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Data Article

# Odor impact of volatiles emitted from marijuana, cocaine, heroin and their surrogate scents

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ABSTRACT

Volatile compounds emitted into headspace from illicit street drugs have been identified, but until now odor impact of these compounds have not been reported. Data in support of identification of these compounds and their odor impact to human nose are presented. In addition, data is reported on odor detection thresholds for canines highlighting differences with human ODTs and needs to address gaps in knowledge. New data presented here include: (1) compound identification, (2) gas chromatography (GC) column retention times, (3) mass spectral data, (4) odor descriptors from 2 databases, (5) human odor detection thresholds from 2 databases, (6) calculated odor activity values, and (7) subsequent ranking of compounds by concentration and ranking of compounds by odor impact (reported as calculated odor activity values). For further interpretation and discussion, see Rice and Koziel [1] and Rice [2].



## Specifications table

| | |
|---|---|
| Subject area | *Chemistry* |
| More specific subject area | *Forensics, Analytical Chemistry, Olfactometry* |
| Type of data | *Table* |

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| | |
|---|---|
| How data was acquired | *Multidimensional gas chromatography (Agilent 6890), mass spectroscopy (Agilent 5973), olfactometry (MOCON, Round Rock, TX).* |
| Data format | *Analyzed mass spec using Automatic Mass Spectral Deconvolution and Identification System (AMDIS) (NIST, Gaithersburg, MD)* |
| Experimental factors | *Volatiles emitted from marijuana, cocaine, and heroin samples were collected on Carboxen/polydimethylsiloxane (PDMS) solid-phase microextraction (SPME) fiber at room temperature, static, for 1 h.* |
| Experimental features | *SPME fibers were thermally desorbed in a multidimensional gas chromatography-mass spectrometry-olfactometry (MDGC-MS-O) instrument, allowing for simultaneous chemical and sensory analysis. Surrogate scents for each drug were also analyzed as previously stated, and aromas were compared using calculated odor activity values (OAVs).* |
| Data source location | *Department of Agricultural and Biosystems Engineering at Iowa State University, Ames, IA 50011* |
| Data accessibility | *Data is with this article.* |

**Value of the data**

- This data is the most comprehensive summary of volatiles emitted from real and surrogate scents of marijuana (221, 78), cocaine (153, 15), and heroin (41, 19), respectively, to date.
- This data includes organoleptic percepts from 2 known databases, odor detection thresholds from 2 benchmark databases, significant ions from mass spectral data, and calculated odor activity values (OAVs, if available) for each compound.
- This data shows rank of drug volatiles by concentration in relation to the rank by odor impact (as calculated OAV).
- Odor activity value data can open up new ways of forensic drug analysis.
- Data from previous research on canine odor detection thresholds (ODTs) is reported for further insight, highlighting differences with human ODTs and needs to address gaps in knowledge.

## 1. Data

### 1.1. CAS Registry Number

A CAS Registry Number is a unique numeric identifier that corresponds to only one substance. The CAS has no chemical significance, but can be used as a link to more information about a specific chemical substance [3]. CAS number is useful to identify a compound that has multiple synonyms. CAS numbers were used in all data tables in this report.

### 1.2. Odor Detection Threshold (ODTs)

Published ODT values are not fixed numbers, but are set to represent the *lowest* concentration that 50% of the population can detect [4]. For the purposes of calculating odor activity values, standardized human ODTs from Devos et al. [5] were used when available. The compilation from Devos et al. contained a total of 2075 ODT values in air for 641 chemical compounds, gathered from 372 references. ODTs were weighted and averaged [5]. If ODT for a compound was not given in Devos et al., the LRI Database [6] was used. LRI database contains 1500+ records on ODT and odor percepts [6]. ODTs for canines were compiled from previous literature. See Rice and Koziel [1] for full discussion on human and canine ODTs. ODTs were used in reporting data in Tables 1–5.

### 1.3. Column retention time in chromatography

Column retention time (RT, min) is the time between sample introduction via thermal desorption in the gas chromatography (GC) inlet and the analyte peak reaching the mass spectrometer and/or

sniff port at the end of the analytical column. It was not appropriate to use retention indexes (Kovats RI) for identification because: (1) the non-polar and polar columns were connected in series when analyzing in multidimensional GC; (2) use of indices of medium polarity column could lead to large errors for compounds that are affected by one of the columns more than the other. Known retention times of standards previously analyzed on this system were used for compound identification, and indicated by + symbol in Tables 3–5. RTs are also reported in Tables 3–5.

### 1.4. Aroma descriptors

Aroma descriptors were compiled from Flavornet and The Good Scents Company. Flavornet has aroma descriptors from 738 compounds, compiled from studies using GC-olfactometry [7]. The Good Scents Company is dedicated to providing organoleptic information to the flavor, food and fragrance industry [8]. Aroma descriptors from these 2 databases were used in reporting data in Tables 3–5.

### 1.5. Sample code

Aromas were characterized by human nose from volatiles emitted into the headspace of illicit marijuana, cocaine, and heroin. Various states of seizure were examined: (1) 50 kg of marijuana in a cloth military style duffel bag (**Sample Code A1–A3**); (2) 1 g marijuana packaged in a plastic zip-top sandwich bag (**Sample Code A4–A5**); (3) 1 g old, desiccated marijuana with no packaging (**Sample Code A6–A7**); (4) plastic zip-top sandwich bag with 1 g marijuana removed (**Sample Code B1–B4**); (5) 1 g crack cocaine packaged as tear drops (**Sample Code D1**); (6) 1 g cocaine adulterated with Levamisole (**Sample Code D2**); (7) 1 kg evidence pack containing cocaine (**Sample Code D3**); (8) 1 g cocaine in an opened plastic bag (**Sample Code D4–D5**); (9) 1 g heroin seized in 1997 (**Sample Code F1**); (10) 1 g heroin seized in 2010 (**Sample Code F2**). Sigma Pseudo™ Narcotic Scent Marijuana formulation (Fluka, P7309) (**Sample Code C1–C3**), Sigma Pseudo™ Narcotic Scent Cocaine formulation (Fluka, P2423) (**Sample Code E1**), and Sigma Pseudo™ Narcotic Scent Heroin formulation (Fluka, P2548) (**Sample Code G1**) were purchased from Sigma-Aldrich (St. Louis, MO). These sample codes were used in reporting data in Tables 3–5.

### 1.6. Target mass spec libraries, models, and net % match, peak area counts

AMDIS (NIST, Gaithersburg, MD) software was used for identification of unknown compounds. Six specialty mass spectral libraries were used for compound identification: NISTEPA (1086 compounds in the EPA's 'list of lists'), NISTDRUG (739 compounds in the Canadian AAFS Toxicology Section MS Database Committee and the Association of Official Racing Chemists libraries), NISTFF (991 compounds in the Philip Morris Flavor and fragrance collection), NISTTOX (1213 compounds represented in Finnigan Corporation's Toxicology library), NISTFDA (415 compounds in an FDA collection of mass spectra), and NISTCW (62 compounds relevant to detection of chemical weapons).

A model is the mass-to-charge ratio ($m/z$) of a deconvoluted peak, and are listed in order of highest to lowest relative abundance. For example, under a 'Models' column heading, 2: 58 88 signifies 2 models with $m/z$ 58 and 88 were used for identification.

Net % Match is the final match quality value (100=perfect match) between the deconvoluted component and the target library spectra. The minimum match value was set at 65 for all analysis of this data.

Peak area counts (PAC) refers to the relative abundance of the analyte, or the area under the chromatographic peak. The mass detector was assumed to have equal response factors for each compound, for the purposes of calculating OAV.

These parameters were used in reporting data in Tables 3–5.

### 1.7. Odor activity values (OAV)

OAV is defined as the unit less ratio of concentration of a compound in gas phase to the odor detection threshold. For illustrative purposes, the PAC was used for the concentration value of each compound. See Rice and Koziel [1] and Rice [2] for further discussion on OAV. This ratio was used to calculate the OAVs reported in Tables 3–5.

### 1.8. Ranking definitions

Compounds from each drug were ranked by concentration (highest concentrated = ranked 1) and then by calculated OAV (highest odor impact = ranked 1). In most cases, there was no apparent correlation between chemical concentration and odor impact, i.e., rank 1 by concentration did not usually rank as 1 by OAV. This ranking and sorting was used to report data in Tables 6–8.

## 2. Experimental design, materials and methods

### 2.1. Surrogate scent formulations

Sigma Pseudo™ Narcotic Scent Marijuana formulation composition is listed as pyrogenic colloidal silica (1%), cellulose (98.5%), butane-2,3-diol (0.4%), and p-mentha-1,4-diene (0.1%). Sigma Pseudo™ Narcotic Scent Cocaine formulation composition is listed as cellulose (98.9%), pyrogenic colloidal silica (1%), and methyl benzoate (0.1%). Sigma Pseudo™ Narcotic Scent Heroin formulation composition is listed as cellulose (74.1%), o-acetylsalicylic acid (25.2%), acetic acid (0.3%), and pyrogenic colloidal silica (0.3%).

### 2.2. Methodology

Carboxen/PDMS, 85 μm Stable-flex, 24 gauge SPME fibers were used (Sigma-Aldrich, St. Louis, MO, USA). Briefly, experimental conditions were as follows: drugs were placed in separate, pre-cleaned and oven-baked 16 ounce mason jars with modified lids. The Carboxen/PDMS SPME fibers were exposed to the headspace and volatiles were passively extracted; equilibration time was the same as extraction time (1 h at ambient temperature). When the extraction step was completed, the SPME fiber was retracted, wrapped in pre-baked aluminum foil, placed in a pre-cleaned mason jar, and transported back to the laboratory in a cooler on ice. In the laboratory, fibers were stored as described above in a 4 °C refrigerator pending placement into the heated injection port of the MDGC-MS-O for thermal desorption and analysis.

MDGC-MS-O analysis was performed on an Agilent 6890 GC, with a restrictor guard column, non-polar capillary column (BP-5, 56 m × 530 μm inner diameter × 1.00 μm thickness, SGE, Austin, TX, USA) and polar capillary column (BP-20, 25 m × 530 μm inner diameter × 1.00 μm thickness, SGE, Austin, TX, USA) connected in series. Outflow from analytical column was held at 7.0 cc/min. Sample flow was split 3:1 via open split interface to the sniff port and mass spectrometer, respectively, as determined by restrictor column inner diameter. Desorption time was 2 min in splitless mode at 270 °C under flow of helium carrier gas (99.995% purity). Analysis of the same fiber immediately after sample injection, revealed no carry over, with all compounds desorbed in the initial analysis. The oven temperature was programmed as follows: 40 °C for 3.00 min, then increased to 220 °C at a rate of 7.00 °C per min, and held for 11.29 min (40 min total run time). The carrier gas was set at constant pressure at the midpoint (junction point of the non-polar and polar column) at 5.8 psi. Transfer line to the MS was set at 240 °C; transfer line to the sniff port was set at 240 °C with humidified air set at 8.00 psi. MS heated zones were 150 °C for the quadrupole and 230 °C for the source. Mass spectrometer parameters were electron impact (EI), electron energy set to 70 eV, with acquisition range m/z 33–280.

The instrument was tuned daily and analysis of column blanks did not show any contaminating compounds. Analysis of blank trip fiber (an unloaded SPME fiber taken to the site and back, stored with fibers to be analyzed) at the end of each sampling run did not demonstrate contaminating compounds. VOCs were identified tentatively using the Automatic Mass Spectral Deconvolution and Identification System (AMDIS) (National Institute of Standards and Technology, Gaithersburg, MD) and six specialty mass spectral libraries provided derived from the NIST05/EPA/NIH mass spectral database. Known retention times of standards previously analyzed on this system were used for identification. Chemical standards available in house were analyzed to match retention times and mass spectra of unknown compounds. Select reference standards were used for identification, purchased from Sigma-Aldrich (St. Louis, MO, USA). These standards are indicated with '+' in Tables 3–5. Each sample (as outlined in Section 1.5) was collected on a single SPME fiber, each fiber sample was analyzed by one panelist. The same panelist analyzed all samples with volatiles from each drug and surrogate scent formulation.

**Table 1**
Comparison of odor detection thresholds and odor activity values between canines (based on Passe and Walker [9]) and humans (based on Devos et al. [5]).

| Source reference in [9] | Methods | Compound | CAS | Canine ODT [9] (ppm) | Human ODT [5] (ppm) | $ODT_C$: $ODT_H$ | Canine OAV of 1 ppm | Human OAV of 1 ppm | $OAV_C$: $OAV_H$ |
|---|---|---|---|---|---|---|---|---|---|
| Neuhaus [10] | Dogs chose from 3 ***odor ports***. Pushing a box behind the correct port uncovered sugar for reward. | Acetic acid | 64-19-7 | 4.99E-11 | 1.45E-01 | 3.44E-10 | 2.00E+10 | 6.90E+00 | 2.90E+09 |
| | | Propanoic acid | 79-09-4 | 3.09E-11 | 3.55E-02 | 8.70E-10 | 3.24E+10 | 2.82E+01 | 1.15E+09 |
| | | Butyric acid | 107-92-6 | 1.46E-12 | 3.89E-03 | 3.76E-10 | 6.84E+11 | 2.57E+02 | 2.66E+09 |
| | | Pentanoic acid | 109-52-4 | 5.36E-12 | 4.79E-03 | 1.12E-09 | 1.87E+11 | 2.09E+02 | 8.94E+08 |
| | | Hexanoic acid | 142-62-1 | 7.67E-12 | 1.26E-02 | 6.09E-10 | 1.30E+11 | 7.94E+01 | 1.64E+09 |
| | | Octanoic acid | 124-07-2 | 1.20E-11 | 3.98E-03 | 3.01E-09 | 8.34E+10 | 2.51E+02 | 3.32E+08 |
| Ashton, Eayrs and Moulton [11] | Crucibles containing odorous solutions was placed on the floor. Dog alerted by sitting when odor was present. | Formic acid | 64-18-6 | 1.30E+03 | 2.82E+01 | 4.60E+01 | 7.71E-04 | 3.55E-02 | 2.17E-02 |
| | | Acetic acid | 64-19-7 | 1.73E+02 | 1.45E-01 | 1.19E+03 | 5.77E-03 | 6.90E+00 | 8.37E-04 |
| | | Propanoic acid | 79-09-4 | 1.78E+01 | 3.55E-02 | 5.01E+02 | 5.63E-02 | 2.82E+01 | 2.00E-03 |
| | | Butyric acid | 107-92-6 | 3.67E+00 | 3.89E-03 | 9.44E+02 | 2.72E-01 | 2.57E+02 | 1.06E-03 |
| | | Pentanoic acid | 109-52-4 | 5.24E+01 | 4.79E-03 | 1.09E+04 | 1.91E-02 | 2.09E+02 | 9.14E-05 |
| | | Hexanoic acid | 142-62-1 | 3.20E+01 | 1.26E-02 | 2.54E+03 | 3.13E-02 | 7.94E+01 | 3.94E-04 |
| | | Heptanoic acid | 111-14-8 | 1.76E+01 | 2.75E-02 | 6.39E+02 | 5.69E-02 | 3.64E+01 | 1.57E-03 |
| | | Octanoic acid | 124-07-2 | 8.11E+00 | 3.98E-03 | 2.04E+03 | 1.23E-01 | 2.51E+02 | 4.91E-04 |
| Moulton, Ashton, and Eayrs [12] | Crucibles containing odorous solutions was placed on the floor. Dog alerted by sitting when odor was present. | Formic acid | 64-18-6 | 1.96E-02 | 2.82E+01 | 6.96E-04 | 5.09E+01 | 3.55E-02 | 1.44E+03 |
| | | Acetic acid | 64-19-7 | 5.73E-04 | 1.45E-01 | 3.95E-03 | 1.74E+03 | 6.90E+00 | 2.53E+02 |
| | | Propanoic acid | 79-09-4 | 1.23E-05 | 3.55E-02 | 3.46E-04 | 8.13E+04 | 2.82E+01 | 2.89E+03 |
| | | Butyric acid | 107-92-6 | 4.95E-07 | 3.89E-03 | 1.27E-04 | 2.02E+06 | 2.57E+02 | 7.85E+03 |
| | | Pentanoic acid | 109-52-4 | 1.55E-05 | 4.79E-03 | 3.23E-03 | 6.47E+04 | 2.09E+02 | 3.10E+02 |
| | | Hexanoic acid | 142-62-1 | 3.13E-06 | 1.26E-02 | 2.48E-04 | 3.20E+05 | 7.94E+01 | 4.03E+03 |
| | | Heptanoic acid | 111-14-8 | 5.55E-07 | 2.75E-02 | 2.02E-05 | 1.80E+06 | 3.64E+01 | 4.95E+04 |
| | | Octanoic acid | 124-07-2 | 1.12E-07 | 3.98E-03 | 2.81E-05 | 8.93E+06 | 2.51E+02 | 3.56E+04 |
| | | Isobutyric acid | 79-31-2 | 5.56E-07 | 1.95E-02 | 2.85E-05 | 1.80E+06 | 5.13E+01 | 3.51E+04 |

**Table 1** (*continued*)

| Source reference in [9] | Methods | Compound | CAS | Canine ODT [9] (ppm) | Human ODT [5] (ppm) | $ODT_C$: $ODT_H$ | Canine OAV of 1 ppm | Human OAV of 1 ppm | $OAV_C$: $OAV_H$ |
|---|---|---|---|---|---|---|---|---|---|
| Moulton and Marshal [13] | Trial was initiated by manipulating a treadle, dogs chose from 3 ***odor ports***. Alert was placing nose in correct odorant for 5 seconds. | α-ionone | 127-41-3 | 4.02E-13 | 5.75E-05 | 6.99E-09 | 2.49E+12 | 1.74E+04 | 1.43E+08 |
| Marshall, Blumer and Moulton [14] | Same test apparatus as Moulton and Marshal (1976). 1 sample port, alert was keeping nose in port for 5 sec. | Pentanoic acid | 109-52-4 | 1.51E-07 | 4.79E-03 | 3.15E-05 | 6.62E+06 | 2.09E+02 | 3.17E+04 |
| Krestel, Passe, Smith and Jonsson [15] | Conditioned suppression using ***odor ports.*** | Amyl acetate | 628-63-7 | 1.93E-07 | 3.09E-02 | 6.23E-06 | 5.19E+06 | 3.24E+01 | 1.60E+05 |

REF=reference; ODT=odor detection threshold; OAV=odor activity value; $ODT_C$=canine odor detection threshold; $ODT_H$=human odor detection threshold; $OAV_C$=odor activity value for canines; $OAV_H$=odor activity value for humans. All gas phase calculations assumed 1 atm at 25 °C.

**Table 2**
Comparison of ODT and OAV in canines vs. humans in two recent field studies.

| REF | Method | Mixture ratio | Compound | CAS | Conc. tested (ppm) | % of canines alerted | Canine ODT (ppm) | Human ODT (ppm) | $ODT_C$: $ODT_H$ | Canine OAV of 1 ppm | Human OAV of 1 ppm | $OAV_C$: $OAV_H$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Lorenzo, Wan, Harper, Hsu, Chow, Rose, Furton [16] | Scent solution was spiked onto filter paper, placed in a metal box with holes drilled on top. | | Insosafrole | 120-58-1 | 6.76E+02 | 0 | | | | | | |
| | | | Phorone | 504-20-1 | 6.27E+02 | 4 | 6.27E+02 | | | 1.60E-03 | | |
| | | | Camphor | 76-22-2 | 6.43E+02 | 0 | | 5.13E-02 | | | 1.95E+01 | |
| | | | Piperonal | 120-57-0 | 6.52E+02 | 17 | 6.52E+02 | 4.79E-03 | 1.36E+05 | 1.53E-03 | 2.09E+02 | 7.35E-06 |
| | | | Safrol | 94-59-7 | 6.61E+02 | 0 | | 9.55E-03 | | | 1.05E+02 | |
| | | | Benzaldehyde | 100-52-7 | 9.63E+02 | 9 | 9.63E+02 | 4.17E-02 | 2.31E+04 | 1.04E-03 | 2.40E+01 | 4.33E-05 |
| | | | Acetic acid | 64-19-7 | 1.71E+03 | 0 | | 1.45E-01 | | | 6.90E+00 | |
| | | | 1-phenyl-2-propanol | 100-86-7 | 6.35E+02 | 9 | 6.35E+02 | | | 1.58E-03 | | |
| | | | Acetophenone | 98-86-2 | 8.37E+02 | 0 | | 3.63E-01 | | | 2.75E+00 | |
| | | 1:1 | MD-P2P | 4676-39-5 | 5.49E+01 | 0 | | | | | | |
| | | | Piperonal | 120-57-0 | 6.52E+01 | 0 | | 4.79E-03 | | | 2.09E+02 | |
| | | 3:1 | MD-P2P | 4676-39-5 | 1.65E+02 | 0 | | | | | | |
| | | | Piperonal | 120-57-0 | 6.52E+01 | 0 | | 4.79E-03 | | | 2.09E+02 | |
| | | 5:1 | MD-P2P | 4676-39-5 | 2.75E+02 | 0 | | | | | | |
| | | | Piperonal | 120-57-0 | 6.52E+01 | 0 | | 4.79E-03 | | | 2.09E+02 | |
| | | 10:1 | MD-P2P | 4676-39-5 | 5.49E+02 | 0 | | | | | | |
| | | | Piperonal | 120-57-0 | 6.52E+01 | 0 | | 4.79E-03 | | | 2.09E+02 | |
| | | 5:1 | MD-P2P | 4676-39-5 | 1.37E+03 | 0 | | | | | | |
| | | | Piperonal | 120-57-0 | 6.52E+01 | 0 | | 4.79E-03 | | | 2.09E+02 | |
| | | | MDMA | NA | 5.07E+00 | 0 | | | | | | |
| | | | MD-P2P | 4676-39-5 | 5.49E+02 | 0 | | | | | | |
| | | | Piperonal | 120-57-0 | 6.52E+03 | 83 | | 4.79E-03 | | | 2.09E+02 | |
| | | | Methamphetamine Pharm Grade | 537-46-2 | 3.28E+05 | 0 | | | | | | |
| | | Unknown mixture | Methamphetamine Street Sample | NA | | 100 | | | | | | |
| Williams and Johnston [17] | Cotton balls were spiked with target odor and placed in a can[Δ]. | | Allyl sulfide | 592-88-1 | 6.01E+05 | >80% | 6.01E+05 | | | 1.66E-06 | | |
| | | | Cumene | 98-82-8 | 5.68E+05 | >80% | 5.68E+05 | 2.40E-02 | 2.37E+07 | 1.76E-06 | 4.17E+01 | 4.22E-08 |
| | | | dimethylthiazole | 541-58-2 | 7.39E+05 | >80% | 7.39E+05 | | | 1.35E-06 | | |
| | | | α-pinene | 80-56-8 | 4.99E+05 | >80% | 4.99E+05 | 6.92E-01 | 7.21E+05 | 2.00E-06 | 1.45E+00 | 1.39E-06 |
| | | | benzaldehyde | 100-52-7 | 7.80E+05 | >80% | 7.80E+05 | 3.00E-03 | 2.60E+08 | 1.28E-06 | 3.33E+02 | 3.85E-09 |

**Table 2** (*continued*)

| REF | Method | Mixture ratio | Compound | CAS | Conc. tested (ppm) | % of canines alerted | Canine ODT (ppm) | Human ODT (ppm) | $ODT_C$: $ODT_H$ | Canine OAV of 1 ppm | Human OAV of 1 ppm | $OAV_C$: $OAV_H$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Menthol | 89-78-1 | 4.51E+05 | >80% | 4.51E+05 | 4.17E-02 | 1.08E+07 | 2.22E-06 | 2.40E+01 | 9.24E-08 |
| | | | Cyclohexanone | 108-91-1 | 7.65E+05 | >80% | 7.65E+05 | 7.08E-01 | 1.08E+06 | 1.31E-06 | 1.41E+00 | 9.25E-07 |
| | | | Eucalyptol | 470-82-6 | 4.74E+05 | >80% | 4.74E+05 | 1.62E-02 | 2.93E+07 | 2.11E-06 | 6.17E+01 | 3.42E-08 |
| | | | Pentanethiol | 110-66-7 | 6.39E+05 | >80% | 6.39E+05 | 1.20E-04 | 5.31E+09 | 1.57E-06 | 8.32E+03 | 1.88E-10 |
| | | | Toluene | 108-88-3 | 7.48E+05 | >80% | 7.48E+05 | 1.55E+00 | 4.83E+05 | 1.34E-06 | 6.45E-01 | 2.07E-06 |

REF=reference; MD-P2P=3,4-methylenedioxyphenyl-2-propanone; Mixture ratio=ratio of MD-P2P to Piperonal; ODT=odor detection threshold; OAV=odor activity value; ODTc=canine odor detection threshold; $ODT_H$=human odor detection threshold; OAVc=odor activity value for canines; $OAV_H$=odor activity value for humans. [Δ]Volume of can was not specified. In this table the can dimensions were assumed to be a cylinder of radius 5.08 cm, 4.62 cm height, displaced volume of cotton balls was not accounted for. All gas phase calculations assumed 1 atm at 25 °C.

**Table 3**
Summary of VOCs emitted from all illicit marijuana samples (sample code A and B in Section 1.5) and Sigma Pseudo™ Narcotic Scent Marijuana formulation (sample code C in Section 1.5) and sampled over 1 h at room temperature. Sigma Pseudo™ Narcotic Scent Marijuana formulation is indicated by underlined fonts.

