,5-dimethyl-	Aromatics	22.58	14.29	25	4.76	
792	Furan, 3-(4-methyl-3-pentenyl)-	Aromatics	25.81				
793	Furan, 3-pentyl-	Aromatics			25		33.33

794	Furan, tetrahydro-2-methyl-	Aromatics	16.13	7.14	50		66.67
795	Furfural	Aromatics	6.45				
796	Glycine, N-(dithiocarboxy)-N-methyl-	Sulfur-containing	19.35	21.43		19.05	
797	Glycolaldehyde dimer	Aldehydes	3.23				
798	Heneicosane	Linear aliphatics		7.14			
799	Heneicosylcyclohexane	Cyclic aliphatics		7.14			
800	Heptacosan-9-ol	Alcohols	3.23	7.14			
801	Heptacosane	Linear aliphatics	25.81	21.43		19.05	33.33
802	Heptadecane	Linear aliphatics	3.23	7.14			
803	Heptadecane, 2,6,10,14-tetramethyl-	Linear aliphatics	6.45				33.33
804	Heptadecane, 2,6,10,15-tetramethyl-	Linear aliphatics	3.23				
805	Heptanal	Aldehydes			25		
806	Heptane	Linear aliphatics	3.23			4.76	
807	Heptane, 1-(methylthio)-	Sulfur-containing	6.45				
808	Heptane, 1-chloro-	Halogen-containing			75		
809	Heptane, 1,1-diphenyl-	Linear aliphatics		7.14			
810	Heptane, 2-methyl-	Linear aliphatics			50		
811	Heptane, 2,2,4-trimethyl-	Linear aliphatics	25.81				
812	Heptane, 2,2,4,6,6-pentamethyl-	Linear aliphatics	25.81			9.52	
813	Heptane, 2,3-dimethyl-	Linear aliphatics	6.45	7.14	25		
814	Heptane, 2,3,6-trimethyl-	Linear aliphatics		7.14		4.76	
815	Heptane, 2,4-dimethyl-	Linear aliphatics	19.35				
816	Heptane, 2,4,6-trimethyl-	Linear aliphatics	3.23				
817	Heptane, 2,5-dimethyl-	Linear aliphatics	32.26	28.57	25	14.29	100
818	Heptane, 2,6-dimethyl-	Linear aliphatics	29.03	21.43	25	23.81	
819	Heptane, 3-ethyl-2-methyl-	Linear aliphatics	3.23	7.14		4.76	33.33
820	Heptane, 3-ethyl-5-methyl-	Linear aliphatics	3.23				
821	Heptane, 3-methyl-	Linear aliphatics	3.23				
822	Heptane, 3-methylene-	Linear aliphatics	3.23				
823	Heptane, 3,4-dimethyl-	Linear aliphatics		7.14			
824	Heptane, 3,5-dimethyl-	Linear aliphatics	3.23	7.14		14.29	
825	Heptane, 4-ethyl-2,2,6,6-tetramethyl-	Linear aliphatics				4.76	
826	Heptane, 4-methyl-	Linear aliphatics	3.23				
827	Heptane, hexadecafluoro-	Halogen-containing		7.14			
828	Heptanoic acid, ethyl ester	Esters and analogues			100		100
829	Heptanonitrile	Nitrogen-containing	16.13				
830	Heptylcyclohexane	Cyclic aliphatics	3.23	7.14			33.33
831	Hexadecanal	Aldehydes	3.23	7.14			
832	Hexadecane	Linear aliphatics	9.68			19.05	33.33
833	Hexadecane, 1-iodo-	Halogen-containing		7.14			
834	Hexadecanoic acid, 1,1-dimethylethyl ester	Esters and analogues	3.23				
835	Hexanal	Aldehydes	3.23		25		
836	Hexanal, 2-ethyl-	Aldehydes		14.29	25	4.76	
837	Hexane, 1-(methylthio)-	Sulfur-containing	6.45				
838	Hexane, 1-chloro-	Halogen-containing	3.23		75		
839	Hexane, 2-methyl-	Linear aliphatics		7.14	50		
840	Hexane, 2-nitro-	Nitrogen-containing	3.23				



841	Hexane, 2,2-dimethyl-	Linear aliphatics	6.45	14.29			33.33
842	Hexane, 2,2,4-trimethyl-	Linear aliphatics	3.23	35.71	50	57.14	66.67
843	Hexane, 2,2,5-trimethyl-	Linear aliphatics	25.81	14.29			33.33
844	Hexane, 2,3-dimethyl-	Linear aliphatics	38.71	21.43	25	4.76	33.33
845	Hexane, 2,3,5-trimethyl-	Linear aliphatics	29.03	7.14		4.76	
846	Hexane, 2,4-dimethyl-	Linear aliphatics	45.16	21.43	25	9.52	33.33
847	Hexane, 2,4,4-trimethyl-	Linear aliphatics	3.23				
848	Hexane, 2,5-dimethyl-	Linear aliphatics	51.61	21.43	25	9.52	33.33
849	Hexane, 3-ethyl-2-methyl-	Linear aliphatics		21.43	25	19.05	33.33
850	Hexane, 3-ethyl-2,5-dimethyl-	Linear aliphatics				4.76	
851	Hexane, 3-methyl-	Linear aliphatics	9.68		25		33.33
852	Hexane, 3,3-dimethyl-	Linear aliphatics	19.35	14.29			
853	Hexane, 3,4-bis(1,1-dimethylethyl)-2,2,5,5-tetramethyl-	Linear aliphatics	6.45				
854	Hexane, 3,4-dimethyl-	Linear aliphatics	41.94	14.29		4.76	
855	Hexanedioic acid, bis(2-ethylhexyl) ester	Esters and analogues	3.23				
856	Hexanenitrile	Nitrogen-containing	38.71		50		33.33
857	Hexanoic acid	Acids	9.68		25		
858	Hexanoic acid, 1-methylethyl ester	Esters and analogues	29.03		50		33.33
859	Hexanoic acid, 2-methyl-	Acids	22.58				
860	Hexanoic acid, 2-methylpropyl ester	Esters and analogues	9.68				
861	Hexanoic acid, butyl ester	Esters and analogues	3.23				
862	Hexanoic acid, ethyl ester	Esters and analogues	25.81		100		100
863	Hexanoic acid, methyl ester	Esters and analogues	9.68		25		66.67
864	Hexanoic acid, pentyl ester	Esters and analogues	12.9				
865	Hexanoic acid, propyl ester	Esters and analogues	9.68				
866	Hexestrol	Alcohols		7.14			
867	Hexestrol, O-trifluoroacetyl-	Halogen-containing		7.14			
868	Homosalate	Esters and analogues	3.23				
869	Hordenine	Aromatics		7.14			
870	Hydrazine	Nitrogen-containing		7.14			
871	Hydrazinecarboxamide	Nitrogen-containing	3.23	7.14	50	4.76	
872	Hydrogen chloride	Halogen-containing		7.14			
873	Hydrogen isocyanate	Nitrogen-containing	3.23				
874	̇± Isomethyl ionone	Ketones	6.45				
875	̇±-Methylstyrene	Aromatics	6.45				
876	̇±-Pinene	Aromatics	16.13				
877	̇±-Pinene	Aromatics	3.23				
878	Indan, 1-methyl-	Aromatics	45.16	21.43	25	4.76	33.33
879	Indane	Aromatics	45.16	21.43	100	14.29	66.67
880	Indene	Aromatics	3.23				
881	Indole	Aromatics	6.45				
882	Indole, 3-methyl-2-(2-dimethylaminopropyl)-	Aromatics		7.14			
883	Isobutyl acetate	Esters and analogues			25		
884	Isobutyl isovalerate	Esters and analogues	16.13				
885	Isobutyronitrile	Nitrogen-containing	35.48			23.81	
886	Isopropyl acetate	Esters and analogues	54.84		100		66.67
887	Isopropyl Alcohol	Alcohols	3.23				

888	Isopropyl butyrate	Esters and analogues	45.16				66.67
889	Isopropyl myristate	Nitrogen-containing	12.9	28.57		4.76	
890	Isopropylcyclobutane	Cyclic aliphatics	29.03	14.29	25		33.33
891	Isothiazole	Aromatics	6.45				
892	Isothiazole, 3-methyl-	Aromatics	25.81				
893	L-Alanine ethylamide	Nitrogen-containing	12.9	35.71		33.33	33.33
894	L-Leucine, n-butoxycarbonyl-N-methyl-, undecyl ester	Esters and analogues	6.45	7.14		4.76	
895	L-Norleucine, N-ethoxycarbonyl-, decyl ester	Esters and analogues		7.14			
896	Levacylmethadol	Alcohols		7.14			
897	Levomenthol	Alcohols	12.9				
898	Limonene	Cyclic aliphatics	3.23	7.14			
899	Linalool	Alcohols				4.76	
900	Linalyl acetate	Esters and analogues	9.68				
901	Longifolene	Aromatics	9.68				
902	m-Anisoyl amide, N-(2-phenylethyl)-N-isobutyl-	Nitrogen-containing		7.14			