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| Ethylene oxide | **75-21-8** | **1.07** | | | | **8.51E+02** | A 1 | 2: 44 45 | 66 | 1.51E+06 | 1.77E+03 |
| | | | | | | | A 3 | | 66 | 2.12E+06 | 2.49E+03 |
| | | | | | | | A 4 | | 65 | 3.37E+06 | 3.96E+03 |
| | | | | | | | A 7 | 2: 43 42 | 89 | 8.62E+03 | 1.01E+01 |
| | | | | | | | B 1 | 2: 44 43 | 66 | 3.75E+06 | 4.40E+03 |
| | | | | | | | B 4 | 4: 44 45 129 43 | 66 | 1.86E+06 | 2.18E+03 |
| | | | | | | | C 1 | 3: 44 45 46 | 66 | 1.35E+06 | 1.59E+03 |
| | | | | | | | C 2 | 2: 44 43 | 85 | 2.14E+05 | 2.51E+02 |
| | | | | | | | C 3 | 4: 44 46 43 131 | 67 | 1.36E+06 | 1.60E+03 |
| +2-nitropropane | 79-46-9 | 1.13 | | | | 7.24E+00 | A 5 | 2: 41 43 | 75 | 6.30E+03 | 8.69E+02 |
| | | | | | | | A 6 | 4: 43 39 56 42 | 83 | 4.16E+04 | 5.74E+03 |
| 2,4-dimethylpentane | 108-08-7 | 1.20 | | | | 8.71E+01 | A 7 | 2: 57 43 | 66 | 8.15E+03 | 9.36E+01 |
| Isobutane | 75-28-5 | 1.22 | | | | 1.00E+01 | A 1 | | 84 | 2.20E+07 | 2.20E+06 |
| | | | | | | | A 2 | 13: 43 41 57 72 39 55 56 38 40 73 62 66 65 | 84 | 2.02E+07 | 2.02E+06 |
| | | | | | | | A 3 | 11: 43 42 41 57 72 40 53 51 38 73 63 | 85 | 1.47E+07 | 1.47E+06 |
| | | | | | | | A 4 | 5: 57 42 43 41 39 | 67 | 2.03E+04 | 2.03E+03 |
| | | | | | | | A 5 | 10: 43 42 41 39 72 55 50 73 71 58 | 84 | 7.18E+06 | 7.18E+05 |
| | | | | | | | A 6 | 4: 43 39 56 42 | 88 | 4.16E+04 | 4.16E+03 |
| | | | | | | | A 7 | 10: 43 42 41 57 39 72 55 56 73 37 | 85 | 2.94E+06 | 2.94E+05 |
| | | | | | | | B 1 | 14: 43 42 41 57 72 39 56 55 71 50 70 53 38 37 | 85 | 2.20E+06 | 2.20E+05 |
| | | | | | | | B 2 | 7: 42 41 72 53 55 56 38 | 84 | 7.00E+05 | 7.00E+04 |
| | | | | | | | B 3 | 4: 43 42 41 39 | 88 | 2.49E+04 | 2.49E+03 |
| | | | | | | | B 4 | 4: 42 43 57 72 | 81 | 6.45E+04 | 6.45E+03 |
| +Acetaldehyde | 75-07-0 | 1.27 | Pungent, Ether | Pungent, Ethereal, Aldehydic, Fruity | 1.50E-02 | 1.86E-01 | A 4 | 2: 44 42 | 91 | 3.10E+04 | 1.67E+05 |
| | | | | | | | A 6 | 2: 43 44 | 90 | 2.69E+04 | 1.44E+05 |
| | | | | | | | A 7 | 2: 43 42 | 88 | 8.62E+03 | 4.63E+04 |
| | | | | | | | B 2 | | 89 | 6.11E+03 | 3.28E+04 |
| | | | | | | | B 3 | | 96 | 2.85E+04 | 1.53E+05 |
| | | | | | | | B 4 | 2: 44 43 | 96 | 8.88E+04 | 4.77E+05 |
| | | | | | | | C 2 | 2: 43 44 | 95 | 2.95E+04 | 1.58E+05 |
| | | | | | | | C 3 | 2: 43 41 | 96 | 6.95E+04 | 3.73E+05 |
| Trichloromonofluoromethane | 75-69-4 | 1.27 | | | | | B 1 | 2: 103 101 | 75 | 4.34E+03 | |
| | | | | | | | B 4 | 2: 101 103 | 81 | 1.72E+04 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| 2,3-dimethylbutane | 79-29-8 | 1.28 | | | | | A 6 | 3: 43 71 42 | 73 | 1.06E+04 | |
| | | | | | | | B 2 | | 66 | 5.01E+03 | |
| | | | | | | | B 3 | 4: 43 42 41 39 | 71 | 2.49E+04 | |
| Ethylenimine | 151-56-4 | 1.30 | | | | | A 5 | 1: 41 | 70 | 5.22E+04 | |
| | | | | | | | A 6 | 3: 43 42 39 | 81 | 2.30E+04 | |
| | | | | | | | B 2 | | 81 | 5.01E+03 | |
| | | | | | | | B 3 | 4: 43 42 41 39 | 83 | 2.49E+04 | |
| +Ethyl ether | 60-29-7 | 1.31 | | Ethereal | | | B 2 | 1: 59 | 86 | 2.37E+04 | |
| Ketene | 463-51-4 | 1.31 | | | | | A 4 | | 80 | 3.54E+03 | |
| | | | | | | | A 7 | 3: 41 42 59 | 74 | 3.81E+04 | |
| | | | | | | | B 1 | 3: 42 41 55 | 72 | 1.04E+05 | |
| | | | | | | | C 2 | 2: 41 42 | 73 | 3.11E+03 | |
| Isoprene | 78-79-5 | 1.33 | | | | | A 4 | 3: 39 53 51 | 85 | 3.34E+04 | |
| | | | | | | | A 5 | 1: 67 | 71 | 1.73E+04 | |
| | | | | | | | A 7 | | 93 | 3.12E+04 | |
| | | | | | | | B 1 | 3: 67 53 65 | 69 | 2.08E+04 | |
| | | | | | | | B 3 | | 77 | 4.59E+03 | |
| | | | | | | | B 4 | 5: 67 51 41 53 66 | 95 | 7.61E+04 | |
| | | | | | | | C 3 | 3: 67 39 53 | 81 | 1.42E+04 | |
| (E)-1,3-Pentadiene | 2004-70-8 | 1.34 | | | | | B 4 | | 94 | 2.13E+04 | |
| +1,3-Pentadiene | 504-60-9 | 1.34 | | | | | B 4 | | 94 | 2.13E+04 | |
| Hexane | 110-54-3 | 1.34 | Alkane | | | 2.19E+01 | A 1 | 7: 41 76 57 56 86 43 39 | 69 | 1.33E+05 | 6.09E+03 |
| | | | | | | | A 2 | 4: 62 56 42 86 | 66 | 2.53E+04 | 1.16E+03 |
| | | | | | | | A 3 | 2: 56 41 | 88 | 8.55E+04 | 3.91E+03 |
| | | | | | | | A 4 | 5: 57 42 43 41 39 | 78 | 2.03E+04 | 9.27E+02 |
| | | | | | | | A 5 | 2: 41 57 | 75 | 1.84E+04 | 8.43E+02 |
| | | | | | | | A 6 | 4: 76 42 56 43 | 74 | 1.57E+05 | 7.18E+03 |
| | | | | | | | A 7 | 1: 86 | 86 | 5.53E+04 | 2.53E+03 |
| | | | | | | | B 1 | 2: 57 56 | 79 | 3.71E+04 | 1.69E+03 |
| | | | | | | | B 2 | 2: 43 57 | 74 | 3.37E+04 | 1.54E+03 |
| | | | | | | | B 3 | | 67 | 2.96E+04 | 1.35E+03 |
| | | | | | | | B 4 | | 81 | 1.82E+04 | 8.32E+02 |
| 4-methyldecane | 2847-72-5 | 1.39 | | | | | A 1 | 12: 43 42 71 41 57 39 70 55 56 86 38 69 | 66 | 2.55E+06 | |
| | | | | | | | A 2 | 13: 43 71 42 41 57 70 39 56 86 85 62 54 63 | 66 | 2.66E+06 | |
| | | | | | | | A 3 | 17: 43 42 41 70 86 56 50 40 57 38 65 63 51 69 37 85 67 | 65 | 4.43E+06 | |
| | | | | | | | A 4 | | 75 | 1.66E+04 | |
| | | | | | | | A 5 | | 66 | 1.35E+06 | |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | 10: 39 57 55 41 86 53 69 38 52 67 | | | |
| | | | | | | | A | 7 | | 65 | 6.20E+05 | |
| | | | | | | | B | 1 | 10: 43 42 41 56 57 39 85 86 69 54 | 65 | 8.52E+05 | |
| 2-methylpentane | 107-83-5 | 1.39 | | | | | A | 1 | 12: 43 42 71 41 57 39 70 55 56 86 38 69 | 98 | 2.55E+06 | |
| | | | | | | | A | 2 | 13: 43 71 42 41 57 70 39 56 86 85 62 54 63 | 98 | 2.66E+06 | |
| | | | | | | | A | 3 | 3: 67 87 85 | 98 | 4.89E+06 | |
| | | | | | | | A | 4 | 2: 43 41 | 80 | 1.89E+04 | |
| | | | | | | | A | 7 | 12: 42 41 55 39 69 72 70 86 56 40 65 50 | 97 | 6.18E+05 | |
| | | | | | | | B | 1 | 10: 43 42 41 56 57 39 85 86 69 54 | 98 | 8.52E+05 | |
| | | | | | | | B | 2 | 6: 43 42 41 70 57 86 | 96 | 2.39E+05 | |
| | | | | | | | B | 4 | 4: 43 57 71 70 | 85 | 3.50E+04 | |
| 3,4,5-trimethyl-1-hexene | 56728-10-0 | 1.39 | | | | | A | 1 | 12: 43 42 71 41 57 39 70 55 56 86 38 69 | 68 | 2.55E+06 | |
| | | | | | | | A | 2 | 13: 43 71 42 41 57 70 39 56 86 85 62 54 63 | 68 | 2.66E+06 | |
| | | | | | | | A | 3 | 3: 67 87 85 | 68 | 4.89E+06 | |
| | | | | | | | A | 5 | 8: 43 71 42 41 57 50 56 86 | 68 | 1.54E+06 | |
| | | | | | | | A | 7 | | 67 | 6.20E+05 | |
| | | | | | | | B | 1 | 1: 70 | 68 | 2.04E+05 | |
| | | | | | | | C | 1 | 7: 85 99 71 110 98 68 39 | 67 | 2.17E+05 | |
| +γ-butyrolactone | 96-48-0 | 1.40 | Caramel, Sweet | Creamy, Oily, Fatty, Caramel | | | A | 7 | 12: 42 41 55 39 69 72 70 86 56 40 65 50 | 71 | 4.33E+05 | |
| Acrylic acid | 79-10-7 | 1.40 | | | 2.95E-01 | 2.95E-01 | B | 1 | 3: 72 55 58 | 65 | 2.17E+04 | 7.36E+04 |
| 2,3,4-trimethylpentane | 565-75-3 | 1.40 | | | | | A | 4 | | 75 | 1.52E+04 | |
| | | | | | | | A | 7 | 9: 43 70 41 55 57 53 56 54 50 | 77 | 2.03E+05 | |
| 3-methylpentane | 96-14-0 | 1.45 | | | | | A | 1 | 5: 57 56 41 58 71 | 98 | 4.98E+05 | |
| | | | | | | | A | 2 | 8: 57 56 41 71 39 58 54 85 | 99 | 5.18E+05 | |
| | | | | | | | A | 3 | | 98 | 6.94E+05 | |
| | | | | | | | A | 4 | | 87 | 2.06E+05 | |
| | | | | | | | A | 6 | 2: 57 39 | 70 | 3.72E+04 | |
| | | | | | | | A | 7 | | 97 | 1.22E+05 | |
| | | | | | | | B | 1 | 6: 57 41 56 58 55 51 | 95 | 2.92E+05 | |
| | | | | | | | B | 2 | 1: 57 | 86 | 6.05E+04 | |
| | | | | | | | B | 4 | 2: 57 56 | 91 | 5.56E+04 | |
| 2-methylaziridine | 75-55-8 | 1.45 | | | | | A | 1 | 5: 57 56 41 58 71 | 86 | 4.98E+05 | |
| | | | | | | | A | 2 | 8: 57 56 41 71 39 58 54 85 | 80 | 5.18E+05 | |
| | | | | | | | A | 3 | | 81 | 6.94E+05 | |
| | | | | | | | A | 4 | 3: 56 41 57 | 77 | 1.54E+04 | |
| | | | | | | | A | 5 | 5: 57 56 55 58 86 | 81 | 4.24E+05 | |
| | | | | | | | A | 7 | 5: 57 56 41 53 39 | 81 | 1.67E+05 | |
| | | | | | | | B | 1 | 6: 57 41 56 58 55 51 | 80 | 2.28E+05 | |
| | | | | | | | B | 2 | 1: 57 | 78 | 6.05E+04 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | B 4 | 2: 57 56 | 80 | 5.56E+04 | |
| Isocyanatomethane | 624-83-9 | 1.46 | | | | | A 3 | | 80 | 1.20E+04 | |
| | | | | | | | A 4 | | 81 | 5.01E+04 | |
| | | | | | | | A 6 | 2: 57 39 | 80 | 1.03E+05 | |
| | | | | | | | A 7 | | 85 | 1.22E+05 | |
| | | | | | | | B 1 | 2: 57 56 | 79 | 7.68E+03 | |
| | | | | | | | B 2 | 2: 56 57 | 79 | 7.77E+03 | |
| | | | | | | | B 4 | 2: 56 57 | 78 | 1.20E+03 | |
| Cyanogen chloride | 506-77-4 | 1.47 | | | | | B 2 | 8: 61 63 62 97 100 35 47 37 | 74 | 1.69E+05 | |
| 1,2-dichloro-, (Z)-ethene | 156-59-2 | 1.47 | | | | 1.91E+01 | B 1 | 4: 60 62 55 86 | 100 | 5.02E+05 | 2.63E+04 |
| | | | | | | | B 2 | 6: 96 98 59 62 60 47 | 91 | 1.71E+05 | 8.96E+03 |
| +Furan | 110-00-9 | 1.47 | | Ethereal | 4.50E+03 | | B 2 | 2: 39 68 | 80 | 9.70E+03 | 2.16E+00 |
| | | | | | | | B 4 | 1: 68 | 68 | 4.04E+04 | 8.99E+00 |
| 1,1-dichloro ethene | 75-35-4 | 1.47 | | | 3.55E+01 | | B 2 | | 99 | 3.57E+05 | 1.01E+04 |
| +Dimethylsulfide | 75-18-3 | 1.51 | Cabbage, Sulfur, Gasoline | Sulfury, Onion, Sweet corn, Vegetable, Cabbage, Tomato, Green, Radish | | 2.24E-03 | A 2 | 3: 47 39 35 | 66 | 5.52E+04 | 2.47E+07 |
| | | | | | | | A 7 | 5: 46 45 47 61 35 | 94 | 9.43E+04 | 4.21E+07 |
| Carbon disulfide | 75-15-0 | 1.52 | | Sulfur, Cabbage, Vegetable | | 9.55E-02 | A 4 | 4: 76 39 86 59 | 82 | 6.35E+04 | 6.65E+05 |
| | | | | | | | A 5 | 2: 44 39 | 84 | 7.99E+04 | 8.36E+05 |
| +3-pentanone | 96-22-0 | 1.53 | Ether | Ethereal, Acetone | | 3.16E-01 | A 4 | 2: 57 86 | 74 | 9.06E+04 | 2.86E+05 |
| | | | | | | | A 6 | | 67 | 3.85E+04 | 1.22E+05 |
| | | | | | | | B 3 | 2: 57 86 | 66 | 2.69E+04 | 8.50E+04 |
| +Butane | 106-97-8 | 1.57 | | | | 2.04E+02 | A 1 | | 79 | 3.90E+05 | 1.91E+03 |
| | | | | | | | A 2 | 2: 43 58 | 78 | 5.36E+05 | 2.62E+03 |
| | | | | | | | A 4 | 2: 43 42 | 83 | 1.85E+04 | 9.04E+01 |
| | | | | | | | A 6 | | 83 | 2.61E+06 | 1.28E+04 |
| | | | | | | | A 7 | 5: 41 59 44 37 60 | 84 | 1.88E+06 | 9.21E+03 |
| | | | | | | | B 1 | 7: 43 58 42 39 37 44 60 | 83 | 2.99E+06 | 1.47E+04 |
| | | | | | | | B 2 | | 77 | 1.35E+05 | 6.62E+02 |
| | | | | | | | B 3 | 6: 43 58 42 39 38 36 | 84 | 1.96E+06 | 9.59E+03 |
| | | | | | | | B 4 | | 87 | 4.62E+04 | 2.26E+02 |
| | | | | | | | C 1 | | 69 | 4.25E+04 | 2.08E+02 |
| | | | | | | | C 2 | 2: 43 42 | 67 | 6.65E+04 | 3.26E+02 |
| | | | | | | | C 3 | 3: 43 58 42 | 68 | 7.06E+04 | 3.46E+02 |
| Hordenine | 539-15-1 | 1.57 | | | | | A 6 | 1: 58 | 66 | 3.41E+04 | |
| +Propanal | 123-38-6 | 1.59 | Solvent, Pungent | Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty | 1.00E-02 | 2.69E-02 | A 1 | 2: 58 42 | 76 | 9.76E+04 | 3.63E+06 |
| | | | | | | | A 6 | | 76 | 1.57E+04 | 5.85E+05 |
| | | | | | | | A 7 | | 76 | 3.30E+04 | 1.23E+06 |
| | | | | | | | B 1 | 2: 57 58 | 75 | 7.59E+04 | 2.82E+06 |
| | | | | | | | B 2 | 1: 58 | 73 | 4.63E+04 | 1.72E+06 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | B | 3 | 2: 58 57 | 77 | 5.57E+04 | 2.07E+06 |
| | | | | | | B | 4 | 1: 58 | 83 | 1.04E+05 | 3.88E+06 |
| 1-Propanamine, 3-dibenzo[b,e] thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide | 1447-71-8 | 1.61 | | | | A | 1 | 2: 58 42 | 75 | 1.50E+05 | |
| | | | | | | A | 2 | 1: 58 | 73 | 7.42E+04 | |
| | | | | | | A | 6 | 5: 58 38 59 52 36 | 71 | 3.95E+05 | |
| | | | | | | A | 7 | | 65 | 3.33E+04 | |
| | | | | | | B | 1 | 2: 57 58 | 68 | 7.59E+04 | |
| | | | | | | B | 2 | 1: 58 | 70 | 4.63E+04 | |
| | | | | | | B | 3 | | 71 | 1.40E+04 | |
| | | | | | | B | 4 | 1: 58 | 68 | 1.24E+05 | |
| +Acetone | 67-64-1 | 1.66 | | Solvent | 1.45E+01 | A | 1 | 4: 43 58 42 37 | 97 | 5.84E+05 | 4.04E+04 |
| | | | | | | A | 2 | 2: 43 58 | 96 | 5.36E+05 | 3.71E+04 |
| | | | | | | A | 3 | 2: 43 58 | 81 | 4.96E+04 | 3.43E+03 |
| | | | | | | A | 4 | | 98 | 8.97E+04 | 6.20E+04 |
| | | | | | | A | 6 | 7: 43 58 42 39 57 38 44 | 99 | 2.71E+06 | 1.88E+05 |
| | | | | | | A | 7 | 10: 43 58 42 39 41 38 37 44 36 59 | 99 | 4.98E+06 | 3.45E+05 |
| | | | | | | B | 1 | 7: 43 58 42 39 37 44 60 | 99 | 2.99E+06 | 2.07E+05 |
| | | | | | | B | 2 | | 93 | 1.35E+05 | 9.35E+03 |
| | | | | | | B | 3 | 6: 43 58 42 39 38 36 | 99 | 1.96E+06 | 1.35E+05 |
| | | | | | | B | 4 | 10: 43 58 59 42 41 39 38 37 36 45 | 99 | 2.96E+06 | 2.05E+05 |
| | | | | | | C | 1 | | 87 | 4.25E+04 | 2.94E+03 |
| | | | | | | C | 2 | 2: 43 42 | 90 | 6.65E+04 | 4.60E+03 |
| | | | | | | C | 3 | 3: 43 58 42 | 88 | 7.06E+04 | 4.88E+03 |
| 2-methyl-2-propanamine | 75-64-9 | 1.67 | | | | A | 2 | 1: 58 | 89 | 7.42E+04 | |
| | | | | | | A | 6 | 3: 60 53 36 | 79 | 9.02E+04 | |
| | | | | | | B | 1 | 3: 42 41 55 | 76 | 9.02E+04 | |
| | | | | | | C | 3 | 2: 58 42 | 70 | 3.20E+04 | |
| +Acetic anhydride | 108-24-7 | 1.70 | | Sharp, Vinegar | 5.89E-01 | A | 1 | 1: 43 | 66 | 9.90E+03 | 1.68E+04 |
| | | | | | | A | 2 | 1: 43 | 72 | 2.31E+05 | 3.93E+05 |
| | | | | | | A | 3 | | 66 | 1.47E+04 | 2.50E+04 |
| | | | | | | A | 4 | 2: 43 41 | 81 | 3.73E+04 | 6.33E+04 |
| | | | | | | A | 5 | 5: 43 42 39 41 37 | 80 | 4.76E+05 | 8.09E+05 |
| | | | | | | A | 6 | | 65 | 2.59E+03 | 4.40E+03 |
| | | | | | | A | 7 | 2: 43 85 | 77 | 5.45E+04 | 9.26E+04 |
| | | | | | | B | 4 | 2: 42 43 | 79 | 8.59E+04 | 1.46E+05 |
| | | | | | | C | 3 | 2: 43 41 | 70 | 3.38E+04 | 5.74E+04 |
| Isobutyraldehyde | 78-84-2 | 1.76 | Pungent, Malt, Green | Spicy | 4.07E-02 | A | 1 | | 78 | 2.20E+07 | 5.40E+08 |
| | | | | | | A | 2 | 13: 43 41 57 72 39 55 56 38 40 73 62 66 65 | 78 | 2.02E+07 | 4.96E+08 |
| | | | | | | A | 3 | 3: 53 73 61 | 80 | 1.63E+06 | 3.99E+07 |
| | | | | | | A | 6 | | 73 | 6.15E+03 | 1.51E+05 |
| | | | | | | A | 7 | | 88 | 1.52E+04 | 3.73E+05 |
| | | | | | | B | 1 | | 93 | 3.08E+04 | 7.55E+05 |
| | | | | | | B | 2 | 7: 42 41 72 53 55 56 38 | 77 | 7.00E+05 | 1.72E+07 |
| | | | | | | B | 3 | | 85 | 7.70E+03 | 1.89E+05 |
| | | | | | | B | 4 | 4: 42 43 57 72 | 75 | 6.45E+04 | 1.58E+06 |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| +Methyl acetate | 79-20-9 | 1.77 | | Ethereal | | | A 1 | | 81 | 2.05E+04 | |
| | | | | | | | A 4 | 1: 43 | 97 | 2.81E+05 | |
| | | | | | | | A 6 | 7: 43 74 59 42 45 72 44 | 94 | 1.54E+06 | |
| | | | | | | | B 3 | 5: 43 41 59 73 75 | 99 | 4.56E+05 | |
| | | | | | | | B 4 | 4: 43 74 42 59 | 95 | 1.24E+05 | |
| Cyclohexene | 110-83-8 | 2.02 | | | | 3.63E-01 | A 7 | 2: 67 82 | 70 | 2.95E+04 | 8.12E+04 |
| Methacrolein | 78-85-3 | 2.14 | | Wild hyacinth foliage | | | A 7 | | 87 | 3.42E+04 | |
| +Butyraldehyde | 123-72-8 | 2.16 | Pungent, Green | Pungent, Cocoa, Musty, Green, Malty, Bread | | | A 6 | | 72 | 4.12E+04 | |
| | | | | | | | B 1 | 3: 41 44 72 | 73 | 1.92E+04 | |
| | | | | | | | B 3 | | 89 | 2.08E+04 | |
| | | | | | | | B 4 | | 91 | 2.41E+04 | |
| +2-butenal | 4170-30-3 | 2.31 | | Flower | | 1.35E-01 | A 7 | | 79 | 3.42E+04 | 2.54E+05 |
| | | | | | | | A 4 | 1: 43 | 68 | 3.13E+05 | 4.03E+04 |
| | | | | | | | A 6 | | 79 | 1.13E+04 | 1.46E+03 |
| | | | | | | | A 7 | 1: 43 | 79 | 2.25E+04 | 2.90E+03 |
| | | | | | | | B 1 | 1: 43 | 76 | 1.16E+05 | 1.49E+04 |
| | | | | | | | B 3 | 3: 72 43 127 | 75 | 3.07E+04 | 3.96E+03 |
| | | | | | | | C 1 | 2: 43 72 | 79 | 1.06E+04 | 1.37E+03 |
| methylhydrazine | 60-34-4 | 2.32 | | | | | A 3 | | 79 | 2.05E+04 | |
| Diazomethane | 334-88-3 | 2.33 | | | | | A 7 | 3: 41 42 59 | 71 | 3.00E+04 | |
| | | | | | | | B 3 | 2: 40 42 | 66 | 1.01E+05 | |
| +Isopropyl alcohol | 67-63-0 | 2.33 | | Alcohol, Musty, Woody | | 1.02E+01 | A 1 | 3: 45 43 41 | 77 | 1.50E+05 | 1.46E+04 |
| | | | | | | | A 3 | 2: 45 42 | 68 | 5.38E+04 | 5.26E+03 |
| | | | | | | | A 6 | 3: 45 44 72 | 75 | 1.43E+05 | 1.40E+04 |
| | | | | | | | B 3 | | 68 | 7.49E+04 | 7.32E+03 |
| | | | | | | | C 1 | 4: 44 90 38 37 | 70 | 6.13E+05 | 5.99E+04 |
| | | | | | | | C 2 | 15: 45 57 44 47 46 42 72 56 73 39 60 89 71 38 74 | 65 | 8.30E+06 | 8.12E+05 |
| | | | | | | | C 3 | 1: 45 | 65 | 1.24E+04 | 1.21E+03 |
| +Formic acid | 64-18-6 | 2.33 | | Acetic | | 2.82E+01 | A 1 | 3: 46 42 45 | 69 | 1.38E+05 | 4.91E+03 |
| | | | | | | | A 2 | 1: 46 | 79 | 6.39E+04 | 2.27E+03 |
| | | | | | | | A 3 | | 79 | 4.06E+04 | 1.44E+03 |
| | | | | | | | A 7 | 6: 45 46 39 42 41 47 | 67 | 4.35E+05 | 1.55E+04 |
| | | | | | | | B 1 | 4: 46 45 39 42 | 67 | 1.45E+05 | 5.14E+03 |
| | | | | | | | B 2 | 2: 45 46 | 77 | 4.31E+04 | 1.53E+03 |
| Nitrogen dioxide | 10102-44-0 | 2.34 | | | | 1.86E-01 | A 1 | 1: 46 | 76 | 2.63E+04 | 1.41E+05 |
| | | | | | | | A 2 | 1: 46 | 76 | 4.35E+04 | 2.34E+05 |
| +Ethanol | 64-17-5 | 2.34 | Sweet | Alcoholic | | 2.88E+01 | A 1 | | 95 | 1.29E+05 | 4.47E+03 |
| | | | | | | | A 2 | | 94 | 1.20E+05 | 4.15E+03 |
| | | | | | | | A 3 | | 95 | 7.50E+04 | 2.60E+03 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | A | 6 | | 72 | 1.69E+05 | 5.86E+03 |
| | | | | | | | A | 7 | 6: 45 46 39 42 41 47 | 99 | 3.01E+05 | 1.04E+04 |
| | | | | | | | B | 1 | 4: 46 45 39 42 | 84 | 9.90E+04 | 3.43E+03 |
| | | | | | | | B | 2 | 2: 45 46 | 78 | 4.31E+04 | 1.49E+03 |
| | | | | | | | B | 3 | 4: 43 207 42 46 | 79 | 5.88E+04 | 2.04E+03 |
| | | | | | | | B | 4 | | 92 | 5.54E+04 | 1.92E+03 |
| +Methylene chloride | 75-09-2 | 2.42 | | | | 2.82E+01 | A | 1 | 2: 86 39 | 94 | 1.76E+05 | 6.23E+03 |
| | | | | | | | A | 2 | 3: 51 48 47 | 97 | 2.98E+05 | 1.06E+04 |
| | | | | | | | A | 4 | 5: 84 51 88 42 50 | 97 | 3.88E+05 | 1.38E+04 |
| | | | | | | | A | 5 | 2: 47 49 | 98 | 2.81E+05 | 9.98E+03 |
| | | | | | | | A | 6 | | 92 | 2.13E+04 | 7.56E+02 |
| | | | | | | | A | 7 | 5: 84 39 86 88 47 | 95 | 7.08E+04 | 2.51E+03 |
| | | | | | | | B | 3 | | 91 | 1.67E+04 | 5.92E+02 |
| | | | | | | | B | 4 | 7: 84 49 88 51 47 83 48 | 97 | 1.62E+05 | 5.74E+03 |
| Amitrole | 61-82-5 | 2.44 | | | | | B | 4 | 1: 84 | 67 | 4.85E+04 | |
| Allyl alcohol | 107-18-6 | 2.75 | | Pungent, Mustard | | 2.69E-01 | A | 6 | | 71 | 1.94E+04 | 7.19E+04 |
| +Methylbutanal | 590-86-3 | 2.75 | Malt | Ethereal, Aldehydic, Chocolate, Peach, Fatty | 1.00E+00 | 2.24E-03 | B | 3 | | 68 | 2.92E+04 | 1.30E+07 |
| Allyl alcohol | 107-18-6 | 2.75 | | Pungent, Mustard | | 2.69E-01 | B | 3 | | 75 | 2.92E+04 | 1.08E+05 |
| Acetonitrile | 75-05-8 | 3.28 | | | 9.77E+01 | | B | 1 | | 96 | 1.18E+05 | 1.20E+03 |
| | | | | | | | B | 2 | | 96 | 9.20E+04 | 9.42E+02 |
| Chloroform | 67-66-3 | 3.78 | | | | | A | 1 | 2: 85 83 | 78 | 3.97E+04 | |
| | | | | | | | A | 2 | | 76 | 1.45E+04 | |
| | | | | | | | A | 4 | | 79 | 1.70E+04 | |
| | | | | | | | A | 5 | | 84 | 2.62E+04 | |
| | | | | | | | A | 6 | | 86 | 2.07E+04 | |
| | | | | | | | B | 4 | 2: 83 47 | 79 | 7.69E+04 | |
| Propyl formate | 110-74-7 | 3.91 | | Sweet, Ethereal, Green, Rum, Fruity, Berry | | 3.39E+00 | A | 7 | 1: 42 | 72 | 1.56E+05 | 4.59E+04 |
| Hydrazine | 302-01-2 | 3.92 | | | | 3.00E+00 | A | 1 | 1: 33 | 77 | 2.35E+03 | 7.85E+02 |
| | | | | | | | A | 2 | 1: 33 | 77 | 1.56E+03 | 5.21E+02 |
| | | | | | | | A | 3 | 1: 33 | 77 | 9.74E+02 | 3.25E+02 |
| | | | | | | | A | 7 | 3: 33 45 37 | 77 | 4.44E+03 | 1.48E+03 |
| | | | | | | | B | 1 | 1: 33 | 77 | 3.54E+03 | 1.18E+03 |
| | | | | | | | B | 4 | 1: 33 | 76 | 8.26E+02 | 2.75E+02 |
| 3-pentanol | 584-02-1 | 3.92 | Fruit | Herbal | | 4.68E-01 | A | 1 | | 69 | 1.14E+05 | 2.43E+05 |
| | | | | | | | A | 2 | 3: 60 59 45 | 68 | 1.06E+05 | 2.27E+05 |
| | | | | | | | A | 3 | | 67 | 6.67E+04 | 1.43E+05 |
| | | | | | | | A | 7 | | 71 | 1.21E+05 | 2.58E+05 |
| | | | | | | | B | 1 | | 70 | 1.01E+05 | 2.17E+05 |
| | | | | | | | B | 3 | 3: 59 60 53 | 77 | 7.79E+05 | 1.67E+06 |
| | | | | | | | B | 4 | 9: 59 42 60 41 57 39 58 40 36 | 75 | 2.14E+06 | 4.58E+06 |
| +1,1-dimethyl-hydrazine | 57-14-7 | 3.92 | | | | | A | 1 | 1: 42 | 76 | 6.10E+04 | |
| | | | | | | | A | 2 | 3: 60 59 45 | 80 | 1.06E+05 | |
| | | | | | | | A | 3 | 1: 42 | 76 | 1.59E+05 | |
| | | | | | | | A | 7 | | 83 | 1.41E+05 | |
| | | | | | | | B | 1 | 2: 59 45 | 77 | 6.29E+04 | |
| | | | | | | | B | 3 | 3: 59 60 33 | 80 | 1.87E+05 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | B 4 | 9: 59 42 60 41 57 39 58 40 36 | 80 | 6.00E+05 | |
| Ethylenediamine | 107-15-3 | 3.92 | | | | | A 1 | | 79 | 7.94E+04 | |
| | | | | | | | A 2 | | 75 | 8.76E+04 | |
| | | | | | | | A 3 | 3: 42 60 59 | 71 | 2.81E+04 | |
| | | | | | | | A 7 | | 75 | 1.41E+05 | |
| | | | | | | | B 1 | | 75 | 1.01E+05 | |
| | | | | | | | B 3 | 3: 59 60 53 | 71 | 4.76E+05 | |
| | | | | | | | B 4 | 7: 41 38 60 61 33 44 58 | 79 | 5.13E+05 | |
| tert-butanol | 75-65-0 | 3.93 | | Camphor | | | A 2 | | 70 | 1.53E+04 | |
| | | | | | | | B 3 | 3: 59 60 53 | 77 | 7.79E+05 | |
| | | | | | | | B 4 | 9: 59 42 60 41 57 39 58 40 36 | 74 | 2.14E+06 | |
| Methyl formate | 107-31-3 | 3.93 | | Fruity, Plum | | 9.33E+01 | A 1 | 1: 33 | 79 | 5.81E+03 | 6.22E+01 |
| | | | | | | | A 4 | 1: 60 | 72 | 3.42E+03 | 3.67E+01 |
| | | | | | | | B 4 | 7: 41 38 60 61 33 44 58 | 71 | 5.62E+05 | 6.02E+03 |
| Propylamine | 107-10-8 | 3.94 | | Ammoniacal | | 1.10E-02 | A 2 | | 76 | 5.74E+04 | 5.23E+06 |
| | | | | | | | B 4 | 9: 59 42 60 41 57 39 58 40 36 | 73 | 2.12E+06 | 1.94E+08 |
| Tetrahydrofurfuryl acetate | 637-64-9 | 4.07 | | Sweet, Fruity, Brown, Rum, Ether, Caramel | | | A 6 | | 70 | 2.00E+04 | |
| | | | | | | | B 3 | 4: 71 55 43 67 | 67 | 1.57E+04 | |
| +Phenylethyl alcohol | 60-12-8 | 5.06 | Honey, Spice, Rose, Lilac | Floral | | 1.70E-02 | A 2 | | 74 | 9.14E+04 | 5.38E+06 |
| +Toluene | 108-88-3 | 5.07 | Paint | Sweet | | 1.55E+00 | A 1 | | 81 | 1.39E+04 | 8.98E+03 |
| | | | | | | | A 2 | | 96 | 9.14E+04 | 5.90E+04 |
| | | | | | | | B 1 | 1: 91 | 79 | 5.82E+04 | 3.76E+04 |
| +Pentanal | 110-62-3 | 5.97 | Almond, Malt, Pungent | Fermented | | 6.03E-03 | B 3 | 3: 44 41 58 | 70 | 3.47E+04 | 5.76E+06 |
| +Hexanal | 66-25-1 | 5.99 | Grass, Tallow, Fat | Green | 4.00E-03 | 1.38E-02 | A 6 | | 85 | 4.12E+04 | 2.98E+06 |
| | | | | | | | A 7 | | 84 | 3.44E+04 | 2.49E+06 |
| | | | | | | | B 1 | 7: 43 41 72 55 45 207 82 | 90 | 1.22E+05 | 8.87E+06 |
| | | | | | | | B 2 | 11: 82 44 55 41 72 39 45 43 81 58 53 | 94 | 5.45E+05 | 3.95E+07 |
| | | | | | | | B 3 | | 73 | 2.30E+04 | 1.66E+06 |
| Glutaraldehyde | 111-30-8 | 6.02 | | | | | B 1 | | 69 | 1.15E+05 | |
| | | | | | | | B 2 | 11: 82 44 55 41 72 39 45 43 81 58 53 | 70 | 5.45E+05 | |
| +1-butanol | 71-36-3 | 6.09 | Medicine, Fruit | Fermented | | 4.90E-01 | A 3 | 2: 56 41 | 79 | 1.25E+05 | 2.54E+05 |
| | | | | | | | A 4 | | 77 | 1.82E+04 | 3.72E+04 |
| | | | | | | | A 6 | 4: 43 39 56 42 | 79 | 3.76E+04 | 7.67E+04 |
| | | | | | | | A 7 | 3: 41 39 56 | 83 | 3.18E+04 | 6.48E+04 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | B | 1 | 3: 56 55 39 | 92 | 1.21E+05 2.47E+05 |
| | | | | | | B | 2 | 2: 57 208 | 66 | 2.51E+05 5.12E+05 |
| | | | | | | B | 3 | 5: 56 43 57 39 72 | 97 | 9.87E+05 2.01E+06 |
| | | | | | | B | 4 | 12: 41 43 55 42 45 39 38 40 33 37 73 49 | 97 | 1.44E+06 2.95E+06 |
| Butyl formate | 592-84-7 | 6.09 | | Fruity | | A | 3 | 2: 56 41 | 67 | 9.56E+04 |
| | | | | | | A | 7 | 3: 41 39 56 | 65 | 2.32E+04 |
| | | | | | | B | 3 | 7: 39 43 56 40 57 41 44 | 82 | 9.78E+05 |
| | | | | | | B | 4 | 16: 56 41 43 55 39 40 46 57 73 38 45 74 51 49 54 50 | 85 | 3.94E+06 |
| +Isobutanol | 78-83-1 | 6.10 | Wine, Solvent, Bitter | Ethereal, Winey | | B | 4 | 2: 59 37 | 85 | 2.76E+05 |
| Propanoic acid, anhydride | 123-62-6 | 6.46 | | | | A | 1 | 1: 57 | 67 | 1.65E+03 |
| | | | | | | A | 2 | 1: 57 | 67 | 3.80E+03 |
| | | | | | | A | 3 | | 68 | 4.04E+03 |
| | | | | | | A | 4 | 3: 57 85 34 | 68 | 7.52E+03 |
| | | | | | | A | 6 | 1: 57 | 76 | 3.42E+04 |
| | | | | | | A | 7 | 1: 57 | 68 | 1.34E+04 |
| | | | | | | B | 2 | | 69 | 4.60E+03 |
| | | | | | | B | 3 | | 77 | 1.89E+04 |
| | | | | | | C | 1 | 1: 57 | 66 | 3.20E+03 |
| | | | | | | C | 2 | 1: 57 | 66 | 4.68E+03 |
| | | | | | | C | 3 | 1: 57 | 66 | 8.12E+03 |
| 4-methyl-3-penten-2-one | 141-79-7 | 6.66 | Sweet, Chemical | Pungent, Earthy, Vegetable, Acrylic | 5.62E-02 | B | 1 | 2: 98 83 | 73 | 3.78E+04 6.72E+05 |