903	m-Anisoyl amide, N-(2-phenylethyl)-N-octyl-	Nitrogen-containing		7.14			
904	Mesitylene	Aromatics	12.9		25	4.76	33.33
905	Methane, bromodichloro-	Halogen-containing	25.81	21.43		4.76	33.33
906	Methane, isothiocyanato-	Nitrogen-containing	3.23	21.43		4.76	
907	Methanesulfonic acid, ethyl ester	Esters and analogues	3.23				
908	Methanesulfonic acid, methyl ester	Esters and analogues	6.45				
909	Methanesulfonic anhydride	Sulfur-containing	41.94	21.43	100	14.29	66.67
910	Methenamine	Nitrogen-containing	22.58	7.14			
911	Methyl Alcohol	Alcohols	19.35	28.57	25	28.57	66.67
912	Methyl ethyl disulfide	Sulfur-containing	19.35				
913	Methyl glyoxal	Aldehydes			25		
914	Methyl Isobutyl Ketone	Ketones	29.03	7.14			
915	Methyl isobutyrate	Esters and analogues	38.71				66.67
916	Methyl isocyanide	Nitrogen-containing	16.13				
917	Methyl isopropyl disulphide	Sulfur-containing	16.13				
918	Methyl isovalerate	Esters and analogues					66.67
919	Methyl n-butyl disulfide	Sulfur-containing	3.23				
920	Methyl propionate	Esters and analogues	16.13		50		
921	Methyl sec-butyl disulphide	Sulfur-containing	3.23				
922	Methyl thioacetate	Esters and analogues	9.68				
923	Methyl valerate	Esters and analogues			25		
924	Methylamine, N,N-dimethyl-	Nitrogen-containing	12.9	7.14			
925	Monoisopropyl carbonotrithioate	Nitrogen-containing		7.14			
926	N-(Cyclohexyl)succinimide	Nitrogen-containing		7.14			
927	n-Butyric acid 2-ethylhexyl ester	Esters and analogues	22.58				
928	N-Cbz-glycylglycine p-nitrophenyl ester	Esters and analogues		7.14			
929	n-Decanoic acid	Acids	3.23		25		
930	N-Dodecylmethylamine	Nitrogen-containing	6.45				
931	n-Hexadecanoic acid	Acids		7.14			
932	n-Hexyl salicylate	Esters and analogues		7.14		4.76	
933	n-Hexylmethylamine	Nitrogen-containing	9.68	7.14			
934	N- $\epsilon$ ,N- $\beta$ -Di-cbz-L-arginine	Nitrogen-containing	3.23				

935	N-Methyltaurine	Nitrogen-containing		7.14			
936	N-(ε-L-N-ε-Di-cbz-L-arginine	Nitrogen-containing		28.57	25	19.05	
937	n-Propyl acetate	Esters and analogues	48.39		100		100
938	N,N-Dimethylacetamide	Nitrogen-containing	3.23				
939	N,N,O-Triacetylhydroxylamine	Nitrogen-containing	12.9		75		66.67
940	Naphthalene, 1,2,3,4-tetrahydro-	Aromatics	45.16		25	4.76	33.33
941	Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	Aromatics	38.71	21.43	25	4.76	
942	Naphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-	Aromatics	12.9	7.14			33.33
943	Naphthalene, 1,2,3,4-tetrahydro-5,6-dimethyl-	Aromatics	3.23	7.14			
944	Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	Aromatics	32.26	7.14		4.76	
945	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	Aromatics		7.14			
946	Naphthalene, 1,6,7-trimethyl-	Aromatics		7.14			
947	Naphthalene, 1,7-dimethyl-	Aromatics	3.23				
948	Naphthalene, 2-methoxy-	Aromatics	19.35	14.29		4.76	
949	Naphthalene, 2-methyl-	Aromatics	35.48	21.43	75	4.76	
950	Naphthalene, 2,3,6-trimethyl-	Aromatics		7.14			
951	Naphthalene, 2,7-dimethyl-	Aromatics	3.23				
952	Naphthalene, decahydro-, trans-	Aromatics	6.45			4.76	
953	Naphtho[2,1-b]furan	Aromatics	3.23				
954	Nitric acid, ethyl ester	Esters and analogues			25		
955	Nitrous oxide	Nitrogen-containing	3.23	7.14			
956	Nonadecane	Linear aliphatics	48.39	21.43	75	23.81	66.67
957	Nonanal	Aldehydes	32.26	28.57	100	28.57	100
958	Nonane	Linear aliphatics	3.23	7.14	25		
959	Nonane, 2-methyl-	Linear aliphatics	22.58	7.14	50	14.29	
960	Nonane, 2,2,4,4,6,8,8-heptamethyl-	Linear aliphatics	3.23	14.29	50	23.81	
961	Nonane, 2,5-dimethyl-	Linear aliphatics	3.23				33.33
962	Nonane, 2,6-dimethyl-	Linear aliphatics	9.68				
963	Nonane, 3-methyl-	Linear aliphatics	32.26	21.43	50	9.52	33.33
964	Nonane, 3,7-dimethyl-	Linear aliphatics	6.45				
965	Nonane, 5-methyl-	Linear aliphatics	6.45				
966	Nonanoic acid	Acids	3.23	7.14	25		
967	Nonanoic acid, ethyl ester	Esters and analogues			100		
968	O-Methylisourea	Nitrogen-containing		7.14			
969	o-Toluyamide, N-(2-phenylethyl)-N-propyl-	Nitrogen-containing	3.23				
970	o-Xylene	Aromatics	41.94	28.57	25	14.29	33.33
971	Octadecane	Linear aliphatics		7.14			
972	Octadecane, 6-methyl-	Linear aliphatics	3.23	7.14		14.29	
973	Octanal	Aldehydes	6.45	14.29	50	4.76	33.33
974	Octanamide, N,N-dimethyl-	Nitrogen-containing		7.14			
975	Octane	Linear aliphatics			25	4.76	
976	Octane, 1-chloro-	Halogen-containing	9.68		75		33.33
977	Octane, 1,1'-oxybis-	Ethers	22.58	35.71	25	23.81	33.33
978	Octane, 2-methyl-	Linear aliphatics	9.68	21.43	50	4.76	33.33
979	Octane, 2,2,6-trimethyl-	Linear aliphatics	9.68	14.29			66.67
980	Octane, 2,3,7-trimethyl-	Linear aliphatics		7.14		4.76	
981	Octane, 2,5-dimethyl-	Linear aliphatics	3.23		25		

982	Octane, 2,6-dimethyl-	Linear aliphatics	19.35	21.43		9.52	66.67
983	Octane, 2,7-dimethyl-	Linear aliphatics		14.29		4.76	
984	Octane, 3-ethyl-	Linear aliphatics	3.23				
985	Octane, 3-methyl-	Linear aliphatics	12.9				
986	Octane, 3,5-dimethyl-	Linear aliphatics	25.81				
987	Octane, 4-ethyl-	Linear aliphatics	9.68	14.29	25	4.76	
988	Octane, 4-methyl-	Linear aliphatics	29.03				
989	Octanoic acid	Acids	9.68				
990	Octanoic acid, ethyl ester	Esters and analogues			100		66.67
991	Octodrine	Nitrogen-containing	3.23	7.14			
992	(E)- Isomethyl ionone	Ketones		14.29		4.76	
993	(E)-Methylstyrene	Aromatics		7.14			
994	(E)-Pinene	Aromatics		35.71	100	47.62	
995	(E)-Dodecalactone	Esters and analogues		7.14			
996	ortho tert-Butyl cyclohexyl acetate	Esters and analogues	3.23				
997	Oxalic acid, diallyl ester	Esters and analogues				4.76	
998	Oxalic acid, isobutyl nonyl ester	Esters and analogues		7.14			33.33
999	Oxepine, 2,7-dimethyl-	Aromatics	3.23				
1000	Oxetane, 3,3-dimethyl-	Ethers			25		
1001	p-Aminotoluene	Aromatics	3.23				
1002	p-Cresol	Alcohols	22.58	7.14			
1003	p-Cymene	Aromatics	22.58	7.14			33.33
1004	Pentadecane	Linear aliphatics	6.45	7.14		4.76	
1005	Pentadecane, 2,6,10-trimethyl-	Linear aliphatics		7.14		9.52	
1006	Pentadecanoic acid, 14-methyl-, methyl ester	Esters and analogues	3.23				
1007	Pentalene, octahydro-	Linear aliphatics	9.68				
1008	Pentalene, octahydro-, cis-	Linear aliphatics	3.23				
1009	Pentalene, octahydro-2-methyl-	Linear aliphatics	12.9				