| | | | | | | B | 3 | | 94 | 1.03E+05 1.83E+06 |
| | | | | | | B | 4 | 4: 55 42 63 77 | 97 | 6.77E+05 1.20E+07 |
| 2,2'-Bioxirane | 1464-53-5 | 6.66 | | | | B | 3 | 3: 55 51 43 | 65 | 9.31E+04 |
| α-angelica lactone | 591-12-8 | 6.66 | | | | B | 3 | 3: 55 51 43 | 82 | 1.17E+05 |
| +Isoamyl alcohol | 123-51-3 | 7.52 | Whiskey, Malt, Burnt | Fusel oil, Alcoholic, Whiskey, Fruity, Banana | 4.47E-02 | A | 6 | | 73 | 3.77E+04 8.43E+05 |
| | | | | | | B | 3 | | 75 | 7.91E+04 1.77E+06 |
| Amyl alcohol | 71-41-0 | 7.52 | Balsamic | Fusel, Oil, Sweet, Balsam | 4.68E-01 | A | 6 | | 78 | 3.77E+04 8.05E+04 |
| | | | | | | B | 3 | | 79 | 7.91E+04 1.69E+05 |
| 2-isopropenyl-3-methylpyrazine | 145984-65-2 | 7.67 | | | | A | 7 | 4: 135 75 134 133 | 73 | 1.03E+05 |
| α-phellandrene | 99-83-2 | 7.89 | Turpentine, Mint, Spice | Terpenic | | A | 1 | 20: 77 40 80 43 121 94 78 92 38 107 136 42 82 90 50 33 137 115 135 117 | 81 | 1.00E+07 |
| | | | | | | A | 2 | 5: 91 107 93 136 92 | 95 | 7.06E+05 |
| | | | | | | A | 3 | 6: 105 107 93 77 81 54 | 74 | 3.57E+05 |
| | | | | | | A | 5 | 13: 94 91 93 55 51 136 92 79 121 77 108 103 122 | 90 | 8.87E+04 |
| | | | | | | A | 6 | 4: 93 55 105 78 | 90 | 9.41E+04 |
| | | | | | | A | 7 | 11: 92 136 91 93 108 78 39 77 107 106 66 | 79 | 1.55E+06 |
| | | | | | | B | 2 | 20: 93 39 67 136 94 77 79 78 92 80 53 41 81 68 137 55 63 95 52 69 | 74 | 1.37E+06 |
| | | | | | | B | 3 | 2: 91 93 | 82 | 1.77E+04 |
| | | | | | | B | 4 | | 85 | 3.25E+04 |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | C 1 | | 90 | 8.81E+04 | |
| | | | | | | | C 2 | | 86 | 3.75E+04 | |
| | | | | | | | C 3 | 7: 136 93 91 92 103 77 94 | 89 | 8.42E+04 | |
| α-pinene | 80-56-8 | 7.90 | Pine, Turpentine | Herbal | | 6.92E-01 | A 1 | 12: 79 93 106 91 78 41 136 51 94 92 77 67 | 93 | 1.05E+06 | 1.52E+06 |
| | | | | | | | A 2 | | 97 | 6.09E+06 | 8.80E+06 |
| | | | | | | | A 3 | 10: 93 91 121 77 43 81 106 94 39 53 | 92 | 2.14E+05 | 3.09E+05 |
| | | | | | | | A 5 | 8: 93 81 68 107 43 105 95 78 | 93 | 3.65E+05 | 5.28E+05 |
| | | | | | | | A 6 | | 93 | 1.61E+05 | 2.33E+05 |
| | | | | | | | A 7 | 11: 92 136 91 93 108 78 39 77 107 106 66 | 97 | 4.88E+05 | 7.05E+05 |
| | | | | | | | B 1 | 11: 92 81 78 39 41 65 107 281 80 122 69 | 98 | 1.79E+06 | 2.58E+06 |
| | | | | | | | B 2 | 20: 93 39 67 136 94 77 79 78 92 80 53 41 81 68 137 55 63 95 52 69 | 98 | 1.24E+06 | 1.79E+06 |
| | | | | | | | B 3 | | 88 | 9.49E+04 | 1.37E+05 |
| | | | | | | | B 4 | | 83 | 3.25E+04 | 4.69E+04 |
| | | | | | | | C 1 | | 71 | 5.23E+04 | 7.56E+04 |
| | | | | | | | C 2 | | 75 | 3.75E+04 | 5.42E+04 |
| | | | | | | | C 3 | 7: 136 93 91 92 103 77 94 | 70 | 8.42E+04 | 1.22E+05 |
| Betahistine | 5638-76-6 | 7.90 | | | | | A 1 | 3: 65 74 104 | 65 | 2.02E+07 | |
| | | | | | | | A 3 | | 69 | 4.37E+04 | |
| | | | | | | | A 4 | | 67 | 1.03E+04 | |
| | | | | | | | A 5 | 8: 136 93 80 43 41 106 65 94 | 70 | 5.56E+05 | |
| | | | | | | | A 6 | 6: 136 94 79 106 93 121 | 73 | 4.42E+05 | |
| | | | | | | | A 7 | | 68 | 5.61E+05 | |
| | | | | | | | B 1 | 18: 77 79 68 80 53 52 121 136 106 105 43 41 64 51 103 66 81 54 | 67 | 1.29E+06 | |
| Conessine | 546-06-5 | 8.31 | | | | | B 3 | 2: 71 84 | 69 | 5.94E+03 | |
| | | | | | | | B 4 | 1: 84 | 74 | 5.31E+04 | |
| 2-formyl pyrrole | 1003-29-8 | 9.09 | | Musty, Beefy, Coffee | | | C 3 | 3: 95 94 81 | 67 | 7.92E+03 | |
| 1,4-dimethoxybenzene | 150-78-7 | 9.19 | | Sweet, Green, New mown hay, Fennel | | | C 1 | | 67 | 1.39E+04 | |
| | | | | | | | C 2 | | 66 | 2.81E+04 | |
| +α-ionol | 25312-34-9 | 9.20 | | Ionone, Tropical, Sweet, Floral, Violet, Woody | | | C 1 | | 73 | 2.42E+04 | |
| | | | | | | | C 3 | 7: 138 95 82 80 55 45 140 | 68 | 1.92E+05 | |
| Menthyl acetate | 16409-45-3 | 9.20 | | Tea cooling, Minty, Fruity, Berry | | 6.17E+00 | C 1 | 5: 138 94 123 95 79 | 74 | 1.46E+05 | 2.37E+04 |
| | | | | | | | C 2 | 2: 138 96 | 79 | 5.85E+04 | 9.49E+03 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | C | 3 | | 77 | 2.29E+04 | 3.71E+03 |
| 4-methyl guaiacol | 93-51-6 | 9.20 | | Spicy | | | C | 1 | 5: 138 94 123 95 79 | 74 | 1.18E+05 | |
| 2-acetyl-6-methyl pyrazine | 22047-26-3 | 9.26 | | Roasted coffee, Cocoa, Popcorn | | | B | 3 | 3: 93 136 41 | 70 | 1.67E+04 | |
| | | | | | | | C | 2 | 15: 93 136 39 80 94 78 67 108 102 104 120 38 75 54 49 | 65 | 3.00E+07 | |
| Tricyclene | 508-32-7 | 9.30 | | | | | A | 2 | 6: 136 133 92 78 107 40 | 81 | 3.13E+05 | |
| | | | | | | | A | 6 | 6: 136 94 79 106 93 121 | 71 | 4.42E+05 | |
| 2-indanone | 615-13-4 | 9.47 | | | | | B | 1 | 6: 104 77 103 39 51 102 | 66 | 1.82E+05 | |
| +Styrene | 100-42-5 | 9.48 | Balsamic, Gasoline | Balsamic | | 1.45E-01 | B | 1 | 6: 104 77 103 39 51 102 | 97 | 1.82E+05 | 1.26E+06 |
| | | | | | | | B | 2 | | 81 | 2.19E+04 | 1.52E+05 |
| β-pinene | 18172-67-3 | 9.90 | Pine, Resin, Turpentine | Terpenic | | | A | 1 | 11: 136 52 128 81 119 78 90 56 83 59 55 | 96 | 2.64E+07 | |
| | | | | | | | A | 2 | 18: 69 41 79 53 39 94 67 80 70 107 66 51 117 137 52 104 37 59 | 97 | 1.09E+07 | |
| | | | | | | | A | 3 | | 93 | 7.03E+05 | |
| | | | | | | | A | 4 | | 67 | 2.39E+04 | |
| | | | | | | | A | 5 | 5: 69 93 121 51 94 | 80 | 5.33E+05 | |
| | | | | | | | A | 6 | | 73 | 8.95E+05 | |
| | | | | | | | A | 7 | | 92 | 5.61E+05 | |
| | | | | | | | B | 1 | 20: 93 69 41 91 39 68 51 92 79 136 77 67 65 94 53 54 107 82 137 52 | 96 | 3.92E+06 | |
| | | | | | | | B | 2 | 20: 69 53 77 78 39 94 121 70 55 42 68 65 89 67 52 40 51 105 66 56 | 95 | 5.72E+06 | |
| | | | | | | | B | 3 | | 75 | 3.51E+04 | |
| +Myrcene | 123-35-3 | 9.94 | Balsamic, Must, Spice | Peppery, Terpene, Spicy, Balsam, Plastic | 1.30E-02 | | A | 1 | 12: 41 92 43 120 80 40 53 51 55 79 52 78 | 88 | 1.86E+06 | 1.43E+08 |
| | | | | | | | A | 2 | 1: 38 | 92 | 1.36E+06 | 1.05E+08 |
| | | | | | | | A | 3 | 12: 93 81 41 94 77 43 91 121 70 79 51 106 | 94 | 1.37E+06 | 1.05E+08 |
| | | | | | | | A | 5 | | 92 | 2.88E+05 | 2.22E+07 |
| | | | | | | | A | 7 | | 94 | 6.11E+05 | 4.70E+07 |
| | | | | | | | B | 1 | 20: 93 69 41 91 39 68 51 92 79 136 77 67 65 94 53 54 107 82 137 52 | 97 | 3.92E+06 | 3.02E+08 |
| | | | | | | | B | 2 | 20: 69 53 77 78 39 94 121 70 55 42 68 65 89 67 52 40 51 105 66 56 | 96 | 5.72E+06 | 4.40E+08 |
| | | | | | | | B | 3 | 3: 93 92 41 | 71 | 3.05E+04 | 2.34E+06 |
| DL-menthol | 89-78-1 | 10.34 | | Peppermint, Cool, Woody | 4.17E-02 | | C | 1 | | 67 | 1.01E+05 | 2.42E+06 |
| | | | | | | | C | 3 | 7: 138 95 82 80 55 45 140 | 66 | 6.55E+04 | 1.57E+06 |
| +(±)-menthol | 1490-04-6 | 10.34 | | Minty | | 4.17E-02 | C | 1 | | 70 | 1.01E+05 | 2.42E+06 |
| | | | | | | | C | 2 | 9: 95 138 139 96 94 67 109 123 68 | 70 | 1.39E+05 | 3.34E+06 |
| | | | | | | | C | 3 | | 69 | 1.90E+05 | 4.56E+06 |
| +o-dimethyl hydroquinone | 91-16-7 | 10.34 | | Vanilla | | | C | 3 | | 69 | 3.63E+05 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | | 9: 95 94 138 96 123 67 53 81 79 | | | |
| (+)-carvomenthene | 1195-31-9 | 10.34 | | | | | C 1 | | 85 | 1.01E+05 | |
| | | | | | | | C 2 | | 85 | 8.21E+04 | |
| | | | | | | | C 3 | | 86 | 1.90E+05 | |
| Menthol | 15356-70-4 | 10.36 | | | 4.17E-02 | | C 3 | | 66 | 8.02E+04 | 1.92E+06 |
| 2,4,6-trimethylphenol | 527-60-6 | 10.48 | | Phenolic | | | C 1 | 6: 57 39 107 135 116 52 | 82 | 4.11E+05 | |
| +α-terpinene | 99-86-5 | 10.50 | Lemon | Woody | | | A 1 | 3: 121 75 68 | 66 | 1.37E+06 | |
| | | | | | | | A 2 | 20: 136 121 93 91 79 77 105 39 51 41 64 120 53 107 106 55 95 50 40 116 | 96 | 4.75E+06 | |
| | | | | | | | A 7 | 13: 121 78 136 68 103 117 80 52 51 77 106 107 81 | 80 | 2.20E+05 | |
| | | | | | | | B 1 | 3: 136 91 107 | 78 | 4.82E+04 | |
| | | | | | | | C 1 | 20: 136 93 53 91 78 41 107 122 137 77 79 105 92 119 50 39 65 108 115 90 | 97 | 2.04E+06 | |
| | | | | | | | C 2 | | 97 | 1.40E+06 | |
| | | | | | | | C 3 | 20: 91 93 79 107 136 92 106 77 95 65 89 51 43 108 137 94 102 68 115 50 | 98 | 1.71E+06 | |
| (+)-4-Carene | 29050-33-7 | 10.50 | | | 4.00E+00 | | A 1 | 7: 93 119 121 137 53 105 136 | 94 | 3.68E+05 | 9.21E+04 |
| | | | | | | | A 2 | 20: 136 121 93 91 79 77 105 39 51 41 64 120 53 107 106 55 95 50 40 116 | 99 | 4.75E+06 | 1.19E+06 |
| | | | | | | | A 3 | | 91 | 3.19E+04 | 7.97E+03 |
| | | | | | | | A 5 | 5: 105 119 121 80 136 | 67 | 7.28E+04 | 1.82E+04 |
| | | | | | | | A 7 | 13: 121 78 136 68 103 117 80 52 51 77 106 107 81 | 82 | 2.20E+05 | 5.49E+04 |
| | | | | | | | B 1 | | 84 | 2.29E+04 | 5.73E+03 |
| | | | | | | | C 1 | 20: 136 93 53 91 78 41 107 122 137 77 79 105 92 119 50 39 65 108 115 90 | 98 | 2.04E+06 | 5.10E+05 |
| | | | | | | | C 2 | | 98 | 1.40E+06 | 3.50E+05 |
| | | | | | | | C 3 | 20: 121 136 122 103 78 77 105 80 41 106 107 39 43 94 120 115 52 135 67 54 | 98 | 1.10E+06 | 2.74E+05 |
| Furfurylmethylamphetamine | 13445-60-8 | 10.50 | | | | | A 1 | 1: 81 | 73 | 5.34E+04 | |
| +Phenylacetic acid | 103-82-2 | 10.53 | Honey, Flower | Sweet, Honey, Floral, Honeysuckle, Sour, Waxy, Civet | | | A 2 | 3: 91 136 43 | 70 | 7.97E+04 | |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| +1-hexanol | 111-27-3 | 10.73 | Resin, Flower, Breen | Herbal | | | 4.37E-02 | A | 6 | | 87 | 5.03E+04 | 1.15E+06 |
| Diacetone alcohol | 123-42-2 | 10.78 | | | | | 8.91E-01 | A | 7 | 2: 59 43 | 77 | 5.51E+04 | 6.18E+04 |
| | | | | | | | | B | 3 | | 87 | 2.54E+05 | 2.85E+05 |
| | | | | | | | | B | 4 | 9: 43 59 101 39 83 55 61 40 45 | 92 | 1.75E+06 | 1.96E+06 |
| (1R)-(+)-trans-isolimonene | 5113-87-1 | 10.85 | | | | | | B | 4 | 8: 79 121 136 105 94 95 108 81 | 71 | 6.65E+04 | |
| 2,2,5-trimethylhexane | 3522-94-9 | 10.88 | | | | | | A | 4 | 4: 56 57 71 136 | 80 | 1.28E+05 | |
| +Limonene | 138-86-3 | 10.89 | Lemon, Orange | Citrus | | 1.00E-02 | 4.37E-01 | A | 1 | 20: 92 105 80 51 117 66 137 122 62 81 64 54 104 63 76 108 103 134 38 43 | 95 | 3.33E+07 | 7.64E+07 |
| | | | | | | | | A | 2 | 20: 68 93 67 94 136 59 107 91 53 39 81 95 105 55 65 66 119 137 52 96 | 95 | 2.21E+07 | 5.05E+07 |
| | | | | | | | | A | 3 | 20: 68 79 93 67 107 115 94 92 77 63 136 39 80 41 91 108 69 95 54 137 | 95 | 1.97E+06 | 4.51E+06 |
| | | | | | | | | A | 4 | 20: 68 92 93 41 67 39 57 71 65 77 55 79 85 94 53 136 91 56 121 191 | 82 | 4.35E+05 | 9.97E+05 |
| | | | | | | | | A | 6 | 8: 92 67 93 65 136 80 107 39 | 87 | 2.06E+05 | 4.71E+05 |
| | | | | | | | | A | 7 | 6: 68 92 80 136 69 41 | 90 | 1.71E+05 | 3.92E+05 |
| | | | | | | | | B | 1 | | 95 | 2.16E+06 | 4.94E+06 |
| | | | | | | | | B | 2 | | 95 | 1.71E+06 | 3.93E+06 |
| | | | | | | | | B | 3 | | 90 | 1.76E+05 | 4.03E+05 |
| | | | | | | | | B | 4 | 3: 67 121 77 | 76 | 8.21E+04 | 1.88E+05 |
| | | | | | | | | C | 1 | 16: 93 67 69 107 39 121 92 136 52 122 41 137 42 77 55 51 | 93 | 3.17E+05 | 7.26E+05 |
| | | | | | | | | C | 2 | 7: 68 91 136 67 121 65 69 | 87 | 1.62E+05 | 3.71E+05 |
| | | | | | | | | C | 3 | | 80 | 3.86E+04 | 8.84E+04 |
| +Camphene | 79-92-5 | 10.93 | Camphor | Woody | | | | A | 1 | 20: 92 105 80 51 117 66 137 122 62 81 64 54 104 63 76 108 103 134 38 43 | 89 | 3.33E+07 | |
| | | | | | | | | A | 2 | 20: 68 93 67 94 136 59 107 91 53 39 81 95 105 55 65 66 119 137 52 96 | 89 | 2.21E+07 | |
| | | | | | | | | A | 3 | 20: 68 79 93 67 107 115 94 92 77 63 136 39 80 41 91 108 69 95 54 137 | 89 | 1.97E+06 | |
| | | | | | | | | A | 4 | 20: 68 92 93 41 67 39 57 71 65 77 55 79 85 94 53 136 91 56 121 191 | 78 | 4.35E+05 | |
| | | | | | | | | A | 5 | 12: 91 53 67 65 121 107 80 105 93 77 41 95 | 87 | 4.38E+05 | |
| | | | | | | | | A | 6 | 8: 92 67 93 65 136 80 107 39 | 82 | 2.06E+05 | |
| | | | | | | | | A | 7 | 7: 79 68 136 107 92 95 91 | 84 | 1.33E+05 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | B 1 | | 90 | 2.16E+06 | |
| | | | | | | | B 2 | | 90 | 1.71E+06 | |
| | | | | | | | B 3 | | 85 | 1.76E+05 | |
| | | | | | | | B 4 | 8: 79 121 136 105 94 95 108 81 | 79 | 3.71E+04 | |
| | | | | | | | C 1 | | 88 | 2.97E+05 | |
| | | | | | | | C 2 | 11: 93 94 120 51 122 77 65 104 108 52 103 | 65 | 2.52E+05 | |
| | | | | | | | C 3 | | 82 | 8.67E+07 | |
| Eucalyptol | 470-82-6 | 10.97 | Mint, Sweet | Eucalyptus, Herbal, Camphor | | 1.62E-02 | A 6 | | 80 | 1.58E+05 | 9.75E+06 |
| | | | | | | | B 3 | | 70 | 1.03E+05 | 6.36E+06 |
| N-Benzyl-2-phenethylamine | 3647-71-0 | 11.32 | | | | | B 3 | 2: 120 91 | 75 | 1.22E+04 | |
| Phenyl propane | 103-65-1 | 11.32 | | | | | B 3 | 2: 120 91 | 70 | 1.22E+04 | |
| 3-ethyl-o-xylene | 933-98-2 | 11.35 | | | | | A 2 | 13: 91 119 78 77 105 55 103 50 104 120 135 133 63 | 81 | 8.85E+05 | |
| m-cymene | 535-77-3 | 11.36 | | | | | A 1 | | 96 | 3.98E+05 | |
| | | | | | | | A 2 | | 98 | 1.76E+06 | |
| | | | | | | | A 3 | 2: 119 91 | 73 | 3.59E+04 | |
| | | | | | | | A 4 | 2: 119 65 | 71 | 4.21E+04 | |
| | | | | | | | A 6 | | 92 | 4.31E+04 | |
| | | | | | | | A 7 | | 86 | 3.49E+04 | |
| | | | | | | | B 1 | | 91 | 5.27E+04 | |
| | | | | | | | B 3 | 3: 119 91 134 | 93 | 9.48E+04 | |
| | | | | | | | C 1 | 19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130 | 99 | 6.79E+07 | |
| | | | | | | | C 2 | | 99 | 3.74E+07 | |
| | | | | | | | C 3 | 20: 119 134 91 77 135 93 92 51 78 116 58 50 128 52 86 87 129 101 131 126 | 97 | 3.94E+07 | |
| +p-cymene | 99-87-6 | 11.36 | Solvent, Gasoline, Citrus | Terpenic | | 2.14E-03 | A 1 | | 93 | 3.98E+05 | 1.86E+08 |
| | | | | | | | A 2 | | 95 | 1.76E+06 | 8.22E+08 |
| | | | | | | | A 3 | 1: 119 | 74 | 5.38E+04 | 2.52E+07 |
| | | | | | | | A 4 | 2: 119 65 | 70 | 5.56E+04 | 2.60E+07 |
| | | | | | | | A 6 | | 91 | 4.31E+04 | 2.01E+07 |
| | | | | | | | A 7 | | 85 | 3.49E+04 | 1.63E+07 |
| | | | | | | | B 1 | | 89 | 5.27E+04 | 2.46E+07 |
| | | | | | | | B 3 | 3: 119 91 134 | 91 | 9.48E+04 | 4.44E+07 |
| | | | | | | | C 1 | 19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130 | 97 | 6.79E+07 | 3.18E+10 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | C | 2 | | 97 | 3.74E+07 1.75E+10 |
| | | | | | | C | 3 | 20: 119 134 91 77 135 93 92 51 78 116 58 50 128 52 86 87 129 101 131 126 | 93 | 3.94E+07 1.84E+10 |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | 11.36 | | Gasoline, Sweet | 2.63E-02 | A | 1 | | 91 | 3.98E+05 1.51E+07 |
| | | | | | | A | 2 | 14: 119 134 117 118 39 135 103 89 116 133 41 78 64 51 | 94 | 1.33E+06 5.06E+07 |
| | | | | | | A | 3 | 2: 134 119 | 72 | 4.73E+04 1.80E+06 |
| | | | | | | A | 4 | 3: 119 117 63 | 67 | 2.58E+04 9.82E+05 |
| | | | | | | A | 5 | 2: 119 134 | 67 | 8.39E+03 3.19E+05 |
| | | | | | | A | 6 | 5: 119 134 120 117 57 | 86 | 1.25E+05 4.77E+06 |
| | | | | | | A | 7 | | 80 | 3.49E+04 1.33E+06 |
| | | | | | | B | 1 | | 85 | 5.27E+04 2.00E+06 |
| | | | | | | B | 3 | 3: 119 91 134 | 87 | 9.48E+04 3.60E+06 |
| | | | | | | C | 1 | 19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130 | 95 | 6.79E+07 2.58E+09 |
| | | | | | | C | 2 | | 95 | 3.74E+07 1.42E+09 |
| | | | | | | C | 3 | 20: 119 134 91 77 135 93 92 51 78 116 58 50 128 52 86 87 129 101 131 126 | 93 | 3.94E+07 1.50E+09 |
| 1-ethyl-2,4-dimethylbenzene | 874-41-9 | 11.36 | | | | A | 1 | 5: 93 78 119 104 106 | 76 | 1.24E+05 |
| | | | | | | A | 3 | 1: 119 | 78 | 5.38E+04 |
| | | | | | | A | 4 | 2: 119 65 | 72 | 5.56E+04 |
| | | | | | | A | 6 | 5: 119 134 120 117 57 | 84 | 1.23E+05 |
| | | | | | | B | 1 | 3: 134 120 77 | 79 | 7.74E+04 |
| | | | | | | B | 3 | 2: 119 120 | 76 | 6.36E+04 |
| 1-phenyl-1-decanone | 6048-82-4 | 11.40 | | | | A | 2 | 6: 57 63 117 58 120 105 | 71 | 2.12E+05 |
| N,N-dimethylbenzenamine | 121-69-7 | 11.40 | | | | A | 2 | 6: 57 63 117 58 120 105 | 71 | 2.12E+05 |
| Isodurene | 527-53-7 | 11.40 | | | | A | 1 | 3: 57 119 134 | 79 | 2.50E+04 |
| | | | | | | A | 2 | 4: 119 39 134 193 | 75 | 3.12E+04 |
| | | | | | | A | 4 | 3: 119 117 63 | 69 | 2.60E+04 |
| | | | | | | B | 1 | 2: 119 134 | 67 | 7.78E+04 |
| | | | | | | C | 1 | 20: 119 134 91 105 103 104 39 75 128 50 53 52 90 76 38 94 106 114 85 98 | 77 | 5.94E+07 |
| 1-(3-methylphenyl)-ethanone | 585-74-0 | 11.41 | | | | A | 1 | 5: 93 78 119 104 106 | 83 | 7.20E+04 |
| | | | | | | A | 3 | 2: 119 91 | 71 | 3.59E+04 |
| | | | | | | B | 1 | 3: 91 120 134 | 76 | 6.51E+04 |
| Dihydromethylcyclopentapyrazine | 23747-48-0 | 11.41 | Roast, Nut | Earthy, Baked potato, Peanut, Roasted | | A | 1 | 3: 57 119 134 | 75 | 1.56E+05 |
| | | | | | | A | 2 | 4: 119 39 134 193 | 69 | 3.12E+04 |
| | | | | | | C | 1 | 19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130 | 70 | 2.87E+07 |
| 1-ethyl-3,5-dimethylbenzene | 934-74-7 | 11.46 | | | | A | 2 | 8: 134 119 116 117 62 102 57 71 | 68 | 3.87E+05 |
| | | | | | | C | 1 | | 82 | 6.16E+07 |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | | 20: 119 134 91 105 103 104 39 75 128 50 53 52 90 76 38 94 106 114 85 98 | | | |
| +Methylisohexenyl ketone | 110-93-0 | 11.51 | Pepper, Mushroom, Rubber | Citrus | | 3.80E-02 | A 4 | | 93 | 3.18E+05 | 8.35E+06 |
| | | | | | | | A 6 | 9: 52 68 65 57 45 77 54 84 50 | 98 | 4.30E+06 | 1.13E+08 |
| | | | | | | | A 7 | | 80 | 4.51E+04 | 1.19E+06 |
| | | | | | | | B 3 | 4: 65 70 82 97 | 98 | 3.30E+06 | 8.67E+07 |
| | | | | | | | B 4 | 7: 93 108 67 117 55 68 126 | 94 | 3.97E+05 | 1.04E+07 |
| 4-ethyl-1,2-dimethylbenzene | 934-80-5 | 11.57 | | | | | A 2 | 8: 134 119 116 117 62 102 57 71 | 67 | 3.91E+05 | |
| +δ-3-carene | 13466-78-9 | 11.57 | Lemon, Resin | Citrus | 4.00E+00 | | A 1 | 4: 108 91 43 105 | 78 | 7.76E+04 | 1.94E+04 |
| | | | | | | | A 2 | 8: 134 119 116 117 62 102 57 71 | 97 | 3.80E+06 | 9.51E+05 |
| | | | | | | | A 3 | | 90 | 7.79E+04 | 1.95E+04 |
| | | | | | | | A 5 | 9: 107 93 92 136 80 118 65 120 79 | 71 | 3.01E+05 | 7.53E+04 |
| | | | | | | | A 6 | | 73 | 9.13E+05 | 2.28E+05 |
| | | | | | | | A 7 | 19: 92 79 94 105 95 91 148 63 65 204 120 41 123 82 135 78 66 39 128 | 70 | 1.42E+06 | 3.56E+05 |
| | | | | | | | B 1 | 11: 137 79 93 136 92 107 94 77 78 81 53 | 96 | 3.24E+05 | 8.11E+04 |
| | | | | | | | B 2 | 7: 79 43 67 51 136 40 105 | 75 | 3.15E+05 | 7.88E+04 |
| | | | | | | | B 3 | | 72 | 8.48E+05 | 2.12E+05 |
| | | | | | | | B 4 | | 71 | 2.10E+05 | 5.25E+04 |
| | | | | | | | C 1 | 4: 90 41 122 107 | 85 | 9.59E+06 | 2.40E+06 |
| | | | | | | | C 2 | 10: 106 122 108 138 135 94 64 68 82 63 | 90 | 2.21E+06 | 5.52E+05 |
| | | | | | | | C 3 | 20: 91 93 79 107 136 92 106 77 95 65 89 51 43 108 137 94 102 68 115 50 | 72 | 1.82E+06 | 4.54E+05 |
| Sabinene | 3387-41-5 | 11.59 | Pepper, Turpentine, Wood | Woody | | | A 1 | 20: 77 40 80 43 121 94 78 92 38 107 136 42 82 90 50 33 137 115 135 117 | 79 | 9.81E+06 | |
| | | | | | | | A 2 | 11: 136 105 92 67 79 43 68 94 51 106 138 | 88 | 1.53E+06 | |
| | | | | | | | A 3 | | 90 | 7.79E+04 | |
| | | | | | | | A 7 | 7: 91 67 107 108 41 94 63 | 69 | 1.09E+05 | |
| | | | | | | | B 1 | 18: 77 79 68 80 53 52 121 136 106 105 43 41 64 51 103 66 54 81 | 75 | 1.30E+06 | |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| γ-terpinene | 99-85-4 | 11.79 | Gasoline, Turpentine | Terpenic | | | A | 2 | | 85 | 5.28E+04 | |
| | | | | | | | A | 7 | 7: 77 107 80 121 92 137 63 | 69 | 1.64E+05 | |
| | | | | | | | C | 1 | 14: 91 136 105 79 78 53 76 80 137 55 81 75 68 127 | 98 | 1.32E+08 | |
| | | | | | | | C | 2 | 18: 91 79 43 107 119 51 103 117 66 55 88 74 135 129 42 123 101 87 | 99 | 1.25E+08 | |
| | | | | | | | C | 3 | 16: 93 91 121 105 41 43 63 122 52 81 76 102 38 42 127 120 | 99 | 8.67E+07 | |
| +Terpinolene | 586-62-9 | 11.83 | Pine, Plastic | Herbal | 2.00E-01 | | A | 1 | 11: 136 52 128 81 119 78 90 56 83 59 55 | 73 | 3.87E+06 | 1.94E+07 |
| | | | | | | | A | 2 | 20: 136 121 93 91 79 77 105 39 51 41 64 120 53 107 106 55 95 50 40 116 | 90 | 6.01E+06 | 3.00E+07 |
| | | | | | | | A | 3 | | 87 | 3.19E+04 | 1.59E+05 |
| | | | | | | | C | 1 | 3: 137 67 104 | 82 | 4.17E+05 | 2.09E+06 |
| | | | | | | | C | 2 | 18: 91 79 43 107 119 51 103 117 66 55 88 74 135 129 42 123 101 87 | 95 | 1.25E+08 | 6.26E+08 |
| | | | | | | | C | 3 | 16: 93 91 121 105 41 43 63 122 52 81 76 102 38 42 127 120 | 95 | 8.67E+07 | 4.33E+08 |
| +Ethyl benzene | 100-41-4 | 11.84 | | | | 2.88E+00 | C | 1 | 14: 91 136 105 79 78 53 76 80 137 55 81 75 68 127 | 67 | 9.64E+07 | 3.34E+07 |
| | | | | | | | C | 2 | 18: 91 79 43 107 119 51 103 117 66 55 88 74 135 129 42 123 101 87 | 71 | 7.80E+07 | 2.70E+07 |
| +Acetic acid | 64-19-7 | 12.23 | Sour | Acidic | | 1.45E-01 | A | 6 | 8: 43 60 45 42 41 44 40 59 | 100 | 2.76E+07 | 1.91E+08 |
| | | | | | | | A | 7 | 3: 43 44 207 | 100 | 7.66E+05 | 5.30E+06 |
| | | | | | | | B | 1 | 3: 45 43 60 | 90 | 1.91E+04 | 1.32E+05 |
| | | | | | | | B | 3 | 4: 43 45 60 42 | 98 | 1.62E+07 | 1.12E+08 |
| N-methyl-N-nitroso urea | 684-93-5 | 12.26 | | | | | A | 7 | 4: 43 60 42 44 | 70 | 1.71E+05 | |
| (z)-rose oxide | 16409-43-1 | 12.28 | | Green, Red rose, Spic, Fresh geranium | | | C | 2 | 14: 69 139 96 97 83 70 95 55 140 207 154 67 71 66 | 66 | 2.19E+05 | |
| | | | | | | | C | 3 | 4: 139 140 96 84 | 68 | 2.25E+05 | |
| Phenetole | 103-73-1 | 12.52 | | | | | A | 2 | 7: 122 107 68 51 50 94 117 | 70 | 1.18E+05 | |
| 2-hydroxyacetophenone | 118-93-4 | 12.53 | | Phenolic | | | A | 1 | | 86 | 7.20E+04 | |
| | | | | | | | A | 2 | 5: 136 107 137 93 122 | 85 | 7.49E+04 | |
| | | | | | | | A | 3 | | 80 | 1.89E+04 | |
| | | | | | | | A | 4 | 2: 121 136 | 75 | 5.91E+04 | |
| | | | | | | | A | 6 | 2: 121 136 | 74 | 9.22E+03 | |
| | | | | | | | A | 7 | 7: 43 136 121 81 92 53 91 | 67 | 2.20E+04 | |
| | | | | | | | C | 1 | 13: 121 93 41 122 136 67 55 108 106 92 104 53 94 | 78 | 8.16E+05 | |
| 1-methyl-2-propyl benzene | 1074-17-5 | 12.63 | | | | | C | 1 | 2: 134 105 | 73 | 1.91E+04 | |
| 2-phenyl propionaldehyde | 93-53-8 | 12.63 | | Fresh, Sharp, Green, Hyacinth, Leaf, Lilac | | | C | 1 | 2: 134 105 | 66 | 1.91E+04 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| +o-xylene | 95-47-6 | 13.07 | Geranium | Geranium | | 8.51E-01 | A 2 | 5: 77 134 106 119 52 | 73 | 9.60E+04 | 1.13E+05 |
| +p-xylene | 106-42-3 | 13.08 | | | | 4.90E-01 | A 2 | | 81 | 4.01E+04 | 8.19E+04 |
| 4-methylphenethylamine | 3261-62-9 | 13.08 | | | | | A 2 | | 69 | 4.01E+04 | |
| 2,3-dimethyl-cyclohexanol | 1502-24-5 | 13.19 | | | | | B 3 | | 68 | 1.94E+04 | |
| Fenchone | 1195-79-5 | 13.47 | | | | 9.33E-02 | A 6 | 6: 81 69 152 53 80 67 | 95 | 2.96E+05 | 3.17E+06 |
| | | | | | | | B 3 | 4: 41 39 109 77 | 91 | 1.41E+05 | 1.51E+06 |
| | | | | | | | C 1 | 19: 81 41 53 55 79 39 82 91 80 137 67 70 42 105 123 85 38 153 77 | 98 | 1.36E+06 | 1.46E+07 |
| | | | | | | | C 2 | 13: 153 152 80 55 77 78 91 42 71 66 52 40 123 | 99 | 1.43E+06 | 1.53E+07 |
| | | | | | | | C 3 | 20: 81 69 152 67 80 41 66 68 82 39 109 72 91 52 55 137 97 42 153 40 | 98 | 1.50E+06 | 1.60E+07 |
| Linalool oxide | 5989-33-3 | 13.67 | Flower, Wood | Earthy, Floral, Sweet, Woody | | | A 5 | 11: 207 266 83 70 79 55 112 67 85 53 97 | 65 | 1.91E+05 | |
| | | | | | | | A 6 | | 83 | 8.06E+04 | |
| | | | | | | | A 7 | 19: 93 55 111 70 92 71 94 43 67 81 83 68 91 69 84 74 57 137 82 | 80 | 3.23E+05 | |
| | | | | | | | B 3 | 5: 111 81 71 95 93 | 82 | 8.43E+04 | |
| 1,3-diethylbenzene | 141-93-5 | 13.81 | | | | | A 2 | 14: 105 93 94 137 81 53 65 119 77 120 82 135 51 39 | 68 | 3.70E+05 | |
| +2-ethylhexanol | 104-76-7 | 13.81 | Rose, Green | Citrus | | 2.45E-01 | A 5 | | 87 | 1.48E+05 | 6.05E+05 |
| | | | | | | | A 6 | | 85 | 9.88E+04 | 4.03E+05 |
| | | | | | | | A 7 | 7: 84 41 54 112 43 56 70 | 91 | 3.39E+05 | 1.38E+06 |
| | | | | | | | B 1 | 3: 82 56 71 | 95 | 5.55E+05 | 2.26E+06 |
| | | | | | | | B 3 | 4: 83 71 57 41 | 92 | 1.23E+05 | 5.01E+05 |
| | | | | | | | B 4 | | 66 | 2.31E+04 | 9.39E+04 |
| +Methyl vinyl ketone | 78-94-4 | 13.82 | | Sweet | | | A 6 | 4: 70 55 39 82 | 67 | 1.34E+04 | |
| Tranylcypromine | 155-09-9 | 13.91 | | | | | A 2 | 7: 132 117 102 118 91 115 99 | 69 | 1.31E+06 | |
| +Propanoic acid | 79-09-4 | 13.91 | Pungent, Rancid, Soy | Pungent, Acidic, Cheesy, Vinegar | | 3.55E-02 | A 6 | 3: 73 74 60 | 65 | 1.76E+05 | 4.97E+06 |
| 5-methylindane | 874-35-1 | 13.91 | | | | | A 1 | | 88 | 2.94E+05 | |
| | | | | | | | A 2 | 5: 132 116 39 131 57 | 90 | 1.91E+06 | |
| | | | | | | | B 1 | 5: 91 132 115 116 64 | 78 | 4.44E+04 | |
| | | | | | | | C 1 | 5: 132 115 131 65 91 | 75 | 1.10E+05 | |
| 2-ethenyl-1,3-dimethylbenzene | 2039-90-9 | 13.91 | | | | | A 1 | | 92 | 2.94E+05 | |
| | | | | | | | A 2 | 7: 132 117 102 118 91 115 99 | 94 | 1.31E+06 | |
| | | | | | | | B 1 | 5: 91 132 115 116 64 | 82 | 4.44E+04 | |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | C | 1 | 5: 132 115 131 65 91 | 82 | 1.10E+05 | | |
| Propylene glycol | 57-55-6 | 13.98 | | | | | A | 1 | 3: 45 43 41 | 72 | 1.50E+05 | | |
| | | | | | | | A | 2 | | 68 | 1.20E+05 | | |
| | | | | | | | A | 3 | | 67 | 7.50E+04 | | |
| | | | | | | | A | 7 | 6: 45 46 39 42 41 47 | 71 | 3.01E+05 | | |
| | | | | | | | B | 3 | | 72 | 4.64E+04 | | |
| | | | | | | | B | 4 | 2: 42 43 | 67 | 7.41E+04 | | |
| | | | | | | | C | 1 | 4: 44 90 38 37 | 69 | 6.13E+05 | | |
| | | | | | | | C | 2 | 17: 45 43 47 44 55 90 76 53 73 115 71 41 60 56 51 54 40 | 69 | 6.30E+06 | | |
| Indane | 496-11-7 | 13.98 | | | | | A | 1 | 3: 118 115 117 | 68 | 1.10E+05 | | |
| 2-chloroacetophenone | 532-27-4 | 14.09 | | Apple blossom | | 2.57E-02 | A | 5 | 6: 105 51 77 52 78 63 | 78 | 6.57E+05 | 2.56E+07 | |
| | | | | | | | A | 7 | | 76 | 1.00E+06 | 3.89E+07 | |
| | | | | | | | B | 1 | 3: 77 78 50 | 76 | 3.34E+05 | 1.30E+07 | |
| | | | | | | | B | 2 | | 71 | 2.25E+04 | 8.76E+05 | |
| | | | | | | | B | 3 | 3: 105 106 107 | 71 | 1.30E+05 | 5.06E+06 | |
| | | | | | | | B | 4 | 6: 105 77 106 78 51 107 | 74 | 1.07E+05 | 4.17E+06 | |
| +Benzaldehyde | 100-52-7 | 14.09 | Almond, Burnt sugar | Fruity | 3.00E-03 | 4.17E-02 | A | 5 | | 98 | 8.98E+05 | 2.15E+07 | |
| | | | | | | | A | 7 | | 98 | 1.00E+06 | 2.40E+07 | |
| | | | | | | | B | 1 | 3: 77 78 50 | 97 | 5.17E+05 | 1.24E+07 | |
| | | | | | | | B | 2 | 3: 106 105 77 | 83 | 4.03E+04 | 9.66E+05 | |
| | | | | | | | B | 3 | 3: 105 106 107 | 89 | 1.30E+05 | 3.12E+06 | |
| | | | | | | | B | 4 | 6: 105 77 106 78 51 107 | 93 | 1.07E+05 | 2.57E+06 | |
| +Ethyl lactate | 97-64-3 | 14.10 | Fruit | Sharp, Tart, Fruity, Buttery, Butterscotch | | 1.62E+00 | A | 6 | 4: 45 46 75 47 | 87 | 2.84E+05 | 1.75E+05 | |
| | | | | | | | B | 3 | 4: 43 207 42 46 | 84 | 5.88E+04 | 3.63E+04 | |
| | | | | | | | C | 1 | 10: 72 90 56 73 37 60 74 48 71 76 | 80 | 9.99E+06 | 6.16E+06 | |
| | | | | | | | C | 2 | 12: 72 39 56 73 41 71 60 53 49 52 48 40 | 80 | 6.67E+06 | 4.11E+06 | |
| | | | | | | | C | 3 | 13: 55 42 58 41 60 56 38 73 91 54 89 74 132 | 79 | 1.64E+07 | 1.01E+07 | |
| Isobutyrophenone | 611-70-1 | 14.10 | | Green | | | B | 1 | 3: 77 78 50 | 69 | 3.34E+05 | | |
| Dimethyl octanol | 106-21-8 | 14.11 | | Waxy, Soapy, Aldehydic, Leathery, Musty, Citrus, Green | | | C | 1 | 8: 54 70 111 67 97 56 53 110 | 82 | 7.44E+05 | | |
| | | | | | | | C | 2 | 6: 70 41 57 79 84 97 | 66 | 2.13E+05 | | |
| 1-Dodecanol | 112-53-8 | 14.11 | Fat, Wax | Earthy, Soapy, Waxy, Fatty, Honey, Coconut | | 1.26E-02 | C | 1 | | 93 | 2.64E+05 | 2.10E+07 | |
| | | | | | | | C | 2 | 6: 70 41 57 79 84 97 | 76 | 1.91E+05 | 1.52E+07 | |
| +1-Decanol | 112-30-1 | 14.11 | Fat | Fatty, Waxy, Floral, Orange, Sweet, Clean, Watery | | 1.82E-02 | C | 1 | | 75 | 6.38E+04 | 3.51E+06 | |
| | | | | | | | C | 2 | 6: 70 41 57 79 84 97 | 86 | 7.90E+04 | 4.34E+06 | |
| 1-Nonanol | 143-08-8 | 14.12 | Fat, Green | Fresh, Clean, Fatty, Floral, Rose, Orange, Dusty, Wet, Oily | 5.00E+01 | 2.24E-03 | C | 1 | | 76 | 3.03E+04 | 1.35E+07 | |
| | | | | | | | C | 2 | | 71 | 7.50E+04 | 3.35E+07 | |
| +Undecane | 1120-21-4 | 14.13 | Alkane | | | 1.17E+00 | C | 1 | 7: 85 99 71 110 98 68 39 | 68 | 2.43E+05 | 2.07E+05 | |
| +Nonane | 111-84-2 | 14.13 | Alkane | Gasoline | | 1.26E+00 | C | 1 | 7: 85 99 71 110 98 68 39 | 77 | 2.17E+05 | 1.72E+05 | |
| +Dodecane | 112-40-3 | 14.13 | Alkane | Alkane | | 2.04E+00 | C | 1 | 7: 85 99 71 110 98 68 39 | 77 | 2.17E+05 | 1.06E+05 | |
| +Tridecane | 629-50-5 | 14.14 | Alkane | Alkane | | 2.14E+00 | A | 4 | | 68 | 1.59E+04 | 7.44E+03 | |
| | | | | | | | C | 1 | 7: 85 99 71 110 98 68 39 | 68 | 2.43E+05 | 1.14E+05 | |
| 2,2-dimethylbutane | 75-83-2 | 14.15 | | | | | A | 4 | | 82 | 1.59E+04 | | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| 3-isopropyl phenol | 618-45-1 | 14.19 | | | | | A 1 | 7: 121 77 55 136 67 120 79 | 77 | 3.82E+05 | |
| | | | | | | | A 2 | 7: 122 105 103 93 121 51 57 | 82 | 7.66E+05 | |
| | | | | | | | C 3 | 20: 121 136 122 103 78 77 105 80 41 106 107 39 43 94 120 115 52 135 67 54 | 81 | 1.39E+06 | |
| 3-(1-methylethyl)-phenol methylcarbamate | 64-00-6 | 14.20 | | | | | A 1 | 8: 121 105 136 106 91 77 79 265 | 76 | 7.43E+05 | |
| | | | | | | | A 2 | 13: 105 121 51 79 136 77 78 53 103 106 39 120 43 | 74 | 7.94E+05 | |
| | | | | | | | A 4 | 2: 136 121 | 65 | 6.07E+04 | |
| | | | | | | | A 7 | 13: 121 78 136 68 103 117 80 52 51 77 106 107 81 | 66 | 3.18E+05 | |
| | | | | | | | B 1 | 3: 136 91 107 | 74 | 4.44E+04 | |
| Acetone cyanohydrin | 75-86-5 | 14.27 | | | | | B 1 | 4: 70 83 112 69 | 69 | 3.20E+04 | |
| | | | | | | | B 3 | 1: 70 | 70 | 8.97E+03 | |
| 1,4-diethylbenzene | 105-05-5 | 14.47 | | | | | A 1 | | 87 | 9.45E+04 | |
| | | | | | | | A 2 | 9: 120 55 115 93 135 52 108 103 133 | 85 | 5.16E+05 | |
| o-cymene | 527-84-4 | 14.47 | | | | 7.94E-04 | A 2 | 18: 91 52 119 106 134 93 55 105 92 115 103 117 79 65 120 63 133 116 | 88 | 4.83E+05 | 6.08E+08 |
| 1,2-diethylbenzene | 135-01-3 | 14.47 | | | | | A 1 | | 85 | 9.45E+04 | |
| | | | | | | | A 2 | 18: 91 52 119 106 134 93 55 105 92 115 103 117 79 65 120 63 133 116 | 84 | 8.70E+05 | |
| p-tert-butylphenol | 98-54-4 | 14.48 | | Leathery | | | A 7 | | 68 | 1.54E+04 | |
| tert-butyl-benzene | 98-06-6 | 14.48 | | | | | A 1 | | 89 | 6.59E+04 | |
| | | | | | | | A 2 | | 86 | 3.38E+05 | |
| | | | | | | | B 1 | 3: 91 120 134 | 76 | 6.51E+04 | |
| o-methylacetophenone | 577-16-2 | 14.48 | | Floral | | 6.61E-03 | A 1 | | 89 | 6.59E+04 | 9.98E+06 |
| 2-methoxyethanol | 109-86-4 | 14.62 | | | | | A 6 | 2: 43 55 | 65 | 1.39E+05 | |
| +2-Butanol | 78-92-2 | 14.66 | Wine | Sweet, Apricot | 1.70E+00 | | C 3 | 13: 45 43 47 44 55 46 42 54 60 58 76 38 86 | 69 | 2.96E+07 | 1.74E+07 |
| Maltol | 118-71-8 | 14.67 | Caramel | Sweet, Caramel, Cotton candy, Jam, Fruity, Baked bread | | | A 4 | 3: 98 126 71 | 66 | 5.65E+03 | |
| Linalyl acetate | 115-95-7 | 15.09 | Sweet, Fruit | Herbal | | 8.91E-03 | A 4 | | 77 | 2.39E+04 | 2.68E+06 |
| | | | | | | | A 6 | 1: 83 | 74 | 4.56E+04 | 5.12E+06 |
| Geranyl butyrate | 106-29-6 | 15.09 | Fruit, Rose, Apple | Sweet, Fruity, Rose, Waxy Raspberry, Tropical | | | A 4 | | 68 | 1.45E+04 | |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Isobornyl thiocyanoacetate | 115-31-1 | 15.11 | | | | | A | 1 | 20: 92 105 80 51 117 66 137 122 62 81 64 54 104 63 76 108 103 134 38 43 | 66 | 3.33E+07 | |
| | | | | | | | A | 2 | 20: 68 93 67 94 136 59 107 91 53 39 81 95 105 55 65 66 119 137 52 96 | 66 | 2.21E+07 | |
| | | | | | | | A | 3 | 9: 81 137 95 106 122 43 42 108 103 | 67 | 9.69E+05 | |
| | | | | | | | A | 6 | 20: 55 65 77 93 39 41 136 80 43 81 121 86 139 97 53 94 91 52 105 84 | 70 | 7.74E+05 | |
| | | | | | | | A | 7 | 20: 93 69 80 71 72 122 41 92 55 107 136 65 94 53 81 105 45 56 96 82 | 68 | 3.68E+05 | |
| | | | | | | | B | 3 | 10: 72 139 94 65 70 57 67 92 52 54 | 73 | 1.18E+06 | |
| Linalyl propionate | 144-39-8 | 15.11 | | Fresh, Bergamot, Lily, Woody, Rose, Rum | | | B | 3 | 17: 121 93 41 82 80 94 70 67 105 68 84 51 56 53 72 137 126 | 67 | 6.45E+05 | |
| Linalool | 78-70-6 | 15.12 | Flower, Lavender | Floral | 6.00E-03 | 5.37E-02 | A | 1 | 3: 69 71 43 | 85 | 9.62E+04 | 1.79E+06 |
| | | | | | | | A | 2 | | 89 | 1.00E+05 | 1.87E+06 |
| | | | | | | | A | 5 | | 91 | 3.31E+05 | 6.16E+06 |
| | | | | | | | A | 6 | | 96 | 8.95E+05 | 1.67E+07 |
| | | | | | | | A | 7 | 20: 93 69 80 71 72 122 41 92 55 107 136 65 94 53 81 105 45 56 96 82 | 95 | 3.68E+05 | 6.85E+06 |
| | | | | | | | B | 3 | 10: 72 139 94 65 70 57 67 92 52 54 | 97 | 1.18E+06 | 2.19E+07 |
| Ethyl cyclohexane | 1678-91-7 | 15.17 | | | | | C | 1 | 6: 55 83 84 67 169 139 | 71 | 3.95E+05 | |
| 1-methyl-1H-imidazole | 616-47-7 | 15.20 | | | | | C | 3 | 3: 82 69 168 | 67 | 1.48E+05 | |
| cis-2-pinanol | 4948-29-2 | 15.41 | | Herbal | | | A | 5 | | 72 | 1.30E+04 | |
| | | | | | | | A | 6 | 20: 81 99 79 97 121 67 77 43 68 83 95 71 86 72 94 108 107 69 57 105 | 95 | 8.31E+05 | |
| | | | | | | | A | 7 | | 79 | 1.66E+04 | |
| | | | | | | | B | 3 | 4: 94 93 58 72 | 92 | 5.15E+05 | |
| trans-carveol | 1197-07-5 | 15.51 | Caraway, Solvent | Caraway, Solvent, Spearmint | | | C | 1 | 19: 109 106 43 137 67 119 69 39 134 65 79 94 110 41 82 105 117 115 121 | 74 | 1.36E+06 | |
| β-cyclocitral | 432-25-7 | 15.52 | Mint | Tropical, Saffron, Herbal, clean, Rose, Sweet, Tobacco, Damascenone, Fruity | | | C | 1 | | 87 | 1.15E+06 | |
| | | | | | | | C | 2 | 20: 95 134 119 138 77 106 121 152 137 67 107 41 79 65 91 78 117 120 110 55 | 87 | 9.49E+05 | |
| | | | | | | | C | 3 | | 86 | 8.54E+05 | |
| tetrahydro-2-methyl-2-furanol | 7326-46-7 | 15.57 | | | | | C | 1 | 7: 71 43 72 78 39 41 82 | 76 | 2.27E+05 | |
| Fenchyl alcohol | 1632-73-1 | 15.72 | Camphor | Camphor, Borneol, Pine, Woody, Dry, Sweet, Lemon | | | A | 1 | | 76 | 4.88E+04 | |
| | | | | | | | A | 2 | 2: 80 81 | 67 | 7.96E+04 | |
| | | | | | | | A | 4 | 12: 81 107 43 41 83 72 71 69 121 53 96 67 | 92 | 2.37E+05 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | A 5 | | 78 | 5.65E+04 | |
| | | | | | | | A 6 | 20: 81 107 72 84 41 69 55 111 92 71 93 123 121 83 122 57 43 95 79 77 | 98 | 1.84E+06 | |
| | | | | | | | A 7 | | 72 | 1.94E+04 | |
| | | | | | | | B 3 | | 99 | 2.28E+06 | |
| | | | | | | | B 4 | | 83 | 2.67E+04 | |
| +1-methyl-1H-pyrrole | 96-54-8 | 15.72 | | Smoky, Woody, Herbal | | | A 2 | 3: 81 80 69 | 69 | 2.65E+04 | |
| (-)-terpinen-4-ol | 20126-76-5 | 16.20 | | | | | A 6 | | 70 | 1.45E+04 | |
| 1-terpinen-4-ol | 562-74-3 | 16.20 | Turpentine, Nutmeg, Must | Woody, Ceding, mentholic, Citrus, Terpiny, Spicy | | | A 6 | | 74 | 1.45E+04 | |
| Thujone | 546-80-5 | 16.22 | | Cedar leaf | | 1.29E-01 | C 3 | | 72 | 8.49E+03 | 6.59E+04 |
| 2-Methyl-4-(1-methylethyl)-2-cyclohexenone | 41469-46-9 | 16.33 | | | | | C 1 | 4: 109 81 95 65 | 77 | 5.92E+04 | |
| | | | | | | | C 2 | | 80 | 3.89E+04 | |
| | | | | | | | C 3 | | 82 | 3.07E+04 | |
| Camphor | 76-22-2 | 16.33 | Camphor | Camphorous | 5.13E-02 | | C 2 | | 69 | 3.89E+04 | 7.58E+05 |
| | | | | | | | C 3 | | 69 | 6.43E+04 | 1.25E+06 |
| Pulegone | 89-82-7 | 16.34 | | Peppermint, Camphor, Fresh, Herbal, Buchu | 3.39E-03 | | C 1 | 4: 152 67 109 81 | 71 | 6.25E+04 | 1.85E+07 |
| | | | | | | | C 2 | | 76 | 3.90E+04 | 1.15E+07 |
| 2,2,4-trimethylpentane | 540-84-1 | 16.57 | | | | | A 4 | 6: 57 99 56 140 183 86 | 77 | 3.93E+05 | |
| γ-hexalactone | 695-06-7 | 17.20 | Coumarin, Sweet | Tonka | | | B 3 | 1: 85 | 78 | 3.62E+04 | |
| Borneol | 507-70-0 | 17.60 | Camphor | Pine, Woody, Camphor | | 2.09E-03 | A 6 | 6: 139 77 110 92 94 91 | 96 | 8.39E+05 | 4.01E+08 |
| | | | | | | | B 3 | | 98 | 7.46E+05 | 3.57E+08 |
| Isobornyl acetate | 125-12-2 | 17.60 | | Balsamic | | | A 6 | 6: 139 77 110 92 94 91 | 77 | 8.39E+05 | |
| | | | | | | | B 3 | | 79 | 7.46E+05 | |
| +Laevo-borneol | 464-45-9 | 17.60 | | Pine, Woody, Camphor | | | A 6 | | 95 | 4.15E+05 | |
| | | | | | | | B 3 | 19: 95 69 121 79 105 140 55 67 92 68 43 110 70 91 111 108 42 57 113 | 98 | 6.63E+05 | |
| +α-terpineol | 98-55-5 | 17.73 | Oil, Anise, Mint | Floral | | 3.72E-02 | A 1 | | 84 | 6.15E+04 | 1.66E+06 |
| | | | | | | | A 2 | | 80 | 3.85E+04 | 1.04E+06 |
| | | | | | | | A 4 | | 83 | 3.03E+04 | 8.17E+05 |
| | | | | | | | A 5 | | 80 | 3.75E+04 | 1.01E+06 |
| | | | | | | | A 6 | | 94 | 7.72E+05 | 2.08E+07 |
| | | | | | | | A 7 | | 80 | 2.54E+04 | 6.84E+05 |
| | | | | | | | B 3 | | 95 | 5.95E+05 | 1.60E+07 |
| α-terpinyl acetate | 80-26-2 | 17.73 | Wax | Herbal, Bergamot, Lavender, Lime, Citrus | | | A 3 | | 67 | 1.20E+06 | |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | 20: 121 136 68 93 41 77 94 51 52 54 78 43 95 80 69 65 42 119 63 103 | | | |
| | | | | | | | A | 4 | 2: 136 121 | 68 | 4.41E+04 | |
| | | | | | | | A | 5 | 7: 136 80 93 95 41 43 81 | 77 | 6.84E+04 | |
| | | | | | | | B | 1 | 6: 136 92 63 119 80 66 | 69 | 4.56E+05 | |
| Terpinyl butyrate | 2153-28-8 | 17.74 | | Sour, Rosemary, Fruity, Balsam | | | A | 7 | 4: 136 94 68 93 | 68 | 1.57E+04 | |
| 2-ethyl-3,5-dimethylpyridine | 1123-96-2 | 17.91 | | | | | A | 1 | 4: 68 82 134 133 | 66 | 1.28E+05 | |
| | | | | | | | B | 1 | 2: 134 135 | 74 | 2.22E+04 | |
| +p-cresyl acetate | 140-39-6 | 18.14 | | Narcissus, Phenolic, Animal | | 7.76E-04 | A | 7 | 1: 108 | 65 | 9.23E+03 | 1.19E+07 |
| m-tert-butylphenol | 585-34-2 | 18.15 | | | | | A | 7 | 5: 135 80 108 79 91 | 68 | 6.76E+04 | |
| Verbenone | 80-57-9 | 18.16 | | Camphor, Menthol, Celery | | | A | 5 | | 75 | 9.46E+03 | |
| | | | | | | | A | 7 | | 82 | 2.55E+04 | |
| 1-Tetradecanol | 112-72-1 | 18.32 | Coconut | Fruity, Waxy, Orris, Coconut | | | C | 1 | | 80 | 8.39E+04 | |
| 3-methylhexane | 589-34-4 | 18.32 | | | | | A | 4 | | 72 | 1.66E+04 | |
| | | | | | | | C | 1 | 10: 57 98 82 71 68 43 67 56 70 127 | 75 | 3.62E+04 | |
| +1-Tridecene | 2437-56-1 | 18.33 | | | | | C | 2 | | 80 | 4.71E+04 | |
| 1-undecanol | 112-42-5 | 18.34 | Mandarin | Waxy | | 6.76E-02 | C | 1 | | 74 | 6.38E+04 | 9.44E+05 |
| | | | | | | | C | 2 | 6: 70 41 57 79 84 97 | 82 | 7.90E+04 | 1.17E+06 |
| Octyl formate | 112-32-3 | 18.34 | | Fruity, rose, Orange, Waxy, Cucumber | | | C | 2 | | 67 | 1.25E+04 | |
| α-copaene | 3856-25-5 | 18.39 | Wood, Spice | Wood | | | A | 1 | | 71 | 3.09E+04 | |
| α-cubebene | 17699-14-8 | 18.50 | Herb, Wax | Herb | | | A | 1 | | 73 | 1.57E+04 | |
| (+)-sativene | 3650-28-0 | 19.40 | | | | | A | 1 | | 78 | 5.89E+04 | |
| | | | | | | | A | 5 | 20: 93 69 120 148 106 68 55 92 189 95 149 175 135 162 190 136 83 91 53 103 | 75 | 2.37E+07 | |
| Nitro cyclohexane | 1122-60-7 | 19.46 | | | | | C | 2 | 2: 83 55 | 67 | 2.04E+04 | |
| β-caryophyllene | 87-44-5 | 19.66 | Wood, Spice | Spice | 6.40E-02 | | A | 1 | 20: 133 69 79 161 105 120 136 81 77 106 119 162 121 39 109 94 175 92 82 123 | 100 | 6.01E+06 | 9.40E+07 |
| | | | | | | | A | 2 | 17: 189 106 92 41 148 190 81 80 93 78 95 121 77 161 94 91 120 | 99 | 2.39E+06 | 3.73E+07 |
| | | | | | | | A | 3 | | 77 | 3.32E+04 | 5.19E+05 |
| | | | | | | | A | 4 | | 80 | 3.35E+04 | 5.24E+05 |
| | | | | | | | A | 6 | 20: 41 133 93 69 107 147 148 120 66 55 121 80 42 176 119 95 53 43 145 136 | 99 | 4.19E+06 | 6.55E+07 |
| | | | | | | | A | 7 | 10: 134 124 96 66 112 190 122 110 177 138 | 89 | 1.05E+06 | 1.64E+07 |
| | | | | | | | B | 3 | | 99 | 3.11E+06 | 4.86E+07 |
| | | | | | | | B | 4 | 14: 94 69 120 135 107 163 80 78 134 176 161 109 63 82 | 99 | 1.37E+06 | 2.14E+07 |
| +Benzyl alcohol | 100-51-6 | 19.74 | | Floral | | | A | 5 | | 96 | 2.16E+07 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | Sweet, Flower | | | | | 11: 78 53 109 149 39 129 66 65 123 134 202 | | | |
| | | | | | | | A 7 | | 96 | 5.83E+06 | |
| | | | | | | | B 1 | 13: 108 79 78 51 91 109 90 39 86 62 92 74 37 | 100 | 3.59E+06 | |
| | | | | | | | B 2 | 11: 108 107 77 80 76 106 49 91 105 53 41 | 99 | 8.86E+05 | |
| Tyramine | 51-67-2 | 19.74 | | Meaty | | | A 5 | 6: 51 85 38 62 90 75 | 70 | 9.20E+06 | |
| | | | | | | | A 7 | 5: 90 62 109 37 61 | 70 | 3.71E+06 | |
| | | | | | | | B 1 | 1: 53 | 70 | 4.00E+06 | |
| | | | | | | | B 2 | | 72 | 6.78E+05 | |
| α-guaiene | 3691-12-1 | 19.85 | Wood, Balsamic | Wood | | | A 1 | | 80 | 2.88E+05 | |
| | | | | | | | A 2 | 13: 106 189 133 123 162 93 204 95 120 108 94 205 105 | 91 | 5.50E+05 | |
| | | | | | | | A 5 | | 72 | 3.36E+05 | |
| | | | | | | | A 6 | 16: 107 147 108 93 94 106 91 67 105 189 121 81 51 69 119 53 | 94 | 4.50E+05 | |
| | | | | | | | B 3 | | 94 | 3.21E+05 | |
| | | | | | | | B 4 | 13: 107 204 135 79 133 119 105 147 81 148 73 65 95 | 88 | 9.51E+04 | |
| +Dimethylsulfone | 67-71-0 | 20.12 | Sulfur, Burnt | Sulfurous, Burnt | | | A 7 | 2: 94 79 | 80 | 1.93E+04 | |
| δ-cadinene | 483-76-1 | 20.20 | Thyme, Medicine, Wood | Herbal | | | A 1 | 20: 161 204 190 122 39 202 107 55 65 134 41 159 69 81 149 67 109 53 78 117 | 66 | 4.74E+05 | |
| | | | | | | | A 5 | | 74 | 1.51E+04 | |
| 2,6-pyridinediamine | 141-86-6 | 20.49 | | | | | A 5 | 1: 109 | 71 | 4.03E+03 | |
| α-humulene | 6753-98-6 | 20.53 | Wood | Wood | 1.20E-01 | | A 1 | 19: 147 93 121 67 92 105 81 109 39 80 91 119 77 57 41 43 135 103 120 | 97 | 1.68E+06 | 1.40E+07 |
| | | | | | | | A 2 | | 91 | 1.76E+05 | 1.47E+06 |
| | | | | | | | A 5 | 20: 93 80 121 107 79 92 147 91 70 41 105 109 205 94 122 189 106 82 204 95 | 98 | 3.99E+06 | 3.32E+07 |
| | | | | | | | A 6 | 20: 107 105 80 67 190 109 94 95 106 147 92 41 68 83 189 108 65 52 42 205 | 96 | 1.55E+06 | 1.29E+07 |
| | | | | | | | A 7 | 19: 92 79 94 105 95 91 148 63 65 204 120 41 123 82 135 78 66 39 128 | 97 | 1.42E+06 | 1.19E+07 |
| | | | | | | | B 3 | | 97 | 1.47E+06 | 1.23E+07 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | 20: 121 93 107 148 91 106 123 66 39 122 42 175 204 95 205 40 73 120 133 129 | | | |
| | | | | | B | 4 | | 93 | 2.10E+05 | 1.75E+06 |
| β-selinene | 17066-67-0 | 21.25 | Herb | Herb | A | 1 | | 93 | 3.35E+05 | |
| | | | | | A | 2 | | 86 | 6.14E+04 | |
| | | | | | A | 6 | 14: 161 135 108 119 163 81 94 109 105 78 41 93 82 149 | 92 | 3.26E+05 | |
| | | | | | A | 7 | 15: 161 162 134 94 190 43 91 81 204 121 123 95 92 131 175 | 72 | 1.56E+05 | |
| | | | | | B | 3 | | 92 | 1.84E+05 | |
| | | | | | B | 4 | | 85 | 4.15E+04 | |
| Longifolene | 475-20-7 | 21.27 | | Wood | A | 1 | 20: 133 69 79 161 105 120 136 81 77 106 119 162 121 39 109 94 175 92 82 123 | 89 | 6.01E+06 | |
| | | | | | A | 2 | 17: 189 106 92 41 148 190 81 80 93 78 95 121 77 161 94 91 120 | 89 | 2.39E+06 | |
| | | | | | A | 5 | 17: 147 205 68 133 161 148 189 105 175 93 107 135 109 123 53 69 134 | 91 | 6.66E+05 | |
| | | | | | A | 6 | 20: 41 133 93 69 107 147 148 120 66 55 121 80 42 176 119 95 53 43 145 136 | 90 | 4.19E+06 | |
| | | | | | A | 7 | | 87 | 1.16E+05 | |
| | | | | | B | 3 | | 90 | 3.11E+06 | |
| | | | | | B | 4 | 14: 94 69 120 135 107 163 80 78 134 176 161 109 63 82 | 88 | 1.37E+06 | |
| Alloaromadendrene | 25246-27-9 | 21.41 | Wood | Wood | B | 3 | 20: 55 135 96 121 79 93 105 161 148 106 204 120 91 80 127 94 77 122 205 104 | 71 | 1.21E+06 | |
| α-bulnescene | 3691-11-0 | 21.41 | | | A | 2 | | 89 | 1.96E+05 | |
| | | | | | A | 6 | 6: 105 136 69 43 42 109 | 94 | 1.08E+06 | |
| | | | | | B | 3 | 20: 55 135 96 121 79 93 105 161 148 106 204 120 91 80 127 94 77 122 205 104 | 96 | 1.07E+06 | |
| | | | | | B | 4 | | 92 | 4.36E+05 | |
| α-gurjunene | 489-40-7 | 21.43 | Wood, Balsamic | Wood | A | 1 | | 85 | 2.68E+05 | |
| | | | | | A | 2 | | 73 | 1.22E+04 | |
| | | | | | A | 5 | | 88 | 2.34E+05 | |
| | | | | | A | 6 | 3: 145 147 109 | 82 | 2.85E+05 | |
| | | | | | A | 7 | 10: 147 131 107 133 109 204 119 79 95 105 | 81 | 1.34E+05 | |
| | | | | | B | 3 | | 81 | 5.86E+04 | |
| | | | | | B | 4 | 9: 106 119 51 149 162 161 123 81 117 | 81 | 3.10E+04 | |
| Aromadendrene | 489-39-4 | 21.48 | Wood | Wood | A | 1 | | 65 | 6.94E+04 | |
| | | | | | A | 2 | | 73 | 1.48E+05 | |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | | 8: 82 93 147 121 162 67 65 133 | | | |
| | | | | | | | A 5 | | 71 | 8.73E+04 | |
| | | | | | | | A 6 | | 81 | 5.80E+04 | |
| | | | | | | | A 7 | | 91 | 1.16E+05 | |
| | | | | | | | B 3 | 19: 161 147 105 129 133 204 106 109 95 77 145 82 92 91 108 190 120 41 117 | 87 | 9.66E+04 | |
| 2,4,6-trimethylpyridine | 108-75-8 | 21.66 | | | | | A 2 | 4: 121 67 39 106 | 65 | 1.24E+05 | |
| | | | | | | | A 6 | | 72 | 1.01E+04 | |
| +Phenol | 108-95-2 | 21.68 | Phenolic | Phenolic | | 1.10E-01 | B 1 | | 78 | 1.73E+04 | 1.58E+05 |
| Dyclocaine | 586-60-7 | 21.69 | | | | | A 1 | | 70 | 6.94E+04 | |
| (-)-Aristolene | 6831-16-9 | 21.74 | | | | | A 1 | 15: 108 119 79 135 204 189 133 187 106 148 67 55 42 43 78 | 74 | 4.92E+05 | |
| | | | | | | | A 6 | | 81 | 5.14E+04 | |
| | | | | | | | B 3 | 11: 161 204 79 148 107 53 109 81 202 108 105 | 83 | 8.64E+04 | |
| +2-ethylphenol | 90-00-6 | 21.91 | | Phenolic | | | A 5 | 2: 122 107 | 71 | 3.34E+03 | |
| (+)-calarene | 17334-55-3 | 22.08 | | | | | A 1 | 20: 121 91 107 162 95 105 189 81 136 135 134 79 39 110 92 57 190 53 160 146 | 73 | 2.22E+06 | |
| | | | | | | | A 2 | | 71 | 2.89E+04 | |
| | | | | | | | A 5 | 17: 147 109 161 91 148 204 135 133 92 189 107 94 93 159 134 41 149 | 78 | 6.42E+05 | |
| | | | | | | | A 6 | 17: 161 121 122 149 136 67 189 55 135 81 145 162 148 39 80 41 134 | 70 | 8.30E+05 | |
| | | | | | | | B 3 | 16: 148 105 161 162 205 92 67 133 107 79 135 115 134 120 93 119 | 78 | 1.44E+05 | |
| | | | | | | | B 4 | 20: 77 147 161 67 134 189 65 121 105 133 82 95 55 79 120 109 43 83 108 78 | 73 | 6.04E+05 | |
| α-cedrene | 469-61-4 | 22.08 | | Woody, Cedar, Sweet, Fresh | | | A 5 | 15: 119 204 161 93 65 69 133 80 121 135 134 41 189 94 79 | 72 | 4.47E+05 | |
| | | | | | | | A 7 | | 72 | 1.74E+04 | |
| Longicyclene | 1137-12-8 | 22.10 | | | | | A 5 | 17: 109 93 189 190 80 131 133 204 55 121 115 79 105 145 82 107 135 | 78 | 1.57E+05 | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | B | 4 | 7: 134 189 81 204 161 106 78 | 72 | 3.50E+05 |
| γ-gurjunene | 22567-17-5 | 22.14 | | Musty | A | 1 | 20: 121 91 107 162 95 105 189 81 136 135 134 79 39 110 92 57 190 53 160 146 | 92 | 2.49E+06 |
| | | | | | A | 2 | | 84 | 6.30E+04 |
| | | | | | A | 5 | 20: 93 147 77 105 129 108 79 189 119 81 91 135 106 175 131 145 205 51 95 109 | 92 | 4.50E+06 |
| | | | | | A | 6 | 18: 161 204 108 105 205 107 122 81 55 53 109 148 39 92 79 77 162 106 | 89 | 9.02E+05 |
| | | | | | A | 7 | | 89 | 5.08E+05 |
| | | | | | B | 3 | 20: 161 122 107 149 204 105 109 205 95 65 79 55 135 134 77 141 91 41 92 108 | 91 | 7.69E+05 |
| | | | | | B | 4 | 20: 148 79 161 107 95 145 204 67 93 120 105 122 41 91 106 162 205 108 39 150 | 90 | 4.49E+05 |
| α-longipinene | 5989-08-2 | 22.18 | | | A | 6 | 20: 93 121 122 204 133 115 119 135 91 205 117 105 77 159 176 54 95 162 51 163 | 70 | 1.01E+06 |
| Cedryl acetate | 77-54-3 | 22.18 | | Wood | B | 4 | 17: 119 105 204 69 55 190 149 107 67 96 95 205 175 106 187 147 109 | 65 | 2.31E+05 |
| Valencene | 4630-07-3 | 22.19 | Green, Oil | Citrus | A | 1 | 20: 133 121 161 92 204 79 107 91 119 52 190 81 93 55 78 53 115 131 206 129 | 96 | 3.06E+06 |
| | | | | | A | 2 | | 88 | 1.47E+05 |
| | | | | | A | 5 | 20: 161 204 131 133 91 53 106 190 68 108 43 66 77 94 162 78 148 73 160 143 | 96 | 3.46E+06 |
| | | | | | A | 6 | 16: 134 78 135 108 204 147 161 39 82 95 79 119 107 175 52 131 | 95 | 1.39E+06 |
| | | | | | A | 7 | | 95 | 8.47E+05 |
| | | | | | B | 3 | 20: 161 91 204 133 145 78 135 81 134 79 55 119 120 63 93 53 107 108 174 122 | 96 | 1.14E+06 |
| | | | | | B | 4 | 20: 77 147 161 67 134 189 65 121 105 133 82 95 55 79 120 109 43 83 108 78 | 94 | 4.66E+05 |
| 2-hydroxyethyl acrylate | 5951-61-1 | 22.61 | | | A | 1 | | 79 | 2.64E+04 |
| | | | | | A | 2 | | 77 | 2.03E+04 |
| | | | | | A | 5 | | 82 | 6.28E+04 |
| | | | | | A | 6 | 4: 133 119 109 161 | 79 | 5.29E+04 |
| | | | | | A | 7 | 13: 107 121 149 81 79 42 189 190 82 161 39 136 97 | 73 | 2.79E+05 |
| | | | | | B | 3 | | 80 | 4.60E+04 |