1010	Pentanal	Aldehydes	12.9				
1011	Pentane, 1-chloro-	Halogen-containing	6.45		75		
1012	Pentane, 1-iodo-	Halogen-containing	6.45				
1013	Pentane, 1-methoxy-	Ethers			100		33.33
1014	Pentane, 2,2,4-trimethyl-	Linear aliphatics	12.9		25		
1015	Pentane, 2,3-dimethyl-	Linear aliphatics	29.03	35.71	50	23.81	66.67
1016	Pentane, 2,3,3-trimethyl-	Linear aliphatics	45.16	21.43	25	9.52	33.33
1017	Pentane, 2,3,4-trimethyl-	Linear aliphatics	48.39	21.43	25	9.52	33.33
1018	Pentane, 3-ethyl-	Linear aliphatics	3.23			9.52	
1019	Pentane, 3,3-dimethyl-	Linear aliphatics	35.48	28.57	25	14.29	33.33
1020	Pentanenitrile	Nitrogen-containing	9.68				
1021	Pentanoic acid	Acids	48.39	7.14	50		66.67
1022	Pentanoic acid, 1-methylethyl ester	Esters and analogues	9.68				
1023	Pentanoic acid, 2-ethylhexyl ester	Esters and analogues	6.45				
1024	Pentanoic acid, 2-methyl-	Acids	3.23				
1025	Pentanoic acid, 2-methylpropyl ester	Esters and analogues	9.68				
1026	Pentanoic acid, 2,2,4-trimethyl-3-hydroxy-, isobutyl ester	Esters and analogues	19.35	14.29		9.52	
1027	Pentanoic acid, 3-methyl-	Acids	12.9				
1028	Pentanoic acid, 4-methyl-	Acids	12.9				

1029	Pentanoic acid, 4-methyl-, ethyl ester	Esters and analogues	22.58				66.67
1030	Pentanoic acid, 4-methyl-, methyl ester	Esters and analogues	12.9				
1031	Pentanoic acid, 4-methyl-, pentyl ester	Esters and analogues	3.23				
1032	Pentanoic acid, butyl ester	Esters and analogues	3.23				
1033	Pentanoic acid, ethyl ester	Esters and analogues	25.81		75		66.67
1034	Pentanoic acid, pentyl ester	Esters and analogues	9.68				
1035	Pentanoic acid, propyl ester	Esters and analogues			25		
1036	Perfluorooctane	Halogen-containing		7.14			
1037	Phenethylamine, p-(E±-dimethyl-	Nitrogen-containing		7.14		4.76	
1038	Phenol	Alcohols	3.23	21.43	25	4.76	
1039	Phenol, 2-(1,1-dimethylethyl)-	Alcohols	6.45	7.14			
1040	Phenol, 2-(1,1-dimethylethyl)-4-(1,1,3,3-tetramethylbutyl)-	Alcohols		7.14			
1041	Phenol, 2-(1,1-dimethylethyl)-5-methyl-	Alcohols		7.14			
1042	phenol, 2-(1,1,3,3-tetramethylbutyl)-	Alcohols		7.14		4.76	
1043	Phenol, 2,4,6-tri-tert-butyl-	Alcohols	3.23				
1044	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate	Esters and analogues		7.14			
1045	Phenol, 3-ethyl-	Alcohols					33.33
1046	Phenol, 4-(1-methylpropyl)-	Alcohols			25		
1047	Phenol, 4-(1,1-dimethylpropyl)-	Alcohols		7.14			
1048	Phenol, 4-[2-(methylamino)ethyl]-	Alcohols	19.35	21.43		4.76	33.33
1049	Phenol, 4-ethyl-	Alcohols	3.23		75		33.33
1050	Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-	Alcohols		7.14			
1051	Phenol, p-tert-butyl-	Alcohols	22.58				
1052	Phenylephrine	Aromatics	22.58	7.14			
1053	Phenylethyl Alcohol	Alcohols	22.58				
1054	Phenylethyne	Aromatics	6.45	7.14	25		
1055	Phenylmaleic anhydride	Esters and analogues	9.68	7.14			
1056	Phosphonic acid, (p-hydroxyphenyl)-	Acids		7.14			
1057	Phosphorocyanidous difluoride	Halogen-containing		7.14			
1058	Phthalic acid, 2-isopropylphenyl methyl ester	Esters and analogues		7.14		4.76	
1059	Phthalic acid, butyl 2-chloropropyl ester	Esters and analogues		7.14			