**Table 3** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | B 4 | 20: 148 79 161 107 95 145 204 67 93 120 105 122 41 91 106 162 205 108 39 150 | 77 | 7.39E+05 | |
| +Butylated Hydroxytoluene | 128-37-0 | 22.66 | | Mild, Phenolic, Camphor | | | B 1 | | 84 | 3.39E+04 | |
| | | | | | | | B 2 | | 90 | 7.76E+04 | |
| Xylazine | 7361-61-7 | 22.67 | | | | | B 2 | | 66 | 7.76E+04 | |
| 2,3,6-trimethylpyridine | 1462-84-6 | 23.95 | | | | | A 2 | 5: 41 134 120 121 83 | 65 | 1.78E+04 | |
| Toluene-2,4-diamine | 95-80-7 | 23.97 | | | | | A 2 | 4: 122 121 105 96 | 70 | 1.18E+04 | |
| Propofol | 2078-54-8 | 23.97 | | Phenolic | | | A 1 | 20: 93 164 108 107 178 80 124 135 79 106 122 145 41 120 55 94 91 103 95 149 | 68 | 7.95E+05 | |
| | | | | | | | A 2 | | 70 | 1.43E+05 | |
| 1-(3,6-Dimethyl-2-pyrazinyl)-2-methyl-1-propanone | 145984-66-3 | 23.98 | | | | | A 2 | 14: 108 123 93 67 163 81 178 107 105 91 79 66 55 145 | 68 | 1.38E+05 | |
| Methyl isoeugenol | 93-16-3 | 23.98 | Clove, Spice | Spice | | | A 1 | 14: 163 41 93 108 107 105 119 115 91 149 95 145 78 160 | 67 | 1.50E+06 | |
| | | | | | | | A 2 | | 66 | 1.43E+05 | |
| Caryophyllene oxide | 1139-30-6 | 24.09 | Herb, Sweet, Spice | Woody | | | A 5 | | 74 | 2.69E+04 | |
| p-acetanisole | 100-06-1 | 24.58 | | Anisic | | | C 1 | 2: 135 150 | 68 | 1.31E+04 | |
| | | | | | | | C 3 | | 69 | 6.11E+03 | |
| 3-methyl-5-(1-methylethyl)-Phenol methylcarbamate | 2631-37-0 | 24.64 | | | | | C 1 | 2: 135 150 | 70 | 1.31E+04 | |
| | | | | | | | C 2 | | 84 | 2.37E+04 | |
| | | | | | | | C 3 | 1: 150 | 73 | 2.09E+04 | |
| Thymol | 89-83-8 | 24.78 | | Herbal | | 1.55E-02 | C 1 | | 91 | 4.48E+04 | 2.89E+06 |
| | | | | | | | C 2 | | 82 | 2.37E+04 | 1.53E+06 |
| | | | | | | | C 3 | | 70 | 6.20E+03 | 4.00E+05 |
| +Carvacrol | 499-75-2 | 24.78 | | Spicy | | 1.12E-02 | C 1 | | 92 | 4.48E+04 | 3.99E+06 |
| | | | | | | | C 2 | | 84 | 2.37E+04 | 2.11E+06 |
| | | | | | | | C 3 | | 72 | 6.20E+03 | 5.53E+05 |
| 2,4-di-tert-butylphenol | 96-76-4 | 26.36 | | Phenolic | | | A 4 | 1: 191 | 68 | 2.90E+04 | |
| α-bisabolol | 72691-24-8 | 26.43 | | | | | A 5 | | 77 | 3.95E+04 | |
| Cyclobarbital | 52-31-3 | 35.80 | | | | | A 7 | 1: 207 | 65 | 9.20E+03 | |
| 1,4-Dioxane | 123-91-1 | 38.37 | | | | 5.50E+00 | B 3 | 2: 58 88 | 71 | 2.39E+03 | 4.34E+02 |

If two references of ODTs are available, ODT from Devos, et al. [5] is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Section 1.5. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are m/z. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. Underlined items highlight the compounds found in Pseudo Scent Marijuana. + Compounds indicate confirmation with reference standards, matching retention time and spectra.

**Table 4**
Summary of VOCs emitted from all illicit cocaine samples (sample code D in Section 1.5) and Sigma Pseudo™ Narcotic Scent Cocaine formulation (sample code E in Section 1.5) and sampled over 1 h at room temperature. **Sigma Pseudo™ Narcotic Scent Cocaine formulation is indicated by underlined fonts.**

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI & Odor [6] | Devos et al. [5] | | | | | |
| Ethylene oxide | 75-21-8 | 1.07 | | | | 8.51E+02 | D 4 | | 66 | 3.83E+06 | 4.50E+03 |
| | | | | | | | E 1 | | 66 | 2.28E+06 | 2.68E+03 |
| +2-nitropropane | 79-46-9 | 1.11 | | | | 7.24E+00 | D 2 | 4: 41 43 56 39 | 88 | 2.92E+04 | 4.03E+03 |
| | | | | | | | D 4 | | 73 | 3.05E+04 | 4.21E+03 |
| | | | | | | | D 5 | 3: 39 43 41 | 83 | 4.84E+03 | 6.69E+02 |
| 2,4-dimethylpentane | 108-08-7 | 1.16 | | | | 8.71E+01 | D 1 | 4: 57 85 43 99 | 70 | 1.41E+05 | 1.62E+03 |
| | | | | | | | D 3 | 5: 53 100 70 86 57 | 83 | 8.33E+05 | 9.57E+03 |
| | | | | | | | D 4 | 4: 43 56 42 84 | 69 | 1.90E+04 | 2.18E+02 |
| 1,2-dimethyl hydrazine | 540-73-8 | 1.18 | | | | | D 1 | 1: 45 | 74 | 1.91E+04 | |
| Ethylenimine | 151-56-4 | 1.20 | | | | | D 2 | 4: 43 42 56 41 | 68 | 7.08E+04 | |
| Isobutane | 75-28-5 | 1.24 | | | | 1.00E+01 | D 1 | 6: 43 42 41 57 72 39 | 83 | 1.26E+06 | 1.26E+05 |
| | | | | | | | D 2 | 9: 43 42 41 57 39 55 56 53 58 | 84 | 1.43E+06 | 1.43E+05 |
| | | | | | | | D 3 | 11: 43 42 41 57 72 56 55 39 38 71 51 | 85 | 3.13E+06 | 3.13E+05 |
| | | | | | | | D 4 | 4: 43 42 41 72 | 82 | 2.27E+05 | 2.27E+04 |
| | | | | | | | D 5 | 7: 41 43 42 39 72 57 55 | 81 | 1.53E+05 | 1.53E+04 |
| Ethyl Chloride | 75-00-3 | 1.26 | | | | | D 1 | 2: 64 66 | 75 | 1.37E+04 | |
| +Butane | 106-97-8 | 1.26 | | | | 2.04E+02 | D 1 | 6: 43 58 42 41 37 45 | 82 | 4.20E+06 | 2.06E+04 |
| | | | | | | | D 2 | 4: 41 43 56 39 | 79 | 2.92E+04 | 1.43E+02 |
| | | | | | | | D 4 | | 91 | 3.05E+04 | 1.49E+02 |
| | | | | | | | D 5 | 3: 43 56 58 | 87 | 5.11E+04 | 2.50E+02 |
| Trichloromonofluoromethane | 75-69-4 | 1.27 | | | | | D 2 | 2: 103 101 | 77 | 5.39E+03 | |
| +Acetaldehyde | 75-07-0 | 1.28 | Pungent, Ether | Pungent, Ethereal, Aldehydic, Fruity | 1.50E-02 | 1.86E-01 | D 1 | 2: 44 43 | 81 | 3.01E+04 | 1.61E+05 |
| | | | | | | | D 2 | 1: 44 | 81 | 2.68E+04 | 1.44E+05 |
| | | | | | | | D 4 | 3: 44 43 42 | 91 | 6.31E+04 | 3.39E+05 |
| | | | | | | | D 5 | | 68 | 2.60E+03 | 1.40E+04 |
| +Ethyl ether | 60-29-7 | 1.31 | | Ethereal | | | D 4 | 2: 59 45 | 86 | 1.43E+04 | |
| Isoprene | 78-79-5 | 1.33 | | | | | D 4 | 2: 53 67 | 82 | 2.29E+04 | |
| 4-methyldecane | 2847-72-5 | 1.39 | | | | | D 1 | 4: 56 57 55 43 | 72 | 7.44E+04 | |
| | | | | | | | D 2 | 8: 43 71 70 41 86 55 57 56 | 65 | 5.04E+05 | |
| | | | | | | | D 3 | 13: 70 56 71 113 99 85 41 69 67 42 72 44 114 | 84 | 8.36E+05 | |
| | | | | | | | D 4 | 2: 42 70 | 65 | 2.98E+05 | |

**Table 4** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI & Odor [6] | Devos et al. [5] | | | | | |
| 2-methylpentane | 107-83-5 | 1.39 | | | | | D 1 | 2: 57 70 | 97 | 3.19E+05 | |
| | | | | | | | D 2 | 8: 43 71 70 41 86 55 57 56 | 98 | 5.04E+05 | |
| | | | | | | | D 3 | 6: 43 71 42 39 55 56 | 97 | 5.78E+05 | |
| | | | | | | | D 4 | 2: 42 70 | 96 | 2.98E+05 | |
| | | | | | | | D 5 | 6: 41 43 71 70 55 39 | 96 | 2.07E+05 | |
| 2,3-dimethylbutane | 79-29-8 | 1.40 | | | | | D 3 | 3: 42 41 43 | 65 | 2.60E+05 | |
| | | | | | | | D 4 | 9: 43 71 41 39 55 86 42 53 72 | 87 | 2.93E+05 | |
| Hexane | 110-54-3 | 1.44 | Alkane | | | 2.19E+01 | D 1 | 2: 43 42 | 96 | 1.06E+05 | 4.83E+03 |
| | | | | | | | D 2 | 4: 43 42 56 41 | 83 | 7.76E+04 | 3.55E+03 |
| | | | | | | | D 3 | 9: 57 43 41 56 86 39 58 55 70 | 99 | 2.29E+06 | 1.05E+05 |
| | | | | | | | D 4 | | 90 | 4.09E+05 | 1.87E+04 |
| | | | | | | | D 5 | 4: 57 56 41 86 | 90 | 3.60E+05 | 1.64E+04 |
| Cyclopentane | 287-92-3 | 1.45 | | Petroleum | | | D 4 | 3: 55 70 53 | 77 | 3.85E+04 | |
| | | | | | | | D 5 | 2: 42 55 | 83 | 2.96E+04 | |
| 2-methylaziridine | 75-55-8 | 1.45 | | | | | D 1 | 3: 56 41 57 | 80 | 7.68E+04 | |
| | | | | | | | D 2 | | 81 | 7.80E+04 | |
| | | | | | | | D 3 | 1: 57 | 79 | 1.35E+05 | |
| | | | | | | | D 4 | | 81 | 6.54E+04 | |
| | | | | | | | D 5 | | 82 | 5.43E+04 | |
| 3-methylpentane | 96-14-0 | 1.45 | | | | | D 1 | 3: 56 41 57 | 87 | 7.68E+04 | |
| | | | | | | | D 2 | | 93 | 7.80E+04 | |
| | | | | | | | D 3 | 1: 57 | 87 | 1.35E+05 | |
| | | | | | | | D 4 | | 96 | 6.37E+04 | |
| | | | | | | | D 5 | 2: 56 55 | 92 | 1.57E+05 | |
| | | | | | | | E 1 | 2: 56 57 | 67 | 3.48E+03 | |
| Isocyanatomethane | 624-83-9 | 1.46 | | | | | D 1 | 4: 56 57 55 43 | 66 | 8.44E+04 | |
| | | | | | | | D 3 | 5: 57 112 85 43 113 | 80 | 8.15E+04 | |
| | | | | | | | D 5 | 2: 56 55 | 80 | 1.23E+05 | |
| | | | | | | | E 1 | 2: 56 57 | 79 | 3.48E+03 | |
| 2-hydroxy propanenitrile | 78-97-7 | 1.48 | | | | | D 3 | 9: 43 56 42 53 55 87 54 85 50 | 73 | 8.86E+05 | |
| | | | | | | | D 5 | 2: 56 55 | 65 | 8.32E+04 | |
| 3,4,5-trimethyl-1-hexene | 56728-10-0 | 1.51 | | | | | D 1 | 9: 43 71 42 56 41 70 57 39 38 | 67 | 3.11E+05 | |
| | | | | | | | D 2 | 8: 43 71 70 41 86 55 57 56 | 67 | 5.04E+05 | |
| | | | | | | | D 3 | | 69 | 4.99E+05 | |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | D 4 | 2: 42 70 | 68 | 2.98E+05 | |
| | | | | | | | D 5 | 3: 43 57 71 | 68 | 1.72E+05 | |
| +Propanal | 123-38-6 | 1.57 | Solvent, Pungent | Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty | 1.00E-02 | 2.69E-02 | D 1 | 3: 58 57 41 | 68 | 1.47E+04 | 5.46E+05 |
| +Acetic anhydride | 108-24-7 | 1.62 | | Sharp, Vinegar | | 5.89E-01 | D 1 | 2: 61 43 | 69 | 2.06E+05 | 3.50E+05 |
| | | | | | | | D 3 | 1: 43 | 81 | 3.68E+04 | 6.25E+04 |
| | | | | | | | D 4 | 3: 43 58 42 | 81 | 3.40E+04 | 5.77E+04 |
| | | | | | | | D 5 | 2: 43 42 | 73 | 4.76E+03 | 8.08E+03 |
| | | | | | | | E 1 | 1: 43 | 65 | 1.08E+03 | 1.83E+03 |
| 2,2,4,4-tetramethyl-3-pentanone | 815-24-7 | 1.65 | | | | | D 1 | 4: 57 85 43 99 | 68 | 1.41E+05 | |
| | | | | | | | D 3 | 5: 112 57 85 41 55 | 75 | 1.28E+05 | |
| 2-methyl-2-propanamine | 75-64-9 | 1.65 | | | | | D 4 | 4: 41 57 37 85 | 91 | 1.22E+05 | |
| 2,2,4,4-tetramethyl-3-pentanone | 815-24-7 | 1.65 | | | | | D 4 | 4: 41 57 37 85 | 73 | 3.53E+04 | |
| +Acetone | 67-64-1 | 1.66 | | Solvent | | 1.45E+01 | D 1 | 6: 43 58 42 41 37 45 | 99 | 4.20E+06 | 2.91E+05 |
| | | | | | | | D 2 | 2: 43 58 | 88 | 1.55E+05 | 1.07E+04 |
| | | | | | | | D 3 | 3: 58 43 42 | 88 | 9.15E+04 | 6.33E+03 |
| | | | | | | | D 4 | 3: 43 58 39 | 97 | 9.33E+05 | 6.46E+04 |
| | | | | | | | D 5 | 6: 43 58 57 42 37 44 | 97 | 5.36E+05 | 3.71E+04 |
| | | | | | | | E 1 | 2: 58 43 | 81 | 1.03E+04 | 7.11E+02 |
| +Methyl acetate | 79-20-9 | 1.68 | | Ethereal | | | D 1 | 1: 43 | 85 | 1.36E+05 | |
| | | | | | | | D 4 | 3: 43 74 39 | 95 | 1.69E+05 | |
| | | | | | | | D 5 | 3: 74 43 42 | 95 | 1.98E+05 | |
| +Acrolein | 107-02-8 | 1.71 | | Almond, Cherry | | 1.74E-01 | D 3 | 1: 56 | 66 | 6.09E+04 | 3.50E+05 |
| +Propene | 115-07-1 | 1.71 | | | | 5.25E+01 | D 3 | 3: 41 39 42 | 77 | 3.28E+04 | 6.25E+02 |
| Methacrylic anhydride | 760-93-0 | 1.71 | | | | | D 3 | 3: 41 39 42 | 75 | 2.28E+04 | |
| Isobutyraldehyde | 78-84-2 | 1.76 | Pungent, Malt, Green | Spicy | | 4.07E-02 | D 1 | | 91 | 4.35E+04 | 1.07E+06 |
| | | | | | | | D 2 | 9: 43 42 41 57 39 55 56 53 58 | 77 | 1.43E+06 | 3.50E+07 |
| | | | | | | | D 3 | 11: 43 42 41 57 72 56 55 39 38 71 51 | 78 | 3.13E+06 | 7.68E+07 |
| | | | | | | | D 4 | 4: 43 42 41 72 | 76 | 2.27E+05 | 5.57E+06 |
| | | | | | | | D 5 | 7: 41 43 42 39 72 57 55 | 75 | 1.53E+05 | 3.77E+06 |
| 1-(ethenyloxy)-butane | 111-34-2 | 1.89 | | | | | D 3 | 5: 53 100 70 86 57 | 69 | 6.85E+05 | |
| +2,4-Pentanedione | 123-54-6 | 1.91 | | | | 3.16E-02 | D 4 | | 69 | 1.34E+04 | 4.25E+05 |
| Mefruside | 7195-27-9 | 1.91 | | | | | D 4 | | 71 | 1.34E+04 | |
| Cyclohexane | 110-82-7 | 1.92 | | | | 2.19E+01 | D 3 | | 82 | 4.27E+04 | 1.95E+03 |
| | | | | | | | D 4 | | 89 | 5.25E+04 | 2.40E+03 |
| | | | | | | | D 5 | 3: 55 42 41 | 86 | 3.56E+04 | 1.63E+03 |
| | | | | | | | E 1 | 2: 41 84 | 76 | 1.34E+04 | 6.13E+02 |
| 2,3,4-trimethylpentane | 565-75-3 | 1.98 | | | | | D 3 | 5: 70 57 39 55 84 | 74 | 4.45E+05 | |
| (S)-2-propylpiperidine | 458-88-8 | 1.99 | | | | | E 1 | | 66 | 3.60E+03 | |
| 2-ethyl-1-butanol | 97-95-0 | 2.00 | | Sweet, Musty, Alcoholic | | 2.34E-01 | D 4 | 3: 84 70 39 | 75 | 1.29E+05 | 5.52E+05 |
| | | | | | | | D 5 | | 74 | 3.28E+04 | 1.40E+05 |
| +Cyclohexanone | 108-94-1 | 2.17 | | Minty, Acetone | | 7.08E-01 | D 4 | 4: 41 55 98 72 | 65 | 9.49E+03 | 1.34E+04 |
| Nimorazole | 6506-37-2 | 2.19 | | | | | D 3 | 1: 100 | 72 | 8.60E+03 | |

**Table 4** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI & Odor [6] | Devos et al. [5] | | | | | |
| 2-(diethylamino)-1-phenyl-1-propanone | 90-84-6 | 2.19 | | | | | D 3 | 1: 100 | 66 | 8.60E+03 | |
| +Heptane | 142-82-5 | 2.22 | Alkane | Sweet, Ethereal | | 9.77E+00 | D 3 | 12: 43 71 41 100 56 55 70 54 39 42 85 40 | 98 | 1.40E+06 | 1.43E+05 |
| +2-methyl-3-pentanone | 565-69-5 | 2.22 | Mint | Mint | | | D 4 | 3: 100 57 41 | 67 | 1.24E+04 | |
| 1,2-diethyl hydrazine | 1615-80-1 | 2.31 | | | | | D 4 | 6: 88 70 89 73 87 60 | 73 | 5.77E+05 | |
| +Ethylacetate | 141-78-6 | 2.31 | Pineapple | Ethereal, Fruity, Sweet, Weedy, Green | | 2.63E+00 | D 1 | 9: 43 61 70 73 62 71 60 89 55 | 99 | 3.08E+06 | 1.17E+06 |
| | | | | | | | D 3 | 6: 61 70 73 62 90 60 | 99 | 4.00E+06 | 1.52E+06 |
| | | | | | | | D 4 | 10: 43 61 42 70 88 45 73 62 87 41 | 99 | 3.29E+06 | 1.25E+06 |
| | | | | | | | D 5 | 7: 70 88 73 42 74 62 59 | 99 | 2.31E+06 | 8.80E+05 |
| +2-butanone | 78-93-3 | 2.33 | Ether | Ethereal, Fruity, Camphor | | 7.76E+00 | D 3 | 4: 43 61 45 60 | 75 | 4.36E+06 | 5.61E+05 |
| | | | | | | | D 4 | 3: 72 57 39 | 67 | 2.54E+05 | 3.27E+04 |
| | | | | | | | D 5 | 5: 43 61 45 73 89 | 76 | 2.23E+06 | 2.88E+05 |
| Methyl thiocyanate | 556-64-9 | 2.33 | Sulfur | Sulfury, Onion | | 1.55E-01 | D 5 | 4: 42 73 46 60 | 66 | 3.15E+05 | 2.03E+06 |
| +Ethanol | 64-17-5 | 2.34 | Sweet | Alcoholic | | 2.88E+01 | D 1 | 2: 45 73 | 87 | 4.09E+05 | 1.42E+04 |
| | | | | | | | D 2 | | 98 | 1.58E+05 | 5.47E+03 |
| +Isopropyl alcohol | 67-63-0 | 2.34 | | Alcohol, Musty, Woody | | 1.02E+01 | D 2 | 1: 45 | 81 | 2.69E+05 | 2.63E+04 |
| | | | | | | | D 4 | | 80 | 5.72E+05 | 5.59E+04 |
| | | | | | | | D 5 | | 82 | 2.92E+05 | 2.86E+04 |
| +Formic acid | 64-18-6 | 2.34 | | Acetic | | 2.82E+01 | D 1 | 2: 45 73 | 78 | 1.00E+06 | 3.56E+04 |
| | | | | | | | D 2 | | 70 | 8.70E+04 | 3.09E+03 |
| Nitrogen dioxide | 10102-44-0 | 2.34 | | | | 1.86E-01 | D 1 | 1: 46 | 75 | 1.36E+05 | 7.28E+05 |
| | | | | | | | D 5 | 2: 46 47 | 76 | 6.16E+03 | 3.31E+04 |
| methylhydrazine | 60-34-4 | 2.35 | | | | | D 1 | 1: 46 | 78 | 1.95E+05 | |
| | | | | | | | D 2 | 2: 45 46 | 77 | 9.05E+04 | |
| Acetic acid ethenyl ester | 108-05-4 | 2.41 | | | | | D 5 | 1: 86 | 68 | 8.39E+04 | |
| +Methylene chloride | 75-09-2 | 2.41 | | | | 2.82E+01 | D 3 | 4: 84 49 48 35 | 97 | 2.87E+05 | 1.02E+04 |
| | | | | | | | D 4 | 6: 84 49 86 51 35 47 | 93 | 2.60E+05 | 9.24E+03 |
| | | | | | | | D 5 | 6: 49 44 57 84 48 35 | 93 | 1.22E+05 | 4.34E+03 |
| Tolycaine | 3686-58-6 | 2.43 | | | | | D 5 | 3: 86 47 35 | 67 | 2.41E+04 | |
| +2-Pentanone | 107-87-9 | 2.43 | Ether, Fruit | Sweet, Fruity, Ethereal, Wine, Banana, Woody | | 1.55E+00 | D 5 | 4: 86 49 84 43 | 72 | 6.97E+04 | 4.50E+04 |
| Amitrole | 61-82-5 | 2.49 | | | | | D 3 | 3: 84 46 57 | 79 | 2.35E+04 | |
| Piperoxan | 59-39-2 | 2.60 | | | | | D 3 | 5: 98 85 84 69 82 | 67 | 3.15E+04 | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Methyl cyclohexane | 108-87-2 | 2.61 | | | | D 3 | 5: 83 56 41 69 39 | 94 | 1.24E+05 | |
| | | | | | | D 4 | 5: 98 55 83 82 56 | 84 | 1.14E+05 | |
| | | | | | | D 5 | 4: 83 69 82 55 | 75 | 2.64E+04 | |
| +n-Propyl acetate | 109-60-4 | 2.68 | Fruit, Apple, Banana | Solvent, Celery, Fruity, Fusel, Raspberry, Pear | 5.75E-01 | D 1 | 9: 43 61 70 73 62 71 60 89 55 | 69 | 4.99E+06 | 8.68E+06 |
| | | | | | | D 3 | 9: 41 33 59 60 39 72 57 74 35 | 97 | 6.43E+06 | 1.12E+07 |
| | | | | | | D 4 | 10: 43 61 42 70 88 45 73 62 87 41 | 69 | 3.29E+06 | 5.71E+06 |
| | | | | | | D 5 | 7: 70 88 73 42 74 62 59 | 69 | 2.31E+06 | 4.02E+06 |
| +1-Heptanol | 111-70-6 | 2.77 | Chemical, Green | Musty, Leafy, Violet, Herbal, Green, Sweet, Woody, Peony | 2.51E-02 | D 3 | | 73 | 3.82E+04 | 1.52E+06 |
| Ethanedinitrile | 460-19-5 | 3.00 | | | | D 5 | 2: 52 61 | 74 | 1.75E+03 | |
| Benzene | 71-43-2 | 3.02 | | Aromatic | 3.63E+00 | D 1 | | 93 | 1.32E+05 | 3.64E+04 |
| | | | | | | D 3 | 4: 78 50 77 79 | 74 | 2.71E+04 | 7.47E+03 |
| 2,5-dimethyl hexane | 592-13-2 | 3.17 | | | | D 3 | 6: 70 53 43 39 99 56 | 84 | 9.76E+05 | |
| 3-methylheptane | 589-81-1 | 3.35 | | | | D 3 | | 93 | 1.29E+05 | |
| Sorbic Acid | 110-44-1 | 3.56 | | | | D 3 | | 67 | 6.14E+04 | |
| +Isothiocyanato methane | 556-61-6 | 3.76 | | Pungent, Mustard, Horseradish | | D 3 | 4: 73 40 72 63 | 67 | 9.72E+05 | |
| Chloroform | 67-66-3 | 3.77 | | | | D 4 | 4: 83 48 61 85 | 79 | 2.12E+05 | |
| | | | | | | D 5 | | 79 | 7.16E+04 | |
| Ethylenediamine | 107-15-3 | 3.93 | | | | D 1 | | 68 | 9.65E+04 | |
| +1,1-dimethyl-hydrazine | 57-14-7 | 3.95 | | | | D 1 | 3: 59 42 60 | 74 | 2.19E+04 | |
| | | | | | | D 2 | | 79 | 4.75E+04 | |
| 3-pentanol | 584-02-1 | 3.95 | Fruit | Herbal | 4.68E-01 | D 2 | | 66 | 4.75E+04 | 1.02E+05 |
| Hydrazine | 302-01-2 | 3.96 | | | 3.00E+00 | D 1 | | 79 | 1.44E+04 | 4.79E+03 |
| | | | | | | D 2 | 1: 33 | 77 | 1.47E+03 | 4.89E+02 |
| | | | | | | D 3 | 1: 33 | 78 | 8.97E+04 | 2.99E+04 |
| | | | | | | D 4 | 2: 111 33 | 78 | 6.05E+03 | 2.02E+03 |
| +Octane | 111-65-9 | 4.00 | Alkane | Gasoline | 5.75E+00 | D 3 | | 91 | 1.90E+05 | 3.30E+04 |
| Tetrahydrofurfuryl acetate | 637-64-9 | 4.07 | | Sweet, Fruity, Brown, Rum, Ether, Caramel | | D 3 | 2: 71 39 | 77 | 1.98E+05 | |
| Isobutyl acetate | 110-19-0 | 4.86 | Fruit, Apple, Banana | Sweet, Fruity, Ethereal, Banana, Tropical | 4.79E-01 | D 1 | | 91 | 2.03E+05 | 4.24E+05 |
| +Isobutyric acid | 79-31-2 | 4.88 | Rancid, Butter, Cheese | | 1.95E-02 | D 1 | 2: 43 41 | 72 | 2.84E+05 | 1.46E+07 |
| +Toluene | 108-88-3 | 5.05 | Paint | Sweet | 1.55E+00 | D 3 | 16: 91 65 93 89 39 50 38 62 77 43 45 74 90 61 46 88 | 100 | 5.76E+06 | 3.72E+06 |
| +Phenylethyl alcohol | 60-12-8 | 5.05 | Honey, Spice, Rose, Lilac | Floral | 1.70E-02 | D 3 | 16: 91 65 93 89 39 50 38 62 77 43 45 74 90 61 46 88 | 75 | 5.76E+06 | 3.39E+08 |
| +1-butanol | 71-36-3 | 6.15 | Medicine, Fruit | Fermented | 4.90E-01 | D 1 | | 80 | 7.81E+03 | 1.59E+04 |
| | | | | | | D 2 | 4: 43 42 56 41 | 68 | 7.76E+04 | 1.58E+05 |
| | | | | | | D 5 | | 73 | 1.90E+04 | 3.88E+04 |
| +Isobutanol | 78-83-1 | 6.17 | Wine, Solvent, Bitter | Ethereal, Winey | | D 1 | 18: 43 41 42 33 39 74 40 72 56 57 38 59 44 53 73 60 51 37 | 97 | 1.29E+07 | |