1060	Phthalic acid, heptyl tridec-2-yn-1-yl ester	Esters and analogues				4.76	
1061	Phthalic anhydride	Esters and analogues	3.23				
1062	Pinocarvone	Ketones	3.23				
1063	Propanal	Aldehydes	22.58				
1064	Propane, 1-(methylthio)-	Sulfur-containing	22.58				
1065	Propane, 1,3-dichloro-	Halogen-containing	3.23				
1066	Propane, 2-(methylthio)-	Sulfur-containing	6.45				
1067	Propane, 2-iodo-	Halogen-containing	3.23				
1068	Propane, 2,2-dimethoxy-	Ethers	41.94				
1069	Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-	Nitrogen-containing	3.23				
1070	Propanedioic acid	Acids	35.48	7.14		9.52	33.33
1071	Propanedioic acid, propyl-	Acids	3.23				
1072	Propanenitrile, 3-hydroxy-	Nitrogen-containing		7.14			
1073	Propanoic acid	Acids	54.84				33.33
1074	Propanoic acid, 1-methylethyl ester	Esters and analogues	45.16				66.67
1075	Propanoic acid, 2-methyl-	Acids	64.52				66.67

1076	Propanoic acid, 2-methyl-, 1-methylethyl ester	Esters and analogues	48.39				
1077	Propanoic acid, 2-methyl-, 2-methylpropyl ester	Esters and analogues	16.13				
1078	Propanoic acid, 2-methyl-, 3-hydroxy-2,2,4-trimethylpentyl ester	Esters and analogues	19.35	14.29		9.52	
1079	Propanoic acid, 2-methyl-, 3-methylbutyl ester	Esters and analogues	9.68				33.33
1080	Propanoic acid, 2-methyl-, anhydride	Esters and analogues		7.14			
1081	Propanoic acid, 2-methyl-, butyl ester	Esters and analogues	25.81				
1082	Propanoic acid, 2-methyl-, ethyl ester	Esters and analogues	38.71		75		100
1083	Propanoic acid, 2-methyl-, hexyl ester	Esters and analogues	3.23				
1084	Propanoic acid, 2-methyl-, pentyl ester	Esters and analogues	6.45				
1085	Propanoic acid, 2-methyl-, propyl ester	Esters and analogues	29.03				66.67
1086	Propanoic acid, 2-methylpropyl ester	Esters and analogues	12.9				
1087	Propanoic acid, 2-oxo-	Acids		7.14			
1088	Propanoic acid, 2-oxo-, methyl ester	Esters and analogues		7.14			
1089	Propanoic acid, 3-amino-2-methyl-	Acids				4.76	
1090	Propanoic acid, butyl ester	Esters and analogues	22.58				66.67
1091	Propanoic acid, ethyl ester	Esters and analogues	38.71		100		
1092	Propanoic acid, pentyl ester	Esters and analogues	9.68				66.67
1093	Propanoic acid, propyl ester	Esters and analogues	35.48		75		
1094	Propene	Linear aliphatics	3.23				
1095	Pyrazine	Aromatics	32.26				
1096	Pyrazine, 2-ethyl-6-methyl-	Aromatics	9.68				
1097	Pyrazine, 2-methoxy-3-(1-methylethyl)-	Aromatics	3.23				
1098	Pyrazine, 2-methoxy-3-(2-methylpropyl)-	Aromatics	3.23				
1099	Pyrazine, 2,3-dimethyl-	Aromatics	19.35				
1100	Pyrazine, 2,5-dimethyl-	Aromatics	12.9				
1101	Pyrazine, 2,6-dimethyl-	Aromatics	9.68				
1102	Pyrazine, 3-ethyl-2,5-dimethyl-	Aromatics	3.23				
1103	Pyrazine, methyl-	Aromatics	29.03				
1104	Pyrazine, tetramethyl-	Aromatics	9.68				
1105	Pyrazine, trimethyl-	Aromatics	22.58				
1106	Pyridine	Aromatics	29.03				
1107	Pyridine, 2-chloro-6-(2-furanylmethoxy)-4-(trichloromethyl)-	Aromatics			25		
1108	Pyridine, 2-ethyl-	Aromatics	12.9				
1109	Pyridine, 2-ethyl-4,6-dimethyl-	Aromatics	3.23				
1110	Pyridine, 2-methyl-	Aromatics	54.84				