**Table 4** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI & Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | D 3 | 3: 42 41 43 | 73 | 2.60E+05 | |
| | | | | | | | D 4 | 6: 43 57 41 42 56 39 | 68 | 1.23E+05 | |
| | | | | | | | D 5 | 3: 39 42 41 | 65 | 5.14E+04 | |
| Propanoic acid, anhydride | 123-62-6 | 6.49 | | | | | D 2 | 1: 57 | 69 | 2.88E+04 | |
| | | | | | | | D 3 | 1: 57 | 76 | 8.26E+04 | |
| | | | | | | | D 5 | 1: 57 | 65 | 3.15E+04 | |
| 4-methyl-3-penten-2-one | 141-79-7 | 6.65 | Sweet, Chemical | Pungent, Earthy, Vegetable, Acrylic | | 5.62E-02 | D 3 | 5: 83 56 41 69 39 | 79 | 1.24E+05 | 2.21E+06 |
| | | | | | | | D 4 | 5: 98 55 83 82 56 | 84 | 6.12E+04 | 1.09E+06 |
| | | | | | | | D 5 | 3: 98 83 55 | 82 | 2.31E+04 | 4.11E+05 |
| +Decane | 124-18-5 | 6.66 | Alkane | | | 7.41E-01 | D 3 | | 69 | 6.62E+04 | 8.93E+04 |
| | | | | | | | E 1 | | 82 | 3.45E+04 | 4.66E+04 |
| +Isoamyl alcohol | 123-51-3 | 7.52 | Whiskey, Malt, Burnt | Fusel oil, Alcoholic, Whiskey, Fruity, Banana | | 4.47E-02 | D 1 | | 69 | 2.43E+04 | 5.45E+05 |
| | | | | | | | D 4 | 3: 55 70 53 | 66 | 1.40E+04 | 3.14E+05 |
| Amyl alcohol | 71-41-0 | 7.54 | Balsamic | Fusel, Oil, Sweet, Balsam | | 4.68E-01 | D 1 | | 77 | 2.43E+04 | 5.20E+04 |
| | | | | | | | D 4 | 3: 55 70 53 | 71 | 1.40E+04 | 3.00E+04 |
| | | | | | | | D 5 | 2: 42 55 | 72 | 2.96E+04 | 6.34E+04 |
| +p-xylene | 106-42-3 | 7.65 | | | | 4.90E-01 | D 3 | 2: 91 105 | 83 | 8.07E+04 | 1.65E+05 |
| α-pinene | 80-56-8 | 7.90 | Pine, Turpentine | Herbal | | 6.92E-01 | D 1 | | 75 | 1.18E+04 | 1.70E+04 |
| α-phellandrene | 99-83-2 | 7.91 | Turpentine, Mint, Spice | Terpenic | | | D 1 | | 79 | 1.18E+04 | |
| +Camphene | 79-92-5 | 10.21 | Camphor | Woody | | | D 1 | | 67 | 1.18E+04 | |
| p-ethyltoluene | 622-96-8 | 10.25 | | | | | D 3 | 5: 120 105 91 155 136 | 76 | 4.89E+04 | |
| 2-ethyltoluene | 611-14-3 | 10.61 | | | | | D 3 | 4: 105 154 77 91 | 75 | 5.10E+04 | |
| 2,2,5-trimethylhexane | 3522-94-9 | 10.67 | | | | | D 3 | 7: 57 70 112 83 69 72 155 | 84 | 8.52E+05 | |
| +1-hexanol | 111-27-3 | 10.73 | Resin, Flower, Green | Herbal | | 4.37E-02 | D 5 | 4: 69 56 41 42 | 66 | 7.45E+04 | 1.71E+06 |
| Diacetone alcohol | 123-42-2 | 10.79 | | | | 8.91E-01 | D 1 | | 89 | 1.90E+05 | 2.14E+05 |
| | | | | | | | D 4 | 10: 43 59 58 42 41 57 98 38 45 61 | 93 | 2.46E+06 | 2.76E+06 |
| | | | | | | | D 5 | 7: 43 59 58 39 55 207 53 | 92 | 1.22E+06 | 1.37E+06 |
| 1,3,5-trimethylbenzene | 108-67-8 | 11.02 | | | | | D 3 | 7: 105 119 120 106 43 77 102 | 83 | 1.34E+05 | |
| +Piperidine | 110-89-4 | 11.20 | | Animal | | 3.72E-01 | D 3 | | 79 | 1.29E+05 | 3.46E+05 |
| 2,4,5-trimethylbenzenamine | 137-17-7 | 11.30 | | | | | D 3 | 1: 120 | 73 | 1.13E+05 | |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| +Durene | 95-93-2 | 11.36 | Rancid, Sweet | Rancid | | 2.63E-02 | D | 1 | 2: 134 119 | 67 | 3.08E+04 | 1.17E+06 |
| Isodurene | 527-53-7 | 11.37 | | | | | D | 1 | 2: 134 119 | 68 | 1.76E+04 | |
| | | | | | | | D | 3 | 2: 119 134 | 70 | 4.14E+04 | |
| 1-ethyl-2,4-dimethylbenzene | 874-41-9 | 11.38 | | | | | D | 3 | 2: 119 134 | 70 | 8.63E+04 | |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | 11.38 | | Gasoline, Sweet | | 2.63E-02 | D | 1 | | 78 | 2.05E+04 | 7.81E+05 |
| | | | | | | | D | 3 | 2: 119 134 | 65 | 8.63E+04 | 3.28E+06 |
| +p-cymene | 99-87-6 | 11.38 | Solvent, Gasoline, Citrus | Terpenic | | 2.14E-03 | D | 1 | | 81 | 2.05E+04 | 9.61E+06 |
| | | | | | | | D | 3 | 2: 119 134 | 67 | 8.63E+04 | 4.04E+07 |
| N,N-dimethylbenzenamine | 121-69-7 | 11.41 | | | | | D | 3 | 9: 120 105 121 103 79 91 97 77 122 | 82 | 2.62E+05 | |
| 3-phenyl propyl isobutyrate | 103-58-2 | 11.41 | | Sweet, Fruity, Balsam | | | D | 3 | 3: 118 117 141 | 69 | 1.09E+04 | |
| 3-phenyl propyl acetate | 122-72-5 | 11.41 | | Sweet, Balsam, Storax, Spicy, Cinnamon | | | D | 3 | 3: 118 117 141 | 67 | 1.09E+04 | |
| 2,4,6-trimethylbenzenamine | 88-05-1 | 11.42 | | | | | D | 1 | | 84 | 8.19E+04 | |
| | | | | | | | D | 3 | 1: 120 | 71 | 1.13E+05 | |
| p-aminotoluene | 106-49-0 | 11.53 | | | | | D | 3 | 4: 107 43 106 93 | 66 | 4.93E+04 | |
| 3,5-dimethylbenzenamine | 108-69-0 | 12.00 | | | | | D | 3 | | 78 | 1.88E+05 | |
| 2,4,6-trimethylpyridine | 108-75-8 | 12.00 | | | | | D | 3 | 7: 120 121 77 56 66 57 122 | 73 | 3.46E+05 | |
| +Acetic acid | 64-19-7 | 12.10 | Sour | Acidic | | 1.45E-01 | D | 3 | 5: 43 60 42 41 61 | 99 | 4.73E+07 | 3.27E+08 |
| | | | | | | | D | 4 | | 100 | 7.03E+07 | 4.87E+08 |
| | | | | | | | D | 5 | 6: 45 43 40 62 56 47 | 100 | 5.47E+07 | 3.78E+08 |
| +o-xylene | 95-47-6 | 13.02 | Geranium | Geranium | | 8.51E-01 | D | 3 | | 73 | 6.49E+03 | 7.63E+03 |
| Benzo[b]thiophene | 95-15-8 | 13.39 | | Solvent, Rubbery, Earthy | | | D | 1 | 1: 134 | 65 | 5.14E+04 | |
| p-Hydroxyamphetamine acetate | 96750-10-6 | 13.39 | | | | | D | 1 | | 66 | 5.86E+04 | |
| +Nonanal | 124-19-6 | 13.64 | Fat, Citrus, Green | Aldehydic | 1.00E-03 | 2.24E-03 | D | 1 | | 69 | 1.28E+04 | 5.73E+06 |
| | | | | | | | E | 1 | | 67 | 9.94E+03 | 4.44E+06 |
| +2-ethylhexanol | 104-76-7 | 13.81 | Rose, Green | Citrus | | 2.45E-01 | D | 1 | | 88 | 2.79E+05 | 1.14E+06 |
| | | | | | | | D | 3 | 14: 42 98 70 112 39 58 113 84 69 72 54 68 99 51 | 98 | 4.65E+06 | 1.90E+07 |
| +Methyl vinyl ketone | 78-94-4 | 13.90 | | Sweet | | | D | 1 | 3: 41 70 55 | 69 | 6.55E+04 | |
| +Propanoic acid | 79-09-4 | 13.90 | Pungent, Rancid, Soy | Pungent, Acidic, Cheesy, Vinegar | | 3.55E-02 | D | 1 | 9: 74 44 55 38 56 57 46 37 58 | 67 | 1.92E+06 | 5.40E+07 |
| | | | | | | | D | 4 | 2: 73 74 | 94 | 2.04E+05 | 5.76E+06 |
| | | | | | | | D | 5 | | 96 | 8.40E+04 | 2.37E+06 |
| Propylene glycol | 57-55-6 | 13.99 | | | | | D | 1 | 2: 45 73 | 66 | 4.09E+05 | |
| | | | | | | | D | 2 | | 74 | 1.58E+05 | |
| | | | | | | | D | 4 | | 96 | 5.72E+05 | |
| | | | | | | | D | 5 | 2: 45 55 | 93 | 2.58E+05 | |
| +Benzaldehyde | 100-52-7 | 14.08 | Almond, Burnt sugar | Fruity | 3.00E-03 | 4.17E-02 | D | 1 | | 97 | 7.61E+05 | 1.83E+07 |
| | | | | | | | D | 2 | 4: 77 105 106 51 | 88 | 3.14E+04 | 7.52E+05 |
| | | | | | | | D | 3 | 10: 107 76 74 52 39 49 108 73 37 64 | 98 | 4.88E+06 | 1.17E+08 |

**Table 4** (*continued*)

| Compound | CAS | RT (min) | Published descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI & Odor [6] | Devos et al. [5] | | | | | |
| | | | | | | | D 4 | 6: 105 77 106 51 50 52 | 95 | 2.19E+05 | 5.25E+06 |
| | | | | | | | D 5 | | 90 | 3.95E+04 | 9.47E+05 |
| Indane | 496-11-7 | 14.10 | | | | | D 3 | 3: 118 117 141 | 67 | 1.09E+04 | |
| Isobutyrophenone | 611-70-1 | 14.10 | | Green | | | D 1 | 13: 105 77 51 78 106 74 75 49 38 50 76 52 39 | 76 | 1.35E+06 | |
| | | | | | | | **E** 1 | 7: 37 105 119 121 118 93 62 | 80 | 4.77E+06 | |
| +Nonane | 111-84-2 | 14.13 | Alkane | Gasoline | | 1.26E+00 | D 3 | | 86 | 5.80E+04 | 4.61E+04 |
| 2-chloroacetophenone | 532-27-4 | 14.14 | | Apple blossom | | 2.57E-02 | D 1 | 13: 105 77 51 78 106 74 75 49 38 50 76 52 39 | 87 | 1.35E+06 | 5.26E+07 |
| | | | | | | | D 2 | | 76 | 4.04E+04 | 1.57E+06 |
| | | | | | | | D 3 | 10: 107 76 74 52 39 49 108 73 37 64 | 76 | 4.88E+06 | 1.90E+08 |
| | | | | | | | D 4 | 6: 105 77 106 51 50 52 | 74 | 2.19E+05 | 8.52E+06 |
| | | | | | | | D 5 | | 69 | 3.95E+04 | 1.54E+06 |
| | | | | | | | E 1 | 7: 37 105 119 121 118 93 62 | 92 | 3.56E+05 | 1.38E+07 |
| +Undecane | 1120-21-4 | 14.14 | Alkane | | | 1.17E+00 | D 3 | 5: 127 53 55 39 72 | 78 | 9.14E+05 | 7.78E+05 |
| 2,2-dimethylbutane | 75-83-2 | 14.15 | | | | | D 3 | 3: 41 71 56 | 84 | 2.69E+05 | |
| +Dodecane | 112-40-3 | 14.15 | Alkane | Alkane | | 2.04E+00 | E 1 | | 95 | 2.59E+05 | 1.27E+05 |
| +Tridecane | 629-50-5 | 14.17 | Alkane | Alkane | | 2.14E+00 | D 1 | 8: 41 56 57 86 85 99 112 70 | 74 | 3.03E+05 | 1.42E+05 |
| | | | | | | | D 3 | 8: 85 127 57 55 82 70 128 126 | 76 | 6.23E+05 | 2.92E+05 |
| Octyl acetate | 112-14-1 | 14.20 | | Green, Earthy, Mushroom, Herbal, Waxy | | 3.98E-03 | D 1 | 4: 56 57 55 43 | 76 | 7.44E+04 | 1.87E+07 |
| N-Nitrosodimethylamine | 62-75-9 | 14.66 | | | | | D 5 | 3: 74 43 57 | 70 | 2.72E+05 | |
| +Ethyl lactate | 97-64-3 | 14.90 | Fruit | Sharp, Tart, Fruity, Buttery, Butterscotch | | 1.62E+00 | D 5 | 2: 45 55 | 68 | 4.23E+05 | 2.61E+05 |
| 2-Hydroxyethylhydrazine | 109-84-2 | 14.91 | | | | | D 4 | | 65 | 5.72E+05 | |
| | | | | | | | D 5 | | 67 | 5.15E+04 | |
| +Ethyl octanoate | 106-32-1 | 15.23 | Fruit, Fat | Fruity, Wine, Waxy, Sweet, Apricot, Banana, Brandy, Pear | | 5.75E-04 | E 1 | 9: 101 43 73 102 88 61 60 129 168 | 87 | 9.77E+04 | 9.77E+04 |
| tetrahydro-2-methyl-2-furanol | 7326-46-7 | 15.59 | | | | | D 3 | 2: 71 69 | 77 | 6.97E+04 | |
| | | | | | | | D 4 | | 76 | 1.27E+04 | |
| +1-methyl-1H-pyrrole | 96-54-8 | 15.72 | | Smoky, Woody, Herbal | | | D 2 | 1: 81 | 69 | 2.94E+04 | |
| 2-ethoxyethanol | 110-80-5 | 15.79 | | | | 1.23E+00 | D 1 | 3: 59 60 37 | 74 | 1.19E+05 | 9.65E+04 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Hexestrol | 84-16-2 | 15.85 | | | | | D | 1 | | 73 | 8.19E+04 | |
| Methyl benzoate | 93-58-3 | 16.30 | Prune, Lettuce, Herb, Sweet | Phenolic | | 1.07E-01 | D | 1 | 11: 105 77 136 76 137 106 39 49 75 74 91 | 99 | 1.81E+06 | 1.69E+07 |
| | | | | | | | E | 1 | 10: 105 77 92 49 52 152 64 181 127 141 | 100 | 1.35E+08 | 1.26E+09 |
| Cumene | 98-82-8 | 16.49 | | | | 2.40E-02 | D | 3 | 5: 105 135 120 77 78 | 77 | 2.84E+05 | 1.18E+07 |
| +Acetophenone | 98-86-2 | 16.49 | Musty, Flower, Almond | Floral | 6.50E-02 | 3.63E-01 | D | 3 | 5: 105 135 120 77 78 | 93 | 2.84E+05 | 7.81E+05 |
| 3-ethyltoluene | 620-14-4 | 16.50 | | | | | D | 3 | 4: 78 105 120 106 | 78 | 1.52E+05 | |
| 2,2,4-trimethylpentane | 540-84-1 | 16.53 | | | | | D | 1 | 4: 56 57 55 43 | 66 | 8.44E+04 | |
| | | | | | | | D | 3 | 3: 41 57 56 | 88 | 2.57E+05 | |
| 2-ethyl-5-methylpyrazine | 13360-64-0 | 16.81 | Fruit, Sweet | Coffee bean, Nutty | | | D | 3 | 3: 121 122 81 | 73 | 3.39E+04 | |
| γ-hexalactone | 695-06-7 | 17.20 | Coumarin, Sweet | Tonka | | | D | 3 | 4: 56 85 69 51 | 68 | 2.89E+05 | |
| 2-ethyl-3,5-dimethylpyridine | 1123-96-2 | 17.90 | | | | | D | 1 | | 91 | 5.86E+04 | |
| | | | | | | | D | 3 | 4: 107 135 134 70 | 86 | 1.49E+05 | |
| +α-α-Dimethylbenzenemethanol | 617-94-7 | 18.05 | | Mild, Green, Sweet, Earthy | | | D | 3 | 6: 122 105 78 77 136 102 | 89 | 1.71E+05 | |
| p-methoxyphenylacetone | 122-84-9 | 18.07 | | Sweet, Fruity, Spicy, Anisic, Balsam | | | D | 3 | | 68 | 9.60E+04 | |
| 3-methylhexane | 589-34-4 | 18.33 | | | | | D | 1 | | 70 | 4.60E+03 | |
| | | | | | | | D | 3 | 7: 43 70 41 56 39 42 100 | 97 | 5.33E+05 | |
| +Tetradecane | 629-59-4 | 18.34 | Alkane | Mild, Waxy | | | D | 1 | 5: 198 140 154 82 100 | 98 | 3.83E+06 | |
| 1-undecanol | 112-42-5 | 18.37 | Mandarin | Waxy | | 6.76E-02 | E | 1 | 4: 111 83 97 106 | 74 | 2.87E+04 | 4.24E+05 |
| Nitrocyclohexane | 1122-60-7 | 19.50 | | | | | D | 3 | 5: 83 56 41 69 39 | 74 | 2.15E+05 | |
| β-caryophyllene | 87-44-5 | 19.68 | Wood, Spice | Spice | 6.40E-02 | | D | 1 | | 66 | 1.51E+04 | 2.36E+05 |
| | | | | | | | D | 2 | | 69 | 1.18E+04 | 1.84E+05 |
| | | | | | | | D | 3 | | 85 | 7.37E+04 | 1.15E+06 |
| +Pentadecane | 629-62-9 | 20.28 | Alkane | Waxy | | | D | 1 | 8: 41 56 57 86 85 99 112 70 | 86 | 1.74E+05 | |
| +Butanoic acid, butyl ester | 109-21-7 | 20.97 | | Fruity, Banana, Pineapple, Sweet | | | D | 1 | | 76 | 3.03E+04 | |
| Longifolene | 475-20-7 | 21.28 | | Wood | | | D | 3 | | 74 | 7.37E+04 | |
| Toluene-2,4-diamine | 95-80-7 | 23.91 | | | | | D | 3 | 3: 121 122 81 | 72 | 3.39E+04 | |
| 2,3,6-trimethylpyridine | 1462-84-6 | 23.96 | | | | | D | 3 | | 74 | 1.06E+05 | |

If two references for ODTs are available, ODT from Devos, et al. [5] is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Section 1.5. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. Underlined items highlight the compounds found in Pseudo Scent Cocaine. + Compounds indicate confirmation with reference standards, matching retention time and spectra.

**Table 5**
Summary of VOCs emitted from all illicit heroin samples (sample code F in Section 1.5) and Sigma Pseudo™ Narcotic Scent Heroin formulation (sample code G in Section 1.5) and sampled over 1 h at room temperature. **Sigma Pseudo™ Narcotic Scent Heroin formulation is indicated by underlined fonts.**

| Compound | CAS | RT (min) | Published Descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Flavornet [7] | TGSC [8] | LRI & Odour [6] | Devos et al. [5] | | | | | |
| Ethylene oxide | 75-21-8 | 1.06 | | | | 8.51E+02 | F 1 | 3: 44 45 46 | 66 | 3.54E+06 | 4.16E+03 |
| | | | | | | | G 1 | 4: 44 45 46 43 | 68 | 1.75E+06 | 2.06E+03 |
| +2-nitropropane | 79-46-9 | 1.12 | | | | 7.24E+00 | F 2 | 3: 43 41 58 | 74 | 1.30E+04 | 1.80E+03 |
| Methyl chloride | 74-87-3 | 1.15 | | | | | F 1 | 2: 50 52 | 73 | 1.00E+04 | |
| +Isobutanol | 78-83-1 | 1.19 | Wine, Solvent, Bitter | Ethereal, Winey | | | F 1 | | 70 | 4.81E+04 | |
| | | | | | | | F 2 | 6: 42 57 43 41 56 39 | 68 | 8.76E+04 | |
| Hexane | 110-54-3 | 1.19 | Alkane | | | 2.19E+01 | F 1 | 6: 43 41 57 42 56 39 | 82 | 7.74E+04 | 3.54E+03 |
| | | | | | | | F 2 | 6: 42 57 43 41 56 39 | 82 | 8.76E+04 | 4.00E+03 |
| Isobutane | 75-28-5 | 1.23 | | | | 1.00E+01 | F 1 | 10: 43 42 41 57 72 39 55 56 38 58 | 83 | 8.96E+05 | 8.96E+04 |
| | | | | | | | F 2 | 13: 43 42 41 72 39 57 56 63 53 38 73 58 37 | 83 | 1.18E+06 | 1.18E+05 |
| Isobutyraldehyde | 78-84-2 | 1.23 | Pungent, Malt, Green | Spicy | | 4.07E-02 | F 1 | 10: 43 42 41 57 72 39 55 56 38 58 | 78 | 8.96E+05 | 2.20E+07 |
| | | | | | | | F 2 | 13: 43 42 41 72 39 57 56 63 53 38 73 58 37 | 77 | 1.18E+06 | 2.89E+07 |
| 4-methyldecane | 2847-72-5 | 1.39 | | | | | F 1 | 4: 71 57 41 72 | 67 | 4.33E+05 | |
| | | | | | | | F 2 | 9: 43 42 41 39 55 85 53 38 69 | 66 | 4.19E+05 | |
| 2-methylpentane | 107-83-5 | 1.39 | | | | | F 1 | 4: 71 57 41 72 | 97 | 4.33E+05 | |
| | | | | | | | F 2 | 9: 43 42 41 39 55 85 53 38 69 | 97 | 4.19E+05 | |
| Ethylenimine | 151-56-4 | 1.40 | | | | | F 2 | 9: 43 42 41 39 55 85 53 38 69 | 86 | 3.48E+05 | |
| 2,3-dimethylbutane | 79-29-8 | 1.40 | | | | | F 2 | 9: 43 42 41 39 55 85 53 38 69 | 81 | 3.48E+05 | |
| 3,4,5-trimethyl-1-hexene | 56728-10-0 | 1.40 | | | | | F 1 | | 68 | 2.72E+05 | |
| | | | | | | | F 2 | 8: 71 43 57 56 70 51 39 86 | 67 | 3.94E+05 | |
| 3-methylhexane | 589-34-4 | 1.40 | | | | | F 2 | 8: 71 43 57 56 70 51 39 86 | 75 | 2.78E+05 | |
| +1-butanol | 71-36-3 | 1.42 | Medicine, Fruit | Fermented | | 4.90E-01 | F 1 | 6: 43 41 57 42 56 39 | 66 | 7.74E+04 | 1.58E+05 |
| | | | | | | | F 2 | | 81 | 1.12E+04 | 2.29E+04 |
| | | | | | | | G 1 | 4: 39 41 69 43 | 72 | 6.39E+04 | 1.30E+05 |
| 3-methylpentane | 96-14-0 | 1.45 | | | | | F 1 | 3: 71 56 57 | 87 | 5.52E+04 | |
| | | | | | | | F 2 | | 88 | 2.45E+04 | |
| 2-methylaziridine | 75-55-8 | 1.49 | | | | | F 1 | 3: 71 56 57 | 79 | 5.52E+04 | |
| | | | | | | | F 2 | 2: 41 56 | 80 | 3.37E+04 | |
| Isocyanatomethane | 624-83-9 | 1.52 | | | | | F 1 | | 77 | 1.32E+04 | |
| Tolycaine | 3686-58-6 | 1.52 | | | | | F 1 | 1: 86 | 67 | 8.96E+02 | |
| +Propene | 115-07-1 | 1.65 | | | | 5.25E+01 | F 2 | 3: 42 39 41 | 73 | 3.41E+04 | 6.50E+02 |
| +Butane | 106-97-8 | 1.66 | | | | 2.04E+02 | F 1 | 4: 58 43 42 38 | 74 | 1.45E+05 | 7.10E+02 |
| | | | | | | | F 2 | | 79 | 2.36E+05 | 1.15E+03 |
| +Acetone | 67-64-1 | 1.66 | | Solvent | | 1.45E+01 | F 1 | 4: 58 43 42 38 | 92 | 1.45E+05 | 1.00E+04 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | F | 2 | 5: 43 58 39 37 38 | 97 | 3.14E+05 | 2.18E+04 |
| Hydrazine | 302-01-2 | 1.97 | | | | 3.00E+00 | F | 1 | 1: 33 | 78 | 1.19E+03 | 3.97E+02 |
| Cyclohexane | 110-82-7 | 1.98 | | | | 2.19E+01 | G | 1 | 9: 39 84 56 42 55 69 85 50 54 | 96 | 2.71E+05 | 1.24E+04 |
| +Ethylacetate | 141-78-6 | 2.32 | Pineapple | Ethereal, Fruity, Sweet, Weedy, Green | | 2.63E+00 | F | 2 | | 96 | 2.41E+05 | 9.17E+04 |
| Propylene glycol | 57-55-6 | 2.33 | | | | | F | 1 | 2: 43 45 | 69 | 5.16E+04 | |
| | | | | | | | F | 2 | 3: 45 61 44 | 65 | 8.74E+04 | |
| +Isopropyl alcohol | 67-63-0 | 2.33 | | Alcohol, Musty, Woody | | 1.02E+01 | F | 1 | 2: 43 45 | 69 | 2.14E+04 | 2.09E+03 |
| +Ethanol | 64-17-5 | 2.33 | Sweet | Alcoholic | | 2.88E+01 | F | 2 | 3: 45 61 44 | 68 | 6.90E+04 | 2.39E+03 |
| +Acetic anhydride | 108-24-7 | 3.66 | | Sharp, Vinegar | | 5.89E-01 | F | 1 | 2: 43 42 | 76 | 6.24E+03 | 1.06E+04 |
| | | | | | | | F | 2 | 4: 43 37 42 38 | 71 | 1.43E+05 | 2.43E+05 |
| | | | | | | | G | 1 | 1: 43 | 69 | 3.64E+04 | 6.18E+04 |
| nitrocyclohexane | 1122-60-7 | 10.29 | | | | | G | 1 | 3: 83 55 41 | 74 | 2.39E+04 | |
| m-cymene | 535-77-3 | 11.33 | | | | | G | 1 | | 93 | 4.08E+04 | |
| 1-(3-methylphenyl)-ethanone | 585-74-0 | 11.34 | | | | | G | 1 | | 86 | 2.84E+04 | |
| tert-butyl-benzene | 98-06-6 | 11.34 | | | | | G | 1 | | 88 | 2.84E+04 | |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | 11.35 | | Gasoline, Sweet | | 2.63E-02 | F | 1 | 3: 120 119 134 | 66 | 2.94E+04 | 1.12E+06 |
| | | | | | | | G | 1 | | 86 | 4.08E+04 | 1.55E+06 |
| +p-cymene | 99-87-6 | 11.35 | Solvent, Gasoline, Citrus | Terpenic | | 2.14E-03 | F | 1 | 3: 120 119 134 | 65 | 2.94E+04 | 1.37E+07 |
| | | | | | | | G | 1 | | 91 | 4.08E+04 | 1.91E+07 |
| Isodurene | 527-53-7 | 11.37 | | | | | F | 1 | 3: 120 119 134 | 69 | 2.94E+04 | |
| +Acetic acid | 64-19-7 | 12.09 | Sour | Acidic | | 1.45E-01 | F | 1 | 5: 43 60 41 59 47 | 97 | 5.74E+07 | 3.97E+08 |
| | | | | | | | F | 2 | | 99 | 2.62E+05 | 1.81E+06 |
| | | | | | | | G | 1 | 5: 45 43 60 46 105 | 100 | 5.84E+07 | 4.04E+08 |
| Nitrogen dioxide | 10102-44-0 | 12.29 | | | | 1.86E-01 | G | 1 | 1: 46 | 76 | 9.21E+02 | 4.95E+03 |
| +Furfural | 98-01-1 | 12.71 | Bread, Almond, Sweet | Sweet, Woody, Almond, Baked bread | | 7.76E-01 | F | 2 | | 93 | 3.22E+04 | 4.15E+04 |
| Fenbendazole | 43210-67-9 | 12.98 | | | | | F | 1 | 3: 267 269 268 | 66 | 5.95E+04 | |
| +Propanoic acid | 79-09-4 | 13.91 | Pungent, Rancid, Soy | Pungent, Acidic, Cheesy, Vinegar | | 3.55E-02 | F | 1 | | 94 | 9.03E+04 | 2.54E+06 |
| Propanoic acid, anhydride | 123-62-6 | 13.91 | | | | | F | 2 | 5: 57 209 193 82 69 | 68 | 3.17E+03 | |
| | | | | | | | G | 1 | 1: 57 | 66 | 4.74E+03 | |
| Benzaldehyde | 100-52-7 | 14.10 | Almond, Burnt sugar | Fruity | 3.00E-03 | 4.17E-02 | G | 1 | 2: 105 77 | 76 | 5.40E+04 | 1.30E+06 |
| 2-chloroacetophenone | 532-27-4 | 14.10 | | Apple blossom | | 2.57E-02 | G | 1 | 2: 105 77 | 77 | 5.40E+04 | 2.10E+06 |
| Isobutyrophenone | 611-70-1 | 14.10 | | Green | | | G | 1 | 2: 105 77 | 66 | 3.06E+04 | |
| Ethyl cyclohexane | 1678-91-7 | 15.20 | | | | | G | 1 | 1: 83 | 70 | 7.33E+04 | |
| Butyric acid | 107-92-6 | 15.53 | Rancid, Cheese, Sweat | Sharp, Acetic, Cheese, Butter, Fruit | | 3.89E-03 | F | 1 | 3: 60 42 37 | 95 | 4.20E+05 | 1.08E+08 |
| +Pentanoic acid | 109-52-4 | 15.53 | Sweat | Sickening, Putrid, Acidic, Sweaty, Rancid | | 4.79E-03 | F | 1 | 5: 60 45 73 43 39 | 89 | 3.45E+05 | 7.22E+07 |
| 2,2-dimethylbutane | 75-83-2 | 15.87 | | | | | F | 1 | | 82 | 1.06E+04 | |
| Methyl benzoate | 93-58-3 | 16.26 | Prune, Lettuce, Herb, Sweet | Phenolic | | 1.07E-01 | G | 1 | | 97 | 1.74E+05 | 1.63E+06 |
| +Toluene | 108-88-3 | 19.16 | Paint | Sweet | | 1.55E+00 | F | 2 | | 80 | 2.84E+04 | 1.84E+04 |