1111	Pyridine, 2-propyl-	Aromatics	3.23				
1112	Pyridine, 2,3,4,5-tetrahydro-	Aromatics	3.23				
1113	Pyridine, 2,4-dimethyl-	Aromatics	61.29	7.14			66.67
1114	Pyridine, 2,4,6-trimethyl-	Aromatics	19.35				33.33
1115	Pyridine, 3-(1a,2,7,7a-tetrahydro-2-methoxy-1-phenyl-1,2,7-metheno-1H-cyclopropa[b]naphthalen-8-yl)-	Aromatics		7.14			
1116	Pyridine, 3-ethyl-	Aromatics	3.23				
1117	Pyridine, 3-methyl-	Aromatics	3.23				
1118	Pyridine, 3,4-dimethyl-	Aromatics	3.23				
1119	Pyridine, 5-ethenyl-2-methyl-	Aromatics	9.68				
1120	Pyrimidine, 4-methyl-	Aromatics	6.45				
1121	Quinoline, 1,2-dihydro-2,2,4-trimethyl-	Aromatics	35.48	42.86	75	52.38	33.33
1122	Quinoline, 2,4-dimethyl-	Aromatics	6.45				

1123	S-Methyl methanethiosulphonate	Sulfur-containing	16.13				
1124	sec-Butyl acetate	Esters and analogues	38.71				
1125	Spiro[3.6]deca-5,7-dien-1-one,5,9,9-trimethyl	Cyclic aliphatics	9.68				33.33
1126	Styrene	Aomatics	29.03	28.57	25	14.29	
1127	Succinic acid, 4-chloro-3-methylphenyl 4-methoxybenzyl ester	Esters and analogues		7.14			
1128	Succinimide	Nitrogen-containing		7.14			
1129	Sulfur, pentafluoro(trifluoromethyl)-, (OC-6-21)-	Sulfur-containing				4.76	
1130	Supraene	Linear aliphatics	3.23				
1131	Tetrachloroethylene	Halogen-containing	19.35				
1132	Tetracosane	Linear aliphatics	16.13	7.14	25	4.76	
1133	Tetracyclo[6.6.1.0(2,7).0(9,14)]pentadeca-4,11-diene	Linear aliphatics		7.14			
1134	Tetradecanal	Aldehydes		7.14			
1135	Tetradecane	Linear aliphatics	12.9	21.43		9.52	
1136	Tetradecane, 1-iodo-	Halogen-containing		7.14			
1137	Tetrafluoroisophthalonitrile	Aromatics	3.23				
1138	Tetrahydrofuran	Aromatics	19.35	14.29	50	19.05	
1139	Tetrahydrofuran, 2,2-dimethyl-	Aromatics			25		
1140	Thiazol-2-amine, N-(4-methoxybenzyl)-	Aromatics		7.14			
1141	Thiazole	Aromatics	16.13				
1142	Thiazole, 2,4-dimethyl-	Aromatics	3.23				
1143	Thiocyanic acid, methyl ester	Esters and analogues	38.71				
1144	Thiophene, 2-ethyl-	Aromatics	3.23				
1145	Thiophene, 2-ethyl-5-propyl-	Aromatics	3.23				
1146	Thiophene, 2-methyl-	Aromatics	25.81				
1147	Thiophene, 2-pentyl-	Aromatics	19.35				
1148	Thiophene, 3-methyl-	Aromatics	9.68	7.14			
1149	Thiourea	Nitrogen-containing	29.03	42.86		19.05	33.33
1150	Thujone	Ketones	6.45				
1151	Toluene	Aromatics	6.45	35.71		33.33	
1152	trans-4-Nonene	Linear aliphatics			25		
1153	trans-1,2-Diethyl cyclopentane	Cyclic aliphatics	3.23			4.76	
1154	trans-1,3-Diethylecyclopentane	Cyclic aliphatics	9.68				
1155	trans-3-Carene-2-ol	Alcohols	3.23				
1156	trans-Calamenene	Aromatics		7.14			
1157	Trichloromethane	Halogen-containing		7.14		9.52	
1158	Tricyclo[2.2.1.0(2,6)]heptane, 1,7,7-trimethyl-	Cyclic aliphatics	3.23	7.14		23.81	33.33
1159	Tridecanal	Aldehydes	3.23	7.14			
1160	Tridecane	Linear aliphatics	38.71	28.57	25	23.81	33.33
1161	Tridecane, 3-methyl-	Linear aliphatics	6.45	7.14			
1162	Tridecanoic acid	Acids		7.14			
1163	Trifluoromethanesulfonic anhydride	Esters and analogues				4.76	
1164	Trioxide, bis(trifluoromethyl)	Halogen-containing				4.76	
1165	Trisulfide, methyl propyl	Sulfur-containing	3.23				
1166	Tuaminoheptane	Nitrogen-containing		7.14			
1167	Undecanal	Aldehydes	3.23	14.29	50	4.76	
1168	Undecane	Linear aliphatics	25.81		25		33.33
1169	Undecane, 2-methyl-	Linear aliphatics	25.81			4.76	33.33

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1170	Undecane, 2,2-dimethyl-	Linear aliphatics	12.9	14.29		4.76	
1171	Undecane, 2,6-dimethyl-	Linear aliphatics	32.26		25	4.76	33.33
1172	Undecane, 3-methyl-	Linear aliphatics	9.68	14.29	25	4.76	33.33
1173	Undecane, 3-methylene-	Linear aliphatics	3.23				
1174	Undecane, 3,7-dimethyl-	Linear aliphatics		7.14			
1175	Undecane, 3,8-dimethyl-	Linear aliphatics	3.23				
1176	Undecane, 4-methyl-	Linear aliphatics	22.58	21.43		4.76	
1177	Undecane, 4,7-dimethyl-	Linear aliphatics	6.45			4.76	33.33
1178	Undecane, 5-methyl-	Linear aliphatics	3.23				
1179	Undecane, 6-methyl-	Linear aliphatics	3.23			4.76	
1180	Undecanoic acid	Acids	12.9				
1181	Urea	Nitrogen-containing		14.29			
1182	Urea, tetramethyl-	Nitrogen-containing	12.9	14.29		4.76	
1183	Urea, trimethylnitroso-	Nitrogen-containing		7.14			



APPENDIX B

**Table B.1** Responses recorded during the dog trials conducted in February 2022 with two OPP cadaver dog-handler teams using training aids.

	Training ID#	Training location and description	Dog Responses	
			Dog 1	Dog 2
Scenario 1	LB7, P1	Imprint Room, boxes	True Positive	True Positive
	LB9, P3	Imprint Room, boxes	True Positive	True Positive
	FB10, P3	Imprint Room, boxes	True Positive	True Positive
	FB3, P4	Carousel Room, metal cans	True Positive	True Positive
	AB8, M	Carousel Room, metal cans	True Positive	True Positive
	LB7, M	Carousel Room, metal cans	True Positive	True Positive
	FB5, D1	Imprint Room, boxes	True Positive	True Positive
	LB7, B1	Imprint Room, boxes	True Positive	True Positive
	AB8, D1	Carousel Room, metal cans	True Positive	True Positive
	FB4, B1	Carousel Room, metal cans	True Positive	True Positive
Scenario 2	FB1, B1, D1	Imprint Room, boxes	True Positive	True Positive
Scenario 3	M1	Imprint Room, box	True Positive	True Positive
	P3	Imprint Room, box	True Positive	True Positive
	B1	Imprint Room, box	True Positive	True Positive
	D1	Carousel Room, metal can	True Positive	True Positive

**Table B.2** Responses recorded during the dog trials conducted in May 2022 with five OPP cadaver dog-handler teams using training aids.

	Training ID#	Training location and description	Dog Responses				
			Dog 1	Dog 2	Dog 3	Dog 4	Dog 5
Scenario 1	FB1, B1	Imprint Room, boxes	True Positive	True Positive	True Positive	True Positive	True Positive
	FB12, P4	Carousel, metal cans	True Positive	True Positive	True Positive	True Positive	True Positive
	AB8, M3	Carousel, metal cans	True Positive	True Positive	True Positive	True Positive	True Positive
	FB2, P4	Imprint Room, boxes	True Positive	True Positive	True Positive	True Positive	True Positive
Scenario 2	FB1, B1, M1	Imprint Room, boxes	True Positive	True Positive	True Positive	True Positive	True Positive
Scenario 3	D1	Imprint Room, box	True Positive	False Positive	True Positive	True Positive	True Positive