**Table 5** (*continued*)

| Compound | CAS | RT (min) | Published Descriptors | | Published ODT (ppm) | | Sample code | Models | Net % match | PAC | OAV |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | **Flavornet** [7] | **TGSC** [8] | **LRI & Odour** [6] | **Devos et al.** [5] | | | | | |
| +Dimethylsulfone | 67-71-0 | 20.11 | Sulfur, Burnt | Sulfurous, Burnt | | | F 2 | 2: 79 62 | 96 | 1.94E+05 | |
| Methyl formate | 107-31-3 | 22.87 | | Fruity, Plum | | 9.33E+01 | G 1 | 1: 60 | 73 | 1.83E+03 | 1.96E+01 |
| Diethyl Phthalate | 84-66-2 | 27.46 | | | | | F 1 | | 69 | 9.71E+03 | |

If two references for ODTs are available, ODT from Devos, et al. [5] is used to calculate OAV. RT=Retention Time. ODT=Odor Detection Threshold. Code, see Section 1.5. Models=significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. Underlined items highlight the compounds found in Pseudo Scent Heroin. + Compounds indicate confirmation with reference standards, matching retention time and spectra.

**Table 6**
Comparing rank of top 10 most concentrated VOCs with the calculated OAV in all marijuana samples. Bolded font signifies 1 g real marijuana (sample code A6/A7). Underlined font signifies 1 g surrogate marijuana (sample code C1–C3).

| Compound | CAS | Sample code | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|---|---|---|---|---|---|
| Limonene | 138-86-3 | A 1 | 1 | 5 | −4 |
| Limonene | 138-86-3 | A 2 | 1 | 6 | −5 |
| Isobutane | 75-28-5 | A 3 | 1 | 6 | −5 |
| Ethylene oxide | 75-21-8 | A 4 | 1 | 17 | −16 |
| (+)-sativene | 3650-28-0 | A 5 | 1 | No ODT | |
| **Acetic acid** | **64-19-7** | **A 6** | **1** | **2** | **−1** |
| **Benzyl alcohol** | **100-51-6** | **A 7** | **1** | **No ODT** | |
| Tyramine | 51-67-2 | B 1 | 1 | No ODT | |
| β-pinene | 18172-67-3 | B 2 | 1 | No ODT | |
| Acetic acid | 64-19-7 | B 3 | 1 | 2 | −1 |
| Butyl formate | 592-84-7 | B 4 | 1 | No ODT | |
| γ-terpinene | 99-85-4 | C 1 | 1 | No ODT | |
| γ-terpinene | 99-85-4 | C 2 | 1 | No ODT | |
| Camphene | 79-92-5 | C 3 | 1 | No ODT | |
| Camphene | 79-92-5 | A 1 | 2 | No ODT | |
| Camphene | 79-92-5 | A 2 | 2 | No ODT | |
| 2-methylpentane | 107-83-5 | A 3 | 2 | No ODT | |
| Acetone | 67-64-1 | A 4 | 2 | 12 | −10 |
| Benzyl alcohol | 100-51-6 | A 5 | 2 | No ODT | |
| **Methylisohexenyl ketone** | **110-93-0** | **A 6** | **2** | **3** | **−1** |
| **Acetone** | **67-64-1** | **A 7** | **2** | **21** | **−19** |
| β-pinene | 18172-67-3 | B 1 | 2 | No ODT | |
| Myrcene | 123-35-3 | B 2 | 2 | 1 | +1 |
| Methylisohexenyl ketone | 110-93-0 | B 3 | 2 | 3 | −1 |
| Acetone | 67-64-1 | B 4 | 2 | 14 | −12 |
| Ethyl benzene | 100-41-4 | C 1 | 2 | 3 | −1 |
| Terpinolene | 586-62-9 | C 2 | 2 | 3 | −1 |
| γ-terpinene | 99-85-4 | C 3 | 2 | No ODT | |
| Isobornyl thiocyanoacetate | 115-31-1 | A 1 | 3 | No ODT | |
| Isobornyl thiocyanoacetate | 115-31-1 | A 2 | 3 | No ODT | |
| 3,4,5-trimethyl-1-hexene | 56728-10-0 | A 3 | 3 | No ODT | |
| Limonene | 138-86-3 | A 4 | 3 | 4 | −1 |
| Tyramine | 51-67-2 | A 5 | 3 | No ODT | |
| **β-caryophyllene** | **87-44-5** | **A 6** | **3** | **4** | **−1** |
| **Tyramine** | **51-67-2** | **A 7** | **3** | **No ODT** | |
| Myrcene | 123-35-3 | B 1 | 3 | 1 | +2 |
| Limonene | 138-86-3 | B 2 | 3 | 4 | −1 |
| β-caryophyllene | 87-44-5 | B 3 | 3 | 4 | −1 |
| 3-pentanol | 584-02-1 | B 4 | 3 | 5 | −2 |
| m-cymene | 535-77-3 | C 1 | 3 | No ODT | |
| Ethyl benzene | 100-41-4 | C 2 | 3 | 5 | −2 |
| Terpinolene | 586-62-9 | C 3 | 3 | 3 | 0 |
| β-pinene | 18172-67-3 | A 1 | 4 | No ODT | |
| Isobutane | 75-28-5 | A 2 | 4 | 13 | −9 |
| 4-methyldecane | 2847-72-5 | A 3 | 4 | No ODT | |
| Camphene | 79-92-5 | A 4 | 4 | No ODT | |
| Isobutane | 75-28-5 | A 5 | 4 | 9 | −5 |
| **Longifolene** | **475-20-7** | **A 6** | **4** | **No ODT** | |
| **Isobutane** | **75-28-5** | **A 7** | **4** | **22** | **−18** |
| Ethylene oxide | 75-21-8 | B 1 | 4 | 28 | −24 |
| Camphene | 79-92-5 | B 2 | 4 | No ODT | |
| Longifolene | 475-20-7 | B 3 | 4 | No ODT | |
| tert-butanol | 75-65-0 | B 4 | 4 | No ODT | |
| p-cymene | 99-87-6 | C 1 | 4 | 1 | +3 |
| m-cymene | 535-77-3 | C 2 | 4 | No ODT | |
| m-cymene | 535-77-3 | C 3 | 4 | No ODT | |
| Isobutane | 75-28-5 | A 1 | 5 | 11 | −6 |
| Isobutyraldehyde | 78-84-2 | A 2 | 5 | 3 | +2 |

**Table 6** (*continued*)

| Compound | CAS | Sample code | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|---|---|---|---|---|---|
| Ethylene oxide | 75-21-8 | A 3 | 5 | 19 | −14 |
| 2,2,4-trimethylpentane | 540-84-1 | A 4 | 5 | No ODT | |
| γ-gurjunene | 22567-17-5 | A 5 | 5 | No ODT | |
| **Acetone** | **67-64-1** | **A 6** | **5** | **22** | **−17** |
| **Butane** | **106-97-8** | **A 7** | **5** | **34** | **−29** |
| Benzyl alcohol | 100-51-6 | B 1 | 5 | No ODT | |
| α-phellandrene | 99-83-2 | B 2 | 5 | No ODT | |
| Fenchyl alcohol | 1632-73-1 | B 3 | 5 | No ODT | |
| Propylamine | 107-10-8 | B 4 | 5 | 1 | +4 |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | C 1 | 5 | 2 | +3 |
| p-cymene | 99-87-6 | C 2 | 5 | 1 | +4 |
| p-cymene | 99-87-6 | C 3 | 5 | 1 | +4 |
| Isobutyraldehyde | 78-84-2 | A 1 | 6 | 1 | +5 |
| β-pinene | 18172-67-3 | A 2 | 6 | No ODT | |
| Limonene | 138-86-3 | A 3 | 6 | 4 | +2 |
| Methylene chloride | 75-09-2 | A 4 | 6 | 15 | −9 |
| α-humulene | 6753-98-6 | A 5 | 6 | 17 | −11 |
| **Butane** | **106-97-8** | **A 6** | **6** | **31** | **−25** |
| **α-phellandrene** | **99-83-2** | **A 7** | **6** | **No ODT** | |
| Butane | 106-97-8 | B 1 | 6 | 25 | −19 |
| α-pinene | 80-56-8 | B 2 | 6 | 5 | +1 |
| Butane | 106-97-8 | B 3 | 6 | 35 | −29 |
| Ethylene oxide | 75-21-8 | B 4 | 6 | 23 | −17 |
| 1-ethyl-3,5-dimethylbenzene | 934-74-7 | C 1 | 6 | No ODT | |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | C 2 | 6 | 2 | +4 |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | C 3 | 6 | 2 | +4 |
| Betahistine | 5638-76-6 | A 1 | 7 | No ODT | |
| α-pinene | 80-56-8 | A 2 | 7 | 10 | −3 |
| Camphene | 79-92-5 | A 3 | 7 | No ODT | |
| Methylisohexenyl ketone | 110-93-0 | A 4 | 7 | 2 | +5 |
| Valencene | 4630-07-3 | A 5 | 7 | No ODT | |
| **Fenchyl alcohol** | **1632-73-1** | **A 6** | **7** | **No ODT** | |
| **δ-3-carene** | **13466-78-9** | **A 7** | **7** | **20** | **−13** |
| Acetone | 67-64-1 | B 1 | 7 | 17 | −10 |
| Benzyl alcohol | 100-51-6 | B 2 | 7 | No ODT | |
| Acetone | 67-64-1 | B 3 | 7 | 31 | -24 |
| Diacetone alcohol | 123-42-2 | B 4 | 7 | 10 | −3 |
| Isodurene | 527-53-7 | C 1 | 7 | No ODT | |
| 2-acetyl-6-methyl pyrazine | 22047-26-3 | C 2 | 7 | No ODT | |
| 2-Butanol | 78-92-2 | C 3 | 7 | 4 | +3 |
| α-phellandrene | 99-83-2 | A 1 | 8 | No ODT | |
| Terpinolene | 586-62-9 | A 2 | 8 | 8 | 0 |
| Isobutyraldehyde | 78-84-2 | A 3 | 8 | 2 | +6 |
| 2-butanone | 78-93-3 | A 4 | 8 | 13 | −5 |
| 3,4,5-trimethyl-1-hexene | 56728-10-0 | A 5 | 8 | No ODT | |
| **α-humulene** | **6753-98-6** | **A 6** | **8** | **8** | **0** |
| **α-humulene** | **6753-98-6** | **A 7** | **8** | **8** | **0** |
| Isobutane | 75-28-5 | B 1 | 8 | 15 | −7 |
| Isobutane | 75-28-5 | B 2 | 8 | 12 | −4 |
| α-humulene | 6753-98-6 | B 3 | 8 | 9 | −1 |
| 1-butanol | 71-36-3 | B 4 | 8 | 8 | 0 |
| Dihydromethylcyclopentapyrazine | 23747-48-0 | C 1 | 8 | No ODT | |
| Isopropyl alcohol | 67-63-0 | C 2 | 8 | 15 | −7 |
| Ethyl lactate | 97-64-3 | C 3 | 8 | 6 | +2 |
| Sabinene | 3387-41-5 | A 1 | 9 | No ODT | |
| α-terpinene | 99-86-5 | A 2 | 9 | No ODT | |
| Myrcene | 123-35-3 | A 3 | 9 | 1 | +8 |
| Methyl acetate | 79-20-9 | A 4 | 9 | No ODT | |
| 4-methyldecane | 2847-72-5 | A 5 | 9 | No ODT | |
| **Methyl acetate** | **79-20-9** | **A 6** | **9** | **No ODT** | |

**Table 6** (*continued*)

| Compound | CAS | Sample code | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|---|---|---|---|---|---|
| **β-caryophyllene** | **87-44-5** | **A 7** | **9** | **5** | **+4** |
| Limonene | 138-86-3 | B 1 | 9 | 6 | +3 |
| Isobutyraldehyde | 78-84-2 | B 2 | 9 | 3 | +6 |
| Alloaromadendrene | 25246-27-9 | B 3 | 9 | No ODT | |
| β-caryophyllene | 87-44-5 | B 4 | 9 | 2 | +7 |
| Ethyl lactate | 97-64-3 | C 1 | 9 | 8 | +1 |
| Ethyl lactate | 97-64-3 | C 2 | 9 | 10 | −1 |
| δ-3-carene | 13466-78-9 | C 3 | 9 | 12 | −3 |
| β-caryophyllene | 87-44-5 | A 1 | 10 | 4 | +6 |
| (+)-4-Carene | 29050-33-7 | A 2 | 10 | 16 | −6 |
| α-terpinyl acetate | 80-26-2 | A 3 | 10 | No ODT | |
| Fenchyl alcohol | 1632-73-1 | A 4 | 10 | No ODT | |
| Benzaldehyde | 100-52-7 | A 5 | 10 | 14 | −4 |
| **Valencene** | **4630-07-3** | **A 6** | **10** | **No ODT** | |
| **2-chloroacetophenone** | **532-27-4** | **A 7** | **10** | **3** | **+7** |
| Camphene | 79-92-5 | B 1 | 10 | No ODT | |
| Tyramine | 51-67-2 | B 2 | 10 | No ODT | |
| Isobornyl thiocyanoacetate | 115-31-1 | B 3 | 10 | No ODT | |
| Longifolene | 475-20-7 | B 4 | 10 | No ODT | |
| δ-3-carene | 13466-78-9 | C 1 | 10 | 14 | −4 |
| Propylene glycol | 57-55-6 | C 2 | 10 | No ODT | |
| α-terpinene | 99-86-5 | C 3 | 10 | No ODT | |

Sample code, see Section 1.5, corresponding to sample identification.
ODT=odor detection threshold from Devos et al. [5].

**Table 7**
Comparing rank of top 10 most concentrated VOCs with the calculated OAV in all cocaine samples. Bolded font signifies 1 g real cocaine (sample code D4/D5). Underlined font signifies 1 g surrogate cocaine (sample code E1).

| Compound | CAS | Sample Code | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|---|---|---|---|---|---|
| Isobutanol | 78-83-1 | D 1 | 1 | 37 | −36 |
| Isobutyraldehyde | 78-84-2 | D 2 | 1 | 1 | 0 |
| Acetic acid | 64-19-7 | D 3 | 1 | 2 | −1 |
| **Acetic acid** | **64-19-7** | **D 4** | **1** | **1** | **0** |
| **Acetic acid** | **64-19-7** | **D 5** | **1** | **1** | **0** |
| Methyl benzoate | 93-58-3 | E 1 | 1 | 1 | 0 |
| n-Propyl acetate | 109-60-4 | D 1 | 2 | 8 | −6 |
| Isobutane | 75-28-5 | D 2 | 2 | 7 | −5 |
| n-Propyl acetate | 109-60-4 | D 3 | 2 | 9 | −7 |
| **Ethylene oxide** | **75-21-8** | **D 4** | **2** | **23** | **−21** |
| **n-Propyl acetate** | **109-60-4** | **D 5** | **2** | **2** | **0** |
| Isobutyrophenone | 611-70-1 | E 1 | 2 | 12 | −10 |
| Acetone | 67-64-1 | D 1 | 3 | 20 | −17 |
| 4-methyldecane | 2847-72-5 | D 2 | 3 | 17 | −14 |
| Phenylethyl alcohol | 60-12-8 | D 3 | 3 | 1 | +2 |
| **n-Propyl acetate** | **109-60-4** | **D 4** | **3** | **4** | **−1** |
| **Ethylacetate** | **141-78-6** | **D 5** | **3** | **10** | **−7** |
| Ethylene oxide | 75-21-8 | E 1 | 3 | 8 | −5 |
| Butane | 106-97-8 | D 1 | 4 | 30 | −26 |
| 2-methylpentane | 107-83-5 | D 2 | 4 | 18 | −14 |
| Toluene | 108-88-3 | D 3 | 4 | 10 | −6 |
| **Ethylacetate** | **141-78-6** | **D 4** | **4** | **8** | **−4** |
| **2-butanone** | **78-93-3** | **D 5** | **4** | **12** | **−8** |
| 2-chloroacetophenone | 532-27-4 | E 1 | 4 | 3 | +1 |
| Tetradecane | 629-59-4 | D 1 | 5 | 38 | −33 |

**Table 7** (*continued*)

| Compound | CAS | Sample Code | | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|---|---|---|---|---|---|---|
| 3,4,5-trimethyl-1-hexene | 56728-10-0 | D | 2 | 5 | 19 | −14 |
| 2-chloroacetophenone | 532-27-4 | D | 3 | 5 | 3 | +2 |
| **Diacetone alcohol** | **123-42-2** | **D** | **4** | **5** | **7** | **−2** |
| **Diacetone alcohol** | **123-42-2** | **D** | **5** | **5** | **8** | **−3** |
| Dodecane | 112-40-3 | E | 1 | 5 | 6 | −1 |
| Ethylacetate | 141-78-6 | D | 1 | 6 | 10 | −4 |
| Isopropyl alcohol | 67-63-0 | D | 2 | 6 | 9 | −3 |
| Benzaldehyde | 100-52-7 | D | 3 | 6 | 4 | +2 |
| **Acetone** | **67-64-1** | **D** | **4** | **6** | **14** | **−8** |
| **Acetone** | **67-64-1** | **D** | **5** | **6** | **18** | **−12** |
| Ethyl octanoate | 106-32-1 | E | 1 | 6 | 2 | +4 |
| Propanoic acid | 79-09-4 | D | 1 | 7 | 1 | +6 |
| Ethanol | 64-17-5 | D | 2 | 7 | 11 | −4 |
| 2-ethylhexanol | 104-76-7 | D | 3 | 7 | 7 | 0 |
| **1,2-diethyl hydrazine** | **1615-80-1** | **D** | **4** | **7** | **29** | **−22** |
| **Ethyl lactate** | **97-64-3** | **D** | **5** | **7** | **13** | **−6** |
| Decane | 124-18-5 | E | 1 | 7 | 7 | 0 |
| Methyl benzoate | 93-58-3 | D | 1 | 8 | 5 | +3 |
| Propylene glycol | 57-55-6 | D | 2 | 8 | 20 | −12 |
| 2-butanone | 78-93-3 | D | 3 | 8 | 18 | −10 |
| **Isopropyl alcohol** | **67-63-0** | **D** | **4** | **8** | **16** | **−8** |
| **Hexane** | **110-54-3** | **D** | **5** | **8** | **21** | **−13** |
| 1-undecanol | 112-42-5 | E | 1 | 8 | 5 | +3 |
| 2-chloroacetophenone | 532-27-4 | D | 1 | 9 | 2 | +7 |
| Acetone | 67-64-1 | D | 2 | 9 | 10 | −1 |
| Ethylacetate | 141-78-6 | D | 3 | 9 | 13 | −4 |
| **Propylene glycol** | **57-55-6** | **D** | **4** | **9** | **30** | **−21** |
| **Methyl thiocyanate** | **556-64-9** | **D** | **5** | **9** | **5** | **+4** |
| Cyclohexane | 110-82-7 | E | 1 | 9 | 11 | −2 |
| Isobutyrophenone | 611-70-1 | D | 1 | 10 | 39 | −29 |
| methylhydrazine | 60-34-4 | D | 2 | 10 | 21 | −11 |
| Isobutyraldehyde | 78-84-2 | D | 3 | 10 | 5 | +5 |
| **2-Hydroxyethylhydrazine** | **109-84-2** | **D** | **4** | **10** | **31** | **−21** |
| **Isopropyl alcohol** | **67-63-0** | **D** | **5** | **10** | **20** | **−10** |
| Acetone | 67-64-1 | E | 1 | 10 | 10 | 0 |

Code, see Section 1.5, corresponding to sample identification. ODT=odor detection threshold from Devos et al., [5].

**Table 8**
Comparing rank of top 10 most concentrated VOCs with the calculated OAV in all heroin samples. Bolded font signifies 1 g real heroin (sample code F1/F2). Underlined font signifies 1 g surrogate marijuana (sample code G1).

| Compound | CAS | Sample Code | | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|---|---|---|---|---|---|---|
| **Acetic acid** | **64-19-7** | **F** | **1** | **1** | **1** | **0** |
| **Isobutyraldehyde** | **78-84-2** | **F** | **2** | **1** | **1** | **0** |
| Acetic acid | 64-19-7 | G | 1 | 1 | 1 | 0 |
| **Ethylene oxide** | **75-21-8** | **F** | **1** | **2** | **12** | **−10** |
| **Isobutane** | **75-28-5** | **F** | **2** | **2** | **4** | **−2** |
| Ethylene oxide | 75-21-8 | G | 1 | 2 | 11 | −9 |
| **Isobutyraldehyde** | **78-84-2** | **F** | **1** | **3** | **4** | **−1** |
| **4-methyldecane** | **2847-72-5** | **F** | **2** | **3** | **No ODT** | |
| Cyclohexane | 110-82-7 | G | 1 | 3 | 9 | −6 |
| **Isobutane** | **75-28-5** | **F** | **1** | **4** | **9** | **−5** |
| **2-methylpentane** | **107-83-5** | **F** | **2** | **4** | **No ODT** | |
| Methyl benzoate | 93-58-3 | G | 1 | 4 | 4 | 0 |
| **4-methyldecane** | **2847-72-5** | **F** | **1** | **5** | **No ODT** | |
| **3,4,5-trimethyl-1-hexene** | **56728-10-0** | **F** | **2** | **5** | **No ODT** | |
| Ethyl cyclohexane | 1678-91-7 | G | 1 | 5 | No ODT | |
| **2-methylpentane** | **107-83-5** | **F** | **1** | **6** | **No ODT** | |
| **Ethylenimine** | **151-56-4** | **F** | **2** | **6** | **No ODT** | |
| 1-butanol | 71-36-3 | G | 1 | 6 | 7 | −1 |
| **Butyric acid** | **107-92-6** | **F** | **1** | **7** | **2** | **+5** |
| **2,3-dimethylbutane** | **79-29-8** | **F** | **2** | **7** | **No ODT** | |
| 2-chloroacetophenone | 532-27-4 | G | 1 | 7 | 3 | +4 |
| **Pentanoic acid** | **109-52-4** | **F** | **1** | **8** | **3** | **+5** |
| **Acetone** | **67-64-1** | **F** | **2** | **8** | **8** | **0** |
| Benzaldehyde | 100-52-7 | G | 1 | 8 | 6 | +2 |
| **3,4,5-trimethyl-1-hexene** | **56728-10-0** | **F** | **1** | **9** | **No ODT** | |
| **3-methylhexane** | **589-34-4** | **F** | **2** | **9** | **No ODT** | |
| p-cymene | 99-87-6 | G | 1 | 9 | 2 | +7 |
| **Acetone** | **67-64-1** | **F** | **1** | **10** | **11** | **−1** |
| **Acetic acid** | **64-19-7** | **F** | **2** | **10** | **2** | **+8** |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | G | 1 | 10 | 5 | +5 |

Code, see Section 1.5, corresponding to sample identification.
ODT=odor detection threshold from Devos et al. [5].

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